



Full wwPDB EM Validation Report ⓘ

Nov 30, 2025 – 03:48 AM JST

PDB ID : 9K9W / pdb_00009k9w
EMDB ID : EMD-62201
Title : structure of bundle-shaped PBS with short rod
Authors : Sui, S.-F.; Ma, J.; You, X.; Sun, S.
Deposited on : 2024-10-28
Resolution : 2.80 Å(reported)
Based on initial model : 6KGX

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

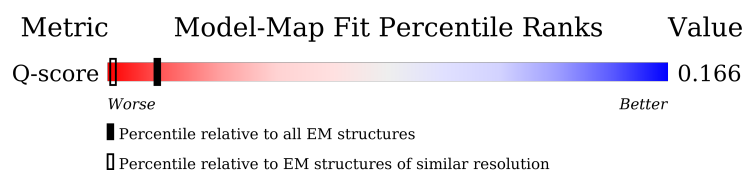
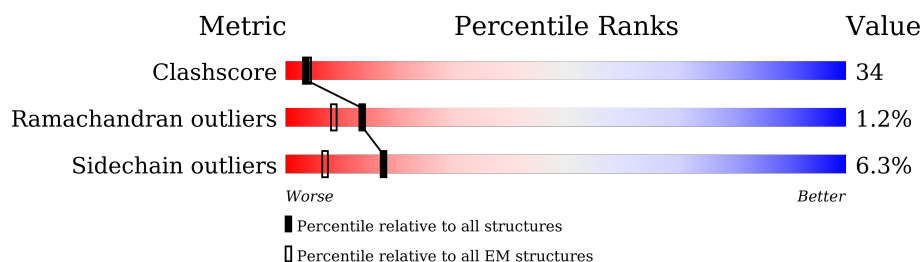
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




























| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore | 210492 | 15764 | - |
| Ramachandran outliers | 207382 | 16835 | - |
| Sidechain outliers | 206894 | 16415 | - |
| Q-score | - | 25397 | 11806 (2.30 - 3.30) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 161 | |
| 1 | B5 | 161 | |
| 1 | B7 | 161 | |
| 1 | D5 | 161 | |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | D7 | 161 |  73% 24% . |
| 1 | F5 | 161 |  77% 21% . |
| 1 | F7 | 161 |  85% 15% |
| 1 | H5 | 161 |  78% 21% . |
| 1 | H7 | 161 |  81% 18% . |
| 1 | J5 | 161 |  66% 24% 8% . |
| 1 | J7 | 161 |  73% 24% . |
| 1 | L5 | 161 |  77% 21% . |
| 1 | L7 | 161 |  85% 15% |
| 1 | N5 | 161 |  84% 15% . |
| 1 | N7 | 161 |  84% 16% |
| 1 | P5 | 161 |  80% 20% |
| 1 | P7 | 161 |  83% 17% |
| 1 | R5 | 161 |  70% 29% . |
| 1 | R7 | 161 |  84% 16% |
| 1 | T5 | 161 |  83% 17% . |
| 1 | T7 | 161 |  81% 19% |
| 1 | V5 | 161 |  80% 20% |
| 1 | V7 | 161 |  83% 16% . |
| 1 | X5 | 161 |  70% 29% . |
| 1 | X7 | 161 |  84% 16% |
| 1 | Z | 161 |  77% 22% . |
| 1 | Z5 | 161 |  80% 20% . |
| 1 | Z7 | 161 |  83% 17% |
| 1 | b5 | 161 |  78% 21% . |



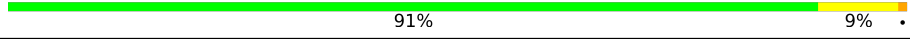
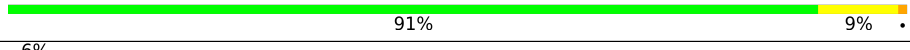
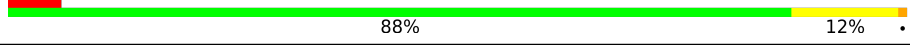








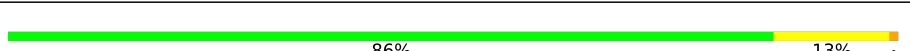
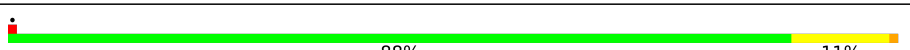

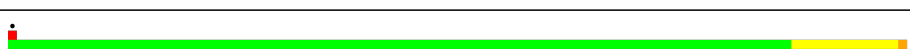




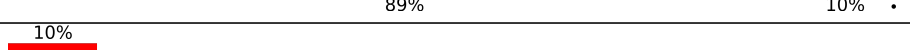
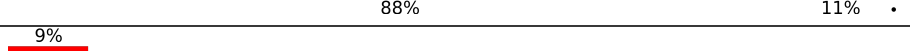

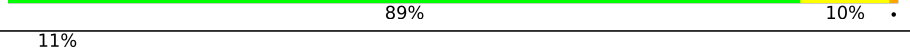
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | b7 | 161 |  |
| 1 | d5 | 161 |  |
| 1 | d7 | 161 |  |
| 1 | f5 | 161 |  |
| 1 | f7 | 161 |  |
| 1 | h7 | 161 |  |
| 1 | j7 | 161 |  |
| 1 | l7 | 161 |  |
| 1 | n7 | 161 |  |
| 1 | p7 | 161 |  |
| 1 | r7 | 161 |  |
| 1 | t7 | 161 |  |
| 1 | v7 | 161 |  |
| 2 | A1 | 162 |  |
| 2 | A2 | 162 |  |
| 2 | A3 | 162 |  |
| 2 | A4 | 162 |  |
| 2 | A6 | 162 |  |
| 2 | A8 | 162 |  |
| 2 | A9 | 162 |  |
| 2 | AA | 162 |  |
| 2 | C1 | 162 |  |
| 2 | C2 | 162 |  |
| 2 | C3 | 162 |  |
| 2 | C4 | 162 |  |



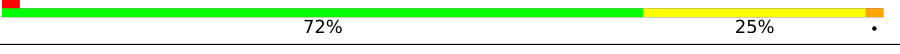

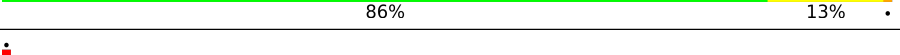
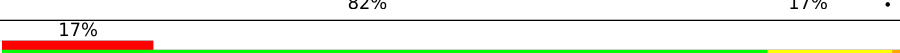
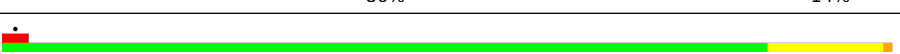
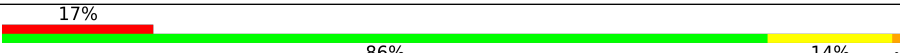


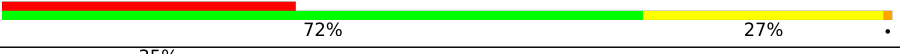




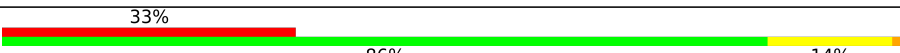


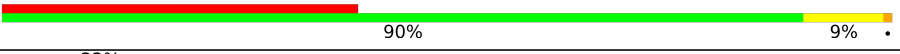


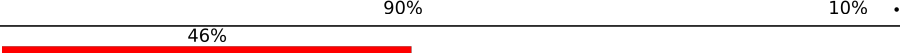



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | C6 | 162 |  |
| 2 | C8 | 162 |  |
| 2 | C9 | 162 |  |
| 2 | CA | 162 |  |
| 2 | E1 | 162 |  |
| 2 | E2 | 162 |  |
| 2 | E3 | 162 |  |
| 2 | E4 | 162 |  |
| 2 | E6 | 162 |  |
| 2 | E8 | 162 |  |
| 2 | E9 | 162 |  |
| 2 | EA | 162 |  |
| 2 | G1 | 162 |  |
| 2 | G2 | 162 |  |
| 2 | G3 | 162 |  |
| 2 | G4 | 162 |  |
| 2 | G6 | 162 |  |
| 2 | G8 | 162 |  |
| 2 | G9 | 162 |  |
| 2 | GA | 162 |  |
| 2 | I1 | 162 |  |
| 2 | I2 | 162 |  |
| 2 | I3 | 162 |  |
| 2 | I4 | 162 |  |
| 2 | I6 | 162 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | I8 | 162 |  89% 10% |
| 2 | I9 | 162 |  75% 22% |
| 2 | IA | 162 |  72% 25% |
| 2 | K1 | 162 |  83% 17% |
| 2 | K2 | 162 |  86% 13% |
| 2 | K3 | 162 |  82% 17% |
| 2 | K4 | 162 |  17% 86% 14% |
| 2 | K6 | 162 |  86% 13% |
| 2 | K8 | 162 |  17% 86% 14% |
| 2 | K9 | 162 |  80% 15% |
| 2 | KA | 162 |  81% 15% |
| 2 | N4 | 162 |  33% 72% 27% |
| 2 | N8 | 162 |  35% 70% 28% |
| 2 | O1 | 162 |  15% 78% 21% |
| 2 | O3 | 162 |  14% 77% 22% |
| 2 | O9 | 162 |  76% 23% |
| 2 | OA | 162 |  77% 22% |
| 2 | P4 | 162 |  33% 86% 14% |
| 2 | P8 | 162 |  33% 88% 11% |
| 2 | Q1 | 162 |  42% 90% 9% |
| 2 | Q3 | 162 |  40% 90% 9% |
| 2 | Q9 | 162 |  22% 87% 12% |
| 2 | QA | 162 |  17% 70% 27% |
| 2 | R4 | 162 |  46% 90% 10% |
| 2 | R8 | 162 |  46% 88% 11% |







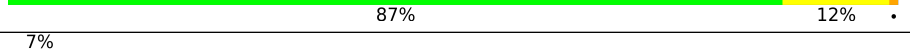
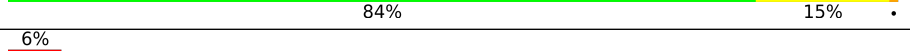
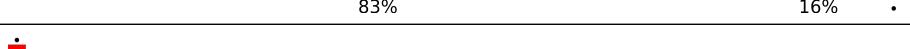
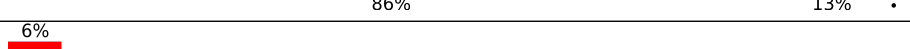
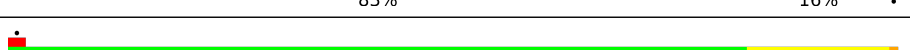

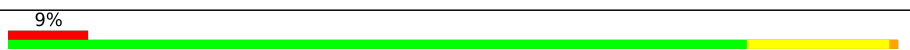

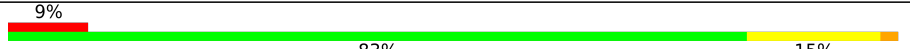





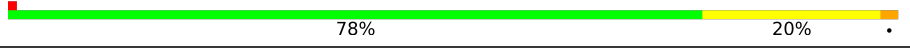
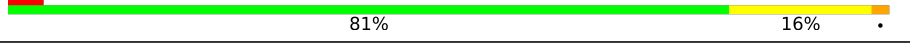



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|----------------------|
| 2 | S1 | 162 | 26% 90% 10% . |
| 2 | S3 | 162 | 25% 89% 10% . |
| 2 | S9 | 162 | 6% 88% 11% . |
| 2 | SA | 162 | 6% 87% 12% . |
| 2 | T4 | 162 | 15% 88% 11% . |
| 2 | T8 | 162 | 14% 88% 10% . |
| 2 | U1 | 162 | 43% 83% 14% . |
| 2 | U3 | 162 | 43% 86% 12% .. |
| 2 | U9 | 162 | 5% 87% 12% . |
| 2 | UA | 162 | 6% 79% 19% . |
| 2 | V4 | 162 | 47% 90% 10% . |
| 2 | V8 | 162 | 47% 91% 9% . |
| 2 | W1 | 162 | 36% 90% 10% . |
| 2 | W3 | 162 | 35% 91% 9% . |
| 2 | W9 | 162 | 54% 88% 11% . |
| 2 | WA | 162 | 54% 88% 11% . |
| 2 | X4 | 162 | 40% 81% 19% . |
| 2 | X8 | 162 | 41% 78% 21% . |
| 2 | Y1 | 162 | 16% 87% 12% . |
| 2 | Y3 | 162 | 16% 88% 11% . |
| 2 | Y9 | 162 | . 87% 12% . |
| 2 | YA | 162 | 5% 86% 13% . |
| 3 | B1 | 172 | . 77% 21% . |
| 3 | B2 | 172 | . 84% 15% .. |
| 3 | B3 | 172 | . 77% 22% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 3 | B4 | 172 |  |
| 3 | B6 | 172 |  |
| 3 | B8 | 172 |  |
| 3 | B9 | 172 |  |
| 3 | BA | 172 |  |
| 3 | D1 | 172 |  |
| 3 | D2 | 172 |  |
| 3 | D3 | 172 |  |
| 3 | D4 | 172 |  |
| 3 | D6 | 172 |  |
| 3 | D8 | 172 |  |
| 3 | D9 | 172 |  |
| 3 | DA | 172 |  |
| 3 | F1 | 172 |  |
| 3 | F2 | 172 |  |
| 3 | F3 | 172 |  |
| 3 | F4 | 172 |  |
| 3 | F6 | 172 |  |
| 3 | F8 | 172 |  |
| 3 | F9 | 172 |  |
| 3 | FA | 172 |  |
| 3 | H1 | 172 |  |
| 3 | H2 | 172 |  |
| 3 | H3 | 172 |  |
| 3 | H4 | 172 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | H6 | 172 | |
| 3 | H8 | 172 | |
| 3 | H9 | 172 | |
| 3 | HA | 172 | |
| 3 | J1 | 172 | |
| 3 | J2 | 172 | |
| 3 | J3 | 172 | |
| 3 | J4 | 172 | |
| 3 | J6 | 172 | |
| 3 | J8 | 172 | |
| 3 | J9 | 172 | |
| 3 | JA | 172 | |
| 3 | L1 | 172 | |
| 3 | L2 | 172 | |
| 3 | L3 | 172 | |
| 3 | L4 | 172 | |
| 3 | L6 | 172 | |
| 3 | L8 | 172 | |
| 3 | L9 | 172 | |
| 3 | LA | 172 | |
| 3 | O4 | 172 | |
| 3 | O8 | 172 | |
| 3 | P1 | 172 | |
| 3 | P3 | 172 | |
| 3 | P9 | 172 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | PA | 172 | |
| 3 | Q4 | 172 | |
| 3 | Q8 | 172 | |
| 3 | R1 | 172 | |
| 3 | R3 | 172 | |
| 3 | R9 | 172 | |
| 3 | RA | 172 | |
| 3 | S4 | 172 | |
| 3 | S8 | 172 | |
| 3 | T1 | 172 | |
| 3 | T3 | 172 | |
| 3 | T9 | 172 | |
| 3 | TA | 172 | |
| 3 | U4 | 172 | |
| 3 | U8 | 172 | |
| 3 | V1 | 172 | |
| 3 | V3 | 172 | |
| 3 | V9 | 172 | |
| 3 | VA | 172 | |
| 3 | W4 | 172 | |
| 3 | W8 | 172 | |
| 3 | X1 | 172 | |
| 3 | X3 | 172 | |
| 3 | X9 | 172 | |
| 3 | XA | 172 | |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | Y4 | 172 | |
| 3 | Y8 | 172 | |
| 3 | Z1 | 172 | |
| 3 | Z3 | 172 | |
| 3 | Z9 | 172 | |
| 3 | ZA | 172 | |
| 4 | M1 | 274 | |
| 4 | M3 | 274 | |
| 4 | M4 | 274 | |
| 4 | M8 | 274 | |
| 4 | M9 | 274 | |
| 4 | MA | 274 | |
| 5 | N1 | 275 | |
| 5 | N3 | 275 | |
| 5 | N9 | 275 | |
| 5 | NA | 275 | |
| 5 | Z4 | 275 | |
| 5 | Z8 | 275 | |
| 6 | M2 | 729 | |
| 6 | M6 | 729 | |
| 7 | N2 | 70 | |
| 7 | N6 | 70 | |
| 8 | A5 | 161 | |
| 8 | A7 | 161 | |
| 8 | C5 | 161 | |





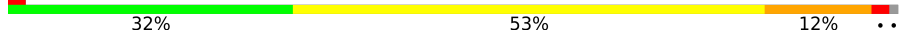


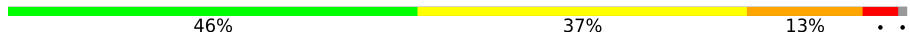


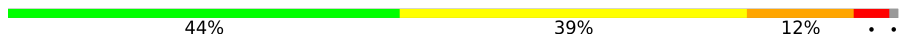
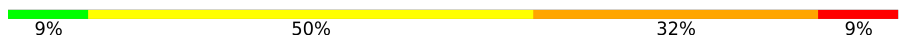







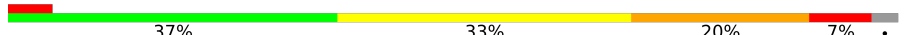
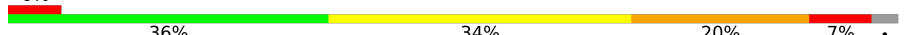
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 8 | C7 | 161 |  63% 34% ... |
| 8 | E5 | 161 |  52% 31% 13% .. |
| 8 | E7 | 161 |  69% 27% .. |
| 8 | G5 | 161 |  53% 39% 7% .. |
| 8 | G7 | 161 |  69% 28% .. |
| 8 | I5 | 161 |  58% 32% 6% .. |
| 8 | I7 | 161 |  61% 35% ... |
| 8 | K5 | 161 |  50% 34% 12% .. |
| 8 | K7 | 161 |  70% 27% .. |
| 8 | M5 | 161 |  66% 30% .. |
| 8 | M7 | 161 |  68% 28% .. |
| 8 | O5 | 161 |  59% 34% |
| 8 | O7 | 161 |  60% 34% |
| 8 | Q5 | 161 |  66% 28% |
| 8 | Q7 | 161 |  66% 30% .. |
| 8 | S5 | 161 |  67% 30% .. |
| 8 | S7 | 161 |  66% 30% .. |
| 8 | U5 | 161 |  54% 40% |
| 8 | U7 | 161 |  62% 32% |
| 8 | W5 | 161 |  66% 29% |
| 8 | W7 | 161 |  66% 30% .. |
| 8 | Y5 | 161 |  71% 26% .. |
| 8 | Y7 | 161 |  70% 27% .. |
| 8 | a5 | 161 |  58% 34% |
| 8 | a7 | 161 |  60% 33% 6% .. |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 8 | c5 | 161 |  |
| 8 | c7 | 161 |  |
| 8 | e5 | 161 |  |
| 8 | e7 | 161 |  |
| 8 | g7 | 161 |  |
| 8 | i7 | 161 |  |
| 8 | k7 | 161 |  |
| 8 | m7 | 161 |  |
| 8 | o7 | 161 |  |
| 8 | q7 | 161 |  |
| 8 | s7 | 161 |  |
| 8 | u7 | 161 |  |
| 9 | i5 | 68 |  |
| 9 | w7 | 68 |  |
| 9 | x7 | 68 |  |
| 9 | y7 | 68 |  |
| 9 | z5 | 68 |  |
| 9 | z7 | 68 |  |
| 10 | j5 | 1155 |  |
| 10 | k5 | 1155 |  |
| 11 | a9 | 824 |  |
| 11 | aA | 824 |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 1 | MEN | D5 | 71 | - | - | X | - |
| 1 | MEN | J5 | 71 | - | - | X | - |
| 1 | MEN | v7 | 71 | - | - | X | - |
| 12 | CYC | A5 | 201 | - | - | X | - |
| 12 | CYC | B1 | 202 | - | - | X | - |
| 12 | CYC | B3 | 202 | - | - | X | - |
| 12 | CYC | B4 | 202 | - | - | X | - |
| 12 | CYC | B5 | 201 | - | - | X | - |
| 12 | CYC | B8 | 202 | - | - | X | - |
| 12 | CYC | D7 | 201 | - | - | X | - |
| 12 | CYC | D8 | 202 | - | - | X | - |
| 12 | CYC | E5 | 201 | - | - | X | - |
| 12 | CYC | F1 | 201 | - | - | X | - |
| 12 | CYC | F2 | 201 | - | - | X | - |
| 12 | CYC | F3 | 201 | - | - | X | - |
| 12 | CYC | F6 | 201 | - | - | X | - |
| 12 | CYC | F9 | 302 | - | - | X | - |
| 12 | CYC | G5 | 201 | - | - | X | - |
| 12 | CYC | H1 | 201 | - | - | X | - |
| 12 | CYC | H4 | 201 | - | - | X | - |
| 12 | CYC | H5 | 201 | - | - | X | - |
| 12 | CYC | H8 | 201 | - | - | X | - |
| 12 | CYC | H9 | 202 | - | - | X | - |
| 12 | CYC | HA | 202 | - | - | X | - |
| 12 | CYC | J3 | 202 | - | - | X | - |
| 12 | CYC | J7 | 201 | - | - | X | - |
| 12 | CYC | J9 | 202 | - | - | X | - |
| 12 | CYC | JA | 202 | - | - | X | - |
| 12 | CYC | K5 | 201 | - | - | X | - |
| 12 | CYC | L3 | 202 | - | - | X | - |
| 12 | CYC | L4 | 202 | - | - | X | - |
| 12 | CYC | L9 | 202 | - | - | X | - |
| 12 | CYC | LA | 202 | - | - | X | - |
| 12 | CYC | M4 | 301 | - | - | X | - |
| 12 | CYC | M8 | 301 | - | - | X | - |
| 12 | CYC | M8 | 302 | - | - | X | - |
| 12 | CYC | O4 | 201 | - | - | X | - |
| 12 | CYC | QA | 201 | - | - | X | - |
| 12 | CYC | R1 | 201 | - | - | X | - |
| 12 | CYC | R3 | 201 | - | - | X | - |
| 12 | CYC | S4 | 202 | - | - | X | - |
| 12 | CYC | T1 | 301 | - | - | X | - |
| 12 | CYC | T3 | 301 | - | - | X | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 12 | CYC | T9 | 301 | - | - | X | - |
| 12 | CYC | TA | 301 | - | - | X | - |
| 12 | CYC | V9 | 201 | - | - | X | - |
| 12 | CYC | VA | 201 | - | - | X | - |
| 12 | CYC | Z1 | 202 | - | - | X | - |
| 12 | CYC | Z3 | 201 | - | - | X | - |
| 12 | CYC | Z4 | 301 | - | - | X | - |
| 12 | CYC | Z8 | 301 | - | - | X | - |
| 12 | CYC | a9 | 901 | - | - | X | - |
| 12 | CYC | aA | 901 | - | - | X | - |
| 12 | CYC | j5 | 1201 | - | - | X | - |
| 12 | CYC | j5 | 1202 | - | - | X | - |
| 12 | CYC | k5 | 1201 | - | - | X | - |
| 12 | CYC | k5 | 1203 | - | - | X | - |
| 12 | CYC | k5 | 1204 | - | - | X | - |
| 12 | CYC | v7 | 201 | - | - | X | - |

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 382772 atoms, of which 76 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Allophycocyanin beta subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1 | A | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | Z | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | L5 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | N5 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | B5 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | D5 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | F5 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | H5 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | J5 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | d5 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | f5 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | P5 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | R5 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | T5 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | V5 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | X5 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | Z5 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1 | b5 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | P7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | R7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | B7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | D7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | F7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | H7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | J7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | L7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | N7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | h7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | j7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | T7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | V7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | X7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | Z7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | b7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | d7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | f7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | l7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | n7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1 | p7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | r7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | t7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |
| 1 | v7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 767 | 202 | 235 | 6 | | |

- Molecule 2 is a protein called Phycocyanin alpha chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | AA | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | CA | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | EA | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | GA | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | IA | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | KA | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | OA | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | QA | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | SA | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | UA | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | WA | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | YA | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | O1 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | Q1 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | S1 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | A1 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | G3 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | I3 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | K3 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | G2 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | I2 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | K2 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | A3 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | C3 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | E3 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | A4 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | C4 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | O3 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | Q3 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | S3 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | U3 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | W3 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | Y3 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | T4 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | V4 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | E4 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | G4 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | I4 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | K4 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | N4 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | P4 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | R4 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | X4 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | C1 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | K6 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | A6 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | C6 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | E6 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | G6 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | I6 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | E1 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | A8 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | C8 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | E8 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | T8 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | V8 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | X8 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | G8 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | I8 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | K8 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | N8 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | P8 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | R8 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | O9 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | Q9 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | A9 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | C9 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | E9 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | G9 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | I9 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | K9 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | S9 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | U9 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | W9 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | Y9 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | G1 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | I1 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | K1 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | U1 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | W1 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | Y1 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | A2 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | C2 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |
| 2 | E2 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1243 | 779 | 217 | 242 | 5 | | |

- Molecule 3 is a protein called Phycocyanin beta chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | BA | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | DA | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | FA | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | HA | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | JA | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | LA | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | PA | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | RA | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | TA | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | VA | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | XA | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | ZA | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | P1 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | R1 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | H3 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | J3 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | H2 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | J2 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | L2 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | B3 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | D3 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | F3 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | Z3 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | B4 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | D4 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | L3 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | P3 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | R3 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | T3 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | V3 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | X3 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | B1 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | S4 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | U4 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | W4 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | F4 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | H4 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | J4 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | L4 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | O4 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | Q4 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | Y4 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | J6 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | L6 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | B6 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | D6 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | F6 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | H6 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | D1 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | B8 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | D8 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | U8 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | W8 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | F8 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | H8 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | J8 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | L8 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | O8 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | Q8 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | S8 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | F1 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | L9 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | P9 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | Y8 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | B9 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | D9 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | F9 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | H9 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | J9 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | R9 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | T9 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | V9 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | X9 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | Z9 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | H1 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | J1 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | L1 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | T1 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | V1 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | X1 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | Z1 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | B2 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | D2 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |
| 3 | F2 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 802 | 229 | 255 | 7 | | |

- Molecule 4 is a protein called Phycocyanin-associated rod linker protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4 | MA | 274 | Total | C | N | O | S | 0 | 0 |
| | | | 2178 | 1383 | 377 | 413 | 5 | | |
| 4 | M3 | 274 | Total | C | N | O | S | 0 | 0 |
| | | | 2178 | 1383 | 377 | 413 | 5 | | |
| 4 | M4 | 274 | Total | C | N | O | S | 0 | 0 |
| | | | 2178 | 1383 | 377 | 413 | 5 | | |
| 4 | M8 | 274 | Total | C | N | O | S | 0 | 0 |
| | | | 2178 | 1383 | 377 | 413 | 5 | | |
| 4 | M9 | 274 | Total | C | N | O | S | 0 | 0 |
| | | | 2178 | 1383 | 377 | 413 | 5 | | |
| 4 | M1 | 274 | Total | C | N | O | S | 0 | 0 |
| | | | 2178 | 1383 | 377 | 413 | 5 | | |

There are 330 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| MA | 1 | MET | - | initiating methionine | UNP Q7NGF2 |
| MA | 2 | ASN | - | expression tag | UNP Q7NGF2 |
| MA | 3 | VAL | - | expression tag | UNP Q7NGF2 |
| MA | 4 | LEU | - | expression tag | UNP Q7NGF2 |
| MA | 5 | THR | - | expression tag | UNP Q7NGF2 |
| MA | 6 | THR | - | expression tag | UNP Q7NGF2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| MA | 7 | SER | - | expression tag | UNP Q7NGF2 |
| MA | 8 | SER | - | expression tag | UNP Q7NGF2 |
| MA | 9 | GLN | - | expression tag | UNP Q7NGF2 |
| MA | 10 | ARG | - | expression tag | UNP Q7NGF2 |
| MA | 11 | GLY | - | expression tag | UNP Q7NGF2 |
| MA | 12 | GLY | - | expression tag | UNP Q7NGF2 |
| MA | 13 | LYS | - | expression tag | UNP Q7NGF2 |
| MA | 14 | LEU | - | expression tag | UNP Q7NGF2 |
| MA | 15 | PHE | - | expression tag | UNP Q7NGF2 |
| MA | 16 | LYS | - | expression tag | UNP Q7NGF2 |
| MA | 17 | VAL | - | expression tag | UNP Q7NGF2 |
| MA | 18 | THR | - | expression tag | UNP Q7NGF2 |
| MA | 19 | MET | - | expression tag | UNP Q7NGF2 |
| MA | 20 | THR | - | expression tag | UNP Q7NGF2 |
| MA | 21 | LEU | - | expression tag | UNP Q7NGF2 |
| MA | 22 | SER | - | expression tag | UNP Q7NGF2 |
| MA | 23 | PRO | - | expression tag | UNP Q7NGF2 |
| MA | 24 | ALA | - | expression tag | UNP Q7NGF2 |
| MA | 25 | LEU | - | expression tag | UNP Q7NGF2 |
| MA | 26 | SER | - | expression tag | UNP Q7NGF2 |
| MA | 27 | HIS | - | expression tag | UNP Q7NGF2 |
| MA | 28 | HIS | - | expression tag | UNP Q7NGF2 |
| MA | 29 | PRO | - | expression tag | UNP Q7NGF2 |
| MA | 30 | TRP | - | expression tag | UNP Q7NGF2 |
| MA | 31 | PRO | - | expression tag | UNP Q7NGF2 |
| MA | 32 | SER | - | expression tag | UNP Q7NGF2 |
| MA | 33 | LEU | - | expression tag | UNP Q7NGF2 |
| MA | 34 | ASP | - | expression tag | UNP Q7NGF2 |
| MA | 35 | THR | - | expression tag | UNP Q7NGF2 |
| MA | 36 | TYR | - | expression tag | UNP Q7NGF2 |
| MA | 37 | GLU | - | expression tag | UNP Q7NGF2 |
| MA | 38 | PRO | - | expression tag | UNP Q7NGF2 |
| MA | 39 | SER | - | expression tag | UNP Q7NGF2 |
| MA | 40 | GLN | - | expression tag | UNP Q7NGF2 |
| MA | 41 | ASN | - | expression tag | UNP Q7NGF2 |
| MA | 42 | SER | - | expression tag | UNP Q7NGF2 |
| MA | 43 | TYR | - | expression tag | UNP Q7NGF2 |
| MA | 44 | SER | - | expression tag | UNP Q7NGF2 |
| MA | 45 | VAL | - | expression tag | UNP Q7NGF2 |
| MA | 46 | VAL | - | expression tag | UNP Q7NGF2 |
| MA | 47 | VAL | - | expression tag | UNP Q7NGF2 |
| MA | 48 | PRO | - | expression tag | UNP Q7NGF2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| MA | 49 | LEU | - | expression tag | UNP Q7NGF2 |
| MA | 50 | ASP | - | expression tag | UNP Q7NGF2 |
| MA | 51 | ARG | - | expression tag | UNP Q7NGF2 |
| MA | 52 | LEU | - | expression tag | UNP Q7NGF2 |
| MA | 53 | LEU | - | expression tag | UNP Q7NGF2 |
| MA | 54 | ALA | - | expression tag | UNP Q7NGF2 |
| MA | 55 | GLU | - | expression tag | UNP Q7NGF2 |
| M3 | 1 | MET | - | initiating methionine | UNP Q7NGF2 |
| M3 | 2 | ASN | - | expression tag | UNP Q7NGF2 |
| M3 | 3 | VAL | - | expression tag | UNP Q7NGF2 |
| M3 | 4 | LEU | - | expression tag | UNP Q7NGF2 |
| M3 | 5 | THR | - | expression tag | UNP Q7NGF2 |
| M3 | 6 | THR | - | expression tag | UNP Q7NGF2 |
| M3 | 7 | SER | - | expression tag | UNP Q7NGF2 |
| M3 | 8 | SER | - | expression tag | UNP Q7NGF2 |
| M3 | 9 | GLN | - | expression tag | UNP Q7NGF2 |
| M3 | 10 | ARG | - | expression tag | UNP Q7NGF2 |
| M3 | 11 | GLY | - | expression tag | UNP Q7NGF2 |
| M3 | 12 | GLY | - | expression tag | UNP Q7NGF2 |
| M3 | 13 | LYS | - | expression tag | UNP Q7NGF2 |
| M3 | 14 | LEU | - | expression tag | UNP Q7NGF2 |
| M3 | 15 | PHE | - | expression tag | UNP Q7NGF2 |
| M3 | 16 | LYS | - | expression tag | UNP Q7NGF2 |
| M3 | 17 | VAL | - | expression tag | UNP Q7NGF2 |
| M3 | 18 | THR | - | expression tag | UNP Q7NGF2 |
| M3 | 19 | MET | - | expression tag | UNP Q7NGF2 |
| M3 | 20 | THR | - | expression tag | UNP Q7NGF2 |
| M3 | 21 | LEU | - | expression tag | UNP Q7NGF2 |
| M3 | 22 | SER | - | expression tag | UNP Q7NGF2 |
| M3 | 23 | PRO | - | expression tag | UNP Q7NGF2 |
| M3 | 24 | ALA | - | expression tag | UNP Q7NGF2 |
| M3 | 25 | LEU | - | expression tag | UNP Q7NGF2 |
| M3 | 26 | SER | - | expression tag | UNP Q7NGF2 |
| M3 | 27 | HIS | - | expression tag | UNP Q7NGF2 |
| M3 | 28 | HIS | - | expression tag | UNP Q7NGF2 |
| M3 | 29 | PRO | - | expression tag | UNP Q7NGF2 |
| M3 | 30 | TRP | - | expression tag | UNP Q7NGF2 |
| M3 | 31 | PRO | - | expression tag | UNP Q7NGF2 |
| M3 | 32 | SER | - | expression tag | UNP Q7NGF2 |
| M3 | 33 | LEU | - | expression tag | UNP Q7NGF2 |
| M3 | 34 | ASP | - | expression tag | UNP Q7NGF2 |
| M3 | 35 | THR | - | expression tag | UNP Q7NGF2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| M3 | 36 | TYR | - | expression tag | UNP Q7NGF2 |
| M3 | 37 | GLU | - | expression tag | UNP Q7NGF2 |
| M3 | 38 | PRO | - | expression tag | UNP Q7NGF2 |
| M3 | 39 | SER | - | expression tag | UNP Q7NGF2 |
| M3 | 40 | GLN | - | expression tag | UNP Q7NGF2 |
| M3 | 41 | ASN | - | expression tag | UNP Q7NGF2 |
| M3 | 42 | SER | - | expression tag | UNP Q7NGF2 |
| M3 | 43 | TYR | - | expression tag | UNP Q7NGF2 |
| M3 | 44 | SER | - | expression tag | UNP Q7NGF2 |
| M3 | 45 | VAL | - | expression tag | UNP Q7NGF2 |
| M3 | 46 | VAL | - | expression tag | UNP Q7NGF2 |
| M3 | 47 | VAL | - | expression tag | UNP Q7NGF2 |
| M3 | 48 | PRO | - | expression tag | UNP Q7NGF2 |
| M3 | 49 | LEU | - | expression tag | UNP Q7NGF2 |
| M3 | 50 | ASP | - | expression tag | UNP Q7NGF2 |
| M3 | 51 | ARG | - | expression tag | UNP Q7NGF2 |
| M3 | 52 | LEU | - | expression tag | UNP Q7NGF2 |
| M3 | 53 | LEU | - | expression tag | UNP Q7NGF2 |
| M3 | 54 | ALA | - | expression tag | UNP Q7NGF2 |
| M3 | 55 | GLU | - | expression tag | UNP Q7NGF2 |
| M4 | 1 | MET | - | initiating methionine | UNP Q7NGF2 |
| M4 | 2 | ASN | - | expression tag | UNP Q7NGF2 |
| M4 | 3 | VAL | - | expression tag | UNP Q7NGF2 |
| M4 | 4 | LEU | - | expression tag | UNP Q7NGF2 |
| M4 | 5 | THR | - | expression tag | UNP Q7NGF2 |
| M4 | 6 | THR | - | expression tag | UNP Q7NGF2 |
| M4 | 7 | SER | - | expression tag | UNP Q7NGF2 |
| M4 | 8 | SER | - | expression tag | UNP Q7NGF2 |
| M4 | 9 | GLN | - | expression tag | UNP Q7NGF2 |
| M4 | 10 | ARG | - | expression tag | UNP Q7NGF2 |
| M4 | 11 | GLY | - | expression tag | UNP Q7NGF2 |
| M4 | 12 | GLY | - | expression tag | UNP Q7NGF2 |
| M4 | 13 | LYS | - | expression tag | UNP Q7NGF2 |
| M4 | 14 | LEU | - | expression tag | UNP Q7NGF2 |
| M4 | 15 | PHE | - | expression tag | UNP Q7NGF2 |
| M4 | 16 | LYS | - | expression tag | UNP Q7NGF2 |
| M4 | 17 | VAL | - | expression tag | UNP Q7NGF2 |
| M4 | 18 | THR | - | expression tag | UNP Q7NGF2 |
| M4 | 19 | MET | - | expression tag | UNP Q7NGF2 |
| M4 | 20 | THR | - | expression tag | UNP Q7NGF2 |
| M4 | 21 | LEU | - | expression tag | UNP Q7NGF2 |
| M4 | 22 | SER | - | expression tag | UNP Q7NGF2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| M4 | 23 | PRO | - | expression tag | UNP Q7NGF2 |
| M4 | 24 | ALA | - | expression tag | UNP Q7NGF2 |
| M4 | 25 | LEU | - | expression tag | UNP Q7NGF2 |
| M4 | 26 | SER | - | expression tag | UNP Q7NGF2 |
| M4 | 27 | HIS | - | expression tag | UNP Q7NGF2 |
| M4 | 28 | HIS | - | expression tag | UNP Q7NGF2 |
| M4 | 29 | PRO | - | expression tag | UNP Q7NGF2 |
| M4 | 30 | TRP | - | expression tag | UNP Q7NGF2 |
| M4 | 31 | PRO | - | expression tag | UNP Q7NGF2 |
| M4 | 32 | SER | - | expression tag | UNP Q7NGF2 |
| M4 | 33 | LEU | - | expression tag | UNP Q7NGF2 |
| M4 | 34 | ASP | - | expression tag | UNP Q7NGF2 |
| M4 | 35 | THR | - | expression tag | UNP Q7NGF2 |
| M4 | 36 | TYR | - | expression tag | UNP Q7NGF2 |
| M4 | 37 | GLU | - | expression tag | UNP Q7NGF2 |
| M4 | 38 | PRO | - | expression tag | UNP Q7NGF2 |
| M4 | 39 | SER | - | expression tag | UNP Q7NGF2 |
| M4 | 40 | GLN | - | expression tag | UNP Q7NGF2 |
| M4 | 41 | ASN | - | expression tag | UNP Q7NGF2 |
| M4 | 42 | SER | - | expression tag | UNP Q7NGF2 |
| M4 | 43 | TYR | - | expression tag | UNP Q7NGF2 |
| M4 | 44 | SER | - | expression tag | UNP Q7NGF2 |
| M4 | 45 | VAL | - | expression tag | UNP Q7NGF2 |
| M4 | 46 | VAL | - | expression tag | UNP Q7NGF2 |
| M4 | 47 | VAL | - | expression tag | UNP Q7NGF2 |
| M4 | 48 | PRO | - | expression tag | UNP Q7NGF2 |
| M4 | 49 | LEU | - | expression tag | UNP Q7NGF2 |
| M4 | 50 | ASP | - | expression tag | UNP Q7NGF2 |
| M4 | 51 | ARG | - | expression tag | UNP Q7NGF2 |
| M4 | 52 | LEU | - | expression tag | UNP Q7NGF2 |
| M4 | 53 | LEU | - | expression tag | UNP Q7NGF2 |
| M4 | 54 | ALA | - | expression tag | UNP Q7NGF2 |
| M4 | 55 | GLU | - | expression tag | UNP Q7NGF2 |
| M8 | 1 | MET | - | initiating methionine | UNP Q7NGF2 |
| M8 | 2 | ASN | - | expression tag | UNP Q7NGF2 |
| M8 | 3 | VAL | - | expression tag | UNP Q7NGF2 |
| M8 | 4 | LEU | - | expression tag | UNP Q7NGF2 |
| M8 | 5 | THR | - | expression tag | UNP Q7NGF2 |
| M8 | 6 | THR | - | expression tag | UNP Q7NGF2 |
| M8 | 7 | SER | - | expression tag | UNP Q7NGF2 |
| M8 | 8 | SER | - | expression tag | UNP Q7NGF2 |
| M8 | 9 | GLN | - | expression tag | UNP Q7NGF2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| M8 | 10 | ARG | - | expression tag | UNP Q7NGF2 |
| M8 | 11 | GLY | - | expression tag | UNP Q7NGF2 |
| M8 | 12 | GLY | - | expression tag | UNP Q7NGF2 |
| M8 | 13 | LYS | - | expression tag | UNP Q7NGF2 |
| M8 | 14 | LEU | - | expression tag | UNP Q7NGF2 |
| M8 | 15 | PHE | - | expression tag | UNP Q7NGF2 |
| M8 | 16 | LYS | - | expression tag | UNP Q7NGF2 |
| M8 | 17 | VAL | - | expression tag | UNP Q7NGF2 |
| M8 | 18 | THR | - | expression tag | UNP Q7NGF2 |
| M8 | 19 | MET | - | expression tag | UNP Q7NGF2 |
| M8 | 20 | THR | - | expression tag | UNP Q7NGF2 |
| M8 | 21 | LEU | - | expression tag | UNP Q7NGF2 |
| M8 | 22 | SER | - | expression tag | UNP Q7NGF2 |
| M8 | 23 | PRO | - | expression tag | UNP Q7NGF2 |
| M8 | 24 | ALA | - | expression tag | UNP Q7NGF2 |
| M8 | 25 | LEU | - | expression tag | UNP Q7NGF2 |
| M8 | 26 | SER | - | expression tag | UNP Q7NGF2 |
| M8 | 27 | HIS | - | expression tag | UNP Q7NGF2 |
| M8 | 28 | HIS | - | expression tag | UNP Q7NGF2 |
| M8 | 29 | PRO | - | expression tag | UNP Q7NGF2 |
| M8 | 30 | TRP | - | expression tag | UNP Q7NGF2 |
| M8 | 31 | PRO | - | expression tag | UNP Q7NGF2 |
| M8 | 32 | SER | - | expression tag | UNP Q7NGF2 |
| M8 | 33 | LEU | - | expression tag | UNP Q7NGF2 |
| M8 | 34 | ASP | - | expression tag | UNP Q7NGF2 |
| M8 | 35 | THR | - | expression tag | UNP Q7NGF2 |
| M8 | 36 | TYR | - | expression tag | UNP Q7NGF2 |
| M8 | 37 | GLU | - | expression tag | UNP Q7NGF2 |
| M8 | 38 | PRO | - | expression tag | UNP Q7NGF2 |
| M8 | 39 | SER | - | expression tag | UNP Q7NGF2 |
| M8 | 40 | GLN | - | expression tag | UNP Q7NGF2 |
| M8 | 41 | ASN | - | expression tag | UNP Q7NGF2 |
| M8 | 42 | SER | - | expression tag | UNP Q7NGF2 |
| M8 | 43 | TYR | - | expression tag | UNP Q7NGF2 |
| M8 | 44 | SER | - | expression tag | UNP Q7NGF2 |
| M8 | 45 | VAL | - | expression tag | UNP Q7NGF2 |
| M8 | 46 | VAL | - | expression tag | UNP Q7NGF2 |
| M8 | 47 | VAL | - | expression tag | UNP Q7NGF2 |
| M8 | 48 | PRO | - | expression tag | UNP Q7NGF2 |
| M8 | 49 | LEU | - | expression tag | UNP Q7NGF2 |
| M8 | 50 | ASP | - | expression tag | UNP Q7NGF2 |
| M8 | 51 | ARG | - | expression tag | UNP Q7NGF2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| M8 | 52 | LEU | - | expression tag | UNP Q7NGF2 |
| M8 | 53 | LEU | - | expression tag | UNP Q7NGF2 |
| M8 | 54 | ALA | - | expression tag | UNP Q7NGF2 |
| M8 | 55 | GLU | - | expression tag | UNP Q7NGF2 |
| M9 | 1 | MET | - | initiating methionine | UNP Q7NGF2 |
| M9 | 2 | ASN | - | expression tag | UNP Q7NGF2 |
| M9 | 3 | VAL | - | expression tag | UNP Q7NGF2 |
| M9 | 4 | LEU | - | expression tag | UNP Q7NGF2 |
| M9 | 5 | THR | - | expression tag | UNP Q7NGF2 |
| M9 | 6 | THR | - | expression tag | UNP Q7NGF2 |
| M9 | 7 | SER | - | expression tag | UNP Q7NGF2 |
| M9 | 8 | SER | - | expression tag | UNP Q7NGF2 |
| M9 | 9 | GLN | - | expression tag | UNP Q7NGF2 |
| M9 | 10 | ARG | - | expression tag | UNP Q7NGF2 |
| M9 | 11 | GLY | - | expression tag | UNP Q7NGF2 |
| M9 | 12 | GLY | - | expression tag | UNP Q7NGF2 |
| M9 | 13 | LYS | - | expression tag | UNP Q7NGF2 |
| M9 | 14 | LEU | - | expression tag | UNP Q7NGF2 |
| M9 | 15 | PHE | - | expression tag | UNP Q7NGF2 |
| M9 | 16 | LYS | - | expression tag | UNP Q7NGF2 |
| M9 | 17 | VAL | - | expression tag | UNP Q7NGF2 |
| M9 | 18 | THR | - | expression tag | UNP Q7NGF2 |
| M9 | 19 | MET | - | expression tag | UNP Q7NGF2 |
| M9 | 20 | THR | - | expression tag | UNP Q7NGF2 |
| M9 | 21 | LEU | - | expression tag | UNP Q7NGF2 |
| M9 | 22 | SER | - | expression tag | UNP Q7NGF2 |
| M9 | 23 | PRO | - | expression tag | UNP Q7NGF2 |
| M9 | 24 | ALA | - | expression tag | UNP Q7NGF2 |
| M9 | 25 | LEU | - | expression tag | UNP Q7NGF2 |
| M9 | 26 | SER | - | expression tag | UNP Q7NGF2 |
| M9 | 27 | HIS | - | expression tag | UNP Q7NGF2 |
| M9 | 28 | HIS | - | expression tag | UNP Q7NGF2 |
| M9 | 29 | PRO | - | expression tag | UNP Q7NGF2 |
| M9 | 30 | TRP | - | expression tag | UNP Q7NGF2 |
| M9 | 31 | PRO | - | expression tag | UNP Q7NGF2 |
| M9 | 32 | SER | - | expression tag | UNP Q7NGF2 |
| M9 | 33 | LEU | - | expression tag | UNP Q7NGF2 |
| M9 | 34 | ASP | - | expression tag | UNP Q7NGF2 |
| M9 | 35 | THR | - | expression tag | UNP Q7NGF2 |
| M9 | 36 | TYR | - | expression tag | UNP Q7NGF2 |
| M9 | 37 | GLU | - | expression tag | UNP Q7NGF2 |
| M9 | 38 | PRO | - | expression tag | UNP Q7NGF2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| M9 | 39 | SER | - | expression tag | UNP Q7NGF2 |
| M9 | 40 | GLN | - | expression tag | UNP Q7NGF2 |
| M9 | 41 | ASN | - | expression tag | UNP Q7NGF2 |
| M9 | 42 | SER | - | expression tag | UNP Q7NGF2 |
| M9 | 43 | TYR | - | expression tag | UNP Q7NGF2 |
| M9 | 44 | SER | - | expression tag | UNP Q7NGF2 |
| M9 | 45 | VAL | - | expression tag | UNP Q7NGF2 |
| M9 | 46 | VAL | - | expression tag | UNP Q7NGF2 |
| M9 | 47 | VAL | - | expression tag | UNP Q7NGF2 |
| M9 | 48 | PRO | - | expression tag | UNP Q7NGF2 |
| M9 | 49 | LEU | - | expression tag | UNP Q7NGF2 |
| M9 | 50 | ASP | - | expression tag | UNP Q7NGF2 |
| M9 | 51 | ARG | - | expression tag | UNP Q7NGF2 |
| M9 | 52 | LEU | - | expression tag | UNP Q7NGF2 |
| M9 | 53 | LEU | - | expression tag | UNP Q7NGF2 |
| M9 | 54 | ALA | - | expression tag | UNP Q7NGF2 |
| M9 | 55 | GLU | - | expression tag | UNP Q7NGF2 |
| M1 | 1 | MET | - | initiating methionine | UNP Q7NGF2 |
| M1 | 2 | ASN | - | expression tag | UNP Q7NGF2 |
| M1 | 3 | VAL | - | expression tag | UNP Q7NGF2 |
| M1 | 4 | LEU | - | expression tag | UNP Q7NGF2 |
| M1 | 5 | THR | - | expression tag | UNP Q7NGF2 |
| M1 | 6 | THR | - | expression tag | UNP Q7NGF2 |
| M1 | 7 | SER | - | expression tag | UNP Q7NGF2 |
| M1 | 8 | SER | - | expression tag | UNP Q7NGF2 |
| M1 | 9 | GLN | - | expression tag | UNP Q7NGF2 |
| M1 | 10 | ARG | - | expression tag | UNP Q7NGF2 |
| M1 | 11 | GLY | - | expression tag | UNP Q7NGF2 |
| M1 | 12 | GLY | - | expression tag | UNP Q7NGF2 |
| M1 | 13 | LYS | - | expression tag | UNP Q7NGF2 |
| M1 | 14 | LEU | - | expression tag | UNP Q7NGF2 |
| M1 | 15 | PHE | - | expression tag | UNP Q7NGF2 |
| M1 | 16 | LYS | - | expression tag | UNP Q7NGF2 |
| M1 | 17 | VAL | - | expression tag | UNP Q7NGF2 |
| M1 | 18 | THR | - | expression tag | UNP Q7NGF2 |
| M1 | 19 | MET | - | expression tag | UNP Q7NGF2 |
| M1 | 20 | THR | - | expression tag | UNP Q7NGF2 |
| M1 | 21 | LEU | - | expression tag | UNP Q7NGF2 |
| M1 | 22 | SER | - | expression tag | UNP Q7NGF2 |
| M1 | 23 | PRO | - | expression tag | UNP Q7NGF2 |
| M1 | 24 | ALA | - | expression tag | UNP Q7NGF2 |
| M1 | 25 | LEU | - | expression tag | UNP Q7NGF2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| M1 | 26 | SER | - | expression tag | UNP Q7NGF2 |
| M1 | 27 | HIS | - | expression tag | UNP Q7NGF2 |
| M1 | 28 | HIS | - | expression tag | UNP Q7NGF2 |
| M1 | 29 | PRO | - | expression tag | UNP Q7NGF2 |
| M1 | 30 | TRP | - | expression tag | UNP Q7NGF2 |
| M1 | 31 | PRO | - | expression tag | UNP Q7NGF2 |
| M1 | 32 | SER | - | expression tag | UNP Q7NGF2 |
| M1 | 33 | LEU | - | expression tag | UNP Q7NGF2 |
| M1 | 34 | ASP | - | expression tag | UNP Q7NGF2 |
| M1 | 35 | THR | - | expression tag | UNP Q7NGF2 |
| M1 | 36 | TYR | - | expression tag | UNP Q7NGF2 |
| M1 | 37 | GLU | - | expression tag | UNP Q7NGF2 |
| M1 | 38 | PRO | - | expression tag | UNP Q7NGF2 |
| M1 | 39 | SER | - | expression tag | UNP Q7NGF2 |
| M1 | 40 | GLN | - | expression tag | UNP Q7NGF2 |
| M1 | 41 | ASN | - | expression tag | UNP Q7NGF2 |
| M1 | 42 | SER | - | expression tag | UNP Q7NGF2 |
| M1 | 43 | TYR | - | expression tag | UNP Q7NGF2 |
| M1 | 44 | SER | - | expression tag | UNP Q7NGF2 |
| M1 | 45 | VAL | - | expression tag | UNP Q7NGF2 |
| M1 | 46 | VAL | - | expression tag | UNP Q7NGF2 |
| M1 | 47 | VAL | - | expression tag | UNP Q7NGF2 |
| M1 | 48 | PRO | - | expression tag | UNP Q7NGF2 |
| M1 | 49 | LEU | - | expression tag | UNP Q7NGF2 |
| M1 | 50 | ASP | - | expression tag | UNP Q7NGF2 |
| M1 | 51 | ARG | - | expression tag | UNP Q7NGF2 |
| M1 | 52 | LEU | - | expression tag | UNP Q7NGF2 |
| M1 | 53 | LEU | - | expression tag | UNP Q7NGF2 |
| M1 | 54 | ALA | - | expression tag | UNP Q7NGF2 |
| M1 | 55 | GLU | - | expression tag | UNP Q7NGF2 |

- Molecule 5 is a protein called Phycocyanin-associated rod linker protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5 | NA | 74 | Total | C | N | O | S | 0 | 0 |
| | | | 578 | 361 | 104 | 111 | 2 | | |
| 5 | N3 | 74 | Total | C | N | O | S | 0 | 0 |
| | | | 578 | 361 | 104 | 111 | 2 | | |
| 5 | Z4 | 74 | Total | C | N | O | S | 0 | 0 |
| | | | 578 | 361 | 104 | 111 | 2 | | |
| 5 | N9 | 74 | Total | C | N | O | S | 0 | 0 |
| | | | 578 | 361 | 104 | 111 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5 | Z8 | 74 | Total | C | N | O | S | 0 | 0 |
| | | | 578 | 361 | 104 | 111 | 2 | | |
| 5 | N1 | 74 | Total | C | N | O | S | 0 | 0 |
| | | | 578 | 361 | 104 | 111 | 2 | | |

There are 336 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| NA | 1 | MET | - | initiating methionine | UNP Q7NM19 |
| NA | 2 | SER | - | expression tag | UNP Q7NM19 |
| NA | 3 | VAL | - | expression tag | UNP Q7NM19 |
| NA | 4 | LEU | - | expression tag | UNP Q7NM19 |
| NA | 5 | THR | - | expression tag | UNP Q7NM19 |
| NA | 6 | GLY | - | expression tag | UNP Q7NM19 |
| NA | 7 | ASP | - | expression tag | UNP Q7NM19 |
| NA | 8 | ASN | - | expression tag | UNP Q7NM19 |
| NA | 9 | GLN | - | expression tag | UNP Q7NM19 |
| NA | 10 | GLN | - | expression tag | UNP Q7NM19 |
| NA | 11 | ARG | - | expression tag | UNP Q7NM19 |
| NA | 12 | GLY | - | expression tag | UNP Q7NM19 |
| NA | 13 | SER | - | expression tag | UNP Q7NM19 |
| NA | 14 | LYS | - | expression tag | UNP Q7NM19 |
| NA | 15 | LEU | - | expression tag | UNP Q7NM19 |
| NA | 16 | PHE | - | expression tag | UNP Q7NM19 |
| NA | 17 | LYS | - | expression tag | UNP Q7NM19 |
| NA | 18 | ILE | - | expression tag | UNP Q7NM19 |
| NA | 19 | THR | - | expression tag | UNP Q7NM19 |
| NA | 20 | ILE | - | expression tag | UNP Q7NM19 |
| NA | 21 | ALA | - | expression tag | UNP Q7NM19 |
| NA | 22 | LEU | - | expression tag | UNP Q7NM19 |
| NA | 23 | SER | - | expression tag | UNP Q7NM19 |
| NA | 24 | PRO | - | expression tag | UNP Q7NM19 |
| NA | 25 | THR | - | expression tag | UNP Q7NM19 |
| NA | 26 | LEU | - | expression tag | UNP Q7NM19 |
| NA | 27 | ALA | - | expression tag | UNP Q7NM19 |
| NA | 28 | HIS | - | expression tag | UNP Q7NM19 |
| NA | 29 | HIS | - | expression tag | UNP Q7NM19 |
| NA | 30 | PRO | - | expression tag | UNP Q7NM19 |
| NA | 31 | TRP | - | expression tag | UNP Q7NM19 |
| NA | 32 | PRO | - | expression tag | UNP Q7NM19 |
| NA | 33 | GLY | - | expression tag | UNP Q7NM19 |
| NA | 34 | LEU | - | expression tag | UNP Q7NM19 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| NA | 35 | ASP | - | expression tag | UNP Q7NM19 |
| NA | 36 | THR | - | expression tag | UNP Q7NM19 |
| NA | 37 | HIS | - | expression tag | UNP Q7NM19 |
| NA | 38 | GLU | - | expression tag | UNP Q7NM19 |
| NA | 39 | PRO | - | expression tag | UNP Q7NM19 |
| NA | 40 | SER | - | expression tag | UNP Q7NM19 |
| NA | 41 | GLN | - | expression tag | UNP Q7NM19 |
| NA | 42 | SER | - | expression tag | UNP Q7NM19 |
| NA | 43 | SER | - | expression tag | UNP Q7NM19 |
| NA | 44 | TYR | - | expression tag | UNP Q7NM19 |
| NA | 45 | SER | - | expression tag | UNP Q7NM19 |
| NA | 46 | THR | - | expression tag | UNP Q7NM19 |
| NA | 47 | ILE | - | expression tag | UNP Q7NM19 |
| NA | 48 | VAL | - | expression tag | UNP Q7NM19 |
| NA | 49 | SER | - | expression tag | UNP Q7NM19 |
| NA | 50 | LEU | - | expression tag | UNP Q7NM19 |
| NA | 51 | GLU | - | expression tag | UNP Q7NM19 |
| NA | 52 | ARG | - | expression tag | UNP Q7NM19 |
| NA | 53 | LEU | - | expression tag | UNP Q7NM19 |
| NA | 54 | LEU | - | expression tag | UNP Q7NM19 |
| NA | 55 | PRO | - | expression tag | UNP Q7NM19 |
| NA | 56 | GLU | - | expression tag | UNP Q7NM19 |
| N3 | 1 | MET | - | initiating methionine | UNP Q7NM19 |
| N3 | 2 | SER | - | expression tag | UNP Q7NM19 |
| N3 | 3 | VAL | - | expression tag | UNP Q7NM19 |
| N3 | 4 | LEU | - | expression tag | UNP Q7NM19 |
| N3 | 5 | THR | - | expression tag | UNP Q7NM19 |
| N3 | 6 | GLY | - | expression tag | UNP Q7NM19 |
| N3 | 7 | ASP | - | expression tag | UNP Q7NM19 |
| N3 | 8 | ASN | - | expression tag | UNP Q7NM19 |
| N3 | 9 | GLN | - | expression tag | UNP Q7NM19 |
| N3 | 10 | GLN | - | expression tag | UNP Q7NM19 |
| N3 | 11 | ARG | - | expression tag | UNP Q7NM19 |
| N3 | 12 | GLY | - | expression tag | UNP Q7NM19 |
| N3 | 13 | SER | - | expression tag | UNP Q7NM19 |
| N3 | 14 | LYS | - | expression tag | UNP Q7NM19 |
| N3 | 15 | LEU | - | expression tag | UNP Q7NM19 |
| N3 | 16 | PHE | - | expression tag | UNP Q7NM19 |
| N3 | 17 | LYS | - | expression tag | UNP Q7NM19 |
| N3 | 18 | ILE | - | expression tag | UNP Q7NM19 |
| N3 | 19 | THR | - | expression tag | UNP Q7NM19 |
| N3 | 20 | ILE | - | expression tag | UNP Q7NM19 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| N3 | 21 | ALA | - | expression tag | UNP Q7NM19 |
| N3 | 22 | LEU | - | expression tag | UNP Q7NM19 |
| N3 | 23 | SER | - | expression tag | UNP Q7NM19 |
| N3 | 24 | PRO | - | expression tag | UNP Q7NM19 |
| N3 | 25 | THR | - | expression tag | UNP Q7NM19 |
| N3 | 26 | LEU | - | expression tag | UNP Q7NM19 |
| N3 | 27 | ALA | - | expression tag | UNP Q7NM19 |
| N3 | 28 | HIS | - | expression tag | UNP Q7NM19 |
| N3 | 29 | HIS | - | expression tag | UNP Q7NM19 |
| N3 | 30 | PRO | - | expression tag | UNP Q7NM19 |
| N3 | 31 | TRP | - | expression tag | UNP Q7NM19 |
| N3 | 32 | PRO | - | expression tag | UNP Q7NM19 |
| N3 | 33 | GLY | - | expression tag | UNP Q7NM19 |
| N3 | 34 | LEU | - | expression tag | UNP Q7NM19 |
| N3 | 35 | ASP | - | expression tag | UNP Q7NM19 |
| N3 | 36 | THR | - | expression tag | UNP Q7NM19 |
| N3 | 37 | HIS | - | expression tag | UNP Q7NM19 |
| N3 | 38 | GLU | - | expression tag | UNP Q7NM19 |
| N3 | 39 | PRO | - | expression tag | UNP Q7NM19 |
| N3 | 40 | SER | - | expression tag | UNP Q7NM19 |
| N3 | 41 | GLN | - | expression tag | UNP Q7NM19 |
| N3 | 42 | SER | - | expression tag | UNP Q7NM19 |
| N3 | 43 | SER | - | expression tag | UNP Q7NM19 |
| N3 | 44 | TYR | - | expression tag | UNP Q7NM19 |
| N3 | 45 | SER | - | expression tag | UNP Q7NM19 |
| N3 | 46 | THR | - | expression tag | UNP Q7NM19 |
| N3 | 47 | ILE | - | expression tag | UNP Q7NM19 |
| N3 | 48 | VAL | - | expression tag | UNP Q7NM19 |
| N3 | 49 | SER | - | expression tag | UNP Q7NM19 |
| N3 | 50 | LEU | - | expression tag | UNP Q7NM19 |
| N3 | 51 | GLU | - | expression tag | UNP Q7NM19 |
| N3 | 52 | ARG | - | expression tag | UNP Q7NM19 |
| N3 | 53 | LEU | - | expression tag | UNP Q7NM19 |
| N3 | 54 | LEU | - | expression tag | UNP Q7NM19 |
| N3 | 55 | PRO | - | expression tag | UNP Q7NM19 |
| N3 | 56 | GLU | - | expression tag | UNP Q7NM19 |
| Z4 | 1 | MET | - | initiating methionine | UNP Q7NM19 |
| Z4 | 2 | SER | - | expression tag | UNP Q7NM19 |
| Z4 | 3 | VAL | - | expression tag | UNP Q7NM19 |
| Z4 | 4 | LEU | - | expression tag | UNP Q7NM19 |
| Z4 | 5 | THR | - | expression tag | UNP Q7NM19 |
| Z4 | 6 | GLY | - | expression tag | UNP Q7NM19 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| Z4 | 7 | ASP | - | expression tag | UNP Q7NM19 |
| Z4 | 8 | ASN | - | expression tag | UNP Q7NM19 |
| Z4 | 9 | GLN | - | expression tag | UNP Q7NM19 |
| Z4 | 10 | GLN | - | expression tag | UNP Q7NM19 |
| Z4 | 11 | ARG | - | expression tag | UNP Q7NM19 |
| Z4 | 12 | GLY | - | expression tag | UNP Q7NM19 |
| Z4 | 13 | SER | - | expression tag | UNP Q7NM19 |
| Z4 | 14 | LYS | - | expression tag | UNP Q7NM19 |
| Z4 | 15 | LEU | - | expression tag | UNP Q7NM19 |
| Z4 | 16 | PHE | - | expression tag | UNP Q7NM19 |
| Z4 | 17 | LYS | - | expression tag | UNP Q7NM19 |
| Z4 | 18 | ILE | - | expression tag | UNP Q7NM19 |
| Z4 | 19 | THR | - | expression tag | UNP Q7NM19 |
| Z4 | 20 | ILE | - | expression tag | UNP Q7NM19 |
| Z4 | 21 | ALA | - | expression tag | UNP Q7NM19 |
| Z4 | 22 | LEU | - | expression tag | UNP Q7NM19 |
| Z4 | 23 | SER | - | expression tag | UNP Q7NM19 |
| Z4 | 24 | PRO | - | expression tag | UNP Q7NM19 |
| Z4 | 25 | THR | - | expression tag | UNP Q7NM19 |
| Z4 | 26 | LEU | - | expression tag | UNP Q7NM19 |
| Z4 | 27 | ALA | - | expression tag | UNP Q7NM19 |
| Z4 | 28 | HIS | - | expression tag | UNP Q7NM19 |
| Z4 | 29 | HIS | - | expression tag | UNP Q7NM19 |
| Z4 | 30 | PRO | - | expression tag | UNP Q7NM19 |
| Z4 | 31 | TRP | - | expression tag | UNP Q7NM19 |
| Z4 | 32 | PRO | - | expression tag | UNP Q7NM19 |
| Z4 | 33 | GLY | - | expression tag | UNP Q7NM19 |
| Z4 | 34 | LEU | - | expression tag | UNP Q7NM19 |
| Z4 | 35 | ASP | - | expression tag | UNP Q7NM19 |
| Z4 | 36 | THR | - | expression tag | UNP Q7NM19 |
| Z4 | 37 | HIS | - | expression tag | UNP Q7NM19 |
| Z4 | 38 | GLU | - | expression tag | UNP Q7NM19 |
| Z4 | 39 | PRO | - | expression tag | UNP Q7NM19 |
| Z4 | 40 | SER | - | expression tag | UNP Q7NM19 |
| Z4 | 41 | GLN | - | expression tag | UNP Q7NM19 |
| Z4 | 42 | SER | - | expression tag | UNP Q7NM19 |
| Z4 | 43 | SER | - | expression tag | UNP Q7NM19 |
| Z4 | 44 | TYR | - | expression tag | UNP Q7NM19 |
| Z4 | 45 | SER | - | expression tag | UNP Q7NM19 |
| Z4 | 46 | THR | - | expression tag | UNP Q7NM19 |
| Z4 | 47 | ILE | - | expression tag | UNP Q7NM19 |
| Z4 | 48 | VAL | - | expression tag | UNP Q7NM19 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| Z4 | 49 | SER | - | expression tag | UNP Q7NM19 |
| Z4 | 50 | LEU | - | expression tag | UNP Q7NM19 |
| Z4 | 51 | GLU | - | expression tag | UNP Q7NM19 |
| Z4 | 52 | ARG | - | expression tag | UNP Q7NM19 |
| Z4 | 53 | LEU | - | expression tag | UNP Q7NM19 |
| Z4 | 54 | LEU | - | expression tag | UNP Q7NM19 |
| Z4 | 55 | PRO | - | expression tag | UNP Q7NM19 |
| Z4 | 56 | GLU | - | expression tag | UNP Q7NM19 |
| N9 | 1 | MET | - | initiating methionine | UNP Q7NM19 |
| N9 | 2 | SER | - | expression tag | UNP Q7NM19 |
| N9 | 3 | VAL | - | expression tag | UNP Q7NM19 |
| N9 | 4 | LEU | - | expression tag | UNP Q7NM19 |
| N9 | 5 | THR | - | expression tag | UNP Q7NM19 |
| N9 | 6 | GLY | - | expression tag | UNP Q7NM19 |
| N9 | 7 | ASP | - | expression tag | UNP Q7NM19 |
| N9 | 8 | ASN | - | expression tag | UNP Q7NM19 |
| N9 | 9 | GLN | - | expression tag | UNP Q7NM19 |
| N9 | 10 | GLN | - | expression tag | UNP Q7NM19 |
| N9 | 11 | ARG | - | expression tag | UNP Q7NM19 |
| N9 | 12 | GLY | - | expression tag | UNP Q7NM19 |
| N9 | 13 | SER | - | expression tag | UNP Q7NM19 |
| N9 | 14 | LYS | - | expression tag | UNP Q7NM19 |
| N9 | 15 | LEU | - | expression tag | UNP Q7NM19 |
| N9 | 16 | PHE | - | expression tag | UNP Q7NM19 |
| N9 | 17 | LYS | - | expression tag | UNP Q7NM19 |
| N9 | 18 | ILE | - | expression tag | UNP Q7NM19 |
| N9 | 19 | THR | - | expression tag | UNP Q7NM19 |
| N9 | 20 | ILE | - | expression tag | UNP Q7NM19 |
| N9 | 21 | ALA | - | expression tag | UNP Q7NM19 |
| N9 | 22 | LEU | - | expression tag | UNP Q7NM19 |
| N9 | 23 | SER | - | expression tag | UNP Q7NM19 |
| N9 | 24 | PRO | - | expression tag | UNP Q7NM19 |
| N9 | 25 | THR | - | expression tag | UNP Q7NM19 |
| N9 | 26 | LEU | - | expression tag | UNP Q7NM19 |
| N9 | 27 | ALA | - | expression tag | UNP Q7NM19 |
| N9 | 28 | HIS | - | expression tag | UNP Q7NM19 |
| N9 | 29 | HIS | - | expression tag | UNP Q7NM19 |
| N9 | 30 | PRO | - | expression tag | UNP Q7NM19 |
| N9 | 31 | TRP | - | expression tag | UNP Q7NM19 |
| N9 | 32 | PRO | - | expression tag | UNP Q7NM19 |
| N9 | 33 | GLY | - | expression tag | UNP Q7NM19 |
| N9 | 34 | LEU | - | expression tag | UNP Q7NM19 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| N9 | 35 | ASP | - | expression tag | UNP Q7NM19 |
| N9 | 36 | THR | - | expression tag | UNP Q7NM19 |
| N9 | 37 | HIS | - | expression tag | UNP Q7NM19 |
| N9 | 38 | GLU | - | expression tag | UNP Q7NM19 |
| N9 | 39 | PRO | - | expression tag | UNP Q7NM19 |
| N9 | 40 | SER | - | expression tag | UNP Q7NM19 |
| N9 | 41 | GLN | - | expression tag | UNP Q7NM19 |
| N9 | 42 | SER | - | expression tag | UNP Q7NM19 |
| N9 | 43 | SER | - | expression tag | UNP Q7NM19 |
| N9 | 44 | TYR | - | expression tag | UNP Q7NM19 |
| N9 | 45 | SER | - | expression tag | UNP Q7NM19 |
| N9 | 46 | THR | - | expression tag | UNP Q7NM19 |
| N9 | 47 | ILE | - | expression tag | UNP Q7NM19 |
| N9 | 48 | VAL | - | expression tag | UNP Q7NM19 |
| N9 | 49 | SER | - | expression tag | UNP Q7NM19 |
| N9 | 50 | LEU | - | expression tag | UNP Q7NM19 |
| N9 | 51 | GLU | - | expression tag | UNP Q7NM19 |
| N9 | 52 | ARG | - | expression tag | UNP Q7NM19 |
| N9 | 53 | LEU | - | expression tag | UNP Q7NM19 |
| N9 | 54 | LEU | - | expression tag | UNP Q7NM19 |
| N9 | 55 | PRO | - | expression tag | UNP Q7NM19 |
| N9 | 56 | GLU | - | expression tag | UNP Q7NM19 |
| Z8 | 1 | MET | - | initiating methionine | UNP Q7NM19 |
| Z8 | 2 | SER | - | expression tag | UNP Q7NM19 |
| Z8 | 3 | VAL | - | expression tag | UNP Q7NM19 |
| Z8 | 4 | LEU | - | expression tag | UNP Q7NM19 |
| Z8 | 5 | THR | - | expression tag | UNP Q7NM19 |
| Z8 | 6 | GLY | - | expression tag | UNP Q7NM19 |
| Z8 | 7 | ASP | - | expression tag | UNP Q7NM19 |
| Z8 | 8 | ASN | - | expression tag | UNP Q7NM19 |
| Z8 | 9 | GLN | - | expression tag | UNP Q7NM19 |
| Z8 | 10 | GLN | - | expression tag | UNP Q7NM19 |
| Z8 | 11 | ARG | - | expression tag | UNP Q7NM19 |
| Z8 | 12 | GLY | - | expression tag | UNP Q7NM19 |
| Z8 | 13 | SER | - | expression tag | UNP Q7NM19 |
| Z8 | 14 | LYS | - | expression tag | UNP Q7NM19 |
| Z8 | 15 | LEU | - | expression tag | UNP Q7NM19 |
| Z8 | 16 | PHE | - | expression tag | UNP Q7NM19 |
| Z8 | 17 | LYS | - | expression tag | UNP Q7NM19 |
| Z8 | 18 | ILE | - | expression tag | UNP Q7NM19 |
| Z8 | 19 | THR | - | expression tag | UNP Q7NM19 |
| Z8 | 20 | ILE | - | expression tag | UNP Q7NM19 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| Z8 | 21 | ALA | - | expression tag | UNP Q7NM19 |
| Z8 | 22 | LEU | - | expression tag | UNP Q7NM19 |
| Z8 | 23 | SER | - | expression tag | UNP Q7NM19 |
| Z8 | 24 | PRO | - | expression tag | UNP Q7NM19 |
| Z8 | 25 | THR | - | expression tag | UNP Q7NM19 |
| Z8 | 26 | LEU | - | expression tag | UNP Q7NM19 |
| Z8 | 27 | ALA | - | expression tag | UNP Q7NM19 |
| Z8 | 28 | HIS | - | expression tag | UNP Q7NM19 |
| Z8 | 29 | HIS | - | expression tag | UNP Q7NM19 |
| Z8 | 30 | PRO | - | expression tag | UNP Q7NM19 |
| Z8 | 31 | TRP | - | expression tag | UNP Q7NM19 |
| Z8 | 32 | PRO | - | expression tag | UNP Q7NM19 |
| Z8 | 33 | GLY | - | expression tag | UNP Q7NM19 |
| Z8 | 34 | LEU | - | expression tag | UNP Q7NM19 |
| Z8 | 35 | ASP | - | expression tag | UNP Q7NM19 |
| Z8 | 36 | THR | - | expression tag | UNP Q7NM19 |
| Z8 | 37 | HIS | - | expression tag | UNP Q7NM19 |
| Z8 | 38 | GLU | - | expression tag | UNP Q7NM19 |
| Z8 | 39 | PRO | - | expression tag | UNP Q7NM19 |
| Z8 | 40 | SER | - | expression tag | UNP Q7NM19 |
| Z8 | 41 | GLN | - | expression tag | UNP Q7NM19 |
| Z8 | 42 | SER | - | expression tag | UNP Q7NM19 |
| Z8 | 43 | SER | - | expression tag | UNP Q7NM19 |
| Z8 | 44 | TYR | - | expression tag | UNP Q7NM19 |
| Z8 | 45 | SER | - | expression tag | UNP Q7NM19 |
| Z8 | 46 | THR | - | expression tag | UNP Q7NM19 |
| Z8 | 47 | ILE | - | expression tag | UNP Q7NM19 |
| Z8 | 48 | VAL | - | expression tag | UNP Q7NM19 |
| Z8 | 49 | SER | - | expression tag | UNP Q7NM19 |
| Z8 | 50 | LEU | - | expression tag | UNP Q7NM19 |
| Z8 | 51 | GLU | - | expression tag | UNP Q7NM19 |
| Z8 | 52 | ARG | - | expression tag | UNP Q7NM19 |
| Z8 | 53 | LEU | - | expression tag | UNP Q7NM19 |
| Z8 | 54 | LEU | - | expression tag | UNP Q7NM19 |
| Z8 | 55 | PRO | - | expression tag | UNP Q7NM19 |
| Z8 | 56 | GLU | - | expression tag | UNP Q7NM19 |
| N1 | 1 | MET | - | initiating methionine | UNP Q7NM19 |
| N1 | 2 | SER | - | expression tag | UNP Q7NM19 |
| N1 | 3 | VAL | - | expression tag | UNP Q7NM19 |
| N1 | 4 | LEU | - | expression tag | UNP Q7NM19 |
| N1 | 5 | THR | - | expression tag | UNP Q7NM19 |
| N1 | 6 | GLY | - | expression tag | UNP Q7NM19 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| N1 | 7 | ASP | - | expression tag | UNP Q7NM19 |
| N1 | 8 | ASN | - | expression tag | UNP Q7NM19 |
| N1 | 9 | GLN | - | expression tag | UNP Q7NM19 |
| N1 | 10 | GLN | - | expression tag | UNP Q7NM19 |
| N1 | 11 | ARG | - | expression tag | UNP Q7NM19 |
| N1 | 12 | GLY | - | expression tag | UNP Q7NM19 |
| N1 | 13 | SER | - | expression tag | UNP Q7NM19 |
| N1 | 14 | LYS | - | expression tag | UNP Q7NM19 |
| N1 | 15 | LEU | - | expression tag | UNP Q7NM19 |
| N1 | 16 | PHE | - | expression tag | UNP Q7NM19 |
| N1 | 17 | LYS | - | expression tag | UNP Q7NM19 |
| N1 | 18 | ILE | - | expression tag | UNP Q7NM19 |
| N1 | 19 | THR | - | expression tag | UNP Q7NM19 |
| N1 | 20 | ILE | - | expression tag | UNP Q7NM19 |
| N1 | 21 | ALA | - | expression tag | UNP Q7NM19 |
| N1 | 22 | LEU | - | expression tag | UNP Q7NM19 |
| N1 | 23 | SER | - | expression tag | UNP Q7NM19 |
| N1 | 24 | PRO | - | expression tag | UNP Q7NM19 |
| N1 | 25 | THR | - | expression tag | UNP Q7NM19 |
| N1 | 26 | LEU | - | expression tag | UNP Q7NM19 |
| N1 | 27 | ALA | - | expression tag | UNP Q7NM19 |
| N1 | 28 | HIS | - | expression tag | UNP Q7NM19 |
| N1 | 29 | HIS | - | expression tag | UNP Q7NM19 |
| N1 | 30 | PRO | - | expression tag | UNP Q7NM19 |
| N1 | 31 | TRP | - | expression tag | UNP Q7NM19 |
| N1 | 32 | PRO | - | expression tag | UNP Q7NM19 |
| N1 | 33 | GLY | - | expression tag | UNP Q7NM19 |
| N1 | 34 | LEU | - | expression tag | UNP Q7NM19 |
| N1 | 35 | ASP | - | expression tag | UNP Q7NM19 |
| N1 | 36 | THR | - | expression tag | UNP Q7NM19 |
| N1 | 37 | HIS | - | expression tag | UNP Q7NM19 |
| N1 | 38 | GLU | - | expression tag | UNP Q7NM19 |
| N1 | 39 | PRO | - | expression tag | UNP Q7NM19 |
| N1 | 40 | SER | - | expression tag | UNP Q7NM19 |
| N1 | 41 | GLN | - | expression tag | UNP Q7NM19 |
| N1 | 42 | SER | - | expression tag | UNP Q7NM19 |
| N1 | 43 | SER | - | expression tag | UNP Q7NM19 |
| N1 | 44 | TYR | - | expression tag | UNP Q7NM19 |
| N1 | 45 | SER | - | expression tag | UNP Q7NM19 |
| N1 | 46 | THR | - | expression tag | UNP Q7NM19 |
| N1 | 47 | ILE | - | expression tag | UNP Q7NM19 |
| N1 | 48 | VAL | - | expression tag | UNP Q7NM19 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| N1 | 49 | SER | - | expression tag | UNP Q7NM19 |
| N1 | 50 | LEU | - | expression tag | UNP Q7NM19 |
| N1 | 51 | GLU | - | expression tag | UNP Q7NM19 |
| N1 | 52 | ARG | - | expression tag | UNP Q7NM19 |
| N1 | 53 | LEU | - | expression tag | UNP Q7NM19 |
| N1 | 54 | LEU | - | expression tag | UNP Q7NM19 |
| N1 | 55 | PRO | - | expression tag | UNP Q7NM19 |
| N1 | 56 | GLU | - | expression tag | UNP Q7NM19 |

- Molecule 6 is a protein called Glr2806 protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6 | M2 | 279 | Total | C | N | O | S | 0 | 0 |
| | | | 2190 | 1381 | 387 | 417 | 5 | | |
| 6 | M6 | 279 | Total | C | N | O | S | 0 | 0 |
| | | | 2190 | 1381 | 387 | 417 | 5 | | |

- Molecule 7 is a protein called CpcD protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 7 | N2 | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 545 | 349 | 91 | 103 | 2 | | |
| 7 | N6 | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 545 | 349 | 91 | 103 | 2 | | |

- Molecule 8 is a protein called Allophycocyanin alpha subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | K5 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | M5 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | O5 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | A5 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | C5 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | E5 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | G5 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | I5 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | c5 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | e5 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | Q5 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | S5 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | U5 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | W5 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | Y5 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | a5 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | A7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | O7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | Q7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | S7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | C7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | E7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | G7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | I7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | K7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | M7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | g7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | i7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | k7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | U7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | W7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | Y7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | a7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | c7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | e7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | m7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | o7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | q7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | s7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |
| 8 | u7 | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 771 | 209 | 237 | 5 | | |

There are 40 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| K5 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| M5 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| O5 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| A5 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| C5 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| E5 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| G5 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| I5 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| c5 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| e5 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| Q5 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| S5 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| U5 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| W5 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| Y5 | 61 | ILE | LYS | conflict | UNP Q7NL80 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| a5 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| A7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| O7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| Q7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| S7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| C7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| E7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| G7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| I7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| K7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| M7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| g7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| i7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| k7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| U7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| W7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| Y7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| a7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| c7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| e7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| m7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| o7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| q7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| s7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |
| u7 | 61 | ILE | LYS | conflict | UNP Q7NL80 |

- Molecule 9 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9 | z5 | 68 | Total | C | N | O | S | 0 | 0 |
| | | | 538 | 345 | 98 | 94 | 1 | | |
| 9 | i5 | 68 | Total | C | N | O | S | 0 | 0 |
| | | | 538 | 345 | 98 | 94 | 1 | | |
| 9 | z7 | 68 | Total | C | N | O | S | 0 | 0 |
| | | | 538 | 345 | 98 | 94 | 1 | | |
| 9 | w7 | 68 | Total | C | N | O | S | 0 | 0 |
| | | | 538 | 345 | 98 | 94 | 1 | | |
| 9 | x7 | 68 | Total | C | N | O | S | 0 | 0 |
| | | | 538 | 345 | 98 | 94 | 1 | | |
| 9 | y7 | 68 | Total | C | N | O | S | 0 | 0 |
| | | | 538 | 345 | 98 | 94 | 1 | | |

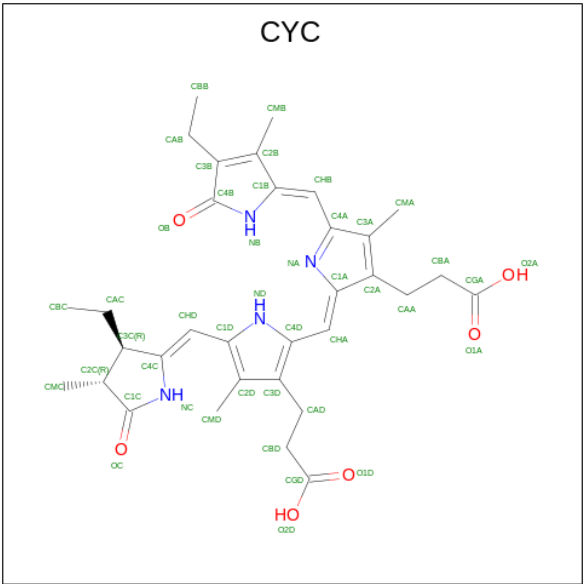
- Molecule 10 is a protein called Phycobiliprotein ApcE.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 10 | j5 | 1108 | Total | C | N | O | S | 0 | 0 |
| | | | 8819 | 5593 | 1559 | 1647 | 20 | | |
| 10 | k5 | 1108 | Total | C | N | O | S | 0 | 0 |
| | | | 8819 | 5593 | 1559 | 1647 | 20 | | |

- Molecule 11 is a protein called Glr1262 protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 11 | a9 | 800 | Total | C | N | O | S | 0 | 0 |
| | | | 6326 | 3959 | 1137 | 1218 | 12 | | |
| 11 | aA | 800 | Total | C | N | O | S | 0 | 0 |
| | | | 6326 | 3959 | 1137 | 1218 | 12 | | |

- Molecule 12 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: C₃₃H₄₀N₄O₆) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 12 | A | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | Z | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | AA | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | BA | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| | | | Total | C | N | O | |
| 12 | BA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | CA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | DA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | DA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | EA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | FA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | GA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | HA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | HA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | IA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | JA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | JA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | KA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | LA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | LA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | OA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | PA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | PA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | QA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | RA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | RA | 1 | 43 | 33 | 4 | 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| | | | Total | C | N | O | |
| 12 | SA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | TA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | TA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | UA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | VA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | VA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | WA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | XA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | XA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | YA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | ZA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | ZA | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | O1 | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | P1 | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | P1 | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | Q1 | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | R1 | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | R1 | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | S1 | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | A1 | 1 | 43 | 33 | 4 | 6 | 0 |
| 12 | G3 | 1 | 43 | 33 | 4 | 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 12 | H3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | H3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | I3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | J3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | J3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | K3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | G2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | H2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | H2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | I2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | J2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | J2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | K2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | L2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | L2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | N2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | A3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | B3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | B3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | C3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | D3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 12 | D3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | E3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | F3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | F3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | Z3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | Z3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | A4 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | B4 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | B4 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | C4 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | D4 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | D4 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | L3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | L3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | O3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | P3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | P3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | Q3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | R3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | R3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | S3 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|
| 12 | T3 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | T3 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | U3 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | V3 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | V3 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | W3 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | X3 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | X3 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | Y3 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | B1 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | B1 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | S4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | S4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | T4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | U4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | U4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | V4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | W4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | W4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | E4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | F4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|
| 12 | F4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | G4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | H4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | H4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | I4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | J4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | J4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | K4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | L4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | L4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | M4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | N4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | O4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | O4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | P4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | Q4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | R4 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | K5 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | L5 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | M5 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | N5 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 12 | O5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | X4 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | Y4 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | Z4 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | A5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | B5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | C5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | D5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | E5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | F5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | G5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | H5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | I5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | J5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | C1 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | c5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | d5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | e5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | f5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | P5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | Q5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|------------------|---|---------|
| 12 | R5 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | S5 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | T5 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | U5 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | V5 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | W5 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | X5 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | Y5 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | Z5 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | a5 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | b5 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | J6 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | J6 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | K6 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | L6 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | L6 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | N6 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | A7 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | j5 | 1 | Total 81 | C 33 | H 38 | N 4 O 6 | 0 | |
| 12 | j5 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 | |
| 12 | k5 | 1 | Total 81 | C 33 | H 38 | N 4 O 6 | 0 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 12 | k5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | k5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | k5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | A6 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | B6 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | C6 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | D6 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | D6 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | E6 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | F6 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | F6 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | G6 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | H6 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | H6 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | I6 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | D1 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | D1 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | O7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | P7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | Q7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | R7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 12 | S7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | B7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | C7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | D7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | E7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | F7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | G7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | H7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | I7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | J7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | K7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | L7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | M7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | N7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | g7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | h7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | i7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | j7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | k7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | T7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | U7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|
| 12 | V7 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | W7 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | X7 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | Y7 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | a7 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | b7 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | c7 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | d7 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | e7 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | f7 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | E1 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | A8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | B8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | B8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | C8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | D8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | D8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | E8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | m7 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | o7 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | p7 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 12 | q7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | r7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | s7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | u7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | v7 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | T8 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | U8 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | U8 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | V8 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | W8 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | W8 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | X8 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | F8 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | F8 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | G8 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | H8 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | H8 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | I8 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | J8 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | J8 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | K8 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|
| 12 | L8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | M8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | M8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | N8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | O8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | O8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | P8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | Q8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | R8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | S8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | F1 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | F1 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | L9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | L9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | O9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | P9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | P9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | Q9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | Y8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | Z8 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | A9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|
| 12 | B9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | B9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | C9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | D9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | D9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | E9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | F9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | F9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | F9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | G9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | H9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | H9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | I9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | J9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | J9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | K9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | R9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | R9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | S9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | T9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | T9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|
| 12 | U9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | V9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | V9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | W9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | X9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | X9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | Y9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | Z9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | Z9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | G1 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | a9 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | aA | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | aA | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | H1 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | H1 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | I1 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | J1 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | K1 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | L1 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | T1 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 12 | T1 | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |

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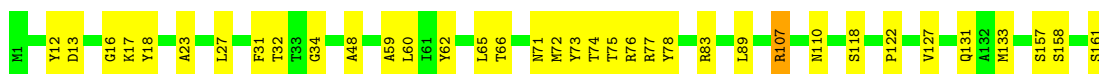
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
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| | | | 43 | 33 | 4 | 6 | |
| 12 | V1 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | V1 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | W1 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | X1 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | X1 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | Y1 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | Z1 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | Z1 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | A2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | B2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | C2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | D2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | D2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | E2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | F2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 12 | F2 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Allophycocyanin beta subunit

Chain A: 




- Molecule 1: Allophycocyanin beta subunit

Chain Z: 




- Molecule 1: Allophycocyanin beta subunit

Chain L5: 




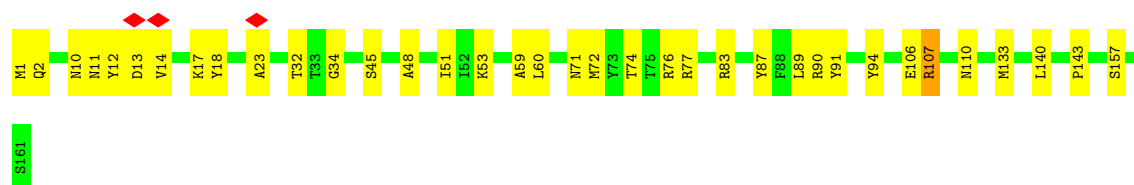
- Molecule 1: Allophycocyanin beta subunit

Chain N5: 



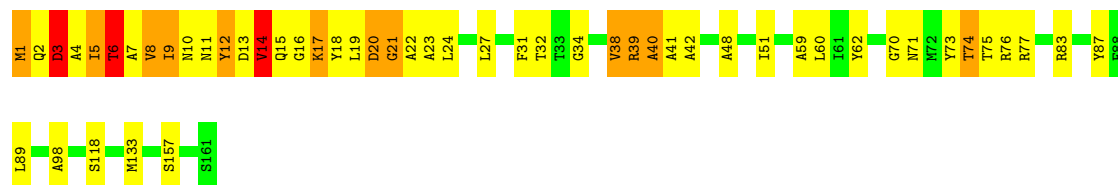
- Molecule 1: Allophycocyanin beta subunit

Chain B5: 



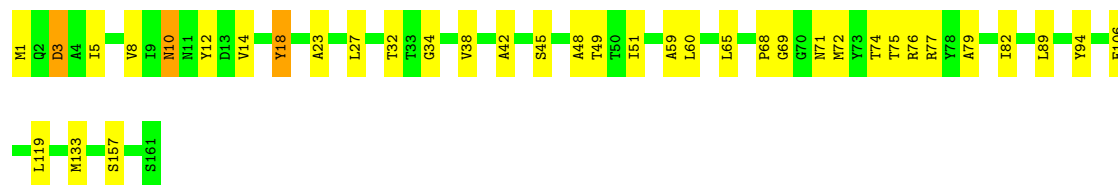
- Molecule 1: Allophycocyanin beta subunit

Chain D5: 68% 23% 7% .



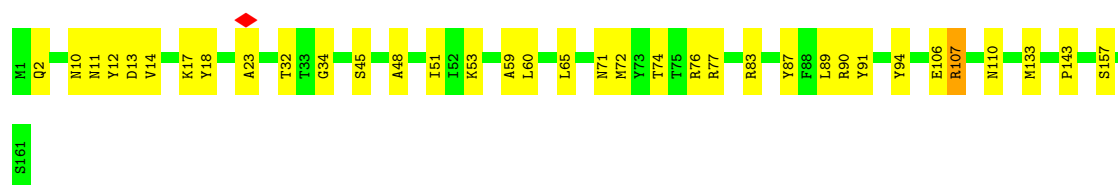
- Molecule 1: Allophycocyanin beta subunit

Chain F5: 77% 21% .



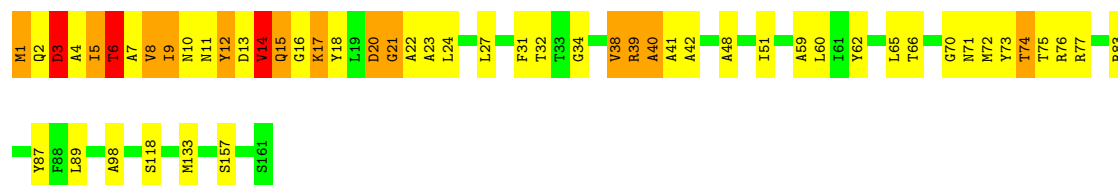
- Molecule 1: Allophycocyanin beta subunit

Chain H5: 78% 21% .



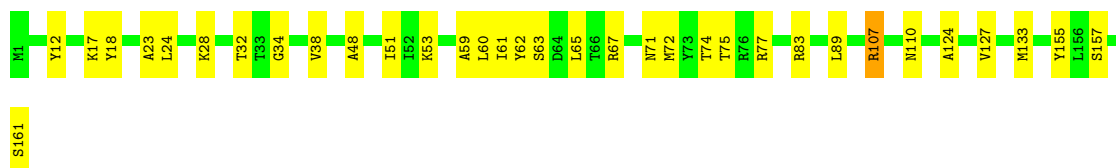
- Molecule 1: Allophycocyanin beta subunit

Chain J5: 66% 24% 8% .

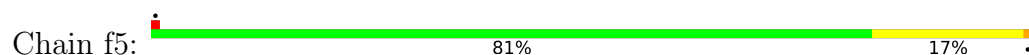


- Molecule 1: Allophycocyanin beta subunit

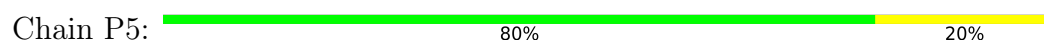
Chain d5: 79% 20% .



- Molecule 1: Allophycocyanin beta subunit



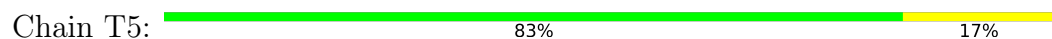
- Molecule 1: Allophycocyanin beta subunit



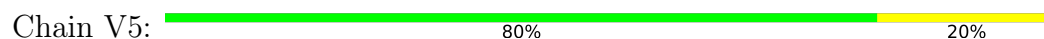
- Molecule 1: Allophycocyanin beta subunit



- Molecule 1: Allophycocyanin beta subunit

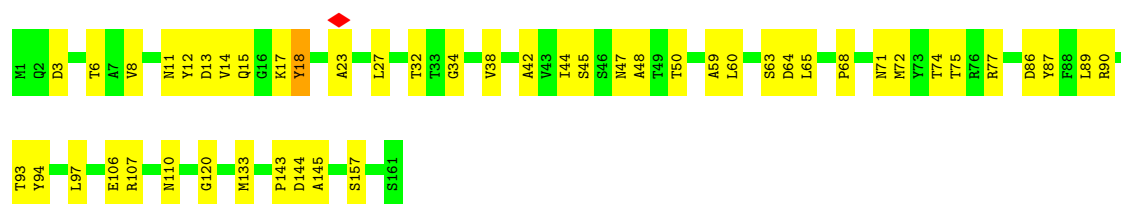


- Molecule 1: Allophycocyanin beta subunit



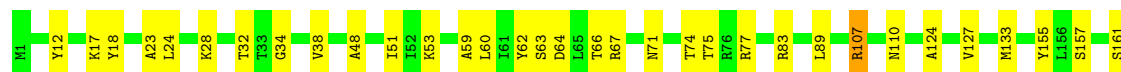
- Molecule 1: Allophycocyanin beta subunit





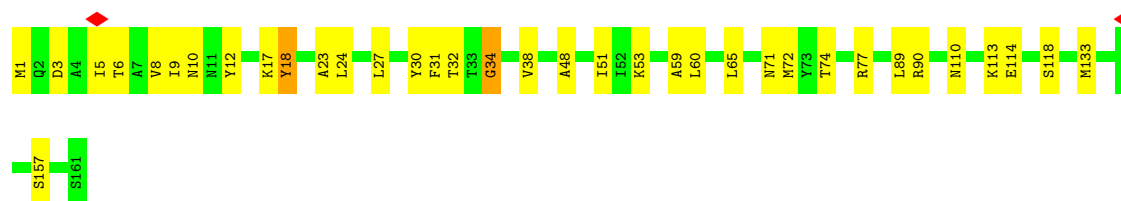
- Molecule 1: Allophycocyanin beta subunit

Chain Z5: 80% 20%



- Molecule 1: Allophycocyanin beta subunit

Chain b5: 78% 21%



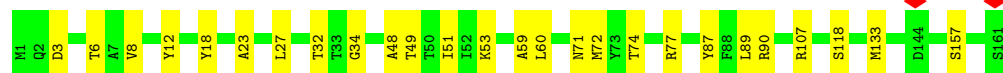
- Molecule 1: Allophycocyanin beta subunit

Chain P7: 83% 17%



- Molecule 1: Allophycocyanin beta subunit

Chain R7: 84% 16%



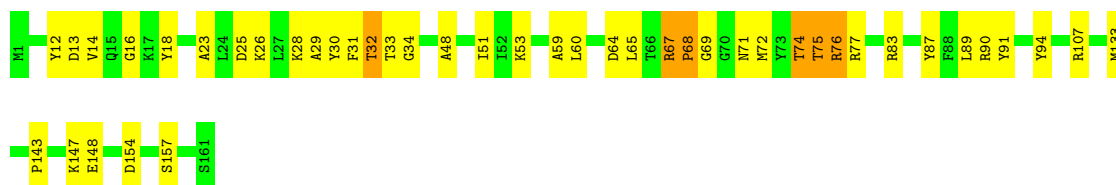
- Molecule 1: Allophycocyanin beta subunit

Chain B7: 83% 17%



- Molecule 1: Allophycocyanin beta subunit

Chain D7: 73% 24%



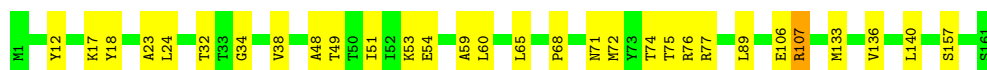
- Molecule 1: Allophycocyanin beta subunit

Chain F7: 85% 15%



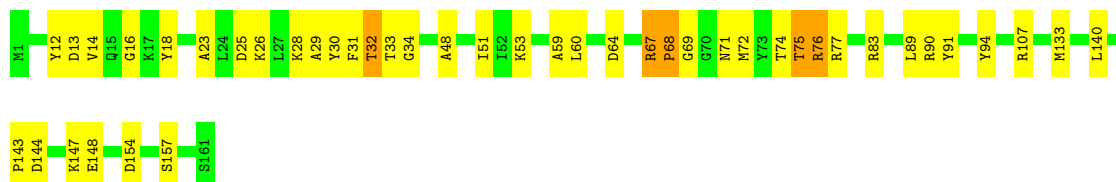
- Molecule 1: Allophycocyanin beta subunit

Chain H7: 81% 18%



- Molecule 1: Allophycocyanin beta subunit

Chain J7: 73% 24%



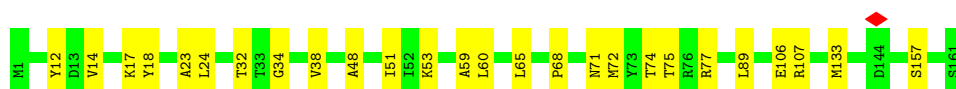
- Molecule 1: Allophycocyanin beta subunit

Chain L7: 85% 15%



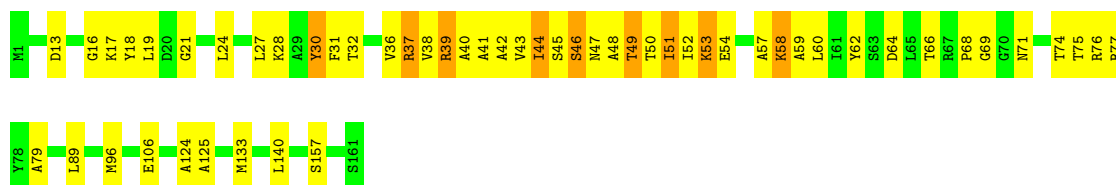
- Molecule 1: Allophycocyanin beta subunit

Chain N7: 84% 16%



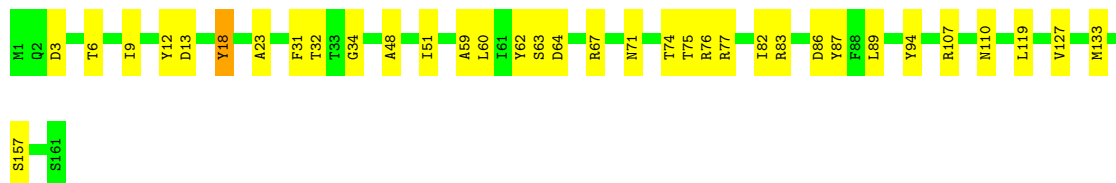
- Molecule 1: Allophycocyanin beta subunit

Chain h7: 66% 28% 6%



- Molecule 1: Allophycocyanin beta subunit

Chain j7: 78% 21% .



- Molecule 1: Allophycocyanin beta subunit

Chain T7: 81% 19%



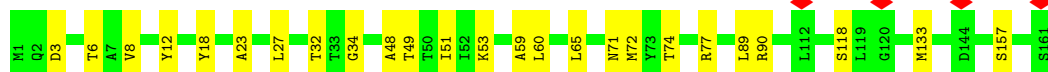
- Molecule 1: Allophycocyanin beta subunit

Chain V7: 83% 16% .



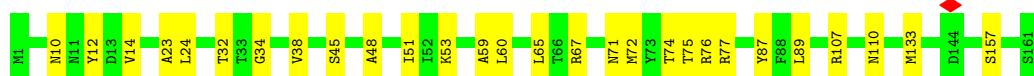
- Molecule 1: Allophycocyanin beta subunit

Chain X7: 84% 16%



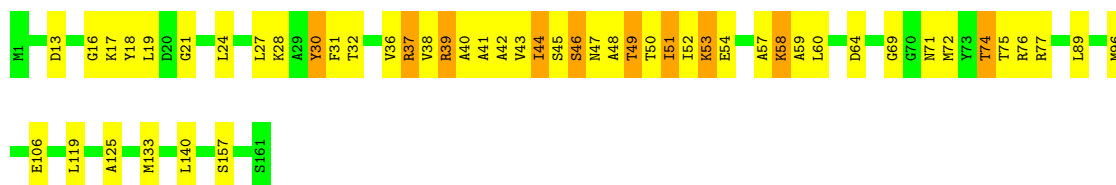
- Molecule 1: Allophycocyanin beta subunit

Chain Z7: 83% 17%



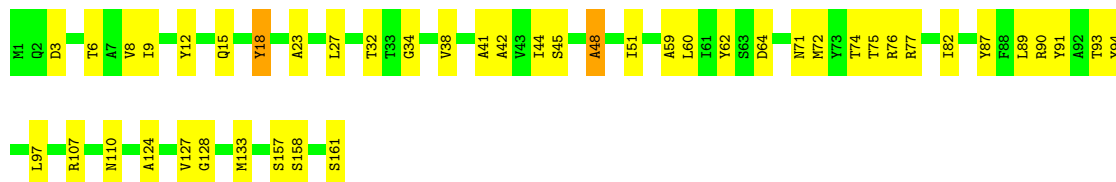
- Molecule 1: Allophycocyanin beta subunit

Chain b7: 68% 25% 6%




- Molecule 1: Allophycocyanin beta subunit

Chain d7:  72% 27% .




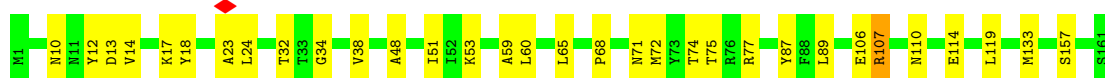
- Molecule 1: Allophycocyanin beta subunit

Chain f7:  83% 17% .




- Molecule 1: Allophycocyanin beta subunit

Chain i7:  80% 19% .



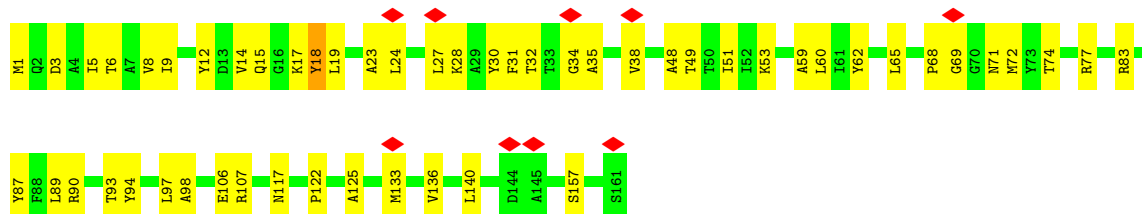
- Molecule 1: Allophycocyanin beta subunit

Chain n7:  79% 21% .




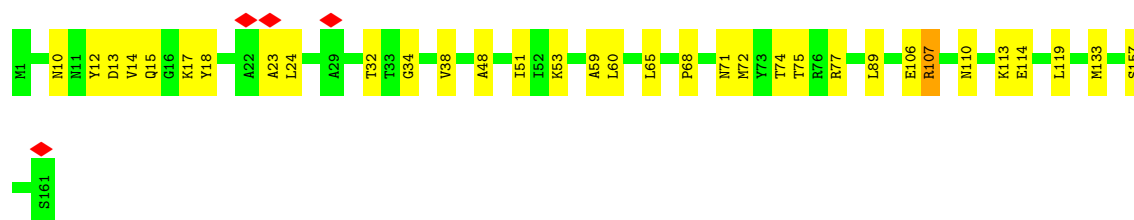
- Molecule 1: Allophycocyanin beta subunit

Chain p7:  6% 67% 32% .




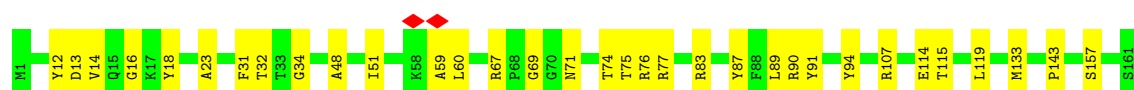
- Molecule 1: Allophycocyanin beta subunit

Chain r7: 



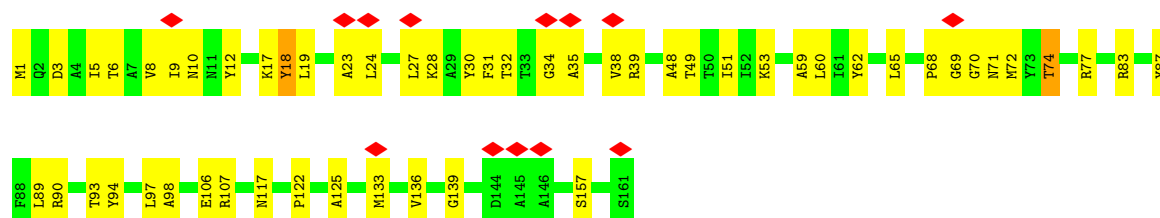
- Molecule 1: Allophycocyanin beta subunit

Chain t7: 




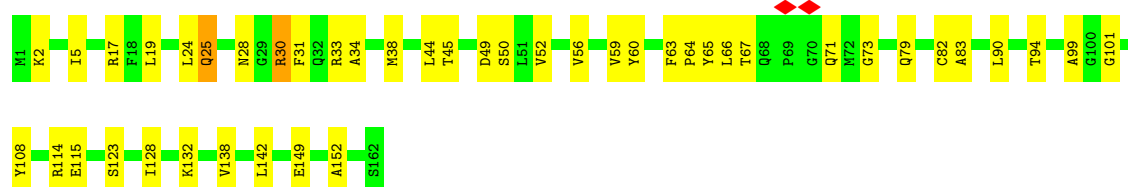
- Molecule 1: Allophycocyanin beta subunit

Chain v7: 



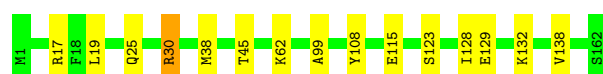
- Molecule 2: Phycocyanin alpha chain

Chain AA: 

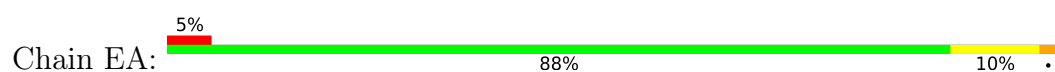


- Molecule 2: Phycocyanin alpha chain

Chain CA: 



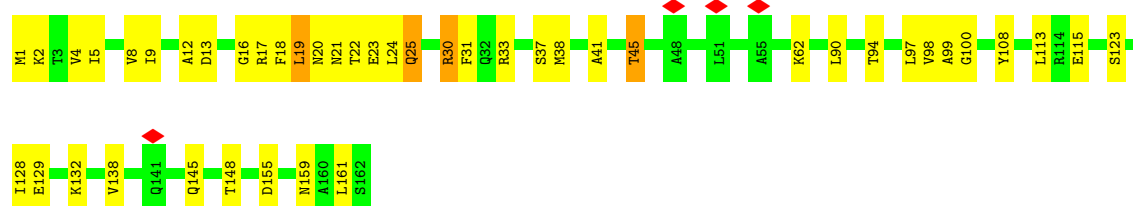
- Molecule 2: Phycocyanin alpha chain



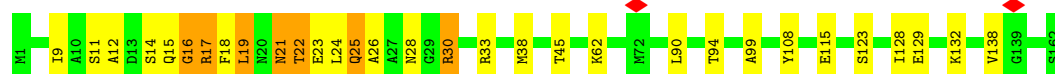
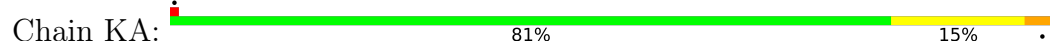
- Molecule 2: Phycocyanin alpha chain



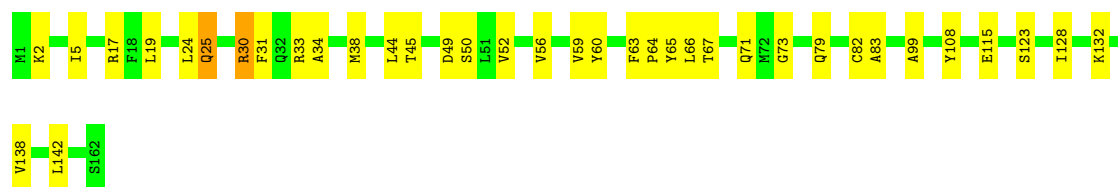
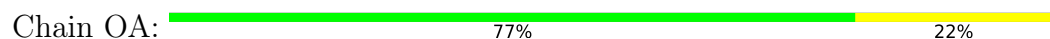
- Molecule 2: Phycocyanin alpha chain



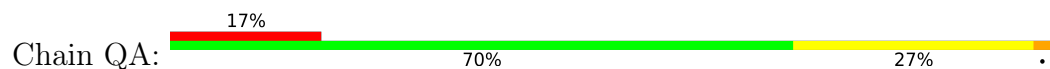
- Molecule 2: Phycocyanin alpha chain



- Molecule 2: Phycocyanin alpha chain

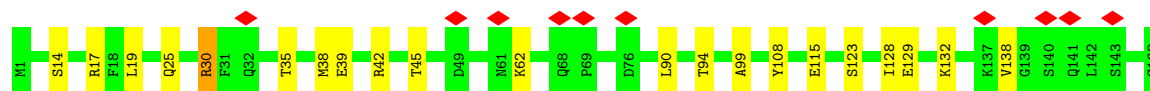
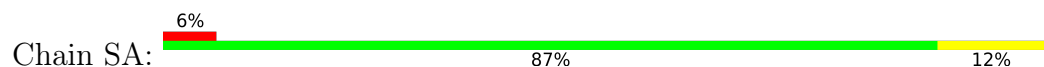


- Molecule 2: Phycocyanin alpha chain

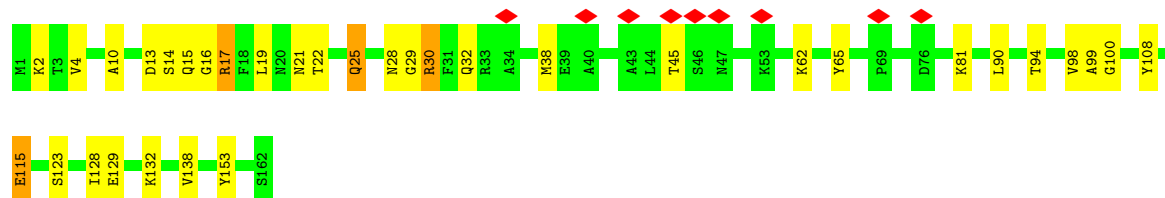
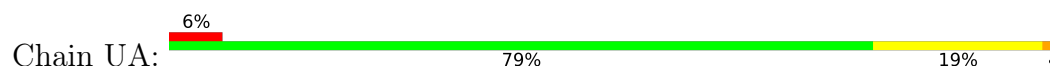




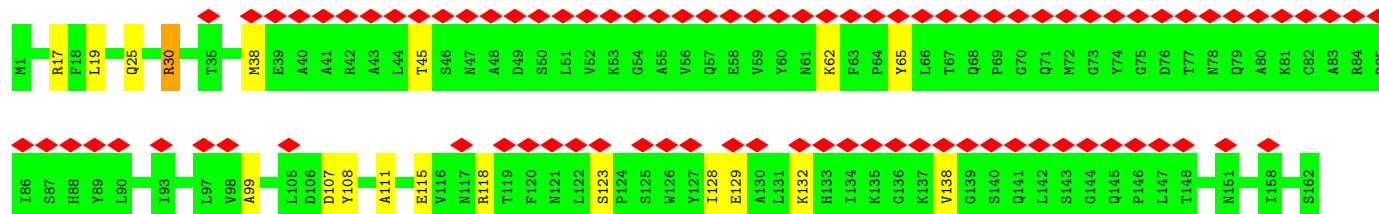
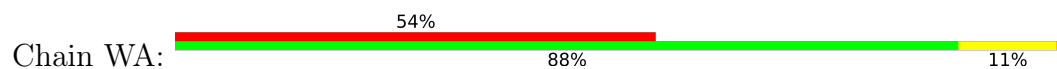
- Molecule 2: Phycocyanin alpha chain



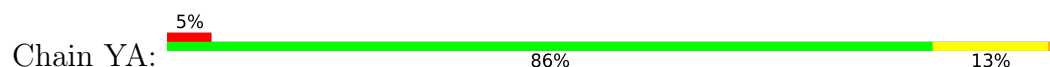
- Molecule 2: Phycocyanin alpha chain



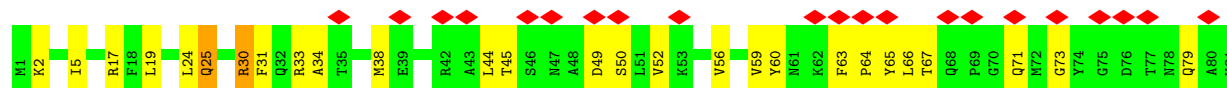
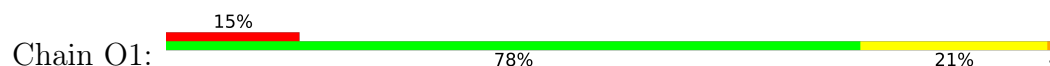
- Molecule 2: Phycocyanin alpha chain

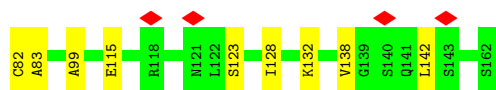


- Molecule 2: Phycocyanin alpha chain

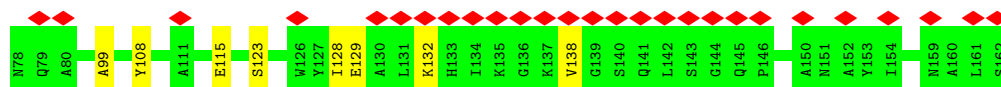
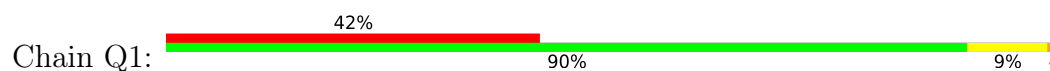


- Molecule 2: Phycocyanin alpha chain

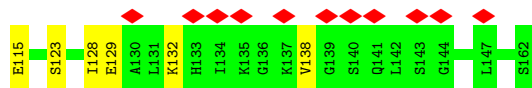
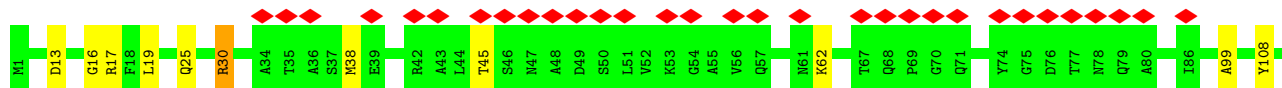
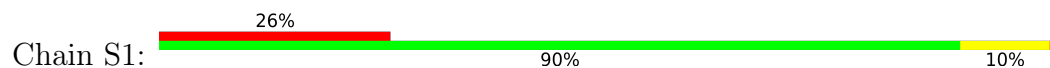




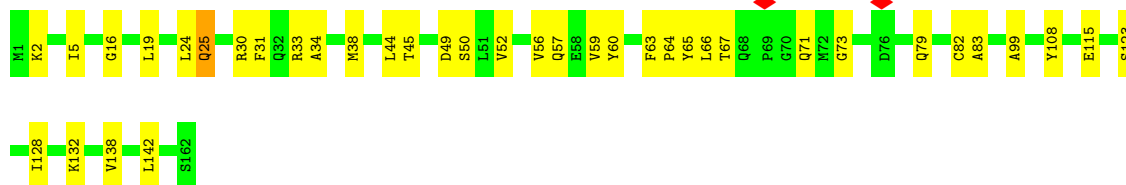
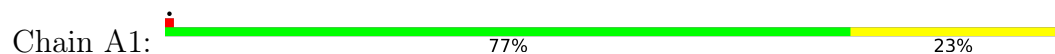
- Molecule 2: Phycocyanin alpha chain



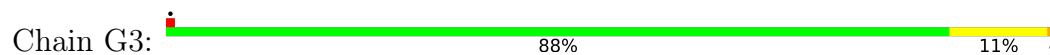
- Molecule 2: Phycocyanin alpha chain



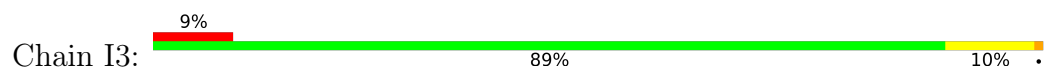
- Molecule 2: Phycocyanin alpha chain

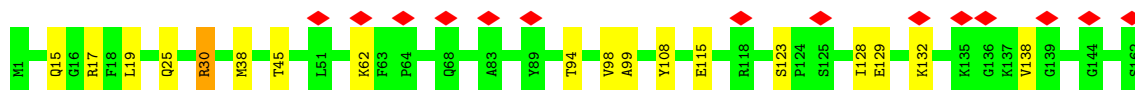


- Molecule 2: Phycocyanin alpha chain

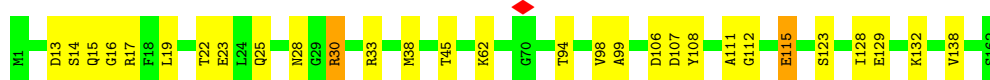
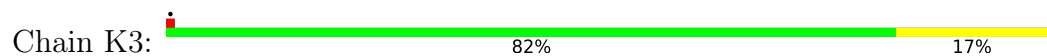


- Molecule 2: Phycocyanin alpha chain

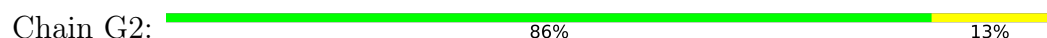




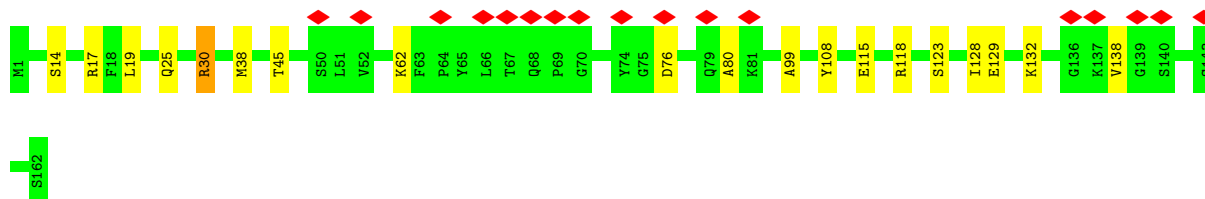
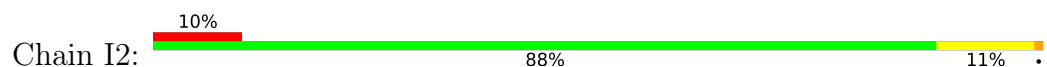
- Molecule 2: Phycocyanin alpha chain



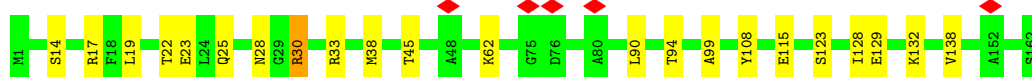
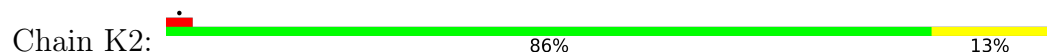
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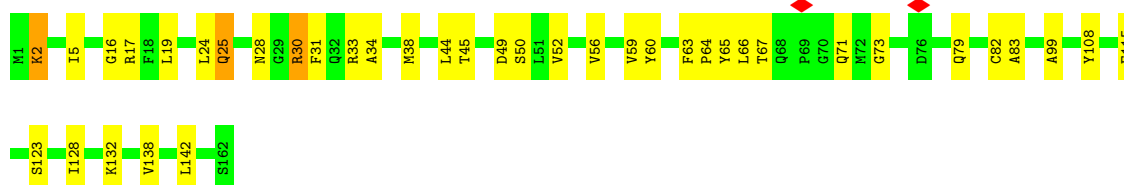
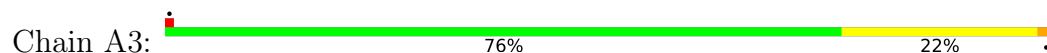
- Molecule 2: Phycocyanin alpha chain



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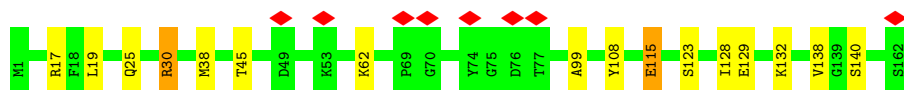


- Molecule 2: Phycocyanin alpha chain

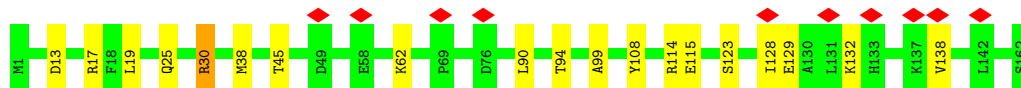
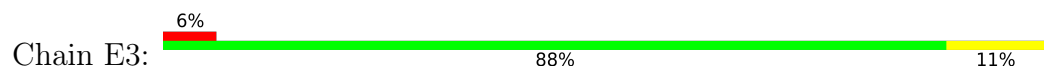


- Molecule 2: Phycocyanin alpha chain

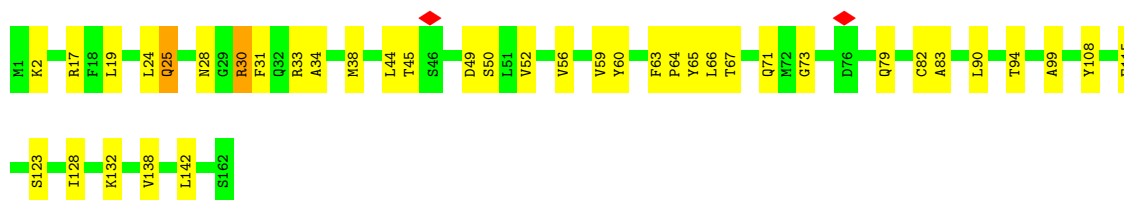
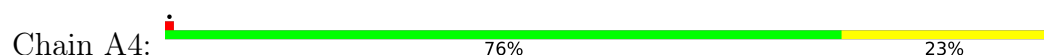




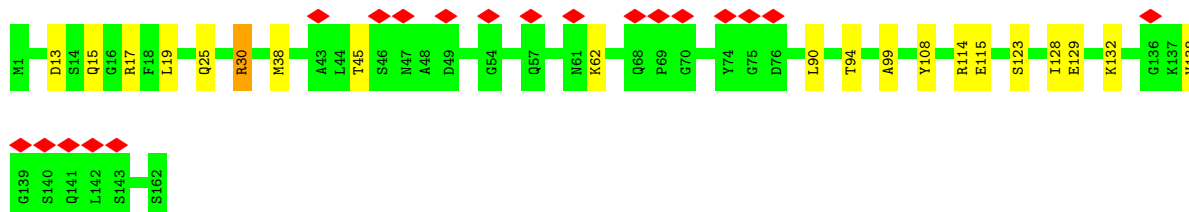
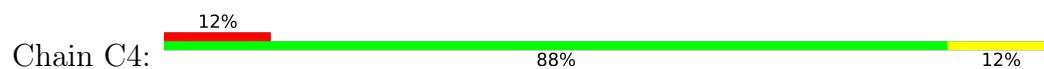
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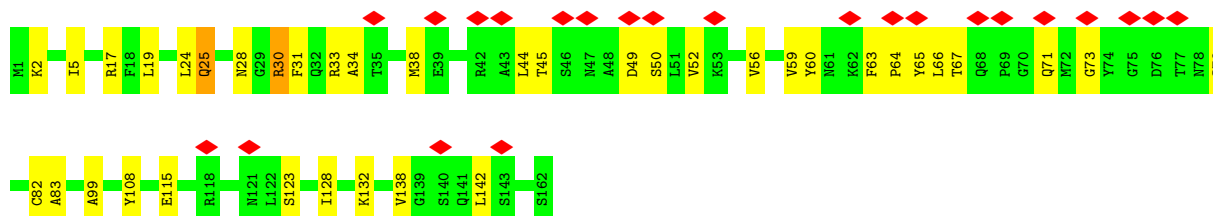
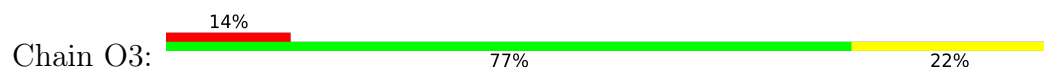
- Molecule 2: Phycocyanin alpha chain



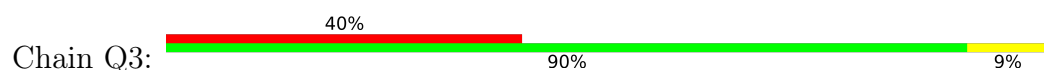
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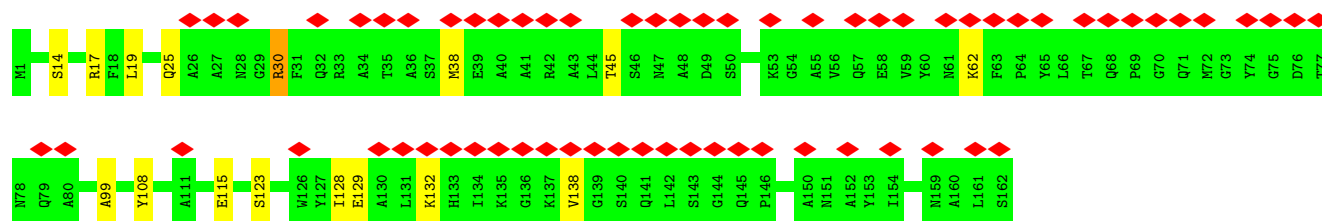


- Molecule 2: Phycocyanin alpha chain

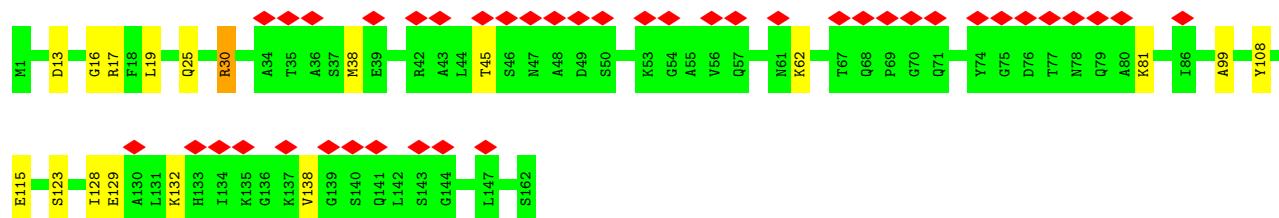
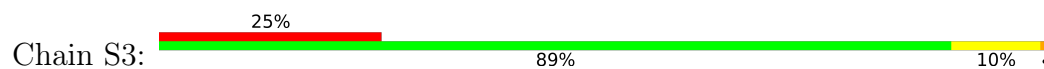


- Molecule 2: Phycocyanin alpha chain

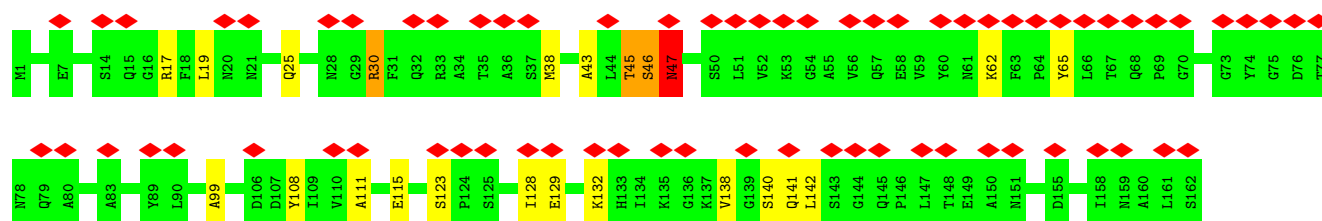
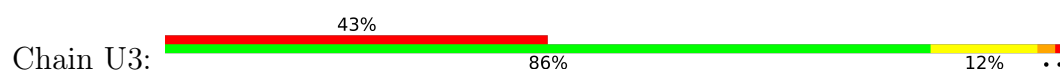




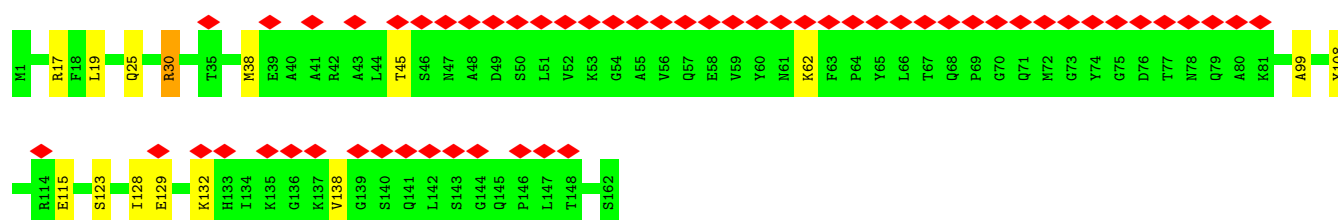
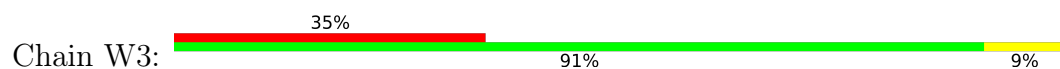
• Molecule 2: Phycocyanin alpha chain



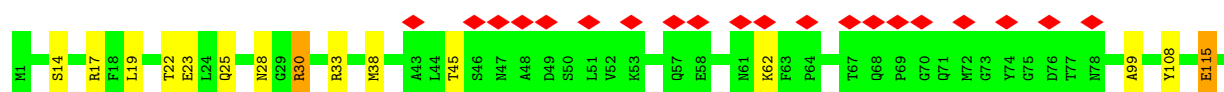
• Molecule 2: Phycocyanin alpha chain



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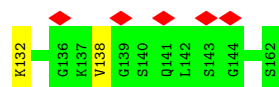
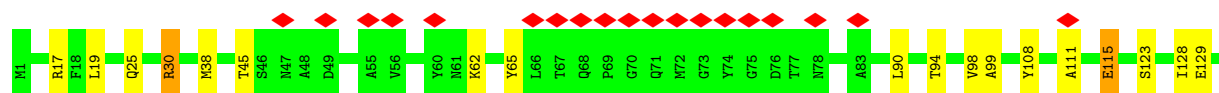
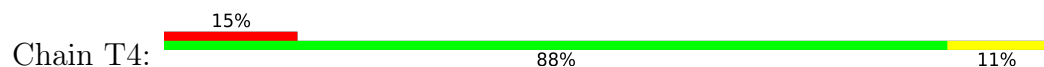


• Molecule 2: Phycocyanin alpha chain

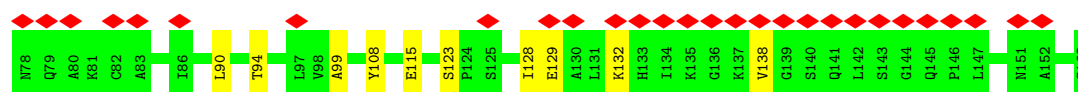
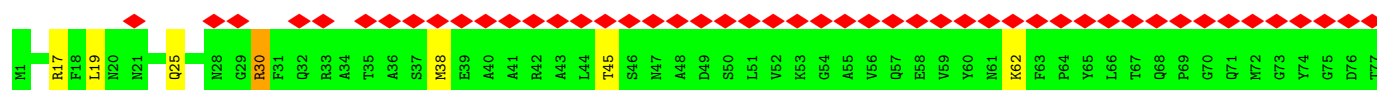
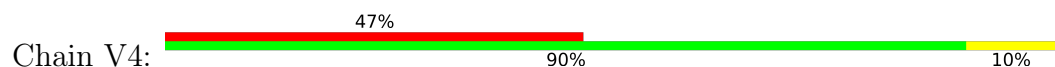




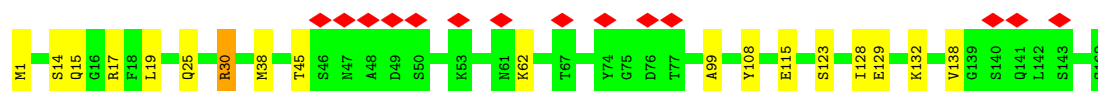
- Molecule 2: Phycocyanin alpha chain



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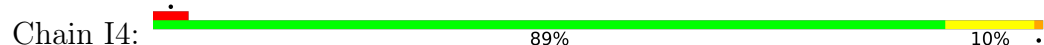
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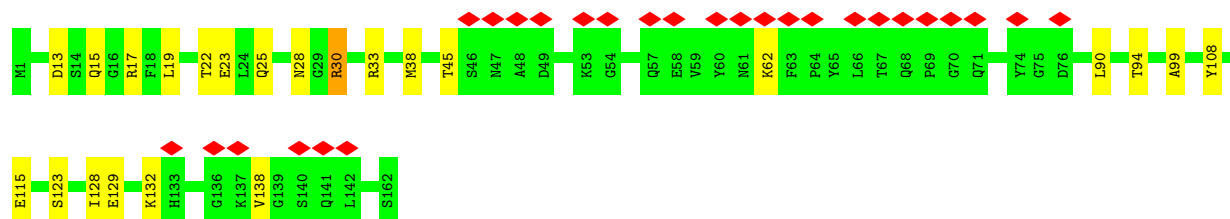
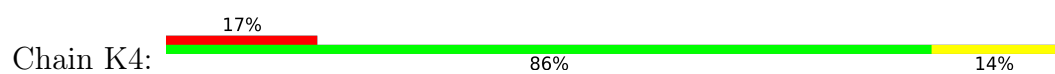
- Molecule 2: Phycocyanin alpha chain



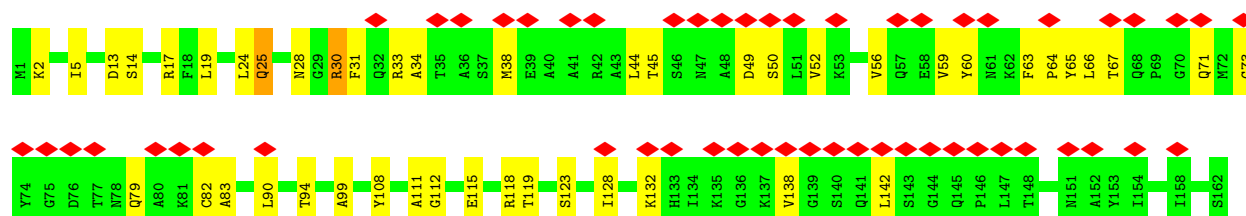
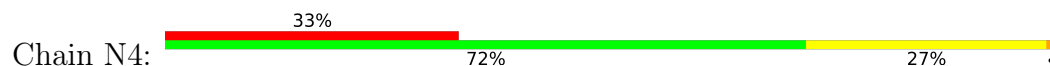
- Molecule 2: Phycocyanin alpha chain



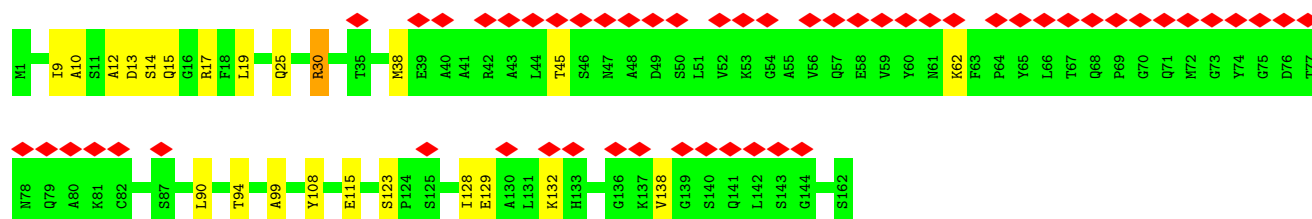
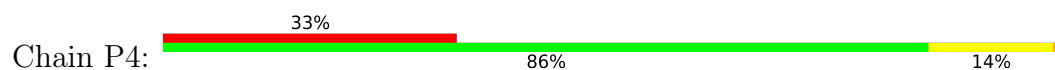
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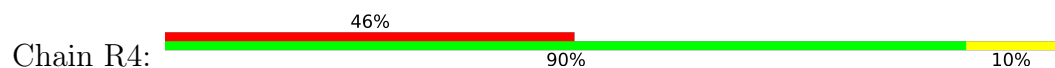
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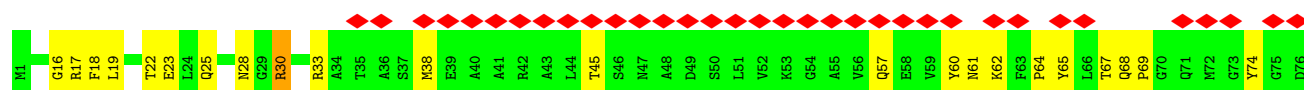
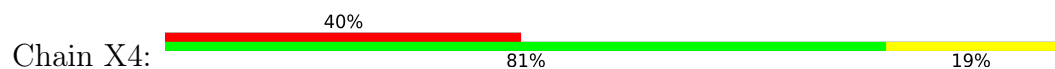
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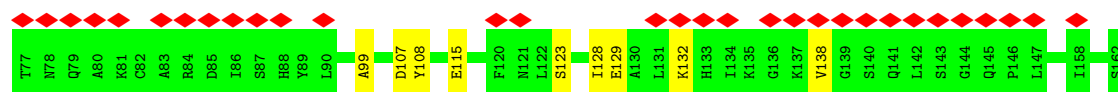


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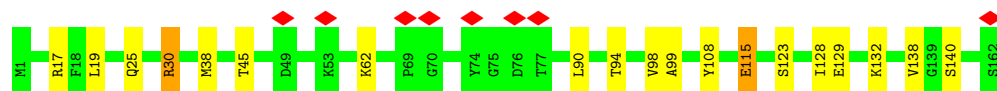
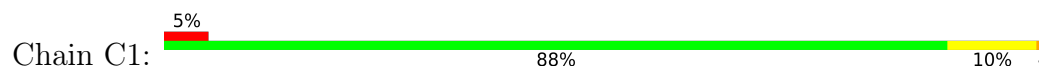


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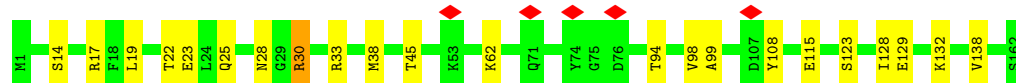




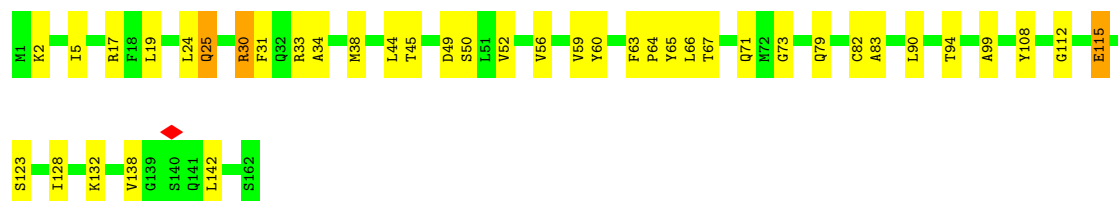
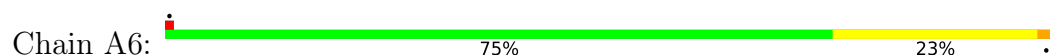
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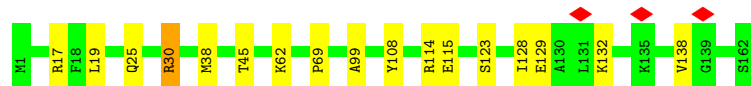
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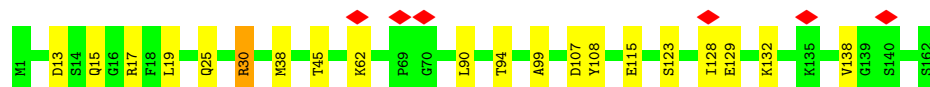
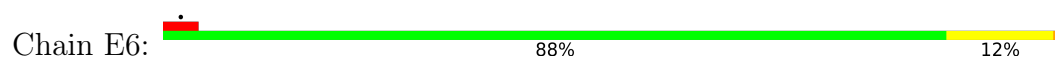
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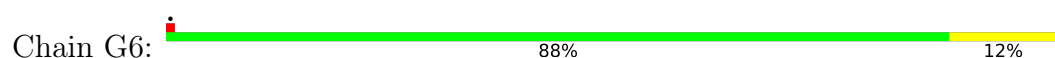
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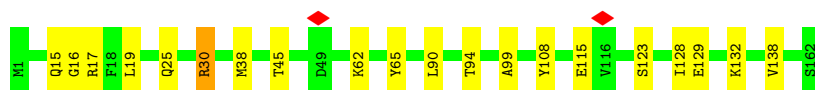


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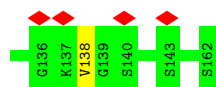
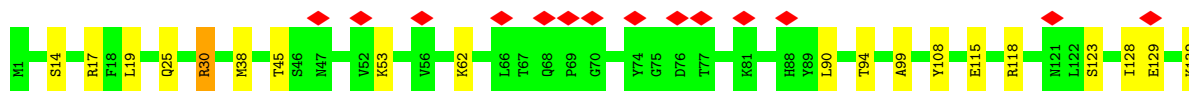
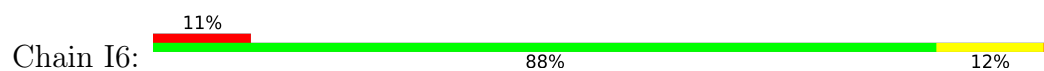


- Molecule 2: Phycocyanin alpha chain

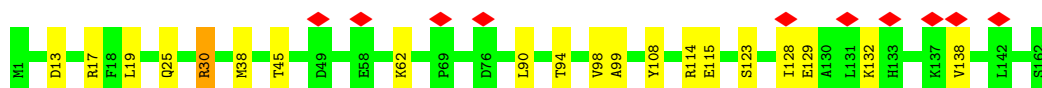
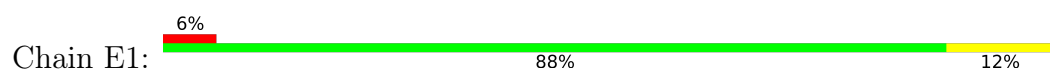




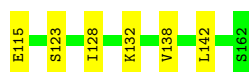
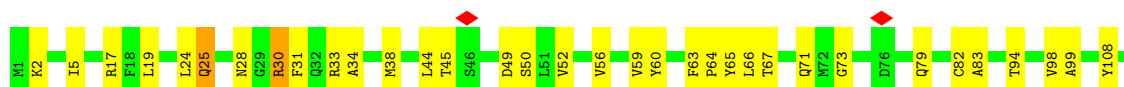
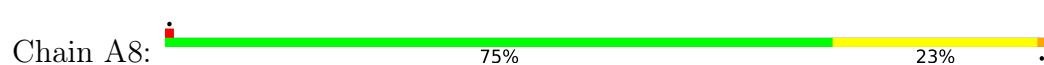
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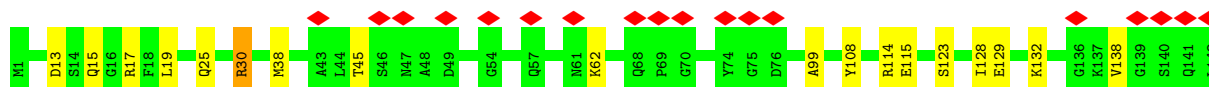
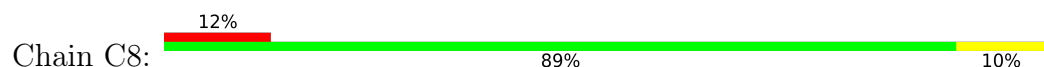
- Molecule 2: Phycocyanin alpha chain



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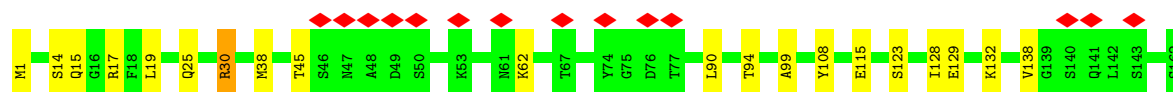


- Molecule 2: Phycocyanin alpha chain

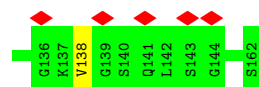
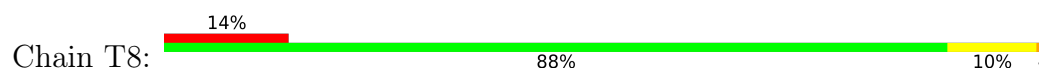


- Molecule 2: Phycocyanin alpha chain

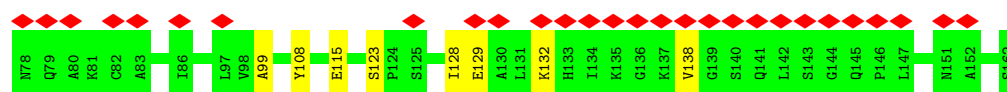
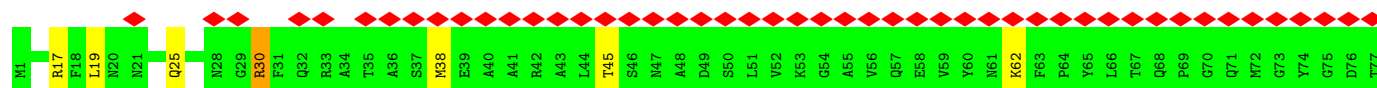
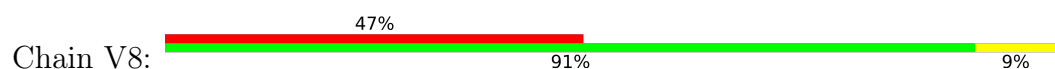




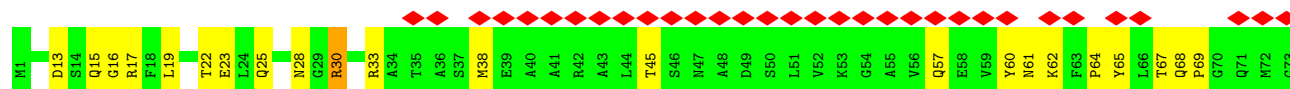
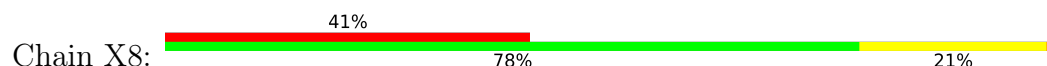
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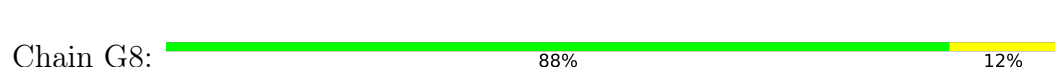
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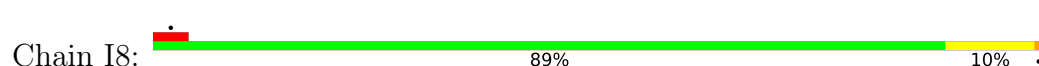
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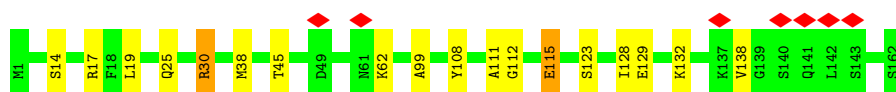


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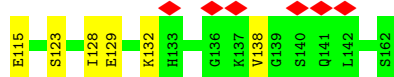
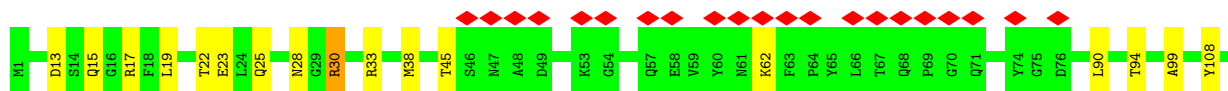
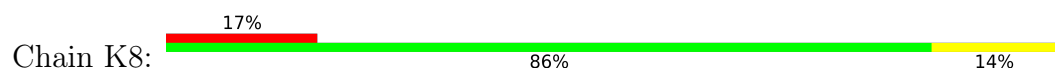


- Molecule 2: Phycocyanin alpha chain

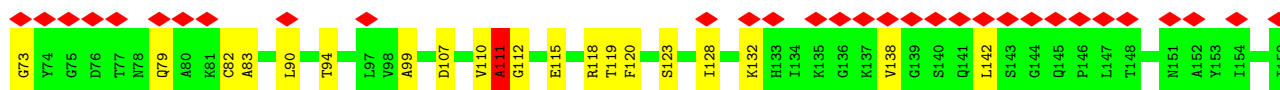
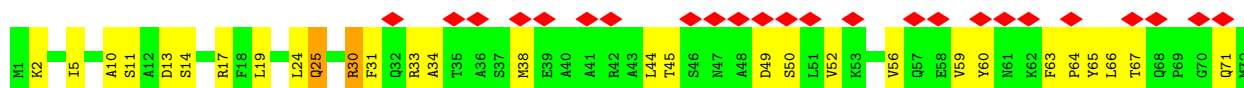




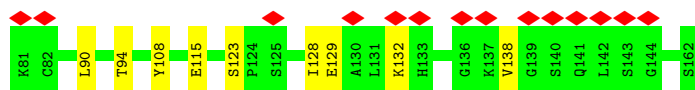
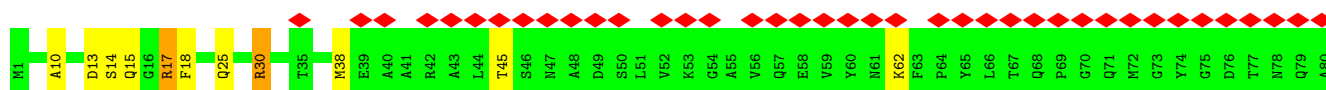
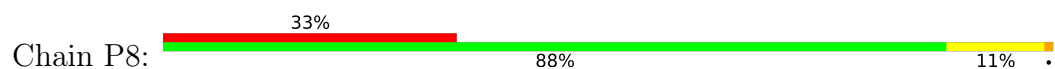
- Molecule 2: Phycocyanin alpha chain



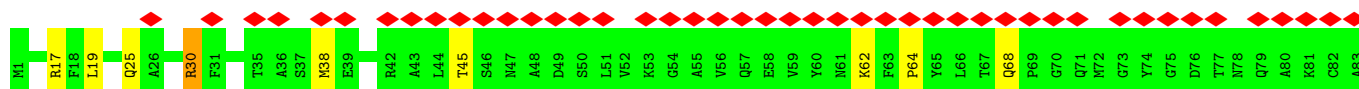
- Molecule 2: Phycocyanin alpha chain

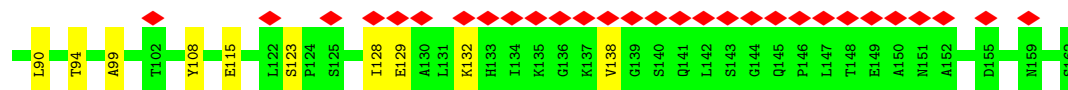


- Molecule 2: Phycocyanin alpha chain



- Molecule 2: Phycocyanin alpha chain





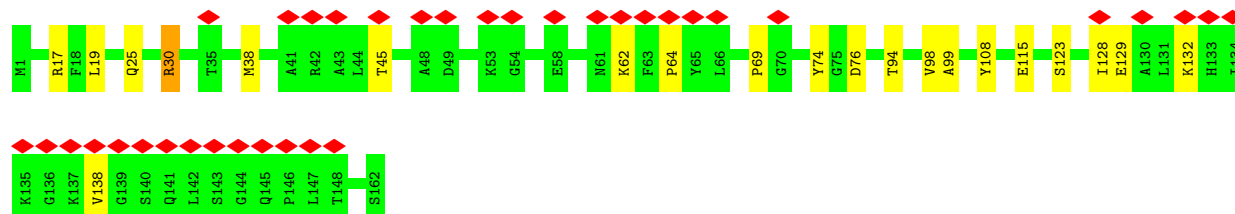
• Molecule 2: Phycocyanin alpha chain

Chain O9:



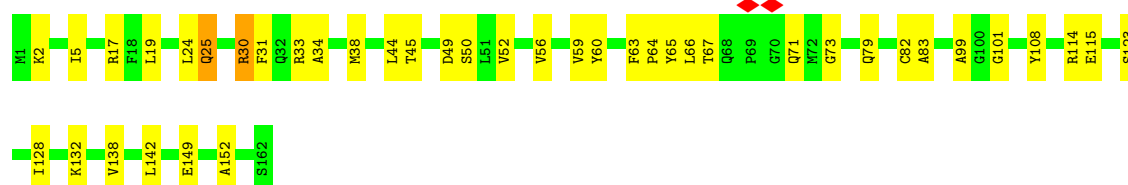
• Molecule 2: Phycocyanin alpha chain

Chain Q9:



• Molecule 2: Phycocyanin alpha chain

Chain A9:



• Molecule 2: Phycocyanin alpha chain

Chain C9:



• Molecule 2: Phycocyanin alpha chain

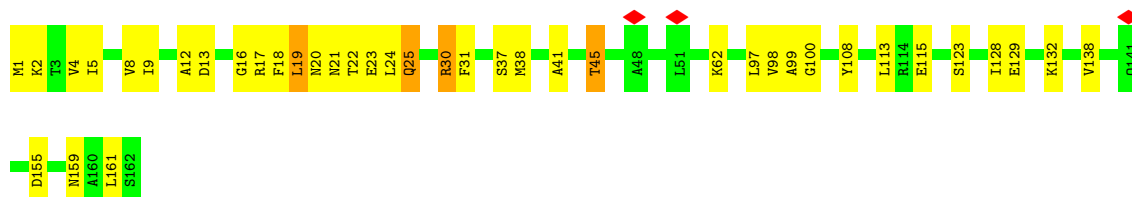
Chain E9:




• Molecule 2: Phycocyanin alpha chain

Chain G9:  89% 10%


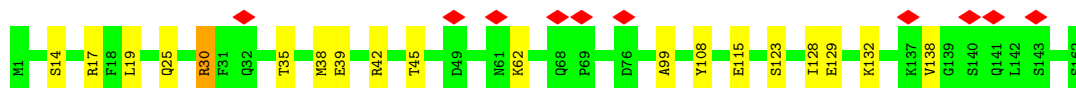
• Molecule 2: Phycocyanin alpha chain

Chain I9:  75% 22%


• Molecule 2: Phycocyanin alpha chain

Chain K9:  80% 15%

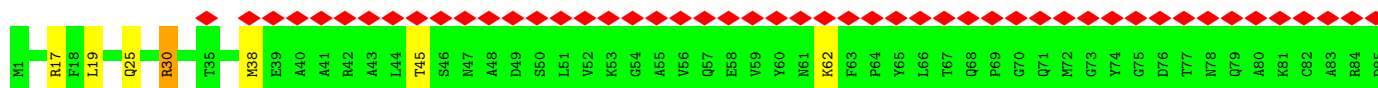
• Molecule 2: Phycocyanin alpha chain

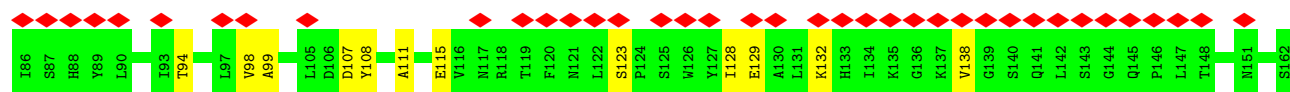
Chain S9:  6% 88% 11%

• Molecule 2: Phycocyanin alpha chain

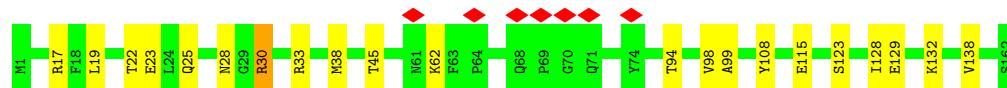
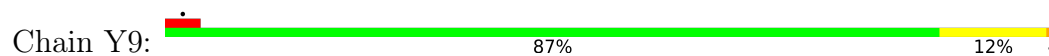
Chain U9:  5% 87% 12%

• Molecule 2: Phycocyanin alpha chain

Chain W9:  54% 88% 11%



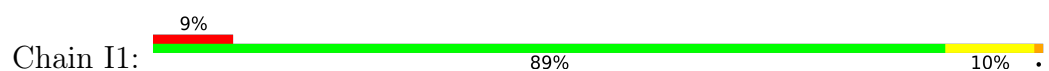
- Molecule 2: Phycocyanin alpha chain



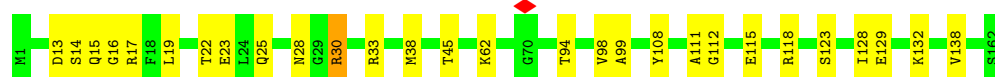
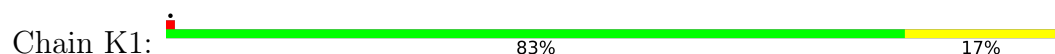
- Molecule 2: Phycocyanin alpha chain



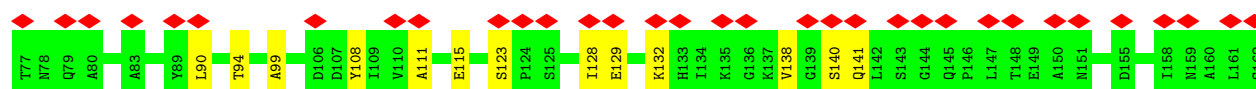
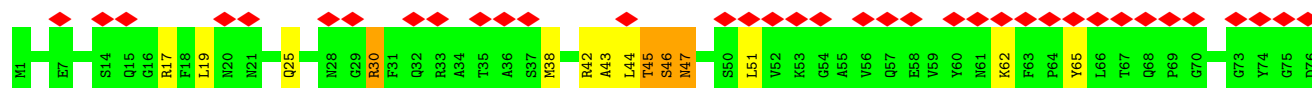
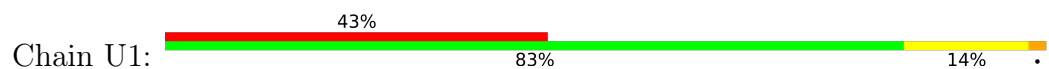
- Molecule 2: Phycocyanin alpha chain



- Molecule 2: Phycocyanin alpha chain

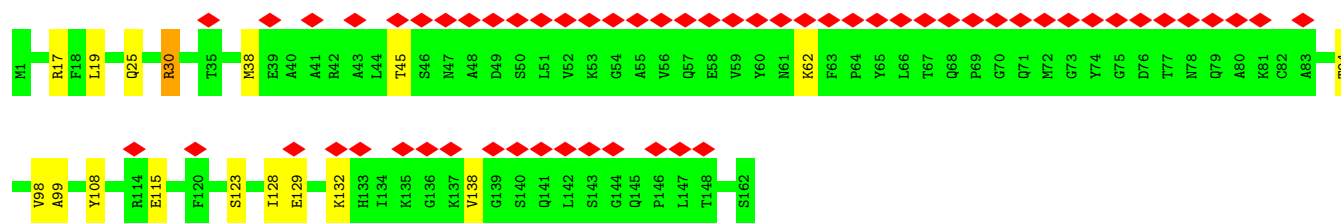


- Molecule 2: Phycocyanin alpha chain

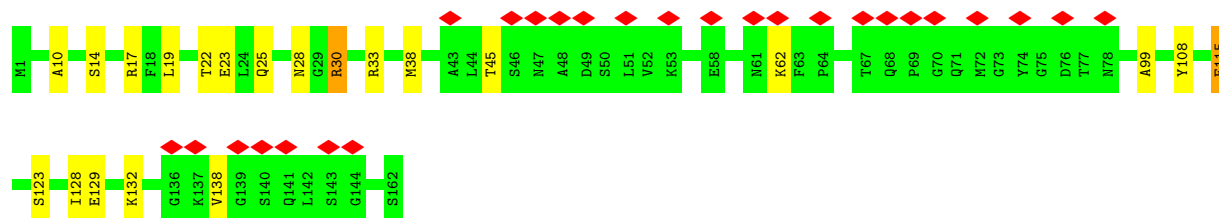
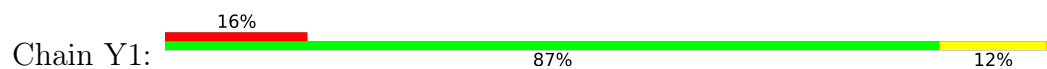


- Molecule 2: Phycocyanin alpha chain

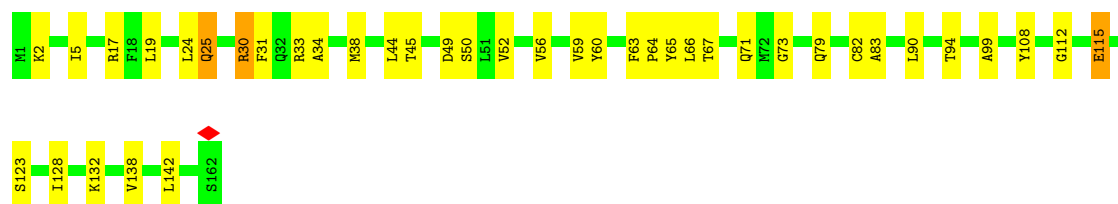
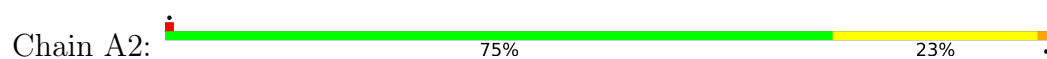




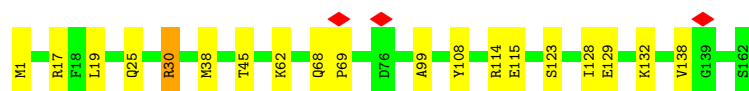
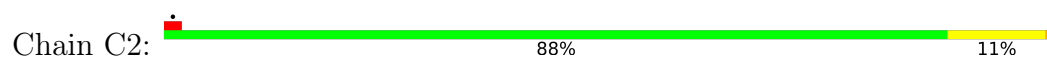
• Molecule 2: Phycocyanin alpha chain



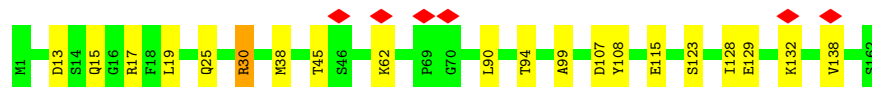
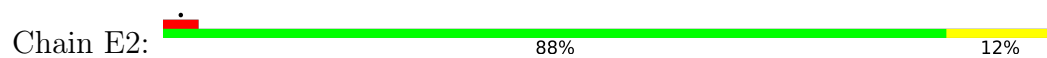
• Molecule 2: Phycocyanin alpha chain



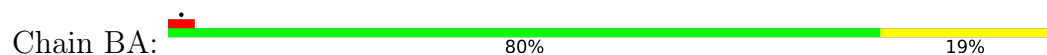
• Molecule 2: Phycocyanin alpha chain



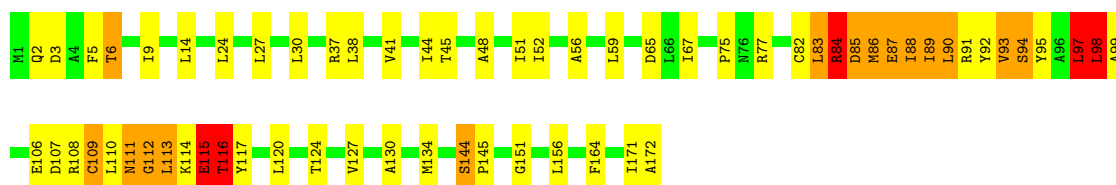
• Molecule 2: Phycocyanin alpha chain




• Molecule 3: Phycocyanin beta chain

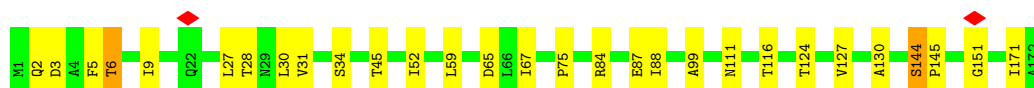


Chain LA:  63% 26% 9% .




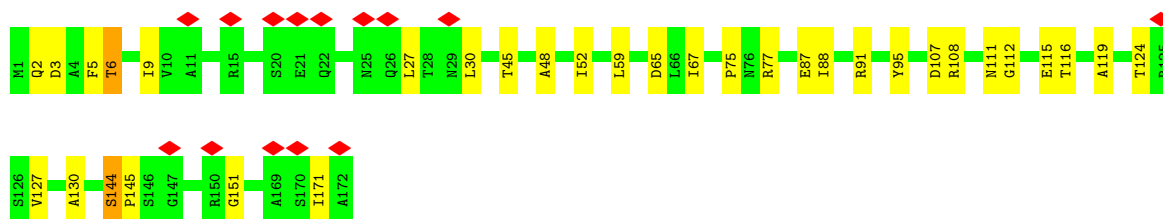
• Molecule 3: Phycocyanin beta chain

Chain PA:  83% 16% .




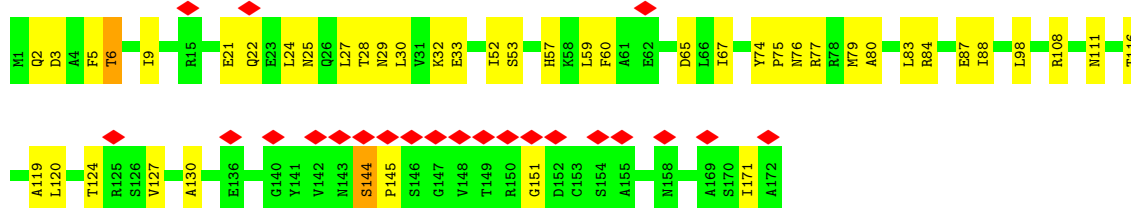
• Molecule 3: Phycocyanin beta chain

Chain RA:  8% 81% 18% .




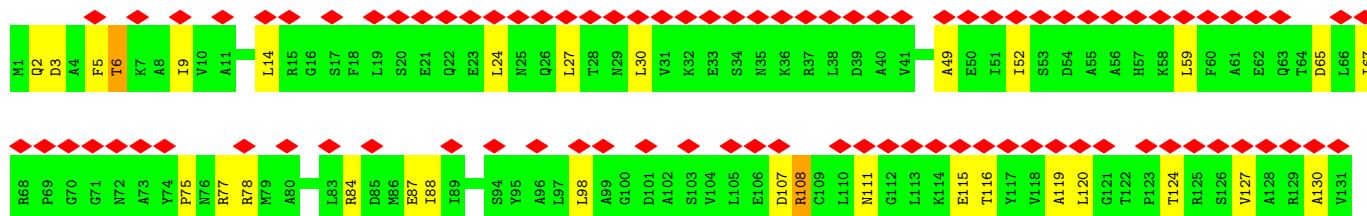
• Molecule 3: Phycocyanin beta chain

Chain TA:  13% 74% 25% .



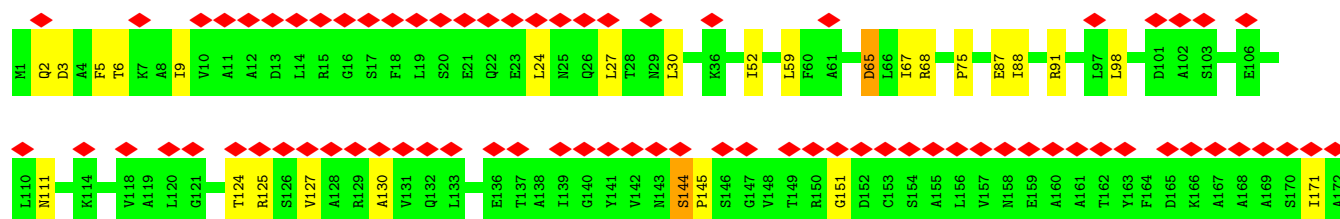
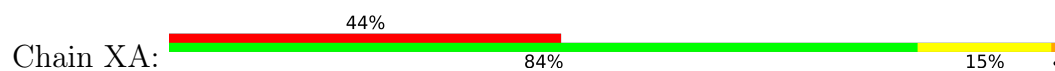
• Molecule 3: Phycocyanin beta chain

Chain VA:  76% 80% 19% .

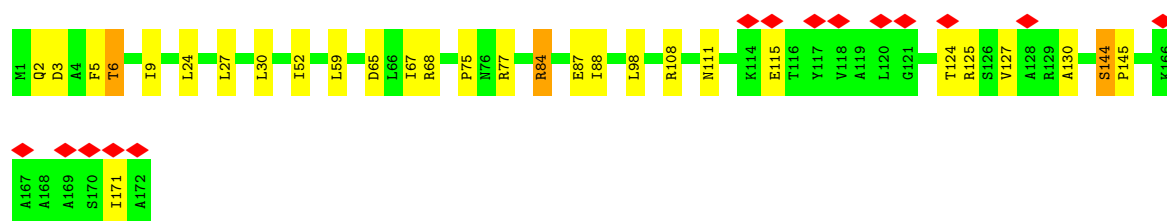
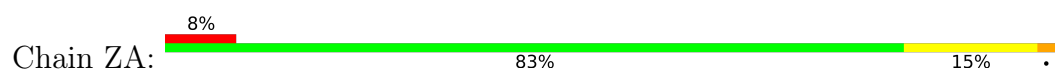




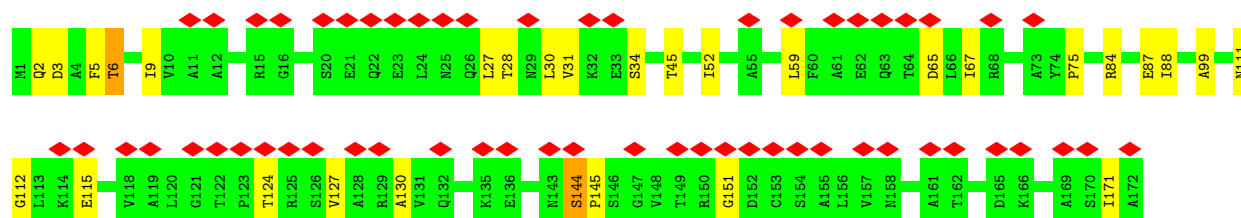
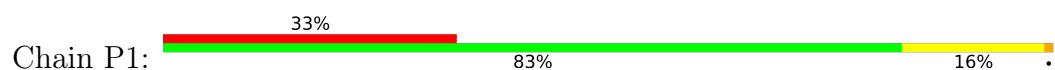
- Molecule 3: Phycocyanin beta chain



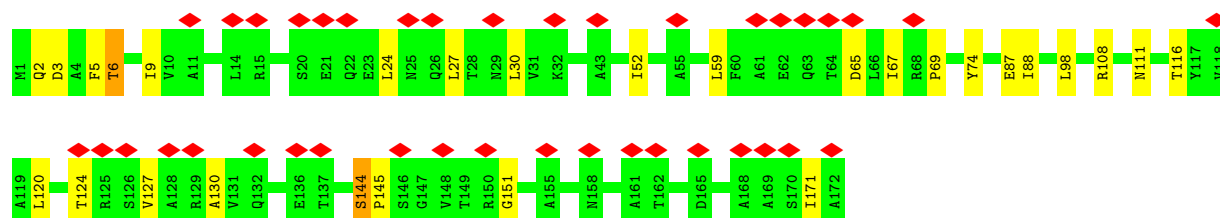
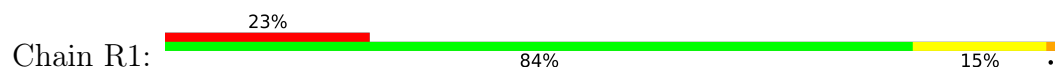
- Molecule 3: Phycocyanin beta chain



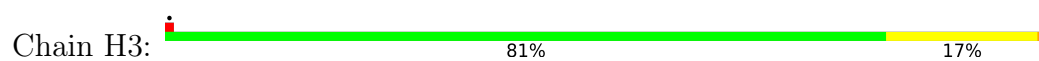
- Molecule 3: Phycocyanin beta chain



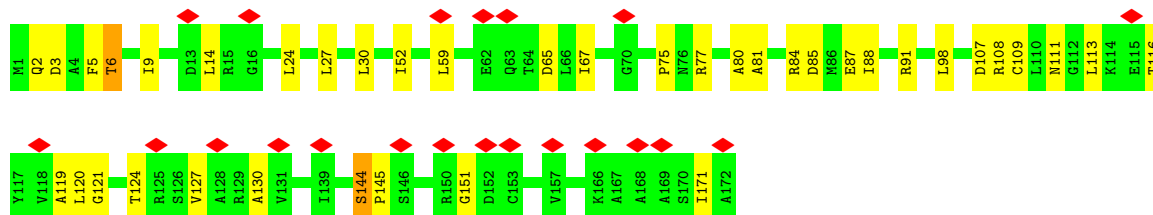
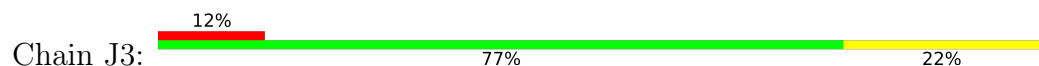
- Molecule 3: Phycocyanin beta chain



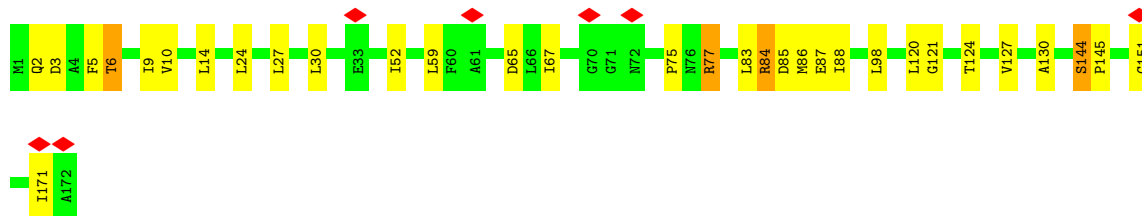
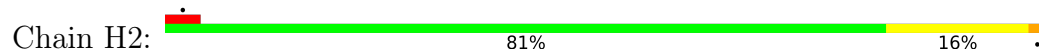
- Molecule 3: Phycocyanin beta chain



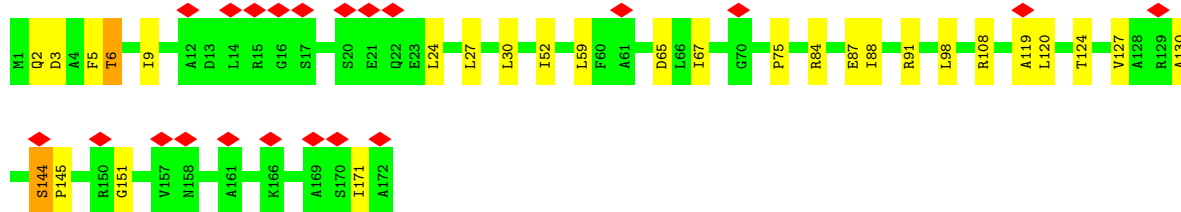
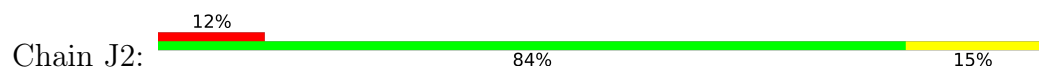
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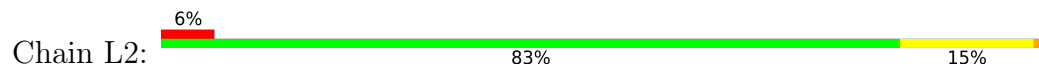
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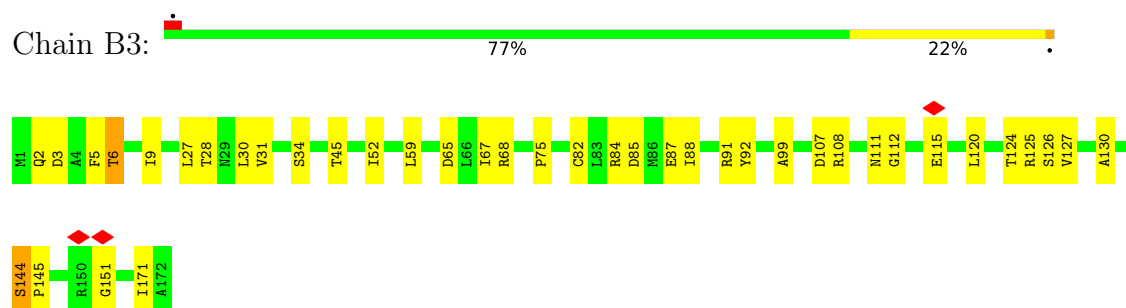
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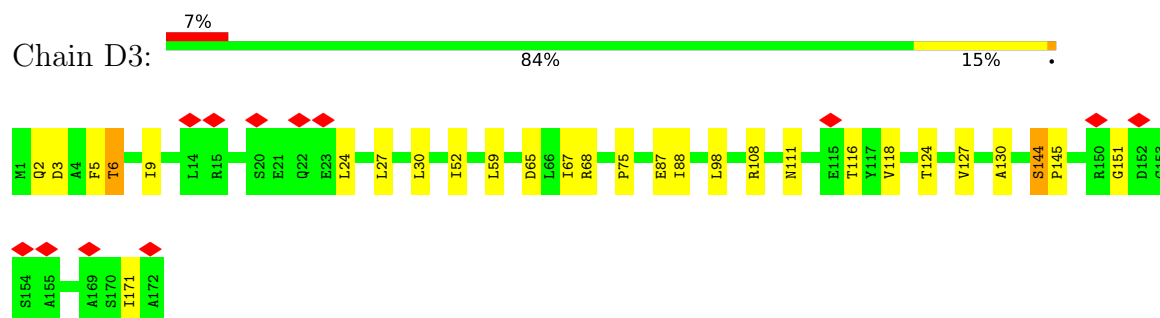
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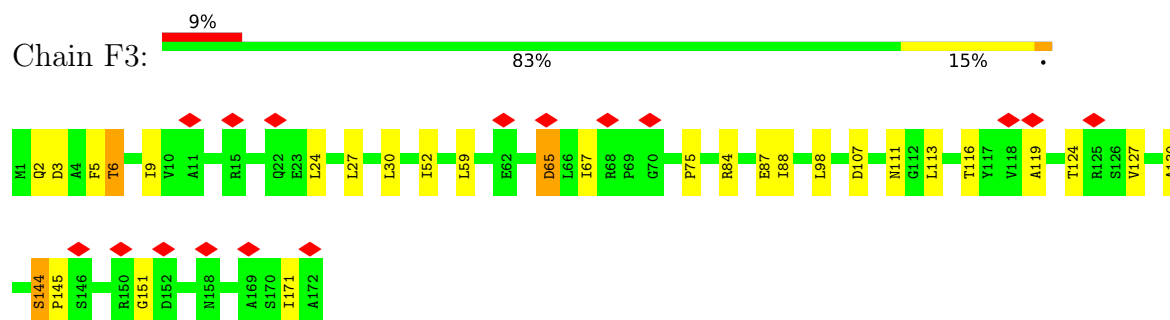
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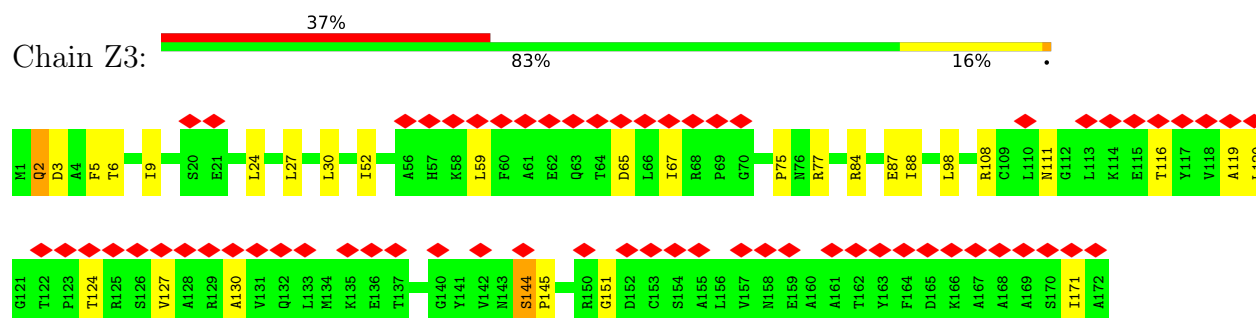
- Molecule 3: Phycocyanin beta chain



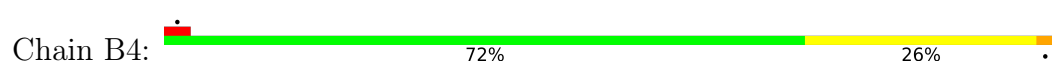
- Molecule 3: Phycocyanin beta chain

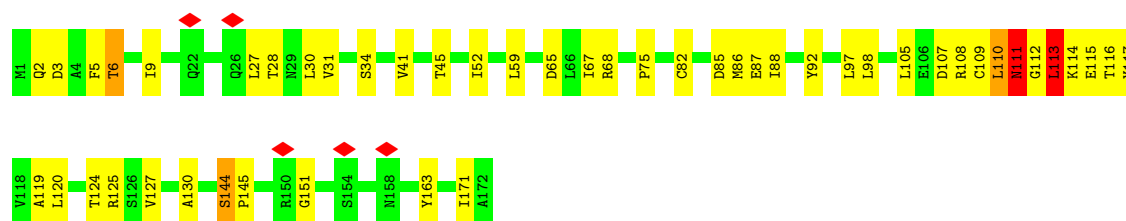


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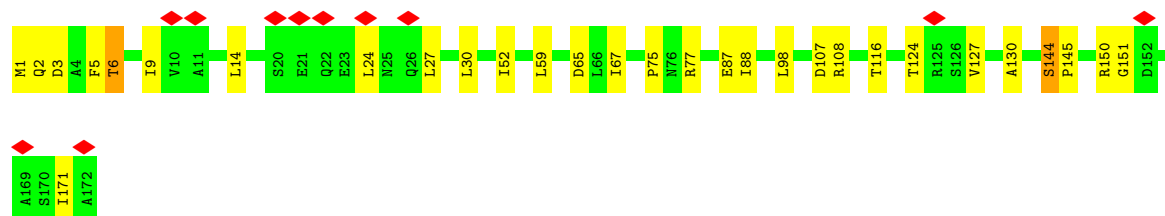
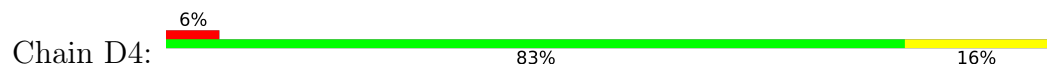


- Molecule 3: Phycocyanin beta chain

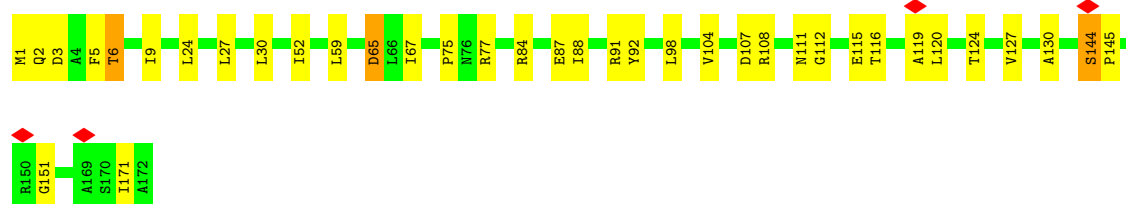
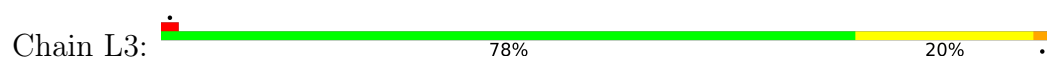




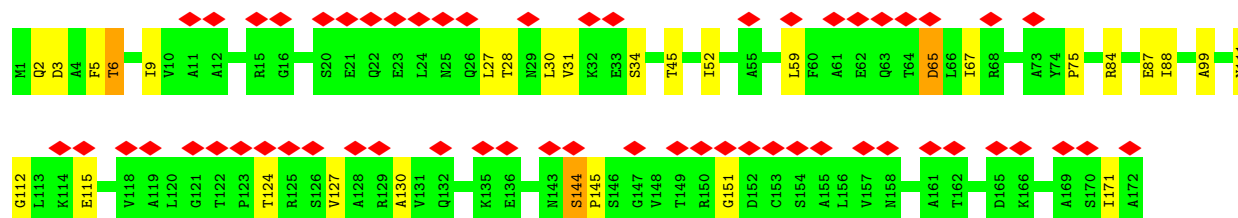
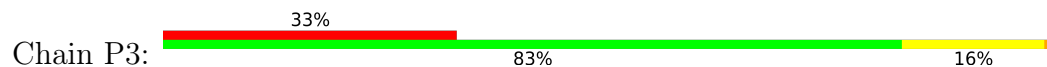
• Molecule 3: Phycocyanin beta chain



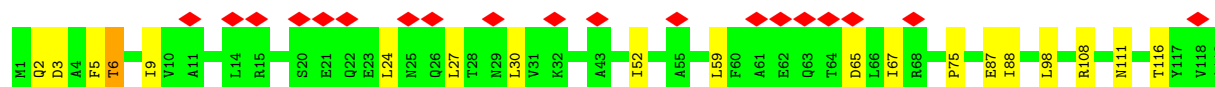
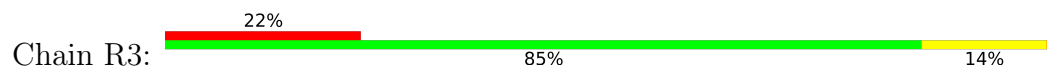
• Molecule 3: Phycocyanin beta chain

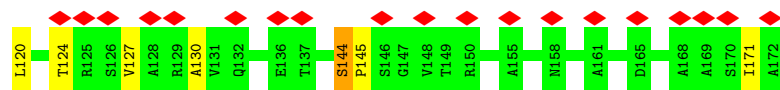


• Molecule 3: Phycocyanin beta chain

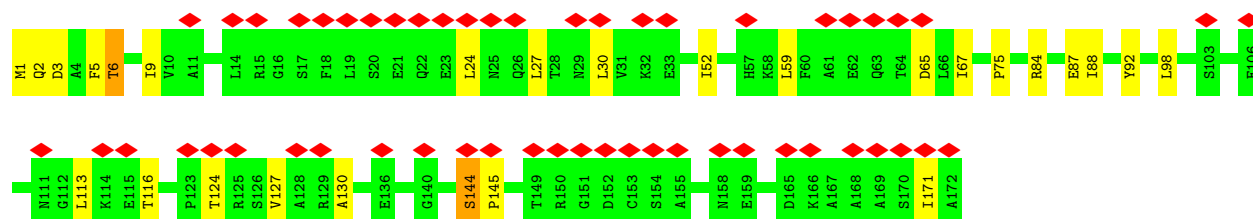
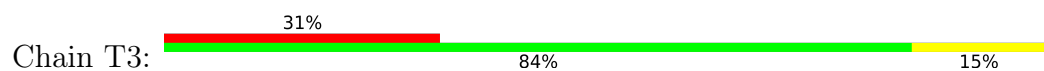


• Molecule 3: Phycocyanin beta chain

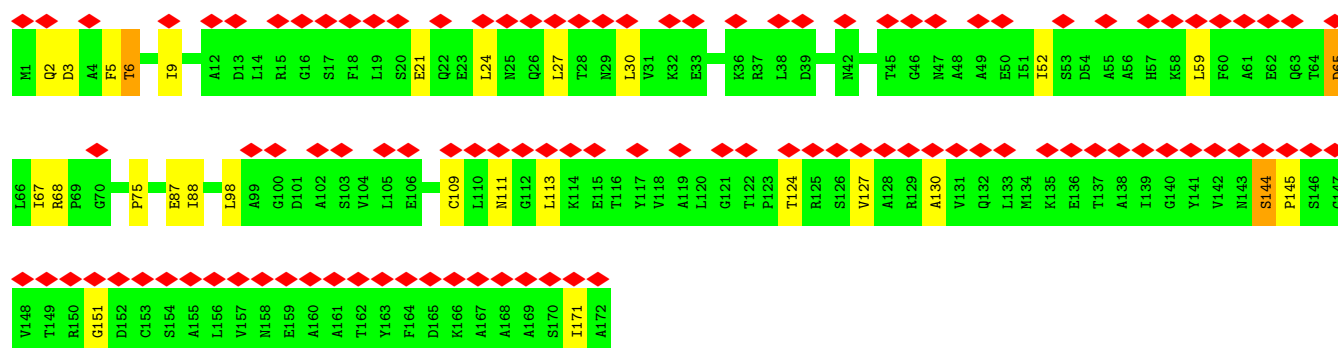
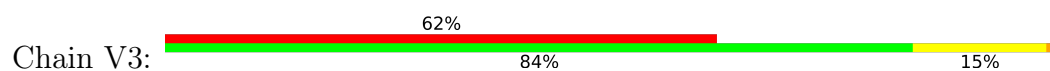




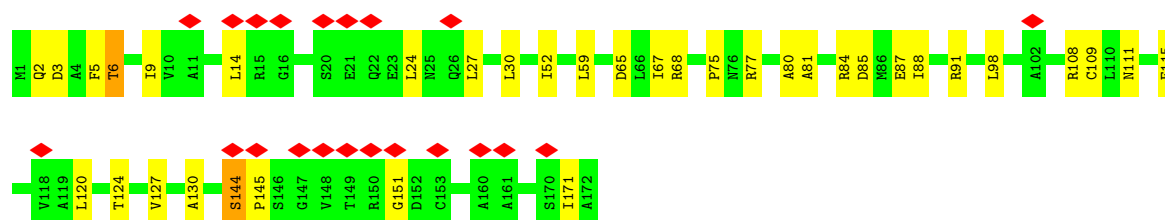
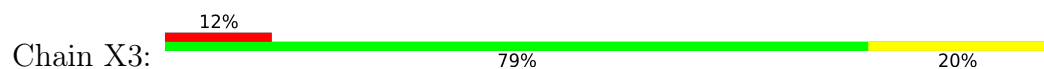
• Molecule 3: Phycocyanin beta chain



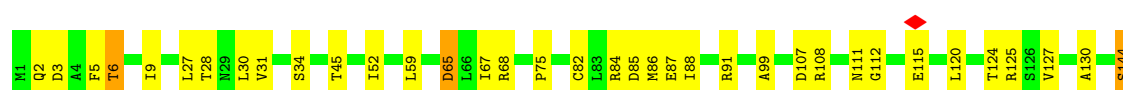
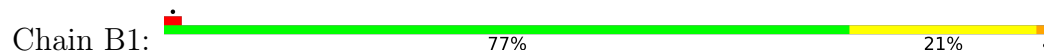
• Molecule 3: Phycocyanin beta chain

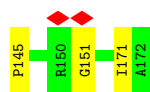


• Molecule 3: Phycocyanin beta chain

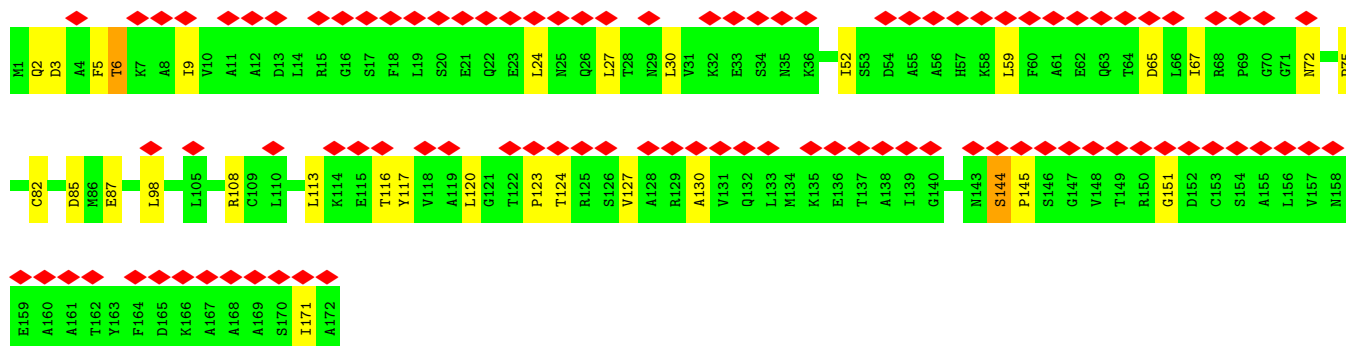
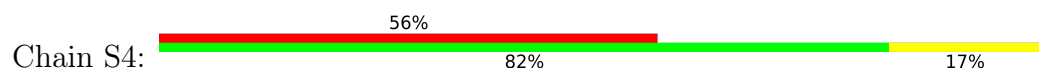


• Molecule 3: Phycocyanin beta chain

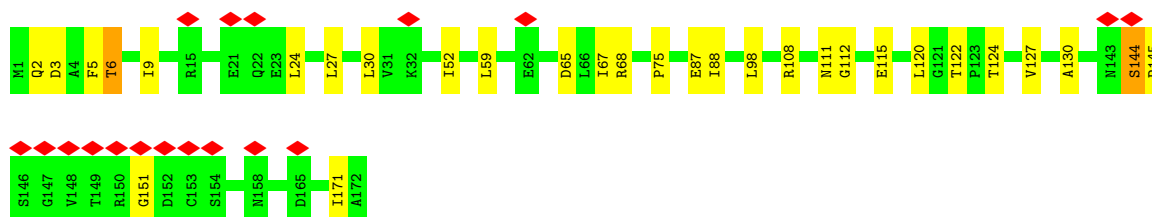
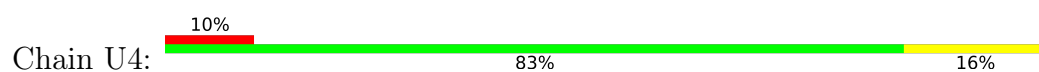




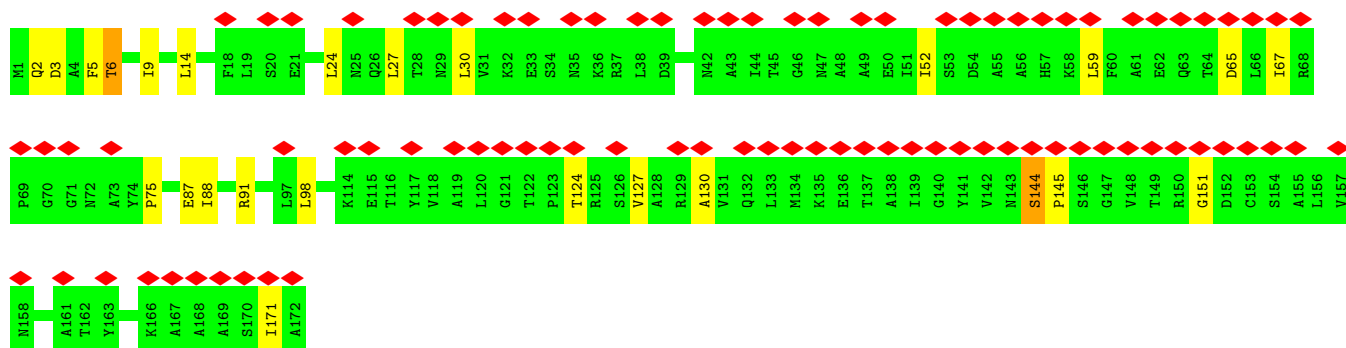
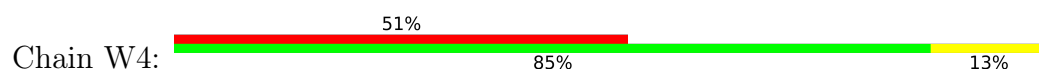
- Molecule 3: Phycocyanin beta chain



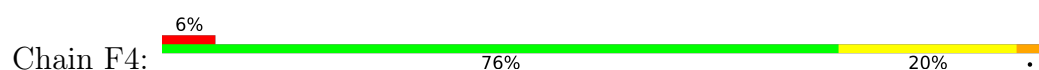
- Molecule 3: Phycocyanin beta chain

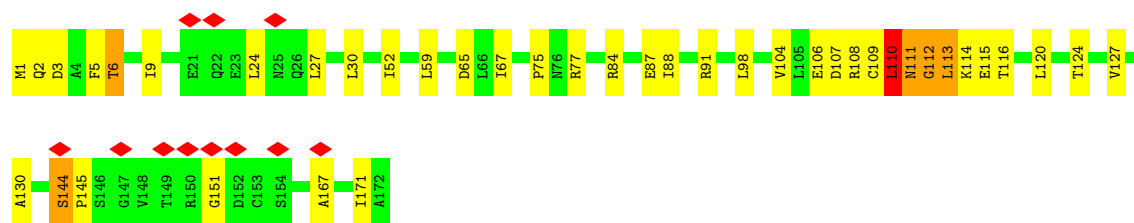


- Molecule 3: Phycocyanin beta chain

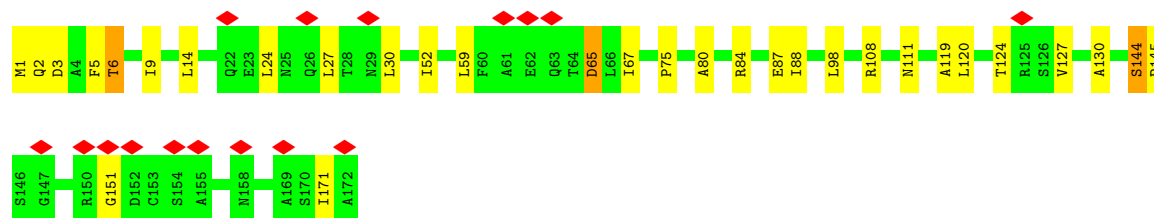
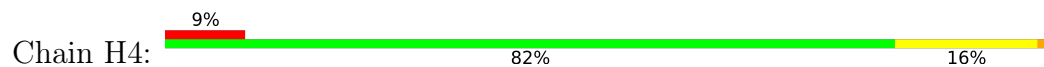


- Molecule 3: Phycocyanin beta chain

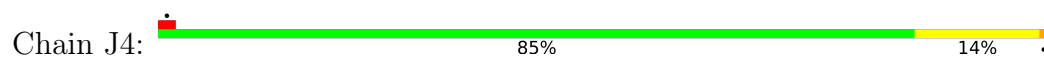




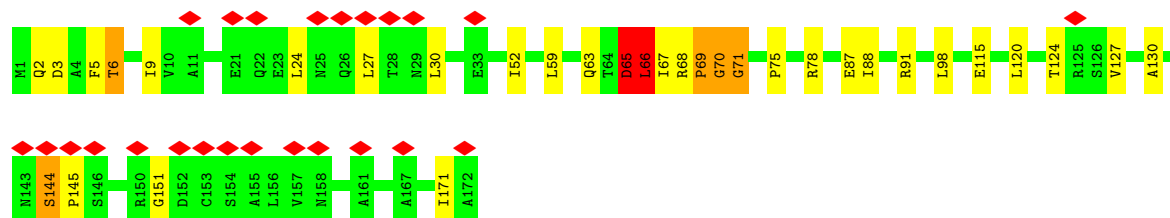
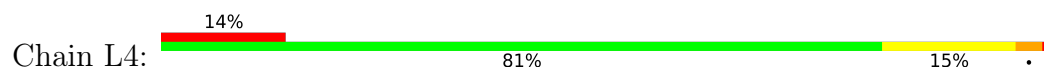
- Molecule 3: Phycocyanin beta chain



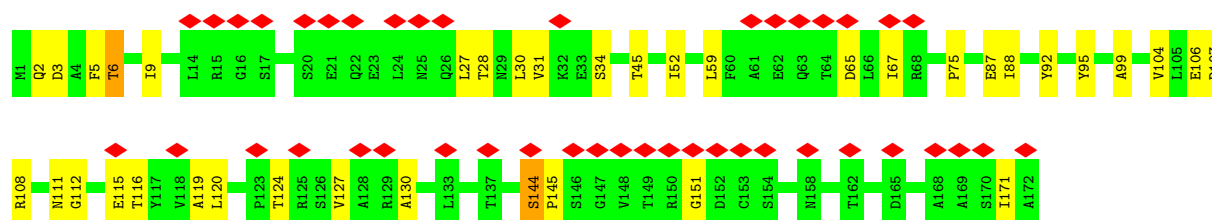
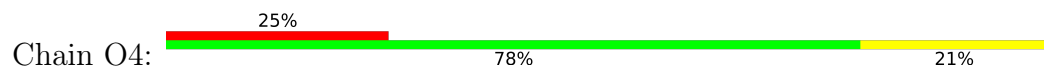
- Molecule 3: Phycocyanin beta chain



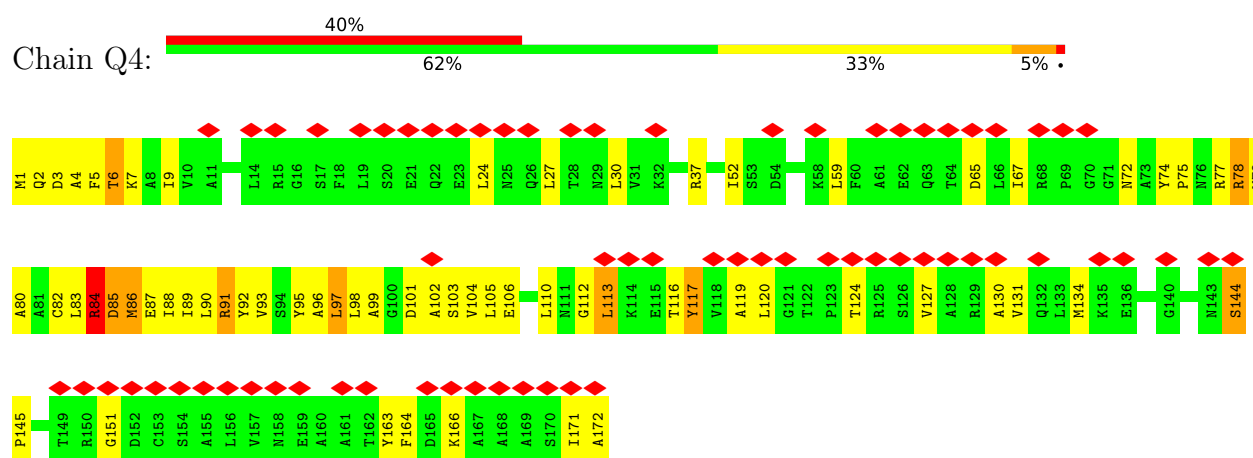
- Molecule 3: Phycocyanin beta chain



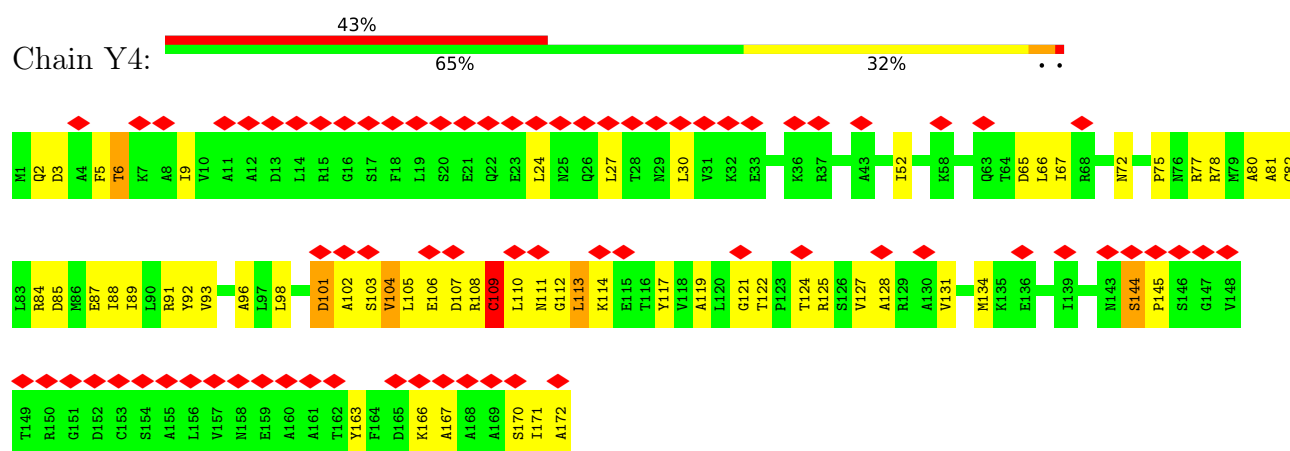
- Molecule 3: Phycocyanin beta chain



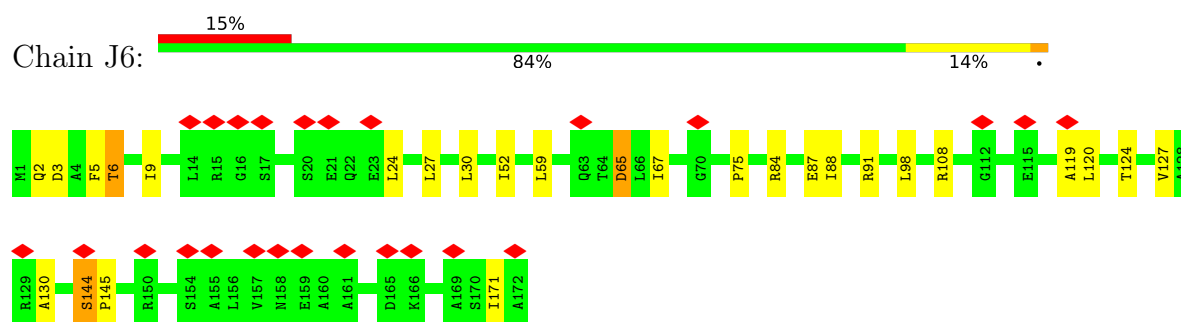
- Molecule 3: Phycocyanin beta chain



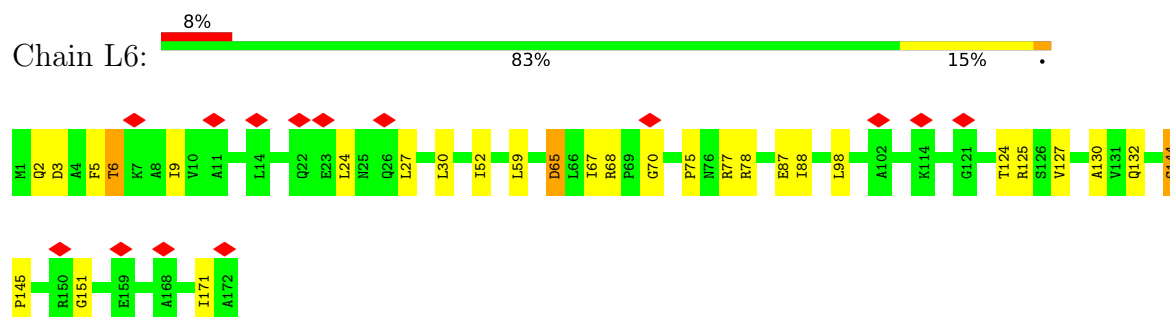
• Molecule 3: Phycocyanin beta chain




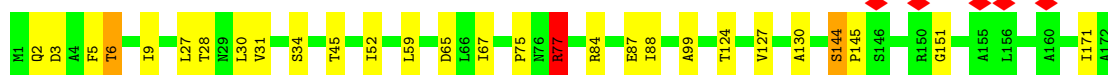
• Molecule 3: Phycocyanin beta chain




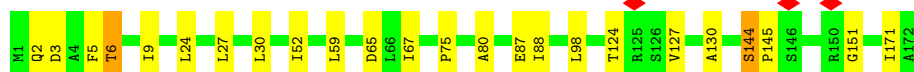
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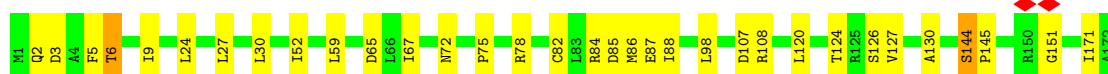
● Molecule 3: Phycocyanin beta chain

Chain B6:  84% 15% ..


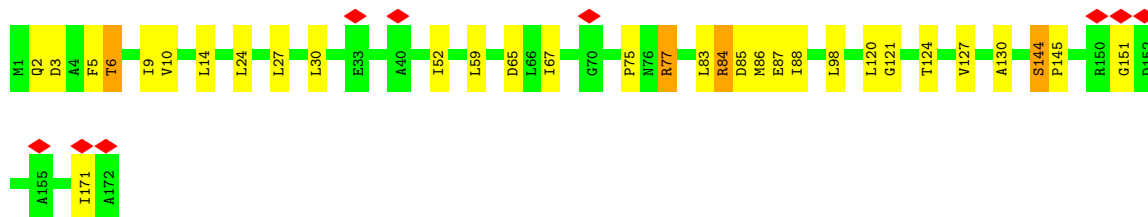
● Molecule 3: Phycocyanin beta chain

Chain D6:  86% 13% .


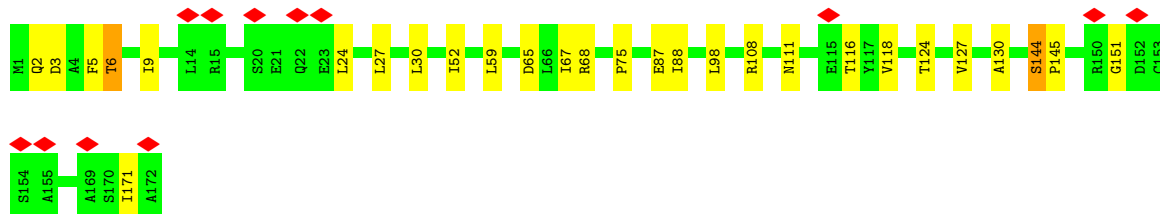
● Molecule 3: Phycocyanin beta chain

Chain F6:  81% 18% .

● Molecule 3: Phycocyanin beta chain

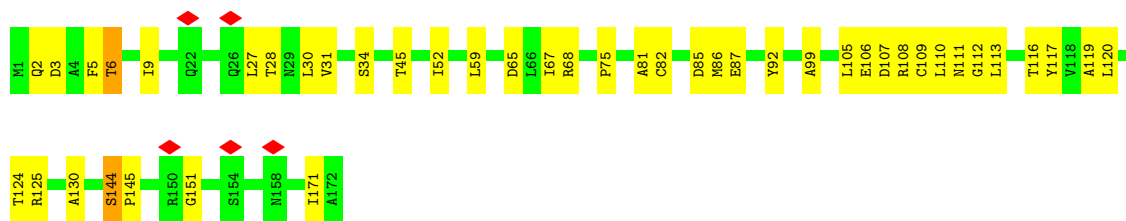
Chain H6:  81% 16% .

● Molecule 3: Phycocyanin beta chain

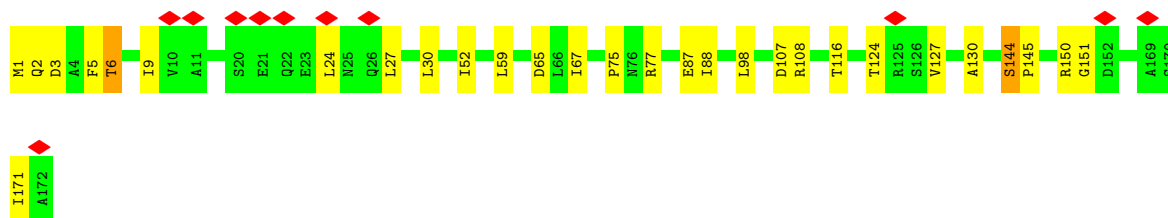
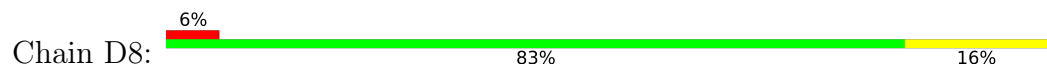
Chain D1:  84% 15% .

● Molecule 3: Phycocyanin beta chain

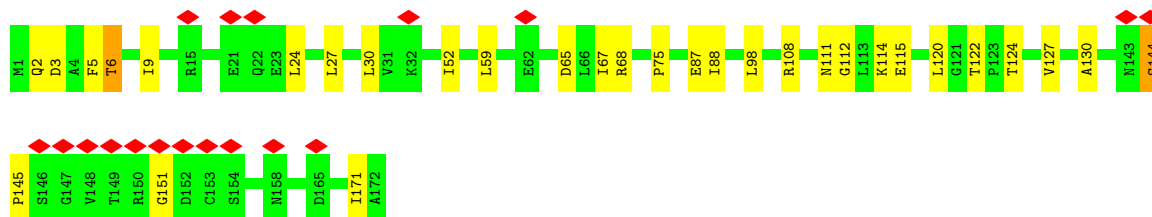
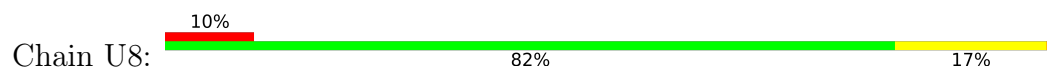
Chain B8:  74% 24% .



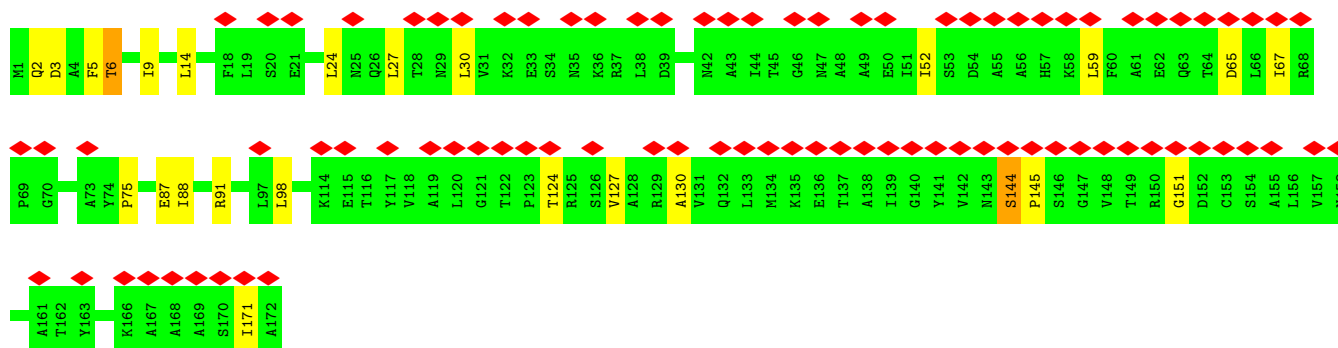
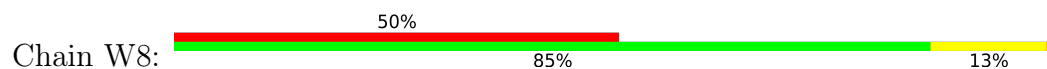
- Molecule 3: Phycocyanin beta chain



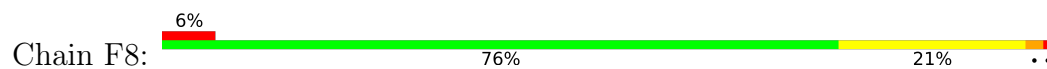
- Molecule 3: Phycocyanin beta chain

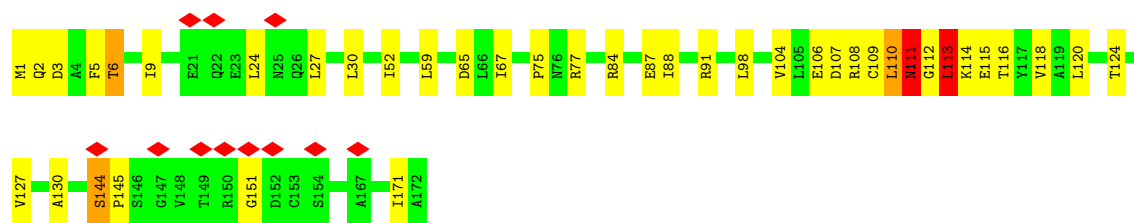


- Molecule 3: Phycocyanin beta chain

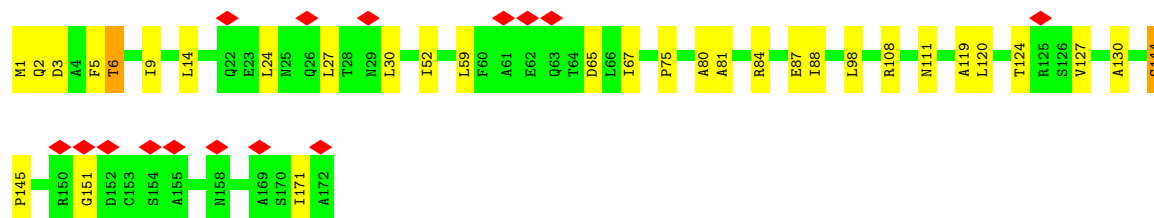
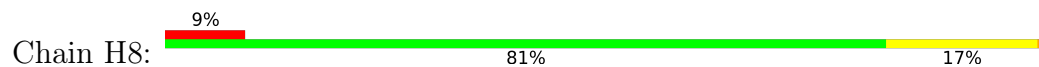


- Molecule 3: Phycocyanin beta chain

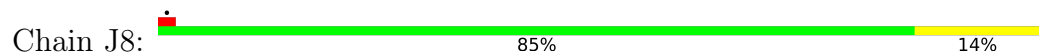




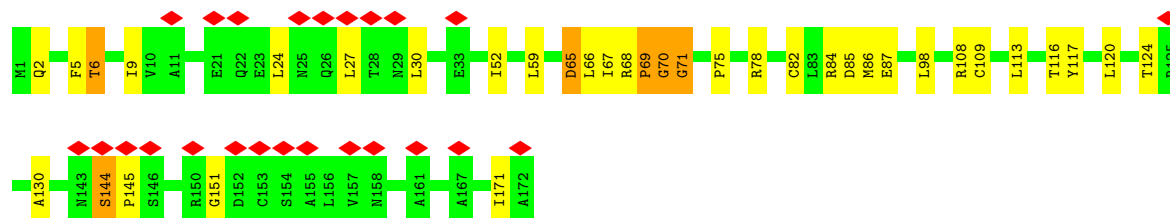
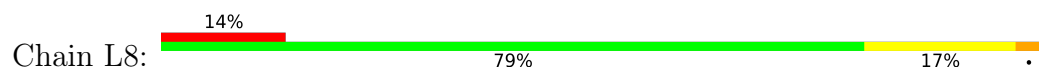
- Molecule 3: Phycocyanin beta chain



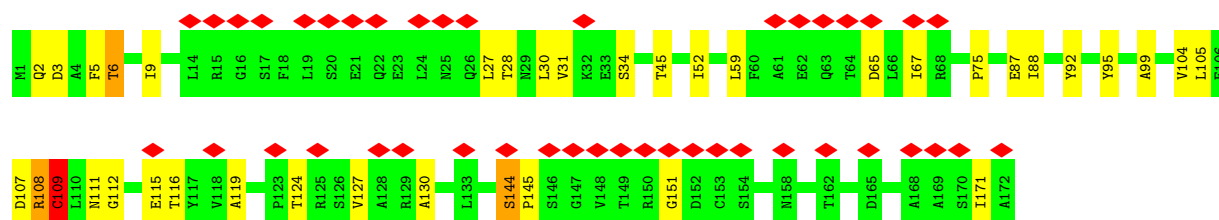
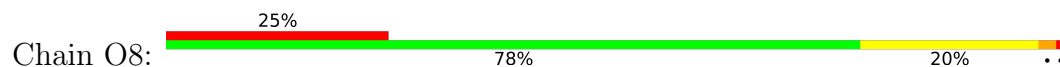
- Molecule 3: Phycocyanin beta chain




- Molecule 3: Phycocyanin beta chain

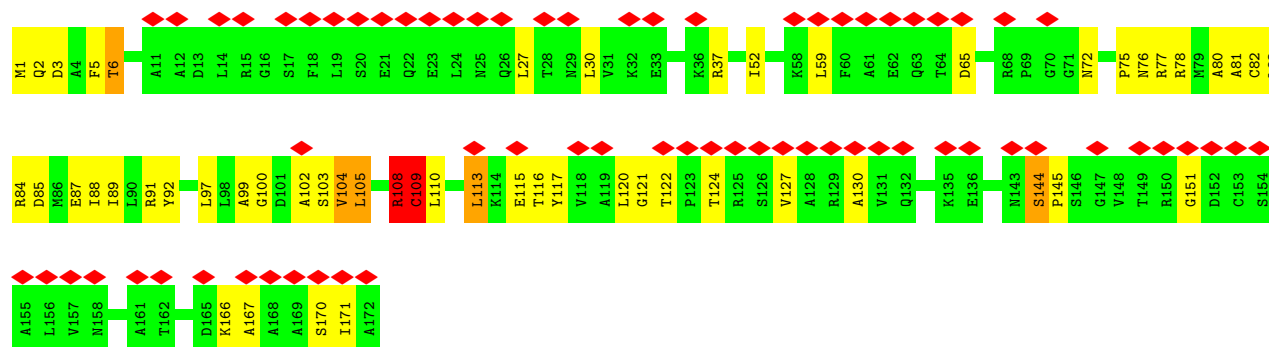


- Molecule 3: Phycocyanin beta chain




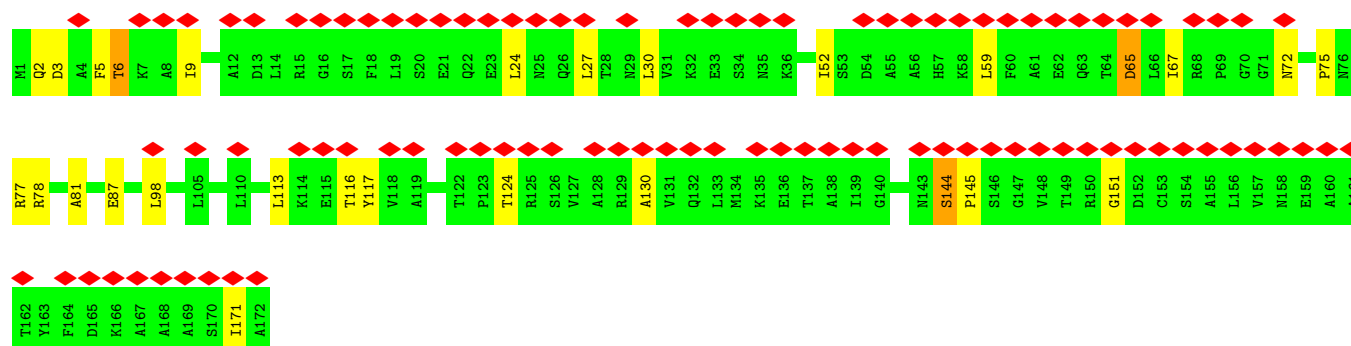
- Molecule 3: Phycocyanin beta chain

Chain Q8: 




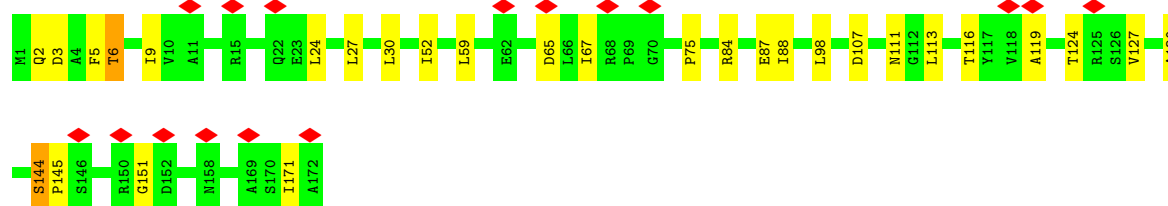
• Molecule 3: Phycocyanin beta chain

Chain S8: 



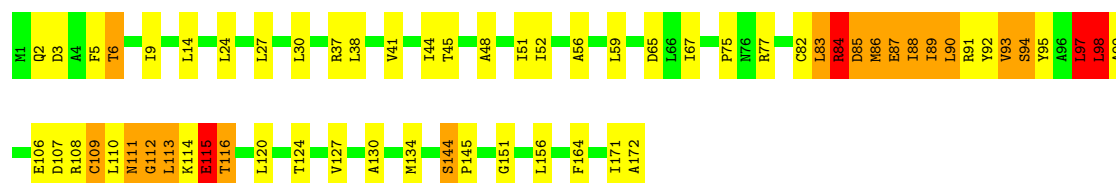
• Molecule 3: Phycocyanin beta chain

Chain F1: 




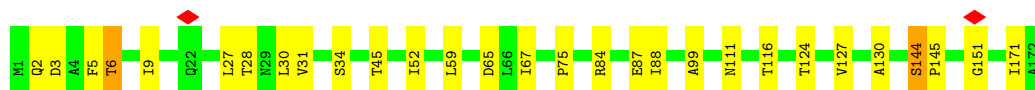
• Molecule 3: Phycocyanin beta chain

Chain L9: 




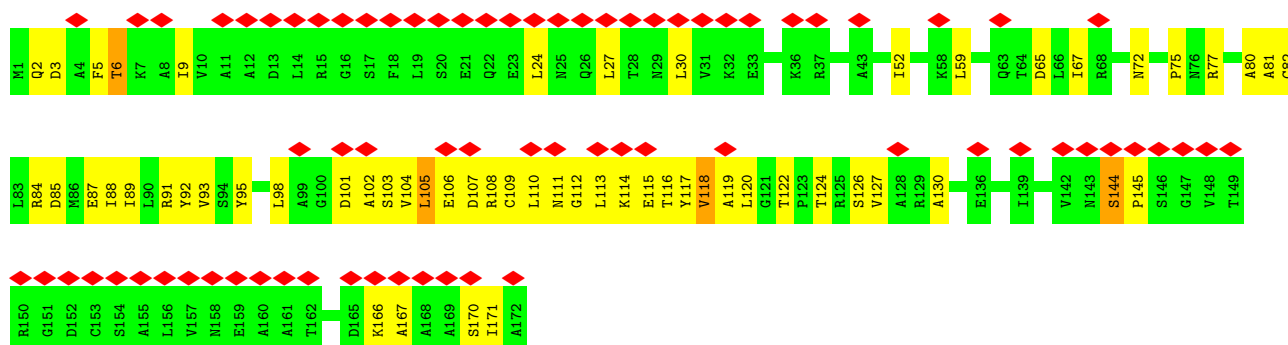
• Molecule 3: Phycocyanin beta chain

Chain P9:  83% 16%




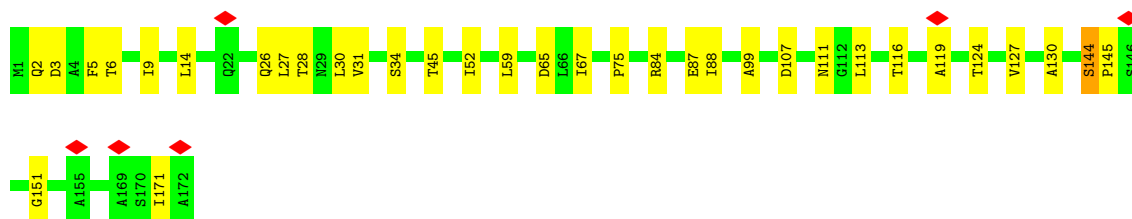
• Molecule 3: Phycocyanin beta chain

Chain Y8:  43% 66% 32%




• Molecule 3: Phycocyanin beta chain

Chain B9:  80% 19%




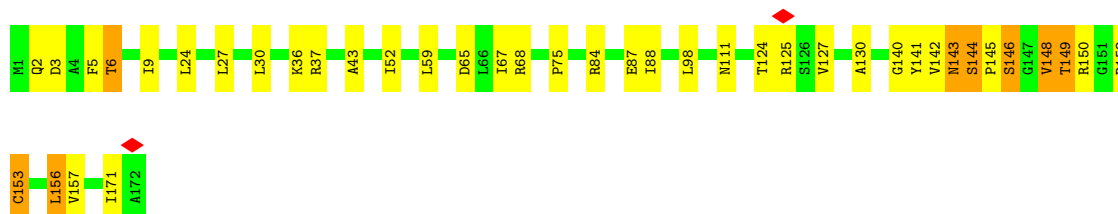
• Molecule 3: Phycocyanin beta chain

Chain D9:  83% 16%

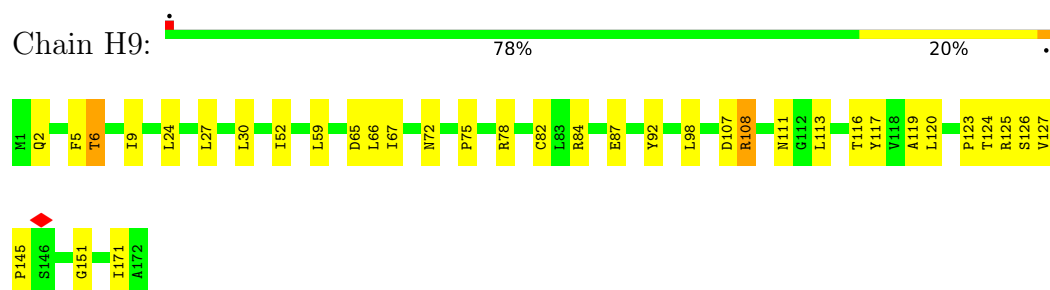


• Molecule 3: Phycocyanin beta chain

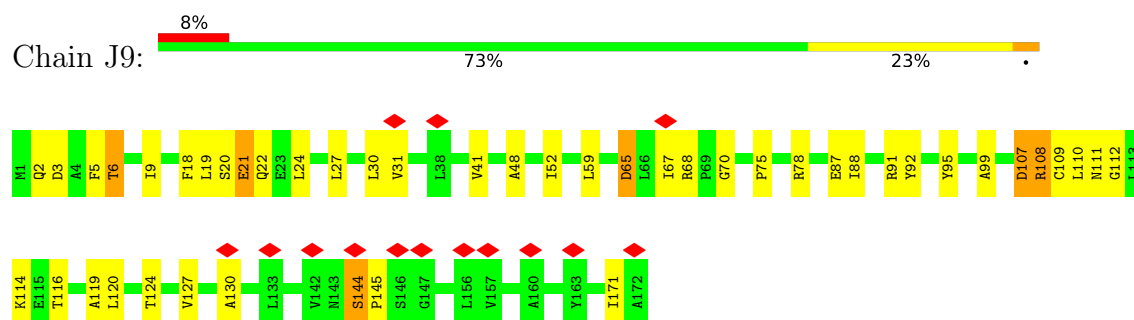
Chain F9:  76% 19% 5%



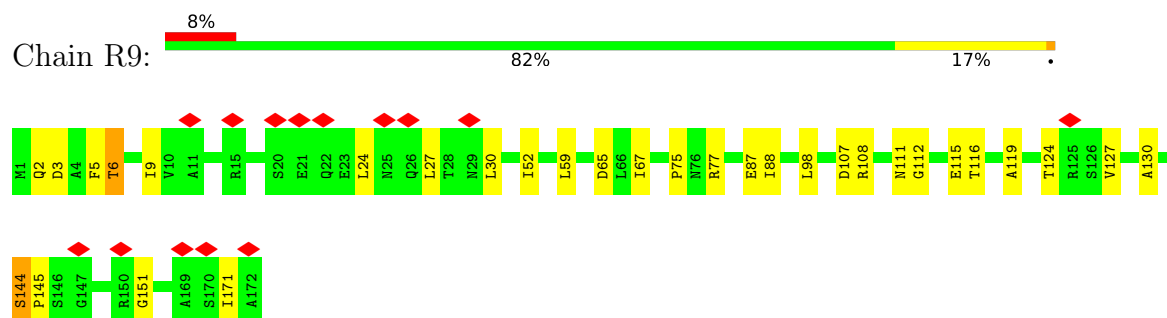
• Molecule 3: Phycocyanin beta chain



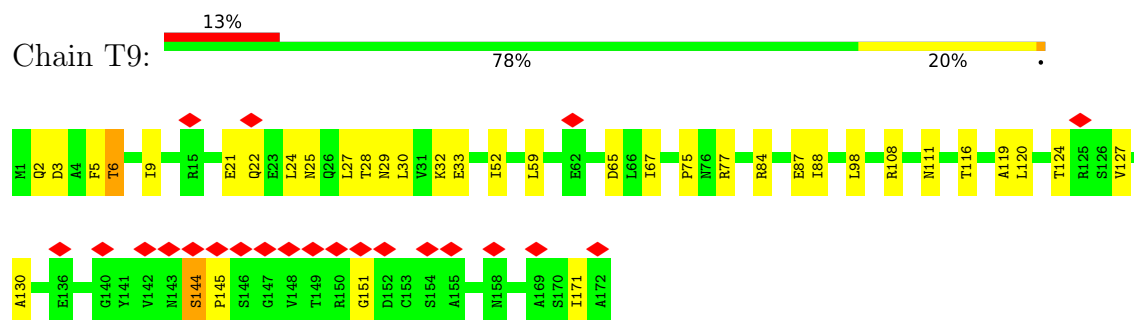
• Molecule 3: Phycocyanin beta chain



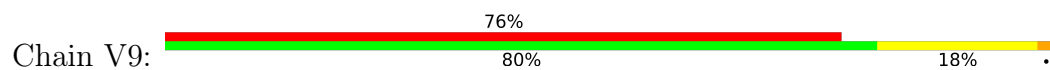
• Molecule 3: Phycocyanin beta chain

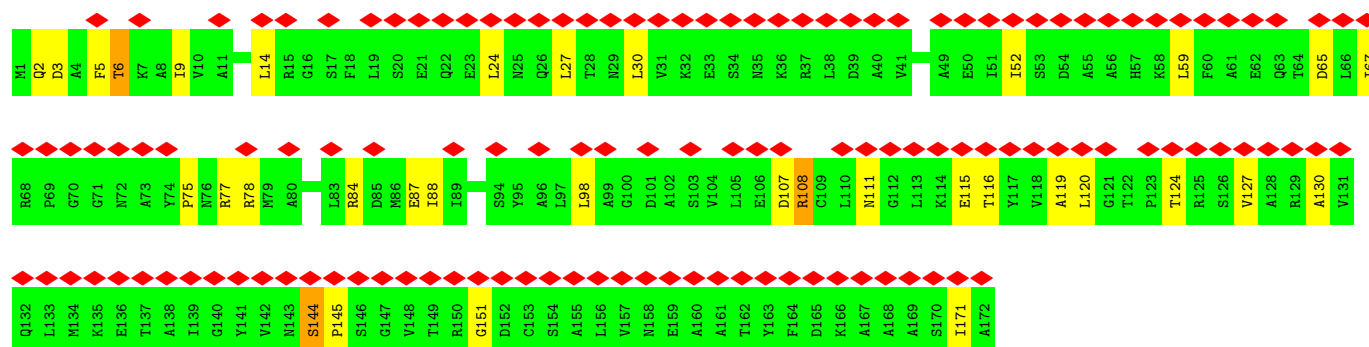


• Molecule 3: Phycocyanin beta chain

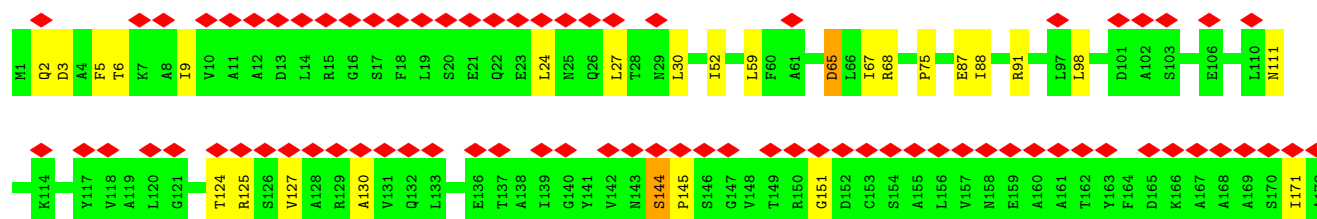
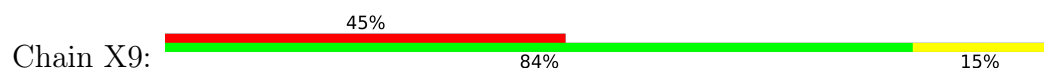


• Molecule 3: Phycocyanin beta chain

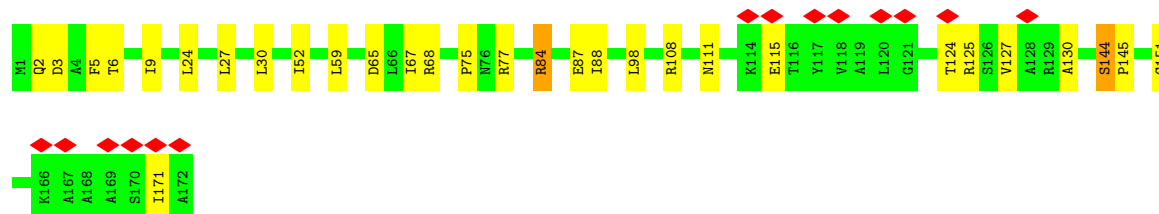
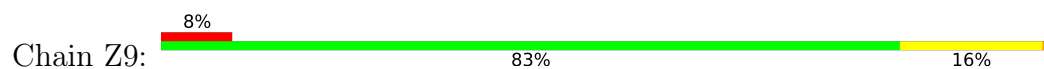




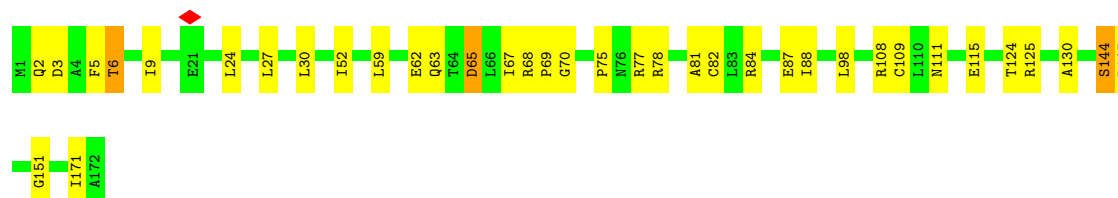
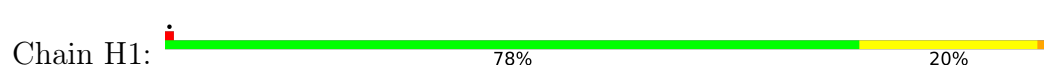
• Molecule 3: Phycocyanin beta chain



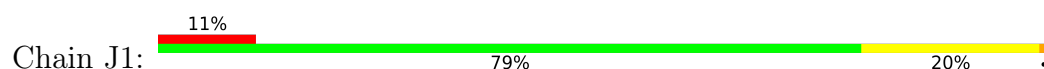
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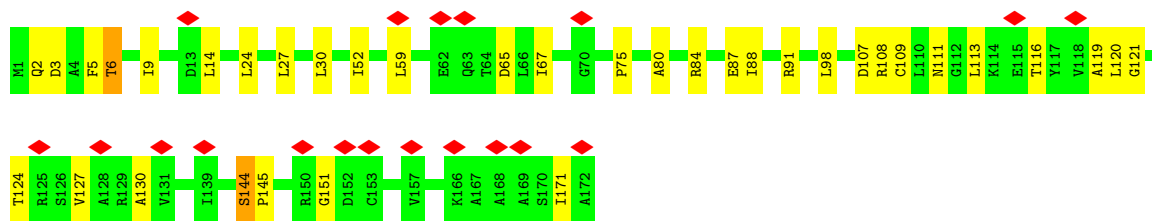


• Molecule 3: Phycocyanin beta chain

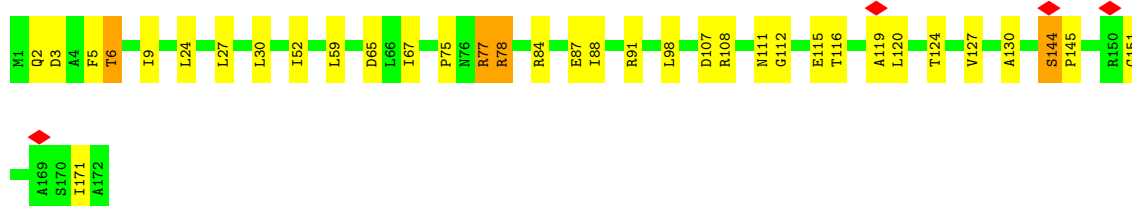
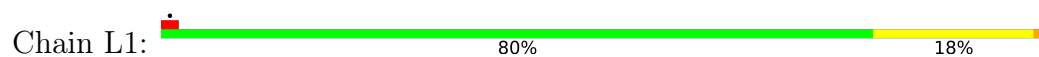


• Molecule 3: Phycocyanin beta chain

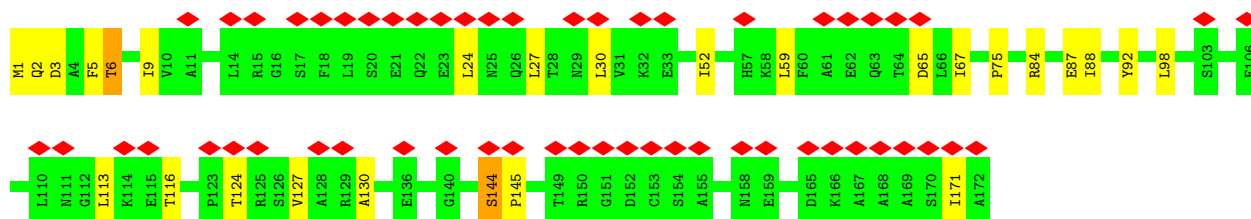
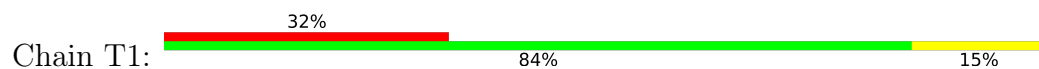




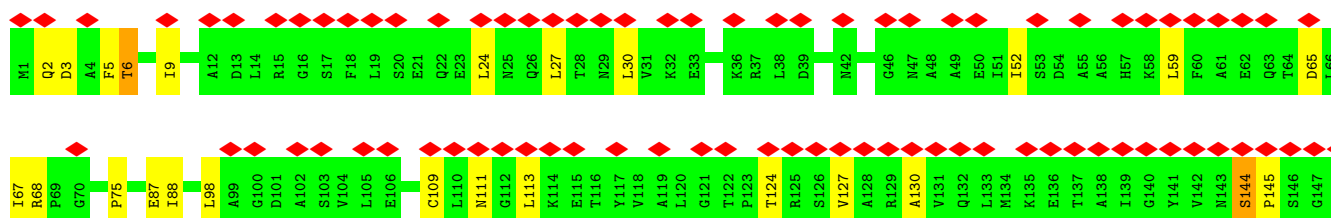
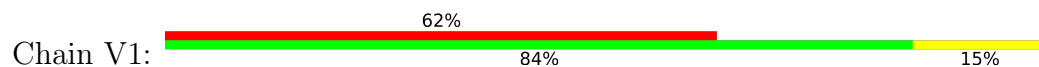
• Molecule 3: Phycocyanin beta chain



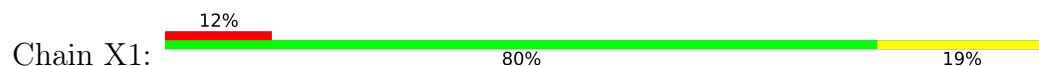
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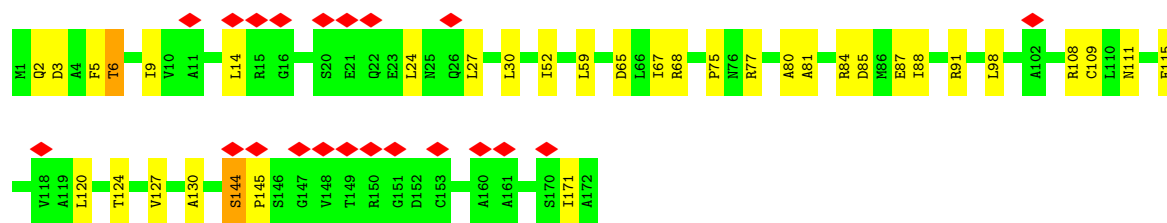


• Molecule 3: Phycocyanin beta chain

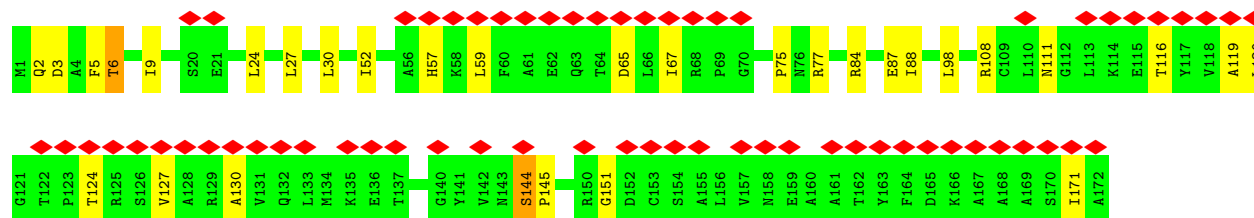
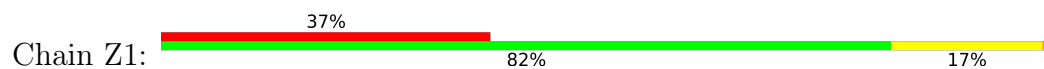


• Molecule 3: Phycocyanin beta chain

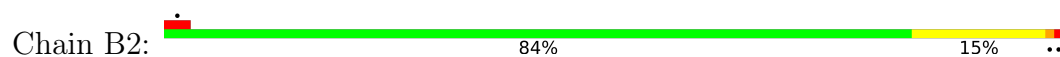




• Molecule 3: Phycocyanin beta chain



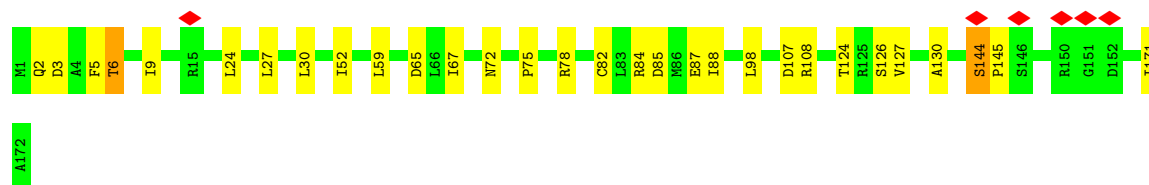
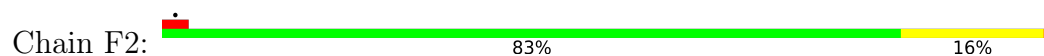
• Molecule 3: Phycocyanin beta chain



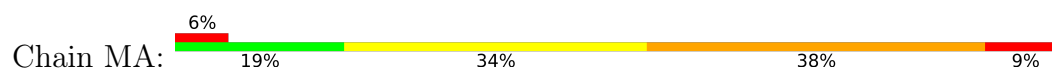
• Molecule 3: Phycocyanin beta chain

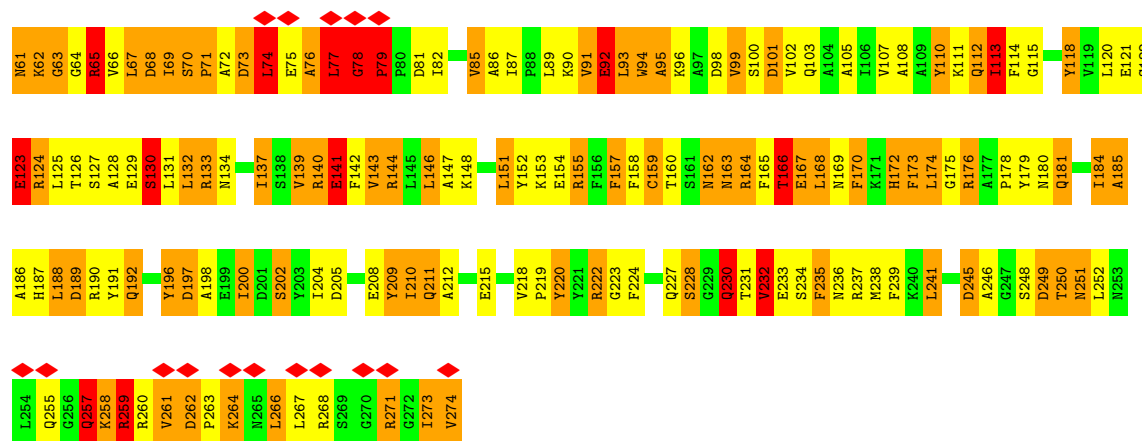


• Molecule 3: Phycocyanin beta chain

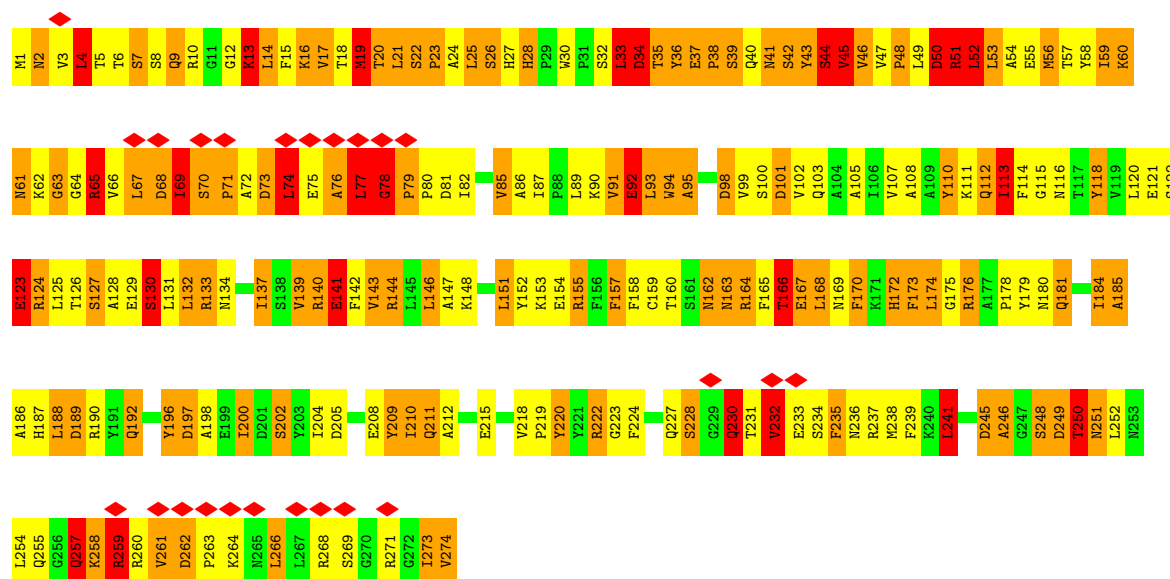
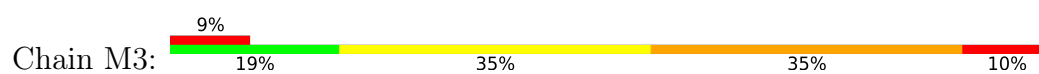


• Molecule 4: Phycocyanin-associated rod linker protein

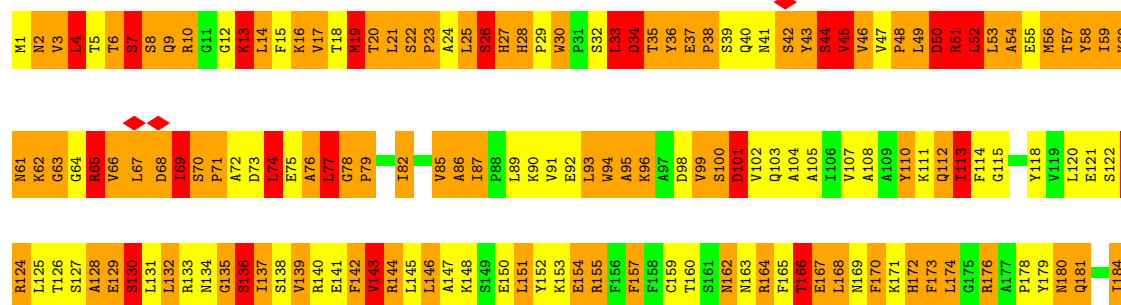


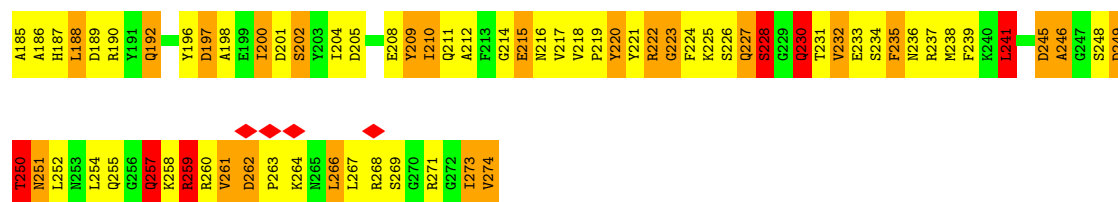


• Molecule 4: Phycocyanin-associated rod linker protein

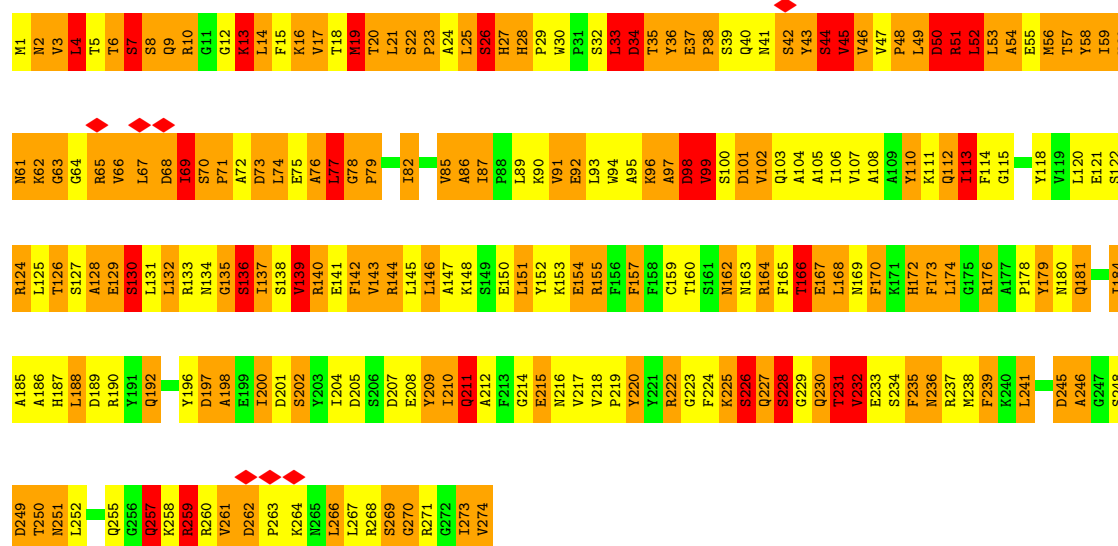


• Molecule 4: Phycocyanin-associated rod linker protein

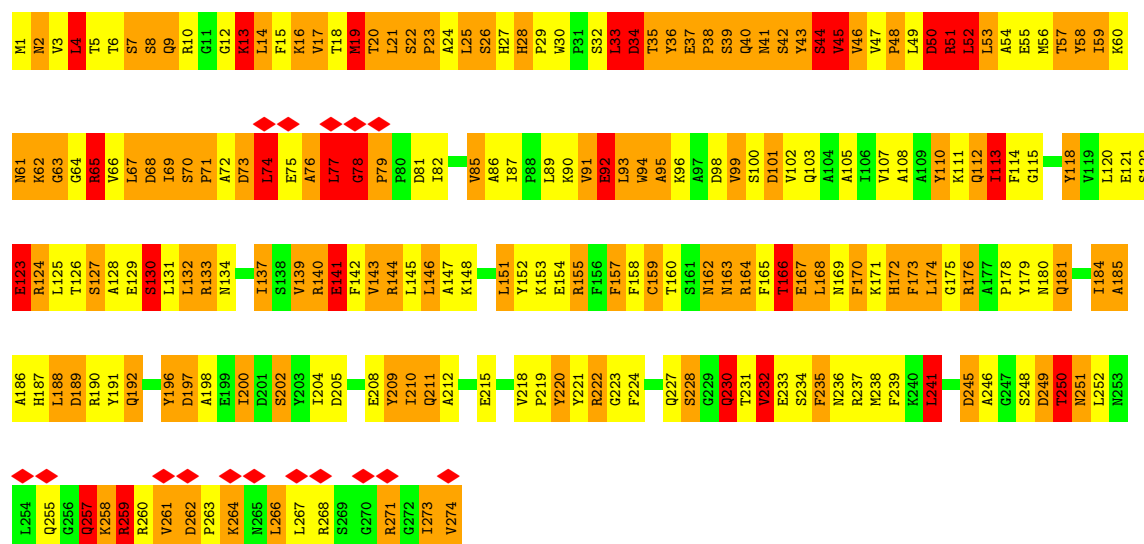
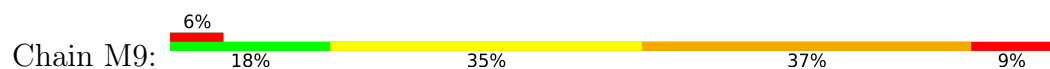




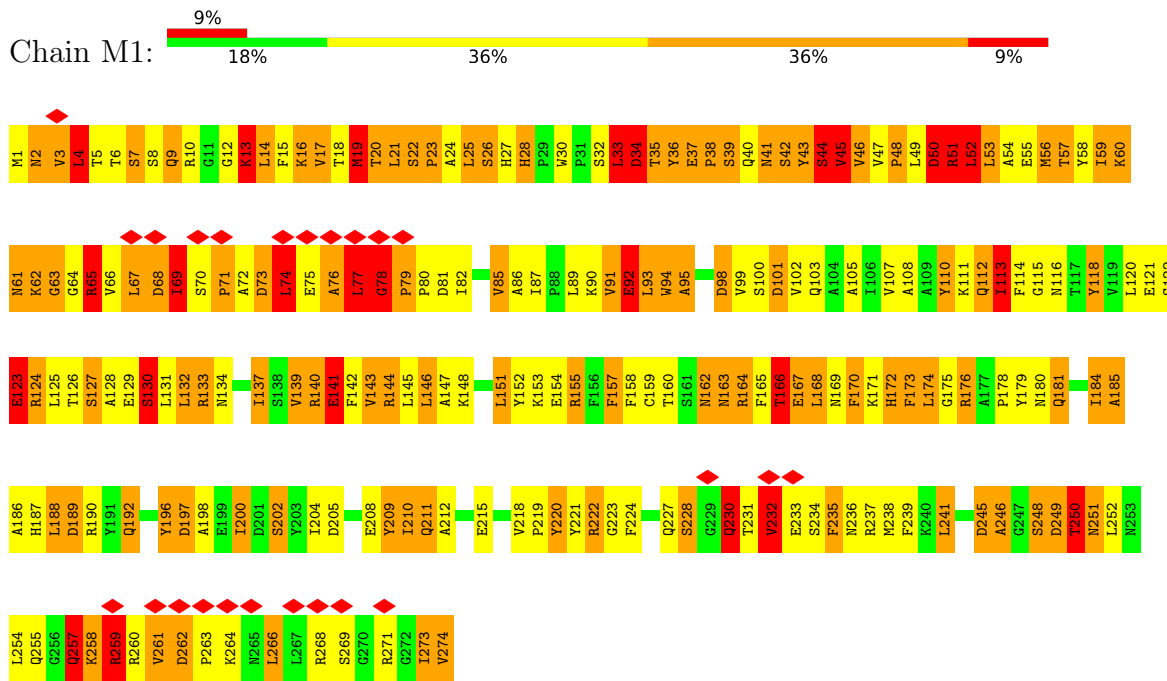
• Molecule 4: Phycocyanin-associated rod linker protein



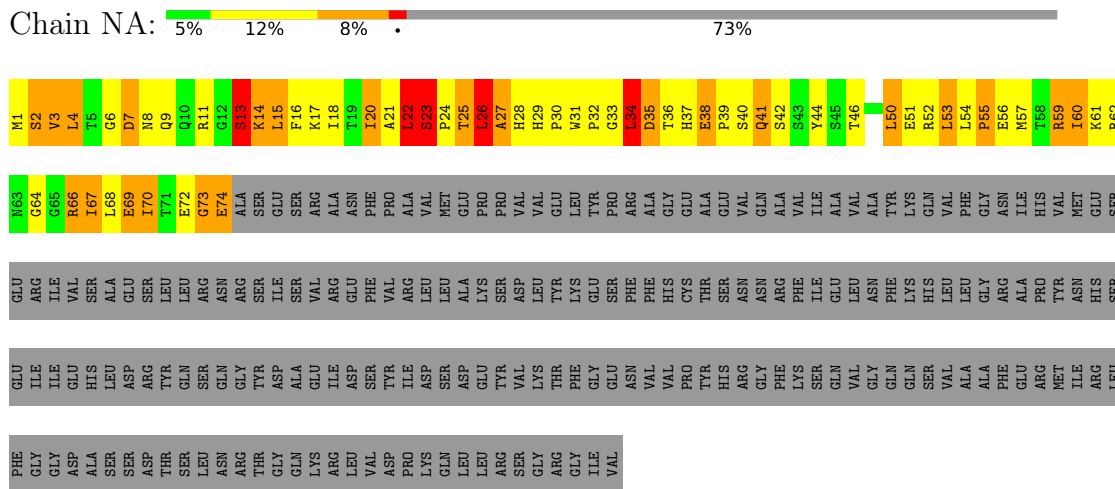
• Molecule 4: Phycocyanin-associated rod linker protein



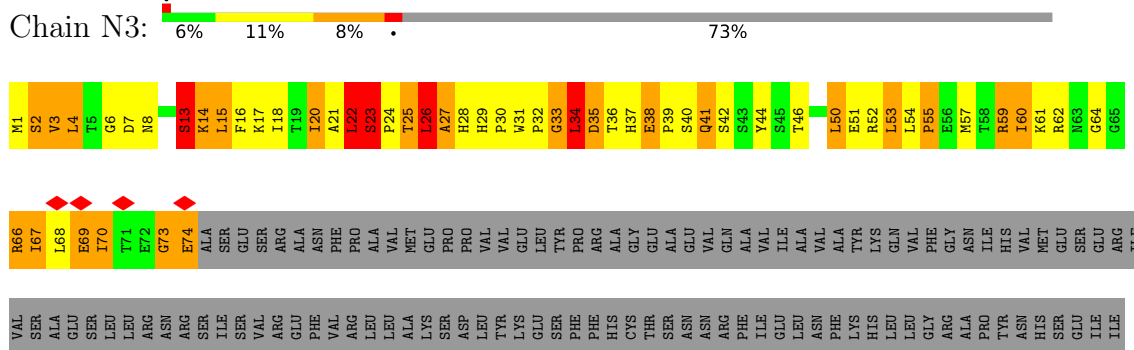
• Molecule 4: Phycocyanin-associated rod linker protein

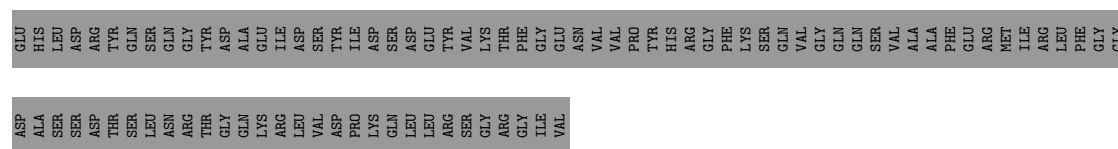


- Molecule 5: Phycocyanin-associated rod linker protein

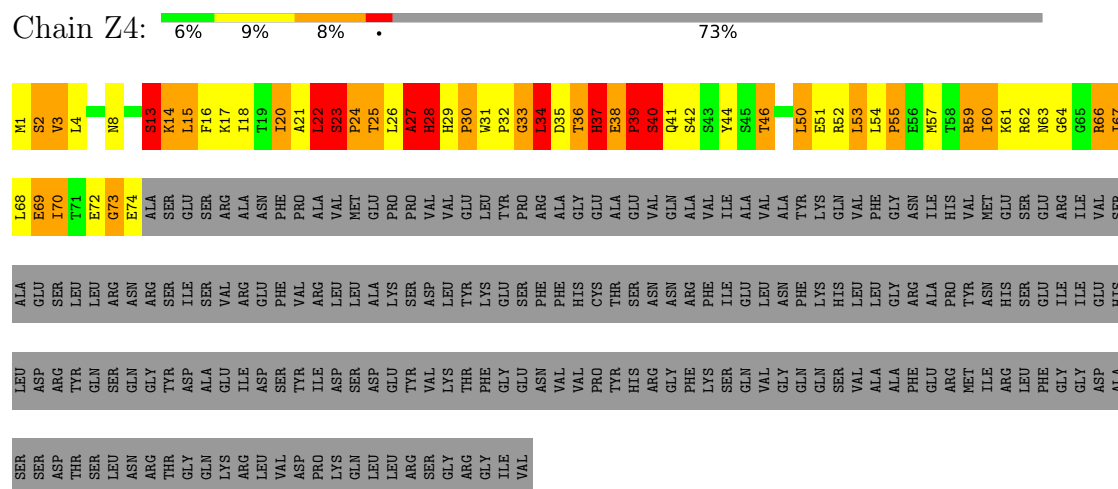


- Molecule 5: Phycocyanin-associated rod linker protein

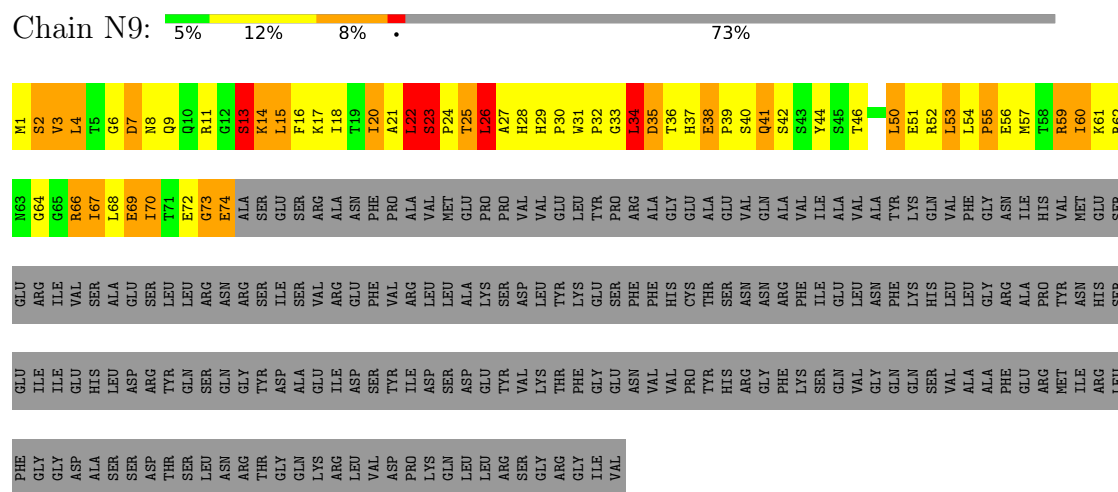




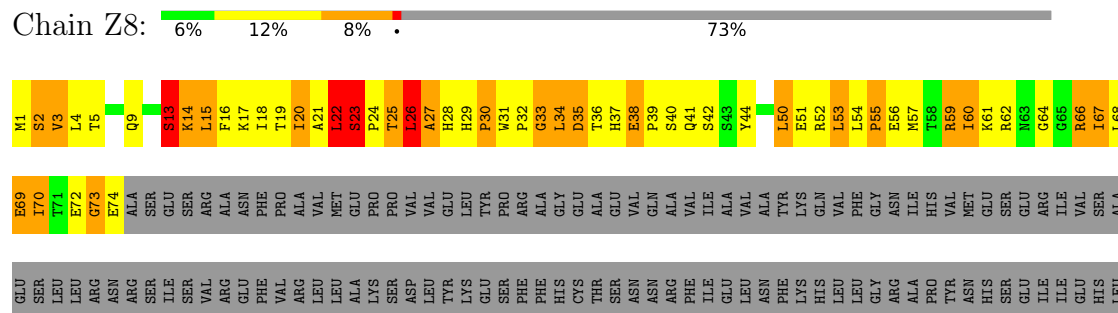
- Molecule 5: Phycocyanin-associated rod linker protein



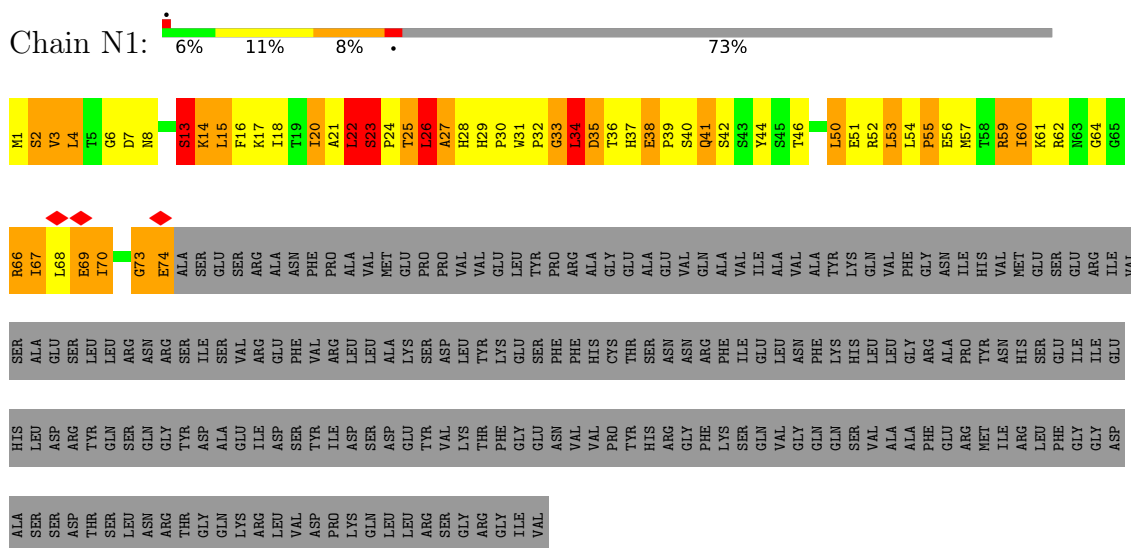
- Molecule 5: Phycocyanin-associated rod linker protein



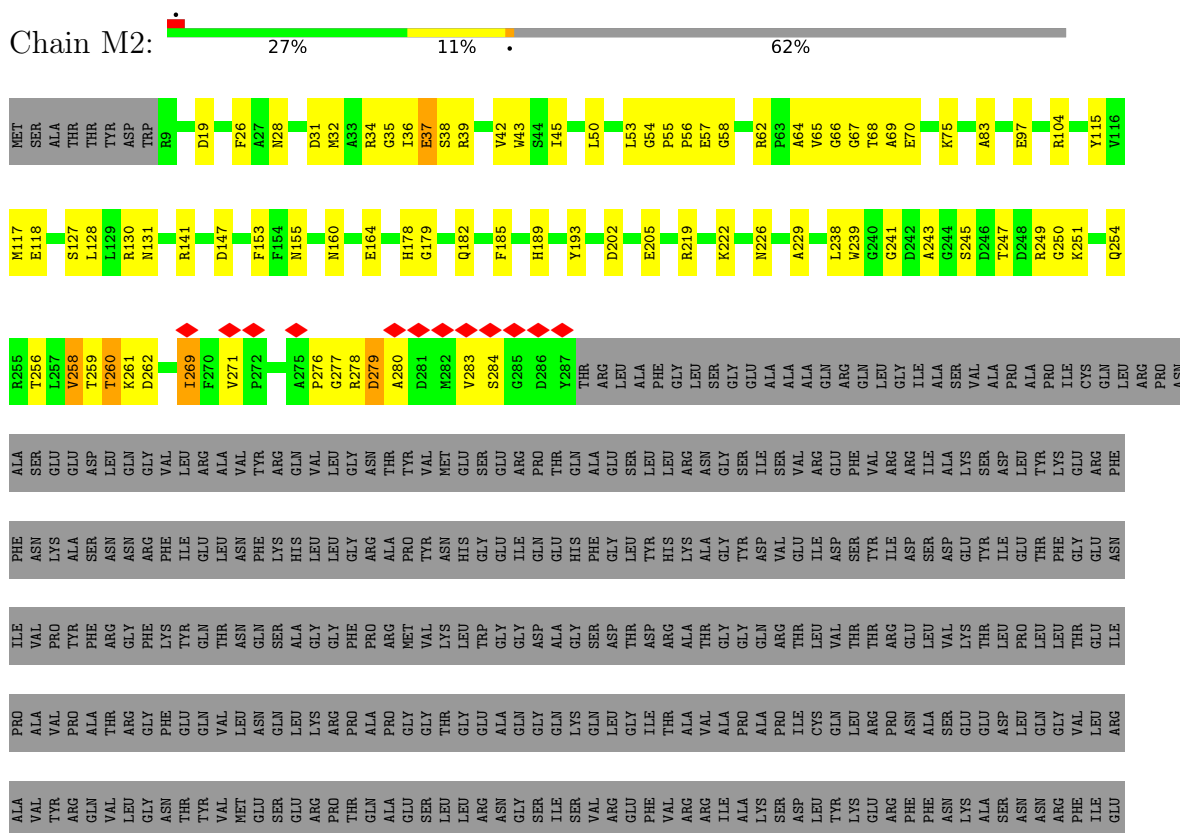
- Molecule 5: Phycocyanin-associated rod linker protein

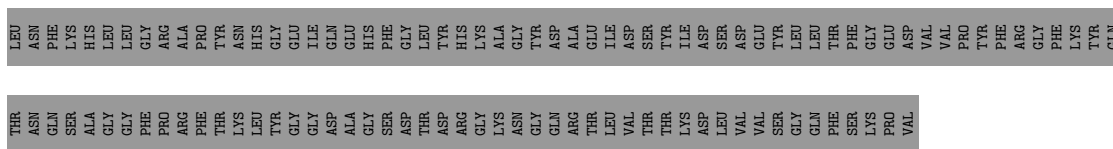


- Molecule 5: Phycocyanin-associated rod linker protein

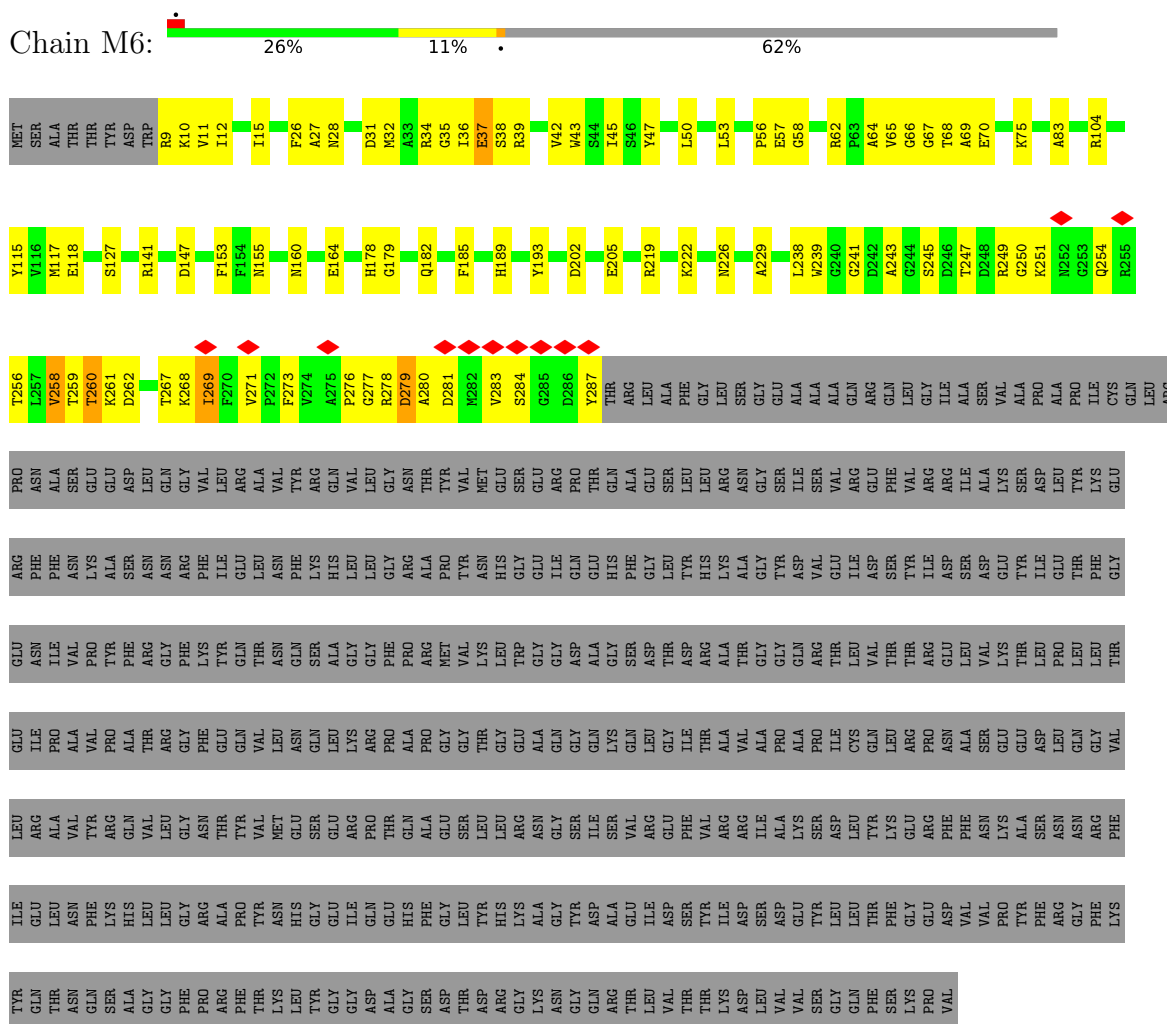


- Molecule 6: Glr2806 protein





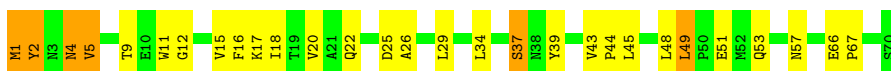
- Molecule 6: Glr2806 protein



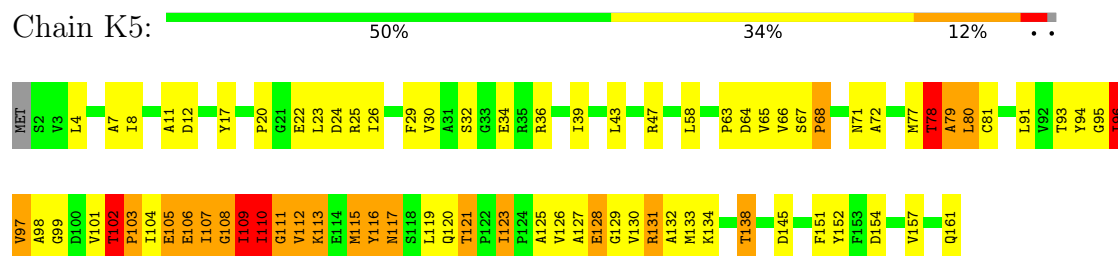
- Molecule 7: CpcD protein



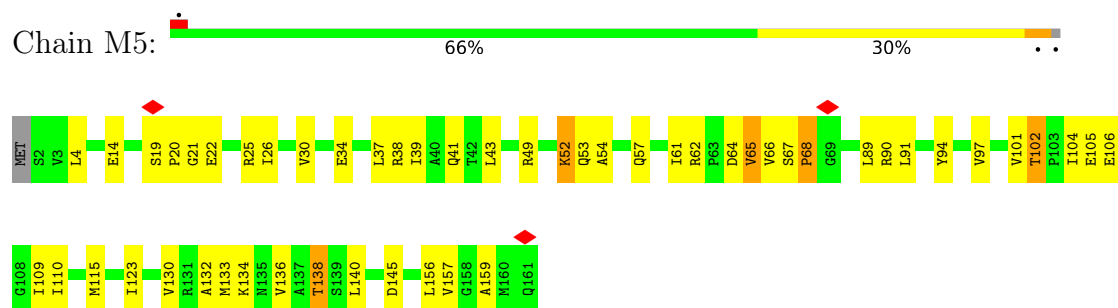
- Molecule 7: CpcD protein



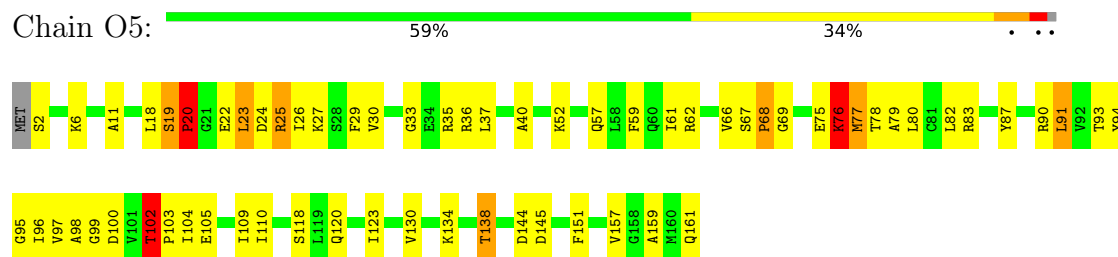
- Molecule 8: Allophycocyanin alpha subunit



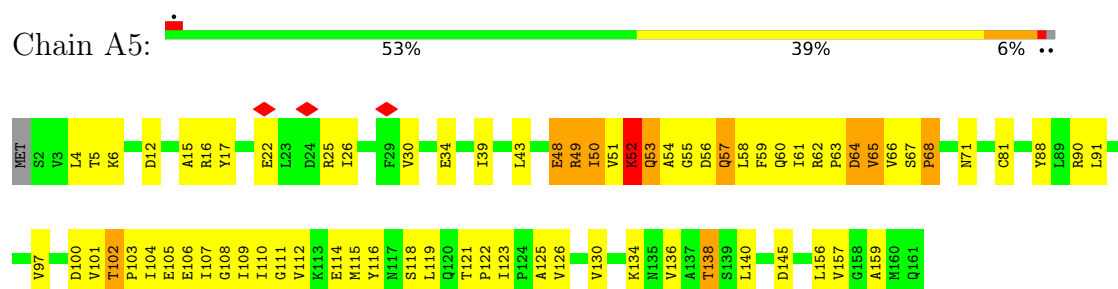
- Molecule 8: Allophycocyanin alpha subunit



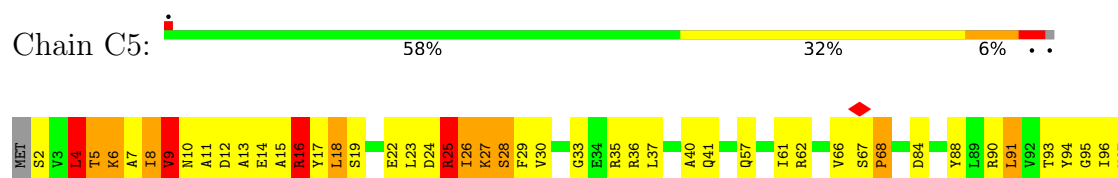
- Molecule 8: Allophycocyanin alpha subunit



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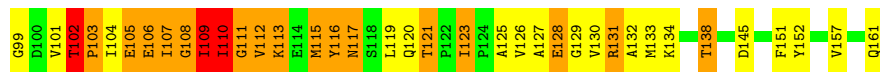


- Molecule 8: Allophycocyanin alpha subunit





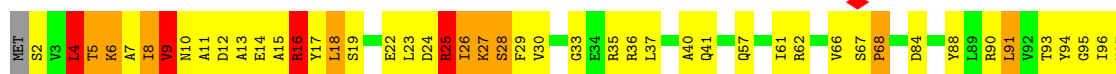
• Molecule 8: Allophycocyanin alpha subunit



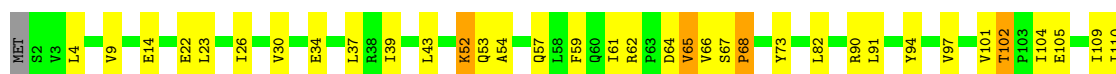
• Molecule 8: Allophycocyanin alpha subunit



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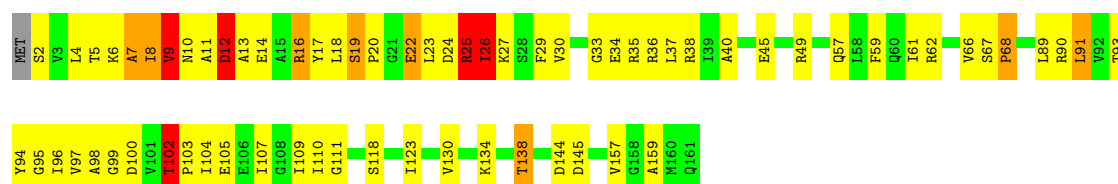


• Molecule 8: Allophycocyanin alpha subunit

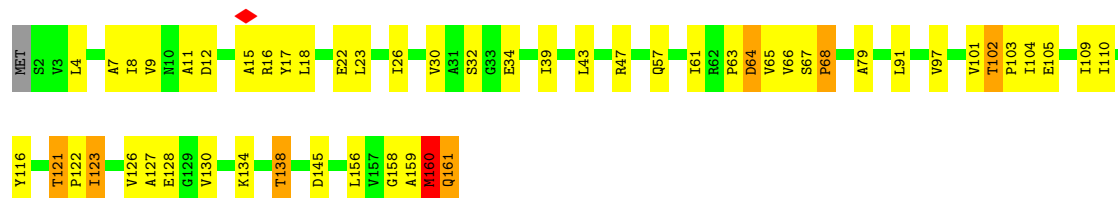


• Molecule 8: Allophycocyanin alpha subunit

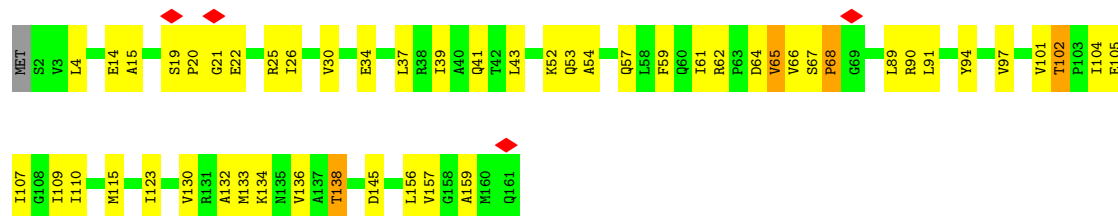




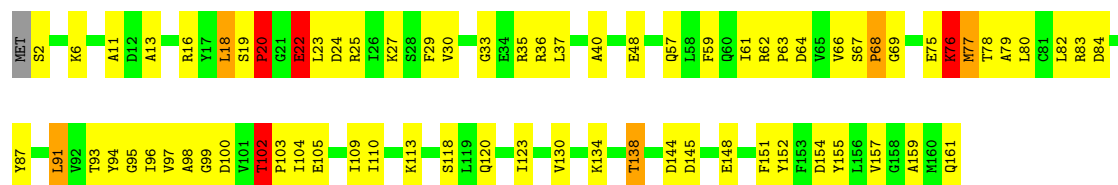
- Molecule 8: Allophycocyanin alpha subunit



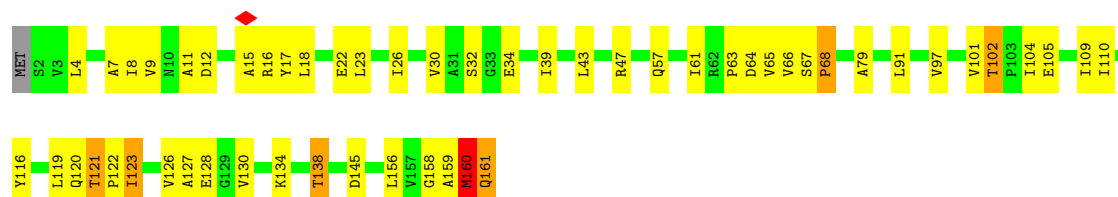
- Molecule 8: Allophycocyanin alpha subunit



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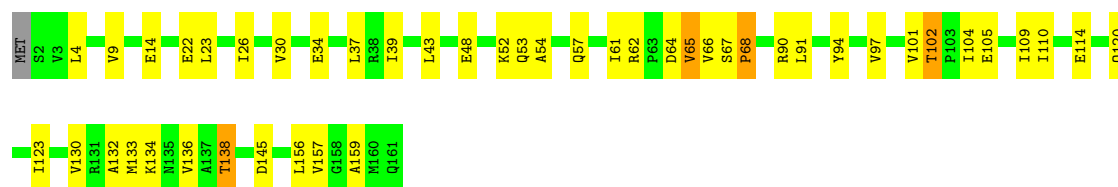


- Molecule 8: Allophycocyanin alpha subunit



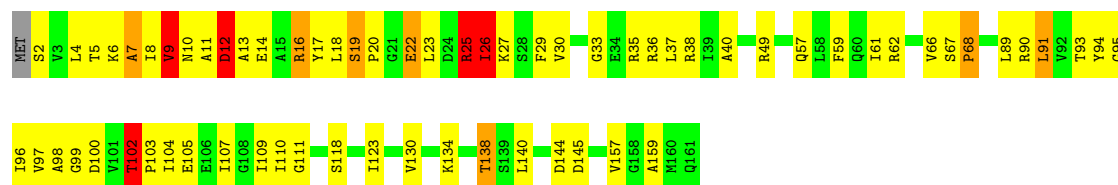
- Molecule 8: Allophycocyanin alpha subunit

Chain Y5:  71% 26% ..



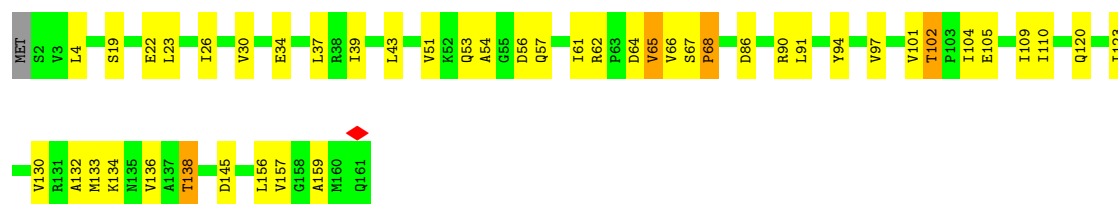
• Molecule 8: Allophycocyanin alpha subunit

Chain a5:  58% 34% . . .



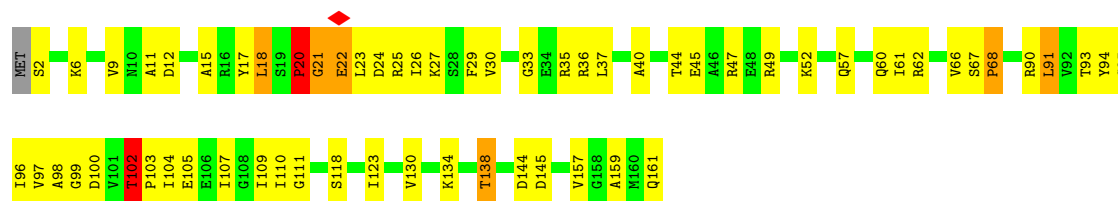
• Molecule 8: Allophycocyanin alpha subunit

Chain A7:  71% 25% ..



• Molecule 8: Allophycocyanin alpha subunit

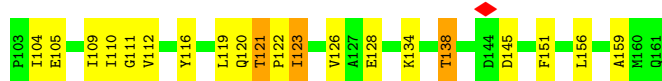
Chain O7:  60% 34% . . .



• Molecule 8: Allophycocyanin alpha subunit

Chain Q7:  66% 30% . . .

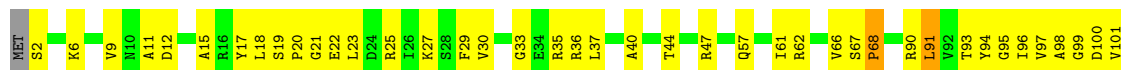




- Molecule 8: Allophycocyanin alpha subunit



- Molecule 8: Allophycocyanin alpha subunit



- Molecule 8: Allophycocyanin alpha subunit

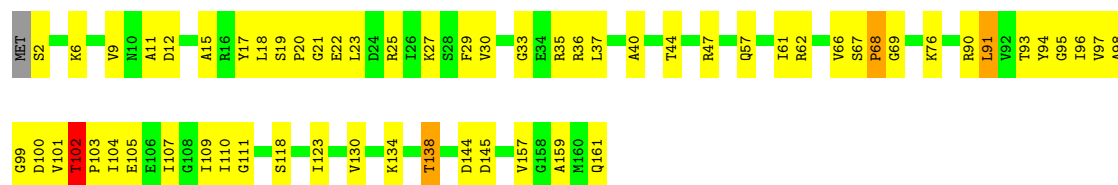


- Molecule 8: Allophycocyanin alpha subunit



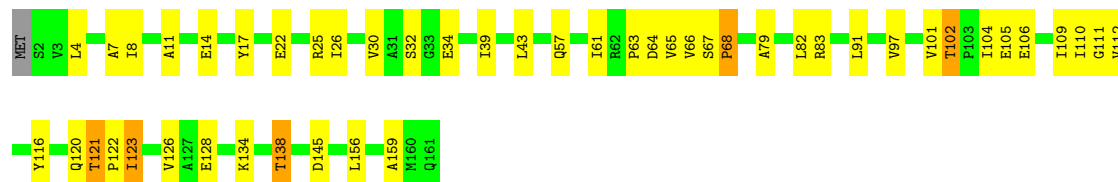
- Molecule 8: Allophycocyanin alpha subunit





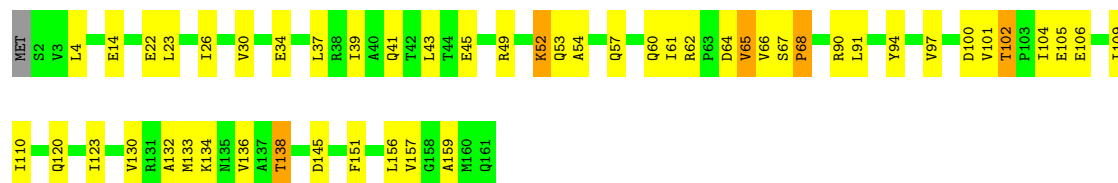
• Molecule 8: Allophycocyanin alpha subunit

Chain K7: 70% 27% ..



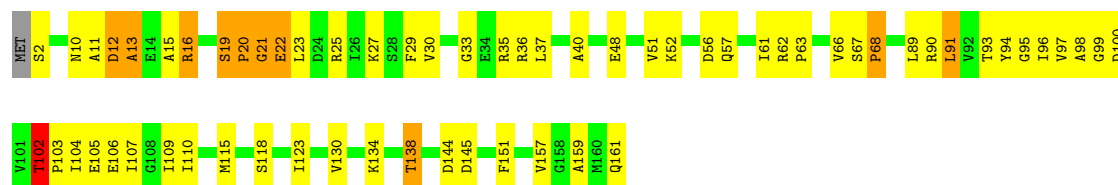
• Molecule 8: Allophycocyanin alpha subunit

Chain M7: 68% 28% ..



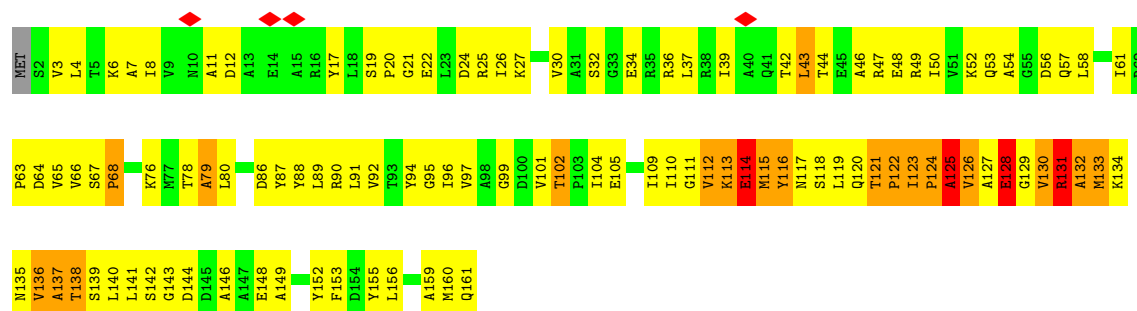
• Molecule 8: Allophycocyanin alpha subunit

Chain g7: 60% 32% 6% ..

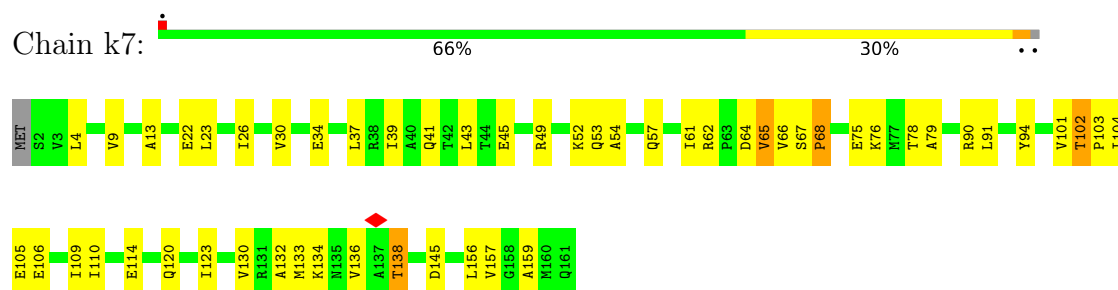


• Molecule 8: Allophycocyanin alpha subunit

Chain i7: 32% 53% 12% ..



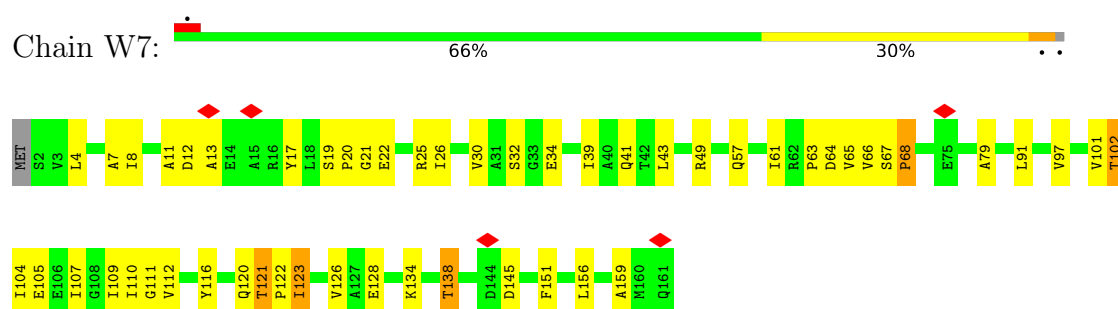
- Molecule 8: Allophycocyanin alpha subunit



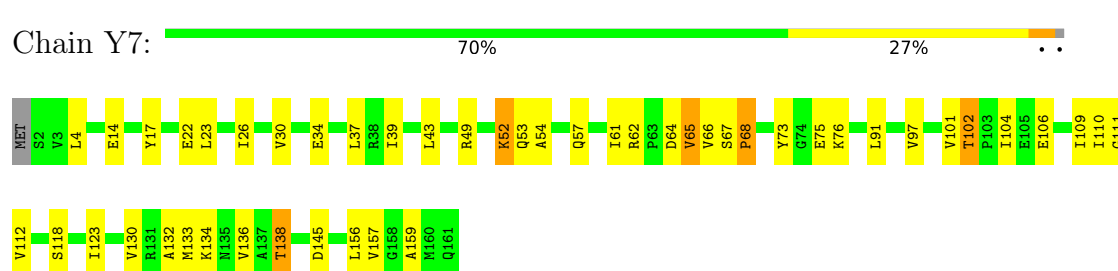
- Molecule 8: Allophycocyanin alpha subunit



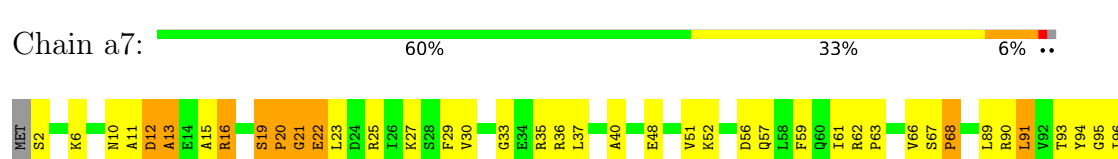
- Molecule 8: Allophycocyanin alpha subunit



- Molecule 8: Allophycocyanin alpha subunit

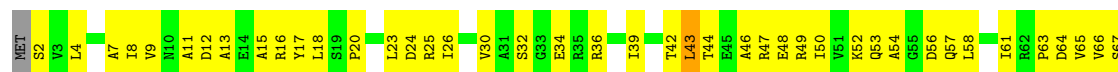


- Molecule 8: Allophycocyanin alpha subunit





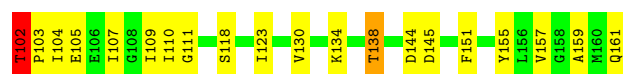
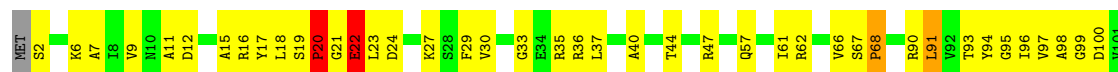
• Molecule 8: Allophycocyanin alpha subunit



• Molecule 8: Allophycocyanin alpha subunit



• Molecule 8: Allophycocyanin alpha subunit

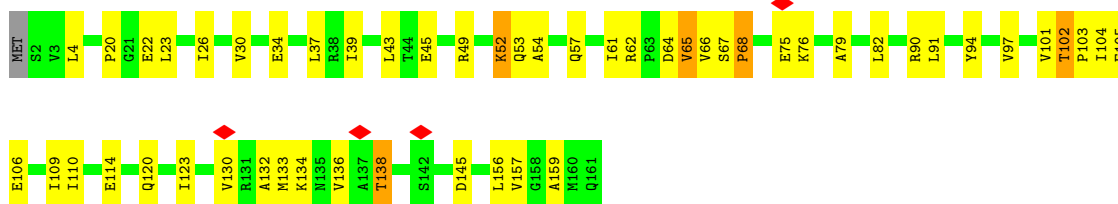


• Molecule 8: Allophycocyanin alpha subunit



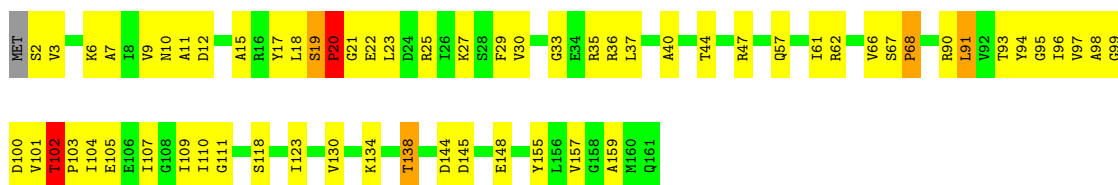
• Molecule 8: Allophycocyanin alpha subunit

Chain q7:  67% 29% ..



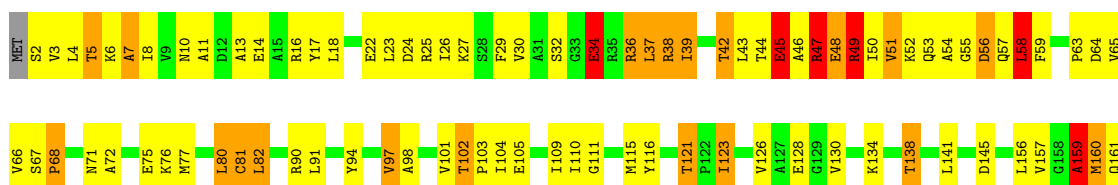
- Molecule 8: Allophycocyanin alpha subunit

Chain s7:  60% 35% ...



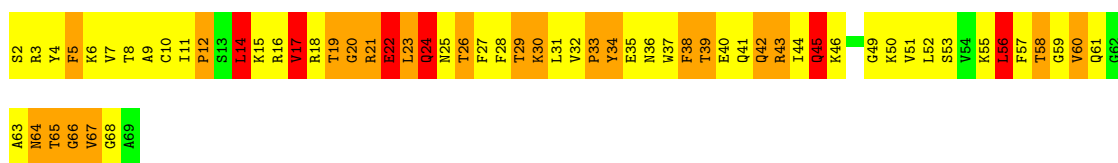
- Molecule 8: Allophycocyanin alpha subunit

Chain u7:  44% 39% 12% ..



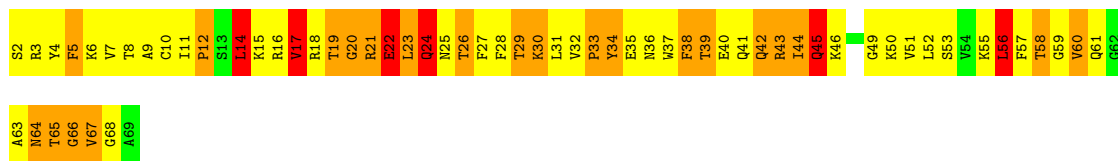
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain z5:  9% 51% 31% 9%

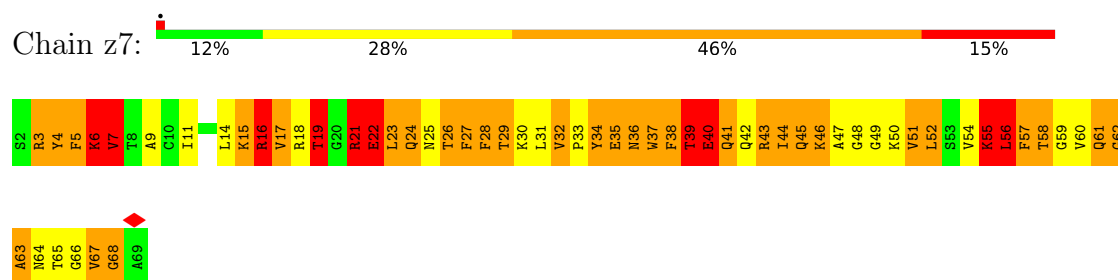


- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

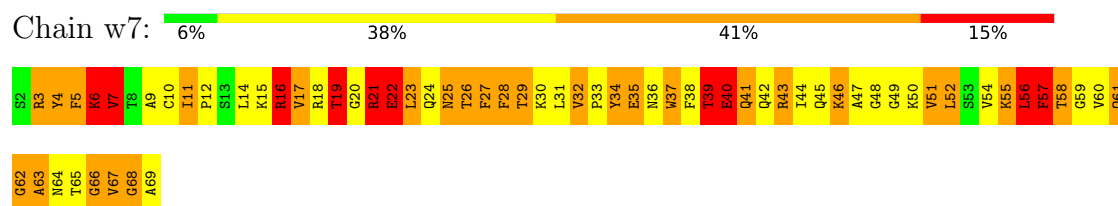
Chain i5:  9% 50% 32% 9%



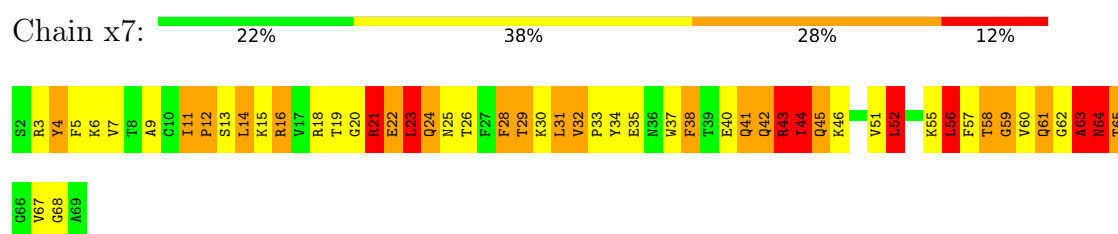
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



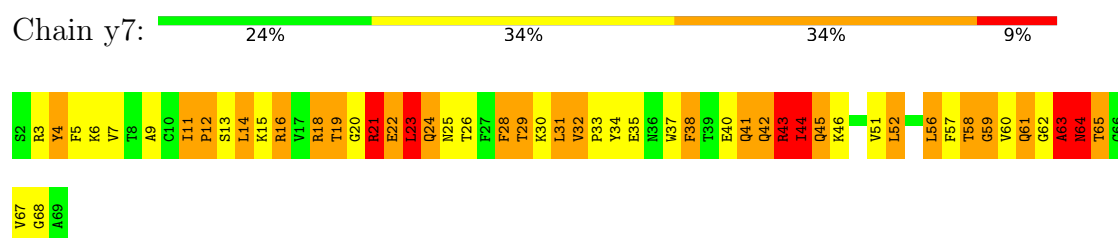
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



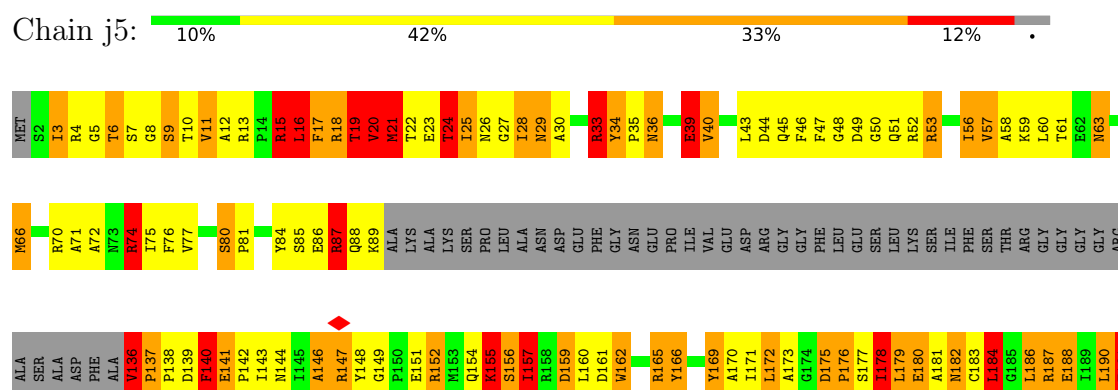
- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

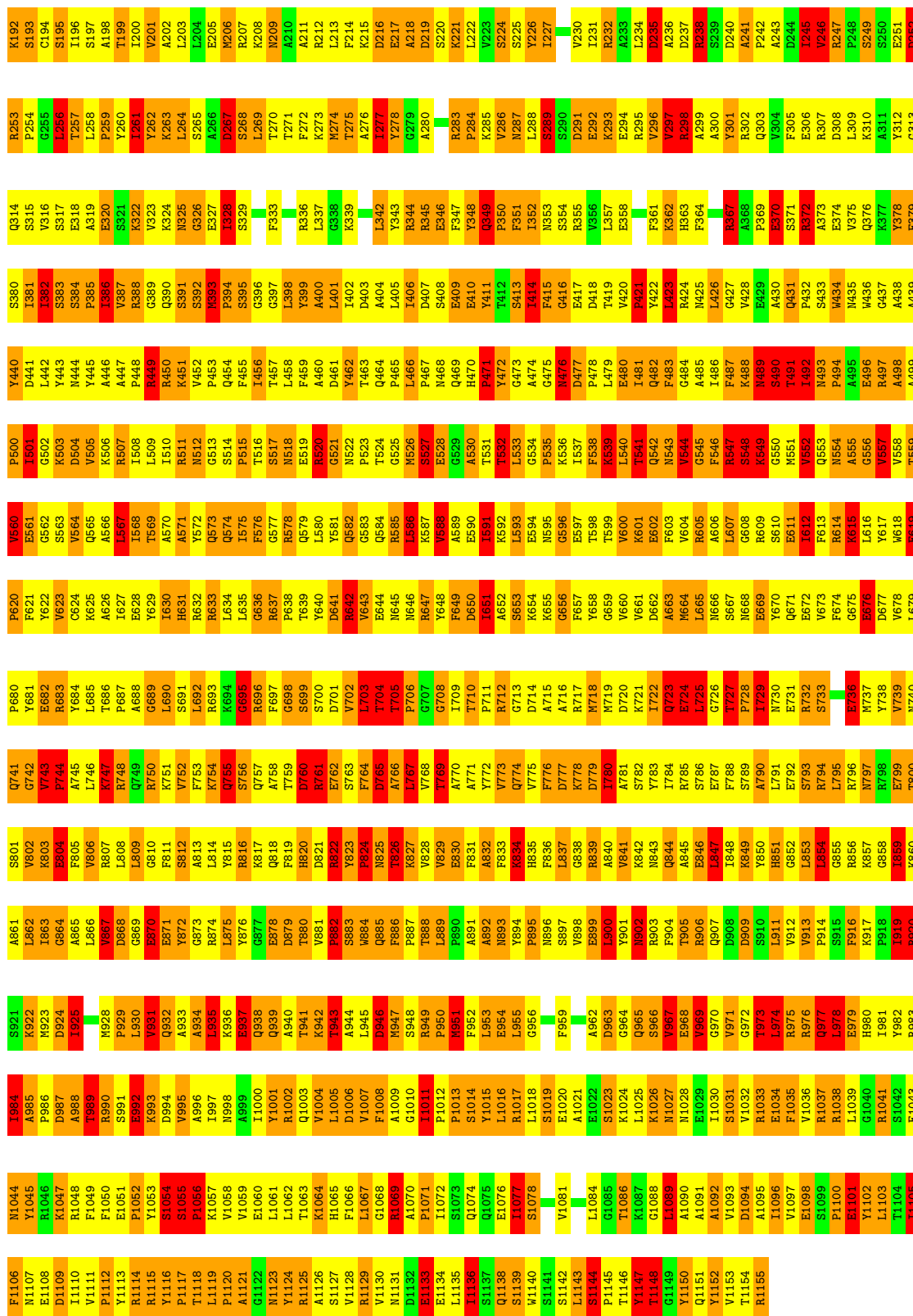


- Molecule 9: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



- Molecule 10: Phycobiliprotein ApcE

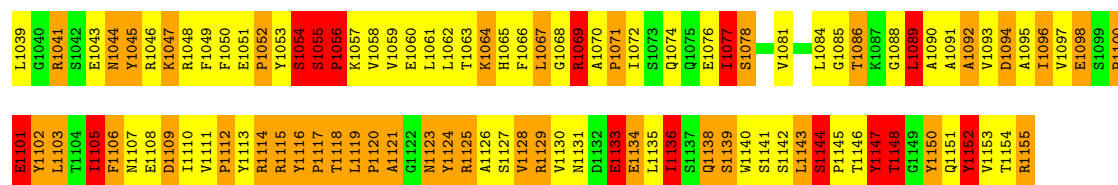




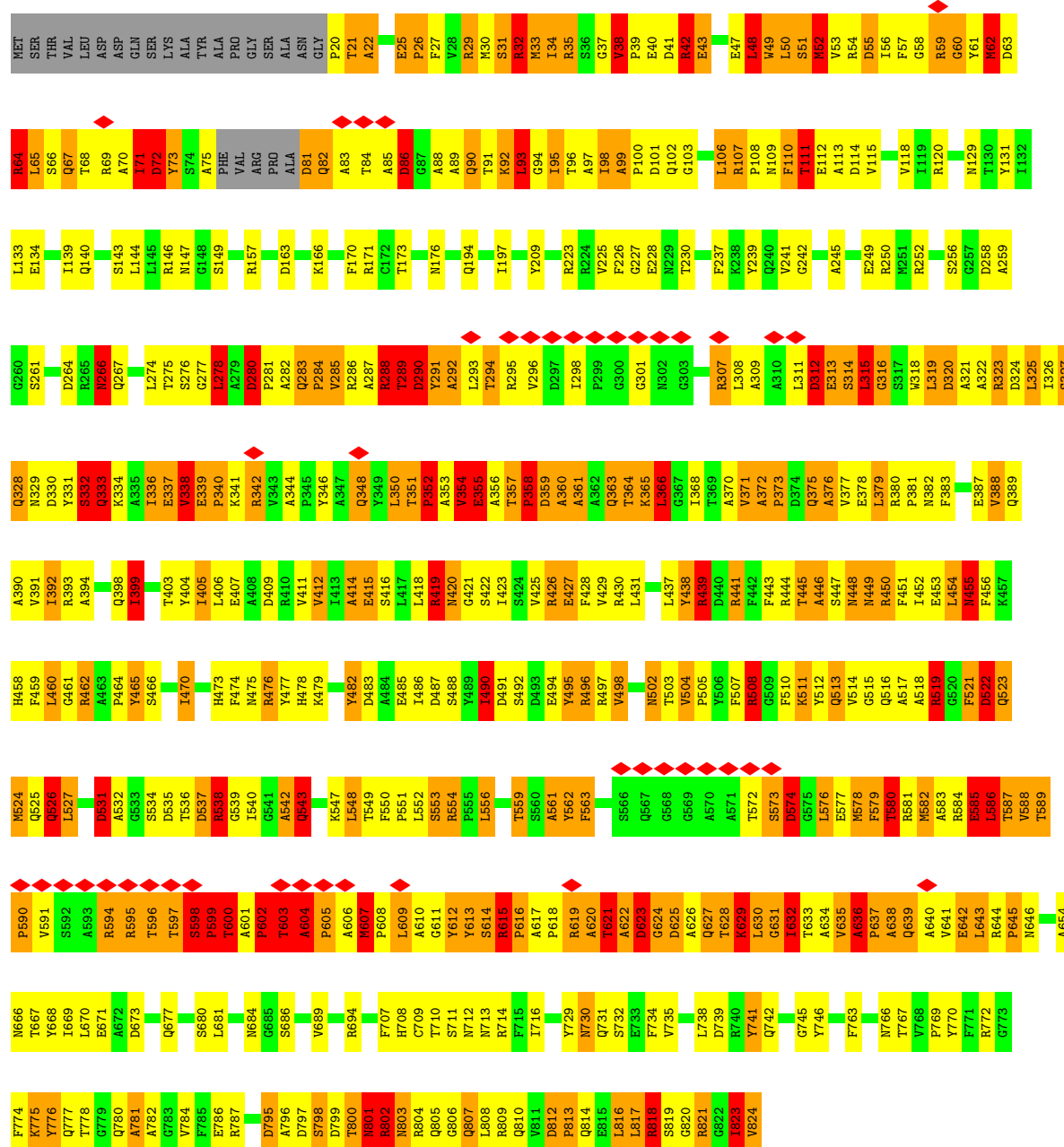
- Molecule 10: Phycobiliprotein ApcE

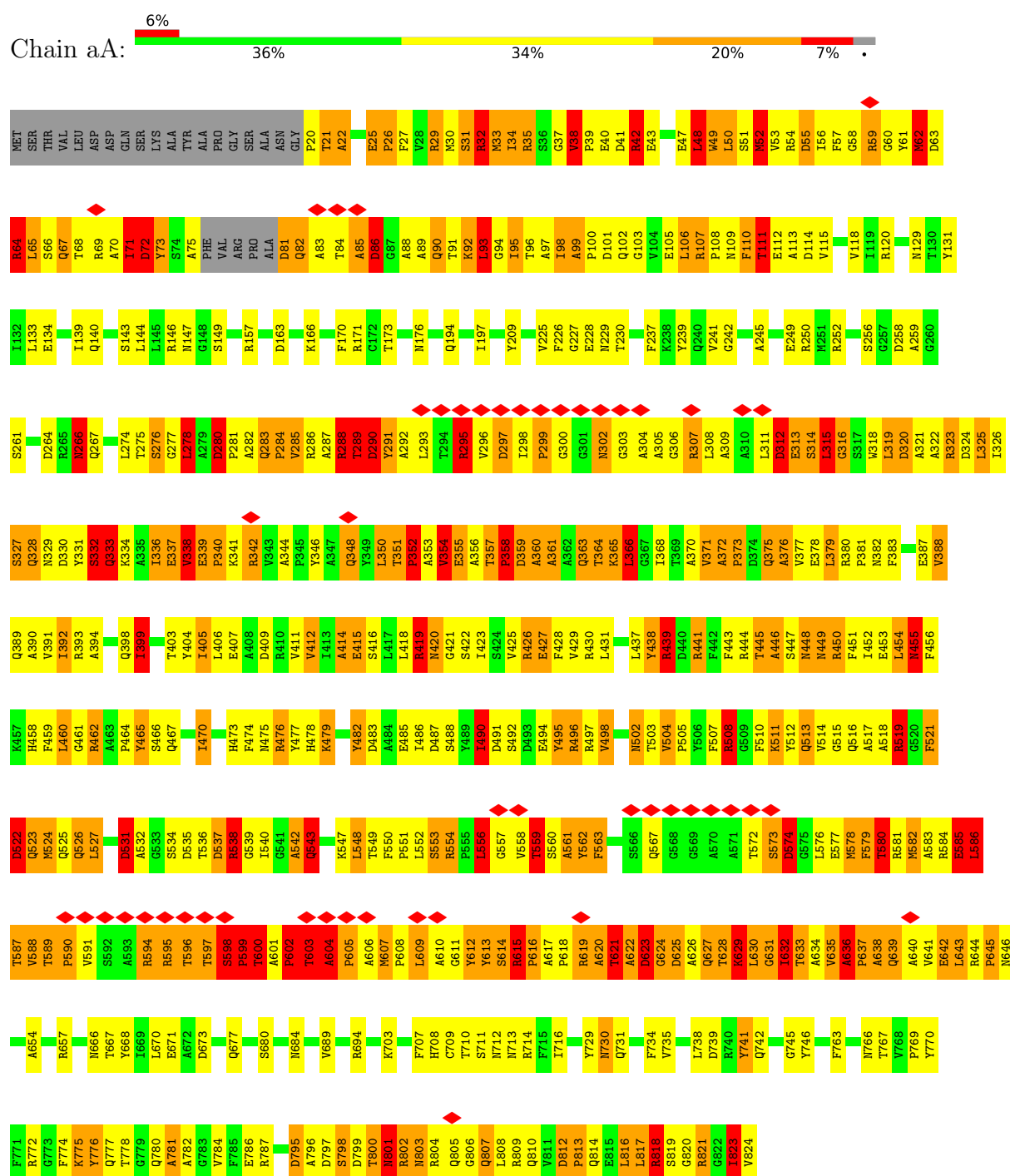


| | | | | | | | | | | | | | | | |
|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|
| E979 | P918 | G858 | R798 | V738 | D677 | V617 | V557 | R497 | G437 | K377 | A311 | S250 | L189 | GLY | MET |
| H980 | I919 | I859 | E799 | V739 | V678 | W618 | V558 | A498 | A438 | Y378 | Y312 | E251 | L190 | ARG | S2 |
| I981 | R920 | R860 | S801 | W740 | L679 | E619 | T559 | A499 | A439 | F379 | Q313 | R252 | L191 | ALA | I3 |
| Y982 | G921 | A861 | S802 | Q741 | P680 | P620 | V560 | P500 | Y440 | S380 | Q314 | R253 | K192 | SER | R4 |
| R983 | K922 | R862 | W802 | G742 | V681 | F621 | E561 | I601 | D441 | I381 | S315 | P254 | G193 | ALA | T5 |
| I984 | N923 | T863 | K803 | V743 | E682 | V622 | G562 | G502 | L442 | I382 | V316 | G255 | C194 | ASP | A71 |
| A985 | N924 | G864 | E804 | V744 | R683 | V623 | S563 | K503 | Y443 | S383 | S317 | L256 | S195 | PHE | S7 |
| P986 | I925 | A865 | F805 | A745 | V684 | C624 | V564 | D504 | N444 | S384 | E318 | T257 | L196 | ALA | G8 |
| D987 | A926 | L866 | W806 | L746 | L685 | K625 | G565 | V505 | Y445 | P385 | A319 | L258 | I197 | W75 | S9 |
| A988 | S927 | V867 | R807 | R747 | T686 | A626 | A566 | K506 | A446 | V387 | S321 | P259 | A198 | F76 | T10 |
| T989 | R928 | D868 | L808 | R748 | P687 | L627 | L567 | R507 | A447 | R388 | G322 | Y260 | T199 | P138 | V11 |
| R990 | P929 | G869 | L809 | G749 | E689 | E628 | I568 | I508 | P448 | G389 | V323 | Y261 | I200 | Y260 | A12 |
| S991 | L930 | E870 | G810 | W750 | G689 | V629 | T569 | L509 | R449 | G390 | V324 | Y262 | I201 | F140 | R13 |
| E992 | V931 | E871 | F811 | K751 | L690 | L630 | A570 | I510 | R450 | Q390 | K324 | K263 | A202 | E141 | F14 |
| K993 | Q932 | W872 | S812 | V752 | S691 | H631 | A571 | R511 | K451 | S391 | N325 | K264 | A203 | P142 | R15 |
| D994 | A933 | G873 | A813 | F753 | L692 | R632 | V572 | N512 | V452 | G392 | G326 | S265 | L204 | I143 | R16 |
| V995 | A934 | R874 | L814 | K754 | R693 | R633 | Q573 | G513 | P453 | E327 | S327 | E266 | E205 | A83 | F17 |
| A996 | L935 | L875 | Y815 | W755 | K694 | L634 | Q574 | S514 | Q454 | P394 | I328 | D267 | M206 | Y84 | R18 |
| A997 | K936 | W876 | R816 | S756 | R695 | L635 | V575 | P515 | F455 | S395 | S329 | S268 | E207 | E86 | R19 |
| N998 | E937 | G877 | K817 | Q757 | R696 | G636 | F576 | T516 | L456 | G396 | F333 | T270 | K208 | R147 | V20 |
| A999 | Q938 | E878 | Q818 | A758 | F697 | R637 | R578 | N518 | L458 | G397 | T271 | T271 | N209 | Q88 | M21 |
| I1000 | Q939 | D879 | F819 | T759 | G698 | P638 | R579 | E519 | F459 | Y399 | R336 | F272 | A211 | K89 | E23 |
| Y1001 | A940 | T880 | H820 | D760 | S699 | T639 | Q579 | A519 | F459 | Y399 | R337 | F273 | E212 | ALA | T22 |
| R1002 | T941 | W881 | D821 | R761 | S700 | Y640 | L580 | R520 | A460 | A400 | L337 | K273 | R123 | LYS | T24 |
| Q1003 | K942 | R822 | R822 | E762 | D701 | D641 | Y581 | G521 | D461 | L401 | G338 | M274 | L213 | ALA | I25 |
| Y1004 | T943 | S823 | Y823 | S763 | V702 | R642 | Q582 | N522 | Y462 | I402 | K339 | T275 | F214 | LYS | N26 |
| L1005 | A944 | W884 | P824 | F764 | L703 | W643 | G583 | P523 | T463 | D403 | L342 | A276 | K215 | SER | G27 |
| D1006 | L945 | K885 | N825 | D765 | T704 | E644 | Q584 | T524 | Q464 | A404 | L343 | T277 | D216 | PRO | I28 |
| Y1007 | R946 | F886 | T826 | A766 | R705 | N645 | R585 | G525 | P465 | L405 | Y343 | G278 | E217 | LEU | N29 |
| F1008 | N947 | R827 | K827 | L767 | T706 | N646 | L586 | M526 | L466 | I406 | R344 | G279 | A218 | ALA | A30 |
| A1009 | S948 | T888 | W828 | V768 | G707 | R647 | K587 | S527 | P467 | D407 | R345 | A280 | D219 | ASN | |
| I1010 | R949 | L889 | W829 | T768 | G708 | V648 | W588 | E528 | N468 | S408 | E346 | | S220 | ASP | R33 |
| P1012 | P951 | F891 | E830 | A770 | L709 | F649 | A589 | G529 | Q469 | E409 | F347 | R283 | K221 | GLU | R34 |
| P1013 | F952 | A892 | F831 | A771 | T710 | D650 | E590 | A530 | H470 | E410 | Y348 | K284 | L222 | PHE | P35 |
| S1014 | L953 | N893 | A832 | V772 | P711 | L651 | E591 | T531 | P471 | Y411 | Q349 | K285 | V223 | GLY | N36 |
| Y1015 | E954 | W894 | R834 | Q774 | R712 | A652 | K592 | T532 | Y472 | T412 | P350 | N267 | S224 | ASN | |
| L1016 | L955 | P895 | H835 | V775 | D714 | K654 | E594 | G534 | A474 | S413 | F351 | N267 | S225 | GLU | E38 |
| R1017 | G956 | K896 | F836 | V776 | A715 | K655 | N595 | P535 | G475 | F415 | N353 | L288 | Y226 | PRO | V40 |
| L1018 | | S897 | L837 | D777 | A716 | G656 | G596 | K536 | R476 | G416 | S354 | S289 | I227 | ILE | |
| S1019 | F959 | W898 | G838 | K778 | R717 | F657 | E597 | F537 | D477 | E417 | R355 | D291 | V230 | GLU | L43 |
| E1020 | G960 | E899 | R839 | D779 | W718 | Y658 | T598 | F538 | P478 | D418 | V356 | E292 | I231 | ASP | D44 |
| A1021 | A961 | L900 | A840 | T780 | W719 | G659 | T599 | K539 | L479 | T419 | L357 | K293 | R232 | ARG | Q45 |
| E1022 | A962 | Y901 | W841 | A781 | D720 | V680 | V600 | L540 | E480 | W420 | E358 | E294 | R233 | GLY | F47 |
| S1023 | D963 | R902 | K842 | S782 | K721 | V661 | K601 | T541 | I481 | P421 | | R295 | L234 | GLY | G48 |
| K1024 | G964 | R903 | N843 | Y783 | I722 | D662 | E602 | Q542 | Q482 | Y422 | F361 | V296 | D235 | PHE | D49 |
| L1025 | Q965 | F904 | Q844 | I784 | Q723 | A663 | F603 | N543 | F483 | L423 | K362 | V297 | A236 | LEU | G50 |
| K1026 | S966 | T905 | A845 | R785 | E724 | N664 | V604 | Y544 | G484 | R424 | H363 | R298 | D237 | GLU | Q51 |
| N1027 | V967 | R906 | E846 | S786 | L725 | L665 | G605 | G545 | A485 | N425 | F364 | A299 | R238 | SER | R52 |
| I1028 | E968 | Q907 | L847 | E787 | G726 | N666 | A606 | F546 | I486 | L426 | | A300 | S239 | LEU | R53 |
| E1029 | V969 | E908 | I848 | F788 | T727 | S667 | L607 | R547 | F487 | Q427 | R387 | Y301 | D240 | LYS | I54 |
| I1030 | G970 | D909 | R849 | S789 | P728 | N668 | G608 | S548 | K488 | W428 | A388 | R302 | A241 | SER | A55 |
| S1031 | V971 | S910 | Y850 | A790 | L729 | E669 | R609 | K549 | N489 | E429 | P369 | Q303 | P242 | ILE | I56 |
| Y1032 | G972 | L911 | H851 | L791 | W730 | V670 | S610 | G550 | A490 | V370 | V304 | A243 | P243 | PHE | V57 |
| R1033 | T973 | V912 | G852 | E792 | E731 | Q671 | E611 | M511 | T491 | Q431 | S371 | F305 | D244 | SER | A58 |
| E1034 | L974 | W913 | L853 | S793 | R732 | E672 | T612 | Y552 | I492 | P432 | R372 | E306 | I245 | THR | K59 |
| F1035 | R975 | P914 | L854 | R794 | S733 | V673 | F613 | Q553 | N493 | S433 | A373 | R307 | V246 | ARG | L60 |
| V1036 | R976 | G915 | G855 | L795 | F674 | F674 | R614 | N554 | P494 | W494 | V374 | D308 | R247 | GLY | T61 |
| R1037 | Q977 | F916 | R856 | R796 | E736 | | A495 | A555 | A495 | V375 | E375 | L309 | P248 | GLY | E62 |
| R1038 | L978 | K917 | K857 | W797 | W737 | E576 | L616 | G556 | E496 | W436 | Q376 | K310 | S249 | GLY | N63 |



• Molecule 11: Glr1262 protein





4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C2 | Depositor |
| Number of particles used | 389430 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TECNAI F30 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 50 | Depositor |
| Minimum defocus (nm) | 1300 | Depositor |
| Maximum defocus (nm) | 2300 | Depositor |
| Magnification | 64000 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 2.900 | Depositor |
| Minimum map value | -1.411 | Depositor |
| Average map value | 0.006 | Depositor |
| Map value standard deviation | 0.067 | Depositor |
| Recommended contour level | 0.15 | Depositor |
| Map size (\AA) | 614.82404, 614.82404, 614.82404 | wwPDB |
| Map dimensions | 560, 560, 560 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.0979, 1.0979, 1.0979 | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MEN, CYC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|---------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 0.73 | 0/1218 | 0.94 | 2/1648 (0.1%) |
| 1 | B5 | 0.74 | 0/1218 | 0.94 | 2/1648 (0.1%) |
| 1 | B7 | 0.74 | 0/1218 | 0.94 | 2/1648 (0.1%) |
| 1 | D5 | 1.39 | 22/1218 (1.8%) | 1.17 | 7/1648 (0.4%) |
| 1 | D7 | 0.98 | 4/1218 (0.3%) | 1.07 | 9/1648 (0.5%) |
| 1 | F5 | 1.04 | 5/1218 (0.4%) | 1.24 | 5/1648 (0.3%) |
| 1 | F7 | 0.90 | 1/1218 (0.1%) | 1.19 | 4/1648 (0.2%) |
| 1 | H5 | 0.74 | 0/1218 | 0.94 | 2/1648 (0.1%) |
| 1 | H7 | 0.74 | 0/1218 | 0.94 | 2/1648 (0.1%) |
| 1 | J5 | 1.39 | 21/1218 (1.7%) | 1.17 | 7/1648 (0.4%) |
| 1 | J7 | 0.98 | 4/1218 (0.3%) | 1.07 | 9/1648 (0.5%) |
| 1 | L5 | 1.05 | 5/1218 (0.4%) | 1.24 | 5/1648 (0.3%) |
| 1 | L7 | 0.90 | 1/1218 (0.1%) | 1.19 | 4/1648 (0.2%) |
| 1 | N5 | 0.74 | 0/1218 | 0.93 | 2/1648 (0.1%) |
| 1 | N7 | 0.74 | 0/1218 | 0.94 | 2/1648 (0.1%) |
| 1 | P5 | 0.75 | 0/1218 | 0.93 | 1/1648 (0.1%) |
| 1 | P7 | 0.74 | 0/1218 | 0.93 | 1/1648 (0.1%) |
| 1 | R5 | 0.90 | 1/1218 (0.1%) | 1.19 | 4/1648 (0.2%) |
| 1 | R7 | 0.90 | 1/1218 (0.1%) | 1.19 | 4/1648 (0.2%) |
| 1 | T5 | 0.74 | 0/1218 | 0.93 | 2/1648 (0.1%) |
| 1 | T7 | 0.74 | 0/1218 | 0.93 | 2/1648 (0.1%) |
| 1 | V5 | 0.75 | 0/1218 | 0.93 | 1/1648 (0.1%) |
| 1 | V7 | 0.75 | 0/1218 | 0.93 | 1/1648 (0.1%) |
| 1 | X5 | 0.91 | 1/1218 (0.1%) | 1.19 | 4/1648 (0.2%) |
| 1 | X7 | 0.90 | 1/1218 (0.1%) | 1.19 | 4/1648 (0.2%) |
| 1 | Z | 0.73 | 0/1218 | 0.94 | 2/1648 (0.1%) |
| 1 | Z5 | 0.73 | 0/1218 | 0.94 | 2/1648 (0.1%) |
| 1 | Z7 | 0.74 | 0/1218 | 0.94 | 2/1648 (0.1%) |
| 1 | b5 | 0.90 | 1/1218 (0.1%) | 1.19 | 4/1648 (0.2%) |
| 1 | b7 | 1.51 | 29/1218 (2.4%) | 1.13 | 3/1648 (0.2%) |
| 1 | d5 | 0.74 | 0/1218 | 0.94 | 2/1648 (0.1%) |
| 1 | d7 | 0.90 | 1/1218 (0.1%) | 1.19 | 4/1648 (0.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | f5 | 0.90 | 1/1218 (0.1%) | 1.19 | 4/1648 (0.2%) |
| 1 | f7 | 0.74 | 0/1218 | 0.93 | 2/1648 (0.1%) |
| 1 | h7 | 1.51 | 29/1218 (2.4%) | 1.13 | 3/1648 (0.2%) |
| 1 | j7 | 0.90 | 1/1218 (0.1%) | 1.19 | 4/1648 (0.2%) |
| 1 | l7 | 0.74 | 0/1218 | 0.94 | 2/1648 (0.1%) |
| 1 | n7 | 0.74 | 0/1218 | 0.93 | 1/1648 (0.1%) |
| 1 | p7 | 0.90 | 1/1218 (0.1%) | 1.19 | 4/1648 (0.2%) |
| 1 | r7 | 0.74 | 0/1218 | 0.94 | 2/1648 (0.1%) |
| 1 | t7 | 0.74 | 0/1218 | 0.92 | 1/1648 (0.1%) |
| 1 | v7 | 0.90 | 1/1218 (0.1%) | 1.19 | 4/1648 (0.2%) |
| 2 | A1 | 0.72 | 0/1265 | 0.86 | 0/1713 |
| 2 | A2 | 0.72 | 0/1265 | 0.86 | 0/1713 |
| 2 | A3 | 0.72 | 0/1265 | 0.86 | 0/1713 |
| 2 | A4 | 0.72 | 0/1265 | 0.86 | 0/1713 |
| 2 | A6 | 0.72 | 0/1265 | 0.86 | 0/1713 |
| 2 | A8 | 0.72 | 0/1265 | 0.86 | 0/1713 |
| 2 | A9 | 0.72 | 0/1265 | 0.86 | 0/1713 |
| 2 | AA | 0.72 | 0/1265 | 0.86 | 0/1713 |
| 2 | C1 | 0.73 | 0/1265 | 0.87 | 0/1713 |
| 2 | C2 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | C3 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | C4 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | C6 | 0.73 | 0/1265 | 0.87 | 0/1713 |
| 2 | C8 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | C9 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | CA | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | E1 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | E2 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | E3 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | E4 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | E6 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | E8 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | E9 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | EA | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | G1 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | G2 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | G3 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | G4 | 0.74 | 0/1265 | 0.86 | 0/1713 |
| 2 | G6 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | G8 | 0.74 | 0/1265 | 0.86 | 0/1713 |
| 2 | G9 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | GA | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | I1 | 0.72 | 0/1265 | 0.87 | 0/1713 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | I2 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | I3 | 0.73 | 0/1265 | 0.87 | 0/1713 |
| 2 | I4 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | I6 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | I8 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | I9 | 0.65 | 0/1265 | 0.84 | 0/1713 |
| 2 | IA | 0.65 | 0/1265 | 0.84 | 0/1713 |
| 2 | K1 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | K2 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | K3 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | K4 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | K6 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | K8 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | K9 | 0.92 | 1/1265 (0.1%) | 1.03 | 6/1713 (0.4%) |
| 2 | KA | 0.92 | 1/1265 (0.1%) | 1.03 | 6/1713 (0.4%) |
| 2 | N4 | 0.72 | 0/1265 | 0.86 | 0/1713 |
| 2 | N8 | 0.72 | 0/1265 | 0.88 | 2/1713 (0.1%) |
| 2 | O1 | 0.72 | 0/1265 | 0.86 | 0/1713 |
| 2 | O3 | 0.72 | 0/1265 | 0.86 | 0/1713 |
| 2 | O9 | 0.72 | 0/1265 | 0.86 | 0/1713 |
| 2 | OA | 0.72 | 0/1265 | 0.86 | 0/1713 |
| 2 | P4 | 0.73 | 0/1265 | 0.87 | 0/1713 |
| 2 | P8 | 0.73 | 0/1265 | 0.87 | 0/1713 |
| 2 | Q1 | 0.73 | 0/1265 | 0.87 | 0/1713 |
| 2 | Q3 | 0.73 | 0/1265 | 0.87 | 0/1713 |
| 2 | Q9 | 0.73 | 0/1265 | 0.87 | 0/1713 |
| 2 | QA | 0.73 | 0/1265 | 0.88 | 0/1713 |
| 2 | R4 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | R8 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | S1 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | S3 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | S9 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | SA | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | T4 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | T8 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | U1 | 0.73 | 0/1265 | 0.90 | 3/1713 (0.2%) |
| 2 | U3 | 0.73 | 0/1265 | 1.09 | 2/1713 (0.1%) |
| 2 | U9 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | UA | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | V4 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | V8 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | W1 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | W3 | 0.73 | 0/1265 | 0.86 | 0/1713 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | W9 | 0.72 | 0/1265 | 0.86 | 0/1713 |
| 2 | WA | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | X4 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | X8 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | Y1 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | Y3 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | Y9 | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 2 | YA | 0.73 | 0/1265 | 0.86 | 0/1713 |
| 3 | B1 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | B2 | 0.82 | 1/1307 (0.1%) | 0.92 | 2/1768 (0.1%) |
| 3 | B3 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | B4 | 0.81 | 0/1307 | 0.94 | 3/1768 (0.2%) |
| 3 | B6 | 0.82 | 1/1307 (0.1%) | 0.92 | 2/1768 (0.1%) |
| 3 | B8 | 0.80 | 0/1307 | 0.92 | 2/1768 (0.1%) |
| 3 | B9 | 0.79 | 0/1307 | 0.91 | 2/1768 (0.1%) |
| 3 | BA | 0.79 | 0/1307 | 0.91 | 2/1768 (0.1%) |
| 3 | D1 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | D2 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | D3 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | D4 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | D6 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | D8 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | D9 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | DA | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | F1 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | F2 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | F3 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | F4 | 0.78 | 0/1307 | 0.96 | 3/1768 (0.2%) |
| 3 | F6 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | F8 | 0.79 | 0/1307 | 0.95 | 4/1768 (0.2%) |
| 3 | F9 | 1.03 | 4/1307 (0.3%) | 1.30 | 9/1768 (0.5%) |
| 3 | FA | 1.04 | 3/1307 (0.2%) | 1.13 | 10/1768 (0.6%) |
| 3 | H1 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | H2 | 0.98 | 4/1307 (0.3%) | 1.05 | 6/1768 (0.3%) |
| 3 | H3 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | H4 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | H6 | 0.98 | 4/1307 (0.3%) | 1.05 | 6/1768 (0.3%) |
| 3 | H8 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | H9 | 0.81 | 0/1307 | 0.91 | 2/1768 (0.1%) |
| 3 | HA | 0.81 | 0/1307 | 0.91 | 2/1768 (0.1%) |
| 3 | J1 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | J2 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | J3 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 3 | J4 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | J6 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | J8 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | J9 | 0.82 | 1/1307 (0.1%) | 0.93 | 4/1768 (0.2%) |
| 3 | JA | 0.82 | 1/1307 (0.1%) | 0.93 | 4/1768 (0.2%) |
| 3 | L1 | 0.78 | 0/1307 | 1.08 | 5/1768 (0.3%) |
| 3 | L2 | 0.80 | 0/1307 | 0.97 | 5/1768 (0.3%) |
| 3 | L3 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | L4 | 0.78 | 0/1307 | 1.12 | 5/1768 (0.3%) |
| 3 | L6 | 0.79 | 0/1307 | 0.91 | 2/1768 (0.1%) |
| 3 | L8 | 0.78 | 0/1307 | 0.91 | 2/1768 (0.1%) |
| 3 | L9 | 1.39 | 24/1307 (1.8%) | 1.11 | 11/1768 (0.6%) |
| 3 | LA | 1.39 | 24/1307 (1.8%) | 1.11 | 11/1768 (0.6%) |
| 3 | O4 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | O8 | 0.79 | 0/1307 | 1.08 | 4/1768 (0.2%) |
| 3 | P1 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | P3 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | P9 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | PA | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | Q4 | 0.84 | 0/1307 | 1.12 | 4/1768 (0.2%) |
| 3 | Q8 | 0.82 | 0/1307 | 1.03 | 4/1768 (0.2%) |
| 3 | R1 | 0.77 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | R3 | 0.78 | 0/1307 | 0.91 | 2/1768 (0.1%) |
| 3 | R9 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | RA | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | S4 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | S8 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | T1 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | T3 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | T9 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | TA | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | U4 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | U8 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | V1 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | V3 | 0.79 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | V9 | 0.79 | 0/1307 | 0.91 | 2/1768 (0.1%) |
| 3 | VA | 0.79 | 0/1307 | 0.91 | 2/1768 (0.1%) |
| 3 | W4 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | W8 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | X1 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | X3 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | X9 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | XA | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 3 | Y4 | 0.82 | 0/1307 | 1.14 | 5/1768 (0.3%) |
| 3 | Y8 | 0.81 | 0/1307 | 0.99 | 2/1768 (0.1%) |
| 3 | Z1 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | Z3 | 0.78 | 0/1307 | 0.90 | 2/1768 (0.1%) |
| 3 | Z9 | 0.79 | 0/1307 | 0.91 | 2/1768 (0.1%) |
| 3 | ZA | 0.79 | 0/1307 | 0.91 | 2/1768 (0.1%) |
| 4 | M1 | 2.88 | 178/2225 (8.0%) | 2.02 | 94/3011 (3.1%) |
| 4 | M3 | 2.88 | 178/2225 (8.0%) | 2.02 | 94/3011 (3.1%) |
| 4 | M4 | 2.85 | 171/2225 (7.7%) | 2.15 | 99/3011 (3.3%) |
| 4 | M8 | 2.85 | 171/2225 (7.7%) | 2.41 | 114/3011 (3.8%) |
| 4 | M9 | 2.88 | 180/2225 (8.1%) | 2.02 | 95/3011 (3.2%) |
| 4 | MA | 2.88 | 178/2225 (8.0%) | 2.02 | 95/3011 (3.2%) |
| 5 | N1 | 1.66 | 3/589 (0.5%) | 1.84 | 13/797 (1.6%) |
| 5 | N3 | 1.66 | 3/589 (0.5%) | 1.84 | 13/797 (1.6%) |
| 5 | N9 | 1.66 | 3/589 (0.5%) | 1.84 | 13/797 (1.6%) |
| 5 | NA | 1.66 | 3/589 (0.5%) | 1.84 | 13/797 (1.6%) |
| 5 | Z4 | 1.66 | 3/589 (0.5%) | 2.83 | 19/797 (2.4%) |
| 5 | Z8 | 1.64 | 3/589 (0.5%) | 1.83 | 13/797 (1.6%) |
| 6 | M2 | 0.34 | 0/2237 | 0.74 | 3/3022 (0.1%) |
| 6 | M6 | 0.34 | 0/2237 | 0.74 | 3/3022 (0.1%) |
| 7 | N2 | 0.43 | 0/555 | 0.90 | 1/755 (0.1%) |
| 7 | N6 | 0.43 | 0/555 | 0.90 | 1/755 (0.1%) |
| 8 | A5 | 1.45 | 28/1239 (2.3%) | 1.12 | 7/1676 (0.4%) |
| 8 | A7 | 0.73 | 2/1239 (0.2%) | 0.99 | 1/1676 (0.1%) |
| 8 | C5 | 1.50 | 30/1239 (2.4%) | 1.28 | 15/1676 (0.9%) |
| 8 | C7 | 0.65 | 1/1239 (0.1%) | 1.00 | 4/1676 (0.2%) |
| 8 | E5 | 1.74 | 34/1239 (2.7%) | 1.40 | 21/1676 (1.3%) |
| 8 | E7 | 0.78 | 3/1239 (0.2%) | 1.12 | 6/1676 (0.4%) |
| 8 | G5 | 1.45 | 28/1239 (2.3%) | 1.12 | 7/1676 (0.4%) |
| 8 | G7 | 0.73 | 2/1239 (0.2%) | 0.99 | 1/1676 (0.1%) |
| 8 | I5 | 1.50 | 29/1239 (2.3%) | 1.28 | 15/1676 (0.9%) |
| 8 | I7 | 0.66 | 1/1239 (0.1%) | 1.01 | 4/1676 (0.2%) |
| 8 | K5 | 1.74 | 34/1239 (2.7%) | 1.39 | 21/1676 (1.3%) |
| 8 | K7 | 0.78 | 3/1239 (0.2%) | 1.12 | 6/1676 (0.4%) |
| 8 | M5 | 0.73 | 2/1239 (0.2%) | 1.00 | 3/1676 (0.2%) |
| 8 | M7 | 0.72 | 2/1239 (0.2%) | 0.98 | 1/1676 (0.1%) |
| 8 | O5 | 0.67 | 1/1239 (0.1%) | 1.15 | 9/1676 (0.5%) |
| 8 | O7 | 0.66 | 1/1239 (0.1%) | 1.01 | 6/1676 (0.4%) |
| 8 | Q5 | 0.85 | 4/1239 (0.3%) | 1.15 | 7/1676 (0.4%) |
| 8 | Q7 | 0.78 | 3/1239 (0.2%) | 1.12 | 6/1676 (0.4%) |
| 8 | S5 | 0.73 | 2/1239 (0.2%) | 0.98 | 1/1676 (0.1%) |
| 8 | S7 | 0.73 | 2/1239 (0.2%) | 0.99 | 1/1676 (0.1%) |
| 8 | U5 | 0.68 | 1/1239 (0.1%) | 1.17 | 8/1676 (0.5%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|--------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 8 | U7 | 0.65 | 1/1239 (0.1%) | 1.03 | 6/1676 (0.4%) |
| 8 | W5 | 0.85 | 4/1239 (0.3%) | 1.15 | 7/1676 (0.4%) |
| 8 | W7 | 0.78 | 3/1239 (0.2%) | 1.12 | 6/1676 (0.4%) |
| 8 | Y5 | 0.72 | 2/1239 (0.2%) | 0.98 | 1/1676 (0.1%) |
| 8 | Y7 | 0.73 | 2/1239 (0.2%) | 0.98 | 1/1676 (0.1%) |
| 8 | a5 | 1.24 | 14/1239 (1.1%) | 1.19 | 7/1676 (0.4%) |
| 8 | a7 | 1.03 | 10/1239 (0.8%) | 1.06 | 7/1676 (0.4%) |
| 8 | c5 | 0.72 | 2/1239 (0.2%) | 0.99 | 1/1676 (0.1%) |
| 8 | c7 | 1.73 | 38/1239 (3.1%) | 1.53 | 21/1676 (1.3%) |
| 8 | e5 | 1.24 | 16/1239 (1.3%) | 1.21 | 8/1676 (0.5%) |
| 8 | e7 | 0.72 | 1/1239 (0.1%) | 0.98 | 1/1676 (0.1%) |
| 8 | g7 | 1.03 | 10/1239 (0.8%) | 1.06 | 7/1676 (0.4%) |
| 8 | i7 | 1.73 | 38/1239 (3.1%) | 1.53 | 21/1676 (1.3%) |
| 8 | k7 | 0.73 | 1/1239 (0.1%) | 1.00 | 1/1676 (0.1%) |
| 8 | m7 | 0.65 | 1/1239 (0.1%) | 1.00 | 4/1676 (0.2%) |
| 8 | o7 | 1.84 | 43/1239 (3.5%) | 1.41 | 18/1676 (1.1%) |
| 8 | q7 | 0.73 | 2/1239 (0.2%) | 1.01 | 1/1676 (0.1%) |
| 8 | s7 | 0.65 | 1/1239 (0.1%) | 1.03 | 5/1676 (0.3%) |
| 8 | u7 | 1.84 | 43/1239 (3.5%) | 1.41 | 18/1676 (1.1%) |
| 9 | i5 | 3.44 | 74/548 (13.5%) | 2.43 | 20/737 (2.7%) |
| 9 | w7 | 3.26 | 66/548 (12.0%) | 2.44 | 37/737 (5.0%) |
| 9 | x7 | 2.30 | 19/548 (3.5%) | 1.99 | 16/737 (2.2%) |
| 9 | y7 | 2.30 | 19/548 (3.5%) | 1.99 | 16/737 (2.2%) |
| 9 | z5 | 3.44 | 77/548 (14.1%) | 2.44 | 20/737 (2.7%) |
| 9 | z7 | 3.26 | 66/548 (12.0%) | 2.44 | 37/737 (5.0%) |
| 10 | j5 | 3.83 | 1446/9003 (16.1%) | 2.36 | 479/12173 (3.9%) |
| 10 | k5 | 3.83 | 1453/9003 (16.1%) | 2.35 | 474/12173 (3.9%) |
| 11 | a9 | 1.67 | 107/6453 (1.7%) | 2.08 | 198/8728 (2.3%) |
| 11 | aA | 1.67 | 107/6453 (1.7%) | 2.09 | 200/8728 (2.3%) |
| All | All | 1.35 | 5153/373432 (1.4%) | 1.21 | 2859/505286 (0.6%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | D5 | 0 | 1 |
| 1 | J5 | 0 | 1 |
| 3 | L9 | 0 | 1 |
| 3 | LA | 0 | 1 |
| 3 | Q4 | 0 | 3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3 | Q8 | 0 | 1 |
| 4 | M1 | 0 | 2 |
| 4 | M3 | 0 | 2 |
| 4 | M4 | 0 | 2 |
| 4 | M8 | 0 | 2 |
| 4 | M9 | 0 | 2 |
| 4 | MA | 0 | 2 |
| 5 | Z4 | 0 | 2 |
| 6 | M2 | 0 | 5 |
| 6 | M6 | 0 | 5 |
| 7 | N2 | 0 | 1 |
| 7 | N6 | 0 | 1 |
| 8 | E7 | 0 | 1 |
| 8 | K7 | 0 | 1 |
| 8 | O5 | 0 | 1 |
| 8 | Q5 | 0 | 1 |
| 8 | Q7 | 0 | 1 |
| 8 | U7 | 0 | 1 |
| 8 | W5 | 0 | 1 |
| 8 | W7 | 0 | 1 |
| 8 | a5 | 0 | 3 |
| 8 | c7 | 0 | 3 |
| 8 | e5 | 0 | 3 |
| 8 | i7 | 0 | 3 |
| 8 | o7 | 0 | 2 |
| 8 | u7 | 0 | 2 |
| 9 | i5 | 0 | 1 |
| 9 | x7 | 0 | 2 |
| 9 | y7 | 0 | 2 |
| 9 | z5 | 0 | 1 |
| 10 | j5 | 0 | 23 |
| 10 | k5 | 0 | 23 |
| 11 | a9 | 0 | 16 |
| 11 | aA | 0 | 17 |
| All | All | 0 | 143 |

All (5153) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 10 | j5 | 897 | SER | C-O | -20.50 | 1.00 | 1.24 |
| 10 | k5 | 897 | SER | C-O | -20.50 | 1.00 | 1.24 |
| 1 | L5 | 18 | TYR | C-N | 18.60 | 1.58 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1 | p7 | 18 | TYR | C-N | 18.58 | 1.58 | 1.33 |
| 1 | v7 | 18 | TYR | C-N | 18.55 | 1.58 | 1.33 |
| 1 | F5 | 18 | TYR | C-N | 18.52 | 1.58 | 1.33 |
| 1 | F7 | 18 | TYR | C-N | 18.46 | 1.58 | 1.33 |
| 1 | R5 | 18 | TYR | C-N | 18.44 | 1.58 | 1.33 |
| 1 | R7 | 18 | TYR | C-N | 18.42 | 1.58 | 1.33 |
| 1 | L7 | 18 | TYR | C-N | 18.42 | 1.58 | 1.33 |
| 1 | X5 | 18 | TYR | C-N | 18.39 | 1.58 | 1.33 |
| 1 | d7 | 18 | TYR | C-N | 18.38 | 1.58 | 1.33 |
| 10 | j5 | 680 | PRO | C-O | -18.37 | 1.01 | 1.23 |
| 10 | k5 | 831 | PHE | C-O | -18.36 | 1.02 | 1.24 |
| 1 | X7 | 18 | TYR | C-N | 18.36 | 1.58 | 1.33 |
| 1 | f5 | 18 | TYR | C-N | 18.33 | 1.58 | 1.33 |
| 1 | j7 | 18 | TYR | C-N | 18.32 | 1.58 | 1.33 |
| 10 | j5 | 831 | PHE | C-O | -18.31 | 1.02 | 1.24 |
| 10 | k5 | 680 | PRO | C-O | -18.31 | 1.01 | 1.23 |
| 1 | b5 | 18 | TYR | C-N | 18.27 | 1.58 | 1.33 |
| 10 | k5 | 629 | TYR | C-O | -17.04 | 1.03 | 1.24 |
| 10 | j5 | 629 | TYR | C-O | -17.00 | 1.03 | 1.24 |
| 10 | k5 | 457 | THR | C-O | -16.92 | 1.03 | 1.24 |
| 10 | j5 | 882 | PRO | C-O | -16.88 | 1.01 | 1.24 |
| 10 | j5 | 457 | THR | C-O | -16.87 | 1.04 | 1.24 |
| 10 | k5 | 882 | PRO | C-O | -16.85 | 1.01 | 1.24 |
| 10 | j5 | 626 | ALA | C-O | -16.79 | 1.04 | 1.24 |
| 10 | k5 | 626 | ALA | C-O | -16.78 | 1.04 | 1.24 |
| 10 | j5 | 839 | ARG | C-O | -16.66 | 1.05 | 1.24 |
| 10 | k5 | 839 | ARG | C-O | -16.61 | 1.05 | 1.24 |
| 10 | j5 | 631 | HIS | C-O | -16.08 | 1.05 | 1.24 |
| 10 | k5 | 631 | HIS | C-O | -16.02 | 1.05 | 1.24 |
| 10 | j5 | 775 | VAL | C-O | -15.62 | 1.05 | 1.24 |
| 10 | k5 | 775 | VAL | C-O | -15.54 | 1.05 | 1.24 |
| 10 | j5 | 828 | VAL | C-O | -15.53 | 1.05 | 1.24 |
| 10 | k5 | 828 | VAL | C-O | -15.46 | 1.05 | 1.24 |
| 10 | k5 | 458 | LEU | C-O | -15.45 | 1.05 | 1.24 |
| 10 | j5 | 458 | LEU | C-O | -15.40 | 1.05 | 1.24 |
| 10 | j5 | 721 | LYS | C-O | -15.34 | 1.06 | 1.24 |
| 10 | k5 | 721 | LYS | C-O | -15.34 | 1.06 | 1.24 |
| 10 | k5 | 572 | TYR | C-O | -15.21 | 1.04 | 1.24 |
| 10 | j5 | 572 | TYR | C-O | -15.18 | 1.04 | 1.24 |
| 10 | j5 | 571 | ALA | C-O | -15.12 | 1.06 | 1.24 |
| 10 | k5 | 571 | ALA | C-O | -15.12 | 1.06 | 1.24 |
| 10 | j5 | 824 | PRO | C-O | -14.97 | 1.05 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 10 | k5 | 824 | PRO | C-O | -14.94 | 1.05 | 1.23 |
| 10 | j5 | 774 | GLN | C-O | -14.85 | 1.11 | 1.23 |
| 10 | k5 | 774 | GLN | C-O | -14.85 | 1.11 | 1.23 |
| 10 | k5 | 649 | PHE | C-O | -14.75 | 1.06 | 1.24 |
| 10 | j5 | 649 | PHE | C-O | -14.66 | 1.06 | 1.24 |
| 10 | j5 | 464 | GLN | C-O | -14.45 | 1.12 | 1.24 |
| 10 | k5 | 464 | GLN | C-O | -14.45 | 1.12 | 1.24 |
| 10 | j5 | 460 | ALA | C-O | -14.44 | 1.06 | 1.24 |
| 10 | j5 | 893 | ASN | C-O | -14.40 | 1.06 | 1.24 |
| 10 | k5 | 460 | ALA | C-O | -14.40 | 1.06 | 1.24 |
| 10 | k5 | 893 | ASN | C-O | -14.38 | 1.07 | 1.24 |
| 10 | j5 | 539 | LYS | C-O | -14.37 | 1.07 | 1.24 |
| 10 | k5 | 539 | LYS | C-O | -14.32 | 1.07 | 1.24 |
| 10 | j5 | 665 | LEU | C-O | -14.14 | 1.06 | 1.24 |
| 10 | k5 | 665 | LEU | C-O | -14.14 | 1.06 | 1.24 |
| 10 | j5 | 830 | GLU | C-O | -14.09 | 1.07 | 1.24 |
| 10 | k5 | 830 | GLU | C-O | -14.05 | 1.07 | 1.24 |
| 10 | j5 | 632 | ARG | C-O | -14.04 | 1.07 | 1.24 |
| 10 | k5 | 632 | ARG | C-O | -14.04 | 1.07 | 1.24 |
| 10 | j5 | 774 | GLN | CA-C | -13.99 | 1.40 | 1.53 |
| 9 | i5 | 42 | GLN | C-O | -13.98 | 1.05 | 1.24 |
| 10 | k5 | 774 | GLN | CA-C | -13.98 | 1.40 | 1.53 |
| 9 | z5 | 42 | GLN | C-O | -13.97 | 1.05 | 1.24 |
| 10 | k5 | 372 | ARG | C-O | -13.78 | 1.06 | 1.24 |
| 10 | j5 | 372 | ARG | C-O | -13.77 | 1.06 | 1.24 |
| 10 | k5 | 768 | VAL | C-O | -13.77 | 1.07 | 1.24 |
| 10 | j5 | 816 | ARG | C-O | -13.75 | 1.08 | 1.24 |
| 10 | k5 | 816 | ARG | C-O | -13.75 | 1.08 | 1.24 |
| 10 | k5 | 619 | GLU | C-O | -13.73 | 1.11 | 1.24 |
| 10 | k5 | 792 | GLU | C-O | -13.72 | 1.08 | 1.24 |
| 10 | j5 | 792 | GLU | C-O | -13.72 | 1.08 | 1.24 |
| 10 | j5 | 768 | VAL | C-O | -13.71 | 1.07 | 1.24 |
| 10 | k5 | 650 | ASP | CB-CG | 13.71 | 1.86 | 1.52 |
| 10 | j5 | 619 | GLU | C-O | -13.68 | 1.11 | 1.24 |
| 10 | j5 | 486 | ILE | C-O | -13.68 | 1.08 | 1.24 |
| 10 | j5 | 650 | ASP | CB-CG | 13.68 | 1.86 | 1.52 |
| 10 | k5 | 486 | ILE | C-O | -13.68 | 1.08 | 1.24 |
| 10 | j5 | 718 | MET | C-O | -13.65 | 1.08 | 1.24 |
| 10 | j5 | 522 | ASN | C-O | -13.65 | 1.10 | 1.24 |
| 10 | k5 | 522 | ASN | C-O | -13.65 | 1.10 | 1.24 |
| 10 | k5 | 637 | ARG | C-O | -13.65 | 1.11 | 1.24 |
| 10 | k5 | 807 | ARG | C-O | -13.62 | 1.07 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 10 | k5 | 718 | MET | C-O | -13.59 | 1.08 | 1.24 |
| 10 | k5 | 1001 | TYR | C-O | -13.58 | 1.08 | 1.24 |
| 10 | j5 | 807 | ARG | C-O | -13.56 | 1.07 | 1.24 |
| 10 | j5 | 1001 | TYR | C-O | -13.55 | 1.08 | 1.24 |
| 10 | k5 | 685 | LEU | C-O | -13.54 | 1.06 | 1.23 |
| 10 | j5 | 661 | VAL | C-O | -13.52 | 1.08 | 1.24 |
| 9 | z5 | 41 | GLN | C-O | -13.51 | 1.08 | 1.24 |
| 10 | j5 | 829 | VAL | C-O | -13.48 | 1.08 | 1.24 |
| 10 | k5 | 829 | VAL | C-O | -13.48 | 1.08 | 1.24 |
| 10 | k5 | 661 | VAL | C-O | -13.47 | 1.08 | 1.24 |
| 9 | i5 | 41 | GLN | C-O | -13.46 | 1.08 | 1.24 |
| 10 | j5 | 685 | LEU | C-O | -13.46 | 1.06 | 1.23 |
| 10 | j5 | 637 | ARG | C-O | -13.45 | 1.12 | 1.24 |
| 10 | j5 | 645 | ASN | C-O | -13.39 | 1.08 | 1.24 |
| 10 | j5 | 659 | GLY | C-O | -13.39 | 1.07 | 1.23 |
| 10 | k5 | 659 | GLY | C-O | -13.39 | 1.07 | 1.23 |
| 10 | k5 | 645 | ASN | C-O | -13.39 | 1.08 | 1.24 |
| 10 | k5 | 804 | GLU | C-O | -13.39 | 1.08 | 1.24 |
| 10 | j5 | 804 | GLU | C-O | -13.38 | 1.08 | 1.24 |
| 10 | j5 | 625 | LYS | C-O | -13.30 | 1.07 | 1.24 |
| 10 | k5 | 625 | LYS | C-O | -13.27 | 1.07 | 1.24 |
| 10 | k5 | 438 | ALA | C-O | -13.23 | 1.08 | 1.24 |
| 10 | k5 | 569 | THR | C-O | -13.22 | 1.06 | 1.24 |
| 10 | j5 | 569 | THR | C-O | -13.21 | 1.06 | 1.24 |
| 10 | j5 | 438 | ALA | C-O | -13.19 | 1.08 | 1.24 |
| 10 | j5 | 771 | ALA | C-O | -13.13 | 1.06 | 1.24 |
| 10 | j5 | 878 | GLU | C-O | -13.12 | 1.08 | 1.24 |
| 10 | k5 | 878 | GLU | C-O | -13.10 | 1.08 | 1.24 |
| 10 | j5 | 601 | LYS | C-O | -13.09 | 1.08 | 1.24 |
| 10 | k5 | 601 | LYS | C-O | -13.09 | 1.08 | 1.24 |
| 10 | k5 | 771 | ALA | C-O | -13.09 | 1.06 | 1.24 |
| 10 | k5 | 482 | GLN | C-O | -13.07 | 1.09 | 1.24 |
| 10 | j5 | 894 | TYR | C-O | -13.06 | 1.11 | 1.24 |
| 10 | j5 | 482 | GLN | C-O | -13.06 | 1.09 | 1.24 |
| 10 | k5 | 719 | MET | C-O | -13.05 | 1.08 | 1.24 |
| 10 | k5 | 894 | TYR | C-O | -13.04 | 1.11 | 1.24 |
| 10 | j5 | 719 | MET | C-O | -13.03 | 1.08 | 1.24 |
| 10 | j5 | 844 | GLN | C-O | -13.01 | 1.06 | 1.24 |
| 10 | k5 | 844 | GLN | C-O | -13.01 | 1.06 | 1.24 |
| 4 | M8 | 47 | VAL | C-O | -12.97 | 1.12 | 1.23 |
| 4 | M4 | 47 | VAL | C-O | -12.91 | 1.12 | 1.23 |
| 10 | k5 | 500 | PRO | C-O | -12.91 | 1.13 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 10 | j5 | 606 | ALA | C-O | -12.87 | 1.08 | 1.24 |
| 4 | M1 | 47 | VAL | C-O | -12.86 | 1.12 | 1.23 |
| 10 | k5 | 876 | TYR | C-O | -12.82 | 1.07 | 1.23 |
| 10 | k5 | 606 | ALA | C-O | -12.82 | 1.08 | 1.24 |
| 10 | j5 | 833 | PHE | C-O | -12.81 | 1.08 | 1.24 |
| 10 | j5 | 628 | GLU | C-O | -12.80 | 1.08 | 1.24 |
| 10 | k5 | 628 | GLU | C-O | -12.80 | 1.08 | 1.24 |
| 10 | k5 | 833 | PHE | C-O | -12.79 | 1.08 | 1.24 |
| 10 | j5 | 876 | TYR | C-O | -12.78 | 1.07 | 1.23 |
| 4 | M3 | 47 | VAL | C-O | -12.77 | 1.12 | 1.23 |
| 4 | MA | 47 | VAL | C-O | -12.77 | 1.12 | 1.23 |
| 4 | M9 | 47 | VAL | C-O | -12.77 | 1.12 | 1.23 |
| 10 | j5 | 663 | ALA | C-O | -12.76 | 1.08 | 1.23 |
| 10 | j5 | 599 | THR | C-O | -12.74 | 1.10 | 1.23 |
| 10 | k5 | 599 | THR | C-O | -12.74 | 1.10 | 1.23 |
| 10 | j5 | 500 | PRO | C-O | -12.68 | 1.14 | 1.24 |
| 10 | k5 | 300 | ALA | C-O | -12.64 | 1.09 | 1.24 |
| 10 | j5 | 619 | GLU | CA-CB | -12.63 | 1.36 | 1.53 |
| 10 | k5 | 663 | ALA | C-O | -12.63 | 1.08 | 1.23 |
| 10 | j5 | 300 | ALA | C-O | -12.61 | 1.09 | 1.24 |
| 10 | j5 | 635 | LEU | C-O | -12.59 | 1.09 | 1.24 |
| 10 | k5 | 635 | LEU | C-O | -12.59 | 1.09 | 1.24 |
| 10 | k5 | 619 | GLU | CA-CB | -12.58 | 1.36 | 1.53 |
| 10 | j5 | 716 | ALA | C-O | -12.56 | 1.09 | 1.24 |
| 10 | k5 | 716 | ALA | C-O | -12.55 | 1.09 | 1.24 |
| 10 | j5 | 538 | PHE | C-O | -12.54 | 1.08 | 1.24 |
| 10 | k5 | 538 | PHE | C-O | -12.54 | 1.08 | 1.24 |
| 10 | j5 | 827 | LYS | C-O | -12.53 | 1.07 | 1.24 |
| 10 | k5 | 827 | LYS | C-O | -12.53 | 1.07 | 1.24 |
| 4 | M3 | 45 | VAL | C-O | -12.51 | 1.11 | 1.24 |
| 10 | k5 | 644 | GLU | C-O | -12.51 | 1.09 | 1.24 |
| 10 | j5 | 644 | GLU | C-O | -12.45 | 1.09 | 1.24 |
| 4 | M1 | 45 | VAL | C-O | -12.43 | 1.11 | 1.24 |
| 4 | MA | 45 | VAL | C-O | -12.42 | 1.11 | 1.24 |
| 4 | M9 | 45 | VAL | C-O | -12.42 | 1.11 | 1.24 |
| 10 | j5 | 510 | ILE | C-O | -12.40 | 1.07 | 1.24 |
| 4 | M8 | 45 | VAL | C-O | -12.39 | 1.11 | 1.24 |
| 4 | M4 | 45 | VAL | C-O | -12.39 | 1.11 | 1.24 |
| 10 | j5 | 764 | PHE | C-O | -12.37 | 1.08 | 1.24 |
| 10 | k5 | 510 | ILE | C-O | -12.37 | 1.07 | 1.24 |
| 10 | k5 | 764 | PHE | C-O | -12.37 | 1.08 | 1.24 |
| 10 | k5 | 847 | LEU | C-O | -12.36 | 1.09 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 10 | k5 | 575 | ILE | C-O | -12.36 | 1.10 | 1.24 |
| 10 | k5 | 753 | PHE | C-O | -12.36 | 1.09 | 1.24 |
| 10 | j5 | 575 | ILE | C-O | -12.36 | 1.10 | 1.24 |
| 10 | j5 | 641 | ASP | CA-C | -12.35 | 1.37 | 1.52 |
| 9 | z7 | 38 | PHE | N-CA | 12.34 | 1.61 | 1.46 |
| 10 | j5 | 439 | ALA | C-O | -12.34 | 1.09 | 1.24 |
| 10 | k5 | 439 | ALA | C-O | -12.34 | 1.09 | 1.24 |
| 9 | w7 | 38 | PHE | N-CA | 12.34 | 1.61 | 1.46 |
| 10 | j5 | 618 | TRP | CA-C | -12.33 | 1.40 | 1.52 |
| 10 | k5 | 618 | TRP | CA-C | -12.33 | 1.40 | 1.52 |
| 10 | j5 | 847 | LEU | C-O | -12.30 | 1.09 | 1.24 |
| 3 | H2 | 77 | ARG | C-O | -12.29 | 1.09 | 1.24 |
| 3 | H6 | 77 | ARG | C-O | -12.29 | 1.09 | 1.24 |
| 10 | j5 | 753 | PHE | C-O | -12.29 | 1.09 | 1.24 |
| 10 | k5 | 641 | ASP | CA-C | -12.29 | 1.37 | 1.52 |
| 1 | J7 | 76 | ARG | C-O | -12.23 | 1.10 | 1.24 |
| 10 | j5 | 301 | TYR | C-O | -12.21 | 1.09 | 1.24 |
| 10 | j5 | 899 | GLU | C-O | -12.21 | 1.09 | 1.24 |
| 10 | k5 | 899 | GLU | C-O | -12.21 | 1.09 | 1.24 |
| 10 | j5 | 456 | ILE | C-O | -12.20 | 1.09 | 1.24 |
| 1 | D7 | 76 | ARG | C-O | -12.20 | 1.10 | 1.24 |
| 10 | k5 | 301 | TYR | C-O | -12.20 | 1.09 | 1.24 |
| 10 | j5 | 746 | LEU | C-O | -12.18 | 1.08 | 1.24 |
| 10 | j5 | 605 | ARG | C-O | -12.14 | 1.09 | 1.24 |
| 10 | k5 | 605 | ARG | C-O | -12.14 | 1.09 | 1.24 |
| 10 | k5 | 746 | LEU | C-O | -12.13 | 1.08 | 1.24 |
| 10 | j5 | 455 | PHE | C-O | -12.12 | 1.06 | 1.23 |
| 10 | k5 | 456 | ILE | C-O | -12.09 | 1.10 | 1.24 |
| 10 | k5 | 455 | PHE | C-O | -12.06 | 1.07 | 1.23 |
| 10 | j5 | 473 | GLY | C-O | -12.06 | 1.09 | 1.23 |
| 10 | j5 | 630 | ILE | C-O | -12.03 | 1.09 | 1.24 |
| 10 | k5 | 630 | ILE | C-O | -12.03 | 1.09 | 1.24 |
| 4 | M3 | 19 | MET | C-O | -12.02 | 1.12 | 1.24 |
| 4 | M1 | 19 | MET | C-O | -12.02 | 1.12 | 1.24 |
| 4 | M8 | 19 | MET | C-O | -12.00 | 1.12 | 1.24 |
| 4 | MA | 19 | MET | C-O | -11.98 | 1.12 | 1.24 |
| 4 | M9 | 19 | MET | C-O | -11.98 | 1.12 | 1.24 |
| 10 | k5 | 473 | GLY | C-O | -11.96 | 1.09 | 1.23 |
| 10 | j5 | 883 | SER | C-O | -11.92 | 1.08 | 1.24 |
| 10 | k5 | 436 | TRP | CA-C | -11.92 | 1.37 | 1.52 |
| 4 | M4 | 19 | MET | C-O | -11.92 | 1.12 | 1.24 |
| 10 | j5 | 591 | ILE | C-O | -11.92 | 1.10 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 10 | k5 | 591 | ILE | C-O | -11.92 | 1.10 | 1.24 |
| 10 | j5 | 693 | ARG | C-O | -11.90 | 1.10 | 1.24 |
| 10 | k5 | 693 | ARG | C-O | -11.90 | 1.10 | 1.24 |
| 10 | k5 | 703 | LEU | C-O | -11.89 | 1.09 | 1.24 |
| 10 | j5 | 436 | TRP | CA-C | -11.88 | 1.37 | 1.52 |
| 10 | k5 | 883 | SER | C-O | -11.85 | 1.09 | 1.24 |
| 4 | M8 | 56 | MET | C-O | -11.84 | 1.10 | 1.24 |
| 10 | k5 | 684 | TYR | C-O | -11.83 | 1.09 | 1.23 |
| 4 | M3 | 56 | MET | C-O | -11.83 | 1.10 | 1.24 |
| 4 | M1 | 56 | MET | C-O | -11.83 | 1.10 | 1.24 |
| 10 | k5 | 571 | ALA | CA-C | -11.83 | 1.38 | 1.52 |
| 4 | M1 | 59 | ILE | C-O | -11.83 | 1.10 | 1.24 |
| 4 | MA | 59 | ILE | C-O | -11.82 | 1.10 | 1.24 |
| 10 | j5 | 684 | TYR | C-O | -11.82 | 1.09 | 1.23 |
| 4 | M9 | 59 | ILE | C-O | -11.82 | 1.10 | 1.24 |
| 4 | M3 | 59 | ILE | C-O | -11.82 | 1.10 | 1.24 |
| 4 | MA | 56 | MET | C-O | -11.82 | 1.10 | 1.24 |
| 4 | M9 | 56 | MET | C-O | -11.82 | 1.10 | 1.24 |
| 4 | M4 | 56 | MET | C-O | -11.80 | 1.10 | 1.24 |
| 10 | j5 | 703 | LEU | C-O | -11.79 | 1.09 | 1.24 |
| 10 | j5 | 571 | ALA | CA-C | -11.79 | 1.38 | 1.52 |
| 4 | M8 | 59 | ILE | C-O | -11.78 | 1.10 | 1.24 |
| 4 | M4 | 59 | ILE | C-O | -11.78 | 1.10 | 1.24 |
| 10 | k5 | 897 | SER | CA-C | -11.78 | 1.37 | 1.52 |
| 10 | j5 | 638 | PRO | C-O | -11.76 | 1.09 | 1.23 |
| 10 | k5 | 638 | PRO | C-O | -11.76 | 1.09 | 1.23 |
| 10 | k5 | 537 | ILE | C-O | -11.74 | 1.11 | 1.24 |
| 10 | j5 | 537 | ILE | C-O | -11.74 | 1.11 | 1.24 |
| 10 | j5 | 715 | ALA | C-O | -11.74 | 1.10 | 1.24 |
| 10 | k5 | 715 | ALA | C-O | -11.74 | 1.10 | 1.24 |
| 10 | k5 | 636 | GLY | C-O | -11.71 | 1.08 | 1.23 |
| 9 | i5 | 37 | TRP | C-O | -11.71 | 1.10 | 1.24 |
| 10 | k5 | 862 | LEU | C-O | -11.71 | 1.10 | 1.24 |
| 10 | j5 | 600 | VAL | C-O | -11.71 | 1.09 | 1.24 |
| 10 | j5 | 862 | LEU | C-O | -11.70 | 1.10 | 1.24 |
| 10 | k5 | 592 | LYS | C-O | -11.69 | 1.09 | 1.24 |
| 10 | j5 | 610 | SER | CA-C | -11.68 | 1.37 | 1.53 |
| 10 | k5 | 600 | VAL | C-O | -11.68 | 1.09 | 1.24 |
| 10 | j5 | 636 | GLY | C-O | -11.67 | 1.08 | 1.23 |
| 10 | j5 | 896 | ASN | C-O | -11.67 | 1.10 | 1.24 |
| 10 | k5 | 896 | ASN | C-O | -11.67 | 1.10 | 1.24 |
| 10 | k5 | 568 | ILE | C-O | -11.67 | 1.09 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 10 | k5 | 610 | SER | CA-C | -11.66 | 1.37 | 1.53 |
| 10 | j5 | 614 | ARG | CA-C | -11.66 | 1.38 | 1.52 |
| 10 | k5 | 614 | ARG | CA-C | -11.66 | 1.38 | 1.52 |
| 10 | j5 | 681 | TYR | C-O | -11.66 | 1.08 | 1.23 |
| 10 | k5 | 681 | TYR | C-O | -11.66 | 1.08 | 1.23 |
| 10 | j5 | 568 | ILE | C-O | -11.64 | 1.09 | 1.24 |
| 10 | j5 | 448 | PRO | C-O | -11.64 | 1.09 | 1.24 |
| 9 | z5 | 37 | TRP | C-O | -11.63 | 1.10 | 1.24 |
| 10 | j5 | 592 | LYS | C-O | -11.64 | 1.09 | 1.24 |
| 10 | j5 | 723 | GLN | CA-C | -11.61 | 1.37 | 1.52 |
| 8 | E5 | 110 | ILE | C-O | -11.60 | 1.11 | 1.24 |
| 10 | j5 | 399 | TYR | C-O | -11.60 | 1.10 | 1.24 |
| 10 | k5 | 399 | TYR | C-O | -11.60 | 1.10 | 1.24 |
| 10 | j5 | 897 | SER | CA-C | -11.57 | 1.37 | 1.52 |
| 10 | k5 | 627 | ILE | C-O | -11.57 | 1.10 | 1.24 |
| 10 | k5 | 723 | GLN | CA-C | -11.56 | 1.37 | 1.52 |
| 10 | k5 | 448 | PRO | C-O | -11.56 | 1.09 | 1.24 |
| 10 | j5 | 802 | VAL | C-O | -11.54 | 1.09 | 1.24 |
| 10 | k5 | 834 | LYS | C-O | -11.53 | 1.08 | 1.24 |
| 10 | j5 | 627 | ILE | C-O | -11.52 | 1.10 | 1.24 |
| 8 | K5 | 110 | ILE | C-O | -11.52 | 1.11 | 1.24 |
| 10 | j5 | 603 | PHE | C-O | -11.51 | 1.09 | 1.24 |
| 10 | j5 | 834 | LYS | C-O | -11.51 | 1.08 | 1.24 |
| 10 | j5 | 598 | THR | C-O | -11.50 | 1.09 | 1.23 |
| 10 | j5 | 831 | PHE | CA-C | -11.49 | 1.38 | 1.52 |
| 10 | k5 | 598 | THR | C-O | -11.49 | 1.09 | 1.23 |
| 10 | k5 | 802 | VAL | C-O | -11.47 | 1.10 | 1.24 |
| 10 | k5 | 603 | PHE | C-O | -11.46 | 1.09 | 1.24 |
| 10 | j5 | 515 | PRO | C-O | -11.46 | 1.09 | 1.24 |
| 10 | k5 | 515 | PRO | C-O | -11.45 | 1.10 | 1.24 |
| 9 | w7 | 42 | GLN | C-O | -11.45 | 1.10 | 1.24 |
| 9 | z7 | 42 | GLN | C-O | -11.44 | 1.10 | 1.24 |
| 10 | k5 | 831 | PHE | CA-C | -11.42 | 1.38 | 1.52 |
| 10 | k5 | 378 | TYR | C-O | -11.40 | 1.10 | 1.24 |
| 10 | j5 | 511 | ARG | C-O | -11.38 | 1.10 | 1.24 |
| 10 | k5 | 511 | ARG | C-O | -11.38 | 1.10 | 1.24 |
| 10 | k5 | 398 | LEU | C-O | -11.38 | 1.10 | 1.24 |
| 10 | j5 | 398 | LEU | C-O | -11.37 | 1.10 | 1.24 |
| 10 | j5 | 378 | TYR | C-O | -11.35 | 1.10 | 1.24 |
| 4 | MA | 69 | ILE | C-O | -11.32 | 1.12 | 1.24 |
| 4 | M9 | 69 | ILE | C-O | -11.32 | 1.12 | 1.24 |
| 10 | k5 | 607 | LEU | C-O | -11.32 | 1.10 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 4 | M4 | 69 | ILE | C-O | -11.27 | 1.12 | 1.24 |
| 10 | j5 | 898 | VAL | C-O | -11.25 | 1.10 | 1.24 |
| 4 | M3 | 69 | ILE | C-O | -11.24 | 1.12 | 1.24 |
| 4 | M1 | 69 | ILE | C-O | -11.24 | 1.12 | 1.24 |
| 10 | k5 | 508 | ILE | C-O | -11.24 | 1.11 | 1.24 |
| 4 | M8 | 69 | ILE | C-O | -11.23 | 1.12 | 1.24 |
| 10 | j5 | 683 | ARG | C-O | -11.22 | 1.09 | 1.24 |
| 10 | j5 | 492 | ILE | C-O | -11.21 | 1.11 | 1.24 |
| 10 | k5 | 492 | ILE | C-O | -11.21 | 1.11 | 1.24 |
| 10 | j5 | 837 | LEU | C-O | -11.20 | 1.09 | 1.24 |
| 10 | k5 | 683 | ARG | C-O | -11.20 | 1.09 | 1.24 |
| 10 | k5 | 898 | VAL | C-O | -11.19 | 1.10 | 1.24 |
| 10 | k5 | 837 | LEU | C-O | -11.18 | 1.09 | 1.24 |
| 10 | j5 | 607 | LEU | C-O | -11.16 | 1.10 | 1.24 |
| 9 | z5 | 45 | GLN | C-O | -11.15 | 1.10 | 1.24 |
| 10 | j5 | 690 | LEU | C-O | -11.15 | 1.09 | 1.24 |
| 10 | k5 | 690 | LEU | C-O | -11.15 | 1.09 | 1.24 |
| 9 | i5 | 44 | ILE | C-O | -11.13 | 1.10 | 1.24 |
| 10 | j5 | 717 | ARG | C-O | -11.12 | 1.10 | 1.24 |
| 10 | j5 | 508 | ILE | C-O | -11.11 | 1.11 | 1.24 |
| 9 | i5 | 45 | GLN | C-O | -11.11 | 1.10 | 1.24 |
| 9 | z5 | 44 | ILE | C-O | -11.11 | 1.10 | 1.24 |
| 10 | j5 | 670 | TYR | C-O | -11.10 | 1.11 | 1.24 |
| 10 | k5 | 670 | TYR | C-O | -11.10 | 1.11 | 1.24 |
| 10 | j5 | 441 | ASP | C-O | -11.10 | 1.10 | 1.24 |
| 10 | k5 | 717 | ARG | C-O | -11.10 | 1.10 | 1.24 |
| 8 | o7 | 52 | LYS | C-O | -11.10 | 1.10 | 1.24 |
| 8 | u7 | 52 | LYS | C-O | -11.08 | 1.10 | 1.24 |
| 10 | k5 | 808 | LEU | C-O | -11.06 | 1.09 | 1.24 |
| 10 | k5 | 466 | LEU | C-O | -11.06 | 1.09 | 1.24 |
| 10 | j5 | 466 | LEU | C-O | -11.04 | 1.09 | 1.24 |
| 10 | j5 | 808 | LEU | C-O | -11.04 | 1.09 | 1.24 |
| 9 | z5 | 38 | PHE | C-O | -11.04 | 1.11 | 1.24 |
| 10 | k5 | 441 | ASP | C-O | -11.03 | 1.10 | 1.24 |
| 10 | j5 | 564 | VAL | C-O | -11.01 | 1.11 | 1.24 |
| 10 | k5 | 564 | VAL | C-O | -11.01 | 1.11 | 1.24 |
| 10 | k5 | 931 | VAL | C-O | -11.01 | 1.11 | 1.24 |
| 10 | j5 | 442 | LEU | C-O | -11.01 | 1.11 | 1.24 |
| 10 | k5 | 442 | LEU | C-O | -11.01 | 1.11 | 1.24 |
| 9 | i5 | 38 | PHE | C-O | -11.00 | 1.11 | 1.24 |
| 10 | k5 | 536 | LYS | C-O | -10.96 | 1.09 | 1.23 |
| 4 | M4 | 51 | ARG | C-O | -10.93 | 1.09 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 10 | j5 | 931 | VAL | C-O | -10.93 | 1.11 | 1.24 |
| 10 | j5 | 373 | ALA | C-O | -10.92 | 1.10 | 1.24 |
| 10 | j5 | 536 | LYS | C-O | -10.91 | 1.09 | 1.23 |
| 10 | j5 | 657 | PHE | C-O | -10.91 | 1.11 | 1.24 |
| 10 | k5 | 657 | PHE | C-O | -10.91 | 1.11 | 1.24 |
| 10 | j5 | 866 | LEU | C-O | -10.90 | 1.11 | 1.24 |
| 9 | z5 | 40 | GLU | CA-C | -10.88 | 1.38 | 1.52 |
| 4 | MA | 51 | ARG | C-O | -10.88 | 1.09 | 1.24 |
| 4 | M9 | 51 | ARG | C-O | -10.88 | 1.09 | 1.24 |
| 10 | k5 | 866 | LEU | C-O | -10.87 | 1.11 | 1.24 |
| 4 | M3 | 51 | ARG | C-O | -10.87 | 1.09 | 1.24 |
| 4 | M1 | 51 | ARG | C-O | -10.87 | 1.09 | 1.24 |
| 4 | M8 | 51 | ARG | C-O | -10.87 | 1.09 | 1.24 |
| 10 | j5 | 905 | THR | C-O | -10.86 | 1.10 | 1.23 |
| 10 | k5 | 373 | ALA | C-O | -10.86 | 1.10 | 1.24 |
| 8 | i7 | 125 | ALA | C-O | -10.85 | 1.11 | 1.24 |
| 4 | M4 | 71 | PRO | C-O | -10.85 | 1.10 | 1.23 |
| 10 | k5 | 623 | VAL | C-O | -10.84 | 1.10 | 1.24 |
| 8 | o7 | 80 | LEU | C-O | -10.84 | 1.11 | 1.24 |
| 4 | M3 | 71 | PRO | C-O | -10.84 | 1.10 | 1.23 |
| 4 | M1 | 71 | PRO | C-O | -10.84 | 1.10 | 1.23 |
| 4 | M8 | 71 | PRO | C-O | -10.84 | 1.10 | 1.23 |
| 10 | k5 | 930 | LEU | C-O | -10.83 | 1.11 | 1.24 |
| 4 | MA | 71 | PRO | C-O | -10.81 | 1.10 | 1.23 |
| 4 | M9 | 71 | PRO | C-O | -10.81 | 1.10 | 1.23 |
| 10 | k5 | 905 | THR | C-O | -10.81 | 1.10 | 1.23 |
| 4 | M8 | 55 | GLU | C-O | -10.81 | 1.11 | 1.24 |
| 10 | j5 | 930 | LEU | C-O | -10.80 | 1.11 | 1.24 |
| 9 | i5 | 40 | GLU | CA-C | -10.79 | 1.38 | 1.52 |
| 9 | i5 | 20 | GLY | C-O | -10.78 | 1.09 | 1.23 |
| 8 | u7 | 80 | LEU | C-O | -10.78 | 1.11 | 1.24 |
| 10 | j5 | 723 | GLN | C-O | -10.78 | 1.11 | 1.24 |
| 10 | k5 | 723 | GLN | C-O | -10.78 | 1.11 | 1.24 |
| 10 | j5 | 642 | ARG | C-O | -10.77 | 1.09 | 1.24 |
| 10 | j5 | 773 | VAL | C-O | -10.77 | 1.11 | 1.24 |
| 10 | k5 | 642 | ARG | C-O | -10.77 | 1.09 | 1.24 |
| 10 | k5 | 773 | VAL | C-O | -10.77 | 1.11 | 1.24 |
| 9 | z5 | 20 | GLY | C-O | -10.76 | 1.09 | 1.23 |
| 10 | j5 | 623 | VAL | C-O | -10.75 | 1.11 | 1.24 |
| 4 | M4 | 55 | GLU | C-O | -10.75 | 1.11 | 1.24 |
| 8 | I5 | 5 | THR | C-O | -10.74 | 1.11 | 1.24 |
| 10 | j5 | 656 | GLY | C-O | -10.74 | 1.09 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 8 | c7 | 125 | ALA | C-O | -10.74 | 1.11 | 1.24 |
| 8 | C5 | 5 | THR | C-O | -10.73 | 1.11 | 1.24 |
| 4 | M3 | 55 | GLU | C-O | -10.73 | 1.11 | 1.24 |
| 10 | k5 | 590 | GLU | C-O | -10.73 | 1.11 | 1.24 |
| 4 | M1 | 55 | GLU | C-O | -10.73 | 1.11 | 1.24 |
| 10 | k5 | 576 | PHE | C-O | -10.72 | 1.09 | 1.24 |
| 4 | MA | 55 | GLU | C-O | -10.71 | 1.11 | 1.24 |
| 10 | j5 | 652 | ALA | CA-C | -10.71 | 1.38 | 1.52 |
| 10 | k5 | 652 | ALA | CA-C | -10.71 | 1.38 | 1.52 |
| 4 | M9 | 55 | GLU | C-O | -10.71 | 1.11 | 1.24 |
| 10 | k5 | 349 | GLN | C-O | -10.71 | 1.14 | 1.24 |
| 10 | j5 | 590 | GLU | C-O | -10.71 | 1.11 | 1.24 |
| 10 | j5 | 741 | GLN | C-O | -10.71 | 1.10 | 1.23 |
| 8 | c7 | 132 | ALA | C-O | -10.70 | 1.11 | 1.24 |
| 10 | k5 | 622 | TYR | C-O | -10.69 | 1.11 | 1.23 |
| 10 | k5 | 656 | GLY | C-O | -10.69 | 1.09 | 1.23 |
| 10 | j5 | 853 | LEU | C-O | -10.69 | 1.10 | 1.24 |
| 10 | k5 | 853 | LEU | C-O | -10.69 | 1.10 | 1.24 |
| 8 | K5 | 104 | ILE | C-O | -10.68 | 1.12 | 1.24 |
| 9 | z5 | 40 | GLU | C-O | -10.68 | 1.11 | 1.24 |
| 10 | j5 | 450 | ARG | C-O | -10.67 | 1.11 | 1.24 |
| 10 | k5 | 450 | ARG | C-O | -10.67 | 1.11 | 1.24 |
| 9 | i5 | 40 | GLU | C-O | -10.67 | 1.11 | 1.24 |
| 8 | i7 | 132 | ALA | C-O | -10.66 | 1.11 | 1.24 |
| 10 | k5 | 741 | GLN | C-O | -10.65 | 1.10 | 1.23 |
| 10 | j5 | 622 | TYR | C-O | -10.65 | 1.11 | 1.23 |
| 8 | E5 | 104 | ILE | C-O | -10.65 | 1.12 | 1.24 |
| 10 | j5 | 349 | GLN | C-O | -10.64 | 1.14 | 1.24 |
| 10 | j5 | 576 | PHE | C-O | -10.62 | 1.10 | 1.24 |
| 10 | k5 | 871 | GLU | C-O | -10.61 | 1.11 | 1.24 |
| 4 | MA | 41 | ASN | C-O | -10.61 | 1.11 | 1.24 |
| 4 | M9 | 41 | ASN | C-O | -10.61 | 1.11 | 1.24 |
| 4 | M3 | 41 | ASN | C-O | -10.61 | 1.11 | 1.24 |
| 10 | k5 | 421 | PRO | C-O | -10.61 | 1.11 | 1.23 |
| 4 | M1 | 41 | ASN | C-O | -10.61 | 1.11 | 1.24 |
| 10 | k5 | 660 | VAL | C-O | -10.60 | 1.11 | 1.24 |
| 10 | j5 | 660 | VAL | C-O | -10.60 | 1.11 | 1.24 |
| 4 | M8 | 41 | ASN | C-O | -10.59 | 1.11 | 1.24 |
| 10 | j5 | 567 | LEU | C-O | -10.59 | 1.10 | 1.24 |
| 10 | k5 | 567 | LEU | C-O | -10.59 | 1.10 | 1.24 |
| 4 | M4 | 41 | ASN | C-O | -10.59 | 1.11 | 1.24 |
| 10 | j5 | 633 | ARG | C-O | -10.58 | 1.11 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 10 | k5 | 651 | ILE | C-O | -10.58 | 1.13 | 1.24 |
| 10 | j5 | 651 | ILE | C-O | -10.58 | 1.13 | 1.24 |
| 10 | j5 | 615 | LYS | CA-CB | -10.54 | 1.36 | 1.53 |
| 10 | k5 | 633 | ARG | C-O | -10.53 | 1.11 | 1.24 |
| 10 | j5 | 421 | PRO | C-O | -10.53 | 1.11 | 1.23 |
| 10 | j5 | 379 | PHE | C-O | -10.53 | 1.10 | 1.24 |
| 10 | j5 | 803 | LYS | C-O | -10.53 | 1.10 | 1.24 |
| 10 | k5 | 379 | PHE | C-O | -10.53 | 1.10 | 1.24 |
| 10 | k5 | 674 | PHE | CA-C | -10.51 | 1.38 | 1.52 |
| 10 | j5 | 566 | ALA | C-O | -10.49 | 1.10 | 1.24 |
| 10 | j5 | 871 | GLU | C-O | -10.49 | 1.11 | 1.24 |
| 10 | k5 | 566 | ALA | C-O | -10.49 | 1.10 | 1.24 |
| 10 | k5 | 615 | LYS | CA-CB | -10.49 | 1.36 | 1.53 |
| 10 | k5 | 803 | LYS | C-O | -10.47 | 1.10 | 1.24 |
| 10 | j5 | 674 | PHE | CA-C | -10.47 | 1.38 | 1.52 |
| 8 | u7 | 55 | GLY | C-O | -10.45 | 1.11 | 1.23 |
| 8 | o7 | 55 | GLY | C-O | -10.44 | 1.11 | 1.23 |
| 10 | j5 | 455 | PHE | CA-C | -10.41 | 1.39 | 1.52 |
| 10 | k5 | 455 | PHE | CA-C | -10.41 | 1.39 | 1.52 |
| 10 | j5 | 801 | SER | C-O | -10.38 | 1.10 | 1.23 |
| 10 | k5 | 801 | SER | C-O | -10.38 | 1.10 | 1.23 |
| 10 | j5 | 937 | GLU | C-O | -10.38 | 1.11 | 1.24 |
| 10 | k5 | 937 | GLU | C-O | -10.38 | 1.11 | 1.24 |
| 10 | k5 | 820 | HIS | C-O | -10.38 | 1.10 | 1.24 |
| 10 | j5 | 836 | PHE | C-O | -10.37 | 1.10 | 1.24 |
| 10 | j5 | 887 | PRO | C-O | -10.37 | 1.11 | 1.23 |
| 10 | k5 | 887 | PRO | C-O | -10.37 | 1.11 | 1.23 |
| 10 | j5 | 647 | ARG | CA-C | -10.36 | 1.39 | 1.52 |
| 8 | u7 | 36 | ARG | C-O | -10.36 | 1.11 | 1.24 |
| 10 | j5 | 852 | GLY | C-O | -10.35 | 1.09 | 1.23 |
| 8 | o7 | 36 | ARG | C-O | -10.35 | 1.11 | 1.24 |
| 10 | j5 | 859 | ILE | C-O | -10.34 | 1.11 | 1.24 |
| 10 | k5 | 852 | GLY | C-O | -10.34 | 1.09 | 1.23 |
| 10 | k5 | 859 | ILE | C-O | -10.34 | 1.11 | 1.24 |
| 10 | j5 | 401 | LEU | C-O | -10.33 | 1.12 | 1.24 |
| 10 | k5 | 401 | LEU | C-O | -10.33 | 1.12 | 1.24 |
| 10 | j5 | 619 | GLU | C-N | -10.32 | 1.25 | 1.33 |
| 10 | k5 | 619 | GLU | C-N | -10.32 | 1.25 | 1.33 |
| 10 | k5 | 836 | PHE | C-O | -10.30 | 1.10 | 1.24 |
| 10 | j5 | 820 | HIS | C-O | -10.30 | 1.10 | 1.24 |
| 10 | k5 | 647 | ARG | CA-C | -10.29 | 1.39 | 1.52 |
| 10 | j5 | 812 | SER | C-O | -10.28 | 1.11 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 10 | k5 | 812 | SER | C-O | -10.28 | 1.11 | 1.23 |
| 10 | k5 | 722 | ILE | C-O | -10.26 | 1.11 | 1.24 |
| 10 | j5 | 485 | ALA | C-O | -10.25 | 1.09 | 1.23 |
| 10 | j5 | 722 | ILE | C-O | -10.24 | 1.11 | 1.24 |
| 10 | j5 | 343 | TYR | C-O | -10.24 | 1.10 | 1.24 |
| 10 | k5 | 673 | VAL | C-O | -10.24 | 1.12 | 1.24 |
| 4 | M3 | 52 | LEU | C-O | -10.22 | 1.12 | 1.24 |
| 4 | M1 | 52 | LEU | C-O | -10.22 | 1.12 | 1.24 |
| 9 | z5 | 41 | GLN | CA-C | -10.22 | 1.39 | 1.52 |
| 9 | i5 | 41 | GLN | CA-C | -10.22 | 1.39 | 1.52 |
| 4 | MA | 52 | LEU | C-O | -10.21 | 1.12 | 1.24 |
| 4 | M9 | 52 | LEU | C-O | -10.21 | 1.12 | 1.24 |
| 10 | j5 | 673 | VAL | C-O | -10.21 | 1.12 | 1.24 |
| 4 | M4 | 52 | LEU | C-O | -10.21 | 1.12 | 1.24 |
| 8 | o7 | 81 | CYS | C-O | -10.18 | 1.11 | 1.24 |
| 10 | k5 | 485 | ALA | C-O | -10.17 | 1.09 | 1.23 |
| 4 | M8 | 52 | LEU | C-O | -10.17 | 1.12 | 1.24 |
| 8 | u7 | 81 | CYS | C-O | -10.15 | 1.12 | 1.24 |
| 10 | j5 | 804 | GLU | CA-C | -10.14 | 1.39 | 1.52 |
| 10 | k5 | 343 | TYR | C-O | -10.14 | 1.10 | 1.24 |
| 10 | j5 | 751 | LYS | C-O | -10.13 | 1.11 | 1.23 |
| 10 | k5 | 751 | LYS | C-O | -10.13 | 1.11 | 1.23 |
| 10 | k5 | 804 | GLU | CA-C | -10.13 | 1.39 | 1.52 |
| 10 | j5 | 628 | GLU | CA-C | -10.12 | 1.39 | 1.52 |
| 9 | w7 | 44 | ILE | C-O | -10.12 | 1.12 | 1.24 |
| 9 | z5 | 22 | GLU | C-O | -10.11 | 1.10 | 1.23 |
| 10 | k5 | 628 | GLU | CA-C | -10.11 | 1.39 | 1.52 |
| 9 | z7 | 44 | ILE | C-O | -10.11 | 1.12 | 1.24 |
| 10 | j5 | 1126 | ALA | C-O | -10.10 | 1.12 | 1.24 |
| 9 | i5 | 22 | GLU | C-O | -10.09 | 1.10 | 1.23 |
| 8 | a5 | 8 | ILE | C-O | -10.08 | 1.10 | 1.24 |
| 4 | M4 | 70 | SER | C-O | -10.07 | 1.11 | 1.24 |
| 10 | k5 | 1127 | SER | C-O | -10.06 | 1.12 | 1.24 |
| 8 | e5 | 8 | ILE | C-O | -10.05 | 1.10 | 1.24 |
| 10 | j5 | 443 | TYR | C-O | -10.05 | 1.11 | 1.24 |
| 10 | j5 | 650 | ASP | C-O | -10.04 | 1.10 | 1.24 |
| 10 | k5 | 650 | ASP | C-O | -10.04 | 1.10 | 1.24 |
| 4 | M1 | 70 | SER | C-O | -10.04 | 1.11 | 1.24 |
| 10 | j5 | 616 | LEU | C-O | -10.04 | 1.12 | 1.24 |
| 10 | k5 | 616 | LEU | C-O | -10.03 | 1.12 | 1.24 |
| 10 | j5 | 1127 | SER | C-O | -10.03 | 1.12 | 1.24 |
| 10 | k5 | 1126 | ALA | C-O | -10.03 | 1.12 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 10 | k5 | 443 | TYR | C-O | -10.03 | 1.11 | 1.24 |
| 4 | MA | 70 | SER | C-O | -10.02 | 1.12 | 1.24 |
| 4 | M9 | 32 | SER | CA-C | -10.02 | 1.40 | 1.52 |
| 4 | M9 | 70 | SER | C-O | -10.02 | 1.12 | 1.24 |
| 4 | M8 | 70 | SER | C-O | -10.02 | 1.12 | 1.24 |
| 4 | M3 | 70 | SER | C-O | -10.01 | 1.12 | 1.24 |
| 4 | M4 | 32 | SER | CA-C | -10.01 | 1.40 | 1.52 |
| 10 | j5 | 646 | ASN | C-O | -10.00 | 1.11 | 1.24 |
| 4 | M8 | 32 | SER | CA-C | -10.00 | 1.40 | 1.52 |
| 10 | j5 | 900 | LEU | C-O | -9.99 | 1.12 | 1.24 |
| 10 | k5 | 646 | ASN | C-O | -9.98 | 1.11 | 1.24 |
| 10 | j5 | 513 | GLY | C-O | -9.96 | 1.11 | 1.23 |
| 10 | k5 | 436 | TRP | C-O | -9.96 | 1.12 | 1.24 |
| 4 | M3 | 32 | SER | CA-C | -9.96 | 1.40 | 1.52 |
| 4 | M1 | 32 | SER | CA-C | -9.96 | 1.40 | 1.52 |
| 4 | MA | 32 | SER | CA-C | -9.95 | 1.40 | 1.52 |
| 10 | j5 | 894 | TYR | CA-C | -9.94 | 1.41 | 1.52 |
| 8 | u7 | 39 | ILE | C-O | -9.94 | 1.11 | 1.24 |
| 10 | k5 | 668 | ASN | C-O | -9.93 | 1.12 | 1.24 |
| 10 | j5 | 436 | TRP | C-O | -9.93 | 1.12 | 1.24 |
| 10 | k5 | 900 | LEU | C-O | -9.92 | 1.12 | 1.24 |
| 10 | k5 | 894 | TYR | CA-C | -9.90 | 1.41 | 1.52 |
| 10 | j5 | 668 | ASN | C-O | -9.90 | 1.12 | 1.24 |
| 9 | w7 | 41 | GLN | C-O | -9.89 | 1.12 | 1.24 |
| 10 | j5 | 796 | ARG | C-O | -9.89 | 1.11 | 1.24 |
| 10 | k5 | 796 | ARG | C-O | -9.89 | 1.11 | 1.24 |
| 10 | j5 | 451 | LYS | C-O | -9.88 | 1.11 | 1.23 |
| 10 | k5 | 451 | LYS | C-O | -9.88 | 1.11 | 1.23 |
| 10 | k5 | 513 | GLY | C-O | -9.88 | 1.11 | 1.23 |
| 10 | j5 | 870 | GLU | C-O | -9.86 | 1.12 | 1.24 |
| 10 | j5 | 665 | LEU | CA-C | -9.86 | 1.39 | 1.52 |
| 10 | k5 | 665 | LEU | CA-C | -9.86 | 1.39 | 1.52 |
| 4 | MA | 54 | ALA | C-O | -9.86 | 1.12 | 1.24 |
| 10 | k5 | 815 | TYR | CA-C | -9.86 | 1.40 | 1.52 |
| 10 | j5 | 597 | GLU | C-O | -9.85 | 1.11 | 1.24 |
| 10 | k5 | 597 | GLU | C-O | -9.85 | 1.11 | 1.24 |
| 10 | k5 | 893 | ASN | CA-C | -9.85 | 1.40 | 1.52 |
| 9 | z7 | 41 | GLN | C-O | -9.85 | 1.12 | 1.24 |
| 9 | z5 | 30 | LYS | C-O | -9.85 | 1.12 | 1.23 |
| 10 | j5 | 815 | TYR | CA-C | -9.85 | 1.40 | 1.52 |
| 4 | M9 | 54 | ALA | C-O | -9.84 | 1.12 | 1.24 |
| 10 | k5 | 870 | GLU | C-O | -9.82 | 1.12 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4 | M3 | 54 | ALA | C-O | -9.82 | 1.12 | 1.24 |
| 9 | i5 | 30 | LYS | C-O | -9.82 | 1.12 | 1.23 |
| 4 | M1 | 54 | ALA | C-O | -9.82 | 1.12 | 1.24 |
| 10 | j5 | 535 | PRO | C-O | -9.81 | 1.12 | 1.23 |
| 10 | k5 | 535 | PRO | C-O | -9.81 | 1.12 | 1.23 |
| 10 | k5 | 811 | PHE | C-O | -9.81 | 1.10 | 1.24 |
| 10 | k5 | 775 | VAL | CA-CB | -9.81 | 1.43 | 1.54 |
| 10 | j5 | 775 | VAL | CA-CB | -9.80 | 1.43 | 1.54 |
| 10 | j5 | 889 | LEU | C-O | -9.80 | 1.12 | 1.24 |
| 10 | k5 | 687 | PRO | C-O | -9.80 | 1.12 | 1.24 |
| 10 | k5 | 889 | LEU | C-O | -9.80 | 1.12 | 1.24 |
| 4 | M4 | 54 | ALA | C-O | -9.80 | 1.12 | 1.24 |
| 10 | j5 | 835 | HIS | C-O | -9.79 | 1.10 | 1.23 |
| 10 | k5 | 643 | VAL | C-O | -9.79 | 1.12 | 1.24 |
| 4 | MA | 48 | PRO | C-O | -9.78 | 1.12 | 1.23 |
| 4 | M9 | 48 | PRO | C-O | -9.78 | 1.12 | 1.23 |
| 10 | j5 | 811 | PHE | C-O | -9.78 | 1.10 | 1.24 |
| 10 | j5 | 893 | ASN | CA-C | -9.78 | 1.40 | 1.52 |
| 10 | k5 | 832 | ALA | C-O | -9.77 | 1.11 | 1.24 |
| 4 | M4 | 48 | PRO | C-O | -9.77 | 1.12 | 1.23 |
| 10 | j5 | 643 | VAL | C-O | -9.77 | 1.12 | 1.24 |
| 10 | j5 | 832 | ALA | C-O | -9.77 | 1.11 | 1.24 |
| 4 | M8 | 54 | ALA | C-O | -9.77 | 1.12 | 1.24 |
| 10 | j5 | 507 | ARG | C-O | -9.77 | 1.11 | 1.23 |
| 10 | k5 | 507 | ARG | C-O | -9.77 | 1.11 | 1.23 |
| 10 | k5 | 835 | HIS | C-O | -9.77 | 1.10 | 1.23 |
| 9 | w7 | 40 | GLU | C-O | -9.77 | 1.11 | 1.24 |
| 8 | C5 | 5 | THR | CA-C | -9.76 | 1.40 | 1.52 |
| 10 | k5 | 692 | LEU | C-O | -9.76 | 1.11 | 1.24 |
| 10 | j5 | 863 | ILE | C-O | -9.76 | 1.12 | 1.24 |
| 10 | k5 | 863 | ILE | C-O | -9.76 | 1.12 | 1.24 |
| 10 | j5 | 687 | PRO | C-O | -9.76 | 1.12 | 1.24 |
| 10 | j5 | 648 | TYR | C-O | -9.74 | 1.12 | 1.24 |
| 10 | k5 | 648 | TYR | C-O | -9.74 | 1.12 | 1.24 |
| 10 | k5 | 648 | TYR | CA-C | -9.74 | 1.40 | 1.52 |
| 10 | j5 | 497 | ARG | C-O | -9.73 | 1.12 | 1.23 |
| 10 | j5 | 788 | PHE | CA-C | -9.73 | 1.41 | 1.53 |
| 10 | j5 | 692 | LEU | C-O | -9.73 | 1.11 | 1.24 |
| 10 | j5 | 648 | TYR | CA-C | -9.73 | 1.40 | 1.52 |
| 10 | j5 | 861 | ALA | C-O | -9.73 | 1.11 | 1.24 |
| 4 | M3 | 48 | PRO | C-O | -9.73 | 1.12 | 1.23 |
| 9 | z7 | 40 | GLU | C-O | -9.73 | 1.11 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4 | M1 | 48 | PRO | C-O | -9.73 | 1.12 | 1.23 |
| 10 | j5 | 936 | LYS | C-O | -9.72 | 1.12 | 1.24 |
| 4 | M8 | 48 | PRO | C-O | -9.72 | 1.12 | 1.23 |
| 10 | j5 | 475 | GLY | C-O | -9.72 | 1.11 | 1.24 |
| 10 | j5 | 608 | GLY | C-O | -9.72 | 1.11 | 1.23 |
| 10 | k5 | 475 | GLY | C-O | -9.72 | 1.11 | 1.24 |
| 10 | k5 | 608 | GLY | C-O | -9.72 | 1.11 | 1.23 |
| 8 | I5 | 5 | THR | CA-C | -9.71 | 1.40 | 1.52 |
| 10 | j5 | 754 | LYS | C-O | -9.71 | 1.11 | 1.23 |
| 10 | k5 | 936 | LYS | C-O | -9.71 | 1.12 | 1.24 |
| 10 | k5 | 754 | LYS | C-O | -9.70 | 1.11 | 1.23 |
| 4 | M4 | 13 | LYS | N-CA | -9.69 | 1.34 | 1.46 |
| 10 | k5 | 861 | ALA | C-O | -9.69 | 1.11 | 1.24 |
| 4 | M3 | 13 | LYS | N-CA | -9.68 | 1.34 | 1.46 |
| 4 | M1 | 13 | LYS | N-CA | -9.68 | 1.34 | 1.46 |
| 10 | j5 | 626 | ALA | CA-C | -9.68 | 1.40 | 1.52 |
| 10 | j5 | 814 | LEU | C-O | -9.68 | 1.12 | 1.24 |
| 10 | k5 | 626 | ALA | CA-C | -9.68 | 1.40 | 1.52 |
| 4 | MA | 13 | LYS | N-CA | -9.67 | 1.34 | 1.46 |
| 10 | k5 | 814 | LEU | C-O | -9.67 | 1.12 | 1.24 |
| 4 | M8 | 13 | LYS | N-CA | -9.66 | 1.34 | 1.46 |
| 10 | k5 | 788 | PHE | CA-C | -9.65 | 1.41 | 1.53 |
| 10 | j5 | 411 | TYR | CA-C | -9.65 | 1.40 | 1.52 |
| 10 | j5 | 637 | ARG | CA-C | -9.64 | 1.43 | 1.52 |
| 10 | k5 | 637 | ARG | CA-C | -9.64 | 1.43 | 1.52 |
| 10 | k5 | 767 | LEU | CA-C | -9.64 | 1.40 | 1.52 |
| 10 | k5 | 497 | ARG | C-O | -9.64 | 1.13 | 1.23 |
| 8 | E5 | 116 | TYR | N-CA | -9.63 | 1.34 | 1.46 |
| 10 | j5 | 767 | LEU | CA-C | -9.63 | 1.40 | 1.52 |
| 10 | j5 | 517 | SER | C-O | -9.63 | 1.11 | 1.24 |
| 10 | k5 | 517 | SER | C-O | -9.63 | 1.11 | 1.24 |
| 4 | M8 | 46 | VAL | C-O | -9.63 | 1.13 | 1.24 |
| 10 | j5 | 690 | LEU | CA-C | -9.62 | 1.39 | 1.52 |
| 10 | k5 | 348 | TYR | C-O | -9.61 | 1.11 | 1.24 |
| 10 | j5 | 865 | ALA | C-O | -9.61 | 1.12 | 1.24 |
| 10 | j5 | 855 | GLY | C-O | -9.61 | 1.12 | 1.23 |
| 10 | k5 | 865 | ALA | C-O | -9.61 | 1.12 | 1.24 |
| 10 | k5 | 855 | GLY | C-O | -9.61 | 1.12 | 1.23 |
| 4 | M9 | 13 | LYS | N-CA | -9.61 | 1.34 | 1.46 |
| 10 | j5 | 613 | PHE | C-O | -9.60 | 1.12 | 1.24 |
| 10 | j5 | 1124 | TYR | C-O | -9.60 | 1.12 | 1.24 |
| 10 | k5 | 411 | TYR | CA-C | -9.60 | 1.40 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | k5 | 1124 | TYR | C-O | -9.60 | 1.12 | 1.24 |
| 5 | Z8 | 13 | SER | CA-C | -9.59 | 1.48 | 1.53 |
| 10 | k5 | 634 | LEU | C-O | -9.59 | 1.11 | 1.24 |
| 10 | j5 | 658 | TYR | CA-C | -9.58 | 1.40 | 1.52 |
| 10 | j5 | 720 | ASP | C-O | -9.58 | 1.12 | 1.24 |
| 10 | k5 | 613 | PHE | C-O | -9.58 | 1.12 | 1.24 |
| 10 | k5 | 658 | TYR | CA-C | -9.58 | 1.40 | 1.52 |
| 4 | MA | 46 | VAL | C-O | -9.57 | 1.13 | 1.24 |
| 10 | j5 | 816 | ARG | CA-C | -9.57 | 1.40 | 1.52 |
| 4 | M9 | 46 | VAL | C-O | -9.57 | 1.13 | 1.24 |
| 10 | k5 | 482 | GLN | CA-C | -9.57 | 1.41 | 1.52 |
| 10 | k5 | 452 | VAL | C-O | -9.56 | 1.12 | 1.24 |
| 10 | j5 | 835 | HIS | CA-C | -9.56 | 1.39 | 1.52 |
| 10 | k5 | 835 | HIS | CA-C | -9.56 | 1.39 | 1.52 |
| 10 | j5 | 482 | GLN | CA-C | -9.56 | 1.41 | 1.52 |
| 10 | k5 | 901 | TYR | CA-C | -9.56 | 1.39 | 1.52 |
| 10 | j5 | 634 | LEU | C-O | -9.55 | 1.11 | 1.24 |
| 10 | j5 | 658 | TYR | C-O | -9.56 | 1.12 | 1.24 |
| 10 | j5 | 795 | LEU | C-O | -9.56 | 1.12 | 1.24 |
| 10 | k5 | 795 | LEU | C-O | -9.56 | 1.12 | 1.24 |
| 4 | M4 | 46 | VAL | C-O | -9.55 | 1.13 | 1.24 |
| 8 | K5 | 116 | TYR | N-CA | -9.55 | 1.34 | 1.46 |
| 10 | k5 | 690 | LEU | CA-C | -9.55 | 1.39 | 1.52 |
| 5 | N3 | 13 | SER | CA-C | -9.55 | 1.48 | 1.53 |
| 5 | N1 | 13 | SER | CA-C | -9.55 | 1.48 | 1.53 |
| 10 | j5 | 884 | TRP | C-O | -9.54 | 1.12 | 1.24 |
| 10 | j5 | 348 | TYR | C-O | -9.54 | 1.11 | 1.24 |
| 5 | Z4 | 13 | SER | CA-C | -9.54 | 1.48 | 1.53 |
| 10 | k5 | 747 | LYS | C-O | -9.54 | 1.12 | 1.24 |
| 10 | k5 | 658 | TYR | C-O | -9.53 | 1.12 | 1.24 |
| 4 | M3 | 46 | VAL | C-O | -9.53 | 1.13 | 1.24 |
| 4 | M1 | 46 | VAL | C-O | -9.53 | 1.13 | 1.24 |
| 10 | j5 | 452 | VAL | C-O | -9.52 | 1.12 | 1.24 |
| 10 | j5 | 901 | TYR | CA-C | -9.52 | 1.39 | 1.52 |
| 10 | k5 | 850 | TYR | C-O | -9.52 | 1.11 | 1.24 |
| 10 | k5 | 1131 | ASN | C-O | -9.52 | 1.11 | 1.24 |
| 10 | j5 | 772 | TYR | C-O | -9.52 | 1.11 | 1.24 |
| 10 | k5 | 772 | TYR | C-O | -9.52 | 1.11 | 1.24 |
| 9 | x7 | 20 | GLY | C-O | -9.52 | 1.12 | 1.23 |
| 10 | k5 | 720 | ASP | C-O | -9.51 | 1.12 | 1.24 |
| 10 | j5 | 688 | ALA | C-O | -9.51 | 1.12 | 1.24 |
| 10 | k5 | 688 | ALA | C-O | -9.51 | 1.12 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | k5 | 381 | ILE | C-O | -9.50 | 1.13 | 1.23 |
| 10 | j5 | 747 | LYS | C-O | -9.50 | 1.13 | 1.24 |
| 9 | y7 | 20 | GLY | C-O | -9.50 | 1.12 | 1.23 |
| 10 | j5 | 1131 | ASN | C-O | -9.50 | 1.11 | 1.24 |
| 10 | k5 | 884 | TRP | C-O | -9.49 | 1.12 | 1.24 |
| 10 | k5 | 816 | ARG | CA-C | -9.48 | 1.40 | 1.52 |
| 5 | NA | 13 | SER | CA-C | -9.48 | 1.48 | 1.53 |
| 5 | N9 | 13 | SER | CA-C | -9.48 | 1.48 | 1.53 |
| 10 | k5 | 732 | ARG | C-O | -9.47 | 1.12 | 1.23 |
| 10 | j5 | 850 | TYR | C-O | -9.46 | 1.11 | 1.24 |
| 8 | i7 | 116 | TYR | C-O | -9.46 | 1.12 | 1.24 |
| 10 | k5 | 610 | SER | C-O | -9.45 | 1.11 | 1.23 |
| 10 | k5 | 674 | PHE | C-O | -9.45 | 1.10 | 1.23 |
| 10 | j5 | 686 | THR | C-O | -9.44 | 1.09 | 1.23 |
| 10 | k5 | 686 | THR | C-O | -9.44 | 1.09 | 1.23 |
| 10 | j5 | 614 | ARG | C-O | -9.43 | 1.13 | 1.24 |
| 10 | j5 | 381 | ILE | C-O | -9.43 | 1.14 | 1.23 |
| 9 | i5 | 39 | THR | C-O | -9.42 | 1.12 | 1.24 |
| 10 | j5 | 693 | ARG | CA-C | -9.42 | 1.41 | 1.52 |
| 10 | j5 | 674 | PHE | C-O | -9.42 | 1.10 | 1.23 |
| 8 | c7 | 116 | TYR | C-O | -9.41 | 1.12 | 1.24 |
| 10 | j5 | 880 | THR | CA-C | -9.41 | 1.40 | 1.52 |
| 10 | k5 | 614 | ARG | C-O | -9.40 | 1.13 | 1.24 |
| 10 | j5 | 793 | SER | C-O | -9.40 | 1.13 | 1.24 |
| 10 | k5 | 793 | SER | C-O | -9.40 | 1.13 | 1.24 |
| 10 | k5 | 399 | TYR | CA-C | -9.40 | 1.40 | 1.52 |
| 10 | j5 | 610 | SER | C-O | -9.39 | 1.11 | 1.23 |
| 10 | k5 | 400 | ALA | C-O | -9.39 | 1.12 | 1.24 |
| 10 | k5 | 929 | PRO | C-O | -9.39 | 1.12 | 1.24 |
| 9 | z5 | 39 | THR | C-O | -9.38 | 1.12 | 1.24 |
| 10 | k5 | 872 | TYR | C-O | -9.37 | 1.12 | 1.24 |
| 10 | k5 | 880 | THR | CA-C | -9.36 | 1.40 | 1.52 |
| 10 | j5 | 404 | ALA | C-O | -9.36 | 1.13 | 1.24 |
| 10 | j5 | 542 | GLN | CA-C | -9.36 | 1.40 | 1.52 |
| 10 | j5 | 872 | TYR | C-O | -9.36 | 1.12 | 1.24 |
| 10 | j5 | 400 | ALA | C-O | -9.35 | 1.12 | 1.24 |
| 10 | j5 | 399 | TYR | CA-C | -9.35 | 1.40 | 1.52 |
| 10 | k5 | 876 | TYR | CA-C | -9.34 | 1.40 | 1.52 |
| 10 | k5 | 542 | GLN | CA-C | -9.34 | 1.40 | 1.52 |
| 10 | k5 | 693 | ARG | CA-C | -9.33 | 1.41 | 1.52 |
| 10 | j5 | 565 | GLN | C-O | -9.33 | 1.11 | 1.24 |
| 10 | j5 | 817 | LYS | C-O | -9.33 | 1.13 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 10 | j5 | 832 | ALA | CA-C | -9.33 | 1.39 | 1.52 |
| 10 | k5 | 817 | LYS | C-O | -9.33 | 1.13 | 1.24 |
| 10 | k5 | 832 | ALA | CA-C | -9.33 | 1.39 | 1.52 |
| 9 | z5 | 23 | LEU | CA-C | -9.32 | 1.40 | 1.52 |
| 9 | i5 | 23 | LEU | CA-C | -9.32 | 1.40 | 1.52 |
| 10 | j5 | 929 | PRO | C-O | -9.32 | 1.13 | 1.24 |
| 10 | k5 | 404 | ALA | C-O | -9.32 | 1.13 | 1.24 |
| 8 | u7 | 58 | LEU | C-O | -9.31 | 1.13 | 1.24 |
| 10 | j5 | 730 | ASN | C-O | -9.31 | 1.12 | 1.24 |
| 10 | j5 | 677 | ASP | CA-C | -9.30 | 1.40 | 1.52 |
| 10 | k5 | 10 | THR | C-O | -9.30 | 1.14 | 1.24 |
| 10 | k5 | 677 | ASP | CA-C | -9.28 | 1.40 | 1.52 |
| 10 | j5 | 876 | TYR | CA-C | -9.28 | 1.40 | 1.52 |
| 10 | k5 | 730 | ASN | C-O | -9.28 | 1.12 | 1.24 |
| 10 | k5 | 490 | SER | C-O | -9.27 | 1.12 | 1.24 |
| 10 | j5 | 850 | TYR | CA-C | -9.27 | 1.40 | 1.52 |
| 10 | j5 | 462 | TYR | CA-C | -9.26 | 1.40 | 1.52 |
| 10 | j5 | 611 | GLU | C-O | -9.26 | 1.13 | 1.24 |
| 10 | k5 | 611 | GLU | C-O | -9.26 | 1.13 | 1.24 |
| 8 | o7 | 58 | LEU | C-O | -9.26 | 1.13 | 1.24 |
| 10 | k5 | 462 | TYR | CA-C | -9.26 | 1.40 | 1.52 |
| 10 | k5 | 615 | LYS | CA-C | -9.25 | 1.40 | 1.52 |
| 10 | k5 | 850 | TYR | CA-C | -9.25 | 1.40 | 1.52 |
| 10 | k5 | 461 | ASP | C-O | -9.24 | 1.12 | 1.24 |
| 10 | j5 | 10 | THR | C-O | -9.23 | 1.14 | 1.24 |
| 10 | j5 | 490 | SER | C-O | -9.23 | 1.12 | 1.24 |
| 10 | j5 | 732 | ARG | CA-C | -9.23 | 1.41 | 1.52 |
| 10 | j5 | 766 | ALA | C-O | -9.23 | 1.13 | 1.24 |
| 10 | k5 | 766 | ALA | C-O | -9.23 | 1.13 | 1.24 |
| 8 | C5 | 11 | ALA | C-O | -9.23 | 1.12 | 1.24 |
| 10 | j5 | 647 | ARG | C-O | -9.21 | 1.13 | 1.24 |
| 10 | k5 | 647 | ARG | C-O | -9.21 | 1.13 | 1.24 |
| 10 | j5 | 615 | LYS | CA-C | -9.21 | 1.40 | 1.52 |
| 10 | k5 | 565 | GLN | C-O | -9.21 | 1.12 | 1.24 |
| 10 | k5 | 689 | GLY | C-O | -9.20 | 1.12 | 1.23 |
| 10 | j5 | 591 | ILE | CA-C | -9.20 | 1.41 | 1.52 |
| 10 | k5 | 484 | GLY | C-O | -9.19 | 1.12 | 1.23 |
| 4 | M3 | 47 | VAL | CA-CB | -9.19 | 1.47 | 1.54 |
| 4 | M1 | 47 | VAL | CA-CB | -9.19 | 1.47 | 1.54 |
| 10 | k5 | 474 | ALA | C-O | -9.19 | 1.12 | 1.24 |
| 10 | k5 | 726 | GLY | C-O | -9.19 | 1.11 | 1.23 |
| 10 | j5 | 474 | ALA | C-O | -9.18 | 1.12 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | j5 | 461 | ASP | C-O | -9.17 | 1.12 | 1.24 |
| 10 | j5 | 525 | GLY | C-O | -9.17 | 1.13 | 1.23 |
| 10 | j5 | 702 | VAL | C-O | -9.17 | 1.13 | 1.24 |
| 10 | k5 | 702 | VAL | C-O | -9.16 | 1.13 | 1.24 |
| 11 | a9 | 818 | ARG | CA-C | -9.16 | 1.41 | 1.52 |
| 11 | aA | 818 | ARG | CA-C | -9.16 | 1.41 | 1.52 |
| 9 | z5 | 34 | TYR | CA-C | -9.16 | 1.40 | 1.52 |
| 9 | z5 | 45 | GLN | CA-C | -9.16 | 1.41 | 1.52 |
| 10 | k5 | 732 | ARG | CA-C | -9.16 | 1.41 | 1.53 |
| 10 | k5 | 525 | GLY | C-O | -9.15 | 1.13 | 1.23 |
| 4 | M4 | 47 | VAL | CA-CB | -9.15 | 1.47 | 1.54 |
| 8 | I5 | 11 | ALA | C-O | -9.15 | 1.12 | 1.24 |
| 9 | i5 | 34 | TYR | CA-C | -9.15 | 1.40 | 1.52 |
| 10 | j5 | 726 | GLY | C-O | -9.15 | 1.11 | 1.23 |
| 10 | k5 | 496 | GLU | C-O | -9.15 | 1.12 | 1.23 |
| 10 | k5 | 615 | LYS | C-O | -9.14 | 1.13 | 1.24 |
| 8 | C5 | 9 | VAL | C-O | -9.14 | 1.13 | 1.24 |
| 8 | I5 | 9 | VAL | C-O | -9.14 | 1.13 | 1.24 |
| 10 | k5 | 403 | ASP | C-O | -9.14 | 1.13 | 1.24 |
| 4 | MA | 25 | LEU | C-O | -9.13 | 1.13 | 1.24 |
| 4 | M9 | 25 | LEU | C-O | -9.13 | 1.13 | 1.24 |
| 10 | j5 | 403 | ASP | C-O | -9.12 | 1.13 | 1.24 |
| 10 | k5 | 769 | THR | C-O | -9.12 | 1.12 | 1.24 |
| 4 | MA | 58 | TYR | C-O | -9.12 | 1.13 | 1.24 |
| 4 | M9 | 58 | TYR | C-O | -9.12 | 1.13 | 1.24 |
| 10 | j5 | 615 | LYS | C-O | -9.12 | 1.13 | 1.24 |
| 10 | j5 | 769 | THR | C-O | -9.12 | 1.12 | 1.24 |
| 10 | j5 | 484 | GLY | C-O | -9.11 | 1.12 | 1.23 |
| 10 | j5 | 1006 | ASP | C-O | -9.11 | 1.13 | 1.24 |
| 10 | k5 | 591 | ILE | CA-C | -9.12 | 1.41 | 1.52 |
| 10 | k5 | 1006 | ASP | C-O | -9.11 | 1.13 | 1.24 |
| 4 | MA | 47 | VAL | CA-CB | -9.11 | 1.47 | 1.54 |
| 4 | M9 | 47 | VAL | CA-CB | -9.11 | 1.47 | 1.54 |
| 9 | z7 | 39 | THR | C-O | -9.11 | 1.11 | 1.24 |
| 4 | M8 | 47 | VAL | CA-CB | -9.11 | 1.47 | 1.54 |
| 10 | j5 | 496 | GLU | C-O | -9.11 | 1.12 | 1.23 |
| 10 | k5 | 575 | ILE | CA-CB | -9.11 | 1.43 | 1.54 |
| 10 | k5 | 935 | LEU | C-O | -9.11 | 1.12 | 1.24 |
| 9 | i5 | 45 | GLN | CA-C | -9.10 | 1.41 | 1.52 |
| 10 | k5 | 489 | ASN | C-O | -9.09 | 1.13 | 1.24 |
| 4 | M3 | 58 | TYR | C-O | -9.09 | 1.13 | 1.24 |
| 4 | M4 | 25 | LEU | C-O | -9.09 | 1.13 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 10 | j5 | 652 | ALA | C-O | -9.09 | 1.12 | 1.24 |
| 10 | j5 | 689 | GLY | C-O | -9.09 | 1.12 | 1.23 |
| 4 | M8 | 25 | LEU | C-O | -9.09 | 1.13 | 1.24 |
| 4 | M1 | 58 | TYR | C-O | -9.09 | 1.13 | 1.24 |
| 10 | j5 | 895 | PRO | C-O | -9.08 | 1.12 | 1.24 |
| 9 | w7 | 39 | THR | C-O | -9.08 | 1.11 | 1.24 |
| 4 | M4 | 58 | TYR | C-O | -9.07 | 1.13 | 1.24 |
| 10 | j5 | 575 | ILE | CA-CB | -9.07 | 1.43 | 1.54 |
| 10 | j5 | 22 | THR | C-O | -9.06 | 1.13 | 1.24 |
| 10 | j5 | 432 | PRO | C-O | -9.05 | 1.13 | 1.23 |
| 10 | j5 | 489 | ASN | C-O | -9.05 | 1.13 | 1.24 |
| 10 | j5 | 935 | LEU | C-O | -9.05 | 1.12 | 1.24 |
| 10 | k5 | 791 | LEU | C-O | -9.05 | 1.13 | 1.24 |
| 10 | k5 | 767 | LEU | C-O | -9.05 | 1.13 | 1.24 |
| 10 | j5 | 464 | GLN | CA-C | -9.04 | 1.42 | 1.52 |
| 10 | k5 | 464 | GLN | CA-C | -9.04 | 1.42 | 1.52 |
| 10 | j5 | 411 | TYR | C-O | -9.04 | 1.13 | 1.24 |
| 10 | j5 | 767 | LEU | C-O | -9.04 | 1.13 | 1.24 |
| 8 | o7 | 39 | ILE | C-O | -9.04 | 1.11 | 1.24 |
| 10 | k5 | 569 | THR | CA-C | -9.04 | 1.40 | 1.52 |
| 10 | k5 | 593 | LEU | C-O | -9.04 | 1.13 | 1.24 |
| 10 | k5 | 895 | PRO | C-O | -9.04 | 1.12 | 1.24 |
| 4 | M8 | 58 | TYR | C-O | -9.03 | 1.13 | 1.24 |
| 10 | j5 | 791 | LEU | C-O | -9.02 | 1.13 | 1.24 |
| 10 | j5 | 745 | ALA | C-O | -9.02 | 1.12 | 1.24 |
| 10 | j5 | 725 | LEU | C-O | -9.01 | 1.11 | 1.24 |
| 10 | j5 | 593 | LEU | C-O | -9.01 | 1.13 | 1.24 |
| 10 | k5 | 725 | LEU | C-O | -9.01 | 1.11 | 1.24 |
| 8 | i7 | 129 | GLY | C-O | -9.00 | 1.12 | 1.23 |
| 10 | k5 | 652 | ALA | C-O | -9.00 | 1.12 | 1.24 |
| 10 | j5 | 569 | THR | CA-C | -8.99 | 1.40 | 1.52 |
| 10 | k5 | 509 | LEU | C-O | -8.99 | 1.12 | 1.24 |
| 8 | c7 | 129 | GLY | C-O | -8.99 | 1.13 | 1.23 |
| 4 | M3 | 25 | LEU | C-O | -8.99 | 1.13 | 1.24 |
| 10 | k5 | 465 | PRO | C-O | -8.99 | 1.12 | 1.23 |
| 10 | k5 | 468 | ASN | C-O | -8.99 | 1.13 | 1.24 |
| 10 | j5 | 449 | ARG | C-O | -8.99 | 1.12 | 1.24 |
| 10 | j5 | 594 | GLU | C-O | -8.99 | 1.12 | 1.24 |
| 10 | k5 | 449 | ARG | C-O | -8.99 | 1.12 | 1.24 |
| 4 | M1 | 25 | LEU | C-O | -8.99 | 1.13 | 1.24 |
| 10 | k5 | 432 | PRO | C-O | -8.98 | 1.13 | 1.23 |
| 10 | j5 | 25 | ILE | C-O | -8.97 | 1.13 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | k5 | 25 | ILE | C-O | -8.97 | 1.13 | 1.24 |
| 10 | k5 | 594 | GLU | C-O | -8.97 | 1.12 | 1.24 |
| 10 | k5 | 411 | TYR | C-O | -8.97 | 1.13 | 1.24 |
| 10 | j5 | 468 | ASN | C-O | -8.96 | 1.13 | 1.24 |
| 8 | c7 | 32 | SER | C-N | 8.96 | 1.46 | 1.33 |
| 10 | j5 | 465 | PRO | C-O | -8.95 | 1.12 | 1.23 |
| 10 | k5 | 745 | ALA | C-O | -8.95 | 1.12 | 1.24 |
| 8 | K5 | 116 | TYR | C-O | -8.94 | 1.13 | 1.24 |
| 8 | i7 | 32 | SER | C-N | 8.93 | 1.46 | 1.33 |
| 10 | j5 | 732 | ARG | C-O | -8.93 | 1.12 | 1.23 |
| 10 | k5 | 755 | GLN | CA-C | -8.93 | 1.40 | 1.52 |
| 9 | i5 | 23 | LEU | C-O | -8.93 | 1.12 | 1.24 |
| 11 | a9 | 603 | THR | CA-C | 8.93 | 1.64 | 1.52 |
| 11 | aA | 603 | THR | CA-C | 8.93 | 1.64 | 1.52 |
| 10 | j5 | 932 | GLN | C-O | -8.92 | 1.12 | 1.24 |
| 8 | E5 | 116 | TYR | C-O | -8.91 | 1.13 | 1.24 |
| 10 | j5 | 580 | LEU | C-O | -8.91 | 1.12 | 1.23 |
| 4 | MA | 38 | PRO | C-O | -8.91 | 1.13 | 1.24 |
| 8 | A5 | 49 | ARG | C-O | -8.91 | 1.13 | 1.24 |
| 4 | M9 | 38 | PRO | C-O | -8.91 | 1.13 | 1.24 |
| 4 | M3 | 38 | PRO | C-O | -8.90 | 1.13 | 1.24 |
| 10 | k5 | 580 | LEU | C-O | -8.90 | 1.12 | 1.23 |
| 8 | E7 | 32 | SER | C-N | 8.89 | 1.46 | 1.33 |
| 8 | K7 | 32 | SER | C-N | 8.89 | 1.46 | 1.33 |
| 10 | j5 | 509 | LEU | C-O | -8.89 | 1.12 | 1.24 |
| 4 | M3 | 66 | VAL | CA-C | -8.88 | 1.42 | 1.52 |
| 4 | M1 | 66 | VAL | CA-C | -8.88 | 1.42 | 1.52 |
| 3 | FA | 148 | VAL | C-O | -8.88 | 1.15 | 1.24 |
| 10 | j5 | 348 | TYR | CA-C | -8.88 | 1.43 | 1.52 |
| 10 | k5 | 380 | SER | C-O | -8.88 | 1.12 | 1.24 |
| 8 | u7 | 32 | SER | C-N | 8.88 | 1.46 | 1.33 |
| 4 | M9 | 66 | VAL | CA-C | -8.88 | 1.42 | 1.52 |
| 4 | M1 | 38 | PRO | C-O | -8.87 | 1.13 | 1.24 |
| 10 | k5 | 1129 | ARG | C-O | -8.87 | 1.13 | 1.24 |
| 8 | Q5 | 32 | SER | C-N | 8.86 | 1.46 | 1.33 |
| 10 | k5 | 348 | TYR | CA-C | -8.86 | 1.43 | 1.52 |
| 10 | j5 | 675 | GLY | C-O | -8.86 | 1.12 | 1.24 |
| 10 | j5 | 903 | ARG | C-O | -8.86 | 1.13 | 1.24 |
| 10 | k5 | 903 | ARG | C-O | -8.86 | 1.13 | 1.24 |
| 4 | MA | 66 | VAL | CA-C | -8.85 | 1.42 | 1.52 |
| 4 | M8 | 38 | PRO | C-O | -8.84 | 1.14 | 1.24 |
| 8 | W5 | 32 | SER | C-N | 8.84 | 1.46 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4 | M4 | 38 | PRO | C-O | -8.84 | 1.14 | 1.24 |
| 10 | j5 | 683 | ARG | CZ-NH2 | -8.83 | 1.22 | 1.33 |
| 10 | j5 | 755 | GLN | CA-C | -8.83 | 1.40 | 1.52 |
| 10 | k5 | 683 | ARG | CZ-NH2 | -8.83 | 1.22 | 1.33 |
| 10 | k5 | 808 | LEU | CA-C | -8.83 | 1.40 | 1.52 |
| 10 | j5 | 380 | SER | C-O | -8.83 | 1.12 | 1.24 |
| 8 | G5 | 49 | ARG | C-O | -8.82 | 1.14 | 1.24 |
| 4 | M8 | 66 | VAL | CA-C | -8.82 | 1.42 | 1.52 |
| 10 | j5 | 808 | LEU | CA-C | -8.82 | 1.40 | 1.52 |
| 4 | M4 | 66 | VAL | CA-C | -8.81 | 1.42 | 1.52 |
| 10 | k5 | 675 | GLY | C-O | -8.81 | 1.12 | 1.24 |
| 10 | k5 | 932 | GLN | C-O | -8.81 | 1.12 | 1.24 |
| 10 | j5 | 588 | VAL | C-O | -8.81 | 1.13 | 1.24 |
| 10 | k5 | 588 | VAL | C-O | -8.81 | 1.13 | 1.24 |
| 10 | j5 | 574 | GLN | C-O | -8.80 | 1.12 | 1.23 |
| 9 | z5 | 23 | LEU | C-O | -8.80 | 1.12 | 1.24 |
| 10 | j5 | 706 | PRO | C-O | -8.80 | 1.12 | 1.24 |
| 10 | j5 | 1129 | ARG | C-O | -8.80 | 1.13 | 1.24 |
| 10 | k5 | 706 | PRO | C-O | -8.80 | 1.12 | 1.24 |
| 10 | k5 | 22 | THR | C-O | -8.79 | 1.13 | 1.24 |
| 10 | k5 | 621 | PHE | C-O | -8.79 | 1.12 | 1.23 |
| 10 | k5 | 574 | GLN | C-O | -8.79 | 1.12 | 1.23 |
| 8 | E5 | 32 | SER | C-N | 8.78 | 1.46 | 1.33 |
| 10 | j5 | 716 | ALA | CA-C | -8.78 | 1.41 | 1.52 |
| 8 | W7 | 32 | SER | C-N | 8.78 | 1.46 | 1.33 |
| 10 | j5 | 756 | SER | C-O | -8.78 | 1.12 | 1.24 |
| 10 | k5 | 716 | ALA | CA-C | -8.78 | 1.41 | 1.52 |
| 10 | k5 | 756 | SER | C-O | -8.78 | 1.12 | 1.24 |
| 8 | Q7 | 32 | SER | C-N | 8.78 | 1.46 | 1.33 |
| 1 | h7 | 40 | ALA | C-O | -8.78 | 1.13 | 1.24 |
| 10 | j5 | 468 | ASN | CA-C | -8.77 | 1.42 | 1.52 |
| 10 | j5 | 710 | THR | C-O | -8.77 | 1.13 | 1.24 |
| 10 | k5 | 468 | ASN | CA-C | -8.77 | 1.42 | 1.52 |
| 10 | k5 | 712 | ARG | CA-C | -8.77 | 1.41 | 1.52 |
| 8 | o7 | 32 | SER | C-N | 8.76 | 1.46 | 1.33 |
| 8 | o7 | 45 | GLU | CA-C | -8.76 | 1.41 | 1.52 |
| 10 | j5 | 438 | ALA | CA-C | -8.75 | 1.41 | 1.52 |
| 1 | b7 | 40 | ALA | C-O | -8.75 | 1.13 | 1.24 |
| 8 | K5 | 32 | SER | C-N | 8.74 | 1.46 | 1.33 |
| 9 | w7 | 33 | PRO | C-O | -8.74 | 1.13 | 1.23 |
| 10 | j5 | 572 | TYR | CA-C | -8.74 | 1.40 | 1.52 |
| 10 | k5 | 710 | THR | C-O | -8.74 | 1.13 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | j5 | 664 | MET | C-O | -8.74 | 1.13 | 1.24 |
| 10 | k5 | 664 | MET | C-O | -8.74 | 1.13 | 1.24 |
| 1 | b7 | 53 | LYS | C-O | -8.73 | 1.12 | 1.24 |
| 8 | u7 | 45 | GLU | CA-C | -8.73 | 1.41 | 1.52 |
| 9 | z7 | 28 | PHE | C-O | -8.73 | 1.12 | 1.23 |
| 10 | j5 | 621 | PHE | C-O | -8.72 | 1.12 | 1.23 |
| 10 | j5 | 807 | ARG | CA-C | -8.72 | 1.41 | 1.52 |
| 10 | k5 | 807 | ARG | CA-C | -8.72 | 1.41 | 1.52 |
| 10 | j5 | 712 | ARG | CA-C | -8.72 | 1.41 | 1.52 |
| 9 | z7 | 33 | PRO | C-O | -8.71 | 1.13 | 1.23 |
| 4 | M8 | 65 | ARG | C-O | -8.71 | 1.14 | 1.24 |
| 10 | k5 | 768 | VAL | CA-C | -8.71 | 1.41 | 1.52 |
| 10 | k5 | 572 | TYR | CA-C | -8.71 | 1.40 | 1.52 |
| 10 | k5 | 1035 | PHE | C-O | -8.71 | 1.14 | 1.24 |
| 10 | j5 | 806 | VAL | C-O | -8.70 | 1.13 | 1.24 |
| 10 | j5 | 459 | PHE | C-O | -8.70 | 1.14 | 1.24 |
| 10 | k5 | 459 | PHE | C-O | -8.70 | 1.14 | 1.24 |
| 10 | j5 | 520 | ARG | C-O | -8.70 | 1.12 | 1.24 |
| 10 | j5 | 768 | VAL | CA-C | -8.70 | 1.41 | 1.52 |
| 10 | j5 | 805 | PHE | C-O | -8.70 | 1.13 | 1.24 |
| 10 | k5 | 520 | ARG | C-O | -8.70 | 1.12 | 1.24 |
| 10 | k5 | 789 | SER | C-O | -8.69 | 1.13 | 1.24 |
| 1 | h7 | 53 | LYS | C-O | -8.69 | 1.12 | 1.24 |
| 4 | MA | 65 | ARG | C-O | -8.69 | 1.14 | 1.24 |
| 10 | j5 | 272 | PHE | C-O | -8.69 | 1.14 | 1.24 |
| 10 | k5 | 438 | ALA | CA-C | -8.69 | 1.41 | 1.52 |
| 4 | M9 | 65 | ARG | C-O | -8.69 | 1.14 | 1.24 |
| 10 | k5 | 565 | GLN | CA-C | -8.68 | 1.40 | 1.52 |
| 9 | w7 | 28 | PHE | C-O | -8.68 | 1.12 | 1.23 |
| 10 | j5 | 856 | ARG | C-O | -8.68 | 1.13 | 1.24 |
| 10 | k5 | 856 | ARG | C-O | -8.68 | 1.13 | 1.24 |
| 10 | j5 | 1035 | PHE | C-O | -8.67 | 1.14 | 1.24 |
| 9 | i5 | 3 | ARG | C-O | -8.66 | 1.12 | 1.23 |
| 10 | j5 | 249 | SER | CA-C | -8.66 | 1.49 | 1.53 |
| 10 | k5 | 805 | PHE | C-O | -8.66 | 1.13 | 1.24 |
| 10 | j5 | 565 | GLN | CA-C | -8.65 | 1.40 | 1.52 |
| 10 | k5 | 806 | VAL | C-O | -8.65 | 1.13 | 1.24 |
| 10 | k5 | 676 | GLU | N-CA | -8.65 | 1.36 | 1.46 |
| 4 | M3 | 53 | LEU | C-O | -8.64 | 1.13 | 1.24 |
| 10 | j5 | 676 | GLU | N-CA | -8.64 | 1.36 | 1.46 |
| 10 | j5 | 344 | ARG | C-O | -8.64 | 1.13 | 1.24 |
| 4 | M1 | 53 | LEU | C-O | -8.64 | 1.13 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 11 | a9 | 632 | ILE | CA-C | -8.64 | 1.40 | 1.52 |
| 11 | aA | 632 | ILE | CA-C | -8.64 | 1.40 | 1.52 |
| 10 | k5 | 573 | GLN | C-O | -8.64 | 1.12 | 1.24 |
| 10 | k5 | 619 | GLU | N-CA | -8.64 | 1.37 | 1.46 |
| 3 | LA | 91 | ARG | C-O | -8.63 | 1.14 | 1.24 |
| 3 | L9 | 91 | ARG | C-O | -8.63 | 1.14 | 1.24 |
| 9 | z5 | 3 | ARG | C-O | -8.63 | 1.12 | 1.23 |
| 10 | k5 | 272 | PHE | C-O | -8.63 | 1.14 | 1.24 |
| 10 | k5 | 792 | GLU | CA-C | -8.63 | 1.41 | 1.52 |
| 10 | j5 | 447 | ALA | CA-C | -8.62 | 1.42 | 1.52 |
| 10 | j5 | 617 | TYR | C-O | -8.62 | 1.12 | 1.24 |
| 10 | k5 | 617 | TYR | C-O | -8.62 | 1.12 | 1.24 |
| 10 | k5 | 699 | SER | C-O | -8.61 | 1.13 | 1.24 |
| 10 | j5 | 619 | GLU | N-CA | -8.61 | 1.37 | 1.46 |
| 10 | j5 | 789 | SER | C-O | -8.61 | 1.13 | 1.24 |
| 9 | w7 | 43 | ARG | C-O | -8.60 | 1.14 | 1.24 |
| 10 | k5 | 447 | ALA | CA-C | -8.60 | 1.42 | 1.52 |
| 4 | M4 | 65 | ARG | C-O | -8.60 | 1.14 | 1.24 |
| 8 | K5 | 95 | GLY | C-O | -8.60 | 1.13 | 1.23 |
| 8 | E5 | 95 | GLY | C-O | -8.59 | 1.13 | 1.23 |
| 10 | k5 | 344 | ARG | C-O | -8.59 | 1.13 | 1.24 |
| 10 | k5 | 590 | GLU | CA-C | -8.59 | 1.41 | 1.52 |
| 9 | z7 | 43 | ARG | C-O | -8.59 | 1.14 | 1.24 |
| 8 | G5 | 55 | GLY | C-O | -8.58 | 1.13 | 1.23 |
| 8 | I5 | 8 | ILE | C-O | -8.58 | 1.14 | 1.24 |
| 10 | j5 | 699 | SER | C-O | -8.58 | 1.13 | 1.24 |
| 10 | j5 | 792 | GLU | CA-C | -8.58 | 1.41 | 1.52 |
| 10 | j5 | 409 | GLU | CA-C | -8.57 | 1.42 | 1.52 |
| 10 | k5 | 409 | GLU | CA-C | -8.57 | 1.42 | 1.52 |
| 8 | A5 | 55 | GLY | C-O | -8.57 | 1.13 | 1.23 |
| 10 | j5 | 573 | GLN | C-O | -8.57 | 1.12 | 1.24 |
| 10 | j5 | 492 | ILE | CA-C | -8.57 | 1.42 | 1.52 |
| 4 | M8 | 53 | LEU | C-O | -8.57 | 1.14 | 1.24 |
| 10 | k5 | 952 | PHE | C-O | -8.56 | 1.14 | 1.24 |
| 10 | k5 | 249 | SER | CA-C | -8.56 | 1.49 | 1.53 |
| 9 | i5 | 37 | TRP | CA-C | -8.56 | 1.41 | 1.52 |
| 10 | j5 | 590 | GLU | CA-C | -8.56 | 1.41 | 1.52 |
| 10 | j5 | 620 | PRO | CA-C | -8.56 | 1.44 | 1.52 |
| 10 | j5 | 952 | PHE | C-O | -8.55 | 1.14 | 1.24 |
| 8 | A5 | 50 | ILE | C-O | -8.55 | 1.14 | 1.24 |
| 9 | z5 | 37 | TRP | CA-C | -8.55 | 1.41 | 1.52 |
| 10 | j5 | 427 | GLY | C-O | -8.55 | 1.13 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 10 | k5 | 427 | GLY | C-O | -8.55 | 1.13 | 1.23 |
| 4 | MA | 53 | LEU | C-O | -8.55 | 1.14 | 1.24 |
| 4 | M9 | 53 | LEU | C-O | -8.55 | 1.14 | 1.24 |
| 4 | M3 | 65 | ARG | C-O | -8.54 | 1.14 | 1.24 |
| 4 | M4 | 53 | LEU | C-O | -8.54 | 1.14 | 1.24 |
| 4 | M1 | 65 | ARG | C-O | -8.54 | 1.14 | 1.24 |
| 10 | j5 | 499 | ALA | CA-C | -8.54 | 1.42 | 1.52 |
| 8 | C5 | 8 | ILE | C-O | -8.53 | 1.14 | 1.24 |
| 8 | G5 | 50 | ILE | C-O | -8.52 | 1.14 | 1.24 |
| 10 | k5 | 492 | ILE | CA-C | -8.52 | 1.42 | 1.52 |
| 8 | C5 | 24 | ASP | CA-C | -8.51 | 1.44 | 1.53 |
| 10 | j5 | 739 | VAL | C-O | -8.51 | 1.14 | 1.24 |
| 10 | j5 | 765 | ASP | C-O | -8.51 | 1.13 | 1.24 |
| 10 | j5 | 917 | LYS | CA-C | -8.50 | 1.44 | 1.53 |
| 10 | j5 | 864 | GLY | C-O | -8.49 | 1.13 | 1.23 |
| 10 | k5 | 864 | GLY | C-O | -8.49 | 1.13 | 1.23 |
| 8 | I5 | 24 | ASP | CA-C | -8.49 | 1.44 | 1.53 |
| 8 | c7 | 123 | ILE | CA-C | -8.49 | 1.44 | 1.52 |
| 8 | I5 | 4 | LEU | C-O | -8.48 | 1.14 | 1.24 |
| 10 | k5 | 434 | TRP | C-O | -8.48 | 1.13 | 1.24 |
| 4 | M1 | 110 | TYR | CA-C | -8.48 | 1.42 | 1.52 |
| 10 | j5 | 854 | LEU | N-CA | -8.48 | 1.35 | 1.46 |
| 10 | k5 | 499 | ALA | CA-C | -8.48 | 1.42 | 1.52 |
| 10 | k5 | 437 | GLY | C-O | -8.47 | 1.13 | 1.23 |
| 10 | k5 | 917 | LYS | CA-C | -8.47 | 1.44 | 1.53 |
| 10 | k5 | 383 | SER | CA-C | -8.47 | 1.40 | 1.52 |
| 8 | A5 | 52 | LYS | C-O | -8.46 | 1.14 | 1.24 |
| 10 | k5 | 765 | ASP | C-O | -8.46 | 1.13 | 1.24 |
| 11 | a9 | 579 | PHE | CA-C | -8.46 | 1.41 | 1.52 |
| 11 | aA | 579 | PHE | CA-C | -8.46 | 1.41 | 1.52 |
| 4 | MA | 110 | TYR | CA-C | -8.46 | 1.42 | 1.52 |
| 4 | M9 | 110 | TYR | CA-C | -8.46 | 1.42 | 1.52 |
| 10 | k5 | 516 | THR | C-O | -8.45 | 1.12 | 1.24 |
| 10 | j5 | 483 | PHE | CA-C | -8.45 | 1.41 | 1.52 |
| 10 | k5 | 483 | PHE | CA-C | -8.45 | 1.41 | 1.52 |
| 8 | i7 | 123 | ILE | CA-C | -8.45 | 1.44 | 1.52 |
| 10 | j5 | 657 | PHE | CA-C | -8.44 | 1.42 | 1.52 |
| 10 | j5 | 594 | GLU | CA-C | -8.43 | 1.41 | 1.52 |
| 10 | k5 | 594 | GLU | CA-C | -8.43 | 1.41 | 1.52 |
| 10 | k5 | 620 | PRO | CA-C | -8.43 | 1.44 | 1.52 |
| 10 | j5 | 434 | TRP | C-O | -8.43 | 1.13 | 1.24 |
| 10 | j5 | 709 | ILE | C-O | -8.43 | 1.14 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | j5 | 383 | SER | CA-C | -8.42 | 1.40 | 1.52 |
| 10 | k5 | 783 | TYR | C-O | -8.42 | 1.12 | 1.24 |
| 10 | k5 | 854 | LEU | N-CA | -8.42 | 1.35 | 1.46 |
| 10 | j5 | 691 | SER | C-O | -8.42 | 1.12 | 1.24 |
| 10 | k5 | 691 | SER | C-O | -8.42 | 1.12 | 1.24 |
| 8 | C5 | 4 | LEU | C-O | -8.42 | 1.14 | 1.24 |
| 8 | G5 | 54 | ALA | C-O | -8.41 | 1.14 | 1.24 |
| 10 | j5 | 516 | THR | C-O | -8.41 | 1.12 | 1.24 |
| 4 | M8 | 110 | TYR | CA-C | -8.41 | 1.42 | 1.52 |
| 4 | M3 | 110 | TYR | CA-C | -8.40 | 1.42 | 1.52 |
| 10 | j5 | 783 | TYR | C-O | -8.39 | 1.13 | 1.24 |
| 10 | j5 | 437 | GLY | C-O | -8.39 | 1.13 | 1.23 |
| 10 | j5 | 409 | GLU | C-O | -8.39 | 1.14 | 1.24 |
| 8 | A5 | 54 | ALA | C-O | -8.39 | 1.14 | 1.24 |
| 10 | j5 | 769 | THR | CA-C | -8.39 | 1.41 | 1.52 |
| 9 | i5 | 32 | VAL | C-O | -8.38 | 1.13 | 1.24 |
| 10 | j5 | 755 | GLN | C-O | -8.38 | 1.13 | 1.24 |
| 10 | k5 | 409 | GLU | C-O | -8.38 | 1.14 | 1.24 |
| 10 | k5 | 755 | GLN | C-O | -8.38 | 1.13 | 1.24 |
| 5 | Z4 | 30 | PRO | N-CD | -8.37 | 1.36 | 1.47 |
| 10 | k5 | 657 | PHE | CA-C | -8.37 | 1.42 | 1.52 |
| 10 | k5 | 997 | ILE | C-O | -8.37 | 1.14 | 1.24 |
| 8 | G5 | 52 | LYS | C-O | -8.37 | 1.14 | 1.24 |
| 10 | j5 | 433 | SER | C-O | -8.37 | 1.12 | 1.24 |
| 10 | k5 | 433 | SER | C-O | -8.37 | 1.12 | 1.24 |
| 10 | k5 | 709 | ILE | C-O | -8.37 | 1.15 | 1.24 |
| 10 | j5 | 825 | ASN | C-O | -8.36 | 1.13 | 1.24 |
| 8 | c7 | 113 | LYS | C-O | -8.36 | 1.14 | 1.24 |
| 4 | M4 | 110 | TYR | CA-C | -8.35 | 1.42 | 1.52 |
| 10 | k5 | 825 | ASN | C-O | -8.35 | 1.13 | 1.24 |
| 4 | M3 | 68 | ASP | CB-CG | -8.35 | 1.31 | 1.52 |
| 4 | M1 | 68 | ASP | CB-CG | -8.35 | 1.31 | 1.52 |
| 4 | M4 | 68 | ASP | CB-CG | -8.35 | 1.31 | 1.52 |
| 10 | j5 | 888 | THR | C-O | -8.35 | 1.13 | 1.23 |
| 9 | z5 | 32 | VAL | C-O | -8.34 | 1.14 | 1.24 |
| 4 | MA | 68 | ASP | CB-CG | -8.34 | 1.31 | 1.52 |
| 8 | i7 | 113 | LYS | C-O | -8.34 | 1.14 | 1.24 |
| 4 | M9 | 68 | ASP | CB-CG | -8.34 | 1.31 | 1.52 |
| 10 | j5 | 444 | ASN | C-O | -8.33 | 1.12 | 1.23 |
| 10 | k5 | 444 | ASN | C-O | -8.33 | 1.12 | 1.23 |
| 10 | k5 | 672 | GLU | C-O | -8.33 | 1.14 | 1.24 |
| 10 | k5 | 1001 | TYR | CA-C | -8.32 | 1.42 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | k5 | 842 | LYS | C-O | -8.32 | 1.14 | 1.24 |
| 10 | j5 | 1001 | TYR | CA-C | -8.31 | 1.42 | 1.52 |
| 4 | M8 | 68 | ASP | CB-CG | -8.31 | 1.31 | 1.52 |
| 10 | k5 | 669 | GLU | C-O | -8.31 | 1.13 | 1.24 |
| 10 | k5 | 769 | THR | CA-C | -8.31 | 1.41 | 1.52 |
| 10 | k5 | 577 | GLY | C-O | -8.30 | 1.12 | 1.24 |
| 8 | u7 | 50 | ILE | C-O | -8.30 | 1.14 | 1.24 |
| 4 | M8 | 230 | GLN | C-O | -8.30 | 1.17 | 1.23 |
| 10 | k5 | 682 | GLU | C-O | -8.30 | 1.14 | 1.24 |
| 10 | k5 | 888 | THR | C-O | -8.29 | 1.13 | 1.23 |
| 11 | a9 | 48 | LEU | C-O | -8.29 | 1.14 | 1.24 |
| 11 | aA | 48 | LEU | C-O | -8.29 | 1.14 | 1.24 |
| 10 | j5 | 997 | ILE | C-O | -8.29 | 1.14 | 1.24 |
| 10 | k5 | 653 | SER | C-O | -8.29 | 1.12 | 1.24 |
| 10 | j5 | 671 | GLN | C-O | -8.29 | 1.14 | 1.24 |
| 10 | k5 | 671 | GLN | C-O | -8.29 | 1.14 | 1.24 |
| 10 | j5 | 724 | GLU | C-O | -8.28 | 1.12 | 1.24 |
| 10 | j5 | 940 | ALA | C-O | -8.28 | 1.14 | 1.24 |
| 8 | u7 | 54 | ALA | C-O | -8.28 | 1.14 | 1.24 |
| 10 | j5 | 682 | GLU | C-O | -8.27 | 1.14 | 1.24 |
| 10 | j5 | 1117 | PRO | C-O | -8.27 | 1.14 | 1.23 |
| 10 | k5 | 1117 | PRO | C-O | -8.27 | 1.14 | 1.23 |
| 10 | k5 | 724 | GLU | C-O | -8.27 | 1.12 | 1.24 |
| 8 | K5 | 94 | TYR | C-O | -8.26 | 1.14 | 1.24 |
| 10 | j5 | 669 | GLU | C-O | -8.26 | 1.13 | 1.24 |
| 4 | M3 | 41 | ASN | N-CA | -8.26 | 1.36 | 1.46 |
| 10 | j5 | 653 | SER | C-O | -8.26 | 1.12 | 1.24 |
| 4 | M1 | 41 | ASN | N-CA | -8.26 | 1.36 | 1.46 |
| 10 | j5 | 672 | GLU | C-O | -8.26 | 1.14 | 1.24 |
| 10 | j5 | 785 | ARG | CA-C | -8.26 | 1.46 | 1.52 |
| 8 | E5 | 94 | TYR | C-O | -8.26 | 1.14 | 1.24 |
| 10 | j5 | 842 | LYS | C-O | -8.25 | 1.14 | 1.24 |
| 4 | M4 | 41 | ASN | N-CA | -8.25 | 1.36 | 1.46 |
| 4 | M8 | 71 | PRO | CA-C | -8.25 | 1.42 | 1.52 |
| 10 | j5 | 933 | ALA | C-O | -8.25 | 1.13 | 1.24 |
| 10 | k5 | 933 | ALA | C-O | -8.25 | 1.13 | 1.24 |
| 8 | o7 | 50 | ILE | C-O | -8.24 | 1.14 | 1.24 |
| 4 | M1 | 71 | PRO | CA-C | -8.24 | 1.42 | 1.52 |
| 10 | k5 | 605 | ARG | CA-C | -8.24 | 1.42 | 1.52 |
| 4 | M3 | 71 | PRO | CA-C | -8.23 | 1.42 | 1.52 |
| 10 | k5 | 785 | ARG | CA-C | -8.23 | 1.46 | 1.52 |
| 10 | k5 | 842 | LYS | CA-C | -8.22 | 1.42 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4 | M8 | 36 | TYR | C-O | -8.22 | 1.13 | 1.23 |
| 10 | j5 | 549 | LYS | N-CA | 8.22 | 1.56 | 1.46 |
| 10 | j5 | 577 | GLY | C-O | -8.22 | 1.12 | 1.24 |
| 10 | k5 | 476 | ASN | CG-ND2 | -8.22 | 1.16 | 1.33 |
| 9 | i5 | 4 | TYR | C-O | -8.21 | 1.13 | 1.23 |
| 8 | K5 | 107 | ILE | C-O | -8.21 | 1.14 | 1.24 |
| 10 | j5 | 668 | ASN | CA-C | -8.21 | 1.42 | 1.52 |
| 10 | j5 | 478 | PRO | CA-C | -8.21 | 1.43 | 1.52 |
| 4 | M4 | 36 | TYR | C-O | -8.20 | 1.13 | 1.23 |
| 4 | M4 | 71 | PRO | CA-C | -8.20 | 1.42 | 1.52 |
| 10 | j5 | 842 | LYS | CA-C | -8.20 | 1.42 | 1.52 |
| 10 | k5 | 538 | PHE | CA-C | -8.20 | 1.42 | 1.52 |
| 8 | o7 | 54 | ALA | C-O | -8.20 | 1.14 | 1.24 |
| 8 | K5 | 116 | TYR | CA-C | -8.20 | 1.42 | 1.52 |
| 1 | D5 | 12 | TYR | C-O | -8.20 | 1.13 | 1.24 |
| 4 | M4 | 66 | VAL | C-O | -8.20 | 1.14 | 1.24 |
| 10 | k5 | 940 | ALA | C-O | -8.20 | 1.14 | 1.24 |
| 8 | c7 | 118 | SER | C-O | -8.20 | 1.14 | 1.24 |
| 10 | k5 | 549 | LYS | N-CA | 8.19 | 1.56 | 1.46 |
| 8 | E5 | 107 | ILE | C-O | -8.19 | 1.14 | 1.24 |
| 10 | j5 | 351 | PHE | C-O | -8.19 | 1.11 | 1.23 |
| 10 | k5 | 351 | PHE | C-O | -8.19 | 1.11 | 1.23 |
| 10 | k5 | 450 | ARG | CZ-NH2 | -8.19 | 1.22 | 1.33 |
| 10 | k5 | 1130 | VAL | C-O | -8.19 | 1.14 | 1.24 |
| 10 | j5 | 490 | SER | CA-C | -8.18 | 1.41 | 1.52 |
| 4 | MA | 41 | ASN | N-CA | -8.18 | 1.36 | 1.46 |
| 10 | k5 | 490 | SER | CA-C | -8.18 | 1.41 | 1.52 |
| 10 | k5 | 854 | LEU | C-O | -8.18 | 1.13 | 1.24 |
| 4 | M9 | 41 | ASN | N-CA | -8.18 | 1.36 | 1.46 |
| 8 | A5 | 56 | ASP | C-O | -8.18 | 1.14 | 1.24 |
| 8 | E5 | 111 | GLY | C-O | -8.18 | 1.12 | 1.23 |
| 10 | j5 | 476 | ASN | CG-ND2 | -8.18 | 1.16 | 1.33 |
| 4 | M4 | 59 | ILE | CA-C | -8.18 | 1.42 | 1.52 |
| 10 | j5 | 854 | LEU | C-O | -8.18 | 1.13 | 1.24 |
| 4 | MA | 71 | PRO | CA-C | -8.18 | 1.42 | 1.52 |
| 4 | M3 | 26 | SER | C-O | -8.18 | 1.13 | 1.24 |
| 10 | j5 | 454 | GLN | C-O | -8.18 | 1.13 | 1.24 |
| 10 | j5 | 780 | ILE | C-O | -8.18 | 1.12 | 1.24 |
| 10 | j5 | 875 | LEU | C-O | -8.18 | 1.14 | 1.24 |
| 10 | k5 | 454 | GLN | C-O | -8.18 | 1.13 | 1.24 |
| 10 | k5 | 780 | ILE | C-O | -8.18 | 1.12 | 1.24 |
| 4 | M9 | 71 | PRO | CA-C | -8.18 | 1.42 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4 | M1 | 26 | SER | C-O | -8.18 | 1.13 | 1.24 |
| 8 | E5 | 116 | TYR | CA-C | -8.17 | 1.42 | 1.52 |
| 10 | j5 | 417 | GLU | C-O | -8.17 | 1.13 | 1.24 |
| 8 | u7 | 7 | ALA | C-O | -8.17 | 1.13 | 1.24 |
| 4 | M4 | 26 | SER | C-O | -8.17 | 1.13 | 1.24 |
| 8 | G5 | 56 | ASP | C-O | -8.17 | 1.14 | 1.24 |
| 4 | M8 | 41 | ASN | N-CA | -8.17 | 1.36 | 1.46 |
| 4 | M8 | 59 | ILE | CA-C | -8.17 | 1.42 | 1.52 |
| 4 | M3 | 59 | ILE | CA-C | -8.17 | 1.42 | 1.52 |
| 4 | M1 | 59 | ILE | CA-C | -8.17 | 1.42 | 1.52 |
| 4 | M3 | 36 | TYR | C-O | -8.16 | 1.13 | 1.23 |
| 10 | j5 | 1130 | VAL | C-O | -8.16 | 1.14 | 1.24 |
| 4 | M1 | 36 | TYR | C-O | -8.16 | 1.13 | 1.23 |
| 4 | MA | 36 | TYR | C-O | -8.16 | 1.13 | 1.23 |
| 10 | j5 | 462 | TYR | C-O | -8.16 | 1.13 | 1.24 |
| 10 | k5 | 462 | TYR | C-O | -8.16 | 1.13 | 1.24 |
| 10 | k5 | 875 | LEU | C-O | -8.16 | 1.14 | 1.24 |
| 10 | k5 | 739 | VAL | C-O | -8.16 | 1.14 | 1.24 |
| 4 | M9 | 36 | TYR | C-O | -8.16 | 1.13 | 1.23 |
| 10 | j5 | 776 | PHE | CA-C | -8.16 | 1.41 | 1.52 |
| 10 | k5 | 776 | PHE | CA-C | -8.16 | 1.41 | 1.52 |
| 1 | J5 | 12 | TYR | C-O | -8.16 | 1.13 | 1.24 |
| 10 | j5 | 605 | ARG | CA-C | -8.16 | 1.42 | 1.52 |
| 10 | j5 | 847 | LEU | N-CA | -8.16 | 1.36 | 1.46 |
| 10 | k5 | 847 | LEU | N-CA | -8.16 | 1.36 | 1.46 |
| 4 | MA | 26 | SER | C-O | -8.15 | 1.13 | 1.24 |
| 8 | K5 | 111 | GLY | C-O | -8.15 | 1.12 | 1.23 |
| 4 | M9 | 26 | SER | C-O | -8.15 | 1.13 | 1.24 |
| 10 | j5 | 408 | SER | CA-C | -8.15 | 1.42 | 1.53 |
| 10 | k5 | 408 | SER | CA-C | -8.15 | 1.42 | 1.53 |
| 8 | i7 | 118 | SER | C-O | -8.15 | 1.14 | 1.24 |
| 8 | I5 | 7 | ALA | C-O | -8.15 | 1.15 | 1.24 |
| 4 | M8 | 26 | SER | C-O | -8.15 | 1.13 | 1.24 |
| 4 | MA | 59 | ILE | CA-C | -8.15 | 1.42 | 1.52 |
| 4 | M9 | 59 | ILE | CA-C | -8.15 | 1.42 | 1.52 |
| 10 | k5 | 668 | ASN | CA-C | -8.15 | 1.42 | 1.52 |
| 8 | o7 | 7 | ALA | C-O | -8.14 | 1.13 | 1.24 |
| 4 | M3 | 62 | LYS | CA-C | -8.14 | 1.41 | 1.52 |
| 4 | M8 | 66 | VAL | C-O | -8.14 | 1.14 | 1.24 |
| 10 | j5 | 1108 | GLU | C-O | -8.14 | 1.14 | 1.24 |
| 4 | M3 | 66 | VAL | C-O | -8.14 | 1.14 | 1.24 |
| 4 | M1 | 66 | VAL | C-O | -8.14 | 1.14 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | j5 | 511 | ARG | CA-C | -8.13 | 1.42 | 1.52 |
| 4 | M4 | 178 | PRO | C-O | -8.13 | 1.17 | 1.24 |
| 10 | k5 | 417 | GLU | C-O | -8.13 | 1.13 | 1.24 |
| 4 | MA | 178 | PRO | C-O | -8.13 | 1.17 | 1.24 |
| 10 | j5 | 450 | ARG | CZ-NH2 | -8.13 | 1.22 | 1.33 |
| 4 | M9 | 178 | PRO | C-O | -8.13 | 1.17 | 1.24 |
| 10 | j5 | 538 | PHE | CA-C | -8.12 | 1.42 | 1.52 |
| 10 | j5 | 760 | ASP | C-O | -8.12 | 1.13 | 1.24 |
| 10 | k5 | 760 | ASP | C-O | -8.12 | 1.13 | 1.24 |
| 8 | G5 | 60 | GLN | C-O | -8.12 | 1.13 | 1.24 |
| 4 | M8 | 62 | LYS | CA-C | -8.12 | 1.41 | 1.52 |
| 10 | j5 | 313 | GLY | C-O | -8.11 | 1.15 | 1.24 |
| 10 | j5 | 806 | VAL | CA-C | -8.11 | 1.42 | 1.52 |
| 10 | k5 | 511 | ARG | CA-C | -8.11 | 1.42 | 1.52 |
| 9 | z5 | 4 | TYR | C-O | -8.11 | 1.13 | 1.23 |
| 10 | j5 | 505 | VAL | C-O | -8.11 | 1.14 | 1.24 |
| 4 | MA | 66 | VAL | C-O | -8.11 | 1.14 | 1.24 |
| 10 | j5 | 641 | ASP | C-O | -8.11 | 1.14 | 1.23 |
| 10 | k5 | 1108 | GLU | C-O | -8.11 | 1.14 | 1.24 |
| 4 | M9 | 66 | VAL | C-O | -8.11 | 1.14 | 1.24 |
| 4 | MA | 62 | LYS | CA-C | -8.10 | 1.42 | 1.52 |
| 4 | M3 | 143 | VAL | C-O | -8.10 | 1.14 | 1.24 |
| 4 | M9 | 62 | LYS | CA-C | -8.10 | 1.42 | 1.52 |
| 4 | M1 | 143 | VAL | C-O | -8.10 | 1.14 | 1.24 |
| 8 | A5 | 60 | GLN | C-O | -8.10 | 1.13 | 1.24 |
| 10 | j5 | 291 | ASP | N-CA | -8.10 | 1.36 | 1.46 |
| 10 | k5 | 291 | ASP | N-CA | -8.10 | 1.36 | 1.46 |
| 10 | j5 | 862 | LEU | CA-C | -8.10 | 1.42 | 1.52 |
| 11 | a9 | 58 | GLY | CA-C | 8.10 | 1.60 | 1.52 |
| 11 | aA | 58 | GLY | CA-C | 8.10 | 1.60 | 1.52 |
| 10 | k5 | 405 | LEU | C-O | -8.10 | 1.14 | 1.24 |
| 10 | k5 | 641 | ASP | C-O | -8.10 | 1.14 | 1.23 |
| 10 | k5 | 478 | PRO | CA-C | -8.09 | 1.43 | 1.52 |
| 8 | C5 | 7 | ALA | C-O | -8.09 | 1.15 | 1.24 |
| 10 | j5 | 405 | LEU | C-O | -8.08 | 1.14 | 1.24 |
| 10 | j5 | 500 | PRO | CA-C | -8.08 | 1.45 | 1.52 |
| 10 | j5 | 860 | LYS | CA-C | -8.08 | 1.41 | 1.52 |
| 10 | j5 | 874 | ARG | CA-C | -8.08 | 1.42 | 1.52 |
| 10 | k5 | 500 | PRO | CA-C | -8.08 | 1.45 | 1.52 |
| 10 | k5 | 874 | ARG | CA-C | -8.08 | 1.42 | 1.52 |
| 10 | k5 | 719 | MET | CA-C | -8.08 | 1.42 | 1.52 |
| 4 | MA | 143 | VAL | C-O | -8.07 | 1.14 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4 | M9 | 143 | VAL | C-O | -8.07 | 1.14 | 1.24 |
| 4 | M1 | 62 | LYS | CA-C | -8.07 | 1.42 | 1.52 |
| 10 | k5 | 901 | TYR | C-O | -8.07 | 1.14 | 1.24 |
| 10 | k5 | 410 | GLU | C-O | -8.07 | 1.14 | 1.24 |
| 4 | M8 | 178 | PRO | C-O | -8.07 | 1.17 | 1.24 |
| 9 | z5 | 43 | ARG | C-O | -8.06 | 1.14 | 1.24 |
| 10 | j5 | 830 | GLU | CA-C | -8.06 | 1.42 | 1.52 |
| 10 | j5 | 881 | VAL | N-CA | -8.06 | 1.38 | 1.47 |
| 10 | k5 | 830 | GLU | CA-C | -8.06 | 1.42 | 1.52 |
| 10 | k5 | 881 | VAL | N-CA | -8.06 | 1.38 | 1.47 |
| 10 | j5 | 640 | TYR | CA-C | -8.06 | 1.42 | 1.52 |
| 10 | k5 | 625 | LYS | CA-C | -8.05 | 1.42 | 1.52 |
| 10 | k5 | 640 | TYR | CA-C | -8.05 | 1.42 | 1.52 |
| 8 | u7 | 51 | VAL | C-O | -8.05 | 1.14 | 1.24 |
| 9 | i5 | 43 | ARG | C-O | -8.05 | 1.14 | 1.24 |
| 10 | k5 | 806 | VAL | CA-C | -8.04 | 1.42 | 1.52 |
| 4 | M3 | 65 | ARG | CA-C | -8.04 | 1.42 | 1.52 |
| 4 | M3 | 178 | PRO | C-O | -8.04 | 1.17 | 1.24 |
| 10 | j5 | 488 | LYS | C-O | -8.04 | 1.13 | 1.23 |
| 10 | k5 | 488 | LYS | C-O | -8.04 | 1.13 | 1.23 |
| 4 | M1 | 178 | PRO | C-O | -8.04 | 1.17 | 1.24 |
| 10 | j5 | 370 | GLU | C-O | -8.04 | 1.13 | 1.24 |
| 10 | k5 | 860 | LYS | CA-C | -8.04 | 1.41 | 1.52 |
| 10 | j5 | 625 | LYS | CA-C | -8.04 | 1.42 | 1.52 |
| 4 | M4 | 62 | LYS | CA-C | -8.03 | 1.42 | 1.52 |
| 9 | z7 | 67 | VAL | C-O | -8.04 | 1.15 | 1.24 |
| 4 | M8 | 65 | ARG | CA-C | -8.04 | 1.42 | 1.52 |
| 10 | j5 | 839 | ARG | CA-C | -8.03 | 1.44 | 1.53 |
| 10 | k5 | 505 | VAL | C-O | -8.03 | 1.15 | 1.24 |
| 10 | k5 | 839 | ARG | CA-C | -8.03 | 1.44 | 1.53 |
| 4 | M1 | 65 | ARG | CA-C | -8.03 | 1.42 | 1.52 |
| 10 | j5 | 410 | GLU | C-O | -8.02 | 1.14 | 1.24 |
| 10 | k5 | 862 | LEU | CA-C | -8.02 | 1.42 | 1.52 |
| 8 | o7 | 51 | VAL | C-O | -8.02 | 1.14 | 1.24 |
| 10 | j5 | 581 | TYR | C-O | -8.02 | 1.13 | 1.23 |
| 10 | j5 | 719 | MET | CA-C | -8.02 | 1.42 | 1.52 |
| 10 | j5 | 677 | ASP | CB-CG | -8.02 | 1.32 | 1.52 |
| 10 | k5 | 677 | ASP | CB-CG | -8.02 | 1.32 | 1.52 |
| 10 | k5 | 677 | ASP | C-O | -8.02 | 1.13 | 1.24 |
| 10 | j5 | 300 | ALA | CA-C | -8.02 | 1.42 | 1.52 |
| 10 | k5 | 446 | ALA | C-O | -8.01 | 1.13 | 1.24 |
| 10 | j5 | 476 | ASN | C-O | -8.01 | 1.13 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | j5 | 1036 | VAL | C-O | -8.00 | 1.14 | 1.24 |
| 10 | k5 | 313 | GLY | C-O | -8.00 | 1.15 | 1.24 |
| 9 | i5 | 5 | PHE | C-O | -8.00 | 1.13 | 1.23 |
| 10 | j5 | 677 | ASP | C-O | -8.00 | 1.14 | 1.24 |
| 10 | j5 | 901 | TYR | C-O | -8.00 | 1.14 | 1.24 |
| 10 | j5 | 5 | GLY | C-O | -8.00 | 1.14 | 1.24 |
| 10 | k5 | 477 | ASP | C-O | -8.00 | 1.15 | 1.24 |
| 10 | k5 | 506 | LYS | C-O | -8.00 | 1.14 | 1.24 |
| 10 | j5 | 477 | ASP | C-O | -7.99 | 1.15 | 1.24 |
| 10 | k5 | 476 | ASN | C-O | -7.99 | 1.13 | 1.24 |
| 4 | MA | 65 | ARG | CA-C | -7.99 | 1.42 | 1.52 |
| 4 | M4 | 65 | ARG | CA-C | -7.99 | 1.42 | 1.52 |
| 10 | k5 | 581 | TYR | C-O | -7.99 | 1.13 | 1.23 |
| 4 | M9 | 65 | ARG | CA-C | -7.99 | 1.42 | 1.52 |
| 9 | w7 | 67 | VAL | C-O | -7.99 | 1.15 | 1.24 |
| 8 | E5 | 80 | LEU | C-O | -7.99 | 1.13 | 1.24 |
| 9 | z5 | 5 | PHE | C-O | -7.99 | 1.13 | 1.23 |
| 8 | K5 | 80 | LEU | C-O | -7.99 | 1.13 | 1.24 |
| 10 | j5 | 972 | GLY | C-O | -7.99 | 1.13 | 1.24 |
| 10 | j5 | 1093 | VAL | C-O | -7.99 | 1.14 | 1.24 |
| 10 | k5 | 1093 | VAL | C-O | -7.99 | 1.14 | 1.24 |
| 10 | j5 | 893 | ASN | N-CA | -7.98 | 1.36 | 1.46 |
| 10 | j5 | 752 | VAL | C-O | -7.98 | 1.15 | 1.24 |
| 10 | k5 | 752 | VAL | C-O | -7.98 | 1.15 | 1.24 |
| 4 | M8 | 143 | VAL | C-O | -7.98 | 1.14 | 1.24 |
| 10 | j5 | 566 | ALA | CA-C | -7.98 | 1.41 | 1.52 |
| 10 | k5 | 566 | ALA | CA-C | -7.98 | 1.41 | 1.52 |
| 10 | j5 | 704 | THR | C-O | -7.98 | 1.14 | 1.24 |
| 10 | k5 | 704 | THR | C-O | -7.98 | 1.14 | 1.24 |
| 9 | i5 | 20 | GLY | CA-C | -7.98 | 1.40 | 1.51 |
| 10 | j5 | 809 | LEU | C-O | -7.97 | 1.12 | 1.23 |
| 10 | k5 | 300 | ALA | CA-C | -7.97 | 1.42 | 1.52 |
| 10 | k5 | 809 | LEU | C-O | -7.97 | 1.12 | 1.23 |
| 10 | j5 | 518 | ASN | C-O | -7.97 | 1.13 | 1.24 |
| 10 | k5 | 518 | ASN | C-O | -7.97 | 1.13 | 1.24 |
| 10 | k5 | 5 | GLY | C-O | -7.97 | 1.14 | 1.24 |
| 10 | j5 | 446 | ALA | C-O | -7.97 | 1.13 | 1.24 |
| 10 | j5 | 528 | GLU | CA-C | -7.96 | 1.43 | 1.52 |
| 10 | k5 | 528 | GLU | CA-C | -7.96 | 1.43 | 1.52 |
| 9 | i5 | 21 | ARG | C-O | -7.96 | 1.14 | 1.24 |
| 10 | k5 | 370 | GLU | C-O | -7.96 | 1.13 | 1.24 |
| 10 | j5 | 715 | ALA | CA-C | -7.96 | 1.42 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9 | w7 | 7 | VAL | C-O | -7.96 | 1.15 | 1.24 |
| 10 | j5 | 701 | ASP | C-O | -7.95 | 1.14 | 1.24 |
| 9 | z7 | 7 | VAL | C-O | -7.95 | 1.15 | 1.24 |
| 8 | G5 | 51 | VAL | C-O | -7.94 | 1.14 | 1.24 |
| 4 | M3 | 209 | TYR | C-O | -7.94 | 1.15 | 1.24 |
| 10 | k5 | 972 | GLY | C-O | -7.94 | 1.13 | 1.24 |
| 4 | M1 | 209 | TYR | C-O | -7.94 | 1.15 | 1.24 |
| 4 | M4 | 209 | TYR | C-O | -7.94 | 1.15 | 1.24 |
| 10 | k5 | 891 | ALA | C-O | -7.94 | 1.14 | 1.23 |
| 4 | M8 | 209 | TYR | C-O | -7.94 | 1.15 | 1.24 |
| 4 | MA | 209 | TYR | C-O | -7.94 | 1.15 | 1.24 |
| 4 | M9 | 209 | TYR | C-O | -7.94 | 1.15 | 1.24 |
| 10 | k5 | 1036 | VAL | C-O | -7.94 | 1.14 | 1.24 |
| 8 | o7 | 52 | LYS | CA-C | -7.93 | 1.42 | 1.52 |
| 1 | J7 | 67 | ARG | C-O | -7.93 | 1.13 | 1.24 |
| 10 | k5 | 893 | ASN | N-CA | -7.93 | 1.36 | 1.46 |
| 4 | M3 | 209 | TYR | CA-C | -7.93 | 1.42 | 1.52 |
| 8 | o7 | 56 | ASP | CA-C | -7.93 | 1.42 | 1.52 |
| 8 | u7 | 56 | ASP | CA-C | -7.93 | 1.42 | 1.52 |
| 4 | M9 | 157 | PHE | CA-C | -7.92 | 1.44 | 1.52 |
| 10 | k5 | 346 | GLU | C-O | -7.92 | 1.12 | 1.23 |
| 9 | z5 | 21 | ARG | C-O | -7.92 | 1.14 | 1.24 |
| 10 | j5 | 678 | VAL | CA-CB | -7.92 | 1.44 | 1.54 |
| 10 | k5 | 678 | VAL | CA-CB | -7.92 | 1.44 | 1.54 |
| 10 | j5 | 891 | ALA | C-O | -7.92 | 1.14 | 1.23 |
| 10 | k5 | 894 | TYR | N-CA | -7.92 | 1.40 | 1.46 |
| 10 | j5 | 902 | ASN | CA-C | -7.91 | 1.43 | 1.53 |
| 9 | z5 | 20 | GLY | CA-C | -7.91 | 1.40 | 1.51 |
| 9 | w7 | 48 | GLY | C-O | -7.91 | 1.15 | 1.24 |
| 10 | j5 | 347 | PHE | C-O | -7.91 | 1.13 | 1.24 |
| 10 | j5 | 742 | GLY | C-O | -7.91 | 1.13 | 1.23 |
| 10 | j5 | 506 | LYS | C-O | -7.90 | 1.14 | 1.24 |
| 10 | k5 | 902 | ASN | CA-C | -7.90 | 1.43 | 1.53 |
| 4 | MA | 209 | TYR | CA-C | -7.90 | 1.42 | 1.52 |
| 8 | c7 | 122 | PRO | C-O | -7.90 | 1.14 | 1.23 |
| 8 | u7 | 52 | LYS | CA-C | -7.90 | 1.42 | 1.52 |
| 4 | M9 | 209 | TYR | CA-C | -7.90 | 1.42 | 1.52 |
| 4 | M1 | 209 | TYR | CA-C | -7.90 | 1.42 | 1.52 |
| 9 | w7 | 5 | PHE | C-O | -7.89 | 1.14 | 1.24 |
| 10 | k5 | 715 | ALA | CA-C | -7.89 | 1.42 | 1.52 |
| 8 | A5 | 51 | VAL | C-O | -7.89 | 1.14 | 1.24 |
| 9 | z5 | 24 | GLN | CA-C | -7.89 | 1.41 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4 | M8 | 157 | PHE | CA-C | -7.89 | 1.44 | 1.52 |
| 4 | M4 | 209 | TYR | CA-C | -7.89 | 1.42 | 1.52 |
| 10 | j5 | 936 | LYS | CA-C | -7.89 | 1.42 | 1.52 |
| 10 | k5 | 701 | ASP | C-O | -7.88 | 1.14 | 1.24 |
| 10 | k5 | 936 | LYS | CA-C | -7.88 | 1.42 | 1.52 |
| 10 | k5 | 743 | VAL | N-CA | -7.88 | 1.37 | 1.46 |
| 1 | D7 | 67 | ARG | C-O | -7.88 | 1.13 | 1.24 |
| 9 | z7 | 5 | PHE | C-O | -7.88 | 1.14 | 1.24 |
| 9 | i5 | 24 | GLN | CA-C | -7.88 | 1.41 | 1.52 |
| 10 | j5 | 874 | ARG | C-O | -7.88 | 1.15 | 1.24 |
| 9 | z7 | 48 | GLY | C-O | -7.87 | 1.15 | 1.24 |
| 10 | j5 | 483 | PHE | C-O | -7.87 | 1.13 | 1.24 |
| 10 | k5 | 301 | TYR | CA-C | -7.87 | 1.42 | 1.52 |
| 10 | k5 | 1128 | VAL | C-O | -7.87 | 1.15 | 1.24 |
| 10 | k5 | 483 | PHE | C-O | -7.87 | 1.13 | 1.24 |
| 9 | w7 | 41 | GLN | CA-C | -7.87 | 1.42 | 1.52 |
| 10 | j5 | 274 | MET | CA-C | -7.87 | 1.45 | 1.53 |
| 8 | A5 | 60 | GLN | CA-C | -7.87 | 1.41 | 1.52 |
| 4 | M8 | 209 | TYR | CA-C | -7.87 | 1.42 | 1.52 |
| 10 | j5 | 457 | THR | CA-C | -7.86 | 1.42 | 1.52 |
| 10 | k5 | 457 | THR | CA-C | -7.86 | 1.42 | 1.52 |
| 10 | k5 | 870 | GLU | CA-C | -7.86 | 1.42 | 1.52 |
| 10 | j5 | 346 | GLU | C-O | -7.86 | 1.12 | 1.23 |
| 10 | j5 | 743 | VAL | N-CA | -7.86 | 1.37 | 1.46 |
| 8 | i7 | 122 | PRO | C-O | -7.86 | 1.14 | 1.23 |
| 9 | z7 | 41 | GLN | CA-C | -7.86 | 1.42 | 1.52 |
| 10 | k5 | 742 | GLY | C-O | -7.86 | 1.13 | 1.23 |
| 8 | G5 | 53 | GLN | CA-C | -7.86 | 1.42 | 1.52 |
| 10 | j5 | 650 | ASP | CA-CB | 7.86 | 1.67 | 1.53 |
| 10 | k5 | 586 | LEU | C-O | -7.85 | 1.12 | 1.23 |
| 4 | MA | 157 | PHE | CA-C | -7.85 | 1.44 | 1.52 |
| 8 | A5 | 53 | GLN | CA-C | -7.85 | 1.42 | 1.52 |
| 10 | k5 | 823 | TYR | CA-C | -7.85 | 1.44 | 1.52 |
| 10 | k5 | 650 | ASP | CA-CB | 7.85 | 1.67 | 1.53 |
| 8 | G5 | 60 | GLN | CA-C | -7.84 | 1.41 | 1.52 |
| 4 | M4 | 157 | PHE | CA-C | -7.84 | 1.44 | 1.52 |
| 10 | j5 | 880 | THR | C-O | -7.84 | 1.14 | 1.24 |
| 10 | j5 | 950 | PRO | C-O | -7.84 | 1.14 | 1.23 |
| 10 | k5 | 539 | LYS | CA-C | -7.83 | 1.43 | 1.52 |
| 10 | k5 | 874 | ARG | C-O | -7.82 | 1.15 | 1.24 |
| 11 | a9 | 629 | LYS | CA-C | -7.82 | 1.42 | 1.52 |
| 11 | aA | 629 | LYS | CA-C | -7.82 | 1.42 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | j5 | 453 | PRO | C-O | -7.82 | 1.14 | 1.23 |
| 10 | j5 | 698 | GLY | CA-C | -7.82 | 1.42 | 1.52 |
| 10 | k5 | 347 | PHE | C-O | -7.82 | 1.13 | 1.24 |
| 10 | k5 | 698 | GLY | CA-C | -7.82 | 1.42 | 1.52 |
| 10 | j5 | 1128 | VAL | C-O | -7.81 | 1.15 | 1.24 |
| 10 | k5 | 274 | MET | CA-C | -7.81 | 1.45 | 1.53 |
| 10 | j5 | 539 | LYS | CA-C | -7.81 | 1.43 | 1.52 |
| 4 | M3 | 157 | PHE | CA-C | -7.80 | 1.44 | 1.52 |
| 10 | j5 | 301 | TYR | CA-C | -7.80 | 1.42 | 1.52 |
| 10 | j5 | 894 | TYR | N-CA | -7.80 | 1.40 | 1.46 |
| 4 | M1 | 157 | PHE | CA-C | -7.80 | 1.44 | 1.52 |
| 10 | k5 | 453 | PRO | C-O | -7.80 | 1.14 | 1.23 |
| 10 | j5 | 586 | LEU | C-O | -7.79 | 1.12 | 1.23 |
| 10 | k5 | 950 | PRO | C-O | -7.79 | 1.14 | 1.23 |
| 1 | L5 | 10 | ASN | C-O | -7.79 | 1.14 | 1.24 |
| 10 | j5 | 823 | TYR | CA-C | -7.78 | 1.44 | 1.52 |
| 10 | j5 | 818 | GLN | C-O | -7.78 | 1.14 | 1.24 |
| 10 | k5 | 540 | LEU | CA-C | -7.78 | 1.43 | 1.53 |
| 10 | j5 | 624 | CYS | CA-C | -7.78 | 1.42 | 1.52 |
| 11 | a9 | 776 | TYR | N-CA | -7.78 | 1.36 | 1.46 |
| 8 | E5 | 106 | GLU | C-O | -7.78 | 1.14 | 1.24 |
| 10 | j5 | 402 | ILE | C-O | -7.77 | 1.14 | 1.24 |
| 10 | k5 | 881 | VAL | C-O | -7.77 | 1.14 | 1.24 |
| 10 | k5 | 880 | THR | C-O | -7.77 | 1.14 | 1.24 |
| 10 | j5 | 897 | SER | CA-CB | -7.77 | 1.41 | 1.53 |
| 10 | k5 | 402 | ILE | C-O | -7.76 | 1.15 | 1.24 |
| 10 | j5 | 881 | VAL | C-O | -7.76 | 1.14 | 1.24 |
| 10 | j5 | 480 | GLU | C-O | -7.76 | 1.13 | 1.23 |
| 10 | k5 | 480 | GLU | C-O | -7.76 | 1.13 | 1.23 |
| 1 | F5 | 10 | ASN | C-O | -7.75 | 1.14 | 1.24 |
| 8 | c7 | 113 | LYS | CA-C | -7.75 | 1.42 | 1.52 |
| 10 | j5 | 870 | GLU | CA-C | -7.75 | 1.42 | 1.52 |
| 10 | j5 | 1093 | VAL | CA-C | -7.75 | 1.43 | 1.52 |
| 10 | k5 | 541 | THR | CA-C | -7.75 | 1.42 | 1.52 |
| 11 | aA | 776 | TYR | N-CA | -7.75 | 1.36 | 1.46 |
| 10 | j5 | 426 | LEU | CA-C | -7.75 | 1.42 | 1.52 |
| 10 | j5 | 568 | ILE | CA-C | -7.75 | 1.41 | 1.52 |
| 8 | c7 | 133 | MET | C-O | -7.75 | 1.14 | 1.24 |
| 8 | K5 | 106 | GLU | C-O | -7.75 | 1.14 | 1.24 |
| 10 | j5 | 504 | ASP | N-CA | -7.75 | 1.36 | 1.46 |
| 10 | k5 | 299 | ALA | C-O | -7.75 | 1.14 | 1.24 |
| 10 | k5 | 504 | ASP | N-CA | -7.75 | 1.36 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9 | z7 | 42 | GLN | CA-C | -7.75 | 1.42 | 1.52 |
| 3 | H2 | 77 | ARG | CA-C | -7.74 | 1.42 | 1.52 |
| 3 | H6 | 77 | ARG | CA-C | -7.74 | 1.42 | 1.52 |
| 10 | j5 | 824 | PRO | CA-C | -7.74 | 1.43 | 1.52 |
| 10 | k5 | 824 | PRO | CA-C | -7.74 | 1.43 | 1.52 |
| 10 | j5 | 441 | ASP | CA-C | -7.74 | 1.42 | 1.52 |
| 10 | j5 | 649 | PHE | CA-C | -7.74 | 1.42 | 1.52 |
| 10 | j5 | 612 | ILE | C-O | -7.74 | 1.14 | 1.24 |
| 10 | k5 | 612 | ILE | C-O | -7.74 | 1.14 | 1.24 |
| 10 | k5 | 624 | CYS | CA-C | -7.73 | 1.42 | 1.52 |
| 4 | M8 | 60 | LYS | CA-C | -7.73 | 1.42 | 1.52 |
| 4 | M4 | 60 | LYS | CA-C | -7.73 | 1.42 | 1.52 |
| 10 | k5 | 676 | GLU | C-O | -7.73 | 1.13 | 1.24 |
| 10 | j5 | 19 | THR | C-O | -7.73 | 1.14 | 1.23 |
| 10 | k5 | 897 | SER | CA-CB | -7.72 | 1.41 | 1.53 |
| 10 | k5 | 639 | THR | C-O | -7.72 | 1.14 | 1.23 |
| 10 | k5 | 649 | PHE | CA-C | -7.71 | 1.42 | 1.52 |
| 1 | D7 | 76 | ARG | N-CA | -7.71 | 1.37 | 1.46 |
| 9 | z7 | 9 | ALA | C-O | -7.71 | 1.14 | 1.23 |
| 9 | w7 | 42 | GLN | CA-C | -7.71 | 1.42 | 1.52 |
| 10 | j5 | 541 | THR | CA-C | -7.71 | 1.42 | 1.52 |
| 1 | J7 | 76 | ARG | N-CA | -7.71 | 1.37 | 1.46 |
| 10 | k5 | 862 | LEU | N-CA | -7.71 | 1.36 | 1.46 |
| 10 | j5 | 540 | LEU | CA-C | -7.71 | 1.43 | 1.53 |
| 10 | j5 | 862 | LEU | N-CA | -7.71 | 1.36 | 1.46 |
| 10 | j5 | 464 | GLN | CA-CB | -7.70 | 1.44 | 1.54 |
| 10 | j5 | 834 | LYS | CA-C | -7.70 | 1.41 | 1.52 |
| 10 | k5 | 464 | GLN | CA-CB | -7.70 | 1.44 | 1.54 |
| 8 | i7 | 113 | LYS | CA-C | -7.70 | 1.42 | 1.52 |
| 10 | j5 | 299 | ALA | C-O | -7.70 | 1.15 | 1.24 |
| 10 | j5 | 602 | GLU | C-O | -7.70 | 1.13 | 1.24 |
| 10 | k5 | 343 | TYR | CA-C | -7.70 | 1.41 | 1.52 |
| 10 | k5 | 602 | GLU | C-O | -7.70 | 1.13 | 1.24 |
| 9 | w7 | 9 | ALA | C-O | -7.70 | 1.14 | 1.23 |
| 10 | k5 | 818 | GLN | C-O | -7.70 | 1.15 | 1.24 |
| 10 | k5 | 1093 | VAL | CA-C | -7.70 | 1.43 | 1.52 |
| 4 | MA | 60 | LYS | CA-C | -7.69 | 1.42 | 1.52 |
| 10 | j5 | 676 | GLU | C-O | -7.69 | 1.13 | 1.24 |
| 4 | M9 | 60 | LYS | CA-C | -7.69 | 1.42 | 1.52 |
| 10 | j5 | 343 | TYR | CA-C | -7.69 | 1.41 | 1.52 |
| 4 | M3 | 60 | LYS | CA-C | -7.69 | 1.42 | 1.52 |
| 10 | k5 | 349 | GLN | CA-C | -7.69 | 1.43 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9 | y7 | 44 | ILE | C-O | -7.69 | 1.15 | 1.24 |
| 4 | M1 | 60 | LYS | CA-C | -7.69 | 1.42 | 1.52 |
| 10 | j5 | 296 | VAL | C-O | -7.68 | 1.15 | 1.24 |
| 10 | k5 | 426 | LEU | CA-C | -7.68 | 1.42 | 1.52 |
| 9 | w7 | 48 | GLY | CA-C | -7.68 | 1.43 | 1.51 |
| 10 | j5 | 1136 | ILE | C-O | -7.68 | 1.16 | 1.24 |
| 10 | k5 | 1136 | ILE | C-O | -7.68 | 1.16 | 1.24 |
| 8 | i7 | 133 | MET | C-O | -7.68 | 1.14 | 1.24 |
| 10 | k5 | 19 | THR | C-O | -7.68 | 1.14 | 1.23 |
| 10 | k5 | 851 | HIS | C-O | -7.68 | 1.13 | 1.24 |
| 10 | j5 | 430 | ALA | C-O | -7.68 | 1.14 | 1.24 |
| 10 | k5 | 441 | ASP | CA-C | -7.67 | 1.43 | 1.52 |
| 9 | z7 | 48 | GLY | CA-C | -7.67 | 1.43 | 1.51 |
| 10 | j5 | 502 | GLY | C-O | -7.67 | 1.09 | 1.23 |
| 10 | j5 | 851 | HIS | C-O | -7.67 | 1.14 | 1.24 |
| 10 | k5 | 502 | GLY | C-O | -7.67 | 1.09 | 1.23 |
| 10 | j5 | 425 | ASN | C-O | -7.67 | 1.14 | 1.24 |
| 10 | k5 | 834 | LYS | CA-C | -7.67 | 1.42 | 1.52 |
| 10 | j5 | 629 | TYR | CA-C | -7.66 | 1.43 | 1.52 |
| 10 | k5 | 629 | TYR | CA-C | -7.66 | 1.43 | 1.52 |
| 9 | i5 | 34 | TYR | C-O | -7.65 | 1.14 | 1.24 |
| 10 | k5 | 350 | PRO | C-O | -7.65 | 1.14 | 1.24 |
| 10 | j5 | 1002 | ARG | C-O | -7.64 | 1.15 | 1.24 |
| 10 | k5 | 1002 | ARG | C-O | -7.64 | 1.15 | 1.24 |
| 10 | j5 | 346 | GLU | CA-C | -7.64 | 1.42 | 1.52 |
| 10 | k5 | 346 | GLU | CA-C | -7.64 | 1.42 | 1.52 |
| 9 | x7 | 44 | ILE | C-O | -7.64 | 1.15 | 1.24 |
| 10 | j5 | 639 | THR | C-O | -7.63 | 1.14 | 1.23 |
| 10 | k5 | 296 | VAL | C-O | -7.63 | 1.15 | 1.24 |
| 10 | j5 | 471 | PRO | CA-CB | -7.63 | 1.43 | 1.53 |
| 10 | j5 | 620 | PRO | N-CA | -7.63 | 1.39 | 1.47 |
| 10 | k5 | 620 | PRO | N-CA | -7.63 | 1.39 | 1.47 |
| 10 | k5 | 793 | SER | CA-C | -7.63 | 1.42 | 1.52 |
| 1 | h7 | 50 | THR | C-O | -7.63 | 1.15 | 1.24 |
| 10 | j5 | 302 | ARG | C-O | -7.63 | 1.14 | 1.24 |
| 8 | a7 | 15 | ALA | CA-C | -7.63 | 1.43 | 1.53 |
| 11 | a9 | 354 | VAL | C-N | 7.62 | 1.44 | 1.33 |
| 11 | aA | 354 | VAL | C-N | 7.62 | 1.44 | 1.33 |
| 10 | j5 | 618 | TRP | C-O | -7.62 | 1.13 | 1.24 |
| 10 | j5 | 815 | TYR | C-O | -7.62 | 1.15 | 1.24 |
| 10 | k5 | 618 | TRP | C-O | -7.62 | 1.13 | 1.24 |
| 10 | k5 | 815 | TYR | C-O | -7.62 | 1.15 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | k5 | 162 | TRP | C-O | -7.62 | 1.15 | 1.24 |
| 10 | k5 | 568 | ILE | CA-C | -7.62 | 1.41 | 1.52 |
| 1 | h7 | 51 | ILE | C-O | -7.62 | 1.15 | 1.24 |
| 10 | k5 | 886 | PHE | C-O | -7.61 | 1.14 | 1.24 |
| 10 | j5 | 886 | PHE | C-O | -7.61 | 1.14 | 1.24 |
| 10 | j5 | 955 | LEU | C-O | -7.61 | 1.14 | 1.24 |
| 10 | k5 | 955 | LEU | C-O | -7.61 | 1.14 | 1.24 |
| 10 | j5 | 349 | GLN | CA-C | -7.61 | 1.43 | 1.52 |
| 10 | j5 | 555 | ALA | C-O | -7.61 | 1.14 | 1.23 |
| 10 | j5 | 640 | TYR | C-O | -7.61 | 1.14 | 1.24 |
| 10 | k5 | 640 | TYR | C-O | -7.61 | 1.14 | 1.24 |
| 10 | k5 | 265 | SER | C-O | -7.60 | 1.14 | 1.24 |
| 4 | M4 | 61 | ASN | C-O | -7.60 | 1.15 | 1.24 |
| 4 | M3 | 61 | ASN | C-O | -7.60 | 1.15 | 1.24 |
| 4 | M1 | 61 | ASN | C-O | -7.60 | 1.15 | 1.24 |
| 10 | k5 | 430 | ALA | C-O | -7.60 | 1.14 | 1.24 |
| 9 | w7 | 67 | VAL | CA-C | -7.59 | 1.43 | 1.52 |
| 10 | k5 | 441 | ASP | CA-CB | -7.59 | 1.41 | 1.53 |
| 10 | k5 | 555 | ALA | C-O | -7.59 | 1.14 | 1.23 |
| 1 | b7 | 50 | THR | C-O | -7.59 | 1.15 | 1.24 |
| 10 | j5 | 793 | SER | CA-C | -7.58 | 1.43 | 1.52 |
| 10 | k5 | 403 | ASP | CA-C | -7.58 | 1.43 | 1.52 |
| 10 | k5 | 776 | PHE | C-O | -7.58 | 1.14 | 1.24 |
| 10 | j5 | 265 | SER | C-O | -7.58 | 1.14 | 1.24 |
| 10 | k5 | 302 | ARG | C-O | -7.58 | 1.14 | 1.24 |
| 4 | M4 | 222 | ARG | C-O | -7.58 | 1.15 | 1.24 |
| 10 | k5 | 520 | ARG | N-CA | -7.57 | 1.36 | 1.46 |
| 10 | j5 | 1003 | GLN | C-O | -7.57 | 1.15 | 1.24 |
| 1 | b7 | 51 | ILE | C-O | -7.57 | 1.15 | 1.24 |
| 10 | j5 | 600 | VAL | CA-C | -7.57 | 1.41 | 1.52 |
| 10 | k5 | 600 | VAL | CA-C | -7.57 | 1.41 | 1.52 |
| 4 | MA | 61 | ASN | C-O | -7.57 | 1.15 | 1.24 |
| 4 | M9 | 61 | ASN | C-O | -7.57 | 1.15 | 1.24 |
| 10 | j5 | 350 | PRO | C-O | -7.56 | 1.14 | 1.24 |
| 10 | j5 | 441 | ASP | CA-CB | -7.56 | 1.41 | 1.53 |
| 10 | k5 | 604 | VAL | C-O | -7.56 | 1.14 | 1.24 |
| 10 | k5 | 471 | PRO | CA-CB | -7.56 | 1.43 | 1.53 |
| 10 | k5 | 843 | ASN | C-O | -7.56 | 1.15 | 1.24 |
| 9 | z5 | 34 | TYR | C-O | -7.56 | 1.14 | 1.24 |
| 10 | k5 | 478 | PRO | C-O | -7.55 | 1.13 | 1.23 |
| 8 | E5 | 94 | TYR | CA-C | -7.55 | 1.43 | 1.52 |
| 10 | j5 | 469 | GLN | C-O | -7.55 | 1.14 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 10 | j5 | 597 | GLU | CA-C | -7.55 | 1.42 | 1.52 |
| 10 | k5 | 469 | GLN | C-O | -7.55 | 1.14 | 1.23 |
| 10 | k5 | 597 | GLU | CA-C | -7.55 | 1.42 | 1.52 |
| 8 | E5 | 97 | VAL | C-O | -7.55 | 1.14 | 1.24 |
| 8 | u7 | 48 | GLU | CA-C | -7.54 | 1.41 | 1.52 |
| 10 | j5 | 611 | GLU | CA-C | -7.54 | 1.43 | 1.52 |
| 10 | k5 | 845 | ALA | CA-C | -7.54 | 1.41 | 1.52 |
| 10 | k5 | 425 | ASN | C-O | -7.54 | 1.14 | 1.24 |
| 8 | o7 | 48 | GLU | CA-C | -7.53 | 1.41 | 1.52 |
| 4 | M8 | 222 | ARG | C-O | -7.53 | 1.15 | 1.24 |
| 10 | j5 | 162 | TRP | C-O | -7.53 | 1.15 | 1.24 |
| 10 | k5 | 159 | ASP | CA-C | -7.53 | 1.43 | 1.52 |
| 9 | z7 | 67 | VAL | CA-C | -7.52 | 1.43 | 1.52 |
| 10 | j5 | 159 | ASP | CA-C | -7.52 | 1.43 | 1.52 |
| 4 | M8 | 61 | ASN | C-O | -7.52 | 1.15 | 1.24 |
| 8 | A5 | 52 | LYS | CA-C | -7.52 | 1.43 | 1.52 |
| 10 | j5 | 761 | ARG | C-O | -7.52 | 1.15 | 1.24 |
| 10 | j5 | 834 | LYS | N-CA | -7.52 | 1.36 | 1.46 |
| 10 | j5 | 871 | GLU | CA-C | -7.52 | 1.43 | 1.52 |
| 10 | k5 | 718 | MET | CA-C | -7.52 | 1.43 | 1.52 |
| 10 | k5 | 761 | ARG | C-O | -7.52 | 1.15 | 1.24 |
| 10 | j5 | 584 | GLN | C-O | -7.52 | 1.15 | 1.24 |
| 10 | j5 | 781 | ALA | C-O | -7.52 | 1.14 | 1.24 |
| 10 | j5 | 520 | ARG | N-CA | -7.51 | 1.36 | 1.46 |
| 10 | k5 | 838 | GLY | C-O | -7.51 | 1.12 | 1.24 |
| 10 | j5 | 556 | GLY | C-O | -7.51 | 1.15 | 1.23 |
| 10 | k5 | 834 | LYS | N-CA | -7.51 | 1.36 | 1.46 |
| 10 | j5 | 776 | PHE | C-O | -7.51 | 1.14 | 1.24 |
| 10 | k5 | 770 | ALA | C-O | -7.51 | 1.14 | 1.24 |
| 10 | j5 | 845 | ALA | CA-C | -7.50 | 1.41 | 1.52 |
| 10 | j5 | 843 | ASN | C-O | -7.50 | 1.15 | 1.24 |
| 10 | k5 | 871 | GLU | CA-C | -7.50 | 1.43 | 1.52 |
| 10 | k5 | 261 | ILE | CA-C | -7.50 | 1.43 | 1.52 |
| 4 | MA | 222 | ARG | C-O | -7.50 | 1.15 | 1.24 |
| 4 | M9 | 222 | ARG | C-O | -7.50 | 1.15 | 1.24 |
| 10 | j5 | 403 | ASP | CA-C | -7.50 | 1.43 | 1.52 |
| 8 | g7 | 15 | ALA | CA-C | -7.50 | 1.43 | 1.53 |
| 10 | j5 | 604 | VAL | C-O | -7.49 | 1.14 | 1.24 |
| 10 | k5 | 630 | ILE | CA-CB | -7.49 | 1.43 | 1.54 |
| 10 | k5 | 996 | ALA | C-O | -7.49 | 1.15 | 1.24 |
| 10 | k5 | 578 | ARG | N-CA | -7.49 | 1.37 | 1.46 |
| 9 | i5 | 46 | LYS | C-O | -7.49 | 1.14 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | j5 | 856 | ARG | CA-C | -7.49 | 1.43 | 1.52 |
| 10 | j5 | 578 | ARG | N-CA | -7.49 | 1.37 | 1.46 |
| 10 | j5 | 795 | LEU | CA-C | -7.49 | 1.43 | 1.52 |
| 10 | k5 | 795 | LEU | CA-C | -7.49 | 1.43 | 1.52 |
| 10 | k5 | 1003 | GLN | C-O | -7.49 | 1.15 | 1.24 |
| 8 | K5 | 94 | TYR | CA-C | -7.49 | 1.43 | 1.52 |
| 10 | k5 | 584 | GLN | C-O | -7.49 | 1.15 | 1.24 |
| 10 | j5 | 822 | ARG | CA-C | -7.48 | 1.43 | 1.52 |
| 10 | k5 | 822 | ARG | CA-C | -7.48 | 1.43 | 1.52 |
| 4 | M3 | 222 | ARG | C-O | -7.48 | 1.15 | 1.24 |
| 9 | z5 | 46 | LYS | C-O | -7.48 | 1.14 | 1.24 |
| 4 | M1 | 222 | ARG | C-O | -7.48 | 1.15 | 1.24 |
| 8 | G5 | 52 | LYS | CA-C | -7.48 | 1.43 | 1.52 |
| 10 | j5 | 478 | PRO | C-O | -7.48 | 1.13 | 1.23 |
| 10 | k5 | 812 | SER | CA-C | -7.48 | 1.42 | 1.52 |
| 10 | j5 | 812 | SER | CA-C | -7.48 | 1.42 | 1.52 |
| 9 | i5 | 31 | LEU | C-O | -7.47 | 1.14 | 1.24 |
| 8 | c7 | 127 | ALA | C-O | -7.47 | 1.14 | 1.24 |
| 10 | j5 | 838 | GLY | C-O | -7.47 | 1.13 | 1.24 |
| 10 | j5 | 849 | LYS | C-O | -7.46 | 1.15 | 1.24 |
| 8 | i7 | 127 | ALA | C-O | -7.46 | 1.14 | 1.24 |
| 9 | z7 | 27 | PHE | C-O | -7.46 | 1.15 | 1.24 |
| 9 | z5 | 31 | LEU | C-O | -7.46 | 1.14 | 1.24 |
| 10 | j5 | 655 | LYS | CA-CB | -7.46 | 1.43 | 1.54 |
| 10 | k5 | 655 | LYS | CA-CB | -7.46 | 1.43 | 1.54 |
| 10 | k5 | 773 | VAL | N-CA | -7.45 | 1.36 | 1.46 |
| 10 | j5 | 784 | ILE | C-O | -7.45 | 1.16 | 1.24 |
| 10 | j5 | 996 | ALA | C-O | -7.45 | 1.15 | 1.24 |
| 11 | a9 | 58 | GLY | N-CA | 7.45 | 1.55 | 1.45 |
| 11 | aA | 58 | GLY | N-CA | 7.45 | 1.55 | 1.45 |
| 10 | j5 | 885 | GLN | C-O | -7.45 | 1.15 | 1.24 |
| 1 | b7 | 48 | ALA | CA-C | -7.45 | 1.43 | 1.52 |
| 9 | y7 | 4 | TYR | CA-C | -7.45 | 1.43 | 1.52 |
| 9 | z5 | 4 | TYR | CA-C | -7.45 | 1.43 | 1.52 |
| 9 | i5 | 4 | TYR | CA-C | -7.45 | 1.43 | 1.52 |
| 10 | j5 | 541 | THR | C-O | -7.45 | 1.14 | 1.24 |
| 10 | j5 | 773 | VAL | N-CA | -7.45 | 1.36 | 1.46 |
| 8 | I5 | 10 | ASN | C-O | -7.44 | 1.14 | 1.24 |
| 10 | j5 | 261 | ILE | CA-C | -7.44 | 1.43 | 1.52 |
| 10 | j5 | 630 | ILE | CA-CB | -7.44 | 1.43 | 1.54 |
| 10 | k5 | 611 | GLU | CA-C | -7.44 | 1.43 | 1.52 |
| 10 | j5 | 653 | SER | CA-C | -7.44 | 1.42 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 10 | k5 | 856 | ARG | CA-C | -7.44 | 1.43 | 1.52 |
| 10 | j5 | 847 | LEU | CA-C | -7.44 | 1.43 | 1.52 |
| 10 | k5 | 847 | LEU | CA-C | -7.44 | 1.43 | 1.52 |
| 10 | j5 | 712 | ARG | C-O | -7.44 | 1.15 | 1.23 |
| 1 | h7 | 48 | ALA | CA-C | -7.44 | 1.43 | 1.52 |
| 8 | c7 | 116 | TYR | CA-C | -7.44 | 1.43 | 1.52 |
| 10 | j5 | 672 | GLU | CA-C | -7.43 | 1.43 | 1.52 |
| 10 | j5 | 7 | SER | C-O | -7.43 | 1.13 | 1.24 |
| 3 | H6 | 84 | ARG | CA-CB | -7.43 | 1.41 | 1.53 |
| 10 | j5 | 613 | PHE | CA-C | -7.43 | 1.43 | 1.52 |
| 10 | k5 | 653 | SER | CA-C | -7.42 | 1.42 | 1.52 |
| 10 | k5 | 613 | PHE | CA-C | -7.42 | 1.43 | 1.52 |
| 10 | k5 | 672 | GLU | CA-C | -7.42 | 1.43 | 1.52 |
| 10 | k5 | 885 | GLN | C-O | -7.42 | 1.15 | 1.24 |
| 8 | K5 | 97 | VAL | C-O | -7.42 | 1.14 | 1.24 |
| 10 | j5 | 718 | MET | CA-C | -7.42 | 1.43 | 1.52 |
| 10 | j5 | 637 | ARG | CZ-NH2 | -7.41 | 1.23 | 1.33 |
| 10 | j5 | 770 | ALA | C-O | -7.41 | 1.14 | 1.24 |
| 10 | j5 | 779 | ASP | C-O | -7.41 | 1.15 | 1.24 |
| 10 | k5 | 499 | ALA | C-O | -7.41 | 1.15 | 1.24 |
| 10 | j5 | 904 | PHE | C-O | -7.41 | 1.13 | 1.23 |
| 10 | j5 | 721 | LYS | N-CA | -7.41 | 1.37 | 1.46 |
| 10 | j5 | 782 | SER | C-O | -7.41 | 1.14 | 1.24 |
| 10 | k5 | 782 | SER | C-O | -7.41 | 1.14 | 1.24 |
| 8 | E5 | 105 | GLU | C-O | -7.40 | 1.15 | 1.24 |
| 10 | k5 | 606 | ALA | CA-C | -7.40 | 1.43 | 1.52 |
| 10 | k5 | 848 | ILE | C-O | -7.40 | 1.15 | 1.24 |
| 10 | j5 | 683 | ARG | CZ-NH1 | -7.40 | 1.22 | 1.32 |
| 10 | k5 | 704 | THR | CB-CG2 | -7.40 | 1.28 | 1.52 |
| 10 | j5 | 873 | GLY | C-O | -7.40 | 1.15 | 1.23 |
| 10 | k5 | 849 | LYS | C-O | -7.39 | 1.15 | 1.24 |
| 9 | w7 | 27 | PHE | C-O | -7.39 | 1.15 | 1.24 |
| 10 | k5 | 896 | ASN | CA-C | -7.39 | 1.43 | 1.52 |
| 10 | k5 | 781 | ALA | C-O | -7.39 | 1.14 | 1.24 |
| 10 | k5 | 860 | LYS | C-O | -7.39 | 1.14 | 1.24 |
| 8 | K5 | 112 | VAL | C-O | -7.39 | 1.14 | 1.24 |
| 3 | H2 | 84 | ARG | CA-CB | -7.38 | 1.41 | 1.53 |
| 10 | k5 | 456 | ILE | CA-C | -7.38 | 1.43 | 1.52 |
| 10 | k5 | 712 | ARG | C-O | -7.38 | 1.15 | 1.23 |
| 10 | k5 | 683 | ARG | CZ-NH1 | -7.38 | 1.22 | 1.32 |
| 10 | j5 | 704 | THR | CB-CG2 | -7.38 | 1.28 | 1.52 |
| 10 | k5 | 652 | ALA | N-CA | -7.38 | 1.36 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 10 | j5 | 499 | ALA | C-O | -7.37 | 1.15 | 1.24 |
| 10 | j5 | 896 | ASN | CA-C | -7.37 | 1.43 | 1.52 |
| 10 | k5 | 830 | GLU | N-CA | -7.37 | 1.37 | 1.46 |
| 4 | M8 | 12 | GLY | N-CA | -7.37 | 1.37 | 1.45 |
| 10 | k5 | 541 | THR | C-O | -7.37 | 1.14 | 1.24 |
| 10 | k5 | 904 | PHE | C-O | -7.37 | 1.13 | 1.23 |
| 10 | k5 | 298 | ARG | C-O | -7.37 | 1.14 | 1.24 |
| 8 | C5 | 10 | ASN | C-O | -7.37 | 1.14 | 1.24 |
| 10 | j5 | 642 | ARG | CA-C | -7.37 | 1.42 | 1.52 |
| 10 | j5 | 848 | ILE | C-O | -7.37 | 1.15 | 1.24 |
| 4 | M4 | 37 | GLU | C-O | -7.37 | 1.14 | 1.24 |
| 10 | k5 | 940 | ALA | CA-C | -7.37 | 1.43 | 1.52 |
| 10 | j5 | 456 | ILE | CA-C | -7.36 | 1.43 | 1.52 |
| 10 | j5 | 783 | TYR | CA-C | -7.36 | 1.42 | 1.52 |
| 10 | k5 | 783 | TYR | CA-C | -7.36 | 1.42 | 1.52 |
| 10 | j5 | 652 | ALA | N-CA | -7.36 | 1.36 | 1.46 |
| 10 | k5 | 637 | ARG | CZ-NH2 | -7.36 | 1.23 | 1.33 |
| 10 | j5 | 860 | LYS | C-O | -7.36 | 1.14 | 1.24 |
| 8 | i7 | 116 | TYR | CA-C | -7.36 | 1.43 | 1.52 |
| 10 | k5 | 556 | GLY | C-O | -7.35 | 1.15 | 1.23 |
| 10 | j5 | 606 | ALA | CA-C | -7.35 | 1.43 | 1.52 |
| 10 | j5 | 528 | GLU | C-O | -7.35 | 1.15 | 1.24 |
| 10 | j5 | 609 | ARG | C-O | -7.35 | 1.14 | 1.24 |
| 11 | a9 | 579 | PHE | C-O | -7.35 | 1.15 | 1.24 |
| 11 | aA | 579 | PHE | C-O | -7.35 | 1.15 | 1.24 |
| 10 | k5 | 779 | ASP | C-O | -7.34 | 1.15 | 1.24 |
| 4 | M8 | 37 | GLU | C-O | -7.34 | 1.14 | 1.24 |
| 10 | k5 | 721 | LYS | N-CA | -7.34 | 1.37 | 1.46 |
| 11 | a9 | 823 | ILE | CA-C | -7.34 | 1.46 | 1.52 |
| 10 | k5 | 873 | GLY | C-O | -7.34 | 1.15 | 1.23 |
| 4 | M4 | 12 | GLY | N-CA | -7.33 | 1.37 | 1.45 |
| 8 | E5 | 112 | VAL | C-O | -7.33 | 1.14 | 1.24 |
| 10 | j5 | 728 | PRO | C-O | -7.33 | 1.15 | 1.24 |
| 4 | M3 | 37 | GLU | C-O | -7.33 | 1.14 | 1.24 |
| 4 | M1 | 37 | GLU | C-O | -7.33 | 1.14 | 1.24 |
| 8 | K5 | 130 | VAL | C-O | -7.33 | 1.15 | 1.24 |
| 8 | E5 | 129 | GLY | C-O | -7.32 | 1.15 | 1.23 |
| 10 | j5 | 261 | ILE | C-O | -7.32 | 1.15 | 1.24 |
| 10 | j5 | 523 | PRO | C-O | -7.32 | 1.14 | 1.24 |
| 10 | k5 | 564 | VAL | CA-C | -7.32 | 1.43 | 1.52 |
| 11 | a9 | 451 | PHE | C-O | -7.32 | 1.15 | 1.24 |
| 11 | aA | 451 | PHE | C-O | -7.32 | 1.15 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4 | M8 | 70 | SER | CA-C | -7.32 | 1.44 | 1.52 |
| 11 | a9 | 586 | LEU | C-O | -7.32 | 1.15 | 1.24 |
| 10 | j5 | 526 | MET | C-O | -7.32 | 1.13 | 1.23 |
| 10 | j5 | 881 | VAL | CA-C | -7.32 | 1.46 | 1.52 |
| 10 | j5 | 454 | GLN | CA-C | -7.31 | 1.43 | 1.52 |
| 10 | j5 | 830 | GLU | N-CA | -7.31 | 1.37 | 1.46 |
| 9 | x7 | 4 | TYR | CA-C | -7.30 | 1.44 | 1.52 |
| 10 | j5 | 940 | ALA | CA-C | -7.30 | 1.43 | 1.52 |
| 10 | k5 | 609 | ARG | C-O | -7.30 | 1.14 | 1.24 |
| 9 | z5 | 29 | THR | C-O | -7.30 | 1.14 | 1.24 |
| 10 | j5 | 298 | ARG | C-O | -7.30 | 1.14 | 1.24 |
| 10 | k5 | 28 | ILE | C-O | -7.29 | 1.15 | 1.24 |
| 8 | K5 | 129 | GLY | C-O | -7.29 | 1.15 | 1.23 |
| 10 | k5 | 474 | ALA | CA-C | -7.29 | 1.42 | 1.52 |
| 8 | K5 | 105 | GLU | C-O | -7.28 | 1.15 | 1.24 |
| 9 | w7 | 4 | TYR | C-O | -7.28 | 1.15 | 1.23 |
| 10 | k5 | 528 | GLU | C-O | -7.28 | 1.15 | 1.24 |
| 8 | A5 | 53 | GLN | C-O | -7.27 | 1.15 | 1.24 |
| 10 | k5 | 7 | SER | C-O | -7.27 | 1.14 | 1.24 |
| 10 | j5 | 1005 | LEU | C-O | -7.27 | 1.15 | 1.24 |
| 10 | k5 | 642 | ARG | CA-C | -7.27 | 1.42 | 1.52 |
| 10 | k5 | 454 | GLN | CA-C | -7.27 | 1.43 | 1.52 |
| 9 | z7 | 4 | TYR | C-O | -7.27 | 1.15 | 1.23 |
| 10 | k5 | 435 | ASN | C-O | -7.27 | 1.12 | 1.23 |
| 1 | F5 | 3 | ASP | CA-C | -7.27 | 1.43 | 1.53 |
| 10 | k5 | 728 | PRO | C-O | -7.26 | 1.15 | 1.24 |
| 10 | j5 | 996 | ALA | CA-C | -7.26 | 1.43 | 1.52 |
| 4 | M3 | 40 | GLN | C-O | -7.26 | 1.13 | 1.23 |
| 8 | G5 | 53 | GLN | C-O | -7.26 | 1.15 | 1.24 |
| 4 | M1 | 40 | GLN | C-O | -7.26 | 1.13 | 1.23 |
| 10 | j5 | 1004 | VAL | C-O | -7.26 | 1.16 | 1.24 |
| 10 | k5 | 256 | LEU | C-O | -7.26 | 1.14 | 1.23 |
| 10 | k5 | 1004 | VAL | C-O | -7.26 | 1.16 | 1.24 |
| 10 | j5 | 659 | GLY | CA-C | -7.26 | 1.43 | 1.52 |
| 10 | k5 | 659 | GLY | CA-C | -7.26 | 1.43 | 1.52 |
| 4 | M4 | 40 | GLN | C-O | -7.26 | 1.13 | 1.23 |
| 4 | M4 | 70 | SER | CA-C | -7.26 | 1.44 | 1.52 |
| 4 | MA | 37 | GLU | C-O | -7.25 | 1.14 | 1.24 |
| 4 | M4 | 34 | ASP | C-O | -7.25 | 1.14 | 1.24 |
| 9 | i5 | 29 | THR | C-O | -7.25 | 1.14 | 1.24 |
| 4 | M9 | 37 | GLU | C-O | -7.25 | 1.14 | 1.24 |
| 4 | M3 | 34 | ASP | C-O | -7.25 | 1.14 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4 | M3 | 70 | SER | CA-C | -7.25 | 1.44 | 1.52 |
| 1 | L5 | 3 | ASP | CA-C | -7.25 | 1.43 | 1.53 |
| 10 | k5 | 526 | MET | C-O | -7.25 | 1.14 | 1.23 |
| 10 | k5 | 682 | GLU | CA-CB | -7.25 | 1.42 | 1.53 |
| 10 | k5 | 794 | ARG | C-O | -7.25 | 1.15 | 1.24 |
| 4 | M8 | 34 | ASP | C-O | -7.25 | 1.14 | 1.24 |
| 4 | M1 | 34 | ASP | C-O | -7.25 | 1.14 | 1.24 |
| 4 | M1 | 70 | SER | CA-C | -7.25 | 1.44 | 1.52 |
| 11 | aA | 586 | LEU | C-O | -7.25 | 1.15 | 1.24 |
| 10 | j5 | 28 | ILE | C-O | -7.25 | 1.15 | 1.24 |
| 10 | j5 | 933 | ALA | CA-C | -7.25 | 1.42 | 1.52 |
| 10 | k5 | 261 | ILE | C-O | -7.25 | 1.15 | 1.24 |
| 4 | MA | 70 | SER | CA-C | -7.25 | 1.44 | 1.52 |
| 8 | E5 | 130 | VAL | C-O | -7.25 | 1.15 | 1.24 |
| 10 | k5 | 842 | LYS | CA-CB | -7.25 | 1.41 | 1.53 |
| 4 | M9 | 70 | SER | CA-C | -7.25 | 1.44 | 1.52 |
| 10 | j5 | 750 | ARG | CZ-NH1 | -7.25 | 1.22 | 1.32 |
| 10 | k5 | 6 | THR | C-O | -7.25 | 1.15 | 1.23 |
| 10 | k5 | 750 | ARG | CZ-NH1 | -7.25 | 1.22 | 1.32 |
| 4 | MA | 12 | GLY | N-CA | -7.24 | 1.37 | 1.45 |
| 4 | M3 | 12 | GLY | N-CA | -7.24 | 1.37 | 1.45 |
| 4 | M8 | 53 | LEU | CA-C | -7.24 | 1.43 | 1.52 |
| 4 | M9 | 12 | GLY | N-CA | -7.24 | 1.37 | 1.45 |
| 4 | M1 | 12 | GLY | N-CA | -7.24 | 1.37 | 1.45 |
| 8 | A5 | 58 | LEU | C-O | -7.24 | 1.15 | 1.24 |
| 10 | k5 | 881 | VAL | CA-C | -7.24 | 1.46 | 1.52 |
| 8 | g7 | 12 | ASP | N-CA | -7.24 | 1.36 | 1.46 |
| 10 | j5 | 738 | TYR | C-O | -7.24 | 1.14 | 1.24 |
| 10 | j5 | 799 | GLU | CA-CB | -7.24 | 1.42 | 1.53 |
| 10 | k5 | 799 | GLU | CA-CB | -7.24 | 1.42 | 1.53 |
| 11 | aA | 823 | ILE | CA-C | -7.24 | 1.46 | 1.53 |
| 8 | a7 | 12 | ASP | N-CA | -7.23 | 1.36 | 1.46 |
| 10 | j5 | 6 | THR | C-O | -7.23 | 1.15 | 1.23 |
| 4 | M4 | 53 | LEU | CA-C | -7.22 | 1.43 | 1.52 |
| 8 | G5 | 58 | LEU | C-O | -7.22 | 1.15 | 1.24 |
| 10 | j5 | 739 | VAL | CA-C | -7.22 | 1.43 | 1.52 |
| 10 | k5 | 996 | ALA | CA-C | -7.22 | 1.43 | 1.52 |
| 4 | M3 | 53 | LEU | CA-C | -7.22 | 1.43 | 1.52 |
| 4 | M1 | 53 | LEU | CA-C | -7.22 | 1.43 | 1.52 |
| 10 | j5 | 794 | ARG | C-O | -7.22 | 1.15 | 1.24 |
| 4 | M8 | 40 | GLN | C-O | -7.22 | 1.13 | 1.23 |
| 10 | j5 | 435 | ASN | C-O | -7.22 | 1.12 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4 | MA | 40 | GLN | C-O | -7.21 | 1.13 | 1.23 |
| 10 | j5 | 428 | VAL | C-O | -7.21 | 1.15 | 1.24 |
| 4 | M9 | 40 | GLN | C-O | -7.21 | 1.13 | 1.23 |
| 10 | j5 | 667 | SER | CA-C | -7.21 | 1.43 | 1.53 |
| 10 | j5 | 564 | VAL | CA-C | -7.21 | 1.43 | 1.52 |
| 10 | j5 | 342 | LEU | C-O | -7.20 | 1.15 | 1.24 |
| 10 | j5 | 682 | GLU | CA-CB | -7.20 | 1.42 | 1.53 |
| 10 | k5 | 713 | GLY | C-O | -7.20 | 1.14 | 1.24 |
| 10 | k5 | 933 | ALA | CA-C | -7.20 | 1.42 | 1.52 |
| 10 | k5 | 1005 | LEU | C-O | -7.20 | 1.15 | 1.24 |
| 10 | j5 | 481 | ILE | C-O | -7.20 | 1.15 | 1.24 |
| 8 | I5 | 11 | ALA | CA-C | -7.20 | 1.43 | 1.52 |
| 10 | j5 | 641 | ASP | CB-CG | -7.20 | 1.34 | 1.52 |
| 1 | h7 | 45 | SER | CA-C | -7.19 | 1.43 | 1.52 |
| 10 | j5 | 842 | LYS | CA-CB | -7.19 | 1.42 | 1.53 |
| 11 | a9 | 578 | MET | C-O | -7.19 | 1.15 | 1.24 |
| 11 | aA | 578 | MET | C-O | -7.19 | 1.15 | 1.24 |
| 10 | j5 | 470 | HIS | C-O | -7.19 | 1.14 | 1.23 |
| 10 | j5 | 534 | GLY | C-O | -7.19 | 1.14 | 1.24 |
| 10 | k5 | 470 | HIS | C-O | -7.19 | 1.14 | 1.23 |
| 10 | k5 | 534 | GLY | C-O | -7.19 | 1.14 | 1.24 |
| 10 | j5 | 492 | ILE | CA-CB | -7.19 | 1.46 | 1.54 |
| 10 | k5 | 492 | ILE | CA-CB | -7.19 | 1.46 | 1.54 |
| 10 | j5 | 256 | LEU | C-O | -7.18 | 1.14 | 1.23 |
| 10 | j5 | 773 | VAL | CA-CB | -7.18 | 1.45 | 1.54 |
| 10 | k5 | 773 | VAL | CA-CB | -7.18 | 1.45 | 1.54 |
| 4 | MA | 53 | LEU | CA-C | -7.18 | 1.43 | 1.52 |
| 10 | k5 | 1090 | ALA | C-O | -7.18 | 1.15 | 1.24 |
| 4 | M9 | 53 | LEU | CA-C | -7.18 | 1.43 | 1.52 |
| 8 | o7 | 57 | GLN | C-O | -7.18 | 1.15 | 1.24 |
| 4 | MA | 34 | ASP | C-O | -7.17 | 1.15 | 1.24 |
| 4 | M9 | 34 | ASP | C-O | -7.17 | 1.15 | 1.24 |
| 10 | k5 | 342 | LEU | C-O | -7.17 | 1.15 | 1.24 |
| 10 | k5 | 667 | SER | CA-C | -7.17 | 1.43 | 1.53 |
| 10 | j5 | 463 | THR | C-O | -7.16 | 1.14 | 1.24 |
| 10 | k5 | 463 | THR | C-O | -7.16 | 1.14 | 1.24 |
| 4 | M4 | 57 | THR | CA-C | -7.16 | 1.43 | 1.52 |
| 10 | j5 | 684 | TYR | CZ-OH | -7.16 | 1.23 | 1.38 |
| 4 | M3 | 57 | THR | CA-C | -7.16 | 1.43 | 1.52 |
| 8 | a5 | 12 | ASP | C-O | -7.16 | 1.15 | 1.24 |
| 9 | z5 | 42 | GLN | CA-C | -7.16 | 1.42 | 1.52 |
| 10 | j5 | 741 | GLN | CD-OE1 | -7.16 | 1.09 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | k5 | 523 | PRO | C-O | -7.16 | 1.14 | 1.24 |
| 8 | c7 | 128 | GLU | CA-C | -7.16 | 1.43 | 1.52 |
| 4 | M1 | 57 | THR | CA-C | -7.16 | 1.43 | 1.52 |
| 8 | e5 | 12 | ASP | C-O | -7.16 | 1.15 | 1.24 |
| 10 | k5 | 641 | ASP | CB-CG | -7.16 | 1.34 | 1.52 |
| 1 | b7 | 45 | SER | CA-C | -7.15 | 1.43 | 1.52 |
| 8 | C5 | 11 | ALA | CA-C | -7.15 | 1.43 | 1.52 |
| 10 | k5 | 663 | ALA | C-N | -7.15 | 1.24 | 1.33 |
| 9 | i5 | 42 | GLN | CA-C | -7.15 | 1.42 | 1.52 |
| 1 | D7 | 76 | ARG | CA-C | -7.15 | 1.43 | 1.52 |
| 10 | k5 | 379 | PHE | CA-C | -7.14 | 1.43 | 1.52 |
| 9 | z5 | 63 | ALA | CA-C | -7.14 | 1.44 | 1.52 |
| 10 | j5 | 431 | GLN | CA-C | -7.14 | 1.43 | 1.53 |
| 10 | k5 | 431 | GLN | CA-C | -7.14 | 1.43 | 1.53 |
| 10 | j5 | 713 | GLY | C-O | -7.14 | 1.14 | 1.24 |
| 10 | j5 | 1090 | ALA | C-O | -7.14 | 1.15 | 1.24 |
| 10 | k5 | 481 | ILE | C-O | -7.14 | 1.15 | 1.24 |
| 10 | k5 | 663 | ALA | N-CA | -7.14 | 1.37 | 1.46 |
| 10 | j5 | 379 | PHE | CA-C | -7.13 | 1.43 | 1.52 |
| 10 | k5 | 848 | ILE | CA-C | -7.13 | 1.43 | 1.52 |
| 3 | F9 | 148 | VAL | C-O | -7.13 | 1.16 | 1.24 |
| 10 | k5 | 684 | TYR | CZ-OH | -7.13 | 1.23 | 1.38 |
| 4 | MA | 57 | THR | CA-C | -7.13 | 1.43 | 1.52 |
| 4 | M3 | 40 | GLN | CA-C | -7.13 | 1.44 | 1.53 |
| 9 | i5 | 63 | ALA | CA-C | -7.13 | 1.44 | 1.52 |
| 10 | j5 | 1124 | TYR | CA-C | -7.13 | 1.43 | 1.52 |
| 10 | k5 | 1124 | TYR | CA-C | -7.13 | 1.43 | 1.52 |
| 4 | M8 | 57 | THR | CA-C | -7.13 | 1.43 | 1.52 |
| 4 | M1 | 40 | GLN | CA-C | -7.13 | 1.44 | 1.53 |
| 10 | j5 | 848 | ILE | CA-C | -7.12 | 1.43 | 1.52 |
| 10 | j5 | 518 | ASN | CA-C | -7.12 | 1.42 | 1.52 |
| 10 | j5 | 883 | SER | N-CA | 7.12 | 1.55 | 1.46 |
| 4 | MA | 40 | GLN | CA-C | -7.12 | 1.44 | 1.53 |
| 10 | j5 | 474 | ALA | CA-C | -7.12 | 1.42 | 1.52 |
| 4 | M9 | 40 | GLN | CA-C | -7.12 | 1.44 | 1.53 |
| 10 | j5 | 381 | ILE | CA-CB | -7.12 | 1.46 | 1.54 |
| 10 | k5 | 448 | PRO | CA-C | -7.12 | 1.43 | 1.52 |
| 10 | k5 | 428 | VAL | C-O | -7.11 | 1.15 | 1.24 |
| 10 | k5 | 400 | ALA | CA-C | -7.10 | 1.43 | 1.52 |
| 10 | k5 | 406 | ILE | C-O | -7.10 | 1.15 | 1.24 |
| 4 | M8 | 40 | GLN | CA-C | -7.10 | 1.44 | 1.53 |
| 10 | j5 | 400 | ALA | CA-C | -7.10 | 1.43 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 9 | z5 | 57 | PHE | N-CA | -7.10 | 1.37 | 1.46 |
| 10 | k5 | 602 | GLU | CA-C | -7.10 | 1.43 | 1.52 |
| 10 | j5 | 448 | PRO | CA-C | -7.09 | 1.43 | 1.52 |
| 10 | k5 | 514 | SER | C-O | -7.09 | 1.14 | 1.24 |
| 10 | k5 | 381 | ILE | CA-CB | -7.09 | 1.46 | 1.54 |
| 10 | k5 | 371 | SER | CA-C | -7.09 | 1.44 | 1.52 |
| 10 | j5 | 514 | SER | C-O | -7.09 | 1.14 | 1.24 |
| 4 | M4 | 40 | GLN | CA-C | -7.09 | 1.44 | 1.53 |
| 8 | a5 | 9 | VAL | C-O | -7.09 | 1.14 | 1.24 |
| 10 | j5 | 371 | SER | CA-C | -7.09 | 1.44 | 1.52 |
| 10 | j5 | 450 | ARG | CA-C | -7.09 | 1.44 | 1.52 |
| 10 | j5 | 645 | ASN | CA-C | -7.09 | 1.43 | 1.52 |
| 10 | k5 | 625 | LYS | CA-CB | -7.09 | 1.41 | 1.53 |
| 10 | k5 | 645 | ASN | CA-C | -7.09 | 1.43 | 1.52 |
| 8 | E5 | 117 | ASN | CA-C | -7.08 | 1.43 | 1.52 |
| 10 | k5 | 450 | ARG | CA-C | -7.08 | 1.44 | 1.52 |
| 8 | i7 | 128 | GLU | CA-C | -7.08 | 1.43 | 1.52 |
| 8 | u7 | 57 | GLN | C-O | -7.08 | 1.15 | 1.24 |
| 9 | i5 | 57 | PHE | N-CA | -7.08 | 1.37 | 1.46 |
| 10 | k5 | 741 | GLN | CD-OE1 | -7.08 | 1.10 | 1.23 |
| 10 | k5 | 518 | ASN | CA-C | -7.08 | 1.42 | 1.52 |
| 10 | k5 | 662 | ASP | C-O | -7.08 | 1.14 | 1.24 |
| 8 | e5 | 9 | VAL | C-O | -7.08 | 1.14 | 1.24 |
| 10 | j5 | 763 | SER | CA-CB | -7.08 | 1.41 | 1.53 |
| 10 | j5 | 1127 | SER | CA-C | -7.08 | 1.43 | 1.52 |
| 10 | k5 | 1130 | VAL | CA-C | -7.08 | 1.43 | 1.52 |
| 4 | M9 | 57 | THR | CA-C | -7.08 | 1.43 | 1.52 |
| 4 | M4 | 39 | SER | C-O | -7.08 | 1.14 | 1.24 |
| 11 | a9 | 523 | GLN | C-O | -7.08 | 1.15 | 1.24 |
| 11 | aA | 523 | GLN | C-O | -7.08 | 1.15 | 1.24 |
| 10 | k5 | 885 | GLN | CA-C | -7.07 | 1.44 | 1.52 |
| 10 | k5 | 579 | GLN | C-O | -7.07 | 1.14 | 1.23 |
| 10 | j5 | 476 | ASN | CG-OD1 | -7.07 | 1.10 | 1.23 |
| 10 | j5 | 1130 | VAL | CA-C | -7.07 | 1.43 | 1.52 |
| 10 | k5 | 476 | ASN | CG-OD1 | -7.07 | 1.10 | 1.23 |
| 10 | j5 | 917 | LYS | C-O | -7.06 | 1.15 | 1.24 |
| 10 | k5 | 917 | LYS | C-O | -7.06 | 1.15 | 1.24 |
| 1 | J7 | 76 | ARG | CA-C | -7.06 | 1.43 | 1.52 |
| 10 | j5 | 602 | GLU | CA-C | -7.06 | 1.43 | 1.52 |
| 10 | j5 | 663 | ALA | N-CA | -7.06 | 1.37 | 1.46 |
| 11 | aA | 339 | GLU | CA-C | -7.06 | 1.44 | 1.52 |
| 10 | j5 | 406 | ILE | C-O | -7.05 | 1.15 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 10 | j5 | 691 | SER | N-CA | -7.05 | 1.37 | 1.46 |
| 10 | k5 | 691 | SER | N-CA | -7.05 | 1.37 | 1.46 |
| 10 | k5 | 883 | SER | N-CA | 7.05 | 1.55 | 1.46 |
| 10 | j5 | 829 | VAL | CA-CB | -7.05 | 1.45 | 1.54 |
| 10 | j5 | 625 | LYS | CA-CB | -7.04 | 1.42 | 1.53 |
| 10 | k5 | 763 | SER | CA-CB | -7.04 | 1.41 | 1.53 |
| 10 | j5 | 373 | ALA | CA-C | -7.04 | 1.43 | 1.52 |
| 10 | j5 | 971 | VAL | C-O | -7.04 | 1.15 | 1.24 |
| 10 | k5 | 819 | PHE | C-O | -7.04 | 1.13 | 1.23 |
| 4 | M8 | 196 | TYR | CA-C | -7.04 | 1.43 | 1.52 |
| 10 | k5 | 971 | VAL | C-O | -7.04 | 1.15 | 1.24 |
| 10 | j5 | 430 | ALA | CA-CB | -7.04 | 1.43 | 1.53 |
| 8 | c7 | 130 | VAL | C-O | -7.04 | 1.15 | 1.24 |
| 9 | z7 | 54 | VAL | C-O | -7.04 | 1.16 | 1.24 |
| 10 | j5 | 761 | ARG | CA-C | -7.03 | 1.43 | 1.52 |
| 4 | MA | 196 | TYR | CA-C | -7.03 | 1.43 | 1.52 |
| 10 | j5 | 826 | THR | C-O | -7.03 | 1.14 | 1.24 |
| 10 | k5 | 826 | THR | C-O | -7.03 | 1.14 | 1.24 |
| 4 | M9 | 196 | TYR | CA-C | -7.03 | 1.43 | 1.52 |
| 10 | j5 | 821 | ASP | C-O | -7.03 | 1.14 | 1.24 |
| 10 | k5 | 821 | ASP | C-O | -7.03 | 1.14 | 1.24 |
| 10 | j5 | 663 | ALA | C-N | -7.03 | 1.24 | 1.33 |
| 10 | k5 | 678 | VAL | C-O | -7.02 | 1.15 | 1.24 |
| 10 | j5 | 320 | GLU | CA-C | -7.02 | 1.43 | 1.52 |
| 10 | j5 | 757 | GLN | N-CA | -7.02 | 1.37 | 1.46 |
| 10 | j5 | 678 | VAL | C-O | -7.02 | 1.15 | 1.24 |
| 10 | j5 | 953 | LEU | C-O | -7.02 | 1.15 | 1.24 |
| 10 | k5 | 953 | LEU | C-O | -7.02 | 1.15 | 1.24 |
| 11 | a9 | 339 | GLU | CA-C | -7.02 | 1.44 | 1.52 |
| 10 | j5 | 579 | GLN | C-O | -7.01 | 1.14 | 1.23 |
| 10 | j5 | 662 | ASP | C-O | -7.01 | 1.15 | 1.24 |
| 10 | j5 | 403 | ASP | CA-CB | -7.01 | 1.42 | 1.53 |
| 10 | j5 | 820 | HIS | CA-C | -7.01 | 1.43 | 1.52 |
| 10 | k5 | 403 | ASP | CA-CB | -7.01 | 1.42 | 1.53 |
| 10 | k5 | 583 | GLY | C-O | -7.01 | 1.15 | 1.23 |
| 10 | k5 | 928 | MET | C-O | -7.01 | 1.15 | 1.23 |
| 4 | M4 | 196 | TYR | CA-C | -7.01 | 1.43 | 1.52 |
| 10 | j5 | 698 | GLY | C-O | -7.01 | 1.13 | 1.24 |
| 10 | k5 | 761 | ARG | CA-C | -7.01 | 1.43 | 1.52 |
| 4 | M3 | 196 | TYR | CA-C | -7.00 | 1.43 | 1.52 |
| 10 | j5 | 654 | LYS | C-O | -7.00 | 1.14 | 1.23 |
| 10 | k5 | 654 | LYS | C-O | -7.00 | 1.14 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4 | M1 | 196 | TYR | CA-C | -7.00 | 1.43 | 1.52 |
| 10 | j5 | 928 | MET | C-O | -7.00 | 1.15 | 1.23 |
| 10 | k5 | 698 | GLY | C-O | -7.00 | 1.13 | 1.24 |
| 10 | j5 | 885 | GLN | CA-C | -7.00 | 1.44 | 1.52 |
| 10 | k5 | 820 | HIS | CA-C | -7.00 | 1.43 | 1.52 |
| 4 | MA | 39 | SER | C-O | -7.00 | 1.14 | 1.24 |
| 10 | k5 | 1127 | SER | CA-C | -7.00 | 1.43 | 1.52 |
| 8 | i7 | 130 | VAL | C-O | -7.00 | 1.15 | 1.24 |
| 4 | M9 | 39 | SER | C-O | -7.00 | 1.14 | 1.24 |
| 10 | j5 | 819 | PHE | C-O | -7.00 | 1.13 | 1.23 |
| 10 | k5 | 758 | ALA | C-O | -7.00 | 1.13 | 1.23 |
| 10 | k5 | 757 | GLN | N-CA | -6.99 | 1.37 | 1.46 |
| 10 | k5 | 858 | GLY | C-O | -6.99 | 1.13 | 1.23 |
| 4 | M3 | 39 | SER | C-O | -6.99 | 1.14 | 1.24 |
| 4 | M4 | 44 | SER | C-O | -6.99 | 1.15 | 1.23 |
| 10 | j5 | 699 | SER | CA-C | -6.99 | 1.44 | 1.52 |
| 10 | k5 | 699 | SER | CA-C | -6.99 | 1.44 | 1.52 |
| 4 | M1 | 39 | SER | C-O | -6.99 | 1.14 | 1.24 |
| 10 | j5 | 494 | PRO | C-O | -6.99 | 1.14 | 1.23 |
| 10 | j5 | 974 | LEU | CA-C | -6.99 | 1.42 | 1.52 |
| 10 | k5 | 316 | VAL | CA-C | -6.99 | 1.46 | 1.53 |
| 10 | k5 | 494 | PRO | C-O | -6.99 | 1.14 | 1.23 |
| 3 | L9 | 97 | LEU | C-O | -6.99 | 1.16 | 1.24 |
| 4 | M8 | 44 | SER | C-O | -6.99 | 1.15 | 1.23 |
| 10 | k5 | 293 | LYS | N-CA | -6.99 | 1.38 | 1.46 |
| 10 | k5 | 833 | PHE | CA-C | -6.99 | 1.43 | 1.52 |
| 10 | j5 | 875 | LEU | N-CA | -6.98 | 1.38 | 1.46 |
| 10 | j5 | 758 | ALA | C-O | -6.98 | 1.13 | 1.23 |
| 4 | M8 | 58 | TYR | CA-C | -6.98 | 1.44 | 1.52 |
| 10 | k5 | 487 | PHE | N-CA | 6.98 | 1.55 | 1.46 |
| 9 | w7 | 34 | TYR | C-O | -6.98 | 1.16 | 1.24 |
| 9 | w7 | 54 | VAL | C-O | -6.98 | 1.16 | 1.24 |
| 10 | j5 | 402 | ILE | CA-CB | -6.97 | 1.45 | 1.54 |
| 10 | j5 | 779 | ASP | CA-C | -6.97 | 1.43 | 1.52 |
| 10 | k5 | 829 | VAL | CA-CB | -6.97 | 1.45 | 1.54 |
| 10 | k5 | 849 | LYS | CA-CB | -6.97 | 1.42 | 1.53 |
| 8 | o7 | 43 | LEU | C-O | -6.97 | 1.15 | 1.24 |
| 4 | M8 | 39 | SER | C-O | -6.97 | 1.14 | 1.24 |
| 8 | K5 | 117 | ASN | CA-C | -6.97 | 1.43 | 1.52 |
| 10 | k5 | 875 | LEU | N-CA | -6.97 | 1.38 | 1.46 |
| 9 | z7 | 67 | VAL | N-CA | -6.97 | 1.38 | 1.46 |
| 10 | j5 | 677 | ASP | CA-CB | -6.97 | 1.41 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 10 | k5 | 430 | ALA | CA-CB | -6.97 | 1.43 | 1.53 |
| 4 | MA | 44 | SER | C-O | -6.96 | 1.15 | 1.23 |
| 10 | j5 | 714 | ASP | C-O | -6.96 | 1.15 | 1.24 |
| 10 | k5 | 714 | ASP | C-O | -6.96 | 1.15 | 1.24 |
| 4 | M9 | 44 | SER | C-O | -6.96 | 1.15 | 1.23 |
| 10 | k5 | 373 | ALA | CA-C | -6.96 | 1.43 | 1.52 |
| 8 | u7 | 43 | LEU | C-O | -6.96 | 1.15 | 1.24 |
| 4 | M3 | 44 | SER | C-O | -6.96 | 1.15 | 1.23 |
| 4 | M1 | 44 | SER | C-O | -6.96 | 1.15 | 1.23 |
| 10 | j5 | 585 | ARG | C-O | -6.96 | 1.15 | 1.23 |
| 9 | w7 | 67 | VAL | N-CA | -6.96 | 1.38 | 1.46 |
| 10 | j5 | 440 | TYR | C-O | -6.95 | 1.15 | 1.24 |
| 10 | k5 | 440 | TYR | C-O | -6.95 | 1.15 | 1.24 |
| 10 | k5 | 681 | TYR | CA-C | -6.95 | 1.43 | 1.52 |
| 4 | M4 | 58 | TYR | CA-C | -6.95 | 1.44 | 1.52 |
| 10 | j5 | 316 | VAL | CA-C | -6.95 | 1.46 | 1.53 |
| 10 | k5 | 677 | ASP | CA-CB | -6.95 | 1.41 | 1.53 |
| 10 | j5 | 367 | ARG | C-O | -6.95 | 1.15 | 1.23 |
| 10 | j5 | 487 | PHE | N-CA | 6.95 | 1.55 | 1.46 |
| 10 | k5 | 367 | ARG | C-O | -6.95 | 1.15 | 1.23 |
| 10 | j5 | 849 | LYS | CA-CB | -6.94 | 1.42 | 1.53 |
| 10 | j5 | 858 | GLY | C-O | -6.94 | 1.13 | 1.23 |
| 10 | k5 | 892 | ALA | CA-C | -6.94 | 1.42 | 1.52 |
| 10 | j5 | 293 | LYS | N-CA | -6.94 | 1.38 | 1.46 |
| 9 | z7 | 25 | ASN | C-O | -6.93 | 1.14 | 1.23 |
| 9 | w7 | 25 | ASN | C-O | -6.93 | 1.14 | 1.23 |
| 10 | j5 | 892 | ALA | CA-C | -6.93 | 1.42 | 1.52 |
| 10 | k5 | 779 | ASP | CA-C | -6.93 | 1.43 | 1.52 |
| 3 | LA | 97 | LEU | C-O | -6.93 | 1.16 | 1.24 |
| 10 | j5 | 757 | GLN | C-O | -6.93 | 1.13 | 1.23 |
| 10 | k5 | 757 | GLN | C-O | -6.93 | 1.13 | 1.23 |
| 4 | M4 | 42 | SER | CA-C | -6.92 | 1.44 | 1.52 |
| 10 | k5 | 585 | ARG | C-O | -6.92 | 1.15 | 1.23 |
| 10 | j5 | 622 | TYR | CA-C | -6.92 | 1.44 | 1.52 |
| 10 | k5 | 622 | TYR | CA-C | -6.92 | 1.44 | 1.52 |
| 9 | z7 | 34 | TYR | C-O | -6.92 | 1.16 | 1.24 |
| 4 | M4 | 62 | LYS | C-O | -6.92 | 1.15 | 1.24 |
| 10 | j5 | 491 | THR | C-O | -6.91 | 1.15 | 1.24 |
| 10 | j5 | 833 | PHE | CA-C | -6.91 | 1.43 | 1.52 |
| 4 | M8 | 62 | LYS | C-O | -6.91 | 1.15 | 1.24 |
| 10 | k5 | 660 | VAL | CA-CB | -6.91 | 1.45 | 1.54 |
| 10 | j5 | 762 | GLU | C-O | -6.91 | 1.16 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | k5 | 762 | GLU | C-O | -6.91 | 1.16 | 1.24 |
| 10 | k5 | 980 | HIS | CA-C | -6.91 | 1.44 | 1.52 |
| 4 | MA | 62 | LYS | C-O | -6.91 | 1.15 | 1.24 |
| 4 | M9 | 62 | LYS | C-O | -6.91 | 1.15 | 1.24 |
| 10 | k5 | 402 | ILE | CA-CB | -6.90 | 1.45 | 1.54 |
| 10 | k5 | 320 | GLU | CA-C | -6.90 | 1.43 | 1.52 |
| 8 | o7 | 82 | LEU | C-O | -6.90 | 1.15 | 1.24 |
| 10 | j5 | 620 | PRO | C-O | -6.89 | 1.16 | 1.23 |
| 10 | k5 | 620 | PRO | C-O | -6.89 | 1.16 | 1.23 |
| 10 | k5 | 728 | PRO | CA-CB | -6.89 | 1.43 | 1.53 |
| 10 | j5 | 476 | ASN | N-CA | -6.89 | 1.36 | 1.46 |
| 10 | j5 | 535 | PRO | CA-C | -6.89 | 1.43 | 1.52 |
| 10 | j5 | 681 | TYR | CA-C | -6.89 | 1.43 | 1.52 |
| 10 | k5 | 535 | PRO | CA-C | -6.89 | 1.43 | 1.52 |
| 10 | j5 | 821 | ASP | CA-C | -6.89 | 1.43 | 1.52 |
| 10 | k5 | 955 | LEU | CA-C | -6.89 | 1.43 | 1.52 |
| 4 | M3 | 42 | SER | CA-C | -6.89 | 1.44 | 1.52 |
| 4 | M1 | 42 | SER | CA-C | -6.89 | 1.44 | 1.52 |
| 4 | M3 | 62 | LYS | C-O | -6.89 | 1.15 | 1.24 |
| 9 | z5 | 5 | PHE | CA-C | -6.89 | 1.44 | 1.52 |
| 10 | k5 | 974 | LEU | CA-C | -6.89 | 1.43 | 1.52 |
| 4 | M1 | 62 | LYS | C-O | -6.89 | 1.15 | 1.24 |
| 9 | i5 | 5 | PHE | C-N | -6.88 | 1.24 | 1.33 |
| 10 | j5 | 1037 | ARG | C-O | -6.88 | 1.16 | 1.24 |
| 10 | k5 | 1037 | ARG | C-O | -6.88 | 1.16 | 1.24 |
| 10 | k5 | 771 | ALA | CA-C | -6.88 | 1.43 | 1.52 |
| 10 | j5 | 181 | ALA | C-O | -6.88 | 1.16 | 1.24 |
| 10 | k5 | 481 | ILE | CA-CB | -6.88 | 1.45 | 1.54 |
| 10 | k5 | 943 | THR | C-O | -6.88 | 1.16 | 1.24 |
| 4 | M8 | 42 | SER | CA-C | -6.88 | 1.44 | 1.52 |
| 8 | u7 | 82 | LEU | C-O | -6.87 | 1.15 | 1.24 |
| 11 | aA | 523 | GLN | CA-C | -6.87 | 1.43 | 1.52 |
| 8 | A5 | 48 | GLU | CA-CB | -6.87 | 1.42 | 1.53 |
| 8 | G5 | 48 | GLU | CA-CB | -6.87 | 1.42 | 1.53 |
| 10 | k5 | 476 | ASN | N-CA | -6.87 | 1.36 | 1.46 |
| 10 | j5 | 445 | TYR | C-O | -6.87 | 1.14 | 1.24 |
| 10 | j5 | 660 | VAL | CA-CB | -6.87 | 1.45 | 1.54 |
| 10 | j5 | 728 | PRO | CA-CB | -6.87 | 1.43 | 1.53 |
| 10 | k5 | 445 | TYR | C-O | -6.87 | 1.14 | 1.24 |
| 4 | M8 | 63 | GLY | C-O | -6.86 | 1.14 | 1.24 |
| 10 | j5 | 352 | ILE | C-N | 6.86 | 1.43 | 1.33 |
| 10 | k5 | 352 | ILE | C-N | 6.86 | 1.43 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4 | MA | 58 | TYR | CA-C | -6.86 | 1.44 | 1.52 |
| 8 | I5 | 19 | SER | CA-C | -6.86 | 1.44 | 1.53 |
| 9 | i5 | 5 | PHE | CA-C | -6.86 | 1.44 | 1.52 |
| 4 | MA | 42 | SER | C-O | -6.86 | 1.16 | 1.24 |
| 10 | j5 | 398 | LEU | CA-C | -6.86 | 1.43 | 1.52 |
| 4 | M9 | 42 | SER | C-O | -6.86 | 1.16 | 1.24 |
| 4 | M4 | 63 | GLY | C-O | -6.86 | 1.14 | 1.24 |
| 1 | J5 | 17 | LYS | C-O | -6.86 | 1.15 | 1.23 |
| 9 | z5 | 5 | PHE | C-N | -6.85 | 1.24 | 1.33 |
| 10 | j5 | 260 | TYR | C-O | -6.85 | 1.15 | 1.24 |
| 10 | k5 | 260 | TYR | C-O | -6.85 | 1.15 | 1.24 |
| 4 | M3 | 58 | TYR | CA-C | -6.85 | 1.44 | 1.52 |
| 4 | M1 | 58 | TYR | CA-C | -6.85 | 1.44 | 1.52 |
| 4 | MA | 42 | SER | CA-C | -6.85 | 1.44 | 1.52 |
| 4 | M9 | 42 | SER | CA-C | -6.85 | 1.44 | 1.52 |
| 4 | M3 | 63 | GLY | C-O | -6.85 | 1.14 | 1.24 |
| 4 | M1 | 63 | GLY | C-O | -6.85 | 1.14 | 1.24 |
| 10 | j5 | 980 | HIS | CA-C | -6.85 | 1.44 | 1.52 |
| 10 | j5 | 930 | LEU | CA-C | -6.84 | 1.44 | 1.52 |
| 10 | k5 | 930 | LEU | CA-C | -6.84 | 1.44 | 1.52 |
| 10 | k5 | 398 | LEU | CA-C | -6.84 | 1.43 | 1.52 |
| 10 | k5 | 679 | LEU | CA-C | -6.84 | 1.44 | 1.53 |
| 11 | a9 | 523 | GLN | CA-C | -6.84 | 1.43 | 1.52 |
| 4 | M4 | 14 | LEU | C-O | -6.84 | 1.15 | 1.23 |
| 9 | z5 | 31 | LEU | CA-C | -6.84 | 1.44 | 1.52 |
| 10 | j5 | 593 | LEU | CA-C | -6.84 | 1.44 | 1.52 |
| 10 | k5 | 491 | THR | C-O | -6.84 | 1.15 | 1.24 |
| 10 | k5 | 799 | GLU | CA-C | -6.84 | 1.43 | 1.52 |
| 10 | k5 | 784 | ILE | CA-CB | -6.84 | 1.46 | 1.54 |
| 10 | j5 | 512 | ASN | C-O | -6.83 | 1.14 | 1.23 |
| 10 | k5 | 512 | ASN | C-O | -6.83 | 1.14 | 1.23 |
| 4 | M9 | 58 | TYR | CA-C | -6.83 | 1.44 | 1.52 |
| 9 | i5 | 46 | LYS | CA-C | -6.83 | 1.43 | 1.52 |
| 10 | j5 | 52 | ARG | CA-C | -6.83 | 1.44 | 1.52 |
| 10 | j5 | 799 | GLU | CA-C | -6.83 | 1.43 | 1.52 |
| 10 | j5 | 863 | ILE | CA-C | -6.83 | 1.44 | 1.52 |
| 10 | j5 | 521 | GLY | C-O | -6.82 | 1.14 | 1.23 |
| 10 | j5 | 679 | LEU | CA-C | -6.82 | 1.44 | 1.53 |
| 10 | j5 | 711 | PRO | C-O | -6.82 | 1.15 | 1.24 |
| 8 | E5 | 131 | ARG | CA-C | -6.82 | 1.43 | 1.52 |
| 9 | z5 | 46 | LYS | CA-C | -6.82 | 1.43 | 1.52 |
| 10 | j5 | 258 | LEU | C-O | -6.82 | 1.15 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 10 | j5 | 547 | ARG | CA-C | -6.82 | 1.44 | 1.52 |
| 10 | k5 | 258 | LEU | C-O | -6.82 | 1.15 | 1.24 |
| 10 | k5 | 595 | ASN | C-O | -6.82 | 1.15 | 1.24 |
| 4 | M9 | 63 | GLY | C-O | -6.82 | 1.14 | 1.24 |
| 10 | j5 | 583 | GLY | C-O | -6.82 | 1.15 | 1.23 |
| 10 | k5 | 821 | ASP | CA-C | -6.82 | 1.43 | 1.52 |
| 10 | j5 | 423 | LEU | C-O | -6.82 | 1.16 | 1.24 |
| 10 | k5 | 593 | LEU | CA-C | -6.82 | 1.44 | 1.52 |
| 4 | M3 | 42 | SER | C-O | -6.81 | 1.16 | 1.24 |
| 10 | j5 | 481 | ILE | CA-CB | -6.81 | 1.45 | 1.54 |
| 10 | j5 | 378 | TYR | CA-C | -6.81 | 1.44 | 1.52 |
| 10 | k5 | 378 | TYR | CA-C | -6.81 | 1.44 | 1.52 |
| 8 | C5 | 19 | SER | CA-C | -6.81 | 1.44 | 1.53 |
| 9 | i5 | 34 | TYR | N-CA | -6.81 | 1.37 | 1.46 |
| 1 | D5 | 10 | ASN | CA-C | -6.80 | 1.43 | 1.52 |
| 10 | j5 | 955 | LEU | CA-C | -6.80 | 1.43 | 1.52 |
| 10 | k5 | 181 | ALA | C-O | -6.80 | 1.16 | 1.24 |
| 11 | a9 | 531 | ASP | C-O | -6.80 | 1.15 | 1.24 |
| 11 | aA | 531 | ASP | C-O | -6.80 | 1.15 | 1.24 |
| 9 | i5 | 31 | LEU | CA-C | -6.79 | 1.44 | 1.52 |
| 10 | k5 | 52 | ARG | CA-C | -6.79 | 1.44 | 1.52 |
| 10 | k5 | 784 | ILE | C-O | -6.79 | 1.16 | 1.24 |
| 4 | MA | 63 | GLY | C-O | -6.79 | 1.14 | 1.24 |
| 10 | j5 | 867 | VAL | C-O | -6.79 | 1.14 | 1.24 |
| 10 | k5 | 485 | ALA | CA-C | -6.79 | 1.44 | 1.53 |
| 10 | k5 | 646 | ASN | CA-C | -6.79 | 1.43 | 1.52 |
| 4 | MA | 72 | ALA | CA-C | -6.79 | 1.44 | 1.52 |
| 4 | M8 | 60 | LYS | C-O | -6.79 | 1.16 | 1.24 |
| 4 | M9 | 72 | ALA | CA-C | -6.79 | 1.44 | 1.52 |
| 1 | J5 | 9 | ILE | C-O | -6.79 | 1.15 | 1.24 |
| 10 | j5 | 259 | PRO | C-O | -6.79 | 1.15 | 1.23 |
| 4 | M3 | 198 | ALA | C-O | -6.79 | 1.16 | 1.24 |
| 10 | k5 | 753 | PHE | CA-CB | -6.79 | 1.43 | 1.53 |
| 4 | M1 | 198 | ALA | C-O | -6.79 | 1.16 | 1.24 |
| 4 | M1 | 42 | SER | C-O | -6.79 | 1.16 | 1.24 |
| 10 | j5 | 656 | GLY | CA-C | -6.78 | 1.42 | 1.51 |
| 10 | j5 | 943 | THR | C-O | -6.78 | 1.16 | 1.24 |
| 4 | M8 | 42 | SER | C-O | -6.78 | 1.16 | 1.24 |
| 11 | a9 | 333 | GLN | CA-C | -6.78 | 1.43 | 1.52 |
| 10 | j5 | 479 | LEU | C-O | -6.78 | 1.15 | 1.23 |
| 10 | k5 | 479 | LEU | C-O | -6.78 | 1.15 | 1.23 |
| 8 | i7 | 134 | LYS | C-O | -6.78 | 1.16 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4 | M3 | 60 | LYS | C-O | -6.78 | 1.16 | 1.24 |
| 4 | M1 | 60 | LYS | C-O | -6.78 | 1.16 | 1.24 |
| 4 | M4 | 42 | SER | C-O | -6.78 | 1.16 | 1.24 |
| 10 | j5 | 771 | ALA | CA-C | -6.78 | 1.43 | 1.52 |
| 10 | k5 | 656 | GLY | CA-C | -6.78 | 1.42 | 1.51 |
| 1 | D5 | 17 | LYS | C-O | -6.77 | 1.15 | 1.23 |
| 10 | j5 | 756 | SER | CA-C | -6.77 | 1.43 | 1.52 |
| 10 | k5 | 756 | SER | CA-C | -6.77 | 1.43 | 1.52 |
| 10 | j5 | 720 | ASP | CA-CB | -6.77 | 1.42 | 1.53 |
| 10 | k5 | 259 | PRO | C-O | -6.77 | 1.15 | 1.23 |
| 10 | k5 | 720 | ASP | CA-CB | -6.77 | 1.42 | 1.53 |
| 4 | MA | 198 | ALA | C-O | -6.77 | 1.16 | 1.24 |
| 4 | M4 | 72 | ALA | CA-C | -6.77 | 1.44 | 1.52 |
| 4 | M9 | 198 | ALA | C-O | -6.77 | 1.16 | 1.24 |
| 4 | M3 | 72 | ALA | CA-C | -6.76 | 1.44 | 1.52 |
| 1 | D5 | 9 | ILE | C-O | -6.76 | 1.15 | 1.24 |
| 10 | k5 | 519 | GLU | C-O | -6.76 | 1.12 | 1.23 |
| 4 | M1 | 72 | ALA | CA-C | -6.76 | 1.44 | 1.52 |
| 10 | j5 | 753 | PHE | CA-CB | -6.76 | 1.43 | 1.53 |
| 10 | k5 | 863 | ILE | CA-C | -6.76 | 1.44 | 1.52 |
| 9 | z5 | 38 | PHE | CA-C | -6.76 | 1.44 | 1.52 |
| 10 | k5 | 521 | GLY | C-O | -6.76 | 1.14 | 1.23 |
| 10 | k5 | 547 | ARG | CA-C | -6.76 | 1.44 | 1.52 |
| 4 | M9 | 14 | LEU | C-O | -6.76 | 1.15 | 1.23 |
| 8 | u7 | 36 | ARG | CA-C | -6.75 | 1.44 | 1.52 |
| 4 | M3 | 14 | LEU | C-O | -6.75 | 1.15 | 1.23 |
| 1 | J5 | 10 | ASN | CA-C | -6.75 | 1.43 | 1.52 |
| 9 | z5 | 34 | TYR | N-CA | -6.75 | 1.37 | 1.46 |
| 4 | M8 | 14 | LEU | C-O | -6.75 | 1.15 | 1.23 |
| 4 | M1 | 14 | LEU | C-O | -6.75 | 1.15 | 1.23 |
| 4 | MA | 14 | LEU | C-O | -6.75 | 1.15 | 1.23 |
| 9 | i5 | 38 | PHE | CA-C | -6.75 | 1.44 | 1.52 |
| 10 | j5 | 485 | ALA | CA-C | -6.75 | 1.44 | 1.53 |
| 10 | j5 | 646 | ASN | CA-C | -6.75 | 1.43 | 1.52 |
| 10 | k5 | 711 | PRO | C-O | -6.75 | 1.15 | 1.24 |
| 10 | k5 | 739 | VAL | CA-C | -6.75 | 1.43 | 1.52 |
| 4 | M8 | 198 | ALA | C-O | -6.75 | 1.16 | 1.24 |
| 10 | j5 | 426 | LEU | C-O | -6.75 | 1.16 | 1.24 |
| 10 | j5 | 595 | ASN | C-O | -6.75 | 1.15 | 1.24 |
| 10 | j5 | 828 | VAL | CA-C | -6.75 | 1.44 | 1.52 |
| 10 | k5 | 423 | LEU | C-O | -6.75 | 1.16 | 1.24 |
| 10 | k5 | 828 | VAL | CA-C | -6.75 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4 | M4 | 198 | ALA | C-O | -6.74 | 1.16 | 1.24 |
| 10 | k5 | 422 | TYR | C-O | -6.74 | 1.15 | 1.23 |
| 8 | o7 | 36 | ARG | CA-C | -6.74 | 1.44 | 1.52 |
| 4 | M8 | 72 | ALA | CA-C | -6.74 | 1.44 | 1.52 |
| 4 | MA | 35 | THR | C-O | -6.74 | 1.15 | 1.23 |
| 10 | k5 | 442 | LEU | CA-C | -6.74 | 1.44 | 1.52 |
| 4 | M9 | 35 | THR | C-O | -6.74 | 1.15 | 1.23 |
| 11 | a9 | 521 | PHE | C-O | -6.74 | 1.16 | 1.24 |
| 11 | aA | 521 | PHE | C-O | -6.74 | 1.16 | 1.24 |
| 10 | k5 | 654 | LYS | CA-C | -6.74 | 1.43 | 1.52 |
| 10 | j5 | 442 | LEU | CA-C | -6.73 | 1.44 | 1.52 |
| 9 | z5 | 21 | ARG | CA-C | -6.73 | 1.43 | 1.52 |
| 10 | k5 | 426 | LEU | C-O | -6.73 | 1.16 | 1.24 |
| 10 | j5 | 422 | TYR | C-O | -6.73 | 1.15 | 1.23 |
| 10 | j5 | 654 | LYS | CA-C | -6.73 | 1.43 | 1.52 |
| 8 | i7 | 123 | ILE | C-O | -6.73 | 1.16 | 1.24 |
| 8 | K5 | 79 | ALA | C-O | -6.73 | 1.16 | 1.24 |
| 4 | M4 | 60 | LYS | C-O | -6.73 | 1.16 | 1.24 |
| 10 | j5 | 519 | GLU | C-O | -6.73 | 1.12 | 1.23 |
| 10 | j5 | 1106 | PHE | C-O | -6.72 | 1.16 | 1.24 |
| 10 | k5 | 709 | ILE | CA-CB | -6.72 | 1.46 | 1.54 |
| 11 | aA | 333 | GLN | CA-C | -6.72 | 1.43 | 1.52 |
| 4 | MA | 60 | LYS | C-O | -6.72 | 1.16 | 1.24 |
| 9 | i5 | 21 | ARG | CA-C | -6.72 | 1.43 | 1.52 |
| 4 | M9 | 60 | LYS | C-O | -6.72 | 1.16 | 1.24 |
| 8 | c7 | 134 | LYS | C-O | -6.72 | 1.16 | 1.24 |
| 10 | j5 | 935 | LEU | N-CA | -6.71 | 1.37 | 1.46 |
| 10 | k5 | 867 | VAL | C-O | -6.71 | 1.14 | 1.24 |
| 11 | a9 | 578 | MET | CA-C | -6.71 | 1.44 | 1.52 |
| 11 | aA | 578 | MET | CA-C | -6.71 | 1.44 | 1.52 |
| 10 | j5 | 878 | GLU | CA-C | -6.71 | 1.44 | 1.52 |
| 10 | j5 | 644 | GLU | CA-C | -6.71 | 1.44 | 1.52 |
| 10 | k5 | 644 | GLU | CA-C | -6.71 | 1.44 | 1.52 |
| 8 | E5 | 79 | ALA | C-O | -6.71 | 1.16 | 1.24 |
| 10 | j5 | 8 | GLY | C-O | -6.71 | 1.15 | 1.23 |
| 10 | k5 | 8 | GLY | C-O | -6.71 | 1.15 | 1.23 |
| 10 | k5 | 878 | GLU | CA-C | -6.71 | 1.44 | 1.52 |
| 8 | c7 | 123 | ILE | C-O | -6.71 | 1.16 | 1.24 |
| 8 | K5 | 131 | ARG | CA-C | -6.70 | 1.43 | 1.52 |
| 10 | j5 | 510 | ILE | CA-CB | -6.70 | 1.46 | 1.54 |
| 9 | w7 | 62 | GLY | C-O | -6.70 | 1.15 | 1.23 |
| 9 | z7 | 62 | GLY | C-O | -6.70 | 1.15 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9 | z7 | 21 | ARG | CA-C | -6.70 | 1.43 | 1.52 |
| 4 | M3 | 35 | THR | C-O | -6.69 | 1.15 | 1.23 |
| 4 | M1 | 35 | THR | C-O | -6.69 | 1.15 | 1.23 |
| 10 | j5 | 738 | TYR | CA-C | -6.69 | 1.43 | 1.52 |
| 4 | M3 | 37 | GLU | CA-C | -6.69 | 1.46 | 1.53 |
| 4 | M1 | 37 | GLU | CA-C | -6.69 | 1.46 | 1.53 |
| 4 | M4 | 54 | ALA | CA-C | -6.69 | 1.44 | 1.52 |
| 10 | j5 | 709 | ILE | CA-CB | -6.69 | 1.46 | 1.54 |
| 1 | D5 | 7 | ALA | C-O | -6.68 | 1.15 | 1.24 |
| 10 | j5 | 624 | CYS | C-O | -6.68 | 1.15 | 1.24 |
| 10 | j5 | 704 | THR | N-CA | -6.68 | 1.38 | 1.46 |
| 9 | z7 | 47 | ALA | C-O | -6.68 | 1.14 | 1.23 |
| 10 | k5 | 693 | ARG | CA-CB | -6.68 | 1.42 | 1.53 |
| 1 | b7 | 43 | VAL | C-O | -6.68 | 1.16 | 1.24 |
| 9 | w7 | 21 | ARG | CA-C | -6.68 | 1.43 | 1.52 |
| 10 | k5 | 763 | SER | C-O | -6.68 | 1.15 | 1.24 |
| 9 | w7 | 46 | LYS | C-O | -6.68 | 1.15 | 1.24 |
| 4 | M8 | 54 | ALA | CA-C | -6.68 | 1.44 | 1.52 |
| 9 | z7 | 46 | LYS | C-O | -6.68 | 1.15 | 1.24 |
| 10 | j5 | 763 | SER | C-O | -6.67 | 1.15 | 1.24 |
| 10 | j5 | 1096 | ILE | C-O | -6.67 | 1.16 | 1.24 |
| 4 | M4 | 35 | THR | C-O | -6.67 | 1.15 | 1.23 |
| 4 | M8 | 35 | THR | C-O | -6.67 | 1.15 | 1.23 |
| 8 | A5 | 64 | ASP | C-O | -6.67 | 1.15 | 1.24 |
| 4 | M4 | 56 | MET | CA-C | -6.67 | 1.44 | 1.52 |
| 8 | K5 | 102 | THR | C-O | -6.67 | 1.18 | 1.24 |
| 9 | i5 | 36 | ASN | C-O | -6.67 | 1.14 | 1.24 |
| 10 | j5 | 902 | ASN | C-O | -6.67 | 1.14 | 1.23 |
| 10 | k5 | 935 | LEU | N-CA | -6.67 | 1.37 | 1.46 |
| 10 | k5 | 1092 | ALA | C-O | -6.67 | 1.16 | 1.24 |
| 9 | i5 | 64 | ASN | C-O | -6.67 | 1.16 | 1.24 |
| 10 | j5 | 678 | VAL | N-CA | -6.66 | 1.38 | 1.46 |
| 10 | k5 | 678 | VAL | N-CA | -6.66 | 1.38 | 1.46 |
| 10 | j5 | 457 | THR | N-CA | -6.66 | 1.38 | 1.46 |
| 10 | j5 | 660 | VAL | CA-C | -6.66 | 1.44 | 1.52 |
| 10 | k5 | 457 | THR | N-CA | -6.66 | 1.38 | 1.46 |
| 10 | k5 | 510 | ILE | CA-CB | -6.66 | 1.46 | 1.54 |
| 8 | G5 | 64 | ASP | C-O | -6.66 | 1.15 | 1.24 |
| 10 | j5 | 740 | ASN | C-O | -6.66 | 1.15 | 1.24 |
| 10 | k5 | 740 | ASN | C-O | -6.66 | 1.15 | 1.24 |
| 10 | k5 | 902 | ASN | C-O | -6.65 | 1.14 | 1.23 |
| 10 | j5 | 319 | ALA | CA-C | -6.65 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | k5 | 319 | ALA | CA-C | -6.65 | 1.44 | 1.52 |
| 4 | M8 | 56 | MET | CA-C | -6.65 | 1.44 | 1.52 |
| 10 | j5 | 763 | SER | CA-C | -6.65 | 1.43 | 1.52 |
| 10 | k5 | 763 | SER | CA-C | -6.65 | 1.43 | 1.52 |
| 11 | a9 | 458 | HIS | C-O | -6.65 | 1.16 | 1.24 |
| 11 | aA | 458 | HIS | C-O | -6.65 | 1.16 | 1.24 |
| 10 | j5 | 1092 | ALA | C-O | -6.64 | 1.16 | 1.24 |
| 10 | k5 | 660 | VAL | CA-C | -6.64 | 1.44 | 1.52 |
| 1 | b7 | 45 | SER | C-O | -6.64 | 1.16 | 1.24 |
| 9 | w7 | 47 | ALA | C-O | -6.64 | 1.14 | 1.23 |
| 8 | E5 | 102 | THR | C-O | -6.64 | 1.18 | 1.24 |
| 10 | j5 | 822 | ARG | C-O | -6.64 | 1.15 | 1.24 |
| 10 | k5 | 822 | ARG | C-O | -6.64 | 1.15 | 1.24 |
| 9 | z7 | 33 | PRO | CA-C | -6.64 | 1.44 | 1.52 |
| 10 | j5 | 746 | LEU | CA-C | -6.64 | 1.43 | 1.52 |
| 10 | k5 | 601 | LYS | CA-C | -6.64 | 1.44 | 1.52 |
| 9 | w7 | 33 | PRO | CA-C | -6.64 | 1.44 | 1.52 |
| 10 | j5 | 27 | GLY | C-O | -6.63 | 1.16 | 1.23 |
| 10 | k5 | 27 | GLY | C-O | -6.63 | 1.16 | 1.23 |
| 10 | k5 | 746 | LEU | CA-C | -6.63 | 1.43 | 1.52 |
| 10 | k5 | 790 | ALA | C-O | -6.63 | 1.15 | 1.24 |
| 8 | c7 | 120 | GLN | CA-C | -6.63 | 1.45 | 1.53 |
| 4 | M3 | 54 | ALA | CA-C | -6.63 | 1.44 | 1.52 |
| 4 | M1 | 54 | ALA | CA-C | -6.63 | 1.44 | 1.52 |
| 10 | j5 | 693 | ARG | CA-CB | -6.62 | 1.42 | 1.53 |
| 10 | k5 | 1118 | THR | CA-C | -6.62 | 1.44 | 1.52 |
| 1 | D5 | 5 | ILE | C-O | -6.62 | 1.15 | 1.24 |
| 10 | k5 | 1096 | ILE | C-O | -6.62 | 1.16 | 1.24 |
| 10 | k5 | 623 | VAL | CA-CB | -6.62 | 1.44 | 1.54 |
| 4 | M3 | 43 | TYR | CB-CG | -6.62 | 1.37 | 1.51 |
| 10 | k5 | 704 | THR | N-CA | -6.62 | 1.38 | 1.46 |
| 4 | M1 | 43 | TYR | CB-CG | -6.62 | 1.37 | 1.51 |
| 8 | E5 | 103 | PRO | C-O | -6.61 | 1.16 | 1.24 |
| 8 | u7 | 49 | ARG | C-O | -6.61 | 1.15 | 1.23 |
| 9 | i5 | 67 | VAL | C-O | -6.61 | 1.16 | 1.24 |
| 10 | j5 | 981 | ILE | C-O | -6.61 | 1.17 | 1.24 |
| 10 | k5 | 624 | CYS | C-O | -6.61 | 1.15 | 1.24 |
| 4 | M4 | 43 | TYR | CB-CG | -6.61 | 1.37 | 1.51 |
| 10 | k5 | 624 | CYS | CA-CB | -6.61 | 1.42 | 1.53 |
| 4 | MA | 54 | ALA | CA-C | -6.61 | 1.44 | 1.52 |
| 4 | MA | 56 | MET | CA-C | -6.61 | 1.44 | 1.52 |
| 9 | i5 | 57 | PHE | CA-C | -6.61 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 9 | i5 | 58 | THR | C-O | -6.61 | 1.15 | 1.23 |
| 1 | h7 | 43 | VAL | C-O | -6.61 | 1.16 | 1.24 |
| 9 | w7 | 24 | GLN | C-O | -6.61 | 1.15 | 1.24 |
| 4 | M9 | 54 | ALA | CA-C | -6.61 | 1.44 | 1.52 |
| 4 | M9 | 56 | MET | CA-C | -6.61 | 1.44 | 1.52 |
| 10 | j5 | 624 | CYS | CA-CB | -6.60 | 1.42 | 1.53 |
| 4 | M4 | 107 | VAL | C-O | -6.60 | 1.16 | 1.24 |
| 10 | k5 | 295 | ARG | C-O | -6.60 | 1.16 | 1.24 |
| 1 | J5 | 5 | ILE | C-O | -6.60 | 1.15 | 1.24 |
| 4 | M8 | 43 | TYR | CB-CG | -6.60 | 1.37 | 1.51 |
| 11 | a9 | 802 | ARG | C-O | -6.60 | 1.15 | 1.24 |
| 11 | aA | 802 | ARG | C-O | -6.60 | 1.15 | 1.24 |
| 4 | MA | 166 | THR | C-O | -6.60 | 1.16 | 1.24 |
| 4 | M9 | 166 | THR | C-O | -6.60 | 1.16 | 1.24 |
| 9 | z5 | 41 | GLN | CD-OE1 | -6.59 | 1.11 | 1.23 |
| 9 | z5 | 64 | ASN | C-O | -6.59 | 1.16 | 1.24 |
| 8 | o7 | 49 | ARG | C-O | -6.59 | 1.15 | 1.23 |
| 9 | z7 | 24 | GLN | C-O | -6.59 | 1.15 | 1.24 |
| 10 | j5 | 522 | ASN | N-CA | -6.59 | 1.41 | 1.46 |
| 4 | MA | 43 | TYR | CB-CG | -6.59 | 1.37 | 1.51 |
| 8 | o7 | 57 | GLN | CA-C | -6.59 | 1.44 | 1.52 |
| 4 | M8 | 57 | THR | C-O | -6.59 | 1.16 | 1.24 |
| 4 | M9 | 43 | TYR | CB-CG | -6.59 | 1.37 | 1.51 |
| 3 | F9 | 157 | VAL | CA-C | 6.59 | 1.60 | 1.52 |
| 3 | LA | 111 | ASN | C-O | -6.59 | 1.16 | 1.24 |
| 1 | h7 | 45 | SER | C-O | -6.59 | 1.16 | 1.24 |
| 1 | b7 | 44 | ILE | C-O | -6.59 | 1.16 | 1.24 |
| 3 | L9 | 111 | ASN | C-O | -6.59 | 1.16 | 1.24 |
| 4 | MA | 37 | GLU | CA-C | -6.59 | 1.46 | 1.53 |
| 10 | j5 | 623 | VAL | CA-CB | -6.59 | 1.44 | 1.54 |
| 4 | M9 | 37 | GLU | CA-C | -6.59 | 1.46 | 1.53 |
| 4 | MA | 19 | MET | CA-C | -6.58 | 1.45 | 1.53 |
| 8 | a5 | 14 | GLU | N-CA | -6.58 | 1.38 | 1.46 |
| 8 | i7 | 137 | ALA | C-O | -6.58 | 1.16 | 1.24 |
| 4 | M9 | 19 | MET | CA-C | -6.58 | 1.45 | 1.53 |
| 9 | z5 | 36 | ASN | C-O | -6.58 | 1.14 | 1.24 |
| 4 | M3 | 19 | MET | CA-C | -6.58 | 1.45 | 1.53 |
| 4 | M3 | 56 | MET | CA-C | -6.58 | 1.44 | 1.52 |
| 10 | j5 | 766 | ALA | CA-C | -6.58 | 1.44 | 1.52 |
| 4 | M1 | 19 | MET | CA-C | -6.58 | 1.45 | 1.53 |
| 4 | M1 | 56 | MET | CA-C | -6.58 | 1.44 | 1.52 |
| 10 | j5 | 451 | LYS | CA-C | -6.58 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | j5 | 790 | ALA | C-O | -6.58 | 1.15 | 1.24 |
| 10 | j5 | 257 | THR | C-O | -6.58 | 1.15 | 1.23 |
| 1 | h7 | 44 | ILE | C-O | -6.58 | 1.16 | 1.24 |
| 8 | I5 | 15 | ALA | C-O | -6.58 | 1.15 | 1.23 |
| 10 | j5 | 635 | LEU | CA-C | -6.58 | 1.44 | 1.52 |
| 1 | J5 | 7 | ALA | C-O | -6.58 | 1.15 | 1.24 |
| 8 | C5 | 15 | ALA | C-O | -6.57 | 1.15 | 1.23 |
| 9 | z7 | 52 | LEU | CA-C | -6.57 | 1.44 | 1.52 |
| 4 | M4 | 57 | THR | C-O | -6.57 | 1.16 | 1.24 |
| 10 | k5 | 522 | ASN | N-CA | -6.57 | 1.41 | 1.46 |
| 9 | w7 | 52 | LEU | CA-C | -6.57 | 1.44 | 1.52 |
| 10 | j5 | 601 | LYS | CA-C | -6.57 | 1.44 | 1.52 |
| 9 | z5 | 67 | VAL | C-O | -6.57 | 1.16 | 1.24 |
| 10 | k5 | 437 | GLY | CA-C | -6.57 | 1.44 | 1.52 |
| 10 | k5 | 753 | PHE | CA-C | -6.57 | 1.44 | 1.52 |
| 11 | a9 | 519 | ARG | CA-C | -6.57 | 1.42 | 1.52 |
| 11 | aA | 519 | ARG | CA-C | -6.57 | 1.42 | 1.52 |
| 4 | M3 | 166 | THR | C-O | -6.57 | 1.16 | 1.24 |
| 10 | j5 | 753 | PHE | CA-C | -6.57 | 1.44 | 1.52 |
| 4 | M1 | 166 | THR | C-O | -6.57 | 1.16 | 1.24 |
| 10 | j5 | 1118 | THR | CA-C | -6.56 | 1.44 | 1.52 |
| 4 | MA | 57 | THR | C-O | -6.56 | 1.16 | 1.24 |
| 4 | M3 | 57 | THR | C-O | -6.56 | 1.16 | 1.24 |
| 4 | M9 | 57 | THR | C-O | -6.56 | 1.16 | 1.24 |
| 4 | M1 | 57 | THR | C-O | -6.56 | 1.16 | 1.24 |
| 10 | j5 | 295 | ARG | C-O | -6.56 | 1.16 | 1.24 |
| 10 | j5 | 727 | THR | CB-CG2 | -6.55 | 1.30 | 1.52 |
| 10 | k5 | 635 | LEU | CA-C | -6.55 | 1.44 | 1.52 |
| 8 | u7 | 37 | LEU | C-O | -6.55 | 1.16 | 1.24 |
| 10 | k5 | 779 | ASP | CA-CB | -6.55 | 1.42 | 1.53 |
| 10 | k5 | 787 | GLU | C-O | -6.55 | 1.16 | 1.24 |
| 8 | i7 | 122 | PRO | CA-C | -6.55 | 1.46 | 1.52 |
| 10 | j5 | 705 | THR | C-O | -6.55 | 1.15 | 1.24 |
| 9 | i5 | 41 | GLN | CD-OE1 | -6.54 | 1.11 | 1.23 |
| 4 | M3 | 107 | VAL | C-O | -6.54 | 1.16 | 1.24 |
| 10 | j5 | 684 | TYR | CA-C | -6.54 | 1.44 | 1.52 |
| 10 | k5 | 684 | TYR | CA-C | -6.54 | 1.44 | 1.52 |
| 8 | c7 | 122 | PRO | CA-C | -6.54 | 1.46 | 1.52 |
| 4 | M1 | 107 | VAL | C-O | -6.54 | 1.16 | 1.24 |
| 8 | K5 | 96 | ILE | C-O | -6.54 | 1.16 | 1.24 |
| 10 | j5 | 637 | ARG | CA-CB | -6.54 | 1.46 | 1.53 |
| 10 | k5 | 637 | ARG | CA-CB | -6.54 | 1.46 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4 | M4 | 173 | PHE | C-O | -6.54 | 1.16 | 1.24 |
| 9 | z5 | 57 | PHE | CA-C | -6.54 | 1.44 | 1.52 |
| 9 | z5 | 58 | THR | C-O | -6.54 | 1.15 | 1.24 |
| 10 | k5 | 727 | THR | CB-CG2 | -6.54 | 1.30 | 1.52 |
| 10 | k5 | 661 | VAL | CA-C | -6.53 | 1.44 | 1.52 |
| 10 | j5 | 171 | ILE | C-O | -6.53 | 1.16 | 1.24 |
| 10 | k5 | 4 | ARG | N-CA | -6.53 | 1.37 | 1.46 |
| 10 | j5 | 349 | GLN | CA-CB | -6.53 | 1.44 | 1.53 |
| 10 | j5 | 787 | GLU | C-O | -6.53 | 1.16 | 1.24 |
| 10 | k5 | 6 | THR | CA-C | -6.53 | 1.44 | 1.52 |
| 10 | k5 | 349 | GLN | CA-CB | -6.53 | 1.44 | 1.53 |
| 4 | M8 | 166 | THR | C-O | -6.53 | 1.16 | 1.24 |
| 4 | M4 | 55 | GLU | CA-C | -6.53 | 1.44 | 1.52 |
| 10 | j5 | 6 | THR | CA-C | -6.53 | 1.44 | 1.52 |
| 10 | j5 | 437 | GLY | CA-C | -6.53 | 1.44 | 1.52 |
| 10 | k5 | 705 | THR | C-O | -6.53 | 1.15 | 1.24 |
| 10 | k5 | 518 | ASN | CG-OD1 | -6.52 | 1.11 | 1.23 |
| 10 | k5 | 981 | ILE | C-O | -6.52 | 1.17 | 1.24 |
| 4 | M4 | 19 | MET | CA-C | -6.52 | 1.45 | 1.53 |
| 8 | e5 | 14 | GLU | N-CA | -6.52 | 1.38 | 1.46 |
| 4 | MA | 107 | VAL | C-O | -6.51 | 1.16 | 1.24 |
| 8 | K5 | 103 | PRO | C-O | -6.51 | 1.16 | 1.24 |
| 10 | j5 | 29 | ASN | C-O | -6.51 | 1.16 | 1.24 |
| 10 | j5 | 764 | PHE | CA-C | -6.51 | 1.44 | 1.52 |
| 10 | j5 | 804 | GLU | CA-CB | -6.51 | 1.43 | 1.53 |
| 10 | k5 | 764 | PHE | CA-C | -6.51 | 1.44 | 1.52 |
| 10 | k5 | 804 | GLU | CA-CB | -6.51 | 1.43 | 1.53 |
| 4 | M8 | 37 | GLU | CA-C | -6.51 | 1.46 | 1.53 |
| 4 | M9 | 107 | VAL | C-O | -6.51 | 1.16 | 1.24 |
| 10 | j5 | 4 | ARG | N-CA | -6.51 | 1.37 | 1.46 |
| 4 | M4 | 166 | THR | C-O | -6.51 | 1.16 | 1.24 |
| 9 | z7 | 49 | GLY | C-O | -6.51 | 1.14 | 1.23 |
| 4 | M8 | 19 | MET | CA-C | -6.51 | 1.45 | 1.53 |
| 4 | M8 | 129 | GLU | C-O | -6.51 | 1.15 | 1.24 |
| 10 | k5 | 29 | ASN | C-O | -6.51 | 1.16 | 1.24 |
| 10 | j5 | 664 | MET | N-CA | -6.51 | 1.38 | 1.46 |
| 10 | k5 | 519 | GLU | CA-CB | -6.51 | 1.46 | 1.54 |
| 10 | k5 | 664 | MET | N-CA | -6.51 | 1.38 | 1.46 |
| 11 | a9 | 487 | ASP | CA-C | -6.51 | 1.44 | 1.52 |
| 11 | aA | 487 | ASP | CA-C | -6.51 | 1.44 | 1.52 |
| 10 | k5 | 451 | LYS | CA-C | -6.50 | 1.44 | 1.52 |
| 10 | k5 | 766 | ALA | CA-C | -6.50 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 10 | j5 | 799 | GLU | C-O | -6.50 | 1.15 | 1.24 |
| 10 | k5 | 171 | ILE | C-O | -6.50 | 1.16 | 1.24 |
| 10 | k5 | 257 | THR | C-O | -6.50 | 1.15 | 1.23 |
| 4 | M9 | 129 | GLU | C-O | -6.50 | 1.15 | 1.24 |
| 4 | MA | 111 | LYS | CA-C | -6.50 | 1.44 | 1.52 |
| 4 | M3 | 110 | TYR | C-O | -6.50 | 1.16 | 1.24 |
| 9 | i5 | 41 | GLN | CA-CB | -6.50 | 1.43 | 1.53 |
| 10 | k5 | 722 | ILE | CA-CB | -6.50 | 1.46 | 1.54 |
| 4 | M9 | 111 | LYS | CA-C | -6.50 | 1.44 | 1.52 |
| 8 | u7 | 57 | GLN | CA-C | -6.50 | 1.44 | 1.52 |
| 4 | MA | 55 | GLU | CA-C | -6.49 | 1.44 | 1.52 |
| 4 | M4 | 129 | GLU | C-O | -6.49 | 1.15 | 1.24 |
| 4 | M9 | 55 | GLU | CA-C | -6.49 | 1.44 | 1.52 |
| 9 | z5 | 41 | GLN | CA-CB | -6.49 | 1.43 | 1.53 |
| 8 | c7 | 137 | ALA | C-O | -6.49 | 1.16 | 1.24 |
| 9 | w7 | 49 | GLY | C-O | -6.49 | 1.14 | 1.23 |
| 4 | M3 | 180 | ASN | CA-C | -6.49 | 1.44 | 1.52 |
| 10 | j5 | 683 | ARG | CA-CB | -6.49 | 1.43 | 1.53 |
| 10 | k5 | 683 | ARG | CA-CB | -6.49 | 1.43 | 1.53 |
| 4 | M1 | 180 | ASN | CA-C | -6.49 | 1.44 | 1.52 |
| 10 | j5 | 159 | ASP | N-CA | -6.48 | 1.38 | 1.46 |
| 10 | j5 | 750 | ARG | C-O | -6.48 | 1.16 | 1.23 |
| 10 | k5 | 159 | ASP | N-CA | -6.48 | 1.38 | 1.46 |
| 4 | M8 | 173 | PHE | C-O | -6.48 | 1.16 | 1.24 |
| 4 | M4 | 37 | GLU | CA-C | -6.48 | 1.46 | 1.53 |
| 10 | j5 | 487 | PHE | C-O | -6.48 | 1.15 | 1.24 |
| 10 | j5 | 519 | GLU | CA-CB | -6.48 | 1.46 | 1.54 |
| 10 | k5 | 487 | PHE | C-O | -6.48 | 1.15 | 1.24 |
| 10 | j5 | 844 | GLN | CA-C | -6.47 | 1.43 | 1.52 |
| 10 | k5 | 844 | GLN | CA-C | -6.47 | 1.43 | 1.52 |
| 4 | M4 | 180 | ASN | CA-C | -6.47 | 1.44 | 1.52 |
| 10 | j5 | 703 | LEU | CA-C | -6.47 | 1.44 | 1.52 |
| 10 | j5 | 779 | ASP | CA-CB | -6.47 | 1.43 | 1.53 |
| 10 | j5 | 661 | VAL | CA-C | -6.47 | 1.44 | 1.52 |
| 10 | k5 | 570 | ALA | C-O | -6.47 | 1.15 | 1.24 |
| 4 | M8 | 55 | GLU | CA-C | -6.47 | 1.44 | 1.52 |
| 10 | j5 | 60 | LEU | C-O | -6.47 | 1.16 | 1.24 |
| 10 | j5 | 371 | SER | N-CA | -6.47 | 1.38 | 1.46 |
| 10 | j5 | 518 | ASN | CG-OD1 | -6.47 | 1.11 | 1.23 |
| 10 | j5 | 642 | ARG | CZ-NH2 | -6.47 | 1.25 | 1.33 |
| 10 | k5 | 60 | LEU | C-O | -6.47 | 1.16 | 1.24 |
| 10 | k5 | 439 | ALA | CA-C | -6.47 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | k5 | 453 | PRO | CA-CB | -6.47 | 1.44 | 1.53 |
| 10 | j5 | 847 | LEU | CA-CB | -6.47 | 1.43 | 1.53 |
| 4 | MA | 173 | PHE | C-O | -6.47 | 1.16 | 1.24 |
| 10 | k5 | 1113 | TYR | C-O | -6.47 | 1.15 | 1.23 |
| 4 | M9 | 173 | PHE | C-O | -6.47 | 1.16 | 1.24 |
| 10 | j5 | 489 | ASN | CA-C | -6.46 | 1.44 | 1.52 |
| 4 | M4 | 111 | LYS | CA-C | -6.46 | 1.44 | 1.52 |
| 4 | M3 | 173 | PHE | C-O | -6.46 | 1.16 | 1.24 |
| 4 | M1 | 173 | PHE | C-O | -6.46 | 1.16 | 1.24 |
| 8 | E5 | 96 | ILE | C-O | -6.46 | 1.16 | 1.24 |
| 10 | k5 | 965 | GLN | C-O | -6.46 | 1.16 | 1.23 |
| 4 | M1 | 110 | TYR | C-O | -6.46 | 1.16 | 1.24 |
| 10 | j5 | 748 | ARG | C-O | -6.46 | 1.15 | 1.24 |
| 10 | k5 | 748 | ARG | C-O | -6.46 | 1.15 | 1.24 |
| 4 | M8 | 107 | VAL | C-O | -6.46 | 1.16 | 1.24 |
| 4 | M8 | 111 | LYS | CA-C | -6.46 | 1.44 | 1.52 |
| 4 | M4 | 110 | TYR | C-O | -6.46 | 1.16 | 1.24 |
| 8 | C5 | 4 | LEU | CA-C | -6.46 | 1.44 | 1.52 |
| 4 | MA | 129 | GLU | C-O | -6.45 | 1.15 | 1.24 |
| 4 | M3 | 55 | GLU | CA-C | -6.45 | 1.44 | 1.52 |
| 8 | I5 | 4 | LEU | CA-C | -6.45 | 1.44 | 1.52 |
| 10 | j5 | 720 | ASP | CA-C | -6.45 | 1.44 | 1.52 |
| 10 | k5 | 720 | ASP | CA-C | -6.45 | 1.44 | 1.52 |
| 10 | k5 | 892 | ALA | C-O | -6.45 | 1.11 | 1.24 |
| 4 | M1 | 55 | GLU | CA-C | -6.45 | 1.44 | 1.52 |
| 4 | M3 | 129 | GLU | C-O | -6.45 | 1.15 | 1.24 |
| 10 | k5 | 500 | PRO | CA-CB | -6.45 | 1.47 | 1.54 |
| 10 | k5 | 750 | ARG | C-O | -6.45 | 1.16 | 1.23 |
| 4 | M1 | 129 | GLU | C-O | -6.45 | 1.15 | 1.24 |
| 4 | M4 | 4 | LEU | C-O | -6.45 | 1.15 | 1.23 |
| 10 | j5 | 439 | ALA | CA-C | -6.45 | 1.44 | 1.52 |
| 10 | j5 | 578 | ARG | C-O | -6.45 | 1.16 | 1.23 |
| 10 | k5 | 371 | SER | N-CA | -6.45 | 1.38 | 1.46 |
| 10 | j5 | 965 | GLN | C-O | -6.44 | 1.16 | 1.23 |
| 10 | k5 | 489 | ASN | CA-C | -6.44 | 1.44 | 1.52 |
| 10 | k5 | 159 | ASP | C-O | -6.44 | 1.16 | 1.24 |
| 4 | M3 | 4 | LEU | C-O | -6.43 | 1.15 | 1.23 |
| 10 | j5 | 573 | GLN | CA-C | -6.43 | 1.43 | 1.52 |
| 4 | M8 | 180 | ASN | CA-C | -6.43 | 1.44 | 1.52 |
| 4 | M1 | 4 | LEU | C-O | -6.43 | 1.15 | 1.23 |
| 10 | k5 | 799 | GLU | C-O | -6.43 | 1.15 | 1.24 |
| 8 | o7 | 37 | LEU | C-O | -6.43 | 1.16 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4 | MA | 180 | ASN | CA-C | -6.43 | 1.44 | 1.52 |
| 4 | M9 | 180 | ASN | CA-C | -6.43 | 1.44 | 1.52 |
| 10 | k5 | 847 | LEU | CA-CB | -6.43 | 1.43 | 1.53 |
| 10 | j5 | 453 | PRO | CA-CB | -6.43 | 1.44 | 1.53 |
| 10 | j5 | 848 | ILE | N-CA | -6.43 | 1.38 | 1.46 |
| 1 | J5 | 39 | ARG | N-CA | -6.42 | 1.38 | 1.46 |
| 10 | k5 | 642 | ARG | CZ-NH2 | -6.42 | 1.25 | 1.33 |
| 10 | j5 | 570 | ALA | C-O | -6.42 | 1.15 | 1.24 |
| 10 | j5 | 589 | ALA | C-O | -6.42 | 1.14 | 1.23 |
| 10 | j5 | 892 | ALA | C-O | -6.42 | 1.11 | 1.24 |
| 10 | j5 | 397 | GLY | C-O | -6.42 | 1.15 | 1.23 |
| 10 | k5 | 397 | GLY | C-O | -6.42 | 1.15 | 1.23 |
| 10 | j5 | 892 | ALA | CA-CB | -6.41 | 1.45 | 1.53 |
| 10 | k5 | 703 | LEU | CA-C | -6.41 | 1.44 | 1.52 |
| 10 | k5 | 892 | ALA | CA-CB | -6.41 | 1.45 | 1.53 |
| 9 | z5 | 33 | PRO | C-O | -6.41 | 1.16 | 1.23 |
| 9 | i5 | 33 | PRO | C-O | -6.41 | 1.16 | 1.23 |
| 4 | M8 | 110 | TYR | C-O | -6.41 | 1.16 | 1.24 |
| 8 | c7 | 114 | GLU | CA-C | -6.41 | 1.44 | 1.52 |
| 11 | a9 | 366 | LEU | CA-C | -6.41 | 1.44 | 1.52 |
| 11 | aA | 366 | LEU | CA-C | -6.41 | 1.44 | 1.52 |
| 10 | j5 | 314 | GLN | CA-C | -6.41 | 1.44 | 1.53 |
| 10 | j5 | 655 | LYS | C-O | -6.41 | 1.15 | 1.24 |
| 10 | k5 | 314 | GLN | CA-C | -6.41 | 1.44 | 1.53 |
| 10 | k5 | 655 | LYS | C-O | -6.41 | 1.15 | 1.24 |
| 4 | M8 | 4 | LEU | C-O | -6.41 | 1.15 | 1.23 |
| 4 | M3 | 111 | LYS | CA-C | -6.40 | 1.44 | 1.52 |
| 4 | M3 | 114 | PHE | C-O | -6.40 | 1.15 | 1.24 |
| 10 | j5 | 868 | ASP | CA-C | -6.40 | 1.44 | 1.52 |
| 10 | k5 | 790 | ALA | N-CA | -6.40 | 1.38 | 1.46 |
| 4 | M1 | 111 | LYS | CA-C | -6.40 | 1.44 | 1.52 |
| 4 | M1 | 114 | PHE | C-O | -6.40 | 1.15 | 1.24 |
| 8 | i7 | 126 | VAL | C-O | -6.40 | 1.16 | 1.24 |
| 10 | j5 | 458 | LEU | CA-C | -6.40 | 1.44 | 1.52 |
| 10 | j5 | 1113 | TYR | C-O | -6.40 | 1.15 | 1.23 |
| 8 | o7 | 54 | ALA | CA-C | -6.40 | 1.44 | 1.52 |
| 4 | MA | 110 | TYR | C-O | -6.39 | 1.16 | 1.24 |
| 10 | j5 | 320 | GLU | C-O | -6.39 | 1.16 | 1.24 |
| 10 | j5 | 500 | PRO | CA-CB | -6.39 | 1.47 | 1.54 |
| 10 | j5 | 515 | PRO | CA-C | -6.39 | 1.41 | 1.52 |
| 10 | j5 | 722 | ILE | CA-CB | -6.39 | 1.46 | 1.54 |
| 10 | k5 | 589 | ALA | C-O | -6.39 | 1.14 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4 | M9 | 110 | TYR | C-O | -6.39 | 1.16 | 1.24 |
| 3 | JA | 108 | ARG | N-CA | -6.39 | 1.38 | 1.46 |
| 4 | M4 | 114 | PHE | C-O | -6.39 | 1.15 | 1.24 |
| 10 | j5 | 1123 | ASN | C-O | -6.39 | 1.15 | 1.24 |
| 10 | k5 | 320 | GLU | C-O | -6.39 | 1.16 | 1.24 |
| 10 | k5 | 1123 | ASN | C-O | -6.39 | 1.15 | 1.24 |
| 3 | J9 | 108 | ARG | N-CA | -6.39 | 1.38 | 1.46 |
| 11 | a9 | 622 | ALA | CA-C | -6.39 | 1.44 | 1.52 |
| 11 | aA | 622 | ALA | CA-C | -6.39 | 1.44 | 1.52 |
| 4 | MA | 4 | LEU | C-O | -6.39 | 1.15 | 1.23 |
| 10 | k5 | 251 | GLU | C-O | -6.39 | 1.15 | 1.24 |
| 4 | M9 | 4 | LEU | C-O | -6.39 | 1.15 | 1.23 |
| 4 | M3 | 51 | ARG | CZ-NH2 | 6.39 | 1.41 | 1.33 |
| 10 | k5 | 626 | ALA | N-CA | -6.39 | 1.38 | 1.46 |
| 10 | k5 | 810 | GLY | C-O | -6.39 | 1.15 | 1.23 |
| 4 | M1 | 51 | ARG | CZ-NH2 | 6.39 | 1.41 | 1.33 |
| 10 | j5 | 184 | LEU | C-O | -6.39 | 1.16 | 1.24 |
| 8 | c7 | 126 | VAL | C-O | -6.39 | 1.16 | 1.24 |
| 1 | D5 | 39 | ARG | N-CA | -6.39 | 1.38 | 1.46 |
| 10 | k5 | 868 | ASP | CA-C | -6.39 | 1.44 | 1.52 |
| 10 | j5 | 1131 | ASN | CA-C | -6.38 | 1.44 | 1.52 |
| 10 | k5 | 515 | PRO | CA-C | -6.38 | 1.41 | 1.52 |
| 10 | j5 | 159 | ASP | C-O | -6.38 | 1.16 | 1.24 |
| 10 | k5 | 778 | LYS | C-O | -6.38 | 1.16 | 1.24 |
| 4 | MA | 34 | ASP | CA-C | -6.38 | 1.44 | 1.52 |
| 10 | k5 | 573 | GLN | N-CA | -6.38 | 1.37 | 1.46 |
| 4 | M9 | 34 | ASP | CA-C | -6.38 | 1.44 | 1.52 |
| 11 | a9 | 22 | ALA | C-O | -6.38 | 1.16 | 1.24 |
| 11 | aA | 22 | ALA | C-O | -6.38 | 1.16 | 1.24 |
| 10 | j5 | 974 | LEU | C-O | -6.38 | 1.15 | 1.23 |
| 10 | j5 | 1033 | ARG | CA-C | -6.38 | 1.44 | 1.52 |
| 10 | k5 | 974 | LEU | C-O | -6.38 | 1.15 | 1.23 |
| 4 | M8 | 114 | PHE | C-O | -6.38 | 1.15 | 1.24 |
| 4 | M1 | 68 | ASP | C-O | -6.38 | 1.16 | 1.23 |
| 4 | M8 | 41 | ASN | CA-C | -6.38 | 1.44 | 1.52 |
| 8 | C5 | 9 | VAL | N-CA | -6.37 | 1.38 | 1.46 |
| 9 | z5 | 65 | THR | C-O | -6.37 | 1.15 | 1.23 |
| 10 | j5 | 995 | VAL | C-O | -6.37 | 1.16 | 1.24 |
| 10 | j5 | 384 | SER | CA-C | -6.37 | 1.46 | 1.52 |
| 10 | k5 | 573 | GLN | CA-C | -6.37 | 1.44 | 1.52 |
| 10 | k5 | 954 | GLU | C-O | -6.37 | 1.15 | 1.24 |
| 4 | M8 | 173 | PHE | CA-C | -6.37 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4 | MA | 114 | PHE | C-O | -6.37 | 1.15 | 1.24 |
| 10 | j5 | 1112 | PRO | C-O | -6.37 | 1.16 | 1.23 |
| 10 | k5 | 578 | ARG | C-O | -6.37 | 1.16 | 1.23 |
| 4 | M9 | 114 | PHE | C-O | -6.37 | 1.15 | 1.24 |
| 10 | k5 | 841 | VAL | C-O | -6.37 | 1.17 | 1.24 |
| 9 | w7 | 14 | LEU | CA-C | -6.37 | 1.44 | 1.52 |
| 3 | LA | 87 | GLU | C-O | -6.36 | 1.16 | 1.24 |
| 8 | I5 | 9 | VAL | N-CA | -6.36 | 1.38 | 1.46 |
| 9 | i5 | 65 | THR | C-O | -6.36 | 1.15 | 1.23 |
| 3 | L9 | 87 | GLU | C-O | -6.36 | 1.16 | 1.24 |
| 4 | M1 | 172 | HIS | CA-C | -6.36 | 1.45 | 1.52 |
| 10 | j5 | 784 | ILE | CA-CB | -6.36 | 1.46 | 1.54 |
| 10 | j5 | 864 | GLY | CA-C | -6.36 | 1.44 | 1.52 |
| 10 | k5 | 1131 | ASN | CA-C | -6.36 | 1.44 | 1.52 |
| 10 | j5 | 540 | LEU | C-O | -6.36 | 1.16 | 1.23 |
| 10 | j5 | 563 | SER | C-O | -6.36 | 1.15 | 1.24 |
| 10 | j5 | 1091 | ALA | C-O | -6.36 | 1.16 | 1.24 |
| 10 | k5 | 540 | LEU | C-O | -6.36 | 1.16 | 1.23 |
| 10 | k5 | 994 | ASP | C-O | -6.36 | 1.16 | 1.24 |
| 10 | j5 | 547 | ARG | N-CA | -6.36 | 1.38 | 1.46 |
| 10 | j5 | 954 | GLU | C-O | -6.36 | 1.15 | 1.24 |
| 10 | k5 | 547 | ARG | N-CA | -6.36 | 1.38 | 1.46 |
| 4 | M8 | 34 | ASP | CA-C | -6.36 | 1.44 | 1.52 |
| 8 | i7 | 120 | GLN | CA-C | -6.35 | 1.45 | 1.53 |
| 4 | MA | 172 | HIS | CA-C | -6.35 | 1.45 | 1.52 |
| 10 | k5 | 184 | LEU | C-O | -6.35 | 1.16 | 1.24 |
| 10 | k5 | 848 | ILE | N-CA | -6.35 | 1.39 | 1.46 |
| 8 | i7 | 114 | GLU | CA-C | -6.35 | 1.44 | 1.52 |
| 9 | z7 | 14 | LEU | CA-C | -6.35 | 1.44 | 1.52 |
| 4 | M9 | 172 | HIS | CA-C | -6.35 | 1.45 | 1.52 |
| 4 | M4 | 34 | ASP | CA-C | -6.35 | 1.44 | 1.52 |
| 4 | MA | 51 | ARG | CZ-NH2 | 6.35 | 1.41 | 1.33 |
| 4 | M9 | 51 | ARG | CZ-NH2 | 6.35 | 1.41 | 1.33 |
| 10 | k5 | 1112 | PRO | C-O | -6.35 | 1.16 | 1.23 |
| 8 | u7 | 54 | ALA | CA-C | -6.34 | 1.44 | 1.52 |
| 10 | j5 | 573 | GLN | N-CA | -6.34 | 1.37 | 1.46 |
| 10 | j5 | 383 | SER | C-O | -6.34 | 1.15 | 1.24 |
| 10 | k5 | 383 | SER | C-O | -6.34 | 1.15 | 1.24 |
| 10 | k5 | 1091 | ALA | C-O | -6.34 | 1.16 | 1.24 |
| 10 | j5 | 251 | GLU | C-O | -6.34 | 1.16 | 1.24 |
| 10 | j5 | 1116 | TYR | C-O | -6.34 | 1.16 | 1.24 |
| 3 | LA | 94 | SER | C-O | -6.34 | 1.15 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | j5 | 418 | ASP | C-O | -6.34 | 1.16 | 1.24 |
| 10 | k5 | 257 | THR | CA-C | -6.34 | 1.45 | 1.52 |
| 3 | L9 | 94 | SER | C-O | -6.34 | 1.15 | 1.24 |
| 10 | j5 | 790 | ALA | N-CA | -6.33 | 1.38 | 1.46 |
| 10 | j5 | 810 | GLY | C-O | -6.33 | 1.15 | 1.23 |
| 10 | k5 | 733 | SER | CA-CB | -6.33 | 1.43 | 1.53 |
| 10 | k5 | 418 | ASP | C-O | -6.33 | 1.16 | 1.24 |
| 10 | k5 | 619 | GLU | CA-C | -6.33 | 1.44 | 1.52 |
| 4 | M1 | 41 | ASN | CA-C | -6.33 | 1.44 | 1.52 |
| 4 | M3 | 173 | PHE | CA-C | -6.33 | 1.44 | 1.52 |
| 9 | z5 | 22 | GLU | CA-C | -6.33 | 1.45 | 1.53 |
| 4 | M1 | 173 | PHE | CA-C | -6.33 | 1.44 | 1.52 |
| 10 | k5 | 458 | LEU | CA-C | -6.32 | 1.44 | 1.52 |
| 10 | k5 | 995 | VAL | C-O | -6.32 | 1.16 | 1.24 |
| 4 | M3 | 172 | HIS | CA-C | -6.32 | 1.45 | 1.52 |
| 4 | M3 | 41 | ASN | CA-C | -6.32 | 1.44 | 1.52 |
| 10 | j5 | 626 | ALA | N-CA | -6.32 | 1.38 | 1.46 |
| 8 | i7 | 117 | ASN | C-O | -6.32 | 1.16 | 1.24 |
| 4 | MA | 41 | ASN | CA-C | -6.32 | 1.44 | 1.52 |
| 4 | M3 | 34 | ASP | CA-C | -6.32 | 1.44 | 1.52 |
| 4 | M9 | 41 | ASN | CA-C | -6.32 | 1.44 | 1.52 |
| 4 | M1 | 34 | ASP | CA-C | -6.32 | 1.44 | 1.52 |
| 10 | k5 | 12 | ALA | CA-C | -6.32 | 1.44 | 1.52 |
| 9 | z7 | 27 | PHE | CA-C | -6.32 | 1.45 | 1.52 |
| 4 | M8 | 68 | ASP | C-O | -6.32 | 1.16 | 1.23 |
| 10 | j5 | 994 | ASP | C-O | -6.31 | 1.16 | 1.24 |
| 10 | k5 | 384 | SER | CA-C | -6.31 | 1.47 | 1.52 |
| 10 | j5 | 471 | PRO | C-O | -6.31 | 1.16 | 1.24 |
| 10 | j5 | 778 | LYS | C-O | -6.31 | 1.16 | 1.24 |
| 10 | k5 | 563 | SER | C-O | -6.31 | 1.15 | 1.24 |
| 4 | MA | 68 | ASP | C-O | -6.31 | 1.16 | 1.23 |
| 10 | j5 | 673 | VAL | CA-CB | -6.31 | 1.46 | 1.54 |
| 4 | M3 | 68 | ASP | C-O | -6.31 | 1.16 | 1.23 |
| 10 | j5 | 472 | TYR | CZ-OH | -6.31 | 1.24 | 1.38 |
| 10 | k5 | 420 | VAL | C-O | -6.31 | 1.16 | 1.24 |
| 4 | M8 | 220 | TYR | C-O | -6.31 | 1.15 | 1.23 |
| 10 | k5 | 909 | ASP | C-O | -6.30 | 1.15 | 1.24 |
| 9 | w7 | 27 | PHE | CA-C | -6.30 | 1.45 | 1.52 |
| 4 | M4 | 220 | TYR | C-O | -6.30 | 1.15 | 1.23 |
| 10 | j5 | 884 | TRP | CB-CG | -6.30 | 1.30 | 1.50 |
| 10 | k5 | 864 | GLY | CA-C | -6.30 | 1.45 | 1.52 |
| 10 | k5 | 1039 | LEU | C-O | -6.30 | 1.16 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4 | M4 | 41 | ASN | CA-C | -6.30 | 1.44 | 1.52 |
| 10 | j5 | 637 | ARG | CZ-NH1 | -6.30 | 1.24 | 1.32 |
| 10 | j5 | 1118 | THR | C-O | -6.30 | 1.16 | 1.24 |
| 10 | k5 | 472 | TYR | CZ-OH | -6.30 | 1.24 | 1.38 |
| 4 | M8 | 128 | ALA | C-O | -6.30 | 1.16 | 1.24 |
| 10 | k5 | 728 | PRO | CA-C | -6.30 | 1.43 | 1.52 |
| 8 | c7 | 117 | ASN | C-O | -6.30 | 1.16 | 1.24 |
| 4 | M4 | 173 | PHE | CA-C | -6.29 | 1.44 | 1.52 |
| 10 | j5 | 868 | ASP | C-O | -6.29 | 1.15 | 1.24 |
| 4 | M9 | 68 | ASP | C-O | -6.29 | 1.16 | 1.23 |
| 10 | k5 | 884 | TRP | CB-CG | -6.29 | 1.30 | 1.50 |
| 4 | M4 | 68 | ASP | C-O | -6.29 | 1.16 | 1.23 |
| 4 | M4 | 51 | ARG | CZ-NH2 | 6.29 | 1.41 | 1.33 |
| 8 | a7 | 20 | PRO | C-O | -6.29 | 1.16 | 1.24 |
| 8 | e5 | 11 | ALA | CA-C | -6.29 | 1.44 | 1.52 |
| 10 | j5 | 733 | SER | CA-CB | -6.29 | 1.43 | 1.53 |
| 10 | j5 | 879 | ASP | C-O | -6.29 | 1.16 | 1.24 |
| 10 | k5 | 637 | ARG | CZ-NH1 | -6.29 | 1.24 | 1.32 |
| 8 | a5 | 11 | ALA | CA-C | -6.28 | 1.44 | 1.52 |
| 10 | j5 | 581 | TYR | CA-CB | -6.28 | 1.44 | 1.53 |
| 10 | k5 | 1116 | TYR | C-O | -6.28 | 1.16 | 1.24 |
| 10 | j5 | 784 | ILE | CA-C | -6.28 | 1.46 | 1.52 |
| 10 | k5 | 818 | GLN | CA-C | -6.28 | 1.44 | 1.52 |
| 10 | k5 | 471 | PRO | C-O | -6.28 | 1.16 | 1.24 |
| 10 | j5 | 420 | VAL | C-O | -6.28 | 1.16 | 1.24 |
| 10 | j5 | 717 | ARG | CA-C | -6.28 | 1.44 | 1.52 |
| 10 | k5 | 4 | ARG | C-O | -6.28 | 1.16 | 1.24 |
| 10 | j5 | 12 | ALA | CA-C | -6.28 | 1.44 | 1.52 |
| 10 | j5 | 1039 | LEU | C-O | -6.28 | 1.16 | 1.24 |
| 10 | k5 | 879 | ASP | C-O | -6.28 | 1.16 | 1.24 |
| 9 | i5 | 35 | GLU | CA-C | -6.27 | 1.43 | 1.52 |
| 10 | j5 | 841 | VAL | C-O | -6.27 | 1.17 | 1.24 |
| 10 | k5 | 866 | LEU | CA-C | -6.27 | 1.44 | 1.52 |
| 10 | k5 | 1118 | THR | C-O | -6.27 | 1.16 | 1.24 |
| 10 | j5 | 488 | LYS | CA-CB | -6.27 | 1.43 | 1.53 |
| 10 | k5 | 488 | LYS | CA-CB | -6.27 | 1.43 | 1.53 |
| 10 | k5 | 994 | ASP | CA-C | -6.27 | 1.44 | 1.52 |
| 10 | j5 | 728 | PRO | CA-C | -6.27 | 1.43 | 1.52 |
| 10 | k5 | 688 | ALA | CA-C | -6.27 | 1.44 | 1.52 |
| 11 | a9 | 625 | ASP | CA-C | -6.27 | 1.44 | 1.52 |
| 11 | a9 | 781 | ALA | C-O | -6.27 | 1.17 | 1.24 |
| 11 | aA | 781 | ALA | C-O | -6.27 | 1.17 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | k5 | 801 | SER | CA-CB | -6.27 | 1.44 | 1.53 |
| 10 | j5 | 666 | ASN | C-O | -6.27 | 1.15 | 1.24 |
| 10 | j5 | 994 | ASP | CA-C | -6.27 | 1.44 | 1.52 |
| 10 | k5 | 666 | ASN | C-O | -6.27 | 1.15 | 1.24 |
| 10 | k5 | 943 | THR | CA-C | -6.27 | 1.45 | 1.52 |
| 10 | j5 | 1004 | VAL | CA-CB | -6.26 | 1.46 | 1.54 |
| 9 | z5 | 57 | PHE | C-O | -6.26 | 1.16 | 1.24 |
| 10 | j5 | 623 | VAL | CA-C | -6.26 | 1.43 | 1.52 |
| 11 | a9 | 464 | PRO | C-O | -6.26 | 1.16 | 1.23 |
| 11 | aA | 464 | PRO | C-O | -6.26 | 1.16 | 1.23 |
| 11 | aA | 625 | ASP | CA-C | -6.26 | 1.44 | 1.52 |
| 10 | j5 | 801 | SER | CA-CB | -6.26 | 1.44 | 1.53 |
| 4 | M8 | 51 | ARG | CZ-NH2 | 6.26 | 1.41 | 1.33 |
| 4 | M8 | 167 | GLU | C-O | -6.26 | 1.16 | 1.24 |
| 9 | z5 | 35 | GLU | CA-C | -6.26 | 1.43 | 1.52 |
| 10 | j5 | 528 | GLU | N-CA | -6.26 | 1.38 | 1.46 |
| 10 | j5 | 849 | LYS | CA-C | -6.26 | 1.44 | 1.52 |
| 10 | j5 | 1111 | VAL | C-O | -6.26 | 1.16 | 1.24 |
| 10 | k5 | 273 | LYS | CA-C | -6.26 | 1.45 | 1.52 |
| 10 | k5 | 617 | TYR | N-CA | -6.26 | 1.38 | 1.46 |
| 10 | k5 | 1111 | VAL | C-O | -6.26 | 1.16 | 1.24 |
| 10 | j5 | 483 | PHE | C-N | -6.25 | 1.26 | 1.33 |
| 10 | k5 | 616 | LEU | CA-C | -6.25 | 1.44 | 1.52 |
| 4 | MA | 173 | PHE | CA-C | -6.25 | 1.44 | 1.52 |
| 8 | G5 | 59 | PHE | C-O | -6.25 | 1.15 | 1.24 |
| 9 | i5 | 22 | GLU | CA-C | -6.25 | 1.45 | 1.53 |
| 10 | j5 | 262 | TYR | C-O | -6.25 | 1.15 | 1.24 |
| 10 | k5 | 673 | VAL | CA-CB | -6.25 | 1.46 | 1.54 |
| 4 | M9 | 173 | PHE | CA-C | -6.25 | 1.44 | 1.52 |
| 4 | MA | 167 | GLU | C-O | -6.25 | 1.16 | 1.24 |
| 10 | k5 | 1033 | ARG | CA-C | -6.25 | 1.44 | 1.52 |
| 4 | M8 | 172 | HIS | CA-C | -6.25 | 1.45 | 1.52 |
| 4 | M9 | 167 | GLU | C-O | -6.25 | 1.16 | 1.24 |
| 4 | M3 | 111 | LYS | C-O | -6.25 | 1.16 | 1.24 |
| 10 | j5 | 670 | TYR | CA-C | -6.25 | 1.44 | 1.52 |
| 4 | M1 | 111 | LYS | C-O | -6.25 | 1.16 | 1.24 |
| 4 | MA | 220 | TYR | C-O | -6.25 | 1.16 | 1.23 |
| 9 | z5 | 64 | ASN | CA-C | -6.25 | 1.44 | 1.52 |
| 10 | j5 | 447 | ALA | C-O | -6.25 | 1.16 | 1.24 |
| 10 | j5 | 619 | GLU | CA-C | -6.25 | 1.44 | 1.52 |
| 4 | M8 | 111 | LYS | C-O | -6.25 | 1.16 | 1.24 |
| 4 | M9 | 220 | TYR | C-O | -6.25 | 1.16 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | j5 | 586 | LEU | CA-C | -6.24 | 1.45 | 1.52 |
| 10 | j5 | 866 | LEU | CA-C | -6.24 | 1.44 | 1.52 |
| 4 | M1 | 139 | VAL | C-O | -6.24 | 1.16 | 1.24 |
| 9 | i5 | 64 | ASN | CA-C | -6.24 | 1.44 | 1.52 |
| 10 | k5 | 581 | TYR | CA-CB | -6.24 | 1.44 | 1.53 |
| 10 | k5 | 1123 | ASN | N-CA | -6.24 | 1.38 | 1.46 |
| 9 | w7 | 26 | THR | C-O | -6.24 | 1.14 | 1.23 |
| 9 | w7 | 60 | VAL | C-O | -6.24 | 1.16 | 1.24 |
| 4 | M4 | 111 | LYS | C-O | -6.24 | 1.16 | 1.24 |
| 10 | j5 | 346 | GLU | CA-CB | -6.24 | 1.43 | 1.53 |
| 10 | k5 | 868 | ASP | C-O | -6.24 | 1.15 | 1.24 |
| 4 | M4 | 167 | GLU | C-O | -6.24 | 1.16 | 1.24 |
| 4 | M8 | 49 | LEU | C-O | -6.24 | 1.16 | 1.24 |
| 1 | h7 | 37 | ARG | C-O | -6.23 | 1.16 | 1.24 |
| 4 | M4 | 49 | LEU | C-O | -6.23 | 1.16 | 1.24 |
| 4 | M4 | 172 | HIS | CA-C | -6.23 | 1.45 | 1.52 |
| 10 | j5 | 257 | THR | CA-C | -6.23 | 1.45 | 1.52 |
| 10 | j5 | 688 | ALA | CA-C | -6.23 | 1.44 | 1.52 |
| 10 | j5 | 721 | LYS | CA-C | -6.23 | 1.45 | 1.52 |
| 10 | j5 | 792 | GLU | CA-CB | -6.23 | 1.43 | 1.53 |
| 11 | a9 | 464 | PRO | CA-C | -6.23 | 1.46 | 1.52 |
| 11 | aA | 464 | PRO | CA-C | -6.23 | 1.46 | 1.52 |
| 8 | e5 | 19 | SER | C-O | -6.23 | 1.16 | 1.24 |
| 10 | j5 | 725 | LEU | N-CA | -6.23 | 1.38 | 1.46 |
| 10 | k5 | 717 | ARG | CA-C | -6.23 | 1.44 | 1.52 |
| 10 | j5 | 596 | GLY | C-O | -6.23 | 1.15 | 1.24 |
| 10 | k5 | 596 | GLY | C-O | -6.23 | 1.15 | 1.24 |
| 10 | j5 | 616 | LEU | CA-C | -6.22 | 1.44 | 1.52 |
| 10 | j5 | 771 | ALA | N-CA | -6.22 | 1.37 | 1.46 |
| 4 | M4 | 128 | ALA | C-O | -6.22 | 1.16 | 1.24 |
| 9 | x7 | 43 | ARG | C-O | -6.22 | 1.16 | 1.24 |
| 4 | MA | 111 | LYS | C-O | -6.22 | 1.16 | 1.24 |
| 4 | M9 | 111 | LYS | C-O | -6.22 | 1.16 | 1.24 |
| 8 | I5 | 18 | LEU | CA-C | -6.21 | 1.44 | 1.52 |
| 10 | j5 | 504 | ASP | C-O | -6.21 | 1.15 | 1.24 |
| 8 | g7 | 16 | ARG | C-O | -6.21 | 1.15 | 1.23 |
| 9 | z7 | 38 | PHE | C-O | -6.21 | 1.16 | 1.24 |
| 8 | A5 | 49 | ARG | N-CA | -6.21 | 1.39 | 1.46 |
| 10 | k5 | 447 | ALA | C-O | -6.21 | 1.16 | 1.24 |
| 11 | a9 | 519 | ARG | C-O | -6.21 | 1.15 | 1.24 |
| 11 | aA | 519 | ARG | C-O | -6.21 | 1.15 | 1.24 |
| 4 | M3 | 49 | LEU | C-O | -6.21 | 1.16 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | k5 | 413 | SER | CA-C | -6.21 | 1.44 | 1.52 |
| 10 | k5 | 917 | LYS | CA-CB | -6.21 | 1.44 | 1.53 |
| 1 | b7 | 47 | ASN | C-O | -6.21 | 1.15 | 1.24 |
| 4 | M1 | 49 | LEU | C-O | -6.21 | 1.16 | 1.24 |
| 10 | j5 | 273 | LYS | CA-C | -6.21 | 1.45 | 1.52 |
| 10 | k5 | 628 | GLU | N-CA | -6.21 | 1.38 | 1.46 |
| 10 | k5 | 787 | GLU | CA-C | -6.21 | 1.44 | 1.52 |
| 11 | aA | 361 | ALA | C-O | -6.21 | 1.17 | 1.24 |
| 3 | LA | 111 | ASN | CA-C | -6.21 | 1.44 | 1.52 |
| 10 | k5 | 528 | GLU | N-CA | -6.21 | 1.38 | 1.46 |
| 8 | g7 | 20 | PRO | C-O | -6.21 | 1.16 | 1.24 |
| 3 | L9 | 111 | ASN | CA-C | -6.21 | 1.44 | 1.52 |
| 10 | j5 | 628 | GLU | N-CA | -6.20 | 1.38 | 1.46 |
| 10 | j5 | 868 | ASP | CA-CB | -6.20 | 1.44 | 1.53 |
| 4 | M3 | 167 | GLU | C-O | -6.20 | 1.16 | 1.24 |
| 8 | C5 | 18 | LEU | CA-C | -6.20 | 1.44 | 1.52 |
| 8 | e5 | 7 | ALA | N-CA | 6.20 | 1.54 | 1.46 |
| 10 | j5 | 1121 | ALA | CA-C | -6.20 | 1.44 | 1.52 |
| 10 | k5 | 262 | TYR | C-O | -6.20 | 1.16 | 1.24 |
| 11 | a9 | 38 | VAL | CA-C | -6.20 | 1.46 | 1.52 |
| 11 | aA | 38 | VAL | CA-C | -6.20 | 1.46 | 1.52 |
| 4 | M1 | 167 | GLU | C-O | -6.20 | 1.16 | 1.24 |
| 4 | M3 | 220 | TYR | C-O | -6.20 | 1.16 | 1.23 |
| 10 | k5 | 346 | GLU | CA-CB | -6.20 | 1.43 | 1.53 |
| 9 | z7 | 26 | THR | C-O | -6.20 | 1.14 | 1.23 |
| 9 | z7 | 60 | VAL | C-O | -6.20 | 1.16 | 1.24 |
| 4 | M1 | 220 | TYR | C-O | -6.20 | 1.16 | 1.23 |
| 10 | k5 | 725 | LEU | N-CA | -6.20 | 1.38 | 1.46 |
| 9 | y7 | 18 | ARG | CA-C | -6.20 | 1.45 | 1.52 |
| 4 | M3 | 139 | VAL | C-O | -6.20 | 1.16 | 1.24 |
| 9 | i5 | 35 | GLU | CA-CB | -6.20 | 1.42 | 1.53 |
| 10 | j5 | 796 | ARG | CA-C | -6.20 | 1.44 | 1.52 |
| 10 | j5 | 818 | GLN | CA-C | -6.20 | 1.44 | 1.52 |
| 10 | j5 | 887 | PRO | CA-C | -6.20 | 1.44 | 1.52 |
| 10 | k5 | 887 | PRO | CA-C | -6.20 | 1.44 | 1.52 |
| 10 | j5 | 345 | ARG | CA-C | -6.19 | 1.44 | 1.52 |
| 10 | k5 | 623 | VAL | CA-C | -6.19 | 1.44 | 1.52 |
| 8 | G5 | 49 | ARG | N-CA | -6.19 | 1.39 | 1.46 |
| 4 | M4 | 49 | LEU | CA-C | -6.19 | 1.44 | 1.52 |
| 10 | k5 | 1123 | ASN | CA-C | -6.19 | 1.44 | 1.52 |
| 8 | i7 | 118 | SER | CA-C | -6.19 | 1.44 | 1.52 |
| 9 | y7 | 43 | ARG | C-O | -6.19 | 1.16 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | j5 | 943 | THR | CA-C | -6.19 | 1.45 | 1.52 |
| 10 | k5 | 1121 | ALA | CA-C | -6.19 | 1.44 | 1.52 |
| 10 | k5 | 586 | LEU | CA-C | -6.19 | 1.45 | 1.52 |
| 10 | k5 | 670 | TYR | CA-C | -6.19 | 1.45 | 1.52 |
| 1 | h7 | 48 | ALA | C-O | -6.18 | 1.16 | 1.24 |
| 10 | k5 | 345 | ARG | CA-C | -6.18 | 1.44 | 1.52 |
| 1 | h7 | 41 | ALA | CA-C | -6.18 | 1.44 | 1.52 |
| 9 | x7 | 18 | ARG | CA-C | -6.18 | 1.45 | 1.52 |
| 4 | MA | 49 | LEU | C-O | -6.18 | 1.16 | 1.24 |
| 10 | j5 | 1123 | ASN | CA-C | -6.18 | 1.44 | 1.52 |
| 4 | M9 | 49 | LEU | C-O | -6.18 | 1.16 | 1.24 |
| 4 | M4 | 157 | PHE | C-O | -6.18 | 1.15 | 1.24 |
| 9 | z5 | 35 | GLU | CA-CB | -6.18 | 1.43 | 1.53 |
| 10 | j5 | 1123 | ASN | N-CA | -6.18 | 1.38 | 1.46 |
| 10 | k5 | 708 | GLY | C-O | -6.18 | 1.14 | 1.23 |
| 10 | k5 | 792 | GLU | CA-CB | -6.18 | 1.43 | 1.53 |
| 10 | k5 | 1004 | VAL | CA-CB | -6.18 | 1.47 | 1.54 |
| 1 | b7 | 37 | ARG | C-O | -6.18 | 1.16 | 1.24 |
| 10 | j5 | 4 | ARG | C-O | -6.17 | 1.16 | 1.24 |
| 10 | k5 | 849 | LYS | CA-C | -6.17 | 1.44 | 1.52 |
| 10 | k5 | 1088 | GLY | C-O | -6.17 | 1.15 | 1.24 |
| 1 | b7 | 41 | ALA | CA-C | -6.17 | 1.44 | 1.52 |
| 9 | i5 | 21 | ARG | CZ-NH1 | -6.17 | 1.24 | 1.32 |
| 10 | j5 | 946 | ASP | C-O | -6.17 | 1.15 | 1.23 |
| 10 | k5 | 483 | PHE | C-N | -6.17 | 1.26 | 1.33 |
| 8 | a5 | 7 | ALA | N-CA | 6.17 | 1.54 | 1.46 |
| 4 | M3 | 157 | PHE | C-O | -6.17 | 1.15 | 1.24 |
| 9 | z5 | 21 | ARG | CZ-NH1 | -6.17 | 1.24 | 1.32 |
| 10 | j5 | 247 | ARG | C-O | -6.17 | 1.17 | 1.24 |
| 10 | k5 | 247 | ARG | C-O | -6.17 | 1.17 | 1.24 |
| 4 | M1 | 157 | PHE | C-O | -6.17 | 1.15 | 1.24 |
| 10 | j5 | 511 | ARG | CZ-NH2 | -6.17 | 1.25 | 1.33 |
| 10 | j5 | 787 | GLU | CA-C | -6.17 | 1.44 | 1.52 |
| 10 | k5 | 424 | ARG | CA-C | -6.17 | 1.46 | 1.53 |
| 10 | k5 | 511 | ARG | CZ-NH2 | -6.17 | 1.25 | 1.33 |
| 10 | k5 | 721 | LYS | CA-C | -6.17 | 1.45 | 1.52 |
| 9 | w7 | 38 | PHE | C-O | -6.17 | 1.17 | 1.24 |
| 4 | M3 | 128 | ALA | C-O | -6.16 | 1.16 | 1.24 |
| 8 | A5 | 60 | GLN | N-CA | -6.16 | 1.38 | 1.46 |
| 10 | j5 | 617 | TYR | N-CA | -6.16 | 1.38 | 1.46 |
| 4 | M8 | 157 | PHE | C-O | -6.16 | 1.15 | 1.24 |
| 4 | M1 | 128 | ALA | C-O | -6.16 | 1.16 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 8 | A5 | 59 | PHE | C-O | -6.16 | 1.15 | 1.24 |
| 8 | G5 | 60 | GLN | N-CA | -6.16 | 1.38 | 1.46 |
| 10 | j5 | 493 | ASN | C-O | -6.16 | 1.17 | 1.24 |
| 10 | j5 | 917 | LYS | CA-CB | -6.16 | 1.44 | 1.53 |
| 10 | k5 | 493 | ASN | C-O | -6.16 | 1.17 | 1.24 |
| 8 | u7 | 160 | MET | C-O | -6.16 | 1.16 | 1.24 |
| 11 | a9 | 614 | SER | N-CA | -6.16 | 1.38 | 1.46 |
| 11 | aA | 614 | SER | N-CA | -6.16 | 1.38 | 1.46 |
| 4 | M3 | 64 | GLY | C-O | -6.16 | 1.14 | 1.23 |
| 8 | a5 | 19 | SER | C-O | -6.16 | 1.16 | 1.24 |
| 11 | a9 | 522 | ASP | CA-C | -6.16 | 1.44 | 1.52 |
| 11 | aA | 522 | ASP | CA-C | -6.16 | 1.44 | 1.52 |
| 10 | j5 | 639 | THR | CB-CG2 | -6.16 | 1.32 | 1.52 |
| 10 | k5 | 639 | THR | CB-CG2 | -6.16 | 1.32 | 1.52 |
| 3 | LA | 112 | GLY | C-O | -6.16 | 1.15 | 1.24 |
| 10 | j5 | 345 | ARG | C-O | -6.16 | 1.16 | 1.24 |
| 10 | j5 | 424 | ARG | CA-C | -6.16 | 1.46 | 1.53 |
| 10 | k5 | 345 | ARG | C-O | -6.16 | 1.16 | 1.24 |
| 1 | h7 | 47 | ASN | C-O | -6.16 | 1.15 | 1.24 |
| 1 | b7 | 39 | ARG | C-O | -6.16 | 1.16 | 1.24 |
| 1 | b7 | 48 | ALA | C-O | -6.16 | 1.17 | 1.24 |
| 3 | L9 | 112 | GLY | C-O | -6.16 | 1.15 | 1.24 |
| 11 | a9 | 361 | ALA | C-O | -6.16 | 1.17 | 1.24 |
| 4 | M1 | 64 | GLY | C-O | -6.16 | 1.14 | 1.23 |
| 4 | MA | 139 | VAL | C-O | -6.15 | 1.16 | 1.24 |
| 4 | M9 | 139 | VAL | C-O | -6.15 | 1.16 | 1.24 |
| 10 | j5 | 802 | VAL | CA-C | -6.15 | 1.44 | 1.52 |
| 1 | h7 | 39 | ARG | C-O | -6.15 | 1.16 | 1.24 |
| 4 | MA | 64 | GLY | C-O | -6.15 | 1.14 | 1.23 |
| 4 | M4 | 43 | TYR | N-CA | -6.15 | 1.38 | 1.45 |
| 10 | j5 | 413 | SER | CA-C | -6.15 | 1.44 | 1.52 |
| 10 | j5 | 786 | SER | C-O | -6.15 | 1.15 | 1.24 |
| 8 | o7 | 7 | ALA | CA-C | -6.15 | 1.43 | 1.52 |
| 4 | M9 | 64 | GLY | C-O | -6.15 | 1.14 | 1.23 |
| 10 | j5 | 587 | LYS | C-N | -6.15 | 1.25 | 1.33 |
| 10 | k5 | 786 | SER | C-O | -6.15 | 1.15 | 1.24 |
| 8 | a7 | 16 | ARG | C-O | -6.15 | 1.16 | 1.23 |
| 9 | w7 | 6 | LYS | C-O | -6.15 | 1.17 | 1.24 |
| 4 | M3 | 57 | THR | CA-CB | -6.14 | 1.43 | 1.53 |
| 10 | j5 | 469 | GLN | CD-NE2 | -6.14 | 1.20 | 1.33 |
| 10 | k5 | 469 | GLN | CD-NE2 | -6.14 | 1.20 | 1.33 |
| 4 | M1 | 57 | THR | CA-CB | -6.14 | 1.43 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | k5 | 916 | PHE | C-O | -6.14 | 1.16 | 1.24 |
| 4 | MA | 128 | ALA | C-O | -6.14 | 1.16 | 1.24 |
| 10 | j5 | 1088 | GLY | C-O | -6.14 | 1.15 | 1.24 |
| 4 | M9 | 128 | ALA | C-O | -6.14 | 1.16 | 1.24 |
| 8 | e5 | 123 | ILE | CA-CB | 6.14 | 1.57 | 1.54 |
| 9 | i5 | 57 | PHE | C-O | -6.14 | 1.16 | 1.24 |
| 8 | c7 | 117 | ASN | CA-C | -6.14 | 1.44 | 1.52 |
| 10 | k5 | 769 | THR | CB-CG2 | -6.14 | 1.32 | 1.52 |
| 4 | M8 | 43 | TYR | N-CA | -6.14 | 1.38 | 1.45 |
| 10 | j5 | 876 | TYR | CA-CB | -6.13 | 1.45 | 1.54 |
| 10 | k5 | 504 | ASP | C-O | -6.13 | 1.15 | 1.24 |
| 10 | k5 | 870 | GLU | N-CA | -6.13 | 1.38 | 1.46 |
| 10 | k5 | 876 | TYR | CA-CB | -6.13 | 1.45 | 1.54 |
| 10 | k5 | 771 | ALA | N-CA | -6.13 | 1.37 | 1.46 |
| 4 | M3 | 43 | TYR | N-CA | -6.13 | 1.38 | 1.45 |
| 11 | a9 | 420 | ASN | C-O | -6.13 | 1.16 | 1.24 |
| 11 | aA | 420 | ASN | C-O | -6.13 | 1.16 | 1.24 |
| 4 | M1 | 43 | TYR | N-CA | -6.13 | 1.38 | 1.45 |
| 10 | j5 | 622 | TYR | CZ-OH | -6.13 | 1.25 | 1.38 |
| 10 | k5 | 622 | TYR | CZ-OH | -6.13 | 1.25 | 1.38 |
| 10 | k5 | 868 | ASP | CA-CB | -6.13 | 1.44 | 1.53 |
| 4 | M8 | 115 | GLY | C-O | -6.13 | 1.17 | 1.24 |
| 4 | MA | 57 | THR | CA-CB | -6.13 | 1.43 | 1.53 |
| 4 | MA | 157 | PHE | C-O | -6.13 | 1.15 | 1.24 |
| 4 | M9 | 57 | THR | CA-CB | -6.13 | 1.43 | 1.53 |
| 4 | M9 | 157 | PHE | C-O | -6.13 | 1.15 | 1.24 |
| 10 | j5 | 645 | ASN | CG-ND2 | -6.12 | 1.20 | 1.33 |
| 8 | C5 | 12 | ASP | C-O | -6.12 | 1.16 | 1.24 |
| 10 | k5 | 796 | ARG | CA-C | -6.12 | 1.44 | 1.52 |
| 4 | M8 | 49 | LEU | CA-C | -6.12 | 1.44 | 1.52 |
| 10 | j5 | 626 | ALA | CA-CB | -6.12 | 1.43 | 1.53 |
| 10 | j5 | 708 | GLY | C-O | -6.12 | 1.14 | 1.23 |
| 10 | j5 | 769 | THR | CB-CG2 | -6.12 | 1.32 | 1.52 |
| 10 | k5 | 802 | VAL | CA-C | -6.12 | 1.44 | 1.52 |
| 8 | u7 | 7 | ALA | CA-C | -6.12 | 1.43 | 1.52 |
| 10 | j5 | 522 | ASN | CA-C | -6.12 | 1.43 | 1.52 |
| 9 | w7 | 61 | GLN | C-O | -6.12 | 1.17 | 1.24 |
| 1 | D5 | 13 | ASP | C-O | -6.12 | 1.15 | 1.23 |
| 8 | I5 | 12 | ASP | C-O | -6.12 | 1.16 | 1.24 |
| 4 | M8 | 64 | GLY | C-O | -6.12 | 1.14 | 1.23 |
| 10 | j5 | 870 | GLU | N-CA | -6.12 | 1.38 | 1.46 |
| 4 | M4 | 64 | GLY | C-O | -6.11 | 1.14 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | k5 | 407 | ASP | C-O | -6.11 | 1.15 | 1.24 |
| 10 | j5 | 680 | PRO | CA-C | -6.11 | 1.45 | 1.52 |
| 4 | MA | 49 | LEU | CA-C | -6.11 | 1.44 | 1.52 |
| 10 | k5 | 413 | SER | C-O | -6.11 | 1.16 | 1.24 |
| 8 | c7 | 118 | SER | CA-C | -6.11 | 1.45 | 1.52 |
| 1 | D5 | 6 | THR | C-O | -6.10 | 1.15 | 1.24 |
| 8 | o7 | 160 | MET | C-O | -6.10 | 1.16 | 1.24 |
| 10 | j5 | 916 | PHE | C-O | -6.10 | 1.16 | 1.24 |
| 10 | j5 | 925 | ILE | C-O | -6.10 | 1.15 | 1.24 |
| 10 | k5 | 680 | PRO | CA-C | -6.10 | 1.45 | 1.52 |
| 10 | j5 | 274 | MET | C-O | -6.10 | 1.16 | 1.23 |
| 9 | z7 | 6 | LYS | C-O | -6.10 | 1.17 | 1.24 |
| 10 | j5 | 459 | PHE | N-CA | -6.10 | 1.39 | 1.46 |
| 10 | k5 | 946 | ASP | C-O | -6.10 | 1.15 | 1.23 |
| 4 | M4 | 115 | GLY | C-O | -6.10 | 1.17 | 1.24 |
| 10 | j5 | 691 | SER | CA-C | -6.09 | 1.43 | 1.52 |
| 10 | k5 | 691 | SER | CA-C | -6.09 | 1.43 | 1.52 |
| 11 | a9 | 419 | ARG | CA-C | -6.09 | 1.45 | 1.52 |
| 11 | aA | 419 | ARG | CA-C | -6.09 | 1.45 | 1.52 |
| 10 | k5 | 954 | GLU | CA-C | -6.09 | 1.44 | 1.52 |
| 8 | A5 | 49 | ARG | CA-C | -6.09 | 1.45 | 1.52 |
| 10 | k5 | 645 | ASN | CG-ND2 | -6.09 | 1.20 | 1.33 |
| 10 | j5 | 633 | ARG | N-CA | -6.09 | 1.38 | 1.46 |
| 10 | j5 | 724 | GLU | CA-C | -6.09 | 1.43 | 1.52 |
| 10 | k5 | 633 | ARG | N-CA | -6.09 | 1.38 | 1.46 |
| 10 | k5 | 724 | GLU | CA-C | -6.09 | 1.43 | 1.52 |
| 10 | k5 | 3 | ILE | CA-C | -6.09 | 1.45 | 1.52 |
| 10 | k5 | 268 | SER | C-O | -6.09 | 1.14 | 1.24 |
| 10 | k5 | 925 | ILE | C-O | -6.09 | 1.15 | 1.24 |
| 9 | z7 | 61 | GLN | C-O | -6.09 | 1.17 | 1.24 |
| 4 | M8 | 57 | THR | CA-CB | -6.09 | 1.43 | 1.53 |
| 4 | M4 | 57 | THR | CA-CB | -6.08 | 1.43 | 1.53 |
| 4 | MA | 43 | TYR | N-CA | -6.08 | 1.38 | 1.45 |
| 9 | z5 | 36 | ASN | CA-C | -6.08 | 1.44 | 1.52 |
| 4 | M9 | 43 | TYR | N-CA | -6.08 | 1.38 | 1.45 |
| 9 | z5 | 39 | THR | CB-CG2 | -6.08 | 1.32 | 1.52 |
| 9 | i5 | 39 | THR | CB-CG2 | -6.08 | 1.32 | 1.52 |
| 10 | j5 | 1010 | GLY | C-O | -6.08 | 1.15 | 1.23 |
| 4 | M3 | 49 | LEU | CA-C | -6.08 | 1.44 | 1.52 |
| 10 | k5 | 587 | LYS | C-N | -6.08 | 1.25 | 1.33 |
| 4 | M1 | 49 | LEU | CA-C | -6.08 | 1.44 | 1.52 |
| 4 | MA | 239 | PHE | C-O | -6.08 | 1.17 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1 | J5 | 6 | THR | C-O | -6.08 | 1.15 | 1.24 |
| 4 | M9 | 239 | PHE | C-O | -6.08 | 1.17 | 1.24 |
| 10 | j5 | 575 | ILE | CA-C | -6.08 | 1.45 | 1.52 |
| 8 | G5 | 49 | ARG | CA-C | -6.07 | 1.45 | 1.52 |
| 1 | J5 | 13 | ASP | C-O | -6.07 | 1.15 | 1.23 |
| 10 | k5 | 522 | ASN | CA-C | -6.07 | 1.43 | 1.52 |
| 3 | LA | 116 | THR | CA-C | -6.07 | 1.45 | 1.52 |
| 10 | j5 | 268 | SER | C-O | -6.07 | 1.14 | 1.24 |
| 3 | L9 | 116 | THR | CA-C | -6.07 | 1.45 | 1.52 |
| 10 | j5 | 954 | GLU | CA-C | -6.07 | 1.44 | 1.52 |
| 8 | i7 | 117 | ASN | CA-C | -6.07 | 1.44 | 1.52 |
| 4 | M4 | 59 | ILE | CA-CB | -6.07 | 1.46 | 1.54 |
| 10 | j5 | 184 | LEU | CA-C | -6.07 | 1.44 | 1.52 |
| 10 | k5 | 184 | LEU | CA-C | -6.07 | 1.44 | 1.52 |
| 10 | j5 | 3 | ILE | CA-C | -6.06 | 1.45 | 1.52 |
| 10 | j5 | 413 | SER | C-O | -6.06 | 1.16 | 1.24 |
| 8 | o7 | 46 | ALA | C-O | -6.06 | 1.16 | 1.24 |
| 9 | x7 | 24 | GLN | CA-C | -6.06 | 1.44 | 1.52 |
| 9 | y7 | 23 | LEU | C-O | -6.06 | 1.16 | 1.24 |
| 10 | j5 | 750 | ARG | CZ-NH2 | -6.06 | 1.25 | 1.33 |
| 9 | y7 | 24 | GLN | CA-C | -6.06 | 1.44 | 1.52 |
| 9 | i5 | 36 | ASN | CA-C | -6.06 | 1.44 | 1.52 |
| 10 | j5 | 219 | ASP | CB-CG | 6.06 | 1.67 | 1.52 |
| 10 | k5 | 1010 | GLY | C-O | -6.06 | 1.15 | 1.23 |
| 4 | M8 | 59 | ILE | CA-CB | -6.06 | 1.46 | 1.54 |
| 4 | MA | 94 | TRP | C-O | -6.06 | 1.15 | 1.23 |
| 10 | j5 | 407 | ASP | C-O | -6.06 | 1.15 | 1.24 |
| 10 | j5 | 612 | ILE | CB-CG1 | -6.06 | 1.41 | 1.53 |
| 10 | k5 | 612 | ILE | CB-CG1 | -6.06 | 1.41 | 1.53 |
| 1 | b7 | 49 | THR | C-O | -6.06 | 1.16 | 1.24 |
| 4 | M9 | 94 | TRP | C-O | -6.06 | 1.15 | 1.23 |
| 1 | b7 | 44 | ILE | CA-CB | -6.05 | 1.46 | 1.54 |
| 10 | k5 | 1044 | ASN | C-O | -6.05 | 1.16 | 1.24 |
| 10 | j5 | 998 | ASN | C-O | -6.05 | 1.17 | 1.24 |
| 10 | k5 | 998 | ASN | C-O | -6.05 | 1.17 | 1.24 |
| 4 | M9 | 49 | LEU | CA-C | -6.05 | 1.44 | 1.52 |
| 8 | W5 | 123 | ILE | CA-CB | 6.05 | 1.57 | 1.54 |
| 1 | h7 | 49 | THR | C-O | -6.05 | 1.16 | 1.24 |
| 10 | j5 | 380 | SER | CA-CB | -6.05 | 1.43 | 1.53 |
| 10 | k5 | 626 | ALA | CA-CB | -6.05 | 1.43 | 1.53 |
| 8 | a5 | 123 | ILE | CA-CB | 6.04 | 1.57 | 1.54 |
| 10 | j5 | 676 | GLU | CA-CB | -6.04 | 1.40 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | k5 | 459 | PHE | N-CA | -6.04 | 1.39 | 1.46 |
| 10 | k5 | 676 | GLU | CA-CB | -6.04 | 1.40 | 1.53 |
| 4 | M3 | 94 | TRP | C-O | -6.04 | 1.15 | 1.23 |
| 8 | G5 | 48 | GLU | C-O | -6.04 | 1.17 | 1.24 |
| 4 | M1 | 94 | TRP | C-O | -6.04 | 1.15 | 1.23 |
| 4 | MA | 115 | GLY | C-O | -6.04 | 1.17 | 1.24 |
| 9 | x7 | 13 | SER | CA-C | -6.04 | 1.44 | 1.52 |
| 4 | M9 | 115 | GLY | C-O | -6.04 | 1.17 | 1.24 |
| 4 | M3 | 59 | ILE | CA-CB | -6.04 | 1.47 | 1.54 |
| 10 | j5 | 765 | ASP | CA-C | -6.04 | 1.44 | 1.52 |
| 10 | k5 | 219 | ASP | CB-CG | 6.04 | 1.67 | 1.52 |
| 10 | k5 | 380 | SER | CA-CB | -6.04 | 1.43 | 1.53 |
| 10 | k5 | 765 | ASP | CA-C | -6.04 | 1.44 | 1.52 |
| 4 | M1 | 59 | ILE | CA-CB | -6.04 | 1.47 | 1.54 |
| 10 | k5 | 370 | GLU | CA-C | -6.04 | 1.43 | 1.52 |
| 10 | k5 | 1114 | ARG | C-O | -6.04 | 1.16 | 1.23 |
| 8 | u7 | 46 | ALA | C-O | -6.04 | 1.16 | 1.24 |
| 10 | j5 | 482 | GLN | CA-CB | -6.04 | 1.44 | 1.53 |
| 9 | y7 | 13 | SER | CA-C | -6.04 | 1.44 | 1.52 |
| 10 | j5 | 216 | ASP | CA-C | -6.03 | 1.44 | 1.53 |
| 4 | MA | 59 | ILE | CA-CB | -6.03 | 1.47 | 1.54 |
| 10 | k5 | 662 | ASP | CA-CB | -6.03 | 1.42 | 1.53 |
| 4 | M9 | 59 | ILE | CA-CB | -6.03 | 1.47 | 1.54 |
| 10 | k5 | 482 | GLN | CA-CB | -6.03 | 1.44 | 1.53 |
| 10 | j5 | 170 | ALA | CA-C | -6.03 | 1.45 | 1.52 |
| 10 | j5 | 472 | TYR | CE1-CZ | -6.03 | 1.23 | 1.38 |
| 1 | h7 | 44 | ILE | CA-CB | -6.03 | 1.46 | 1.54 |
| 4 | M3 | 239 | PHE | C-O | -6.03 | 1.17 | 1.24 |
| 4 | M4 | 239 | PHE | C-O | -6.03 | 1.17 | 1.24 |
| 10 | j5 | 783 | TYR | CA-CB | -6.03 | 1.43 | 1.53 |
| 10 | k5 | 783 | TYR | CA-CB | -6.03 | 1.43 | 1.53 |
| 10 | j5 | 431 | GLN | C-O | -6.02 | 1.15 | 1.23 |
| 10 | j5 | 615 | LYS | N-CA | -6.02 | 1.39 | 1.46 |
| 10 | k5 | 901 | TYR | CZ-OH | -6.02 | 1.25 | 1.38 |
| 4 | M8 | 68 | ASP | CA-CB | -6.02 | 1.43 | 1.53 |
| 10 | k5 | 472 | TYR | CE1-CZ | -6.02 | 1.23 | 1.38 |
| 10 | k5 | 575 | ILE | CA-C | -6.02 | 1.45 | 1.52 |
| 10 | j5 | 435 | ASN | CG-OD1 | -6.02 | 1.12 | 1.23 |
| 10 | j5 | 901 | TYR | CZ-OH | -6.02 | 1.25 | 1.38 |
| 10 | k5 | 435 | ASN | CG-OD1 | -6.02 | 1.12 | 1.23 |
| 4 | M4 | 94 | TRP | C-O | -6.01 | 1.15 | 1.23 |
| 8 | A5 | 123 | ILE | CA-CB | 6.01 | 1.57 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | k5 | 455 | PHE | N-CA | -6.01 | 1.38 | 1.46 |
| 10 | k5 | 779 | ASP | CB-CG | -6.01 | 1.37 | 1.52 |
| 10 | j5 | 152 | ARG | C-O | -6.01 | 1.17 | 1.24 |
| 10 | j5 | 511 | ARG | CD-NE | -6.01 | 1.37 | 1.46 |
| 10 | j5 | 632 | ARG | CZ-NH1 | -6.01 | 1.24 | 1.32 |
| 10 | j5 | 1044 | ASN | C-O | -6.01 | 1.16 | 1.24 |
| 10 | k5 | 632 | ARG | CZ-NH1 | -6.01 | 1.24 | 1.32 |
| 9 | z7 | 63 | ALA | C-O | -6.01 | 1.16 | 1.24 |
| 10 | k5 | 797 | ASN | N-CA | -6.01 | 1.38 | 1.46 |
| 10 | j5 | 36 | ASN | CA-C | -6.01 | 1.45 | 1.53 |
| 10 | j5 | 370 | GLU | CA-C | -6.01 | 1.43 | 1.52 |
| 10 | j5 | 900 | LEU | CA-C | -6.01 | 1.45 | 1.52 |
| 10 | k5 | 467 | PRO | CA-CB | -6.01 | 1.44 | 1.53 |
| 9 | w7 | 41 | GLN | CD-NE2 | -6.01 | 1.20 | 1.33 |
| 10 | k5 | 371 | SER | C-O | -6.00 | 1.16 | 1.23 |
| 10 | k5 | 729 | ILE | N-CA | 6.00 | 1.53 | 1.46 |
| 10 | k5 | 750 | ARG | CZ-NH2 | -6.00 | 1.25 | 1.33 |
| 1 | b7 | 41 | ALA | C-O | -6.00 | 1.16 | 1.24 |
| 4 | M3 | 115 | GLY | C-O | -6.00 | 1.17 | 1.24 |
| 10 | j5 | 662 | ASP | CA-CB | -6.00 | 1.42 | 1.53 |
| 10 | k5 | 615 | LYS | N-CA | -6.00 | 1.39 | 1.46 |
| 10 | k5 | 800 | THR | C-O | -6.00 | 1.16 | 1.23 |
| 10 | k5 | 882 | PRO | N-CA | -6.00 | 1.39 | 1.47 |
| 9 | z7 | 41 | GLN | CD-NE2 | -6.00 | 1.20 | 1.33 |
| 4 | M1 | 115 | GLY | C-O | -6.00 | 1.17 | 1.24 |
| 10 | k5 | 274 | MET | C-O | -6.00 | 1.16 | 1.23 |
| 4 | M1 | 239 | PHE | C-O | -6.00 | 1.17 | 1.24 |
| 10 | j5 | 800 | THR | C-O | -6.00 | 1.16 | 1.23 |
| 10 | k5 | 216 | ASP | CA-C | -6.00 | 1.44 | 1.53 |
| 4 | M8 | 48 | PRO | CA-CB | -6.00 | 1.45 | 1.53 |
| 11 | a9 | 473 | HIS | CA-C | -6.00 | 1.45 | 1.52 |
| 11 | aA | 473 | HIS | CA-C | -6.00 | 1.45 | 1.52 |
| 8 | K5 | 117 | ASN | C-O | -6.00 | 1.17 | 1.24 |
| 10 | k5 | 900 | LEU | CA-C | -6.00 | 1.45 | 1.52 |
| 4 | M4 | 68 | ASP | CA-CB | -5.99 | 1.43 | 1.53 |
| 10 | j5 | 467 | PRO | CA-CB | -5.99 | 1.44 | 1.53 |
| 10 | j5 | 779 | ASP | CB-CG | -5.99 | 1.37 | 1.52 |
| 10 | k5 | 36 | ASN | CA-C | -5.99 | 1.45 | 1.53 |
| 8 | c7 | 115 | MET | C-O | -5.99 | 1.17 | 1.24 |
| 10 | k5 | 701 | ASP | N-CA | -5.99 | 1.39 | 1.46 |
| 11 | a9 | 802 | ARG | CA-C | -5.99 | 1.45 | 1.52 |
| 11 | aA | 802 | ARG | CA-C | -5.99 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 8 | O7 | 123 | ILE | CA-CB | 5.98 | 1.57 | 1.54 |
| 10 | j5 | 17 | PHE | C-O | -5.98 | 1.16 | 1.23 |
| 10 | j5 | 788 | PHE | C-O | -5.98 | 1.15 | 1.23 |
| 10 | k5 | 17 | PHE | C-O | -5.98 | 1.16 | 1.23 |
| 1 | D5 | 12 | TYR | N-CA | -5.98 | 1.38 | 1.46 |
| 10 | j5 | 1114 | ARG | C-O | -5.98 | 1.16 | 1.23 |
| 8 | E5 | 117 | ASN | C-O | -5.98 | 1.17 | 1.24 |
| 10 | j5 | 992 | GLU | C-O | -5.98 | 1.17 | 1.24 |
| 10 | k5 | 431 | GLN | C-O | -5.98 | 1.15 | 1.23 |
| 9 | w7 | 32 | VAL | C-O | -5.98 | 1.16 | 1.24 |
| 4 | M3 | 68 | ASP | CA-CB | -5.98 | 1.43 | 1.53 |
| 8 | A5 | 48 | GLU | C-O | -5.98 | 1.17 | 1.24 |
| 10 | j5 | 712 | ARG | CZ-NH2 | -5.98 | 1.25 | 1.33 |
| 9 | w7 | 40 | GLU | N-CA | -5.98 | 1.38 | 1.46 |
| 4 | M1 | 68 | ASP | CA-CB | -5.98 | 1.43 | 1.53 |
| 4 | M4 | 48 | PRO | CA-CB | -5.97 | 1.45 | 1.53 |
| 10 | k5 | 855 | GLY | CA-C | -5.97 | 1.45 | 1.52 |
| 1 | h7 | 41 | ALA | C-O | -5.97 | 1.16 | 1.24 |
| 1 | L5 | 3 | ASP | C-O | -5.97 | 1.15 | 1.24 |
| 8 | o7 | 58 | LEU | N-CA | -5.97 | 1.39 | 1.46 |
| 3 | L9 | 90 | LEU | C-O | -5.97 | 1.17 | 1.24 |
| 10 | k5 | 784 | ILE | CA-C | -5.97 | 1.46 | 1.52 |
| 10 | j5 | 555 | ALA | CA-C | -5.97 | 1.45 | 1.52 |
| 9 | w7 | 63 | ALA | C-O | -5.97 | 1.16 | 1.24 |
| 10 | k5 | 788 | PHE | C-O | -5.97 | 1.15 | 1.23 |
| 9 | z7 | 32 | VAL | C-O | -5.97 | 1.17 | 1.24 |
| 10 | j5 | 855 | GLY | CA-C | -5.96 | 1.45 | 1.52 |
| 4 | M8 | 239 | PHE | C-O | -5.96 | 1.17 | 1.24 |
| 8 | u7 | 81 | CYS | CA-C | -5.96 | 1.45 | 1.52 |
| 8 | i7 | 115 | MET | C-O | -5.96 | 1.17 | 1.24 |
| 10 | j5 | 371 | SER | C-O | -5.96 | 1.16 | 1.23 |
| 10 | k5 | 515 | PRO | CA-CB | -5.96 | 1.45 | 1.53 |
| 9 | z7 | 26 | THR | CA-C | -5.96 | 1.44 | 1.52 |
| 4 | M3 | 48 | PRO | CA-CB | -5.96 | 1.45 | 1.53 |
| 4 | M1 | 48 | PRO | CA-CB | -5.96 | 1.45 | 1.53 |
| 10 | j5 | 455 | PHE | N-CA | -5.95 | 1.38 | 1.46 |
| 10 | j5 | 729 | ILE | N-CA | 5.95 | 1.53 | 1.46 |
| 10 | k5 | 511 | ARG | CD-NE | -5.95 | 1.38 | 1.46 |
| 9 | w7 | 26 | THR | CA-C | -5.95 | 1.44 | 1.52 |
| 4 | M4 | 236 | ASN | C-O | -5.95 | 1.16 | 1.24 |
| 10 | k5 | 574 | GLN | CA-C | -5.95 | 1.46 | 1.52 |
| 10 | j5 | 524 | THR | C-O | -5.95 | 1.15 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | j5 | 770 | ALA | CA-CB | -5.95 | 1.43 | 1.53 |
| 10 | k5 | 584 | GLN | CA-C | -5.95 | 1.45 | 1.52 |
| 1 | F5 | 3 | ASP | C-O | -5.95 | 1.15 | 1.24 |
| 10 | k5 | 152 | ARG | C-O | -5.95 | 1.17 | 1.24 |
| 1 | J5 | 12 | TYR | N-CA | -5.95 | 1.38 | 1.46 |
| 10 | j5 | 618 | TRP | C-N | -5.95 | 1.25 | 1.33 |
| 9 | x7 | 23 | LEU | C-O | -5.95 | 1.17 | 1.24 |
| 10 | k5 | 575 | ILE | N-CA | -5.94 | 1.39 | 1.46 |
| 10 | k5 | 914 | PRO | C-O | -5.94 | 1.16 | 1.24 |
| 3 | FA | 152 | ASP | C-O | -5.94 | 1.17 | 1.24 |
| 10 | j5 | 584 | GLN | CA-C | -5.94 | 1.45 | 1.52 |
| 10 | k5 | 733 | SER | C-O | -5.94 | 1.16 | 1.24 |
| 9 | z7 | 57 | PHE | C-O | -5.94 | 1.16 | 1.24 |
| 10 | j5 | 537 | ILE | CA-C | -5.94 | 1.44 | 1.52 |
| 10 | j5 | 575 | ILE | N-CA | -5.94 | 1.39 | 1.46 |
| 10 | k5 | 449 | ARG | N-CA | -5.94 | 1.38 | 1.46 |
| 10 | k5 | 537 | ILE | CA-C | -5.94 | 1.44 | 1.52 |
| 10 | k5 | 555 | ALA | CA-C | -5.94 | 1.45 | 1.52 |
| 10 | k5 | 770 | ALA | CA-CB | -5.94 | 1.43 | 1.53 |
| 9 | w7 | 57 | PHE | C-O | -5.94 | 1.16 | 1.24 |
| 3 | LA | 90 | LEU | C-O | -5.93 | 1.17 | 1.24 |
| 4 | M3 | 52 | LEU | CA-C | -5.93 | 1.45 | 1.52 |
| 10 | k5 | 712 | ARG | CZ-NH2 | -5.93 | 1.25 | 1.33 |
| 1 | h7 | 30 | TYR | C-O | -5.93 | 1.17 | 1.24 |
| 4 | M1 | 52 | LEU | CA-C | -5.93 | 1.45 | 1.52 |
| 4 | M3 | 45 | VAL | CA-C | -5.93 | 1.45 | 1.52 |
| 10 | j5 | 549 | LYS | CA-C | 5.93 | 1.60 | 1.52 |
| 10 | j5 | 607 | LEU | CA-C | -5.93 | 1.45 | 1.52 |
| 10 | k5 | 549 | LYS | CA-C | 5.93 | 1.60 | 1.52 |
| 10 | k5 | 1101 | GLU | C-O | -5.93 | 1.17 | 1.24 |
| 4 | M1 | 45 | VAL | CA-C | -5.93 | 1.45 | 1.52 |
| 10 | k5 | 731 | GLU | C-O | -5.93 | 1.16 | 1.23 |
| 1 | D5 | 2 | GLN | C-O | -5.93 | 1.16 | 1.23 |
| 10 | j5 | 797 | ASN | N-CA | -5.93 | 1.38 | 1.46 |
| 10 | j5 | 857 | LYS | C-O | -5.93 | 1.15 | 1.24 |
| 10 | k5 | 857 | LYS | C-O | -5.93 | 1.15 | 1.24 |
| 1 | h7 | 36 | VAL | C-O | -5.93 | 1.16 | 1.24 |
| 9 | z7 | 40 | GLU | N-CA | -5.93 | 1.38 | 1.46 |
| 4 | M3 | 230 | GLN | C-O | -5.93 | 1.16 | 1.24 |
| 4 | M1 | 230 | GLN | C-O | -5.93 | 1.16 | 1.24 |
| 1 | J5 | 2 | GLN | C-O | -5.93 | 1.16 | 1.23 |
| 10 | j5 | 576 | PHE | CA-CB | -5.93 | 1.45 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 10 | j5 | 731 | GLU | C-O | -5.92 | 1.16 | 1.23 |
| 10 | k5 | 817 | LYS | CA-C | -5.92 | 1.45 | 1.52 |
| 8 | S7 | 123 | ILE | CA-CB | 5.92 | 1.57 | 1.54 |
| 4 | M8 | 236 | ASN | C-O | -5.92 | 1.16 | 1.24 |
| 4 | MA | 236 | ASN | C-O | -5.92 | 1.16 | 1.24 |
| 1 | b7 | 36 | VAL | C-O | -5.92 | 1.16 | 1.24 |
| 4 | M9 | 236 | ASN | C-O | -5.92 | 1.16 | 1.24 |
| 10 | k5 | 170 | ALA | C-O | -5.92 | 1.17 | 1.24 |
| 10 | k5 | 246 | VAL | C-O | -5.92 | 1.17 | 1.24 |
| 4 | MA | 72 | ALA | C-O | -5.92 | 1.17 | 1.24 |
| 10 | j5 | 935 | LEU | CA-C | -5.92 | 1.44 | 1.52 |
| 10 | k5 | 935 | LEU | CA-C | -5.92 | 1.44 | 1.52 |
| 4 | M9 | 72 | ALA | C-O | -5.92 | 1.17 | 1.24 |
| 4 | MA | 48 | PRO | CA-CB | -5.92 | 1.45 | 1.53 |
| 10 | j5 | 584 | GLN | N-CA | -5.92 | 1.39 | 1.46 |
| 10 | k5 | 584 | GLN | N-CA | -5.92 | 1.39 | 1.46 |
| 4 | M9 | 48 | PRO | CA-CB | -5.92 | 1.45 | 1.53 |
| 3 | LA | 83 | LEU | C-O | -5.92 | 1.16 | 1.24 |
| 4 | MA | 68 | ASP | CA-CB | -5.92 | 1.43 | 1.53 |
| 10 | j5 | 714 | ASP | CA-C | -5.92 | 1.44 | 1.52 |
| 10 | k5 | 714 | ASP | CA-C | -5.92 | 1.44 | 1.52 |
| 4 | M9 | 68 | ASP | CA-CB | -5.92 | 1.43 | 1.53 |
| 9 | z7 | 23 | LEU | C-O | -5.92 | 1.16 | 1.24 |
| 10 | k5 | 524 | THR | C-O | -5.91 | 1.15 | 1.23 |
| 4 | M8 | 72 | ALA | C-O | -5.91 | 1.17 | 1.24 |
| 3 | L9 | 83 | LEU | C-O | -5.91 | 1.16 | 1.24 |
| 10 | j5 | 574 | GLN | CA-C | -5.91 | 1.46 | 1.52 |
| 10 | j5 | 727 | THR | C-O | -5.91 | 1.18 | 1.24 |
| 10 | k5 | 727 | THR | C-O | -5.91 | 1.18 | 1.24 |
| 10 | k5 | 907 | GLN | CA-C | -5.91 | 1.45 | 1.52 |
| 8 | q7 | 123 | ILE | CA-CB | 5.91 | 1.57 | 1.54 |
| 10 | j5 | 582 | GLN | CA-CB | -5.91 | 1.44 | 1.53 |
| 10 | j5 | 914 | PRO | C-O | -5.91 | 1.16 | 1.24 |
| 10 | k5 | 582 | GLN | CA-CB | -5.91 | 1.44 | 1.53 |
| 8 | c7 | 136 | VAL | CA-CB | -5.90 | 1.47 | 1.54 |
| 4 | MA | 52 | LEU | CA-C | -5.90 | 1.45 | 1.52 |
| 10 | j5 | 507 | ARG | CZ-NH2 | -5.90 | 1.25 | 1.33 |
| 10 | j5 | 515 | PRO | CA-CB | -5.90 | 1.45 | 1.53 |
| 10 | j5 | 683 | ARG | N-CA | -5.90 | 1.38 | 1.46 |
| 10 | j5 | 882 | PRO | N-CA | -5.90 | 1.39 | 1.47 |
| 10 | j5 | 907 | GLN | CA-C | -5.90 | 1.45 | 1.52 |
| 10 | k5 | 683 | ARG | N-CA | -5.90 | 1.38 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4 | M9 | 52 | LEU | CA-C | -5.90 | 1.45 | 1.52 |
| 4 | M1 | 72 | ALA | C-O | -5.90 | 1.17 | 1.24 |
| 10 | j5 | 701 | ASP | N-CA | -5.90 | 1.39 | 1.46 |
| 10 | j5 | 996 | ALA | N-CA | -5.90 | 1.39 | 1.46 |
| 10 | k5 | 996 | ALA | N-CA | -5.90 | 1.39 | 1.46 |
| 8 | i7 | 136 | VAL | CA-CB | -5.90 | 1.47 | 1.54 |
| 11 | a9 | 490 | ILE | CA-C | -5.90 | 1.45 | 1.52 |
| 11 | aA | 490 | ILE | CA-C | -5.90 | 1.45 | 1.52 |
| 8 | Q5 | 123 | ILE | CA-CB | 5.90 | 1.57 | 1.54 |
| 10 | k5 | 170 | ALA | CA-C | -5.90 | 1.45 | 1.52 |
| 10 | j5 | 449 | ARG | N-CA | -5.90 | 1.38 | 1.46 |
| 10 | j5 | 690 | LEU | C-N | -5.90 | 1.25 | 1.33 |
| 10 | j5 | 778 | LYS | CA-C | -5.90 | 1.44 | 1.52 |
| 10 | k5 | 690 | LEU | C-N | -5.90 | 1.25 | 1.33 |
| 8 | C5 | 24 | ASP | C-O | -5.89 | 1.17 | 1.23 |
| 10 | j5 | 343 | TYR | CA-CB | -5.89 | 1.44 | 1.53 |
| 10 | k5 | 398 | LEU | CA-CB | -5.89 | 1.44 | 1.53 |
| 10 | k5 | 956 | GLY | C-O | -5.89 | 1.16 | 1.23 |
| 10 | k5 | 992 | GLU | C-O | -5.89 | 1.17 | 1.24 |
| 4 | M4 | 45 | VAL | CA-C | -5.89 | 1.45 | 1.52 |
| 10 | j5 | 979 | GLU | C-O | -5.89 | 1.17 | 1.24 |
| 10 | k5 | 836 | PHE | CA-C | -5.89 | 1.45 | 1.52 |
| 10 | k5 | 979 | GLU | C-O | -5.89 | 1.17 | 1.24 |
| 8 | o7 | 81 | CYS | CA-C | -5.89 | 1.45 | 1.52 |
| 9 | w7 | 23 | LEU | C-O | -5.88 | 1.16 | 1.24 |
| 10 | j5 | 457 | THR | CB-CG2 | -5.88 | 1.33 | 1.52 |
| 9 | z7 | 3 | ARG | C-O | -5.88 | 1.16 | 1.23 |
| 10 | j5 | 824 | PRO | CA-CB | -5.88 | 1.45 | 1.53 |
| 10 | k5 | 343 | TYR | CA-CB | -5.88 | 1.44 | 1.53 |
| 10 | k5 | 618 | TRP | C-N | -5.88 | 1.25 | 1.33 |
| 4 | M8 | 17 | VAL | CA-C | -5.88 | 1.45 | 1.52 |
| 10 | k5 | 607 | LEU | CA-C | -5.88 | 1.45 | 1.52 |
| 8 | Q7 | 123 | ILE | CA-CB | 5.87 | 1.57 | 1.54 |
| 4 | M3 | 72 | ALA | C-O | -5.87 | 1.17 | 1.24 |
| 8 | I5 | 24 | ASP | C-O | -5.87 | 1.17 | 1.23 |
| 10 | j5 | 733 | SER | C-O | -5.87 | 1.16 | 1.24 |
| 10 | k5 | 507 | ARG | CZ-NH2 | -5.87 | 1.25 | 1.33 |
| 10 | j5 | 13 | ARG | C-O | -5.87 | 1.20 | 1.25 |
| 10 | j5 | 687 | PRO | CA-C | -5.87 | 1.43 | 1.52 |
| 10 | k5 | 13 | ARG | C-O | -5.87 | 1.20 | 1.25 |
| 10 | k5 | 457 | THR | CB-CG2 | -5.87 | 1.33 | 1.52 |
| 4 | M8 | 52 | LEU | CA-C | -5.87 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4 | MA | 45 | VAL | CA-C | -5.87 | 1.45 | 1.52 |
| 10 | j5 | 1089 | LEU | C-O | -5.87 | 1.17 | 1.24 |
| 9 | x7 | 7 | VAL | C-O | -5.87 | 1.17 | 1.24 |
| 4 | M9 | 45 | VAL | CA-C | -5.87 | 1.45 | 1.52 |
| 10 | j5 | 817 | LYS | CA-C | -5.86 | 1.45 | 1.52 |
| 10 | k5 | 514 | SER | CA-C | -5.86 | 1.45 | 1.53 |
| 10 | k5 | 576 | PHE | CA-CB | -5.86 | 1.45 | 1.54 |
| 8 | u7 | 123 | ILE | CA-CB | 5.86 | 1.57 | 1.54 |
| 8 | S5 | 123 | ILE | CA-CB | 5.86 | 1.57 | 1.54 |
| 10 | j5 | 169 | TYR | C-O | -5.86 | 1.17 | 1.24 |
| 9 | w7 | 3 | ARG | C-O | -5.86 | 1.16 | 1.23 |
| 8 | u7 | 58 | LEU | N-CA | -5.86 | 1.39 | 1.46 |
| 4 | M3 | 236 | ASN | C-O | -5.85 | 1.16 | 1.24 |
| 4 | M4 | 52 | LEU | CA-C | -5.85 | 1.45 | 1.52 |
| 4 | M8 | 45 | VAL | CA-C | -5.85 | 1.45 | 1.52 |
| 4 | M1 | 236 | ASN | C-O | -5.85 | 1.16 | 1.24 |
| 9 | z5 | 59 | GLY | C-O | -5.85 | 1.18 | 1.23 |
| 10 | j5 | 978 | LEU | CA-C | -5.85 | 1.44 | 1.52 |
| 10 | j5 | 956 | GLY | C-O | -5.85 | 1.16 | 1.23 |
| 1 | b7 | 30 | TYR | C-O | -5.85 | 1.17 | 1.24 |
| 10 | j5 | 514 | SER | CA-C | -5.85 | 1.45 | 1.53 |
| 10 | j5 | 413 | SER | N-CA | -5.85 | 1.38 | 1.46 |
| 10 | k5 | 978 | LEU | CA-C | -5.84 | 1.44 | 1.52 |
| 4 | MA | 43 | TYR | C-O | -5.84 | 1.16 | 1.23 |
| 10 | j5 | 314 | GLN | C-O | -5.84 | 1.16 | 1.23 |
| 10 | k5 | 314 | GLN | C-O | -5.84 | 1.16 | 1.23 |
| 8 | a7 | 123 | ILE | CA-CB | 5.84 | 1.57 | 1.54 |
| 4 | M9 | 43 | TYR | C-O | -5.84 | 1.16 | 1.23 |
| 4 | M8 | 174 | LEU | C-O | -5.84 | 1.16 | 1.24 |
| 10 | k5 | 169 | TYR | C-O | -5.84 | 1.17 | 1.24 |
| 4 | M3 | 43 | TYR | C-O | -5.83 | 1.16 | 1.23 |
| 10 | k5 | 413 | SER | N-CA | -5.83 | 1.38 | 1.46 |
| 4 | M8 | 230 | GLN | CA-C | -5.83 | 1.47 | 1.53 |
| 4 | M1 | 43 | TYR | C-O | -5.83 | 1.16 | 1.23 |
| 4 | M4 | 72 | ALA | C-O | -5.83 | 1.17 | 1.24 |
| 8 | e5 | 16 | ARG | C-O | -5.83 | 1.16 | 1.24 |
| 10 | j5 | 900 | LEU | N-CA | -5.83 | 1.39 | 1.46 |
| 4 | M3 | 181 | GLN | C-O | -5.83 | 1.16 | 1.24 |
| 4 | M4 | 230 | GLN | C-O | -5.83 | 1.17 | 1.24 |
| 9 | z5 | 46 | LYS | CA-CB | -5.83 | 1.43 | 1.53 |
| 10 | j5 | 398 | LEU | CA-CB | -5.83 | 1.44 | 1.53 |
| 10 | j5 | 1101 | GLU | C-O | -5.83 | 1.17 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4 | M1 | 181 | GLN | C-O | -5.83 | 1.16 | 1.24 |
| 4 | MA | 230 | GLN | C-O | -5.83 | 1.17 | 1.24 |
| 10 | k5 | 778 | LYS | CA-C | -5.83 | 1.45 | 1.52 |
| 9 | x7 | 32 | VAL | C-O | -5.83 | 1.17 | 1.24 |
| 4 | M9 | 230 | GLN | C-O | -5.83 | 1.17 | 1.24 |
| 8 | U5 | 123 | ILE | CA-CB | 5.83 | 1.57 | 1.54 |
| 10 | j5 | 170 | ALA | C-O | -5.83 | 1.17 | 1.24 |
| 10 | j5 | 632 | ARG | C-N | -5.83 | 1.26 | 1.33 |
| 8 | k7 | 123 | ILE | CA-CB | 5.83 | 1.57 | 1.54 |
| 3 | F9 | 152 | ASP | C-O | -5.83 | 1.17 | 1.24 |
| 10 | j5 | 246 | VAL | C-O | -5.83 | 1.17 | 1.24 |
| 10 | k5 | 263 | LYS | N-CA | -5.83 | 1.38 | 1.46 |
| 10 | k5 | 687 | PRO | CA-C | -5.83 | 1.43 | 1.52 |
| 1 | J5 | 5 | ILE | CA-C | -5.83 | 1.44 | 1.52 |
| 10 | j5 | 373 | ALA | C-N | -5.83 | 1.25 | 1.34 |
| 10 | k5 | 373 | ALA | C-N | -5.83 | 1.25 | 1.34 |
| 8 | g7 | 123 | ILE | CA-CB | 5.83 | 1.57 | 1.54 |
| 8 | o7 | 47 | ARG | CA-C | -5.83 | 1.45 | 1.52 |
| 4 | M8 | 36 | TYR | CA-C | -5.83 | 1.45 | 1.53 |
| 4 | MA | 17 | VAL | CA-C | -5.82 | 1.45 | 1.52 |
| 10 | j5 | 597 | GLU | CA-CB | -5.82 | 1.43 | 1.53 |
| 10 | k5 | 519 | GLU | CA-C | -5.82 | 1.42 | 1.53 |
| 8 | W7 | 123 | ILE | CA-CB | 5.82 | 1.57 | 1.54 |
| 4 | M9 | 17 | VAL | CA-C | -5.82 | 1.45 | 1.52 |
| 8 | a5 | 16 | ARG | C-O | -5.82 | 1.16 | 1.24 |
| 10 | j5 | 979 | GLU | CA-C | -5.82 | 1.45 | 1.52 |
| 10 | j5 | 486 | ILE | CA-C | -5.82 | 1.45 | 1.52 |
| 10 | j5 | 836 | PHE | CA-C | -5.82 | 1.45 | 1.52 |
| 10 | k5 | 486 | ILE | CA-C | -5.82 | 1.45 | 1.52 |
| 10 | k5 | 865 | ALA | CA-C | -5.82 | 1.45 | 1.52 |
| 8 | u7 | 47 | ARG | CA-C | -5.82 | 1.45 | 1.52 |
| 4 | M8 | 43 | TYR | C-O | -5.82 | 1.16 | 1.23 |
| 8 | I5 | 16 | ARG | C-O | -5.81 | 1.16 | 1.24 |
| 10 | j5 | 263 | LYS | N-CA | -5.81 | 1.38 | 1.46 |
| 11 | a9 | 49 | TRP | CA-C | -5.81 | 1.44 | 1.52 |
| 11 | aA | 49 | TRP | CA-C | -5.81 | 1.44 | 1.52 |
| 10 | j5 | 151 | GLU | C-O | -5.81 | 1.17 | 1.24 |
| 9 | x7 | 25 | ASN | N-CA | -5.81 | 1.39 | 1.46 |
| 4 | M8 | 62 | LYS | N-CA | -5.81 | 1.38 | 1.46 |
| 1 | D5 | 7 | ALA | CA-CB | -5.81 | 1.44 | 1.53 |
| 10 | k5 | 644 | GLU | CA-CB | -5.81 | 1.44 | 1.53 |
| 3 | H2 | 84 | ARG | C-O | -5.81 | 1.17 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4 | M3 | 163 | ASN | CA-C | -5.81 | 1.45 | 1.52 |
| 10 | k5 | 344 | ARG | CA-C | -5.81 | 1.45 | 1.52 |
| 3 | H6 | 84 | ARG | C-O | -5.81 | 1.17 | 1.24 |
| 4 | M1 | 163 | ASN | CA-C | -5.81 | 1.45 | 1.52 |
| 4 | M3 | 174 | LEU | C-O | -5.81 | 1.16 | 1.24 |
| 4 | M1 | 174 | LEU | C-O | -5.81 | 1.16 | 1.24 |
| 4 | M4 | 36 | TYR | CA-C | -5.80 | 1.45 | 1.53 |
| 10 | j5 | 519 | GLU | CA-C | -5.80 | 1.42 | 1.53 |
| 9 | y7 | 7 | VAL | C-O | -5.80 | 1.17 | 1.24 |
| 4 | M1 | 36 | TYR | CA-C | -5.80 | 1.45 | 1.53 |
| 10 | j5 | 678 | VAL | CA-C | -5.80 | 1.46 | 1.52 |
| 10 | j5 | 876 | TYR | CB-CG | -5.80 | 1.38 | 1.51 |
| 10 | k5 | 498 | ALA | CA-CB | -5.80 | 1.42 | 1.53 |
| 10 | k5 | 876 | TYR | CB-CG | -5.80 | 1.38 | 1.51 |
| 4 | M8 | 130 | SER | CA-C | -5.80 | 1.45 | 1.52 |
| 1 | J5 | 7 | ALA | CA-CB | -5.80 | 1.44 | 1.53 |
| 4 | M4 | 43 | TYR | C-O | -5.80 | 1.16 | 1.23 |
| 10 | j5 | 1105 | ILE | CA-CB | -5.80 | 1.47 | 1.54 |
| 10 | k5 | 900 | LEU | N-CA | -5.80 | 1.39 | 1.46 |
| 10 | j5 | 382 | ILE | CB-CG1 | -5.80 | 1.41 | 1.53 |
| 10 | k5 | 382 | ILE | CB-CG1 | -5.80 | 1.41 | 1.53 |
| 9 | z7 | 51 | VAL | C-O | -5.80 | 1.17 | 1.24 |
| 10 | k5 | 979 | GLU | CA-C | -5.79 | 1.45 | 1.52 |
| 10 | k5 | 1089 | LEU | C-O | -5.79 | 1.17 | 1.24 |
| 9 | i5 | 46 | LYS | CA-CB | -5.79 | 1.43 | 1.53 |
| 10 | j5 | 533 | LEU | C-O | -5.79 | 1.16 | 1.24 |
| 10 | k5 | 533 | LEU | C-O | -5.79 | 1.16 | 1.24 |
| 10 | j5 | 934 | ALA | C-O | -5.79 | 1.16 | 1.24 |
| 8 | M7 | 123 | ILE | CA-CB | 5.79 | 1.57 | 1.54 |
| 10 | j5 | 183 | CYS | CA-C | -5.79 | 1.45 | 1.52 |
| 10 | j5 | 371 | SER | CA-CB | -5.79 | 1.44 | 1.53 |
| 8 | m7 | 123 | ILE | CA-CB | 5.79 | 1.57 | 1.54 |
| 3 | LA | 91 | ARG | CA-C | -5.79 | 1.45 | 1.52 |
| 4 | MA | 174 | LEU | C-O | -5.79 | 1.16 | 1.24 |
| 9 | i5 | 59 | GLY | C-O | -5.79 | 1.18 | 1.23 |
| 10 | k5 | 824 | PRO | CA-CB | -5.79 | 1.45 | 1.53 |
| 10 | k5 | 1000 | ILE | C-O | -5.79 | 1.17 | 1.24 |
| 3 | L9 | 91 | ARG | CA-C | -5.79 | 1.45 | 1.52 |
| 4 | M9 | 174 | LEU | C-O | -5.79 | 1.16 | 1.24 |
| 11 | a9 | 627 | GLN | C-O | -5.79 | 1.17 | 1.24 |
| 11 | aA | 627 | GLN | C-O | -5.79 | 1.17 | 1.24 |
| 4 | M4 | 62 | LYS | N-CA | -5.78 | 1.38 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 9 | z5 | 3 | ARG | CA-C | -5.78 | 1.45 | 1.52 |
| 10 | j5 | 507 | ARG | CA-C | -5.78 | 1.45 | 1.52 |
| 10 | k5 | 597 | GLU | CA-CB | -5.78 | 1.43 | 1.53 |
| 9 | z7 | 50 | LYS | C-O | -5.78 | 1.16 | 1.23 |
| 9 | y7 | 32 | VAL | C-O | -5.78 | 1.17 | 1.24 |
| 4 | M4 | 17 | VAL | CA-C | -5.78 | 1.45 | 1.52 |
| 10 | j5 | 6 | THR | CB-CG2 | -5.78 | 1.33 | 1.52 |
| 10 | k5 | 6 | THR | CB-CG2 | -5.78 | 1.33 | 1.52 |
| 8 | O5 | 123 | ILE | CA-CB | 5.78 | 1.57 | 1.54 |
| 1 | D5 | 5 | ILE | CA-C | -5.78 | 1.44 | 1.52 |
| 8 | G5 | 123 | ILE | CA-CB | 5.78 | 1.57 | 1.54 |
| 9 | z5 | 68 | GLY | CA-C | -5.78 | 1.43 | 1.51 |
| 8 | o7 | 123 | ILE | CA-CB | 5.78 | 1.57 | 1.54 |
| 10 | j5 | 498 | ALA | CA-CB | -5.78 | 1.42 | 1.53 |
| 10 | k5 | 632 | ARG | C-N | -5.78 | 1.26 | 1.33 |
| 10 | j5 | 630 | ILE | CA-C | -5.77 | 1.44 | 1.52 |
| 8 | s7 | 123 | ILE | CA-CB | 5.77 | 1.57 | 1.54 |
| 4 | M8 | 163 | ASN | CA-C | -5.77 | 1.45 | 1.52 |
| 4 | MA | 36 | TYR | CA-C | -5.77 | 1.45 | 1.53 |
| 10 | k5 | 507 | ARG | CA-C | -5.77 | 1.45 | 1.52 |
| 4 | M9 | 36 | TYR | CA-C | -5.77 | 1.45 | 1.53 |
| 4 | M3 | 12 | GLY | C-N | -5.77 | 1.25 | 1.33 |
| 10 | j5 | 644 | GLU | CA-CB | -5.77 | 1.44 | 1.53 |
| 10 | j5 | 722 | ILE | CA-C | -5.77 | 1.45 | 1.52 |
| 4 | M1 | 12 | GLY | C-N | -5.77 | 1.25 | 1.33 |
| 10 | j5 | 423 | LEU | CA-C | -5.77 | 1.45 | 1.52 |
| 10 | k5 | 396 | GLY | C-O | -5.77 | 1.16 | 1.23 |
| 10 | k5 | 423 | LEU | CA-C | -5.77 | 1.45 | 1.52 |
| 4 | M3 | 17 | VAL | CA-C | -5.77 | 1.45 | 1.52 |
| 4 | M1 | 17 | VAL | CA-C | -5.77 | 1.45 | 1.52 |
| 4 | M4 | 174 | LEU | C-O | -5.76 | 1.16 | 1.24 |
| 10 | j5 | 865 | ALA | CA-C | -5.76 | 1.45 | 1.52 |
| 4 | MA | 163 | ASN | CA-C | -5.76 | 1.45 | 1.52 |
| 10 | k5 | 1105 | ILE | CA-CB | -5.76 | 1.47 | 1.54 |
| 9 | w7 | 14 | LEU | C-O | -5.76 | 1.16 | 1.24 |
| 4 | M9 | 163 | ASN | CA-C | -5.76 | 1.45 | 1.52 |
| 4 | MA | 62 | LYS | N-CA | -5.76 | 1.38 | 1.46 |
| 8 | C5 | 16 | ARG | C-O | -5.76 | 1.16 | 1.24 |
| 4 | M9 | 62 | LYS | N-CA | -5.76 | 1.38 | 1.46 |
| 10 | k5 | 678 | VAL | CA-C | -5.76 | 1.46 | 1.52 |
| 9 | z7 | 14 | LEU | C-O | -5.76 | 1.16 | 1.24 |
| 4 | M4 | 37 | GLU | CA-CB | -5.76 | 1.45 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4 | M4 | 130 | SER | CA-C | -5.76 | 1.45 | 1.52 |
| 9 | i5 | 68 | GLY | CA-C | -5.76 | 1.43 | 1.51 |
| 1 | b7 | 42 | ALA | C-O | -5.76 | 1.17 | 1.24 |
| 4 | M8 | 181 | GLN | C-O | -5.76 | 1.16 | 1.24 |
| 8 | u7 | 58 | LEU | CA-C | -5.75 | 1.45 | 1.52 |
| 9 | w7 | 50 | LYS | C-O | -5.75 | 1.16 | 1.23 |
| 9 | w7 | 51 | VAL | C-O | -5.75 | 1.18 | 1.24 |
| 1 | b7 | 44 | ILE | N-CA | -5.75 | 1.39 | 1.46 |
| 4 | M3 | 62 | LYS | N-CA | -5.75 | 1.38 | 1.46 |
| 10 | j5 | 344 | ARG | CA-C | -5.75 | 1.45 | 1.52 |
| 8 | o7 | 7 | ALA | C-N | -5.75 | 1.26 | 1.33 |
| 11 | a9 | 496 | ARG | CA-C | -5.75 | 1.45 | 1.52 |
| 11 | aA | 496 | ARG | CA-C | -5.75 | 1.45 | 1.52 |
| 4 | M1 | 62 | LYS | N-CA | -5.75 | 1.38 | 1.46 |
| 4 | MA | 181 | GLN | C-O | -5.74 | 1.16 | 1.24 |
| 4 | M3 | 36 | TYR | CA-C | -5.74 | 1.45 | 1.53 |
| 10 | j5 | 512 | ASN | CG-ND2 | -5.74 | 1.21 | 1.33 |
| 10 | k5 | 479 | LEU | CA-C | -5.74 | 1.45 | 1.52 |
| 10 | k5 | 497 | ARG | CA-C | -5.74 | 1.45 | 1.52 |
| 10 | k5 | 722 | ILE | CA-C | -5.74 | 1.45 | 1.52 |
| 4 | M9 | 181 | GLN | C-O | -5.74 | 1.16 | 1.24 |
| 4 | M1 | 196 | TYR | C-O | -5.74 | 1.17 | 1.24 |
| 10 | k5 | 512 | ASN | CG-ND2 | -5.74 | 1.21 | 1.33 |
| 8 | I7 | 123 | ILE | CA-CB | 5.74 | 1.57 | 1.54 |
| 3 | LA | 116 | THR | N-CA | -5.74 | 1.39 | 1.46 |
| 4 | M4 | 181 | GLN | C-O | -5.74 | 1.16 | 1.24 |
| 10 | j5 | 178 | ILE | C-O | -5.74 | 1.15 | 1.24 |
| 10 | k5 | 630 | ILE | CA-C | -5.74 | 1.44 | 1.52 |
| 9 | y7 | 25 | ASN | N-CA | -5.74 | 1.39 | 1.46 |
| 3 | L9 | 116 | THR | N-CA | -5.74 | 1.39 | 1.46 |
| 11 | aA | 394 | ALA | CA-C | -5.74 | 1.45 | 1.52 |
| 10 | j5 | 570 | ALA | CA-CB | -5.74 | 1.44 | 1.53 |
| 10 | j5 | 571 | ALA | CA-CB | -5.74 | 1.44 | 1.53 |
| 10 | j5 | 706 | PRO | N-CA | -5.74 | 1.40 | 1.47 |
| 10 | k5 | 934 | ALA | C-O | -5.74 | 1.16 | 1.24 |
| 1 | h7 | 42 | ALA | C-O | -5.74 | 1.17 | 1.24 |
| 4 | M3 | 264 | LYS | C-O | -5.74 | 1.17 | 1.24 |
| 10 | j5 | 766 | ALA | CA-CB | -5.74 | 1.44 | 1.53 |
| 10 | k5 | 766 | ALA | CA-CB | -5.74 | 1.44 | 1.53 |
| 4 | M1 | 264 | LYS | C-O | -5.74 | 1.17 | 1.24 |
| 10 | j5 | 348 | TYR | CA-CB | -5.74 | 1.44 | 1.54 |
| 10 | j5 | 527 | SER | C-O | -5.74 | 1.16 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 10 | j5 | 730 | ASN | CA-C | -5.74 | 1.45 | 1.52 |
| 10 | k5 | 348 | TYR | CA-CB | -5.74 | 1.44 | 1.54 |
| 10 | k5 | 527 | SER | C-O | -5.74 | 1.16 | 1.24 |
| 8 | o7 | 58 | LEU | CA-C | -5.74 | 1.45 | 1.52 |
| 4 | MA | 37 | GLU | CA-CB | -5.73 | 1.45 | 1.53 |
| 8 | M5 | 123 | ILE | CA-CB | 5.73 | 1.57 | 1.54 |
| 4 | M9 | 37 | GLU | CA-CB | -5.73 | 1.45 | 1.53 |
| 4 | MA | 130 | SER | CA-C | -5.73 | 1.45 | 1.52 |
| 10 | j5 | 479 | LEU | CA-C | -5.73 | 1.45 | 1.52 |
| 10 | j5 | 885 | GLN | CA-CB | -5.73 | 1.45 | 1.53 |
| 4 | M9 | 130 | SER | CA-C | -5.73 | 1.45 | 1.52 |
| 8 | A5 | 62 | ARG | C-O | -5.73 | 1.17 | 1.24 |
| 8 | I5 | 123 | ILE | CA-CB | 5.73 | 1.57 | 1.54 |
| 10 | j5 | 39 | GLU | CA-C | -5.73 | 1.45 | 1.52 |
| 9 | z7 | 45 | GLN | C-O | -5.73 | 1.16 | 1.24 |
| 9 | w7 | 25 | ASN | N-CA | -5.73 | 1.38 | 1.46 |
| 4 | M8 | 37 | GLU | CA-CB | -5.73 | 1.45 | 1.53 |
| 9 | z5 | 21 | ARG | N-CA | -5.73 | 1.38 | 1.46 |
| 10 | k5 | 939 | GLN | CA-CB | -5.73 | 1.44 | 1.53 |
| 8 | C7 | 123 | ILE | CA-CB | 5.73 | 1.57 | 1.54 |
| 10 | j5 | 447 | ALA | N-CA | -5.73 | 1.38 | 1.46 |
| 10 | k5 | 447 | ALA | N-CA | -5.73 | 1.38 | 1.46 |
| 8 | U7 | 123 | ILE | CA-CB | 5.73 | 1.57 | 1.54 |
| 10 | j5 | 645 | ASN | CG-OD1 | -5.73 | 1.12 | 1.23 |
| 10 | k5 | 571 | ALA | CA-CB | -5.73 | 1.44 | 1.53 |
| 10 | k5 | 645 | ASN | CG-OD1 | -5.73 | 1.12 | 1.23 |
| 8 | G7 | 123 | ILE | CA-CB | 5.73 | 1.57 | 1.54 |
| 4 | MA | 12 | GLY | C-N | -5.72 | 1.25 | 1.33 |
| 9 | z7 | 43 | ARG | CZ-NH1 | 5.72 | 1.40 | 1.32 |
| 4 | M9 | 12 | GLY | C-N | -5.72 | 1.25 | 1.33 |
| 3 | LA | 115 | GLU | CA-C | -5.72 | 1.45 | 1.52 |
| 8 | K5 | 117 | ASN | C-N | -5.72 | 1.26 | 1.33 |
| 1 | D5 | 8 | VAL | C-O | -5.72 | 1.16 | 1.23 |
| 10 | k5 | 178 | ILE | C-O | -5.72 | 1.15 | 1.24 |
| 3 | L9 | 115 | GLU | CA-C | -5.72 | 1.45 | 1.52 |
| 9 | w7 | 45 | GLN | C-O | -5.72 | 1.16 | 1.24 |
| 8 | K5 | 93 | THR | C-O | -5.72 | 1.16 | 1.23 |
| 1 | h7 | 44 | ILE | N-CA | -5.72 | 1.39 | 1.46 |
| 4 | M3 | 37 | GLU | CA-CB | -5.72 | 1.45 | 1.53 |
| 8 | I5 | 13 | ALA | C-O | -5.72 | 1.16 | 1.24 |
| 10 | j5 | 396 | GLY | C-O | -5.72 | 1.16 | 1.23 |
| 9 | z7 | 25 | ASN | N-CA | -5.72 | 1.38 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4 | M8 | 46 | VAL | CA-CB | -5.72 | 1.47 | 1.54 |
| 4 | M1 | 37 | GLU | CA-CB | -5.72 | 1.45 | 1.53 |
| 4 | M3 | 130 | SER | CA-C | -5.71 | 1.45 | 1.52 |
| 4 | M1 | 130 | SER | CA-C | -5.71 | 1.45 | 1.52 |
| 8 | Y5 | 123 | ILE | CA-CB | 5.71 | 1.57 | 1.54 |
| 8 | A7 | 123 | ILE | CA-CB | 5.71 | 1.57 | 1.54 |
| 11 | a9 | 629 | LYS | C-O | -5.71 | 1.17 | 1.24 |
| 11 | aA | 629 | LYS | C-O | -5.71 | 1.17 | 1.24 |
| 10 | k5 | 315 | SER | C-O | -5.71 | 1.17 | 1.23 |
| 10 | k5 | 371 | SER | CA-CB | -5.71 | 1.44 | 1.53 |
| 10 | k5 | 905 | THR | CA-C | -5.71 | 1.45 | 1.52 |
| 9 | x7 | 45 | GLN | C-O | -5.71 | 1.16 | 1.24 |
| 10 | j5 | 157 | ILE | C-O | -5.71 | 1.17 | 1.24 |
| 10 | k5 | 157 | ILE | C-O | -5.71 | 1.17 | 1.24 |
| 10 | k5 | 183 | CYS | CA-C | -5.71 | 1.45 | 1.52 |
| 8 | u7 | 7 | ALA | C-N | -5.71 | 1.26 | 1.33 |
| 9 | y7 | 45 | GLN | C-O | -5.71 | 1.16 | 1.24 |
| 4 | M3 | 196 | TYR | C-O | -5.71 | 1.17 | 1.24 |
| 10 | j5 | 967 | VAL | C-O | -5.71 | 1.17 | 1.24 |
| 10 | k5 | 967 | VAL | C-O | -5.71 | 1.17 | 1.24 |
| 10 | j5 | 466 | LEU | CA-C | -5.71 | 1.47 | 1.53 |
| 10 | k5 | 466 | LEU | CA-C | -5.71 | 1.47 | 1.53 |
| 9 | z7 | 44 | ILE | CA-C | -5.71 | 1.45 | 1.52 |
| 11 | a9 | 818 | ARG | C-O | -5.71 | 1.17 | 1.24 |
| 11 | aA | 818 | ARG | C-O | -5.71 | 1.17 | 1.24 |
| 4 | MA | 118 | TYR | CA-C | -5.70 | 1.45 | 1.52 |
| 8 | C5 | 13 | ALA | C-O | -5.70 | 1.16 | 1.24 |
| 9 | i5 | 21 | ARG | N-CA | -5.70 | 1.38 | 1.46 |
| 10 | j5 | 619 | GLU | CG-CD | -5.70 | 1.37 | 1.52 |
| 10 | k5 | 619 | GLU | CG-CD | -5.70 | 1.37 | 1.52 |
| 10 | k5 | 730 | ASN | CA-C | -5.70 | 1.45 | 1.52 |
| 4 | M9 | 118 | TYR | CA-C | -5.70 | 1.45 | 1.52 |
| 4 | M3 | 56 | MET | CA-CB | -5.70 | 1.44 | 1.53 |
| 4 | M4 | 46 | VAL | CA-CB | -5.70 | 1.47 | 1.54 |
| 10 | j5 | 315 | SER | C-O | -5.70 | 1.17 | 1.23 |
| 10 | k5 | 483 | PHE | N-CA | -5.70 | 1.37 | 1.45 |
| 10 | k5 | 982 | TYR | CA-C | -5.70 | 1.46 | 1.52 |
| 9 | z7 | 29 | THR | C-O | -5.70 | 1.16 | 1.23 |
| 10 | k5 | 570 | ALA | CA-CB | -5.70 | 1.44 | 1.53 |
| 8 | c7 | 113 | LYS | CA-CB | -5.70 | 1.44 | 1.53 |
| 4 | M4 | 196 | TYR | C-O | -5.70 | 1.17 | 1.24 |
| 10 | k5 | 151 | GLU | C-O | -5.70 | 1.17 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4 | M4 | 12 | GLY | C-N | -5.69 | 1.26 | 1.33 |
| 10 | k5 | 557 | VAL | C-O | -5.69 | 1.16 | 1.24 |
| 9 | w7 | 43 | ARG | CZ-NH1 | 5.69 | 1.40 | 1.32 |
| 4 | M3 | 46 | VAL | CA-CB | -5.69 | 1.47 | 1.54 |
| 4 | M4 | 56 | MET | CA-CB | -5.69 | 1.44 | 1.53 |
| 8 | E5 | 93 | THR | C-O | -5.69 | 1.16 | 1.23 |
| 10 | k5 | 39 | GLU | CA-C | -5.69 | 1.45 | 1.52 |
| 4 | M8 | 196 | TYR | C-O | -5.69 | 1.17 | 1.24 |
| 4 | M1 | 46 | VAL | CA-CB | -5.69 | 1.47 | 1.54 |
| 4 | MA | 196 | TYR | C-O | -5.69 | 1.17 | 1.24 |
| 8 | c7 | 136 | VAL | C-O | -5.69 | 1.17 | 1.24 |
| 4 | M9 | 196 | TYR | C-O | -5.69 | 1.17 | 1.24 |
| 8 | G5 | 62 | ARG | C-O | -5.69 | 1.17 | 1.24 |
| 10 | k5 | 807 | ARG | CA-CB | -5.69 | 1.44 | 1.53 |
| 4 | M8 | 12 | GLY | C-N | -5.69 | 1.26 | 1.33 |
| 11 | a9 | 496 | ARG | C-O | -5.69 | 1.17 | 1.24 |
| 11 | aA | 496 | ARG | C-O | -5.69 | 1.17 | 1.24 |
| 9 | w7 | 44 | ILE | CA-C | -5.69 | 1.45 | 1.52 |
| 11 | a9 | 521 | PHE | CA-C | -5.69 | 1.45 | 1.52 |
| 11 | aA | 521 | PHE | CA-C | -5.69 | 1.45 | 1.52 |
| 4 | M1 | 56 | MET | CA-CB | -5.69 | 1.44 | 1.53 |
| 8 | i7 | 136 | VAL | C-O | -5.68 | 1.17 | 1.24 |
| 4 | MA | 56 | MET | CA-CB | -5.68 | 1.44 | 1.53 |
| 4 | M4 | 163 | ASN | CA-C | -5.68 | 1.45 | 1.52 |
| 10 | j5 | 468 | ASN | CB-CG | -5.68 | 1.37 | 1.52 |
| 10 | j5 | 520 | ARG | CZ-NH2 | -5.68 | 1.26 | 1.33 |
| 10 | j5 | 723 | GLN | C-N | -5.68 | 1.26 | 1.33 |
| 10 | j5 | 1000 | ILE | C-O | -5.68 | 1.17 | 1.24 |
| 10 | k5 | 468 | ASN | CB-CG | -5.68 | 1.37 | 1.52 |
| 10 | k5 | 520 | ARG | CZ-NH2 | -5.68 | 1.26 | 1.33 |
| 10 | k5 | 723 | GLN | C-N | -5.68 | 1.26 | 1.33 |
| 4 | M8 | 168 | LEU | C-O | -5.68 | 1.17 | 1.24 |
| 4 | M9 | 56 | MET | CA-CB | -5.68 | 1.44 | 1.53 |
| 8 | I5 | 17 | TYR | C-O | -5.68 | 1.17 | 1.23 |
| 9 | i5 | 3 | ARG | CA-C | -5.68 | 1.45 | 1.52 |
| 4 | M8 | 144 | ARG | C-O | -5.68 | 1.17 | 1.24 |
| 9 | z7 | 6 | LYS | CA-C | -5.68 | 1.45 | 1.52 |
| 9 | w7 | 29 | THR | C-O | -5.68 | 1.16 | 1.23 |
| 4 | M4 | 139 | VAL | C-O | -5.68 | 1.16 | 1.24 |
| 10 | k5 | 885 | GLN | CA-CB | -5.68 | 1.45 | 1.53 |
| 4 | MA | 144 | ARG | C-O | -5.67 | 1.17 | 1.24 |
| 4 | M3 | 118 | TYR | CA-C | -5.67 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | j5 | 30 | ALA | N-CA | -5.67 | 1.38 | 1.46 |
| 10 | k5 | 30 | ALA | N-CA | -5.67 | 1.38 | 1.46 |
| 4 | M9 | 144 | ARG | C-O | -5.67 | 1.17 | 1.24 |
| 11 | a9 | 522 | ASP | C-O | -5.67 | 1.17 | 1.24 |
| 11 | aA | 522 | ASP | C-O | -5.67 | 1.17 | 1.24 |
| 4 | M1 | 118 | TYR | CA-C | -5.67 | 1.45 | 1.52 |
| 10 | j5 | 15 | ARG | C-O | -5.67 | 1.17 | 1.24 |
| 10 | k5 | 15 | ARG | C-O | -5.67 | 1.17 | 1.24 |
| 10 | k5 | 408 | SER | C-O | -5.67 | 1.16 | 1.23 |
| 10 | k5 | 462 | TYR | N-CA | -5.67 | 1.39 | 1.46 |
| 10 | j5 | 807 | ARG | CA-CB | -5.67 | 1.44 | 1.53 |
| 8 | a7 | 19 | SER | CA-C | -5.67 | 1.45 | 1.52 |
| 10 | j5 | 605 | ARG | N-CA | -5.67 | 1.39 | 1.46 |
| 10 | j5 | 905 | THR | CA-C | -5.67 | 1.45 | 1.52 |
| 10 | k5 | 721 | LYS | CA-CB | -5.67 | 1.44 | 1.53 |
| 3 | B2 | 77 | ARG | C-O | -5.67 | 1.17 | 1.24 |
| 10 | j5 | 939 | GLN | CA-CB | -5.67 | 1.44 | 1.53 |
| 10 | j5 | 981 | ILE | CA-C | -5.67 | 1.45 | 1.52 |
| 10 | j5 | 1038 | ARG | C-O | -5.67 | 1.17 | 1.24 |
| 11 | a9 | 394 | ALA | CA-C | -5.67 | 1.45 | 1.52 |
| 4 | M4 | 188 | LEU | C-O | -5.66 | 1.17 | 1.24 |
| 10 | j5 | 982 | TYR | CA-C | -5.66 | 1.46 | 1.52 |
| 4 | M8 | 264 | LYS | C-O | -5.66 | 1.17 | 1.24 |
| 10 | j5 | 462 | TYR | N-CA | -5.66 | 1.39 | 1.46 |
| 4 | M4 | 105 | ALA | C-O | -5.66 | 1.17 | 1.24 |
| 11 | a9 | 522 | ASP | CB-CG | -5.66 | 1.37 | 1.52 |
| 11 | aA | 522 | ASP | CB-CG | -5.66 | 1.37 | 1.52 |
| 4 | M4 | 165 | PHE | C-O | -5.66 | 1.17 | 1.24 |
| 10 | k5 | 750 | ARG | CA-C | -5.66 | 1.45 | 1.52 |
| 8 | i7 | 113 | LYS | CA-CB | -5.66 | 1.44 | 1.53 |
| 8 | u7 | 55 | GLY | CA-C | -5.66 | 1.45 | 1.52 |
| 11 | a9 | 473 | HIS | C-O | -5.66 | 1.17 | 1.24 |
| 11 | aA | 473 | HIS | C-O | -5.66 | 1.17 | 1.24 |
| 4 | M3 | 105 | ALA | C-O | -5.66 | 1.17 | 1.24 |
| 10 | k5 | 703 | LEU | N-CA | -5.66 | 1.39 | 1.46 |
| 4 | M1 | 105 | ALA | C-O | -5.66 | 1.17 | 1.24 |
| 1 | J5 | 8 | VAL | C-O | -5.65 | 1.16 | 1.23 |
| 10 | j5 | 780 | ILE | N-CA | -5.65 | 1.38 | 1.46 |
| 10 | j5 | 888 | THR | CB-CG2 | -5.65 | 1.33 | 1.52 |
| 10 | k5 | 888 | THR | CB-CG2 | -5.65 | 1.33 | 1.52 |
| 4 | M3 | 165 | PHE | C-O | -5.65 | 1.17 | 1.24 |
| 10 | j5 | 483 | PHE | N-CA | -5.65 | 1.38 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | j5 | 815 | TYR | CZ-OH | -5.65 | 1.26 | 1.38 |
| 10 | k5 | 815 | TYR | CZ-OH | -5.65 | 1.26 | 1.38 |
| 4 | M1 | 165 | PHE | C-O | -5.65 | 1.17 | 1.24 |
| 10 | j5 | 155 | LYS | C-O | -5.65 | 1.17 | 1.24 |
| 10 | j5 | 730 | ASN | N-CA | 5.65 | 1.53 | 1.46 |
| 10 | j5 | 1078 | SER | CB-OG | 5.65 | 1.53 | 1.42 |
| 10 | k5 | 155 | LYS | C-O | -5.65 | 1.17 | 1.24 |
| 10 | k5 | 780 | ILE | N-CA | -5.65 | 1.38 | 1.46 |
| 11 | aA | 448 | ASN | C-O | -5.65 | 1.17 | 1.24 |
| 4 | M4 | 19 | MET | CA-CB | -5.65 | 1.46 | 1.54 |
| 4 | M8 | 56 | MET | CA-CB | -5.65 | 1.44 | 1.53 |
| 1 | J5 | 10 | ASN | C-O | -5.65 | 1.16 | 1.24 |
| 8 | g7 | 19 | SER | CA-C | -5.65 | 1.45 | 1.52 |
| 3 | LA | 93 | VAL | C-O | -5.64 | 1.17 | 1.24 |
| 1 | D5 | 10 | ASN | C-O | -5.64 | 1.16 | 1.24 |
| 8 | G5 | 57 | GLN | C-O | -5.64 | 1.17 | 1.24 |
| 8 | a5 | 7 | ALA | C-O | -5.64 | 1.15 | 1.23 |
| 3 | L9 | 93 | VAL | C-O | -5.64 | 1.17 | 1.24 |
| 4 | MA | 105 | ALA | C-O | -5.64 | 1.17 | 1.24 |
| 8 | E5 | 117 | ASN | C-N | -5.64 | 1.26 | 1.33 |
| 10 | j5 | 165 | ARG | C-O | -5.64 | 1.17 | 1.24 |
| 10 | j5 | 497 | ARG | CA-C | -5.64 | 1.45 | 1.52 |
| 10 | j5 | 621 | PHE | CA-C | -5.64 | 1.45 | 1.52 |
| 10 | k5 | 165 | ARG | C-O | -5.64 | 1.17 | 1.24 |
| 10 | k5 | 621 | PHE | CA-C | -5.64 | 1.45 | 1.52 |
| 8 | E7 | 123 | ILE | CA-CB | 5.64 | 1.57 | 1.54 |
| 9 | w7 | 6 | LYS | CA-C | -5.64 | 1.46 | 1.52 |
| 4 | M9 | 105 | ALA | C-O | -5.64 | 1.17 | 1.24 |
| 4 | M8 | 66 | VAL | CA-CB | -5.64 | 1.47 | 1.54 |
| 11 | a9 | 615 | ARG | CA-C | -5.64 | 1.46 | 1.53 |
| 11 | aA | 615 | ARG | CA-C | -5.64 | 1.46 | 1.53 |
| 10 | j5 | 408 | SER | C-O | -5.64 | 1.16 | 1.23 |
| 10 | j5 | 686 | THR | CB-CG2 | -5.64 | 1.33 | 1.52 |
| 10 | j5 | 913 | VAL | C-O | -5.64 | 1.17 | 1.24 |
| 10 | j5 | 993 | LYS | C-O | -5.64 | 1.17 | 1.24 |
| 10 | k5 | 981 | ILE | CA-C | -5.64 | 1.45 | 1.52 |
| 10 | k5 | 1038 | ARG | C-O | -5.64 | 1.17 | 1.24 |
| 4 | MA | 264 | LYS | C-O | -5.64 | 1.17 | 1.24 |
| 10 | j5 | 1133 | GLU | C-O | -5.64 | 1.16 | 1.24 |
| 10 | k5 | 605 | ARG | N-CA | -5.64 | 1.39 | 1.46 |
| 10 | k5 | 1078 | SER | CB-OG | 5.64 | 1.53 | 1.42 |
| 4 | M9 | 264 | LYS | C-O | -5.64 | 1.17 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 8 | K7 | 123 | ILE | CA-CB | 5.64 | 1.57 | 1.54 |
| 4 | MA | 46 | VAL | CA-CB | -5.63 | 1.47 | 1.54 |
| 4 | M9 | 46 | VAL | CA-CB | -5.63 | 1.47 | 1.54 |
| 8 | o7 | 56 | ASP | C-O | -5.63 | 1.17 | 1.24 |
| 10 | j5 | 544 | VAL | CA-CB | -5.63 | 1.46 | 1.54 |
| 4 | M4 | 264 | LYS | C-O | -5.63 | 1.17 | 1.24 |
| 10 | j5 | 1102 | TYR | CA-C | -5.63 | 1.45 | 1.52 |
| 4 | M8 | 165 | PHE | C-O | -5.63 | 1.17 | 1.24 |
| 11 | a9 | 490 | ILE | C-O | -5.63 | 1.17 | 1.24 |
| 11 | aA | 490 | ILE | C-O | -5.63 | 1.17 | 1.24 |
| 4 | M3 | 144 | ARG | C-O | -5.63 | 1.17 | 1.24 |
| 4 | M1 | 144 | ARG | C-O | -5.63 | 1.17 | 1.24 |
| 1 | D5 | 15 | GLN | C-O | -5.62 | 1.16 | 1.24 |
| 1 | J5 | 3 | ASP | C-O | -5.62 | 1.16 | 1.24 |
| 10 | k5 | 706 | PRO | N-CA | -5.62 | 1.40 | 1.47 |
| 9 | x7 | 56 | LEU | CA-C | -5.62 | 1.45 | 1.52 |
| 4 | M9 | 168 | LEU | C-O | -5.62 | 1.17 | 1.24 |
| 10 | j5 | 503 | LYS | CA-CB | -5.62 | 1.44 | 1.54 |
| 10 | j5 | 703 | LEU | N-CA | -5.62 | 1.39 | 1.46 |
| 10 | k5 | 686 | THR | CB-CG2 | -5.62 | 1.33 | 1.52 |
| 11 | a9 | 448 | ASN | C-O | -5.62 | 1.17 | 1.24 |
| 4 | M3 | 19 | MET | CA-CB | -5.62 | 1.46 | 1.54 |
| 10 | k5 | 903 | ARG | CA-C | -5.62 | 1.45 | 1.52 |
| 4 | M8 | 241 | LEU | C-O | -5.62 | 1.17 | 1.24 |
| 11 | a9 | 632 | ILE | C-O | -5.62 | 1.18 | 1.24 |
| 8 | K5 | 109 | ILE | N-CA | -5.62 | 1.38 | 1.46 |
| 8 | u7 | 56 | ASP | C-O | -5.62 | 1.17 | 1.24 |
| 1 | D5 | 3 | ASP | C-O | -5.62 | 1.17 | 1.24 |
| 10 | j5 | 683 | ARG | CA-C | -5.62 | 1.44 | 1.52 |
| 4 | MA | 19 | MET | CA-CB | -5.61 | 1.46 | 1.54 |
| 8 | C5 | 123 | ILE | CA-CB | 5.61 | 1.57 | 1.54 |
| 1 | J5 | 15 | GLN | C-O | -5.61 | 1.17 | 1.24 |
| 10 | j5 | 293 | LYS | C-O | -5.61 | 1.17 | 1.24 |
| 8 | o7 | 55 | GLY | CA-C | -5.61 | 1.45 | 1.52 |
| 4 | M9 | 19 | MET | CA-CB | -5.61 | 1.46 | 1.54 |
| 10 | k5 | 503 | LYS | CA-CB | -5.61 | 1.44 | 1.54 |
| 10 | j5 | 518 | ASN | N-CA | -5.61 | 1.39 | 1.46 |
| 11 | a9 | 439 | ARG | C-O | -5.61 | 1.17 | 1.24 |
| 11 | aA | 439 | ARG | C-O | -5.61 | 1.17 | 1.24 |
| 4 | M1 | 19 | MET | CA-CB | -5.61 | 1.46 | 1.54 |
| 4 | M8 | 249 | ASP | C-O | -5.61 | 1.17 | 1.24 |
| 4 | MA | 188 | LEU | C-O | -5.61 | 1.17 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | j5 | 774 | GLN | N-CA | -5.61 | 1.40 | 1.47 |
| 10 | j5 | 783 | TYR | N-CA | -5.61 | 1.38 | 1.46 |
| 10 | k5 | 783 | TYR | N-CA | -5.61 | 1.38 | 1.46 |
| 4 | M9 | 188 | LEU | C-O | -5.61 | 1.17 | 1.24 |
| 4 | MA | 66 | VAL | CA-CB | -5.61 | 1.47 | 1.54 |
| 10 | k5 | 993 | LYS | C-O | -5.61 | 1.17 | 1.24 |
| 4 | M9 | 66 | VAL | CA-CB | -5.61 | 1.47 | 1.54 |
| 4 | M4 | 23 | PRO | C-O | -5.60 | 1.16 | 1.24 |
| 4 | M4 | 168 | LEU | C-O | -5.60 | 1.17 | 1.24 |
| 1 | D5 | 12 | TYR | CA-C | -5.60 | 1.44 | 1.52 |
| 10 | k5 | 544 | VAL | CA-CB | -5.60 | 1.46 | 1.54 |
| 10 | k5 | 702 | VAL | CA-CB | -5.60 | 1.46 | 1.54 |
| 4 | MA | 168 | LEU | C-O | -5.60 | 1.17 | 1.24 |
| 4 | M3 | 66 | VAL | CA-CB | -5.60 | 1.47 | 1.54 |
| 4 | M9 | 12 | GLY | CA-C | -5.60 | 1.45 | 1.51 |
| 4 | M1 | 66 | VAL | CA-CB | -5.60 | 1.47 | 1.54 |
| 4 | M4 | 249 | ASP | C-O | -5.60 | 1.17 | 1.24 |
| 8 | e5 | 7 | ALA | C-O | -5.60 | 1.15 | 1.23 |
| 10 | k5 | 774 | GLN | N-CA | -5.60 | 1.40 | 1.47 |
| 11 | a9 | 614 | SER | C-O | -5.60 | 1.17 | 1.24 |
| 11 | aA | 614 | SER | C-O | -5.60 | 1.17 | 1.24 |
| 1 | h7 | 46 | SER | C-O | -5.59 | 1.16 | 1.24 |
| 1 | b7 | 46 | SER | C-O | -5.59 | 1.16 | 1.24 |
| 4 | MA | 23 | PRO | C-O | -5.59 | 1.16 | 1.24 |
| 10 | k5 | 730 | ASN | N-CA | -5.59 | 1.53 | 1.46 |
| 10 | k5 | 1133 | GLU | C-O | -5.59 | 1.17 | 1.24 |
| 4 | M9 | 23 | PRO | C-O | -5.59 | 1.16 | 1.24 |
| 4 | M3 | 249 | ASP | C-O | -5.59 | 1.17 | 1.24 |
| 9 | z7 | 55 | LYS | CA-C | -5.59 | 1.45 | 1.52 |
| 4 | M1 | 249 | ASP | C-O | -5.59 | 1.17 | 1.24 |
| 10 | k5 | 463 | THR | N-CA | -5.59 | 1.39 | 1.46 |
| 9 | y7 | 56 | LEU | CA-C | -5.59 | 1.45 | 1.52 |
| 8 | C5 | 17 | TYR | C-O | -5.59 | 1.17 | 1.23 |
| 10 | j5 | 980 | HIS | C-O | -5.59 | 1.16 | 1.23 |
| 11 | a9 | 626 | ALA | C-O | -5.58 | 1.17 | 1.24 |
| 11 | aA | 626 | ALA | C-O | -5.58 | 1.17 | 1.24 |
| 10 | j5 | 253 | ARG | CA-C | -5.58 | 1.47 | 1.52 |
| 10 | j5 | 721 | LYS | CA-CB | -5.58 | 1.44 | 1.53 |
| 4 | M3 | 133 | ARG | C-O | -5.58 | 1.17 | 1.24 |
| 10 | j5 | 699 | SER | N-CA | -5.58 | 1.39 | 1.46 |
| 10 | k5 | 274 | MET | N-CA | -5.58 | 1.39 | 1.46 |
| 10 | j5 | 1032 | VAL | C-O | -5.58 | 1.17 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4 | M8 | 19 | MET | CA-CB | -5.58 | 1.46 | 1.54 |
| 10 | j5 | 776 | PHE | C-N | -5.58 | 1.27 | 1.33 |
| 10 | k5 | 683 | ARG | CA-C | -5.58 | 1.45 | 1.52 |
| 10 | k5 | 744 | PRO | CA-CB | -5.58 | 1.45 | 1.53 |
| 4 | MA | 12 | GLY | CA-C | -5.58 | 1.45 | 1.51 |
| 8 | c7 | 134 | LYS | CA-C | -5.58 | 1.45 | 1.52 |
| 11 | a9 | 466 | SER | CA-C | -5.58 | 1.45 | 1.52 |
| 11 | aA | 466 | SER | CA-C | -5.58 | 1.45 | 1.52 |
| 8 | A5 | 57 | GLN | C-O | -5.58 | 1.17 | 1.24 |
| 4 | M3 | 168 | LEU | C-O | -5.57 | 1.17 | 1.24 |
| 8 | E5 | 109 | ILE | N-CA | -5.57 | 1.39 | 1.46 |
| 10 | j5 | 424 | ARG | C-O | -5.57 | 1.16 | 1.23 |
| 10 | k5 | 424 | ARG | C-O | -5.57 | 1.16 | 1.23 |
| 10 | k5 | 776 | PHE | C-N | -5.57 | 1.27 | 1.33 |
| 4 | M1 | 168 | LEU | C-O | -5.57 | 1.17 | 1.24 |
| 4 | MA | 192 | GLN | C-O | -5.57 | 1.17 | 1.24 |
| 10 | j5 | 702 | VAL | CA-CB | -5.57 | 1.46 | 1.54 |
| 4 | M9 | 192 | GLN | C-O | -5.57 | 1.17 | 1.24 |
| 4 | M3 | 188 | LEU | C-O | -5.57 | 1.17 | 1.24 |
| 4 | M4 | 133 | ARG | C-O | -5.57 | 1.17 | 1.24 |
| 10 | j5 | 440 | TYR | CA-C | -5.57 | 1.45 | 1.52 |
| 10 | j5 | 903 | ARG | CA-C | -5.57 | 1.46 | 1.52 |
| 10 | k5 | 440 | TYR | CA-C | -5.57 | 1.45 | 1.52 |
| 8 | u7 | 48 | GLU | C-O | -5.57 | 1.16 | 1.24 |
| 11 | aA | 632 | ILE | C-O | -5.57 | 1.18 | 1.24 |
| 4 | M1 | 188 | LEU | C-O | -5.57 | 1.17 | 1.24 |
| 10 | k5 | 913 | VAL | C-O | -5.57 | 1.17 | 1.24 |
| 10 | k5 | 1102 | TYR | CA-C | -5.57 | 1.45 | 1.52 |
| 8 | o7 | 45 | GLU | C-O | -5.57 | 1.17 | 1.24 |
| 11 | a9 | 525 | GLN | C-O | -5.57 | 1.17 | 1.24 |
| 4 | M3 | 186 | ALA | C-O | -5.57 | 1.17 | 1.24 |
| 9 | z5 | 67 | VAL | N-CA | -5.57 | 1.39 | 1.46 |
| 10 | j5 | 166 | TYR | C-O | -5.57 | 1.17 | 1.24 |
| 10 | k5 | 478 | PRO | CA-CB | -5.57 | 1.44 | 1.53 |
| 10 | k5 | 725 | LEU | CB-CG | -5.57 | 1.42 | 1.53 |
| 3 | B6 | 77 | ARG | C-O | -5.57 | 1.17 | 1.24 |
| 4 | M8 | 12 | GLY | CA-C | -5.57 | 1.45 | 1.51 |
| 4 | M1 | 186 | ALA | C-O | -5.57 | 1.17 | 1.24 |
| 4 | MA | 165 | PHE | C-O | -5.57 | 1.17 | 1.24 |
| 4 | M3 | 23 | PRO | C-O | -5.57 | 1.16 | 1.24 |
| 10 | j5 | 750 | ARG | CA-C | -5.57 | 1.45 | 1.52 |
| 8 | o7 | 48 | GLU | C-O | -5.57 | 1.16 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4 | M9 | 165 | PHE | C-O | -5.57 | 1.17 | 1.24 |
| 4 | M1 | 23 | PRO | C-O | -5.57 | 1.16 | 1.24 |
| 10 | j5 | 531 | THR | CB-CG2 | -5.56 | 1.34 | 1.52 |
| 4 | MA | 133 | ARG | C-O | -5.56 | 1.17 | 1.24 |
| 10 | j5 | 554 | ASN | CA-C | -5.56 | 1.45 | 1.52 |
| 4 | M9 | 133 | ARG | C-O | -5.56 | 1.17 | 1.24 |
| 11 | a9 | 48 | LEU | N-CA | -5.56 | 1.39 | 1.46 |
| 10 | k5 | 568 | ILE | N-CA | -5.56 | 1.39 | 1.46 |
| 11 | a9 | 616 | PRO | CA-C | -5.56 | 1.45 | 1.52 |
| 11 | aA | 616 | PRO | CA-C | -5.56 | 1.45 | 1.52 |
| 4 | MA | 249 | ASP | C-O | -5.56 | 1.17 | 1.24 |
| 10 | j5 | 879 | ASP | CA-C | -5.56 | 1.46 | 1.52 |
| 8 | i7 | 134 | LYS | CA-C | -5.56 | 1.45 | 1.52 |
| 9 | w7 | 55 | LYS | CA-C | -5.56 | 1.45 | 1.52 |
| 4 | M9 | 241 | LEU | C-O | -5.56 | 1.17 | 1.24 |
| 4 | M9 | 249 | ASP | C-O | -5.56 | 1.17 | 1.24 |
| 4 | M4 | 186 | ALA | C-O | -5.56 | 1.17 | 1.24 |
| 10 | j5 | 776 | PHE | CA-CB | 5.56 | 1.62 | 1.53 |
| 10 | k5 | 776 | PHE | CA-CB | 5.56 | 1.62 | 1.53 |
| 10 | k5 | 879 | ASP | CA-C | -5.56 | 1.46 | 1.52 |
| 4 | M1 | 133 | ARG | C-O | -5.56 | 1.17 | 1.24 |
| 4 | M4 | 118 | TYR | CA-C | -5.55 | 1.45 | 1.52 |
| 10 | k5 | 1032 | VAL | C-O | -5.55 | 1.17 | 1.24 |
| 9 | z7 | 11 | ILE | C-O | -5.55 | 1.18 | 1.24 |
| 5 | N3 | 22 | LEU | CA-C | -5.55 | 1.45 | 1.52 |
| 10 | k5 | 699 | SER | N-CA | -5.55 | 1.39 | 1.46 |
| 4 | M8 | 118 | TYR | CA-C | -5.55 | 1.45 | 1.52 |
| 4 | M8 | 105 | ALA | C-O | -5.55 | 1.17 | 1.24 |
| 4 | M4 | 66 | VAL | CA-CB | -5.55 | 1.47 | 1.54 |
| 10 | k5 | 609 | ARG | CA-C | -5.55 | 1.44 | 1.52 |
| 10 | j5 | 291 | ASP | C-O | -5.55 | 1.17 | 1.24 |
| 10 | k5 | 291 | ASP | C-O | -5.55 | 1.17 | 1.24 |
| 10 | k5 | 531 | THR | CB-CG2 | -5.55 | 1.34 | 1.52 |
| 11 | a9 | 483 | ASP | C-O | -5.55 | 1.17 | 1.24 |
| 11 | aA | 483 | ASP | C-O | -5.55 | 1.17 | 1.24 |
| 4 | M3 | 12 | GLY | CA-C | -5.54 | 1.45 | 1.51 |
| 4 | M4 | 12 | GLY | CA-C | -5.54 | 1.45 | 1.51 |
| 10 | j5 | 738 | TYR | N-CA | -5.54 | 1.38 | 1.46 |
| 4 | M1 | 12 | GLY | CA-C | -5.54 | 1.45 | 1.51 |
| 9 | i5 | 67 | VAL | N-CA | -5.54 | 1.39 | 1.46 |
| 10 | k5 | 1106 | PHE | C-O | -5.54 | 1.16 | 1.23 |
| 11 | a9 | 42 | ARG | N-CA | -5.54 | 1.39 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 11 | aA | 42 | ARG | N-CA | -5.54 | 1.39 | 1.46 |
| 8 | Y7 | 123 | ILE | CA-CB | 5.54 | 1.57 | 1.54 |
| 11 | aA | 525 | GLN | C-O | -5.54 | 1.17 | 1.24 |
| 4 | M1 | 94 | TRP | CA-C | -5.54 | 1.45 | 1.53 |
| 4 | MA | 94 | TRP | CA-C | -5.54 | 1.45 | 1.53 |
| 4 | M4 | 248 | SER | C-O | -5.54 | 1.17 | 1.23 |
| 10 | j5 | 591 | ILE | CA-CB | -5.54 | 1.48 | 1.54 |
| 10 | j5 | 870 | GLU | CA-CB | -5.54 | 1.44 | 1.53 |
| 10 | k5 | 498 | ALA | N-CA | -5.54 | 1.39 | 1.45 |
| 10 | k5 | 518 | ASN | N-CA | -5.54 | 1.39 | 1.46 |
| 10 | k5 | 870 | GLU | CA-CB | -5.54 | 1.44 | 1.53 |
| 4 | M9 | 94 | TRP | CA-C | -5.54 | 1.45 | 1.53 |
| 4 | M4 | 94 | TRP | CA-C | -5.54 | 1.45 | 1.53 |
| 8 | A5 | 58 | LEU | CA-C | -5.54 | 1.45 | 1.52 |
| 4 | M4 | 170 | PHE | C-O | -5.54 | 1.17 | 1.24 |
| 10 | k5 | 253 | ARG | CA-C | -5.54 | 1.47 | 1.52 |
| 4 | M3 | 241 | LEU | C-O | -5.53 | 1.17 | 1.24 |
| 1 | J5 | 12 | TYR | CA-C | -5.53 | 1.45 | 1.52 |
| 10 | j5 | 478 | PRO | CA-CB | -5.53 | 1.45 | 1.53 |
| 10 | k5 | 609 | ARG | N-CA | -5.53 | 1.39 | 1.46 |
| 4 | M1 | 241 | LEU | C-O | -5.53 | 1.17 | 1.24 |
| 8 | o7 | 47 | ARG | C-O | -5.53 | 1.17 | 1.24 |
| 4 | M8 | 170 | PHE | C-O | -5.53 | 1.17 | 1.24 |
| 1 | D5 | 17 | LYS | CA-C | -5.53 | 1.45 | 1.53 |
| 10 | j5 | 445 | TYR | CZ-OH | -5.53 | 1.26 | 1.38 |
| 10 | k5 | 445 | TYR | CZ-OH | -5.53 | 1.26 | 1.38 |
| 11 | aA | 48 | LEU | N-CA | -5.53 | 1.39 | 1.46 |
| 10 | j5 | 809 | LEU | CA-C | -5.53 | 1.45 | 1.52 |
| 10 | k5 | 809 | LEU | CA-C | -5.53 | 1.45 | 1.52 |
| 2 | KA | 19 | LEU | CA-C | -5.53 | 1.45 | 1.52 |
| 10 | j5 | 646 | ASN | CA-CB | -5.53 | 1.43 | 1.53 |
| 10 | k5 | 646 | ASN | CA-CB | -5.53 | 1.43 | 1.53 |
| 2 | K9 | 19 | LEU | CA-C | -5.53 | 1.45 | 1.52 |
| 8 | E5 | 123 | ILE | CA-CB | 5.53 | 1.57 | 1.54 |
| 10 | j5 | 384 | SER | C-O | -5.53 | 1.16 | 1.24 |
| 10 | k5 | 384 | SER | C-O | -5.53 | 1.16 | 1.24 |
| 8 | g7 | 12 | ASP | C-O | -5.53 | 1.17 | 1.24 |
| 10 | j5 | 609 | ARG | N-CA | -5.52 | 1.39 | 1.46 |
| 3 | F9 | 144 | SER | CA-C | -5.52 | 1.48 | 1.52 |
| 4 | MA | 241 | LEU | C-O | -5.52 | 1.17 | 1.24 |
| 4 | M4 | 163 | ASN | C-O | -5.52 | 1.17 | 1.24 |
| 8 | c5 | 123 | ILE | CA-CB | 5.52 | 1.57 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | j5 | 671 | GLN | CA-CB | -5.52 | 1.44 | 1.53 |
| 10 | j5 | 715 | ALA | N-CA | -5.52 | 1.39 | 1.46 |
| 10 | j5 | 830 | GLU | CA-CB | -5.52 | 1.44 | 1.53 |
| 10 | k5 | 441 | ASP | CB-CG | -5.52 | 1.38 | 1.52 |
| 10 | k5 | 715 | ALA | N-CA | -5.52 | 1.39 | 1.46 |
| 10 | k5 | 776 | PHE | N-CA | 5.52 | 1.53 | 1.46 |
| 10 | k5 | 1031 | SER | C-O | -5.52 | 1.16 | 1.23 |
| 1 | b7 | 45 | SER | N-CA | -5.52 | 1.39 | 1.46 |
| 4 | M4 | 192 | GLN | C-O | -5.52 | 1.17 | 1.24 |
| 4 | M1 | 192 | GLN | C-O | -5.52 | 1.17 | 1.24 |
| 10 | j5 | 274 | MET | N-CA | -5.52 | 1.39 | 1.46 |
| 10 | k5 | 293 | LYS | C-O | -5.52 | 1.17 | 1.24 |
| 9 | w7 | 11 | ILE | C-O | -5.52 | 1.18 | 1.24 |
| 10 | j5 | 744 | PRO | CA-CB | -5.52 | 1.46 | 1.53 |
| 9 | w7 | 28 | PHE | CA-C | -5.51 | 1.45 | 1.52 |
| 4 | M8 | 186 | ALA | C-O | -5.51 | 1.17 | 1.24 |
| 10 | k5 | 587 | LYS | CA-C | -5.51 | 1.45 | 1.53 |
| 1 | h7 | 44 | ILE | CA-C | -5.51 | 1.45 | 1.52 |
| 10 | j5 | 951 | MET | C-O | -5.51 | 1.17 | 1.24 |
| 10 | k5 | 658 | TYR | N-CA | -5.51 | 1.39 | 1.46 |
| 8 | u7 | 45 | GLU | C-O | -5.51 | 1.17 | 1.24 |
| 4 | M8 | 23 | PRO | C-O | -5.51 | 1.16 | 1.24 |
| 11 | a9 | 439 | ARG | CA-C | -5.51 | 1.45 | 1.52 |
| 11 | aA | 439 | ARG | CA-C | -5.51 | 1.45 | 1.52 |
| 4 | MA | 186 | ALA | C-O | -5.51 | 1.17 | 1.24 |
| 4 | M4 | 28 | HIS | C-O | -5.51 | 1.16 | 1.23 |
| 9 | i5 | 41 | GLN | CD-NE2 | -5.51 | 1.21 | 1.33 |
| 10 | k5 | 980 | HIS | C-O | -5.51 | 1.16 | 1.23 |
| 4 | M9 | 186 | ALA | C-O | -5.51 | 1.17 | 1.24 |
| 3 | FA | 144 | SER | CA-C | -5.51 | 1.46 | 1.52 |
| 4 | M8 | 188 | LEU | C-O | -5.51 | 1.17 | 1.24 |
| 10 | k5 | 166 | TYR | C-O | -5.50 | 1.17 | 1.24 |
| 4 | MA | 165 | PHE | CA-C | -5.50 | 1.45 | 1.52 |
| 10 | j5 | 441 | ASP | CB-CG | -5.50 | 1.38 | 1.52 |
| 10 | j5 | 733 | SER | N-CA | -5.50 | 1.38 | 1.46 |
| 10 | j5 | 790 | ALA | CA-C | -5.50 | 1.45 | 1.52 |
| 10 | k5 | 371 | SER | CB-OG | -5.50 | 1.31 | 1.42 |
| 10 | k5 | 733 | SER | N-CA | -5.50 | 1.38 | 1.46 |
| 4 | M9 | 165 | PHE | CA-C | -5.50 | 1.45 | 1.52 |
| 4 | M3 | 192 | GLN | C-O | -5.50 | 1.17 | 1.24 |
| 10 | j5 | 631 | HIS | CA-C | -5.50 | 1.45 | 1.52 |
| 10 | k5 | 806 | VAL | CA-CB | -5.50 | 1.47 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | k5 | 790 | ALA | CA-C | -5.50 | 1.45 | 1.52 |
| 4 | M3 | 165 | PHE | CA-C | -5.50 | 1.46 | 1.52 |
| 8 | K5 | 123 | ILE | CA-CB | 5.50 | 1.57 | 1.54 |
| 10 | j5 | 695 | GLY | CA-C | -5.50 | 1.44 | 1.51 |
| 5 | Z8 | 22 | LEU | CA-C | -5.50 | 1.45 | 1.52 |
| 11 | a9 | 524 | MET | C-O | -5.50 | 1.17 | 1.24 |
| 4 | M1 | 165 | PHE | CA-C | -5.50 | 1.46 | 1.52 |
| 8 | G5 | 58 | LEU | CA-C | -5.50 | 1.45 | 1.52 |
| 10 | j5 | 512 | ASN | CG-OD1 | -5.50 | 1.13 | 1.23 |
| 10 | j5 | 725 | LEU | CB-CG | -5.50 | 1.42 | 1.53 |
| 10 | k5 | 566 | ALA | N-CA | -5.50 | 1.38 | 1.46 |
| 4 | M8 | 248 | SER | C-O | -5.50 | 1.17 | 1.23 |
| 10 | j5 | 245 | ILE | C-O | -5.49 | 1.18 | 1.24 |
| 10 | k5 | 587 | LYS | C-O | -5.49 | 1.16 | 1.23 |
| 10 | j5 | 780 | ILE | CB-CG1 | -5.49 | 1.42 | 1.53 |
| 9 | x7 | 31 | LEU | C-O | -5.49 | 1.17 | 1.23 |
| 10 | k5 | 631 | HIS | CA-C | -5.49 | 1.45 | 1.52 |
| 11 | a9 | 438 | TYR | CA-C | -5.49 | 1.45 | 1.52 |
| 4 | M4 | 241 | LEU | C-O | -5.49 | 1.17 | 1.24 |
| 10 | j5 | 463 | THR | N-CA | -5.49 | 1.39 | 1.46 |
| 10 | j5 | 498 | ALA | N-CA | -5.49 | 1.39 | 1.45 |
| 9 | z7 | 41 | GLN | N-CA | -5.49 | 1.39 | 1.46 |
| 9 | w7 | 41 | GLN | N-CA | -5.49 | 1.39 | 1.46 |
| 4 | M8 | 133 | ARG | C-O | -5.49 | 1.17 | 1.24 |
| 10 | k5 | 554 | ASN | CA-C | -5.49 | 1.45 | 1.52 |
| 10 | k5 | 1008 | PHE | C-O | -5.49 | 1.17 | 1.24 |
| 10 | j5 | 405 | LEU | CA-C | -5.49 | 1.46 | 1.52 |
| 10 | k5 | 828 | VAL | N-CA | -5.49 | 1.39 | 1.46 |
| 11 | aA | 438 | TYR | CA-C | -5.49 | 1.45 | 1.52 |
| 1 | J5 | 17 | LYS | CA-C | -5.48 | 1.45 | 1.53 |
| 10 | j5 | 568 | ILE | N-CA | -5.48 | 1.39 | 1.46 |
| 10 | j5 | 609 | ARG | CA-C | -5.48 | 1.44 | 1.52 |
| 10 | k5 | 643 | VAL | CA-C | -5.48 | 1.45 | 1.52 |
| 10 | k5 | 695 | GLY | CA-C | -5.48 | 1.44 | 1.51 |
| 10 | k5 | 723 | GLN | CA-CB | -5.48 | 1.44 | 1.53 |
| 4 | M1 | 248 | SER | C-O | -5.48 | 1.17 | 1.23 |
| 3 | LA | 115 | GLU | C-O | -5.48 | 1.17 | 1.24 |
| 10 | k5 | 591 | ILE | CA-CB | -5.48 | 1.48 | 1.54 |
| 8 | a7 | 12 | ASP | C-O | -5.48 | 1.17 | 1.24 |
| 3 | L9 | 115 | GLU | C-O | -5.48 | 1.17 | 1.24 |
| 5 | N1 | 22 | LEU | CA-C | -5.48 | 1.45 | 1.52 |
| 10 | j5 | 172 | LEU | C-O | -5.48 | 1.17 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | j5 | 464 | GLN | CG-CD | -5.48 | 1.38 | 1.52 |
| 10 | j5 | 587 | LYS | C-O | -5.48 | 1.16 | 1.23 |
| 10 | k5 | 464 | GLN | CG-CD | -5.48 | 1.38 | 1.52 |
| 4 | M3 | 28 | HIS | C-O | -5.48 | 1.16 | 1.23 |
| 8 | I5 | 8 | ILE | N-CA | -5.48 | 1.39 | 1.46 |
| 10 | j5 | 53 | ARG | C-O | -5.48 | 1.17 | 1.24 |
| 10 | k5 | 53 | ARG | C-O | -5.48 | 1.17 | 1.24 |
| 10 | k5 | 671 | GLN | CA-CB | -5.48 | 1.44 | 1.53 |
| 8 | g7 | 19 | SER | C-O | -5.48 | 1.15 | 1.23 |
| 9 | z7 | 28 | PHE | CA-C | -5.48 | 1.45 | 1.52 |
| 11 | a9 | 547 | LYS | C-O | -5.48 | 1.17 | 1.24 |
| 11 | aA | 547 | LYS | C-O | -5.48 | 1.17 | 1.24 |
| 4 | M1 | 28 | HIS | C-O | -5.48 | 1.16 | 1.23 |
| 4 | M3 | 94 | TRP | CA-C | -5.48 | 1.45 | 1.53 |
| 10 | j5 | 187 | ARG | C-O | -5.47 | 1.17 | 1.24 |
| 10 | j5 | 806 | VAL | CA-CB | -5.47 | 1.47 | 1.54 |
| 10 | k5 | 23 | GLU | CA-C | -5.47 | 1.45 | 1.52 |
| 10 | k5 | 187 | ARG | C-O | -5.47 | 1.17 | 1.24 |
| 10 | j5 | 23 | GLU | CA-C | -5.47 | 1.45 | 1.52 |
| 10 | j5 | 532 | THR | C-O | -5.47 | 1.16 | 1.24 |
| 10 | k5 | 532 | THR | C-O | -5.47 | 1.16 | 1.24 |
| 10 | k5 | 573 | GLN | CD-OE1 | -5.47 | 1.13 | 1.23 |
| 1 | b7 | 44 | ILE | CA-C | -5.47 | 1.45 | 1.52 |
| 9 | z5 | 41 | GLN | CD-NE2 | -5.47 | 1.21 | 1.33 |
| 10 | j5 | 776 | PHE | N-CA | 5.47 | 1.53 | 1.46 |
| 10 | k5 | 53 | ARG | CA-C | -5.47 | 1.45 | 1.52 |
| 8 | a7 | 19 | SER | C-O | -5.47 | 1.15 | 1.23 |
| 10 | j5 | 510 | ILE | CA-C | -5.47 | 1.46 | 1.52 |
| 10 | k5 | 1034 | GLU | C-O | -5.47 | 1.17 | 1.24 |
| 8 | i7 | 119 | LEU | C-O | -5.47 | 1.16 | 1.24 |
| 4 | MA | 248 | SER | C-O | -5.46 | 1.17 | 1.23 |
| 4 | M8 | 192 | GLN | C-O | -5.46 | 1.17 | 1.24 |
| 4 | M9 | 248 | SER | C-O | -5.46 | 1.17 | 1.23 |
| 11 | aA | 524 | MET | C-O | -5.46 | 1.17 | 1.24 |
| 10 | j5 | 296 | VAL | CA-CB | -5.46 | 1.47 | 1.54 |
| 10 | j5 | 566 | ALA | N-CA | -5.46 | 1.38 | 1.46 |
| 10 | j5 | 587 | LYS | CA-C | -5.46 | 1.45 | 1.53 |
| 4 | M4 | 238 | MET | C-O | -5.46 | 1.17 | 1.24 |
| 10 | k5 | 830 | GLU | CA-CB | -5.46 | 1.44 | 1.53 |
| 1 | h7 | 45 | SER | N-CA | -5.46 | 1.39 | 1.46 |
| 4 | M3 | 170 | PHE | C-O | -5.46 | 1.17 | 1.24 |
| 10 | j5 | 53 | ARG | CA-C | -5.46 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | k5 | 780 | ILE | CB-CG1 | -5.46 | 1.42 | 1.53 |
| 4 | M1 | 170 | PHE | C-O | -5.46 | 1.17 | 1.24 |
| 10 | j5 | 177 | SER | C-O | -5.46 | 1.17 | 1.24 |
| 11 | a9 | 476 | ARG | C-O | -5.46 | 1.17 | 1.24 |
| 11 | a9 | 483 | ASP | CA-C | -5.46 | 1.45 | 1.52 |
| 11 | aA | 483 | ASP | CA-C | -5.46 | 1.45 | 1.52 |
| 4 | M4 | 165 | PHE | CA-C | -5.45 | 1.46 | 1.52 |
| 10 | j5 | 535 | PRO | CA-CB | -5.45 | 1.46 | 1.53 |
| 10 | j5 | 739 | VAL | CA-CB | -5.45 | 1.47 | 1.54 |
| 10 | k5 | 512 | ASN | CG-OD1 | -5.45 | 1.13 | 1.23 |
| 9 | z5 | 37 | TRP | CA-CB | -5.45 | 1.44 | 1.53 |
| 11 | a9 | 452 | ILE | C-O | -5.45 | 1.17 | 1.24 |
| 11 | aA | 452 | ILE | C-O | -5.45 | 1.17 | 1.24 |
| 10 | j5 | 322 | LYS | C-O | -5.45 | 1.17 | 1.24 |
| 10 | j5 | 371 | SER | CB-OG | -5.45 | 1.31 | 1.42 |
| 10 | j5 | 469 | GLN | CD-OE1 | -5.45 | 1.13 | 1.23 |
| 10 | k5 | 322 | LYS | C-O | -5.45 | 1.17 | 1.24 |
| 10 | k5 | 434 | TRP | CB-CG | -5.45 | 1.33 | 1.50 |
| 10 | k5 | 469 | GLN | CD-OE1 | -5.45 | 1.13 | 1.23 |
| 8 | c7 | 119 | LEU | C-O | -5.45 | 1.16 | 1.24 |
| 4 | MA | 170 | PHE | C-O | -5.45 | 1.17 | 1.24 |
| 4 | M9 | 170 | PHE | C-O | -5.45 | 1.17 | 1.24 |
| 4 | MA | 238 | MET | C-O | -5.45 | 1.17 | 1.24 |
| 10 | j5 | 506 | LYS | CA-C | -5.45 | 1.46 | 1.52 |
| 10 | j5 | 1031 | SER | C-O | -5.45 | 1.16 | 1.23 |
| 10 | k5 | 506 | LYS | CA-C | -5.45 | 1.46 | 1.52 |
| 4 | M9 | 238 | MET | C-O | -5.45 | 1.17 | 1.24 |
| 4 | M4 | 185 | ALA | CA-C | -5.44 | 1.45 | 1.52 |
| 10 | j5 | 573 | GLN | CD-OE1 | -5.44 | 1.13 | 1.23 |
| 4 | M3 | 40 | GLN | CA-CB | -5.44 | 1.45 | 1.53 |
| 8 | C5 | 8 | ILE | N-CA | -5.44 | 1.39 | 1.46 |
| 10 | j5 | 476 | ASN | CB-CG | -5.44 | 1.38 | 1.52 |
| 10 | k5 | 15 | ARG | CA-C | -5.44 | 1.45 | 1.52 |
| 10 | k5 | 454 | GLN | CA-CB | -5.44 | 1.45 | 1.53 |
| 11 | aA | 476 | ARG | C-O | -5.44 | 1.17 | 1.24 |
| 4 | M1 | 40 | GLN | CA-CB | -5.44 | 1.45 | 1.53 |
| 4 | MA | 67 | LEU | C-O | -5.44 | 1.16 | 1.23 |
| 10 | j5 | 723 | GLN | CA-CB | -5.44 | 1.44 | 1.53 |
| 10 | j5 | 924 | ASP | C-O | -5.44 | 1.17 | 1.23 |
| 10 | k5 | 172 | LEU | C-O | -5.44 | 1.17 | 1.24 |
| 4 | M8 | 28 | HIS | C-O | -5.44 | 1.16 | 1.23 |
| 4 | M8 | 165 | PHE | CA-C | -5.44 | 1.46 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4 | M8 | 185 | ALA | CA-C | -5.44 | 1.45 | 1.52 |
| 4 | M9 | 67 | LEU | C-O | -5.44 | 1.16 | 1.23 |
| 4 | M4 | 67 | LEU | C-O | -5.44 | 1.16 | 1.23 |
| 8 | E5 | 108 | GLY | C-O | -5.44 | 1.16 | 1.23 |
| 10 | j5 | 15 | ARG | CA-C | -5.44 | 1.45 | 1.52 |
| 10 | j5 | 643 | VAL | CA-C | -5.44 | 1.45 | 1.52 |
| 10 | j5 | 995 | VAL | CA-CB | -5.44 | 1.47 | 1.54 |
| 10 | j5 | 1034 | GLU | C-O | -5.44 | 1.17 | 1.24 |
| 4 | MA | 40 | GLN | CA-CB | -5.43 | 1.45 | 1.53 |
| 4 | M3 | 140 | ARG | C-O | -5.43 | 1.17 | 1.24 |
| 10 | j5 | 893 | ASN | CG-ND2 | -5.43 | 1.21 | 1.33 |
| 4 | M9 | 40 | GLN | CA-CB | -5.43 | 1.45 | 1.53 |
| 4 | M1 | 140 | ARG | C-O | -5.43 | 1.17 | 1.24 |
| 9 | y7 | 31 | LEU | CA-C | -5.43 | 1.45 | 1.52 |
| 10 | j5 | 406 | ILE | CA-C | -5.43 | 1.44 | 1.52 |
| 4 | M3 | 51 | ARG | CA-C | -5.43 | 1.45 | 1.52 |
| 10 | k5 | 476 | ASN | CB-CG | -5.43 | 1.38 | 1.52 |
| 4 | M1 | 51 | ARG | CA-C | -5.43 | 1.45 | 1.52 |
| 4 | M1 | 185 | ALA | CA-C | -5.43 | 1.45 | 1.52 |
| 4 | M3 | 163 | ASN | C-O | -5.43 | 1.17 | 1.24 |
| 4 | M1 | 163 | ASN | C-O | -5.43 | 1.17 | 1.24 |
| 5 | NA | 22 | LEU | CA-C | -5.43 | 1.45 | 1.52 |
| 10 | j5 | 21 | MET | C-O | -5.43 | 1.17 | 1.24 |
| 10 | j5 | 198 | ALA | C-O | -5.43 | 1.17 | 1.24 |
| 10 | j5 | 592 | LYS | CA-CB | -5.43 | 1.44 | 1.53 |
| 10 | j5 | 670 | TYR | CZ-OH | -5.43 | 1.26 | 1.38 |
| 10 | j5 | 824 | PRO | C-N | -5.43 | 1.26 | 1.33 |
| 10 | k5 | 592 | LYS | CA-CB | -5.43 | 1.44 | 1.53 |
| 4 | M3 | 185 | ALA | CA-C | -5.42 | 1.45 | 1.52 |
| 10 | k5 | 405 | LEU | CA-C | -5.42 | 1.46 | 1.52 |
| 4 | M8 | 246 | ALA | C-O | -5.42 | 1.16 | 1.24 |
| 4 | MA | 185 | ALA | CA-C | -5.42 | 1.45 | 1.52 |
| 4 | M3 | 238 | MET | C-O | -5.42 | 1.17 | 1.24 |
| 10 | k5 | 995 | VAL | CA-CB | -5.42 | 1.47 | 1.54 |
| 4 | M9 | 185 | ALA | CA-C | -5.42 | 1.45 | 1.52 |
| 4 | M1 | 238 | MET | C-O | -5.42 | 1.17 | 1.24 |
| 4 | M4 | 40 | GLN | CA-CB | -5.42 | 1.45 | 1.53 |
| 10 | j5 | 905 | THR | CB-CG2 | -5.42 | 1.34 | 1.52 |
| 10 | k5 | 296 | VAL | CA-CB | -5.42 | 1.47 | 1.54 |
| 10 | k5 | 905 | THR | CB-CG2 | -5.42 | 1.34 | 1.52 |
| 10 | j5 | 434 | TRP | CB-CG | -5.42 | 1.33 | 1.50 |
| 10 | j5 | 552 | VAL | C-O | -5.42 | 1.18 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | k5 | 893 | ASN | CG-ND2 | -5.42 | 1.21 | 1.33 |
| 4 | M9 | 28 | HIS | C-O | -5.42 | 1.16 | 1.23 |
| 4 | M3 | 248 | SER | C-O | -5.42 | 1.17 | 1.23 |
| 10 | j5 | 226 | TYR | C-O | -5.42 | 1.17 | 1.24 |
| 10 | k5 | 492 | ILE | N-CA | -5.42 | 1.40 | 1.46 |
| 1 | h7 | 51 | ILE | CA-C | -5.42 | 1.45 | 1.52 |
| 4 | M8 | 163 | ASN | C-O | -5.41 | 1.17 | 1.24 |
| 10 | k5 | 1126 | ALA | CA-C | -5.41 | 1.46 | 1.52 |
| 4 | M1 | 67 | LEU | C-O | -5.41 | 1.16 | 1.23 |
| 10 | j5 | 454 | GLN | CA-CB | -5.41 | 1.45 | 1.53 |
| 10 | j5 | 701 | ASP | CA-C | -5.41 | 1.45 | 1.52 |
| 10 | k5 | 535 | PRO | CA-CB | -5.41 | 1.46 | 1.53 |
| 10 | k5 | 701 | ASP | CA-C | -5.41 | 1.45 | 1.52 |
| 10 | k5 | 824 | PRO | C-N | -5.41 | 1.26 | 1.33 |
| 4 | M8 | 40 | GLN | CA-CB | -5.41 | 1.45 | 1.53 |
| 5 | Z4 | 22 | LEU | CA-C | -5.41 | 1.45 | 1.52 |
| 10 | j5 | 576 | PHE | CG-CD1 | -5.41 | 1.27 | 1.38 |
| 10 | j5 | 658 | TYR | N-CA | -5.41 | 1.39 | 1.46 |
| 10 | k5 | 439 | ALA | CA-CB | -5.41 | 1.44 | 1.53 |
| 4 | M9 | 113 | ILE | C-O | -5.41 | 1.17 | 1.24 |
| 4 | MA | 163 | ASN | C-O | -5.41 | 1.17 | 1.24 |
| 4 | M3 | 113 | ILE | C-O | -5.41 | 1.17 | 1.24 |
| 8 | K5 | 108 | GLY | C-O | -5.41 | 1.16 | 1.23 |
| 8 | E5 | 106 | GLU | CA-C | -5.41 | 1.45 | 1.52 |
| 10 | j5 | 29 | ASN | CA-C | -5.41 | 1.45 | 1.52 |
| 10 | k5 | 29 | ASN | CA-C | -5.41 | 1.45 | 1.52 |
| 10 | k5 | 245 | ILE | C-O | -5.41 | 1.18 | 1.24 |
| 4 | M8 | 67 | LEU | C-O | -5.41 | 1.16 | 1.23 |
| 4 | M9 | 163 | ASN | C-O | -5.41 | 1.17 | 1.24 |
| 4 | M1 | 113 | ILE | C-O | -5.41 | 1.17 | 1.24 |
| 10 | k5 | 827 | LYS | CA-CB | -5.40 | 1.44 | 1.53 |
| 10 | k5 | 370 | GLU | CA-CB | -5.40 | 1.44 | 1.53 |
| 10 | k5 | 951 | MET | C-O | -5.40 | 1.17 | 1.24 |
| 8 | u7 | 47 | ARG | C-O | -5.40 | 1.17 | 1.24 |
| 10 | k5 | 21 | MET | C-O | -5.40 | 1.17 | 1.24 |
| 9 | i5 | 37 | TRP | CA-CB | -5.40 | 1.44 | 1.53 |
| 10 | k5 | 576 | PHE | CG-CD1 | -5.40 | 1.27 | 1.38 |
| 10 | k5 | 670 | TYR | CZ-OH | -5.40 | 1.26 | 1.38 |
| 11 | a9 | 320 | ASP | CA-C | -5.40 | 1.46 | 1.52 |
| 11 | a9 | 800 | THR | CA-C | -5.40 | 1.45 | 1.52 |
| 11 | aA | 320 | ASP | CA-C | -5.40 | 1.46 | 1.52 |
| 8 | a5 | 12 | ASP | CA-CB | -5.40 | 1.44 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | k5 | 552 | VAL | C-O | -5.40 | 1.18 | 1.24 |
| 10 | k5 | 924 | ASP | C-O | -5.40 | 1.17 | 1.23 |
| 4 | MA | 22 | SER | N-CA | -5.39 | 1.38 | 1.45 |
| 10 | k5 | 510 | ILE | CA-C | -5.39 | 1.46 | 1.52 |
| 10 | k5 | 627 | ILE | CA-C | -5.39 | 1.46 | 1.52 |
| 4 | M9 | 22 | SER | N-CA | -5.39 | 1.38 | 1.45 |
| 4 | M3 | 16 | LYS | CA-C | -5.39 | 1.46 | 1.52 |
| 4 | M8 | 238 | MET | C-O | -5.39 | 1.17 | 1.24 |
| 4 | M1 | 16 | LYS | CA-C | -5.39 | 1.46 | 1.52 |
| 10 | j5 | 627 | ILE | CA-C | -5.39 | 1.46 | 1.52 |
| 4 | M8 | 22 | SER | N-CA | -5.39 | 1.38 | 1.45 |
| 3 | LA | 113 | LEU | C-O | -5.39 | 1.17 | 1.24 |
| 8 | e5 | 12 | ASP | CA-CB | -5.39 | 1.44 | 1.53 |
| 10 | j5 | 370 | GLU | C-N | -5.39 | 1.26 | 1.33 |
| 10 | j5 | 797 | ASN | C-O | -5.39 | 1.16 | 1.24 |
| 10 | k5 | 198 | ALA | C-O | -5.39 | 1.17 | 1.24 |
| 10 | k5 | 797 | ASN | C-O | -5.39 | 1.16 | 1.24 |
| 3 | L9 | 113 | LEU | C-O | -5.39 | 1.17 | 1.24 |
| 10 | j5 | 505 | VAL | CA-C | -5.39 | 1.46 | 1.52 |
| 10 | j5 | 1008 | PHE | C-O | -5.39 | 1.17 | 1.24 |
| 10 | j5 | 893 | ASN | CA-CB | -5.39 | 1.44 | 1.53 |
| 10 | k5 | 406 | ILE | CA-C | -5.39 | 1.44 | 1.52 |
| 1 | b7 | 51 | ILE | CA-C | -5.39 | 1.45 | 1.52 |
| 5 | N9 | 22 | LEU | CA-C | -5.39 | 1.45 | 1.52 |
| 8 | K5 | 106 | GLU | CA-C | -5.38 | 1.45 | 1.52 |
| 10 | k5 | 530 | ALA | C-O | -5.38 | 1.17 | 1.24 |
| 10 | j5 | 1120 | PRO | CA-CB | -5.38 | 1.46 | 1.53 |
| 10 | k5 | 226 | TYR | C-O | -5.38 | 1.17 | 1.24 |
| 10 | k5 | 706 | PRO | CA-CB | -5.38 | 1.46 | 1.53 |
| 4 | MA | 16 | LYS | CA-C | -5.38 | 1.46 | 1.52 |
| 4 | MA | 246 | ALA | C-O | -5.38 | 1.16 | 1.24 |
| 4 | M3 | 180 | ASN | C-O | -5.38 | 1.17 | 1.23 |
| 4 | M1 | 180 | ASN | C-O | -5.38 | 1.17 | 1.23 |
| 4 | MA | 140 | ARG | C-O | -5.38 | 1.17 | 1.24 |
| 10 | j5 | 416 | GLY | CA-C | -5.38 | 1.44 | 1.51 |
| 10 | j5 | 530 | ALA | C-O | -5.38 | 1.17 | 1.24 |
| 4 | M9 | 140 | ARG | C-O | -5.38 | 1.17 | 1.24 |
| 11 | a9 | 523 | GLN | CA-CB | -5.38 | 1.45 | 1.53 |
| 11 | aA | 523 | GLN | CA-CB | -5.38 | 1.45 | 1.53 |
| 10 | j5 | 738 | TYR | CZ-OH | -5.38 | 1.26 | 1.38 |
| 10 | j5 | 828 | VAL | N-CA | -5.38 | 1.40 | 1.46 |
| 9 | y7 | 31 | LEU | C-O | -5.38 | 1.17 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4 | M9 | 16 | LYS | CA-C | -5.38 | 1.46 | 1.52 |
| 4 | MA | 28 | HIS | C-O | -5.38 | 1.16 | 1.23 |
| 10 | j5 | 439 | ALA | CA-CB | -5.38 | 1.44 | 1.53 |
| 4 | M3 | 246 | ALA | C-O | -5.38 | 1.16 | 1.24 |
| 10 | j5 | 370 | GLU | CA-CB | -5.38 | 1.44 | 1.53 |
| 10 | k5 | 893 | ASN | CA-CB | -5.38 | 1.44 | 1.53 |
| 10 | j5 | 492 | ILE | N-CA | -5.37 | 1.40 | 1.46 |
| 10 | j5 | 751 | LYS | CA-C | -5.37 | 1.46 | 1.52 |
| 10 | k5 | 1120 | PRO | CA-CB | -5.37 | 1.46 | 1.53 |
| 8 | K7 | 97 | VAL | CA-CB | 5.37 | 1.61 | 1.54 |
| 4 | M9 | 246 | ALA | C-O | -5.37 | 1.16 | 1.24 |
| 10 | j5 | 398 | LEU | N-CA | -5.37 | 1.39 | 1.46 |
| 10 | j5 | 720 | ASP | CB-CG | -5.37 | 1.38 | 1.52 |
| 10 | k5 | 373 | ALA | CA-CB | -5.37 | 1.44 | 1.53 |
| 10 | k5 | 398 | LEU | N-CA | -5.37 | 1.39 | 1.46 |
| 10 | k5 | 462 | TYR | CA-CB | -5.37 | 1.44 | 1.53 |
| 11 | aA | 800 | THR | CA-C | -5.37 | 1.45 | 1.52 |
| 10 | j5 | 373 | ALA | CA-CB | -5.37 | 1.44 | 1.53 |
| 10 | j5 | 768 | VAL | CA-CB | -5.37 | 1.47 | 1.54 |
| 10 | j5 | 1098 | GLU | C-O | -5.37 | 1.16 | 1.24 |
| 10 | k5 | 768 | VAL | CA-CB | -5.37 | 1.47 | 1.54 |
| 10 | k5 | 1098 | GLU | C-O | -5.37 | 1.16 | 1.24 |
| 1 | b7 | 47 | ASN | CA-C | -5.37 | 1.45 | 1.52 |
| 4 | M8 | 92 | GLU | C-O | -5.37 | 1.18 | 1.24 |
| 9 | z5 | 35 | GLU | C-O | -5.37 | 1.16 | 1.24 |
| 10 | k5 | 902 | ASN | N-CA | -5.37 | 1.40 | 1.46 |
| 8 | C5 | 4 | LEU | N-CA | -5.37 | 1.40 | 1.46 |
| 10 | k5 | 11 | VAL | CA-CB | -5.37 | 1.47 | 1.54 |
| 8 | I5 | 14 | GLU | CA-C | -5.36 | 1.45 | 1.52 |
| 10 | j5 | 445 | TYR | CE1-CZ | -5.36 | 1.25 | 1.38 |
| 10 | k5 | 177 | SER | C-O | -5.36 | 1.17 | 1.24 |
| 10 | k5 | 445 | TYR | CE1-CZ | -5.36 | 1.25 | 1.38 |
| 8 | c7 | 97 | VAL | CA-CB | 5.36 | 1.61 | 1.54 |
| 11 | a9 | 508 | ARG | C-O | -5.36 | 1.16 | 1.24 |
| 11 | aA | 508 | ARG | C-O | -5.36 | 1.16 | 1.24 |
| 8 | I5 | 4 | LEU | N-CA | -5.36 | 1.40 | 1.46 |
| 10 | j5 | 802 | VAL | CA-CB | -5.36 | 1.46 | 1.54 |
| 10 | j5 | 827 | LYS | N-CA | -5.36 | 1.39 | 1.46 |
| 10 | k5 | 642 | ARG | CA-CB | -5.36 | 1.44 | 1.53 |
| 10 | k5 | 827 | LYS | N-CA | -5.36 | 1.39 | 1.46 |
| 4 | M1 | 246 | ALA | C-O | -5.36 | 1.16 | 1.24 |
| 4 | M4 | 144 | ARG | C-O | -5.36 | 1.17 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | k5 | 505 | VAL | CA-C | -5.36 | 1.46 | 1.52 |
| 10 | k5 | 1103 | LEU | CA-C | -5.36 | 1.45 | 1.52 |
| 4 | MA | 113 | ILE | C-O | -5.36 | 1.17 | 1.24 |
| 10 | j5 | 938 | GLN | C-O | -5.36 | 1.17 | 1.24 |
| 10 | k5 | 641 | ASP | CA-CB | -5.36 | 1.44 | 1.53 |
| 10 | k5 | 938 | GLN | C-O | -5.36 | 1.17 | 1.24 |
| 10 | k5 | 719 | MET | CA-CB | -5.36 | 1.44 | 1.53 |
| 10 | j5 | 839 | ARG | CA-CB | -5.35 | 1.46 | 1.53 |
| 10 | k5 | 839 | ARG | CA-CB | -5.35 | 1.46 | 1.53 |
| 4 | MA | 51 | ARG | CA-C | -5.35 | 1.45 | 1.52 |
| 10 | j5 | 531 | THR | CA-C | -5.35 | 1.45 | 1.53 |
| 4 | M8 | 16 | LYS | CA-C | -5.35 | 1.46 | 1.52 |
| 4 | M9 | 51 | ARG | CA-C | -5.35 | 1.45 | 1.52 |
| 4 | M3 | 67 | LEU | C-O | -5.35 | 1.16 | 1.23 |
| 9 | i5 | 35 | GLU | C-O | -5.35 | 1.16 | 1.24 |
| 10 | k5 | 1094 | ASP | C-O | -5.35 | 1.17 | 1.24 |
| 4 | M8 | 14 | LEU | N-CA | -5.35 | 1.39 | 1.46 |
| 9 | x7 | 31 | LEU | CA-C | -5.35 | 1.45 | 1.52 |
| 4 | M4 | 113 | ILE | C-O | -5.34 | 1.17 | 1.24 |
| 10 | j5 | 856 | ARG | CA-CB | -5.34 | 1.44 | 1.53 |
| 10 | j5 | 462 | TYR | CA-CB | -5.34 | 1.44 | 1.53 |
| 10 | k5 | 372 | ARG | CZ-NH1 | -5.34 | 1.25 | 1.32 |
| 10 | k5 | 416 | GLY | C-O | -5.34 | 1.16 | 1.23 |
| 8 | o7 | 160 | MET | CA-C | -5.34 | 1.45 | 1.52 |
| 4 | M8 | 51 | ARG | CA-C | -5.34 | 1.45 | 1.52 |
| 11 | a9 | 492 | SER | CA-C | -5.34 | 1.46 | 1.52 |
| 11 | aA | 492 | SER | CA-C | -5.34 | 1.46 | 1.52 |
| 10 | j5 | 56 | ILE | C-O | -5.34 | 1.18 | 1.24 |
| 10 | j5 | 297 | VAL | C-O | -5.34 | 1.16 | 1.24 |
| 10 | j5 | 719 | MET | CA-CB | -5.34 | 1.44 | 1.53 |
| 10 | j5 | 827 | LYS | CA-CB | -5.34 | 1.44 | 1.53 |
| 10 | k5 | 297 | VAL | C-O | -5.34 | 1.16 | 1.24 |
| 8 | E7 | 97 | VAL | CA-CB | 5.34 | 1.61 | 1.54 |
| 4 | M4 | 246 | ALA | C-O | -5.34 | 1.16 | 1.24 |
| 10 | j5 | 476 | ASN | CA-CB | -5.34 | 1.44 | 1.53 |
| 8 | u7 | 160 | MET | CA-C | -5.34 | 1.45 | 1.52 |
| 8 | e7 | 123 | ILE | CA-CB | 5.33 | 1.57 | 1.54 |
| 4 | MA | 185 | ALA | C-O | -5.33 | 1.17 | 1.24 |
| 10 | j5 | 578 | ARG | CZ-NH2 | -5.33 | 1.26 | 1.33 |
| 10 | j5 | 783 | TYR | CB-CG | -5.33 | 1.40 | 1.51 |
| 10 | k5 | 472 | TYR | CA-CB | -5.33 | 1.44 | 1.53 |
| 10 | k5 | 783 | TYR | CB-CG | -5.33 | 1.40 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4 | M9 | 185 | ALA | C-O | -5.33 | 1.17 | 1.24 |
| 10 | j5 | 616 | LEU | N-CA | -5.33 | 1.39 | 1.46 |
| 10 | k5 | 616 | LEU | N-CA | -5.33 | 1.39 | 1.46 |
| 9 | x7 | 19 | THR | CA-C | -5.33 | 1.45 | 1.52 |
| 4 | M3 | 7 | SER | C-O | 5.33 | 1.30 | 1.24 |
| 8 | G5 | 48 | GLU | CA-C | -5.33 | 1.46 | 1.52 |
| 10 | j5 | 706 | PRO | CA-CB | -5.33 | 1.46 | 1.53 |
| 10 | k5 | 691 | SER | CA-CB | -5.33 | 1.44 | 1.53 |
| 11 | a9 | 495 | TYR | CA-C | -5.33 | 1.46 | 1.52 |
| 4 | M1 | 7 | SER | C-O | 5.33 | 1.30 | 1.24 |
| 9 | z5 | 22 | GLU | N-CA | -5.33 | 1.40 | 1.46 |
| 10 | j5 | 511 | ARG | NE-CZ | -5.33 | 1.27 | 1.33 |
| 10 | j5 | 1126 | ALA | CA-C | -5.33 | 1.46 | 1.52 |
| 10 | k5 | 511 | ARG | NE-CZ | -5.33 | 1.27 | 1.33 |
| 10 | k5 | 802 | VAL | CA-CB | -5.33 | 1.46 | 1.54 |
| 9 | y7 | 24 | GLN | C-O | -5.33 | 1.17 | 1.24 |
| 11 | a9 | 805 | GLN | C-O | -5.33 | 1.17 | 1.24 |
| 11 | aA | 805 | GLN | C-O | -5.33 | 1.17 | 1.24 |
| 4 | M4 | 51 | ARG | N-CA | -5.32 | 1.39 | 1.46 |
| 8 | C5 | 14 | GLU | CA-C | -5.32 | 1.45 | 1.52 |
| 10 | j5 | 677 | ASP | N-CA | -5.32 | 1.39 | 1.46 |
| 10 | j5 | 885 | GLN | CD-OE1 | -5.32 | 1.13 | 1.23 |
| 10 | k5 | 531 | THR | CA-C | -5.32 | 1.45 | 1.53 |
| 10 | k5 | 962 | ALA | CA-C | -5.32 | 1.45 | 1.52 |
| 8 | Q5 | 97 | VAL | CA-CB | 5.32 | 1.61 | 1.54 |
| 4 | M4 | 22 | SER | N-CA | -5.32 | 1.38 | 1.45 |
| 10 | j5 | 641 | ASP | CA-CB | -5.32 | 1.44 | 1.53 |
| 10 | k5 | 751 | LYS | CA-C | -5.32 | 1.46 | 1.52 |
| 9 | x7 | 24 | GLN | C-O | -5.32 | 1.17 | 1.24 |
| 4 | M8 | 113 | ILE | C-O | -5.32 | 1.17 | 1.24 |
| 4 | M4 | 51 | ARG | CA-C | -5.32 | 1.45 | 1.52 |
| 8 | G5 | 63 | PRO | C-O | -5.32 | 1.17 | 1.24 |
| 10 | k5 | 476 | ASN | CA-CB | -5.32 | 1.44 | 1.53 |
| 8 | i7 | 97 | VAL | CA-CB | 5.32 | 1.61 | 1.54 |
| 10 | j5 | 579 | GLN | CA-C | -5.31 | 1.45 | 1.53 |
| 10 | j5 | 902 | ASN | N-CA | -5.31 | 1.40 | 1.46 |
| 10 | k5 | 981 | ILE | CA-CB | -5.31 | 1.47 | 1.54 |
| 11 | a9 | 37 | GLY | C-O | -5.31 | 1.16 | 1.23 |
| 11 | aA | 37 | GLY | C-O | -5.31 | 1.16 | 1.23 |
| 9 | i5 | 22 | GLU | N-CA | -5.31 | 1.40 | 1.46 |
| 11 | a9 | 511 | LYS | CA-C | -5.31 | 1.46 | 1.52 |
| 11 | aA | 511 | LYS | CA-C | -5.31 | 1.46 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4 | M4 | 16 | LYS | CA-C | -5.31 | 1.46 | 1.52 |
| 4 | M3 | 51 | ARG | N-CA | -5.31 | 1.39 | 1.46 |
| 8 | E5 | 78 | THR | C-O | -5.31 | 1.17 | 1.24 |
| 8 | W5 | 97 | VAL | CA-CB | 5.31 | 1.61 | 1.54 |
| 10 | j5 | 970 | GLY | CA-C | -5.31 | 1.44 | 1.51 |
| 10 | k5 | 856 | ARG | CA-CB | -5.31 | 1.44 | 1.53 |
| 10 | k5 | 970 | GLY | CA-C | -5.31 | 1.44 | 1.51 |
| 1 | h7 | 47 | ASN | CA-C | -5.31 | 1.45 | 1.52 |
| 4 | M1 | 51 | ARG | N-CA | -5.31 | 1.39 | 1.46 |
| 4 | M3 | 22 | SER | N-CA | -5.31 | 1.38 | 1.45 |
| 10 | j5 | 372 | ARG | CZ-NH1 | -5.31 | 1.25 | 1.32 |
| 10 | k5 | 885 | GLN | CD-OE1 | -5.31 | 1.13 | 1.23 |
| 1 | h7 | 43 | VAL | CA-C | -5.31 | 1.46 | 1.52 |
| 4 | M1 | 22 | SER | N-CA | -5.31 | 1.38 | 1.45 |
| 4 | M4 | 180 | ASN | C-O | -5.30 | 1.17 | 1.23 |
| 8 | M5 | 97 | VAL | CA-CB | 5.30 | 1.61 | 1.54 |
| 10 | j5 | 265 | SER | CA-C | -5.30 | 1.45 | 1.52 |
| 10 | j5 | 772 | TYR | CA-C | -5.30 | 1.45 | 1.52 |
| 1 | b7 | 43 | VAL | CA-C | -5.30 | 1.46 | 1.52 |
| 4 | M9 | 7 | SER | C-O | 5.30 | 1.30 | 1.24 |
| 4 | MA | 51 | ARG | N-CA | -5.30 | 1.39 | 1.46 |
| 10 | j5 | 585 | ARG | CA-C | -5.30 | 1.46 | 1.52 |
| 4 | M9 | 51 | ARG | N-CA | -5.30 | 1.39 | 1.46 |
| 10 | j5 | 11 | VAL | CA-CB | -5.30 | 1.47 | 1.54 |
| 10 | k5 | 370 | GLU | C-N | -5.30 | 1.26 | 1.33 |
| 10 | k5 | 720 | ASP | CB-CG | -5.30 | 1.38 | 1.52 |
| 11 | a9 | 527 | LEU | C-O | -5.30 | 1.18 | 1.24 |
| 11 | aA | 527 | LEU | C-O | -5.30 | 1.18 | 1.24 |
| 10 | j5 | 1094 | ASP | C-O | -5.30 | 1.17 | 1.24 |
| 3 | LA | 84 | ARG | C-O | -5.30 | 1.17 | 1.24 |
| 10 | j5 | 642 | ARG | CA-CB | -5.30 | 1.44 | 1.53 |
| 3 | L9 | 84 | ARG | C-O | -5.30 | 1.17 | 1.24 |
| 10 | j5 | 416 | GLY | C-O | -5.29 | 1.16 | 1.23 |
| 8 | K5 | 131 | ARG | C-O | -5.29 | 1.17 | 1.24 |
| 4 | M8 | 185 | ALA | C-O | -5.29 | 1.17 | 1.24 |
| 10 | j5 | 997 | ILE | CA-C | -5.29 | 1.46 | 1.52 |
| 10 | k5 | 973 | THR | C-O | -5.29 | 1.17 | 1.24 |
| 10 | k5 | 997 | ILE | CA-C | -5.29 | 1.46 | 1.52 |
| 4 | M9 | 215 | GLU | C-O | -5.29 | 1.17 | 1.24 |
| 4 | MA | 180 | ASN | C-O | -5.29 | 1.17 | 1.23 |
| 10 | k5 | 1045 | TYR | CA-C | -5.29 | 1.45 | 1.52 |
| 8 | o7 | 53 | GLN | C-O | -5.29 | 1.17 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4 | M9 | 180 | ASN | C-O | -5.29 | 1.17 | 1.23 |
| 8 | A5 | 63 | PRO | C-O | -5.29 | 1.17 | 1.24 |
| 10 | j5 | 160 | LEU | C-O | -5.29 | 1.18 | 1.24 |
| 10 | k5 | 854 | LEU | CA-CB | -5.29 | 1.45 | 1.53 |
| 11 | a9 | 461 | GLY | C-O | -5.29 | 1.18 | 1.24 |
| 11 | aA | 461 | GLY | C-O | -5.29 | 1.18 | 1.24 |
| 11 | aA | 495 | TYR | CA-C | -5.29 | 1.46 | 1.52 |
| 10 | k5 | 677 | ASP | N-CA | -5.29 | 1.39 | 1.46 |
| 4 | M3 | 185 | ALA | C-O | -5.29 | 1.17 | 1.24 |
| 4 | M4 | 14 | LEU | N-CA | -5.29 | 1.39 | 1.46 |
| 4 | M1 | 185 | ALA | C-O | -5.29 | 1.17 | 1.24 |
| 10 | j5 | 848 | ILE | CA-CB | -5.28 | 1.47 | 1.54 |
| 10 | k5 | 56 | ILE | C-O | -5.28 | 1.18 | 1.24 |
| 10 | k5 | 792 | GLU | N-CA | -5.28 | 1.40 | 1.46 |
| 9 | y7 | 19 | THR | CA-C | -5.28 | 1.45 | 1.52 |
| 10 | j5 | 180 | GLU | C-O | -5.28 | 1.17 | 1.24 |
| 10 | k5 | 180 | GLU | C-O | -5.28 | 1.17 | 1.24 |
| 10 | k5 | 416 | GLY | CA-C | -5.28 | 1.44 | 1.51 |
| 10 | j5 | 785 | ARG | C-O | -5.28 | 1.17 | 1.23 |
| 10 | k5 | 772 | TYR | N-CA | -5.28 | 1.39 | 1.46 |
| 10 | k5 | 785 | ARG | C-O | -5.28 | 1.17 | 1.23 |
| 4 | M1 | 215 | GLU | C-O | -5.28 | 1.17 | 1.24 |
| 10 | j5 | 328 | ILE | C-O | -5.28 | 1.18 | 1.24 |
| 10 | j5 | 602 | GLU | CA-CB | -5.28 | 1.44 | 1.53 |
| 10 | k5 | 328 | ILE | C-O | -5.28 | 1.18 | 1.24 |
| 10 | j5 | 397 | GLY | N-CA | -5.28 | 1.37 | 1.45 |
| 10 | j5 | 692 | LEU | CA-C | -5.28 | 1.45 | 1.52 |
| 10 | j5 | 770 | ALA | CA-C | -5.28 | 1.45 | 1.52 |
| 10 | k5 | 397 | GLY | N-CA | -5.28 | 1.37 | 1.45 |
| 10 | k5 | 578 | ARG | CZ-NH2 | -5.28 | 1.26 | 1.33 |
| 10 | k5 | 803 | LYS | CA-CB | -5.28 | 1.44 | 1.53 |
| 8 | u7 | 53 | GLN | C-O | -5.28 | 1.17 | 1.24 |
| 8 | C5 | 14 | GLU | C-O | -5.27 | 1.17 | 1.24 |
| 10 | k5 | 11 | VAL | C-O | -5.27 | 1.17 | 1.24 |
| 10 | j5 | 401 | LEU | CA-C | -5.27 | 1.46 | 1.52 |
| 10 | j5 | 538 | PHE | N-CA | -5.27 | 1.39 | 1.46 |
| 10 | k5 | 401 | LEU | CA-C | -5.27 | 1.46 | 1.52 |
| 10 | k5 | 538 | PHE | N-CA | -5.27 | 1.39 | 1.46 |
| 10 | k5 | 692 | LEU | CA-C | -5.27 | 1.45 | 1.52 |
| 10 | j5 | 733 | SER | CB-OG | -5.27 | 1.31 | 1.42 |
| 4 | M3 | 14 | LEU | N-CA | -5.27 | 1.39 | 1.46 |
| 10 | j5 | 271 | THR | C-O | -5.27 | 1.17 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | j5 | 298 | ARG | CA-C | -5.27 | 1.45 | 1.52 |
| 10 | j5 | 691 | SER | CA-CB | -5.27 | 1.44 | 1.53 |
| 10 | j5 | 977 | GLN | C-O | -5.27 | 1.17 | 1.24 |
| 10 | j5 | 1100 | PRO | C-O | -5.27 | 1.17 | 1.24 |
| 10 | k5 | 298 | ARG | CA-C | -5.27 | 1.45 | 1.52 |
| 10 | k5 | 977 | GLN | C-O | -5.27 | 1.17 | 1.24 |
| 10 | k5 | 1100 | PRO | C-O | -5.27 | 1.17 | 1.24 |
| 10 | k5 | 317 | SER | C-O | -5.27 | 1.18 | 1.24 |
| 8 | i7 | 114 | GLU | C-O | -5.27 | 1.17 | 1.24 |
| 4 | M1 | 14 | LEU | N-CA | -5.27 | 1.39 | 1.46 |
| 4 | M4 | 185 | ALA | C-O | -5.27 | 1.17 | 1.24 |
| 10 | j5 | 883 | SER | CA-CB | -5.27 | 1.44 | 1.53 |
| 10 | j5 | 854 | LEU | CA-CB | -5.26 | 1.45 | 1.53 |
| 3 | LA | 86 | MET | CA-C | -5.26 | 1.46 | 1.52 |
| 4 | MA | 41 | ASN | CA-CB | -5.26 | 1.45 | 1.53 |
| 10 | j5 | 982 | TYR | C-O | -5.26 | 1.17 | 1.24 |
| 3 | L9 | 86 | MET | CA-C | -5.26 | 1.46 | 1.52 |
| 4 | M9 | 41 | ASN | CA-CB | -5.26 | 1.45 | 1.53 |
| 4 | MA | 215 | GLU | C-O | -5.26 | 1.17 | 1.24 |
| 8 | K5 | 78 | THR | C-O | -5.26 | 1.17 | 1.24 |
| 10 | j5 | 1045 | TYR | CA-C | -5.26 | 1.45 | 1.52 |
| 4 | M3 | 215 | GLU | C-O | -5.26 | 1.17 | 1.24 |
| 8 | A5 | 51 | VAL | CA-C | -5.26 | 1.46 | 1.52 |
| 4 | M8 | 7 | SER | C-O | 5.26 | 1.30 | 1.24 |
| 8 | A5 | 48 | GLU | CA-C | -5.26 | 1.46 | 1.52 |
| 4 | M8 | 180 | ASN | C-O | -5.26 | 1.17 | 1.23 |
| 8 | I5 | 14 | GLU | C-O | -5.25 | 1.17 | 1.24 |
| 10 | j5 | 792 | GLU | N-CA | -5.25 | 1.40 | 1.46 |
| 10 | k5 | 7 | SER | CA-C | -5.25 | 1.45 | 1.52 |
| 8 | I5 | 6 | LYS | C-O | -5.25 | 1.15 | 1.23 |
| 10 | j5 | 517 | SER | N-CA | -5.25 | 1.40 | 1.46 |
| 10 | j5 | 572 | TYR | C-N | -5.25 | 1.25 | 1.33 |
| 10 | k5 | 420 | VAL | CA-CB | -5.25 | 1.47 | 1.54 |
| 10 | k5 | 517 | SER | N-CA | -5.25 | 1.40 | 1.46 |
| 10 | k5 | 572 | TYR | C-N | -5.25 | 1.25 | 1.33 |
| 10 | k5 | 883 | SER | CA-CB | -5.25 | 1.44 | 1.53 |
| 8 | Q7 | 97 | VAL | CA-CB | 5.25 | 1.61 | 1.54 |
| 10 | j5 | 367 | ARG | CZ-NH2 | -5.25 | 1.26 | 1.33 |
| 10 | k5 | 367 | ARG | CZ-NH2 | -5.25 | 1.26 | 1.33 |
| 4 | M8 | 51 | ARG | N-CA | -5.25 | 1.39 | 1.46 |
| 11 | a9 | 327 | SER | C-O | -5.25 | 1.18 | 1.24 |
| 11 | aA | 327 | SER | C-O | -5.25 | 1.18 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 5 | Z8 | 26 | LEU | N-CA | -5.25 | 1.39 | 1.45 |
| 4 | MA | 234 | SER | N-CA | -5.25 | 1.39 | 1.46 |
| 10 | k5 | 372 | ARG | CZ-NH2 | -5.25 | 1.26 | 1.33 |
| 4 | M9 | 234 | SER | N-CA | -5.25 | 1.39 | 1.46 |
| 8 | E5 | 131 | ARG | C-O | -5.24 | 1.17 | 1.24 |
| 10 | k5 | 265 | SER | CA-C | -5.24 | 1.45 | 1.52 |
| 10 | k5 | 537 | ILE | N-CA | -5.24 | 1.39 | 1.46 |
| 10 | k5 | 772 | TYR | CA-C | -5.24 | 1.45 | 1.52 |
| 4 | MA | 7 | SER | C-O | 5.24 | 1.30 | 1.24 |
| 10 | j5 | 372 | ARG | CZ-NH2 | -5.24 | 1.26 | 1.33 |
| 10 | j5 | 962 | ALA | CA-C | -5.24 | 1.45 | 1.52 |
| 10 | k5 | 733 | SER | CB-OG | -5.24 | 1.31 | 1.42 |
| 4 | M4 | 234 | SER | N-CA | -5.24 | 1.39 | 1.46 |
| 8 | S5 | 97 | VAL | CA-CB | 5.24 | 1.61 | 1.54 |
| 10 | j5 | 7 | SER | CA-CB | -5.24 | 1.45 | 1.53 |
| 10 | j5 | 973 | THR | C-O | -5.24 | 1.17 | 1.24 |
| 10 | k5 | 271 | THR | C-O | -5.24 | 1.17 | 1.23 |
| 8 | C5 | 8 | ILE | CA-CB | -5.24 | 1.47 | 1.54 |
| 8 | W5 | 160 | MET | N-CA | -5.24 | 1.39 | 1.46 |
| 10 | j5 | 226 | TYR | CA-C | -5.24 | 1.46 | 1.52 |
| 10 | j5 | 772 | TYR | N-CA | -5.24 | 1.39 | 1.46 |
| 10 | k5 | 160 | LEU | C-O | -5.24 | 1.18 | 1.24 |
| 10 | k5 | 1023 | SER | CB-OG | 5.24 | 1.52 | 1.42 |
| 10 | j5 | 472 | TYR | CA-CB | -5.23 | 1.44 | 1.53 |
| 10 | k5 | 462 | TYR | CZ-OH | -5.23 | 1.27 | 1.38 |
| 11 | a9 | 43 | GLU | C-O | -5.23 | 1.17 | 1.23 |
| 11 | aA | 43 | GLU | C-O | -5.23 | 1.17 | 1.23 |
| 10 | j5 | 758 | ALA | CA-C | -5.23 | 1.46 | 1.52 |
| 10 | j5 | 946 | ASP | CA-C | -5.23 | 1.46 | 1.53 |
| 10 | k5 | 585 | ARG | CA-C | -5.23 | 1.46 | 1.52 |
| 8 | q7 | 97 | VAL | CA-CB | 5.23 | 1.61 | 1.54 |
| 4 | M4 | 7 | SER | C-O | 5.23 | 1.30 | 1.24 |
| 10 | j5 | 859 | ILE | CA-C | -5.23 | 1.45 | 1.52 |
| 10 | k5 | 859 | ILE | CA-C | -5.23 | 1.45 | 1.52 |
| 8 | c7 | 114 | GLU | C-O | -5.23 | 1.17 | 1.24 |
| 4 | M8 | 234 | SER | N-CA | -5.23 | 1.39 | 1.46 |
| 4 | MA | 14 | LEU | N-CA | -5.23 | 1.39 | 1.46 |
| 10 | k5 | 946 | ASP | CA-C | -5.23 | 1.46 | 1.53 |
| 4 | M9 | 14 | LEU | N-CA | -5.23 | 1.39 | 1.46 |
| 10 | j5 | 508 | ILE | CA-CB | -5.23 | 1.48 | 1.54 |
| 10 | j5 | 840 | ALA | CA-CB | -5.23 | 1.45 | 1.53 |
| 10 | j5 | 997 | ILE | CA-CB | -5.23 | 1.48 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10 | j5 | 1023 | SER | CB-OG | 5.23 | 1.52 | 1.42 |
| 10 | k5 | 508 | ILE | CA-CB | -5.23 | 1.48 | 1.54 |
| 10 | k5 | 997 | ILE | CA-CB | -5.23 | 1.48 | 1.54 |
| 10 | k5 | 840 | ALA | CA-CB | -5.23 | 1.45 | 1.53 |
| 8 | Y5 | 97 | VAL | CA-CB | 5.22 | 1.61 | 1.54 |
| 5 | NA | 26 | LEU | N-CA | -5.22 | 1.39 | 1.45 |
| 10 | j5 | 682 | GLU | CG-CD | -5.22 | 1.39 | 1.52 |
| 10 | j5 | 884 | TRP | CA-C | -5.22 | 1.46 | 1.52 |
| 10 | k5 | 884 | TRP | CA-C | -5.22 | 1.46 | 1.52 |
| 8 | u7 | 97 | VAL | CA-CB | 5.22 | 1.61 | 1.54 |
| 5 | N9 | 26 | LEU | N-CA | -5.22 | 1.39 | 1.45 |
| 10 | k5 | 226 | TYR | CA-C | -5.22 | 1.46 | 1.52 |
| 10 | k5 | 579 | GLN | CA-C | -5.22 | 1.45 | 1.53 |
| 10 | k5 | 816 | ARG | CA-CB | -5.22 | 1.45 | 1.53 |
| 8 | i7 | 125 | ALA | CA-C | -5.22 | 1.46 | 1.52 |
| 8 | o7 | 97 | VAL | CA-CB | 5.22 | 1.61 | 1.54 |
| 10 | j5 | 981 | ILE | CA-CB | -5.22 | 1.47 | 1.54 |
| 10 | j5 | 1102 | TYR | C-O | -5.22 | 1.18 | 1.24 |
| 10 | k5 | 1102 | TYR | C-O | -5.22 | 1.18 | 1.24 |
| 10 | j5 | 537 | ILE | N-CA | -5.21 | 1.39 | 1.46 |
| 10 | k5 | 770 | ALA | CA-C | -5.21 | 1.45 | 1.52 |
| 10 | k5 | 848 | ILE | CA-CB | -5.21 | 1.48 | 1.54 |
| 10 | j5 | 939 | GLN | CA-C | -5.21 | 1.46 | 1.52 |
| 10 | k5 | 682 | GLU | CG-CD | -5.21 | 1.39 | 1.52 |
| 10 | k5 | 939 | GLN | CA-C | -5.21 | 1.46 | 1.52 |
| 8 | Q5 | 160 | MET | N-CA | -5.21 | 1.39 | 1.46 |
| 10 | j5 | 542 | GLN | C-O | -5.21 | 1.17 | 1.23 |
| 10 | j5 | 1027 | ASN | N-CA | -5.21 | 1.39 | 1.46 |
| 10 | k5 | 542 | GLN | C-O | -5.21 | 1.17 | 1.23 |
| 10 | k5 | 10 | THR | CA-C | -5.21 | 1.48 | 1.53 |
| 10 | k5 | 602 | GLU | CA-CB | -5.21 | 1.44 | 1.53 |
| 4 | M4 | 222 | ARG | CA-C | -5.21 | 1.47 | 1.52 |
| 10 | j5 | 195 | SER | CA-C | -5.21 | 1.46 | 1.52 |
| 10 | j5 | 1103 | LEU | C-O | -5.21 | 1.18 | 1.24 |
| 10 | k5 | 195 | SER | CA-C | -5.21 | 1.46 | 1.52 |
| 10 | k5 | 1103 | LEU | C-O | -5.21 | 1.18 | 1.24 |
| 1 | h7 | 50 | THR | CA-C | -5.21 | 1.46 | 1.52 |
| 9 | z7 | 58 | THR | N-CA | -5.21 | 1.40 | 1.46 |
| 11 | a9 | 776 | TYR | C-O | -5.21 | 1.18 | 1.24 |
| 10 | j5 | 1103 | LEU | CA-C | -5.21 | 1.46 | 1.52 |
| 10 | j5 | 816 | ARG | CA-CB | -5.20 | 1.45 | 1.53 |
| 8 | u7 | 38 | ARG | C-O | -5.20 | 1.18 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 11 | a9 | 420 | ASN | CG-OD1 | -5.20 | 1.13 | 1.23 |
| 11 | aA | 420 | ASN | CG-OD1 | -5.20 | 1.13 | 1.23 |
| 5 | N3 | 26 | LEU | N-CA | -5.20 | 1.39 | 1.45 |
| 1 | J5 | 6 | THR | CB-CG2 | -5.20 | 1.35 | 1.52 |
| 8 | e5 | 22 | GLU | CA-C | -5.20 | 1.45 | 1.52 |
| 10 | k5 | 758 | ALA | CA-C | -5.20 | 1.46 | 1.52 |
| 10 | k5 | 1135 | LEU | CA-C | -5.20 | 1.46 | 1.53 |
| 5 | N1 | 26 | LEU | N-CA | -5.20 | 1.39 | 1.45 |
| 8 | I5 | 8 | ILE | CA-CB | -5.20 | 1.47 | 1.54 |
| 10 | j5 | 803 | LYS | CA-CB | -5.20 | 1.44 | 1.53 |
| 9 | z7 | 35 | GLU | C-O | -5.20 | 1.17 | 1.24 |
| 10 | j5 | 11 | VAL | C-O | -5.20 | 1.17 | 1.24 |
| 10 | j5 | 574 | GLN | CD-NE2 | -5.20 | 1.22 | 1.33 |
| 10 | j5 | 1133 | GLU | CA-C | -5.20 | 1.45 | 1.52 |
| 10 | k5 | 574 | GLN | CD-NE2 | -5.20 | 1.22 | 1.33 |
| 11 | a9 | 582 | MET | C-O | -5.20 | 1.17 | 1.24 |
| 11 | aA | 582 | MET | C-O | -5.20 | 1.17 | 1.24 |
| 10 | j5 | 462 | TYR | CZ-OH | -5.20 | 1.27 | 1.38 |
| 10 | k5 | 629 | TYR | CA-CB | -5.20 | 1.45 | 1.53 |
| 4 | M8 | 245 | ASP | C-O | -5.20 | 1.18 | 1.24 |
| 1 | F5 | 10 | ASN | CA-C | -5.19 | 1.46 | 1.52 |
| 8 | G5 | 51 | VAL | CA-C | -5.19 | 1.46 | 1.52 |
| 4 | MA | 164 | ARG | C-O | -5.19 | 1.18 | 1.24 |
| 10 | j5 | 4 | ARG | CA-C | -5.19 | 1.45 | 1.52 |
| 10 | j5 | 457 | THR | CB-OG1 | -5.19 | 1.35 | 1.43 |
| 10 | k5 | 457 | THR | CB-OG1 | -5.19 | 1.35 | 1.43 |
| 10 | k5 | 913 | VAL | N-CA | -5.19 | 1.40 | 1.46 |
| 4 | M9 | 164 | ARG | C-O | -5.19 | 1.18 | 1.24 |
| 4 | M3 | 234 | SER | N-CA | -5.19 | 1.39 | 1.46 |
| 8 | C5 | 6 | LYS | C-O | -5.19 | 1.15 | 1.23 |
| 4 | M1 | 234 | SER | N-CA | -5.19 | 1.39 | 1.46 |
| 4 | M3 | 41 | ASN | CA-CB | -5.19 | 1.45 | 1.53 |
| 10 | j5 | 863 | ILE | C-N | -5.19 | 1.27 | 1.33 |
| 10 | k5 | 863 | ILE | C-N | -5.19 | 1.27 | 1.33 |
| 4 | M1 | 41 | ASN | CA-CB | -5.19 | 1.45 | 1.53 |
| 10 | j5 | 317 | SER | C-O | -5.19 | 1.18 | 1.24 |
| 10 | j5 | 728 | PRO | N-CA | -5.19 | 1.40 | 1.47 |
| 10 | j5 | 913 | VAL | N-CA | -5.19 | 1.40 | 1.46 |
| 9 | i5 | 60 | VAL | C-O | -5.18 | 1.18 | 1.24 |
| 10 | j5 | 897 | SER | CB-OG | -5.18 | 1.31 | 1.42 |
| 10 | k5 | 728 | PRO | N-CA | -5.18 | 1.40 | 1.47 |
| 10 | k5 | 897 | SER | CB-OG | -5.18 | 1.31 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 9 | z7 | 36 | ASN | N-CA | -5.18 | 1.40 | 1.46 |
| 10 | j5 | 526 | MET | N-CA | -5.18 | 1.39 | 1.46 |
| 10 | j5 | 680 | PRO | CA-CB | -5.18 | 1.46 | 1.53 |
| 10 | k5 | 433 | SER | CA-CB | -5.18 | 1.45 | 1.53 |
| 10 | k5 | 982 | TYR | C-O | -5.18 | 1.17 | 1.24 |
| 8 | a5 | 22 | GLU | CA-C | -5.18 | 1.45 | 1.52 |
| 1 | L5 | 10 | ASN | CA-C | -5.18 | 1.46 | 1.52 |
| 8 | a5 | 10 | ASN | C-O | -5.18 | 1.17 | 1.24 |
| 9 | z5 | 22 | GLU | CA-CB | -5.18 | 1.46 | 1.53 |
| 10 | j5 | 10 | THR | CA-C | -5.18 | 1.48 | 1.53 |
| 10 | j5 | 476 | ASN | CA-C | -5.18 | 1.45 | 1.52 |
| 10 | j5 | 537 | ILE | CA-CB | -5.18 | 1.47 | 1.54 |
| 10 | k5 | 4 | ARG | CA-C | -5.18 | 1.45 | 1.52 |
| 3 | LA | 89 | ILE | C-O | -5.18 | 1.18 | 1.24 |
| 10 | j5 | 1001 | TYR | N-CA | -5.18 | 1.40 | 1.46 |
| 3 | L9 | 89 | ILE | C-O | -5.18 | 1.18 | 1.24 |
| 8 | e5 | 17 | TYR | CA-CB | -5.18 | 1.44 | 1.53 |
| 8 | M7 | 97 | VAL | CA-CB | 5.18 | 1.61 | 1.54 |
| 10 | k5 | 463 | THR | CB-CG2 | -5.17 | 1.35 | 1.52 |
| 8 | C5 | 22 | GLU | CA-CB | -5.17 | 1.47 | 1.54 |
| 10 | k5 | 497 | ARG | CA-CB | -5.17 | 1.45 | 1.53 |
| 10 | k5 | 860 | LYS | N-CA | -5.17 | 1.39 | 1.46 |
| 4 | M4 | 215 | GLU | C-O | -5.17 | 1.17 | 1.24 |
| 8 | a5 | 17 | TYR | CA-CB | -5.17 | 1.44 | 1.53 |
| 10 | j5 | 629 | TYR | CA-CB | -5.17 | 1.45 | 1.53 |
| 10 | j5 | 633 | ARG | CA-C | -5.17 | 1.46 | 1.52 |
| 10 | k5 | 632 | ARG | CZ-NH2 | -5.17 | 1.26 | 1.33 |
| 10 | k5 | 633 | ARG | CA-C | -5.17 | 1.46 | 1.52 |
| 8 | G7 | 97 | VAL | CA-CB | 5.17 | 1.61 | 1.54 |
| 8 | o7 | 38 | ARG | C-O | -5.17 | 1.18 | 1.24 |
| 9 | w7 | 35 | GLU | C-O | -5.17 | 1.17 | 1.24 |
| 4 | MA | 235 | PHE | C-O | -5.17 | 1.17 | 1.24 |
| 4 | M4 | 44 | SER | N-CA | -5.17 | 1.39 | 1.46 |
| 1 | D5 | 6 | THR | CB-CG2 | -5.17 | 1.35 | 1.52 |
| 9 | i5 | 20 | GLY | N-CA | -5.17 | 1.37 | 1.45 |
| 4 | M9 | 235 | PHE | C-O | -5.17 | 1.17 | 1.24 |
| 11 | a9 | 455 | ASN | C-O | -5.17 | 1.18 | 1.24 |
| 11 | aA | 455 | ASN | C-O | -5.17 | 1.18 | 1.24 |
| 10 | j5 | 7 | SER | CA-C | -5.17 | 1.45 | 1.52 |
| 10 | j5 | 433 | SER | CA-CB | -5.17 | 1.45 | 1.53 |
| 10 | j5 | 724 | GLU | N-CA | -5.17 | 1.39 | 1.46 |
| 1 | b7 | 50 | THR | CA-C | -5.17 | 1.46 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 8 | u7 | 56 | ASP | CA-CB | -5.17 | 1.45 | 1.53 |
| 4 | M8 | 41 | ASN | CA-CB | -5.17 | 1.45 | 1.53 |
| 10 | j5 | 822 | ARG | CA-CB | -5.17 | 1.45 | 1.53 |
| 10 | k5 | 822 | ARG | CA-CB | -5.17 | 1.45 | 1.53 |
| 10 | k5 | 823 | TYR | CB-CG | -5.17 | 1.40 | 1.51 |
| 9 | w7 | 36 | ASN | N-CA | -5.17 | 1.40 | 1.46 |
| 10 | k5 | 452 | VAL | CA-C | -5.17 | 1.47 | 1.52 |
| 8 | S7 | 97 | VAL | CA-CB | 5.16 | 1.61 | 1.54 |
| 8 | g7 | 22 | GLU | CA-C | -5.16 | 1.44 | 1.52 |
| 9 | w7 | 58 | THR | N-CA | -5.16 | 1.40 | 1.46 |
| 4 | MA | 222 | ARG | CA-C | -5.16 | 1.47 | 1.52 |
| 4 | M9 | 222 | ARG | CA-C | -5.16 | 1.47 | 1.52 |
| 3 | LA | 110 | LEU | N-CA | -5.16 | 1.39 | 1.46 |
| 4 | M3 | 44 | SER | N-CA | -5.16 | 1.39 | 1.46 |
| 4 | M4 | 41 | ASN | CA-CB | -5.16 | 1.45 | 1.53 |
| 3 | L9 | 110 | LEU | N-CA | -5.16 | 1.39 | 1.46 |
| 11 | a9 | 464 | PRO | CA-CB | -5.16 | 1.47 | 1.53 |
| 11 | aA | 464 | PRO | CA-CB | -5.16 | 1.47 | 1.53 |
| 4 | M1 | 44 | SER | N-CA | -5.16 | 1.39 | 1.46 |
| 10 | j5 | 195 | SER | C-O | -5.16 | 1.17 | 1.24 |
| 10 | k5 | 680 | PRO | CA-CB | -5.16 | 1.46 | 1.53 |
| 8 | i7 | 131 | ARG | C-O | -5.16 | 1.17 | 1.24 |
| 4 | M8 | 222 | ARG | CA-C | -5.16 | 1.47 | 1.52 |
| 10 | j5 | 732 | ARG | CA-CB | -5.16 | 1.46 | 1.52 |
| 10 | k5 | 476 | ASN | CA-C | -5.16 | 1.45 | 1.52 |
| 11 | a9 | 803 | ASN | N-CA | -5.16 | 1.39 | 1.46 |
| 11 | aA | 803 | ASN | N-CA | -5.16 | 1.39 | 1.46 |
| 4 | M3 | 222 | ARG | CA-C | -5.15 | 1.47 | 1.52 |
| 10 | k5 | 537 | ILE | CA-CB | -5.15 | 1.47 | 1.54 |
| 4 | M1 | 222 | ARG | CA-C | -5.15 | 1.47 | 1.52 |
| 4 | M3 | 164 | ARG | C-O | -5.15 | 1.18 | 1.24 |
| 4 | M4 | 164 | ARG | C-O | -5.15 | 1.18 | 1.24 |
| 8 | c5 | 97 | VAL | CA-CB | 5.15 | 1.61 | 1.54 |
| 10 | k5 | 863 | ILE | CA-CB | -5.15 | 1.47 | 1.54 |
| 11 | aA | 776 | TYR | C-O | -5.15 | 1.18 | 1.24 |
| 4 | M1 | 164 | ARG | C-O | -5.15 | 1.18 | 1.24 |
| 1 | D5 | 14 | VAL | C-O | -5.15 | 1.18 | 1.24 |
| 10 | j5 | 891 | ALA | CA-CB | -5.15 | 1.44 | 1.53 |
| 4 | M8 | 164 | ARG | C-O | -5.15 | 1.18 | 1.24 |
| 10 | k5 | 318 | GLU | C-O | -5.15 | 1.18 | 1.24 |
| 4 | MA | 245 | ASP | C-O | -5.15 | 1.18 | 1.24 |
| 10 | j5 | 420 | VAL | CA-CB | -5.15 | 1.47 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | j5 | 860 | LYS | N-CA | -5.15 | 1.39 | 1.46 |
| 4 | M8 | 44 | SER | N-CA | -5.15 | 1.39 | 1.46 |
| 4 | M3 | 9 | GLN | CA-C | 5.15 | 1.57 | 1.52 |
| 10 | j5 | 675 | GLY | CA-C | -5.15 | 1.44 | 1.52 |
| 10 | k5 | 675 | GLY | CA-C | -5.15 | 1.44 | 1.52 |
| 10 | k5 | 724 | GLU | N-CA | -5.15 | 1.39 | 1.46 |
| 4 | M1 | 9 | GLN | CA-C | 5.15 | 1.57 | 1.52 |
| 4 | M3 | 235 | PHE | C-O | -5.14 | 1.17 | 1.24 |
| 8 | e5 | 10 | ASN | C-O | -5.14 | 1.17 | 1.24 |
| 10 | j5 | 861 | ALA | CA-CB | -5.14 | 1.45 | 1.53 |
| 10 | k5 | 777 | ASP | N-CA | -5.14 | 1.39 | 1.46 |
| 9 | z5 | 20 | GLY | N-CA | -5.14 | 1.38 | 1.45 |
| 10 | j5 | 632 | ARG | CA-C | -5.14 | 1.46 | 1.52 |
| 10 | k5 | 440 | TYR | CZ-OH | -5.14 | 1.27 | 1.38 |
| 8 | a7 | 22 | GLU | C-O | -5.14 | 1.15 | 1.23 |
| 1 | J5 | 14 | VAL | C-O | -5.14 | 1.18 | 1.24 |
| 10 | k5 | 18 | ARG | CA-CB | -5.14 | 1.45 | 1.53 |
| 8 | K5 | 128 | GLU | C-O | -5.14 | 1.17 | 1.24 |
| 10 | j5 | 502 | GLY | CA-C | -5.14 | 1.44 | 1.52 |
| 10 | j5 | 760 | ASP | CA-C | -5.14 | 1.45 | 1.52 |
| 10 | k5 | 502 | GLY | CA-C | -5.14 | 1.44 | 1.52 |
| 4 | M4 | 245 | ASP | C-O | -5.14 | 1.18 | 1.24 |
| 10 | j5 | 440 | TYR | CZ-OH | -5.14 | 1.27 | 1.38 |
| 10 | k5 | 1027 | ASN | N-CA | -5.14 | 1.39 | 1.46 |
| 10 | k5 | 1133 | GLU | CA-C | -5.14 | 1.45 | 1.52 |
| 10 | j5 | 610 | SER | C-N | -5.13 | 1.26 | 1.33 |
| 10 | k5 | 610 | SER | C-N | -5.13 | 1.26 | 1.33 |
| 8 | a7 | 22 | GLU | CA-C | -5.13 | 1.44 | 1.52 |
| 8 | c7 | 131 | ARG | C-O | -5.13 | 1.17 | 1.24 |
| 10 | j5 | 463 | THR | CB-CG2 | -5.13 | 1.35 | 1.52 |
| 10 | j5 | 611 | GLU | CA-CB | -5.13 | 1.45 | 1.53 |
| 9 | z7 | 40 | GLU | CA-CB | -5.13 | 1.45 | 1.53 |
| 4 | MA | 44 | SER | N-CA | -5.13 | 1.39 | 1.46 |
| 4 | M9 | 44 | SER | N-CA | -5.13 | 1.39 | 1.46 |
| 4 | M1 | 235 | PHE | C-O | -5.13 | 1.17 | 1.24 |
| 10 | j5 | 840 | ALA | C-O | -5.13 | 1.17 | 1.23 |
| 1 | h7 | 51 | ILE | CA-CB | -5.13 | 1.47 | 1.54 |
| 1 | b7 | 51 | ILE | CA-CB | -5.13 | 1.47 | 1.54 |
| 10 | k5 | 739 | VAL | CA-CB | -5.13 | 1.47 | 1.54 |
| 10 | k5 | 866 | LEU | C-N | -5.13 | 1.28 | 1.34 |
| 9 | w7 | 22 | GLU | C-O | -5.13 | 1.17 | 1.24 |
| 8 | I5 | 22 | GLU | CA-CB | -5.13 | 1.47 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 10 | j5 | 497 | ARG | CA-CB | -5.13 | 1.45 | 1.53 |
| 4 | M3 | 262 | ASP | CA-C | -5.12 | 1.47 | 1.53 |
| 4 | M1 | 262 | ASP | CA-C | -5.12 | 1.47 | 1.53 |
| 4 | M4 | 262 | ASP | CA-C | -5.12 | 1.47 | 1.53 |
| 10 | j5 | 823 | TYR | CB-CG | -5.12 | 1.40 | 1.51 |
| 10 | j5 | 866 | LEU | C-N | -5.12 | 1.28 | 1.34 |
| 8 | c7 | 125 | ALA | CA-C | -5.12 | 1.46 | 1.52 |
| 8 | o7 | 56 | ASP | CA-CB | -5.12 | 1.45 | 1.53 |
| 10 | j5 | 396 | GLY | CA-C | -5.12 | 1.44 | 1.51 |
| 10 | j5 | 849 | LYS | N-CA | -5.12 | 1.40 | 1.46 |
| 10 | k5 | 396 | GLY | CA-C | -5.12 | 1.44 | 1.51 |
| 10 | k5 | 849 | LYS | N-CA | -5.12 | 1.40 | 1.46 |
| 4 | M9 | 245 | ASP | C-O | -5.12 | 1.18 | 1.24 |
| 4 | MA | 262 | ASP | CA-C | -5.12 | 1.47 | 1.53 |
| 9 | i5 | 22 | GLU | CA-CB | -5.12 | 1.46 | 1.53 |
| 10 | j5 | 206 | MET | C-O | -5.12 | 1.18 | 1.24 |
| 10 | j5 | 763 | SER | N-CA | -5.12 | 1.39 | 1.46 |
| 10 | k5 | 206 | MET | C-O | -5.12 | 1.18 | 1.24 |
| 4 | M8 | 262 | ASP | CA-C | -5.12 | 1.47 | 1.53 |
| 4 | M9 | 262 | ASP | CA-C | -5.12 | 1.47 | 1.53 |
| 9 | z5 | 60 | VAL | C-O | -5.12 | 1.18 | 1.24 |
| 10 | j5 | 318 | GLU | CA-C | -5.12 | 1.46 | 1.52 |
| 10 | j5 | 610 | SER | CA-CB | -5.12 | 1.45 | 1.53 |
| 10 | j5 | 789 | SER | CA-C | -5.12 | 1.44 | 1.52 |
| 10 | k5 | 318 | GLU | CA-C | -5.12 | 1.46 | 1.52 |
| 10 | k5 | 610 | SER | CA-CB | -5.12 | 1.45 | 1.53 |
| 8 | g7 | 22 | GLU | C-O | -5.12 | 1.15 | 1.23 |
| 11 | a9 | 399 | ILE | C-O | -5.12 | 1.19 | 1.24 |
| 11 | aA | 399 | ILE | C-O | -5.12 | 1.19 | 1.24 |
| 10 | j5 | 452 | VAL | CA-C | -5.12 | 1.47 | 1.52 |
| 10 | k5 | 891 | ALA | CA-CB | -5.12 | 1.44 | 1.53 |
| 3 | LA | 87 | GLU | N-CA | -5.11 | 1.40 | 1.46 |
| 10 | j5 | 554 | ASN | C-O | -5.11 | 1.17 | 1.24 |
| 10 | j5 | 845 | ALA | C-O | -5.11 | 1.17 | 1.24 |
| 10 | k5 | 554 | ASN | C-O | -5.11 | 1.17 | 1.24 |
| 9 | z7 | 22 | GLU | C-O | -5.11 | 1.17 | 1.24 |
| 3 | L9 | 87 | GLU | N-CA | -5.11 | 1.40 | 1.46 |
| 10 | j5 | 347 | PHE | CA-C | -5.11 | 1.46 | 1.52 |
| 10 | j5 | 641 | ASP | N-CA | -5.11 | 1.40 | 1.46 |
| 10 | k5 | 195 | SER | C-O | -5.11 | 1.17 | 1.24 |
| 10 | k5 | 347 | PHE | CA-C | -5.11 | 1.46 | 1.52 |
| 4 | M8 | 215 | GLU | C-O | -5.11 | 1.17 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4 | MA | 232 | VAL | C-O | -5.11 | 1.17 | 1.24 |
| 4 | M3 | 74 | LEU | C-O | -5.11 | 1.18 | 1.24 |
| 10 | j5 | 777 | ASP | N-CA | -5.11 | 1.40 | 1.46 |
| 10 | k5 | 7 | SER | CA-CB | -5.11 | 1.45 | 1.53 |
| 4 | M9 | 232 | VAL | C-O | -5.11 | 1.17 | 1.24 |
| 4 | M1 | 74 | LEU | C-O | -5.11 | 1.18 | 1.24 |
| 10 | k5 | 410 | GLU | N-CA | -5.11 | 1.40 | 1.46 |
| 10 | k5 | 1001 | TYR | CA-CB | -5.11 | 1.45 | 1.53 |
| 11 | a9 | 315 | LEU | C-O | -5.11 | 1.18 | 1.24 |
| 11 | aA | 315 | LEU | C-O | -5.11 | 1.18 | 1.24 |
| 10 | j5 | 732 | ARG | CZ-NH1 | -5.10 | 1.25 | 1.32 |
| 10 | k5 | 402 | ILE | N-CA | -5.10 | 1.40 | 1.46 |
| 10 | k5 | 526 | MET | N-CA | -5.10 | 1.39 | 1.46 |
| 10 | k5 | 712 | ARG | CZ-NH1 | -5.10 | 1.25 | 1.32 |
| 11 | a9 | 495 | TYR | C-O | -5.10 | 1.18 | 1.24 |
| 11 | aA | 495 | TYR | C-O | -5.10 | 1.18 | 1.24 |
| 8 | A5 | 97 | VAL | CA-CB | 5.10 | 1.61 | 1.54 |
| 8 | E5 | 128 | GLU | C-O | -5.10 | 1.17 | 1.24 |
| 10 | j5 | 642 | ARG | N-CA | -5.10 | 1.39 | 1.46 |
| 10 | k5 | 611 | GLU | CA-CB | -5.10 | 1.45 | 1.53 |
| 3 | LA | 92 | TYR | C-O | -5.10 | 1.18 | 1.24 |
| 4 | M3 | 232 | VAL | C-O | -5.10 | 1.17 | 1.24 |
| 8 | A7 | 97 | VAL | CA-CB | 5.10 | 1.61 | 1.54 |
| 9 | z5 | 42 | GLN | CA-CB | -5.10 | 1.44 | 1.53 |
| 10 | j5 | 863 | ILE | CA-CB | -5.10 | 1.47 | 1.54 |
| 10 | j5 | 1001 | TYR | CA-CB | -5.10 | 1.45 | 1.53 |
| 10 | k5 | 632 | ARG | CA-C | -5.10 | 1.46 | 1.52 |
| 10 | k5 | 642 | ARG | N-CA | -5.10 | 1.39 | 1.46 |
| 8 | i7 | 128 | GLU | C-O | -5.10 | 1.18 | 1.24 |
| 3 | L9 | 92 | TYR | C-O | -5.10 | 1.18 | 1.24 |
| 4 | M1 | 232 | VAL | C-O | -5.10 | 1.17 | 1.24 |
| 10 | k5 | 763 | SER | N-CA | -5.10 | 1.39 | 1.46 |
| 4 | M4 | 9 | GLN | CA-C | 5.09 | 1.57 | 1.52 |
| 10 | j5 | 402 | ILE | N-CA | -5.09 | 1.40 | 1.46 |
| 8 | c7 | 128 | GLU | C-O | -5.09 | 1.18 | 1.24 |
| 11 | a9 | 497 | ARG | C-O | -5.09 | 1.18 | 1.24 |
| 11 | aA | 497 | ARG | C-O | -5.09 | 1.18 | 1.24 |
| 10 | k5 | 975 | ARG | C-O | -5.09 | 1.17 | 1.24 |
| 9 | y7 | 38 | PHE | C-O | -5.09 | 1.18 | 1.24 |
| 4 | M3 | 245 | ASP | C-O | -5.09 | 1.18 | 1.24 |
| 10 | j5 | 18 | ARG | CA-CB | -5.09 | 1.45 | 1.53 |
| 10 | j5 | 632 | ARG | CZ-NH2 | -5.09 | 1.26 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | j5 | 799 | GLU | N-CA | -5.09 | 1.39 | 1.46 |
| 10 | j5 | 1135 | LEU | CA-C | -5.09 | 1.46 | 1.53 |
| 10 | k5 | 799 | GLU | N-CA | -5.09 | 1.39 | 1.46 |
| 10 | k5 | 24 | THR | C-O | -5.09 | 1.18 | 1.24 |
| 10 | j5 | 516 | THR | N-CA | -5.09 | 1.39 | 1.46 |
| 10 | j5 | 772 | TYR | CZ-OH | -5.09 | 1.27 | 1.38 |
| 10 | k5 | 516 | THR | N-CA | -5.09 | 1.39 | 1.46 |
| 9 | y7 | 41 | GLN | C-O | -5.08 | 1.18 | 1.24 |
| 10 | j5 | 1041 | ARG | CA-C | -5.08 | 1.46 | 1.53 |
| 10 | k5 | 502 | GLY | C-N | -5.08 | 1.26 | 1.33 |
| 10 | k5 | 641 | ASP | N-CA | -5.08 | 1.40 | 1.46 |
| 10 | k5 | 760 | ASP | CA-C | -5.08 | 1.46 | 1.52 |
| 11 | a9 | 465 | TYR | CA-C | -5.08 | 1.45 | 1.52 |
| 10 | j5 | 568 | ILE | CA-CB | -5.08 | 1.47 | 1.54 |
| 10 | j5 | 612 | ILE | CA-C | -5.08 | 1.45 | 1.52 |
| 10 | k5 | 1001 | TYR | N-CA | -5.08 | 1.40 | 1.46 |
| 11 | aA | 465 | TYR | CA-C | -5.08 | 1.45 | 1.52 |
| 10 | j5 | 984 | ILE | C-O | -5.08 | 1.18 | 1.24 |
| 10 | k5 | 658 | TYR | CB-CG | -5.08 | 1.40 | 1.51 |
| 10 | k5 | 984 | ILE | C-O | -5.08 | 1.18 | 1.24 |
| 11 | a9 | 580 | THR | CA-C | -5.08 | 1.46 | 1.52 |
| 11 | aA | 580 | THR | CA-C | -5.08 | 1.46 | 1.52 |
| 3 | LA | 113 | LEU | CA-C | -5.08 | 1.46 | 1.52 |
| 10 | k5 | 944 | ALA | N-CA | -5.08 | 1.40 | 1.46 |
| 3 | L9 | 113 | LEU | CA-C | -5.08 | 1.46 | 1.52 |
| 4 | M8 | 10 | ARG | C-O | -5.08 | 1.18 | 1.24 |
| 4 | MA | 9 | GLN | CA-C | 5.08 | 1.57 | 1.52 |
| 4 | MA | 55 | GLU | CA-CB | -5.08 | 1.45 | 1.53 |
| 4 | M3 | 141 | GLU | C-O | -5.08 | 1.18 | 1.24 |
| 10 | j5 | 382 | ILE | CA-CB | -5.08 | 1.48 | 1.54 |
| 10 | j5 | 667 | SER | CB-OG | -5.08 | 1.31 | 1.42 |
| 10 | k5 | 1095 | ALA | CA-C | -5.08 | 1.46 | 1.52 |
| 4 | M9 | 9 | GLN | CA-C | 5.08 | 1.57 | 1.52 |
| 4 | M9 | 55 | GLU | CA-CB | -5.08 | 1.45 | 1.53 |
| 4 | M1 | 141 | GLU | C-O | -5.08 | 1.18 | 1.24 |
| 4 | MA | 143 | VAL | CA-CB | -5.07 | 1.48 | 1.54 |
| 8 | e5 | 17 | TYR | CZ-OH | -5.07 | 1.27 | 1.38 |
| 10 | j5 | 642 | ARG | CZ-NH1 | -5.07 | 1.25 | 1.32 |
| 10 | k5 | 789 | SER | CA-C | -5.07 | 1.45 | 1.52 |
| 4 | M9 | 143 | VAL | CA-CB | -5.07 | 1.48 | 1.54 |
| 4 | M1 | 245 | ASP | C-O | -5.07 | 1.18 | 1.24 |
| 10 | j5 | 832 | ALA | CA-CB | -5.07 | 1.44 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10 | k5 | 832 | ALA | CA-CB | -5.07 | 1.44 | 1.53 |
| 10 | k5 | 843 | ASN | CG-OD1 | -5.07 | 1.14 | 1.23 |
| 4 | M4 | 235 | PHE | C-O | -5.07 | 1.17 | 1.24 |
| 10 | j5 | 894 | TYR | CZ-OH | -5.07 | 1.27 | 1.38 |
| 10 | j5 | 900 | LEU | CB-CG | -5.07 | 1.43 | 1.53 |
| 10 | k5 | 900 | LEU | CB-CG | -5.07 | 1.43 | 1.53 |
| 9 | w7 | 40 | GLU | CA-CB | -5.07 | 1.45 | 1.53 |
| 4 | MA | 141 | GLU | C-O | -5.07 | 1.18 | 1.24 |
| 10 | k5 | 568 | ILE | CA-CB | -5.07 | 1.47 | 1.54 |
| 4 | M9 | 141 | GLU | C-O | -5.07 | 1.18 | 1.24 |
| 4 | M4 | 10 | ARG | C-O | -5.07 | 1.18 | 1.24 |
| 9 | z5 | 63 | ALA | C-O | -5.07 | 1.17 | 1.24 |
| 10 | j5 | 808 | LEU | C-N | -5.07 | 1.26 | 1.33 |
| 4 | M3 | 143 | VAL | CA-CB | -5.07 | 1.48 | 1.54 |
| 8 | C5 | 9 | VAL | CA-CB | -5.07 | 1.48 | 1.54 |
| 10 | j5 | 692 | LEU | CA-CB | -5.07 | 1.46 | 1.53 |
| 10 | k5 | 692 | LEU | CA-CB | -5.07 | 1.46 | 1.53 |
| 10 | k5 | 1041 | ARG | CA-C | -5.07 | 1.46 | 1.53 |
| 4 | M1 | 143 | VAL | CA-CB | -5.07 | 1.48 | 1.54 |
| 10 | j5 | 318 | GLU | C-O | -5.06 | 1.18 | 1.24 |
| 10 | j5 | 658 | TYR | CB-CG | -5.06 | 1.40 | 1.51 |
| 10 | j5 | 696 | ARG | CZ-NH2 | -5.06 | 1.26 | 1.33 |
| 10 | k5 | 696 | ARG | CZ-NH2 | -5.06 | 1.26 | 1.33 |
| 4 | M3 | 55 | GLU | CA-CB | -5.06 | 1.45 | 1.53 |
| 4 | M4 | 55 | GLU | CA-CB | -5.06 | 1.45 | 1.53 |
| 10 | j5 | 410 | GLU | N-CA | -5.06 | 1.40 | 1.46 |
| 10 | j5 | 843 | ASN | CG-OD1 | -5.06 | 1.14 | 1.23 |
| 10 | k5 | 732 | ARG | CZ-NH1 | -5.06 | 1.25 | 1.32 |
| 10 | k5 | 1120 | PRO | C-O | -5.06 | 1.17 | 1.24 |
| 4 | M1 | 55 | GLU | CA-CB | -5.06 | 1.45 | 1.53 |
| 9 | i5 | 63 | ALA | C-O | -5.06 | 1.17 | 1.24 |
| 10 | j5 | 711 | PRO | CA-CB | -5.06 | 1.48 | 1.53 |
| 10 | j5 | 382 | ILE | CA-C | -5.06 | 1.46 | 1.52 |
| 10 | k5 | 382 | ILE | CA-C | -5.06 | 1.46 | 1.52 |
| 10 | j5 | 630 | ILE | CB-CG1 | -5.06 | 1.43 | 1.53 |
| 10 | j5 | 895 | PRO | CA-CB | -5.06 | 1.46 | 1.53 |
| 10 | k5 | 711 | PRO | CA-CB | -5.06 | 1.48 | 1.53 |
| 10 | k5 | 772 | TYR | CZ-OH | -5.06 | 1.27 | 1.38 |
| 10 | k5 | 840 | ALA | C-O | -5.06 | 1.17 | 1.23 |
| 10 | k5 | 894 | TYR | CZ-OH | -5.06 | 1.27 | 1.38 |
| 4 | M8 | 235 | PHE | C-O | -5.06 | 1.17 | 1.24 |
| 11 | a9 | 450 | ARG | C-O | -5.06 | 1.18 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 11 | aA | 450 | ARG | C-O | -5.06 | 1.18 | 1.24 |
| 4 | M4 | 74 | LEU | C-O | -5.06 | 1.18 | 1.24 |
| 9 | i5 | 34 | TYR | CB-CG | -5.06 | 1.40 | 1.51 |
| 10 | j5 | 396 | GLY | N-CA | -5.05 | 1.38 | 1.45 |
| 10 | k5 | 396 | GLY | N-CA | -5.05 | 1.38 | 1.45 |
| 4 | M9 | 234 | SER | C-O | -5.05 | 1.17 | 1.24 |
| 4 | MA | 74 | LEU | C-O | -5.05 | 1.18 | 1.24 |
| 4 | M4 | 61 | ASN | CA-CB | -5.05 | 1.45 | 1.53 |
| 10 | j5 | 502 | GLY | C-N | -5.05 | 1.26 | 1.33 |
| 4 | M9 | 74 | LEU | C-O | -5.05 | 1.18 | 1.24 |
| 10 | j5 | 712 | ARG | CZ-NH1 | -5.05 | 1.25 | 1.32 |
| 10 | j5 | 1114 | ARG | CA-C | -5.05 | 1.46 | 1.52 |
| 10 | k5 | 732 | ARG | CA-CB | -5.05 | 1.46 | 1.53 |
| 4 | M8 | 55 | GLU | CA-CB | -5.05 | 1.45 | 1.53 |
| 10 | j5 | 460 | ALA | CA-C | -5.05 | 1.46 | 1.52 |
| 10 | j5 | 544 | VAL | CA-C | -5.05 | 1.46 | 1.52 |
| 10 | k5 | 826 | THR | CB-CG2 | -5.05 | 1.35 | 1.52 |
| 4 | M8 | 9 | GLN | CA-C | 5.05 | 1.57 | 1.52 |
| 11 | a9 | 32 | ARG | CA-C | -5.05 | 1.46 | 1.52 |
| 11 | a9 | 51 | SER | C-O | -5.05 | 1.17 | 1.24 |
| 11 | aA | 32 | ARG | CA-C | -5.05 | 1.46 | 1.52 |
| 11 | aA | 51 | SER | C-O | -5.05 | 1.17 | 1.24 |
| 10 | j5 | 505 | VAL | CA-CB | -5.05 | 1.47 | 1.54 |
| 10 | k5 | 505 | VAL | CA-CB | -5.05 | 1.47 | 1.54 |
| 10 | k5 | 807 | ARG | N-CA | -5.05 | 1.40 | 1.46 |
| 8 | C5 | 25 | ARG | C-O | -5.05 | 1.17 | 1.24 |
| 10 | j5 | 319 | ALA | C-O | -5.05 | 1.18 | 1.24 |
| 10 | j5 | 852 | GLY | CA-C | -5.05 | 1.44 | 1.51 |
| 10 | k5 | 852 | GLY | CA-C | -5.05 | 1.44 | 1.51 |
| 8 | c7 | 120 | GLN | C-O | -5.05 | 1.17 | 1.23 |
| 4 | M9 | 127 | SER | C-O | -5.05 | 1.18 | 1.24 |
| 10 | j5 | 700 | SER | CA-C | -5.04 | 1.46 | 1.52 |
| 10 | j5 | 789 | SER | CA-CB | -5.04 | 1.46 | 1.54 |
| 10 | j5 | 1095 | ALA | CA-C | -5.04 | 1.46 | 1.52 |
| 10 | k5 | 700 | SER | CA-C | -5.04 | 1.46 | 1.52 |
| 10 | k5 | 789 | SER | CA-CB | -5.04 | 1.46 | 1.54 |
| 4 | MA | 61 | ASN | CA-C | -5.04 | 1.46 | 1.52 |
| 10 | k5 | 3 | ILE | C-O | -5.04 | 1.18 | 1.24 |
| 10 | k5 | 808 | LEU | C-N | -5.04 | 1.26 | 1.33 |
| 4 | M9 | 61 | ASN | CA-C | -5.04 | 1.46 | 1.52 |
| 11 | a9 | 588 | VAL | C-O | 5.04 | 1.31 | 1.24 |
| 11 | aA | 588 | VAL | C-O | 5.04 | 1.31 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4 | M3 | 223 | GLY | C-O | -5.04 | 1.17 | 1.24 |
| 10 | k5 | 612 | ILE | CA-C | -5.04 | 1.45 | 1.52 |
| 10 | k5 | 845 | ALA | C-O | -5.04 | 1.17 | 1.24 |
| 10 | k5 | 1144 | SER | CA-C | -5.04 | 1.46 | 1.52 |
| 11 | a9 | 38 | VAL | C-O | -5.04 | 1.18 | 1.24 |
| 11 | aA | 38 | VAL | C-O | -5.04 | 1.18 | 1.24 |
| 4 | M1 | 223 | GLY | C-O | -5.04 | 1.17 | 1.24 |
| 10 | j5 | 572 | TYR | CZ-OH | -5.04 | 1.27 | 1.38 |
| 10 | k5 | 23 | GLU | C-O | -5.04 | 1.18 | 1.24 |
| 4 | MA | 169 | ASN | C-O | -5.04 | 1.18 | 1.24 |
| 9 | z5 | 34 | TYR | CB-CG | -5.04 | 1.40 | 1.51 |
| 9 | i5 | 42 | GLN | CA-CB | -5.04 | 1.44 | 1.53 |
| 10 | j5 | 907 | GLN | CA-CB | -5.04 | 1.45 | 1.53 |
| 10 | k5 | 414 | ILE | C-O | -5.04 | 1.18 | 1.24 |
| 10 | k5 | 1114 | ARG | CA-C | -5.04 | 1.46 | 1.52 |
| 9 | x7 | 41 | GLN | C-O | -5.04 | 1.18 | 1.24 |
| 4 | M9 | 169 | ASN | C-O | -5.04 | 1.18 | 1.24 |
| 10 | j5 | 826 | THR | CB-CG2 | -5.04 | 1.35 | 1.52 |
| 10 | k5 | 544 | VAL | CA-C | -5.04 | 1.46 | 1.52 |
| 10 | k5 | 895 | PRO | CA-CB | -5.04 | 1.46 | 1.53 |
| 11 | a9 | 494 | GLU | C-O | -5.04 | 1.18 | 1.24 |
| 4 | M3 | 140 | ARG | CA-C | -5.03 | 1.46 | 1.52 |
| 10 | j5 | 24 | THR | C-O | -5.03 | 1.18 | 1.24 |
| 10 | j5 | 414 | ILE | C-O | -5.03 | 1.18 | 1.24 |
| 10 | j5 | 975 | ARG | C-O | -5.03 | 1.17 | 1.24 |
| 10 | k5 | 382 | ILE | CA-CB | -5.03 | 1.48 | 1.54 |
| 10 | k5 | 460 | ALA | CA-C | -5.03 | 1.46 | 1.52 |
| 10 | k5 | 907 | GLN | CA-CB | -5.03 | 1.45 | 1.53 |
| 8 | i7 | 117 | ASN | CA-CB | -5.03 | 1.45 | 1.53 |
| 4 | M1 | 140 | ARG | CA-C | -5.03 | 1.46 | 1.52 |
| 10 | k5 | 861 | ALA | CA-CB | -5.03 | 1.45 | 1.53 |
| 8 | c7 | 117 | ASN | CA-CB | -5.03 | 1.45 | 1.53 |
| 10 | j5 | 3 | ILE | C-O | -5.03 | 1.18 | 1.24 |
| 10 | k5 | 445 | TYR | CA-C | -5.03 | 1.45 | 1.52 |
| 10 | k5 | 572 | TYR | CZ-OH | -5.03 | 1.27 | 1.38 |
| 10 | k5 | 1034 | GLU | CA-C | -5.03 | 1.46 | 1.52 |
| 4 | M4 | 169 | ASN | C-O | -5.03 | 1.18 | 1.24 |
| 10 | j5 | 241 | ALA | C-O | -5.03 | 1.21 | 1.23 |
| 10 | j5 | 1034 | GLU | CA-C | -5.03 | 1.46 | 1.52 |
| 10 | k5 | 241 | ALA | C-O | -5.03 | 1.21 | 1.23 |
| 10 | k5 | 515 | PRO | C-N | -5.03 | 1.26 | 1.33 |
| 10 | k5 | 640 | TYR | CA-CB | -5.03 | 1.45 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | D5 | 38 | VAL | C-N | -5.03 | 1.27 | 1.33 |
| 10 | j5 | 944 | ALA | N-CA | -5.02 | 1.40 | 1.46 |
| 10 | k5 | 768 | VAL | C-N | -5.02 | 1.26 | 1.33 |
| 3 | LA | 111 | ASN | N-CA | -5.02 | 1.40 | 1.46 |
| 4 | M4 | 223 | GLY | C-O | -5.02 | 1.17 | 1.24 |
| 3 | L9 | 111 | ASN | N-CA | -5.02 | 1.40 | 1.46 |
| 4 | MA | 140 | ARG | CA-C | -5.02 | 1.46 | 1.52 |
| 4 | M3 | 175 | GLY | C-O | -5.02 | 1.17 | 1.23 |
| 10 | j5 | 731 | GLU | CA-CB | -5.02 | 1.44 | 1.53 |
| 10 | j5 | 1130 | VAL | CA-CB | -5.02 | 1.48 | 1.54 |
| 10 | k5 | 731 | GLU | CA-CB | -5.02 | 1.44 | 1.53 |
| 4 | M9 | 140 | ARG | CA-C | -5.02 | 1.46 | 1.52 |
| 11 | a9 | 449 | ASN | CA-C | -5.02 | 1.46 | 1.52 |
| 11 | aA | 449 | ASN | CA-C | -5.02 | 1.46 | 1.52 |
| 4 | M1 | 175 | GLY | C-O | -5.02 | 1.17 | 1.23 |
| 8 | I5 | 9 | VAL | CA-CB | -5.02 | 1.48 | 1.54 |
| 10 | j5 | 712 | ARG | N-CA | -5.02 | 1.40 | 1.46 |
| 10 | k5 | 712 | ARG | N-CA | -5.02 | 1.40 | 1.46 |
| 10 | k5 | 836 | PHE | N-CA | -5.02 | 1.39 | 1.45 |
| 8 | Y7 | 97 | VAL | CA-CB | 5.02 | 1.61 | 1.54 |
| 11 | a9 | 613 | TYR | CA-C | -5.02 | 1.46 | 1.53 |
| 11 | aA | 613 | TYR | CA-C | -5.02 | 1.46 | 1.53 |
| 10 | k5 | 419 | THR | CA-C | -5.01 | 1.46 | 1.52 |
| 10 | k5 | 630 | ILE | CB-CG1 | -5.01 | 1.43 | 1.53 |
| 4 | M3 | 10 | ARG | C-O | -5.01 | 1.18 | 1.24 |
| 10 | j5 | 933 | ALA | N-CA | -5.01 | 1.39 | 1.46 |
| 10 | k5 | 933 | ALA | N-CA | -5.01 | 1.39 | 1.46 |
| 4 | M1 | 10 | ARG | C-O | -5.01 | 1.18 | 1.24 |
| 10 | j5 | 1000 | ILE | CA-C | -5.01 | 1.46 | 1.52 |
| 10 | j5 | 1144 | SER | CA-C | -5.01 | 1.46 | 1.52 |
| 10 | k5 | 642 | ARG | CZ-NH1 | -5.01 | 1.25 | 1.32 |
| 11 | aA | 494 | GLU | C-O | -5.01 | 1.18 | 1.24 |
| 10 | j5 | 419 | THR | CA-C | -5.01 | 1.46 | 1.52 |
| 10 | k5 | 926 | ALA | C-O | -5.01 | 1.17 | 1.24 |
| 4 | M8 | 169 | ASN | C-O | -5.01 | 1.18 | 1.24 |
| 4 | M8 | 61 | ASN | CA-CB | -5.01 | 1.45 | 1.53 |
| 4 | M8 | 232 | VAL | C-O | -5.01 | 1.17 | 1.24 |
| 4 | M3 | 127 | SER | C-O | -5.01 | 1.18 | 1.24 |
| 4 | M3 | 169 | ASN | C-O | -5.01 | 1.18 | 1.24 |
| 8 | e5 | 12 | ASP | CB-CG | -5.01 | 1.39 | 1.52 |
| 9 | z5 | 37 | TRP | CD2-CE2 | -5.01 | 1.32 | 1.41 |
| 9 | z5 | 37 | TRP | N-CA | -5.01 | 1.40 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 10 | j5 | 482 | GLN | CD-OE1 | -5.01 | 1.14 | 1.23 |
| 10 | k5 | 54 | ILE | N-CA | -5.01 | 1.40 | 1.46 |
| 10 | k5 | 277 | ILE | CA-C | 5.01 | 1.59 | 1.52 |
| 8 | W7 | 97 | VAL | CA-CB | 5.01 | 1.61 | 1.54 |
| 9 | z7 | 15 | LYS | C-O | -5.01 | 1.18 | 1.24 |
| 9 | w7 | 12 | PRO | C-O | -5.01 | 1.17 | 1.23 |
| 4 | M8 | 50 | ASP | CB-CG | -5.01 | 1.39 | 1.52 |
| 4 | M1 | 127 | SER | C-O | -5.01 | 1.18 | 1.24 |
| 4 | M1 | 169 | ASN | C-O | -5.01 | 1.18 | 1.24 |
| 4 | MA | 175 | GLY | C-O | -5.00 | 1.17 | 1.23 |
| 4 | MA | 223 | GLY | C-O | -5.00 | 1.17 | 1.24 |
| 10 | j5 | 531 | THR | C-O | -5.00 | 1.17 | 1.24 |
| 10 | k5 | 667 | SER | CB-OG | -5.00 | 1.32 | 1.42 |
| 4 | M9 | 175 | GLY | C-O | -5.00 | 1.17 | 1.23 |
| 4 | M9 | 223 | GLY | C-O | -5.00 | 1.17 | 1.24 |
| 10 | j5 | 23 | GLU | C-O | -5.00 | 1.18 | 1.24 |
| 10 | k5 | 49 | ASP | CA-C | -5.00 | 1.46 | 1.52 |
| 10 | k5 | 168 | THR | C-O | -5.00 | 1.18 | 1.24 |
| 10 | k5 | 684 | TYR | CE1-CZ | -5.00 | 1.26 | 1.38 |
| 8 | i7 | 120 | GLN | C-O | -5.00 | 1.17 | 1.23 |
| 9 | x7 | 38 | PHE | C-O | -5.00 | 1.18 | 1.24 |
| 4 | M9 | 210 | ILE | C-O | -5.00 | 1.18 | 1.24 |
| 4 | MA | 210 | ILE | C-O | -5.00 | 1.18 | 1.24 |
| 8 | G5 | 52 | LYS | CA-CB | -5.00 | 1.45 | 1.53 |
| 9 | z5 | 67 | VAL | CA-C | -5.00 | 1.46 | 1.52 |
| 10 | k5 | 444 | ASN | CA-CB | -5.00 | 1.45 | 1.53 |

All (2859) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 11 | aA | 354 | VAL | O-C-N | -47.09 | 63.71 | 122.57 |
| 11 | a9 | 354 | VAL | O-C-N | -47.06 | 63.75 | 122.57 |
| 5 | Z4 | 23 | SER | CA-C-N | 36.90 | 155.98 | 119.82 |
| 5 | Z4 | 23 | SER | C-N-CA | 36.90 | 155.98 | 119.82 |
| 10 | j5 | 743 | VAL | CA-C-N | 33.24 | 161.38 | 119.84 |
| 10 | j5 | 743 | VAL | C-N-CA | 33.24 | 161.38 | 119.84 |
| 10 | k5 | 743 | VAL | CA-C-N | 33.23 | 161.38 | 119.84 |
| 10 | k5 | 743 | VAL | C-N-CA | 33.23 | 161.38 | 119.84 |
| 11 | a9 | 351 | THR | CA-C-N | 28.61 | 155.60 | 119.84 |
| 11 | a9 | 351 | THR | C-N-CA | 28.61 | 155.60 | 119.84 |
| 11 | aA | 351 | THR | CA-C-N | 28.57 | 155.56 | 119.84 |
| 11 | aA | 351 | THR | C-N-CA | 28.57 | 155.56 | 119.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 10 | j5 | 701 | ASP | N-CA-C | 28.28 | 142.11 | 111.28 |
| 10 | k5 | 701 | ASP | N-CA-C | 28.24 | 142.06 | 111.28 |
| 4 | M8 | 269 | SER | N-CA-C | -26.07 | 74.38 | 110.35 |
| 10 | j5 | 489 | ASN | N-CA-C | 25.54 | 139.19 | 111.36 |
| 10 | k5 | 489 | ASN | N-CA-C | 25.53 | 139.19 | 111.36 |
| 4 | M8 | 231 | THR | N-CA-CB | 25.47 | 153.54 | 110.49 |
| 4 | M8 | 6 | THR | N-CA-C | 25.33 | 152.22 | 113.72 |
| 4 | M4 | 6 | THR | N-CA-C | 25.32 | 152.21 | 113.72 |
| 11 | a9 | 372 | ALA | CA-C-N | 25.15 | 154.20 | 120.25 |
| 11 | a9 | 372 | ALA | C-N-CA | 25.15 | 154.20 | 120.25 |
| 11 | aA | 372 | ALA | CA-C-N | 25.15 | 154.20 | 120.25 |
| 11 | aA | 372 | ALA | C-N-CA | 25.15 | 154.20 | 120.25 |
| 10 | k5 | 1055 | SER | O-C-N | -24.40 | 93.26 | 121.32 |
| 10 | j5 | 1055 | SER | O-C-N | -24.35 | 93.31 | 121.32 |
| 10 | j5 | 484 | GLY | N-CA-C | 23.77 | 141.25 | 112.49 |
| 10 | k5 | 484 | GLY | N-CA-C | 23.75 | 141.23 | 112.49 |
| 10 | j5 | 175 | ASP | CA-C-N | 23.67 | 146.39 | 120.12 |
| 10 | j5 | 175 | ASP | C-N-CA | 23.67 | 146.39 | 120.12 |
| 10 | k5 | 175 | ASP | CA-C-N | 23.67 | 146.39 | 120.12 |
| 10 | k5 | 175 | ASP | C-N-CA | 23.67 | 146.39 | 120.12 |
| 9 | z5 | 24 | GLN | N-CA-C | -23.64 | 84.59 | 113.20 |
| 9 | i5 | 24 | GLN | N-CA-C | -23.60 | 84.64 | 113.20 |
| 11 | a9 | 638 | ALA | N-CA-C | 23.10 | 141.03 | 111.24 |
| 11 | aA | 638 | ALA | N-CA-C | 23.10 | 141.03 | 111.24 |
| 10 | k5 | 919 | ILE | N-CA-C | 22.52 | 133.47 | 110.72 |
| 10 | j5 | 919 | ILE | N-CA-C | 22.50 | 133.45 | 110.72 |
| 11 | a9 | 283 | GLN | CA-C-N | 22.46 | 147.91 | 119.84 |
| 11 | a9 | 283 | GLN | C-N-CA | 22.46 | 147.91 | 119.84 |
| 11 | aA | 283 | GLN | CA-C-N | 22.46 | 147.91 | 119.84 |
| 11 | aA | 283 | GLN | C-N-CA | 22.46 | 147.91 | 119.84 |
| 9 | z5 | 24 | GLN | CA-C-N | -22.39 | 82.30 | 120.58 |
| 9 | z5 | 24 | GLN | C-N-CA | -22.39 | 82.30 | 120.58 |
| 9 | i5 | 24 | GLN | CA-C-N | -22.37 | 82.33 | 120.58 |
| 9 | i5 | 24 | GLN | C-N-CA | -22.37 | 82.33 | 120.58 |
| 3 | O8 | 108 | ARG | N-CA-C | -22.18 | 77.54 | 110.14 |
| 2 | U3 | 46 | SER | N-CA-C | -22.04 | 74.68 | 110.17 |
| 8 | U5 | 20 | PRO | N-CA-CB | -21.47 | 80.70 | 103.25 |
| 3 | L4 | 65 | ASP | N-CA-C | -21.25 | 75.95 | 110.17 |
| 4 | M8 | 135 | GLY | N-CA-C | -21.07 | 77.01 | 112.83 |
| 4 | M4 | 135 | GLY | N-CA-C | -21.05 | 77.05 | 112.83 |
| 11 | a9 | 573 | SER | O-C-N | 20.78 | 150.29 | 122.03 |
| 11 | aA | 573 | SER | O-C-N | 20.78 | 150.29 | 122.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 4 | M8 | 211 | GLN | N-CA-CB | 20.57 | 145.25 | 110.49 |
| 4 | M8 | 136 | SER | N-CA-CB | 19.39 | 143.26 | 110.49 |
| 4 | M4 | 136 | SER | N-CA-CB | 19.37 | 143.23 | 110.49 |
| 5 | Z4 | 28 | HIS | N-CA-CB | 19.33 | 143.16 | 110.49 |
| 4 | M8 | 78 | GLY | CA-C-N | 19.32 | 140.28 | 120.38 |
| 4 | M8 | 78 | GLY | C-N-CA | 19.32 | 140.28 | 120.38 |
| 4 | M4 | 78 | GLY | CA-C-N | 19.27 | 140.22 | 120.38 |
| 4 | M4 | 78 | GLY | C-N-CA | 19.27 | 140.22 | 120.38 |
| 4 | MA | 78 | GLY | CA-C-N | 19.25 | 140.21 | 120.38 |
| 4 | MA | 78 | GLY | C-N-CA | 19.25 | 140.21 | 120.38 |
| 4 | M9 | 78 | GLY | CA-C-N | 19.23 | 140.19 | 120.38 |
| 4 | M9 | 78 | GLY | C-N-CA | 19.23 | 140.19 | 120.38 |
| 4 | M3 | 78 | GLY | CA-C-N | 19.21 | 140.17 | 120.38 |
| 4 | M3 | 78 | GLY | C-N-CA | 19.21 | 140.17 | 120.38 |
| 4 | M1 | 78 | GLY | CA-C-N | 19.21 | 140.17 | 120.38 |
| 4 | M1 | 78 | GLY | C-N-CA | 19.21 | 140.17 | 120.38 |
| 10 | k5 | 486 | ILE | N-CA-C | 18.98 | 128.37 | 110.53 |
| 10 | j5 | 486 | ILE | N-CA-C | 18.97 | 128.36 | 110.53 |
| 11 | a9 | 621 | THR | N-CA-C | 18.80 | 137.62 | 109.24 |
| 3 | F9 | 157 | VAL | N-CA-C | 18.79 | 128.46 | 110.42 |
| 11 | aA | 621 | THR | N-CA-C | 18.77 | 137.58 | 109.24 |
| 4 | M8 | 225 | LYS | N-CA-C | 18.74 | 137.60 | 112.68 |
| 11 | a9 | 604 | ALA | CA-C-N | 18.39 | 142.83 | 119.84 |
| 11 | a9 | 604 | ALA | C-N-CA | 18.39 | 142.83 | 119.84 |
| 11 | aA | 604 | ALA | CA-C-N | 18.39 | 142.83 | 119.84 |
| 11 | aA | 604 | ALA | C-N-CA | 18.39 | 142.83 | 119.84 |
| 1 | F7 | 18 | TYR | CA-C-N | -18.20 | 95.47 | 120.95 |
| 1 | F7 | 18 | TYR | C-N-CA | -18.20 | 95.47 | 120.95 |
| 1 | X7 | 18 | TYR | CA-C-N | -18.18 | 95.49 | 120.95 |
| 1 | X7 | 18 | TYR | C-N-CA | -18.18 | 95.49 | 120.95 |
| 1 | X5 | 18 | TYR | CA-C-N | -18.17 | 95.52 | 120.95 |
| 1 | X5 | 18 | TYR | C-N-CA | -18.17 | 95.52 | 120.95 |
| 1 | d7 | 18 | TYR | CA-C-N | -18.16 | 95.53 | 120.95 |
| 1 | d7 | 18 | TYR | C-N-CA | -18.16 | 95.53 | 120.95 |
| 1 | R5 | 18 | TYR | CA-C-N | -18.16 | 95.53 | 120.95 |
| 1 | R5 | 18 | TYR | C-N-CA | -18.16 | 95.53 | 120.95 |
| 1 | p7 | 18 | TYR | CA-C-N | -18.14 | 95.55 | 120.95 |
| 1 | p7 | 18 | TYR | C-N-CA | -18.14 | 95.55 | 120.95 |
| 1 | j7 | 18 | TYR | CA-C-N | -18.14 | 95.56 | 120.95 |
| 1 | j7 | 18 | TYR | C-N-CA | -18.14 | 95.56 | 120.95 |
| 1 | L7 | 18 | TYR | CA-C-N | -18.14 | 95.56 | 120.95 |
| 1 | L7 | 18 | TYR | C-N-CA | -18.14 | 95.56 | 120.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1 | v7 | 18 | TYR | CA-C-N | -18.13 | 95.56 | 120.95 |
| 1 | v7 | 18 | TYR | C-N-CA | -18.13 | 95.56 | 120.95 |
| 1 | R7 | 18 | TYR | CA-C-N | -18.13 | 95.57 | 120.95 |
| 1 | R7 | 18 | TYR | C-N-CA | -18.13 | 95.57 | 120.95 |
| 1 | L5 | 18 | TYR | CA-C-N | -18.12 | 95.58 | 120.95 |
| 1 | L5 | 18 | TYR | C-N-CA | -18.12 | 95.58 | 120.95 |
| 10 | k5 | 882 | PRO | CA-C-O | -18.10 | 91.45 | 120.05 |
| 10 | j5 | 882 | PRO | CA-C-O | -18.09 | 91.46 | 120.05 |
| 1 | F5 | 18 | TYR | CA-C-N | -18.09 | 95.62 | 120.95 |
| 1 | F5 | 18 | TYR | C-N-CA | -18.09 | 95.62 | 120.95 |
| 1 | b5 | 18 | TYR | CA-C-N | -18.04 | 95.69 | 120.95 |
| 1 | b5 | 18 | TYR | C-N-CA | -18.04 | 95.69 | 120.95 |
| 1 | f5 | 18 | TYR | CA-C-N | -18.00 | 95.75 | 120.95 |
| 1 | f5 | 18 | TYR | C-N-CA | -18.00 | 95.75 | 120.95 |
| 3 | L4 | 66 | LEU | N-CA-CB | 17.25 | 139.65 | 110.49 |
| 3 | L1 | 78 | ARG | N-CA-CB | 17.04 | 139.29 | 110.49 |
| 4 | M8 | 226 | SER | N-CA-CB | 16.75 | 138.79 | 110.49 |
| 11 | a9 | 313 | GLU | N-CA-C | -16.62 | 90.48 | 111.75 |
| 11 | aA | 313 | GLU | N-CA-C | -16.62 | 90.48 | 111.75 |
| 11 | a9 | 573 | SER | N-CA-C | 16.59 | 135.00 | 112.93 |
| 11 | aA | 573 | SER | N-CA-C | 16.59 | 135.00 | 112.93 |
| 5 | Z4 | 40 | SER | N-CA-CB | 16.57 | 138.49 | 110.49 |
| 10 | j5 | 1004 | VAL | N-CA-C | 16.54 | 126.07 | 110.53 |
| 10 | k5 | 1004 | VAL | N-CA-C | 16.53 | 126.07 | 110.53 |
| 10 | k5 | 384 | SER | CA-C-N | 16.39 | 136.91 | 119.87 |
| 10 | k5 | 384 | SER | C-N-CA | 16.39 | 136.91 | 119.87 |
| 10 | j5 | 384 | SER | CA-C-N | 16.36 | 136.89 | 119.87 |
| 10 | j5 | 384 | SER | C-N-CA | 16.36 | 136.89 | 119.87 |
| 4 | M8 | 210 | ILE | N-CA-C | -16.34 | 87.01 | 109.55 |
| 10 | j5 | 704 | THR | N-CA-C | 16.32 | 128.76 | 111.14 |
| 3 | Y4 | 109 | CYS | CB-CA-C | -16.31 | 77.96 | 110.42 |
| 10 | k5 | 704 | THR | N-CA-C | 16.30 | 128.75 | 111.14 |
| 2 | U3 | 47 | ASN | N-CA-CB | 16.27 | 137.98 | 110.49 |
| 3 | F9 | 144 | SER | CA-C-N | 16.22 | 140.12 | 119.84 |
| 3 | F9 | 144 | SER | C-N-CA | 16.22 | 140.12 | 119.84 |
| 3 | L1 | 77 | ARG | N-CA-C | -15.90 | 85.07 | 110.20 |
| 5 | Z4 | 27 | ALA | CB-CA-C | 15.78 | 141.82 | 110.42 |
| 1 | j7 | 18 | TYR | O-C-N | 15.59 | 141.98 | 122.81 |
| 1 | d7 | 18 | TYR | O-C-N | 15.58 | 141.97 | 122.81 |
| 1 | F7 | 18 | TYR | O-C-N | 15.57 | 141.96 | 122.81 |
| 1 | L7 | 18 | TYR | O-C-N | 15.57 | 141.96 | 122.81 |
| 1 | X5 | 18 | TYR | O-C-N | 15.54 | 141.92 | 122.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 10 | j5 | 728 | PRO | CA-C-O | -15.54 | 95.62 | 119.86 |
| 1 | X7 | 18 | TYR | O-C-N | 15.52 | 141.90 | 122.81 |
| 10 | k5 | 728 | PRO | CA-C-O | -15.51 | 95.66 | 119.86 |
| 1 | R7 | 18 | TYR | O-C-N | 15.51 | 141.89 | 122.81 |
| 11 | a9 | 615 | ARG | CA-C-N | 15.46 | 135.69 | 119.76 |
| 11 | a9 | 615 | ARG | C-N-CA | 15.46 | 135.69 | 119.76 |
| 11 | aA | 615 | ARG | CA-C-N | 15.46 | 135.69 | 119.76 |
| 11 | aA | 615 | ARG | C-N-CA | 15.46 | 135.69 | 119.76 |
| 1 | R5 | 18 | TYR | O-C-N | 15.46 | 141.82 | 122.81 |
| 1 | p7 | 18 | TYR | O-C-N | 15.46 | 141.82 | 122.81 |
| 10 | j5 | 291 | ASP | N-CA-C | -15.44 | 95.29 | 114.75 |
| 10 | k5 | 291 | ASP | N-CA-C | -15.44 | 95.29 | 114.75 |
| 1 | v7 | 18 | TYR | O-C-N | 15.44 | 141.80 | 122.81 |
| 1 | b5 | 18 | TYR | O-C-N | 15.43 | 141.79 | 122.81 |
| 1 | F5 | 18 | TYR | O-C-N | 15.41 | 141.76 | 122.81 |
| 1 | L5 | 18 | TYR | O-C-N | 15.40 | 141.75 | 122.81 |
| 1 | f5 | 18 | TYR | O-C-N | 15.38 | 141.72 | 122.81 |
| 11 | a9 | 282 | ALA | N-CA-C | 15.30 | 127.95 | 111.28 |
| 11 | aA | 282 | ALA | N-CA-C | 15.30 | 127.95 | 111.28 |
| 10 | j5 | 743 | VAL | N-CA-C | 15.28 | 130.68 | 112.35 |
| 10 | k5 | 777 | ASP | N-CA-C | 15.27 | 128.77 | 110.91 |
| 10 | k5 | 743 | VAL | N-CA-C | 15.27 | 130.67 | 112.35 |
| 10 | j5 | 1106 | PHE | N-CA-C | -15.25 | 82.99 | 108.76 |
| 10 | j5 | 428 | VAL | N-CA-C | 15.24 | 126.17 | 110.62 |
| 10 | j5 | 18 | ARG | N-CA-C | 15.21 | 127.94 | 111.36 |
| 10 | j5 | 777 | ASP | N-CA-C | 15.20 | 128.70 | 110.91 |
| 10 | k5 | 428 | VAL | N-CA-C | 15.20 | 126.12 | 110.62 |
| 10 | k5 | 18 | ARG | N-CA-C | 15.19 | 127.92 | 111.36 |
| 9 | z5 | 61 | GLN | N-CA-C | 15.00 | 127.62 | 111.28 |
| 9 | i5 | 61 | GLN | N-CA-C | 14.98 | 127.61 | 111.28 |
| 11 | a9 | 58 | GLY | N-CA-C | 14.93 | 130.56 | 112.49 |
| 11 | aA | 58 | GLY | N-CA-C | 14.93 | 130.56 | 112.49 |
| 10 | j5 | 501 | ILE | N-CA-C | 14.88 | 127.24 | 111.77 |
| 10 | k5 | 501 | ILE | N-CA-C | 14.86 | 127.22 | 111.77 |
| 10 | j5 | 1143 | LEU | N-CA-C | 14.52 | 126.82 | 111.14 |
| 10 | k5 | 1143 | LEU | N-CA-C | 14.49 | 126.79 | 111.14 |
| 11 | a9 | 354 | VAL | CA-C-N | 14.46 | 147.73 | 121.70 |
| 11 | a9 | 354 | VAL | C-N-CA | 14.46 | 147.73 | 121.70 |
| 11 | aA | 354 | VAL | CA-C-N | 14.44 | 147.70 | 121.70 |
| 11 | aA | 354 | VAL | C-N-CA | 14.44 | 147.70 | 121.70 |
| 11 | aA | 32 | ARG | N-CA-C | -14.39 | 95.60 | 111.14 |
| 11 | a9 | 32 | ARG | N-CA-C | -14.38 | 95.61 | 111.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 8 | O5 | 20 | PRO | N-CA-CB | -14.36 | 88.17 | 103.25 |
| 11 | a9 | 631 | GLY | N-CA-C | -14.35 | 79.18 | 113.18 |
| 11 | aA | 631 | GLY | N-CA-C | -14.35 | 79.18 | 113.18 |
| 9 | z7 | 58 | THR | N-CA-C | 14.32 | 126.61 | 111.14 |
| 9 | w7 | 58 | THR | N-CA-C | 14.28 | 126.56 | 111.14 |
| 8 | a5 | 7 | ALA | N-CA-C | 14.18 | 131.42 | 113.55 |
| 8 | e5 | 7 | ALA | N-CA-C | 14.13 | 131.35 | 113.55 |
| 3 | Y4 | 109 | CYS | N-CA-C | 14.11 | 140.86 | 110.80 |
| 10 | k5 | 1011 | ILE | CA-C-N | 14.09 | 134.90 | 120.38 |
| 10 | k5 | 1011 | ILE | C-N-CA | 14.09 | 134.90 | 120.38 |
| 10 | j5 | 1011 | ILE | CA-C-N | 14.07 | 134.87 | 120.38 |
| 10 | j5 | 1011 | ILE | C-N-CA | 14.07 | 134.87 | 120.38 |
| 3 | H2 | 83 | LEU | O-C-N | -13.97 | 107.31 | 122.12 |
| 8 | c7 | 124 | PRO | CA-C-N | -13.88 | 102.40 | 120.44 |
| 8 | c7 | 124 | PRO | C-N-CA | -13.88 | 102.40 | 120.44 |
| 3 | H6 | 83 | LEU | O-C-N | -13.87 | 107.42 | 122.12 |
| 8 | i7 | 124 | PRO | CA-C-N | -13.86 | 102.42 | 120.44 |
| 8 | i7 | 124 | PRO | C-N-CA | -13.86 | 102.42 | 120.44 |
| 11 | a9 | 280 | ASP | CA-C-N | 13.79 | 134.22 | 119.87 |
| 11 | a9 | 280 | ASP | C-N-CA | 13.79 | 134.22 | 119.87 |
| 11 | aA | 280 | ASP | CA-C-N | 13.77 | 134.19 | 119.87 |
| 11 | aA | 280 | ASP | C-N-CA | 13.77 | 134.19 | 119.87 |
| 9 | w7 | 38 | PHE | N-CA-C | 13.61 | 126.11 | 111.28 |
| 9 | z7 | 38 | PHE | N-CA-C | 13.61 | 126.11 | 111.28 |
| 8 | c7 | 124 | PRO | N-CA-C | -13.48 | 97.01 | 113.86 |
| 8 | i7 | 124 | PRO | N-CA-C | -13.44 | 97.06 | 113.86 |
| 11 | a9 | 540 | ILE | CB-CA-C | -13.44 | 98.40 | 111.30 |
| 11 | aA | 540 | ILE | CB-CA-C | -13.44 | 98.40 | 111.30 |
| 8 | s7 | 20 | PRO | N-CA-CB | -13.35 | 89.24 | 103.25 |
| 10 | k5 | 1147 | TYR | N-CA-C | 13.28 | 125.83 | 111.36 |
| 10 | j5 | 1147 | TYR | N-CA-C | 13.25 | 125.80 | 111.36 |
| 4 | M4 | 6 | THR | CB-CA-C | -13.08 | 85.15 | 110.65 |
| 4 | M8 | 6 | THR | CB-CA-C | -13.07 | 85.15 | 110.65 |
| 4 | M8 | 270 | GLY | N-CA-C | 13.00 | 132.40 | 112.51 |
| 4 | M8 | 4 | LEU | N-CA-C | 12.93 | 127.60 | 110.53 |
| 4 | M4 | 4 | LEU | N-CA-C | 12.93 | 127.60 | 110.53 |
| 10 | k5 | 673 | VAL | N-CA-C | 12.92 | 122.68 | 110.53 |
| 4 | M8 | 142 | PHE | N-CA-C | -12.92 | 96.85 | 111.71 |
| 4 | M3 | 4 | LEU | N-CA-C | 12.92 | 127.58 | 110.53 |
| 4 | M1 | 4 | LEU | N-CA-C | 12.92 | 127.58 | 110.53 |
| 10 | j5 | 673 | VAL | N-CA-C | 12.91 | 122.67 | 110.53 |
| 10 | j5 | 426 | LEU | N-CA-C | 12.90 | 125.34 | 111.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 4 | MA | 4 | LEU | N-CA-C | 12.90 | 127.56 | 110.53 |
| 4 | M9 | 4 | LEU | N-CA-C | 12.90 | 127.56 | 110.53 |
| 10 | k5 | 426 | LEU | N-CA-C | 12.86 | 125.30 | 111.28 |
| 11 | a9 | 82 | GLN | N-CA-CB | -12.79 | 88.45 | 109.56 |
| 11 | aA | 82 | GLN | N-CA-CB | -12.79 | 88.45 | 109.56 |
| 8 | O5 | 22 | GLU | CB-CA-C | -12.60 | 88.87 | 110.17 |
| 11 | aA | 299 | PRO | N-CA-C | -12.54 | 95.06 | 113.75 |
| 11 | aA | 625 | ASP | N-CA-C | -12.44 | 97.80 | 111.36 |
| 11 | a9 | 625 | ASP | N-CA-C | -12.43 | 97.81 | 111.36 |
| 4 | M4 | 63 | GLY | N-CA-C | 12.41 | 131.78 | 115.40 |
| 4 | MA | 63 | GLY | N-CA-C | 12.38 | 131.75 | 115.40 |
| 4 | M9 | 63 | GLY | N-CA-C | 12.38 | 131.75 | 115.40 |
| 4 | M8 | 63 | GLY | N-CA-C | 12.38 | 131.74 | 115.40 |
| 4 | M3 | 63 | GLY | N-CA-C | 12.36 | 131.71 | 115.40 |
| 10 | k5 | 136 | VAL | CA-C-N | 12.36 | 133.11 | 120.38 |
| 10 | k5 | 136 | VAL | C-N-CA | 12.36 | 133.11 | 120.38 |
| 4 | M1 | 63 | GLY | N-CA-C | 12.36 | 131.71 | 115.40 |
| 10 | j5 | 136 | VAL | CA-C-N | 12.34 | 133.09 | 120.38 |
| 10 | j5 | 136 | VAL | C-N-CA | 12.34 | 133.09 | 120.38 |
| 10 | k5 | 1115 | ARG | N-CA-C | 12.31 | 128.94 | 113.43 |
| 11 | a9 | 67 | GLN | CA-C-N | -12.31 | 98.03 | 121.54 |
| 11 | a9 | 67 | GLN | C-N-CA | -12.31 | 98.03 | 121.54 |
| 11 | aA | 67 | GLN | CA-C-N | -12.31 | 98.03 | 121.54 |
| 11 | aA | 67 | GLN | C-N-CA | -12.31 | 98.03 | 121.54 |
| 10 | j5 | 1115 | ARG | N-CA-C | 12.30 | 128.92 | 113.43 |
| 8 | I5 | 24 | ASP | N-CA-C | -12.28 | 94.65 | 111.96 |
| 8 | C5 | 24 | ASP | N-CA-C | -12.24 | 94.70 | 111.96 |
| 10 | j5 | 395 | SER | N-CA-C | -12.22 | 89.73 | 108.67 |
| 10 | k5 | 395 | SER | N-CA-C | -12.21 | 89.74 | 108.67 |
| 9 | i5 | 26 | THR | N-CA-C | 12.09 | 124.46 | 111.28 |
| 10 | j5 | 611 | GLU | N-CA-C | 12.08 | 124.52 | 111.36 |
| 5 | Z4 | 25 | THR | N-CA-C | -12.07 | 98.21 | 111.36 |
| 10 | k5 | 611 | GLU | N-CA-C | 12.07 | 124.51 | 111.36 |
| 10 | k5 | 317 | SER | N-CA-C | 12.04 | 124.14 | 111.14 |
| 10 | j5 | 317 | SER | N-CA-C | 12.03 | 124.14 | 111.14 |
| 9 | z5 | 26 | THR | N-CA-C | 11.98 | 124.34 | 111.28 |
| 4 | M9 | 33 | LEU | N-CA-C | 11.91 | 131.82 | 113.72 |
| 4 | MA | 33 | LEU | N-CA-C | 11.91 | 131.82 | 113.72 |
| 4 | M4 | 33 | LEU | N-CA-C | 11.90 | 131.81 | 113.72 |
| 4 | M3 | 33 | LEU | N-CA-C | 11.89 | 131.79 | 113.72 |
| 4 | M1 | 33 | LEU | N-CA-C | 11.89 | 131.79 | 113.72 |
| 4 | M8 | 33 | LEU | N-CA-C | 11.87 | 131.77 | 113.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 3 | F9 | 141 | TYR | N-CA-C | 11.83 | 124.17 | 111.28 |
| 10 | k5 | 1119 | LEU | N-CA-C | 11.82 | 135.94 | 109.81 |
| 10 | j5 | 1119 | LEU | N-CA-C | 11.80 | 135.88 | 109.81 |
| 10 | k5 | 584 | GLN | N-CA-C | 11.74 | 124.08 | 111.28 |
| 10 | j5 | 584 | GLN | N-CA-C | 11.71 | 124.05 | 111.28 |
| 10 | k5 | 247 | ARG | CA-C-N | 11.70 | 131.46 | 119.76 |
| 10 | k5 | 247 | ARG | C-N-CA | 11.70 | 131.46 | 119.76 |
| 5 | NA | 34 | LEU | N-CA-C | 11.69 | 127.44 | 111.54 |
| 5 | N9 | 34 | LEU | N-CA-C | 11.69 | 127.44 | 111.54 |
| 5 | N3 | 34 | LEU | N-CA-C | 11.69 | 127.44 | 111.54 |
| 10 | j5 | 19 | THR | N-CA-C | 11.69 | 127.65 | 111.17 |
| 5 | N1 | 34 | LEU | N-CA-C | 11.69 | 127.44 | 111.54 |
| 10 | k5 | 19 | THR | N-CA-C | 11.69 | 127.64 | 111.17 |
| 10 | k5 | 140 | PHE | N-CA-C | -11.68 | 84.70 | 108.18 |
| 4 | M8 | 231 | THR | N-CA-C | -11.67 | 85.93 | 110.80 |
| 10 | j5 | 140 | PHE | N-CA-C | -11.66 | 84.73 | 108.18 |
| 10 | j5 | 247 | ARG | CA-C-N | 11.66 | 131.42 | 119.76 |
| 10 | j5 | 247 | ARG | C-N-CA | 11.66 | 131.42 | 119.76 |
| 11 | a9 | 289 | THR | N-CA-C | 11.65 | 127.38 | 111.54 |
| 11 | aA | 289 | THR | N-CA-C | 11.65 | 127.38 | 111.54 |
| 5 | Z8 | 34 | LEU | N-CA-C | 11.64 | 127.37 | 111.54 |
| 10 | j5 | 268 | SER | N-CA-C | 11.61 | 127.03 | 112.86 |
| 5 | Z4 | 34 | LEU | N-CA-C | 11.60 | 127.40 | 111.39 |
| 10 | k5 | 268 | SER | N-CA-C | 11.60 | 127.01 | 112.86 |
| 11 | a9 | 553 | SER | N-CA-C | 11.47 | 125.13 | 111.82 |
| 8 | m7 | 20 | PRO | N-CA-CB | -11.42 | 91.26 | 103.25 |
| 10 | k5 | 889 | LEU | CA-C-N | 11.41 | 154.39 | 127.00 |
| 10 | k5 | 889 | LEU | C-N-CA | 11.41 | 154.39 | 127.00 |
| 10 | j5 | 889 | LEU | CA-C-N | 11.40 | 154.36 | 127.00 |
| 10 | j5 | 889 | LEU | C-N-CA | 11.40 | 154.36 | 127.00 |
| 10 | k5 | 728 | PRO | N-CA-C | 11.37 | 129.34 | 113.53 |
| 10 | j5 | 728 | PRO | N-CA-C | 11.37 | 129.34 | 113.53 |
| 10 | k5 | 823 | TYR | CA-C-N | 11.33 | 131.45 | 119.78 |
| 10 | k5 | 823 | TYR | C-N-CA | 11.33 | 131.45 | 119.78 |
| 10 | j5 | 823 | TYR | CA-C-N | 11.26 | 131.38 | 119.78 |
| 10 | j5 | 823 | TYR | C-N-CA | 11.26 | 131.38 | 119.78 |
| 5 | NA | 23 | SER | CA-C-N | -11.24 | 101.55 | 120.88 |
| 5 | NA | 23 | SER | C-N-CA | -11.24 | 101.55 | 120.88 |
| 5 | N9 | 23 | SER | CA-C-N | -11.24 | 101.55 | 120.88 |
| 5 | N9 | 23 | SER | C-N-CA | -11.24 | 101.55 | 120.88 |
| 5 | N3 | 23 | SER | CA-C-N | -11.23 | 101.56 | 120.88 |
| 5 | N3 | 23 | SER | C-N-CA | -11.23 | 101.56 | 120.88 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 5 | N1 | 23 | SER | CA-C-N | -11.23 | 101.56 | 120.88 |
| 5 | N1 | 23 | SER | C-N-CA | -11.23 | 101.56 | 120.88 |
| 5 | Z8 | 23 | SER | CA-C-N | -11.22 | 101.59 | 120.88 |
| 5 | Z8 | 23 | SER | C-N-CA | -11.22 | 101.59 | 120.88 |
| 1 | F5 | 3 | ASP | CB-CA-C | -11.18 | 95.37 | 113.37 |
| 1 | L5 | 3 | ASP | CB-CA-C | -11.16 | 95.39 | 113.37 |
| 10 | j5 | 1006 | ASP | N-CA-C | 11.07 | 124.40 | 111.11 |
| 10 | k5 | 1006 | ASP | N-CA-C | 11.07 | 124.40 | 111.11 |
| 11 | aA | 602 | PRO | CA-C-O | 11.07 | 133.83 | 121.43 |
| 10 | j5 | 663 | ALA | CA-C-N | -11.07 | 105.45 | 120.28 |
| 10 | j5 | 663 | ALA | C-N-CA | -11.07 | 105.45 | 120.28 |
| 11 | a9 | 602 | PRO | CA-C-O | 11.03 | 133.78 | 121.43 |
| 10 | j5 | 397 | GLY | N-CA-C | -11.02 | 87.07 | 113.18 |
| 10 | k5 | 397 | GLY | N-CA-C | -11.02 | 87.07 | 113.18 |
| 10 | k5 | 663 | ALA | CA-C-N | -11.01 | 105.52 | 120.28 |
| 10 | k5 | 663 | ALA | C-N-CA | -11.01 | 105.52 | 120.28 |
| 10 | j5 | 33 | ARG | N-CA-C | 11.00 | 134.23 | 110.80 |
| 10 | k5 | 33 | ARG | N-CA-C | 10.99 | 134.22 | 110.80 |
| 11 | a9 | 359 | ASP | CA-C-N | 10.97 | 135.87 | 120.29 |
| 11 | a9 | 359 | ASP | C-N-CA | 10.97 | 135.87 | 120.29 |
| 11 | aA | 359 | ASP | CA-C-N | 10.97 | 135.87 | 120.29 |
| 11 | aA | 359 | ASP | C-N-CA | 10.97 | 135.87 | 120.29 |
| 10 | k5 | 371 | SER | N-CA-CB | -10.96 | 94.57 | 111.56 |
| 10 | j5 | 371 | SER | N-CA-CB | -10.95 | 94.58 | 111.56 |
| 11 | a9 | 351 | THR | C-N-CD | -10.85 | 80.50 | 125.00 |
| 11 | aA | 351 | THR | C-N-CD | -10.85 | 80.50 | 125.00 |
| 11 | a9 | 110 | PHE | N-CA-C | 10.84 | 126.25 | 112.92 |
| 11 | aA | 110 | PHE | N-CA-C | 10.84 | 126.25 | 112.92 |
| 10 | j5 | 146 | ALA | N-CA-C | 10.84 | 122.84 | 111.14 |
| 10 | j5 | 492 | ILE | N-CA-C | 10.83 | 120.82 | 110.42 |
| 10 | k5 | 146 | ALA | N-CA-C | 10.82 | 122.82 | 111.14 |
| 11 | a9 | 630 | LEU | N-CA-C | 10.80 | 122.63 | 111.07 |
| 3 | FA | 141 | TYR | N-CA-C | 10.79 | 124.12 | 111.71 |
| 10 | k5 | 492 | ILE | N-CA-C | 10.79 | 120.77 | 110.42 |
| 10 | j5 | 847 | LEU | N-CA-C | -10.78 | 98.17 | 111.11 |
| 10 | k5 | 847 | LEU | N-CA-C | -10.78 | 98.17 | 111.11 |
| 11 | aA | 630 | LEU | N-CA-C | 10.78 | 122.60 | 111.07 |
| 4 | M4 | 95 | ALA | N-CA-C | -10.74 | 91.91 | 109.96 |
| 11 | a9 | 574 | ASP | N-CA-C | 10.73 | 124.69 | 110.53 |
| 11 | aA | 574 | ASP | N-CA-C | 10.73 | 124.69 | 110.53 |
| 10 | j5 | 373 | ALA | CA-C-N | 10.72 | 136.61 | 120.31 |
| 10 | j5 | 373 | ALA | C-N-CA | 10.72 | 136.61 | 120.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 4 | M8 | 47 | VAL | N-CA-CB | -10.72 | 101.01 | 112.37 |
| 4 | M4 | 47 | VAL | N-CA-CB | -10.72 | 101.01 | 112.37 |
| 10 | k5 | 373 | ALA | CA-C-N | 10.70 | 136.57 | 120.31 |
| 10 | k5 | 373 | ALA | C-N-CA | 10.70 | 136.57 | 120.31 |
| 4 | MA | 47 | VAL | N-CA-CB | -10.66 | 101.07 | 112.37 |
| 4 | M9 | 47 | VAL | N-CA-CB | -10.66 | 101.07 | 112.37 |
| 4 | M3 | 47 | VAL | N-CA-CB | -10.66 | 101.07 | 112.37 |
| 4 | M1 | 47 | VAL | N-CA-CB | -10.66 | 101.07 | 112.37 |
| 3 | F4 | 110 | LEU | N-CA-CB | -10.65 | 92.49 | 110.49 |
| 9 | z7 | 22 | GLU | N-CA-C | 10.62 | 133.43 | 110.80 |
| 9 | w7 | 22 | GLU | N-CA-C | 10.61 | 133.41 | 110.80 |
| 10 | j5 | 253 | ARG | CA-C-N | 10.61 | 131.27 | 119.92 |
| 10 | j5 | 253 | ARG | C-N-CA | 10.61 | 131.27 | 119.92 |
| 10 | k5 | 582 | GLN | N-CA-C | 10.58 | 122.82 | 111.28 |
| 10 | k5 | 253 | ARG | CA-C-N | 10.58 | 131.24 | 119.92 |
| 10 | k5 | 253 | ARG | C-N-CA | 10.58 | 131.24 | 119.92 |
| 10 | j5 | 582 | GLN | N-CA-C | 10.57 | 122.80 | 111.28 |
| 11 | a9 | 52 | MET | N-CA-C | -10.45 | 99.80 | 112.54 |
| 11 | aA | 52 | MET | N-CA-C | -10.45 | 99.80 | 112.54 |
| 10 | k5 | 842 | LYS | N-CA-C | 10.44 | 122.41 | 111.14 |
| 10 | j5 | 842 | LYS | N-CA-C | 10.38 | 122.35 | 111.14 |
| 10 | j5 | 776 | PHE | N-CA-CB | 10.33 | 127.95 | 110.49 |
| 3 | Q8 | 109 | CYS | N-CA-C | 10.32 | 132.79 | 110.80 |
| 10 | k5 | 776 | PHE | N-CA-CB | 10.30 | 127.89 | 110.49 |
| 10 | k5 | 467 | PRO | CA-C-N | -10.29 | 109.08 | 122.77 |
| 10 | k5 | 467 | PRO | C-N-CA | -10.29 | 109.08 | 122.77 |
| 3 | O8 | 109 | CYS | N-CA-C | 10.29 | 132.72 | 110.80 |
| 10 | j5 | 467 | PRO | CA-C-N | -10.26 | 109.13 | 122.77 |
| 10 | j5 | 467 | PRO | C-N-CA | -10.26 | 109.13 | 122.77 |
| 10 | j5 | 988 | ALA | N-CA-C | 10.25 | 128.61 | 109.24 |
| 10 | k5 | 641 | ASP | CB-CA-C | -10.24 | 91.10 | 111.17 |
| 10 | k5 | 988 | ALA | N-CA-C | 10.24 | 128.59 | 109.24 |
| 11 | a9 | 288 | ARG | CA-C-N | 10.23 | 136.71 | 122.07 |
| 11 | a9 | 288 | ARG | C-N-CA | 10.23 | 136.71 | 122.07 |
| 11 | aA | 288 | ARG | CA-C-N | 10.23 | 136.71 | 122.07 |
| 11 | aA | 288 | ARG | C-N-CA | 10.23 | 136.71 | 122.07 |
| 4 | MA | 179 | TYR | N-CA-C | 10.23 | 123.48 | 111.71 |
| 10 | j5 | 641 | ASP | CB-CA-C | -10.23 | 91.12 | 111.17 |
| 4 | M9 | 179 | TYR | N-CA-C | 10.23 | 123.48 | 111.71 |
| 10 | j5 | 191 | GLU | N-CA-C | 10.22 | 124.85 | 112.38 |
| 10 | k5 | 191 | GLU | N-CA-C | 10.22 | 124.85 | 112.38 |
| 10 | k5 | 261 | ILE | N-CA-C | -10.22 | 100.21 | 112.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 4 | M4 | 179 | TYR | N-CA-C | 10.22 | 123.46 | 111.71 |
| 4 | M3 | 179 | TYR | N-CA-C | 10.21 | 123.46 | 111.71 |
| 4 | M1 | 179 | TYR | N-CA-C | 10.21 | 123.46 | 111.71 |
| 10 | j5 | 261 | ILE | N-CA-C | -10.21 | 100.22 | 112.98 |
| 10 | j5 | 486 | ILE | CA-C-O | -10.20 | 109.73 | 121.05 |
| 10 | k5 | 486 | ILE | CA-C-O | -10.20 | 109.73 | 121.05 |
| 10 | k5 | 393 | MET | CA-C-N | 10.19 | 132.58 | 119.84 |
| 10 | k5 | 393 | MET | C-N-CA | 10.19 | 132.58 | 119.84 |
| 10 | k5 | 889 | LEU | C-N-CD | -10.19 | 98.19 | 120.60 |
| 4 | M8 | 179 | TYR | N-CA-C | 10.18 | 123.42 | 111.71 |
| 10 | j5 | 889 | LEU | C-N-CD | -10.16 | 98.25 | 120.60 |
| 10 | j5 | 393 | MET | CA-C-N | 10.15 | 132.53 | 119.84 |
| 10 | j5 | 393 | MET | C-N-CA | 10.15 | 132.53 | 119.84 |
| 10 | j5 | 947 | MET | N-CA-C | 10.11 | 132.33 | 110.80 |
| 10 | k5 | 947 | MET | N-CA-C | 10.10 | 132.32 | 110.80 |
| 8 | a5 | 25 | ARG | N-CA-C | -10.10 | 100.11 | 111.82 |
| 4 | M8 | 122 | SER | CA-C-N | 10.08 | 133.79 | 120.28 |
| 4 | M8 | 122 | SER | C-N-CA | 10.08 | 133.79 | 120.28 |
| 10 | j5 | 730 | ASN | N-CA-CB | 10.07 | 127.52 | 110.49 |
| 10 | k5 | 730 | ASN | N-CA-CB | 10.07 | 127.51 | 110.49 |
| 4 | MA | 122 | SER | CA-C-N | 10.05 | 133.75 | 120.28 |
| 4 | MA | 122 | SER | C-N-CA | 10.05 | 133.75 | 120.28 |
| 9 | x7 | 19 | THR | N-CA-C | 10.05 | 125.83 | 113.17 |
| 4 | M9 | 122 | SER | CA-C-N | 10.05 | 133.75 | 120.28 |
| 4 | M9 | 122 | SER | C-N-CA | 10.05 | 133.75 | 120.28 |
| 9 | y7 | 19 | THR | N-CA-C | 10.01 | 125.79 | 113.17 |
| 9 | z5 | 58 | THR | N-CA-C | 9.99 | 125.78 | 113.50 |
| 10 | j5 | 969 | VAL | N-CA-C | 9.95 | 125.97 | 112.04 |
| 10 | k5 | 969 | VAL | N-CA-C | 9.93 | 125.94 | 112.04 |
| 10 | j5 | 743 | VAL | C-N-CD | -9.90 | 84.40 | 125.00 |
| 10 | k5 | 743 | VAL | C-N-CD | -9.89 | 84.44 | 125.00 |
| 10 | k5 | 370 | GLU | N-CA-C | 9.83 | 125.02 | 112.92 |
| 11 | a9 | 823 | ILE | N-CA-C | -9.83 | 95.69 | 106.21 |
| 10 | j5 | 370 | GLU | N-CA-C | 9.81 | 124.99 | 112.92 |
| 10 | k5 | 1118 | THR | N-CA-C | 9.81 | 122.05 | 111.36 |
| 8 | K5 | 121 | THR | CA-C-N | -9.81 | 108.04 | 120.79 |
| 8 | K5 | 121 | THR | C-N-CA | -9.81 | 108.04 | 120.79 |
| 8 | E5 | 121 | THR | CA-C-N | -9.81 | 108.04 | 120.79 |
| 8 | E5 | 121 | THR | C-N-CA | -9.81 | 108.04 | 120.79 |
| 8 | W7 | 121 | THR | CA-C-N | -9.81 | 108.04 | 120.79 |
| 8 | W7 | 121 | THR | C-N-CA | -9.81 | 108.04 | 120.79 |
| 8 | E7 | 121 | THR | CA-C-N | -9.80 | 108.05 | 120.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 8 | E7 | 121 | THR | C-N-CA | -9.80 | 108.05 | 120.79 |
| 10 | j5 | 619 | GLU | CB-CG-CD | -9.79 | 95.97 | 112.60 |
| 8 | K7 | 121 | THR | CA-C-N | -9.79 | 108.07 | 120.79 |
| 8 | K7 | 121 | THR | C-N-CA | -9.79 | 108.07 | 120.79 |
| 10 | k5 | 619 | GLU | CB-CG-CD | -9.78 | 95.97 | 112.60 |
| 9 | z5 | 56 | LEU | O-C-N | 9.77 | 132.13 | 122.07 |
| 10 | j5 | 1118 | THR | N-CA-C | 9.76 | 122.00 | 111.36 |
| 9 | i5 | 56 | LEU | O-C-N | 9.76 | 132.12 | 122.07 |
| 10 | j5 | 564 | VAL | CB-CA-C | -9.75 | 98.77 | 112.22 |
| 4 | MA | 98 | ASP | N-CA-C | 9.74 | 125.16 | 113.28 |
| 4 | M9 | 98 | ASP | N-CA-C | 9.74 | 125.16 | 113.28 |
| 8 | W5 | 121 | THR | CA-C-N | -9.73 | 108.14 | 120.79 |
| 8 | W5 | 121 | THR | C-N-CA | -9.73 | 108.14 | 120.79 |
| 8 | Q7 | 121 | THR | CA-C-N | -9.72 | 108.15 | 120.79 |
| 8 | Q7 | 121 | THR | C-N-CA | -9.72 | 108.15 | 120.79 |
| 4 | M8 | 99 | VAL | N-CA-CB | 9.72 | 127.27 | 111.23 |
| 10 | k5 | 564 | VAL | CB-CA-C | -9.72 | 98.81 | 112.22 |
| 8 | Q5 | 121 | THR | CA-C-N | -9.72 | 108.16 | 120.79 |
| 8 | Q5 | 121 | THR | C-N-CA | -9.72 | 108.16 | 120.79 |
| 4 | M3 | 98 | ASP | N-CA-C | 9.72 | 125.13 | 113.28 |
| 4 | M1 | 98 | ASP | N-CA-C | 9.72 | 125.13 | 113.28 |
| 10 | k5 | 1105 | ILE | N-CA-C | 9.67 | 119.62 | 110.53 |
| 11 | a9 | 57 | PHE | N-CA-C | 9.67 | 126.79 | 114.31 |
| 11 | aA | 57 | PHE | N-CA-C | 9.67 | 126.79 | 114.31 |
| 8 | u7 | 121 | THR | CA-C-N | -9.67 | 108.22 | 120.79 |
| 8 | u7 | 121 | THR | C-N-CA | -9.67 | 108.22 | 120.79 |
| 8 | o7 | 121 | THR | CA-C-N | -9.67 | 108.22 | 120.79 |
| 8 | o7 | 121 | THR | C-N-CA | -9.67 | 108.22 | 120.79 |
| 10 | j5 | 1105 | ILE | N-CA-C | 9.66 | 119.61 | 110.53 |
| 10 | j5 | 391 | SER | N-CA-C | -9.65 | 100.84 | 111.36 |
| 10 | j5 | 701 | ASP | CA-C-O | -9.63 | 110.34 | 120.55 |
| 9 | z7 | 11 | ILE | N-CA-C | 9.61 | 117.88 | 107.60 |
| 10 | k5 | 701 | ASP | CA-C-O | -9.61 | 110.37 | 120.55 |
| 11 | a9 | 620 | ALA | N-CA-C | 9.60 | 131.24 | 110.80 |
| 11 | aA | 620 | ALA | N-CA-C | 9.60 | 131.24 | 110.80 |
| 10 | k5 | 391 | SER | N-CA-C | -9.59 | 100.91 | 111.36 |
| 10 | k5 | 492 | ILE | CA-C-O | -9.59 | 111.00 | 121.17 |
| 9 | w7 | 11 | ILE | N-CA-C | 9.58 | 117.85 | 107.60 |
| 4 | M8 | 61 | ASN | CB-CA-C | -9.58 | 95.77 | 110.90 |
| 11 | aA | 637 | PRO | CA-C-N | 9.57 | 136.38 | 120.88 |
| 11 | aA | 637 | PRO | C-N-CA | 9.57 | 136.38 | 120.88 |
| 11 | a9 | 637 | PRO | CA-C-N | 9.56 | 136.37 | 120.88 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11 | a9 | 637 | PRO | C-N-CA | 9.56 | 136.37 | 120.88 |
| 8 | e5 | 25 | ARG | N-CA-C | -9.56 | 100.73 | 111.82 |
| 10 | j5 | 492 | ILE | CA-C-O | -9.56 | 111.04 | 121.17 |
| 4 | MA | 61 | ASN | CB-CA-C | -9.55 | 95.80 | 110.90 |
| 4 | M9 | 61 | ASN | CB-CA-C | -9.55 | 95.80 | 110.90 |
| 1 | D5 | 38 | VAL | CA-C-N | -9.55 | 108.05 | 120.65 |
| 1 | D5 | 38 | VAL | C-N-CA | -9.55 | 108.05 | 120.65 |
| 4 | M4 | 61 | ASN | CB-CA-C | -9.54 | 95.82 | 110.90 |
| 1 | J5 | 38 | VAL | CA-C-N | -9.54 | 108.06 | 120.65 |
| 1 | J5 | 38 | VAL | C-N-CA | -9.54 | 108.06 | 120.65 |
| 4 | M3 | 61 | ASN | CB-CA-C | -9.53 | 95.84 | 110.90 |
| 4 | M1 | 61 | ASN | CB-CA-C | -9.53 | 95.84 | 110.90 |
| 5 | Z4 | 24 | PRO | CA-C-N | 9.51 | 133.80 | 120.29 |
| 5 | Z4 | 24 | PRO | C-N-CA | 9.51 | 133.80 | 120.29 |
| 5 | Z8 | 25 | THR | CB-CA-C | -9.50 | 95.89 | 110.90 |
| 5 | NA | 25 | THR | CB-CA-C | -9.48 | 95.92 | 110.90 |
| 5 | N3 | 25 | THR | CB-CA-C | -9.48 | 95.93 | 110.90 |
| 5 | N1 | 25 | THR | CB-CA-C | -9.48 | 95.93 | 110.90 |
| 5 | N9 | 25 | THR | CB-CA-C | -9.47 | 95.94 | 110.90 |
| 10 | k5 | 740 | ASN | N-CA-C | 9.46 | 124.89 | 113.16 |
| 10 | j5 | 740 | ASN | N-CA-C | 9.46 | 124.88 | 113.16 |
| 4 | M8 | 269 | SER | CB-CA-C | 9.44 | 132.77 | 111.71 |
| 10 | k5 | 775 | VAL | O-C-N | -9.44 | 112.33 | 122.61 |
| 9 | z5 | 14 | LEU | N-CA-C | 9.43 | 121.64 | 111.36 |
| 10 | j5 | 285 | LYS | CA-C-N | 9.40 | 138.90 | 121.97 |
| 10 | j5 | 285 | LYS | C-N-CA | 9.40 | 138.90 | 121.97 |
| 9 | i5 | 14 | LEU | N-CA-C | 9.39 | 121.60 | 111.36 |
| 11 | aA | 632 | ILE | CA-C-N | -9.39 | 110.24 | 123.20 |
| 11 | aA | 632 | ILE | C-N-CA | -9.39 | 110.24 | 123.20 |
| 4 | MA | 126 | THR | N-CA-C | 9.39 | 121.59 | 111.36 |
| 4 | M9 | 126 | THR | N-CA-C | 9.39 | 121.59 | 111.36 |
| 10 | j5 | 775 | VAL | O-C-N | -9.38 | 112.39 | 122.61 |
| 11 | a9 | 632 | ILE | CA-C-N | -9.38 | 110.26 | 123.20 |
| 11 | a9 | 632 | ILE | C-N-CA | -9.38 | 110.26 | 123.20 |
| 4 | M4 | 126 | THR | N-CA-C | 9.37 | 121.58 | 111.36 |
| 4 | M3 | 126 | THR | N-CA-C | 9.37 | 121.57 | 111.36 |
| 11 | a9 | 340 | PRO | N-CA-C | -9.37 | 96.66 | 110.80 |
| 11 | aA | 340 | PRO | N-CA-C | -9.37 | 96.66 | 110.80 |
| 4 | M3 | 122 | SER | CA-C-N | 9.36 | 133.75 | 120.28 |
| 4 | M3 | 122 | SER | C-N-CA | 9.36 | 133.75 | 120.28 |
| 4 | M1 | 122 | SER | CA-C-N | 9.36 | 133.75 | 120.28 |
| 4 | M1 | 122 | SER | C-N-CA | 9.36 | 133.75 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4 | M1 | 126 | THR | N-CA-C | 9.35 | 121.55 | 111.36 |
| 4 | M4 | 122 | SER | CA-C-N | 9.34 | 133.73 | 120.28 |
| 4 | M4 | 122 | SER | C-N-CA | 9.34 | 133.73 | 120.28 |
| 10 | k5 | 285 | LYS | CA-C-N | 9.33 | 138.77 | 121.97 |
| 10 | k5 | 285 | LYS | C-N-CA | 9.33 | 138.77 | 121.97 |
| 4 | M8 | 126 | THR | N-CA-C | 9.33 | 121.53 | 111.36 |
| 9 | w7 | 7 | VAL | N-CA-C | 9.26 | 123.10 | 108.85 |
| 4 | M4 | 101 | ASP | N-CA-C | -9.24 | 101.16 | 111.14 |
| 8 | K5 | 115 | MET | O-C-N | 9.24 | 131.58 | 122.07 |
| 9 | z7 | 7 | VAL | N-CA-C | 9.23 | 123.07 | 108.85 |
| 4 | M3 | 101 | ASP | N-CA-C | -9.23 | 101.17 | 111.14 |
| 4 | M1 | 101 | ASP | N-CA-C | -9.23 | 101.17 | 111.14 |
| 4 | MA | 101 | ASP | N-CA-C | -9.22 | 101.18 | 111.14 |
| 11 | aA | 800 | THR | N-CA-C | 9.21 | 124.58 | 113.16 |
| 4 | M9 | 101 | ASP | N-CA-C | -9.19 | 101.22 | 111.14 |
| 11 | a9 | 800 | THR | N-CA-C | 9.19 | 124.55 | 113.16 |
| 11 | a9 | 618 | PRO | CA-C-N | -9.19 | 104.00 | 121.54 |
| 11 | a9 | 618 | PRO | C-N-CA | -9.19 | 104.00 | 121.54 |
| 11 | aA | 618 | PRO | CA-C-N | -9.19 | 104.00 | 121.54 |
| 11 | aA | 618 | PRO | C-N-CA | -9.19 | 104.00 | 121.54 |
| 8 | E5 | 115 | MET | O-C-N | 9.18 | 131.52 | 122.07 |
| 10 | k5 | 945 | LEU | N-CA-C | 9.18 | 123.74 | 109.52 |
| 10 | j5 | 369 | PRO | CA-C-N | -9.17 | 107.97 | 122.65 |
| 10 | j5 | 369 | PRO | C-N-CA | -9.17 | 107.97 | 122.65 |
| 10 | j5 | 945 | LEU | N-CA-C | 9.17 | 123.73 | 109.52 |
| 10 | j5 | 1071 | PRO | CA-N-CD | -9.16 | 99.17 | 112.00 |
| 10 | k5 | 1071 | PRO | CA-N-CD | -9.16 | 99.17 | 112.00 |
| 10 | k5 | 561 | GLU | N-CA-C | -9.16 | 89.77 | 108.18 |
| 11 | aA | 278 | LEU | N-CA-C | 9.15 | 121.26 | 111.28 |
| 9 | i5 | 58 | THR | N-CA-C | 9.15 | 125.68 | 113.97 |
| 10 | k5 | 369 | PRO | CA-C-N | -9.13 | 108.04 | 122.65 |
| 10 | k5 | 369 | PRO | C-N-CA | -9.13 | 108.04 | 122.65 |
| 11 | a9 | 278 | LEU | N-CA-C | 9.12 | 121.22 | 111.28 |
| 9 | y7 | 16 | ARG | N-CA-C | 9.10 | 130.19 | 110.80 |
| 9 | x7 | 16 | ARG | N-CA-C | 9.10 | 130.17 | 110.80 |
| 9 | x7 | 52 | LEU | N-CA-C | 9.09 | 121.27 | 111.36 |
| 10 | j5 | 643 | VAL | CB-CA-C | -9.08 | 99.69 | 112.22 |
| 9 | z7 | 56 | LEU | N-CA-C | 9.08 | 120.79 | 111.07 |
| 11 | a9 | 37 | GLY | N-CA-C | 9.08 | 134.70 | 113.18 |
| 11 | a9 | 332 | SER | N-CA-C | -9.08 | 102.78 | 114.04 |
| 11 | aA | 37 | GLY | N-CA-C | 9.08 | 134.70 | 113.18 |
| 11 | aA | 332 | SER | N-CA-C | -9.08 | 102.78 | 114.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9 | w7 | 56 | LEU | N-CA-C | 9.08 | 120.78 | 111.07 |
| 9 | y7 | 52 | LEU | N-CA-C | 9.07 | 121.24 | 111.36 |
| 11 | a9 | 360 | ALA | N-CA-C | 9.05 | 121.23 | 111.36 |
| 11 | aA | 360 | ALA | N-CA-C | 9.05 | 121.23 | 111.36 |
| 2 | KA | 25 | GLN | CA-C-N | -9.05 | 107.25 | 120.82 |
| 2 | KA | 25 | GLN | C-N-CA | -9.05 | 107.25 | 120.82 |
| 2 | K9 | 25 | GLN | CA-C-N | -9.05 | 107.25 | 120.82 |
| 2 | K9 | 25 | GLN | C-N-CA | -9.05 | 107.25 | 120.82 |
| 3 | FA | 143 | ASN | N-CA-C | 9.04 | 121.13 | 111.28 |
| 10 | k5 | 369 | PRO | O-C-N | -9.04 | 112.98 | 123.10 |
| 10 | k5 | 643 | VAL | CB-CA-C | -9.03 | 99.76 | 112.22 |
| 1 | h7 | 21 | GLY | N-CA-C | 9.02 | 123.55 | 112.73 |
| 10 | j5 | 369 | PRO | O-C-N | -9.00 | 113.02 | 123.10 |
| 8 | i7 | 125 | ALA | CA-C-N | 8.99 | 132.78 | 120.46 |
| 8 | i7 | 125 | ALA | C-N-CA | 8.99 | 132.78 | 120.46 |
| 8 | c7 | 125 | ALA | CA-C-N | 8.99 | 132.77 | 120.46 |
| 8 | c7 | 125 | ALA | C-N-CA | 8.99 | 132.77 | 120.46 |
| 10 | j5 | 589 | ALA | N-CA-C | -8.97 | 101.25 | 113.18 |
| 11 | a9 | 409 | ASP | N-CA-C | 8.96 | 123.52 | 112.59 |
| 10 | k5 | 589 | ALA | N-CA-C | -8.96 | 101.27 | 113.18 |
| 11 | aA | 409 | ASP | N-CA-C | 8.96 | 123.52 | 112.59 |
| 1 | b7 | 21 | GLY | N-CA-C | 8.94 | 123.46 | 112.73 |
| 3 | Q8 | 108 | ARG | CB-CA-C | 8.93 | 128.18 | 110.42 |
| 10 | j5 | 883 | SER | N-CA-C | 8.90 | 129.75 | 110.80 |
| 11 | aA | 292 | ALA | N-CA-C | -8.89 | 102.35 | 113.55 |
| 10 | k5 | 883 | SER | N-CA-C | 8.88 | 129.72 | 110.80 |
| 10 | k5 | 1056 | PRO | CA-N-CD | -8.88 | 99.56 | 112.00 |
| 10 | j5 | 1056 | PRO | CA-N-CD | -8.87 | 99.58 | 112.00 |
| 10 | k5 | 269 | LEU | N-CA-C | 8.87 | 129.69 | 110.80 |
| 10 | j5 | 269 | LEU | N-CA-C | 8.86 | 129.67 | 110.80 |
| 9 | y7 | 63 | ALA | N-CA-C | 8.85 | 129.65 | 110.80 |
| 10 | k5 | 597 | GLU | N-CA-C | 8.84 | 122.07 | 111.82 |
| 10 | k5 | 149 | GLY | CA-C-N | -8.83 | 108.80 | 119.84 |
| 10 | k5 | 149 | GLY | C-N-CA | -8.83 | 108.80 | 119.84 |
| 10 | k5 | 1109 | ASP | N-CA-C | 8.83 | 123.75 | 111.56 |
| 9 | w7 | 16 | ARG | N-CA-C | 8.83 | 131.57 | 113.20 |
| 9 | x7 | 63 | ALA | N-CA-C | 8.82 | 129.59 | 110.80 |
| 11 | a9 | 563 | PHE | CA-C-N | 8.81 | 128.67 | 120.21 |
| 11 | a9 | 563 | PHE | C-N-CA | 8.81 | 128.67 | 120.21 |
| 11 | aA | 563 | PHE | CA-C-N | 8.81 | 128.67 | 120.21 |
| 11 | aA | 563 | PHE | C-N-CA | 8.81 | 128.67 | 120.21 |
| 10 | j5 | 1109 | ASP | N-CA-C | 8.81 | 123.72 | 111.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9 | z7 | 16 | ARG | N-CA-C | 8.81 | 131.52 | 113.20 |
| 10 | k5 | 619 | GLU | N-CA-CB | -8.80 | 96.79 | 110.43 |
| 5 | Z4 | 23 | SER | O-C-N | 8.79 | 129.34 | 120.99 |
| 10 | j5 | 149 | GLY | CA-C-N | -8.79 | 108.85 | 119.84 |
| 10 | j5 | 149 | GLY | C-N-CA | -8.79 | 108.85 | 119.84 |
| 10 | j5 | 597 | GLU | N-CA-C | 8.79 | 122.02 | 111.82 |
| 10 | j5 | 484 | GLY | CA-C-O | -8.79 | 111.06 | 120.90 |
| 10 | k5 | 484 | GLY | CA-C-O | -8.77 | 111.07 | 120.90 |
| 11 | a9 | 632 | ILE | CB-CA-C | -8.77 | 97.86 | 111.71 |
| 11 | aA | 632 | ILE | CB-CA-C | -8.77 | 97.86 | 111.71 |
| 4 | MA | 123 | GLU | N-CA-C | 8.76 | 120.83 | 111.28 |
| 10 | j5 | 619 | GLU | N-CA-CB | -8.76 | 96.85 | 110.43 |
| 4 | M3 | 52 | LEU | N-CA-C | 8.75 | 120.82 | 111.28 |
| 8 | i7 | 128 | GLU | CB-CA-C | -8.75 | 97.14 | 110.88 |
| 4 | M8 | 52 | LEU | N-CA-C | 8.75 | 120.82 | 111.28 |
| 4 | M1 | 52 | LEU | N-CA-C | 8.75 | 120.82 | 111.28 |
| 10 | j5 | 615 | LYS | N-CA-C | 8.75 | 120.82 | 111.28 |
| 11 | a9 | 55 | ASP | N-CA-C | 8.75 | 120.59 | 111.14 |
| 10 | k5 | 615 | LYS | N-CA-C | 8.75 | 120.81 | 111.28 |
| 11 | aA | 55 | ASP | N-CA-C | 8.74 | 120.58 | 111.14 |
| 4 | MA | 43 | TYR | N-CA-CB | -8.74 | 96.13 | 111.08 |
| 4 | M9 | 43 | TYR | N-CA-CB | -8.74 | 96.13 | 111.08 |
| 4 | M8 | 123 | GLU | N-CA-C | 8.74 | 120.81 | 111.28 |
| 4 | MA | 52 | LEU | N-CA-C | 8.74 | 120.80 | 111.28 |
| 4 | M4 | 52 | LEU | N-CA-C | 8.74 | 120.80 | 111.28 |
| 4 | M9 | 123 | GLU | N-CA-C | 8.74 | 120.80 | 111.28 |
| 8 | c7 | 128 | GLU | CB-CA-C | -8.74 | 97.17 | 110.88 |
| 4 | M9 | 52 | LEU | N-CA-C | 8.74 | 120.80 | 111.28 |
| 4 | M4 | 43 | TYR | N-CA-CB | -8.73 | 96.15 | 111.08 |
| 4 | M8 | 43 | TYR | N-CA-CB | -8.73 | 96.15 | 111.08 |
| 4 | M3 | 43 | TYR | N-CA-CB | -8.72 | 96.17 | 111.08 |
| 4 | M1 | 43 | TYR | N-CA-CB | -8.72 | 96.17 | 111.08 |
| 10 | k5 | 1077 | ILE | CA-C-N | -8.70 | 97.53 | 122.15 |
| 10 | k5 | 1077 | ILE | C-N-CA | -8.70 | 97.53 | 122.15 |
| 5 | N3 | 64 | GLY | N-CA-C | 8.70 | 125.04 | 114.69 |
| 5 | N1 | 64 | GLY | N-CA-C | 8.70 | 125.04 | 114.69 |
| 5 | Z4 | 64 | GLY | N-CA-C | 8.69 | 125.04 | 114.69 |
| 10 | j5 | 1077 | ILE | CA-C-N | -8.69 | 97.55 | 122.15 |
| 10 | j5 | 1077 | ILE | C-N-CA | -8.69 | 97.55 | 122.15 |
| 10 | k5 | 1118 | THR | CB-CA-C | -8.68 | 96.09 | 110.85 |
| 8 | e5 | 24 | ASP | N-CA-C | -8.68 | 103.28 | 114.04 |
| 10 | j5 | 1118 | THR | CB-CA-C | -8.67 | 96.11 | 110.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 5 | NA | 64 | GLY | N-CA-C | 8.66 | 125.00 | 114.69 |
| 5 | N9 | 64 | GLY | N-CA-C | 8.66 | 125.00 | 114.69 |
| 10 | j5 | 984 | ILE | N-CA-C | 8.65 | 127.34 | 109.34 |
| 4 | M4 | 143 | VAL | N-CA-C | -8.64 | 101.80 | 110.62 |
| 10 | k5 | 984 | ILE | N-CA-C | 8.64 | 127.31 | 109.34 |
| 10 | j5 | 1107 | ASN | N-CA-CB | -8.63 | 95.90 | 110.49 |
| 8 | U7 | 22 | GLU | N-CA-C | -8.62 | 101.36 | 112.23 |
| 5 | Z8 | 64 | GLY | N-CA-C | 8.62 | 124.94 | 114.69 |
| 10 | j5 | 725 | LEU | CB-CG-CD2 | -8.60 | 84.89 | 110.70 |
| 8 | i7 | 124 | PRO | O-C-N | -8.60 | 110.60 | 122.30 |
| 10 | j5 | 880 | THR | N-CA-CB | 8.60 | 125.03 | 110.49 |
| 8 | c7 | 126 | VAL | CB-CA-C | -8.60 | 100.53 | 112.14 |
| 10 | k5 | 725 | LEU | CB-CG-CD2 | -8.59 | 84.93 | 110.70 |
| 8 | c7 | 124 | PRO | O-C-N | -8.59 | 110.62 | 122.30 |
| 8 | i7 | 126 | VAL | CB-CA-C | -8.57 | 100.57 | 112.14 |
| 10 | k5 | 880 | THR | N-CA-CB | 8.57 | 124.97 | 110.49 |
| 4 | MA | 154 | GLU | N-CA-C | 8.56 | 120.70 | 111.36 |
| 4 | M9 | 154 | GLU | N-CA-C | 8.56 | 120.70 | 111.36 |
| 4 | M3 | 154 | GLU | N-CA-C | 8.56 | 120.69 | 111.36 |
| 4 | M8 | 154 | GLU | N-CA-C | 8.54 | 120.66 | 111.36 |
| 11 | a9 | 344 | ALA | N-CA-C | -8.54 | 96.95 | 109.50 |
| 11 | aA | 344 | ALA | N-CA-C | -8.54 | 96.95 | 109.50 |
| 4 | M1 | 154 | GLU | N-CA-C | 8.53 | 120.66 | 111.36 |
| 4 | MA | 3 | VAL | CA-C-N | 8.53 | 136.50 | 120.97 |
| 4 | MA | 3 | VAL | C-N-CA | 8.53 | 136.50 | 120.97 |
| 4 | M3 | 3 | VAL | CA-C-N | 8.53 | 136.49 | 120.97 |
| 4 | M3 | 3 | VAL | C-N-CA | 8.53 | 136.49 | 120.97 |
| 4 | M9 | 3 | VAL | CA-C-N | 8.53 | 136.50 | 120.97 |
| 4 | M9 | 3 | VAL | C-N-CA | 8.53 | 136.50 | 120.97 |
| 4 | M1 | 3 | VAL | CA-C-N | 8.53 | 136.49 | 120.97 |
| 4 | M1 | 3 | VAL | C-N-CA | 8.53 | 136.49 | 120.97 |
| 10 | j5 | 511 | ARG | CG-CD-NE | -8.53 | 93.24 | 112.00 |
| 4 | M4 | 154 | GLU | N-CA-C | 8.53 | 120.65 | 111.36 |
| 10 | k5 | 56 | ILE | CB-CA-C | -8.52 | 100.64 | 112.14 |
| 10 | k5 | 520 | ARG | N-CA-C | -8.52 | 103.03 | 113.50 |
| 11 | a9 | 292 | ALA | N-CA-C | -8.52 | 103.42 | 113.21 |
| 4 | M4 | 3 | VAL | CA-C-N | 8.51 | 136.46 | 120.97 |
| 4 | M4 | 3 | VAL | C-N-CA | 8.51 | 136.46 | 120.97 |
| 10 | k5 | 511 | ARG | CG-CD-NE | -8.51 | 93.28 | 112.00 |
| 10 | k5 | 777 | ASP | N-CA-CB | -8.50 | 97.42 | 111.53 |
| 10 | j5 | 56 | ILE | CB-CA-C | -8.49 | 100.67 | 112.14 |
| 10 | k5 | 261 | ILE | O-C-N | -8.48 | 111.74 | 122.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4 | M8 | 3 | VAL | CA-C-N | 8.48 | 136.41 | 120.97 |
| 4 | M8 | 3 | VAL | C-N-CA | 8.48 | 136.41 | 120.97 |
| 10 | j5 | 777 | ASP | N-CA-CB | -8.48 | 97.45 | 111.53 |
| 10 | k5 | 417 | GLU | N-CA-C | 8.48 | 128.86 | 110.80 |
| 10 | j5 | 261 | ILE | O-C-N | -8.48 | 111.74 | 122.17 |
| 10 | j5 | 417 | GLU | N-CA-C | 8.48 | 128.85 | 110.80 |
| 8 | c7 | 32 | SER | CA-C-N | 8.46 | 138.00 | 121.41 |
| 8 | c7 | 32 | SER | C-N-CA | 8.46 | 138.00 | 121.41 |
| 8 | O7 | 20 | PRO | N-CA-CB | -8.46 | 94.37 | 103.25 |
| 8 | c7 | 7 | ALA | N-CA-C | 8.45 | 120.57 | 111.36 |
| 11 | a9 | 50 | LEU | CA-C-N | 8.45 | 132.45 | 120.28 |
| 11 | a9 | 50 | LEU | C-N-CA | 8.45 | 132.45 | 120.28 |
| 11 | aA | 50 | LEU | CA-C-N | 8.45 | 132.45 | 120.28 |
| 11 | aA | 50 | LEU | C-N-CA | 8.45 | 132.45 | 120.28 |
| 10 | j5 | 520 | ARG | N-CA-C | -8.45 | 103.11 | 113.50 |
| 10 | j5 | 842 | LYS | CB-CA-C | -8.44 | 97.56 | 110.90 |
| 8 | K5 | 7 | ALA | N-CA-C | 8.43 | 120.55 | 111.36 |
| 10 | k5 | 842 | LYS | CB-CA-C | -8.43 | 97.58 | 110.90 |
| 8 | i7 | 7 | ALA | N-CA-C | 8.43 | 120.54 | 111.36 |
| 10 | j5 | 1152 | TYR | N-CA-C | 8.42 | 123.71 | 110.32 |
| 8 | i7 | 32 | SER | CA-C-N | 8.42 | 137.92 | 121.41 |
| 8 | i7 | 32 | SER | C-N-CA | 8.42 | 137.92 | 121.41 |
| 8 | o7 | 32 | SER | CA-C-N | 8.42 | 137.91 | 121.41 |
| 8 | o7 | 32 | SER | C-N-CA | 8.42 | 137.91 | 121.41 |
| 4 | M4 | 68 | ASP | N-CA-C | 8.41 | 122.19 | 108.99 |
| 4 | M3 | 68 | ASP | N-CA-C | 8.40 | 122.18 | 108.99 |
| 8 | E7 | 32 | SER | CA-C-N | 8.40 | 137.87 | 121.41 |
| 8 | E7 | 32 | SER | C-N-CA | 8.40 | 137.87 | 121.41 |
| 4 | M9 | 68 | ASP | N-CA-C | 8.40 | 122.17 | 108.99 |
| 8 | E5 | 32 | SER | CA-C-N | 8.39 | 137.86 | 121.41 |
| 8 | E5 | 32 | SER | C-N-CA | 8.39 | 137.86 | 121.41 |
| 8 | E5 | 7 | ALA | N-CA-C | 8.39 | 120.51 | 111.36 |
| 8 | W5 | 7 | ALA | N-CA-C | 8.39 | 120.50 | 111.36 |
| 10 | k5 | 663 | ALA | N-CA-C | -8.39 | 99.96 | 112.04 |
| 4 | MA | 68 | ASP | N-CA-C | 8.39 | 122.16 | 108.99 |
| 8 | Q5 | 7 | ALA | N-CA-C | 8.39 | 120.50 | 111.36 |
| 10 | j5 | 663 | ALA | N-CA-C | -8.39 | 99.96 | 112.04 |
| 4 | M1 | 68 | ASP | N-CA-C | 8.39 | 122.16 | 108.99 |
| 8 | u7 | 32 | SER | CA-C-N | 8.38 | 137.84 | 121.41 |
| 8 | u7 | 32 | SER | C-N-CA | 8.38 | 137.84 | 121.41 |
| 8 | K5 | 32 | SER | CA-C-N | 8.38 | 137.84 | 121.41 |
| 8 | K5 | 32 | SER | C-N-CA | 8.38 | 137.84 | 121.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8 | K7 | 32 | SER | CA-C-N | 8.38 | 137.84 | 121.41 |
| 8 | K7 | 32 | SER | C-N-CA | 8.38 | 137.84 | 121.41 |
| 11 | a9 | 288 | ARG | O-C-N | 8.38 | 133.73 | 122.59 |
| 11 | aA | 288 | ARG | O-C-N | 8.38 | 133.73 | 122.59 |
| 4 | M8 | 68 | ASP | N-CA-C | 8.38 | 122.14 | 108.99 |
| 10 | j5 | 428 | VAL | CB-CA-C | -8.37 | 100.84 | 112.14 |
| 8 | Q5 | 32 | SER | CA-C-N | 8.37 | 137.81 | 121.41 |
| 8 | Q5 | 32 | SER | C-N-CA | 8.37 | 137.81 | 121.41 |
| 8 | W7 | 32 | SER | CA-C-N | 8.37 | 137.81 | 121.41 |
| 8 | W7 | 32 | SER | C-N-CA | 8.37 | 137.81 | 121.41 |
| 10 | k5 | 428 | VAL | CB-CA-C | -8.36 | 100.85 | 112.14 |
| 8 | Q7 | 32 | SER | CA-C-N | 8.36 | 137.79 | 121.41 |
| 8 | W5 | 32 | SER | CA-C-N | 8.36 | 137.79 | 121.41 |
| 8 | W5 | 32 | SER | C-N-CA | 8.36 | 137.79 | 121.41 |
| 10 | j5 | 1005 | LEU | N-CA-C | -8.36 | 95.61 | 109.07 |
| 8 | Q7 | 32 | SER | C-N-CA | 8.36 | 137.79 | 121.41 |
| 8 | W7 | 7 | ALA | N-CA-C | 8.36 | 120.47 | 111.36 |
| 8 | K7 | 7 | ALA | N-CA-C | 8.35 | 120.46 | 111.36 |
| 9 | w7 | 38 | PHE | CB-CA-C | -8.35 | 96.92 | 110.79 |
| 10 | k5 | 1005 | LEU | N-CA-C | -8.34 | 95.64 | 109.07 |
| 9 | z7 | 38 | PHE | CB-CA-C | -8.34 | 96.95 | 110.79 |
| 8 | Q7 | 7 | ALA | N-CA-C | 8.33 | 120.44 | 111.36 |
| 8 | E7 | 7 | ALA | N-CA-C | 8.31 | 120.42 | 111.36 |
| 10 | k5 | 696 | ARG | N-CA-C | -8.31 | 97.99 | 110.28 |
| 8 | c7 | 32 | SER | O-C-N | -8.31 | 111.73 | 122.37 |
| 10 | k5 | 487 | PHE | N-CA-C | 8.30 | 128.48 | 110.80 |
| 8 | i7 | 32 | SER | O-C-N | -8.29 | 111.75 | 122.37 |
| 10 | j5 | 487 | PHE | N-CA-C | 8.29 | 128.46 | 110.80 |
| 10 | j5 | 696 | ARG | N-CA-C | -8.29 | 98.01 | 110.28 |
| 8 | E7 | 32 | SER | O-C-N | -8.27 | 111.78 | 122.37 |
| 8 | Q7 | 32 | SER | O-C-N | -8.25 | 111.81 | 122.37 |
| 8 | c7 | 144 | ASP | N-CA-C | 8.25 | 120.35 | 111.36 |
| 4 | M8 | 68 | ASP | CB-CA-C | -8.24 | 92.39 | 109.94 |
| 4 | M4 | 68 | ASP | CB-CA-C | -8.24 | 92.39 | 109.94 |
| 4 | M3 | 68 | ASP | CB-CA-C | -8.24 | 92.39 | 109.94 |
| 4 | M1 | 68 | ASP | CB-CA-C | -8.24 | 92.40 | 109.94 |
| 10 | k5 | 619 | GLU | N-CA-C | 8.23 | 124.85 | 113.16 |
| 4 | MA | 68 | ASP | CB-CA-C | -8.23 | 92.41 | 109.94 |
| 4 | M9 | 68 | ASP | CB-CA-C | -8.23 | 92.41 | 109.94 |
| 11 | a9 | 81 | ASP | N-CA-C | -8.23 | 87.96 | 111.00 |
| 11 | aA | 81 | ASP | N-CA-C | -8.23 | 87.96 | 111.00 |
| 10 | k5 | 141 | GLU | CA-C-N | -8.22 | 111.51 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10 | k5 | 141 | GLU | C-N-CA | -8.22 | 111.51 | 119.90 |
| 8 | i7 | 144 | ASP | N-CA-C | 8.22 | 120.33 | 111.36 |
| 4 | M8 | 142 | PHE | CA-C-N | -8.22 | 108.74 | 120.42 |
| 4 | M8 | 142 | PHE | C-N-CA | -8.22 | 108.74 | 120.42 |
| 5 | Z8 | 38 | GLU | CA-C-N | 8.22 | 128.32 | 119.28 |
| 5 | Z8 | 38 | GLU | C-N-CA | 8.22 | 128.32 | 119.28 |
| 10 | k5 | 1152 | TYR | N-CA-C | 8.21 | 123.76 | 109.96 |
| 8 | u7 | 32 | SER | O-C-N | -8.21 | 111.86 | 122.37 |
| 10 | j5 | 141 | GLU | CA-C-N | -8.21 | 111.53 | 119.90 |
| 10 | j5 | 141 | GLU | C-N-CA | -8.21 | 111.53 | 119.90 |
| 10 | j5 | 619 | GLU | N-CA-C | 8.21 | 124.81 | 113.16 |
| 8 | K7 | 32 | SER | O-C-N | -8.21 | 111.86 | 122.37 |
| 11 | a9 | 59 | ARG | CA-C-N | 8.21 | 129.26 | 119.99 |
| 11 | a9 | 59 | ARG | C-N-CA | 8.21 | 129.26 | 119.99 |
| 11 | aA | 59 | ARG | CA-C-N | 8.21 | 129.26 | 119.99 |
| 11 | aA | 59 | ARG | C-N-CA | 8.21 | 129.26 | 119.99 |
| 8 | E5 | 32 | SER | O-C-N | -8.19 | 111.89 | 122.37 |
| 8 | W5 | 32 | SER | O-C-N | -8.19 | 111.89 | 122.37 |
| 10 | j5 | 732 | ARG | N-CA-C | -8.18 | 93.59 | 107.99 |
| 1 | D7 | 67 | ARG | CB-CA-C | -8.18 | 99.25 | 109.31 |
| 8 | K5 | 32 | SER | O-C-N | -8.18 | 111.90 | 122.37 |
| 8 | W7 | 32 | SER | O-C-N | -8.16 | 111.92 | 122.37 |
| 8 | o7 | 32 | SER | O-C-N | -8.16 | 111.92 | 122.37 |
| 8 | Q5 | 32 | SER | O-C-N | -8.16 | 111.93 | 122.37 |
| 11 | aA | 812 | ASP | CA-C-N | 8.16 | 127.74 | 118.85 |
| 11 | aA | 812 | ASP | C-N-CA | 8.16 | 127.74 | 118.85 |
| 11 | a9 | 812 | ASP | CA-C-N | 8.15 | 127.73 | 118.85 |
| 11 | a9 | 812 | ASP | C-N-CA | 8.15 | 127.73 | 118.85 |
| 11 | a9 | 585 | GLU | CB-CA-C | -8.15 | 97.26 | 110.79 |
| 11 | a9 | 638 | ALA | N-CA-CB | -8.14 | 98.10 | 110.07 |
| 11 | aA | 638 | ALA | N-CA-CB | -8.14 | 98.10 | 110.07 |
| 10 | j5 | 84 | TYR | N-CA-C | 8.14 | 120.15 | 111.28 |
| 5 | N3 | 38 | GLU | CA-C-N | 8.13 | 128.23 | 119.28 |
| 5 | N3 | 38 | GLU | C-N-CA | 8.13 | 128.23 | 119.28 |
| 10 | k5 | 84 | TYR | N-CA-C | 8.13 | 120.14 | 111.28 |
| 1 | J7 | 67 | ARG | CB-CA-C | -8.13 | 99.31 | 109.31 |
| 11 | aA | 585 | GLU | CB-CA-C | -8.13 | 97.30 | 110.79 |
| 4 | M3 | 85 | VAL | N-CA-C | 8.12 | 119.89 | 112.17 |
| 4 | M1 | 85 | VAL | N-CA-C | 8.12 | 119.89 | 112.17 |
| 8 | E5 | 113 | LYS | CA-C-N | 8.12 | 137.25 | 122.79 |
| 8 | E5 | 113 | LYS | C-N-CA | 8.12 | 137.25 | 122.79 |
| 5 | NA | 38 | GLU | CA-C-N | 8.11 | 128.20 | 119.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 5 | NA | 38 | GLU | C-N-CA | 8.11 | 128.20 | 119.28 |
| 5 | N9 | 38 | GLU | CA-C-N | 8.11 | 128.20 | 119.28 |
| 5 | N9 | 38 | GLU | C-N-CA | 8.11 | 128.20 | 119.28 |
| 5 | N1 | 38 | GLU | CA-C-N | 8.11 | 128.20 | 119.28 |
| 5 | N1 | 38 | GLU | C-N-CA | 8.11 | 128.20 | 119.28 |
| 8 | K5 | 113 | LYS | CA-C-N | 8.11 | 137.22 | 122.79 |
| 8 | K5 | 113 | LYS | C-N-CA | 8.11 | 137.22 | 122.79 |
| 10 | j5 | 289 | SER | N-CA-C | 8.10 | 122.59 | 112.87 |
| 10 | k5 | 864 | GLY | CA-C-O | -8.10 | 112.07 | 120.66 |
| 9 | x7 | 21 | ARG | N-CA-C | 8.10 | 128.06 | 110.80 |
| 4 | M8 | 8 | SER | N-CA-C | 8.10 | 122.07 | 109.52 |
| 9 | y7 | 21 | ARG | N-CA-C | 8.10 | 128.04 | 110.80 |
| 4 | M4 | 8 | SER | N-CA-C | 8.09 | 122.05 | 109.52 |
| 10 | k5 | 20 | VAL | N-CA-C | 8.09 | 126.16 | 109.34 |
| 4 | M8 | 85 | VAL | N-CA-C | 8.09 | 119.85 | 112.17 |
| 11 | a9 | 57 | PHE | O-C-N | -8.09 | 113.44 | 122.34 |
| 11 | aA | 57 | PHE | O-C-N | -8.09 | 113.44 | 122.34 |
| 10 | j5 | 761 | ARG | N-CA-C | 8.08 | 120.09 | 111.28 |
| 4 | M3 | 8 | SER | N-CA-C | 8.08 | 122.05 | 109.52 |
| 4 | M1 | 8 | SER | N-CA-C | 8.08 | 122.05 | 109.52 |
| 8 | Q5 | 160 | MET | N-CA-C | -8.07 | 93.61 | 110.80 |
| 10 | k5 | 289 | SER | N-CA-C | 8.07 | 122.56 | 112.87 |
| 10 | j5 | 1119 | LEU | CA-C-N | -8.07 | 111.91 | 119.82 |
| 10 | j5 | 1119 | LEU | C-N-CA | -8.07 | 111.91 | 119.82 |
| 4 | MA | 8 | SER | N-CA-C | 8.07 | 122.02 | 109.52 |
| 8 | K5 | 104 | ILE | CB-CA-C | -8.06 | 101.65 | 111.97 |
| 10 | j5 | 20 | VAL | N-CA-C | 8.06 | 126.11 | 109.34 |
| 10 | j5 | 842 | LYS | CB-CG-CD | -8.06 | 92.76 | 111.30 |
| 10 | j5 | 864 | GLY | CA-C-O | -8.06 | 112.12 | 120.66 |
| 10 | k5 | 845 | ALA | N-CA-C | -8.05 | 103.36 | 113.02 |
| 4 | MA | 85 | VAL | N-CA-C | 8.05 | 119.82 | 112.17 |
| 8 | W5 | 160 | MET | N-CA-C | -8.05 | 93.66 | 110.80 |
| 10 | k5 | 761 | ARG | N-CA-C | 8.05 | 120.05 | 111.28 |
| 4 | M9 | 8 | SER | N-CA-C | 8.05 | 122.00 | 109.52 |
| 10 | j5 | 1096 | ILE | N-CA-C | 8.04 | 118.84 | 110.72 |
| 10 | k5 | 842 | LYS | CB-CG-CD | -8.04 | 92.80 | 111.30 |
| 10 | j5 | 494 | PRO | N-CA-C | 8.04 | 124.37 | 111.26 |
| 4 | M4 | 85 | VAL | N-CA-C | 8.04 | 119.81 | 112.17 |
| 8 | E5 | 104 | ILE | CB-CA-C | -8.04 | 101.68 | 111.97 |
| 3 | FA | 144 | SER | CA-C-N | 8.03 | 129.88 | 119.84 |
| 3 | FA | 144 | SER | C-N-CA | 8.03 | 129.88 | 119.84 |
| 5 | Z4 | 39 | PRO | N-CD-CG | -8.03 | 91.15 | 103.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4 | M9 | 85 | VAL | N-CA-C | 8.03 | 119.80 | 112.17 |
| 10 | k5 | 1119 | LEU | CA-C-N | -8.03 | 111.95 | 119.82 |
| 10 | k5 | 1119 | LEU | C-N-CA | -8.03 | 111.95 | 119.82 |
| 10 | j5 | 845 | ALA | N-CA-C | -8.02 | 103.40 | 113.02 |
| 9 | w7 | 19 | THR | N-CA-C | 8.02 | 125.64 | 113.61 |
| 10 | k5 | 494 | PRO | N-CA-C | 8.01 | 124.32 | 111.26 |
| 11 | a9 | 107 | ARG | CA-C-N | 8.00 | 128.48 | 119.92 |
| 11 | a9 | 107 | ARG | C-N-CA | 8.00 | 128.48 | 119.92 |
| 9 | z7 | 19 | THR | N-CA-C | 8.00 | 125.60 | 113.61 |
| 10 | k5 | 1096 | ILE | N-CA-C | 7.99 | 118.79 | 110.72 |
| 11 | aA | 107 | ARG | CA-C-N | 7.98 | 128.45 | 119.92 |
| 11 | aA | 107 | ARG | C-N-CA | 7.98 | 128.45 | 119.92 |
| 11 | a9 | 98 | ILE | CA-C-N | -7.97 | 102.36 | 121.80 |
| 11 | a9 | 98 | ILE | C-N-CA | -7.97 | 102.36 | 121.80 |
| 3 | Q4 | 86 | MET | N-CA-C | -7.96 | 102.55 | 111.14 |
| 11 | aA | 98 | ILE | CA-C-N | -7.96 | 102.39 | 121.80 |
| 11 | aA | 98 | ILE | C-N-CA | -7.96 | 102.39 | 121.80 |
| 3 | L1 | 77 | ARG | CB-CA-C | -7.94 | 96.11 | 109.53 |
| 4 | M3 | 123 | GLU | N-CA-C | 7.94 | 120.84 | 111.71 |
| 4 | M1 | 123 | GLU | N-CA-C | 7.94 | 120.84 | 111.71 |
| 8 | I7 | 22 | GLU | N-CA-C | -7.94 | 103.75 | 113.19 |
| 4 | M4 | 123 | GLU | N-CA-C | 7.92 | 120.82 | 111.71 |
| 3 | Q4 | 84 | ARG | CB-CA-C | -7.91 | 98.46 | 110.88 |
| 4 | MA | 108 | ALA | N-CA-C | 7.91 | 119.98 | 111.36 |
| 4 | M9 | 108 | ALA | N-CA-C | 7.91 | 119.98 | 111.36 |
| 4 | M8 | 211 | GLN | N-CA-C | -7.91 | 93.96 | 110.80 |
| 4 | M8 | 108 | ALA | N-CA-C | 7.90 | 119.97 | 111.36 |
| 10 | j5 | 635 | LEU | N-CA-C | -7.89 | 95.39 | 108.34 |
| 4 | M4 | 108 | ALA | N-CA-C | 7.89 | 119.96 | 111.36 |
| 10 | k5 | 635 | LEU | N-CA-C | -7.89 | 95.40 | 108.34 |
| 4 | M3 | 108 | ALA | N-CA-C | 7.88 | 119.95 | 111.36 |
| 4 | M1 | 108 | ALA | N-CA-C | 7.88 | 119.95 | 111.36 |
| 10 | j5 | 729 | ILE | N-CA-CB | 7.86 | 124.19 | 111.23 |
| 4 | MA | 259 | ARG | N-CA-C | 7.83 | 127.48 | 110.80 |
| 4 | M8 | 259 | ARG | N-CA-C | 7.83 | 127.49 | 110.80 |
| 4 | M9 | 259 | ARG | N-CA-C | 7.83 | 127.48 | 110.80 |
| 4 | M3 | 259 | ARG | N-CA-C | 7.83 | 127.47 | 110.80 |
| 4 | M1 | 259 | ARG | N-CA-C | 7.83 | 127.47 | 110.80 |
| 10 | k5 | 729 | ILE | N-CA-CB | 7.82 | 124.13 | 111.23 |
| 11 | aA | 633 | THR | N-CA-C | -7.81 | 97.52 | 108.54 |
| 4 | M4 | 259 | ARG | N-CA-C | 7.81 | 127.44 | 110.80 |
| 11 | a9 | 621 | THR | CA-C-N | 7.81 | 136.45 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 11 | a9 | 621 | THR | C-N-CA | 7.81 | 136.45 | 121.54 |
| 11 | aA | 621 | THR | CA-C-N | 7.81 | 136.45 | 121.54 |
| 11 | aA | 621 | THR | C-N-CA | 7.81 | 136.45 | 121.54 |
| 10 | k5 | 677 | ASP | CB-CA-C | -7.80 | 94.89 | 110.42 |
| 10 | k5 | 16 | LEU | N-CA-C | 7.80 | 119.86 | 111.36 |
| 10 | j5 | 16 | LEU | N-CA-C | 7.79 | 119.86 | 111.36 |
| 10 | j5 | 677 | ASP | CB-CA-C | -7.79 | 94.91 | 110.42 |
| 10 | j5 | 1120 | PRO | N-CA-C | 7.79 | 124.03 | 113.98 |
| 10 | j5 | 326 | GLY | N-CA-C | 7.79 | 125.72 | 115.36 |
| 11 | a9 | 633 | THR | N-CA-C | -7.79 | 97.56 | 108.54 |
| 10 | k5 | 1120 | PRO | N-CA-C | 7.78 | 124.02 | 113.98 |
| 10 | j5 | 939 | GLN | CB-CA-C | -7.78 | 98.67 | 110.88 |
| 10 | k5 | 939 | GLN | CB-CA-C | -7.78 | 98.67 | 110.88 |
| 10 | k5 | 743 | VAL | O-C-N | -7.75 | 115.46 | 120.42 |
| 8 | o7 | 48 | GLU | CA-C-N | -7.75 | 109.39 | 122.11 |
| 8 | o7 | 48 | GLU | C-N-CA | -7.75 | 109.39 | 122.11 |
| 10 | k5 | 141 | GLU | N-CA-C | 7.75 | 126.94 | 109.81 |
| 10 | k5 | 326 | GLY | N-CA-C | 7.75 | 125.67 | 115.36 |
| 10 | j5 | 141 | GLU | N-CA-C | 7.75 | 126.93 | 109.81 |
| 10 | j5 | 743 | VAL | O-C-N | -7.74 | 115.46 | 120.42 |
| 8 | u7 | 48 | GLU | CA-C-N | -7.74 | 109.42 | 122.11 |
| 8 | u7 | 48 | GLU | C-N-CA | -7.74 | 109.42 | 122.11 |
| 9 | w7 | 35 | GLU | N-CA-C | 7.73 | 120.60 | 111.71 |
| 11 | a9 | 602 | PRO | N-CA-C | 7.73 | 123.39 | 111.11 |
| 11 | aA | 602 | PRO | N-CA-C | 7.73 | 123.39 | 111.11 |
| 5 | Z4 | 23 | SER | C-N-CD | -7.71 | 93.37 | 125.00 |
| 9 | z7 | 35 | GLU | N-CA-C | 7.71 | 120.58 | 111.71 |
| 11 | aA | 380 | ARG | CA-C-N | 7.71 | 127.64 | 119.85 |
| 11 | aA | 380 | ARG | C-N-CA | 7.71 | 127.64 | 119.85 |
| 11 | a9 | 806 | GLY | N-CA-C | 7.71 | 131.44 | 113.18 |
| 11 | aA | 806 | GLY | N-CA-C | 7.71 | 131.44 | 113.18 |
| 10 | j5 | 651 | ILE | CG1-CB-CG2 | -7.70 | 87.61 | 110.70 |
| 10 | k5 | 651 | ILE | CG1-CB-CG2 | -7.70 | 87.61 | 110.70 |
| 3 | F9 | 143 | ASN | N-CA-C | 7.70 | 119.67 | 111.28 |
| 10 | k5 | 705 | THR | N-CA-CB | 7.69 | 124.05 | 110.37 |
| 9 | z7 | 36 | ASN | CA-C-N | -7.68 | 106.86 | 121.54 |
| 9 | z7 | 36 | ASN | C-N-CA | -7.68 | 106.86 | 121.54 |
| 3 | L2 | 77 | ARG | CA-C-N | -7.68 | 109.39 | 120.29 |
| 3 | L2 | 77 | ARG | C-N-CA | -7.68 | 109.39 | 120.29 |
| 5 | NA | 27 | ALA | N-CA-C | 7.68 | 122.10 | 111.74 |
| 5 | N9 | 27 | ALA | N-CA-C | 7.68 | 122.10 | 111.74 |
| 10 | j5 | 972 | GLY | CA-C-N | 7.67 | 136.19 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10 | j5 | 972 | GLY | C-N-CA | 7.67 | 136.19 | 121.54 |
| 9 | w7 | 36 | ASN | CA-C-N | -7.67 | 106.89 | 121.54 |
| 9 | w7 | 36 | ASN | C-N-CA | -7.67 | 106.89 | 121.54 |
| 11 | a9 | 380 | ARG | CA-C-N | 7.67 | 127.60 | 119.85 |
| 11 | a9 | 380 | ARG | C-N-CA | 7.67 | 127.60 | 119.85 |
| 10 | k5 | 972 | GLY | CA-C-N | 7.66 | 136.18 | 121.54 |
| 10 | k5 | 972 | GLY | C-N-CA | 7.66 | 136.18 | 121.54 |
| 5 | Z8 | 27 | ALA | N-CA-C | 7.66 | 122.08 | 111.74 |
| 5 | N3 | 27 | ALA | N-CA-C | 7.65 | 122.07 | 111.74 |
| 10 | k5 | 427 | GLY | CA-C-N | 7.65 | 130.94 | 120.46 |
| 10 | k5 | 427 | GLY | C-N-CA | 7.65 | 130.94 | 120.46 |
| 5 | N1 | 27 | ALA | N-CA-C | 7.65 | 122.07 | 111.74 |
| 10 | k5 | 277 | ILE | N-CA-C | 7.65 | 125.25 | 109.34 |
| 10 | j5 | 277 | ILE | N-CA-C | 7.65 | 125.24 | 109.34 |
| 10 | j5 | 427 | GLY | CA-C-N | 7.65 | 130.94 | 120.46 |
| 10 | j5 | 427 | GLY | C-N-CA | 7.65 | 130.94 | 120.46 |
| 10 | k5 | 1130 | VAL | N-CA-C | 7.64 | 118.44 | 110.72 |
| 10 | j5 | 561 | GLU | N-CA-C | -7.64 | 94.53 | 110.80 |
| 10 | j5 | 856 | ARG | N-CA-C | 7.63 | 119.68 | 111.36 |
| 10 | j5 | 705 | THR | N-CA-CB | 7.63 | 123.96 | 110.37 |
| 8 | i7 | 126 | VAL | N-CA-C | 7.63 | 118.40 | 110.62 |
| 10 | k5 | 732 | ARG | N-CA-C | -7.62 | 93.58 | 107.75 |
| 10 | j5 | 1130 | VAL | N-CA-C | 7.61 | 118.41 | 110.72 |
| 10 | k5 | 1006 | ASP | CA-C-O | -7.61 | 112.76 | 120.90 |
| 4 | MA | 59 | ILE | CB-CA-C | -7.61 | 101.87 | 112.14 |
| 10 | k5 | 856 | ARG | N-CA-C | 7.61 | 119.65 | 111.36 |
| 4 | M9 | 59 | ILE | CB-CA-C | -7.61 | 101.87 | 112.14 |
| 11 | a9 | 521 | PHE | N-CA-C | 7.60 | 119.20 | 111.07 |
| 11 | aA | 521 | PHE | N-CA-C | 7.60 | 119.20 | 111.07 |
| 4 | M8 | 59 | ILE | CB-CA-C | -7.60 | 101.88 | 112.14 |
| 4 | M8 | 78 | GLY | N-CA-C | 7.60 | 127.84 | 112.34 |
| 4 | M4 | 59 | ILE | CB-CA-C | -7.59 | 101.89 | 112.14 |
| 4 | M3 | 78 | GLY | N-CA-C | 7.59 | 127.83 | 112.34 |
| 4 | M1 | 78 | GLY | N-CA-C | 7.59 | 127.83 | 112.34 |
| 10 | j5 | 1006 | ASP | CA-C-O | -7.59 | 112.78 | 120.90 |
| 11 | a9 | 351 | THR | CB-CA-C | -7.59 | 97.51 | 109.42 |
| 11 | aA | 351 | THR | CB-CA-C | -7.59 | 97.51 | 109.42 |
| 4 | M4 | 78 | GLY | N-CA-C | 7.58 | 127.81 | 112.34 |
| 4 | MA | 78 | GLY | N-CA-C | 7.58 | 127.81 | 112.34 |
| 4 | M9 | 78 | GLY | N-CA-C | 7.58 | 127.81 | 112.34 |
| 4 | M3 | 59 | ILE | CB-CA-C | -7.58 | 101.91 | 112.14 |
| 4 | M1 | 59 | ILE | CB-CA-C | -7.58 | 101.91 | 112.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 11 | aA | 531 | ASP | N-CA-C | 7.56 | 120.40 | 111.71 |
| 4 | M4 | 23 | PRO | N-CA-C | -7.56 | 96.90 | 112.47 |
| 4 | M8 | 23 | PRO | N-CA-C | -7.55 | 96.91 | 112.47 |
| 11 | a9 | 613 | TYR | N-CA-C | -7.55 | 97.90 | 108.54 |
| 11 | aA | 613 | TYR | N-CA-C | -7.55 | 97.90 | 108.54 |
| 8 | c7 | 126 | VAL | N-CA-C | 7.55 | 118.32 | 110.62 |
| 8 | C7 | 22 | GLU | N-CA-C | -7.54 | 104.22 | 113.19 |
| 11 | a9 | 531 | ASP | N-CA-C | 7.53 | 120.37 | 111.71 |
| 4 | MA | 23 | PRO | N-CA-C | -7.53 | 96.96 | 112.47 |
| 4 | M9 | 23 | PRO | N-CA-C | -7.53 | 96.96 | 112.47 |
| 4 | M3 | 23 | PRO | N-CA-C | -7.52 | 96.97 | 112.47 |
| 9 | x7 | 26 | THR | N-CA-C | 7.52 | 122.59 | 113.41 |
| 4 | M1 | 23 | PRO | N-CA-C | -7.52 | 96.97 | 112.47 |
| 9 | z7 | 31 | LEU | O-C-N | -7.51 | 113.73 | 122.89 |
| 9 | y7 | 26 | THR | N-CA-C | 7.51 | 122.57 | 113.41 |
| 10 | j5 | 409 | GLU | CB-CA-C | -7.50 | 99.11 | 110.88 |
| 10 | j5 | 393 | MET | CB-CG-SD | -7.50 | 90.21 | 112.70 |
| 10 | k5 | 393 | MET | CB-CG-SD | -7.49 | 90.22 | 112.70 |
| 4 | MA | 47 | VAL | N-CA-C | 7.49 | 116.52 | 107.61 |
| 4 | M9 | 47 | VAL | N-CA-C | 7.49 | 116.52 | 107.61 |
| 4 | M4 | 49 | LEU | N-CA-C | 7.48 | 120.38 | 111.33 |
| 11 | aA | 823 | ILE | N-CA-C | -7.48 | 95.71 | 106.55 |
| 9 | w7 | 31 | LEU | O-C-N | -7.47 | 113.78 | 122.89 |
| 10 | k5 | 409 | GLU | CB-CA-C | -7.47 | 99.15 | 110.88 |
| 4 | M3 | 47 | VAL | N-CA-C | 7.46 | 116.49 | 107.61 |
| 4 | M1 | 17 | VAL | CA-C-N | -7.46 | 110.65 | 122.73 |
| 4 | M1 | 17 | VAL | C-N-CA | -7.46 | 110.65 | 122.73 |
| 4 | M1 | 47 | VAL | N-CA-C | 7.46 | 116.49 | 107.61 |
| 4 | M3 | 49 | LEU | N-CA-C | 7.45 | 120.35 | 111.33 |
| 4 | M1 | 49 | LEU | N-CA-C | 7.45 | 120.35 | 111.33 |
| 10 | j5 | 623 | VAL | N-CA-C | 7.45 | 121.45 | 111.17 |
| 4 | M4 | 47 | VAL | N-CA-C | 7.45 | 116.47 | 107.61 |
| 8 | a7 | 21 | GLY | N-CA-C | 7.44 | 122.30 | 112.77 |
| 3 | H2 | 84 | ARG | CA-C-N | -7.44 | 107.33 | 121.54 |
| 3 | H2 | 84 | ARG | C-N-CA | -7.44 | 107.33 | 121.54 |
| 3 | H6 | 84 | ARG | CA-C-N | -7.44 | 107.33 | 121.54 |
| 3 | H6 | 84 | ARG | C-N-CA | -7.44 | 107.33 | 121.54 |
| 4 | MA | 17 | VAL | CA-C-N | -7.44 | 110.68 | 122.73 |
| 4 | MA | 17 | VAL | C-N-CA | -7.44 | 110.68 | 122.73 |
| 4 | M9 | 17 | VAL | CA-C-N | -7.44 | 110.68 | 122.73 |
| 4 | M9 | 17 | VAL | C-N-CA | -7.44 | 110.68 | 122.73 |
| 4 | M3 | 17 | VAL | CA-C-N | -7.43 | 110.69 | 122.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | M3 | 17 | VAL | C-N-CA | -7.43 | 110.69 | 122.73 |
| 4 | M8 | 49 | LEU | N-CA-C | 7.43 | 120.32 | 111.33 |
| 10 | j5 | 847 | LEU | CB-CA-C | -7.43 | 98.92 | 110.81 |
| 10 | j5 | 941 | THR | N-CA-C | 7.43 | 119.38 | 111.28 |
| 11 | a9 | 283 | GLN | N-CA-C | 7.43 | 126.22 | 109.81 |
| 10 | j5 | 882 | PRO | N-CA-C | 7.42 | 125.81 | 113.78 |
| 4 | MA | 49 | LEU | N-CA-C | 7.42 | 120.31 | 111.33 |
| 4 | M4 | 17 | VAL | CA-C-N | -7.42 | 110.72 | 122.73 |
| 4 | M4 | 17 | VAL | C-N-CA | -7.42 | 110.72 | 122.73 |
| 9 | z5 | 46 | LYS | N-CA-C | 7.41 | 121.91 | 113.01 |
| 4 | M8 | 47 | VAL | N-CA-C | 7.41 | 116.43 | 107.61 |
| 11 | aA | 283 | GLN | N-CA-C | 7.41 | 126.20 | 109.81 |
| 10 | k5 | 623 | VAL | N-CA-C | 7.41 | 121.40 | 111.17 |
| 10 | k5 | 882 | PRO | N-CA-C | 7.41 | 125.78 | 113.78 |
| 10 | j5 | 52 | ARG | CB-CA-C | -7.41 | 99.25 | 110.88 |
| 10 | k5 | 941 | THR | N-CA-C | 7.41 | 119.35 | 111.28 |
| 10 | k5 | 847 | LEU | CB-CA-C | -7.40 | 98.97 | 110.81 |
| 4 | M9 | 49 | LEU | N-CA-C | 7.40 | 120.29 | 111.33 |
| 8 | g7 | 21 | GLY | N-CA-C | 7.40 | 122.24 | 112.77 |
| 9 | i5 | 46 | LYS | N-CA-C | 7.40 | 121.89 | 113.01 |
| 10 | j5 | 650 | ASP | CB-CA-C | 7.40 | 123.33 | 110.01 |
| 2 | KA | 22 | THR | CB-CA-C | -7.39 | 98.52 | 110.79 |
| 2 | K9 | 22 | THR | CB-CA-C | -7.39 | 98.52 | 110.79 |
| 10 | k5 | 52 | ARG | CB-CA-C | -7.38 | 99.28 | 110.88 |
| 4 | M8 | 17 | VAL | CA-C-N | -7.38 | 110.77 | 122.73 |
| 4 | M8 | 17 | VAL | C-N-CA | -7.38 | 110.77 | 122.73 |
| 11 | a9 | 603 | THR | N-CA-C | -7.37 | 95.11 | 110.80 |
| 11 | aA | 603 | THR | N-CA-C | -7.37 | 95.11 | 110.80 |
| 10 | k5 | 650 | ASP | CB-CA-C | 7.36 | 123.26 | 110.01 |
| 10 | j5 | 885 | GLN | CA-C-O | -7.35 | 112.42 | 120.43 |
| 10 | k5 | 557 | VAL | N-CA-C | 7.35 | 120.28 | 111.09 |
| 4 | MA | 35 | THR | N-CA-CB | -7.34 | 97.87 | 111.53 |
| 4 | M9 | 35 | THR | N-CA-CB | -7.34 | 97.87 | 111.53 |
| 10 | k5 | 874 | ARG | CB-CA-C | -7.33 | 99.32 | 110.90 |
| 10 | k5 | 414 | ILE | CB-CA-C | -7.33 | 102.11 | 112.22 |
| 4 | M3 | 35 | THR | N-CA-CB | -7.32 | 97.91 | 111.53 |
| 10 | k5 | 329 | SER | N-CA-C | 7.32 | 119.78 | 110.33 |
| 4 | M1 | 35 | THR | N-CA-CB | -7.32 | 97.91 | 111.53 |
| 9 | x7 | 22 | GLU | N-CA-C | 7.32 | 121.94 | 113.38 |
| 4 | M8 | 77 | LEU | N-CA-C | -7.32 | 98.84 | 109.59 |
| 10 | k5 | 885 | GLN | CA-C-O | -7.31 | 112.46 | 120.43 |
| 4 | M4 | 35 | THR | N-CA-CB | -7.31 | 97.94 | 111.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9 | y7 | 22 | GLU | N-CA-C | 7.30 | 121.92 | 113.38 |
| 8 | C5 | 15 | ALA | CA-C-N | -7.30 | 107.59 | 121.54 |
| 8 | C5 | 15 | ALA | C-N-CA | -7.30 | 107.59 | 121.54 |
| 10 | j5 | 414 | ILE | CB-CA-C | -7.30 | 102.15 | 112.22 |
| 4 | M8 | 35 | THR | N-CA-CB | -7.30 | 97.96 | 111.53 |
| 10 | j5 | 874 | ARG | CB-CA-C | -7.29 | 99.38 | 110.90 |
| 10 | j5 | 329 | SER | N-CA-C | 7.29 | 119.74 | 110.33 |
| 4 | MA | 95 | ALA | N-CA-C | 7.29 | 118.87 | 111.07 |
| 10 | k5 | 640 | TYR | CB-CA-C | -7.29 | 96.02 | 109.29 |
| 1 | D7 | 67 | ARG | CA-C-N | 7.29 | 128.95 | 119.84 |
| 1 | D7 | 67 | ARG | C-N-CA | 7.29 | 128.95 | 119.84 |
| 4 | M9 | 95 | ALA | N-CA-C | 7.29 | 118.87 | 111.07 |
| 11 | a9 | 312 | ASP | CA-C-N | 7.29 | 131.02 | 120.38 |
| 11 | a9 | 312 | ASP | C-N-CA | 7.29 | 131.02 | 120.38 |
| 11 | aA | 312 | ASP | CA-C-N | 7.29 | 131.02 | 120.38 |
| 11 | aA | 312 | ASP | C-N-CA | 7.29 | 131.02 | 120.38 |
| 10 | j5 | 403 | ASP | CB-CA-C | -7.29 | 98.69 | 110.79 |
| 4 | MA | 77 | LEU | N-CA-C | -7.28 | 98.88 | 109.59 |
| 4 | M3 | 77 | LEU | N-CA-C | -7.28 | 98.89 | 109.59 |
| 4 | M4 | 77 | LEU | N-CA-C | -7.28 | 98.89 | 109.59 |
| 4 | M1 | 77 | LEU | N-CA-C | -7.28 | 98.89 | 109.59 |
| 8 | I5 | 15 | ALA | CA-C-N | -7.28 | 107.64 | 121.54 |
| 8 | I5 | 15 | ALA | C-N-CA | -7.28 | 107.64 | 121.54 |
| 10 | k5 | 403 | ASP | CB-CA-C | -7.28 | 98.70 | 110.79 |
| 4 | M1 | 95 | ALA | N-CA-C | 7.28 | 118.86 | 111.07 |
| 10 | j5 | 640 | TYR | CB-CA-C | -7.28 | 96.04 | 109.29 |
| 8 | o7 | 36 | ARG | CB-CA-C | -7.28 | 98.48 | 110.85 |
| 4 | M3 | 95 | ALA | N-CA-C | 7.27 | 118.85 | 111.07 |
| 4 | M9 | 77 | LEU | N-CA-C | -7.26 | 98.92 | 109.59 |
| 9 | i5 | 65 | THR | CB-CA-C | -7.26 | 96.60 | 110.24 |
| 8 | u7 | 36 | ARG | CB-CA-C | -7.25 | 98.52 | 110.85 |
| 11 | a9 | 498 | VAL | N-CA-C | 7.25 | 119.27 | 111.58 |
| 11 | aA | 498 | VAL | N-CA-C | 7.25 | 119.27 | 111.58 |
| 9 | z5 | 65 | THR | CB-CA-C | -7.25 | 96.61 | 110.24 |
| 10 | j5 | 775 | VAL | CB-CA-C | -7.24 | 100.25 | 111.26 |
| 8 | M5 | 65 | VAL | N-CA-C | -7.24 | 103.24 | 110.62 |
| 1 | J7 | 67 | ARG | CA-C-N | 7.24 | 128.89 | 119.84 |
| 1 | J7 | 67 | ARG | C-N-CA | 7.24 | 128.89 | 119.84 |
| 10 | j5 | 34 | TYR | N-CA-CB | 7.22 | 123.22 | 110.37 |
| 10 | k5 | 34 | TYR | N-CA-CB | 7.21 | 123.21 | 110.37 |
| 5 | N3 | 25 | THR | N-CA-C | -7.21 | 103.36 | 111.14 |
| 10 | k5 | 775 | VAL | CB-CA-C | -7.21 | 100.30 | 111.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8 | G7 | 65 | VAL | N-CA-C | -7.21 | 103.27 | 110.62 |
| 4 | MA | 86 | ALA | N-CA-C | -7.20 | 103.36 | 111.14 |
| 4 | M9 | 86 | ALA | N-CA-C | -7.20 | 103.36 | 111.14 |
| 4 | M3 | 86 | ALA | N-CA-C | -7.20 | 103.37 | 111.14 |
| 4 | M1 | 86 | ALA | N-CA-C | -7.20 | 103.37 | 111.14 |
| 8 | S5 | 65 | VAL | N-CA-C | -7.19 | 103.29 | 110.62 |
| 5 | N1 | 25 | THR | N-CA-C | -7.18 | 103.38 | 111.14 |
| 8 | c5 | 65 | VAL | N-CA-C | -7.18 | 103.29 | 110.62 |
| 11 | a9 | 459 | PHE | N-CA-C | 7.17 | 122.42 | 112.45 |
| 11 | aA | 459 | PHE | N-CA-C | 7.17 | 122.42 | 112.45 |
| 11 | aA | 612 | TYR | N-CA-C | 7.16 | 119.16 | 111.36 |
| 8 | A7 | 65 | VAL | N-CA-C | -7.16 | 103.32 | 110.62 |
| 3 | FA | 160 | ALA | N-CA-C | 7.15 | 118.72 | 111.07 |
| 10 | j5 | 692 | LEU | N-CA-C | -7.15 | 104.69 | 113.41 |
| 2 | N8 | 111 | ALA | CB-CA-C | 7.15 | 124.65 | 110.42 |
| 8 | Y7 | 65 | VAL | N-CA-C | -7.15 | 103.33 | 110.62 |
| 10 | j5 | 468 | ASN | N-CA-CB | 7.14 | 122.07 | 110.42 |
| 5 | NA | 25 | THR | N-CA-C | -7.14 | 103.43 | 111.14 |
| 4 | M4 | 86 | ALA | N-CA-C | -7.14 | 103.43 | 111.14 |
| 11 | a9 | 612 | TYR | N-CA-C | 7.14 | 119.14 | 111.36 |
| 10 | k5 | 692 | LEU | N-CA-C | -7.14 | 104.70 | 113.41 |
| 8 | e7 | 65 | VAL | N-CA-C | -7.14 | 103.34 | 110.62 |
| 8 | Y5 | 65 | VAL | N-CA-C | -7.13 | 103.34 | 110.62 |
| 4 | M8 | 21 | LEU | N-CA-C | 7.13 | 121.45 | 109.76 |
| 5 | N9 | 25 | THR | N-CA-C | -7.12 | 103.44 | 111.14 |
| 2 | KA | 14 | SER | O-C-N | 7.12 | 132.83 | 122.43 |
| 10 | k5 | 468 | ASN | N-CA-CB | 7.12 | 122.03 | 110.42 |
| 4 | MA | 21 | LEU | N-CA-C | 7.12 | 121.44 | 109.76 |
| 4 | M3 | 21 | LEU | N-CA-C | 7.12 | 121.43 | 109.76 |
| 4 | M1 | 21 | LEU | N-CA-C | 7.12 | 121.43 | 109.76 |
| 10 | j5 | 534 | GLY | CA-C-N | 7.11 | 127.07 | 120.03 |
| 10 | j5 | 534 | GLY | C-N-CA | 7.11 | 127.07 | 120.03 |
| 4 | M8 | 136 | SER | N-CA-C | -7.11 | 95.65 | 110.80 |
| 4 | M9 | 21 | LEU | N-CA-C | 7.11 | 121.42 | 109.76 |
| 4 | M4 | 21 | LEU | N-CA-C | 7.11 | 121.41 | 109.76 |
| 8 | U5 | 22 | GLU | CB-CA-C | -7.11 | 97.29 | 109.65 |
| 10 | j5 | 1106 | PHE | CB-CA-C | -7.11 | 96.84 | 109.70 |
| 4 | M8 | 86 | ALA | N-CA-C | -7.10 | 103.47 | 111.14 |
| 9 | z5 | 67 | VAL | CB-CA-C | -7.10 | 102.43 | 112.22 |
| 2 | K9 | 14 | SER | O-C-N | 7.10 | 132.79 | 122.43 |
| 8 | S7 | 65 | VAL | N-CA-C | -7.09 | 103.38 | 110.62 |
| 8 | k7 | 65 | VAL | N-CA-C | -7.09 | 103.39 | 110.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9 | i5 | 67 | VAL | CB-CA-C | -7.09 | 102.44 | 112.22 |
| 5 | NA | 35 | ASP | N-CA-C | 7.08 | 121.17 | 111.39 |
| 5 | N9 | 35 | ASP | N-CA-C | 7.08 | 121.17 | 111.39 |
| 4 | M4 | 136 | SER | N-CA-C | -7.08 | 95.72 | 110.80 |
| 10 | k5 | 534 | GLY | CA-C-N | 7.08 | 127.04 | 120.03 |
| 10 | k5 | 534 | GLY | C-N-CA | 7.08 | 127.04 | 120.03 |
| 10 | k5 | 725 | LEU | CB-CA-C | 7.07 | 122.52 | 110.56 |
| 8 | q7 | 65 | VAL | N-CA-C | -7.07 | 103.41 | 110.62 |
| 10 | j5 | 725 | LEU | CB-CA-C | 7.07 | 122.51 | 110.56 |
| 5 | N3 | 35 | ASP | N-CA-C | 7.07 | 121.14 | 111.39 |
| 5 | Z8 | 25 | THR | N-CA-C | -7.07 | 103.51 | 111.14 |
| 5 | N1 | 35 | ASP | N-CA-C | 7.07 | 121.14 | 111.39 |
| 5 | Z8 | 35 | ASP | N-CA-C | 7.06 | 121.13 | 111.39 |
| 10 | j5 | 849 | LYS | N-CA-C | 7.05 | 119.05 | 111.36 |
| 9 | z7 | 21 | ARG | CA-C-N | -7.05 | 108.06 | 121.54 |
| 9 | z7 | 21 | ARG | C-N-CA | -7.05 | 108.06 | 121.54 |
| 9 | w7 | 63 | ALA | N-CA-C | 7.05 | 125.82 | 110.80 |
| 9 | z7 | 63 | ALA | N-CA-C | 7.05 | 125.82 | 110.80 |
| 9 | w7 | 21 | ARG | CA-C-N | -7.05 | 108.07 | 121.54 |
| 9 | w7 | 21 | ARG | C-N-CA | -7.05 | 108.07 | 121.54 |
| 10 | k5 | 530 | ALA | N-CA-C | -7.04 | 95.80 | 110.80 |
| 8 | M7 | 65 | VAL | N-CA-C | -7.04 | 103.43 | 110.62 |
| 4 | M4 | 45 | VAL | N-CA-CB | -7.04 | 99.90 | 111.45 |
| 10 | j5 | 530 | ALA | N-CA-C | -7.04 | 95.80 | 110.80 |
| 10 | j5 | 501 | ILE | CB-CA-C | -7.04 | 103.10 | 112.46 |
| 10 | j5 | 751 | LYS | N-CA-C | 7.04 | 121.15 | 109.95 |
| 10 | k5 | 751 | LYS | N-CA-C | 7.03 | 121.13 | 109.95 |
| 4 | MA | 45 | VAL | N-CA-CB | -7.03 | 99.92 | 111.45 |
| 4 | M9 | 45 | VAL | N-CA-CB | -7.03 | 99.92 | 111.45 |
| 4 | M8 | 45 | VAL | N-CA-CB | -7.03 | 99.93 | 111.45 |
| 4 | M1 | 45 | VAL | N-CA-CB | -7.03 | 99.93 | 111.45 |
| 8 | u7 | 56 | ASP | N-CA-C | 7.02 | 118.94 | 111.28 |
| 8 | i7 | 114 | GLU | CB-CA-C | -7.02 | 98.91 | 110.85 |
| 11 | aA | 482 | TYR | N-CA-C | 7.02 | 118.93 | 111.28 |
| 10 | j5 | 1010 | GLY | CA-C-N | 7.02 | 135.11 | 122.13 |
| 10 | j5 | 1010 | GLY | C-N-CA | 7.02 | 135.11 | 122.13 |
| 10 | j5 | 291 | ASP | CA-C-N | -7.01 | 109.65 | 120.31 |
| 10 | j5 | 291 | ASP | C-N-CA | -7.01 | 109.65 | 120.31 |
| 10 | k5 | 291 | ASP | CA-C-N | -7.01 | 109.65 | 120.31 |
| 10 | k5 | 291 | ASP | C-N-CA | -7.01 | 109.65 | 120.31 |
| 8 | a7 | 22 | GLU | CA-C-N | 7.01 | 134.94 | 121.54 |
| 8 | a7 | 22 | GLU | C-N-CA | 7.01 | 134.94 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10 | j5 | 633 | ARG | N-CA-C | 7.01 | 119.00 | 111.36 |
| 10 | k5 | 633 | ARG | N-CA-C | 7.01 | 119.00 | 111.36 |
| 8 | g7 | 22 | GLU | CA-C-N | 7.01 | 134.93 | 121.54 |
| 8 | g7 | 22 | GLU | C-N-CA | 7.01 | 134.93 | 121.54 |
| 10 | k5 | 1120 | PRO | CA-C-O | -7.01 | 108.31 | 118.89 |
| 8 | c7 | 114 | GLU | CB-CA-C | -7.01 | 98.93 | 110.85 |
| 10 | k5 | 849 | LYS | N-CA-C | 7.01 | 119.00 | 111.36 |
| 4 | M3 | 45 | VAL | N-CA-CB | -7.01 | 99.96 | 111.45 |
| 10 | k5 | 1010 | GLY | CA-C-N | 7.00 | 135.09 | 122.13 |
| 10 | k5 | 1010 | GLY | C-N-CA | 7.00 | 135.09 | 122.13 |
| 10 | k5 | 238 | ARG | N-CA-C | -7.00 | 103.87 | 113.18 |
| 10 | j5 | 1120 | PRO | CA-C-O | -7.00 | 108.32 | 118.89 |
| 11 | a9 | 482 | TYR | N-CA-C | 7.00 | 118.91 | 111.28 |
| 2 | KA | 16 | GLY | N-CA-C | 7.00 | 123.69 | 113.48 |
| 2 | K9 | 16 | GLY | N-CA-C | 7.00 | 123.69 | 113.48 |
| 10 | k5 | 501 | ILE | CB-CA-C | -6.99 | 103.16 | 112.46 |
| 8 | o7 | 56 | ASP | N-CA-C | 6.99 | 118.90 | 111.28 |
| 10 | k5 | 723 | GLN | CB-CA-C | -6.99 | 98.97 | 110.85 |
| 11 | a9 | 372 | ALA | C-N-CD | -6.97 | 96.40 | 125.00 |
| 11 | aA | 372 | ALA | C-N-CD | -6.97 | 96.40 | 125.00 |
| 10 | j5 | 506 | LYS | CA-C-N | 6.97 | 130.77 | 120.87 |
| 10 | j5 | 506 | LYS | C-N-CA | 6.97 | 130.77 | 120.87 |
| 11 | a9 | 776 | TYR | CB-CA-C | -6.97 | 99.80 | 110.26 |
| 11 | aA | 776 | TYR | CB-CA-C | -6.97 | 99.81 | 110.26 |
| 4 | M8 | 197 | ASP | N-CA-C | 6.97 | 118.95 | 111.36 |
| 10 | j5 | 238 | ARG | N-CA-C | -6.97 | 103.92 | 113.18 |
| 10 | k5 | 257 | THR | CB-CA-C | -6.96 | 94.83 | 109.38 |
| 4 | MA | 212 | ALA | N-CA-C | 6.96 | 118.95 | 111.36 |
| 4 | M9 | 212 | ALA | N-CA-C | 6.96 | 118.95 | 111.36 |
| 4 | M4 | 197 | ASP | N-CA-C | 6.96 | 118.94 | 111.36 |
| 10 | j5 | 723 | GLN | CB-CA-C | -6.96 | 99.02 | 110.85 |
| 10 | j5 | 257 | THR | CB-CA-C | -6.96 | 94.84 | 109.38 |
| 9 | z7 | 11 | ILE | CB-CA-C | -6.95 | 103.19 | 111.18 |
| 4 | MA | 197 | ASP | N-CA-C | 6.95 | 118.94 | 111.36 |
| 10 | k5 | 506 | LYS | CA-C-N | 6.95 | 130.74 | 120.87 |
| 10 | k5 | 506 | LYS | C-N-CA | 6.95 | 130.74 | 120.87 |
| 10 | k5 | 973 | THR | N-CA-CB | 6.95 | 122.23 | 110.49 |
| 4 | M1 | 197 | ASP | N-CA-C | 6.95 | 118.94 | 111.36 |
| 10 | j5 | 188 | GLU | N-CA-C | 6.94 | 118.85 | 111.28 |
| 4 | M9 | 197 | ASP | N-CA-C | 6.93 | 118.92 | 111.36 |
| 4 | M8 | 212 | ALA | N-CA-C | 6.93 | 118.92 | 111.36 |
| 4 | M8 | 230 | GLN | N-CA-C | 6.93 | 124.01 | 110.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | M3 | 197 | ASP | N-CA-C | 6.93 | 118.91 | 111.36 |
| 9 | w7 | 11 | ILE | CB-CA-C | -6.93 | 103.21 | 111.18 |
| 10 | j5 | 973 | THR | N-CA-CB | 6.92 | 122.18 | 110.49 |
| 4 | M3 | 212 | ALA | N-CA-C | 6.91 | 118.89 | 111.36 |
| 10 | k5 | 778 | LYS | N-CA-C | 6.91 | 125.52 | 110.80 |
| 4 | M1 | 212 | ALA | N-CA-C | 6.91 | 118.89 | 111.36 |
| 4 | M4 | 212 | ALA | N-CA-C | 6.91 | 118.89 | 111.36 |
| 10 | j5 | 778 | LYS | N-CA-C | 6.91 | 125.51 | 110.80 |
| 10 | j5 | 483 | PHE | N-CA-C | 6.90 | 124.80 | 113.89 |
| 10 | k5 | 483 | PHE | N-CA-C | 6.90 | 124.79 | 113.89 |
| 11 | a9 | 464 | PRO | CA-C-O | -6.90 | 112.85 | 120.92 |
| 11 | aA | 464 | PRO | CA-C-O | -6.90 | 112.85 | 120.92 |
| 10 | k5 | 188 | GLU | N-CA-C | 6.89 | 118.80 | 111.28 |
| 10 | k5 | 190 | LEU | N-CA-C | 6.89 | 118.87 | 111.36 |
| 4 | M9 | 13 | LYS | N-CA-C | -6.89 | 97.18 | 108.41 |
| 11 | a9 | 801 | ASN | N-CA-C | 6.89 | 120.91 | 111.54 |
| 11 | aA | 801 | ASN | N-CA-C | 6.89 | 120.91 | 111.54 |
| 9 | w7 | 67 | VAL | N-CA-CB | -6.88 | 102.50 | 110.55 |
| 10 | j5 | 190 | LEU | N-CA-C | 6.88 | 118.85 | 111.36 |
| 4 | MA | 13 | LYS | N-CA-C | -6.87 | 97.20 | 108.41 |
| 11 | a9 | 47 | GLU | CB-CA-C | -6.87 | 100.10 | 110.88 |
| 11 | aA | 47 | GLU | CB-CA-C | -6.87 | 100.10 | 110.88 |
| 4 | M3 | 50 | ASP | N-CA-C | 6.87 | 118.84 | 111.36 |
| 4 | M1 | 50 | ASP | N-CA-C | 6.87 | 118.84 | 111.36 |
| 11 | a9 | 642 | GLU | N-CA-C | 6.86 | 117.64 | 108.38 |
| 11 | aA | 642 | GLU | N-CA-C | 6.86 | 117.64 | 108.38 |
| 9 | z7 | 67 | VAL | N-CA-CB | -6.86 | 102.52 | 110.55 |
| 4 | M4 | 30 | TRP | CA-C-N | 6.86 | 127.00 | 119.87 |
| 4 | M4 | 30 | TRP | C-N-CA | 6.86 | 127.00 | 119.87 |
| 10 | j5 | 36 | ASN | CB-CA-C | -6.86 | 95.62 | 109.68 |
| 4 | M4 | 13 | LYS | N-CA-C | -6.85 | 97.24 | 108.41 |
| 4 | MA | 32 | SER | CB-CA-C | -6.85 | 98.31 | 109.89 |
| 9 | i5 | 43 | ARG | CA-C-N | 6.85 | 130.15 | 120.42 |
| 9 | i5 | 43 | ARG | C-N-CA | 6.85 | 130.15 | 120.42 |
| 10 | j5 | 480 | GLU | N-CA-C | 6.85 | 120.48 | 108.56 |
| 10 | j5 | 556 | GLY | CA-C-N | -6.85 | 112.41 | 122.68 |
| 10 | j5 | 556 | GLY | C-N-CA | -6.85 | 112.41 | 122.68 |
| 4 | M8 | 30 | TRP | CA-C-N | 6.85 | 126.99 | 119.87 |
| 4 | M8 | 30 | TRP | C-N-CA | 6.85 | 126.99 | 119.87 |
| 4 | MA | 50 | ASP | N-CA-C | 6.84 | 118.82 | 111.36 |
| 4 | M9 | 32 | SER | CB-CA-C | -6.84 | 98.32 | 109.89 |
| 4 | M9 | 50 | ASP | N-CA-C | 6.84 | 118.82 | 111.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11 | a9 | 624 | GLY | N-CA-C | -6.84 | 106.02 | 114.92 |
| 11 | aA | 624 | GLY | N-CA-C | -6.84 | 106.02 | 114.92 |
| 4 | M4 | 249 | ASP | N-CA-C | 6.84 | 119.75 | 111.82 |
| 10 | j5 | 381 | ILE | N-CA-C | -6.84 | 105.93 | 111.81 |
| 10 | j5 | 583 | GLY | CA-C-N | 6.84 | 129.44 | 120.28 |
| 10 | j5 | 583 | GLY | C-N-CA | 6.84 | 129.44 | 120.28 |
| 10 | k5 | 583 | GLY | CA-C-N | 6.84 | 129.44 | 120.28 |
| 10 | k5 | 583 | GLY | C-N-CA | 6.84 | 129.44 | 120.28 |
| 4 | M8 | 13 | LYS | N-CA-C | -6.83 | 97.27 | 108.41 |
| 4 | M3 | 13 | LYS | N-CA-C | -6.83 | 97.28 | 108.41 |
| 4 | M4 | 32 | SER | CB-CA-C | -6.83 | 98.35 | 109.89 |
| 10 | j5 | 320 | GLU | N-CA-C | 6.83 | 118.72 | 111.28 |
| 4 | M8 | 249 | ASP | N-CA-C | 6.83 | 119.74 | 111.82 |
| 4 | M1 | 13 | LYS | N-CA-C | -6.83 | 97.28 | 108.41 |
| 9 | y7 | 28 | PHE | N-CA-C | 6.82 | 119.70 | 108.99 |
| 4 | M8 | 32 | SER | CB-CA-C | -6.82 | 98.36 | 109.89 |
| 4 | M3 | 32 | SER | CB-CA-C | -6.81 | 98.38 | 109.89 |
| 4 | M1 | 32 | SER | CB-CA-C | -6.81 | 98.38 | 109.89 |
| 11 | a9 | 607 | MET | N-CA-C | 6.81 | 121.88 | 107.91 |
| 11 | aA | 607 | MET | N-CA-C | 6.81 | 121.88 | 107.91 |
| 10 | k5 | 480 | GLU | N-CA-C | 6.81 | 120.41 | 108.56 |
| 9 | z5 | 43 | ARG | CA-C-N | 6.81 | 130.09 | 120.42 |
| 9 | z5 | 43 | ARG | C-N-CA | 6.81 | 130.09 | 120.42 |
| 10 | k5 | 627 | ILE | N-CA-C | 6.81 | 117.57 | 110.62 |
| 4 | MA | 30 | TRP | CA-C-N | 6.81 | 126.95 | 119.87 |
| 4 | MA | 30 | TRP | C-N-CA | 6.81 | 126.95 | 119.87 |
| 4 | M9 | 30 | TRP | CA-C-N | 6.81 | 126.95 | 119.87 |
| 4 | M9 | 30 | TRP | C-N-CA | 6.81 | 126.95 | 119.87 |
| 4 | M4 | 50 | ASP | N-CA-C | 6.81 | 118.78 | 111.36 |
| 10 | k5 | 818 | GLN | N-CA-C | 6.80 | 118.78 | 111.36 |
| 10 | j5 | 818 | GLN | N-CA-C | 6.80 | 118.77 | 111.36 |
| 10 | k5 | 381 | ILE | N-CA-C | -6.79 | 105.97 | 111.81 |
| 10 | j5 | 231 | ILE | CB-CA-C | -6.79 | 103.12 | 112.02 |
| 10 | k5 | 231 | ILE | CB-CA-C | -6.79 | 103.12 | 112.02 |
| 9 | x7 | 28 | PHE | N-CA-C | 6.79 | 119.66 | 108.99 |
| 4 | M8 | 50 | ASP | N-CA-C | 6.79 | 118.76 | 111.36 |
| 11 | a9 | 563 | PHE | CB-CA-C | 6.79 | 118.59 | 109.42 |
| 11 | aA | 563 | PHE | CB-CA-C | 6.79 | 118.59 | 109.42 |
| 10 | j5 | 1055 | SER | CA-C-N | -6.79 | 111.36 | 119.84 |
| 10 | j5 | 1055 | SER | C-N-CA | -6.79 | 111.36 | 119.84 |
| 4 | M1 | 241 | LEU | N-CA-C | 6.78 | 118.75 | 111.36 |
| 10 | k5 | 320 | GLU | N-CA-C | 6.78 | 118.67 | 111.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4 | M3 | 30 | TRP | CA-C-N | 6.78 | 126.92 | 119.87 |
| 4 | M3 | 30 | TRP | C-N-CA | 6.78 | 126.92 | 119.87 |
| 4 | M1 | 30 | TRP | CA-C-N | 6.78 | 126.92 | 119.87 |
| 4 | M1 | 30 | TRP | C-N-CA | 6.78 | 126.92 | 119.87 |
| 10 | j5 | 804 | GLU | CB-CA-C | -6.78 | 99.33 | 110.85 |
| 10 | k5 | 1111 | VAL | N-CA-CB | -6.77 | 103.78 | 110.08 |
| 10 | j5 | 350 | PRO | CA-C-O | -6.76 | 110.73 | 118.98 |
| 10 | j5 | 557 | VAL | CB-CA-C | 6.76 | 121.83 | 110.95 |
| 10 | k5 | 1055 | SER | CA-C-N | -6.76 | 111.39 | 119.84 |
| 10 | k5 | 1055 | SER | C-N-CA | -6.76 | 111.39 | 119.84 |
| 10 | j5 | 1111 | VAL | N-CA-CB | -6.76 | 103.80 | 110.08 |
| 4 | M8 | 7 | SER | N-CA-C | 6.76 | 125.19 | 110.80 |
| 5 | Z8 | 73 | GLY | N-CA-C | 6.75 | 120.84 | 112.73 |
| 4 | MA | 241 | LEU | N-CA-C | 6.75 | 118.72 | 111.36 |
| 4 | M8 | 241 | LEU | N-CA-C | 6.75 | 118.72 | 111.36 |
| 4 | M9 | 241 | LEU | N-CA-C | 6.75 | 118.72 | 111.36 |
| 4 | M3 | 241 | LEU | N-CA-C | 6.75 | 118.72 | 111.36 |
| 10 | j5 | 431 | GLN | CB-CA-C | -6.75 | 99.35 | 108.87 |
| 10 | k5 | 804 | GLU | CB-CA-C | -6.75 | 99.37 | 110.85 |
| 4 | M4 | 7 | SER | N-CA-C | 6.75 | 125.18 | 110.80 |
| 4 | MA | 249 | ASP | N-CA-C | 6.75 | 119.65 | 111.82 |
| 10 | j5 | 627 | ILE | N-CA-C | 6.75 | 117.50 | 110.62 |
| 10 | k5 | 431 | GLN | CB-CA-C | -6.75 | 99.36 | 108.87 |
| 4 | M9 | 249 | ASP | N-CA-C | 6.75 | 119.65 | 111.82 |
| 10 | k5 | 878 | GLU | CB-CA-C | -6.74 | 100.26 | 110.90 |
| 4 | M3 | 249 | ASP | N-CA-C | 6.73 | 119.62 | 111.82 |
| 4 | M1 | 249 | ASP | N-CA-C | 6.73 | 119.62 | 111.82 |
| 4 | M4 | 241 | LEU | N-CA-C | 6.72 | 118.69 | 111.36 |
| 4 | MA | 258 | LYS | N-CA-C | 6.72 | 119.36 | 108.34 |
| 4 | M9 | 258 | LYS | N-CA-C | 6.72 | 119.36 | 108.34 |
| 4 | M4 | 258 | LYS | N-CA-C | 6.72 | 119.36 | 108.34 |
| 10 | k5 | 84 | TYR | CB-CA-C | -6.71 | 99.64 | 110.79 |
| 4 | M4 | 41 | ASN | CA-C-O | -6.71 | 113.44 | 120.55 |
| 10 | j5 | 878 | GLU | CB-CA-C | -6.71 | 100.30 | 110.90 |
| 10 | k5 | 493 | ASN | N-CA-C | -6.71 | 97.75 | 108.82 |
| 10 | j5 | 901 | TYR | CB-CA-C | -6.71 | 97.79 | 110.67 |
| 4 | M8 | 258 | LYS | N-CA-C | 6.71 | 119.34 | 108.34 |
| 10 | k5 | 901 | TYR | CB-CA-C | -6.71 | 97.80 | 110.67 |
| 4 | M3 | 258 | LYS | N-CA-C | 6.70 | 119.33 | 108.34 |
| 10 | k5 | 350 | PRO | CA-C-O | -6.70 | 110.80 | 118.98 |
| 10 | j5 | 84 | TYR | CB-CA-C | -6.70 | 99.68 | 110.79 |
| 4 | M1 | 258 | LYS | N-CA-C | 6.70 | 119.32 | 108.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4 | M8 | 41 | ASN | CA-C-O | -6.69 | 113.46 | 120.55 |
| 10 | k5 | 526 | MET | CB-CG-SD | 6.69 | 132.77 | 112.70 |
| 10 | j5 | 863 | ILE | CB-CA-C | -6.69 | 102.99 | 112.22 |
| 10 | k5 | 863 | ILE | CB-CA-C | -6.69 | 102.99 | 112.22 |
| 5 | N1 | 73 | GLY | N-CA-C | 6.68 | 120.75 | 112.73 |
| 11 | a9 | 598 | SER | CA-C-N | 6.68 | 128.19 | 119.84 |
| 11 | a9 | 598 | SER | C-N-CA | 6.68 | 128.19 | 119.84 |
| 10 | j5 | 984 | ILE | CA-C-O | -6.68 | 112.43 | 120.78 |
| 10 | k5 | 984 | ILE | CA-C-O | -6.68 | 112.43 | 120.78 |
| 10 | j5 | 493 | ASN | N-CA-C | -6.68 | 97.80 | 108.82 |
| 10 | j5 | 526 | MET | CB-CG-SD | 6.68 | 132.73 | 112.70 |
| 4 | M3 | 41 | ASN | CA-C-O | -6.67 | 113.47 | 120.55 |
| 10 | j5 | 919 | ILE | CA-C-O | -6.67 | 113.78 | 120.85 |
| 4 | M1 | 41 | ASN | CA-C-O | -6.67 | 113.48 | 120.55 |
| 5 | NA | 73 | GLY | N-CA-C | 6.67 | 120.73 | 112.73 |
| 10 | k5 | 36 | ASN | CB-CA-C | -6.67 | 95.65 | 110.19 |
| 4 | M8 | 17 | VAL | N-CA-C | 6.67 | 119.12 | 108.85 |
| 5 | N3 | 73 | GLY | N-CA-C | 6.66 | 120.72 | 112.73 |
| 3 | JA | 107 | ASP | CA-C-N | -6.66 | 110.17 | 122.09 |
| 3 | JA | 107 | ASP | C-N-CA | -6.66 | 110.17 | 122.09 |
| 3 | J9 | 107 | ASP | CA-C-N | -6.66 | 110.17 | 122.09 |
| 3 | J9 | 107 | ASP | C-N-CA | -6.66 | 110.17 | 122.09 |
| 5 | Z4 | 73 | GLY | N-CA-C | 6.66 | 120.72 | 112.73 |
| 8 | i7 | 120 | GLN | N-CA-C | 6.66 | 120.73 | 111.74 |
| 5 | N9 | 73 | GLY | N-CA-C | 6.66 | 120.72 | 112.73 |
| 11 | aA | 598 | SER | CA-C-N | 6.65 | 128.16 | 119.84 |
| 11 | aA | 598 | SER | C-N-CA | 6.65 | 128.16 | 119.84 |
| 4 | MA | 41 | ASN | CA-C-O | -6.65 | 113.50 | 120.55 |
| 10 | j5 | 523 | PRO | N-CA-C | 6.65 | 122.49 | 113.84 |
| 4 | M9 | 41 | ASN | CA-C-O | -6.65 | 113.50 | 120.55 |
| 10 | j5 | 440 | TYR | CA-CB-CG | -6.65 | 101.93 | 113.90 |
| 10 | k5 | 763 | SER | CA-CB-OG | -6.65 | 97.80 | 111.10 |
| 10 | k5 | 919 | ILE | CA-C-O | -6.65 | 113.81 | 120.85 |
| 10 | j5 | 947 | MET | CB-CG-SD | -6.64 | 92.79 | 112.70 |
| 10 | k5 | 878 | GLU | N-CA-C | 6.64 | 118.31 | 111.14 |
| 10 | k5 | 947 | MET | CB-CG-SD | -6.64 | 92.79 | 112.70 |
| 4 | M3 | 17 | VAL | N-CA-C | 6.63 | 119.07 | 108.85 |
| 4 | M4 | 17 | VAL | N-CA-C | 6.63 | 119.07 | 108.85 |
| 10 | k5 | 523 | PRO | N-CA-C | 6.63 | 122.47 | 113.84 |
| 4 | M1 | 17 | VAL | N-CA-C | 6.63 | 119.07 | 108.85 |
| 4 | MA | 98 | ASP | CA-C-N | 6.63 | 133.91 | 121.97 |
| 4 | MA | 98 | ASP | C-N-CA | 6.63 | 133.91 | 121.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 10 | k5 | 440 | TYR | CA-CB-CG | -6.63 | 101.96 | 113.90 |
| 4 | M9 | 98 | ASP | CA-C-N | 6.63 | 133.91 | 121.97 |
| 4 | M9 | 98 | ASP | C-N-CA | 6.63 | 133.91 | 121.97 |
| 4 | MA | 17 | VAL | N-CA-C | 6.63 | 119.06 | 108.85 |
| 4 | M3 | 98 | ASP | CA-C-N | 6.63 | 133.90 | 121.97 |
| 4 | M3 | 98 | ASP | C-N-CA | 6.63 | 133.90 | 121.97 |
| 4 | M9 | 17 | VAL | N-CA-C | 6.63 | 119.06 | 108.85 |
| 4 | M1 | 98 | ASP | CA-C-N | 6.63 | 133.90 | 121.97 |
| 4 | M1 | 98 | ASP | C-N-CA | 6.63 | 133.90 | 121.97 |
| 10 | k5 | 662 | ASP | N-CA-C | 6.62 | 120.95 | 113.01 |
| 10 | k5 | 750 | ARG | NE-CZ-NH2 | 6.62 | 125.16 | 119.20 |
| 3 | LA | 86 | MET | CB-CG-SD | -6.62 | 92.85 | 112.70 |
| 3 | L9 | 86 | MET | CB-CG-SD | -6.62 | 92.85 | 112.70 |
| 10 | j5 | 763 | SER | CA-CB-OG | -6.61 | 97.87 | 111.10 |
| 10 | j5 | 641 | ASP | N-CA-C | 6.60 | 118.24 | 108.60 |
| 10 | j5 | 729 | ILE | CB-CA-C | -6.60 | 100.46 | 111.29 |
| 10 | j5 | 249 | SER | N-CA-C | 6.60 | 114.19 | 108.78 |
| 8 | c7 | 120 | GLN | N-CA-C | 6.60 | 120.76 | 111.52 |
| 11 | a9 | 580 | THR | CB-CA-C | -6.59 | 99.84 | 110.79 |
| 3 | LA | 88 | ILE | CB-CA-C | -6.59 | 103.24 | 112.14 |
| 3 | L9 | 88 | ILE | CB-CA-C | -6.59 | 103.24 | 112.14 |
| 1 | J5 | 7 | ALA | N-CA-C | -6.59 | 105.40 | 113.50 |
| 4 | M4 | 143 | VAL | CA-C-N | -6.59 | 109.32 | 120.58 |
| 4 | M4 | 143 | VAL | C-N-CA | -6.59 | 109.32 | 120.58 |
| 9 | x7 | 59 | GLY | N-CA-C | 6.58 | 120.97 | 112.54 |
| 11 | aA | 580 | THR | CB-CA-C | -6.58 | 99.86 | 110.79 |
| 10 | j5 | 750 | ARG | NE-CZ-NH2 | 6.58 | 125.12 | 119.20 |
| 1 | D5 | 7 | ALA | N-CA-C | -6.58 | 105.41 | 113.50 |
| 10 | j5 | 420 | VAL | CA-C-N | 6.58 | 126.53 | 119.76 |
| 10 | j5 | 420 | VAL | C-N-CA | 6.58 | 126.53 | 119.76 |
| 10 | j5 | 560 | VAL | CB-CA-C | 6.58 | 122.07 | 111.29 |
| 10 | k5 | 664 | MET | CB-CA-C | 6.58 | 121.70 | 110.79 |
| 10 | k5 | 729 | ILE | CB-CA-C | -6.58 | 100.51 | 111.29 |
| 10 | j5 | 278 | TYR | N-CA-C | 6.57 | 120.06 | 109.02 |
| 10 | k5 | 278 | TYR | N-CA-C | 6.57 | 120.05 | 109.02 |
| 9 | y7 | 59 | GLY | N-CA-C | 6.57 | 120.95 | 112.54 |
| 8 | C5 | 7 | ALA | N-CA-C | -6.57 | 106.48 | 114.75 |
| 8 | A5 | 48 | GLU | CB-CA-C | -6.56 | 99.69 | 110.85 |
| 4 | M8 | 226 | SER | N-CA-C | -6.56 | 96.82 | 110.80 |
| 10 | k5 | 641 | ASP | N-CA-C | 6.56 | 118.18 | 108.60 |
| 10 | j5 | 878 | GLU | N-CA-C | 6.56 | 118.22 | 111.14 |
| 10 | k5 | 859 | ILE | N-CA-C | 6.56 | 119.25 | 111.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 11 | a9 | 111 | THR | CB-CA-C | -6.55 | 109.03 | 116.63 |
| 11 | aA | 111 | THR | CB-CA-C | -6.55 | 109.03 | 116.63 |
| 8 | I5 | 7 | ALA | N-CA-C | -6.55 | 106.50 | 114.75 |
| 8 | G5 | 48 | GLU | CB-CA-C | -6.55 | 99.72 | 110.85 |
| 10 | j5 | 664 | MET | CB-CA-C | 6.55 | 121.66 | 110.79 |
| 10 | j5 | 859 | ILE | N-CA-C | 6.55 | 119.24 | 111.05 |
| 10 | j5 | 984 | ILE | N-CA-CB | 6.55 | 122.04 | 111.23 |
| 10 | k5 | 984 | ILE | N-CA-CB | 6.55 | 122.03 | 111.23 |
| 10 | k5 | 458 | LEU | N-CA-C | 6.54 | 118.49 | 111.36 |
| 10 | k5 | 420 | VAL | CA-C-N | 6.54 | 126.50 | 119.76 |
| 10 | k5 | 420 | VAL | C-N-CA | 6.54 | 126.50 | 119.76 |
| 9 | i5 | 45 | GLN | CB-CA-C | -6.54 | 99.74 | 110.85 |
| 10 | j5 | 662 | ASP | N-CA-C | 6.54 | 120.85 | 113.01 |
| 10 | k5 | 664 | MET | N-CA-C | -6.53 | 104.16 | 111.28 |
| 10 | k5 | 667 | SER | CB-CA-C | -6.53 | 96.29 | 109.68 |
| 10 | k5 | 1138 | GLN | N-CA-C | 6.53 | 124.71 | 110.80 |
| 10 | j5 | 1138 | GLN | N-CA-C | 6.53 | 124.71 | 110.80 |
| 10 | j5 | 588 | VAL | N-CA-CB | 6.53 | 122.00 | 111.23 |
| 10 | k5 | 500 | PRO | N-CA-CB | -6.53 | 99.27 | 102.92 |
| 10 | j5 | 667 | SER | CB-CA-C | -6.52 | 96.31 | 109.68 |
| 10 | k5 | 249 | SER | N-CA-C | 6.52 | 114.13 | 108.78 |
| 11 | aA | 559 | THR | N-CA-C | -6.52 | 96.91 | 110.80 |
| 11 | a9 | 537 | ASP | N-CA-C | 6.52 | 121.25 | 113.16 |
| 10 | j5 | 216 | ASP | N-CA-C | 6.52 | 120.50 | 111.90 |
| 9 | z5 | 45 | GLN | CB-CA-C | -6.52 | 99.77 | 110.85 |
| 10 | j5 | 500 | PRO | N-CA-CB | -6.51 | 99.27 | 102.92 |
| 8 | O5 | 23 | LEU | N-CA-C | -6.51 | 104.91 | 112.92 |
| 10 | j5 | 458 | LEU | N-CA-C | 6.51 | 118.46 | 111.36 |
| 11 | aA | 537 | ASP | N-CA-C | 6.51 | 121.23 | 113.16 |
| 11 | a9 | 606 | ALA | N-CA-C | 6.51 | 120.13 | 109.85 |
| 11 | aA | 606 | ALA | N-CA-C | 6.51 | 120.13 | 109.85 |
| 10 | k5 | 216 | ASP | N-CA-C | 6.51 | 120.49 | 111.90 |
| 4 | MA | 47 | VAL | CB-CA-C | -6.50 | 103.82 | 110.13 |
| 4 | M9 | 47 | VAL | CB-CA-C | -6.50 | 103.82 | 110.13 |
| 4 | M4 | 47 | VAL | CB-CA-C | -6.50 | 103.82 | 110.13 |
| 10 | k5 | 699 | SER | CA-C-N | 6.50 | 130.19 | 120.31 |
| 10 | k5 | 699 | SER | C-N-CA | 6.50 | 130.19 | 120.31 |
| 10 | j5 | 838 | GLY | CA-C-O | -6.50 | 112.53 | 119.55 |
| 10 | k5 | 838 | GLY | CA-C-O | -6.50 | 112.53 | 119.55 |
| 10 | j5 | 557 | VAL | CA-CB-CG2 | 6.50 | 121.44 | 110.40 |
| 10 | j5 | 973 | THR | CB-CA-C | -6.49 | 97.50 | 110.42 |
| 11 | a9 | 392 | ILE | N-CA-C | 6.49 | 117.28 | 110.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 11 | aA | 392 | ILE | N-CA-C | 6.49 | 117.28 | 110.72 |
| 11 | a9 | 588 | VAL | N-CA-C | -6.49 | 98.92 | 108.97 |
| 11 | aA | 588 | VAL | N-CA-C | -6.49 | 98.92 | 108.97 |
| 10 | k5 | 588 | VAL | N-CA-CB | 6.48 | 121.93 | 111.23 |
| 10 | j5 | 699 | SER | CA-C-N | 6.48 | 130.16 | 120.31 |
| 10 | j5 | 699 | SER | C-N-CA | 6.48 | 130.16 | 120.31 |
| 10 | j5 | 664 | MET | N-CA-C | -6.47 | 104.22 | 111.28 |
| 10 | j5 | 984 | ILE | CB-CA-C | -6.47 | 100.68 | 111.29 |
| 11 | a9 | 607 | MET | CA-C-N | 6.47 | 127.93 | 119.84 |
| 11 | a9 | 607 | MET | C-N-CA | 6.47 | 127.93 | 119.84 |
| 11 | aA | 607 | MET | CA-C-N | 6.47 | 127.93 | 119.84 |
| 11 | aA | 607 | MET | C-N-CA | 6.47 | 127.93 | 119.84 |
| 10 | k5 | 973 | THR | CB-CA-C | -6.47 | 97.54 | 110.42 |
| 10 | k5 | 984 | ILE | CB-CA-C | -6.47 | 100.69 | 111.29 |
| 4 | M1 | 4 | LEU | CB-CA-C | -6.46 | 96.44 | 109.68 |
| 4 | M3 | 4 | LEU | CB-CA-C | -6.46 | 96.44 | 109.68 |
| 4 | M3 | 47 | VAL | CB-CA-C | -6.45 | 103.87 | 110.13 |
| 4 | M1 | 47 | VAL | CB-CA-C | -6.45 | 103.87 | 110.13 |
| 10 | j5 | 19 | THR | CA-C-O | -6.45 | 114.79 | 122.27 |
| 10 | j5 | 421 | PRO | CA-C-O | -6.44 | 114.00 | 121.34 |
| 4 | M4 | 4 | LEU | CB-CA-C | -6.44 | 96.48 | 109.68 |
| 4 | M8 | 47 | VAL | CB-CA-C | -6.44 | 103.88 | 110.13 |
| 4 | M8 | 4 | LEU | CB-CA-C | -6.43 | 96.49 | 109.68 |
| 4 | MA | 4 | LEU | CB-CA-C | -6.43 | 96.50 | 109.68 |
| 9 | y7 | 20 | GLY | CA-C-O | -6.43 | 115.69 | 121.47 |
| 4 | M9 | 4 | LEU | CB-CA-C | -6.43 | 96.50 | 109.68 |
| 9 | i5 | 19 | THR | N-CA-C | 6.43 | 118.08 | 111.14 |
| 11 | a9 | 25 | GLU | O-C-N | -6.43 | 115.30 | 120.38 |
| 1 | J5 | 20 | ASP | N-CA-C | 6.42 | 119.20 | 108.73 |
| 10 | j5 | 663 | ALA | O-C-N | -6.42 | 113.63 | 122.30 |
| 10 | k5 | 19 | THR | CA-C-O | -6.42 | 114.82 | 122.27 |
| 1 | D5 | 20 | ASP | N-CA-C | 6.42 | 119.19 | 108.73 |
| 10 | k5 | 421 | PRO | CA-C-O | -6.42 | 114.03 | 121.34 |
| 9 | x7 | 20 | GLY | CA-C-O | -6.42 | 115.70 | 121.47 |
| 10 | j5 | 464 | GLN | CA-CB-CG | -6.41 | 101.28 | 114.10 |
| 6 | M2 | 269 | ILE | CB-CA-C | -6.41 | 106.26 | 111.71 |
| 10 | k5 | 663 | ALA | O-C-N | -6.41 | 113.65 | 122.30 |
| 8 | I5 | 19 | SER | CB-CA-C | -6.40 | 99.64 | 108.86 |
| 10 | k5 | 660 | VAL | CB-CA-C | -6.40 | 103.50 | 112.14 |
| 10 | j5 | 660 | VAL | CB-CA-C | -6.40 | 103.50 | 112.14 |
| 9 | z5 | 19 | THR | N-CA-C | 6.40 | 118.05 | 111.14 |
| 10 | j5 | 966 | SER | N-CA-CB | -6.40 | 101.29 | 110.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 10 | k5 | 464 | GLN | CA-CB-CG | -6.40 | 101.31 | 114.10 |
| 10 | k5 | 929 | PRO | N-CA-C | 6.39 | 121.96 | 113.40 |
| 10 | k5 | 87 | ARG | N-CA-C | -6.39 | 104.24 | 111.14 |
| 10 | k5 | 617 | TYR | N-CA-C | 6.38 | 121.12 | 112.88 |
| 8 | C5 | 19 | SER | CB-CA-C | -6.38 | 99.67 | 108.86 |
| 8 | O5 | 20 | PRO | CB-CG-CD | -6.38 | 85.69 | 106.10 |
| 6 | M6 | 269 | ILE | CB-CA-C | -6.38 | 106.29 | 111.71 |
| 10 | k5 | 995 | VAL | CB-CA-C | -6.38 | 103.53 | 112.14 |
| 8 | i7 | 135 | ASN | N-CA-C | 6.38 | 118.23 | 111.28 |
| 10 | j5 | 87 | ARG | N-CA-C | -6.37 | 104.26 | 111.14 |
| 10 | j5 | 995 | VAL | CB-CA-C | -6.37 | 103.54 | 112.14 |
| 10 | k5 | 966 | SER | N-CA-CB | -6.37 | 101.33 | 110.44 |
| 8 | A5 | 65 | VAL | N-CA-C | -6.37 | 103.36 | 110.62 |
| 11 | aA | 446 | ALA | CA-C-N | -6.36 | 110.22 | 121.29 |
| 11 | aA | 446 | ALA | C-N-CA | -6.36 | 110.22 | 121.29 |
| 11 | a9 | 446 | ALA | CA-C-N | -6.36 | 110.23 | 121.29 |
| 11 | a9 | 446 | ALA | C-N-CA | -6.36 | 110.23 | 121.29 |
| 8 | c7 | 135 | ASN | N-CA-C | 6.36 | 118.21 | 111.28 |
| 8 | K5 | 94 | TYR | N-CA-C | -6.35 | 104.28 | 111.14 |
| 10 | j5 | 929 | PRO | N-CA-C | 6.35 | 121.90 | 113.40 |
| 10 | j5 | 917 | LYS | CB-CA-C | -6.34 | 99.50 | 109.52 |
| 8 | G5 | 65 | VAL | N-CA-C | -6.33 | 103.40 | 110.62 |
| 9 | w7 | 41 | GLN | CA-C-O | -6.33 | 113.71 | 120.42 |
| 8 | E5 | 94 | TYR | N-CA-C | -6.33 | 104.31 | 111.14 |
| 9 | z7 | 41 | GLN | CA-C-O | -6.33 | 113.71 | 120.42 |
| 10 | j5 | 617 | TYR | N-CA-C | 6.32 | 121.04 | 112.88 |
| 9 | w7 | 7 | VAL | CB-CA-C | -6.32 | 101.09 | 110.82 |
| 10 | j5 | 1111 | VAL | CB-CA-C | -6.31 | 104.07 | 110.89 |
| 10 | j5 | 267 | ASP | N-CA-C | 6.31 | 124.24 | 110.80 |
| 10 | k5 | 917 | LYS | CB-CA-C | -6.31 | 99.55 | 109.52 |
| 11 | a9 | 98 | ILE | N-CA-C | 6.30 | 119.88 | 111.44 |
| 11 | aA | 98 | ILE | N-CA-C | 6.30 | 119.88 | 111.44 |
| 4 | M4 | 19 | MET | CB-CA-C | -6.30 | 99.93 | 114.41 |
| 9 | z7 | 7 | VAL | CB-CA-C | -6.30 | 101.12 | 110.82 |
| 4 | MA | 19 | MET | CB-CA-C | -6.29 | 99.94 | 114.41 |
| 4 | M9 | 19 | MET | CB-CA-C | -6.29 | 99.94 | 114.41 |
| 3 | LA | 116 | THR | CB-CA-C | -6.29 | 101.01 | 110.88 |
| 3 | L9 | 116 | THR | CB-CA-C | -6.29 | 101.01 | 110.88 |
| 10 | k5 | 1111 | VAL | CB-CA-C | -6.28 | 104.11 | 110.89 |
| 8 | o7 | 56 | ASP | CB-CA-C | -6.28 | 100.36 | 110.79 |
| 4 | M1 | 19 | MET | CB-CA-C | -6.28 | 99.97 | 114.41 |
| 10 | k5 | 831 | PHE | CA-C-O | -6.27 | 113.77 | 120.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | M8 | 19 | MET | CB-CA-C | -6.27 | 99.98 | 114.41 |
| 11 | a9 | 602 | PRO | CA-C-N | 6.27 | 133.51 | 121.54 |
| 11 | a9 | 602 | PRO | C-N-CA | 6.27 | 133.51 | 121.54 |
| 11 | aA | 602 | PRO | CA-C-N | 6.27 | 133.51 | 121.54 |
| 11 | aA | 602 | PRO | C-N-CA | 6.27 | 133.51 | 121.54 |
| 10 | k5 | 267 | ASP | N-CA-C | 6.27 | 124.15 | 110.80 |
| 4 | MA | 93 | LEU | N-CA-C | 6.26 | 118.49 | 108.41 |
| 9 | z7 | 66 | GLY | CA-C-N | 6.26 | 128.45 | 120.56 |
| 9 | z7 | 66 | GLY | C-N-CA | 6.26 | 128.45 | 120.56 |
| 4 | M9 | 93 | LEU | N-CA-C | 6.26 | 118.49 | 108.41 |
| 4 | M3 | 19 | MET | CB-CA-C | -6.26 | 100.01 | 114.41 |
| 11 | a9 | 490 | ILE | CB-CA-C | -6.26 | 103.82 | 112.02 |
| 11 | aA | 490 | ILE | CB-CA-C | -6.26 | 103.82 | 112.02 |
| 4 | M3 | 93 | LEU | N-CA-C | 6.25 | 118.48 | 108.41 |
| 4 | M1 | 93 | LEU | N-CA-C | 6.25 | 118.48 | 108.41 |
| 8 | u7 | 56 | ASP | CB-CA-C | -6.25 | 100.42 | 110.79 |
| 11 | a9 | 324 | ASP | N-CA-C | 6.25 | 118.89 | 111.71 |
| 11 | aA | 324 | ASP | N-CA-C | 6.25 | 118.89 | 111.71 |
| 11 | a9 | 604 | ALA | N-CA-C | 6.24 | 123.60 | 109.81 |
| 11 | aA | 604 | ALA | N-CA-C | 6.24 | 123.60 | 109.81 |
| 11 | a9 | 419 | ARG | CB-CA-C | -6.24 | 101.28 | 110.95 |
| 11 | aA | 419 | ARG | CB-CA-C | -6.24 | 101.28 | 110.95 |
| 10 | k5 | 919 | ILE | CB-CA-C | -6.23 | 103.62 | 112.22 |
| 10 | j5 | 919 | ILE | CB-CA-C | -6.23 | 103.62 | 112.22 |
| 10 | j5 | 453 | PRO | CA-C-O | -6.23 | 114.34 | 121.56 |
| 10 | j5 | 831 | PHE | CA-C-O | -6.22 | 113.83 | 120.42 |
| 9 | w7 | 66 | GLY | CA-C-N | 6.22 | 128.40 | 120.56 |
| 9 | w7 | 66 | GLY | C-N-CA | 6.22 | 128.40 | 120.56 |
| 4 | M8 | 7 | SER | N-CA-CB | 6.22 | 121.00 | 110.49 |
| 8 | a7 | 13 | ALA | N-CA-C | 6.21 | 120.12 | 112.54 |
| 8 | C5 | 25 | ARG | N-CA-C | 6.21 | 124.03 | 110.80 |
| 1 | d5 | 107 | ARG | N-CA-C | 6.21 | 120.99 | 113.17 |
| 4 | M4 | 7 | SER | N-CA-CB | 6.20 | 120.97 | 110.49 |
| 10 | j5 | 880 | THR | N-CA-C | -6.20 | 97.59 | 110.80 |
| 10 | k5 | 453 | PRO | CA-C-O | -6.20 | 114.37 | 121.56 |
| 10 | k5 | 651 | ILE | CB-CA-C | -6.20 | 101.78 | 110.95 |
| 8 | g7 | 13 | ALA | N-CA-C | 6.19 | 120.10 | 112.54 |
| 10 | k5 | 880 | THR | N-CA-C | -6.19 | 97.61 | 110.80 |
| 1 | Z | 107 | ARG | N-CA-C | 6.19 | 120.97 | 113.17 |
| 8 | C5 | 27 | LYS | CA-C-N | -6.19 | 109.72 | 121.54 |
| 8 | C5 | 27 | LYS | C-N-CA | -6.19 | 109.72 | 121.54 |
| 10 | j5 | 651 | ILE | CB-CA-C | -6.19 | 101.79 | 110.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10 | j5 | 488 | LYS | N-CA-C | 6.19 | 119.22 | 110.50 |
| 1 | Z7 | 107 | ARG | N-CA-C | 6.19 | 120.97 | 113.17 |
| 8 | C5 | 23 | LEU | N-CA-C | -6.18 | 105.38 | 113.17 |
| 8 | I5 | 25 | ARG | N-CA-C | 6.18 | 123.97 | 110.80 |
| 1 | Z5 | 107 | ARG | N-CA-C | 6.18 | 120.96 | 113.17 |
| 1 | A | 107 | ARG | N-CA-C | 6.18 | 120.96 | 113.17 |
| 1 | N5 | 107 | ARG | N-CA-C | 6.18 | 120.95 | 113.17 |
| 10 | j5 | 857 | LYS | N-CA-C | 6.18 | 122.23 | 113.02 |
| 10 | k5 | 488 | LYS | N-CA-C | 6.18 | 119.21 | 110.50 |
| 10 | k5 | 857 | LYS | N-CA-C | 6.18 | 122.23 | 113.02 |
| 11 | aA | 540 | ILE | N-CA-C | -6.18 | 106.89 | 111.90 |
| 9 | z7 | 68 | GLY | N-CA-C | 6.17 | 121.33 | 113.24 |
| 8 | I5 | 27 | LYS | CA-C-N | -6.17 | 109.75 | 121.54 |
| 8 | I5 | 27 | LYS | C-N-CA | -6.17 | 109.75 | 121.54 |
| 9 | w7 | 68 | GLY | N-CA-C | 6.17 | 121.32 | 113.24 |
| 8 | A5 | 55 | GLY | O-C-N | -6.17 | 116.27 | 122.19 |
| 11 | a9 | 540 | ILE | N-CA-C | -6.17 | 106.90 | 111.90 |
| 4 | MA | 121 | GLU | N-CA-C | 6.17 | 118.80 | 111.71 |
| 5 | NA | 3 | VAL | N-CA-C | -6.17 | 96.51 | 109.34 |
| 4 | M9 | 121 | GLU | N-CA-C | 6.17 | 118.80 | 111.71 |
| 5 | N9 | 3 | VAL | N-CA-C | -6.17 | 96.51 | 109.34 |
| 1 | T5 | 107 | ARG | N-CA-C | 6.16 | 120.94 | 113.17 |
| 10 | k5 | 280 | ALA | N-CA-C | 6.16 | 117.80 | 111.14 |
| 10 | k5 | 586 | LEU | N-CA-C | 6.16 | 119.57 | 107.98 |
| 9 | z7 | 40 | GLU | N-CA-C | -6.16 | 105.92 | 113.50 |
| 10 | j5 | 947 | MET | CA-C-N | 6.16 | 131.86 | 122.37 |
| 10 | j5 | 947 | MET | C-N-CA | 6.16 | 131.86 | 122.37 |
| 4 | M8 | 121 | GLU | N-CA-C | 6.16 | 118.79 | 111.71 |
| 5 | Z8 | 3 | VAL | N-CA-C | -6.16 | 96.53 | 109.34 |
| 5 | N1 | 3 | VAL | N-CA-C | -6.16 | 96.53 | 109.34 |
| 8 | I5 | 23 | LEU | N-CA-C | -6.16 | 105.41 | 113.17 |
| 10 | k5 | 184 | LEU | N-CA-C | 6.16 | 118.79 | 111.71 |
| 10 | k5 | 295 | ARG | N-CA-C | -6.16 | 104.65 | 111.36 |
| 10 | k5 | 947 | MET | CA-C-N | 6.16 | 131.85 | 122.37 |
| 10 | k5 | 947 | MET | C-N-CA | 6.16 | 131.85 | 122.37 |
| 5 | Z4 | 3 | VAL | N-CA-C | -6.15 | 96.54 | 109.34 |
| 11 | aA | 621 | THR | CB-CA-C | -6.15 | 96.53 | 110.07 |
| 11 | a9 | 621 | THR | CB-CA-C | -6.15 | 96.53 | 110.07 |
| 9 | w7 | 40 | GLU | N-CA-C | -6.15 | 105.94 | 113.50 |
| 5 | N3 | 3 | VAL | N-CA-C | -6.14 | 96.56 | 109.34 |
| 10 | j5 | 586 | LEU | N-CA-C | 6.14 | 119.53 | 107.98 |
| 10 | j5 | 184 | LEU | N-CA-C | 6.14 | 118.77 | 111.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 8 | E5 | 133 | MET | N-CA-C | -6.14 | 105.50 | 112.87 |
| 10 | j5 | 280 | ALA | N-CA-C | 6.14 | 117.77 | 111.14 |
| 4 | M8 | 139 | VAL | N-CA-C | 6.14 | 116.88 | 110.62 |
| 1 | B5 | 107 | ARG | N-CA-C | 6.13 | 120.90 | 113.17 |
| 1 | T7 | 107 | ARG | N-CA-C | 6.13 | 120.90 | 113.17 |
| 3 | LA | 98 | LEU | CA-C-N | -6.13 | 111.43 | 120.38 |
| 3 | LA | 98 | LEU | C-N-CA | -6.13 | 111.43 | 120.38 |
| 4 | M4 | 121 | GLU | N-CA-C | 6.13 | 118.75 | 111.71 |
| 3 | H2 | 84 | ARG | O-C-N | -6.12 | 115.17 | 122.15 |
| 10 | j5 | 722 | ILE | CB-CA-C | -6.12 | 103.77 | 112.22 |
| 3 | H6 | 84 | ARG | O-C-N | -6.12 | 115.17 | 122.15 |
| 4 | M8 | 66 | VAL | CB-CA-C | -6.12 | 103.19 | 111.15 |
| 4 | M8 | 140 | ARG | N-CA-C | 6.12 | 117.62 | 111.07 |
| 3 | L9 | 98 | LEU | CA-C-N | -6.12 | 111.45 | 120.38 |
| 3 | L9 | 98 | LEU | C-N-CA | -6.12 | 111.45 | 120.38 |
| 1 | H7 | 107 | ARG | N-CA-C | 6.12 | 120.88 | 113.17 |
| 1 | H5 | 107 | ARG | N-CA-C | 6.11 | 120.87 | 113.17 |
| 10 | k5 | 704 | THR | CA-C-O | -6.11 | 114.40 | 120.70 |
| 4 | M9 | 66 | VAL | CB-CA-C | -6.11 | 103.21 | 111.15 |
| 1 | f7 | 107 | ARG | N-CA-C | 6.11 | 120.87 | 113.17 |
| 11 | a9 | 813 | PRO | N-CA-C | -6.11 | 105.22 | 113.40 |
| 4 | M3 | 121 | GLU | N-CA-C | 6.11 | 118.73 | 111.71 |
| 10 | j5 | 501 | ILE | CG1-CB-CG2 | 6.11 | 129.01 | 110.70 |
| 11 | aA | 813 | PRO | N-CA-C | -6.11 | 105.22 | 113.40 |
| 4 | M1 | 121 | GLU | N-CA-C | 6.11 | 118.73 | 111.71 |
| 8 | G5 | 55 | GLY | O-C-N | -6.10 | 116.33 | 122.19 |
| 10 | j5 | 704 | THR | CA-C-O | -6.10 | 114.41 | 120.70 |
| 8 | E5 | 108 | GLY | N-CA-C | 6.10 | 127.64 | 113.18 |
| 4 | MA | 66 | VAL | CB-CA-C | -6.10 | 103.22 | 111.15 |
| 8 | K5 | 108 | GLY | N-CA-C | 6.10 | 127.63 | 113.18 |
| 10 | k5 | 501 | ILE | CG1-CB-CG2 | 6.10 | 129.00 | 110.70 |
| 10 | k5 | 692 | LEU | CA-CB-CG | 6.10 | 137.64 | 116.30 |
| 10 | j5 | 692 | LEU | CA-CB-CG | 6.09 | 137.63 | 116.30 |
| 10 | j5 | 655 | LYS | N-CA-C | 6.09 | 122.59 | 114.12 |
| 10 | k5 | 722 | ILE | CB-CA-C | -6.09 | 103.82 | 112.22 |
| 4 | M4 | 66 | VAL | CB-CA-C | -6.09 | 103.24 | 111.15 |
| 1 | B7 | 107 | ARG | N-CA-C | 6.08 | 120.84 | 113.17 |
| 10 | k5 | 536 | LYS | N-CA-CB | -6.08 | 101.41 | 110.17 |
| 10 | k5 | 847 | LEU | CA-C-O | -6.08 | 114.39 | 120.90 |
| 8 | U7 | 23 | LEU | CA-C-N | -6.08 | 111.97 | 122.79 |
| 8 | U7 | 23 | LEU | C-N-CA | -6.08 | 111.97 | 122.79 |
| 1 | N7 | 107 | ARG | N-CA-C | 6.08 | 120.82 | 113.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 10 | j5 | 573 | GLN | CA-CB-CG | 6.07 | 126.25 | 114.10 |
| 10 | j5 | 847 | LEU | CA-C-O | -6.07 | 114.40 | 120.90 |
| 9 | x7 | 26 | THR | CB-CA-C | -6.07 | 98.61 | 109.24 |
| 4 | M3 | 46 | VAL | N-CA-CB | -6.07 | 104.11 | 111.21 |
| 10 | j5 | 295 | ARG | N-CA-C | -6.07 | 104.74 | 111.36 |
| 4 | M1 | 46 | VAL | N-CA-CB | -6.07 | 104.11 | 111.21 |
| 4 | MA | 25 | LEU | N-CA-C | -6.07 | 98.62 | 108.52 |
| 10 | k5 | 573 | GLN | CA-CB-CG | 6.07 | 126.24 | 114.10 |
| 4 | M9 | 25 | LEU | N-CA-C | -6.07 | 98.62 | 108.52 |
| 1 | h7 | 48 | ALA | N-CA-C | 6.07 | 117.89 | 111.28 |
| 8 | i7 | 143 | GLY | N-CA-C | 6.07 | 120.23 | 112.83 |
| 1 | b7 | 48 | ALA | N-CA-C | 6.06 | 117.89 | 111.28 |
| 4 | M3 | 66 | VAL | CB-CA-C | -6.06 | 103.27 | 111.15 |
| 4 | M1 | 66 | VAL | CB-CA-C | -6.06 | 103.27 | 111.15 |
| 10 | j5 | 461 | ASP | CB-CA-C | -6.06 | 99.42 | 110.63 |
| 10 | j5 | 571 | ALA | N-CA-C | -6.06 | 104.60 | 111.14 |
| 4 | M9 | 46 | VAL | N-CA-CB | -6.06 | 104.12 | 111.21 |
| 10 | j5 | 536 | LYS | N-CA-CB | -6.06 | 101.45 | 110.17 |
| 10 | k5 | 461 | ASP | CB-CA-C | -6.06 | 99.43 | 110.63 |
| 8 | c7 | 143 | GLY | N-CA-C | 6.05 | 120.22 | 112.83 |
| 4 | M8 | 25 | LEU | N-CA-C | -6.05 | 98.65 | 108.52 |
| 4 | MA | 46 | VAL | N-CA-CB | -6.05 | 104.13 | 111.21 |
| 4 | M3 | 25 | LEU | N-CA-C | -6.05 | 98.65 | 108.52 |
| 1 | r7 | 107 | ARG | N-CA-C | 6.05 | 120.80 | 113.17 |
| 4 | M1 | 25 | LEU | N-CA-C | -6.05 | 98.65 | 108.52 |
| 10 | j5 | 514 | SER | CA-C-O | -6.05 | 115.15 | 120.60 |
| 9 | y7 | 26 | THR | CB-CA-C | -6.05 | 98.65 | 109.24 |
| 11 | a9 | 623 | ASP | N-CA-C | -6.05 | 98.22 | 108.26 |
| 11 | aA | 623 | ASP | N-CA-C | -6.05 | 98.22 | 108.26 |
| 10 | k5 | 655 | LYS | N-CA-C | 6.05 | 122.52 | 114.12 |
| 1 | l7 | 107 | ARG | N-CA-C | 6.05 | 120.79 | 113.17 |
| 10 | k5 | 494 | PRO | CB-CA-C | -6.04 | 103.97 | 111.64 |
| 10 | k5 | 537 | ILE | N-CA-CB | -6.04 | 103.79 | 111.64 |
| 4 | M4 | 25 | LEU | N-CA-C | -6.04 | 98.68 | 108.52 |
| 10 | j5 | 614 | ARG | CB-CA-C | -6.04 | 101.40 | 110.88 |
| 10 | k5 | 614 | ARG | CB-CA-C | -6.04 | 101.40 | 110.88 |
| 4 | M4 | 46 | VAL | N-CA-CB | -6.03 | 104.15 | 111.21 |
| 10 | k5 | 824 | PRO | CA-C-O | -6.03 | 114.56 | 121.56 |
| 10 | k5 | 492 | ILE | N-CA-CB | 6.03 | 117.61 | 110.55 |
| 8 | i7 | 136 | VAL | CB-CA-C | -6.03 | 104.25 | 111.97 |
| 10 | k5 | 15 | ARG | N-CA-C | 6.03 | 118.47 | 109.25 |
| 8 | e5 | 13 | ALA | N-CA-C | -6.03 | 105.93 | 113.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10 | j5 | 15 | ARG | N-CA-C | 6.02 | 118.47 | 109.25 |
| 10 | k5 | 571 | ALA | N-CA-C | -6.02 | 104.64 | 111.14 |
| 10 | j5 | 537 | ILE | N-CA-CB | -6.02 | 103.81 | 111.64 |
| 10 | k5 | 589 | ALA | CA-C-N | 6.02 | 128.83 | 120.29 |
| 10 | k5 | 589 | ALA | C-N-CA | 6.02 | 128.83 | 120.29 |
| 3 | L9 | 144 | SER | CA-C-N | 6.02 | 127.36 | 119.84 |
| 3 | L9 | 144 | SER | C-N-CA | 6.02 | 127.36 | 119.84 |
| 4 | M8 | 46 | VAL | N-CA-CB | -6.01 | 104.17 | 111.21 |
| 10 | k5 | 854 | LEU | N-CA-C | -6.01 | 104.09 | 112.45 |
| 10 | j5 | 824 | PRO | CA-C-O | -6.01 | 114.59 | 121.56 |
| 10 | j5 | 779 | ASP | N-CA-C | 6.01 | 117.91 | 111.36 |
| 9 | x7 | 63 | ALA | CA-C-N | 6.01 | 133.01 | 121.54 |
| 9 | x7 | 63 | ALA | C-N-CA | 6.01 | 133.01 | 121.54 |
| 11 | a9 | 423 | ILE | N-CA-C | 6.01 | 118.36 | 108.99 |
| 11 | aA | 423 | ILE | N-CA-C | 6.01 | 118.36 | 108.99 |
| 11 | a9 | 807 | GLN | N-CA-C | -6.00 | 98.29 | 108.26 |
| 11 | aA | 807 | GLN | N-CA-C | -6.00 | 98.29 | 108.26 |
| 8 | a5 | 13 | ALA | N-CA-C | -6.00 | 105.96 | 113.28 |
| 10 | j5 | 494 | PRO | CB-CA-C | -6.00 | 104.02 | 111.64 |
| 3 | H6 | 144 | SER | CA-C-N | 6.00 | 127.34 | 119.84 |
| 3 | H6 | 144 | SER | C-N-CA | 6.00 | 127.34 | 119.84 |
| 11 | aA | 800 | THR | CB-CA-C | -6.00 | 99.20 | 110.01 |
| 10 | j5 | 492 | ILE | N-CA-CB | 6.00 | 117.57 | 110.55 |
| 10 | k5 | 883 | SER | CB-CA-C | -6.00 | 98.48 | 110.42 |
| 8 | U5 | 22 | GLU | N-CA-C | -6.00 | 106.00 | 113.38 |
| 10 | j5 | 733 | SER | N-CA-CB | -6.00 | 101.59 | 110.53 |
| 3 | L4 | 144 | SER | CA-C-N | 6.00 | 127.33 | 119.84 |
| 3 | L4 | 144 | SER | C-N-CA | 6.00 | 127.33 | 119.84 |
| 3 | L8 | 144 | SER | CA-C-N | 6.00 | 127.33 | 119.84 |
| 3 | L8 | 144 | SER | C-N-CA | 6.00 | 127.33 | 119.84 |
| 10 | j5 | 589 | ALA | CA-C-N | 5.99 | 128.80 | 120.29 |
| 10 | j5 | 589 | ALA | C-N-CA | 5.99 | 128.80 | 120.29 |
| 3 | LA | 144 | SER | CA-C-N | 5.99 | 127.33 | 119.84 |
| 3 | LA | 144 | SER | C-N-CA | 5.99 | 127.33 | 119.84 |
| 10 | j5 | 767 | LEU | CB-CA-C | -5.99 | 101.48 | 110.88 |
| 11 | a9 | 538 | ARG | N-CA-C | 5.99 | 119.41 | 111.75 |
| 11 | aA | 538 | ARG | N-CA-C | 5.99 | 119.41 | 111.75 |
| 9 | y7 | 63 | ALA | CA-C-N | 5.99 | 132.97 | 121.54 |
| 9 | y7 | 63 | ALA | C-N-CA | 5.99 | 132.97 | 121.54 |
| 3 | H2 | 144 | SER | CA-C-N | 5.98 | 127.32 | 119.84 |
| 3 | H2 | 144 | SER | C-N-CA | 5.98 | 127.32 | 119.84 |
| 10 | k5 | 779 | ASP | N-CA-C | 5.98 | 117.88 | 111.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | X3 | 144 | SER | CA-C-N | 5.98 | 127.31 | 119.84 |
| 3 | X3 | 144 | SER | C-N-CA | 5.98 | 127.31 | 119.84 |
| 10 | k5 | 411 | TYR | CB-CA-C | -5.98 | 101.50 | 110.88 |
| 3 | X1 | 144 | SER | CA-C-N | 5.98 | 127.31 | 119.84 |
| 3 | X1 | 144 | SER | C-N-CA | 5.98 | 127.31 | 119.84 |
| 3 | H4 | 144 | SER | CA-C-N | 5.98 | 127.31 | 119.84 |
| 3 | H4 | 144 | SER | C-N-CA | 5.98 | 127.31 | 119.84 |
| 10 | j5 | 883 | SER | CB-CA-C | -5.98 | 98.53 | 110.42 |
| 11 | a9 | 800 | THR | CB-CA-C | -5.97 | 99.26 | 110.01 |
| 10 | j5 | 411 | TYR | CB-CA-C | -5.97 | 101.50 | 110.88 |
| 10 | k5 | 767 | LEU | CB-CA-C | -5.97 | 101.51 | 110.88 |
| 8 | c7 | 136 | VAL | CB-CA-C | -5.96 | 104.34 | 111.97 |
| 10 | k5 | 893 | ASN | CA-C-O | -5.96 | 114.10 | 120.42 |
| 8 | U5 | 18 | LEU | O-C-N | 5.96 | 130.14 | 122.81 |
| 8 | O7 | 20 | PRO | N-CA-C | 5.96 | 124.74 | 112.47 |
| 10 | k5 | 511 | ARG | N-CA-CB | -5.95 | 100.72 | 110.43 |
| 3 | H8 | 144 | SER | CA-C-N | 5.95 | 127.28 | 119.84 |
| 3 | H8 | 144 | SER | C-N-CA | 5.95 | 127.28 | 119.84 |
| 3 | L4 | 66 | LEU | N-CA-C | -5.95 | 98.12 | 110.80 |
| 10 | j5 | 511 | ARG | N-CA-CB | -5.95 | 100.73 | 110.43 |
| 3 | D3 | 144 | SER | CA-C-N | 5.95 | 127.28 | 119.84 |
| 3 | D3 | 144 | SER | C-N-CA | 5.95 | 127.28 | 119.84 |
| 9 | z7 | 17 | VAL | N-CA-C | 5.95 | 121.72 | 109.34 |
| 9 | z7 | 62 | GLY | N-CA-C | 5.95 | 120.39 | 112.77 |
| 4 | M4 | 93 | LEU | N-CA-C | 5.95 | 118.43 | 108.02 |
| 10 | k5 | 733 | SER | N-CA-CB | -5.95 | 101.67 | 110.53 |
| 11 | a9 | 636 | ALA | CA-C-N | 5.95 | 127.55 | 120.23 |
| 11 | a9 | 636 | ALA | C-N-CA | 5.95 | 127.55 | 120.23 |
| 3 | T1 | 144 | SER | CA-C-N | 5.95 | 127.27 | 119.84 |
| 3 | T1 | 144 | SER | C-N-CA | 5.95 | 127.27 | 119.84 |
| 10 | k5 | 557 | VAL | CA-C-O | -5.94 | 114.05 | 120.47 |
| 3 | F3 | 144 | SER | CA-C-N | 5.94 | 127.27 | 119.84 |
| 3 | F3 | 144 | SER | C-N-CA | 5.94 | 127.27 | 119.84 |
| 10 | j5 | 854 | LEU | N-CA-C | -5.94 | 104.19 | 112.45 |
| 10 | k5 | 514 | SER | CA-C-O | -5.94 | 115.25 | 120.60 |
| 9 | w7 | 17 | VAL | N-CA-C | 5.94 | 121.70 | 109.34 |
| 3 | F1 | 144 | SER | CA-C-N | 5.94 | 127.27 | 119.84 |
| 3 | F1 | 144 | SER | C-N-CA | 5.94 | 127.27 | 119.84 |
| 10 | j5 | 544 | VAL | N-CA-C | -5.94 | 96.99 | 109.34 |
| 3 | D1 | 144 | SER | CA-C-N | 5.94 | 127.26 | 119.84 |
| 3 | D1 | 144 | SER | C-N-CA | 5.94 | 127.26 | 119.84 |
| 3 | L1 | 144 | SER | CA-C-N | 5.94 | 127.26 | 119.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | L1 | 144 | SER | C-N-CA | 5.94 | 127.26 | 119.84 |
| 3 | L6 | 144 | SER | CA-C-N | 5.93 | 127.26 | 119.84 |
| 3 | L6 | 144 | SER | C-N-CA | 5.93 | 127.26 | 119.84 |
| 10 | j5 | 893 | ASN | CA-C-O | -5.93 | 114.13 | 120.42 |
| 4 | M8 | 92 | GLU | N-CA-C | 5.93 | 118.08 | 108.41 |
| 3 | H3 | 144 | SER | CA-C-N | 5.93 | 127.25 | 119.84 |
| 3 | H3 | 144 | SER | C-N-CA | 5.93 | 127.25 | 119.84 |
| 4 | M8 | 173 | PHE | N-CA-C | 5.93 | 117.82 | 111.36 |
| 11 | a9 | 616 | PRO | CB-CA-C | -5.93 | 103.81 | 111.46 |
| 11 | aA | 616 | PRO | CB-CA-C | -5.93 | 103.81 | 111.46 |
| 3 | H1 | 144 | SER | CA-C-N | 5.93 | 127.25 | 119.84 |
| 3 | H1 | 144 | SER | C-N-CA | 5.93 | 127.25 | 119.84 |
| 3 | F9 | 157 | VAL | N-CA-CB | -5.93 | 103.61 | 110.55 |
| 11 | a9 | 444 | ARG | N-CA-C | 5.92 | 117.74 | 111.28 |
| 3 | L2 | 144 | SER | CA-C-N | 5.92 | 127.24 | 119.84 |
| 3 | L2 | 144 | SER | C-N-CA | 5.92 | 127.24 | 119.84 |
| 10 | k5 | 544 | VAL | N-CA-C | -5.92 | 97.02 | 109.34 |
| 11 | aA | 444 | ARG | N-CA-C | 5.92 | 117.73 | 111.28 |
| 8 | I5 | 11 | ALA | N-CA-C | -5.92 | 104.41 | 111.69 |
| 3 | T3 | 144 | SER | CA-C-N | 5.92 | 127.24 | 119.84 |
| 3 | T3 | 144 | SER | C-N-CA | 5.92 | 127.24 | 119.84 |
| 1 | T7 | 34 | GLY | N-CA-C | 5.92 | 119.36 | 112.50 |
| 11 | aA | 636 | ALA | CA-C-N | 5.92 | 127.51 | 120.23 |
| 11 | aA | 636 | ALA | C-N-CA | 5.92 | 127.51 | 120.23 |
| 4 | M3 | 112 | GLN | N-CA-C | 5.92 | 117.53 | 111.14 |
| 4 | M4 | 173 | PHE | N-CA-C | 5.92 | 117.81 | 111.36 |
| 9 | w7 | 62 | GLY | N-CA-C | 5.91 | 120.34 | 112.77 |
| 11 | a9 | 583 | ALA | CA-C-N | -5.91 | 111.89 | 120.29 |
| 11 | a9 | 583 | ALA | C-N-CA | -5.91 | 111.89 | 120.29 |
| 11 | aA | 583 | ALA | CA-C-N | -5.91 | 111.89 | 120.29 |
| 11 | aA | 583 | ALA | C-N-CA | -5.91 | 111.89 | 120.29 |
| 1 | L5 | 34 | GLY | N-CA-C | 5.91 | 119.36 | 112.50 |
| 3 | XA | 144 | SER | CA-C-N | 5.91 | 127.22 | 119.84 |
| 3 | XA | 144 | SER | C-N-CA | 5.91 | 127.22 | 119.84 |
| 3 | L3 | 144 | SER | CA-C-N | 5.91 | 127.23 | 119.84 |
| 3 | L3 | 144 | SER | C-N-CA | 5.91 | 127.23 | 119.84 |
| 10 | k5 | 544 | VAL | N-CA-CB | 5.91 | 120.98 | 111.23 |
| 3 | F6 | 144 | SER | CA-C-N | 5.91 | 127.22 | 119.84 |
| 3 | F6 | 144 | SER | C-N-CA | 5.91 | 127.22 | 119.84 |
| 11 | a9 | 542 | ALA | N-CA-C | 5.91 | 117.80 | 111.36 |
| 11 | aA | 542 | ALA | N-CA-C | 5.91 | 117.80 | 111.36 |
| 1 | d5 | 34 | GLY | N-CA-C | 5.90 | 119.35 | 112.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3 | X9 | 144 | SER | CA-C-N | 5.90 | 127.22 | 119.84 |
| 3 | X9 | 144 | SER | C-N-CA | 5.90 | 127.22 | 119.84 |
| 10 | k5 | 751 | LYS | CA-C-O | -5.90 | 114.50 | 121.16 |
| 3 | J3 | 144 | SER | CA-C-N | 5.89 | 127.21 | 119.84 |
| 3 | J3 | 144 | SER | C-N-CA | 5.89 | 127.21 | 119.84 |
| 10 | j5 | 751 | LYS | CA-C-O | -5.89 | 114.50 | 121.16 |
| 1 | T5 | 34 | GLY | N-CA-C | 5.89 | 119.33 | 112.50 |
| 4 | M3 | 228 | SER | O-C-N | -5.89 | 116.62 | 123.27 |
| 10 | j5 | 385 | PRO | O-C-N | -5.89 | 114.11 | 122.35 |
| 8 | C5 | 11 | ALA | N-CA-C | -5.89 | 104.45 | 111.69 |
| 4 | M3 | 57 | THR | CB-CA-C | -5.88 | 101.02 | 110.79 |
| 4 | M4 | 57 | THR | CB-CA-C | -5.88 | 101.02 | 110.79 |
| 1 | B7 | 34 | GLY | N-CA-C | 5.88 | 119.33 | 112.50 |
| 3 | F8 | 113 | LEU | CA-C-N | -5.88 | 110.40 | 122.58 |
| 3 | F8 | 113 | LEU | C-N-CA | -5.88 | 110.40 | 122.58 |
| 3 | F9 | 153 | CYS | CA-CB-SG | 5.88 | 127.93 | 114.40 |
| 11 | a9 | 51 | SER | CA-C-O | -5.88 | 113.45 | 120.10 |
| 11 | aA | 51 | SER | CA-C-O | -5.88 | 113.45 | 120.10 |
| 4 | M1 | 57 | THR | CB-CA-C | -5.88 | 101.02 | 110.79 |
| 3 | Q8 | 144 | SER | CA-C-N | 5.88 | 127.19 | 119.84 |
| 3 | Q8 | 144 | SER | C-N-CA | 5.88 | 127.19 | 119.84 |
| 3 | Q4 | 144 | SER | CA-C-N | 5.88 | 127.19 | 119.84 |
| 3 | Q4 | 144 | SER | C-N-CA | 5.88 | 127.19 | 119.84 |
| 1 | D5 | 34 | GLY | N-CA-C | 5.88 | 119.32 | 112.50 |
| 3 | H9 | 144 | SER | CA-C-N | 5.88 | 127.19 | 119.84 |
| 3 | H9 | 144 | SER | C-N-CA | 5.88 | 127.19 | 119.84 |
| 4 | MA | 57 | THR | CB-CA-C | -5.88 | 101.03 | 110.79 |
| 3 | Y4 | 144 | SER | CA-C-N | 5.88 | 127.19 | 119.84 |
| 3 | Y4 | 144 | SER | C-N-CA | 5.88 | 127.19 | 119.84 |
| 1 | N7 | 34 | GLY | N-CA-C | 5.88 | 119.32 | 112.50 |
| 1 | r7 | 34 | GLY | N-CA-C | 5.88 | 119.32 | 112.50 |
| 3 | FA | 153 | CYS | CA-CB-SG | 5.88 | 127.92 | 114.40 |
| 10 | j5 | 544 | VAL | N-CA-CB | 5.88 | 120.93 | 111.23 |
| 10 | k5 | 548 | SER | CA-C-N | 5.88 | 132.76 | 121.54 |
| 10 | k5 | 548 | SER | C-N-CA | 5.88 | 132.76 | 121.54 |
| 3 | HA | 144 | SER | CA-C-N | 5.87 | 127.18 | 119.84 |
| 3 | HA | 144 | SER | C-N-CA | 5.87 | 127.18 | 119.84 |
| 1 | H5 | 34 | GLY | N-CA-C | 5.87 | 119.31 | 112.50 |
| 1 | J5 | 34 | GLY | N-CA-C | 5.87 | 119.31 | 112.50 |
| 3 | PA | 144 | SER | CA-C-N | 5.87 | 127.18 | 119.84 |
| 3 | PA | 144 | SER | C-N-CA | 5.87 | 127.18 | 119.84 |
| 1 | P7 | 34 | GLY | N-CA-C | 5.87 | 119.31 | 112.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | R7 | 34 | GLY | N-CA-C | 5.87 | 119.31 | 112.50 |
| 3 | P9 | 144 | SER | CA-C-N | 5.87 | 127.18 | 119.84 |
| 3 | P9 | 144 | SER | C-N-CA | 5.87 | 127.18 | 119.84 |
| 3 | B3 | 144 | SER | CA-C-N | 5.87 | 127.17 | 119.84 |
| 3 | B3 | 144 | SER | C-N-CA | 5.87 | 127.17 | 119.84 |
| 3 | B1 | 144 | SER | CA-C-N | 5.87 | 127.17 | 119.84 |
| 3 | B1 | 144 | SER | C-N-CA | 5.87 | 127.17 | 119.84 |
| 3 | RA | 144 | SER | CA-C-N | 5.87 | 127.17 | 119.84 |
| 3 | RA | 144 | SER | C-N-CA | 5.87 | 127.17 | 119.84 |
| 4 | M3 | 173 | PHE | N-CA-C | 5.87 | 117.75 | 111.36 |
| 1 | N5 | 34 | GLY | N-CA-C | 5.87 | 119.31 | 112.50 |
| 1 | F5 | 34 | GLY | N-CA-C | 5.87 | 119.30 | 112.50 |
| 1 | Z5 | 34 | GLY | N-CA-C | 5.87 | 119.30 | 112.50 |
| 3 | R9 | 144 | SER | CA-C-N | 5.87 | 127.17 | 119.84 |
| 3 | R9 | 144 | SER | C-N-CA | 5.87 | 127.17 | 119.84 |
| 4 | M1 | 173 | PHE | N-CA-C | 5.87 | 117.75 | 111.36 |
| 1 | l7 | 34 | GLY | N-CA-C | 5.86 | 119.30 | 112.50 |
| 8 | u7 | 50 | ILE | CB-CA-C | -5.86 | 104.13 | 112.22 |
| 9 | z7 | 67 | VAL | CB-CA-C | -5.86 | 104.47 | 111.97 |
| 4 | M8 | 57 | THR | CB-CA-C | -5.86 | 101.06 | 110.79 |
| 4 | M9 | 57 | THR | CB-CA-C | -5.86 | 101.06 | 110.79 |
| 3 | J1 | 144 | SER | CA-C-N | 5.86 | 127.17 | 119.84 |
| 3 | J1 | 144 | SER | C-N-CA | 5.86 | 127.17 | 119.84 |
| 4 | M1 | 228 | SER | O-C-N | -5.86 | 116.64 | 123.27 |
| 1 | H7 | 34 | GLY | N-CA-C | 5.86 | 119.30 | 112.50 |
| 4 | MA | 112 | GLN | N-CA-C | 5.86 | 117.47 | 111.14 |
| 4 | MA | 173 | PHE | N-CA-C | 5.86 | 117.75 | 111.36 |
| 4 | M4 | 112 | GLN | N-CA-C | 5.86 | 117.47 | 111.14 |
| 9 | w7 | 67 | VAL | CB-CA-C | -5.86 | 104.47 | 111.97 |
| 4 | M9 | 112 | GLN | N-CA-C | 5.86 | 117.47 | 111.14 |
| 4 | M9 | 173 | PHE | N-CA-C | 5.86 | 117.75 | 111.36 |
| 11 | aA | 557 | GLY | N-CA-C | -5.86 | 99.29 | 113.18 |
| 4 | M1 | 112 | GLN | N-CA-C | 5.86 | 117.47 | 111.14 |
| 1 | Z | 34 | GLY | N-CA-C | 5.86 | 119.30 | 112.50 |
| 3 | TA | 144 | SER | CA-C-N | 5.86 | 127.16 | 119.84 |
| 3 | TA | 144 | SER | C-N-CA | 5.86 | 127.16 | 119.84 |
| 3 | Y8 | 144 | SER | CA-C-N | 5.86 | 127.16 | 119.84 |
| 3 | Y8 | 144 | SER | C-N-CA | 5.86 | 127.16 | 119.84 |
| 3 | T9 | 144 | SER | CA-C-N | 5.86 | 127.16 | 119.84 |
| 3 | T9 | 144 | SER | C-N-CA | 5.86 | 127.16 | 119.84 |
| 10 | j5 | 741 | GLN | CA-C-O | -5.86 | 115.18 | 121.56 |
| 1 | A | 34 | GLY | N-CA-C | 5.85 | 119.29 | 112.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3 | Z3 | 144 | SER | CA-C-N | 5.85 | 127.15 | 119.84 |
| 3 | Z3 | 144 | SER | C-N-CA | 5.85 | 127.15 | 119.84 |
| 10 | k5 | 1086 | THR | N-CA-C | 5.85 | 120.43 | 113.12 |
| 3 | Z1 | 144 | SER | CA-C-N | 5.85 | 127.15 | 119.84 |
| 3 | Z1 | 144 | SER | C-N-CA | 5.85 | 127.15 | 119.84 |
| 1 | V5 | 34 | GLY | N-CA-C | 5.85 | 119.28 | 112.50 |
| 3 | B6 | 144 | SER | CA-C-N | 5.85 | 127.15 | 119.84 |
| 3 | B6 | 144 | SER | C-N-CA | 5.85 | 127.15 | 119.84 |
| 8 | o7 | 50 | ILE | N-CA-C | -5.85 | 104.81 | 110.72 |
| 4 | M8 | 112 | GLN | N-CA-C | 5.85 | 117.45 | 111.14 |
| 2 | U1 | 44 | LEU | CA-C-N | 5.85 | 128.70 | 120.28 |
| 2 | U1 | 44 | LEU | C-N-CA | 5.85 | 128.70 | 120.28 |
| 10 | k5 | 385 | PRO | O-C-N | -5.85 | 114.17 | 122.35 |
| 3 | V3 | 144 | SER | CA-C-N | 5.84 | 127.15 | 119.84 |
| 3 | V3 | 144 | SER | C-N-CA | 5.84 | 127.15 | 119.84 |
| 3 | U4 | 144 | SER | CA-C-N | 5.84 | 127.14 | 119.84 |
| 3 | U4 | 144 | SER | C-N-CA | 5.84 | 127.14 | 119.84 |
| 1 | B5 | 34 | GLY | N-CA-C | 5.84 | 119.28 | 112.50 |
| 3 | U8 | 144 | SER | CA-C-N | 5.84 | 127.14 | 119.84 |
| 3 | U8 | 144 | SER | C-N-CA | 5.84 | 127.14 | 119.84 |
| 3 | O8 | 144 | SER | CA-C-N | 5.84 | 127.14 | 119.84 |
| 3 | O8 | 144 | SER | C-N-CA | 5.84 | 127.14 | 119.84 |
| 3 | V1 | 144 | SER | CA-C-N | 5.84 | 127.15 | 119.84 |
| 3 | V1 | 144 | SER | C-N-CA | 5.84 | 127.15 | 119.84 |
| 10 | j5 | 157 | ILE | N-CA-C | 5.84 | 116.62 | 110.72 |
| 3 | B4 | 144 | SER | CA-C-N | 5.84 | 127.14 | 119.84 |
| 3 | B4 | 144 | SER | C-N-CA | 5.84 | 127.14 | 119.84 |
| 3 | B2 | 144 | SER | CA-C-N | 5.84 | 127.14 | 119.84 |
| 3 | B2 | 144 | SER | C-N-CA | 5.84 | 127.14 | 119.84 |
| 1 | b5 | 34 | GLY | N-CA-C | 5.84 | 119.27 | 112.50 |
| 10 | k5 | 848 | ILE | CB-CA-C | -5.84 | 104.26 | 112.14 |
| 1 | n7 | 34 | GLY | N-CA-C | 5.84 | 119.27 | 112.50 |
| 3 | W4 | 144 | SER | CA-C-N | 5.83 | 127.13 | 119.84 |
| 3 | W4 | 144 | SER | C-N-CA | 5.83 | 127.13 | 119.84 |
| 10 | j5 | 548 | SER | CA-C-N | 5.83 | 132.69 | 121.54 |
| 10 | j5 | 548 | SER | C-N-CA | 5.83 | 132.69 | 121.54 |
| 3 | W8 | 144 | SER | CA-C-N | 5.83 | 127.13 | 119.84 |
| 3 | W8 | 144 | SER | C-N-CA | 5.83 | 127.13 | 119.84 |
| 1 | P5 | 34 | GLY | N-CA-C | 5.83 | 119.27 | 112.50 |
| 3 | B8 | 144 | SER | CA-C-N | 5.83 | 127.13 | 119.84 |
| 3 | B8 | 144 | SER | C-N-CA | 5.83 | 127.13 | 119.84 |
| 11 | aA | 376 | ALA | N-CA-C | 5.83 | 117.86 | 110.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11 | a9 | 338 | VAL | N-CA-C | -5.83 | 107.01 | 111.62 |
| 11 | aA | 338 | VAL | N-CA-C | -5.83 | 107.01 | 111.62 |
| 10 | j5 | 252 | ASP | N-CA-C | 5.83 | 120.53 | 112.90 |
| 1 | Z7 | 34 | GLY | N-CA-C | 5.83 | 119.26 | 112.50 |
| 3 | F2 | 144 | SER | CA-C-N | 5.83 | 127.12 | 119.84 |
| 3 | F2 | 144 | SER | C-N-CA | 5.83 | 127.12 | 119.84 |
| 11 | a9 | 280 | ASP | N-CA-C | 5.83 | 122.69 | 109.81 |
| 11 | aA | 280 | ASP | N-CA-C | 5.83 | 122.69 | 109.81 |
| 10 | j5 | 1086 | THR | N-CA-C | 5.83 | 120.40 | 113.12 |
| 3 | F4 | 144 | SER | CA-C-N | 5.82 | 127.12 | 119.84 |
| 3 | F4 | 144 | SER | C-N-CA | 5.82 | 127.12 | 119.84 |
| 10 | j5 | 152 | ARG | CB-CA-C | -5.82 | 101.12 | 110.79 |
| 3 | F8 | 144 | SER | CA-C-N | 5.82 | 127.12 | 119.84 |
| 3 | F8 | 144 | SER | C-N-CA | 5.82 | 127.12 | 119.84 |
| 4 | M9 | 228 | SER | O-C-N | -5.82 | 116.69 | 123.27 |
| 3 | R1 | 144 | SER | CA-C-N | 5.82 | 127.11 | 119.84 |
| 3 | R1 | 144 | SER | C-N-CA | 5.82 | 127.11 | 119.84 |
| 10 | k5 | 1103 | LEU | N-CA-C | 5.82 | 117.62 | 111.28 |
| 3 | D4 | 144 | SER | CA-C-N | 5.82 | 127.11 | 119.84 |
| 3 | D4 | 144 | SER | C-N-CA | 5.82 | 127.11 | 119.84 |
| 3 | J4 | 144 | SER | CA-C-N | 5.82 | 127.11 | 119.84 |
| 3 | J4 | 144 | SER | C-N-CA | 5.82 | 127.11 | 119.84 |
| 3 | D8 | 144 | SER | CA-C-N | 5.82 | 127.11 | 119.84 |
| 3 | D8 | 144 | SER | C-N-CA | 5.82 | 127.11 | 119.84 |
| 11 | aA | 25 | GLU | O-C-N | -5.82 | 115.30 | 120.48 |
| 3 | BA | 144 | SER | CA-C-N | 5.82 | 127.11 | 119.84 |
| 3 | BA | 144 | SER | C-N-CA | 5.82 | 127.11 | 119.84 |
| 4 | MA | 228 | SER | O-C-N | -5.82 | 116.70 | 123.27 |
| 1 | v7 | 34 | GLY | N-CA-C | 5.82 | 119.25 | 112.50 |
| 3 | B9 | 144 | SER | CA-C-N | 5.82 | 127.11 | 119.84 |
| 3 | B9 | 144 | SER | C-N-CA | 5.82 | 127.11 | 119.84 |
| 3 | O4 | 144 | SER | CA-C-N | 5.81 | 127.11 | 119.84 |
| 3 | O4 | 144 | SER | C-N-CA | 5.81 | 127.11 | 119.84 |
| 3 | ZA | 144 | SER | CA-C-N | 5.81 | 127.11 | 119.84 |
| 3 | ZA | 144 | SER | C-N-CA | 5.81 | 127.11 | 119.84 |
| 10 | k5 | 157 | ILE | N-CA-C | 5.81 | 116.59 | 110.72 |
| 8 | o7 | 50 | ILE | CB-CA-C | -5.81 | 104.20 | 112.22 |
| 8 | u7 | 34 | GLU | CA-C-N | 5.81 | 128.54 | 120.29 |
| 8 | u7 | 34 | GLU | C-N-CA | 5.81 | 128.54 | 120.29 |
| 3 | Z9 | 144 | SER | CA-C-N | 5.81 | 127.11 | 119.84 |
| 3 | Z9 | 144 | SER | C-N-CA | 5.81 | 127.11 | 119.84 |
| 3 | D2 | 144 | SER | CA-C-N | 5.81 | 127.11 | 119.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3 | D2 | 144 | SER | C-N-CA | 5.81 | 127.11 | 119.84 |
| 3 | FA | 154 | SER | N-CA-C | 5.81 | 117.61 | 111.28 |
| 11 | a9 | 376 | ALA | N-CA-C | 5.81 | 117.83 | 110.33 |
| 3 | R3 | 144 | SER | CA-C-N | 5.81 | 127.10 | 119.84 |
| 3 | R3 | 144 | SER | C-N-CA | 5.81 | 127.10 | 119.84 |
| 10 | k5 | 636 | GLY | N-CA-C | 5.81 | 126.95 | 113.18 |
| 10 | k5 | 741 | GLN | CA-C-O | -5.81 | 115.23 | 121.56 |
| 3 | D6 | 144 | SER | CA-C-N | 5.81 | 127.10 | 119.84 |
| 3 | D6 | 144 | SER | C-N-CA | 5.81 | 127.10 | 119.84 |
| 10 | j5 | 848 | ILE | CB-CA-C | -5.81 | 104.30 | 112.14 |
| 10 | j5 | 983 | ARG | N-CA-C | 5.81 | 120.66 | 112.93 |
| 10 | k5 | 983 | ARG | N-CA-C | 5.81 | 120.66 | 112.93 |
| 1 | F7 | 34 | GLY | N-CA-C | 5.81 | 119.24 | 112.50 |
| 3 | V9 | 144 | SER | CA-C-N | 5.81 | 127.10 | 119.84 |
| 3 | V9 | 144 | SER | C-N-CA | 5.81 | 127.10 | 119.84 |
| 4 | MA | 8 | SER | N-CA-CB | -5.80 | 101.45 | 111.55 |
| 4 | M4 | 228 | SER | O-C-N | -5.80 | 116.71 | 123.27 |
| 1 | f5 | 34 | GLY | N-CA-C | 5.80 | 119.23 | 112.50 |
| 10 | j5 | 983 | ARG | CA-C-N | 5.80 | 132.42 | 121.97 |
| 10 | j5 | 983 | ARG | C-N-CA | 5.80 | 132.42 | 121.97 |
| 1 | t7 | 34 | GLY | N-CA-C | 5.80 | 119.23 | 112.50 |
| 11 | a9 | 419 | ARG | O-C-N | -5.80 | 115.76 | 122.03 |
| 11 | aA | 419 | ARG | O-C-N | -5.80 | 115.76 | 122.03 |
| 4 | M3 | 8 | SER | N-CA-CB | -5.80 | 101.45 | 111.55 |
| 10 | j5 | 489 | ASN | CA-C-O | -5.80 | 114.27 | 120.42 |
| 8 | u7 | 50 | ILE | N-CA-C | -5.80 | 104.86 | 110.72 |
| 4 | M1 | 8 | SER | N-CA-CB | -5.80 | 101.45 | 111.55 |
| 3 | VA | 144 | SER | CA-C-N | 5.80 | 127.09 | 119.84 |
| 3 | VA | 144 | SER | C-N-CA | 5.80 | 127.09 | 119.84 |
| 10 | k5 | 152 | ARG | CB-CA-C | -5.80 | 101.16 | 110.79 |
| 10 | k5 | 489 | ASN | CA-C-O | -5.80 | 114.27 | 120.42 |
| 10 | j5 | 650 | ASP | OD1-CG-OD2 | -5.80 | 108.98 | 122.90 |
| 10 | j5 | 1011 | ILE | CB-CA-C | -5.80 | 100.81 | 111.36 |
| 1 | X7 | 34 | GLY | N-CA-C | 5.80 | 119.23 | 112.50 |
| 1 | p7 | 34 | GLY | N-CA-C | 5.80 | 119.23 | 112.50 |
| 3 | J8 | 144 | SER | CA-C-N | 5.80 | 127.09 | 119.84 |
| 3 | J8 | 144 | SER | C-N-CA | 5.80 | 127.09 | 119.84 |
| 3 | D9 | 144 | SER | CA-C-N | 5.80 | 127.09 | 119.84 |
| 3 | D9 | 144 | SER | C-N-CA | 5.80 | 127.09 | 119.84 |
| 4 | M4 | 8 | SER | N-CA-CB | -5.80 | 101.47 | 111.55 |
| 1 | j7 | 34 | GLY | N-CA-C | 5.80 | 119.22 | 112.50 |
| 8 | U5 | 76 | LYS | N-CA-C | -5.79 | 103.77 | 111.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9 | w7 | 59 | GLY | N-CA-C | 5.79 | 122.05 | 112.66 |
| 4 | M9 | 8 | SER | N-CA-CB | -5.79 | 101.47 | 111.55 |
| 4 | MA | 37 | GLU | N-CA-CB | -5.79 | 100.89 | 109.98 |
| 3 | P1 | 144 | SER | CA-C-N | 5.79 | 127.08 | 119.84 |
| 3 | P1 | 144 | SER | C-N-CA | 5.79 | 127.08 | 119.84 |
| 3 | P3 | 144 | SER | CA-C-N | 5.79 | 127.08 | 119.84 |
| 3 | P3 | 144 | SER | C-N-CA | 5.79 | 127.08 | 119.84 |
| 8 | O5 | 76 | LYS | N-CA-C | -5.79 | 103.77 | 111.24 |
| 1 | X5 | 34 | GLY | N-CA-C | 5.79 | 119.22 | 112.50 |
| 4 | M9 | 37 | GLU | N-CA-CB | -5.79 | 100.89 | 109.98 |
| 10 | k5 | 983 | ARG | CA-C-N | 5.79 | 132.39 | 121.97 |
| 10 | k5 | 983 | ARG | C-N-CA | 5.79 | 132.39 | 121.97 |
| 3 | S4 | 144 | SER | CA-C-N | 5.79 | 127.08 | 119.84 |
| 3 | S4 | 144 | SER | C-N-CA | 5.79 | 127.08 | 119.84 |
| 10 | j5 | 636 | GLY | N-CA-C | 5.79 | 126.90 | 113.18 |
| 10 | k5 | 457 | THR | CA-C-O | -5.79 | 114.28 | 120.42 |
| 1 | D7 | 34 | GLY | N-CA-C | 5.79 | 119.22 | 112.50 |
| 4 | M8 | 8 | SER | N-CA-CB | -5.79 | 101.48 | 111.55 |
| 3 | S8 | 144 | SER | CA-C-N | 5.79 | 127.08 | 119.84 |
| 3 | S8 | 144 | SER | C-N-CA | 5.79 | 127.08 | 119.84 |
| 11 | a9 | 799 | ASP | N-CA-C | -5.79 | 98.47 | 110.80 |
| 11 | aA | 799 | ASP | N-CA-C | -5.79 | 98.47 | 110.80 |
| 3 | J6 | 144 | SER | CA-C-N | 5.79 | 127.07 | 119.84 |
| 3 | J6 | 144 | SER | C-N-CA | 5.79 | 127.07 | 119.84 |
| 10 | j5 | 457 | THR | CA-C-O | -5.79 | 114.29 | 120.42 |
| 10 | k5 | 1011 | ILE | CB-CA-C | -5.79 | 100.83 | 111.36 |
| 3 | J2 | 144 | SER | CA-C-N | 5.79 | 127.07 | 119.84 |
| 3 | J2 | 144 | SER | C-N-CA | 5.79 | 127.07 | 119.84 |
| 1 | J7 | 34 | GLY | N-CA-C | 5.78 | 119.21 | 112.50 |
| 1 | f7 | 34 | GLY | N-CA-C | 5.78 | 119.21 | 112.50 |
| 5 | Z4 | 39 | PRO | N-CA-CB | -5.78 | 97.18 | 103.25 |
| 10 | k5 | 252 | ASP | N-CA-C | 5.78 | 120.47 | 112.90 |
| 4 | M8 | 37 | GLU | N-CA-CB | -5.78 | 100.90 | 109.98 |
| 1 | d7 | 34 | GLY | N-CA-C | 5.78 | 119.20 | 112.50 |
| 8 | o7 | 34 | GLU | CA-C-N | 5.78 | 128.49 | 120.29 |
| 8 | o7 | 34 | GLU | C-N-CA | 5.78 | 128.49 | 120.29 |
| 11 | a9 | 502 | ASN | N-CA-C | 5.78 | 121.76 | 114.31 |
| 11 | aA | 502 | ASN | N-CA-C | 5.78 | 121.76 | 114.31 |
| 5 | N3 | 33 | GLY | N-CA-C | 5.78 | 126.87 | 113.18 |
| 4 | M3 | 37 | GLU | N-CA-CB | -5.77 | 100.92 | 109.98 |
| 10 | j5 | 1103 | LEU | N-CA-C | 5.77 | 117.57 | 111.28 |
| 4 | M1 | 37 | GLU | N-CA-CB | -5.77 | 100.92 | 109.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 10 | k5 | 383 | SER | N-CA-C | 5.77 | 120.32 | 113.16 |
| 9 | z7 | 59 | GLY | N-CA-C | 5.77 | 122.01 | 112.66 |
| 10 | j5 | 751 | LYS | N-CA-CB | -5.77 | 101.62 | 110.85 |
| 3 | DA | 144 | SER | CA-C-N | 5.77 | 127.05 | 119.84 |
| 3 | DA | 144 | SER | C-N-CA | 5.77 | 127.05 | 119.84 |
| 3 | J9 | 144 | SER | CA-C-N | 5.77 | 127.05 | 119.84 |
| 3 | J9 | 144 | SER | C-N-CA | 5.77 | 127.05 | 119.84 |
| 10 | k5 | 650 | ASP | OD1-CG-OD2 | -5.77 | 109.06 | 122.90 |
| 4 | M4 | 94 | TRP | N-CA-C | 5.76 | 117.50 | 110.41 |
| 10 | j5 | 750 | ARG | O-C-N | -5.76 | 117.25 | 123.42 |
| 5 | N1 | 33 | GLY | N-CA-C | 5.76 | 126.84 | 113.18 |
| 4 | MA | 94 | TRP | N-CA-C | 5.76 | 117.50 | 110.41 |
| 10 | k5 | 750 | ARG | O-C-N | -5.76 | 117.26 | 123.42 |
| 4 | M9 | 94 | TRP | N-CA-C | 5.76 | 117.50 | 110.41 |
| 5 | Z8 | 33 | GLY | N-CA-C | 5.76 | 126.83 | 113.18 |
| 10 | j5 | 592 | LYS | N-CA-C | 5.76 | 118.50 | 111.82 |
| 10 | k5 | 235 | ASP | O-C-N | 5.76 | 129.35 | 122.79 |
| 11 | aA | 412 | VAL | N-CA-C | 5.76 | 118.25 | 111.05 |
| 11 | a9 | 587 | THR | O-C-N | 5.75 | 128.25 | 122.03 |
| 11 | aA | 587 | THR | O-C-N | 5.75 | 128.25 | 122.03 |
| 1 | R5 | 34 | GLY | N-CA-C | 5.75 | 119.17 | 112.50 |
| 4 | M1 | 94 | TRP | N-CA-C | 5.75 | 117.48 | 110.41 |
| 5 | Z4 | 33 | GLY | N-CA-C | 5.75 | 126.81 | 113.18 |
| 8 | I5 | 26 | ILE | CA-C-N | 5.75 | 132.52 | 121.54 |
| 8 | I5 | 26 | ILE | C-N-CA | 5.75 | 132.52 | 121.54 |
| 10 | j5 | 383 | SER | N-CA-C | 5.75 | 120.29 | 113.16 |
| 4 | M3 | 94 | TRP | N-CA-C | 5.75 | 117.48 | 110.41 |
| 10 | j5 | 1103 | LEU | CA-CB-CG | -5.74 | 96.20 | 116.30 |
| 10 | k5 | 751 | LYS | N-CA-CB | -5.74 | 101.66 | 110.85 |
| 1 | L7 | 34 | GLY | N-CA-C | 5.74 | 119.16 | 112.50 |
| 4 | M8 | 228 | SER | O-C-N | -5.74 | 116.78 | 123.27 |
| 3 | JA | 144 | SER | CA-C-N | 5.74 | 127.02 | 119.84 |
| 3 | JA | 144 | SER | C-N-CA | 5.74 | 127.02 | 119.84 |
| 5 | NA | 33 | GLY | N-CA-C | 5.74 | 126.79 | 113.18 |
| 10 | j5 | 899 | GLU | CB-CA-C | -5.74 | 101.26 | 110.79 |
| 5 | N9 | 33 | GLY | N-CA-C | 5.74 | 126.79 | 113.18 |
| 10 | k5 | 899 | GLU | CB-CA-C | -5.74 | 101.26 | 110.79 |
| 8 | O7 | 102 | THR | CA-C-N | 5.74 | 125.42 | 119.05 |
| 8 | O7 | 102 | THR | C-N-CA | 5.74 | 125.42 | 119.05 |
| 10 | j5 | 803 | LYS | CB-CG-CD | -5.74 | 98.10 | 111.30 |
| 10 | k5 | 1103 | LEU | CA-CB-CG | -5.74 | 96.22 | 116.30 |
| 8 | C5 | 26 | ILE | CA-C-N | 5.74 | 132.49 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 8 | C5 | 26 | ILE | C-N-CA | 5.74 | 132.49 | 121.54 |
| 10 | j5 | 235 | ASP | O-C-N | 5.74 | 129.33 | 122.79 |
| 8 | K5 | 80 | LEU | N-CA-C | -5.73 | 105.99 | 112.87 |
| 4 | M4 | 37 | GLU | N-CA-CB | -5.73 | 100.98 | 109.98 |
| 8 | U5 | 102 | THR | CA-C-N | 5.73 | 125.41 | 119.05 |
| 8 | U5 | 102 | THR | C-N-CA | 5.73 | 125.41 | 119.05 |
| 11 | a9 | 412 | VAL | N-CA-C | 5.73 | 118.22 | 111.05 |
| 10 | j5 | 1120 | PRO | CA-C-N | 5.73 | 132.49 | 121.54 |
| 10 | j5 | 1120 | PRO | C-N-CA | 5.73 | 132.49 | 121.54 |
| 4 | M4 | 228 | SER | N-CA-C | 5.73 | 118.58 | 109.24 |
| 10 | k5 | 592 | LYS | N-CA-C | 5.72 | 118.46 | 111.82 |
| 10 | j5 | 935 | LEU | N-CA-C | -5.72 | 104.50 | 112.45 |
| 5 | Z4 | 39 | PRO | CA-C-N | -5.72 | 110.61 | 121.54 |
| 5 | Z4 | 39 | PRO | C-N-CA | -5.72 | 110.61 | 121.54 |
| 4 | M8 | 113 | ILE | N-CA-C | 5.72 | 116.50 | 110.72 |
| 10 | k5 | 803 | LYS | CB-CG-CD | -5.72 | 98.15 | 111.30 |
| 8 | E5 | 80 | LEU | N-CA-C | -5.72 | 106.01 | 112.87 |
| 4 | MA | 228 | SER | N-CA-C | 5.71 | 118.55 | 109.24 |
| 1 | V7 | 34 | GLY | N-CA-C | 5.71 | 119.13 | 112.50 |
| 4 | M9 | 228 | SER | N-CA-C | 5.71 | 118.55 | 109.24 |
| 4 | M8 | 228 | SER | N-CA-C | 5.71 | 118.55 | 109.24 |
| 4 | M3 | 228 | SER | N-CA-C | 5.71 | 118.54 | 109.24 |
| 4 | M1 | 228 | SER | N-CA-C | 5.71 | 118.54 | 109.24 |
| 8 | O5 | 102 | THR | CA-C-N | 5.70 | 125.38 | 119.05 |
| 8 | O5 | 102 | THR | C-N-CA | 5.70 | 125.38 | 119.05 |
| 4 | M8 | 61 | ASN | N-CA-C | 5.70 | 117.30 | 111.14 |
| 8 | i7 | 119 | LEU | CA-C-N | 5.70 | 130.22 | 122.19 |
| 8 | i7 | 119 | LEU | C-N-CA | 5.70 | 130.22 | 122.19 |
| 8 | U7 | 102 | THR | CA-C-N | 5.70 | 125.37 | 119.05 |
| 8 | U7 | 102 | THR | C-N-CA | 5.70 | 125.37 | 119.05 |
| 4 | MA | 82 | ILE | CB-CA-C | -5.70 | 104.70 | 111.65 |
| 4 | M9 | 82 | ILE | CB-CA-C | -5.70 | 104.70 | 111.65 |
| 10 | k5 | 1120 | PRO | CA-C-N | 5.69 | 132.41 | 121.54 |
| 10 | k5 | 1120 | PRO | C-N-CA | 5.69 | 132.41 | 121.54 |
| 11 | a9 | 352 | PRO | N-CA-C | 5.69 | 124.19 | 112.47 |
| 11 | aA | 352 | PRO | N-CA-C | 5.69 | 124.19 | 112.47 |
| 4 | MA | 61 | ASN | N-CA-C | 5.69 | 117.28 | 111.14 |
| 10 | k5 | 935 | LEU | N-CA-C | -5.69 | 104.54 | 112.45 |
| 9 | w7 | 51 | VAL | N-CA-CB | 5.69 | 118.63 | 111.46 |
| 4 | M9 | 61 | ASN | N-CA-C | 5.69 | 117.28 | 111.14 |
| 4 | M4 | 113 | ILE | N-CA-C | 5.68 | 116.46 | 110.72 |
| 4 | MA | 113 | ILE | N-CA-C | 5.68 | 116.46 | 110.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10 | k5 | 731 | GLU | N-CA-CB | -5.68 | 101.25 | 109.83 |
| 10 | j5 | 731 | GLU | N-CA-CB | -5.68 | 101.25 | 109.83 |
| 11 | a9 | 443 | PHE | N-CA-C | 5.68 | 117.55 | 111.36 |
| 9 | z7 | 51 | VAL | N-CA-CB | 5.67 | 118.61 | 111.46 |
| 4 | M8 | 82 | ILE | CB-CA-C | -5.67 | 104.73 | 111.65 |
| 8 | c7 | 119 | LEU | CA-C-N | 5.67 | 130.23 | 122.34 |
| 8 | c7 | 119 | LEU | C-N-CA | 5.67 | 130.23 | 122.34 |
| 4 | M4 | 61 | ASN | N-CA-C | 5.67 | 117.26 | 111.14 |
| 11 | a9 | 487 | ASP | CB-CA-C | -5.67 | 101.38 | 110.79 |
| 11 | aA | 487 | ASP | CB-CA-C | -5.67 | 101.38 | 110.79 |
| 4 | M3 | 113 | ILE | N-CA-C | 5.67 | 116.45 | 110.72 |
| 10 | k5 | 1136 | ILE | CB-CA-C | -5.67 | 104.45 | 111.08 |
| 8 | I7 | 102 | THR | CA-C-N | 5.67 | 125.34 | 119.05 |
| 8 | I7 | 102 | THR | C-N-CA | 5.67 | 125.34 | 119.05 |
| 8 | s7 | 102 | THR | CA-C-N | 5.67 | 125.34 | 119.05 |
| 8 | s7 | 102 | THR | C-N-CA | 5.67 | 125.34 | 119.05 |
| 4 | M1 | 113 | ILE | N-CA-C | 5.67 | 116.45 | 110.72 |
| 10 | j5 | 573 | GLN | N-CA-CB | -5.67 | 101.56 | 110.46 |
| 8 | g7 | 102 | THR | CA-C-N | 5.67 | 125.34 | 119.05 |
| 8 | g7 | 102 | THR | C-N-CA | 5.67 | 125.34 | 119.05 |
| 10 | k5 | 831 | PHE | CB-CA-C | -5.67 | 101.22 | 110.85 |
| 11 | aA | 443 | PHE | N-CA-C | 5.67 | 117.53 | 111.36 |
| 4 | M1 | 10 | ARG | N-CA-C | -5.67 | 105.19 | 111.36 |
| 4 | M8 | 10 | ARG | N-CA-C | -5.66 | 105.19 | 111.36 |
| 8 | a5 | 102 | THR | CA-C-N | 5.66 | 125.33 | 119.05 |
| 8 | a5 | 102 | THR | C-N-CA | 5.66 | 125.33 | 119.05 |
| 10 | j5 | 831 | PHE | CB-CA-C | -5.66 | 101.23 | 110.85 |
| 4 | M9 | 113 | ILE | N-CA-C | 5.66 | 116.43 | 110.72 |
| 10 | k5 | 573 | GLN | N-CA-CB | -5.65 | 101.59 | 110.46 |
| 4 | M8 | 14 | LEU | CA-C-N | 5.65 | 131.41 | 122.94 |
| 4 | M8 | 14 | LEU | C-N-CA | 5.65 | 131.41 | 122.94 |
| 4 | M3 | 61 | ASN | N-CA-C | 5.65 | 117.24 | 111.14 |
| 4 | M1 | 61 | ASN | N-CA-C | 5.65 | 117.24 | 111.14 |
| 10 | j5 | 456 | ILE | CA-C-O | -5.65 | 115.08 | 120.95 |
| 10 | k5 | 456 | ILE | CA-C-O | -5.64 | 115.08 | 120.95 |
| 4 | M3 | 4 | LEU | N-CA-CB | -5.64 | 102.29 | 110.36 |
| 8 | M5 | 52 | LYS | CA-C-N | -5.64 | 111.09 | 120.68 |
| 8 | M5 | 52 | LYS | C-N-CA | -5.64 | 111.09 | 120.68 |
| 8 | C7 | 102 | THR | CA-C-N | 5.64 | 125.31 | 119.05 |
| 8 | C7 | 102 | THR | C-N-CA | 5.64 | 125.31 | 119.05 |
| 1 | J7 | 75 | THR | CA-C-N | 5.64 | 127.77 | 120.44 |
| 1 | J7 | 75 | THR | C-N-CA | 5.64 | 127.77 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8 | a7 | 102 | THR | CA-C-N | 5.64 | 125.31 | 119.05 |
| 8 | a7 | 102 | THR | C-N-CA | 5.64 | 125.31 | 119.05 |
| 4 | M4 | 10 | ARG | N-CA-C | -5.63 | 105.22 | 111.36 |
| 8 | C5 | 102 | THR | CA-C-N | 5.63 | 125.31 | 119.05 |
| 8 | C5 | 102 | THR | C-N-CA | 5.63 | 125.31 | 119.05 |
| 8 | e5 | 102 | THR | CA-C-N | 5.63 | 125.31 | 119.05 |
| 8 | e5 | 102 | THR | C-N-CA | 5.63 | 125.31 | 119.05 |
| 10 | k5 | 40 | VAL | CB-CA-C | -5.63 | 104.53 | 112.14 |
| 10 | j5 | 763 | SER | N-CA-C | 5.63 | 118.35 | 111.82 |
| 4 | M3 | 10 | ARG | N-CA-C | -5.63 | 105.22 | 111.36 |
| 1 | D7 | 75 | THR | CA-C-N | 5.63 | 127.76 | 120.44 |
| 1 | D7 | 75 | THR | C-N-CA | 5.63 | 127.76 | 120.44 |
| 4 | MA | 10 | ARG | N-CA-C | -5.63 | 105.22 | 111.36 |
| 4 | M8 | 4 | LEU | N-CA-CB | -5.63 | 102.31 | 110.36 |
| 4 | M9 | 10 | ARG | N-CA-C | -5.63 | 105.22 | 111.36 |
| 4 | M4 | 14 | LEU | CA-C-N | 5.63 | 131.38 | 122.94 |
| 4 | M4 | 14 | LEU | C-N-CA | 5.63 | 131.38 | 122.94 |
| 8 | o7 | 51 | VAL | CB-CA-C | -5.62 | 104.46 | 112.22 |
| 10 | k5 | 296 | VAL | N-CA-C | 5.62 | 116.40 | 110.72 |
| 10 | k5 | 471 | PRO | CA-C-N | 5.62 | 132.28 | 121.54 |
| 10 | k5 | 471 | PRO | C-N-CA | 5.62 | 132.28 | 121.54 |
| 4 | M1 | 4 | LEU | N-CA-CB | -5.62 | 102.32 | 110.36 |
| 9 | z7 | 5 | PHE | CA-C-N | -5.62 | 114.86 | 123.07 |
| 9 | z7 | 5 | PHE | C-N-CA | -5.62 | 114.86 | 123.07 |
| 10 | j5 | 296 | VAL | N-CA-C | 5.62 | 116.39 | 110.72 |
| 10 | k5 | 1047 | LYS | CA-C-N | 5.62 | 132.51 | 122.06 |
| 10 | k5 | 1047 | LYS | C-N-CA | 5.62 | 132.51 | 122.06 |
| 4 | M3 | 196 | TYR | CB-CA-C | -5.62 | 101.47 | 110.79 |
| 4 | M3 | 82 | ILE | CB-CA-C | -5.62 | 104.80 | 111.65 |
| 8 | m7 | 102 | THR | CA-C-N | 5.62 | 125.28 | 119.05 |
| 8 | m7 | 102 | THR | C-N-CA | 5.62 | 125.28 | 119.05 |
| 4 | M1 | 82 | ILE | CB-CA-C | -5.62 | 104.80 | 111.65 |
| 8 | G5 | 64 | ASP | N-CA-C | 5.61 | 119.39 | 112.54 |
| 10 | j5 | 471 | PRO | CA-C-N | 5.61 | 132.26 | 121.54 |
| 10 | j5 | 471 | PRO | C-N-CA | 5.61 | 132.26 | 121.54 |
| 10 | k5 | 641 | ASP | N-CA-CB | -5.61 | 102.81 | 111.46 |
| 4 | M4 | 82 | ILE | CB-CA-C | -5.61 | 104.81 | 111.65 |
| 1 | D5 | 8 | VAL | N-CA-C | -5.61 | 105.64 | 111.58 |
| 8 | I5 | 102 | THR | CA-C-N | 5.61 | 125.27 | 119.05 |
| 8 | I5 | 102 | THR | C-N-CA | 5.61 | 125.27 | 119.05 |
| 10 | j5 | 1047 | LYS | CA-C-N | 5.61 | 132.49 | 122.06 |
| 10 | j5 | 1047 | LYS | C-N-CA | 5.61 | 132.49 | 122.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4 | M1 | 196 | TYR | CB-CA-C | -5.61 | 101.48 | 110.79 |
| 8 | u7 | 51 | VAL | CB-CA-C | -5.60 | 104.49 | 112.22 |
| 3 | LA | 115 | GLU | CB-CA-C | -5.60 | 101.49 | 110.79 |
| 3 | L9 | 115 | GLU | CB-CA-C | -5.60 | 101.49 | 110.79 |
| 11 | a9 | 547 | LYS | N-CA-C | 5.60 | 117.47 | 111.36 |
| 11 | aA | 547 | LYS | N-CA-C | 5.60 | 117.47 | 111.36 |
| 4 | M3 | 14 | LEU | CA-C-N | 5.60 | 131.34 | 122.94 |
| 4 | M3 | 14 | LEU | C-N-CA | 5.60 | 131.34 | 122.94 |
| 4 | M1 | 14 | LEU | CA-C-N | 5.60 | 131.34 | 122.94 |
| 4 | M1 | 14 | LEU | C-N-CA | 5.60 | 131.34 | 122.94 |
| 4 | MA | 4 | LEU | N-CA-CB | -5.60 | 102.35 | 110.36 |
| 10 | k5 | 763 | SER | N-CA-C | 5.60 | 118.32 | 111.82 |
| 9 | w7 | 5 | PHE | CA-C-N | -5.60 | 114.89 | 123.07 |
| 9 | w7 | 5 | PHE | C-N-CA | -5.60 | 114.89 | 123.07 |
| 4 | M9 | 4 | LEU | N-CA-CB | -5.60 | 102.35 | 110.36 |
| 10 | j5 | 378 | TYR | N-CA-C | 5.60 | 117.46 | 111.36 |
| 10 | k5 | 378 | TYR | N-CA-C | 5.60 | 117.46 | 111.36 |
| 10 | j5 | 40 | VAL | CB-CA-C | -5.59 | 104.59 | 112.14 |
| 10 | j5 | 641 | ASP | N-CA-CB | -5.59 | 102.84 | 111.46 |
| 10 | k5 | 683 | ARG | N-CA-C | 5.59 | 120.24 | 113.41 |
| 4 | M4 | 4 | LEU | N-CA-CB | -5.59 | 102.36 | 110.36 |
| 10 | j5 | 1002 | ARG | N-CA-C | 5.59 | 117.38 | 111.28 |
| 10 | j5 | 1136 | ILE | CB-CA-C | -5.59 | 104.54 | 111.08 |
| 11 | a9 | 60 | GLY | CA-C-O | -5.59 | 115.29 | 121.05 |
| 11 | aA | 60 | GLY | CA-C-O | -5.59 | 115.29 | 121.05 |
| 10 | j5 | 853 | LEU | N-CA-C | -5.59 | 106.36 | 114.12 |
| 4 | M9 | 257 | GLN | CB-CA-C | -5.59 | 102.18 | 110.67 |
| 10 | k5 | 1002 | ARG | N-CA-C | 5.58 | 117.37 | 111.28 |
| 11 | a9 | 806 | GLY | CA-C-N | -5.58 | 114.13 | 122.39 |
| 11 | a9 | 806 | GLY | C-N-CA | -5.58 | 114.13 | 122.39 |
| 11 | aA | 806 | GLY | CA-C-N | -5.58 | 114.13 | 122.39 |
| 11 | aA | 806 | GLY | C-N-CA | -5.58 | 114.13 | 122.39 |
| 4 | MA | 196 | TYR | CB-CA-C | -5.58 | 101.53 | 110.79 |
| 10 | k5 | 853 | LEU | N-CA-C | -5.58 | 106.37 | 114.12 |
| 4 | M9 | 196 | TYR | CB-CA-C | -5.58 | 101.53 | 110.79 |
| 1 | J5 | 8 | VAL | N-CA-C | -5.58 | 105.67 | 111.58 |
| 4 | MA | 14 | LEU | CA-C-N | 5.57 | 131.30 | 122.94 |
| 4 | MA | 14 | LEU | C-N-CA | 5.57 | 131.30 | 122.94 |
| 4 | M3 | 257 | GLN | CB-CA-C | -5.57 | 102.20 | 110.67 |
| 10 | j5 | 642 | ARG | CB-CG-CD | -5.57 | 98.48 | 111.30 |
| 4 | M8 | 196 | TYR | CB-CA-C | -5.57 | 101.54 | 110.79 |
| 4 | M9 | 14 | LEU | CA-C-N | 5.57 | 131.30 | 122.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 4 | M9 | 14 | LEU | C-N-CA | 5.57 | 131.30 | 122.94 |
| 4 | M1 | 257 | GLN | CB-CA-C | -5.57 | 102.20 | 110.67 |
| 10 | j5 | 1005 | LEU | CA-C-O | -5.57 | 114.31 | 120.38 |
| 4 | M4 | 196 | TYR | CB-CA-C | -5.57 | 101.55 | 110.79 |
| 4 | MA | 257 | GLN | CB-CA-C | -5.57 | 102.21 | 110.67 |
| 10 | j5 | 683 | ARG | N-CA-C | 5.57 | 120.20 | 113.41 |
| 8 | A5 | 64 | ASP | N-CA-C | 5.56 | 119.33 | 112.54 |
| 8 | E5 | 94 | TYR | CA-C-N | 5.56 | 126.15 | 119.98 |
| 8 | E5 | 94 | TYR | C-N-CA | 5.56 | 126.15 | 119.98 |
| 4 | M3 | 76 | ALA | N-CA-C | -5.56 | 106.62 | 113.41 |
| 4 | M1 | 76 | ALA | N-CA-C | -5.56 | 106.62 | 113.41 |
| 4 | M4 | 257 | GLN | CB-CA-C | -5.56 | 102.22 | 110.67 |
| 4 | M9 | 76 | ALA | N-CA-C | -5.56 | 106.63 | 113.41 |
| 10 | j5 | 679 | LEU | CB-CA-C | -5.55 | 100.87 | 108.86 |
| 4 | MA | 76 | ALA | N-CA-C | -5.54 | 106.65 | 113.41 |
| 10 | j5 | 637 | ARG | CA-C-N | 5.54 | 125.52 | 120.03 |
| 10 | j5 | 637 | ARG | C-N-CA | 5.54 | 125.52 | 120.03 |
| 9 | w7 | 61 | GLN | N-CA-C | 5.54 | 117.32 | 111.28 |
| 10 | j5 | 635 | LEU | O-C-N | -5.54 | 116.79 | 123.27 |
| 4 | M8 | 257 | GLN | CB-CA-C | -5.54 | 102.25 | 110.67 |
| 10 | k5 | 1005 | LEU | CA-C-O | -5.54 | 114.34 | 120.38 |
| 10 | j5 | 1010 | GLY | CA-C-O | -5.54 | 110.94 | 120.57 |
| 8 | E5 | 110 | ILE | CG1-CB-CG2 | -5.54 | 94.09 | 110.70 |
| 9 | z7 | 52 | LEU | N-CA-C | 5.54 | 118.50 | 111.69 |
| 4 | M3 | 250 | THR | N-CA-C | 5.53 | 122.59 | 110.80 |
| 8 | K5 | 110 | ILE | CG1-CB-CG2 | -5.53 | 94.10 | 110.70 |
| 10 | k5 | 249 | SER | CA-C-N | 5.53 | 131.26 | 121.80 |
| 10 | k5 | 249 | SER | C-N-CA | 5.53 | 131.26 | 121.80 |
| 9 | x7 | 28 | PHE | N-CA-CB | -5.53 | 101.23 | 111.52 |
| 4 | M1 | 250 | THR | N-CA-C | 5.53 | 122.59 | 110.80 |
| 9 | z7 | 61 | GLN | N-CA-C | 5.53 | 117.31 | 111.28 |
| 11 | aA | 429 | VAL | CB-CA-C | -5.53 | 104.89 | 111.97 |
| 10 | j5 | 249 | SER | CA-C-N | 5.53 | 131.25 | 121.80 |
| 10 | j5 | 249 | SER | C-N-CA | 5.53 | 131.25 | 121.80 |
| 4 | M8 | 76 | ALA | N-CA-C | -5.53 | 106.67 | 113.41 |
| 4 | M8 | 250 | THR | N-CA-C | 5.53 | 122.58 | 110.80 |
| 4 | MA | 250 | THR | N-CA-C | 5.53 | 122.57 | 110.80 |
| 10 | k5 | 342 | LEU | N-CA-C | 5.53 | 118.23 | 111.82 |
| 4 | M9 | 250 | THR | N-CA-C | 5.53 | 122.57 | 110.80 |
| 10 | k5 | 642 | ARG | CB-CG-CD | -5.52 | 98.61 | 111.30 |
| 10 | k5 | 679 | LEU | CB-CA-C | -5.52 | 100.91 | 108.86 |
| 4 | M4 | 76 | ALA | N-CA-C | -5.52 | 106.68 | 113.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 10 | k5 | 1010 | GLY | CA-C-O | -5.52 | 110.97 | 120.57 |
| 11 | a9 | 429 | VAL | CB-CA-C | -5.52 | 104.91 | 111.97 |
| 10 | k5 | 635 | LEU | O-C-N | -5.52 | 116.82 | 123.27 |
| 11 | a9 | 66 | SER | N-CA-C | 5.52 | 121.26 | 110.56 |
| 10 | k5 | 1105 | ILE | CB-CA-C | -5.51 | 104.80 | 112.02 |
| 9 | y7 | 28 | PHE | N-CA-CB | -5.51 | 101.26 | 111.52 |
| 10 | j5 | 454 | GLN | N-CA-C | 5.51 | 121.88 | 113.61 |
| 9 | w7 | 52 | LEU | N-CA-C | 5.51 | 118.47 | 111.69 |
| 11 | a9 | 72 | ASP | CA-C-N | 5.51 | 131.62 | 121.70 |
| 11 | a9 | 72 | ASP | C-N-CA | 5.51 | 131.62 | 121.70 |
| 11 | aA | 72 | ASP | CA-C-N | 5.51 | 131.62 | 121.70 |
| 11 | aA | 72 | ASP | C-N-CA | 5.51 | 131.62 | 121.70 |
| 3 | FA | 159 | GLU | N-CA-CB | 5.51 | 118.22 | 110.12 |
| 10 | k5 | 881 | VAL | CB-CA-C | -5.51 | 105.60 | 111.00 |
| 10 | k5 | 1069 | ARG | N-CA-C | 5.51 | 115.83 | 108.23 |
| 11 | a9 | 673 | ASP | CA-CB-CG | 5.51 | 118.11 | 112.60 |
| 11 | aA | 673 | ASP | CA-CB-CG | 5.51 | 118.11 | 112.60 |
| 11 | a9 | 441 | ARG | N-CA-C | 5.50 | 117.36 | 111.36 |
| 11 | aA | 66 | SER | N-CA-C | 5.50 | 121.24 | 110.56 |
| 10 | j5 | 878 | GLU | CA-C-O | -5.50 | 115.03 | 120.70 |
| 8 | K5 | 94 | TYR | CA-C-N | 5.50 | 126.08 | 119.98 |
| 8 | K5 | 94 | TYR | C-N-CA | 5.50 | 126.08 | 119.98 |
| 10 | j5 | 1105 | ILE | CB-CA-C | -5.50 | 104.82 | 112.02 |
| 10 | k5 | 878 | GLU | CA-C-O | -5.50 | 115.04 | 120.70 |
| 10 | j5 | 1069 | ARG | N-CA-C | 5.50 | 115.81 | 108.23 |
| 10 | k5 | 454 | GLN | N-CA-C | 5.50 | 121.85 | 113.61 |
| 4 | M4 | 250 | THR | N-CA-C | 5.49 | 122.50 | 110.80 |
| 10 | j5 | 175 | ASP | C-N-CD | -5.49 | 102.48 | 125.00 |
| 1 | D7 | 76 | ARG | CA-C-N | 5.49 | 131.63 | 121.52 |
| 1 | D7 | 76 | ARG | C-N-CA | 5.49 | 131.63 | 121.52 |
| 10 | k5 | 175 | ASP | C-N-CD | -5.49 | 102.49 | 125.00 |
| 4 | MA | 75 | GLU | N-CA-C | 5.49 | 119.61 | 113.02 |
| 10 | j5 | 291 | ASP | O-C-N | -5.49 | 114.89 | 121.64 |
| 10 | k5 | 291 | ASP | O-C-N | -5.49 | 114.89 | 121.64 |
| 4 | M4 | 75 | GLU | N-CA-C | 5.49 | 119.60 | 113.02 |
| 10 | k5 | 637 | ARG | CA-C-N | 5.49 | 125.46 | 120.03 |
| 10 | k5 | 637 | ARG | C-N-CA | 5.49 | 125.46 | 120.03 |
| 11 | a9 | 730 | ASN | CA-CB-CG | 5.48 | 118.08 | 112.60 |
| 11 | aA | 730 | ASN | CA-CB-CG | 5.48 | 118.08 | 112.60 |
| 10 | j5 | 382 | ILE | CB-CA-C | -5.48 | 95.09 | 111.05 |
| 10 | j5 | 881 | VAL | CB-CA-C | -5.48 | 105.63 | 111.00 |
| 10 | k5 | 736 | GLU | CB-CA-C | -5.48 | 99.51 | 110.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | M9 | 75 | GLU | N-CA-C | 5.48 | 119.60 | 113.02 |
| 11 | aA | 441 | ARG | N-CA-C | 5.48 | 117.34 | 111.36 |
| 9 | z5 | 44 | ILE | CB-CA-C | -5.48 | 104.66 | 112.22 |
| 10 | k5 | 382 | ILE | CB-CA-C | -5.48 | 95.10 | 111.05 |
| 1 | J7 | 76 | ARG | CA-C-N | 5.48 | 131.60 | 121.52 |
| 1 | J7 | 76 | ARG | C-N-CA | 5.48 | 131.60 | 121.52 |
| 2 | KA | 21 | ASN | N-CA-C | 5.48 | 118.76 | 111.75 |
| 2 | K9 | 21 | ASN | N-CA-C | 5.48 | 118.76 | 111.75 |
| 4 | M8 | 102 | VAL | N-CA-C | -5.47 | 105.04 | 110.62 |
| 9 | i5 | 44 | ILE | CB-CA-C | -5.47 | 104.67 | 112.22 |
| 10 | j5 | 920 | ARG | N-CA-CB | 5.47 | 119.74 | 110.49 |
| 10 | j5 | 825 | ASN | N-CA-C | 5.47 | 119.06 | 112.38 |
| 4 | M3 | 75 | GLU | N-CA-C | 5.47 | 119.58 | 113.02 |
| 4 | M1 | 75 | GLU | N-CA-C | 5.47 | 119.58 | 113.02 |
| 4 | M8 | 159 | CYS | N-CA-C | 5.46 | 120.05 | 113.17 |
| 8 | O5 | 20 | PRO | CB-CA-C | -5.46 | 102.55 | 111.56 |
| 10 | k5 | 535 | PRO | CB-CA-C | -5.46 | 103.80 | 110.95 |
| 11 | a9 | 266 | ASN | OD1-CG-ND2 | -5.46 | 117.14 | 122.60 |
| 11 | aA | 266 | ASN | OD1-CG-ND2 | -5.46 | 117.14 | 122.60 |
| 11 | a9 | 266 | ASN | CA-CB-CG | 5.45 | 118.05 | 112.60 |
| 11 | aA | 266 | ASN | CA-CB-CG | 5.45 | 118.05 | 112.60 |
| 10 | k5 | 386 | ILE | CA-C-N | 5.45 | 131.78 | 121.97 |
| 10 | k5 | 386 | ILE | C-N-CA | 5.45 | 131.78 | 121.97 |
| 10 | k5 | 575 | ILE | CA-C-O | -5.45 | 115.39 | 121.17 |
| 10 | k5 | 320 | GLU | CB-CA-C | -5.44 | 101.76 | 110.79 |
| 4 | M8 | 75 | GLU | N-CA-C | 5.44 | 119.55 | 113.02 |
| 11 | aA | 775 | LYS | CA-C-N | -5.44 | 113.41 | 121.24 |
| 11 | aA | 775 | LYS | C-N-CA | -5.44 | 113.41 | 121.24 |
| 10 | k5 | 920 | ARG | N-CA-CB | 5.44 | 119.68 | 110.49 |
| 4 | M3 | 159 | CYS | N-CA-C | 5.43 | 120.01 | 113.17 |
| 1 | D7 | 67 | ARG | N-CA-C | 5.43 | 117.50 | 109.62 |
| 4 | M1 | 159 | CYS | N-CA-C | 5.43 | 120.01 | 113.17 |
| 8 | K5 | 133 | MET | N-CA-C | -5.43 | 105.75 | 112.38 |
| 10 | j5 | 320 | GLU | CB-CA-C | -5.43 | 101.78 | 110.79 |
| 10 | j5 | 342 | LEU | N-CA-C | 5.43 | 118.12 | 111.82 |
| 10 | k5 | 775 | VAL | CA-C-O | -5.43 | 115.42 | 121.23 |
| 10 | j5 | 549 | LYS | CA-C-N | 5.42 | 132.04 | 121.41 |
| 10 | j5 | 549 | LYS | C-N-CA | 5.42 | 132.04 | 121.41 |
| 10 | j5 | 774 | GLN | N-CA-C | -5.42 | 100.04 | 110.56 |
| 10 | j5 | 775 | VAL | CA-C-O | -5.42 | 115.43 | 121.23 |
| 4 | MA | 159 | CYS | N-CA-C | 5.42 | 120.00 | 113.17 |
| 4 | M9 | 159 | CYS | N-CA-C | 5.42 | 120.00 | 113.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4 | M3 | 91 | VAL | O-C-N | -5.42 | 117.45 | 123.20 |
| 1 | J7 | 67 | ARG | N-CA-C | 5.42 | 117.48 | 109.62 |
| 4 | M1 | 91 | VAL | O-C-N | -5.42 | 117.45 | 123.20 |
| 10 | k5 | 774 | GLN | N-CA-C | -5.42 | 100.05 | 110.56 |
| 10 | k5 | 825 | ASN | N-CA-C | 5.42 | 118.99 | 112.38 |
| 10 | j5 | 386 | ILE | CA-C-N | 5.42 | 131.72 | 121.97 |
| 10 | j5 | 386 | ILE | C-N-CA | 5.42 | 131.72 | 121.97 |
| 10 | j5 | 535 | PRO | CB-CA-C | -5.42 | 103.85 | 110.95 |
| 10 | j5 | 406 | ILE | N-CA-C | 5.42 | 117.86 | 111.09 |
| 4 | M4 | 159 | CYS | N-CA-C | 5.41 | 119.99 | 113.17 |
| 10 | k5 | 549 | LYS | CA-C-N | 5.41 | 132.02 | 121.41 |
| 10 | k5 | 549 | LYS | C-N-CA | 5.41 | 132.02 | 121.41 |
| 11 | a9 | 775 | LYS | CA-C-N | -5.41 | 113.44 | 121.24 |
| 11 | a9 | 775 | LYS | C-N-CA | -5.41 | 113.44 | 121.24 |
| 10 | j5 | 507 | ARG | N-CA-C | 5.41 | 118.29 | 110.28 |
| 11 | a9 | 283 | GLN | C-N-CD | -5.41 | 102.82 | 125.00 |
| 11 | aA | 283 | GLN | C-N-CD | -5.41 | 102.82 | 125.00 |
| 10 | j5 | 571 | ALA | CA-C-O | -5.41 | 115.13 | 120.70 |
| 8 | O7 | 18 | LEU | O-C-N | -5.41 | 116.43 | 122.75 |
| 10 | k5 | 346 | GLU | N-CA-CB | -5.40 | 102.15 | 110.42 |
| 10 | k5 | 406 | ILE | N-CA-C | 5.40 | 117.84 | 111.09 |
| 8 | s7 | 102 | THR | N-CA-C | 5.40 | 121.75 | 109.81 |
| 4 | M8 | 91 | VAL | O-C-N | -5.40 | 117.47 | 123.20 |
| 10 | k5 | 1007 | VAL | N-CA-C | 5.40 | 120.57 | 109.34 |
| 8 | u7 | 159 | ALA | CA-C-N | 5.40 | 127.77 | 120.38 |
| 8 | u7 | 159 | ALA | C-N-CA | 5.40 | 127.77 | 120.38 |
| 8 | m7 | 102 | THR | N-CA-C | 5.39 | 121.73 | 109.81 |
| 10 | j5 | 700 | SER | N-CA-C | 5.39 | 118.08 | 111.82 |
| 10 | j5 | 1007 | VAL | N-CA-C | 5.39 | 120.56 | 109.34 |
| 10 | k5 | 507 | ARG | N-CA-C | 5.39 | 118.26 | 110.28 |
| 10 | k5 | 700 | SER | N-CA-C | 5.39 | 118.07 | 111.82 |
| 10 | j5 | 575 | ILE | CA-C-O | -5.39 | 115.46 | 121.17 |
| 10 | k5 | 894 | TYR | CA-C-O | -5.39 | 113.62 | 118.79 |
| 8 | U7 | 102 | THR | N-CA-C | 5.39 | 121.72 | 109.81 |
| 11 | a9 | 548 | LEU | N-CA-C | 5.39 | 119.72 | 113.20 |
| 11 | aA | 548 | LEU | N-CA-C | 5.39 | 119.72 | 113.20 |
| 8 | s7 | 22 | GLU | N-CA-C | -5.38 | 106.78 | 113.19 |
| 10 | k5 | 547 | ARG | CA-C-O | -5.38 | 114.85 | 120.55 |
| 10 | k5 | 701 | ASP | CB-CA-C | -5.38 | 101.86 | 110.79 |
| 8 | o7 | 159 | ALA | CA-C-N | 5.38 | 127.75 | 120.38 |
| 8 | o7 | 159 | ALA | C-N-CA | 5.38 | 127.75 | 120.38 |
| 8 | O5 | 102 | THR | N-CA-C | 5.38 | 121.70 | 109.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 8 | O7 | 102 | THR | N-CA-C | 5.38 | 121.69 | 109.81 |
| 3 | FA | 159 | GLU | CB-CG-CD | 5.38 | 121.74 | 112.60 |
| 10 | k5 | 1011 | ILE | CG1-CB-CG2 | -5.38 | 94.57 | 110.70 |
| 10 | j5 | 701 | ASP | CB-CA-C | -5.37 | 101.87 | 110.79 |
| 10 | j5 | 1011 | ILE | CG1-CB-CG2 | -5.37 | 94.58 | 110.70 |
| 10 | k5 | 571 | ALA | CA-C-O | -5.37 | 115.17 | 120.70 |
| 3 | LA | 113 | LEU | N-CA-C | 5.37 | 117.21 | 111.36 |
| 3 | L9 | 113 | LEU | N-CA-C | 5.37 | 117.21 | 111.36 |
| 8 | I5 | 102 | THR | N-CA-C | 5.37 | 121.67 | 109.81 |
| 10 | j5 | 894 | TYR | CA-C-O | -5.37 | 113.64 | 118.79 |
| 8 | C5 | 102 | THR | N-CA-C | 5.36 | 121.67 | 109.81 |
| 8 | a5 | 102 | THR | N-CA-C | 5.36 | 121.66 | 109.81 |
| 8 | e5 | 102 | THR | N-CA-C | 5.36 | 121.66 | 109.81 |
| 8 | U5 | 102 | THR | N-CA-C | 5.36 | 121.66 | 109.81 |
| 10 | j5 | 989 | THR | N-CA-CB | 5.36 | 119.55 | 110.49 |
| 10 | j5 | 547 | ARG | CA-C-O | -5.35 | 114.88 | 120.55 |
| 10 | k5 | 385 | PRO | CA-C-N | -5.35 | 112.34 | 121.97 |
| 10 | k5 | 385 | PRO | C-N-CA | -5.35 | 112.34 | 121.97 |
| 10 | k5 | 989 | THR | N-CA-CB | 5.35 | 119.53 | 110.49 |
| 8 | C7 | 102 | THR | N-CA-C | 5.35 | 121.64 | 109.81 |
| 10 | j5 | 385 | PRO | CA-C-N | -5.35 | 112.34 | 121.97 |
| 10 | j5 | 385 | PRO | C-N-CA | -5.35 | 112.34 | 121.97 |
| 8 | a7 | 102 | THR | N-CA-C | 5.35 | 121.63 | 109.81 |
| 4 | MA | 91 | VAL | O-C-N | -5.35 | 117.53 | 123.20 |
| 9 | z5 | 21 | ARG | CA-CB-CG | -5.35 | 103.41 | 114.10 |
| 10 | k5 | 812 | SER | CA-C-O | -5.35 | 114.94 | 121.36 |
| 4 | M9 | 91 | VAL | O-C-N | -5.35 | 117.53 | 123.20 |
| 8 | G5 | 48 | GLU | N-CA-C | 5.34 | 117.19 | 111.36 |
| 9 | i5 | 21 | ARG | CA-CB-CG | -5.34 | 103.41 | 114.10 |
| 10 | j5 | 719 | MET | CB-CA-C | -5.34 | 101.77 | 110.85 |
| 10 | j5 | 812 | SER | CA-C-O | -5.34 | 114.95 | 121.36 |
| 8 | g7 | 102 | THR | N-CA-C | 5.34 | 121.61 | 109.81 |
| 3 | LA | 110 | LEU | N-CA-C | -5.34 | 105.87 | 112.38 |
| 10 | k5 | 482 | GLN | CA-C-N | -5.34 | 113.66 | 121.99 |
| 10 | k5 | 482 | GLN | C-N-CA | -5.34 | 113.66 | 121.99 |
| 3 | L9 | 110 | LEU | N-CA-C | -5.34 | 105.87 | 112.38 |
| 11 | a9 | 373 | PRO | CB-CA-C | -5.34 | 101.76 | 110.25 |
| 11 | aA | 373 | PRO | CB-CA-C | -5.34 | 101.76 | 110.25 |
| 10 | j5 | 346 | GLU | N-CA-CB | -5.34 | 102.25 | 110.42 |
| 10 | j5 | 482 | GLN | CA-C-N | -5.33 | 113.67 | 121.99 |
| 10 | j5 | 482 | GLN | C-N-CA | -5.33 | 113.67 | 121.99 |
| 10 | j5 | 968 | GLU | N-CA-C | 5.33 | 118.89 | 112.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8 | I7 | 102 | THR | N-CA-C | 5.33 | 121.59 | 109.81 |
| 11 | a9 | 277 | GLY | N-CA-C | 5.33 | 119.59 | 112.77 |
| 11 | aA | 277 | GLY | N-CA-C | 5.33 | 119.59 | 112.77 |
| 10 | j5 | 1032 | VAL | N-CA-C | 5.32 | 118.52 | 111.17 |
| 10 | k5 | 719 | MET | CB-CA-C | -5.32 | 101.81 | 110.85 |
| 10 | k5 | 1032 | VAL | N-CA-C | 5.31 | 118.50 | 111.17 |
| 10 | k5 | 215 | LYS | CA-C-N | 5.31 | 129.89 | 122.08 |
| 10 | k5 | 215 | LYS | C-N-CA | 5.31 | 129.89 | 122.08 |
| 10 | j5 | 666 | ASN | N-CA-C | 5.31 | 119.45 | 112.92 |
| 10 | k5 | 968 | GLU | N-CA-C | 5.31 | 118.86 | 112.38 |
| 4 | MA | 92 | GLU | N-CA-C | 5.31 | 118.05 | 109.40 |
| 8 | A5 | 48 | GLU | N-CA-C | 5.31 | 117.14 | 111.36 |
| 10 | k5 | 6 | THR | CB-CA-C | -5.31 | 97.78 | 109.56 |
| 4 | M9 | 92 | GLU | N-CA-C | 5.31 | 118.05 | 109.40 |
| 3 | Y4 | 104 | VAL | N-CA-C | -5.31 | 107.58 | 112.83 |
| 11 | aA | 341 | LYS | CA-C-N | 5.30 | 131.66 | 121.54 |
| 11 | aA | 341 | LYS | C-N-CA | 5.30 | 131.66 | 121.54 |
| 10 | j5 | 6 | THR | CB-CA-C | -5.30 | 97.79 | 109.56 |
| 11 | a9 | 341 | LYS | CA-C-N | 5.30 | 131.66 | 121.54 |
| 11 | a9 | 341 | LYS | C-N-CA | 5.30 | 131.66 | 121.54 |
| 4 | M9 | 12 | GLY | CA-C-O | 5.30 | 126.74 | 121.60 |
| 10 | j5 | 1001 | TYR | CA-C-O | -5.29 | 115.26 | 120.82 |
| 10 | j5 | 680 | PRO | CB-CA-C | -5.29 | 104.46 | 111.23 |
| 10 | k5 | 864 | GLY | CA-C-N | 5.29 | 127.80 | 120.29 |
| 10 | k5 | 864 | GLY | C-N-CA | 5.29 | 127.80 | 120.29 |
| 9 | w7 | 41 | GLN | N-CA-C | -5.29 | 105.59 | 111.36 |
| 4 | M8 | 12 | GLY | CA-C-O | 5.29 | 126.73 | 121.60 |
| 10 | k5 | 733 | SER | N-CA-C | 5.29 | 119.88 | 113.38 |
| 10 | j5 | 351 | PHE | CA-C-N | 5.29 | 129.69 | 122.34 |
| 10 | j5 | 351 | PHE | C-N-CA | 5.29 | 129.69 | 122.34 |
| 11 | a9 | 439 | ARG | CB-CA-C | -5.29 | 102.02 | 110.79 |
| 11 | aA | 439 | ARG | CB-CA-C | -5.29 | 102.02 | 110.79 |
| 10 | j5 | 548 | SER | N-CA-CB | 5.28 | 119.42 | 110.49 |
| 4 | M1 | 92 | GLU | N-CA-C | 5.28 | 118.01 | 109.40 |
| 10 | k5 | 553 | GLN | N-CA-C | 5.28 | 117.72 | 111.33 |
| 10 | k5 | 351 | PHE | CA-C-N | 5.28 | 129.68 | 122.34 |
| 10 | k5 | 351 | PHE | C-N-CA | 5.28 | 129.68 | 122.34 |
| 10 | k5 | 548 | SER | N-CA-CB | 5.28 | 119.42 | 110.49 |
| 10 | k5 | 680 | PRO | CB-CA-C | -5.28 | 104.47 | 111.23 |
| 9 | z7 | 41 | GLN | N-CA-C | -5.28 | 105.60 | 111.36 |
| 10 | j5 | 643 | VAL | CA-C-N | 5.28 | 127.79 | 120.29 |
| 10 | j5 | 643 | VAL | C-N-CA | 5.28 | 127.79 | 120.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 11 | a9 | 414 | ALA | O-C-N | 5.27 | 127.78 | 122.09 |
| 11 | a9 | 513 | GLN | CB-CA-C | -5.27 | 99.89 | 109.38 |
| 11 | aA | 414 | ALA | O-C-N | 5.27 | 127.78 | 122.09 |
| 11 | aA | 513 | GLN | CB-CA-C | -5.27 | 99.89 | 109.38 |
| 10 | j5 | 215 | LYS | CA-C-N | 5.27 | 129.83 | 122.08 |
| 10 | j5 | 215 | LYS | C-N-CA | 5.27 | 129.83 | 122.08 |
| 10 | k5 | 546 | PHE | CB-CA-C | 5.27 | 120.20 | 112.09 |
| 2 | U1 | 44 | LEU | O-C-N | 5.27 | 127.71 | 122.12 |
| 10 | j5 | 29 | ASN | CB-CA-C | -5.27 | 102.05 | 110.79 |
| 10 | j5 | 733 | SER | N-CA-C | 5.27 | 119.86 | 113.38 |
| 10 | k5 | 29 | ASN | CB-CA-C | -5.27 | 102.05 | 110.79 |
| 10 | k5 | 666 | ASN | N-CA-C | 5.26 | 119.40 | 112.92 |
| 10 | k5 | 1001 | TYR | CA-C-O | -5.26 | 115.29 | 120.82 |
| 10 | k5 | 550 | GLY | N-CA-C | -5.26 | 100.71 | 113.18 |
| 4 | M3 | 92 | GLU | N-CA-C | 5.26 | 117.98 | 109.40 |
| 10 | j5 | 553 | GLN | N-CA-C | 5.26 | 117.69 | 111.33 |
| 4 | MA | 12 | GLY | CA-C-O | 5.26 | 126.70 | 121.60 |
| 10 | j5 | 546 | PHE | CB-CA-C | 5.26 | 120.19 | 112.09 |
| 8 | G5 | 60 | GLN | CB-CA-C | -5.25 | 100.05 | 109.24 |
| 4 | M8 | 32 | SER | N-CA-C | 5.25 | 116.94 | 108.32 |
| 10 | j5 | 550 | GLY | N-CA-C | -5.25 | 100.74 | 113.18 |
| 9 | i5 | 44 | ILE | CA-C-O | -5.25 | 115.29 | 120.85 |
| 1 | h7 | 38 | VAL | N-CA-C | 5.25 | 116.02 | 110.72 |
| 4 | M4 | 12 | GLY | CA-C-O | 5.25 | 126.69 | 121.60 |
| 10 | j5 | 864 | GLY | CA-C-N | 5.25 | 127.74 | 120.29 |
| 10 | j5 | 864 | GLY | C-N-CA | 5.25 | 127.74 | 120.29 |
| 10 | k5 | 643 | VAL | CA-C-N | 5.25 | 127.74 | 120.29 |
| 10 | k5 | 643 | VAL | C-N-CA | 5.25 | 127.74 | 120.29 |
| 8 | K5 | 96 | ILE | CG1-CB-CG2 | -5.25 | 94.97 | 110.70 |
| 10 | k5 | 245 | ILE | CB-CA-C | -5.24 | 103.52 | 111.33 |
| 10 | j5 | 703 | LEU | N-CA-CB | -5.24 | 101.72 | 110.37 |
| 10 | k5 | 946 | ASP | CB-CA-C | -5.24 | 100.02 | 111.71 |
| 2 | N8 | 111 | ALA | N-CA-C | 5.24 | 121.97 | 110.80 |
| 4 | M4 | 32 | SER | N-CA-C | 5.24 | 116.91 | 108.32 |
| 8 | A5 | 60 | GLN | CB-CA-C | -5.24 | 100.07 | 109.24 |
| 10 | k5 | 703 | LEU | N-CA-CB | -5.24 | 101.73 | 110.37 |
| 10 | k5 | 1112 | PRO | N-CA-C | 5.24 | 119.53 | 111.21 |
| 4 | M9 | 32 | SER | N-CA-C | 5.24 | 116.91 | 108.32 |
| 11 | a9 | 316 | GLY | CA-C-O | -5.24 | 115.36 | 120.75 |
| 1 | b7 | 38 | VAL | N-CA-C | 5.23 | 116.01 | 110.72 |
| 6 | M2 | 56 | PRO | CA-C-N | 5.23 | 131.54 | 121.54 |
| 6 | M2 | 56 | PRO | C-N-CA | 5.23 | 131.54 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 8 | E5 | 108 | GLY | CA-C-N | -5.23 | 114.55 | 122.76 |
| 8 | E5 | 108 | GLY | C-N-CA | -5.23 | 114.55 | 122.76 |
| 9 | z5 | 44 | ILE | CA-C-O | -5.23 | 115.30 | 120.85 |
| 10 | k5 | 415 | PHE | CB-CA-C | -5.23 | 102.54 | 111.02 |
| 8 | K5 | 108 | GLY | CA-C-N | -5.23 | 114.55 | 122.76 |
| 8 | K5 | 108 | GLY | C-N-CA | -5.23 | 114.55 | 122.76 |
| 11 | aA | 637 | PRO | CA-C-O | 5.23 | 127.04 | 120.92 |
| 4 | M4 | 130 | SER | N-CA-C | -5.23 | 105.48 | 111.07 |
| 10 | j5 | 245 | ILE | CB-CA-C | -5.22 | 103.55 | 111.33 |
| 10 | j5 | 946 | ASP | CB-CA-C | -5.22 | 100.06 | 111.71 |
| 10 | j5 | 1112 | PRO | N-CA-C | 5.22 | 119.52 | 111.21 |
| 10 | k5 | 692 | LEU | CB-CA-C | -5.22 | 100.10 | 109.24 |
| 11 | a9 | 453 | GLU | CB-CA-C | -5.22 | 102.68 | 110.88 |
| 11 | aA | 453 | GLU | CB-CA-C | -5.22 | 102.68 | 110.88 |
| 11 | aA | 618 | PRO | N-CA-C | 5.22 | 123.23 | 112.47 |
| 10 | j5 | 415 | PHE | CB-CA-C | -5.22 | 102.56 | 111.02 |
| 4 | M3 | 32 | SER | N-CA-C | 5.22 | 116.88 | 108.32 |
| 4 | M1 | 32 | SER | N-CA-C | 5.22 | 116.88 | 108.32 |
| 10 | k5 | 74 | ARG | N-CA-C | 5.22 | 119.27 | 113.01 |
| 11 | a9 | 618 | PRO | N-CA-C | 5.22 | 123.22 | 112.47 |
| 6 | M6 | 56 | PRO | CA-C-N | 5.21 | 131.50 | 121.54 |
| 6 | M6 | 56 | PRO | C-N-CA | 5.21 | 131.50 | 121.54 |
| 8 | E5 | 116 | TYR | CA-C-O | -5.21 | 115.33 | 120.70 |
| 4 | M8 | 99 | VAL | N-CA-C | -5.21 | 98.50 | 109.34 |
| 4 | MA | 32 | SER | N-CA-C | 5.21 | 116.86 | 108.32 |
| 8 | E5 | 96 | ILE | CG1-CB-CG2 | -5.21 | 95.07 | 110.70 |
| 11 | a9 | 637 | PRO | CA-C-O | 5.21 | 127.01 | 120.92 |
| 11 | a9 | 817 | LEU | CA-C-N | -5.21 | 113.67 | 120.44 |
| 11 | a9 | 817 | LEU | C-N-CA | -5.21 | 113.67 | 120.44 |
| 11 | aA | 817 | LEU | CA-C-N | -5.21 | 113.67 | 120.44 |
| 11 | aA | 817 | LEU | C-N-CA | -5.21 | 113.67 | 120.44 |
| 11 | aA | 316 | GLY | CA-C-O | -5.21 | 115.39 | 120.75 |
| 4 | M8 | 130 | SER | N-CA-C | -5.21 | 105.50 | 111.07 |
| 10 | j5 | 692 | LEU | CB-CA-C | -5.20 | 100.14 | 109.24 |
| 10 | j5 | 389 | GLY | N-CA-C | 5.20 | 125.51 | 113.18 |
| 10 | k5 | 994 | ASP | N-CA-C | 5.20 | 116.95 | 111.28 |
| 10 | k5 | 462 | TYR | CB-CA-C | -5.20 | 100.69 | 110.67 |
| 10 | j5 | 74 | ARG | N-CA-C | 5.19 | 119.24 | 113.01 |
| 10 | j5 | 462 | TYR | CB-CA-C | -5.19 | 100.70 | 110.67 |
| 10 | j5 | 994 | ASP | N-CA-C | 5.19 | 116.94 | 111.28 |
| 11 | aA | 37 | GLY | CA-C-N | 5.19 | 131.73 | 122.13 |
| 11 | aA | 37 | GLY | C-N-CA | 5.19 | 131.73 | 122.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 10 | j5 | 488 | LYS | CA-C-N | 5.19 | 127.66 | 120.29 |
| 10 | j5 | 488 | LYS | C-N-CA | 5.19 | 127.66 | 120.29 |
| 3 | B4 | 111 | ASN | N-CA-C | -5.19 | 105.71 | 111.36 |
| 10 | j5 | 645 | ASN | CB-CA-C | -5.18 | 102.03 | 110.85 |
| 10 | k5 | 389 | GLY | N-CA-C | 5.18 | 125.47 | 113.18 |
| 4 | M8 | 3 | VAL | O-C-N | 5.18 | 128.64 | 122.83 |
| 8 | K5 | 116 | TYR | CA-C-O | -5.18 | 115.36 | 120.70 |
| 10 | j5 | 756 | SER | N-CA-C | 5.18 | 119.47 | 113.20 |
| 4 | M3 | 210 | ILE | N-CA-C | 5.18 | 115.91 | 110.62 |
| 10 | k5 | 944 | ALA | N-CA-C | 5.18 | 116.93 | 111.28 |
| 4 | M1 | 210 | ILE | N-CA-C | 5.18 | 115.91 | 110.62 |
| 11 | a9 | 37 | GLY | CA-C-N | 5.18 | 131.71 | 122.13 |
| 11 | a9 | 37 | GLY | C-N-CA | 5.18 | 131.71 | 122.13 |
| 9 | z5 | 66 | GLY | CA-C-O | 5.18 | 124.87 | 119.07 |
| 4 | MA | 130 | SER | N-CA-C | -5.17 | 105.53 | 111.07 |
| 10 | k5 | 645 | ASN | CB-CA-C | -5.17 | 102.06 | 110.85 |
| 9 | y7 | 64 | ASN | N-CA-C | 5.17 | 121.82 | 110.80 |
| 4 | M9 | 130 | SER | N-CA-C | -5.17 | 105.53 | 111.07 |
| 9 | x7 | 64 | ASN | N-CA-C | 5.17 | 121.82 | 110.80 |
| 8 | A5 | 61 | ILE | CB-CG1-CD1 | 5.17 | 124.66 | 113.80 |
| 11 | a9 | 290 | ASP | N-CA-C | -5.17 | 99.96 | 108.49 |
| 11 | aA | 290 | ASP | N-CA-C | -5.17 | 99.96 | 108.49 |
| 4 | M3 | 130 | SER | N-CA-C | -5.17 | 105.54 | 111.07 |
| 8 | G5 | 61 | ILE | CB-CG1-CD1 | 5.17 | 124.66 | 113.80 |
| 10 | j5 | 881 | VAL | N-CA-CB | -5.17 | 104.67 | 109.99 |
| 10 | k5 | 881 | VAL | N-CA-CB | -5.17 | 104.67 | 109.99 |
| 4 | M9 | 210 | ILE | N-CA-C | 5.17 | 115.89 | 110.62 |
| 4 | M1 | 130 | SER | N-CA-C | -5.17 | 105.54 | 111.07 |
| 10 | k5 | 902 | ASN | N-CA-C | 5.17 | 119.76 | 111.81 |
| 10 | k5 | 193 | SER | N-CA-C | 5.16 | 119.32 | 112.30 |
| 11 | aA | 561 | ALA | N-CA-C | -5.16 | 99.81 | 110.80 |
| 10 | j5 | 976 | ARG | N-CA-CB | 5.16 | 118.81 | 110.40 |
| 4 | M8 | 42 | SER | N-CA-C | -5.16 | 99.88 | 108.34 |
| 10 | j5 | 193 | SER | N-CA-C | 5.16 | 119.32 | 112.30 |
| 10 | j5 | 855 | GLY | N-CA-C | -5.16 | 106.17 | 112.77 |
| 10 | j5 | 944 | ALA | N-CA-C | 5.16 | 116.90 | 111.28 |
| 4 | M8 | 187 | HIS | N-CA-C | 5.16 | 116.98 | 111.36 |
| 11 | a9 | 561 | ALA | N-CA-C | -5.16 | 99.82 | 110.80 |
| 10 | j5 | 1129 | ARG | N-CA-C | 5.15 | 116.98 | 111.36 |
| 4 | M8 | 101 | ASP | N-CA-C | -5.15 | 105.57 | 111.14 |
| 11 | a9 | 371 | VAL | N-CA-C | 5.15 | 120.06 | 109.34 |
| 4 | MA | 42 | SER | N-CA-C | -5.15 | 99.89 | 108.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4 | M4 | 42 | SER | N-CA-C | -5.15 | 99.89 | 108.34 |
| 10 | j5 | 29 | ASN | N-CA-C | 5.15 | 116.90 | 111.28 |
| 10 | j5 | 902 | ASN | N-CA-C | 5.15 | 119.75 | 111.81 |
| 4 | M9 | 42 | SER | N-CA-C | -5.15 | 99.89 | 108.34 |
| 9 | i5 | 66 | GLY | CA-C-O | 5.15 | 124.84 | 119.07 |
| 3 | F9 | 140 | GLY | O-C-N | -5.15 | 116.00 | 122.70 |
| 4 | MA | 27 | HIS | O-C-N | -5.15 | 117.38 | 123.25 |
| 4 | M9 | 27 | HIS | O-C-N | -5.15 | 117.38 | 123.25 |
| 10 | j5 | 709 | ILE | CB-CA-C | -5.15 | 103.93 | 110.98 |
| 4 | M3 | 42 | SER | N-CA-C | -5.14 | 99.90 | 108.34 |
| 1 | D5 | 16 | GLY | N-CA-C | -5.14 | 108.18 | 115.43 |
| 4 | M3 | 12 | GLY | CA-C-O | 5.14 | 126.59 | 121.60 |
| 4 | M4 | 210 | ILE | N-CA-C | 5.14 | 115.86 | 110.62 |
| 10 | k5 | 488 | LYS | CA-C-N | 5.14 | 127.59 | 120.29 |
| 10 | k5 | 488 | LYS | C-N-CA | 5.14 | 127.59 | 120.29 |
| 4 | M1 | 12 | GLY | CA-C-O | 5.14 | 126.59 | 121.60 |
| 4 | MA | 187 | HIS | N-CA-C | 5.14 | 116.96 | 111.36 |
| 10 | k5 | 1129 | ARG | N-CA-C | 5.14 | 116.96 | 111.36 |
| 8 | u7 | 159 | ALA | O-C-N | 5.14 | 127.64 | 122.09 |
| 4 | M9 | 187 | HIS | N-CA-C | 5.14 | 116.96 | 111.36 |
| 3 | FA | 140 | GLY | O-C-N | -5.14 | 116.02 | 122.70 |
| 4 | MA | 210 | ILE | N-CA-C | 5.14 | 115.86 | 110.62 |
| 10 | k5 | 63 | ASN | N-CA-C | -5.14 | 102.50 | 109.54 |
| 10 | k5 | 756 | SER | N-CA-C | 5.14 | 119.42 | 113.20 |
| 11 | aA | 371 | VAL | N-CA-C | 5.14 | 120.03 | 109.34 |
| 4 | M4 | 27 | HIS | O-C-N | -5.14 | 117.39 | 123.25 |
| 10 | k5 | 467 | PRO | CA-C-O | -5.14 | 115.37 | 122.15 |
| 10 | k5 | 625 | LYS | CG-CD-CE | -5.14 | 99.49 | 111.30 |
| 4 | M8 | 89 | LEU | N-CA-C | -5.14 | 100.80 | 109.07 |
| 4 | M4 | 187 | HIS | N-CA-C | 5.13 | 116.96 | 111.36 |
| 10 | j5 | 63 | ASN | N-CA-C | -5.13 | 102.50 | 109.54 |
| 10 | j5 | 80 | SER | CA-C-N | 5.13 | 124.45 | 118.85 |
| 10 | j5 | 80 | SER | C-N-CA | 5.13 | 124.45 | 118.85 |
| 10 | j5 | 545 | GLY | CA-C-O | -5.13 | 113.32 | 119.02 |
| 10 | k5 | 80 | SER | CA-C-N | 5.13 | 124.45 | 118.85 |
| 10 | k5 | 80 | SER | C-N-CA | 5.13 | 124.45 | 118.85 |
| 10 | j5 | 58 | ALA | O-C-N | 5.13 | 127.36 | 122.07 |
| 4 | MA | 169 | ASN | CB-CA-C | -5.13 | 102.27 | 110.79 |
| 4 | M4 | 3 | VAL | O-C-N | 5.13 | 128.58 | 122.83 |
| 4 | M4 | 169 | ASN | CB-CA-C | -5.13 | 102.27 | 110.79 |
| 4 | M8 | 27 | HIS | O-C-N | -5.13 | 117.40 | 123.25 |
| 4 | M8 | 169 | ASN | CB-CA-C | -5.13 | 102.27 | 110.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4 | M9 | 169 | ASN | CB-CA-C | -5.13 | 102.27 | 110.79 |
| 11 | a9 | 315 | LEU | N-CA-C | -5.13 | 105.69 | 111.28 |
| 11 | aA | 315 | LEU | N-CA-C | -5.13 | 105.69 | 111.28 |
| 4 | M1 | 42 | SER | N-CA-C | -5.13 | 99.93 | 108.34 |
| 4 | M1 | 89 | LEU | N-CA-C | -5.13 | 100.81 | 109.07 |
| 10 | k5 | 58 | ALA | O-C-N | 5.13 | 127.35 | 122.07 |
| 4 | M3 | 169 | ASN | CB-CA-C | -5.13 | 102.28 | 110.79 |
| 10 | j5 | 736 | GLU | CB-CA-C | -5.13 | 100.21 | 110.42 |
| 10 | k5 | 345 | ARG | N-CA-C | 5.13 | 117.77 | 111.82 |
| 4 | M1 | 169 | ASN | CB-CA-C | -5.13 | 102.28 | 110.79 |
| 4 | MA | 89 | LEU | N-CA-C | -5.13 | 100.82 | 109.07 |
| 8 | o7 | 159 | ALA | O-C-N | 5.13 | 127.63 | 122.09 |
| 4 | M9 | 89 | LEU | N-CA-C | -5.13 | 100.82 | 109.07 |
| 4 | M3 | 3 | VAL | O-C-N | 5.12 | 128.57 | 122.83 |
| 10 | j5 | 1154 | THR | N-CA-C | 5.12 | 117.66 | 110.23 |
| 10 | k5 | 29 | ASN | N-CA-C | 5.12 | 116.86 | 111.28 |
| 10 | k5 | 1154 | THR | N-CA-C | 5.12 | 117.66 | 110.23 |
| 4 | M1 | 3 | VAL | O-C-N | 5.12 | 128.57 | 122.83 |
| 4 | M3 | 27 | HIS | O-C-N | -5.12 | 117.41 | 123.25 |
| 4 | M3 | 187 | HIS | N-CA-C | 5.12 | 116.94 | 111.36 |
| 9 | z5 | 41 | GLN | CB-CA-C | -5.12 | 102.84 | 110.88 |
| 10 | k5 | 1004 | VAL | CB-CA-C | -5.12 | 105.31 | 112.02 |
| 9 | x7 | 56 | LEU | CA-CB-CG | -5.12 | 98.38 | 116.30 |
| 4 | M1 | 27 | HIS | O-C-N | -5.12 | 117.41 | 123.25 |
| 4 | M1 | 187 | HIS | N-CA-C | 5.12 | 116.94 | 111.36 |
| 4 | M3 | 89 | LEU | N-CA-C | -5.12 | 100.83 | 109.07 |
| 4 | M4 | 89 | LEU | N-CA-C | -5.12 | 100.83 | 109.07 |
| 9 | i5 | 41 | GLN | CB-CA-C | -5.12 | 102.84 | 110.88 |
| 10 | k5 | 855 | GLY | N-CA-C | -5.12 | 106.22 | 112.77 |
| 10 | k5 | 976 | ARG | N-CA-CB | 5.12 | 118.74 | 110.40 |
| 8 | e5 | 7 | ALA | CB-CA-C | -5.11 | 101.41 | 109.34 |
| 9 | y7 | 56 | LEU | CA-CB-CG | -5.11 | 98.40 | 116.30 |
| 11 | a9 | 504 | VAL | CA-C-N | 5.11 | 125.03 | 119.76 |
| 11 | a9 | 504 | VAL | C-N-CA | 5.11 | 125.03 | 119.76 |
| 11 | aA | 504 | VAL | CA-C-N | 5.11 | 125.03 | 119.76 |
| 11 | aA | 504 | VAL | C-N-CA | 5.11 | 125.03 | 119.76 |
| 10 | j5 | 467 | PRO | CA-C-O | -5.11 | 115.40 | 122.15 |
| 10 | j5 | 625 | LYS | CG-CD-CE | -5.11 | 99.54 | 111.30 |
| 10 | j5 | 586 | LEU | CA-CB-CG | 5.11 | 134.19 | 116.30 |
| 1 | J5 | 16 | GLY | N-CA-C | -5.11 | 108.23 | 115.43 |
| 10 | j5 | 345 | ARG | N-CA-C | 5.11 | 117.75 | 111.82 |
| 10 | j5 | 603 | PHE | N-CA-C | -5.11 | 105.79 | 112.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 10 | j5 | 1004 | VAL | CB-CA-C | -5.11 | 105.33 | 112.02 |
| 11 | a9 | 364 | THR | CA-C-N | 5.11 | 127.54 | 120.29 |
| 11 | a9 | 364 | THR | C-N-CA | 5.11 | 127.54 | 120.29 |
| 11 | aA | 364 | THR | CA-C-N | 5.11 | 127.54 | 120.29 |
| 11 | aA | 364 | THR | C-N-CA | 5.11 | 127.54 | 120.29 |
| 7 | N2 | 37 | SER | N-CA-C | 5.10 | 117.50 | 109.39 |
| 4 | MA | 3 | VAL | O-C-N | 5.10 | 128.54 | 122.83 |
| 10 | k5 | 709 | ILE | CB-CA-C | -5.10 | 103.99 | 110.98 |
| 4 | M9 | 3 | VAL | O-C-N | 5.10 | 128.54 | 122.83 |
| 8 | a5 | 7 | ALA | CB-CA-C | -5.10 | 101.44 | 109.34 |
| 10 | k5 | 461 | ASP | N-CA-C | 5.10 | 117.57 | 111.71 |
| 11 | aA | 85 | ALA | CA-C-O | -5.09 | 115.26 | 121.88 |
| 10 | j5 | 461 | ASP | N-CA-C | 5.09 | 117.56 | 111.71 |
| 10 | k5 | 1143 | LEU | CA-CB-CG | -5.09 | 98.48 | 116.30 |
| 10 | k5 | 586 | LEU | CA-CB-CG | 5.09 | 134.11 | 116.30 |
| 10 | k5 | 518 | ASN | CA-C-O | -5.09 | 113.34 | 119.49 |
| 3 | F9 | 146 | SER | N-CA-C | 5.09 | 117.05 | 108.96 |
| 7 | N6 | 37 | SER | N-CA-C | 5.08 | 117.47 | 109.39 |
| 10 | k5 | 545 | GLY | CA-C-O | -5.08 | 113.38 | 119.02 |
| 4 | M3 | 48 | PRO | CA-C-O | -5.08 | 115.58 | 122.08 |
| 4 | M1 | 48 | PRO | CA-C-O | -5.08 | 115.58 | 122.08 |
| 10 | j5 | 1143 | LEU | CA-CB-CG | -5.08 | 98.52 | 116.30 |
| 3 | L9 | 85 | ASP | CB-CA-C | -5.08 | 102.91 | 110.88 |
| 10 | k5 | 222 | LEU | N-CA-C | 5.08 | 116.50 | 111.07 |
| 11 | a9 | 498 | VAL | CB-CA-C | -5.08 | 105.54 | 111.94 |
| 11 | aA | 498 | VAL | CB-CA-C | -5.08 | 105.54 | 111.94 |
| 10 | k5 | 603 | PHE | N-CA-C | -5.07 | 105.84 | 112.23 |
| 11 | a9 | 526 | GLN | CB-CA-C | -5.07 | 102.23 | 110.85 |
| 11 | aA | 526 | GLN | CB-CA-C | -5.07 | 102.23 | 110.85 |
| 10 | j5 | 349 | GLN | N-CA-C | 5.07 | 120.36 | 113.16 |
| 4 | M4 | 48 | PRO | CA-C-O | -5.07 | 115.59 | 122.08 |
| 9 | z7 | 41 | GLN | CA-CB-CG | 5.07 | 124.24 | 114.10 |
| 3 | LA | 85 | ASP | CB-CA-C | -5.07 | 102.93 | 110.88 |
| 3 | L2 | 77 | ARG | N-CA-C | -5.07 | 105.76 | 111.28 |
| 10 | k5 | 176 | PRO | N-CA-C | -5.07 | 108.12 | 114.20 |
| 10 | k5 | 349 | GLN | N-CA-C | 5.07 | 120.35 | 113.16 |
| 9 | z7 | 21 | ARG | N-CA-CB | 5.07 | 119.05 | 110.49 |
| 9 | z7 | 33 | PRO | CB-CA-C | -5.07 | 104.58 | 111.12 |
| 9 | w7 | 21 | ARG | N-CA-CB | 5.06 | 119.04 | 110.49 |
| 10 | j5 | 987 | ASP | N-CA-CB | -5.06 | 104.36 | 110.53 |
| 10 | k5 | 985 | ALA | CA-C-N | 5.06 | 126.16 | 119.84 |
| 10 | k5 | 985 | ALA | C-N-CA | 5.06 | 126.16 | 119.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 9 | w7 | 33 | PRO | CB-CA-C | -5.06 | 104.59 | 111.12 |
| 10 | j5 | 222 | LEU | N-CA-C | 5.05 | 116.48 | 111.07 |
| 9 | w7 | 41 | GLN | CA-CB-CG | 5.05 | 124.21 | 114.10 |
| 10 | j5 | 649 | PHE | CA-C-O | -5.05 | 115.20 | 120.55 |
| 4 | M8 | 48 | PRO | CA-C-O | -5.05 | 115.62 | 122.08 |
| 11 | aA | 496 | ARG | N-CA-C | 5.05 | 116.86 | 111.36 |
| 10 | j5 | 718 | MET | CA-C-O | -5.05 | 115.20 | 120.55 |
| 10 | j5 | 634 | LEU | N-CA-C | 5.04 | 119.51 | 112.90 |
| 4 | MA | 48 | PRO | CA-C-O | -5.04 | 115.62 | 122.08 |
| 10 | j5 | 176 | PRO | N-CA-C | -5.04 | 108.15 | 114.20 |
| 4 | M9 | 48 | PRO | CA-C-O | -5.04 | 115.62 | 122.08 |
| 10 | k5 | 987 | ASP | N-CA-CB | -5.04 | 104.38 | 110.53 |
| 10 | j5 | 599 | THR | N-CA-C | 5.03 | 117.64 | 109.79 |
| 11 | a9 | 824 | VAL | N-CA-C | -5.03 | 96.91 | 111.00 |
| 10 | j5 | 518 | ASN | CA-C-O | -5.03 | 113.41 | 119.49 |
| 4 | MA | 172 | HIS | N-CA-C | 5.03 | 116.61 | 111.03 |
| 10 | j5 | 985 | ALA | CA-C-N | 5.03 | 126.12 | 119.84 |
| 10 | j5 | 985 | ALA | C-N-CA | 5.03 | 126.12 | 119.84 |
| 10 | j5 | 1148 | THR | N-CA-C | 5.03 | 123.34 | 113.29 |
| 4 | M9 | 172 | HIS | N-CA-C | 5.03 | 116.61 | 111.03 |
| 10 | k5 | 925 | ILE | N-CA-C | 5.02 | 119.53 | 113.00 |
| 11 | a9 | 496 | ARG | N-CA-C | 5.02 | 116.84 | 111.36 |
| 10 | k5 | 260 | TYR | N-CA-C | 5.02 | 117.48 | 111.71 |
| 10 | k5 | 1148 | THR | N-CA-C | 5.02 | 123.33 | 113.29 |
| 10 | j5 | 704 | THR | OG1-CB-CG2 | -5.02 | 99.26 | 109.30 |
| 10 | j5 | 1047 | LYS | N-CA-C | 5.02 | 116.44 | 111.07 |
| 10 | k5 | 704 | THR | OG1-CB-CG2 | -5.01 | 99.27 | 109.30 |
| 10 | k5 | 634 | LEU | N-CA-C | 5.01 | 119.47 | 112.90 |
| 11 | a9 | 798 | SER | O-C-N | 5.01 | 129.13 | 123.27 |
| 11 | aA | 798 | SER | O-C-N | 5.01 | 129.13 | 123.27 |
| 10 | k5 | 649 | PHE | CA-C-O | -5.01 | 115.24 | 120.55 |
| 10 | k5 | 778 | LYS | CD-CE-NZ | -5.01 | 95.88 | 111.90 |
| 10 | k5 | 1047 | LYS | N-CA-C | 5.00 | 116.42 | 111.07 |

There are no chirality outliers.

All (143) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | D5 | 6 | THR | Mainchain |
| 8 | E7 | 79 | ALA | Mainchain |
| 1 | J5 | 6 | THR | Mainchain |
| 8 | K7 | 79 | ALA | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 3 | L9 | 109 | CYS | Mainchain |
| 3 | LA | 109 | CYS | Mainchain |
| 4 | M1 | 20 | THR | Mainchain |
| 4 | M1 | 228 | SER | Mainchain |
| 6 | M2 | 269 | ILE | Peptide |
| 6 | M2 | 279 | ASP | Peptide |
| 6 | M2 | 280 | ALA | Peptide |
| 6 | M2 | 37 | GLU | Peptide |
| 6 | M2 | 58 | GLY | Peptide |
| 4 | M3 | 20 | THR | Mainchain |
| 4 | M3 | 228 | SER | Mainchain |
| 4 | M4 | 20 | THR | Mainchain |
| 4 | M4 | 228 | SER | Mainchain |
| 6 | M6 | 269 | ILE | Peptide |
| 6 | M6 | 279 | ASP | Peptide |
| 6 | M6 | 280 | ALA | Peptide |
| 6 | M6 | 37 | GLU | Peptide |
| 6 | M6 | 58 | GLY | Peptide |
| 4 | M8 | 20 | THR | Mainchain |
| 4 | M8 | 228 | SER | Mainchain |
| 4 | M9 | 20 | THR | Mainchain |
| 4 | M9 | 228 | SER | Mainchain |
| 4 | MA | 20 | THR | Mainchain |
| 4 | MA | 228 | SER | Mainchain |
| 7 | N2 | 26 | ALA | Peptide |
| 7 | N6 | 26 | ALA | Peptide |
| 8 | O5 | 19 | SER | Mainchain |
| 3 | Q4 | 78 | ARG | Sidechain |
| 3 | Q4 | 84 | ARG | Sidechain |
| 3 | Q4 | 91 | ARG | Sidechain |
| 8 | Q5 | 79 | ALA | Mainchain |
| 8 | Q7 | 79 | ALA | Mainchain |
| 3 | Q8 | 108 | ARG | Sidechain |
| 8 | U7 | 18 | LEU | Mainchain |
| 8 | W5 | 79 | ALA | Mainchain |
| 8 | W7 | 79 | ALA | Mainchain |
| 5 | Z4 | 23 | SER | Mainchain |
| 5 | Z4 | 34 | LEU | Mainchain |
| 8 | a5 | 23 | LEU | Mainchain |
| 8 | a5 | 25 | ARG | Sidechain |
| 8 | a5 | 6 | LYS | Mainchain |
| 11 | a9 | 157 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-------------------|
| 11 | a9 | 354 | VAL | Mainchain,Peptide |
| 11 | a9 | 372 | ALA | Peptide |
| 11 | a9 | 554 | ARG | Sidechain |
| 11 | a9 | 559 | THR | Mainchain |
| 11 | a9 | 595 | ARG | Peptide |
| 11 | a9 | 596 | THR | Peptide |
| 11 | a9 | 598 | SER | Peptide |
| 11 | a9 | 599 | PRO | Mainchain |
| 11 | a9 | 603 | THR | Peptide |
| 11 | a9 | 604 | ALA | Peptide |
| 11 | a9 | 636 | ALA | Peptide |
| 11 | a9 | 64 | ARG | Sidechain |
| 11 | a9 | 72 | ASP | Peptide |
| 11 | a9 | 741 | TYR | Sidechain |
| 11 | aA | 157 | ARG | Sidechain |
| 11 | aA | 295 | ARG | Sidechain |
| 11 | aA | 354 | VAL | Mainchain,Peptide |
| 11 | aA | 372 | ALA | Peptide |
| 11 | aA | 554 | ARG | Sidechain |
| 11 | aA | 559 | THR | Mainchain |
| 11 | aA | 595 | ARG | Peptide |
| 11 | aA | 596 | THR | Peptide |
| 11 | aA | 598 | SER | Peptide |
| 11 | aA | 599 | PRO | Mainchain |
| 11 | aA | 603 | THR | Peptide |
| 11 | aA | 604 | ALA | Peptide |
| 11 | aA | 636 | ALA | Peptide |
| 11 | aA | 64 | ARG | Sidechain |
| 11 | aA | 72 | ASP | Peptide |
| 11 | aA | 741 | TYR | Sidechain |
| 8 | c7 | 112 | VAL | Mainchain |
| 8 | c7 | 125 | ALA | Mainchain |
| 8 | c7 | 79 | ALA | Mainchain |
| 8 | e5 | 23 | LEU | Mainchain |
| 8 | e5 | 25 | ARG | Sidechain |
| 8 | e5 | 6 | LYS | Mainchain |
| 9 | i5 | 33 | PRO | Mainchain |
| 8 | i7 | 112 | VAL | Mainchain |
| 8 | i7 | 125 | ALA | Mainchain |
| 8 | i7 | 79 | ALA | Mainchain |
| 10 | j5 | 1026 | LYS | Mainchain |
| 10 | j5 | 1031 | SER | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 10 | j5 | 1055 | SER | Mainchain |
| 10 | j5 | 1077 | ILE | Mainchain |
| 10 | j5 | 1139 | SER | Mainchain |
| 10 | j5 | 137 | PRO | Peptide |
| 10 | j5 | 284 | PRO | Peptide |
| 10 | j5 | 289 | SER | Mainchain |
| 10 | j5 | 291 | ASP | Mainchain |
| 10 | j5 | 518 | ASN | Mainchain |
| 10 | j5 | 543 | ASN | Mainchain |
| 10 | j5 | 571 | ALA | Mainchain |
| 10 | j5 | 615 | LYS | Mainchain |
| 10 | j5 | 695 | GLY | Mainchain |
| 10 | j5 | 743 | VAL | Peptide |
| 10 | j5 | 765 | ASP | Mainchain |
| 10 | j5 | 812 | SER | Mainchain |
| 10 | j5 | 824 | PRO | Mainchain |
| 10 | j5 | 832 | ALA | Mainchain |
| 10 | j5 | 846 | GLU | Mainchain |
| 10 | j5 | 847 | LEU | Mainchain |
| 10 | j5 | 864 | GLY | Mainchain |
| 10 | j5 | 882 | PRO | Mainchain |
| 10 | k5 | 1026 | LYS | Mainchain |
| 10 | k5 | 1031 | SER | Mainchain |
| 10 | k5 | 1055 | SER | Mainchain |
| 10 | k5 | 1077 | ILE | Mainchain |
| 10 | k5 | 1139 | SER | Mainchain |
| 10 | k5 | 137 | PRO | Peptide |
| 10 | k5 | 284 | PRO | Peptide |
| 10 | k5 | 289 | SER | Mainchain |
| 10 | k5 | 291 | ASP | Mainchain |
| 10 | k5 | 518 | ASN | Mainchain |
| 10 | k5 | 543 | ASN | Mainchain |
| 10 | k5 | 571 | ALA | Mainchain |
| 10 | k5 | 615 | LYS | Mainchain |
| 10 | k5 | 695 | GLY | Mainchain |
| 10 | k5 | 743 | VAL | Peptide |
| 10 | k5 | 765 | ASP | Mainchain |
| 10 | k5 | 812 | SER | Mainchain |
| 10 | k5 | 824 | PRO | Mainchain |
| 10 | k5 | 832 | ALA | Mainchain |
| 10 | k5 | 846 | GLU | Mainchain |
| 10 | k5 | 847 | LEU | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 10 | k5 | 864 | GLY | Mainchain |
| 10 | k5 | 882 | PRO | Mainchain |
| 8 | o7 | 159 | ALA | Mainchain |
| 8 | o7 | 5 | THR | Mainchain |
| 8 | u7 | 159 | ALA | Mainchain |
| 8 | u7 | 5 | THR | Mainchain |
| 9 | x7 | 21 | ARG | Mainchain |
| 9 | x7 | 61 | GLN | Mainchain |
| 9 | y7 | 21 | ARG | Mainchain |
| 9 | y7 | 61 | GLN | Mainchain |
| 9 | z5 | 33 | PRO | Mainchain |

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1210 | 0 | 1220 | 112 | 0 |
| 1 | B5 | 1210 | 0 | 1218 | 97 | 0 |
| 1 | B7 | 1210 | 0 | 1219 | 59 | 0 |
| 1 | D5 | 1210 | 0 | 1219 | 89 | 0 |
| 1 | D7 | 1210 | 0 | 1219 | 151 | 0 |
| 1 | F5 | 1210 | 0 | 1220 | 69 | 0 |
| 1 | F7 | 1210 | 0 | 1220 | 21 | 0 |
| 1 | H5 | 1210 | 0 | 1218 | 77 | 0 |
| 1 | H7 | 1210 | 0 | 1219 | 59 | 0 |
| 1 | J5 | 1210 | 0 | 1219 | 91 | 0 |
| 1 | J7 | 1210 | 0 | 1220 | 149 | 0 |
| 1 | L5 | 1210 | 0 | 1220 | 74 | 0 |
| 1 | L7 | 1210 | 0 | 1220 | 19 | 0 |
| 1 | N5 | 1210 | 0 | 1220 | 82 | 0 |
| 1 | N7 | 1210 | 0 | 1218 | 28 | 0 |
| 1 | P5 | 1210 | 0 | 1218 | 63 | 0 |
| 1 | P7 | 1210 | 0 | 1220 | 51 | 0 |
| 1 | R5 | 1210 | 0 | 1216 | 184 | 0 |
| 1 | R7 | 1210 | 0 | 1219 | 31 | 0 |
| 1 | T5 | 1210 | 0 | 1220 | 90 | 0 |
| 1 | T7 | 1210 | 0 | 1218 | 44 | 0 |
| 1 | V5 | 1210 | 0 | 1219 | 64 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | V7 | 1210 | 0 | 1220 | 51 | 0 |
| 1 | X5 | 1210 | 0 | 1219 | 181 | 0 |
| 1 | X7 | 1210 | 0 | 1219 | 30 | 0 |
| 1 | Z | 1210 | 0 | 1219 | 115 | 0 |
| 1 | Z5 | 1210 | 0 | 1215 | 100 | 0 |
| 1 | Z7 | 1210 | 0 | 1218 | 44 | 0 |
| 1 | b5 | 1210 | 0 | 1218 | 118 | 0 |
| 1 | b7 | 1210 | 0 | 1219 | 105 | 0 |
| 1 | d5 | 1210 | 0 | 1217 | 91 | 0 |
| 1 | d7 | 1210 | 0 | 1215 | 163 | 0 |
| 1 | f5 | 1210 | 0 | 1219 | 110 | 0 |
| 1 | f7 | 1210 | 0 | 1218 | 46 | 0 |
| 1 | h7 | 1210 | 0 | 1219 | 108 | 0 |
| 1 | j7 | 1210 | 0 | 1217 | 100 | 0 |
| 1 | l7 | 1210 | 0 | 1217 | 73 | 0 |
| 1 | n7 | 1210 | 0 | 1220 | 109 | 0 |
| 1 | p7 | 1210 | 0 | 1219 | 339 | 0 |
| 1 | r7 | 1210 | 0 | 1219 | 55 | 0 |
| 1 | t7 | 1210 | 0 | 1218 | 126 | 0 |
| 1 | v7 | 1210 | 0 | 1218 | 335 | 0 |
| 2 | A1 | 1243 | 0 | 1225 | 84 | 0 |
| 2 | A2 | 1243 | 0 | 1225 | 84 | 0 |
| 2 | A3 | 1243 | 0 | 1225 | 87 | 0 |
| 2 | A4 | 1243 | 0 | 1225 | 82 | 0 |
| 2 | A6 | 1243 | 0 | 1225 | 84 | 0 |
| 2 | A8 | 1243 | 0 | 1225 | 83 | 0 |
| 2 | A9 | 1243 | 0 | 1225 | 85 | 0 |
| 2 | AA | 1243 | 0 | 1225 | 84 | 0 |
| 2 | C1 | 1243 | 0 | 1225 | 29 | 0 |
| 2 | C2 | 1243 | 0 | 1225 | 17 | 0 |
| 2 | C3 | 1243 | 0 | 1225 | 26 | 0 |
| 2 | C4 | 1243 | 0 | 1225 | 18 | 0 |
| 2 | C6 | 1243 | 0 | 1225 | 15 | 0 |
| 2 | C8 | 1243 | 0 | 1225 | 17 | 0 |
| 2 | C9 | 1243 | 0 | 1225 | 12 | 0 |
| 2 | CA | 1243 | 0 | 1225 | 12 | 0 |
| 2 | E1 | 1243 | 0 | 1225 | 19 | 0 |
| 2 | E2 | 1243 | 0 | 1225 | 17 | 0 |
| 2 | E3 | 1243 | 0 | 1225 | 19 | 0 |
| 2 | E4 | 1243 | 0 | 1224 | 32 | 0 |
| 2 | E6 | 1243 | 0 | 1225 | 17 | 0 |
| 2 | E8 | 1243 | 0 | 1224 | 27 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | E9 | 1243 | 0 | 1225 | 40 | 0 |
| 2 | EA | 1243 | 0 | 1225 | 40 | 0 |
| 2 | G1 | 1243 | 0 | 1225 | 43 | 0 |
| 2 | G2 | 1243 | 0 | 1225 | 34 | 0 |
| 2 | G3 | 1243 | 0 | 1225 | 42 | 0 |
| 2 | G4 | 1243 | 0 | 1225 | 21 | 0 |
| 2 | G6 | 1243 | 0 | 1225 | 26 | 0 |
| 2 | G8 | 1243 | 0 | 1225 | 20 | 0 |
| 2 | G9 | 1243 | 0 | 1225 | 20 | 0 |
| 2 | GA | 1243 | 0 | 1225 | 21 | 0 |
| 2 | I1 | 1243 | 0 | 1225 | 15 | 0 |
| 2 | I2 | 1243 | 0 | 1225 | 18 | 0 |
| 2 | I3 | 1243 | 0 | 1225 | 15 | 0 |
| 2 | I4 | 1243 | 0 | 1225 | 25 | 0 |
| 2 | I6 | 1243 | 0 | 1225 | 17 | 0 |
| 2 | I8 | 1243 | 0 | 1225 | 27 | 0 |
| 2 | I9 | 1243 | 0 | 1225 | 99 | 0 |
| 2 | IA | 1243 | 0 | 1225 | 106 | 0 |
| 2 | K1 | 1243 | 0 | 1224 | 68 | 0 |
| 2 | K2 | 1243 | 0 | 1225 | 29 | 0 |
| 2 | K3 | 1243 | 0 | 1224 | 91 | 0 |
| 2 | K4 | 1243 | 0 | 1225 | 32 | 0 |
| 2 | K6 | 1243 | 0 | 1225 | 30 | 0 |
| 2 | K8 | 1243 | 0 | 1225 | 32 | 0 |
| 2 | K9 | 1243 | 0 | 1225 | 76 | 0 |
| 2 | KA | 1243 | 0 | 1225 | 58 | 0 |
| 2 | N4 | 1243 | 0 | 1225 | 152 | 0 |
| 2 | N8 | 1243 | 0 | 1225 | 174 | 0 |
| 2 | O1 | 1243 | 0 | 1225 | 78 | 0 |
| 2 | O3 | 1243 | 0 | 1225 | 82 | 0 |
| 2 | O9 | 1243 | 0 | 1225 | 81 | 0 |
| 2 | OA | 1243 | 0 | 1225 | 80 | 0 |
| 2 | P4 | 1243 | 0 | 1223 | 67 | 0 |
| 2 | P8 | 1243 | 0 | 1223 | 54 | 0 |
| 2 | Q1 | 1243 | 0 | 1225 | 19 | 0 |
| 2 | Q3 | 1243 | 0 | 1225 | 18 | 0 |
| 2 | Q9 | 1243 | 0 | 1224 | 39 | 0 |
| 2 | QA | 1243 | 0 | 1223 | 164 | 0 |
| 2 | R4 | 1243 | 0 | 1225 | 18 | 0 |
| 2 | R8 | 1243 | 0 | 1225 | 18 | 0 |
| 2 | S1 | 1243 | 0 | 1225 | 21 | 0 |
| 2 | S3 | 1243 | 0 | 1225 | 22 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | S9 | 1243 | 0 | 1223 | 60 | 0 |
| 2 | SA | 1243 | 0 | 1223 | 59 | 0 |
| 2 | T4 | 1243 | 0 | 1225 | 19 | 0 |
| 2 | T8 | 1243 | 0 | 1225 | 18 | 0 |
| 2 | U1 | 1243 | 0 | 1224 | 45 | 0 |
| 2 | U3 | 1243 | 0 | 1222 | 42 | 0 |
| 2 | U9 | 1243 | 0 | 1225 | 29 | 0 |
| 2 | UA | 1243 | 0 | 1225 | 67 | 0 |
| 2 | V4 | 1243 | 0 | 1225 | 13 | 0 |
| 2 | V8 | 1243 | 0 | 1225 | 11 | 0 |
| 2 | W1 | 1243 | 0 | 1225 | 12 | 0 |
| 2 | W3 | 1243 | 0 | 1225 | 11 | 0 |
| 2 | W9 | 1243 | 0 | 1225 | 22 | 0 |
| 2 | WA | 1243 | 0 | 1225 | 30 | 0 |
| 2 | X4 | 1243 | 0 | 1224 | 152 | 0 |
| 2 | X8 | 1243 | 0 | 1224 | 162 | 0 |
| 2 | Y1 | 1243 | 0 | 1225 | 32 | 0 |
| 2 | Y3 | 1243 | 0 | 1225 | 32 | 0 |
| 2 | Y9 | 1243 | 0 | 1225 | 29 | 0 |
| 2 | YA | 1243 | 0 | 1225 | 30 | 0 |
| 3 | B1 | 1293 | 0 | 1300 | 113 | 0 |
| 3 | B2 | 1293 | 0 | 1301 | 42 | 0 |
| 3 | B3 | 1293 | 0 | 1301 | 108 | 0 |
| 3 | B4 | 1293 | 0 | 1300 | 216 | 0 |
| 3 | B6 | 1293 | 0 | 1301 | 42 | 0 |
| 3 | B8 | 1293 | 0 | 1298 | 136 | 0 |
| 3 | B9 | 1293 | 0 | 1301 | 67 | 0 |
| 3 | BA | 1293 | 0 | 1301 | 66 | 0 |
| 3 | D1 | 1293 | 0 | 1301 | 42 | 0 |
| 3 | D2 | 1293 | 0 | 1301 | 19 | 0 |
| 3 | D3 | 1293 | 0 | 1301 | 41 | 0 |
| 3 | D4 | 1293 | 0 | 1301 | 54 | 0 |
| 3 | D6 | 1293 | 0 | 1301 | 20 | 0 |
| 3 | D8 | 1293 | 0 | 1301 | 46 | 0 |
| 3 | D9 | 1293 | 0 | 1300 | 62 | 0 |
| 3 | DA | 1293 | 0 | 1300 | 63 | 0 |
| 3 | F1 | 1293 | 0 | 1301 | 37 | 0 |
| 3 | F2 | 1293 | 0 | 1302 | 62 | 0 |
| 3 | F3 | 1293 | 0 | 1301 | 39 | 0 |
| 3 | F4 | 1293 | 0 | 1298 | 175 | 0 |
| 3 | F6 | 1293 | 0 | 1302 | 81 | 0 |
| 3 | F8 | 1293 | 0 | 1299 | 145 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | F9 | 1293 | 0 | 1301 | 122 | 0 |
| 3 | FA | 1293 | 0 | 1302 | 133 | 0 |
| 3 | H1 | 1293 | 0 | 1301 | 81 | 0 |
| 3 | H2 | 1293 | 0 | 1301 | 55 | 0 |
| 3 | H3 | 1293 | 0 | 1299 | 52 | 0 |
| 3 | H4 | 1293 | 0 | 1299 | 104 | 0 |
| 3 | H6 | 1293 | 0 | 1301 | 56 | 0 |
| 3 | H8 | 1293 | 0 | 1300 | 100 | 0 |
| 3 | H9 | 1293 | 0 | 1301 | 120 | 0 |
| 3 | HA | 1293 | 0 | 1300 | 123 | 0 |
| 3 | J1 | 1293 | 0 | 1297 | 82 | 0 |
| 3 | J2 | 1293 | 0 | 1301 | 43 | 0 |
| 3 | J3 | 1293 | 0 | 1300 | 148 | 0 |
| 3 | J4 | 1293 | 0 | 1301 | 33 | 0 |
| 3 | J6 | 1293 | 0 | 1301 | 42 | 0 |
| 3 | J8 | 1293 | 0 | 1301 | 31 | 0 |
| 3 | J9 | 1293 | 0 | 1294 | 144 | 0 |
| 3 | JA | 1293 | 0 | 1294 | 150 | 0 |
| 3 | L1 | 1293 | 0 | 1301 | 140 | 0 |
| 3 | L2 | 1293 | 0 | 1301 | 82 | 0 |
| 3 | L3 | 1293 | 0 | 1301 | 137 | 0 |
| 3 | L4 | 1293 | 0 | 1301 | 100 | 0 |
| 3 | L6 | 1293 | 0 | 1301 | 45 | 0 |
| 3 | L8 | 1293 | 0 | 1302 | 139 | 0 |
| 3 | L9 | 1293 | 0 | 1301 | 154 | 0 |
| 3 | LA | 1293 | 0 | 1301 | 156 | 0 |
| 3 | O4 | 1293 | 0 | 1299 | 122 | 0 |
| 3 | O8 | 1293 | 0 | 1298 | 145 | 0 |
| 3 | P1 | 1293 | 0 | 1301 | 40 | 0 |
| 3 | P3 | 1293 | 0 | 1301 | 41 | 0 |
| 3 | P9 | 1293 | 0 | 1301 | 37 | 0 |
| 3 | PA | 1293 | 0 | 1301 | 38 | 0 |
| 3 | Q4 | 1293 | 0 | 1301 | 208 | 0 |
| 3 | Q8 | 1293 | 0 | 1301 | 243 | 0 |
| 3 | R1 | 1293 | 0 | 1301 | 34 | 0 |
| 3 | R3 | 1293 | 0 | 1301 | 30 | 0 |
| 3 | R9 | 1293 | 0 | 1301 | 46 | 0 |
| 3 | RA | 1293 | 0 | 1301 | 52 | 0 |
| 3 | S4 | 1293 | 0 | 1302 | 57 | 0 |
| 3 | S8 | 1293 | 0 | 1302 | 77 | 0 |
| 3 | T1 | 1293 | 0 | 1301 | 41 | 0 |
| 3 | T3 | 1293 | 0 | 1301 | 43 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | T9 | 1293 | 0 | 1297 | 144 | 0 |
| 3 | TA | 1293 | 0 | 1297 | 238 | 0 |
| 3 | U4 | 1293 | 0 | 1299 | 92 | 0 |
| 3 | U8 | 1293 | 0 | 1301 | 103 | 0 |
| 3 | V1 | 1293 | 0 | 1301 | 39 | 0 |
| 3 | V3 | 1293 | 0 | 1301 | 41 | 0 |
| 3 | V9 | 1293 | 0 | 1298 | 143 | 0 |
| 3 | VA | 1293 | 0 | 1298 | 146 | 0 |
| 3 | W4 | 1293 | 0 | 1301 | 21 | 0 |
| 3 | W8 | 1293 | 0 | 1301 | 21 | 0 |
| 3 | X1 | 1293 | 0 | 1301 | 77 | 0 |
| 3 | X3 | 1293 | 0 | 1301 | 77 | 0 |
| 3 | X9 | 1293 | 0 | 1301 | 45 | 0 |
| 3 | XA | 1293 | 0 | 1301 | 46 | 0 |
| 3 | Y4 | 1293 | 0 | 1301 | 221 | 0 |
| 3 | Y8 | 1293 | 0 | 1299 | 162 | 0 |
| 3 | Z1 | 1293 | 0 | 1299 | 48 | 0 |
| 3 | Z3 | 1293 | 0 | 1299 | 46 | 0 |
| 3 | Z9 | 1293 | 0 | 1301 | 52 | 0 |
| 3 | ZA | 1293 | 0 | 1301 | 51 | 0 |
| 4 | M1 | 2178 | 0 | 2143 | 394 | 0 |
| 4 | M3 | 2178 | 0 | 2143 | 377 | 0 |
| 4 | M4 | 2178 | 0 | 2139 | 967 | 0 |
| 4 | M8 | 2178 | 0 | 2139 | 873 | 0 |
| 4 | M9 | 2178 | 0 | 2140 | 513 | 0 |
| 4 | MA | 2178 | 0 | 2140 | 513 | 0 |
| 5 | N1 | 578 | 0 | 587 | 206 | 0 |
| 5 | N3 | 578 | 0 | 587 | 201 | 0 |
| 5 | N9 | 578 | 0 | 584 | 235 | 0 |
| 5 | NA | 578 | 0 | 584 | 231 | 0 |
| 5 | Z4 | 578 | 0 | 584 | 469 | 0 |
| 5 | Z8 | 578 | 0 | 584 | 536 | 0 |
| 6 | M2 | 2190 | 0 | 2142 | 289 | 0 |
| 6 | M6 | 2190 | 0 | 2137 | 317 | 0 |
| 7 | N2 | 545 | 0 | 552 | 43 | 0 |
| 7 | N6 | 545 | 0 | 552 | 43 | 0 |
| 8 | A5 | 1222 | 0 | 1234 | 174 | 0 |
| 8 | A7 | 1222 | 0 | 1233 | 50 | 0 |
| 8 | C5 | 1222 | 0 | 1232 | 109 | 0 |
| 8 | C7 | 1222 | 0 | 1231 | 119 | 0 |
| 8 | E5 | 1222 | 0 | 1231 | 105 | 0 |
| 8 | E7 | 1222 | 0 | 1231 | 76 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8 | G5 | 1222 | 0 | 1234 | 216 | 0 |
| 8 | G7 | 1222 | 0 | 1233 | 68 | 0 |
| 8 | I5 | 1222 | 0 | 1232 | 109 | 0 |
| 8 | I7 | 1222 | 0 | 1232 | 130 | 0 |
| 8 | K5 | 1222 | 0 | 1231 | 123 | 0 |
| 8 | K7 | 1222 | 0 | 1231 | 77 | 0 |
| 8 | M5 | 1222 | 0 | 1233 | 110 | 0 |
| 8 | M7 | 1222 | 0 | 1233 | 64 | 0 |
| 8 | O5 | 1222 | 0 | 1233 | 176 | 0 |
| 8 | O7 | 1222 | 0 | 1230 | 131 | 0 |
| 8 | Q5 | 1222 | 0 | 1230 | 125 | 0 |
| 8 | Q7 | 1222 | 0 | 1231 | 105 | 0 |
| 8 | S5 | 1222 | 0 | 1233 | 127 | 0 |
| 8 | S7 | 1222 | 0 | 1233 | 85 | 0 |
| 8 | U5 | 1222 | 0 | 1230 | 222 | 0 |
| 8 | U7 | 1222 | 0 | 1231 | 120 | 0 |
| 8 | W5 | 1222 | 0 | 1230 | 123 | 0 |
| 8 | W7 | 1222 | 0 | 1231 | 96 | 0 |
| 8 | Y5 | 1222 | 0 | 1233 | 55 | 0 |
| 8 | Y7 | 1222 | 0 | 1233 | 59 | 0 |
| 8 | a5 | 1222 | 0 | 1232 | 126 | 0 |
| 8 | a7 | 1222 | 0 | 1230 | 173 | 0 |
| 8 | c5 | 1222 | 0 | 1233 | 64 | 0 |
| 8 | c7 | 1222 | 0 | 1228 | 335 | 0 |
| 8 | e5 | 1222 | 0 | 1232 | 124 | 0 |
| 8 | e7 | 1222 | 0 | 1233 | 51 | 0 |
| 8 | g7 | 1222 | 0 | 1232 | 175 | 0 |
| 8 | i7 | 1222 | 0 | 1229 | 362 | 0 |
| 8 | k7 | 1222 | 0 | 1233 | 107 | 0 |
| 8 | m7 | 1222 | 0 | 1232 | 123 | 0 |
| 8 | o7 | 1222 | 0 | 1226 | 310 | 0 |
| 8 | q7 | 1222 | 0 | 1233 | 105 | 0 |
| 8 | s7 | 1222 | 0 | 1229 | 172 | 0 |
| 8 | u7 | 1222 | 0 | 1228 | 301 | 0 |
| 9 | i5 | 538 | 0 | 555 | 145 | 0 |
| 9 | w7 | 538 | 0 | 552 | 106 | 0 |
| 9 | x7 | 538 | 0 | 552 | 115 | 0 |
| 9 | y7 | 538 | 0 | 553 | 99 | 0 |
| 9 | z5 | 538 | 0 | 555 | 152 | 0 |
| 9 | z7 | 538 | 0 | 554 | 99 | 0 |
| 10 | j5 | 8819 | 0 | 8820 | 1743 | 0 |
| 10 | k5 | 8819 | 0 | 8823 | 1832 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11 | a9 | 6326 | 0 | 6124 | 1826 | 0 |
| 11 | aA | 6326 | 0 | 6123 | 1862 | 0 |
| 12 | A | 43 | 0 | 37 | 9 | 0 |
| 12 | A1 | 43 | 0 | 37 | 8 | 0 |
| 12 | A2 | 43 | 0 | 37 | 8 | 0 |
| 12 | A3 | 43 | 0 | 37 | 8 | 0 |
| 12 | A4 | 43 | 0 | 37 | 8 | 0 |
| 12 | A5 | 43 | 0 | 38 | 69 | 0 |
| 12 | A6 | 43 | 0 | 37 | 8 | 0 |
| 12 | A7 | 43 | 0 | 37 | 3 | 0 |
| 12 | A8 | 43 | 0 | 37 | 8 | 0 |
| 12 | A9 | 43 | 0 | 37 | 8 | 0 |
| 12 | AA | 43 | 0 | 37 | 8 | 0 |
| 12 | B1 | 86 | 0 | 74 | 75 | 0 |
| 12 | B2 | 43 | 0 | 37 | 7 | 0 |
| 12 | B3 | 86 | 0 | 75 | 75 | 0 |
| 12 | B4 | 86 | 0 | 69 | 124 | 0 |
| 12 | B5 | 43 | 0 | 37 | 26 | 0 |
| 12 | B6 | 43 | 0 | 37 | 7 | 0 |
| 12 | B7 | 43 | 0 | 37 | 12 | 0 |
| 12 | B8 | 86 | 0 | 68 | 92 | 0 |
| 12 | B9 | 86 | 0 | 74 | 27 | 0 |
| 12 | BA | 86 | 0 | 74 | 26 | 0 |
| 12 | C1 | 43 | 0 | 37 | 8 | 0 |
| 12 | C2 | 43 | 0 | 37 | 8 | 0 |
| 12 | C3 | 43 | 0 | 37 | 8 | 0 |
| 12 | C4 | 43 | 0 | 37 | 8 | 0 |
| 12 | C5 | 43 | 0 | 37 | 7 | 0 |
| 12 | C6 | 43 | 0 | 37 | 8 | 0 |
| 12 | C7 | 43 | 0 | 37 | 4 | 0 |
| 12 | C8 | 43 | 0 | 37 | 8 | 0 |
| 12 | C9 | 43 | 0 | 37 | 8 | 0 |
| 12 | CA | 43 | 0 | 37 | 8 | 0 |
| 12 | D1 | 86 | 0 | 74 | 15 | 0 |
| 12 | D2 | 86 | 0 | 74 | 15 | 0 |
| 12 | D3 | 86 | 0 | 74 | 15 | 0 |
| 12 | D4 | 86 | 0 | 73 | 15 | 0 |
| 12 | D5 | 43 | 0 | 37 | 11 | 0 |
| 12 | D6 | 86 | 0 | 74 | 14 | 0 |
| 12 | D7 | 43 | 0 | 35 | 32 | 0 |
| 12 | D8 | 86 | 0 | 73 | 27 | 0 |
| 12 | D9 | 86 | 0 | 74 | 21 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 12 | DA | 86 | 0 | 74 | 20 | 0 |
| 12 | E1 | 43 | 0 | 37 | 8 | 0 |
| 12 | E2 | 43 | 0 | 37 | 7 | 0 |
| 12 | E3 | 43 | 0 | 37 | 8 | 0 |
| 12 | E4 | 43 | 0 | 37 | 8 | 0 |
| 12 | E5 | 43 | 0 | 37 | 27 | 0 |
| 12 | E6 | 43 | 0 | 37 | 8 | 0 |
| 12 | E7 | 43 | 0 | 37 | 13 | 0 |
| 12 | E8 | 43 | 0 | 37 | 8 | 0 |
| 12 | E9 | 43 | 0 | 37 | 7 | 0 |
| 12 | EA | 43 | 0 | 37 | 7 | 0 |
| 12 | F1 | 86 | 0 | 74 | 31 | 0 |
| 12 | F2 | 86 | 0 | 75 | 59 | 0 |
| 12 | F3 | 86 | 0 | 74 | 31 | 0 |
| 12 | F4 | 86 | 0 | 70 | 17 | 0 |
| 12 | F5 | 43 | 0 | 37 | 17 | 0 |
| 12 | F6 | 86 | 0 | 75 | 69 | 0 |
| 12 | F7 | 43 | 0 | 37 | 17 | 0 |
| 12 | F8 | 86 | 0 | 70 | 14 | 0 |
| 12 | F9 | 129 | 0 | 112 | 73 | 0 |
| 12 | FA | 43 | 0 | 37 | 19 | 0 |
| 12 | G1 | 43 | 0 | 37 | 8 | 0 |
| 12 | G2 | 43 | 0 | 37 | 11 | 0 |
| 12 | G3 | 43 | 0 | 37 | 8 | 0 |
| 12 | G4 | 43 | 0 | 37 | 8 | 0 |
| 12 | G5 | 43 | 0 | 38 | 70 | 0 |
| 12 | G6 | 43 | 0 | 37 | 8 | 0 |
| 12 | G7 | 43 | 0 | 37 | 3 | 0 |
| 12 | G8 | 43 | 0 | 37 | 8 | 0 |
| 12 | G9 | 43 | 0 | 37 | 8 | 0 |
| 12 | GA | 43 | 0 | 37 | 8 | 0 |
| 12 | H1 | 86 | 0 | 73 | 62 | 0 |
| 12 | H2 | 86 | 0 | 74 | 27 | 0 |
| 12 | H3 | 86 | 0 | 74 | 20 | 0 |
| 12 | H4 | 86 | 0 | 74 | 35 | 0 |
| 12 | H5 | 43 | 0 | 37 | 21 | 0 |
| 12 | H6 | 86 | 0 | 74 | 25 | 0 |
| 12 | H7 | 43 | 0 | 37 | 11 | 0 |
| 12 | H8 | 86 | 0 | 74 | 34 | 0 |
| 12 | H9 | 86 | 0 | 72 | 88 | 0 |
| 12 | HA | 86 | 0 | 73 | 88 | 0 |
| 12 | I1 | 43 | 0 | 37 | 8 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 12 | I2 | 43 | 0 | 37 | 8 | 0 |
| 12 | I3 | 43 | 0 | 37 | 8 | 0 |
| 12 | I4 | 43 | 0 | 37 | 8 | 0 |
| 12 | I5 | 43 | 0 | 37 | 8 | 0 |
| 12 | I6 | 43 | 0 | 37 | 8 | 0 |
| 12 | I7 | 43 | 0 | 37 | 3 | 0 |
| 12 | I8 | 43 | 0 | 37 | 8 | 0 |
| 12 | I9 | 43 | 0 | 37 | 8 | 0 |
| 12 | IA | 43 | 0 | 37 | 8 | 0 |
| 12 | J1 | 43 | 0 | 37 | 7 | 0 |
| 12 | J2 | 86 | 0 | 74 | 18 | 0 |
| 12 | J3 | 86 | 0 | 74 | 51 | 0 |
| 12 | J4 | 86 | 0 | 74 | 18 | 0 |
| 12 | J5 | 43 | 0 | 37 | 12 | 0 |
| 12 | J6 | 86 | 0 | 74 | 17 | 0 |
| 12 | J7 | 43 | 0 | 35 | 23 | 0 |
| 12 | J8 | 86 | 0 | 74 | 20 | 0 |
| 12 | J9 | 86 | 0 | 73 | 48 | 0 |
| 12 | JA | 86 | 0 | 73 | 47 | 0 |
| 12 | K1 | 43 | 0 | 37 | 8 | 0 |
| 12 | K2 | 43 | 0 | 37 | 8 | 0 |
| 12 | K3 | 43 | 0 | 37 | 8 | 0 |
| 12 | K4 | 43 | 0 | 37 | 8 | 0 |
| 12 | K5 | 43 | 0 | 37 | 28 | 0 |
| 12 | K6 | 43 | 0 | 37 | 8 | 0 |
| 12 | K7 | 43 | 0 | 37 | 14 | 0 |
| 12 | K8 | 43 | 0 | 37 | 8 | 0 |
| 12 | K9 | 43 | 0 | 37 | 8 | 0 |
| 12 | KA | 43 | 0 | 37 | 8 | 0 |
| 12 | L1 | 43 | 0 | 37 | 9 | 0 |
| 12 | L2 | 86 | 0 | 74 | 18 | 0 |
| 12 | L3 | 86 | 0 | 71 | 30 | 0 |
| 12 | L4 | 86 | 0 | 74 | 30 | 0 |
| 12 | L5 | 43 | 0 | 37 | 14 | 0 |
| 12 | L6 | 86 | 0 | 74 | 18 | 0 |
| 12 | L7 | 43 | 0 | 37 | 13 | 0 |
| 12 | L8 | 43 | 0 | 37 | 10 | 0 |
| 12 | L9 | 86 | 0 | 74 | 35 | 0 |
| 12 | LA | 86 | 0 | 74 | 33 | 0 |
| 12 | M4 | 43 | 0 | 37 | 76 | 0 |
| 12 | M5 | 43 | 0 | 37 | 4 | 0 |
| 12 | M7 | 43 | 0 | 37 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 12 | M8 | 86 | 0 | 72 | 181 | 0 |
| 12 | N2 | 43 | 0 | 37 | 13 | 0 |
| 12 | N4 | 43 | 0 | 37 | 8 | 0 |
| 12 | N5 | 43 | 0 | 37 | 14 | 0 |
| 12 | N6 | 43 | 0 | 37 | 13 | 0 |
| 12 | N7 | 43 | 0 | 37 | 10 | 0 |
| 12 | N8 | 43 | 0 | 37 | 12 | 0 |
| 12 | O1 | 43 | 0 | 37 | 11 | 0 |
| 12 | O3 | 43 | 0 | 37 | 8 | 0 |
| 12 | O4 | 86 | 0 | 74 | 32 | 0 |
| 12 | O5 | 43 | 0 | 37 | 4 | 0 |
| 12 | O7 | 43 | 0 | 37 | 3 | 0 |
| 12 | O8 | 86 | 0 | 74 | 27 | 0 |
| 12 | O9 | 43 | 0 | 37 | 8 | 0 |
| 12 | OA | 43 | 0 | 37 | 8 | 0 |
| 12 | P1 | 86 | 0 | 74 | 25 | 0 |
| 12 | P3 | 86 | 0 | 74 | 25 | 0 |
| 12 | P4 | 43 | 0 | 37 | 8 | 0 |
| 12 | P5 | 43 | 0 | 37 | 18 | 0 |
| 12 | P7 | 43 | 0 | 37 | 13 | 0 |
| 12 | P8 | 43 | 0 | 37 | 8 | 0 |
| 12 | P9 | 86 | 0 | 74 | 20 | 0 |
| 12 | PA | 86 | 0 | 74 | 19 | 0 |
| 12 | Q1 | 43 | 0 | 37 | 8 | 0 |
| 12 | Q3 | 43 | 0 | 37 | 8 | 0 |
| 12 | Q4 | 43 | 0 | 37 | 6 | 0 |
| 12 | Q5 | 43 | 0 | 37 | 15 | 0 |
| 12 | Q7 | 43 | 0 | 37 | 14 | 0 |
| 12 | Q8 | 43 | 0 | 37 | 6 | 0 |
| 12 | Q9 | 43 | 0 | 37 | 8 | 0 |
| 12 | QA | 43 | 0 | 37 | 49 | 0 |
| 12 | R1 | 86 | 0 | 74 | 33 | 0 |
| 12 | R3 | 86 | 0 | 74 | 32 | 0 |
| 12 | R4 | 43 | 0 | 37 | 8 | 0 |
| 12 | R5 | 43 | 0 | 37 | 15 | 0 |
| 12 | R7 | 43 | 0 | 37 | 9 | 0 |
| 12 | R8 | 43 | 0 | 37 | 8 | 0 |
| 12 | R9 | 86 | 0 | 74 | 25 | 0 |
| 12 | RA | 86 | 0 | 74 | 27 | 0 |
| 12 | S1 | 43 | 0 | 37 | 8 | 0 |
| 12 | S3 | 43 | 0 | 37 | 9 | 0 |
| 12 | S4 | 86 | 0 | 75 | 39 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 12 | S5 | 43 | 0 | 37 | 3 | 0 |
| 12 | S7 | 43 | 0 | 37 | 4 | 0 |
| 12 | S8 | 43 | 0 | 37 | 6 | 0 |
| 12 | S9 | 43 | 0 | 37 | 8 | 0 |
| 12 | SA | 43 | 0 | 37 | 8 | 0 |
| 12 | T1 | 86 | 0 | 74 | 28 | 0 |
| 12 | T3 | 86 | 0 | 74 | 28 | 0 |
| 12 | T4 | 43 | 0 | 37 | 8 | 0 |
| 12 | T5 | 43 | 0 | 37 | 19 | 0 |
| 12 | T7 | 43 | 0 | 37 | 16 | 0 |
| 12 | T8 | 43 | 0 | 37 | 8 | 0 |
| 12 | T9 | 86 | 0 | 74 | 52 | 0 |
| 12 | TA | 86 | 0 | 74 | 53 | 0 |
| 12 | U1 | 43 | 0 | 37 | 8 | 0 |
| 12 | U3 | 43 | 0 | 37 | 8 | 0 |
| 12 | U4 | 86 | 0 | 74 | 19 | 0 |
| 12 | U5 | 43 | 0 | 37 | 3 | 0 |
| 12 | U7 | 43 | 0 | 37 | 3 | 0 |
| 12 | U8 | 86 | 0 | 74 | 21 | 0 |
| 12 | U9 | 43 | 0 | 37 | 8 | 0 |
| 12 | UA | 43 | 0 | 37 | 9 | 0 |
| 12 | V1 | 86 | 0 | 74 | 13 | 0 |
| 12 | V3 | 86 | 0 | 74 | 13 | 0 |
| 12 | V4 | 43 | 0 | 37 | 8 | 0 |
| 12 | V5 | 43 | 0 | 37 | 18 | 0 |
| 12 | V7 | 43 | 0 | 37 | 10 | 0 |
| 12 | V8 | 43 | 0 | 37 | 8 | 0 |
| 12 | V9 | 86 | 0 | 74 | 48 | 0 |
| 12 | VA | 86 | 0 | 74 | 60 | 0 |
| 12 | W1 | 43 | 0 | 37 | 8 | 0 |
| 12 | W3 | 43 | 0 | 37 | 8 | 0 |
| 12 | W4 | 86 | 0 | 74 | 14 | 0 |
| 12 | W5 | 43 | 0 | 37 | 14 | 0 |
| 12 | W7 | 43 | 0 | 37 | 14 | 0 |
| 12 | W8 | 86 | 0 | 74 | 15 | 0 |
| 12 | W9 | 43 | 0 | 37 | 8 | 0 |
| 12 | WA | 43 | 0 | 37 | 8 | 0 |
| 12 | X1 | 86 | 0 | 74 | 23 | 0 |
| 12 | X3 | 86 | 0 | 74 | 26 | 0 |
| 12 | X4 | 43 | 0 | 37 | 8 | 0 |
| 12 | X5 | 43 | 0 | 37 | 16 | 0 |
| 12 | X7 | 43 | 0 | 37 | 8 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 12 | X8 | 43 | 0 | 37 | 8 | 0 |
| 12 | X9 | 86 | 0 | 74 | 15 | 0 |
| 12 | XA | 86 | 0 | 74 | 13 | 0 |
| 12 | Y1 | 43 | 0 | 37 | 8 | 0 |
| 12 | Y3 | 43 | 0 | 37 | 8 | 0 |
| 12 | Y4 | 43 | 0 | 37 | 8 | 0 |
| 12 | Y5 | 43 | 0 | 37 | 3 | 0 |
| 12 | Y7 | 43 | 0 | 37 | 3 | 0 |
| 12 | Y8 | 43 | 0 | 37 | 10 | 0 |
| 12 | Y9 | 43 | 0 | 37 | 8 | 0 |
| 12 | YA | 43 | 0 | 37 | 8 | 0 |
| 12 | Z | 43 | 0 | 37 | 8 | 0 |
| 12 | Z1 | 86 | 0 | 74 | 37 | 0 |
| 12 | Z3 | 86 | 0 | 74 | 38 | 0 |
| 12 | Z4 | 43 | 0 | 38 | 104 | 0 |
| 12 | Z5 | 43 | 0 | 37 | 15 | 0 |
| 12 | Z8 | 43 | 0 | 37 | 163 | 0 |
| 12 | Z9 | 86 | 0 | 74 | 20 | 0 |
| 12 | ZA | 86 | 0 | 74 | 21 | 0 |
| 12 | a5 | 43 | 0 | 37 | 8 | 0 |
| 12 | a7 | 43 | 0 | 37 | 3 | 0 |
| 12 | a9 | 43 | 0 | 36 | 106 | 0 |
| 12 | aA | 86 | 0 | 71 | 72 | 0 |
| 12 | b5 | 43 | 0 | 37 | 7 | 0 |
| 12 | b7 | 43 | 0 | 37 | 18 | 0 |
| 12 | c5 | 43 | 0 | 37 | 3 | 0 |
| 12 | c7 | 43 | 0 | 37 | 10 | 0 |
| 12 | d5 | 43 | 0 | 37 | 16 | 0 |
| 12 | d7 | 43 | 0 | 37 | 19 | 0 |
| 12 | e5 | 43 | 0 | 37 | 8 | 0 |
| 12 | e7 | 43 | 0 | 37 | 3 | 0 |
| 12 | f5 | 43 | 0 | 37 | 6 | 0 |
| 12 | f7 | 43 | 0 | 35 | 16 | 0 |
| 12 | g7 | 43 | 0 | 37 | 3 | 0 |
| 12 | h7 | 43 | 0 | 37 | 15 | 0 |
| 12 | i7 | 43 | 0 | 37 | 13 | 0 |
| 12 | j5 | 86 | 38 | 75 | 57 | 0 |
| 12 | j7 | 43 | 0 | 37 | 15 | 0 |
| 12 | k5 | 172 | 38 | 147 | 119 | 0 |
| 12 | k7 | 43 | 0 | 37 | 3 | 0 |
| 12 | m7 | 43 | 0 | 37 | 4 | 0 |
| 12 | o7 | 43 | 0 | 35 | 18 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 12 | p7 | 43 | 0 | 37 | 16 | 0 |
| 12 | q7 | 43 | 0 | 37 | 3 | 0 |
| 12 | r7 | 43 | 0 | 37 | 17 | 0 |
| 12 | s7 | 43 | 0 | 37 | 3 | 0 |
| 12 | u7 | 43 | 0 | 35 | 19 | 0 |
| 12 | v7 | 43 | 0 | 37 | 22 | 0 |
| All | All | 382696 | 76 | 379888 | 26296 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (26296) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:73:TYR:HE1 | 10:k5:162:TRP:CZ2 | 1.10 | 1.70 |
| 10:k5:1152:TYR:CE2 | 8:G7:68:PRO:HG2 | 1.24 | 1.70 |
| 10:k5:1008:PHE:CE1 | 1:p7:87:TYR:CE2 | 1.76 | 1.68 |
| 10:j5:1008:PHE:CE1 | 1:v7:87:TYR:CE2 | 1.77 | 1.68 |
| 3:TA:32:LYS:HE3 | 2:X4:60:TYR:CD2 | 1.25 | 1.68 |
| 2:X8:60:TYR:CD2 | 3:T9:32:LYS:HE3 | 1.25 | 1.68 |
| 8:i7:47:ARG:HD3 | 1:j7:18:TYR:CE2 | 1.27 | 1.67 |
| 3:B3:82:CYS:SG | 12:B3:202:CYC:HAC2 | 1.26 | 1.65 |
| 8:i7:47:ARG:CD | 1:j7:18:TYR:CZ | 1.75 | 1.65 |
| 3:B4:120:LEU:CD1 | 4:M4:53:LEU:HB2 | 1.23 | 1.64 |
| 3:B4:116:THR:HB | 4:M4:56:MET:CB | 1.25 | 1.63 |
| 11:a9:275:THR:CA | 11:a9:278:LEU:HD11 | 1.25 | 1.63 |
| 11:aA:742:GLN:HG2 | 3:L1:88:ILE:CD1 | 1.19 | 1.63 |
| 3:Q8:102:ALA:CB | 3:Q8:166:LYS:HE2 | 1.26 | 1.63 |
| 2:SA:35:THR:HG23 | 2:X4:74:TYR:CE1 | 1.29 | 1.62 |
| 3:U8:115:GLU:CB | 4:M8:74:LEU:HD12 | 1.29 | 1.62 |
| 8:c7:20:PRO:CG | 8:m7:155:TYR:HB2 | 1.16 | 1.62 |
| 3:F2:82:CYS:SG | 12:F2:201:CYC:HAC2 | 1.39 | 1.62 |
| 2:I9:37:SER:C | 2:I9:97:LEU:HD11 | 1.24 | 1.62 |
| 12:B1:202:CYC:CBA | 11:aA:684:ASN:HB2 | 1.17 | 1.61 |
| 2:N4:111:ALA:CB | 5:Z4:34:LEU:HG | 1.16 | 1.61 |
| 3:B4:85:ASP:CB | 12:B4:202:CYC:HAC1 | 1.25 | 1.61 |
| 2:X8:74:TYR:CE1 | 2:S9:35:THR:HG23 | 1.29 | 1.61 |
| 8:u7:27:LYS:CE | 1:v7:35:ALA:HB1 | 1.30 | 1.61 |
| 1:A:161:SER:HB2 | 1:R5:14:VAL:CB | 1.29 | 1.61 |
| 9:z5:6:LYS:HB3 | 9:z5:55:LYS:CB | 1.30 | 1.60 |
| 10:k5:889:LEU:CD2 | 12:D7:201:CYC:CBB | 1.74 | 1.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:u7:29:PHE:CE2 | 1:v7:31:PHE:HE1 | 1.07 | 1.60 |
| 8:u7:37:LEU:CD2 | 1:v7:24:LEU:HD22 | 1.20 | 1.60 |
| 4:M8:214:GLY:HA2 | 5:Z8:28:HIS:CD2 | 1.14 | 1.59 |
| 5:Z8:41:GLN:CB | 12:Z8:301:CYC:C2B | 1.81 | 1.59 |
| 8:o7:29:PHE:CE2 | 1:p7:31:PHE:HE1 | 1.07 | 1.59 |
| 12:J9:202:CYC:CBA | 11:a9:511:LYS:HA | 1.28 | 1.59 |
| 8:o7:37:LEU:CD2 | 1:p7:24:LEU:HD22 | 1.20 | 1.59 |
| 2:N8:112:GLY:CA | 5:Z8:34:LEU:H | 1.00 | 1.59 |
| 1:P5:114:GLU:CG | 10:k5:496:GLU:HG3 | 1.21 | 1.59 |
| 3:FA:153:CYS:SG | 12:F9:302:CYC:HAC1 | 1.36 | 1.59 |
| 3:U4:115:GLU:CB | 4:M4:74:LEU:HD12 | 1.25 | 1.59 |
| 8:Q7:13:ALA:CA | 9:z7:46:LYS:HZ3 | 1.02 | 1.59 |
| 1:A:73:TYR:CE1 | 10:k5:162:TRP:CZ2 | 1.82 | 1.58 |
| 12:JA:202:CYC:CBA | 11:aA:511:LYS:HA | 1.30 | 1.58 |
| 8:u7:29:PHE:CE2 | 1:v7:31:PHE:CE1 | 1.91 | 1.58 |
| 1:A:161:SER:HB2 | 1:R5:14:VAL:CG2 | 1.14 | 1.58 |
| 1:P5:114:GLU:HG2 | 10:k5:496:GLU:CD | 1.24 | 1.58 |
| 1:V5:114:GLU:HG2 | 10:j5:496:GLU:CG | 1.20 | 1.58 |
| 10:k5:934:ALA:CB | 1:D7:32:THR:HG21 | 1.19 | 1.58 |
| 5:Z8:38:GLU:HB2 | 12:Z8:301:CYC:CMB | 1.19 | 1.58 |
| 1:A:161:SER:CB | 1:R5:14:VAL:CG2 | 1.76 | 1.58 |
| 9:z5:6:LYS:CB | 9:z5:55:LYS:HB2 | 1.23 | 1.58 |
| 3:L9:14:LEU:HD21 | 11:a9:358:PRO:CB | 1.19 | 1.58 |
| 4:MA:274:VAL:HG13 | 3:VA:77:ARG:CD | 1.18 | 1.58 |
| 3:TA:32:LYS:CE | 2:X4:60:TYR:HD2 | 1.06 | 1.58 |
| 3:U8:108:ARG:HA | 4:M8:246:ALA:CB | 1.32 | 1.58 |
| 5:Z8:41:GLN:HG2 | 12:Z8:301:CYC:C3B | 1.18 | 1.58 |
| 2:X8:60:TYR:HD2 | 3:T9:32:LYS:CE | 1.06 | 1.57 |
| 5:Z8:22:LEU:HD22 | 5:Z8:26:LEU:CD1 | 1.34 | 1.57 |
| 12:J3:202:CYC:CBA | 11:a9:667:THR:HG22 | 1.19 | 1.57 |
| 12:B3:202:CYC:CBA | 11:a9:684:ASN:HB3 | 1.12 | 1.57 |
| 2:N4:111:ALA:C | 5:Z4:34:LEU:HB2 | 1.24 | 1.57 |
| 11:a9:275:THR:HA | 11:a9:278:LEU:CD1 | 1.31 | 1.57 |
| 3:FA:150:ARG:HG2 | 3:F9:150:ARG:CG | 1.18 | 1.57 |
| 3:LA:14:LEU:HD21 | 11:aA:358:PRO:CB | 1.20 | 1.57 |
| 4:M9:274:VAL:CG1 | 3:V9:77:ARG:HD3 | 1.12 | 1.57 |
| 11:aA:667:THR:CG2 | 12:aA:901:CYC:HBA2 | 1.23 | 1.57 |
| 4:M4:27:HIS:CE1 | 4:M4:34:ASP:CA | 1.76 | 1.57 |
| 8:i7:25:ARG:CZ | 8:s7:6:LYS:HB3 | 1.10 | 1.57 |
| 12:M8:302:CYC:CMC | 3:S8:72:ASN:CG | 1.76 | 1.57 |
| 5:Z8:22:LEU:CD2 | 5:Z8:26:LEU:CD1 | 1.83 | 1.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:N3:22:LEU:CD2 | 5:N3:26:LEU:CD1 | 1.83 | 1.56 |
| 5:NA:22:LEU:HD22 | 5:NA:26:LEU:CD1 | 1.35 | 1.56 |
| 10:k5:934:ALA:CB | 1:D7:32:THR:CG2 | 1.79 | 1.56 |
| 3:H8:84:ARG:CD | 11:a9:131:TYR:CG | 1.88 | 1.56 |
| 3:B4:116:THR:HB | 4:M4:56:MET:CG | 1.11 | 1.56 |
| 1:V5:114:GLU:HG2 | 10:j5:496:GLU:CD | 1.30 | 1.56 |
| 11:aA:621:THR:HG22 | 3:J1:14:LEU:CD2 | 1.28 | 1.56 |
| 12:J3:202:CYC:HBA2 | 11:a9:667:THR:CG2 | 1.23 | 1.56 |
| 3:H4:84:ARG:CD | 11:aA:131:TYR:CG | 1.81 | 1.56 |
| 10:j5:1025:LEU:CD2 | 10:j5:1035:PHE:HB2 | 1.23 | 1.56 |
| 4:M8:127:SER:CA | 12:M8:302:CYC:CMA | 1.80 | 1.56 |
| 4:M8:217:VAL:CG2 | 5:Z8:30:PRO:HG3 | 1.11 | 1.56 |
| 11:a9:403:THR:HG22 | 11:a9:536:THR:CG2 | 1.33 | 1.56 |
| 1:Z:161:SER:HB2 | 1:X5:14:VAL:CG2 | 1.33 | 1.55 |
| 5:N9:22:LEU:CD2 | 5:N9:26:LEU:CD1 | 1.83 | 1.55 |
| 3:H4:84:ARG:HD3 | 11:aA:131:TYR:CD2 | 1.39 | 1.55 |
| 9:i5:6:LYS:HB3 | 9:i5:55:LYS:CB | 1.30 | 1.55 |
| 1:Z:73:TYR:HE1 | 10:j5:162:TRP:CZ2 | 1.20 | 1.55 |
| 8:o7:27:LYS:CE | 1:p7:35:ALA:HB1 | 1.30 | 1.55 |
| 3:U8:115:GLU:CB | 4:M8:74:LEU:CD1 | 1.82 | 1.55 |
| 11:aA:275:THR:CA | 11:aA:278:LEU:HD11 | 1.25 | 1.55 |
| 10:j5:1008:PHE:CZ | 1:v7:87:TYR:CE2 | 1.95 | 1.55 |
| 3:Y8:89:ILE:HA | 3:Y8:92:TYR:CE2 | 1.03 | 1.55 |
| 5:Z8:29:HIS:CE1 | 5:Z8:31:TRP:HB2 | 1.36 | 1.55 |
| 11:aA:798:SER:CB | 11:aA:800:THR:HG23 | 1.32 | 1.55 |
| 4:M8:87:ILE:CD1 | 3:Y8:77:ARG:HG3 | 1.14 | 1.55 |
| 11:a9:710:THR:HG22 | 11:a9:807:GLN:CG | 1.35 | 1.55 |
| 11:aA:667:THR:HG22 | 12:aA:901:CYC:CBA | 1.18 | 1.55 |
| 3:D4:108:ARG:CD | 11:aA:107:ARG:HH12 | 1.17 | 1.54 |
| 5:N3:22:LEU:HD22 | 5:N3:26:LEU:CD1 | 1.35 | 1.54 |
| 3:L4:68:ARG:CB | 11:aA:82:GLN:H | 1.19 | 1.54 |
| 3:Q8:120:LEU:HD11 | 3:Q8:122:THR:CB | 1.29 | 1.54 |
| 1:f7:67:ARG:CD | 11:aA:311:LEU:HD22 | 1.36 | 1.54 |
| 8:u7:23:LEU:CB | 1:v7:38:VAL:HG13 | 1.35 | 1.54 |
| 5:Z8:41:GLN:HB3 | 12:Z8:301:CYC:C1B | 1.12 | 1.54 |
| 3:J3:14:LEU:CD2 | 11:a9:621:THR:HG22 | 1.28 | 1.54 |
| 12:B4:202:CYC:HBB2 | 4:M4:61:ASN:CB | 1.37 | 1.54 |
| 9:i5:6:LYS:CB | 9:i5:55:LYS:HB2 | 1.23 | 1.54 |
| 10:k5:820:HIS:CE1 | 10:k5:859:ILE:HD11 | 1.42 | 1.54 |
| 8:c7:15:ALA:HA | 1:d7:90:ARG:CZ | 1.37 | 1.54 |
| 4:M9:274:VAL:HG13 | 3:V9:77:ARG:CD | 1.17 | 1.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:Z8:41:GLN:CD | 12:Z8:301:CYC:HBB2 | 1.22 | 1.54 |
| 1:V5:114:GLU:CG | 10:j5:496:GLU:HG3 | 1.38 | 1.54 |
| 10:k5:966:SER:HA | 1:p7:14:VAL:CG1 | 1.11 | 1.54 |
| 8:i7:42:THR:HG21 | 8:i7:141:LEU:CD2 | 1.37 | 1.54 |
| 3:D8:108:ARG:CD | 11:a9:107:ARG:HH12 | 1.17 | 1.54 |
| 4:M4:104:ALA:CB | 2:P4:14:SER:CA | 1.76 | 1.54 |
| 3:Q4:102:ALA:CB | 3:Q4:166:LYS:HE2 | 1.37 | 1.54 |
| 5:Z4:41:GLN:HB2 | 12:Z4:301:CYC:C1B | 1.34 | 1.54 |
| 1:V5:83:ARG:NH1 | 10:j5:649:PHE:CE2 | 1.75 | 1.54 |
| 10:k5:175:ASP:HB2 | 10:k5:176:PRO:CD | 1.28 | 1.54 |
| 10:k5:1025:LEU:CD2 | 10:k5:1035:PHE:HB2 | 1.23 | 1.54 |
| 3:L8:68:ARG:CB | 11:a9:82:GLN:H | 1.21 | 1.54 |
| 4:M4:27:HIS:CE1 | 4:M4:35:THR:N | 1.75 | 1.53 |
| 5:NA:54:LEU:HD22 | 3:TA:84:ARG:CZ | 1.37 | 1.53 |
| 2:G3:107:ASP:HA | 3:L3:77:ARG:CZ | 1.37 | 1.53 |
| 3:Y4:89:ILE:HA | 3:Y4:92:TYR:CE2 | 1.03 | 1.53 |
| 3:Q8:89:ILE:HA | 3:Q8:92:TYR:CE2 | 1.05 | 1.53 |
| 3:O4:107:ASP:CG | 5:Z4:66:ARG:HD2 | 1.30 | 1.53 |
| 11:aA:275:THR:HA | 11:aA:278:LEU:CD1 | 1.31 | 1.53 |
| 2:K3:112:GLY:CA | 11:a9:670:LEU:HD22 | 1.36 | 1.53 |
| 8:a7:48:GLU:HA | 11:a9:318:TRP:CH2 | 1.44 | 1.53 |
| 11:aA:710:THR:HG22 | 11:aA:807:GLN:CG | 1.35 | 1.53 |
| 10:k5:966:SER:CA | 1:p7:14:VAL:CG1 | 1.77 | 1.52 |
| 11:a9:312:ASP:HB2 | 11:a9:315:LEU:CB | 1.37 | 1.52 |
| 11:aA:403:THR:HG22 | 11:aA:536:THR:CG2 | 1.33 | 1.52 |
| 1:B7:136:VAL:HG13 | 11:a9:563:PHE:CZ | 1.44 | 1.52 |
| 3:F4:113:LEU:CB | 4:M4:5:THR:HG23 | 1.37 | 1.52 |
| 3:H4:84:ARG:HD3 | 11:aA:131:TYR:CG | 1.02 | 1.52 |
| 8:c7:42:THR:HG21 | 8:c7:141:LEU:CD2 | 1.37 | 1.52 |
| 4:M8:87:ILE:HD13 | 3:Y8:77:ARG:CG | 1.38 | 1.52 |
| 5:N9:54:LEU:HD22 | 3:T9:84:ARG:CZ | 1.37 | 1.52 |
| 11:a9:75:ALA:CB | 11:a9:81:ASP:CG | 1.81 | 1.52 |
| 4:M4:144:ARG:HE | 4:M4:204:ILE:CG2 | 1.20 | 1.52 |
| 10:j5:1008:PHE:CE1 | 1:v7:87:TYR:CZ | 1.97 | 1.52 |
| 3:B8:82:CYS:HA | 12:B8:202:CYC:C1C | 1.39 | 1.52 |
| 3:H8:84:ARG:HD2 | 11:a9:131:TYR:CG | 1.03 | 1.52 |
| 4:M8:104:ALA:CB | 2:P8:14:SER:HB3 | 1.06 | 1.52 |
| 2:G1:107:ASP:HA | 3:L1:77:ARG:CZ | 1.37 | 1.52 |
| 6:M6:53:LEU:HD23 | 8:c7:80:LEU:CD2 | 1.37 | 1.52 |
| 12:B8:202:CYC:HBB2 | 4:M8:61:ASN:CB | 1.37 | 1.52 |
| 11:a9:280:ASP:HB3 | 11:a9:281:PRO:CD | 1.37 | 1.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:aA:742:GLN:CG | 3:L1:88:ILE:HD11 | 1.06 | 1.52 |
| 1:T5:110:ASN:HD21 | 10:j5:692:LEU:CB | 1.22 | 1.51 |
| 8:g7:63:PRO:CD | 11:aA:336:ILE:CG2 | 1.83 | 1.51 |
| 4:MA:274:VAL:CA | 3:VA:77:ARG:HG2 | 1.08 | 1.51 |
| 2:QA:119:THR:CB | 3:TA:83:LEU:HD13 | 1.37 | 1.51 |
| 1:Z5:28:LYS:NZ | 1:t7:143:PRO:CG | 1.70 | 1.51 |
| 11:a9:588:VAL:C | 11:a9:590:PRO:HD3 | 1.34 | 1.51 |
| 4:M1:158:PHE:CD1 | 3:Z1:108:ARG:NH1 | 1.74 | 1.51 |
| 5:N1:22:LEU:HD22 | 5:N1:26:LEU:CD1 | 1.35 | 1.51 |
| 10:j5:820:HIS:CE1 | 10:j5:859:ILE:CD1 | 1.93 | 1.51 |
| 4:M9:274:VAL:CA | 3:V9:77:ARG:HG2 | 1.04 | 1.51 |
| 4:M4:27:HIS:CE1 | 4:M4:34:ASP:HA | 1.00 | 1.51 |
| 4:M4:27:HIS:NE2 | 4:M4:34:ASP:HA | 1.23 | 1.51 |
| 4:M4:104:ALA:HB1 | 2:P4:14:SER:CA | 1.03 | 1.51 |
| 8:o7:29:PHE:CE2 | 1:p7:31:PHE:CE1 | 1.91 | 1.51 |
| 3:H8:119:ALA:CB | 11:a9:266:ASN:HD22 | 1.22 | 1.51 |
| 8:a7:63:PRO:CD | 11:a9:336:ILE:CG2 | 1.86 | 1.51 |
| 3:Z3:108:ARG:NH1 | 4:M3:158:PHE:CD1 | 1.74 | 1.50 |
| 1:N5:53:LYS:NZ | 8:O5:120:GLN:HE21 | 1.01 | 1.50 |
| 10:j5:820:HIS:CE1 | 10:j5:859:ILE:HD11 | 1.42 | 1.50 |
| 12:M8:302:CYC:C1C | 3:S8:78:ARG:CD | 1.85 | 1.50 |
| 11:a9:75:ALA:HB1 | 11:a9:81:ASP:CG | 1.09 | 1.50 |
| 1:A:158:SER:CB | 1:R5:11:ASN:ND2 | 1.71 | 1.50 |
| 2:IA:37:SER:C | 2:IA:97:LEU:HD11 | 1.24 | 1.50 |
| 3:F4:113:LEU:HB2 | 4:M4:5:THR:CG2 | 1.37 | 1.50 |
| 3:O4:119:ALA:HB1 | 5:Z4:72:GLU:CG | 1.33 | 1.50 |
| 4:M8:217:VAL:CG2 | 5:Z8:30:PRO:CG | 1.84 | 1.50 |
| 11:aA:312:ASP:HB2 | 11:aA:315:LEU:CB | 1.37 | 1.50 |
| 11:aA:798:SER:CB | 11:aA:800:THR:CG2 | 1.87 | 1.50 |
| 3:J3:77:ARG:CZ | 2:K3:107:ASP:HA | 1.37 | 1.50 |
| 2:X8:74:TYR:CZ | 2:S9:35:THR:HG23 | 1.47 | 1.50 |
| 11:aA:312:ASP:CB | 11:aA:315:LEU:HB3 | 1.04 | 1.50 |
| 5:N1:22:LEU:CD2 | 5:N1:26:LEU:HD11 | 1.02 | 1.50 |
| 6:M6:117:MET:CE | 3:H6:77:ARG:HH11 | 1.21 | 1.50 |
| 10:j5:934:ALA:CB | 1:J7:32:THR:HG21 | 1.36 | 1.50 |
| 10:j5:978:LEU:CD2 | 1:v7:107:ARG:NH2 | 1.70 | 1.50 |
| 10:k5:820:HIS:CE1 | 10:k5:859:ILE:CD1 | 1.93 | 1.50 |
| 8:Q7:25:ARG:CB | 8:C7:25:ARG:HH21 | 1.22 | 1.50 |
| 8:o7:23:LEU:CB | 1:p7:38:VAL:HG13 | 1.35 | 1.50 |
| 2:N8:115:GLU:CG | 5:Z8:32:PRO:HG2 | 1.04 | 1.50 |
| 11:aA:75:ALA:HB1 | 11:aA:81:ASP:CG | 1.09 | 1.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:131:GLN:CG | 1:R5:17:LYS:NZ | 1.70 | 1.50 |
| 1:Z:161:SER:CB | 1:X5:14:VAL:CG2 | 1.90 | 1.50 |
| 6:M2:28:ASN:HB3 | 8:O5:80:LEU:CD2 | 1.38 | 1.50 |
| 5:NA:22:LEU:CD2 | 5:NA:26:LEU:HD11 | 1.02 | 1.49 |
| 3:F4:84:ARG:CD | 11:aA:139:ILE:HG22 | 1.42 | 1.49 |
| 8:U5:83:ARG:HB3 | 6:M6:26:PHE:CE1 | 1.48 | 1.49 |
| 10:j5:1050:PHE:CE2 | 1:r7:107:ARG:NH2 | 1.79 | 1.49 |
| 5:Z8:37:HIS:NE2 | 12:Z8:301:CYC:C3A | 1.74 | 1.49 |
| 3:LA:14:LEU:CG | 11:aA:358:PRO:HB3 | 1.40 | 1.49 |
| 3:H2:77:ARG:HH11 | 6:M2:117:MET:CE | 1.21 | 1.49 |
| 5:N9:22:LEU:HD22 | 5:N9:26:LEU:CD1 | 1.35 | 1.49 |
| 11:aA:75:ALA:CB | 11:aA:81:ASP:CG | 1.81 | 1.49 |
| 3:H4:119:ALA:CB | 11:aA:266:ASN:HD22 | 1.24 | 1.49 |
| 10:k5:650:ASP:CB | 10:k5:650:ASP:CG | 1.86 | 1.49 |
| 3:B8:81:ALA:CB | 12:B8:202:CYC:CMD | 1.84 | 1.49 |
| 2:N8:115:GLU:CB | 5:Z8:32:PRO:HG2 | 1.38 | 1.49 |
| 3:Y8:89:ILE:CA | 3:Y8:92:TYR:CE2 | 1.94 | 1.49 |
| 11:aA:670:LEU:HD22 | 2:K1:112:GLY:CA | 1.36 | 1.49 |
| 4:M4:104:ALA:HB1 | 2:P4:14:SER:CB | 1.04 | 1.49 |
| 10:j5:650:ASP:CG | 10:j5:650:ASP:CB | 1.86 | 1.49 |
| 1:d7:87:TYR:OH | 9:x7:38:PHE:CE2 | 1.65 | 1.49 |
| 3:U8:108:ARG:CA | 4:M8:246:ALA:HB2 | 1.37 | 1.49 |
| 3:H8:84:ARG:HD2 | 11:a9:131:TYR:CD1 | 1.47 | 1.49 |
| 5:Z8:41:GLN:CG | 12:Z8:301:CYC:C3B | 1.90 | 1.49 |
| 2:E9:2:LYS:NZ | 2:I9:17:ARG:HH12 | 1.08 | 1.49 |
| 5:N9:22:LEU:CD2 | 5:N9:26:LEU:HD11 | 1.02 | 1.49 |
| 3:B4:120:LEU:HD11 | 4:M4:53:LEU:CA | 1.42 | 1.48 |
| 1:T5:83:ARG:NH1 | 10:j5:483:PHE:CZ | 1.75 | 1.48 |
| 8:c7:42:THR:CG2 | 8:c7:141:LEU:HD23 | 1.44 | 1.48 |
| 4:M4:104:ALA:CB | 2:P4:14:SER:CB | 1.84 | 1.48 |
| 3:Y4:89:ILE:CA | 3:Y4:92:TYR:CE2 | 1.94 | 1.48 |
| 1:f5:18:TYR:CD1 | 10:j5:165:ARG:HD3 | 1.48 | 1.48 |
| 8:o7:23:LEU:CG | 1:p7:38:VAL:HG13 | 1.44 | 1.48 |
| 3:FA:150:ARG:CG | 3:F9:150:ARG:HG2 | 1.01 | 1.48 |
| 8:S7:49:ARG:HD2 | 11:aA:550:PHE:CE1 | 1.45 | 1.48 |
| 3:L9:14:LEU:CG | 11:a9:358:PRO:HB3 | 1.39 | 1.48 |
| 10:k5:1146:THR:HB | 1:p7:77:ARG:NH2 | 1.28 | 1.48 |
| 3:H8:84:ARG:HB3 | 11:a9:131:TYR:CE1 | 1.48 | 1.48 |
| 2:K9:15:GLN:CA | 11:a9:393:ARG:HH11 | 1.24 | 1.48 |
| 1:Z:73:TYR:CE1 | 10:j5:162:TRP:CZ2 | 1.99 | 1.48 |
| 4:MA:274:VAL:CG1 | 3:VA:77:ARG:HD3 | 1.01 | 1.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:T5:53:LYS:NZ | 8:U5:120:GLN:HE21 | 1.01 | 1.48 |
| 1:Z7:67:ARG:CD | 11:a9:311:LEU:HD22 | 1.40 | 1.48 |
| 8:a7:63:PRO:HD2 | 11:a9:336:ILE:CG2 | 1.01 | 1.48 |
| 11:a9:312:ASP:CB | 11:a9:315:LEU:HB3 | 1.04 | 1.48 |
| 5:N3:22:LEU:CD2 | 5:N3:26:LEU:HD11 | 1.02 | 1.47 |
| 8:u7:23:LEU:HB3 | 1:v7:38:VAL:CG1 | 1.02 | 1.47 |
| 5:N1:22:LEU:CD2 | 5:N1:26:LEU:CD1 | 1.83 | 1.47 |
| 2:SA:35:THR:HG23 | 2:X4:74:TYR:CZ | 1.47 | 1.47 |
| 3:O4:119:ALA:CB | 5:Z4:72:GLU:HG3 | 1.40 | 1.47 |
| 3:F8:84:ARG:CD | 11:a9:139:ILE:HG22 | 1.43 | 1.47 |
| 4:M8:214:GLY:CA | 5:Z8:28:HIS:NE2 | 1.76 | 1.47 |
| 4:M9:263:PRO:HB2 | 3:V9:119:ALA:CB | 1.44 | 1.47 |
| 3:B4:116:THR:CB | 4:M4:56:MET:CB | 1.91 | 1.47 |
| 3:U4:112:GLY:CA | 4:M4:74:LEU:HD21 | 1.42 | 1.47 |
| 10:k5:284:PRO:CG | 10:k5:326:GLY:HA3 | 1.15 | 1.47 |
| 8:q7:76:LYS:NZ | 11:aA:605:PRO:HB3 | 1.28 | 1.47 |
| 11:a9:283:GLN:HB3 | 11:a9:284:PRO:CD | 1.33 | 1.47 |
| 1:d5:28:LYS:NZ | 1:n7:143:PRO:CB | 1.76 | 1.47 |
| 1:Z5:28:LYS:NZ | 1:t7:143:PRO:CB | 1.78 | 1.47 |
| 8:g7:63:PRO:HD2 | 11:aA:336:ILE:CG2 | 1.01 | 1.47 |
| 3:B4:86:MET:N | 12:B4:202:CYC:HBC1 | 1.16 | 1.47 |
| 1:Z5:28:LYS:CD | 1:t7:143:PRO:HG3 | 1.42 | 1.47 |
| 3:J9:119:ALA:O | 11:a9:365:LYS:CE | 1.63 | 1.47 |
| 11:aA:588:VAL:C | 11:aA:590:PRO:HD3 | 1.34 | 1.47 |
| 10:k5:1025:LEU:HD21 | 10:k5:1035:PHE:CB | 1.42 | 1.46 |
| 8:i7:42:THR:CG2 | 8:i7:141:LEU:HD23 | 1.44 | 1.46 |
| 4:MA:29:PRO:HD3 | 11:aA:378:GLU:CD | 1.41 | 1.46 |
| 2:N4:111:ALA:C | 5:Z4:34:LEU:CB | 1.88 | 1.46 |
| 3:O8:107:ASP:CB | 5:Z8:66:ARG:HB3 | 1.43 | 1.46 |
| 5:Z8:41:GLN:HB3 | 12:Z8:301:CYC:C2B | 1.33 | 1.46 |
| 11:a9:55:ASP:CB | 11:a9:612:TYR:HB2 | 1.31 | 1.46 |
| 11:aA:280:ASP:HB3 | 11:aA:281:PRO:CD | 1.37 | 1.46 |
| 3:B1:82:CYS:SG | 12:B1:202:CYC:CAC | 2.03 | 1.46 |
| 3:F4:108:ARG:NE | 4:M4:9:GLN:CG | 1.74 | 1.46 |
| 4:M4:228:SER:HB2 | 2:X4:16:GLY:CA | 1.44 | 1.46 |
| 1:P5:114:GLU:HG2 | 10:k5:496:GLU:CG | 1.00 | 1.46 |
| 8:g7:48:GLU:HA | 11:aA:318:TRP:CH2 | 1.47 | 1.46 |
| 2:P8:18:PHE:N | 3:Q8:91:ARG:NH2 | 1.60 | 1.46 |
| 4:MA:274:VAL:HA | 3:VA:77:ARG:CG | 1.01 | 1.46 |
| 12:QA:201:CYC:HBB2 | 3:TA:75:PRO:CB | 1.45 | 1.46 |
| 1:d7:87:TYR:OH | 9:x7:38:PHE:CZ | 1.68 | 1.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:H4:84:ARG:HB3 | 11:aA:131:TYR:CE1 | 1.48 | 1.46 |
| 10:j5:1025:LEU:HD21 | 10:j5:1035:PHE:CB | 1.42 | 1.46 |
| 10:k5:931:VAL:HG22 | 1:D7:29:ALA:C | 1.36 | 1.46 |
| 4:M9:274:VAL:HA | 3:V9:77:ARG:CG | 1.00 | 1.46 |
| 3:LA:14:LEU:HD11 | 11:aA:358:PRO:CG | 1.44 | 1.45 |
| 1:X5:50:THR:HG21 | 8:a5:49:ARG:CZ | 1.42 | 1.45 |
| 10:k5:1008:PHE:HE1 | 1:p7:87:TYR:CE2 | 1.18 | 1.45 |
| 3:H4:84:ARG:HD3 | 11:aA:131:TYR:CD1 | 1.48 | 1.45 |
| 8:o7:23:LEU:HB3 | 1:p7:38:VAL:CG1 | 1.02 | 1.45 |
| 5:Z8:22:LEU:CD2 | 5:Z8:26:LEU:HD11 | 1.02 | 1.45 |
| 3:J3:84:ARG:CD | 11:a9:668:TYR:CD1 | 1.74 | 1.45 |
| 3:F4:115:GLU:CD | 4:M4:3:VAL:HG22 | 1.37 | 1.45 |
| 3:L4:68:ARG:HH11 | 11:aA:81:ASP:N | 1.10 | 1.45 |
| 4:M4:87:ILE:CD1 | 3:Y4:77:ARG:HG3 | 1.44 | 1.45 |
| 4:M4:104:ALA:CB | 2:P4:14:SER:N | 1.76 | 1.45 |
| 5:Z4:41:GLN:HB2 | 12:Z4:301:CYC:C2B | 1.47 | 1.45 |
| 5:Z8:29:HIS:ND1 | 5:Z8:31:TRP:HB2 | 1.25 | 1.45 |
| 11:a9:280:ASP:CB | 11:a9:281:PRO:HD2 | 1.38 | 1.45 |
| 1:Z:158:SER:HB3 | 1:X5:11:ASN:ND2 | 1.16 | 1.45 |
| 5:NA:22:LEU:CD2 | 5:NA:26:LEU:CD1 | 1.83 | 1.45 |
| 3:U4:108:ARG:HA | 4:M4:246:ALA:CB | 1.46 | 1.45 |
| 3:H4:84:ARG:CD | 11:aA:131:TYR:CD2 | 1.94 | 1.45 |
| 11:aA:55:ASP:CB | 11:aA:612:TYR:HB2 | 1.31 | 1.45 |
| 3:FA:68:ARG:NH1 | 3:ZA:68:ARG:HH12 | 0.97 | 1.45 |
| 10:k5:284:PRO:HG2 | 10:k5:326:GLY:CA | 1.37 | 1.45 |
| 8:i7:25:ARG:NH2 | 8:s7:6:LYS:HB3 | 1.28 | 1.45 |
| 8:u7:23:LEU:CG | 1:v7:38:VAL:HG13 | 1.44 | 1.45 |
| 2:X8:67:THR:CB | 3:T9:28:THR:CG2 | 1.94 | 1.45 |
| 3:Q8:87:GLU:OE1 | 5:Z8:31:TRP:CH2 | 1.68 | 1.45 |
| 2:EA:2:LYS:NZ | 2:IA:17:ARG:HH12 | 1.08 | 1.44 |
| 10:k5:1152:TYR:CD2 | 8:G7:68:PRO:CG | 1.99 | 1.44 |
| 3:H8:84:ARG:HD2 | 11:a9:131:TYR:CD2 | 1.50 | 1.44 |
| 3:L9:14:LEU:CD2 | 11:a9:358:PRO:HB3 | 0.97 | 1.44 |
| 3:L9:14:LEU:HD11 | 11:a9:358:PRO:CG | 1.43 | 1.44 |
| 5:N9:66:ARG:NH1 | 3:T9:111:ASN:ND2 | 1.62 | 1.44 |
| 11:aA:742:GLN:CD | 3:L1:88:ILE:CG1 | 1.87 | 1.44 |
| 4:M4:104:ALA:CB | 2:P4:14:SER:HB3 | 1.43 | 1.44 |
| 8:U5:48:GLU:HB3 | 6:M6:34:ARG:NH2 | 1.19 | 1.44 |
| 10:j5:971:VAL:CG1 | 1:t7:76:ARG:HH12 | 1.26 | 1.44 |
| 8:i7:20:PRO:HD3 | 8:s7:155:TYR:CE1 | 1.49 | 1.44 |
| 3:B8:81:ALA:CB | 12:B8:202:CYC:HMD1 | 1.40 | 1.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:M9:53:LEU:HD13 | 12:F9:301:CYC:NB | 1.20 | 1.44 |
| 12:FA:301:CYC:NB | 4:MA:53:LEU:HD13 | 1.20 | 1.44 |
| 4:MA:263:PRO:HB2 | 3:VA:119:ALA:CB | 1.44 | 1.44 |
| 3:L4:71:GLY:N | 11:aA:82:GLN:HG2 | 1.32 | 1.44 |
| 8:U5:48:GLU:CB | 6:M6:34:ARG:HH22 | 1.28 | 1.44 |
| 3:Q8:102:ALA:CB | 3:Q8:166:LYS:CE | 1.92 | 1.44 |
| 3:Y8:89:ILE:HG23 | 3:Y8:92:TYR:CZ | 1.52 | 1.44 |
| 3:LA:14:LEU:CD2 | 11:aA:358:PRO:HB3 | 0.98 | 1.44 |
| 3:TA:28:THR:CG2 | 2:X4:67:THR:CB | 1.94 | 1.44 |
| 2:N4:111:ALA:O | 5:Z4:34:LEU:CD1 | 1.65 | 1.44 |
| 11:a9:312:ASP:CA | 11:a9:315:LEU:CB | 1.96 | 1.44 |
| 4:M1:120:LEU:HD21 | 3:X1:84:ARG:NH1 | 1.32 | 1.44 |
| 3:U4:115:GLU:HB3 | 4:M4:74:LEU:CD1 | 1.47 | 1.44 |
| 3:F4:115:GLU:HG2 | 4:M4:3:VAL:CG1 | 1.47 | 1.44 |
| 10:j5:965:GLN:H | 1:t7:69:GLY:CA | 1.27 | 1.44 |
| 3:Q8:89:ILE:CA | 3:Q8:92:TYR:CE2 | 1.97 | 1.44 |
| 11:aA:283:GLN:HB3 | 11:aA:284:PRO:CD | 1.33 | 1.44 |
| 3:TA:28:THR:CG2 | 2:X4:67:THR:HB | 1.49 | 1.43 |
| 4:M4:27:HIS:CE1 | 4:M4:35:THR:H | 1.23 | 1.43 |
| 8:A7:56:ASP:OD1 | 11:aA:586:LEU:CD1 | 1.64 | 1.43 |
| 10:j5:175:ASP:HB2 | 10:j5:176:PRO:CD | 1.28 | 1.43 |
| 10:j5:284:PRO:CG | 10:j5:326:GLY:HA3 | 1.15 | 1.43 |
| 4:M9:77:LEU:CD1 | 3:Z9:115:GLU:OE2 | 1.63 | 1.43 |
| 11:aA:800:THR:CG2 | 12:aA:901:CYC:HAA1 | 1.47 | 1.43 |
| 5:NA:66:ARG:NH1 | 3:TA:111:ASN:ND2 | 1.62 | 1.43 |
| 4:M3:120:LEU:HD21 | 3:X3:84:ARG:NH1 | 1.32 | 1.43 |
| 1:J5:71:MEN:CA | 1:J5:77:ARG:NH1 | 1.81 | 1.43 |
| 1:T5:110:ASN:ND2 | 10:j5:692:LEU:HB3 | 1.29 | 1.43 |
| 2:N8:112:GLY:CA | 5:Z8:34:LEU:N | 1.76 | 1.43 |
| 10:j5:175:ASP:CB | 10:j5:176:PRO:HD2 | 1.09 | 1.43 |
| 1:B7:136:VAL:HG13 | 11:a9:563:PHE:CE2 | 1.53 | 1.43 |
| 8:i7:96:ILE:HG13 | 8:i7:152:TYR:CG | 1.53 | 1.43 |
| 8:o7:23:LEU:CB | 1:p7:38:VAL:CG1 | 1.88 | 1.43 |
| 11:aA:742:GLN:NE2 | 3:L1:88:ILE:CG1 | 1.82 | 1.43 |
| 12:FA:301:CYC:C4B | 4:MA:53:LEU:CD1 | 1.96 | 1.43 |
| 4:M4:82:ILE:CD1 | 12:M4:301:CYC:O2D | 1.64 | 1.43 |
| 8:W5:11:ALA:HB3 | 1:X5:94:TYR:CE1 | 1.53 | 1.43 |
| 8:c7:15:ALA:CA | 1:d7:90:ARG:NH2 | 1.81 | 1.43 |
| 4:M3:51:ARG:HH21 | 11:a9:694:ARG:CZ | 1.31 | 1.43 |
| 10:j5:1050:PHE:CZ | 1:r7:107:ARG:NH2 | 1.84 | 1.43 |
| 4:M9:53:LEU:CD1 | 12:F9:301:CYC:C4B | 1.96 | 1.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:aA:312:ASP:CA | 11:aA:315:LEU:CB | 1.96 | 1.43 |
| 3:H2:77:ARG:NH1 | 6:M2:117:MET:CE | 1.79 | 1.42 |
| 1:D5:71:MEN:CA | 1:D5:77:ARG:NH1 | 1.82 | 1.42 |
| 1:Z:161:SER:HB2 | 1:X5:14:VAL:CB | 1.48 | 1.42 |
| 3:Y4:89:ILE:HG23 | 3:Y4:92:TYR:CZ | 1.52 | 1.42 |
| 5:Z4:22:LEU:CD1 | 12:Z4:301:CYC:OB | 1.66 | 1.42 |
| 8:Q5:11:ALA:HB3 | 1:R5:94:TYR:CE1 | 1.54 | 1.42 |
| 10:k5:175:ASP:CB | 10:k5:176:PRO:HD2 | 1.09 | 1.42 |
| 8:c7:96:ILE:HG13 | 8:c7:152:TYR:CG | 1.53 | 1.42 |
| 11:aA:694:ARG:CZ | 4:M1:51:ARG:HH21 | 1.31 | 1.42 |
| 12:L4:202:CYC:OB | 11:aA:239:TYR:CD1 | 1.69 | 1.42 |
| 4:M8:91:VAL:CG2 | 2:P8:14:SER:O | 1.66 | 1.42 |
| 12:QA:201:CYC:O2D | 3:TA:57:HIS:CD2 | 1.70 | 1.42 |
| 4:M4:138:SER:CB | 4:M4:215:GLU:OE2 | 1.68 | 1.42 |
| 8:e5:45:GLU:OE1 | 1:R5:139:GLY:CA | 1.66 | 1.42 |
| 3:L8:71:GLY:N | 11:a9:82:GLN:HG2 | 1.20 | 1.42 |
| 4:M8:230:GLN:CB | 12:M8:301:CYC:OB | 1.65 | 1.42 |
| 4:M8:231:THR:N | 12:M8:301:CYC:HBB3 | 1.10 | 1.42 |
| 4:MA:77:LEU:CD1 | 3:ZA:115:GLU:OE2 | 1.63 | 1.41 |
| 12:B3:202:CYC:HBA2 | 11:a9:684:ASN:CB | 1.47 | 1.41 |
| 3:B4:120:LEU:CD1 | 4:M4:53:LEU:CB | 1.97 | 1.41 |
| 8:i7:96:ILE:HA | 8:i7:152:TYR:CZ | 1.53 | 1.41 |
| 1:d7:77:ARG:NH2 | 9:x7:63:ALA:HB3 | 1.25 | 1.41 |
| 12:D8:202:CYC:CBA | 4:M8:35:THR:OG1 | 1.67 | 1.41 |
| 3:Q8:89:ILE:HG23 | 3:Q8:92:TYR:CZ | 1.55 | 1.41 |
| 3:B4:85:ASP:HB2 | 12:B4:202:CYC:C3C | 1.32 | 1.41 |
| 3:F4:109:CYS:C | 4:M4:6:THR:HG22 | 1.39 | 1.41 |
| 4:M4:29:PRO:CB | 11:aA:225:VAL:O | 1.67 | 1.41 |
| 4:M9:53:LEU:CD1 | 12:F9:301:CYC:OB | 1.67 | 1.41 |
| 4:M1:158:PHE:HD1 | 3:Z1:108:ARG:NH1 | 0.94 | 1.41 |
| 2:K3:112:GLY:HA2 | 11:a9:670:LEU:CD2 | 1.25 | 1.41 |
| 1:N5:110:ASN:HD21 | 10:k5:692:LEU:CB | 1.28 | 1.41 |
| 1:T5:83:ARG:NH1 | 10:j5:483:PHE:HZ | 1.08 | 1.41 |
| 10:j5:974:LEU:HG | 1:v7:1:MET:N | 1.10 | 1.41 |
| 10:j5:1018:LEU:CD1 | 10:j5:1035:PHE:CZ | 2.03 | 1.41 |
| 3:JA:119:ALA:O | 11:aA:365:LYS:CE | 1.64 | 1.41 |
| 1:N5:113:LYS:NZ | 1:Z5:155:TYR:CE2 | 1.89 | 1.41 |
| 1:d7:87:TYR:CZ | 9:x7:38:PHE:CZ | 2.09 | 1.41 |
| 8:W5:16:ARG:CA | 1:X5:90:ARG:HH11 | 1.32 | 1.41 |
| 10:j5:965:GLN:N | 1:t7:69:GLY:HA2 | 1.14 | 1.41 |
| 10:k5:1018:LEU:CD1 | 10:k5:1035:PHE:CZ | 2.03 | 1.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:M9:29:PRO:HD3 | 11:a9:378:GLU:CD | 1.40 | 1.41 |
| 11:aA:670:LEU:CD2 | 2:K1:112:GLY:HA2 | 1.23 | 1.41 |
| 3:B4:85:ASP:HB2 | 12:B4:202:CYC:CAC | 0.96 | 1.40 |
| 3:L8:82:CYS:SG | 12:a9:901:CYC:HAC2 | 1.61 | 1.40 |
| 4:M8:214:GLY:HA2 | 5:Z8:28:HIS:NE2 | 1.10 | 1.40 |
| 3:O8:108:ARG:HB2 | 5:Z8:61:LYS:CD | 1.11 | 1.40 |
| 11:aA:798:SER:HB3 | 11:aA:800:THR:CG2 | 0.94 | 1.40 |
| 3:Z3:108:ARG:NH1 | 4:M3:158:PHE:HD1 | 0.94 | 1.40 |
| 1:B5:10:ASN:OD1 | 10:k5:557:VAL:CB | 1.66 | 1.40 |
| 8:Q7:13:ALA:HA | 9:z7:46:LYS:NZ | 1.24 | 1.40 |
| 3:F9:68:ARG:NH1 | 3:Z9:68:ARG:HH12 | 0.97 | 1.40 |
| 2:SA:35:THR:CG2 | 2:X4:74:TYR:CZ | 2.03 | 1.40 |
| 6:M2:127:SER:HB3 | 3:F2:84:ARG:CZ | 1.50 | 1.40 |
| 2:E4:1:MET:N | 4:M4:10:ARG:HH21 | 0.94 | 1.40 |
| 3:F4:113:LEU:CA | 4:M4:5:THR:HG23 | 1.47 | 1.40 |
| 3:B8:81:ALA:HB1 | 12:B8:202:CYC:CMD | 0.93 | 1.40 |
| 2:N8:115:GLU:CG | 5:Z8:32:PRO:CG | 1.97 | 1.40 |
| 6:M2:62:ARG:HH21 | 1:h7:58:LYS:C | 1.27 | 1.40 |
| 3:Q4:120:LEU:CD2 | 5:Z4:42:SER:HB2 | 1.48 | 1.40 |
| 1:Z7:67:ARG:NH2 | 11:a9:307:ARG:HB3 | 1.32 | 1.40 |
| 3:H8:84:ARG:CD | 11:a9:131:TYR:CD2 | 2.02 | 1.40 |
| 11:aA:312:ASP:CB | 11:aA:315:LEU:CB | 1.92 | 1.40 |
| 3:U4:112:GLY:HA2 | 4:M4:74:LEU:CD2 | 1.52 | 1.40 |
| 1:d5:28:LYS:NZ | 1:n7:143:PRO:HB2 | 1.14 | 1.40 |
| 1:f5:18:TYR:CZ | 10:j5:165:ARG:HB2 | 1.57 | 1.40 |
| 6:M6:117:MET:CE | 3:H6:77:ARG:NH1 | 1.79 | 1.40 |
| 4:M8:214:GLY:CA | 5:Z8:28:HIS:CE1 | 2.04 | 1.40 |
| 2:N8:14:SER:CB | 5:Z8:62:ARG:NE | 1.85 | 1.40 |
| 5:Z8:41:GLN:CD | 12:Z8:301:CYC:CBB | 1.93 | 1.40 |
| 3:B3:88:ILE:CG2 | 12:B3:202:CYC:HAB2 | 1.49 | 1.39 |
| 8:W5:11:ALA:CB | 1:X5:94:TYR:CE1 | 2.04 | 1.39 |
| 8:c7:15:ALA:HA | 1:d7:90:ARG:NH2 | 1.10 | 1.39 |
| 8:c7:39:ILE:CD1 | 8:c7:148:GLU:CG | 2.00 | 1.39 |
| 2:X8:67:THR:HB | 3:T9:28:THR:CG2 | 1.48 | 1.39 |
| 4:M8:104:ALA:HB1 | 2:P8:14:SER:CB | 0.92 | 1.39 |
| 2:N4:111:ALA:CB | 5:Z4:34:LEU:CG | 1.98 | 1.39 |
| 3:O4:107:ASP:CB | 5:Z4:66:ARG:HB3 | 1.51 | 1.39 |
| 8:Q5:16:ARG:CA | 1:R5:90:ARG:HH11 | 1.33 | 1.39 |
| 8:Q7:25:ARG:CB | 8:C7:25:ARG:NH2 | 1.85 | 1.39 |
| 3:Q8:127:VAL:HG22 | 12:Z8:301:CYC:CMC | 1.51 | 1.39 |
| 1:Z:131:GLN:CG | 1:X5:17:LYS:NZ | 1.82 | 1.39 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:J3:14:LEU:HD13 | 11:a9:621:THR:CG2 | 1.51 | 1.39 |
| 3:U4:115:GLU:CB | 4:M4:74:LEU:CD1 | 1.95 | 1.39 |
| 3:H4:119:ALA:C | 11:aA:266:ASN:HB3 | 1.47 | 1.39 |
| 1:N5:110:ASN:ND2 | 10:k5:692:LEU:HB3 | 1.27 | 1.39 |
| 8:I7:25:ARG:HH21 | 8:W7:25:ARG:CB | 1.33 | 1.39 |
| 8:i7:96:ILE:HG12 | 8:i7:152:TYR:CD1 | 1.57 | 1.39 |
| 8:c7:96:ILE:HA | 8:c7:152:TYR:CZ | 1.53 | 1.39 |
| 1:X5:50:THR:HG21 | 8:a5:49:ARG:NH1 | 1.36 | 1.39 |
| 8:i7:47:ARG:HD3 | 1:j7:18:TYR:CZ | 0.88 | 1.39 |
| 2:X8:74:TYR:CZ | 2:S9:35:THR:CG2 | 2.03 | 1.39 |
| 5:Z8:42:SER:CA | 12:Z8:301:CYC:HMA2 | 1.49 | 1.39 |
| 11:aA:312:ASP:CA | 11:aA:315:LEU:HB3 | 1.51 | 1.39 |
| 11:aA:621:THR:CG2 | 3:J1:14:LEU:HD13 | 1.49 | 1.39 |
| 11:aA:776:TYR:CE1 | 12:H1:201:CYC:OB | 1.74 | 1.39 |
| 1:Z:158:SER:CB | 1:X5:11:ASN:ND2 | 1.84 | 1.39 |
| 3:J3:84:ARG:HH22 | 11:a9:669:ILE:C | 1.31 | 1.39 |
| 2:P4:19:LEU:CG | 3:Q4:95:TYR:HE1 | 1.35 | 1.39 |
| 8:Q5:11:ALA:CB | 1:R5:94:TYR:CE1 | 2.04 | 1.39 |
| 8:a7:52:LYS:HD2 | 11:a9:321:ALA:CB | 1.51 | 1.39 |
| 4:M8:138:SER:CB | 4:M8:215:GLU:OE2 | 1.68 | 1.39 |
| 12:M8:302:CYC:HMD3 | 3:S8:77:ARG:NH2 | 1.28 | 1.39 |
| 3:B4:85:ASP:CB | 12:B4:202:CYC:CAC | 1.83 | 1.38 |
| 3:B4:116:THR:CB | 4:M4:56:MET:HB3 | 1.45 | 1.38 |
| 8:I5:27:LYS:O | 8:I5:29:PHE:N | 1.56 | 1.38 |
| 2:X8:16:GLY:CA | 4:M8:228:SER:HB2 | 1.52 | 1.38 |
| 12:FA:301:CYC:OB | 4:MA:53:LEU:CD1 | 1.67 | 1.38 |
| 2:SA:38:MET:C | 2:X4:69:PRO:HG2 | 1.48 | 1.38 |
| 3:B4:85:ASP:CA | 12:B4:202:CYC:HAC1 | 1.51 | 1.38 |
| 2:U3:46:SER:O | 2:Q9:74:TYR:CZ | 1.75 | 1.38 |
| 1:Z5:28:LYS:NZ | 1:t7:143:PRO:HG2 | 1.20 | 1.38 |
| 10:j5:934:ALA:CB | 1:J7:32:THR:CG2 | 2.01 | 1.38 |
| 3:L3:84:ARG:HG2 | 11:a9:742:GLN:OE1 | 1.24 | 1.38 |
| 6:M6:127:SER:HB3 | 3:F6:84:ARG:CZ | 1.50 | 1.38 |
| 10:j5:931:VAL:HG22 | 1:J7:29:ALA:C | 1.47 | 1.38 |
| 10:k5:1008:PHE:CE1 | 1:p7:87:TYR:CZ | 2.11 | 1.38 |
| 3:F6:78:ARG:CD | 12:F6:201:CYC:O2D | 1.71 | 1.38 |
| 8:i7:21:GLY:N | 8:s7:101:VAL:HG22 | 1.35 | 1.38 |
| 8:i7:39:ILE:CD1 | 8:i7:148:GLU:CG | 1.99 | 1.38 |
| 3:D4:108:ARG:CD | 11:aA:107:ARG:NH1 | 1.76 | 1.38 |
| 10:j5:190:LEU:HB3 | 10:j5:194:CYS:SG | 1.62 | 1.38 |
| 8:i7:20:PRO:HG3 | 8:s7:155:TYR:CG | 1.58 | 1.38 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:X8:13:ASP:OD1 | 4:M8:229:GLY:CA | 1.69 | 1.38 |
| 11:aA:280:ASP:CB | 11:aA:281:PRO:HD2 | 1.38 | 1.38 |
| 1:A:110:ASN:ND2 | 10:k5:462:TYR:CE2 | 1.92 | 1.38 |
| 3:L3:119:ALA:HB2 | 11:a9:813:PRO:CB | 1.51 | 1.38 |
| 12:B1:202:CYC:HAA1 | 11:aA:684:ASN:CG | 1.48 | 1.38 |
| 1:P5:114:GLU:CG | 10:k5:496:GLU:CG | 1.83 | 1.38 |
| 1:T5:53:LYS:NZ | 8:U5:120:GLN:NE2 | 1.72 | 1.38 |
| 1:b5:18:TYR:CD1 | 10:k5:165:ARG:HD3 | 1.57 | 1.38 |
| 11:aA:742:GLN:CG | 3:L1:88:ILE:CD1 | 1.74 | 1.38 |
| 3:B1:88:ILE:HG21 | 12:B1:202:CYC:CMB | 1.50 | 1.37 |
| 8:C5:27:LYS:O | 8:C5:29:PHE:N | 1.56 | 1.37 |
| 8:i7:21:GLY:H | 8:s7:101:VAL:CG2 | 1.36 | 1.37 |
| 11:aA:586:LEU:O | 11:aA:590:PRO:CG | 1.73 | 1.37 |
| 1:Z:131:GLN:CG | 1:X5:17:LYS:HZ1 | 1.35 | 1.37 |
| 1:d5:28:LYS:HZ3 | 1:n7:143:PRO:CB | 1.35 | 1.37 |
| 8:W5:15:ALA:O | 1:X5:90:ARG:CD | 1.72 | 1.37 |
| 6:M6:283:VAL:CG1 | 8:Y7:75:GLU:HB3 | 1.53 | 1.37 |
| 10:k5:1143:LEU:HD12 | 8:k7:106:GLU:OE1 | 1.22 | 1.37 |
| 10:k5:1152:TYR:CD2 | 8:G7:68:PRO:HG2 | 1.55 | 1.37 |
| 11:aA:742:GLN:CD | 3:L1:88:ILE:HD11 | 1.44 | 1.37 |
| 1:b5:18:TYR:CZ | 10:k5:165:ARG:HB2 | 1.57 | 1.37 |
| 8:c7:96:ILE:HG12 | 8:c7:152:TYR:CD1 | 1.57 | 1.37 |
| 3:F8:107:ASP:CB | 4:M8:8:SER:O | 1.72 | 1.37 |
| 4:M8:127:SER:HA | 12:M8:302:CYC:CMA | 1.41 | 1.37 |
| 10:j5:156:SER:OG | 12:j5:1201:CYC:H3C | 1.25 | 1.37 |
| 10:k5:190:LEU:HB3 | 10:k5:194:CYS:SG | 1.62 | 1.37 |
| 8:g7:52:LYS:HD2 | 11:aA:321:ALA:CB | 1.53 | 1.37 |
| 12:M8:302:CYC:CMC | 3:S8:72:ASN:ND2 | 1.82 | 1.37 |
| 8:U5:59:PHE:CD2 | 6:M6:37:GLU:OE2 | 1.77 | 1.36 |
| 10:k5:1055:SER:OG | 12:k5:1203:CYC:CBB | 1.71 | 1.36 |
| 3:D8:108:ARG:CD | 11:a9:107:ARG:NH1 | 1.77 | 1.36 |
| 11:a9:586:LEU:O | 11:a9:590:PRO:CG | 1.73 | 1.36 |
| 1:N5:53:LYS:NZ | 8:O5:120:GLN:NE2 | 1.72 | 1.36 |
| 10:j5:136:VAL:HG12 | 10:j5:137:PRO:CD | 1.56 | 1.36 |
| 10:j5:1018:LEU:HB3 | 10:j5:1021:ALA:CB | 1.55 | 1.36 |
| 4:M8:91:VAL:CG1 | 2:P8:14:SER:O | 1.71 | 1.36 |
| 1:A:161:SER:CB | 1:R5:14:VAL:HG23 | 1.43 | 1.36 |
| 3:DA:108:ARG:O | 4:MA:6:THR:HG22 | 1.23 | 1.36 |
| 6:M2:28:ASN:CB | 8:O5:80:LEU:CD2 | 2.04 | 1.36 |
| 1:Z:131:GLN:HG3 | 1:X5:17:LYS:NZ | 1.08 | 1.36 |
| 3:DA:68:ARG:HH22 | 3:XA:68:ARG:NH1 | 1.22 | 1.36 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:1146:THR:HB | 1:v7:77:ARG:NH2 | 1.33 | 1.36 |
| 3:H8:119:ALA:HB3 | 11:a9:266:ASN:ND2 | 1.37 | 1.36 |
| 4:M8:127:SER:CB | 12:M8:302:CYC:CMA | 2.00 | 1.36 |
| 3:H9:120:LEU:HD11 | 12:H9:202:CYC:CAA | 1.53 | 1.36 |
| 11:a9:31:SER:OG | 11:a9:34:ILE:HB | 1.22 | 1.36 |
| 11:a9:624:GLY:O | 11:a9:628:THR:HG22 | 1.19 | 1.36 |
| 11:aA:666:ASN:HB3 | 12:aA:901:CYC:C4B | 1.56 | 1.36 |
| 11:aA:813:PRO:CB | 3:L1:119:ALA:HB2 | 1.53 | 1.36 |
| 1:B5:10:ASN:CG | 10:k5:557:VAL:HB | 1.48 | 1.36 |
| 6:M6:127:SER:CB | 3:F6:84:ARG:CZ | 2.03 | 1.36 |
| 10:j5:974:LEU:CG | 1:v7:1:MET:N | 1.88 | 1.36 |
| 1:f7:67:ARG:NH2 | 11:aA:307:ARG:HB3 | 1.33 | 1.36 |
| 3:H8:119:ALA:C | 11:a9:266:ASN:HB3 | 1.48 | 1.36 |
| 8:Q5:15:ALA:O | 1:R5:90:ARG:CD | 1.72 | 1.35 |
| 8:U5:76:LYS:HD2 | 8:U5:77:MET:CE | 1.56 | 1.35 |
| 12:B8:202:CYC:CBB | 4:M8:61:ASN:CB | 2.04 | 1.35 |
| 3:Q8:85:ASP:CB | 12:Z8:301:CYC:HBC1 | 1.55 | 1.35 |
| 3:Q8:102:ALA:HB2 | 3:Q8:166:LYS:CE | 1.53 | 1.35 |
| 5:Z8:38:GLU:CB | 12:Z8:301:CYC:HMB2 | 1.55 | 1.35 |
| 11:a9:312:ASP:CB | 11:a9:315:LEU:CB | 1.92 | 1.35 |
| 3:F4:107:ASP:CB | 4:M4:8:SER:OG | 1.73 | 1.35 |
| 4:M4:232:VAL:O | 4:M4:235:PHE:CE2 | 1.78 | 1.35 |
| 10:k5:935:LEU:CD1 | 1:D7:29:ALA:HB2 | 1.53 | 1.35 |
| 2:E1:13:ASP:CG | 11:aA:644:ARG:NH1 | 1.84 | 1.35 |
| 2:X8:69:PRO:HG2 | 2:S9:38:MET:C | 1.48 | 1.35 |
| 4:M8:232:VAL:O | 4:M8:235:PHE:CE2 | 1.78 | 1.35 |
| 6:M2:127:SER:HB2 | 3:F2:84:ARG:NH2 | 1.42 | 1.35 |
| 10:k5:965:GLN:N | 1:n7:69:GLY:HA2 | 1.38 | 1.35 |
| 8:I7:76:LYS:NZ | 11:aA:567:GLN:HE21 | 1.22 | 1.35 |
| 8:g7:63:PRO:CD | 11:aA:336:ILE:HG22 | 1.47 | 1.35 |
| 4:M8:127:SER:CA | 12:M8:302:CYC:HMA1 | 1.40 | 1.35 |
| 8:O5:76:LYS:HD2 | 8:O5:77:MET:CE | 1.56 | 1.35 |
| 10:k5:136:VAL:HG12 | 10:k5:137:PRO:CD | 1.56 | 1.35 |
| 10:k5:935:LEU:HD13 | 1:D7:29:ALA:CB | 1.56 | 1.35 |
| 1:R7:118:SER:O | 9:z7:61:GLN:CD | 1.70 | 1.35 |
| 3:L9:14:LEU:HD21 | 11:a9:358:PRO:CA | 1.57 | 1.35 |
| 11:a9:312:ASP:CA | 11:a9:315:LEU:HB3 | 1.51 | 1.35 |
| 3:HA:120:LEU:HD11 | 12:HA:202:CYC:CAA | 1.55 | 1.35 |
| 3:HA:126:SER:CB | 12:HA:202:CYC:HMC3 | 1.55 | 1.35 |
| 6:M2:127:SER:CB | 3:F2:84:ARG:CZ | 2.03 | 1.35 |
| 3:B4:120:LEU:HD11 | 4:M4:53:LEU:CB | 1.53 | 1.35 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:b5:38:VAL:HG13 | 10:k5:40:VAL:CG1 | 1.55 | 1.35 |
| 10:k5:820:HIS:ND1 | 10:k5:859:ILE:CD1 | 1.89 | 1.35 |
| 10:k5:1016:LEU:HD12 | 10:k5:1017:ARG:N | 1.40 | 1.35 |
| 4:M8:205:ASP:CB | 5:Z8:59:ARG:HE | 1.36 | 1.35 |
| 12:M8:302:CYC:C1C | 3:S8:78:ARG:HD3 | 0.89 | 1.35 |
| 4:M9:6:THR:HG22 | 3:D9:108:ARG:O | 1.23 | 1.35 |
| 11:a9:239:TYR:HE2 | 12:a9:901:CYC:C4B | 1.38 | 1.35 |
| 5:Z4:41:GLN:CB | 12:Z4:301:CYC:C2B | 2.04 | 1.34 |
| 12:B5:201:CYC:CBA | 9:z5:26:THR:HG21 | 1.53 | 1.34 |
| 10:j5:820:HIS:ND1 | 10:j5:859:ILE:CD1 | 1.89 | 1.34 |
| 5:Z8:34:LEU:O | 5:Z8:34:LEU:HD23 | 1.23 | 1.34 |
| 3:JA:20:SER:O | 3:JA:22:GLN:N | 1.58 | 1.34 |
| 3:B3:82:CYS:SG | 12:B3:202:CYC:CAC | 2.13 | 1.34 |
| 12:B4:202:CYC:CBB | 4:M4:61:ASN:CB | 2.04 | 1.34 |
| 2:P4:19:LEU:HG | 3:Q4:95:TYR:CE1 | 1.60 | 1.34 |
| 8:e5:49:ARG:CZ | 1:R5:50:THR:HG21 | 1.57 | 1.34 |
| 10:k5:924:ASP:OD1 | 1:D7:26:LYS:NZ | 1.56 | 1.34 |
| 10:k5:1018:LEU:HB3 | 10:k5:1021:ALA:CB | 1.55 | 1.34 |
| 8:g7:25:ARG:NH2 | 8:u7:25:ARG:NH1 | 1.69 | 1.34 |
| 3:Y8:87:GLU:OE2 | 3:Y8:91:ARG:NH2 | 1.59 | 1.34 |
| 11:aA:776:TYR:CD1 | 12:H1:201:CYC:OB | 1.79 | 1.34 |
| 2:QA:71:GLN:N | 2:QA:74:TYR:CE2 | 1.92 | 1.34 |
| 1:D5:71:MEN:CA | 1:D5:77:ARG:HH11 | 1.38 | 1.34 |
| 6:M6:127:SER:HB2 | 3:F6:84:ARG:NH2 | 1.42 | 1.34 |
| 6:M6:277:GLY:CA | 1:d7:62:TYR:O | 1.74 | 1.34 |
| 1:H7:136:VAL:HG13 | 11:aA:563:PHE:CE2 | 1.62 | 1.34 |
| 8:i7:47:ARG:HD3 | 1:j7:18:TYR:CE1 | 1.62 | 1.34 |
| 1:d7:87:TYR:CZ | 9:x7:38:PHE:HZ | 1.39 | 1.34 |
| 8:u7:23:LEU:CB | 1:v7:38:VAL:CG1 | 1.88 | 1.34 |
| 4:M8:87:ILE:CD1 | 3:Y8:77:ARG:CG | 1.97 | 1.34 |
| 11:a9:283:GLN:CB | 11:a9:284:PRO:HD2 | 1.57 | 1.34 |
| 3:U4:111:ASN:OD1 | 4:M4:77:LEU:HD13 | 1.23 | 1.34 |
| 1:N5:83:ARG:NH1 | 10:k5:483:PHE:HZ | 1.25 | 1.34 |
| 1:J5:71:MEN:HA | 1:J5:77:ARG:NH1 | 1.02 | 1.34 |
| 10:j5:934:ALA:HB1 | 1:J7:32:THR:CG2 | 1.58 | 1.34 |
| 4:M8:197:ASP:HB3 | 5:Z8:52:ARG:CG | 1.54 | 1.34 |
| 3:J9:20:SER:O | 3:J9:22:GLN:N | 1.58 | 1.34 |
| 11:a9:403:THR:CG2 | 11:a9:536:THR:CG2 | 2.06 | 1.34 |
| 12:J3:202:CYC:C4B | 11:a9:666:ASN:HB3 | 1.57 | 1.34 |
| 3:H4:119:ALA:HB3 | 11:aA:266:ASN:ND2 | 1.37 | 1.34 |
| 12:M4:301:CYC:CMC | 3:Y4:72:ASN:HB3 | 1.56 | 1.34 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:M5:20:PRO:HG2 | 8:A5:100:ASP:OD1 | 1.26 | 1.34 |
| 10:k5:1074:GLN:OE1 | 1:l7:119:LEU:HD21 | 1.23 | 1.34 |
| 3:S8:113:LEU:O | 3:S8:116:THR:HG22 | 1.22 | 1.34 |
| 11:a9:710:THR:HG22 | 11:a9:807:GLN:CB | 1.58 | 1.34 |
| 11:aA:312:ASP:HA | 11:aA:315:LEU:CB | 1.53 | 1.34 |
| 3:LA:14:LEU:HD21 | 11:aA:358:PRO:CA | 1.58 | 1.33 |
| 3:J3:84:ARG:HD2 | 11:a9:668:TYR:CG | 1.61 | 1.33 |
| 10:j5:1016:LEU:HD12 | 10:j5:1017:ARG:N | 1.40 | 1.33 |
| 10:k5:978:LEU:HD21 | 1:p7:107:ARG:NH2 | 1.39 | 1.33 |
| 4:M8:223:GLY:O | 12:M8:301:CYC:HBA2 | 1.19 | 1.33 |
| 3:F9:68:ARG:HH12 | 3:Z9:68:ARG:NH1 | 0.85 | 1.33 |
| 11:aA:621:THR:CG2 | 3:J1:14:LEU:CD1 | 2.05 | 1.33 |
| 4:MA:274:VAL:CG1 | 3:VA:77:ARG:CD | 1.84 | 1.33 |
| 5:NA:54:LEU:HD22 | 3:TA:84:ARG:NE | 1.43 | 1.33 |
| 2:SA:35:THR:HG22 | 2:X4:74:TYR:OH | 1.27 | 1.33 |
| 12:O4:201:CYC:CMA | 5:Z4:53:LEU:HD13 | 1.56 | 1.33 |
| 10:k5:934:ALA:HB1 | 1:D7:32:THR:CG2 | 1.41 | 1.33 |
| 8:M7:49:ARG:HD2 | 11:a9:550:PHE:CE1 | 1.63 | 1.33 |
| 4:M8:29:PRO:HB3 | 11:a9:225:VAL:O | 1.22 | 1.33 |
| 2:N8:112:GLY:HA3 | 5:Z8:34:LEU:N | 1.28 | 1.33 |
| 3:O8:104:VAL:O | 5:Z8:61:LYS:HE2 | 1.20 | 1.33 |
| 5:Z8:42:SER:HA | 12:Z8:301:CYC:CMA | 1.57 | 1.33 |
| 11:a9:239:TYR:CE2 | 12:a9:901:CYC:OB | 1.80 | 1.33 |
| 11:aA:403:THR:CG2 | 11:aA:536:THR:CG2 | 2.06 | 1.33 |
| 5:NA:22:LEU:CD2 | 5:NA:26:LEU:HD21 | 1.57 | 1.33 |
| 3:J3:14:LEU:CD1 | 11:a9:621:THR:CG2 | 2.06 | 1.33 |
| 1:D5:71:MEN:HA | 1:D5:77:ARG:NH1 | 1.02 | 1.33 |
| 8:i7:25:ARG:CZ | 8:s7:6:LYS:CB | 2.04 | 1.33 |
| 8:c7:96:ILE:HA | 8:c7:152:TYR:CE2 | 1.63 | 1.33 |
| 12:D8:202:CYC:CBA | 4:M8:35:THR:CB | 2.04 | 1.33 |
| 11:aA:742:GLN:CD | 3:L1:88:ILE:CD1 | 1.90 | 1.33 |
| 3:TA:32:LYS:HE2 | 2:X4:57:GLN:OE1 | 1.23 | 1.33 |
| 3:L3:88:ILE:CG1 | 11:a9:742:GLN:NE2 | 1.82 | 1.33 |
| 1:Z5:127:VAL:HG11 | 10:k5:698:GLY:N | 1.42 | 1.33 |
| 1:b5:30:TYR:OH | 10:k5:47:PHE:CZ | 1.72 | 1.33 |
| 10:j5:284:PRO:HG2 | 10:j5:326:GLY:CA | 1.37 | 1.33 |
| 3:U8:114:LYS:NZ | 4:M8:13:LYS:CE | 1.90 | 1.33 |
| 5:N9:61:LYS:HD3 | 3:T9:108:ARG:O | 1.27 | 1.33 |
| 5:Z8:22:LEU:CD1 | 12:Z8:301:CYC:OB | 1.75 | 1.33 |
| 5:Z8:41:GLN:CG | 12:Z8:301:CYC:C4B | 2.04 | 1.33 |
| 11:a9:312:ASP:HA | 11:a9:315:LEU:CB | 1.53 | 1.33 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:110:ASN:ND2 | 10:k5:462:TYR:CZ | 1.91 | 1.33 |
| 2:OA:33:ARG:NH1 | 12:ZA:201:CYC:OB | 1.62 | 1.33 |
| 6:M2:39:ARG:NE | 8:O5:66:VAL:HG11 | 1.38 | 1.33 |
| 2:E3:13:ASP:CG | 11:a9:644:ARG:HH11 | 1.32 | 1.33 |
| 2:N4:111:ALA:HB3 | 5:Z4:34:LEU:CD1 | 1.58 | 1.33 |
| 10:k5:1013:PRO:HB3 | 8:k7:114:GLU:OE2 | 1.27 | 1.33 |
| 4:M8:214:GLY:CA | 5:Z8:28:HIS:CD2 | 2.06 | 1.33 |
| 4:M8:235:PHE:HB3 | 12:M8:301:CYC:C3A | 1.57 | 1.33 |
| 3:B9:107:ASP:CB | 11:a9:382:ASN:HD22 | 1.41 | 1.33 |
| 11:aA:817:LEU:CD1 | 3:L1:119:ALA:O | 1.77 | 1.33 |
| 3:FA:68:ARG:HH12 | 3:ZA:68:ARG:NH1 | 0.85 | 1.32 |
| 3:F4:84:ARG:HD3 | 11:aA:139:ILE:CG2 | 1.59 | 1.32 |
| 8:c7:20:PRO:CG | 8:m7:155:TYR:CB | 2.05 | 1.32 |
| 8:m7:29:PHE:CZ | 8:m7:98:ALA:O | 1.82 | 1.32 |
| 2:N8:115:GLU:HB2 | 5:Z8:32:PRO:CB | 1.56 | 1.32 |
| 3:Q8:102:ALA:HB2 | 3:Q8:166:LYS:NZ | 1.39 | 1.32 |
| 3:Y8:89:ILE:CG2 | 3:Y8:92:TYR:OH | 1.77 | 1.32 |
| 5:Z8:41:GLN:HG2 | 12:Z8:301:CYC:C4B | 1.57 | 1.32 |
| 11:aA:621:THR:HG22 | 3:J1:14:LEU:CG | 1.57 | 1.32 |
| 11:aA:776:TYR:H | 12:H1:201:CYC:CBA | 1.40 | 1.32 |
| 3:H1:77:ARG:HH12 | 12:H1:201:CYC:CGD | 1.40 | 1.32 |
| 3:J3:14:LEU:CG | 11:a9:621:THR:HG22 | 1.59 | 1.32 |
| 3:J3:120:LEU:HD21 | 11:a9:800:THR:CG2 | 1.60 | 1.32 |
| 3:L3:119:ALA:O | 11:a9:817:LEU:CD1 | 1.76 | 1.32 |
| 3:F4:108:ARG:NH2 | 4:M4:9:GLN:HG2 | 1.43 | 1.32 |
| 8:e5:38:ARG:NH2 | 1:R5:144:ASP:OD1 | 1.62 | 1.32 |
| 8:U7:29:PHE:CZ | 8:U7:98:ALA:O | 1.83 | 1.32 |
| 3:O8:107:ASP:CG | 5:Z8:66:ARG:HD2 | 1.53 | 1.32 |
| 11:aA:710:THR:HG22 | 11:aA:807:GLN:CB | 1.58 | 1.32 |
| 12:B1:202:CYC:HBA2 | 11:aA:684:ASN:CB | 1.57 | 1.32 |
| 2:N4:112:GLY:N | 5:Z4:34:LEU:HB2 | 1.41 | 1.32 |
| 10:k5:1143:LEU:CD1 | 8:k7:106:GLU:OE1 | 1.77 | 1.32 |
| 8:g7:25:ARG:HH21 | 8:u7:25:ARG:NH1 | 1.23 | 1.32 |
| 8:i7:96:ILE:HA | 8:i7:152:TYR:CE2 | 1.63 | 1.32 |
| 8:u7:6:LYS:NZ | 8:u7:102:THR:OG1 | 1.60 | 1.32 |
| 11:a9:351:THR:CB | 11:a9:352:PRO:HD2 | 1.40 | 1.32 |
| 2:A1:33:ARG:NH1 | 12:L1:201:CYC:OB | 1.62 | 1.32 |
| 2:E3:13:ASP:CG | 11:a9:644:ARG:NH1 | 1.87 | 1.32 |
| 4:M4:27:HIS:CE1 | 4:M4:34:ASP:C | 2.04 | 1.32 |
| 4:M4:29:PRO:HB3 | 11:aA:225:VAL:C | 1.51 | 1.32 |
| 1:d5:28:LYS:CD | 1:n7:143:PRO:HB3 | 1.60 | 1.32 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:j5:1009:ALA:HB2 | 1:v7:87:TYR:CE1 | 1.63 | 1.32 |
| 8:O7:29:PHE:CZ | 8:O7:98:ALA:O | 1.83 | 1.32 |
| 2:N8:33:ARG:NH1 | 12:Y8:201:CYC:OB | 1.62 | 1.32 |
| 3:D9:68:ARG:HH22 | 3:X9:68:ARG:NH1 | 1.22 | 1.32 |
| 3:H4:111:ASN:CG | 11:aA:291:TYR:OH | 1.72 | 1.32 |
| 8:I5:29:PHE:CZ | 8:I5:98:ALA:O | 1.83 | 1.32 |
| 8:W5:16:ARG:CA | 1:X5:90:ARG:HD3 | 1.60 | 1.32 |
| 3:Q8:85:ASP:CB | 12:Z8:301:CYC:CBC | 2.07 | 1.32 |
| 3:Q8:85:ASP:HB2 | 12:Z8:301:CYC:CBC | 1.59 | 1.32 |
| 3:F2:78:ARG:CD | 12:F2:201:CYC:O2D | 1.75 | 1.32 |
| 4:MA:232:VAL:HG13 | 3:XA:111:ASN:O | 1.14 | 1.31 |
| 2:QA:68:GLN:CA | 2:U1:46:SER:HB3 | 1.60 | 1.31 |
| 12:L2:202:CYC:OB | 2:A2:33:ARG:NH1 | 1.62 | 1.31 |
| 6:M2:53:LEU:HD23 | 8:i7:80:LEU:CD2 | 1.59 | 1.31 |
| 2:U3:46:SER:OG | 2:Q9:74:TYR:CD1 | 1.70 | 1.31 |
| 3:Y4:89:ILE:CG2 | 3:Y4:92:TYR:OH | 1.77 | 1.31 |
| 5:Z4:24:PRO:CG | 12:Z4:301:CYC:O2A | 1.78 | 1.31 |
| 1:f5:19:LEU:CD1 | 10:j5:172:LEU:CD1 | 2.06 | 1.31 |
| 3:L6:125:ARG:HD2 | 1:b7:69:GLY:CA | 1.57 | 1.31 |
| 8:a7:29:PHE:CZ | 8:a7:98:ALA:O | 1.83 | 1.31 |
| 4:M8:235:PHE:HB3 | 12:M8:301:CYC:C2A | 1.60 | 1.31 |
| 12:M8:302:CYC:CMC | 3:S8:72:ASN:OD1 | 1.68 | 1.31 |
| 11:aA:290:ASP:O | 11:aA:291:TYR:CD1 | 1.82 | 1.31 |
| 3:F4:115:GLU:OE2 | 4:M4:3:VAL:HG22 | 1.23 | 1.31 |
| 8:C5:29:PHE:CZ | 8:C5:98:ALA:O | 1.83 | 1.31 |
| 8:i7:20:PRO:HD3 | 8:s7:155:TYR:CD1 | 1.65 | 1.31 |
| 8:i7:37:LEU:HD11 | 1:j7:31:PHE:CE2 | 1.63 | 1.31 |
| 3:U8:115:GLU:HB2 | 4:M8:74:LEU:CD1 | 1.50 | 1.31 |
| 12:FA:301:CYC:NB | 4:MA:53:LEU:CD1 | 1.93 | 1.31 |
| 2:C3:115:GLU:OE2 | 4:M3:33:LEU:HD23 | 1.15 | 1.31 |
| 3:B4:116:THR:OG1 | 4:M4:56:MET:HB3 | 1.31 | 1.31 |
| 3:L4:68:ARG:CB | 11:aA:82:GLN:N | 1.92 | 1.31 |
| 2:N4:33:ARG:NH1 | 12:Y4:201:CYC:OB | 1.62 | 1.31 |
| 8:M5:41:GLN:OE1 | 1:J7:143:PRO:HG3 | 1.25 | 1.31 |
| 8:O5:29:PHE:CZ | 8:O5:98:ALA:O | 1.83 | 1.31 |
| 5:Z4:34:LEU:O | 5:Z4:34:LEU:HD23 | 1.23 | 1.31 |
| 10:j5:284:PRO:CG | 10:j5:326:GLY:CA | 1.93 | 1.31 |
| 8:O7:49:ARG:NH1 | 1:r7:114:GLU:CD | 1.87 | 1.31 |
| 8:I7:29:PHE:CZ | 8:I7:98:ALA:O | 1.82 | 1.31 |
| 8:g7:29:PHE:CZ | 8:g7:98:ALA:O | 1.83 | 1.31 |
| 8:i7:3:VAL:HG13 | 8:s7:25:ARG:NH2 | 1.41 | 1.31 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:O9:33:ARG:NH1 | 12:Z9:201:CYC:OB | 1.62 | 1.31 |
| 11:aA:107:ARG:CG | 11:aA:108:PRO:HD2 | 1.60 | 1.31 |
| 12:Z3:202:CYC:OB | 2:O3:33:ARG:NH1 | 1.62 | 1.31 |
| 4:M4:104:ALA:CA | 2:P4:14:SER:HB3 | 1.61 | 1.31 |
| 8:e5:29:PHE:CZ | 8:e5:98:ALA:O | 1.83 | 1.31 |
| 10:j5:965:GLN:HG3 | 1:t7:69:GLY:O | 1.28 | 1.31 |
| 3:U8:120:LEU:HD21 | 12:U8:201:CYC:CBD | 1.61 | 1.31 |
| 2:X8:57:GLN:OE1 | 3:T9:32:LYS:HE2 | 1.23 | 1.31 |
| 3:F8:115:GLU:HG2 | 4:M8:3:VAL:CG1 | 1.59 | 1.31 |
| 11:a9:107:ARG:CG | 11:a9:108:PRO:HD2 | 1.60 | 1.31 |
| 11:aA:668:TYR:OH | 2:K1:115:GLU:HG3 | 1.14 | 1.31 |
| 4:M4:232:VAL:O | 4:M4:235:PHE:CD2 | 1.83 | 1.31 |
| 8:U5:83:ARG:CB | 6:M6:26:PHE:CE1 | 2.14 | 1.31 |
| 8:a5:29:PHE:CZ | 8:a5:98:ALA:O | 1.83 | 1.31 |
| 8:C7:29:PHE:CZ | 8:C7:98:ALA:O | 1.82 | 1.31 |
| 8:i7:12:ASP:OD2 | 9:y7:46:LYS:NZ | 1.64 | 1.31 |
| 4:M8:225:LYS:N | 12:M8:301:CYC:O1A | 1.59 | 1.31 |
| 12:O8:201:CYC:CMA | 5:Z8:53:LEU:HD13 | 1.60 | 1.31 |
| 11:a9:275:THR:CA | 11:a9:278:LEU:CD1 | 1.96 | 1.31 |
| 5:N1:36:THR:OG1 | 12:T1:301:CYC:NB | 1.64 | 1.31 |
| 1:A:122:PRO:HB3 | 1:P5:64:ASP:OD2 | 1.16 | 1.30 |
| 3:BA:107:ASP:CB | 11:aA:382:ASN:HD22 | 1.42 | 1.30 |
| 3:FA:145:PRO:CG | 12:F9:302:CYC:HMC2 | 1.60 | 1.30 |
| 3:F4:113:LEU:N | 4:M4:5:THR:HA | 1.43 | 1.30 |
| 10:k5:978:LEU:CD2 | 1:p7:107:ARG:NH2 | 1.92 | 1.30 |
| 8:O7:49:ARG:HH12 | 1:r7:114:GLU:CD | 1.37 | 1.30 |
| 2:A8:33:ARG:NH1 | 12:L8:201:CYC:OB | 1.62 | 1.30 |
| 3:L8:65:ASP:O | 11:a9:82:GLN:NE2 | 1.63 | 1.30 |
| 4:M8:127:SER:N | 12:M8:302:CYC:HMA2 | 1.42 | 1.30 |
| 5:Z8:22:LEU:CD2 | 5:Z8:26:LEU:HD21 | 1.57 | 1.30 |
| 11:aA:75:ALA:HB1 | 11:aA:81:ASP:CB | 1.61 | 1.30 |
| 11:aA:283:GLN:CB | 11:aA:284:PRO:HD2 | 1.57 | 1.30 |
| 3:TA:21:GLU:CB | 2:R4:64:PRO:HG2 | 1.60 | 1.30 |
| 1:D5:73:TYR:O | 1:D5:77:ARG:HD3 | 1.30 | 1.30 |
| 1:f5:161:SER:O | 1:V5:101:PRO:HG3 | 1.26 | 1.30 |
| 12:L6:202:CYC:OB | 2:A6:33:ARG:NH1 | 1.62 | 1.30 |
| 4:M8:1:MET:N | 11:a9:149:SER:O | 1.63 | 1.30 |
| 4:M8:232:VAL:O | 4:M8:235:PHE:CD2 | 1.84 | 1.30 |
| 5:N9:22:LEU:CD2 | 5:N9:26:LEU:HD21 | 1.57 | 1.30 |
| 11:a9:75:ALA:HB1 | 11:a9:81:ASP:CB | 1.61 | 1.30 |
| 10:j5:1150:TYR:CE2 | 1:v7:69:GLY:O | 1.84 | 1.30 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:1153:VAL:CG2 | 1:v7:125:ALA:CB | 2.07 | 1.30 |
| 12:B8:202:CYC:CMA | 4:M8:58:TYR:H | 1.43 | 1.30 |
| 8:s7:29:PHE:CZ | 8:s7:98:ALA:O | 1.82 | 1.30 |
| 3:L8:68:ARG:CB | 11:a9:82:GLN:N | 1.94 | 1.30 |
| 4:M8:205:ASP:HB3 | 5:Z8:59:ARG:NE | 1.41 | 1.30 |
| 4:M8:214:GLY:N | 5:Z8:28:HIS:CE1 | 1.98 | 1.30 |
| 12:M8:302:CYC:OC | 3:S8:78:ARG:HD3 | 1.19 | 1.30 |
| 2:R8:64:PRO:HG2 | 3:T9:21:GLU:CB | 1.60 | 1.30 |
| 5:Z8:37:HIS:CD2 | 12:Z8:301:CYC:C4A | 2.12 | 1.30 |
| 11:a9:93:LEU:HD23 | 11:a9:252:ARG:NH1 | 1.44 | 1.30 |
| 11:a9:290:ASP:O | 11:a9:291:TYR:CD1 | 1.82 | 1.30 |
| 3:F2:82:CYS:SG | 12:F2:201:CYC:CAC | 2.18 | 1.30 |
| 3:F4:108:ARG:CZ | 4:M4:9:GLN:CG | 2.10 | 1.30 |
| 4:M4:29:PRO:HG3 | 11:aA:226:PHE:C | 1.54 | 1.30 |
| 3:O4:119:ALA:HB1 | 5:Z4:72:GLU:CB | 1.62 | 1.30 |
| 1:f7:67:ARG:HD3 | 11:aA:311:LEU:CD2 | 1.62 | 1.30 |
| 3:H8:111:ASN:CG | 11:a9:291:TYR:OH | 1.72 | 1.30 |
| 4:M8:104:ALA:HB1 | 2:P8:14:SER:CA | 1.59 | 1.30 |
| 2:N8:115:GLU:HG3 | 5:Z8:32:PRO:CG | 1.57 | 1.30 |
| 2:AA:33:ARG:NH1 | 12:LA:201:CYC:OB | 1.62 | 1.30 |
| 5:NA:61:LYS:NZ | 12:TA:301:CYC:HBB2 | 1.47 | 1.30 |
| 3:J3:84:ARG:HD2 | 11:a9:668:TYR:CB | 1.60 | 1.30 |
| 3:J3:85:ASP:OD1 | 11:a9:668:TYR:HE2 | 1.14 | 1.30 |
| 3:B4:86:MET:N | 12:B4:202:CYC:CBC | 1.95 | 1.30 |
| 5:N3:22:LEU:CD2 | 5:N3:26:LEU:HD21 | 1.58 | 1.30 |
| 2:N4:13:ASP:CG | 3:O4:108:ARG:NH1 | 1.90 | 1.30 |
| 8:Q5:17:TYR:CE2 | 1:R5:44:ILE:CG2 | 2.15 | 1.30 |
| 6:M6:50:LEU:CD2 | 8:c7:79:ALA:O | 1.79 | 1.30 |
| 10:k5:1018:LEU:CB | 10:k5:1021:ALA:HB3 | 1.62 | 1.30 |
| 8:i7:21:GLY:HA3 | 8:s7:100:ASP:OD1 | 1.17 | 1.30 |
| 1:f7:67:ARG:HH22 | 11:aA:307:ARG:CB | 1.44 | 1.30 |
| 3:TA:28:THR:HG21 | 2:X4:67:THR:C | 1.56 | 1.29 |
| 4:M4:87:ILE:HD13 | 3:Y4:77:ARG:CG | 1.61 | 1.29 |
| 8:M5:41:GLN:CD | 1:J7:143:PRO:HG3 | 1.55 | 1.29 |
| 8:Q5:16:ARG:N | 1:R5:90:ARG:HD3 | 1.46 | 1.29 |
| 10:k5:743:VAL:N | 12:D7:201:CYC:O2D | 1.63 | 1.29 |
| 2:N8:13:ASP:CG | 3:O8:108:ARG:NH1 | 1.89 | 1.29 |
| 3:O8:107:ASP:OD1 | 5:Z8:66:ARG:CD | 1.80 | 1.29 |
| 3:Q8:127:VAL:CG2 | 12:Z8:301:CYC:CMC | 2.09 | 1.29 |
| 12:L9:201:CYC:OB | 2:A9:33:ARG:NH1 | 1.62 | 1.29 |
| 2:G3:107:ASP:HA | 3:L3:77:ARG:NH2 | 1.47 | 1.29 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:L2:77:ARG:NH1 | 6:M2:70:GLU:OE2 | 1.65 | 1.29 |
| 10:j5:741:GLN:HG3 | 1:J7:77:ARG:NH2 | 1.48 | 1.29 |
| 8:o7:6:LYS:NZ | 8:o7:102:THR:OG1 | 1.59 | 1.29 |
| 12:M8:302:CYC:HMC3 | 3:S8:72:ASN:ND2 | 1.43 | 1.29 |
| 2:I9:37:SER:O | 2:I9:97:LEU:HD11 | 1.12 | 1.29 |
| 2:G1:107:ASP:HA | 3:L1:77:ARG:NH2 | 1.47 | 1.29 |
| 8:Q5:17:TYR:CE2 | 1:R5:93:THR:OG1 | 1.82 | 1.29 |
| 10:j5:1018:LEU:CB | 10:j5:1021:ALA:HB3 | 1.62 | 1.29 |
| 10:k5:1119:LEU:HD12 | 12:k5:1204:CYC:C4B | 1.60 | 1.29 |
| 8:g7:25:ARG:HH21 | 8:u7:25:ARG:CZ | 1.42 | 1.29 |
| 4:M8:127:SER:HB3 | 12:M8:302:CYC:CMA | 1.59 | 1.29 |
| 3:O8:108:ARG:CB | 5:Z8:61:LYS:CD | 1.97 | 1.29 |
| 4:M9:53:LEU:HD11 | 12:F9:301:CYC:C4B | 1.59 | 1.29 |
| 5:N9:53:LEU:HB3 | 12:T9:301:CYC:CBA | 1.62 | 1.29 |
| 2:K9:15:GLN:O | 11:a9:393:ARG:NH1 | 1.63 | 1.29 |
| 11:aA:476:ARG:NH1 | 11:aA:488:SER:CB | 1.95 | 1.29 |
| 2:O1:33:ARG:NH1 | 12:Z1:201:CYC:OB | 1.62 | 1.29 |
| 4:M4:82:ILE:CD1 | 12:M4:301:CYC:CGD | 2.10 | 1.29 |
| 2:P4:19:LEU:CG | 3:Q4:95:TYR:CE1 | 2.14 | 1.29 |
| 8:O5:29:PHE:CE1 | 8:O5:98:ALA:O | 1.86 | 1.29 |
| 1:J5:71:MEN:CA | 1:J5:77:ARG:HH11 | 1.38 | 1.29 |
| 8:U5:29:PHE:CZ | 8:U5:98:ALA:O | 1.83 | 1.29 |
| 8:U5:83:ARG:CB | 6:M6:26:PHE:HE1 | 1.44 | 1.29 |
| 8:W5:17:TYR:CE2 | 1:X5:44:ILE:CG2 | 2.15 | 1.29 |
| 8:a5:29:PHE:CE1 | 8:a5:98:ALA:O | 1.86 | 1.29 |
| 8:U7:29:PHE:CE1 | 8:U7:98:ALA:O | 1.86 | 1.29 |
| 4:M8:231:THR:H | 12:M8:301:CYC:CBB | 1.44 | 1.29 |
| 5:N9:61:LYS:NZ | 12:T9:301:CYC:HBB2 | 1.47 | 1.29 |
| 11:a9:239:TYR:CE2 | 12:a9:901:CYC:C4B | 2.15 | 1.29 |
| 3:JA:70:GLY:HA2 | 11:aA:357:THR:O | 1.23 | 1.29 |
| 2:A3:33:ARG:NH1 | 12:L3:201:CYC:OB | 1.62 | 1.29 |
| 2:A4:33:ARG:NH1 | 12:L4:201:CYC:OB | 1.62 | 1.29 |
| 3:L3:119:ALA:CB | 11:a9:813:PRO:CB | 2.11 | 1.29 |
| 3:L8:109:CYS:HA | 12:a9:901:CYC:CBB | 1.63 | 1.29 |
| 3:Q8:84:ARG:HG3 | 5:Z8:31:TRP:NE1 | 1.48 | 1.29 |
| 4:M9:53:LEU:HD11 | 12:F9:301:CYC:OB | 1.21 | 1.29 |
| 5:N9:1:MET:CG | 3:R9:119:ALA:CB | 2.11 | 1.29 |
| 11:aA:93:LEU:HD23 | 11:aA:252:ARG:NH1 | 1.44 | 1.29 |
| 2:K3:112:GLY:CA | 11:a9:670:LEU:CD2 | 1.97 | 1.28 |
| 4:M4:144:ARG:HH22 | 5:Z4:59:ARG:NH1 | 1.28 | 1.28 |
| 4:M4:197:ASP:OD1 | 5:Z4:52:ARG:NE | 1.65 | 1.28 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:Q5:16:ARG:CA | 1:R5:90:ARG:HD3 | 1.60 | 1.28 |
| 5:Z8:37:HIS:NE2 | 12:Z8:301:CYC:C4A | 1.96 | 1.28 |
| 11:aA:624:GLY:O | 11:aA:628:THR:CG2 | 1.81 | 1.28 |
| 4:MA:274:VAL:N | 3:VA:77:ARG:HG2 | 1.47 | 1.28 |
| 12:B4:202:CYC:CMA | 4:M4:58:TYR:H | 1.43 | 1.28 |
| 3:B1:88:ILE:HD13 | 12:B1:202:CYC:C3B | 1.63 | 1.28 |
| 8:I7:29:PHE:CE1 | 8:I7:98:ALA:O | 1.86 | 1.28 |
| 2:E1:13:ASP:CG | 11:aA:644:ARG:HH11 | 1.30 | 1.28 |
| 2:X8:67:THR:C | 3:T9:28:THR:HG21 | 1.56 | 1.28 |
| 11:aA:351:THR:CB | 11:aA:352:PRO:HD2 | 1.40 | 1.28 |
| 4:MA:274:VAL:HA | 3:VA:77:ARG:CD | 1.60 | 1.28 |
| 4:M4:227:GLN:O | 3:Y4:88:ILE:HG22 | 1.30 | 1.28 |
| 1:J5:20:ASP:O | 1:J5:22:ALA:N | 1.65 | 1.28 |
| 1:Z7:67:ARG:HH22 | 11:a9:307:ARG:CB | 1.44 | 1.28 |
| 4:M8:104:ALA:CA | 2:P8:14:SER:HB3 | 1.64 | 1.28 |
| 11:a9:476:ARG:NH1 | 11:a9:488:SER:CB | 1.95 | 1.28 |
| 3:J3:77:ARG:NH2 | 2:K3:107:ASP:HA | 1.48 | 1.28 |
| 5:N3:36:THR:OG1 | 12:T3:301:CYC:NB | 1.64 | 1.28 |
| 2:N4:13:ASP:OD2 | 3:O4:108:ARG:NH1 | 1.63 | 1.28 |
| 8:U5:29:PHE:CE1 | 8:U5:98:ALA:O | 1.86 | 1.28 |
| 10:j5:362:LYS:HD3 | 10:j5:363:HIS:CD2 | 1.69 | 1.28 |
| 8:c7:42:THR:CG2 | 8:c7:141:LEU:CD2 | 2.04 | 1.28 |
| 5:N1:22:LEU:CD2 | 5:N1:26:LEU:HD21 | 1.58 | 1.28 |
| 3:HA:126:SER:HB2 | 12:HA:202:CYC:CMC | 1.62 | 1.28 |
| 2:SA:42:ARG:NH1 | 3:TA:21:GLU:OE1 | 1.66 | 1.28 |
| 3:L4:71:GLY:CA | 11:aA:82:GLN:HG2 | 1.61 | 1.28 |
| 5:Z4:41:GLN:O | 12:Z4:301:CYC:HMA3 | 1.12 | 1.28 |
| 1:D5:20:ASP:O | 1:D5:22:ALA:N | 1.65 | 1.28 |
| 8:W5:16:ARG:N | 1:X5:90:ARG:HD3 | 1.46 | 1.28 |
| 8:W5:17:TYR:CE2 | 1:X5:44:ILE:HG21 | 1.68 | 1.28 |
| 10:k5:931:VAL:HG22 | 1:D7:29:ALA:O | 1.30 | 1.28 |
| 1:H7:136:VAL:HG13 | 11:aA:563:PHE:CZ | 1.68 | 1.28 |
| 8:W7:13:ALA:HA | 9:w7:46:LYS:NZ | 1.45 | 1.28 |
| 8:a7:63:PRO:CD | 11:a9:336:ILE:HG22 | 1.50 | 1.28 |
| 2:N8:14:SER:HB3 | 5:Z8:62:ARG:CZ | 1.64 | 1.28 |
| 11:aA:586:LEU:O | 11:aA:590:PRO:HG3 | 1.14 | 1.28 |
| 3:D4:14:LEU:CD1 | 3:Y4:125:ARG:HD2 | 1.62 | 1.27 |
| 1:d5:127:VAL:HG11 | 10:j5:698:GLY:N | 1.48 | 1.27 |
| 3:L6:125:ARG:CD | 1:b7:69:GLY:CA | 2.08 | 1.27 |
| 6:M6:283:VAL:HG12 | 8:Y7:75:GLU:CB | 1.64 | 1.27 |
| 8:C7:29:PHE:CE1 | 8:C7:98:ALA:O | 1.86 | 1.27 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:I7:76:LYS:HZ2 | 11:aA:567:GLN:NE2 | 1.28 | 1.27 |
| 8:c7:20:PRO:HG2 | 8:m7:155:TYR:CB | 1.63 | 1.27 |
| 3:D8:108:ARG:HD3 | 11:a9:107:ARG:NH1 | 0.94 | 1.27 |
| 3:H8:119:ALA:C | 11:a9:266:ASN:CB | 2.07 | 1.27 |
| 3:L9:14:LEU:HD11 | 11:a9:358:PRO:CB | 1.64 | 1.27 |
| 11:aA:798:SER:OG | 12:aA:901:CYC:HMA1 | 1.17 | 1.27 |
| 3:FA:150:ARG:HG2 | 3:F9:150:ARG:CB | 1.62 | 1.27 |
| 3:TA:32:LYS:HZ1 | 2:X4:57:GLN:CA | 1.46 | 1.27 |
| 3:TA:32:LYS:HD3 | 2:X4:57:GLN:NE2 | 1.46 | 1.27 |
| 12:J3:202:CYC:HMA1 | 11:a9:798:SER:OG | 1.18 | 1.27 |
| 6:M2:62:ARG:NH2 | 1:h7:58:LYS:HA | 1.49 | 1.27 |
| 5:Z4:41:GLN:CG | 12:Z4:301:CYC:CMB | 2.11 | 1.27 |
| 8:I5:29:PHE:CE1 | 8:I5:98:ALA:O | 1.86 | 1.27 |
| 8:e5:29:PHE:CE1 | 8:e5:98:ALA:O | 1.86 | 1.27 |
| 1:f5:18:TYR:CE1 | 10:j5:165:ARG:HD3 | 1.68 | 1.27 |
| 8:m7:29:PHE:CE1 | 8:m7:98:ALA:O | 1.86 | 1.27 |
| 2:X8:57:GLN:NE2 | 3:T9:32:LYS:HD3 | 1.46 | 1.27 |
| 3:F8:84:ARG:HD3 | 11:a9:139:ILE:CG2 | 1.61 | 1.27 |
| 3:F8:109:CYS:C | 4:M8:6:THR:HG22 | 1.58 | 1.27 |
| 5:N9:54:LEU:HD22 | 3:T9:84:ARG:NE | 1.43 | 1.27 |
| 3:L2:77:ARG:CZ | 6:M2:70:GLU:OE2 | 1.81 | 1.27 |
| 2:E4:1:MET:N | 4:M4:10:ARG:NH2 | 1.78 | 1.27 |
| 4:M4:226:SER:HB2 | 3:Y4:85:ASP:OD1 | 1.21 | 1.27 |
| 1:Z5:28:LYS:CD | 1:t7:143:PRO:CG | 2.09 | 1.27 |
| 8:O7:29:PHE:CE1 | 8:O7:98:ALA:O | 1.86 | 1.27 |
| 8:g7:29:PHE:CE1 | 8:g7:98:ALA:O | 1.86 | 1.27 |
| 3:F8:115:GLU:CD | 4:M8:3:VAL:HG22 | 1.58 | 1.27 |
| 2:N8:115:GLU:CB | 5:Z8:32:PRO:CG | 2.11 | 1.27 |
| 3:O8:107:ASP:CG | 5:Z8:66:ARG:HB3 | 1.59 | 1.27 |
| 3:J9:70:GLY:HA2 | 11:a9:357:THR:O | 1.21 | 1.27 |
| 11:a9:50:LEU:O | 11:a9:53:VAL:HB | 1.29 | 1.27 |
| 3:LA:14:LEU:HD11 | 11:aA:358:PRO:CB | 1.65 | 1.27 |
| 5:NA:53:LEU:HB3 | 12:TA:301:CYC:CBA | 1.62 | 1.27 |
| 3:D4:108:ARG:HD3 | 11:aA:107:ARG:NH1 | 0.95 | 1.27 |
| 4:M4:138:SER:HB2 | 4:M4:215:GLU:OE2 | 1.21 | 1.27 |
| 8:G5:61:ILE:HD11 | 8:o7:67:SER:CB | 1.64 | 1.27 |
| 8:U5:75:GLU:OE1 | 6:M6:43:TRP:CZ2 | 1.87 | 1.27 |
| 3:B8:120:LEU:CD1 | 4:M8:53:LEU:HB2 | 1.64 | 1.27 |
| 3:Q8:89:ILE:CG2 | 3:Q8:92:TYR:OH | 1.81 | 1.27 |
| 3:L9:52:ILE:CD1 | 3:L9:87:GLU:HB2 | 1.64 | 1.27 |
| 4:M9:53:LEU:CD1 | 12:F9:301:CYC:NB | 1.93 | 1.27 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:a9:624:GLY:O | 11:a9:628:THR:CG2 | 1.81 | 1.27 |
| 11:aA:624:GLY:O | 11:aA:628:THR:HG22 | 1.19 | 1.27 |
| 1:A:73:TYR:HE1 | 10:k5:162:TRP:CH2 | 1.52 | 1.27 |
| 3:HA:66:LEU:HD22 | 12:HA:202:CYC:OC | 1.18 | 1.27 |
| 2:IA:37:SER:O | 2:IA:97:LEU:HD11 | 1.12 | 1.27 |
| 3:J3:14:LEU:HD22 | 11:a9:621:THR:CG2 | 1.64 | 1.27 |
| 6:M2:127:SER:O | 12:F2:201:CYC:CBA | 1.82 | 1.27 |
| 3:S4:113:LEU:O | 3:S4:116:THR:HG22 | 1.22 | 1.27 |
| 2:N4:63:PHE:HB2 | 2:N4:66:LEU:CD1 | 1.64 | 1.27 |
| 1:N5:53:LYS:HD3 | 8:O5:118:SER:O | 1.12 | 1.27 |
| 8:C5:29:PHE:CE1 | 8:C5:98:ALA:O | 1.86 | 1.27 |
| 6:M6:127:SER:HB3 | 3:F6:84:ARG:NH1 | 1.50 | 1.27 |
| 10:j5:978:LEU:HD21 | 1:v7:107:ARG:NH2 | 0.96 | 1.27 |
| 10:k5:362:LYS:HD3 | 10:k5:363:HIS:CD2 | 1.69 | 1.27 |
| 8:i7:25:ARG:NH2 | 8:s7:6:LYS:CB | 1.98 | 1.27 |
| 8:s7:29:PHE:CE1 | 8:s7:98:ALA:O | 1.86 | 1.27 |
| 2:N8:13:ASP:OD2 | 3:O8:108:ARG:NH1 | 1.63 | 1.27 |
| 3:H9:66:LEU:HD22 | 12:H9:202:CYC:OC | 1.18 | 1.27 |
| 2:S9:42:ARG:NH1 | 3:T9:21:GLU:OE1 | 1.66 | 1.27 |
| 4:M1:232:VAL:HG13 | 3:V1:111:ASN:O | 1.25 | 1.27 |
| 3:B4:82:CYS:HA | 12:B4:202:CYC:C1C | 1.64 | 1.26 |
| 1:J5:73:TYR:O | 1:J5:77:ARG:HD3 | 1.30 | 1.26 |
| 8:o7:27:LYS:CE | 1:p7:35:ALA:CB | 2.13 | 1.26 |
| 8:q7:66:VAL:O | 11:aA:65:LEU:HD21 | 1.32 | 1.26 |
| 2:X8:64:PRO:C | 3:T9:25:ASN:HB3 | 1.60 | 1.26 |
| 2:X8:69:PRO:HG2 | 2:S9:38:MET:O | 1.27 | 1.26 |
| 3:Q8:85:ASP:CG | 12:Z8:301:CYC:CBC | 2.07 | 1.26 |
| 4:M9:181:GLN:NE2 | 3:V9:120:LEU:HD21 | 1.50 | 1.26 |
| 11:aA:50:LEU:O | 11:aA:53:VAL:HB | 1.29 | 1.26 |
| 12:FA:301:CYC:C4B | 4:MA:53:LEU:HD11 | 1.59 | 1.26 |
| 12:R1:201:CYC:NB | 5:N1:54:LEU:HD12 | 1.48 | 1.26 |
| 3:D4:108:ARG:HD3 | 11:aA:107:ARG:CZ | 1.59 | 1.26 |
| 5:N3:54:LEU:HD12 | 12:R3:201:CYC:NB | 1.48 | 1.26 |
| 4:M4:101:ASP:HA | 2:P4:13:ASP:CB | 1.63 | 1.26 |
| 2:C1:115:GLU:OE2 | 4:M1:33:LEU:HD23 | 1.15 | 1.26 |
| 8:c7:15:ALA:C | 1:d7:90:ARG:NE | 1.93 | 1.26 |
| 4:M8:126:THR:HB | 12:M8:302:CYC:O2A | 1.20 | 1.26 |
| 11:aA:742:GLN:OE1 | 3:L1:84:ARG:HG2 | 1.26 | 1.26 |
| 1:Z:158:SER:CB | 1:X5:11:ASN:HD21 | 1.40 | 1.26 |
| 2:O1:63:PHE:HB2 | 2:O1:66:LEU:CD1 | 1.64 | 1.26 |
| 2:A4:63:PHE:HB2 | 2:A4:66:LEU:CD1 | 1.64 | 1.26 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:O7:49:ARG:NH1 | 1:r7:114:GLU:OE2 | 1.69 | 1.26 |
| 8:a7:29:PHE:CE1 | 8:a7:98:ALA:O | 1.86 | 1.26 |
| 1:f7:10:ASN:HB2 | 9:y7:65:THR:OG1 | 1.36 | 1.26 |
| 2:X8:74:TYR:OH | 2:S9:35:THR:HG22 | 1.27 | 1.26 |
| 3:F8:107:ASP:CG | 4:M8:8:SER:O | 1.78 | 1.26 |
| 3:J3:84:ARG:C | 11:a9:668:TYR:OH | 1.78 | 1.26 |
| 3:B3:88:ILE:HG21 | 12:B3:202:CYC:CAB | 1.65 | 1.26 |
| 3:B1:88:ILE:CG2 | 12:B1:202:CYC:CMB | 2.13 | 1.26 |
| 3:L4:68:ARG:NH1 | 11:aA:81:ASP:N | 1.82 | 1.26 |
| 8:Q5:17:TYR:CE2 | 1:R5:44:ILE:HG21 | 1.68 | 1.26 |
| 10:j5:138:PRO:CB | 10:j5:201:VAL:HG11 | 1.65 | 1.26 |
| 12:M8:302:CYC:C2C | 3:S8:78:ARG:CD | 2.13 | 1.26 |
| 2:N8:63:PHE:HB2 | 2:N8:66:LEU:CD1 | 1.64 | 1.26 |
| 5:NA:1:MET:CG | 3:RA:119:ALA:CB | 2.11 | 1.26 |
| 3:B4:116:THR:CB | 4:M4:56:MET:CG | 2.03 | 1.26 |
| 12:L3:202:CYC:OB | 11:a9:738:LEU:HD22 | 1.09 | 1.26 |
| 1:d5:161:SER:CB | 10:j5:695:GLY:O | 1.81 | 1.26 |
| 1:b5:18:TYR:CE2 | 10:k5:165:ARG:HA | 1.70 | 1.26 |
| 10:j5:386:ILE:HG22 | 10:j5:395:SER:O | 1.36 | 1.26 |
| 10:k5:1077:ILE:C | 12:k5:1203:CYC:HBA2 | 1.57 | 1.26 |
| 4:M8:139:VAL:CG2 | 4:M8:216:ASN:HA | 1.65 | 1.26 |
| 4:M8:224:PHE:C | 12:M8:301:CYC:O1A | 1.76 | 1.26 |
| 2:O9:63:PHE:HB2 | 2:O9:66:LEU:CD1 | 1.64 | 1.26 |
| 2:A9:63:PHE:HB2 | 2:A9:66:LEU:CD1 | 1.64 | 1.26 |
| 3:HA:126:SER:CB | 12:HA:202:CYC:CMC | 2.11 | 1.25 |
| 3:LA:52:ILE:CD1 | 3:LA:87:GLU:HB2 | 1.64 | 1.25 |
| 2:QA:119:THR:HB | 3:TA:83:LEU:CD1 | 1.62 | 1.25 |
| 3:B4:116:THR:CB | 4:M4:56:MET:HG2 | 1.61 | 1.25 |
| 4:M3:77:LEU:HD11 | 3:X3:115:GLU:OE2 | 1.09 | 1.25 |
| 4:M3:232:VAL:HG13 | 3:V3:111:ASN:O | 1.25 | 1.25 |
| 2:O3:63:PHE:HB2 | 2:O3:66:LEU:CD1 | 1.64 | 1.25 |
| 2:C1:115:GLU:OE2 | 4:M1:33:LEU:CD2 | 1.83 | 1.25 |
| 1:d5:28:LYS:HZ2 | 1:n7:143:PRO:CG | 1.45 | 1.25 |
| 8:S5:41:GLN:OE1 | 1:D7:143:PRO:HG3 | 1.20 | 1.25 |
| 10:j5:1008:PHE:CZ | 1:v7:87:TYR:HE2 | 1.37 | 1.25 |
| 8:i7:20:PRO:HG3 | 8:s7:155:TYR:CD2 | 1.69 | 1.25 |
| 8:u7:27:LYS:CE | 1:v7:35:ALA:CB | 2.13 | 1.25 |
| 4:MA:181:GLN:NE2 | 3:VA:120:LEU:HD21 | 1.50 | 1.25 |
| 5:NA:61:LYS:HD3 | 3:TA:108:ARG:O | 1.27 | 1.25 |
| 2:A3:63:PHE:HB2 | 2:A3:66:LEU:CD1 | 1.64 | 1.25 |
| 10:k5:1150:TYR:CE1 | 11:a9:38:VAL:HG22 | 1.71 | 1.25 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:U8:108:ARG:CA | 4:M8:246:ALA:CB | 2.01 | 1.25 |
| 2:K9:15:GLN:CB | 11:a9:393:ARG:NH1 | 1.98 | 1.25 |
| 2:A2:63:PHE:HB2 | 2:A2:66:LEU:CD1 | 1.64 | 1.25 |
| 1:Z:110:ASN:OD1 | 10:j5:462:TYR:CE1 | 1.90 | 1.25 |
| 2:AA:63:PHE:HB2 | 2:AA:66:LEU:CD1 | 1.64 | 1.25 |
| 2:G2:113:LEU:HA | 3:L2:76:ASN:ND2 | 1.51 | 1.25 |
| 2:C3:115:GLU:OE2 | 4:M3:33:LEU:CD2 | 1.83 | 1.25 |
| 3:F4:109:CYS:C | 4:M4:6:THR:CG2 | 2.08 | 1.25 |
| 5:NA:54:LEU:HD12 | 12:TA:301:CYC:NB | 1.51 | 1.25 |
| 3:H4:119:ALA:C | 11:aA:266:ASN:CB | 2.07 | 1.25 |
| 4:M4:144:ARG:NH2 | 5:Z4:59:ARG:NH1 | 1.81 | 1.25 |
| 1:T5:53:LYS:HD3 | 8:U5:118:SER:O | 1.12 | 1.25 |
| 8:W5:15:ALA:C | 1:X5:90:ARG:HD3 | 1.59 | 1.25 |
| 10:j5:1119:LEU:HD22 | 1:t7:87:TYR:OH | 1.37 | 1.25 |
| 4:M4:215:GLU:CD | 12:Z4:301:CYC:HAB1 | 1.58 | 1.25 |
| 10:j5:974:LEU:HD12 | 1:v7:106:GLU:OE2 | 1.31 | 1.25 |
| 10:j5:1015:TYR:O | 10:j5:1017:ARG:CG | 1.85 | 1.25 |
| 10:k5:138:PRO:CB | 10:k5:201:VAL:HG11 | 1.65 | 1.25 |
| 2:A6:63:PHE:HB2 | 2:A6:66:LEU:CD1 | 1.64 | 1.25 |
| 8:k7:76:LYS:NZ | 11:a9:605:PRO:HB3 | 1.51 | 1.25 |
| 8:u7:37:LEU:CD2 | 1:v7:24:LEU:CD2 | 2.14 | 1.25 |
| 4:M8:217:VAL:HG22 | 5:Z8:30:PRO:CG | 1.49 | 1.25 |
| 12:O8:201:CYC:HMA1 | 5:Z8:53:LEU:CD1 | 1.65 | 1.25 |
| 3:Q8:120:LEU:HD12 | 3:Q8:122:THR:N | 1.50 | 1.25 |
| 3:L9:14:LEU:CG | 11:a9:358:PRO:CB | 2.10 | 1.25 |
| 3:F9:153:CYS:CB | 12:F9:303:CYC:HAC1 | 1.66 | 1.25 |
| 11:a9:586:LEU:O | 11:a9:590:PRO:HG3 | 1.14 | 1.25 |
| 11:aA:30:MET:HB3 | 11:aA:34:ILE:O | 1.31 | 1.25 |
| 3:Q8:120:LEU:CD1 | 3:Q8:122:THR:N | 1.98 | 1.25 |
| 4:M9:232:VAL:CG1 | 3:X9:111:ASN:O | 1.84 | 1.25 |
| 11:aA:621:THR:CG2 | 3:J1:14:LEU:HD22 | 1.64 | 1.25 |
| 2:A1:63:PHE:HB2 | 2:A1:66:LEU:CD1 | 1.64 | 1.25 |
| 3:F4:115:GLU:CG | 4:M4:3:VAL:CG1 | 2.15 | 1.25 |
| 8:Q5:15:ALA:C | 1:R5:90:ARG:HD3 | 1.59 | 1.25 |
| 1:V5:107:ARG:NH2 | 10:j5:619:GLU:OE1 | 1.70 | 1.25 |
| 8:W5:17:TYR:CE2 | 1:X5:93:THR:OG1 | 1.82 | 1.25 |
| 10:j5:868:ASP:O | 9:w7:43:ARG:HD2 | 1.12 | 1.25 |
| 10:j5:868:ASP:O | 9:w7:43:ARG:CD | 1.84 | 1.25 |
| 10:k5:803:LYS:NZ | 9:z7:40:GLU:OE1 | 1.65 | 1.25 |
| 8:Q7:25:ARG:HB3 | 8:C7:25:ARG:NH2 | 1.42 | 1.25 |
| 1:d7:87:TYR:CE2 | 9:x7:38:PHE:CZ | 2.24 | 1.25 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:A8:63:PHE:HB2 | 2:A8:66:LEU:CD1 | 1.64 | 1.25 |
| 3:H8:84:ARG:HB3 | 11:a9:131:TYR:CZ | 1.71 | 1.25 |
| 4:M8:226:SER:HB2 | 3:Y8:85:ASP:OD1 | 1.08 | 1.25 |
| 5:N9:54:LEU:HD12 | 12:T9:301:CYC:NB | 1.51 | 1.25 |
| 12:B1:202:CYC:CBA | 11:aA:684:ASN:CB | 2.12 | 1.25 |
| 8:O5:76:LYS:CD | 8:O5:77:MET:CE | 2.15 | 1.25 |
| 1:V5:114:GLU:CG | 10:j5:496:GLU:CG | 2.04 | 1.25 |
| 10:j5:803:LYS:NZ | 9:w7:40:GLU:OE1 | 1.67 | 1.25 |
| 10:j5:1146:THR:CB | 1:v7:77:ARG:NH2 | 1.99 | 1.25 |
| 10:k5:1152:TYR:CE2 | 8:G7:68:PRO:CG | 2.16 | 1.25 |
| 3:L8:86:MET:CG | 12:a9:901:CYC:HBC1 | 1.66 | 1.25 |
| 12:M8:302:CYC:C2C | 3:S8:78:ARG:HD3 | 1.65 | 1.25 |
| 11:aA:742:GLN:NE2 | 3:L1:88:ILE:HG13 | 0.93 | 1.25 |
| 11:aA:813:PRO:CB | 3:L1:119:ALA:CB | 2.13 | 1.25 |
| 2:OA:63:PHE:HB2 | 2:OA:66:LEU:CD1 | 1.64 | 1.24 |
| 3:TA:25:ASN:HB3 | 2:X4:64:PRO:C | 1.60 | 1.24 |
| 8:U5:76:LYS:CD | 8:U5:77:MET:CE | 2.15 | 1.24 |
| 10:j5:743:VAL:N | 12:J7:201:CYC:O2D | 1.70 | 1.24 |
| 10:j5:935:LEU:CD1 | 1:J7:29:ALA:HB2 | 1.67 | 1.24 |
| 8:i7:47:ARG:CD | 1:j7:18:TYR:CE2 | 2.05 | 1.24 |
| 9:x7:3:ARG:CZ | 9:x7:67:VAL:CG1 | 2.14 | 1.24 |
| 4:M8:138:SER:HB2 | 4:M8:215:GLU:OE2 | 1.21 | 1.24 |
| 11:a9:95:ILE:HD11 | 11:a9:237:PHE:CE1 | 1.73 | 1.24 |
| 4:MA:232:VAL:CG1 | 3:XA:111:ASN:O | 1.84 | 1.24 |
| 3:J3:14:LEU:CD2 | 11:a9:621:THR:CG2 | 2.15 | 1.24 |
| 3:B4:82:CYS:O | 12:B4:202:CYC:HAC2 | 1.10 | 1.24 |
| 8:G5:61:ILE:CG1 | 8:o7:68:PRO:HD2 | 1.65 | 1.24 |
| 1:Z5:127:VAL:HG11 | 10:k5:698:GLY:CA | 1.66 | 1.24 |
| 1:b5:3:ASP:OD2 | 10:k5:21:MET:HB3 | 1.35 | 1.24 |
| 8:i7:39:ILE:HD13 | 8:i7:148:GLU:CG | 1.63 | 1.24 |
| 2:N8:14:SER:HB3 | 5:Z8:62:ARG:CD | 1.64 | 1.24 |
| 3:Q8:85:ASP:OD2 | 12:Z8:301:CYC:HBC3 | 1.08 | 1.24 |
| 3:F9:150:ARG:NH1 | 12:F9:302:CYC:C1C | 2.00 | 1.24 |
| 11:aA:31:SER:OG | 11:aA:34:ILE:HB | 1.22 | 1.24 |
| 6:M2:28:ASN:CB | 8:O5:80:LEU:HD21 | 1.61 | 1.24 |
| 5:Z4:24:PRO:HG2 | 12:Z4:301:CYC:O2A | 1.33 | 1.24 |
| 1:b5:38:VAL:CG1 | 10:k5:40:VAL:CG1 | 2.16 | 1.24 |
| 10:k5:386:ILE:HG22 | 10:k5:395:SER:O | 1.36 | 1.24 |
| 10:k5:978:LEU:CD2 | 1:p7:107:ARG:HH21 | 1.49 | 1.24 |
| 10:k5:1008:PHE:CZ | 1:p7:87:TYR:HE2 | 1.55 | 1.24 |
| 10:k5:1077:ILE:O | 12:k5:1203:CYC:CBA | 1.85 | 1.24 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M8:104:ALA:CB | 2:P8:14:SER:CB | 1.78 | 1.24 |
| 3:LA:14:LEU:CG | 11:aA:358:PRO:CB | 2.11 | 1.24 |
| 2:A1:16:GLY:HA2 | 11:aA:677:GLN:NE2 | 1.52 | 1.24 |
| 5:Z4:42:SER:HA | 12:Z4:301:CYC:CMA | 1.68 | 1.24 |
| 8:G5:61:ILE:CD1 | 8:o7:67:SER:HB3 | 1.66 | 1.24 |
| 10:k5:1049:PHE:CE1 | 10:k5:1065:HIS:HE1 | 1.55 | 1.24 |
| 8:i7:47:ARG:CD | 1:j7:18:TYR:CE1 | 2.18 | 1.24 |
| 12:B8:202:CYC:CBB | 4:M8:61:ASN:HB2 | 1.66 | 1.24 |
| 8:o7:37:LEU:HD22 | 1:p7:24:LEU:CD2 | 1.68 | 1.24 |
| 3:Q8:120:LEU:CD1 | 3:Q8:122:THR:H | 1.50 | 1.24 |
| 4:M9:274:VAL:HA | 3:V9:77:ARG:CD | 1.68 | 1.24 |
| 3:B9:26:GLN:O | 3:B9:30:LEU:CD1 | 1.86 | 1.24 |
| 4:M4:223:GLY:O | 12:M4:301:CYC:HBA2 | 1.33 | 1.24 |
| 3:O4:107:ASP:OD1 | 5:Z4:66:ARG:HD2 | 1.11 | 1.24 |
| 6:M6:277:GLY:HA2 | 1:d7:62:TYR:O | 1.08 | 1.24 |
| 10:k5:1015:TYR:O | 10:k5:1017:ARG:CG | 1.85 | 1.24 |
| 3:H9:126:SER:HB2 | 12:H9:202:CYC:CMC | 1.67 | 1.24 |
| 11:aA:707:PHE:CE2 | 3:L1:108:ARG:NH1 | 2.06 | 1.24 |
| 2:QA:76:ASP:HB3 | 2:U1:140:SER:O | 1.34 | 1.23 |
| 3:TA:28:THR:HG21 | 2:X4:67:THR:CB | 1.61 | 1.23 |
| 6:M2:127:SER:HB3 | 3:F2:84:ARG:NH1 | 1.50 | 1.23 |
| 3:S4:72:ASN:ND2 | 3:S4:123:PRO:HD3 | 1.49 | 1.23 |
| 3:U4:108:ARG:CA | 4:M4:246:ALA:CB | 2.16 | 1.23 |
| 1:f5:161:SER:O | 1:V5:101:PRO:CG | 1.86 | 1.23 |
| 1:b5:3:ASP:OD2 | 10:k5:21:MET:CB | 1.83 | 1.23 |
| 10:j5:924:ASP:OD1 | 1:J7:26:LYS:NZ | 1.68 | 1.23 |
| 8:u7:90:ARG:HD3 | 1:v7:18:TYR:CE1 | 1.73 | 1.23 |
| 9:z7:4:TYR:O | 9:z7:56:LEU:O | 1.56 | 1.23 |
| 9:y7:3:ARG:CZ | 9:y7:67:VAL:CG1 | 2.14 | 1.23 |
| 2:QA:68:GLN:HA | 2:U1:46:SER:CB | 1.66 | 1.23 |
| 4:M4:100:SER:N | 3:Q4:1:MET:CE | 2.00 | 1.23 |
| 3:Q4:72:ASN:CG | 12:Z4:301:CYC:HMD2 | 1.61 | 1.23 |
| 1:d5:28:LYS:CD | 1:n7:143:PRO:CB | 2.16 | 1.23 |
| 8:i7:42:THR:CG2 | 8:i7:141:LEU:CD2 | 2.04 | 1.23 |
| 3:H9:126:SER:CB | 12:H9:202:CYC:CMC | 2.15 | 1.23 |
| 4:M1:77:LEU:HD11 | 3:X1:115:GLU:OE2 | 1.09 | 1.23 |
| 3:DA:115:GLU:OE2 | 4:MA:76:ALA:O | 1.56 | 1.23 |
| 3:FA:150:ARG:HA | 3:F9:150:ARG:CG | 1.69 | 1.23 |
| 3:TA:32:LYS:NZ | 2:X4:57:GLN:HA | 1.52 | 1.23 |
| 1:d5:161:SER:HB3 | 10:j5:695:GLY:O | 1.35 | 1.23 |
| 8:A7:56:ASP:OD1 | 11:aA:586:LEU:HD11 | 1.10 | 1.23 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:1049:PHE:CE1 | 10:j5:1065:HIS:HE1 | 1.55 | 1.23 |
| 10:j5:1150:TYR:CE1 | 11:aA:38:VAL:HG22 | 1.74 | 1.23 |
| 8:u7:90:ARG:HD3 | 1:v7:18:TYR:CD1 | 1.73 | 1.23 |
| 4:M9:232:VAL:HG13 | 3:X9:111:ASN:O | 1.14 | 1.23 |
| 11:a9:56:ILE:HD11 | 11:a9:612:TYR:CE2 | 1.74 | 1.23 |
| 2:SA:38:MET:O | 2:X4:69:PRO:HG2 | 1.27 | 1.23 |
| 1:Z5:110:ASN:HD21 | 10:k5:451:LYS:CB | 1.51 | 1.23 |
| 10:k5:966:SER:CA | 1:p7:14:VAL:HG11 | 1.51 | 1.23 |
| 8:o7:37:LEU:CD2 | 1:p7:24:LEU:CD2 | 2.14 | 1.23 |
| 1:p7:136:VAL:HG13 | 11:a9:342:ARG:NH1 | 1.52 | 1.23 |
| 3:F8:84:ARG:CD | 11:a9:139:ILE:CG2 | 2.15 | 1.23 |
| 11:aA:55:ASP:HB3 | 11:aA:612:TYR:CB | 1.68 | 1.23 |
| 3:H4:84:ARG:NE | 11:aA:131:TYR:CD2 | 2.04 | 1.23 |
| 5:Z4:44:TYR:CE2 | 5:Z4:46:THR:OG1 | 1.91 | 1.23 |
| 6:M6:127:SER:O | 12:F6:201:CYC:HBA1 | 1.39 | 1.23 |
| 8:o7:90:ARG:HD3 | 1:p7:18:TYR:CD1 | 1.73 | 1.23 |
| 2:X8:57:GLN:CA | 3:T9:32:LYS:HZ1 | 1.52 | 1.23 |
| 11:aA:95:ILE:HD11 | 11:aA:237:PHE:CE1 | 1.72 | 1.23 |
| 2:EA:115:GLU:OE2 | 4:MA:33:LEU:HD23 | 1.39 | 1.22 |
| 12:B4:202:CYC:CBB | 4:M4:61:ASN:HB2 | 1.66 | 1.22 |
| 3:U4:108:ARG:CA | 4:M4:246:ALA:HB2 | 1.67 | 1.22 |
| 12:L4:202:CYC:OB | 11:aA:239:TYR:HD1 | 1.06 | 1.22 |
| 11:aA:745:GLY:HA3 | 2:K1:15:GLN:CA | 1.69 | 1.22 |
| 4:MA:157:PHE:O | 3:VA:108:ARG:HD2 | 1.06 | 1.22 |
| 3:L2:77:ARG:HH22 | 6:M2:70:GLU:CD | 1.45 | 1.22 |
| 3:Z3:119:ALA:CB | 4:M3:263:PRO:HB2 | 1.70 | 1.22 |
| 3:H4:84:ARG:HB3 | 11:aA:131:TYR:CZ | 1.72 | 1.22 |
| 1:X5:110:ASN:OD1 | 10:j5:466:LEU:HB2 | 1.33 | 1.22 |
| 1:Z5:28:LYS:NZ | 1:t7:143:PRO:HB2 | 1.40 | 1.22 |
| 10:k5:156:SER:OG | 12:k5:1201:CYC:H3C | 1.35 | 1.22 |
| 10:k5:362:LYS:CD | 10:k5:363:HIS:CD2 | 2.21 | 1.22 |
| 10:k5:889:LEU:HD23 | 12:D7:201:CYC:CBB | 1.49 | 1.22 |
| 8:O7:52:LYS:HE3 | 11:aA:29:ARG:NH1 | 1.53 | 1.22 |
| 8:o7:90:ARG:HD3 | 1:p7:18:TYR:CE1 | 1.73 | 1.22 |
| 3:Q8:89:ILE:HG23 | 3:Q8:92:TYR:OH | 1.10 | 1.22 |
| 4:M9:274:VAL:N | 3:V9:77:ARG:HG2 | 1.53 | 1.22 |
| 11:aA:621:THR:CG2 | 3:J1:14:LEU:CD2 | 2.15 | 1.22 |
| 11:aA:710:THR:CG2 | 11:aA:807:GLN:CG | 2.16 | 1.22 |
| 11:aA:817:LEU:HD12 | 3:L1:119:ALA:O | 1.33 | 1.22 |
| 3:BA:26:GLN:O | 3:BA:30:LEU:CD1 | 1.86 | 1.22 |
| 2:A3:16:GLY:HA2 | 11:a9:677:GLN:NE2 | 1.51 | 1.22 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:X5:63:SER:OG | 10:j5:706:PRO:HA | 1.35 | 1.22 |
| 8:O7:25:ARG:HH21 | 8:E7:25:ARG:CB | 1.52 | 1.22 |
| 8:i7:94:TYR:CZ | 1:j7:9:ILE:HG23 | 1.73 | 1.22 |
| 2:E8:1:MET:N | 4:M8:10:ARG:HH21 | 1.37 | 1.22 |
| 2:X8:57:GLN:HA | 3:T9:32:LYS:NZ | 1.52 | 1.22 |
| 3:F8:115:GLU:OE2 | 4:M8:3:VAL:HG22 | 1.38 | 1.22 |
| 11:a9:30:MET:HB3 | 11:a9:34:ILE:O | 1.31 | 1.22 |
| 11:a9:55:ASP:HB3 | 11:a9:612:TYR:CB | 1.68 | 1.22 |
| 11:a9:239:TYR:HE2 | 12:a9:901:CYC:OB | 0.90 | 1.22 |
| 11:aA:738:LEU:HD22 | 12:aA:902:CYC:OB | 1.08 | 1.22 |
| 3:L4:66:LEU:N | 11:aA:82:GLN:OE1 | 1.72 | 1.22 |
| 8:U5:83:ARG:CG | 6:M6:31:ASP:OD1 | 1.87 | 1.22 |
| 1:Z5:28:LYS:CE | 1:t7:143:PRO:CG | 2.18 | 1.22 |
| 8:o7:121:THR:CG2 | 12:o7:201:CYC:HMC3 | 1.68 | 1.22 |
| 8:u7:121:THR:CG2 | 12:u7:201:CYC:HMC3 | 1.68 | 1.22 |
| 3:L8:82:CYS:SG | 12:a9:901:CYC:CAC | 2.28 | 1.22 |
| 3:L9:14:LEU:CD2 | 11:a9:358:PRO:CB | 1.86 | 1.22 |
| 6:M2:37:GLU:OE2 | 8:O5:59:PHE:CD2 | 1.92 | 1.22 |
| 3:B4:120:LEU:HD11 | 4:M4:53:LEU:N | 1.54 | 1.22 |
| 12:B4:202:CYC:HMA2 | 4:M4:58:TYR:N | 1.55 | 1.22 |
| 1:B5:14:VAL:CG1 | 10:k5:554:ASN:O | 1.85 | 1.22 |
| 1:T5:110:ASN:CG | 10:j5:692:LEU:O | 1.80 | 1.22 |
| 8:W5:15:ALA:C | 1:X5:90:ARG:CD | 2.12 | 1.22 |
| 8:c7:96:ILE:CG1 | 8:c7:152:TYR:CD1 | 2.22 | 1.22 |
| 12:D8:202:CYC:O2A | 4:M8:35:THR:HB | 1.38 | 1.22 |
| 3:Q8:120:LEU:CD1 | 3:Q8:122:THR:CB | 2.16 | 1.22 |
| 2:I9:37:SER:O | 2:I9:97:LEU:CD1 | 1.88 | 1.22 |
| 11:a9:239:TYR:CE2 | 12:a9:901:CYC:NB | 2.08 | 1.22 |
| 6:M2:26:PHE:CZ | 8:O5:87:TYR:HD1 | 1.40 | 1.21 |
| 3:L4:68:ARG:HB2 | 11:aA:82:GLN:N | 1.50 | 1.21 |
| 10:j5:766:ALA:CB | 8:K7:14:GLU:OE2 | 1.88 | 1.21 |
| 10:j5:1018:LEU:HD13 | 10:j5:1035:PHE:CE2 | 1.74 | 1.21 |
| 10:k5:743:VAL:CG1 | 12:D7:201:CYC:O2D | 1.87 | 1.21 |
| 10:k5:966:SER:CA | 1:p7:14:VAL:HG12 | 1.52 | 1.21 |
| 8:i7:96:ILE:CG1 | 8:i7:152:TYR:CD1 | 2.22 | 1.21 |
| 4:M8:91:VAL:HG22 | 2:P8:14:SER:O | 1.27 | 1.21 |
| 11:aA:56:ILE:HD11 | 11:aA:612:TYR:CE2 | 1.74 | 1.21 |
| 11:aA:742:GLN:CD | 3:L1:88:ILE:HG13 | 1.58 | 1.21 |
| 11:aA:800:THR:CG2 | 12:aA:901:CYC:CAA | 2.18 | 1.21 |
| 3:HA:116:THR:OG1 | 11:aA:449:ASN:ND2 | 1.73 | 1.21 |
| 3:H3:78:ARG:NH2 | 11:a9:623:ASP:CB | 2.03 | 1.21 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:Q5:15:ALA:C | 1:R5:90:ARG:CD | 2.12 | 1.21 |
| 10:j5:362:LYS:CD | 10:j5:363:HIS:CD2 | 2.21 | 1.21 |
| 10:j5:978:LEU:HD21 | 1:v7:107:ARG:CZ | 1.69 | 1.21 |
| 10:k5:741:GLN:O | 1:D7:77:ARG:NH2 | 1.71 | 1.21 |
| 8:o7:23:LEU:HD22 | 1:p7:38:VAL:CA | 1.69 | 1.21 |
| 8:u7:37:LEU:HD22 | 1:v7:24:LEU:CD2 | 1.68 | 1.21 |
| 4:M8:231:THR:N | 12:M8:301:CYC:CBB | 1.98 | 1.21 |
| 5:Z8:38:GLU:CB | 12:Z8:301:CYC:CMB | 2.11 | 1.21 |
| 3:F9:153:CYS:HB2 | 12:F9:303:CYC:CAC | 1.67 | 1.21 |
| 5:NA:1:MET:SD | 3:RA:119:ALA:HB1 | 1.81 | 1.21 |
| 5:N3:62:ARG:NH2 | 2:Q3:14:SER:HB3 | 1.54 | 1.21 |
| 4:M4:27:HIS:ND1 | 4:M4:35:THR:N | 1.83 | 1.21 |
| 10:j5:1055:SER:OG | 12:r7:201:CYC:HBB2 | 1.33 | 1.21 |
| 10:k5:974:LEU:HG | 1:p7:1:MET:N | 1.53 | 1.21 |
| 10:k5:1018:LEU:HD13 | 10:k5:1035:PHE:CE2 | 1.74 | 1.21 |
| 8:q7:75:GLU:O | 11:aA:53:VAL:HG11 | 1.34 | 1.21 |
| 3:L9:14:LEU:CD1 | 11:a9:358:PRO:CB | 2.19 | 1.21 |
| 2:E9:2:LYS:NZ | 2:I9:17:ARG:NH1 | 1.88 | 1.21 |
| 11:aA:708:HIS:CB | 3:L1:108:ARG:HH21 | 1.52 | 1.21 |
| 12:B3:202:CYC:CAA | 11:a9:684:ASN:HB3 | 1.70 | 1.21 |
| 3:F4:1:MET:CA | 4:M4:10:ARG:O | 1.74 | 1.21 |
| 1:N5:53:LYS:HZ1 | 8:O5:120:GLN:NE2 | 1.27 | 1.21 |
| 10:k5:284:PRO:CG | 10:k5:326:GLY:CA | 1.93 | 1.21 |
| 10:k5:978:LEU:HD21 | 1:p7:107:ARG:CZ | 1.69 | 1.21 |
| 10:k5:1013:PRO:CB | 8:k7:114:GLU:OE2 | 1.88 | 1.21 |
| 1:Z7:67:ARG:HD3 | 11:a9:311:LEU:CD2 | 1.70 | 1.21 |
| 1:d7:77:ARG:NH2 | 9:x7:63:ALA:CB | 2.03 | 1.21 |
| 8:u7:23:LEU:HD22 | 1:v7:38:VAL:CA | 1.69 | 1.21 |
| 3:U8:114:LYS:HZ1 | 4:M8:13:LYS:CD | 1.54 | 1.21 |
| 3:F8:109:CYS:CA | 4:M8:6:THR:HG22 | 1.69 | 1.21 |
| 4:M9:76:ALA:O | 3:D9:115:GLU:OE2 | 1.56 | 1.21 |
| 4:M9:157:PHE:O | 3:V9:108:ARG:HD2 | 1.06 | 1.21 |
| 2:K9:15:GLN:CA | 11:a9:393:ARG:NH1 | 2.03 | 1.21 |
| 2:IA:37:SER:O | 2:IA:97:LEU:CD1 | 1.88 | 1.21 |
| 6:M2:26:PHE:CE1 | 8:O5:87:TYR:CD1 | 2.12 | 1.21 |
| 6:M2:37:GLU:OE2 | 8:O5:59:PHE:HD2 | 1.18 | 1.21 |
| 6:M2:127:SER:O | 12:F2:201:CYC:HBA1 | 1.03 | 1.21 |
| 3:B4:119:ALA:CB | 4:M4:69:ILE:HG21 | 1.70 | 1.21 |
| 3:L3:104:VAL:HB | 3:L3:108:ARG:NH2 | 1.56 | 1.21 |
| 8:M5:66:VAL:CG1 | 8:K7:68:PRO:HG3 | 1.70 | 1.21 |
| 10:j5:935:LEU:HD13 | 1:J7:29:ALA:CB | 1.70 | 1.21 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:c7:96:ILE:CG1 | 8:c7:152:TYR:CG | 2.24 | 1.21 |
| 2:N8:14:SER:HB3 | 5:Z8:62:ARG:NE | 0.88 | 1.21 |
| 11:aA:403:THR:CG2 | 11:aA:536:THR:HG22 | 1.65 | 1.21 |
| 3:DA:108:ARG:O | 4:MA:6:THR:CG2 | 1.90 | 1.20 |
| 3:FA:151:GLY:CA | 3:F9:150:ARG:HH21 | 1.52 | 1.20 |
| 3:TA:28:THR:HG22 | 2:X4:67:THR:CB | 1.62 | 1.20 |
| 12:B3:202:CYC:CBA | 11:a9:684:ASN:CB | 2.08 | 1.20 |
| 3:F4:109:CYS:N | 4:M4:6:THR:CG2 | 2.03 | 1.20 |
| 2:N4:14:SER:CB | 5:Z4:62:ARG:HD2 | 1.71 | 1.20 |
| 1:N5:83:ARG:NH1 | 10:k5:483:PHE:CZ | 2.09 | 1.20 |
| 3:Y4:88:ILE:HG22 | 3:Y4:91:ARG:NH2 | 1.56 | 1.20 |
| 1:d5:28:LYS:CD | 1:n7:143:PRO:HG3 | 1.71 | 1.20 |
| 8:Q5:16:ARG:HA | 1:R5:90:ARG:NH1 | 1.54 | 1.20 |
| 10:j5:387:VAL:O | 10:j5:394:PRO:HG2 | 1.41 | 1.20 |
| 10:k5:1152:TYR:CD2 | 8:G7:68:PRO:HG3 | 1.70 | 1.20 |
| 3:Q8:85:ASP:OD2 | 12:Z8:301:CYC:CBC | 1.87 | 1.20 |
| 3:H9:116:THR:OG1 | 11:a9:449:ASN:ND2 | 1.72 | 1.20 |
| 11:aA:666:ASN:HB3 | 12:aA:901:CYC:NB | 1.56 | 1.20 |
| 11:aA:800:THR:HG21 | 12:aA:901:CYC:CAA | 1.68 | 1.20 |
| 2:Q1:14:SER:HB3 | 5:N1:62:ARG:NH2 | 1.54 | 1.20 |
| 6:M2:39:ARG:CZ | 8:O5:66:VAL:HG11 | 1.70 | 1.20 |
| 6:M2:62:ARG:NH2 | 1:h7:58:LYS:CA | 2.02 | 1.20 |
| 12:L3:202:CYC:HB | 11:a9:738:LEU:HD13 | 1.06 | 1.20 |
| 8:W5:16:ARG:HA | 1:X5:90:ARG:NH1 | 1.54 | 1.20 |
| 8:i7:20:PRO:CG | 8:s7:155:TYR:CD2 | 2.23 | 1.20 |
| 8:c7:39:ILE:HD13 | 8:c7:148:GLU:CG | 1.63 | 1.20 |
| 8:o7:97:VAL:HG21 | 1:p7:19:LEU:CD1 | 1.71 | 1.20 |
| 2:X8:60:TYR:CD2 | 3:T9:32:LYS:CE | 1.97 | 1.20 |
| 4:M8:126:THR:CB | 12:M8:302:CYC:O2A | 1.87 | 1.20 |
| 3:O8:108:ARG:CB | 5:Z8:61:LYS:HD3 | 1.61 | 1.20 |
| 3:L9:52:ILE:CD1 | 3:L9:87:GLU:CB | 2.20 | 1.20 |
| 3:J9:111:ASN:O | 11:a9:518:ALA:C | 1.82 | 1.20 |
| 3:TA:32:LYS:CE | 2:X4:60:TYR:CD2 | 1.97 | 1.20 |
| 12:R1:201:CYC:NB | 5:N1:54:LEU:CD1 | 2.04 | 1.20 |
| 3:J3:120:LEU:CD2 | 11:a9:800:THR:HG21 | 1.72 | 1.20 |
| 2:K3:15:GLN:CA | 11:a9:745:GLY:HA3 | 1.70 | 1.20 |
| 6:M2:276:PRO:HB2 | 1:j7:63:SER:OG | 1.40 | 1.20 |
| 3:B3:88:ILE:HG21 | 12:B3:202:CYC:C3B | 1.71 | 1.20 |
| 5:N3:54:LEU:CD1 | 12:R3:201:CYC:NB | 2.04 | 1.20 |
| 3:Y4:89:ILE:HG23 | 3:Y4:92:TYR:OH | 1.05 | 1.20 |
| 8:C5:2:SER:OG | 1:D5:3:ASP:OD2 | 1.59 | 1.20 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:j7:77:ARG:NH2 | 9:y7:63:ALA:HB3 | 1.54 | 1.20 |
| 3:Y8:89:ILE:HG23 | 3:Y8:92:TYR:OH | 1.05 | 1.20 |
| 11:a9:710:THR:CG2 | 11:a9:807:GLN:CG | 2.16 | 1.20 |
| 11:aA:283:GLN:CB | 11:aA:284:PRO:CD | 2.01 | 1.20 |
| 1:A:107:ARG:NH2 | 8:a5:12:ASP:OD2 | 1.75 | 1.20 |
| 12:J3:202:CYC:CMA | 11:a9:798:SER:OG | 1.90 | 1.20 |
| 3:F4:84:ARG:CD | 11:aA:139:ILE:CG2 | 2.14 | 1.20 |
| 3:Q4:102:ALA:HB2 | 3:Q4:166:LYS:CE | 1.71 | 1.20 |
| 8:W5:12:ASP:CA | 1:X5:94:TYR:CE2 | 2.25 | 1.20 |
| 10:k5:930:LEU:C | 1:D7:33:THR:HG21 | 1.65 | 1.20 |
| 10:k5:938:GLN:OE1 | 1:D7:28:LYS:CD | 1.90 | 1.20 |
| 12:M8:302:CYC:CMD | 3:S8:77:ARG:HH22 | 1.55 | 1.20 |
| 5:Z8:41:GLN:HG2 | 12:Z8:301:CYC:CBB | 1.70 | 1.20 |
| 11:aA:776:TYR:N | 12:H1:201:CYC:HBA1 | 1.56 | 1.20 |
| 3:LA:14:LEU:CD1 | 11:aA:358:PRO:CB | 2.20 | 1.20 |
| 6:M2:26:PHE:CZ | 8:O5:87:TYR:CD1 | 2.17 | 1.20 |
| 10:k5:938:GLN:OE1 | 1:D7:28:LYS:CG | 1.90 | 1.20 |
| 8:i7:96:ILE:CG1 | 8:i7:152:TYR:CG | 2.24 | 1.20 |
| 3:U8:115:GLU:HB3 | 4:M8:74:LEU:CD1 | 1.49 | 1.20 |
| 3:F8:107:ASP:HB2 | 4:M8:8:SER:C | 1.40 | 1.20 |
| 4:M9:6:THR:CG2 | 3:D9:108:ARG:O | 1.90 | 1.20 |
| 4:M9:158:PHE:C | 3:V9:108:ARG:HD3 | 1.67 | 1.20 |
| 11:a9:275:THR:C | 11:a9:278:LEU:CD1 | 2.15 | 1.20 |
| 2:EA:2:LYS:NZ | 2:IA:17:ARG:NH1 | 1.88 | 1.19 |
| 2:A3:63:PHE:HB2 | 2:A3:66:LEU:HD11 | 1.20 | 1.19 |
| 5:Z4:41:GLN:CG | 12:Z4:301:CYC:C2B | 2.20 | 1.19 |
| 1:f5:114:GLU:HG2 | 10:j5:491:THR:OG1 | 1.37 | 1.19 |
| 8:W5:16:ARG:CA | 1:X5:90:ARG:NH1 | 2.06 | 1.19 |
| 10:k5:931:VAL:HG13 | 1:D7:29:ALA:CB | 1.72 | 1.19 |
| 8:c7:16:ARG:C | 1:d7:90:ARG:CD | 2.16 | 1.19 |
| 8:c7:20:PRO:CD | 8:m7:155:TYR:HB2 | 1.72 | 1.19 |
| 12:B8:202:CYC:CMA | 4:M8:58:TYR:N | 2.02 | 1.19 |
| 3:U8:108:ARG:CB | 4:M8:246:ALA:HB2 | 1.71 | 1.19 |
| 3:U8:120:LEU:CD2 | 12:U8:201:CYC:HBD1 | 1.70 | 1.19 |
| 3:F8:108:ARG:C | 4:M8:6:THR:HG21 | 1.67 | 1.19 |
| 4:M8:91:VAL:CB | 2:P8:14:SER:O | 1.90 | 1.19 |
| 11:aA:798:SER:OG | 12:aA:901:CYC:CMA | 1.89 | 1.19 |
| 4:M1:263:PRO:HB2 | 3:Z1:119:ALA:CB | 1.70 | 1.19 |
| 2:K3:13:ASP:OD2 | 11:a9:707:PHE:CZ | 1.95 | 1.19 |
| 3:U4:120:LEU:CD1 | 12:U4:201:CYC:HBD1 | 1.69 | 1.19 |
| 3:F4:109:CYS:CA | 4:M4:6:THR:HG22 | 1.72 | 1.19 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:U8:114:LYS:NZ | 4:M8:13:LYS:CD | 2.05 | 1.19 |
| 3:U8:114:LYS:CE | 4:M8:13:LYS:NZ | 2.04 | 1.19 |
| 4:M9:274:VAL:C | 3:V9:77:ARG:HE | 1.51 | 1.19 |
| 5:Z8:41:GLN:HG2 | 12:Z8:301:CYC:CAB | 1.72 | 1.19 |
| 5:Z8:41:GLN:CG | 12:Z8:301:CYC:CBB | 2.17 | 1.19 |
| 12:J9:202:CYC:CGA | 11:a9:511:LYS:HD3 | 1.71 | 1.19 |
| 11:aA:666:ASN:HB3 | 12:aA:901:CYC:OB | 1.40 | 1.19 |
| 11:aA:670:LEU:CD2 | 2:K1:112:GLY:CA | 1.96 | 1.19 |
| 3:FA:150:ARG:HA | 3:F9:150:ARG:NE | 1.58 | 1.19 |
| 3:JA:111:ASN:O | 11:aA:518:ALA:C | 1.82 | 1.19 |
| 3:LA:52:ILE:CD1 | 3:LA:87:GLU:CB | 2.20 | 1.19 |
| 2:S1:16:GLY:CA | 5:N1:31:TRP:CD1 | 2.25 | 1.19 |
| 3:H4:119:ALA:O | 11:aA:266:ASN:CB | 1.89 | 1.19 |
| 4:M4:214:GLY:CA | 5:Z4:27:ALA:O | 1.90 | 1.19 |
| 8:e5:45:GLU:OE1 | 1:R5:139:GLY:HA2 | 1.17 | 1.19 |
| 1:f5:114:GLU:CG | 10:j5:491:THR:OG1 | 1.90 | 1.19 |
| 8:Q5:12:ASP:CA | 1:R5:94:TYR:CE2 | 2.25 | 1.19 |
| 10:j5:971:VAL:HG12 | 12:j5:1202:CYC:O1D | 1.43 | 1.19 |
| 8:c7:11:ALA:C | 1:d7:94:TYR:OH | 1.85 | 1.19 |
| 12:B8:202:CYC:O1A | 4:M8:54:ALA:CB | 1.73 | 1.19 |
| 8:o7:103:PRO:HG3 | 1:p7:9:ILE:HD13 | 1.23 | 1.19 |
| 9:w7:4:TYR:O | 9:w7:56:LEU:O | 1.56 | 1.19 |
| 4:M8:197:ASP:CB | 5:Z8:52:ARG:HG3 | 1.73 | 1.19 |
| 12:M8:301:CYC:H3C | 3:Y8:127:VAL:CG2 | 1.72 | 1.19 |
| 11:aA:623:ASP:CB | 3:H1:78:ARG:NH2 | 2.04 | 1.19 |
| 11:aA:694:ARG:NH2 | 4:M1:51:ARG:HH21 | 1.39 | 1.19 |
| 4:MA:160:THR:O | 3:VA:108:ARG:NH2 | 1.74 | 1.19 |
| 12:J3:202:CYC:OB | 11:a9:666:ASN:HB3 | 1.41 | 1.19 |
| 6:M2:28:ASN:HB2 | 8:O5:80:LEU:HG | 1.23 | 1.19 |
| 12:B4:202:CYC:CMA | 4:M4:58:TYR:N | 2.02 | 1.19 |
| 3:U4:108:ARG:CB | 4:M4:246:ALA:HB2 | 1.71 | 1.19 |
| 3:F4:113:LEU:H | 4:M4:5:THR:CA | 1.56 | 1.19 |
| 1:Z5:83:ARG:NH1 | 10:k5:379:PHE:HE2 | 1.38 | 1.19 |
| 1:b5:6:THR:HG22 | 10:k5:19:THR:OG1 | 1.42 | 1.19 |
| 10:k5:1119:LEU:HD12 | 12:k5:1204:CYC:OB | 1.02 | 1.19 |
| 8:g7:25:ARG:NH2 | 8:u7:25:ARG:CZ | 2.03 | 1.19 |
| 8:i7:25:ARG:NH1 | 8:s7:6:LYS:CB | 2.06 | 1.19 |
| 3:F8:107:ASP:C | 4:M8:6:THR:O | 1.86 | 1.19 |
| 5:N9:1:MET:SD | 3:R9:119:ALA:HB1 | 1.81 | 1.19 |
| 3:H9:120:LEU:CD1 | 12:H9:202:CYC:CAA | 2.20 | 1.19 |
| 11:a9:601:ALA:O | 11:a9:604:ALA:HB2 | 1.39 | 1.19 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A:161:SER:OG | 1:R5:14:VAL:HG23 | 1.37 | 1.19 |
| 12:B4:202:CYC:O1A | 4:M4:54:ALA:CB | 1.73 | 1.19 |
| 3:F4:115:GLU:OE2 | 4:M4:3:VAL:CG2 | 1.91 | 1.19 |
| 8:M5:19:SER:OG | 8:A5:6:LYS:NZ | 1.76 | 1.19 |
| 8:S5:41:GLN:CD | 1:D7:143:PRO:HG3 | 1.66 | 1.19 |
| 6:M6:53:LEU:HD23 | 8:c7:80:LEU:CG | 1.73 | 1.19 |
| 1:f7:64:ASP:OD2 | 11:aA:307:ARG:NE | 1.57 | 1.19 |
| 8:u7:103:PRO:HG3 | 1:v7:9:ILE:HD13 | 1.23 | 1.19 |
| 4:M8:128:ALA:O | 4:M8:142:PHE:CE1 | 1.96 | 1.19 |
| 2:N8:115:GLU:OE1 | 5:Z8:33:GLY:N | 1.76 | 1.19 |
| 2:N8:115:GLU:CD | 5:Z8:32:PRO:HD2 | 1.67 | 1.19 |
| 3:F1:116:THR:OG1 | 4:M1:38:PRO:O | 1.58 | 1.19 |
| 1:Z:127:VAL:HG11 | 1:X5:15:GLN:CG | 1.74 | 1.18 |
| 3:J3:84:ARG:CD | 11:a9:668:TYR:HD1 | 1.18 | 1.18 |
| 5:N3:31:TRP:CD1 | 2:S3:16:GLY:CA | 2.25 | 1.18 |
| 5:N3:66:ARG:NH1 | 3:R3:111:ASN:HD21 | 1.39 | 1.18 |
| 4:M4:228:SER:CB | 2:X4:16:GLY:HA2 | 1.71 | 1.18 |
| 3:Q4:120:LEU:HD11 | 5:Z4:40:SER:N | 1.57 | 1.18 |
| 8:K5:36:ARG:NH1 | 8:U5:24:ASP:OD2 | 1.76 | 1.18 |
| 10:j5:974:LEU:CG | 1:v7:1:MET:H3 | 1.51 | 1.18 |
| 10:k5:974:LEU:HD12 | 1:p7:106:GLU:OE2 | 1.40 | 1.18 |
| 3:B8:68:ARG:CZ | 3:U8:68:ARG:HH22 | 1.55 | 1.18 |
| 3:H8:119:ALA:O | 11:a9:266:ASN:CB | 1.87 | 1.18 |
| 11:a9:75:ALA:CB | 11:a9:81:ASP:CB | 2.19 | 1.18 |
| 11:a9:632:ILE:HG22 | 11:a9:634:ALA:N | 1.57 | 1.18 |
| 11:aA:707:PHE:CZ | 2:K1:13:ASP:OD2 | 1.96 | 1.18 |
| 3:TA:28:THR:CG2 | 2:X4:67:THR:OG1 | 1.92 | 1.18 |
| 6:M2:277:GLY:CA | 1:j7:62:TYR:O | 1.91 | 1.18 |
| 3:F4:107:ASP:CA | 4:M4:8:SER:H | 1.55 | 1.18 |
| 3:F4:108:ARG:NE | 4:M4:9:GLN:HG3 | 0.87 | 1.18 |
| 4:M4:144:ARG:NE | 4:M4:204:ILE:CG2 | 2.06 | 1.18 |
| 1:d5:28:LYS:HD3 | 1:n7:143:PRO:CB | 1.72 | 1.18 |
| 1:R5:110:ASN:OD1 | 10:k5:466:LEU:HB2 | 1.43 | 1.18 |
| 8:U5:75:GLU:CD | 6:M6:32:MET:HE1 | 1.68 | 1.18 |
| 11:a9:351:THR:HB | 11:a9:352:PRO:CD | 1.74 | 1.18 |
| 11:aA:275:THR:C | 11:aA:278:LEU:CD1 | 2.15 | 1.18 |
| 11:aA:601:ALA:O | 11:aA:604:ALA:HB2 | 1.39 | 1.18 |
| 11:aA:621:THR:HG22 | 3:J1:14:LEU:CD1 | 1.70 | 1.18 |
| 4:MA:58:TYR:CG | 11:aA:496:ARG:NH2 | 2.12 | 1.18 |
| 3:TA:28:THR:HG22 | 2:X4:67:THR:OG1 | 1.42 | 1.18 |
| 3:J3:84:ARG:HH22 | 11:a9:670:LEU:N | 1.41 | 1.18 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:B4:68:ARG:CZ | 3:U4:68:ARG:HH22 | 1.55 | 1.18 |
| 3:L3:119:ALA:O | 11:a9:817:LEU:HD12 | 1.32 | 1.18 |
| 3:O4:107:ASP:OD1 | 5:Z4:66:ARG:CD | 1.90 | 1.18 |
| 8:I5:27:LYS:HA | 8:I5:30:VAL:HG22 | 1.20 | 1.18 |
| 1:d5:28:LYS:CD | 1:n7:143:PRO:CG | 2.21 | 1.18 |
| 1:X5:110:ASN:OD1 | 10:j5:466:LEU:CB | 1.90 | 1.18 |
| 10:k5:966:SER:CB | 1:p7:14:VAL:HG11 | 1.74 | 1.18 |
| 8:c7:16:ARG:N | 1:d7:90:ARG:NE | 1.92 | 1.18 |
| 3:D8:108:ARG:HD3 | 11:a9:107:ARG:CZ | 1.59 | 1.18 |
| 8:q7:45:GLU:OE1 | 3:H1:125:ARG:NH2 | 1.74 | 1.18 |
| 8:u7:18:LEU:HD13 | 1:v7:97:LEU:CD1 | 1.74 | 1.18 |
| 2:A9:63:PHE:HB2 | 2:A9:66:LEU:HD11 | 1.20 | 1.18 |
| 3:H9:78:ARG:NH1 | 12:H9:202:CYC:O2D | 1.76 | 1.18 |
| 11:aA:75:ALA:HB1 | 11:aA:81:ASP:OD1 | 1.43 | 1.18 |
| 5:N1:22:LEU:HD22 | 5:N1:26:LEU:CG | 1.74 | 1.18 |
| 12:FA:301:CYC:OB | 4:MA:53:LEU:HD11 | 1.21 | 1.18 |
| 12:JA:202:CYC:CGA | 11:aA:511:LYS:HD3 | 1.72 | 1.18 |
| 2:O1:63:PHE:HB2 | 2:O1:66:LEU:HD11 | 1.20 | 1.18 |
| 12:J3:202:CYC:NB | 11:a9:666:ASN:HB3 | 1.57 | 1.18 |
| 3:B1:88:ILE:HD13 | 12:B1:202:CYC:C2B | 1.72 | 1.18 |
| 4:M4:82:ILE:HD11 | 12:M4:301:CYC:CGD | 1.71 | 1.18 |
| 4:M4:138:SER:CB | 12:Z4:301:CYC:HBB1 | 1.72 | 1.18 |
| 5:Z4:41:GLN:HG3 | 12:Z4:301:CYC:HMB1 | 1.26 | 1.18 |
| 1:b5:5:ILE:CD1 | 10:k5:46:PHE:CZ | 2.27 | 1.18 |
| 8:u7:97:VAL:HG21 | 1:v7:19:LEU:CD1 | 1.71 | 1.18 |
| 2:X8:67:THR:OG1 | 3:T9:28:THR:HG22 | 1.42 | 1.18 |
| 3:O8:104:VAL:HA | 5:Z8:61:LYS:NZ | 1.55 | 1.18 |
| 3:Q8:127:VAL:HG22 | 12:Z8:301:CYC:HMC1 | 1.23 | 1.18 |
| 5:Z8:41:GLN:OE1 | 12:Z8:301:CYC:HBB2 | 1.03 | 1.18 |
| 3:B3:88:ILE:CG2 | 12:B3:202:CYC:CAB | 2.19 | 1.18 |
| 3:F4:108:ARG:HE | 4:M4:9:GLN:CG | 1.43 | 1.18 |
| 3:Q4:120:LEU:HD21 | 5:Z4:42:SER:CB | 1.74 | 1.18 |
| 12:H5:201:CYC:CBA | 9:i5:26:THR:HG21 | 1.74 | 1.18 |
| 10:k5:387:VAL:O | 10:k5:394:PRO:HG2 | 1.41 | 1.18 |
| 2:N8:115:GLU:HB2 | 5:Z8:32:PRO:CG | 1.71 | 1.18 |
| 4:M9:33:LEU:HD23 | 2:E9:115:GLU:OE2 | 1.39 | 1.18 |
| 4:M9:162:ASN:H | 12:V9:201:CYC:HBB3 | 1.07 | 1.18 |
| 5:N9:22:LEU:HD22 | 5:N9:26:LEU:CG | 1.74 | 1.18 |
| 3:FA:153:CYS:SG | 12:F9:302:CYC:CAC | 2.32 | 1.17 |
| 4:M3:205:ASP:OD2 | 5:N3:52:ARG:NH1 | 1.76 | 1.17 |
| 3:Q4:78:ARG:HD3 | 12:Z4:301:CYC:HAD1 | 1.24 | 1.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:Z4:26:LEU:HD21 | 5:Z4:63:ASN:CB | 1.73 | 1.17 |
| 3:J6:108:ARG:NE | 6:M6:155:ASN:O | 1.76 | 1.17 |
| 6:M6:277:GLY:HA2 | 1:d7:62:TYR:C | 1.67 | 1.17 |
| 10:j5:387:VAL:O | 10:j5:394:PRO:CG | 1.92 | 1.17 |
| 3:U8:112:GLY:CA | 4:M8:74:LEU:HD21 | 1.74 | 1.17 |
| 3:F8:109:CYS:N | 4:M8:6:THR:HG22 | 1.57 | 1.17 |
| 3:J3:84:ARG:NH2 | 11:a9:669:ILE:O | 1.77 | 1.17 |
| 6:M2:62:ARG:NH2 | 1:h7:58:LYS:C | 2.01 | 1.17 |
| 2:N4:111:ALA:O | 5:Z4:34:LEU:HB2 | 1.43 | 1.17 |
| 8:I5:2:SER:OG | 1:J5:3:ASP:OD2 | 1.59 | 1.17 |
| 8:U5:76:LYS:CG | 8:U5:77:MET:HE2 | 1.74 | 1.17 |
| 10:j5:971:VAL:CG1 | 1:t7:76:ARG:NH1 | 2.05 | 1.17 |
| 10:k5:1037:ARG:NH1 | 10:k5:1098:GLU:OE2 | 1.76 | 1.17 |
| 8:Q7:12:ASP:O | 9:z7:46:LYS:NZ | 1.76 | 1.17 |
| 1:R7:118:SER:O | 9:z7:61:GLN:NE2 | 1.77 | 1.17 |
| 1:f7:10:ASN:CB | 9:y7:65:THR:OG1 | 1.93 | 1.17 |
| 3:B8:119:ALA:CB | 4:M8:69:ILE:HG21 | 1.74 | 1.17 |
| 8:o7:103:PRO:CB | 1:p7:9:ILE:HG21 | 1.75 | 1.17 |
| 4:M8:56:MET:HE1 | 4:M8:66:VAL:CG2 | 1.74 | 1.17 |
| 1:A:158:SER:HB3 | 1:R5:11:ASN:ND2 | 1.31 | 1.17 |
| 12:J3:202:CYC:O1D | 11:a9:802:ARG:NE | 1.76 | 1.17 |
| 3:D4:108:ARG:HD2 | 11:aA:107:ARG:HH12 | 1.08 | 1.17 |
| 3:B1:115:GLU:OE2 | 4:M1:76:ALA:O | 1.63 | 1.17 |
| 12:U4:201:CYC:HBA2 | 4:M4:252:LEU:O | 1.40 | 1.17 |
| 4:M4:29:PRO:HG3 | 11:aA:226:PHE:CA | 1.72 | 1.17 |
| 4:M4:138:SER:HB3 | 12:Z4:301:CYC:HBB1 | 1.20 | 1.17 |
| 8:O5:76:LYS:CG | 8:O5:77:MET:HE2 | 1.74 | 1.17 |
| 3:Y4:89:ILE:HA | 3:Y4:92:TYR:CD2 | 1.79 | 1.17 |
| 8:Q5:16:ARG:CB | 1:R5:90:ARG:NH1 | 2.07 | 1.17 |
| 8:W5:16:ARG:CB | 1:X5:90:ARG:NH1 | 2.07 | 1.17 |
| 1:b5:18:TYR:CZ | 10:k5:165:ARG:CB | 2.26 | 1.17 |
| 10:k5:1008:PHE:CZ | 1:p7:87:TYR:CE2 | 2.30 | 1.17 |
| 12:M8:302:CYC:CMD | 3:S8:77:ARG:NH2 | 2.08 | 1.17 |
| 4:M9:160:THR:O | 3:V9:108:ARG:NH2 | 1.74 | 1.17 |
| 5:N9:22:LEU:CD2 | 5:N9:26:LEU:CD2 | 2.23 | 1.17 |
| 3:H9:120:LEU:CD1 | 12:H9:202:CYC:C2A | 2.21 | 1.17 |
| 11:a9:280:ASP:OD1 | 11:a9:281:PRO:HD3 | 1.45 | 1.17 |
| 11:aA:249:GLU:O | 11:aA:285:VAL:HG21 | 1.41 | 1.17 |
| 11:aA:666:ASN:CB | 12:aA:901:CYC:OB | 1.91 | 1.17 |
| 3:B3:115:GLU:OE2 | 4:M3:76:ALA:O | 1.63 | 1.17 |
| 4:M3:51:ARG:HH21 | 11:a9:694:ARG:NH2 | 1.40 | 1.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:N3:22:LEU:CD2 | 5:N3:26:LEU:CD2 | 2.23 | 1.17 |
| 10:j5:1150:TYR:HE2 | 1:v7:69:GLY:C | 1.52 | 1.17 |
| 3:F6:78:ARG:HD3 | 12:F6:201:CYC:CGD | 1.75 | 1.17 |
| 8:i7:3:VAL:CG1 | 8:s7:25:ARG:NH2 | 2.07 | 1.17 |
| 8:c7:15:ALA:CA | 1:d7:90:ARG:CZ | 2.11 | 1.17 |
| 8:o7:18:LEU:HD13 | 1:p7:97:LEU:CD1 | 1.74 | 1.17 |
| 3:U8:114:LYS:NZ | 4:M8:13:LYS:HD3 | 1.58 | 1.17 |
| 2:X8:74:TYR:OH | 2:S9:35:THR:CG2 | 1.91 | 1.17 |
| 3:Q8:85:ASP:CG | 12:Z8:301:CYC:HBC3 | 1.67 | 1.17 |
| 12:S8:201:CYC:HMD1 | 12:S8:201:CYC:HC | 1.10 | 1.17 |
| 5:Z8:37:HIS:CG | 12:Z8:301:CYC:NB | 2.13 | 1.17 |
| 11:a9:403:THR:CG2 | 11:a9:536:THR:HG22 | 1.65 | 1.17 |
| 5:NA:22:LEU:CD2 | 5:NA:26:LEU:CD2 | 2.23 | 1.17 |
| 3:R1:111:ASN:HD21 | 5:N1:66:ARG:NH1 | 1.39 | 1.17 |
| 12:J3:202:CYC:OB | 11:a9:666:ASN:CB | 1.93 | 1.17 |
| 5:N3:22:LEU:HD22 | 5:N3:26:LEU:CG | 1.74 | 1.17 |
| 3:B1:91:ARG:NH2 | 11:aA:677:GLN:NE2 | 1.91 | 1.17 |
| 8:G5:100:ASP:OD1 | 8:S5:20:PRO:CG | 1.91 | 1.17 |
| 10:k5:387:VAL:O | 10:k5:394:PRO:CG | 1.92 | 1.17 |
| 2:X8:74:TYR:CE1 | 2:S9:35:THR:CG2 | 2.25 | 1.17 |
| 5:Z8:41:GLN:CB | 12:Z8:301:CYC:C1B | 2.09 | 1.17 |
| 4:M1:205:ASP:OD2 | 5:N1:52:ARG:NH1 | 1.76 | 1.17 |
| 2:A2:63:PHE:HB2 | 2:A2:66:LEU:HD11 | 1.19 | 1.17 |
| 12:QA:201:CYC:HBB2 | 3:TA:75:PRO:CA | 1.74 | 1.16 |
| 12:QA:201:CYC:CBB | 3:TA:75:PRO:CB | 2.20 | 1.16 |
| 3:J3:84:ARG:HD3 | 11:a9:668:TYR:CD1 | 1.50 | 1.16 |
| 2:U3:46:SER:O | 2:Q9:74:TYR:CE1 | 1.98 | 1.16 |
| 3:H4:119:ALA:CB | 11:aA:266:ASN:ND2 | 1.99 | 1.16 |
| 4:M4:140:ARG:NH1 | 4:M4:144:ARG:NH1 | 1.92 | 1.16 |
| 4:M4:215:GLU:N | 5:Z4:27:ALA:C | 2.03 | 1.16 |
| 12:M4:301:CYC:HBC1 | 3:Y4:82:CYS:SG | 1.84 | 1.16 |
| 1:d5:28:LYS:NZ | 1:n7:143:PRO:CG | 2.04 | 1.16 |
| 1:V5:83:ARG:NH1 | 10:j5:649:PHE:HE2 | 1.17 | 1.16 |
| 3:L6:125:ARG:CD | 1:b7:69:GLY:HA2 | 1.69 | 1.16 |
| 3:L8:82:CYS:SG | 12:a9:901:CYC:C4C | 2.33 | 1.16 |
| 4:M9:58:TYR:CG | 11:a9:496:ARG:NH2 | 2.12 | 1.16 |
| 11:aA:632:ILE:HG22 | 11:aA:634:ALA:N | 1.57 | 1.16 |
| 3:F4:108:ARG:C | 4:M4:6:THR:HG21 | 1.67 | 1.16 |
| 8:Q5:16:ARG:CA | 1:R5:90:ARG:NH1 | 2.06 | 1.16 |
| 1:T5:53:LYS:HZ2 | 8:U5:120:GLN:NE2 | 1.37 | 1.16 |
| 8:Q7:13:ALA:CA | 9:z7:46:LYS:NZ | 1.90 | 1.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:I7:25:ARG:NH2 | 8:W7:25:ARG:CD | 2.09 | 1.16 |
| 8:W7:13:ALA:CA | 9:w7:46:LYS:HZ2 | 1.56 | 1.16 |
| 8:c7:25:ARG:HH22 | 8:m7:6:LYS:NZ | 1.39 | 1.16 |
| 3:B8:108:ARG:HA | 4:M8:61:ASN:HA | 1.25 | 1.16 |
| 12:B8:202:CYC:HMA2 | 4:M8:58:TYR:N | 1.55 | 1.16 |
| 2:X8:67:THR:OG1 | 3:T9:28:THR:CG2 | 1.92 | 1.16 |
| 5:Z8:22:LEU:HD22 | 5:Z8:26:LEU:CG | 1.73 | 1.16 |
| 11:a9:249:GLU:O | 11:a9:285:VAL:HG21 | 1.41 | 1.16 |
| 1:A:73:TYR:CE1 | 10:k5:162:TRP:CH2 | 2.29 | 1.16 |
| 2:K3:28:ASN:OD1 | 2:A3:33:ARG:NH2 | 1.79 | 1.16 |
| 3:O4:112:GLY:O | 5:Z4:70:ILE:HB | 1.44 | 1.16 |
| 5:Z4:22:LEU:HD11 | 12:Z4:301:CYC:C4B | 1.75 | 1.16 |
| 1:D5:75:THR:HG21 | 8:E5:112:VAL:HG23 | 1.18 | 1.16 |
| 7:N6:2:TYR:OH | 3:F6:107:ASP:O | 1.64 | 1.16 |
| 10:j5:742:GLY:HA2 | 12:J7:201:CYC:CGD | 1.75 | 1.16 |
| 10:k5:357:LEU:HD11 | 10:k5:379:PHE:HA | 1.28 | 1.16 |
| 10:k5:938:GLN:CD | 1:D7:28:LYS:HD2 | 1.68 | 1.16 |
| 10:k5:1119:LEU:CD1 | 12:k5:1204:CYC:OB | 1.93 | 1.16 |
| 1:B7:68:PRO:CB | 1:D7:14:VAL:O | 1.94 | 1.16 |
| 8:i7:3:VAL:CG1 | 8:s7:25:ARG:HH21 | 1.58 | 1.16 |
| 1:l7:17:LYS:NZ | 11:a9:41:ASP:OD2 | 1.79 | 1.16 |
| 8:q7:66:VAL:HG11 | 11:aA:61:TYR:CE1 | 1.80 | 1.16 |
| 4:M8:225:LYS:N | 12:M8:301:CYC:CGA | 2.07 | 1.16 |
| 5:Z8:29:HIS:CE1 | 5:Z8:31:TRP:CB | 2.27 | 1.16 |
| 3:H9:113:LEU:HD11 | 12:H9:202:CYC:HMB3 | 1.23 | 1.16 |
| 11:a9:75:ALA:HB1 | 11:a9:81:ASP:OD1 | 1.43 | 1.16 |
| 11:a9:588:VAL:C | 11:a9:590:PRO:CD | 2.18 | 1.16 |
| 5:N1:22:LEU:CD2 | 5:N1:26:LEU:CD2 | 2.23 | 1.16 |
| 3:FA:151:GLY:C | 3:F9:150:ARG:NH2 | 2.03 | 1.16 |
| 2:OA:33:ARG:NH2 | 2:YA:28:ASN:OD1 | 1.79 | 1.16 |
| 8:W5:16:ARG:HA | 1:X5:90:ARG:CD | 1.76 | 1.16 |
| 9:z5:18:ARG:HB3 | 9:z5:22:GLU:OE2 | 1.45 | 1.16 |
| 1:d7:87:TYR:CE2 | 9:x7:38:PHE:HZ | 1.62 | 1.16 |
| 2:X8:67:THR:CB | 3:T9:28:THR:HG22 | 1.62 | 1.16 |
| 4:M8:104:ALA:CB | 2:P8:14:SER:CA | 2.15 | 1.16 |
| 11:aA:351:THR:HB | 11:aA:352:PRO:CD | 1.74 | 1.16 |
| 4:M1:252:LEU:HD13 | 12:X1:201:CYC:O1D | 1.43 | 1.16 |
| 1:A:131:GLN:HG3 | 1:R5:17:LYS:NZ | 0.83 | 1.16 |
| 1:Z:73:TYR:HE1 | 10:j5:162:TRP:CH2 | 1.63 | 1.16 |
| 3:FA:145:PRO:CG | 12:F9:302:CYC:CMC | 2.24 | 1.16 |
| 3:HA:120:LEU:CD1 | 12:HA:202:CYC:CAA | 2.23 | 1.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:MA:158:PHE:C | 3:VA:108:ARG:HD3 | 1.67 | 1.16 |
| 2:QA:119:THR:HG21 | 3:TA:83:LEU:CD2 | 1.76 | 1.16 |
| 12:QA:201:CYC:CBB | 3:TA:75:PRO:HB3 | 1.76 | 1.16 |
| 3:J3:14:LEU:CD1 | 11:a9:621:THR:HG22 | 1.72 | 1.16 |
| 3:B4:82:CYS:O | 12:B4:202:CYC:CAC | 1.93 | 1.16 |
| 3:S4:120:LEU:HD22 | 12:S4:202:CYC:CBD | 1.73 | 1.16 |
| 2:N4:33:ARG:NH2 | 2:X4:28:ASN:OD1 | 1.79 | 1.16 |
| 1:R5:124:ALA:HB3 | 1:Z5:64:ASP:OD1 | 1.46 | 1.16 |
| 8:S5:68:PRO:CB | 8:a5:59:PHE:HB2 | 1.76 | 1.16 |
| 10:j5:1037:ARG:NH1 | 10:j5:1098:GLU:OE2 | 1.76 | 1.16 |
| 10:j5:1119:LEU:HD12 | 12:j5:1202:CYC:C4B | 1.74 | 1.16 |
| 12:F1:202:CYC:HMD1 | 12:F1:202:CYC:HC | 1.10 | 1.16 |
| 12:X1:202:CYC:HMD1 | 12:X1:202:CYC:HC | 1.10 | 1.16 |
| 3:FA:150:ARG:CB | 3:F9:150:ARG:HG2 | 1.74 | 1.15 |
| 5:NA:22:LEU:HD22 | 5:NA:26:LEU:CG | 1.74 | 1.15 |
| 6:M2:276:PRO:O | 1:j7:63:SER:HA | 1.43 | 1.15 |
| 3:B3:91:ARG:NH2 | 11:a9:677:GLN:NE2 | 1.92 | 1.15 |
| 3:B4:119:ALA:CB | 4:M4:52:LEU:HD11 | 1.76 | 1.15 |
| 4:M3:51:ARG:NH2 | 11:a9:694:ARG:NH1 | 1.92 | 1.15 |
| 4:M3:252:LEU:HD13 | 12:X3:201:CYC:O1D | 1.43 | 1.15 |
| 4:M4:128:ALA:HB1 | 4:M4:142:PHE:CE1 | 1.81 | 1.15 |
| 2:N4:63:PHE:HB2 | 2:N4:66:LEU:HD11 | 1.20 | 1.15 |
| 8:M5:20:PRO:CG | 8:A5:100:ASP:OD1 | 1.93 | 1.15 |
| 8:G5:61:ILE:HG13 | 8:o7:68:PRO:CD | 1.76 | 1.15 |
| 8:I5:27:LYS:O | 8:I5:28:SER:C | 1.86 | 1.15 |
| 1:P5:114:GLU:CG | 10:k5:496:GLU:CD | 2.06 | 1.15 |
| 10:j5:1119:LEU:HD12 | 12:j5:1202:CYC:OB | 1.45 | 1.15 |
| 1:r7:68:PRO:CB | 1:t7:14:VAL:O | 1.94 | 1.15 |
| 8:u7:97:VAL:HG21 | 1:v7:19:LEU:HD13 | 1.16 | 1.15 |
| 4:M8:225:LYS:CA | 12:M8:301:CYC:O1A | 1.94 | 1.15 |
| 3:Q8:84:ARG:HG3 | 5:Z8:31:TRP:CE2 | 1.80 | 1.15 |
| 2:O9:33:ARG:NH2 | 2:Y9:28:ASN:OD1 | 1.79 | 1.15 |
| 3:Y8:89:ILE:HA | 3:Y8:92:TYR:CD2 | 1.79 | 1.15 |
| 11:a9:312:ASP:HB2 | 11:a9:315:LEU:CD1 | 1.75 | 1.15 |
| 4:MA:263:PRO:HB2 | 3:VA:119:ALA:HB2 | 1.24 | 1.15 |
| 6:M2:277:GLY:HA2 | 1:j7:62:TYR:O | 0.98 | 1.15 |
| 12:S4:201:CYC:HMD1 | 12:S4:201:CYC:HC | 1.10 | 1.15 |
| 3:L4:69:PRO:O | 11:aA:82:GLN:HB3 | 1.45 | 1.15 |
| 8:U5:83:ARG:CD | 6:M6:27:ALA:O | 1.93 | 1.15 |
| 1:Z5:28:LYS:HD3 | 1:t7:143:PRO:HB3 | 1.17 | 1.15 |
| 1:b5:30:TYR:OH | 10:k5:47:PHE:HZ | 1.05 | 1.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:k5:938:GLN:OE1 | 1:D7:28:LYS:HG2 | 1.42 | 1.15 |
| 10:k5:1153:VAL:CG2 | 1:p7:125:ALA:CB | 2.22 | 1.15 |
| 8:c7:39:ILE:CD1 | 8:c7:148:GLU:HG2 | 1.75 | 1.15 |
| 8:c7:39:ILE:HD13 | 8:c7:148:GLU:HG3 | 1.27 | 1.15 |
| 5:Z8:22:LEU:CD2 | 5:Z8:26:LEU:CD2 | 2.23 | 1.15 |
| 11:aA:312:ASP:HB2 | 11:aA:315:LEU:CD1 | 1.75 | 1.15 |
| 11:aA:588:VAL:C | 11:aA:590:PRO:CD | 2.18 | 1.15 |
| 5:NA:54:LEU:N | 12:TA:301:CYC:HBA1 | 1.61 | 1.15 |
| 3:J2:108:ARG:NE | 6:M2:155:ASN:O | 1.76 | 1.15 |
| 3:F3:116:THR:OG1 | 4:M3:38:PRO:O | 1.58 | 1.15 |
| 3:D4:150:ARG:HG3 | 2:C1:140:SER:HB3 | 1.15 | 1.15 |
| 5:N3:62:ARG:NH2 | 2:Q3:14:SER:CB | 2.08 | 1.15 |
| 1:f5:30:TYR:OH | 10:j5:47:PHE:CZ | 2.00 | 1.15 |
| 8:U5:59:PHE:HB3 | 6:M6:39:ARG:HD3 | 1.28 | 1.15 |
| 10:j5:938:GLN:OE1 | 1:J7:28:LYS:CD | 1.95 | 1.15 |
| 10:j5:1151:GLN:HA | 1:v7:122:PRO:HB3 | 1.17 | 1.15 |
| 10:k5:889:LEU:HD21 | 12:D7:201:CYC:CBB | 1.76 | 1.15 |
| 10:k5:970:GLY:N | 1:n7:77:ARG:NH2 | 1.93 | 1.15 |
| 10:k5:1153:VAL:HG23 | 1:p7:125:ALA:HB2 | 1.26 | 1.15 |
| 3:F6:82:CYS:HB2 | 12:F6:201:CYC:HMD3 | 1.26 | 1.15 |
| 1:P7:14:VAL:O | 1:N7:68:PRO:CB | 1.94 | 1.15 |
| 8:o7:17:TYR:HE2 | 1:p7:93:THR:OG1 | 1.30 | 1.15 |
| 5:N9:53:LEU:CB | 12:T9:301:CYC:HBA2 | 1.75 | 1.15 |
| 2:A9:33:ARG:NH2 | 2:K9:28:ASN:OD1 | 1.79 | 1.15 |
| 2:E9:33:ARG:HG2 | 2:I9:25:GLN:CD | 1.72 | 1.15 |
| 11:aA:275:THR:CA | 11:aA:278:LEU:CD1 | 1.96 | 1.15 |
| 11:aA:280:ASP:OD1 | 11:aA:281:PRO:HD3 | 1.45 | 1.15 |
| 11:aA:694:ARG:NH2 | 4:M1:51:ARG:NH2 | 1.93 | 1.15 |
| 3:HA:119:ALA:HA | 8:S7:49:ARG:NH1 | 1.60 | 1.15 |
| 12:HA:201:CYC:HC | 12:HA:201:CYC:HMD1 | 1.10 | 1.15 |
| 2:IA:37:SER:C | 2:IA:97:LEU:CD1 | 2.20 | 1.15 |
| 3:J3:84:ARG:NH2 | 11:a9:669:ILE:C | 2.03 | 1.15 |
| 12:Z3:202:CYC:C4B | 2:O3:33:ARG:HH12 | 1.60 | 1.15 |
| 2:A4:33:ARG:NH2 | 2:K4:28:ASN:OD1 | 1.79 | 1.15 |
| 3:F4:115:GLU:CD | 4:M4:3:VAL:CG2 | 2.19 | 1.15 |
| 3:H4:119:ALA:O | 11:aA:266:ASN:HB3 | 0.98 | 1.15 |
| 4:M4:101:ASP:CA | 2:P4:13:ASP:HB3 | 1.75 | 1.15 |
| 1:D5:71:MEN:C | 1:D5:77:ARG:HH11 | 1.59 | 1.15 |
| 1:H5:143:PRO:HG3 | 8:Q7:41:GLN:HE22 | 1.12 | 1.15 |
| 8:Q5:12:ASP:HB2 | 1:R5:94:TYR:CE2 | 1.81 | 1.15 |
| 8:U5:79:ALA:HB2 | 6:M6:32:MET:HA | 1.22 | 1.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:K6:28:ASN:OD1 | 2:A6:33:ARG:NH2 | 1.79 | 1.15 |
| 10:j5:1009:ALA:CB | 1:v7:87:TYR:HE1 | 1.58 | 1.15 |
| 3:F6:130:ALA:CB | 12:F6:201:CYC:HBC2 | 1.76 | 1.15 |
| 2:A8:33:ARG:NH2 | 2:K8:28:ASN:OD1 | 1.79 | 1.15 |
| 3:D8:108:ARG:HD2 | 11:a9:107:ARG:HH12 | 1.09 | 1.15 |
| 1:l7:68:PRO:CB | 1:n7:14:VAL:O | 1.94 | 1.15 |
| 8:u7:103:PRO:CB | 1:v7:9:ILE:HG21 | 1.75 | 1.15 |
| 3:L9:14:LEU:CD1 | 11:a9:358:PRO:HG3 | 1.76 | 1.15 |
| 4:M9:160:THR:HG22 | 4:M9:257:GLN:HB2 | 1.27 | 1.15 |
| 5:N9:53:LEU:HD13 | 12:T9:301:CYC:HAA1 | 1.21 | 1.15 |
| 11:a9:245:ALA:CB | 12:a9:901:CYC:HBB3 | 1.77 | 1.15 |
| 1:Z:161:SER:CB | 1:X5:14:VAL:HG21 | 1.60 | 1.15 |
| 7:N2:2:TYR:OH | 3:F2:107:ASP:O | 1.64 | 1.15 |
| 2:C3:140:SER:HB3 | 3:D8:150:ARG:HG3 | 1.15 | 1.15 |
| 8:M5:110:ILE:CD1 | 10:k5:533:LEU:HD11 | 1.77 | 1.15 |
| 8:C5:27:LYS:HA | 8:C5:30:VAL:HG22 | 1.20 | 1.15 |
| 10:k5:386:ILE:HG21 | 10:k5:395:SER:N | 1.42 | 1.15 |
| 10:k5:386:ILE:CG2 | 10:k5:387:VAL:H | 1.59 | 1.15 |
| 10:k5:779:ASP:OD2 | 12:F7:201:CYC:HMA2 | 1.47 | 1.15 |
| 2:X8:28:ASN:OD1 | 2:N8:33:ARG:NH2 | 1.79 | 1.15 |
| 2:X8:67:THR:CB | 3:T9:28:THR:HG21 | 1.61 | 1.15 |
| 4:M8:91:VAL:HG13 | 2:P8:14:SER:O | 1.35 | 1.15 |
| 4:M8:205:ASP:CB | 5:Z8:59:ARG:NE | 2.03 | 1.15 |
| 3:Q8:89:ILE:HA | 3:Q8:92:TYR:CD2 | 1.80 | 1.15 |
| 3:DA:112:GLY:N | 4:MA:76:ALA:HB1 | 1.62 | 1.14 |
| 5:NA:53:LEU:CB | 12:TA:301:CYC:HBA2 | 1.75 | 1.14 |
| 2:Q1:14:SER:CB | 5:N1:62:ARG:NH2 | 2.08 | 1.14 |
| 2:K2:28:ASN:OD1 | 2:A2:33:ARG:NH2 | 1.79 | 1.14 |
| 6:M2:26:PHE:CB | 8:O5:87:TYR:OH | 1.93 | 1.14 |
| 8:K5:112:VAL:HG23 | 1:J5:75:THR:HG21 | 1.18 | 1.14 |
| 1:N5:110:ASN:CG | 10:k5:692:LEU:O | 1.90 | 1.14 |
| 1:Z5:127:VAL:CG1 | 10:k5:698:GLY:HA3 | 1.76 | 1.14 |
| 10:k5:970:GLY:CA | 1:n7:77:ARG:HH21 | 1.60 | 1.14 |
| 10:k5:1150:TYR:CE2 | 1:p7:69:GLY:O | 1.99 | 1.14 |
| 8:c7:16:ARG:N | 1:d7:90:ARG:CD | 2.10 | 1.14 |
| 8:u7:121:THR:HG23 | 12:u7:201:CYC:HMC3 | 1.24 | 1.14 |
| 12:L8:201:CYC:HMD1 | 12:L8:201:CYC:HC | 1.10 | 1.14 |
| 3:O8:107:ASP:CB | 5:Z8:66:ARG:CB | 2.25 | 1.14 |
| 11:a9:403:THR:HG21 | 11:a9:536:THR:HG22 | 1.28 | 1.14 |
| 11:aA:632:ILE:CG2 | 11:aA:634:ALA:H | 1.60 | 1.14 |
| 11:aA:694:ARG:NH1 | 4:M1:51:ARG:NH2 | 1.94 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AA:33:ARG:HH12 | 12:LA:201:CYC:C4B | 1.60 | 1.14 |
| 2:AA:33:ARG:NH2 | 2:KA:28:ASN:OD1 | 1.79 | 1.14 |
| 3:JA:109:CYS:O | 11:aA:518:ALA:HB2 | 1.47 | 1.14 |
| 4:M3:51:ARG:HH21 | 11:a9:694:ARG:NH1 | 1.42 | 1.14 |
| 3:F4:108:ARG:CZ | 4:M4:9:GLN:HG3 | 1.73 | 1.14 |
| 4:M4:138:SER:HB3 | 12:Z4:301:CYC:CBB | 1.77 | 1.14 |
| 4:M4:232:VAL:HB | 12:M4:301:CYC:HBB2 | 1.17 | 1.14 |
| 8:G5:126:VAL:HG22 | 12:G5:201:CYC:H3C | 1.25 | 1.14 |
| 1:J5:71:MEN:C | 1:J5:77:ARG:HH11 | 1.59 | 1.14 |
| 1:Z5:64:ASP:HB2 | 10:k5:705:THR:CG2 | 1.76 | 1.14 |
| 10:j5:357:LEU:HD11 | 10:j5:379:PHE:HA | 1.28 | 1.14 |
| 10:j5:1047:LYS:O | 10:j5:1051:GLU:HB3 | 1.47 | 1.14 |
| 1:v7:62:TYR:CB | 11:aA:602:PRO:HD2 | 1.39 | 1.14 |
| 2:P8:18:PHE:CA | 3:Q8:91:ARG:NH2 | 2.10 | 1.14 |
| 5:N9:1:MET:HG3 | 3:R9:119:ALA:HB2 | 1.29 | 1.14 |
| 5:N9:22:LEU:HD22 | 5:N9:26:LEU:CD2 | 1.77 | 1.14 |
| 12:T9:302:CYC:HMD1 | 12:T9:302:CYC:HC | 1.10 | 1.14 |
| 11:a9:239:TYR:CE1 | 12:a9:901:CYC:HBA1 | 1.80 | 1.14 |
| 11:a9:632:ILE:CG2 | 11:a9:634:ALA:H | 1.60 | 1.14 |
| 1:Z:122:PRO:HB3 | 1:V5:64:ASP:OD2 | 1.46 | 1.14 |
| 2:SA:35:THR:CG2 | 2:X4:74:TYR:CE1 | 2.25 | 1.14 |
| 2:O1:33:ARG:NH2 | 2:Y1:28:ASN:OD1 | 1.79 | 1.14 |
| 2:O1:33:ARG:HH12 | 12:Z1:201:CYC:C4B | 1.60 | 1.14 |
| 3:J3:14:LEU:CD1 | 11:a9:621:THR:HG21 | 1.72 | 1.14 |
| 3:J3:85:ASP:OD1 | 11:a9:668:TYR:CE2 | 2.00 | 1.14 |
| 8:W5:12:ASP:HB2 | 1:X5:94:TYR:CE2 | 1.81 | 1.14 |
| 1:Z5:161:SER:CB | 10:k5:695:GLY:O | 1.96 | 1.14 |
| 10:j5:729:ILE:HD12 | 1:J7:64:ASP:OD1 | 1.46 | 1.14 |
| 1:H7:68:PRO:CB | 1:J7:14:VAL:O | 1.94 | 1.14 |
| 8:i7:96:ILE:CA | 8:i7:152:TYR:CE2 | 2.31 | 1.14 |
| 8:c7:16:ARG:CA | 1:d7:90:ARG:CD | 2.25 | 1.14 |
| 4:M8:104:ALA:HB2 | 2:P8:10:ALA:O | 1.43 | 1.14 |
| 5:N9:54:LEU:N | 12:T9:301:CYC:HBA1 | 1.61 | 1.14 |
| 3:H9:126:SER:CB | 12:H9:202:CYC:HMC1 | 1.73 | 1.14 |
| 11:aA:708:HIS:HB3 | 3:L1:108:ARG:NH2 | 1.61 | 1.14 |
| 2:IA:113:LEU:HD21 | 2:IA:161:LEU:HD23 | 1.25 | 1.14 |
| 5:NA:22:LEU:HD22 | 5:NA:26:LEU:CD2 | 1.77 | 1.14 |
| 2:A3:33:ARG:HH12 | 12:L3:201:CYC:C4B | 1.60 | 1.14 |
| 3:F4:107:ASP:HB3 | 4:M4:8:SER:CB | 1.68 | 1.14 |
| 3:Q4:72:ASN:OD1 | 12:Z4:301:CYC:HMD2 | 1.48 | 1.14 |
| 1:d5:127:VAL:HG11 | 10:j5:698:GLY:CA | 1.77 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:Q5:16:ARG:HA | 1:R5:90:ARG:CD | 1.76 | 1.14 |
| 1:R5:110:ASN:OD1 | 10:k5:466:LEU:CB | 1.96 | 1.14 |
| 8:U5:59:PHE:CE2 | 6:M6:37:GLU:OE2 | 1.99 | 1.14 |
| 6:M6:53:LEU:CD2 | 8:c7:80:LEU:HG | 1.75 | 1.14 |
| 10:j5:152:ARG:NH2 | 10:j5:193:SER:O | 1.79 | 1.14 |
| 10:j5:1067:LEU:CD1 | 10:j5:1101:GLU:HG2 | 1.78 | 1.14 |
| 1:T7:68:PRO:CB | 1:V7:14:VAL:O | 1.94 | 1.14 |
| 3:U8:114:LYS:HE2 | 4:M8:13:LYS:NZ | 1.61 | 1.14 |
| 3:Q8:120:LEU:CD1 | 3:Q8:122:THR:OG1 | 1.96 | 1.14 |
| 12:J9:202:CYC:CBA | 11:a9:511:LYS:CA | 2.24 | 1.14 |
| 11:a9:245:ALA:HB2 | 12:a9:901:CYC:HBB3 | 1.27 | 1.14 |
| 1:Z:107:ARG:NH2 | 8:e5:12:ASP:OD2 | 1.79 | 1.14 |
| 4:M3:51:ARG:NH2 | 11:a9:694:ARG:NH2 | 1.94 | 1.14 |
| 8:C5:27:LYS:O | 8:C5:28:SER:C | 1.86 | 1.14 |
| 8:G5:100:ASP:OD1 | 8:S5:20:PRO:HG2 | 1.44 | 1.14 |
| 1:d5:83:ARG:NH1 | 10:j5:379:PHE:HE2 | 1.45 | 1.14 |
| 8:Q5:11:ALA:CB | 1:R5:94:TYR:HE1 | 1.48 | 1.14 |
| 12:L6:202:CYC:HMD1 | 12:L6:202:CYC:HC | 1.10 | 1.14 |
| 6:M6:65:VAL:HG12 | 1:b7:59:ALA:C | 1.71 | 1.14 |
| 9:z5:6:LYS:CB | 9:z5:55:LYS:CB | 2.02 | 1.14 |
| 9:i5:18:ARG:HB3 | 9:i5:22:GLU:OE2 | 1.45 | 1.14 |
| 3:H8:84:ARG:CB | 11:a9:131:TYR:CE1 | 2.31 | 1.14 |
| 3:L8:69:PRO:O | 11:a9:82:GLN:HB3 | 1.47 | 1.14 |
| 3:L8:108:ARG:O | 12:a9:901:CYC:HBB1 | 1.48 | 1.14 |
| 5:Z8:29:HIS:ND1 | 5:Z8:31:TRP:CB | 2.11 | 1.14 |
| 2:I9:37:SER:C | 2:I9:97:LEU:CD1 | 2.20 | 1.14 |
| 3:J9:119:ALA:C | 11:a9:365:LYS:CE | 2.20 | 1.14 |
| 12:J9:202:CYC:HBA1 | 11:a9:511:LYS:CA | 1.78 | 1.14 |
| 11:a9:239:TYR:HE1 | 12:a9:901:CYC:HBA1 | 1.06 | 1.14 |
| 11:aA:338:VAL:HG22 | 11:aA:340:PRO:CG | 1.77 | 1.14 |
| 12:LA:201:CYC:HC | 12:LA:201:CYC:HMD1 | 1.09 | 1.13 |
| 5:NA:53:LEU:HD13 | 12:TA:301:CYC:HAA1 | 1.21 | 1.13 |
| 2:O3:33:ARG:NH2 | 2:Y3:28:ASN:OD1 | 1.79 | 1.13 |
| 1:d5:53:LYS:HD3 | 8:e5:118:SER:O | 1.46 | 1.13 |
| 8:S5:66:VAL:HG11 | 8:E7:68:PRO:HG3 | 1.29 | 1.13 |
| 12:L6:202:CYC:C4B | 2:A6:33:ARG:HH12 | 1.60 | 1.13 |
| 10:k5:152:ARG:NH2 | 10:k5:193:SER:O | 1.79 | 1.13 |
| 10:k5:825:ASN:OD1 | 10:k5:854:LEU:HD13 | 1.47 | 1.13 |
| 10:k5:1056:PRO:HD2 | 10:k5:1057:LYS:H | 1.14 | 1.13 |
| 3:F8:109:CYS:N | 4:M8:6:THR:CG2 | 2.11 | 1.13 |
| 12:B9:202:CYC:HMD1 | 12:B9:202:CYC:HC | 1.10 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 11:a9:710:THR:HG22 | 11:a9:807:GLN:CD | 1.72 | 1.13 |
| 11:aA:280:ASP:CB | 11:aA:281:PRO:CD | 2.03 | 1.13 |
| 11:aA:312:ASP:HB2 | 11:aA:315:LEU:CG | 1.79 | 1.13 |
| 4:M1:258:LYS:NZ | 3:Z1:111:ASN:HD21 | 1.46 | 1.13 |
| 3:HA:120:LEU:CD1 | 12:HA:202:CYC:C2A | 2.26 | 1.13 |
| 2:OA:33:ARG:HH12 | 12:ZA:201:CYC:C4B | 1.60 | 1.13 |
| 4:M4:144:ARG:HG2 | 4:M4:204:ILE:HD13 | 1.14 | 1.13 |
| 4:M4:217:VAL:HG22 | 5:Z4:30:PRO:CD | 1.78 | 1.13 |
| 8:G5:100:ASP:OD2 | 8:S5:20:PRO:HB2 | 1.46 | 1.13 |
| 1:d5:110:ASN:HD21 | 10:j5:451:LYS:CB | 1.60 | 1.13 |
| 1:Z5:110:ASN:ND2 | 10:k5:451:LYS:HB3 | 1.61 | 1.13 |
| 10:j5:1067:LEU:HD11 | 10:j5:1101:GLU:HG2 | 1.20 | 1.13 |
| 10:j5:1153:VAL:CG2 | 1:v7:125:ALA:HB1 | 1.73 | 1.13 |
| 3:D1:68:ARG:CZ | 3:X1:68:ARG:HH22 | 1.62 | 1.13 |
| 3:B8:81:ALA:HB1 | 12:B8:202:CYC:HMD3 | 1.30 | 1.13 |
| 8:o7:97:VAL:HG21 | 1:p7:19:LEU:HD13 | 1.16 | 1.13 |
| 4:M9:274:VAL:CG1 | 3:V9:77:ARG:CD | 1.87 | 1.13 |
| 2:O9:33:ARG:HH12 | 12:Z9:201:CYC:C4B | 1.60 | 1.13 |
| 12:Z9:201:CYC:HMD1 | 12:Z9:201:CYC:HC | 1.10 | 1.13 |
| 11:a9:312:ASP:HB2 | 11:a9:315:LEU:CG | 1.79 | 1.13 |
| 11:aA:621:THR:HG21 | 3:J1:14:LEU:CD1 | 1.71 | 1.13 |
| 1:Z:127:VAL:HG11 | 1:X5:15:GLN:HG2 | 1.16 | 1.13 |
| 2:EA:33:ARG:HG2 | 2:IA:25:GLN:CD | 1.72 | 1.13 |
| 3:LA:14:LEU:CD1 | 11:aA:358:PRO:HG3 | 1.77 | 1.13 |
| 2:QA:76:ASP:CB | 2:U1:140:SER:O | 1.95 | 1.13 |
| 3:H3:78:ARG:NH2 | 11:a9:623:ASP:HB3 | 1.63 | 1.13 |
| 3:J3:85:ASP:N | 11:a9:668:TYR:OH | 1.80 | 1.13 |
| 3:B3:108:ARG:O | 4:M3:6:THR:HG22 | 1.47 | 1.13 |
| 12:T3:302:CYC:HMD1 | 12:T3:302:CYC:HC | 1.10 | 1.13 |
| 12:U4:202:CYC:HMD1 | 12:U4:202:CYC:HC | 1.10 | 1.13 |
| 5:Z4:41:GLN:CG | 12:Z4:301:CYC:HMB1 | 1.75 | 1.13 |
| 8:S5:68:PRO:HB3 | 8:a5:59:PHE:CB | 1.77 | 1.13 |
| 1:b5:18:TYR:CE1 | 10:k5:165:ARG:HD3 | 1.83 | 1.13 |
| 10:j5:136:VAL:CG1 | 10:j5:137:PRO:CD | 2.24 | 1.13 |
| 10:j5:138:PRO:HB3 | 10:j5:201:VAL:HG11 | 1.30 | 1.13 |
| 10:j5:1151:GLN:O | 1:v7:122:PRO:HB2 | 1.47 | 1.13 |
| 8:i7:25:ARG:NH1 | 8:s7:6:LYS:HB3 | 1.59 | 1.13 |
| 2:A8:33:ARG:HH12 | 12:L8:201:CYC:C4B | 1.60 | 1.13 |
| 3:U8:112:GLY:HA2 | 4:M8:74:LEU:CD2 | 1.79 | 1.13 |
| 12:F8:201:CYC:HMD1 | 12:F8:201:CYC:HC | 1.10 | 1.13 |
| 3:L8:68:ARG:HB2 | 11:a9:82:GLN:N | 1.57 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:L8:71:GLY:CA | 11:a9:82:GLN:HG2 | 1.76 | 1.13 |
| 3:O8:112:GLY:O | 5:Z8:70:ILE:HB | 1.47 | 1.13 |
| 4:M9:76:ALA:HB1 | 3:D9:112:GLY:N | 1.62 | 1.13 |
| 3:FA:150:ARG:CA | 3:F9:150:ARG:CG | 2.27 | 1.13 |
| 3:HA:78:ARG:NH1 | 12:HA:202:CYC:O2D | 1.80 | 1.13 |
| 2:A1:33:ARG:HH12 | 12:L1:201:CYC:C4B | 1.60 | 1.13 |
| 2:A1:33:ARG:NH2 | 2:K1:28:ASN:OD1 | 1.79 | 1.13 |
| 3:D3:68:ARG:CZ | 3:X3:68:ARG:HH22 | 1.62 | 1.13 |
| 12:L3:202:CYC:OB | 11:a9:738:LEU:CD2 | 1.97 | 1.13 |
| 3:B1:108:ARG:O | 4:M1:6:THR:HG22 | 1.47 | 1.13 |
| 2:N4:33:ARG:HH12 | 12:Y4:201:CYC:C4B | 1.60 | 1.13 |
| 8:A5:107:ILE:HG12 | 1:B5:13:ASP:OD2 | 1.48 | 1.13 |
| 1:d5:28:LYS:CE | 1:n7:143:PRO:CB | 2.26 | 1.13 |
| 1:V5:114:GLU:CG | 10:j5:496:GLU:CD | 2.18 | 1.13 |
| 10:j5:931:VAL:HG13 | 1:J7:29:ALA:HB1 | 1.31 | 1.13 |
| 10:k5:136:VAL:CG1 | 10:k5:137:PRO:CD | 2.24 | 1.13 |
| 10:k5:1067:LEU:HD11 | 10:k5:1101:GLU:HG2 | 1.20 | 1.13 |
| 10:k5:1153:VAL:HG21 | 1:p7:125:ALA:HB1 | 1.31 | 1.13 |
| 12:H6:202:CYC:HMD1 | 12:H6:202:CYC:HC | 1.10 | 1.13 |
| 1:H7:140:LEU:HD11 | 11:aA:561:ALA:CB | 1.78 | 1.13 |
| 8:i7:39:ILE:CD1 | 8:i7:148:GLU:CB | 2.27 | 1.13 |
| 8:a7:63:PRO:HD3 | 11:a9:336:ILE:HG22 | 1.30 | 1.13 |
| 12:B2:201:CYC:HMD1 | 12:B2:201:CYC:HC | 1.10 | 1.13 |
| 5:NA:16:PHE:CE1 | 3:TA:120:LEU:HD23 | 1.83 | 1.13 |
| 2:SA:35:THR:CG2 | 2:X4:74:TYR:OH | 1.91 | 1.12 |
| 2:A1:63:PHE:HB2 | 2:A1:66:LEU:HD11 | 1.20 | 1.13 |
| 12:L2:202:CYC:C4B | 2:A2:33:ARG:HH12 | 1.60 | 1.12 |
| 2:A4:33:ARG:HH12 | 12:L4:201:CYC:C4B | 1.60 | 1.13 |
| 4:M4:100:SER:HB3 | 3:Q4:1:MET:CE | 1.78 | 1.12 |
| 12:M4:301:CYC:CAC | 3:Y4:82:CYS:SG | 2.38 | 1.12 |
| 2:N4:111:ALA:O | 5:Z4:34:LEU:HD12 | 1.29 | 1.12 |
| 5:Z4:42:SER:HA | 12:Z4:301:CYC:HMA1 | 1.26 | 1.12 |
| 8:E5:80:LEU:CD1 | 12:E5:201:CYC:HAD2 | 1.79 | 1.12 |
| 8:I5:41:GLN:HB2 | 1:J5:24:LEU:HD11 | 1.31 | 1.13 |
| 8:S5:14:GLU:HG2 | 10:j5:538:PHE:CE2 | 1.84 | 1.12 |
| 8:W5:12:ASP:CA | 1:X5:94:TYR:HE2 | 1.60 | 1.12 |
| 1:b5:114:GLU:HG2 | 10:k5:491:THR:OG1 | 1.49 | 1.12 |
| 10:j5:56:ILE:CD1 | 10:j5:219:ASP:HB3 | 1.79 | 1.12 |
| 10:j5:1143:LEU:HD12 | 8:q7:106:GLU:HB2 | 1.19 | 1.13 |
| 10:j5:1146:THR:N | 1:v7:77:ARG:HH22 | 1.44 | 1.13 |
| 8:c7:39:ILE:CD1 | 8:c7:148:GLU:CB | 2.27 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:c7:96:ILE:CA | 8:c7:152:TYR:CE2 | 2.31 | 1.13 |
| 12:B8:202:CYC:O1A | 4:M8:54:ALA:HB2 | 1.31 | 1.12 |
| 8:u7:27:LYS:HE2 | 1:v7:35:ALA:HB1 | 1.16 | 1.13 |
| 3:J3:14:LEU:HD22 | 11:a9:621:THR:HG22 | 1.18 | 1.12 |
| 2:K3:14:SER:HB2 | 11:a9:746:TYR:CB | 1.79 | 1.12 |
| 3:F4:109:CYS:CA | 4:M4:6:THR:CG2 | 2.25 | 1.12 |
| 10:k5:1118:THR:O | 12:k5:1204:CYC:HMA2 | 1.48 | 1.12 |
| 8:o7:27:LYS:HE2 | 1:p7:35:ALA:HB1 | 1.16 | 1.12 |
| 4:M8:217:VAL:HG22 | 5:Z8:30:PRO:HG2 | 1.14 | 1.12 |
| 3:L9:52:ILE:HD11 | 3:L9:87:GLU:CB | 1.78 | 1.12 |
| 5:N9:16:PHE:CE1 | 3:T9:120:LEU:HD23 | 1.83 | 1.12 |
| 5:Z8:22:LEU:HD22 | 5:Z8:26:LEU:CD2 | 1.77 | 1.12 |
| 5:Z8:41:GLN:HB2 | 12:Z8:301:CYC:C2B | 1.68 | 1.12 |
| 3:H9:126:SER:HB2 | 12:H9:202:CYC:HMC1 | 1.21 | 1.12 |
| 12:V9:202:CYC:HMD1 | 12:V9:202:CYC:HC | 1.11 | 1.12 |
| 11:aA:710:THR:HG22 | 11:aA:807:GLN:CD | 1.72 | 1.12 |
| 3:LA:52:ILE:HD11 | 3:LA:87:GLU:CB | 1.78 | 1.12 |
| 2:A4:63:PHE:HB2 | 2:A4:66:LEU:HD11 | 1.20 | 1.12 |
| 3:U4:115:GLU:HB3 | 4:M4:74:LEU:HD11 | 1.12 | 1.12 |
| 3:O4:107:ASP:HB3 | 5:Z4:66:ARG:CB | 1.77 | 1.12 |
| 5:Z4:25:THR:CG2 | 5:Z4:63:ASN:O | 1.95 | 1.12 |
| 1:X5:65:LEU:HD12 | 10:j5:706:PRO:HG3 | 1.15 | 1.12 |
| 1:Z5:53:LYS:HD3 | 8:a5:118:SER:O | 1.46 | 1.12 |
| 10:j5:386:ILE:CG2 | 10:j5:387:VAL:H | 1.59 | 1.12 |
| 10:j5:1018:LEU:HD11 | 10:j5:1035:PHE:CZ | 1.78 | 1.12 |
| 8:U7:60:GLN:OE1 | 1:p7:117:ASN:CB | 1.97 | 1.12 |
| 3:F8:115:GLU:HG2 | 4:M8:3:VAL:HG11 | 1.24 | 1.12 |
| 2:N8:112:GLY:HA2 | 5:Z8:34:LEU:H | 1.02 | 1.12 |
| 12:L9:201:CYC:C4B | 2:A9:33:ARG:HH12 | 1.60 | 1.12 |
| 5:Z8:38:GLU:HB2 | 12:Z8:301:CYC:HMB3 | 1.22 | 1.12 |
| 11:aA:738:LEU:CD2 | 12:aA:902:CYC:OB | 1.97 | 1.12 |
| 5:NA:1:MET:HB3 | 5:NA:3:VAL:HG23 | 1.30 | 1.12 |
| 3:J3:77:ARG:CZ | 2:K3:107:ASP:CA | 2.27 | 1.12 |
| 5:N3:22:LEU:HD22 | 5:N3:26:LEU:CD2 | 1.77 | 1.12 |
| 2:U3:45:THR:O | 2:Q9:69:PRO:HG2 | 1.48 | 1.12 |
| 3:L4:88:ILE:HD11 | 11:aA:239:TYR:CE2 | 1.82 | 1.12 |
| 12:Q4:201:CYC:HMD1 | 12:Q4:201:CYC:HC | 1.11 | 1.12 |
| 5:Z4:41:GLN:HG3 | 12:Z4:301:CYC:CMB | 1.76 | 1.12 |
| 1:d5:28:LYS:HD2 | 1:n7:143:PRO:CG | 1.76 | 1.12 |
| 1:R5:63:SER:OG | 10:k5:706:PRO:HA | 1.49 | 1.12 |
| 10:j5:1146:THR:CA | 1:v7:77:ARG:HH22 | 1.62 | 1.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:F8:84:ARG:HD2 | 11:a9:139:ILE:HG22 | 1.17 | 1.12 |
| 3:H8:119:ALA:O | 11:a9:266:ASN:HB3 | 0.96 | 1.12 |
| 4:M8:226:SER:CB | 3:Y8:85:ASP:OD1 | 1.96 | 1.12 |
| 4:M9:158:PHE:CA | 3:V9:108:ARG:HD3 | 1.79 | 1.12 |
| 4:M9:274:VAL:HG11 | 2:W9:111:ALA:HB1 | 1.14 | 1.12 |
| 5:N9:66:ARG:HB2 | 3:T9:111:ASN:ND2 | 1.64 | 1.12 |
| 2:O9:63:PHE:HB2 | 2:O9:66:LEU:HD11 | 1.20 | 1.12 |
| 5:Z8:41:GLN:O | 12:Z8:301:CYC:HMA1 | 1.47 | 1.12 |
| 11:a9:710:THR:HG22 | 11:a9:807:GLN:HB3 | 1.32 | 1.12 |
| 11:aA:30:MET:CB | 11:aA:34:ILE:O | 1.97 | 1.12 |
| 1:A:122:PRO:CB | 1:P5:64:ASP:OD2 | 1.96 | 1.12 |
| 3:FA:150:ARG:CG | 3:F9:150:ARG:CG | 1.90 | 1.12 |
| 4:MA:185:ALA:HA | 12:VA:201:CYC:CGA | 1.79 | 1.12 |
| 4:MA:274:VAL:CA | 3:VA:77:ARG:CG | 1.85 | 1.12 |
| 2:QA:119:THR:CG2 | 3:TA:83:LEU:HD22 | 1.78 | 1.12 |
| 12:P1:202:CYC:HMD1 | 12:P1:202:CYC:HC | 1.10 | 1.12 |
| 6:M2:50:LEU:HD22 | 8:i7:79:ALA:O | 1.48 | 1.12 |
| 5:N3:1:MET:HB3 | 5:N3:3:VAL:HG23 | 1.30 | 1.12 |
| 4:M4:100:SER:CB | 3:Q4:1:MET:HE3 | 1.77 | 1.12 |
| 4:M4:160:THR:HG22 | 4:M4:257:GLN:HB2 | 1.27 | 1.12 |
| 8:A5:126:VAL:HG22 | 12:A5:201:CYC:H3C | 1.24 | 1.12 |
| 1:B5:87:TYR:CE1 | 9:z5:19:THR:O | 2.01 | 1.12 |
| 8:e5:49:ARG:NH1 | 1:R5:50:THR:HG21 | 1.63 | 1.12 |
| 8:W5:15:ALA:O | 1:X5:90:ARG:NE | 1.82 | 1.12 |
| 8:W5:17:TYR:HE2 | 1:X5:93:THR:OG1 | 1.21 | 1.12 |
| 10:j5:825:ASN:OD1 | 10:j5:854:LEU:HD13 | 1.47 | 1.12 |
| 10:k5:741:GLN:HG3 | 1:D7:77:ARG:NH2 | 1.65 | 1.12 |
| 10:k5:965:GLN:H | 1:n7:69:GLY:CA | 1.61 | 1.12 |
| 1:B7:140:LEU:HD11 | 11:a9:561:ALA:CB | 1.79 | 1.12 |
| 8:I7:25:ARG:NH2 | 8:W7:25:ARG:CB | 2.11 | 1.12 |
| 8:I7:25:ARG:HH22 | 8:W7:25:ARG:CD | 1.60 | 1.12 |
| 3:Q8:110:LEU:HD21 | 3:Q8:167:ALA:HA | 1.22 | 1.12 |
| 11:aA:615:ARG:O | 3:H1:68:ARG:HD3 | 1.48 | 1.12 |
| 11:aA:746:TYR:CB | 2:K1:14:SER:HB2 | 1.78 | 1.12 |
| 5:N1:39:PRO:HB3 | 3:T1:113:LEU:HA | 1.28 | 1.12 |
| 1:A:161:SER:CB | 1:R5:14:VAL:HG21 | 1.74 | 1.12 |
| 12:DA:202:CYC:HMD1 | 12:DA:202:CYC:HC | 1.10 | 1.12 |
| 3:JA:119:ALA:C | 11:aA:365:LYS:CE | 2.21 | 1.12 |
| 12:JA:202:CYC:CBA | 11:aA:511:LYS:CA | 2.26 | 1.12 |
| 4:MA:113:ILE:HD11 | 4:MA:143:VAL:HG13 | 1.13 | 1.12 |
| 3:Z3:111:ASN:HD21 | 4:M3:258:LYS:NZ | 1.46 | 1.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:B4:108:ARG:HA | 4:M4:61:ASN:CA | 1.79 | 1.12 |
| 12:D4:201:CYC:HMD1 | 12:D4:201:CYC:HC | 1.11 | 1.12 |
| 3:F4:77:ARG:HD2 | 11:aA:146:ARG:HH12 | 0.96 | 1.12 |
| 4:M4:235:PHE:HB2 | 12:M4:301:CYC:HAA1 | 1.16 | 1.12 |
| 2:N4:14:SER:CB | 5:Z4:62:ARG:CD | 2.28 | 1.12 |
| 5:Z4:22:LEU:HD11 | 12:Z4:301:CYC:OB | 0.96 | 1.12 |
| 6:M6:278:ARG:NH2 | 1:d7:64:ASP:OD1 | 1.83 | 1.12 |
| 10:j5:1050:PHE:CZ | 1:r7:107:ARG:CZ | 2.33 | 1.12 |
| 10:k5:1018:LEU:CD1 | 10:k5:1035:PHE:CE2 | 2.31 | 1.12 |
| 10:k5:1119:LEU:CD1 | 12:k5:1204:CYC:C4B | 2.28 | 1.12 |
| 8:U7:52:LYS:CE | 11:a9:29:ARG:HH12 | 1.63 | 1.12 |
| 12:b7:201:CYC:HBB2 | 9:x7:21:ARG:CD | 1.78 | 1.12 |
| 8:o7:90:ARG:HA | 1:p7:18:TYR:CE2 | 1.84 | 1.12 |
| 8:u7:90:ARG:HA | 1:v7:18:TYR:CE2 | 1.84 | 1.12 |
| 3:L8:68:ARG:HB3 | 11:a9:82:GLN:N | 1.64 | 1.12 |
| 4:M8:160:THR:HG22 | 4:M8:257:GLN:HB2 | 1.27 | 1.12 |
| 4:M8:230:GLN:HB3 | 12:M8:301:CYC:OB | 0.94 | 1.12 |
| 2:N8:33:ARG:HH12 | 12:Y8:201:CYC:C4B | 1.60 | 1.12 |
| 5:Z8:1:MET:HB3 | 5:Z8:3:VAL:HG23 | 1.30 | 1.12 |
| 11:a9:30:MET:CB | 11:a9:34:ILE:O | 1.97 | 1.12 |
| 4:MA:163:ASN:HD21 | 12:VA:201:CYC:CMA | 1.62 | 1.11 |
| 4:M3:134:ASN:HB2 | 12:P3:201:CYC:CAA | 1.80 | 1.11 |
| 4:M4:100:SER:H | 3:Q4:1:MET:CE | 1.60 | 1.11 |
| 4:M4:225:LYS:HE3 | 3:Y4:81:ALA:HB2 | 1.30 | 1.11 |
| 5:Z4:41:GLN:CB | 12:Z4:301:CYC:C1B | 2.27 | 1.11 |
| 1:B5:87:TYR:HE1 | 9:z5:19:THR:O | 1.32 | 1.11 |
| 8:G5:107:ILE:HG12 | 1:H5:13:ASP:OD2 | 1.48 | 1.11 |
| 1:f5:38:VAL:HG13 | 10:j5:40:VAL:CG1 | 1.78 | 1.11 |
| 10:j5:766:ALA:HB1 | 8:K7:14:GLU:OE2 | 1.43 | 1.11 |
| 10:k5:1052:PRO:HB3 | 1:l7:106:GLU:OE2 | 1.50 | 1.11 |
| 10:k5:1067:LEU:CD1 | 10:k5:1101:GLU:HG2 | 1.78 | 1.11 |
| 3:F6:130:ALA:CB | 12:F6:201:CYC:CBC | 2.28 | 1.11 |
| 8:i7:25:ARG:NH1 | 8:s7:6:LYS:HG2 | 1.64 | 1.11 |
| 8:u7:17:TYR:HE2 | 1:v7:93:THR:OG1 | 1.30 | 1.11 |
| 1:v7:62:TYR:HB3 | 11:aA:602:PRO:HD2 | 1.15 | 1.11 |
| 3:U8:111:ASN:OD1 | 4:M8:77:LEU:HD13 | 1.46 | 1.11 |
| 4:M8:128:ALA:C | 4:M8:142:PHE:CE1 | 2.28 | 1.11 |
| 4:M8:197:ASP:O | 5:Z8:52:ARG:CZ | 1.98 | 1.11 |
| 4:M9:148:LYS:HD3 | 4:M9:197:ASP:OD1 | 1.50 | 1.11 |
| 11:a9:338:VAL:HG22 | 11:a9:340:PRO:CG | 1.77 | 1.11 |
| 5:N1:22:LEU:HD22 | 5:N1:26:LEU:CD2 | 1.77 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:FA:150:ARG:CD | 3:F9:150:ARG:HG2 | 1.79 | 1.11 |
| 5:NA:1:MET:HG3 | 3:RA:119:ALA:HB2 | 1.29 | 1.11 |
| 5:NA:70:ILE:HG21 | 3:TA:116:THR:HA | 1.26 | 1.11 |
| 4:M3:51:ARG:NH2 | 11:a9:694:ARG:CZ | 2.13 | 1.11 |
| 3:S4:120:LEU:CD2 | 12:S4:202:CYC:HBD1 | 1.80 | 1.11 |
| 4:M4:225:LYS:CE | 3:Y4:81:ALA:HB2 | 1.80 | 1.11 |
| 2:N4:111:ALA:C | 5:Z4:34:LEU:CG | 2.23 | 1.11 |
| 3:O4:107:ASP:CG | 5:Z4:66:ARG:CD | 2.23 | 1.11 |
| 10:j5:793:SER:HB3 | 12:T7:201:CYC:O2A | 1.50 | 1.11 |
| 10:j5:931:VAL:HG13 | 1:J7:29:ALA:CB | 1.78 | 1.11 |
| 10:k5:1047:LYS:O | 10:k5:1051:GLU:HB3 | 1.47 | 1.11 |
| 12:d7:201:CYC:CBB | 9:x7:42:GLN:OE1 | 1.98 | 1.11 |
| 8:u7:103:PRO:HB3 | 1:v7:9:ILE:HG21 | 1.12 | 1.11 |
| 3:U8:108:ARG:O | 4:M8:246:ALA:HB1 | 1.48 | 1.11 |
| 4:M8:141:GLU:HB2 | 4:M8:144:ARG:HH21 | 1.13 | 1.11 |
| 4:M9:185:ALA:HA | 12:V9:201:CYC:CGA | 1.79 | 1.11 |
| 3:J9:109:CYS:O | 11:a9:518:ALA:HB2 | 1.46 | 1.11 |
| 11:aA:694:ARG:NH1 | 4:M1:51:ARG:HH21 | 1.44 | 1.11 |
| 11:aA:710:THR:HG22 | 11:aA:807:GLN:HB3 | 1.32 | 1.11 |
| 12:V1:202:CYC:HMD1 | 12:V1:202:CYC:HC | 1.10 | 1.11 |
| 3:FA:36:LYS:HB3 | 3:FA:156:LEU:HD13 | 1.31 | 1.11 |
| 4:M3:148:LYS:HD3 | 4:M3:197:ASP:OD1 | 1.49 | 1.11 |
| 3:S4:72:ASN:HD22 | 3:S4:123:PRO:CD | 1.61 | 1.11 |
| 3:L4:68:ARG:HD2 | 11:aA:81:ASP:CA | 1.80 | 1.11 |
| 8:Q5:15:ALA:O | 1:R5:90:ARG:NE | 1.82 | 1.11 |
| 1:T5:53:LYS:CD | 8:U5:118:SER:O | 1.99 | 1.11 |
| 8:U5:76:LYS:HG3 | 8:U5:77:MET:HE2 | 1.31 | 1.11 |
| 8:U5:79:ALA:CB | 6:M6:32:MET:HA | 1.79 | 1.11 |
| 10:j5:1018:LEU:CD1 | 10:j5:1035:PHE:CE2 | 2.31 | 1.11 |
| 10:k5:1009:ALA:HB2 | 1:p7:87:TYR:CE1 | 1.85 | 1.11 |
| 1:B7:136:VAL:CG1 | 11:a9:563:PHE:CZ | 2.33 | 1.11 |
| 3:O8:111:ASN:O | 5:Z8:67:ILE:CG2 | 1.99 | 1.11 |
| 4:M9:7:SER:N | 3:D9:107:ASP:O | 1.83 | 1.11 |
| 5:Z8:41:GLN:CB | 12:Z8:301:CYC:C3B | 2.18 | 1.11 |
| 3:H9:116:THR:HG21 | 12:H9:202:CYC:HMA3 | 1.26 | 1.11 |
| 1:Z:161:SER:OG | 1:X5:14:VAL:CG2 | 1.99 | 1.11 |
| 12:H3:202:CYC:O2A | 11:a9:776:TYR:CD2 | 2.04 | 1.11 |
| 6:M2:53:LEU:CD2 | 8:i7:80:LEU:HG | 1.80 | 1.11 |
| 8:G5:119:LEU:HD13 | 12:G5:201:CYC:CHA | 1.81 | 1.11 |
| 1:b5:17:LYS:O | 10:k5:169:TYR:OH | 1.66 | 1.11 |
| 1:H7:140:LEU:CD1 | 11:aA:561:ALA:CB | 2.28 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:I7:25:ARG:NH2 | 8:W7:25:ARG:HD3 | 1.65 | 1.11 |
| 8:q7:68:PRO:HG2 | 11:aA:334:LYS:HD3 | 1.13 | 1.11 |
| 4:M8:144:ARG:HG2 | 4:M8:204:ILE:HD13 | 1.24 | 1.11 |
| 3:O8:107:ASP:OD1 | 5:Z8:66:ARG:HD2 | 0.93 | 1.11 |
| 4:M9:113:ILE:HD11 | 4:M9:143:VAL:HG13 | 1.13 | 1.11 |
| 5:N9:22:LEU:CD1 | 5:N9:26:LEU:HD21 | 1.80 | 1.11 |
| 3:J9:119:ALA:C | 11:a9:365:LYS:HE2 | 1.76 | 1.11 |
| 11:a9:245:ALA:HB2 | 12:a9:901:CYC:CBB | 1.80 | 1.11 |
| 11:aA:694:ARG:CZ | 4:M1:51:ARG:NH2 | 2.14 | 1.11 |
| 12:JA:202:CYC:HBA2 | 11:aA:511:LYS:HA | 1.18 | 1.11 |
| 4:MA:58:TYR:CD2 | 11:aA:496:ARG:NH2 | 2.19 | 1.11 |
| 4:MA:158:PHE:CA | 3:VA:108:ARG:HD3 | 1.79 | 1.11 |
| 3:B4:68:ARG:NH1 | 3:U4:68:ARG:HH22 | 1.47 | 1.11 |
| 12:H4:202:CYC:HMD1 | 12:H4:202:CYC:HC | 1.11 | 1.11 |
| 12:L5:201:CYC:HB | 12:L5:201:CYC:HMA1 | 1.06 | 1.11 |
| 9:i5:6:LYS:CG | 9:i5:55:LYS:HB2 | 1.81 | 1.11 |
| 1:R7:49:THR:HG21 | 8:C7:161:GLN:HG2 | 1.28 | 1.11 |
| 2:N8:11:SER:HA | 5:Z8:62:ARG:HH21 | 1.11 | 1.11 |
| 2:N8:112:GLY:N | 5:Z8:34:LEU:CA | 2.14 | 1.11 |
| 3:Q8:120:LEU:HD11 | 3:Q8:122:THR:CA | 1.80 | 1.11 |
| 3:Q8:127:VAL:CG2 | 12:Z8:301:CYC:HMC1 | 1.77 | 1.11 |
| 5:Z8:37:HIS:CD2 | 12:Z8:301:CYC:CHB | 2.34 | 1.11 |
| 2:I9:31:PHE:CE2 | 3:J9:31:VAL:HA | 1.62 | 1.11 |
| 2:I9:113:LEU:HD21 | 2:I9:161:LEU:HD23 | 1.25 | 1.11 |
| 2:G1:107:ASP:CA | 3:L1:77:ARG:CZ | 2.27 | 1.11 |
| 5:N1:22:LEU:CD1 | 5:N1:26:LEU:HD21 | 1.81 | 1.11 |
| 3:FA:145:PRO:HG2 | 12:F9:302:CYC:HMC2 | 1.22 | 1.10 |
| 3:JA:78:ARG:HH12 | 11:aA:359:ASP:HA | 1.15 | 1.10 |
| 5:NA:66:ARG:HB2 | 3:TA:111:ASN:ND2 | 1.64 | 1.10 |
| 2:QA:69:PRO:HB3 | 2:U1:47:ASN:HA | 1.32 | 1.10 |
| 2:G3:107:ASP:CA | 3:L3:77:ARG:CZ | 2.27 | 1.10 |
| 3:H3:68:ARG:HD3 | 11:a9:615:ARG:O | 1.47 | 1.10 |
| 2:O3:63:PHE:HB2 | 2:O3:66:LEU:HD11 | 1.20 | 1.10 |
| 3:F4:115:GLU:CB | 4:M4:3:VAL:HG13 | 1.80 | 1.10 |
| 4:M4:140:ARG:HH11 | 4:M4:144:ARG:CZ | 1.64 | 1.10 |
| 4:M4:144:ARG:HE | 4:M4:204:ILE:HG22 | 0.96 | 1.10 |
| 5:Z4:1:MET:HB3 | 5:Z4:3:VAL:HG23 | 1.30 | 1.10 |
| 8:A5:64:ASP:HA | 8:A5:67:SER:OG | 1.49 | 1.10 |
| 1:B5:10:ASN:OD1 | 10:k5:557:VAL:HB | 0.93 | 1.10 |
| 8:G5:64:ASP:HA | 8:G5:67:SER:OG | 1.49 | 1.10 |
| 8:Q5:11:ALA:HB1 | 1:R5:94:TYR:HE1 | 1.13 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:974:LEU:CD2 | 1:v7:1:MET:H3 | 1.63 | 1.10 |
| 10:k5:362:LYS:HE2 | 10:k5:363:HIS:NE2 | 1.66 | 1.10 |
| 8:k7:68:PRO:HG2 | 11:a9:334:LYS:CD | 1.80 | 1.10 |
| 8:u7:29:PHE:CD2 | 1:v7:31:PHE:HE1 | 1.69 | 1.10 |
| 3:F8:107:ASP:CA | 4:M8:8:SER:H | 1.63 | 1.10 |
| 4:M8:104:ALA:CB | 2:P8:14:SER:N | 2.13 | 1.10 |
| 12:L9:201:CYC:HMD1 | 12:L9:201:CYC:HC | 1.09 | 1.10 |
| 5:Z8:22:LEU:CD1 | 5:Z8:26:LEU:HD21 | 1.81 | 1.10 |
| 3:J9:119:ALA:O | 11:a9:365:LYS:NZ | 1.81 | 1.10 |
| 11:a9:91:THR:HG22 | 11:a9:96:THR:HA | 1.31 | 1.10 |
| 4:M1:258:LYS:HZ2 | 3:Z1:111:ASN:ND2 | 1.48 | 1.10 |
| 12:Z1:201:CYC:HMD1 | 12:Z1:201:CYC:HC | 1.10 | 1.10 |
| 12:F2:202:CYC:HMD1 | 12:F2:202:CYC:HC | 1.10 | 1.10 |
| 2:EA:33:ARG:HG2 | 2:IA:25:GLN:OE1 | 1.48 | 1.10 |
| 3:TA:25:ASN:OD1 | 2:X4:68:GLN:CG | 1.99 | 1.10 |
| 12:L2:202:CYC:HMD1 | 12:L2:202:CYC:HC | 1.10 | 1.10 |
| 3:B3:88:ILE:HG23 | 12:B3:202:CYC:HAB2 | 1.28 | 1.10 |
| 4:M3:113:ILE:HD11 | 4:M3:143:VAL:HG13 | 1.13 | 1.10 |
| 3:U4:120:LEU:HD11 | 12:U4:201:CYC:CBD | 1.79 | 1.10 |
| 3:H4:84:ARG:CB | 11:aA:131:TYR:CE1 | 2.32 | 1.10 |
| 1:N5:113:LYS:NZ | 1:Z5:155:TYR:CZ | 2.19 | 1.10 |
| 6:M6:53:LEU:HD23 | 8:c7:80:LEU:HD23 | 1.20 | 1.10 |
| 10:k5:743:VAL:HG12 | 12:D7:201:CYC:O2D | 1.48 | 1.10 |
| 3:H8:119:ALA:CB | 11:a9:266:ASN:ND2 | 1.98 | 1.10 |
| 3:L8:59:LEU:HD21 | 12:a9:901:CYC:HMC3 | 1.32 | 1.10 |
| 4:M8:101:ASP:HA | 2:P8:13:ASP:HB3 | 1.30 | 1.10 |
| 3:O8:104:VAL:HA | 5:Z8:61:LYS:HZ1 | 1.05 | 1.10 |
| 4:M9:163:ASN:HD21 | 12:V9:201:CYC:CMA | 1.62 | 1.10 |
| 4:M9:263:PRO:HB2 | 3:V9:119:ALA:HB2 | 1.24 | 1.10 |
| 2:E9:33:ARG:HG2 | 2:I9:25:GLN:OE1 | 1.48 | 1.10 |
| 2:K9:15:GLN:HA | 11:a9:393:ARG:HH11 | 1.16 | 1.10 |
| 11:a9:95:ILE:CD1 | 11:a9:237:PHE:CE1 | 2.33 | 1.10 |
| 11:a9:283:GLN:CB | 11:a9:284:PRO:CD | 2.01 | 1.10 |
| 3:HA:113:LEU:HD11 | 12:HA:202:CYC:HMB3 | 1.25 | 1.10 |
| 3:JA:119:ALA:C | 11:aA:365:LYS:HE2 | 1.77 | 1.10 |
| 12:JA:202:CYC:HBA1 | 11:aA:511:LYS:CA | 1.79 | 1.10 |
| 4:MA:29:PRO:CD | 11:aA:378:GLU:CD | 2.24 | 1.10 |
| 12:P1:201:CYC:CAA | 4:M1:134:ASN:HB2 | 1.80 | 1.10 |
| 3:L2:75:PRO:CG | 3:L2:78:ARG:HB2 | 1.80 | 1.10 |
| 6:M2:57:GLU:OE1 | 8:i7:76:LYS:CE | 1.99 | 1.10 |
| 3:L3:108:ARG:O | 11:a9:712:ASN:OD1 | 1.67 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M4:1:MET:N | 11:aA:149:SER:O | 1.83 | 1.10 |
| 8:K5:80:LEU:CD1 | 12:K5:201:CYC:HAD2 | 1.79 | 1.10 |
| 1:f5:114:GLU:HB3 | 10:j5:491:THR:CG2 | 1.82 | 1.10 |
| 1:b5:38:VAL:HG13 | 10:k5:40:VAL:HG13 | 1.16 | 1.10 |
| 9:z5:6:LYS:CG | 9:z5:55:LYS:HB2 | 1.81 | 1.10 |
| 10:k5:56:ILE:CD1 | 10:k5:219:ASP:HB3 | 1.79 | 1.10 |
| 3:B8:68:ARG:NH1 | 3:U8:68:ARG:HH22 | 1.47 | 1.10 |
| 3:F8:77:ARG:HD2 | 11:a9:146:ARG:HH12 | 0.98 | 1.10 |
| 3:Q8:102:ALA:HB1 | 3:Q8:166:LYS:HE2 | 1.24 | 1.10 |
| 4:M9:29:PRO:CD | 11:a9:378:GLU:CD | 2.23 | 1.10 |
| 5:N9:1:MET:HB3 | 5:N9:3:VAL:HG23 | 1.30 | 1.10 |
| 12:R9:202:CYC:HMD1 | 12:R9:202:CYC:HC | 1.11 | 1.10 |
| 11:aA:312:ASP:C | 11:aA:315:LEU:N | 2.10 | 1.10 |
| 11:aA:640:ALA:HB1 | 11:aA:767:THR:CG2 | 1.82 | 1.10 |
| 3:F2:78:ARG:HD3 | 12:F2:201:CYC:O2D | 0.92 | 1.10 |
| 4:MA:160:THR:HG22 | 4:MA:257:GLN:HB2 | 1.27 | 1.10 |
| 3:H3:78:ARG:HH22 | 11:a9:623:ASP:CB | 1.64 | 1.10 |
| 3:L2:77:ARG:NH2 | 6:M2:70:GLU:CD | 2.09 | 1.10 |
| 6:M2:26:PHE:CE1 | 8:O5:87:TYR:HD1 | 1.54 | 1.10 |
| 6:M2:53:LEU:HD23 | 8:i7:80:LEU:CG | 1.82 | 1.10 |
| 12:P3:202:CYC:HMD1 | 12:P3:202:CYC:HC | 1.10 | 1.10 |
| 3:Q4:7:LYS:CE | 3:Q4:101:ASP:OD1 | 1.99 | 1.10 |
| 1:N5:53:LYS:CD | 8:O5:118:SER:O | 1.99 | 1.10 |
| 8:G5:6:LYS:NZ | 8:S5:19:SER:CB | 2.14 | 1.10 |
| 8:Q5:12:ASP:CA | 1:R5:94:TYR:HE2 | 1.60 | 1.10 |
| 1:X5:144:ASP:HB3 | 8:a5:38:ARG:NH2 | 1.66 | 1.10 |
| 9:i5:6:LYS:CB | 9:i5:55:LYS:CB | 2.02 | 1.10 |
| 10:k5:1146:THR:CB | 1:p7:77:ARG:NH2 | 2.15 | 1.10 |
| 3:F6:82:CYS:SG | 12:F6:201:CYC:HAC2 | 1.92 | 1.10 |
| 1:H7:140:LEU:CD1 | 11:aA:561:ALA:HB1 | 1.81 | 1.10 |
| 8:I7:76:LYS:NZ | 11:aA:567:GLN:NE2 | 1.89 | 1.10 |
| 12:D8:202:CYC:HBA2 | 4:M8:35:THR:HA | 1.22 | 1.10 |
| 4:M8:128:ALA:HB1 | 4:M8:142:PHE:CE1 | 1.85 | 1.10 |
| 4:M8:225:LYS:HA | 12:M8:301:CYC:O1A | 1.52 | 1.10 |
| 4:M8:235:PHE:CB | 12:M8:301:CYC:C2A | 2.30 | 1.10 |
| 4:M9:157:PHE:O | 3:V9:108:ARG:CD | 2.00 | 1.10 |
| 2:K9:15:GLN:C | 11:a9:393:ARG:NH1 | 2.08 | 1.10 |
| 11:aA:95:ILE:CD1 | 11:aA:237:PHE:CE1 | 2.33 | 1.10 |
| 4:M1:113:ILE:HD11 | 4:M1:143:VAL:HG13 | 1.13 | 1.10 |
| 3:FA:145:PRO:CD | 12:F9:302:CYC:HMC3 | 1.81 | 1.10 |
| 3:JA:119:ALA:O | 11:aA:365:LYS:NZ | 1.82 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 12:PA:202:CYC:HMD1 | 12:PA:202:CYC:HC | 1.10 | 1.10 |
| 3:L2:75:PRO:CD | 3:L2:78:ARG:HB2 | 1.81 | 1.10 |
| 6:M2:50:LEU:CD2 | 8:i7:79:ALA:O | 2.00 | 1.10 |
| 3:Z3:111:ASN:ND2 | 4:M3:258:LYS:HZ2 | 1.48 | 1.10 |
| 3:B4:68:ARG:NH2 | 3:U4:68:ARG:NH2 | 2.00 | 1.10 |
| 3:D4:1:MET:N | 11:aA:111:THR:OG1 | 1.84 | 1.10 |
| 4:M4:87:ILE:CD1 | 3:Y4:77:ARG:CG | 2.23 | 1.10 |
| 3:Y4:124:THR:HB | 3:Y4:172:ALA:CA | 1.78 | 1.10 |
| 8:U5:83:ARG:HG2 | 6:M6:31:ASP:OD1 | 0.92 | 1.10 |
| 8:U5:83:ARG:NE | 6:M6:27:ALA:O | 1.85 | 1.10 |
| 6:M6:50:LEU:HD22 | 8:c7:79:ALA:O | 1.43 | 1.10 |
| 10:j5:1118:THR:OG1 | 12:j5:1202:CYC:O2A | 1.70 | 1.10 |
| 10:k5:489:ASN:O | 10:k5:490:SER:OG | 1.69 | 1.10 |
| 10:k5:1018:LEU:HD11 | 10:k5:1035:PHE:CZ | 1.77 | 1.10 |
| 10:k5:1045:TYR:OH | 10:k5:1062:LEU:HD23 | 1.52 | 1.10 |
| 10:k5:1143:LEU:HD13 | 8:k7:103:PRO:HA | 1.29 | 1.10 |
| 12:H7:201:CYC:HMA1 | 12:H7:201:CYC:HB | 1.06 | 1.10 |
| 8:o7:29:PHE:CD2 | 1:p7:31:PHE:HE1 | 1.69 | 1.10 |
| 8:o7:103:PRO:HG3 | 1:p7:9:ILE:CD1 | 1.81 | 1.10 |
| 2:X8:16:GLY:CA | 4:M8:228:SER:CB | 2.28 | 1.10 |
| 2:X8:68:GLN:CG | 3:T9:25:ASN:OD1 | 1.99 | 1.10 |
| 4:M8:56:MET:HE1 | 4:M8:66:VAL:HG21 | 1.23 | 1.10 |
| 4:M9:58:TYR:CD2 | 11:a9:496:ARG:NH2 | 2.19 | 1.10 |
| 3:J9:111:ASN:O | 11:a9:519:ARG:N | 1.84 | 1.10 |
| 3:DA:107:ASP:O | 4:MA:7:SER:N | 1.83 | 1.09 |
| 3:HA:120:LEU:HD11 | 12:HA:202:CYC:HAA1 | 1.10 | 1.09 |
| 4:MA:148:LYS:HD3 | 4:MA:197:ASP:OD1 | 1.49 | 1.09 |
| 4:MA:162:ASN:H | 12:VA:201:CYC:HBB3 | 1.07 | 1.09 |
| 4:MA:274:VAL:OXT | 3:VA:77:ARG:NE | 1.85 | 1.09 |
| 5:NA:22:LEU:CD1 | 5:NA:26:LEU:HD21 | 1.80 | 1.09 |
| 12:J3:201:CYC:HMD1 | 12:J3:201:CYC:HC | 1.10 | 1.09 |
| 12:B4:201:CYC:HMD1 | 12:B4:201:CYC:HC | 1.10 | 1.09 |
| 12:L3:201:CYC:HMD1 | 12:L3:201:CYC:HC | 1.10 | 1.09 |
| 5:N3:22:LEU:CD1 | 5:N3:26:LEU:HD21 | 1.81 | 1.09 |
| 12:B1:201:CYC:HMD1 | 12:B1:201:CYC:HC | 1.10 | 1.09 |
| 3:F4:107:ASP:HA | 4:M4:8:SER:H | 0.98 | 1.09 |
| 8:M5:19:SER:CB | 8:A5:6:LYS:NZ | 2.14 | 1.09 |
| 8:c5:9:VAL:CG1 | 10:j5:344:ARG:CZ | 2.30 | 1.09 |
| 8:Q5:16:ARG:HA | 1:R5:90:ARG:HD3 | 1.23 | 1.09 |
| 10:j5:489:ASN:O | 10:j5:490:SER:OG | 1.69 | 1.09 |
| 10:j5:1045:TYR:OH | 10:j5:1062:LEU:HD23 | 1.52 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:1105:ILE:CD1 | 10:j5:1115:ARG:NH2 | 2.15 | 1.09 |
| 8:i7:25:ARG:HH22 | 8:s7:6:LYS:N | 1.46 | 1.09 |
| 8:i7:39:ILE:CD1 | 8:i7:148:GLU:HG2 | 1.75 | 1.09 |
| 8:u7:103:PRO:HG3 | 1:v7:9:ILE:CD1 | 1.81 | 1.09 |
| 3:U8:114:LYS:HE2 | 4:M8:13:LYS:HZ1 | 1.04 | 1.09 |
| 4:M8:126:THR:HB | 12:M8:302:CYC:CGA | 1.80 | 1.09 |
| 3:O8:104:VAL:HA | 5:Z8:61:LYS:CE | 1.82 | 1.09 |
| 3:J9:88:ILE:HD11 | 11:a9:512:TYR:CE1 | 1.86 | 1.09 |
| 11:a9:312:ASP:C | 11:a9:315:LEU:N | 2.10 | 1.09 |
| 11:aA:708:HIS:HB3 | 3:L1:108:ARG:HH21 | 0.96 | 1.09 |
| 11:aA:712:ASN:OD1 | 3:L1:108:ARG:O | 1.68 | 1.09 |
| 4:M1:148:LYS:HD3 | 4:M1:197:ASP:OD1 | 1.49 | 1.09 |
| 1:A:161:SER:HB2 | 1:R5:14:VAL:HB | 1.18 | 1.09 |
| 3:JA:119:ALA:O | 11:aA:365:LYS:HE3 | 1.35 | 1.09 |
| 12:JA:202:CYC:NB | 11:aA:512:TYR:HB2 | 1.44 | 1.09 |
| 5:NA:54:LEU:CD2 | 3:TA:84:ARG:NE | 2.14 | 1.09 |
| 4:M4:205:ASP:HB3 | 5:Z4:59:ARG:HE | 1.10 | 1.09 |
| 4:M4:230:GLN:HG2 | 12:M4:301:CYC:OB | 1.50 | 1.09 |
| 3:Q4:77:ARG:HG3 | 5:Z4:34:LEU:O | 1.50 | 1.09 |
| 1:X5:106:GLU:HG2 | 10:j5:504:ASP:O | 1.50 | 1.09 |
| 10:k5:741:GLN:HG3 | 1:D7:77:ARG:HH22 | 1.08 | 1.09 |
| 10:k5:889:LEU:HA | 12:D7:201:CYC:OB | 1.52 | 1.09 |
| 3:B8:81:ALA:CB | 12:B8:202:CYC:HMD3 | 1.79 | 1.09 |
| 12:D8:201:CYC:HMD1 | 12:D8:201:CYC:HC | 1.11 | 1.09 |
| 8:u7:27:LYS:HE3 | 1:v7:35:ALA:HB1 | 1.09 | 1.09 |
| 3:Q8:127:VAL:HG22 | 12:Z8:301:CYC:HMC3 | 1.31 | 1.09 |
| 11:a9:99:ALA:HB1 | 11:a9:100:PRO:HD3 | 1.34 | 1.09 |
| 12:T1:302:CYC:HMD1 | 12:T1:302:CYC:HC | 1.10 | 1.09 |
| 5:NA:1:MET:HG2 | 3:RA:119:ALA:HB3 | 1.33 | 1.09 |
| 2:QA:33:ARG:NE | 12:VA:202:CYC:HBB3 | 1.67 | 1.09 |
| 3:B3:88:ILE:HD13 | 12:B3:202:CYC:C3B | 1.80 | 1.09 |
| 2:N4:112:GLY:CA | 5:Z4:34:LEU:HB2 | 1.83 | 1.09 |
| 2:P4:19:LEU:CD2 | 3:Q4:95:TYR:HE1 | 1.64 | 1.09 |
| 3:Q4:77:ARG:HA | 5:Z4:34:LEU:HB3 | 1.26 | 1.09 |
| 8:W5:11:ALA:HB1 | 1:X5:94:TYR:HE1 | 1.13 | 1.09 |
| 1:Z5:28:LYS:HD3 | 1:t7:143:PRO:CB | 1.82 | 1.09 |
| 1:b5:114:GLU:HB3 | 10:k5:491:THR:HG23 | 1.22 | 1.09 |
| 10:k5:56:ILE:HD13 | 10:k5:219:ASP:HB3 | 1.09 | 1.09 |
| 8:O7:25:ARG:NH2 | 8:E7:25:ARG:CB | 2.14 | 1.09 |
| 8:O7:52:LYS:CE | 11:aA:29:ARG:HH12 | 1.64 | 1.09 |
| 8:I7:25:ARG:HH21 | 8:W7:25:ARG:HB3 | 1.07 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:i7:21:GLY:CA | 8:s7:100:ASP:OD1 | 1.99 | 1.09 |
| 8:i7:39:ILE:HD13 | 8:i7:148:GLU:HG3 | 1.26 | 1.09 |
| 8:c7:20:PRO:HG2 | 8:m7:155:TYR:HB2 | 1.13 | 1.09 |
| 3:B8:82:CYS:CA | 12:B8:202:CYC:C1C | 2.30 | 1.09 |
| 8:o7:5:THR:OG1 | 1:p7:6:THR:HG21 | 1.52 | 1.09 |
| 8:o7:23:LEU:HD22 | 1:p7:38:VAL:HA | 1.17 | 1.09 |
| 8:o7:121:THR:HG23 | 12:o7:201:CYC:HMC3 | 1.24 | 1.09 |
| 8:q7:79:ALA:HB2 | 11:aA:53:VAL:HG21 | 1.13 | 1.09 |
| 1:r7:17:LYS:NZ | 11:aA:41:ASP:OD2 | 1.82 | 1.09 |
| 2:N8:63:PHE:HB2 | 2:N8:66:LEU:HD11 | 1.20 | 1.09 |
| 3:Q8:78:ARG:CD | 12:Z8:301:CYC:HAD1 | 1.81 | 1.09 |
| 4:M9:274:VAL:HG22 | 3:V9:77:ARG:HB2 | 1.12 | 1.09 |
| 5:N9:54:LEU:CD2 | 3:T9:84:ARG:NE | 2.14 | 1.09 |
| 3:H9:117:TYR:CE1 | 12:H9:202:CYC:HBB | 1.87 | 1.09 |
| 12:J9:202:CYC:NB | 11:a9:512:TYR:HB2 | 1.44 | 1.09 |
| 11:a9:331:TYR:HA | 11:a9:333:GLN:NE2 | 1.67 | 1.09 |
| 11:aA:99:ALA:CB | 11:aA:100:PRO:CD | 2.30 | 1.09 |
| 11:aA:586:LEU:C | 11:aA:590:PRO:HG3 | 1.76 | 1.09 |
| 3:JA:111:ASN:O | 11:aA:519:ARG:N | 1.85 | 1.09 |
| 2:OA:63:PHE:HB2 | 2:OA:66:LEU:HD11 | 1.20 | 1.09 |
| 3:D4:14:LEU:CD1 | 3:Y4:125:ARG:CD | 2.29 | 1.09 |
| 3:B1:91:ARG:CZ | 11:aA:677:GLN:NE2 | 2.15 | 1.09 |
| 12:M4:301:CYC:C1C | 3:Y4:72:ASN:OD1 | 2.01 | 1.09 |
| 2:N4:111:ALA:C | 5:Z4:34:LEU:HD12 | 1.78 | 1.09 |
| 3:O4:107:ASP:CB | 5:Z4:66:ARG:CB | 2.30 | 1.09 |
| 3:O4:115:GLU:HB2 | 5:Z4:70:ILE:O | 1.51 | 1.09 |
| 3:Q4:120:LEU:CD2 | 5:Z4:42:SER:CB | 2.31 | 1.09 |
| 5:Z4:26:LEU:HD21 | 5:Z4:63:ASN:HB3 | 1.13 | 1.09 |
| 12:B5:201:CYC:HBB2 | 9:z5:21:ARG:HA | 1.34 | 1.09 |
| 10:k5:889:LEU:HD22 | 12:D7:201:CYC:CBB | 1.81 | 1.09 |
| 10:k5:1105:ILE:HD12 | 10:k5:1115:ARG:NH2 | 1.68 | 1.09 |
| 2:A6:63:PHE:HB2 | 2:A6:66:LEU:HD11 | 1.19 | 1.09 |
| 8:O7:25:ARG:NH2 | 8:E7:25:ARG:HB3 | 1.65 | 1.09 |
| 8:g7:63:PRO:HD3 | 11:aA:336:ILE:HG22 | 1.25 | 1.09 |
| 8:i7:39:ILE:HD13 | 8:i7:148:GLU:CB | 1.83 | 1.09 |
| 8:i7:94:TYR:CE1 | 1:j7:9:ILE:HG23 | 1.86 | 1.09 |
| 8:o7:97:VAL:CG2 | 1:p7:19:LEU:CD1 | 2.30 | 1.09 |
| 12:M8:301:CYC:ND | 3:Y8:85:ASP:OD2 | 1.85 | 1.09 |
| 3:Q8:78:ARG:HD3 | 12:Z8:301:CYC:CAD | 1.80 | 1.09 |
| 11:a9:99:ALA:CB | 11:a9:100:PRO:CD | 2.30 | 1.09 |
| 11:a9:640:ALA:HB1 | 11:a9:767:THR:CG2 | 1.82 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 11:aA:666:ASN:CG | 12:aA:901:CYC:OB | 1.94 | 1.09 |
| 12:L1:201:CYC:HMD1 | 12:L1:201:CYC:HC | 1.10 | 1.09 |
| 12:BA:202:CYC:HMD1 | 12:BA:202:CYC:HC | 1.10 | 1.09 |
| 12:J3:202:CYC:OB | 11:a9:666:ASN:CG | 1.96 | 1.09 |
| 4:M3:120:LEU:CD2 | 3:X3:84:ARG:NH1 | 2.15 | 1.09 |
| 4:M3:160:THR:HG22 | 4:M3:257:GLN:HB2 | 1.27 | 1.09 |
| 4:M3:190:ARG:NH1 | 4:M3:202:SER:CB | 2.16 | 1.09 |
| 12:J4:202:CYC:HC | 12:J4:202:CYC:HMD1 | 1.10 | 1.09 |
| 4:M4:140:ARG:HH12 | 4:M4:144:ARG:NH1 | 1.50 | 1.09 |
| 3:Q4:72:ASN:HD21 | 12:Z4:301:CYC:HBD2 | 1.12 | 1.09 |
| 5:Z4:41:GLN:HG3 | 12:Z4:301:CYC:C2B | 1.82 | 1.09 |
| 8:A5:122:PRO:O | 12:A5:201:CYC:CMC | 2.00 | 1.09 |
| 8:G5:122:PRO:O | 12:G5:201:CYC:CMC | 2.00 | 1.09 |
| 1:H5:87:TYR:CE1 | 9:i5:19:THR:O | 2.06 | 1.09 |
| 1:T5:53:LYS:HZ2 | 8:U5:120:GLN:CD | 1.60 | 1.09 |
| 8:U5:75:GLU:HG3 | 6:M6:36:ILE:HG13 | 1.26 | 1.09 |
| 1:Z5:161:SER:HB3 | 10:k5:695:GLY:O | 1.51 | 1.09 |
| 10:j5:362:LYS:HE2 | 10:j5:363:HIS:NE2 | 1.66 | 1.09 |
| 10:j5:386:ILE:CD1 | 10:j5:395:SER:OG | 1.82 | 1.09 |
| 10:k5:1077:ILE:O | 12:k5:1203:CYC:HBA1 | 1.52 | 1.09 |
| 10:k5:1153:VAL:CG2 | 1:p7:125:ALA:HB2 | 1.82 | 1.09 |
| 8:I7:25:ARG:HH22 | 8:W7:25:ARG:HD3 | 0.95 | 1.09 |
| 8:o7:18:LEU:HD13 | 1:p7:97:LEU:HD12 | 1.33 | 1.09 |
| 8:u7:23:LEU:HD22 | 1:v7:38:VAL:HA | 1.17 | 1.09 |
| 3:L8:109:CYS:HA | 12:a9:901:CYC:HBB1 | 1.28 | 1.09 |
| 4:M8:113:ILE:HD11 | 4:M8:143:VAL:HG13 | 1.13 | 1.09 |
| 3:Q8:77:ARG:HG3 | 5:Z8:34:LEU:O | 1.33 | 1.09 |
| 4:M1:120:LEU:CD2 | 3:X1:84:ARG:NH1 | 2.15 | 1.09 |
| 5:N1:1:MET:HB3 | 5:N1:3:VAL:HG23 | 1.30 | 1.09 |
| 3:FA:68:ARG:HH12 | 3:ZA:68:ARG:CZ | 1.66 | 1.08 |
| 12:JA:201:CYC:HMD1 | 12:JA:201:CYC:HC | 1.10 | 1.08 |
| 4:MA:273:ILE:CD1 | 3:VA:75:PRO:CD | 2.31 | 1.08 |
| 4:M4:226:SER:CB | 3:Y4:85:ASP:OD1 | 2.01 | 1.08 |
| 8:A5:119:LEU:HD13 | 12:A5:201:CYC:CHA | 1.81 | 1.08 |
| 9:i5:6:LYS:N | 9:i5:55:LYS:O | 1.86 | 1.08 |
| 10:j5:742:GLY:C | 12:J7:201:CYC:O2D | 1.95 | 1.08 |
| 10:k5:53:ARG:O | 10:k5:56:ILE:HG22 | 1.53 | 1.08 |
| 10:k5:1025:LEU:CD2 | 10:k5:1035:PHE:CB | 2.14 | 1.08 |
| 10:k5:1105:ILE:CD1 | 10:k5:1115:ARG:NH2 | 2.15 | 1.08 |
| 12:F6:202:CYC:HMD1 | 12:F6:202:CYC:HC | 1.10 | 1.08 |
| 12:Q7:201:CYC:HMD1 | 12:Q7:201:CYC:HC | 1.18 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:i7:39:ILE:CD1 | 8:i7:148:GLU:HB3 | 1.82 | 1.08 |
| 3:D8:1:MET:N | 11:a9:111:THR:OG1 | 1.85 | 1.08 |
| 8:o7:103:PRO:HB3 | 1:p7:9:ILE:HG21 | 1.12 | 1.08 |
| 1:p7:136:VAL:HG13 | 11:a9:342:ARG:HH12 | 0.94 | 1.08 |
| 2:R8:64:PRO:HG2 | 3:T9:21:GLU:HB3 | 1.10 | 1.08 |
| 4:M9:263:PRO:HB2 | 3:V9:119:ALA:HB3 | 1.23 | 1.08 |
| 12:H9:201:CYC:HMD1 | 12:H9:201:CYC:HC | 1.10 | 1.08 |
| 11:aA:622:ALA:H | 3:J1:14:LEU:HD21 | 1.18 | 1.08 |
| 11:aA:798:SER:CB | 12:aA:901:CYC:HAA1 | 1.83 | 1.08 |
| 1:Z:161:SER:HB2 | 1:X5:14:VAL:HB | 1.29 | 1.08 |
| 3:JA:88:ILE:HD11 | 11:aA:512:TYR:CE1 | 1.88 | 1.08 |
| 4:MA:190:ARG:NH1 | 4:MA:202:SER:CB | 2.16 | 1.08 |
| 5:NA:54:LEU:CD2 | 3:TA:84:ARG:CZ | 2.30 | 1.08 |
| 6:M2:26:PHE:HB3 | 8:O5:83:ARG:HD2 | 1.18 | 1.08 |
| 3:L3:88:ILE:HG13 | 11:a9:742:GLN:NE2 | 0.92 | 1.08 |
| 3:H4:119:ALA:HB1 | 11:aA:266:ASN:HB2 | 1.29 | 1.08 |
| 4:M4:148:LYS:HZ2 | 5:Z4:52:ARG:HD2 | 1.07 | 1.08 |
| 3:Q4:120:LEU:HD11 | 5:Z4:40:SER:H | 0.94 | 1.08 |
| 8:W5:11:ALA:HB1 | 1:X5:94:TYR:CE1 | 1.83 | 1.08 |
| 10:k5:778:LYS:NZ | 12:F7:201:CYC:HBB2 | 1.68 | 1.08 |
| 12:B6:201:CYC:HMD1 | 12:B6:201:CYC:HC | 1.10 | 1.08 |
| 3:L8:71:GLY:N | 11:a9:82:GLN:CG | 2.16 | 1.08 |
| 4:M8:190:ARG:NH1 | 4:M8:202:SER:CB | 2.16 | 1.08 |
| 2:P8:17:ARG:C | 3:Q8:91:ARG:NH2 | 2.10 | 1.08 |
| 4:M9:134:ASN:HB2 | 12:R9:201:CYC:HAA1 | 1.35 | 1.08 |
| 11:aA:643:LEU:HD21 | 11:aA:689:VAL:HG23 | 1.35 | 1.08 |
| 1:Z:161:SER:CB | 1:X5:14:VAL:HG23 | 1.78 | 1.08 |
| 3:FA:68:ARG:NH1 | 3:ZA:68:ARG:NH1 | 1.66 | 1.08 |
| 2:KA:18:PHE:CE2 | 3:LA:48:ALA:CB | 2.37 | 1.08 |
| 4:MA:189:ASP:OD1 | 3:VA:84:ARG:NH1 | 1.85 | 1.08 |
| 4:MA:263:PRO:HB2 | 3:VA:119:ALA:HB3 | 1.23 | 1.08 |
| 4:MA:273:ILE:HD11 | 3:VA:75:PRO:HD3 | 1.33 | 1.08 |
| 12:ZA:201:CYC:HMD1 | 12:ZA:201:CYC:HC | 1.10 | 1.08 |
| 3:L2:75:PRO:HD2 | 3:L2:78:ARG:HB2 | 1.35 | 1.08 |
| 12:B3:201:CYC:HMD1 | 12:B3:201:CYC:HC | 1.10 | 1.08 |
| 3:B4:120:LEU:HD13 | 4:M4:53:LEU:HB2 | 1.16 | 1.08 |
| 4:M4:140:ARG:NH1 | 4:M4:144:ARG:CZ | 2.17 | 1.08 |
| 4:M4:214:GLY:HA2 | 5:Z4:27:ALA:O | 1.50 | 1.08 |
| 12:M4:301:CYC:HMB2 | 3:Y4:89:ILE:HD11 | 1.30 | 1.08 |
| 3:Q4:102:ALA:HB1 | 3:Q4:166:LYS:HE2 | 1.33 | 1.08 |
| 8:C5:41:GLN:HB2 | 1:D5:24:LEU:HD11 | 1.31 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:H5:14:VAL:CG1 | 10:j5:554:ASN:O | 1.99 | 1.08 |
| 1:d5:110:ASN:ND2 | 10:j5:451:LYS:HB3 | 1.69 | 1.08 |
| 1:Z5:28:LYS:CE | 1:t7:143:PRO:CB | 2.31 | 1.08 |
| 10:j5:929:PRO:CG | 1:J7:147:LYS:HE2 | 1.83 | 1.08 |
| 10:j5:938:GLN:CD | 1:J7:28:LYS:HD2 | 1.78 | 1.08 |
| 10:j5:971:VAL:HG11 | 1:t7:76:ARG:HH12 | 1.15 | 1.08 |
| 10:k5:931:VAL:HG13 | 1:D7:29:ALA:HB1 | 1.22 | 1.08 |
| 8:c7:39:ILE:CD1 | 8:c7:148:GLU:HB3 | 1.82 | 1.08 |
| 12:B8:201:CYC:HMD1 | 12:B8:201:CYC:HC | 1.10 | 1.08 |
| 2:X8:16:GLY:HA2 | 4:M8:228:SER:HB2 | 1.23 | 1.08 |
| 4:M8:205:ASP:HB3 | 5:Z8:59:ARG:CZ | 1.83 | 1.08 |
| 3:O8:104:VAL:HG23 | 5:Z8:61:LYS:HE3 | 1.30 | 1.08 |
| 4:M9:29:PRO:HD3 | 11:a9:378:GLU:OE2 | 1.53 | 1.08 |
| 4:M9:190:ARG:NH1 | 4:M9:202:SER:CB | 2.16 | 1.08 |
| 11:a9:798:SER:HB3 | 11:a9:800:THR:HB | 1.29 | 1.08 |
| 11:aA:621:THR:HG22 | 3:J1:14:LEU:HD22 | 1.19 | 1.08 |
| 11:aA:632:ILE:HG12 | 3:J1:107:ASP:OD1 | 1.52 | 1.08 |
| 4:M1:263:PRO:HB2 | 3:Z1:119:ALA:HB2 | 1.34 | 1.08 |
| 4:MA:37:GLU:OE1 | 4:MA:40:GLN:NE2 | 1.86 | 1.08 |
| 4:MA:160:THR:HG22 | 4:MA:257:GLN:CB | 1.84 | 1.08 |
| 4:MA:274:VAL:HG11 | 2:WA:111:ALA:HB1 | 1.14 | 1.08 |
| 3:J3:84:ARG:HD2 | 11:a9:668:TYR:HB3 | 1.18 | 1.08 |
| 3:B3:91:ARG:CZ | 11:a9:677:GLN:NE2 | 2.16 | 1.08 |
| 3:B4:120:LEU:CD2 | 4:M4:52:LEU:HB3 | 1.81 | 1.08 |
| 3:Q4:72:ASN:ND2 | 12:Z4:301:CYC:HBD2 | 1.68 | 1.08 |
| 3:Y4:113:LEU:HG | 3:Y4:171:ILE:HG12 | 1.33 | 1.08 |
| 12:B5:201:CYC:HB | 12:B5:201:CYC:HMA1 | 1.06 | 1.08 |
| 12:H5:201:CYC:HBA2 | 9:i5:26:THR:HG21 | 1.29 | 1.08 |
| 1:f5:38:VAL:HG13 | 10:j5:40:VAL:HG13 | 1.25 | 1.08 |
| 9:z5:22:GLU:C | 9:z5:25:ASN:H | 1.61 | 1.08 |
| 10:j5:1020:GLU:HG3 | 1:f7:87:TYR:CZ | 1.87 | 1.08 |
| 10:k5:148:TYR:O | 10:k5:152:ARG:HG3 | 1.54 | 1.08 |
| 10:k5:931:VAL:CG2 | 1:D7:29:ALA:O | 2.00 | 1.08 |
| 12:B7:201:CYC:HB | 12:B7:201:CYC:HMA1 | 1.06 | 1.08 |
| 12:K7:201:CYC:HMD1 | 12:K7:201:CYC:HC | 1.18 | 1.08 |
| 8:g7:52:LYS:HD2 | 11:aA:321:ALA:HB1 | 1.13 | 1.08 |
| 3:B8:68:ARG:NH2 | 3:U8:68:ARG:NH2 | 2.00 | 1.08 |
| 8:u7:5:THR:OG1 | 1:v7:6:THR:HG21 | 1.52 | 1.08 |
| 3:L8:82:CYS:SG | 12:a9:901:CYC:C3C | 2.41 | 1.08 |
| 3:O8:111:ASN:OD1 | 5:Z8:68:LEU:HA | 1.35 | 1.08 |
| 3:F9:68:ARG:HH12 | 3:Z9:68:ARG:CZ | 1.66 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:a9:107:ARG:HG2 | 11:a9:108:PRO:HD2 | 1.25 | 1.08 |
| 3:FA:151:GLY:N | 3:F9:150:ARG:HH21 | 1.51 | 1.08 |
| 4:MA:157:PHE:O | 3:VA:108:ARG:CD | 2.00 | 1.08 |
| 12:QA:201:CYC:OB | 3:TA:75:PRO:HA | 1.51 | 1.08 |
| 3:Z3:119:ALA:HB2 | 4:M3:263:PRO:HB2 | 1.34 | 1.08 |
| 3:B4:82:CYS:HA | 12:B4:202:CYC:C2C | 1.83 | 1.08 |
| 3:L3:119:ALA:CB | 11:a9:813:PRO:HB3 | 1.77 | 1.08 |
| 4:M3:77:LEU:CD1 | 3:X3:115:GLU:OE2 | 2.00 | 1.08 |
| 3:B1:88:ILE:HG21 | 12:B1:202:CYC:C2B | 1.82 | 1.08 |
| 4:M4:128:ALA:C | 4:M4:142:PHE:CZ | 2.30 | 1.08 |
| 4:M4:144:ARG:NE | 4:M4:204:ILE:HG22 | 1.67 | 1.08 |
| 3:O4:119:ALA:HB3 | 5:Z4:72:GLU:HG3 | 1.36 | 1.08 |
| 1:B5:14:VAL:HG11 | 10:k5:554:ASN:O | 1.49 | 1.08 |
| 8:G5:6:LYS:NZ | 8:S5:19:SER:OG | 1.87 | 1.08 |
| 12:G5:201:CYC:HMD1 | 12:G5:201:CYC:HC | 1.18 | 1.08 |
| 8:Q5:12:ASP:CB | 1:R5:94:TYR:CE2 | 2.36 | 1.08 |
| 8:Q5:17:TYR:CE2 | 1:R5:44:ILE:HG22 | 1.88 | 1.08 |
| 1:T5:110:ASN:CG | 10:j5:692:LEU:HB3 | 1.79 | 1.08 |
| 1:T5:110:ASN:OD1 | 10:j5:692:LEU:O | 1.71 | 1.08 |
| 8:U5:76:LYS:HG3 | 8:U5:77:MET:N | 1.67 | 1.08 |
| 1:V5:114:GLU:CD | 10:j5:496:GLU:HG3 | 1.77 | 1.08 |
| 8:W5:12:ASP:CB | 1:X5:94:TYR:CE2 | 2.35 | 1.08 |
| 9:z5:6:LYS:N | 9:z5:55:LYS:O | 1.86 | 1.08 |
| 10:j5:965:GLN:N | 1:t7:69:GLY:CA | 1.95 | 1.08 |
| 10:j5:1015:TYR:O | 10:j5:1017:ARG:HG2 | 0.90 | 1.08 |
| 10:k5:1076:GLU:C | 10:k5:1078:SER:H | 1.51 | 1.08 |
| 8:O7:49:ARG:NH1 | 1:r7:114:GLU:OE1 | 1.83 | 1.08 |
| 8:I7:161:GLN:HG2 | 1:X7:49:THR:CG2 | 1.83 | 1.08 |
| 8:i7:25:ARG:HH22 | 8:s7:6:LYS:CA | 1.66 | 1.08 |
| 8:u7:97:VAL:CG2 | 1:v7:19:LEU:CD1 | 2.30 | 1.08 |
| 12:H8:202:CYC:HMD1 | 12:H8:202:CYC:HC | 1.11 | 1.08 |
| 3:L9:48:ALA:CB | 2:K9:18:PHE:CE2 | 2.37 | 1.08 |
| 11:a9:586:LEU:C | 11:a9:590:PRO:HG3 | 1.76 | 1.08 |
| 2:AA:63:PHE:HB2 | 2:AA:66:LEU:HD11 | 1.20 | 1.07 |
| 3:DA:68:ARG:NH2 | 3:XA:68:ARG:HH12 | 1.52 | 1.07 |
| 12:R1:201:CYC:C4B | 5:N1:54:LEU:CD1 | 2.32 | 1.07 |
| 3:U4:108:ARG:HA | 4:M4:246:ALA:HB3 | 1.21 | 1.07 |
| 3:H4:80:ALA:CB | 3:H4:84:ARG:HH12 | 1.66 | 1.07 |
| 4:M4:201:ASP:HB3 | 5:Z4:59:ARG:HD2 | 1.36 | 1.07 |
| 12:M4:301:CYC:CMB | 3:Y4:89:ILE:HD11 | 1.84 | 1.07 |
| 12:O4:201:CYC:HMA3 | 5:Z4:53:LEU:HD13 | 1.14 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:O5:76:LYS:HG3 | 8:O5:77:MET:HE2 | 1.31 | 1.07 |
| 8:G5:71:ASN:OD1 | 12:G5:201:CYC:CMD | 2.02 | 1.07 |
| 8:Q5:11:ALA:HB1 | 1:R5:94:TYR:CE1 | 1.83 | 1.07 |
| 10:k5:971:VAL:CG1 | 1:n7:76:ARG:HH12 | 1.67 | 1.07 |
| 10:k5:1023:SER:HB3 | 12:k5:1202:CYC:HMA2 | 1.34 | 1.07 |
| 1:R7:118:SER:O | 9:z7:61:GLN:CG | 2.02 | 1.07 |
| 8:c7:16:ARG:C | 1:d7:90:ARG:HD2 | 1.76 | 1.07 |
| 2:A8:63:PHE:HB2 | 2:A8:66:LEU:HD11 | 1.20 | 1.07 |
| 8:u7:18:LEU:HD13 | 1:v7:97:LEU:HD12 | 1.33 | 1.07 |
| 3:H8:84:ARG:HD3 | 11:a9:131:TYR:CD2 | 1.88 | 1.07 |
| 5:Z8:41:GLN:OE1 | 12:Z8:301:CYC:CBB | 1.94 | 1.07 |
| 11:a9:585:GLU:C | 11:a9:588:VAL:O | 1.97 | 1.07 |
| 11:aA:331:TYR:HA | 11:aA:333:GLN:NE2 | 1.67 | 1.07 |
| 3:HA:116:THR:HG21 | 12:HA:202:CYC:HMA3 | 1.30 | 1.07 |
| 4:MA:134:ASN:HB2 | 12:RA:201:CYC:HAA1 | 1.35 | 1.07 |
| 6:M2:127:SER:C | 12:F2:201:CYC:HBA1 | 1.79 | 1.07 |
| 12:V3:202:CYC:HC | 12:V3:202:CYC:HMD1 | 1.10 | 1.07 |
| 3:H4:14:LEU:HD22 | 11:aA:85:ALA:HA | 1.36 | 1.07 |
| 4:M4:144:ARG:HE | 4:M4:204:ILE:HG21 | 1.09 | 1.07 |
| 4:M4:210:ILE:O | 5:Z4:28:HIS:NE2 | 1.87 | 1.07 |
| 1:N5:53:LYS:HZ2 | 8:O5:120:GLN:CG | 1.67 | 1.07 |
| 3:Y4:109:CYS:SG | 3:Y4:109:CYS:O | 2.05 | 1.07 |
| 12:Y4:201:CYC:HMD1 | 12:Y4:201:CYC:HC | 1.10 | 1.07 |
| 10:j5:930:LEU:HD13 | 1:J7:33:THR:HB | 1.35 | 1.07 |
| 10:j5:1153:VAL:HG23 | 1:v7:125:ALA:HB2 | 1.30 | 1.07 |
| 10:k5:1054:SER:OG | 1:l7:110:ASN:HB3 | 1.53 | 1.07 |
| 8:Q7:25:ARG:CD | 8:C7:25:ARG:HH22 | 1.67 | 1.07 |
| 1:B7:140:LEU:HD12 | 11:a9:561:ALA:HA | 1.32 | 1.07 |
| 8:U7:60:GLN:OE1 | 1:p7:117:ASN:HB3 | 1.26 | 1.07 |
| 3:B8:81:ALA:HB1 | 12:B8:202:CYC:HMD2 | 1.36 | 1.07 |
| 3:B8:108:ARG:HA | 4:M8:61:ASN:CA | 1.83 | 1.07 |
| 3:B8:119:ALA:CB | 4:M8:52:LEU:HD11 | 1.84 | 1.07 |
| 8:u7:90:ARG:HB2 | 1:v7:18:TYR:CZ | 1.90 | 1.07 |
| 3:F8:115:GLU:CG | 4:M8:3:VAL:CG1 | 2.32 | 1.07 |
| 3:L8:68:ARG:HB3 | 11:a9:82:GLN:H | 1.12 | 1.07 |
| 5:N9:54:LEU:CD2 | 3:T9:84:ARG:CZ | 2.30 | 1.07 |
| 11:a9:710:THR:CG2 | 11:a9:807:GLN:CD | 2.28 | 1.07 |
| 11:aA:91:THR:HG22 | 11:aA:96:THR:HA | 1.31 | 1.07 |
| 4:M1:77:LEU:CD1 | 3:X1:115:GLU:OE2 | 2.00 | 1.07 |
| 4:M1:160:THR:HG22 | 4:M1:257:GLN:CB | 1.84 | 1.07 |
| 1:A:158:SER:HB2 | 1:R5:11:ASN:ND2 | 1.57 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:FA:145:PRO:CD | 12:F9:302:CYC:CMC | 2.31 | 1.07 |
| 3:LA:52:ILE:HD11 | 3:LA:87:GLU:HA | 1.37 | 1.07 |
| 4:MA:158:PHE:HA | 3:VA:108:ARG:HD3 | 1.34 | 1.07 |
| 4:MA:163:ASN:ND2 | 12:VA:201:CYC:CMA | 2.18 | 1.07 |
| 5:N3:39:PRO:HB3 | 3:T3:113:LEU:HA | 1.28 | 1.07 |
| 5:N3:54:LEU:CD1 | 12:R3:201:CYC:C4B | 2.32 | 1.07 |
| 4:M4:214:GLY:C | 5:Z4:27:ALA:O | 1.98 | 1.07 |
| 3:O4:115:GLU:CB | 5:Z4:70:ILE:O | 2.03 | 1.07 |
| 5:Z4:25:THR:HG21 | 5:Z4:63:ASN:O | 1.54 | 1.07 |
| 1:B5:53:LYS:HD3 | 8:C5:118:SER:O | 1.54 | 1.07 |
| 8:G5:61:ILE:HG21 | 8:o7:68:PRO:HG2 | 1.31 | 1.07 |
| 8:S5:68:PRO:HB3 | 8:a5:59:PHE:HB2 | 1.09 | 1.07 |
| 8:W5:17:TYR:CZ | 1:X5:44:ILE:CG2 | 2.37 | 1.07 |
| 10:j5:386:ILE:HG21 | 10:j5:395:SER:N | 1.41 | 1.07 |
| 12:D1:201:CYC:HMD1 | 12:D1:201:CYC:HC | 1.11 | 1.07 |
| 1:T7:106:GLU:CG | 9:w7:58:THR:HG23 | 1.84 | 1.07 |
| 8:o7:94:TYR:OH | 1:p7:17:LYS:O | 1.73 | 1.07 |
| 4:M9:189:ASP:OD1 | 3:V9:84:ARG:NH1 | 1.85 | 1.07 |
| 4:M9:273:ILE:CD1 | 3:V9:75:PRO:CD | 2.31 | 1.07 |
| 5:Z8:22:LEU:HD11 | 12:Z8:301:CYC:OB | 0.91 | 1.07 |
| 11:aA:107:ARG:HG2 | 11:aA:108:PRO:HD2 | 1.25 | 1.07 |
| 11:aA:623:ASP:HB3 | 3:H1:78:ARG:NH2 | 1.65 | 1.07 |
| 11:aA:813:PRO:HB3 | 3:L1:119:ALA:CB | 1.79 | 1.07 |
| 3:TA:21:GLU:HB3 | 2:R4:64:PRO:HG2 | 1.10 | 1.07 |
| 3:B4:119:ALA:HB1 | 4:M4:52:LEU:HD11 | 1.28 | 1.07 |
| 5:Z4:41:GLN:C | 12:Z4:301:CYC:HMA3 | 1.79 | 1.07 |
| 1:X5:65:LEU:HD12 | 10:j5:706:PRO:CG | 1.85 | 1.07 |
| 8:i7:25:ARG:NH1 | 8:s7:6:LYS:CG | 2.18 | 1.07 |
| 8:i7:54:ALA:CB | 8:i7:133:MET:HG3 | 1.83 | 1.07 |
| 8:c7:54:ALA:CB | 8:c7:133:MET:HG3 | 1.83 | 1.07 |
| 8:o7:27:LYS:HD2 | 1:p7:35:ALA:HA | 1.34 | 1.07 |
| 8:u7:18:LEU:HD22 | 1:v7:97:LEU:HD13 | 1.34 | 1.07 |
| 3:F8:91:ARG:NH2 | 11:a9:140:GLN:NE2 | 2.03 | 1.07 |
| 3:Q8:84:ARG:CG | 5:Z8:31:TRP:NE1 | 2.17 | 1.07 |
| 12:Q8:201:CYC:HMD1 | 12:Q8:201:CYC:HC | 1.11 | 1.07 |
| 4:M9:274:VAL:HG22 | 3:V9:77:ARG:CB | 1.85 | 1.07 |
| 12:J9:202:CYC:HBA2 | 11:a9:511:LYS:HA | 1.17 | 1.07 |
| 11:aA:275:THR:HA | 11:aA:278:LEU:HD13 | 1.35 | 1.07 |
| 11:aA:585:GLU:C | 11:aA:588:VAL:O | 1.97 | 1.07 |
| 12:H3:201:CYC:HC | 12:H3:201:CYC:HMD1 | 1.10 | 1.07 |
| 3:F4:1:MET:HA | 4:M4:10:ARG:O | 1.37 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:M4:190:ARG:NH1 | 4:M4:202:SER:CB | 2.16 | 1.07 |
| 4:M4:228:SER:CB | 2:X4:16:GLY:CA | 2.27 | 1.07 |
| 8:K5:112:VAL:HG23 | 1:J5:75:THR:CG2 | 1.85 | 1.07 |
| 1:f5:18:TYR:CZ | 10:j5:165:ARG:CB | 2.36 | 1.07 |
| 8:Q5:16:ARG:HB2 | 1:R5:90:ARG:NH1 | 1.69 | 1.07 |
| 10:j5:148:TYR:O | 10:j5:152:ARG:HG3 | 1.54 | 1.07 |
| 10:j5:931:VAL:HG22 | 1:J7:29:ALA:O | 1.52 | 1.07 |
| 10:j5:938:GLN:OE1 | 1:J7:28:LYS:CG | 2.03 | 1.07 |
| 10:k5:841:VAL:HG13 | 10:k5:846:GLU:OE1 | 1.54 | 1.07 |
| 8:M7:49:ARG:HH12 | 3:H9:119:ALA:HA | 0.94 | 1.07 |
| 12:i7:201:CYC:HMD1 | 12:i7:201:CYC:HC | 1.18 | 1.07 |
| 8:k7:79:ALA:HB2 | 11:a9:53:VAL:HG21 | 1.29 | 1.07 |
| 8:c7:20:PRO:HG3 | 8:m7:155:TYR:HB2 | 1.21 | 1.07 |
| 8:c7:39:ILE:HD13 | 8:c7:148:GLU:CB | 1.83 | 1.07 |
| 3:J8:108:ARG:NH2 | 11:a9:171:ARG:HB3 | 1.69 | 1.07 |
| 4:M8:160:THR:HG22 | 4:M8:257:GLN:CB | 1.84 | 1.07 |
| 12:M8:302:CYC:H2C | 3:S8:78:ARG:CD | 1.81 | 1.07 |
| 3:O8:107:ASP:HB3 | 5:Z8:66:ARG:HB3 | 1.13 | 1.07 |
| 3:Q8:120:LEU:HD13 | 3:Q8:122:THR:OG1 | 1.53 | 1.07 |
| 4:M9:158:PHE:C | 3:V9:108:ARG:CD | 2.27 | 1.07 |
| 3:B9:107:ASP:HB3 | 11:a9:382:ASN:ND2 | 1.69 | 1.07 |
| 3:H9:113:LEU:HD11 | 12:H9:202:CYC:CMB | 1.84 | 1.07 |
| 11:a9:643:LEU:HD21 | 11:a9:689:VAL:HG23 | 1.36 | 1.07 |
| 11:aA:403:THR:HG21 | 11:aA:536:THR:HG22 | 1.28 | 1.07 |
| 11:aA:798:SER:CB | 11:aA:800:THR:HG21 | 1.78 | 1.07 |
| 4:M1:190:ARG:NH1 | 4:M1:202:SER:CB | 2.16 | 1.07 |
| 4:MA:274:VAL:HG22 | 3:VA:77:ARG:CB | 1.85 | 1.06 |
| 3:L2:77:ARG:HH12 | 6:M2:70:GLU:CG | 1.65 | 1.06 |
| 12:B1:202:CYC:HBA1 | 11:aA:684:ASN:HB2 | 1.36 | 1.06 |
| 12:B1:202:CYC:CAA | 11:aA:684:ASN:HB2 | 1.84 | 1.06 |
| 3:U4:120:LEU:HG | 4:M4:254:LEU:HD21 | 1.34 | 1.06 |
| 3:F4:84:ARG:HD2 | 11:aA:139:ILE:HG22 | 1.18 | 1.06 |
| 3:F4:115:GLU:CG | 4:M4:3:VAL:HG13 | 1.82 | 1.06 |
| 12:M4:301:CYC:HMC3 | 3:Y4:72:ASN:HB3 | 1.19 | 1.06 |
| 2:N4:111:ALA:HB3 | 5:Z4:34:LEU:CG | 1.73 | 1.06 |
| 8:A5:71:ASN:OD1 | 12:A5:201:CYC:CMD | 2.02 | 1.06 |
| 12:B5:201:CYC:HBA2 | 9:z5:26:THR:HG21 | 1.20 | 1.06 |
| 1:D5:75:THR:CG2 | 8:E5:112:VAL:HG23 | 1.85 | 1.06 |
| 1:H5:53:LYS:HD3 | 8:I5:118:SER:O | 1.54 | 1.06 |
| 10:j5:741:GLN:O | 1:J7:77:ARG:NH2 | 1.87 | 1.06 |
| 10:k5:1025:LEU:HD23 | 10:k5:1030:ILE:CG2 | 1.85 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 12:D6:202:CYC:HMD1 | 12:D6:202:CYC:HC | 1.10 | 1.06 |
| 12:R7:201:CYC:O1A | 9:z7:34:TYR:OH | 1.72 | 1.06 |
| 8:u7:94:TYR:OH | 1:v7:17:LYS:O | 1.73 | 1.06 |
| 2:X8:13:ASP:OD1 | 4:M8:229:GLY:HA3 | 0.89 | 1.06 |
| 2:X8:67:THR:CA | 3:T9:28:THR:HG21 | 1.86 | 1.06 |
| 3:H8:84:ARG:HG2 | 11:a9:131:TYR:CE2 | 1.90 | 1.06 |
| 12:H8:201:CYC:HBB2 | 11:a9:259:ALA:HB2 | 1.37 | 1.06 |
| 3:O8:119:ALA:HB1 | 5:Z8:72:GLU:HB2 | 1.35 | 1.06 |
| 4:M9:163:ASN:ND2 | 12:V9:201:CYC:CMA | 2.18 | 1.06 |
| 11:aA:312:ASP:HA | 11:aA:315:LEU:HB2 | 1.07 | 1.06 |
| 11:aA:707:PHE:HE2 | 3:L1:108:ARG:NH1 | 1.47 | 1.06 |
| 11:aA:710:THR:CG2 | 11:aA:807:GLN:HG3 | 1.82 | 1.06 |
| 11:aA:738:LEU:HD13 | 12:aA:902:CYC:HB | 1.05 | 1.06 |
| 11:aA:746:TYR:HB3 | 2:K1:14:SER:HB2 | 1.07 | 1.06 |
| 4:MA:29:PRO:HD3 | 11:aA:378:GLU:OE2 | 1.54 | 1.06 |
| 4:MA:158:PHE:C | 3:VA:108:ARG:CD | 2.27 | 1.06 |
| 12:B4:202:CYC:O1A | 4:M4:54:ALA:HB2 | 1.31 | 1.06 |
| 5:N3:33:GLY:O | 3:T3:84:ARG:HD2 | 1.56 | 1.06 |
| 2:U3:141:GLN:O | 2:Q9:76:ASP:N | 1.88 | 1.06 |
| 2:I4:115:GLU:OE1 | 11:aA:133:LEU:HD23 | 1.55 | 1.06 |
| 12:L4:201:CYC:HMD1 | 12:L4:201:CYC:HC | 1.10 | 1.06 |
| 4:M4:232:VAL:CB | 12:M4:301:CYC:HBB2 | 1.86 | 1.06 |
| 3:Q4:7:LYS:NZ | 3:Q4:101:ASP:OD1 | 1.89 | 1.06 |
| 8:Q5:17:TYR:CZ | 1:R5:44:ILE:CG2 | 2.37 | 1.06 |
| 12:W5:201:CYC:HC | 12:W5:201:CYC:HMD1 | 1.18 | 1.06 |
| 6:M6:53:LEU:CD2 | 8:c7:80:LEU:CD2 | 2.33 | 1.06 |
| 9:i5:22:GLU:C | 9:i5:25:ASN:H | 1.61 | 1.06 |
| 10:j5:53:ARG:O | 10:j5:56:ILE:HG22 | 1.52 | 1.06 |
| 10:j5:820:HIS:CE1 | 10:j5:859:ILE:HD13 | 1.87 | 1.06 |
| 10:j5:965:GLN:CG | 1:t7:69:GLY:O | 2.03 | 1.06 |
| 10:j5:1051:GLU:OE2 | 11:aA:32:ARG:NH2 | 1.89 | 1.06 |
| 10:j5:1105:ILE:HD12 | 10:j5:1115:ARG:NH2 | 1.67 | 1.06 |
| 10:j5:1150:TYR:HE1 | 11:aA:38:VAL:HG22 | 1.08 | 1.06 |
| 10:k5:631:HIS:CD2 | 10:k5:664:MET:CE | 2.38 | 1.06 |
| 10:k5:970:GLY:N | 1:n7:77:ARG:HH21 | 1.52 | 1.06 |
| 10:k5:1051:GLU:OE2 | 11:a9:32:ARG:NH2 | 1.88 | 1.06 |
| 8:a7:25:ARG:HE | 8:o7:25:ARG:CZ | 1.67 | 1.06 |
| 1:l7:68:PRO:HB2 | 1:n7:14:VAL:O | 1.56 | 1.06 |
| 8:o7:90:ARG:HB2 | 1:p7:18:TYR:CZ | 1.89 | 1.06 |
| 3:H8:119:ALA:HB1 | 11:a9:266:ASN:HB2 | 1.30 | 1.06 |
| 11:aA:710:THR:CG2 | 11:aA:807:GLN:CD | 2.28 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 12:H1:202:CYC:HMD1 | 12:H1:202:CYC:HC | 1.10 | 1.06 |
| 2:IA:16:GLY:HA2 | 3:JA:91:ARG:NH1 | 1.69 | 1.06 |
| 3:LA:111:ASN:O | 11:aA:532:ALA:CB | 2.04 | 1.06 |
| 3:L2:75:PRO:HG2 | 3:L2:78:ARG:HB2 | 1.36 | 1.06 |
| 12:B4:202:CYC:CMA | 4:M4:58:TYR:HB2 | 1.85 | 1.06 |
| 4:M3:160:THR:HG22 | 4:M3:257:GLN:CB | 1.84 | 1.06 |
| 3:U4:111:ASN:OD1 | 4:M4:77:LEU:CD1 | 2.03 | 1.06 |
| 1:B5:143:PRO:HG3 | 8:W7:41:GLN:NE2 | 1.70 | 1.06 |
| 1:f5:114:GLU:HB3 | 10:j5:491:THR:HG23 | 1.13 | 1.06 |
| 6:M6:117:MET:HE2 | 3:H6:77:ARG:NH1 | 1.65 | 1.06 |
| 10:j5:386:ILE:HD13 | 10:j5:395:SER:OG | 1.38 | 1.06 |
| 12:j5:1202:CYC:HMA1 | 12:j5:1202:CYC:HB | 1.06 | 1.06 |
| 3:D1:68:ARG:NH1 | 3:X1:68:ARG:HH22 | 1.53 | 1.06 |
| 1:H7:140:LEU:HG | 11:aA:561:ALA:HB2 | 1.36 | 1.06 |
| 8:i7:25:ARG:HH12 | 8:s7:6:LYS:C | 1.62 | 1.06 |
| 9:x7:4:TYR:HB2 | 9:x7:58:THR:OG1 | 1.54 | 1.06 |
| 4:M8:225:LYS:HE3 | 3:Y8:81:ALA:HB2 | 1.36 | 1.06 |
| 2:N8:112:GLY:H | 5:Z8:34:LEU:HB2 | 1.17 | 1.06 |
| 3:O8:104:VAL:CG2 | 5:Z8:61:LYS:HE3 | 1.83 | 1.06 |
| 3:O8:119:ALA:HB1 | 5:Z8:72:GLU:CB | 1.86 | 1.06 |
| 4:M9:37:GLU:OE1 | 4:M9:40:GLN:NE2 | 1.86 | 1.06 |
| 4:M9:163:ASN:ND2 | 12:V9:201:CYC:HMA1 | 1.71 | 1.06 |
| 5:Z8:34:LEU:O | 5:Z8:34:LEU:CD2 | 2.04 | 1.06 |
| 3:J9:70:GLY:CA | 11:a9:357:THR:O | 2.04 | 1.06 |
| 1:Z:76:ARG:NH1 | 10:j5:262:TYR:CE2 | 2.22 | 1.06 |
| 12:JA:202:CYC:CBA | 11:aA:511:LYS:HD3 | 1.85 | 1.06 |
| 4:MA:274:VAL:HG22 | 3:VA:77:ARG:HB2 | 1.11 | 1.06 |
| 5:N3:34:LEU:O | 3:T3:84:ARG:NH1 | 1.89 | 1.06 |
| 3:L4:68:ARG:HB3 | 11:aA:82:GLN:H | 1.19 | 1.06 |
| 1:L5:75:THR:HG22 | 8:G5:115:MET:CE | 1.85 | 1.06 |
| 1:F5:119:LEU:HD21 | 10:k5:546:PHE:HD2 | 1.19 | 1.06 |
| 8:c5:9:VAL:HG11 | 10:j5:344:ARG:NH2 | 1.70 | 1.06 |
| 8:Q5:12:ASP:HA | 1:R5:94:TYR:HE2 | 1.20 | 1.06 |
| 1:R5:106:GLU:HG2 | 10:k5:504:ASP:O | 1.56 | 1.06 |
| 10:j5:631:HIS:CD2 | 10:j5:664:MET:CE | 2.38 | 1.06 |
| 10:j5:820:HIS:ND1 | 10:j5:859:ILE:HD12 | 1.68 | 1.06 |
| 10:j5:841:VAL:HG13 | 10:j5:846:GLU:OE1 | 1.54 | 1.06 |
| 10:k5:56:ILE:HD13 | 10:k5:219:ASP:CB | 1.86 | 1.06 |
| 10:k5:1017:ARG:HB3 | 10:k5:1017:ARG:HH21 | 1.20 | 1.06 |
| 10:k5:1052:PRO:CB | 1:l7:106:GLU:OE2 | 2.03 | 1.06 |
| 12:B8:202:CYC:CMA | 4:M8:58:TYR:HB2 | 1.85 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:F8:84:ARG:HD3 | 11:a9:139:ILE:HG22 | 1.13 | 1.06 |
| 3:H8:14:LEU:HD22 | 11:a9:85:ALA:HA | 1.36 | 1.06 |
| 3:O8:111:ASN:HB3 | 5:Z8:67:ILE:HB | 1.36 | 1.06 |
| 4:M9:273:ILE:HD11 | 3:V9:75:PRO:HD3 | 1.33 | 1.06 |
| 11:a9:93:LEU:CD2 | 11:a9:252:ARG:NH1 | 2.19 | 1.06 |
| 11:a9:287:ALA:C | 11:a9:289:THR:H | 1.53 | 1.06 |
| 11:aA:738:LEU:HD22 | 12:aA:902:CYC:C4B | 1.86 | 1.06 |
| 4:MA:163:ASN:ND2 | 12:VA:201:CYC:HMA1 | 1.71 | 1.06 |
| 12:J3:202:CYC:HAA1 | 11:a9:798:SER:CB | 1.84 | 1.06 |
| 12:D3:201:CYC:HC | 12:D3:201:CYC:HMD1 | 1.11 | 1.06 |
| 3:F4:115:GLU:HG2 | 4:M4:3:VAL:HG11 | 1.13 | 1.06 |
| 4:M4:214:GLY:C | 5:Z4:27:ALA:C | 2.24 | 1.06 |
| 1:P5:114:GLU:CD | 10:k5:496:GLU:HG3 | 1.80 | 1.06 |
| 8:U5:75:GLU:OE2 | 6:M6:32:MET:HE3 | 1.53 | 1.06 |
| 1:X5:50:THR:CG2 | 8:a5:49:ARG:CZ | 2.32 | 1.06 |
| 10:k5:386:ILE:HD13 | 10:k5:395:SER:OG | 1.38 | 1.06 |
| 10:k5:822:ARG:HB2 | 10:k5:822:ARG:HH11 | 1.20 | 1.06 |
| 10:k5:1015:TYR:O | 10:k5:1017:ARG:HG2 | 0.90 | 1.06 |
| 1:B7:140:LEU:HD11 | 11:a9:561:ALA:HB1 | 1.06 | 1.06 |
| 8:c7:16:ARG:O | 1:d7:90:ARG:HD2 | 1.55 | 1.06 |
| 3:U8:115:GLU:OE1 | 4:M8:74:LEU:HD13 | 1.54 | 1.06 |
| 4:M8:214:GLY:HA2 | 5:Z8:28:HIS:CG | 1.91 | 1.06 |
| 2:P8:18:PHE:CA | 3:Q8:91:ARG:HH21 | 1.64 | 1.06 |
| 12:L9:202:CYC:O2A | 11:a9:404:TYR:HB2 | 1.55 | 1.06 |
| 4:M9:263:PRO:CB | 3:V9:119:ALA:CB | 2.33 | 1.06 |
| 3:D9:68:ARG:NH2 | 3:X9:68:ARG:HH12 | 1.52 | 1.06 |
| 11:a9:75:ALA:CA | 11:a9:81:ASP:CG | 2.29 | 1.06 |
| 11:aA:98:ILE:HD12 | 11:aA:101:ASP:HB2 | 1.37 | 1.06 |
| 11:aA:775:LYS:HA | 12:H1:201:CYC:HBA2 | 1.36 | 1.06 |
| 3:FA:145:PRO:HD3 | 12:F9:302:CYC:HMC3 | 1.38 | 1.05 |
| 2:IA:31:PHE:CE2 | 3:JA:31:VAL:HA | 1.62 | 1.05 |
| 12:XA:202:CYC:HMD1 | 12:XA:202:CYC:HC | 1.10 | 1.05 |
| 3:B1:88:ILE:HG21 | 12:B1:202:CYC:HMB1 | 1.30 | 1.05 |
| 4:M4:217:VAL:HG21 | 5:Z4:30:PRO:CA | 1.86 | 1.05 |
| 2:N4:112:GLY:HA2 | 5:Z4:34:LEU:N | 1.71 | 1.05 |
| 8:M5:66:VAL:HG11 | 8:K7:68:PRO:CG | 1.86 | 1.05 |
| 3:Y4:87:GLU:HG2 | 3:Y4:91:ARG:HH11 | 1.20 | 1.05 |
| 5:Z4:34:LEU:O | 5:Z4:34:LEU:CD2 | 2.04 | 1.05 |
| 1:F5:119:LEU:HD21 | 10:k5:546:PHE:CD2 | 1.91 | 1.05 |
| 1:f5:161:SER:C | 1:V5:101:PRO:HG3 | 1.81 | 1.05 |
| 1:R5:65:LEU:HD12 | 10:k5:706:PRO:HG3 | 1.13 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:b5:18:TYR:CE2 | 10:k5:165:ARG:CA | 2.39 | 1.05 |
| 10:j5:56:ILE:HD13 | 10:j5:219:ASP:HB3 | 1.09 | 1.05 |
| 10:j5:822:ARG:HH11 | 10:j5:822:ARG:HB2 | 1.20 | 1.05 |
| 10:k5:136:VAL:CG1 | 10:k5:137:PRO:HD2 | 1.84 | 1.05 |
| 10:k5:1074:GLN:CD | 1:l7:119:LEU:HD21 | 1.80 | 1.05 |
| 10:k5:1152:TYR:HD2 | 8:G7:68:PRO:CG | 1.46 | 1.05 |
| 3:D1:68:ARG:HH22 | 3:X1:68:ARG:CZ | 1.70 | 1.05 |
| 8:u7:17:TYR:CD2 | 1:v7:93:THR:HG21 | 1.90 | 1.05 |
| 8:u7:37:LEU:HD23 | 1:v7:24:LEU:HD22 | 1.33 | 1.05 |
| 4:M8:197:ASP:HB3 | 5:Z8:52:ARG:HG3 | 1.14 | 1.05 |
| 3:O8:111:ASN:ND2 | 5:Z8:68:LEU:HD23 | 1.70 | 1.05 |
| 3:Q8:78:ARG:NH1 | 12:Z8:301:CYC:O1D | 1.87 | 1.05 |
| 4:M9:274:VAL:CG1 | 2:W9:111:ALA:HB1 | 1.86 | 1.05 |
| 5:N9:70:ILE:HG21 | 3:T9:116:THR:HA | 1.26 | 1.05 |
| 3:B9:107:ASP:HB3 | 11:a9:382:ASN:HD22 | 0.92 | 1.05 |
| 3:J9:78:ARG:HH12 | 11:a9:359:ASP:HA | 1.16 | 1.05 |
| 11:a9:312:ASP:O | 11:a9:315:LEU:N | 1.82 | 1.05 |
| 11:a9:403:THR:HG22 | 11:a9:536:THR:HG23 | 1.07 | 1.05 |
| 3:LA:52:ILE:HD11 | 3:LA:87:GLU:CA | 1.85 | 1.05 |
| 3:H2:77:ARG:NH1 | 6:M2:117:MET:HE2 | 1.65 | 1.05 |
| 3:L4:68:ARG:HB3 | 11:aA:82:GLN:N | 1.69 | 1.05 |
| 4:M4:113:ILE:HD11 | 4:M4:143:VAL:HG22 | 1.36 | 1.05 |
| 8:O5:76:LYS:HD2 | 8:O5:77:MET:HE3 | 1.38 | 1.05 |
| 3:Y4:103:SER:HA | 3:Y4:107:ASP:HB3 | 1.36 | 1.05 |
| 12:A5:201:CYC:HMD1 | 12:A5:201:CYC:HC | 1.18 | 1.05 |
| 8:G5:6:LYS:HZ1 | 8:S5:19:SER:CB | 1.68 | 1.05 |
| 8:G5:6:LYS:HZ3 | 8:S5:19:SER:HB3 | 1.21 | 1.05 |
| 8:U5:76:LYS:HD2 | 8:U5:77:MET:HE3 | 1.38 | 1.05 |
| 1:b5:5:ILE:HD12 | 10:k5:46:PHE:CE1 | 1.91 | 1.05 |
| 10:j5:156:SER:OG | 12:j5:1201:CYC:C3C | 2.03 | 1.05 |
| 10:j5:175:ASP:CB | 10:j5:176:PRO:CD | 1.97 | 1.05 |
| 10:k5:138:PRO:HB3 | 10:k5:201:VAL:HG11 | 1.31 | 1.05 |
| 10:k5:386:ILE:HG23 | 10:k5:387:VAL:N | 1.64 | 1.05 |
| 8:M7:49:ARG:NH1 | 3:H9:119:ALA:HA | 1.70 | 1.05 |
| 8:a7:52:LYS:HD2 | 11:a9:321:ALA:HB1 | 1.13 | 1.05 |
| 8:c7:11:ALA:HB3 | 1:d7:94:TYR:CE1 | 1.90 | 1.05 |
| 2:X8:69:PRO:CG | 2:S9:38:MET:C | 2.29 | 1.05 |
| 3:H8:111:ASN:CG | 11:a9:291:TYR:HH | 1.51 | 1.05 |
| 3:Q8:72:ASN:HD21 | 12:Z8:301:CYC:HBD2 | 1.15 | 1.05 |
| 3:L9:111:ASN:ND2 | 11:a9:531:ASP:OD1 | 1.89 | 1.05 |
| 5:Z8:22:LEU:HD11 | 12:Z8:301:CYC:C4B | 1.85 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 5:Z8:29:HIS:HD2 | 5:Z8:36:THR:HG23 | 1.15 | 1.05 |
| 3:H9:120:LEU:HD11 | 12:H9:202:CYC:C2A | 1.82 | 1.05 |
| 3:J9:119:ALA:O | 11:a9:365:LYS:HE3 | 1.35 | 1.05 |
| 12:J9:202:CYC:CBA | 11:a9:511:LYS:HD3 | 1.85 | 1.05 |
| 11:a9:98:ILE:HD12 | 11:a9:101:ASP:HB2 | 1.37 | 1.05 |
| 11:a9:275:THR:HA | 11:a9:278:LEU:HD13 | 1.35 | 1.05 |
| 11:a9:280:ASP:CB | 11:a9:281:PRO:CD | 2.03 | 1.05 |
| 11:aA:623:ASP:CB | 3:H1:78:ARG:HH22 | 1.65 | 1.05 |
| 5:N1:34:LEU:O | 3:T1:84:ARG:NH1 | 1.89 | 1.05 |
| 4:MA:263:PRO:CB | 3:VA:119:ALA:CB | 2.33 | 1.05 |
| 3:J3:107:ASP:OD1 | 11:a9:632:ILE:HG12 | 1.54 | 1.05 |
| 2:K3:14:SER:HB2 | 11:a9:746:TYR:HB3 | 1.08 | 1.05 |
| 3:B4:120:LEU:HD12 | 4:M4:53:LEU:HB2 | 1.38 | 1.05 |
| 3:B1:88:ILE:CG2 | 12:B1:202:CYC:HMB1 | 1.78 | 1.05 |
| 3:L4:68:ARG:NH1 | 11:aA:75:ALA:HB3 | 1.71 | 1.05 |
| 3:L4:68:ARG:HB2 | 11:aA:82:GLN:HB2 | 1.36 | 1.05 |
| 3:L4:68:ARG:HB3 | 11:aA:81:ASP:CA | 1.86 | 1.05 |
| 4:M4:273:ILE:HD12 | 2:X4:108:TYR:CZ | 1.91 | 1.05 |
| 8:A5:115:MET:CE | 1:F5:75:THR:HG22 | 1.85 | 1.05 |
| 1:d5:127:VAL:CG1 | 10:j5:698:GLY:HA3 | 1.85 | 1.05 |
| 1:f5:114:GLU:CB | 10:j5:491:THR:HG23 | 1.85 | 1.05 |
| 8:Q5:17:TYR:HE2 | 1:R5:93:THR:OG1 | 1.21 | 1.05 |
| 8:W5:11:ALA:CB | 1:X5:94:TYR:HE1 | 1.48 | 1.05 |
| 10:j5:230:VAL:O | 10:j5:234:LEU:HG | 1.57 | 1.05 |
| 10:j5:1017:ARG:HB3 | 10:j5:1017:ARG:HH21 | 1.20 | 1.05 |
| 10:j5:1023:SER:HB3 | 12:f7:201:CYC:HMA2 | 1.36 | 1.05 |
| 10:k5:362:LYS:HE2 | 10:k5:363:HIS:HE2 | 1.19 | 1.05 |
| 10:k5:386:ILE:CG2 | 10:k5:395:SER:O | 2.05 | 1.05 |
| 10:k5:742:GLY:C | 12:D7:201:CYC:O2D | 1.99 | 1.05 |
| 8:S7:49:ARG:CD | 11:aA:550:PHE:CE1 | 2.40 | 1.05 |
| 8:U7:49:ARG:HH12 | 1:l7:114:GLU:CD | 1.64 | 1.05 |
| 8:U7:52:LYS:HE3 | 11:a9:29:ARG:NH1 | 1.71 | 1.05 |
| 8:q7:66:VAL:HG11 | 11:aA:61:TYR:HE1 | 1.12 | 1.05 |
| 8:u7:27:LYS:HD2 | 1:v7:35:ALA:HA | 1.34 | 1.05 |
| 9:y7:4:TYR:HB2 | 9:y7:58:THR:OG1 | 1.54 | 1.05 |
| 2:X8:16:GLY:HA2 | 4:M8:228:SER:CB | 1.85 | 1.05 |
| 4:M8:56:MET:CE | 4:M8:66:VAL:HG21 | 1.84 | 1.05 |
| 3:Q8:78:ARG:HH11 | 12:Z8:301:CYC:CAD | 1.69 | 1.05 |
| 3:L9:51:ILE:HG21 | 3:L9:90:LEU:CD1 | 1.85 | 1.05 |
| 3:L9:52:ILE:HD11 | 3:L9:87:GLU:HA | 1.36 | 1.05 |
| 3:Y8:89:ILE:CG2 | 3:Y8:92:TYR:CZ | 2.37 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:J9:88:ILE:CD1 | 11:a9:512:TYR:CE1 | 2.39 | 1.05 |
| 11:aA:742:GLN:CB | 3:L1:88:ILE:HD11 | 1.85 | 1.05 |
| 11:aA:798:SER:HB3 | 11:aA:800:THR:HG21 | 1.24 | 1.05 |
| 5:N1:33:GLY:O | 3:T1:84:ARG:HD2 | 1.56 | 1.05 |
| 3:BA:107:ASP:HB3 | 11:aA:382:ASN:ND2 | 1.71 | 1.05 |
| 3:FA:150:ARG:HA | 3:F9:150:ARG:CD | 1.85 | 1.05 |
| 3:LA:51:ILE:HG21 | 3:LA:90:LEU:CD1 | 1.85 | 1.05 |
| 4:MA:274:VAL:CG1 | 2:WA:111:ALA:HB1 | 1.86 | 1.05 |
| 2:K3:13:ASP:OD2 | 11:a9:707:PHE:HZ | 1.33 | 1.05 |
| 4:M3:134:ASN:HB2 | 12:P3:201:CYC:HAA1 | 1.05 | 1.05 |
| 5:N3:62:ARG:HH21 | 2:Q3:14:SER:HB3 | 0.89 | 1.05 |
| 3:S4:82:CYS:CB | 12:S4:202:CYC:HAC2 | 1.85 | 1.05 |
| 3:H4:111:ASN:ND2 | 11:aA:291:TYR:CZ | 2.25 | 1.05 |
| 4:M4:29:PRO:HB3 | 11:aA:225:VAL:O | 0.87 | 1.05 |
| 4:M4:100:SER:N | 3:Q4:1:MET:HE1 | 1.65 | 1.05 |
| 3:Y4:124:THR:HB | 3:Y4:172:ALA:HA | 1.36 | 1.05 |
| 8:I5:37:LEU:HD21 | 1:J5:27:LEU:HD13 | 1.37 | 1.05 |
| 1:Z5:127:VAL:CG1 | 10:k5:698:GLY:CA | 2.30 | 1.05 |
| 1:T7:106:GLU:HG3 | 9:w7:58:THR:HG23 | 1.35 | 1.05 |
| 8:a7:25:ARG:HE | 8:o7:25:ARG:NE | 1.54 | 1.05 |
| 8:a7:48:GLU:CA | 11:a9:318:TRP:HH2 | 1.69 | 1.05 |
| 3:B8:120:LEU:HD11 | 4:M8:53:LEU:HB2 | 1.37 | 1.05 |
| 3:U8:108:ARG:HA | 4:M8:246:ALA:HB3 | 1.25 | 1.05 |
| 3:U8:114:LYS:HZ1 | 4:M8:13:LYS:CE | 1.57 | 1.05 |
| 2:I8:14:SER:HA | 11:a9:170:PHE:CZ | 1.92 | 1.05 |
| 3:B9:107:ASP:CB | 11:a9:382:ASN:ND2 | 2.17 | 1.05 |
| 3:F9:68:ARG:NH1 | 3:Z9:68:ARG:NH1 | 1.66 | 1.05 |
| 3:H9:120:LEU:HD11 | 12:H9:202:CYC:HAA1 | 1.09 | 1.05 |
| 11:a9:75:ALA:HA | 11:a9:81:ASP:OD2 | 1.57 | 1.05 |
| 11:aA:75:ALA:CA | 11:aA:81:ASP:CG | 2.29 | 1.05 |
| 3:L2:65:ASP:OD2 | 1:h7:64:ASP:OD2 | 1.74 | 1.05 |
| 12:F3:201:CYC:O2A | 4:M3:35:THR:HA | 1.57 | 1.05 |
| 12:L3:202:CYC:C4B | 11:a9:738:LEU:HD22 | 1.85 | 1.05 |
| 12:L3:202:CYC:HBA2 | 11:a9:735:VAL:N | 1.70 | 1.05 |
| 4:M3:81:ASP:H | 3:X3:111:ASN:ND2 | 1.54 | 1.05 |
| 2:E4:15:GLN:HG2 | 11:aA:163:ASP:HB2 | 1.39 | 1.05 |
| 3:F4:106:GLU:O | 4:M4:6:THR:O | 1.72 | 1.05 |
| 3:F4:107:ASP:HA | 4:M4:8:SER:N | 1.72 | 1.05 |
| 4:M4:142:PHE:O | 4:M4:146:LEU:HG | 1.57 | 1.05 |
| 4:M4:160:THR:HG22 | 4:M4:257:GLN:CB | 1.84 | 1.05 |
| 1:L5:119:LEU:HD21 | 10:j5:546:PHE:CD2 | 1.91 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:P5:114:GLU:CB | 10:k5:496:GLU:HG3 | 1.86 | 1.05 |
| 1:b5:5:ILE:HD12 | 10:k5:46:PHE:CZ | 1.89 | 1.05 |
| 10:j5:743:VAL:CG1 | 12:J7:201:CYC:O2D | 2.05 | 1.05 |
| 10:j5:1025:LEU:HD23 | 10:j5:1030:ILE:CG2 | 1.85 | 1.05 |
| 10:j5:1153:VAL:HG23 | 1:v7:125:ALA:CB | 1.77 | 1.05 |
| 10:k5:1055:SER:CB | 12:k5:1203:CYC:HBB2 | 1.86 | 1.05 |
| 1:H7:140:LEU:HD12 | 11:aA:561:ALA:HA | 1.39 | 1.05 |
| 8:g7:48:GLU:CA | 11:aA:318:TRP:HH2 | 1.69 | 1.05 |
| 8:i7:20:PRO:CG | 8:s7:155:TYR:CG | 2.39 | 1.05 |
| 8:o7:17:TYR:CD2 | 1:p7:93:THR:HG21 | 1.90 | 1.05 |
| 3:L8:82:CYS:SG | 12:a9:901:CYC:NC | 2.29 | 1.05 |
| 4:M8:205:ASP:OD2 | 5:Z8:59:ARG:CG | 2.03 | 1.05 |
| 12:F1:201:CYC:O2A | 4:M1:35:THR:HA | 1.57 | 1.05 |
| 2:I9:16:GLY:HA2 | 3:J9:91:ARG:NH1 | 1.69 | 1.05 |
| 11:aA:99:ALA:HB1 | 11:aA:100:PRO:HD3 | 1.34 | 1.05 |
| 11:aA:426:ARG:HH21 | 11:aA:496:ARG:HD3 | 1.15 | 1.05 |
| 4:M1:160:THR:HG22 | 4:M1:257:GLN:HB2 | 1.27 | 1.05 |
| 3:FA:150:ARG:CA | 3:F9:150:ARG:HG3 | 1.87 | 1.04 |
| 3:TA:28:THR:HG21 | 2:X4:67:THR:CA | 1.86 | 1.04 |
| 2:K3:13:ASP:OD1 | 11:a9:741:TYR:OH | 1.74 | 1.04 |
| 3:D3:68:ARG:HH22 | 3:X3:68:ARG:CZ | 1.70 | 1.04 |
| 12:B4:202:CYC:HBB3 | 4:M4:61:ASN:ND2 | 1.72 | 1.04 |
| 3:F4:91:ARG:NH2 | 11:aA:140:GLN:NE2 | 2.05 | 1.04 |
| 2:I4:14:SER:HA | 11:aA:170:PHE:CZ | 1.92 | 1.04 |
| 4:M4:104:ALA:HB3 | 2:P4:14:SER:CA | 1.85 | 1.04 |
| 3:Q4:104:VAL:CG2 | 3:Q4:105:LEU:HD12 | 1.87 | 1.04 |
| 1:Z5:83:ARG:NH1 | 10:k5:379:PHE:CE2 | 2.24 | 1.04 |
| 10:j5:275:THR:CG2 | 10:j5:286:VAL:HG13 | 1.87 | 1.04 |
| 10:k5:66:MET:HA | 10:k5:66:MET:HE3 | 1.39 | 1.04 |
| 10:k5:275:THR:CG2 | 10:k5:286:VAL:HG13 | 1.86 | 1.04 |
| 10:k5:974:LEU:CD2 | 1:p7:1:MET:H3 | 1.69 | 1.04 |
| 10:k5:1081:VAL:HG11 | 12:k5:1203:CYC:HMA2 | 1.33 | 1.04 |
| 8:o7:27:LYS:HD2 | 1:p7:35:ALA:CA | 1.87 | 1.04 |
| 8:o7:37:LEU:HD23 | 1:p7:24:LEU:HD22 | 1.33 | 1.04 |
| 8:q7:49:ARG:NH2 | 3:H1:62:GLU:OE1 | 1.87 | 1.04 |
| 2:X8:16:GLY:HA3 | 4:M8:228:SER:HB2 | 1.35 | 1.04 |
| 3:L9:111:ASN:O | 11:a9:532:ALA:CB | 2.03 | 1.04 |
| 4:M9:274:VAL:CA | 3:V9:77:ARG:CG | 1.84 | 1.04 |
| 5:N9:1:MET:HG2 | 3:R9:119:ALA:HB3 | 1.33 | 1.04 |
| 5:N9:22:LEU:HD21 | 5:N9:26:LEU:HD21 | 1.38 | 1.04 |
| 11:a9:50:LEU:O | 11:a9:53:VAL:CB | 2.06 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:a9:239:TYR:CZ | 12:a9:901:CYC:NB | 2.21 | 1.04 |
| 11:a9:312:ASP:HA | 11:a9:315:LEU:HB2 | 1.07 | 1.04 |
| 11:aA:287:ALA:C | 11:aA:289:THR:H | 1.53 | 1.04 |
| 3:FA:151:GLY:H | 3:F9:150:ARG:NE | 1.53 | 1.04 |
| 3:LA:111:ASN:ND2 | 11:aA:531:ASP:OD1 | 1.91 | 1.04 |
| 5:NA:53:LEU:HB3 | 12:TA:301:CYC:HBA2 | 1.04 | 1.04 |
| 4:M4:227:GLN:O | 3:Y4:88:ILE:CG2 | 2.04 | 1.04 |
| 2:N4:111:ALA:HB1 | 5:Z4:34:LEU:CG | 1.73 | 1.04 |
| 8:U5:83:ARG:HG2 | 6:M6:31:ASP:CG | 1.81 | 1.04 |
| 1:V5:83:ARG:NH1 | 10:j5:649:PHE:CZ | 2.25 | 1.04 |
| 1:Z5:64:ASP:HB2 | 10:k5:705:THR:HG23 | 1.06 | 1.04 |
| 10:j5:136:VAL:HG12 | 10:j5:137:PRO:HD3 | 1.08 | 1.04 |
| 10:j5:362:LYS:HE2 | 10:j5:363:HIS:HE2 | 1.19 | 1.04 |
| 10:k5:742:GLY:HA2 | 12:D7:201:CYC:CGD | 1.87 | 1.04 |
| 10:k5:931:VAL:CG2 | 1:D7:30:TYR:HA | 1.87 | 1.04 |
| 8:c7:15:ALA:C | 1:d7:90:ARG:CZ | 2.29 | 1.04 |
| 12:J8:201:CYC:CMA | 11:a9:176:ASN:HD21 | 1.71 | 1.04 |
| 3:L9:52:ILE:HD11 | 3:L9:87:GLU:CA | 1.85 | 1.04 |
| 4:M9:158:PHE:HA | 3:V9:108:ARG:HD3 | 1.34 | 1.04 |
| 11:a9:710:THR:CG2 | 11:a9:807:GLN:HG3 | 1.82 | 1.04 |
| 11:aA:93:LEU:CD2 | 11:aA:252:ARG:NH1 | 2.19 | 1.04 |
| 4:M1:81:ASP:H | 3:X1:111:ASN:ND2 | 1.55 | 1.04 |
| 4:M1:258:LYS:NZ | 3:Z1:111:ASN:ND2 | 2.05 | 1.04 |
| 3:HA:120:LEU:HD11 | 12:HA:202:CYC:C2A | 1.86 | 1.04 |
| 5:NA:1:MET:SD | 3:RA:119:ALA:CB | 2.44 | 1.04 |
| 12:P1:201:CYC:HAA1 | 4:M1:134:ASN:HB2 | 1.05 | 1.04 |
| 2:U3:45:THR:O | 2:Q9:69:PRO:CG | 1.95 | 1.04 |
| 4:M4:29:PRO:CG | 11:aA:226:PHE:HA | 1.87 | 1.04 |
| 4:M4:100:SER:H | 3:Q4:1:MET:HE1 | 1.15 | 1.04 |
| 8:O5:102:THR:HB | 8:O5:103:PRO:CD | 1.88 | 1.04 |
| 8:U5:75:GLU:CD | 6:M6:32:MET:CE | 2.31 | 1.04 |
| 10:j5:56:ILE:HD13 | 10:j5:219:ASP:CB | 1.86 | 1.04 |
| 10:k5:136:VAL:HG12 | 10:k5:137:PRO:HD3 | 1.08 | 1.04 |
| 10:k5:1150:TYR:HE2 | 1:p7:69:GLY:C | 1.64 | 1.04 |
| 8:O7:102:THR:HB | 8:O7:103:PRO:CD | 1.88 | 1.04 |
| 1:P7:14:VAL:O | 1:N7:68:PRO:HB2 | 1.56 | 1.04 |
| 1:B7:140:LEU:CD1 | 11:a9:561:ALA:CB | 2.35 | 1.04 |
| 12:d7:201:CYC:NB | 9:x7:38:PHE:CE1 | 2.24 | 1.04 |
| 2:X8:60:TYR:CD2 | 3:T9:32:LYS:NZ | 2.25 | 1.04 |
| 3:F8:107:ASP:HB2 | 4:M8:8:SER:O | 1.30 | 1.04 |
| 3:L8:82:CYS:CB | 12:a9:901:CYC:HMD3 | 1.87 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M9:160:THR:HG22 | 4:M9:257:GLN:CB | 1.84 | 1.04 |
| 5:Z8:41:GLN:O | 12:Z8:301:CYC:CMA | 2.04 | 1.04 |
| 3:J9:111:ASN:N | 11:a9:518:ALA:HB3 | 1.73 | 1.04 |
| 1:A:161:SER:OG | 1:R5:14:VAL:CG2 | 1.91 | 1.04 |
| 3:FA:68:ARG:NH1 | 3:ZA:68:ARG:CZ | 2.21 | 1.04 |
| 3:HA:126:SER:HB2 | 12:HA:202:CYC:HMC2 | 1.34 | 1.04 |
| 12:JA:202:CYC:HBA1 | 11:aA:511:LYS:HA | 1.06 | 1.04 |
| 3:J3:84:ARG:C | 11:a9:668:TYR:CZ | 2.31 | 1.04 |
| 12:J3:202:CYC:CBA | 11:a9:667:THR:CG2 | 1.99 | 1.04 |
| 3:J4:108:ARG:NH2 | 11:aA:171:ARG:HB3 | 1.71 | 1.04 |
| 4:M4:104:ALA:CB | 2:P4:14:SER:HA | 1.81 | 1.04 |
| 2:N4:14:SER:HB3 | 5:Z4:62:ARG:HD2 | 1.35 | 1.04 |
| 5:Z4:41:GLN:O | 12:Z4:301:CYC:CMA | 2.05 | 1.04 |
| 10:j5:951:MET:CE | 10:j5:955:LEU:HG | 1.88 | 1.04 |
| 10:k5:283:ARG:HB2 | 10:k5:284:PRO:HD2 | 1.39 | 1.04 |
| 10:k5:729:ILE:HD12 | 1:D7:64:ASP:OD1 | 1.56 | 1.04 |
| 10:k5:820:HIS:CE1 | 10:k5:859:ILE:HD13 | 1.87 | 1.04 |
| 8:I7:161:GLN:CD | 1:X7:49:THR:HG22 | 1.81 | 1.04 |
| 8:i7:20:PRO:CD | 8:s7:155:TYR:CE1 | 2.41 | 1.04 |
| 8:a7:102:THR:HB | 8:a7:103:PRO:CD | 1.88 | 1.04 |
| 3:B8:68:ARG:HH22 | 3:U8:68:ARG:CZ | 1.70 | 1.04 |
| 3:B8:116:THR:HA | 4:M8:56:MET:HG3 | 1.38 | 1.04 |
| 8:u7:27:LYS:HD2 | 1:v7:35:ALA:CA | 1.87 | 1.04 |
| 3:H8:84:ARG:CB | 11:a9:131:TYR:CZ | 2.40 | 1.04 |
| 3:H8:111:ASN:ND2 | 11:a9:291:TYR:CZ | 2.26 | 1.04 |
| 12:M8:301:CYC:C3C | 3:Y8:127:VAL:HG22 | 1.88 | 1.04 |
| 3:Q8:110:LEU:HD22 | 3:Q8:170:SER:HB3 | 1.40 | 1.04 |
| 3:Q8:120:LEU:HD11 | 3:Q8:122:THR:HB | 1.12 | 1.04 |
| 5:N9:1:MET:SD | 3:R9:119:ALA:CB | 2.44 | 1.04 |
| 3:J9:88:ILE:HD13 | 11:a9:512:TYR:CE2 | 1.91 | 1.04 |
| 3:F2:78:ARG:HG2 | 12:F2:201:CYC:CGD | 1.86 | 1.04 |
| 3:DA:115:GLU:OE2 | 4:MA:78:GLY:N | 1.90 | 1.04 |
| 12:LA:202:CYC:O2A | 11:aA:404:TYR:HB2 | 1.55 | 1.04 |
| 2:SA:38:MET:C | 2:X4:69:PRO:CG | 2.29 | 1.04 |
| 3:B4:116:THR:HB | 4:M4:56:MET:HG2 | 1.07 | 1.04 |
| 5:N3:31:TRP:CD1 | 2:S3:16:GLY:HA2 | 1.93 | 1.04 |
| 8:M5:19:SER:HB3 | 8:A5:6:LYS:HZ1 | 1.16 | 1.04 |
| 8:C5:102:THR:HB | 8:C5:103:PRO:CD | 1.88 | 1.04 |
| 1:Z5:28:LYS:CD | 1:t7:143:PRO:CB | 2.34 | 1.04 |
| 10:j5:386:ILE:HG21 | 10:j5:395:SER:H | 0.91 | 1.04 |
| 8:I7:102:THR:HB | 8:I7:103:PRO:CD | 1.88 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:h7:75:THR:HG22 | 8:i7:115:MET:HE2 | 1.37 | 1.04 |
| 8:i7:86:ASP:OD1 | 1:j7:18:TYR:OH | 1.74 | 1.04 |
| 8:c7:16:ARG:C | 1:d7:90:ARG:HD3 | 1.78 | 1.04 |
| 8:c7:92:VAL:HG23 | 8:c7:156:LEU:CD1 | 1.88 | 1.04 |
| 3:O8:107:ASP:HB3 | 5:Z8:66:ARG:CB | 1.88 | 1.04 |
| 3:O8:119:ALA:O | 5:Z8:72:GLU:OE2 | 1.74 | 1.04 |
| 4:M9:53:LEU:HD12 | 12:F9:301:CYC:OB | 1.56 | 1.04 |
| 4:M9:274:VAL:OXT | 3:V9:77:ARG:NE | 1.90 | 1.04 |
| 5:N9:70:ILE:HG22 | 3:T9:119:ALA:CB | 1.87 | 1.04 |
| 3:D9:68:ARG:NH2 | 3:X9:68:ARG:NH1 | 2.06 | 1.04 |
| 11:a9:448:ASN:OD1 | 11:a9:474:PHE:CE1 | 2.11 | 1.04 |
| 11:a9:602:PRO:O | 11:a9:604:ALA:N | 1.91 | 1.04 |
| 11:aA:50:LEU:O | 11:aA:53:VAL:CB | 2.06 | 1.04 |
| 11:aA:403:THR:HG22 | 11:aA:536:THR:HG23 | 1.07 | 1.04 |
| 11:aA:741:TYR:OH | 2:K1:13:ASP:OD1 | 1.74 | 1.04 |
| 3:BA:107:ASP:CB | 11:aA:382:ASN:ND2 | 2.19 | 1.03 |
| 5:NA:22:LEU:HD21 | 5:NA:26:LEU:HD21 | 1.38 | 1.03 |
| 3:D3:68:ARG:NH1 | 3:X3:68:ARG:HH22 | 1.53 | 1.03 |
| 3:B4:68:ARG:HH22 | 3:U4:68:ARG:CZ | 1.70 | 1.03 |
| 3:F4:115:GLU:HB3 | 4:M4:3:VAL:HG13 | 1.35 | 1.03 |
| 4:M4:211:GLN:O | 5:Z4:28:HIS:HE1 | 1.40 | 1.03 |
| 8:O5:76:LYS:HG3 | 8:O5:77:MET:N | 1.67 | 1.03 |
| 8:C5:37:LEU:HD21 | 1:D5:27:LEU:HD13 | 1.37 | 1.03 |
| 8:W5:16:ARG:HA | 1:X5:90:ARG:HD3 | 1.23 | 1.03 |
| 10:j5:386:ILE:CG2 | 10:j5:395:SER:O | 2.05 | 1.03 |
| 10:j5:990:ARG:HE | 10:j5:1026:LYS:NZ | 1.55 | 1.03 |
| 10:j5:1023:SER:OG | 12:f7:201:CYC:O2A | 1.74 | 1.03 |
| 10:j5:1056:PRO:HD2 | 10:j5:1057:LYS:H | 1.14 | 1.03 |
| 10:j5:1153:VAL:HG22 | 1:v7:65:LEU:HD11 | 1.40 | 1.03 |
| 10:k5:230:VAL:O | 10:k5:234:LEU:HG | 1.57 | 1.03 |
| 8:g7:102:THR:HB | 8:g7:103:PRO:CD | 1.88 | 1.03 |
| 8:c7:16:ARG:CA | 1:d7:90:ARG:HD3 | 1.83 | 1.03 |
| 12:B8:202:CYC:HBB3 | 4:M8:61:ASN:ND2 | 1.72 | 1.03 |
| 3:H9:84:ARG:HA | 11:a9:478:HIS:NE2 | 1.71 | 1.03 |
| 11:aA:75:ALA:HA | 11:aA:81:ASP:OD2 | 1.56 | 1.03 |
| 11:aA:776:TYR:H | 12:H1:201:CYC:HBA1 | 0.89 | 1.03 |
| 12:FA:301:CYC:OB | 4:MA:53:LEU:HD12 | 1.56 | 1.03 |
| 3:HA:117:TYR:CE1 | 12:HA:202:CYC:HHB | 1.92 | 1.03 |
| 3:JA:88:ILE:HD13 | 11:aA:512:TYR:CE2 | 1.93 | 1.03 |
| 5:NA:70:ILE:HG22 | 3:TA:119:ALA:CB | 1.87 | 1.03 |
| 2:SA:42:ARG:CD | 2:X4:69:PRO:O | 2.07 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 6:M2:26:PHE:HE2 | 8:O5:90:ARG:NH2 | 1.56 | 1.03 |
| 3:B4:119:ALA:HB2 | 4:M4:69:ILE:HG21 | 1.03 | 1.03 |
| 8:K5:112:VAL:CG2 | 1:J5:75:THR:HG21 | 1.87 | 1.03 |
| 8:G5:100:ASP:CG | 8:S5:20:PRO:HB2 | 1.83 | 1.03 |
| 1:H5:87:TYR:HE1 | 9:i5:19:THR:O | 1.39 | 1.03 |
| 12:Q5:201:CYC:HMD1 | 12:Q5:201:CYC:HC | 1.18 | 1.03 |
| 10:k5:190:LEU:CB | 10:k5:194:CYS:SG | 2.46 | 1.03 |
| 10:k5:974:LEU:CG | 1:p7:1:MET:N | 2.21 | 1.03 |
| 10:k5:990:ARG:HE | 10:k5:1026:LYS:NZ | 1.55 | 1.03 |
| 8:o7:18:LEU:HD22 | 1:p7:97:LEU:HD13 | 1.34 | 1.03 |
| 8:s7:102:THR:HB | 8:s7:103:PRO:CD | 1.88 | 1.03 |
| 3:Q8:77:ARG:HA | 5:Z8:34:LEU:HB3 | 1.04 | 1.03 |
| 4:M9:78:GLY:N | 3:D9:115:GLU:OE2 | 1.90 | 1.03 |
| 4:M9:273:ILE:HD13 | 3:V9:75:PRO:CG | 1.88 | 1.03 |
| 4:M9:274:VAL:CB | 3:V9:77:ARG:HG2 | 1.89 | 1.03 |
| 3:BA:107:ASP:HB3 | 11:aA:382:ASN:HD22 | 0.93 | 1.03 |
| 4:MA:273:ILE:HD13 | 3:VA:75:PRO:CG | 1.88 | 1.03 |
| 3:TA:32:LYS:NZ | 2:X4:60:TYR:CD2 | 2.25 | 1.03 |
| 3:B4:82:CYS:C | 12:B4:202:CYC:HAC2 | 1.83 | 1.03 |
| 4:M4:104:ALA:HB1 | 2:P4:14:SER:N | 1.52 | 1.03 |
| 4:M4:134:ASN:OD1 | 5:Z4:1:MET:HE1 | 1.58 | 1.03 |
| 4:M4:235:PHE:HB2 | 12:M4:301:CYC:CAA | 1.70 | 1.03 |
| 8:I5:102:THR:HB | 8:I5:103:PRO:CD | 1.88 | 1.03 |
| 8:Y5:9:VAL:CG1 | 10:k5:344:ARG:CZ | 2.36 | 1.03 |
| 1:b5:5:ILE:CD1 | 10:k5:46:PHE:CE1 | 2.42 | 1.03 |
| 10:j5:1025:LEU:CD2 | 10:j5:1035:PHE:CB | 2.14 | 1.03 |
| 10:j5:1153:VAL:HG21 | 1:v7:125:ALA:HB1 | 1.35 | 1.03 |
| 8:a7:25:ARG:NE | 8:o7:25:ARG:CZ | 2.17 | 1.03 |
| 8:c7:47:ARG:HD3 | 1:d7:18:TYR:CZ | 1.93 | 1.03 |
| 3:B8:120:LEU:HD11 | 4:M8:53:LEU:CB | 1.88 | 1.03 |
| 8:o7:29:PHE:CZ | 1:p7:31:PHE:CE1 | 2.47 | 1.03 |
| 1:r7:68:PRO:HB2 | 1:t7:14:VAL:O | 1.56 | 1.03 |
| 2:X8:57:GLN:NE2 | 3:T9:32:LYS:CD | 2.21 | 1.03 |
| 3:Q8:117:TYR:HD1 | 3:Q8:120:LEU:HD21 | 1.23 | 1.03 |
| 3:H9:113:LEU:CD2 | 12:H9:202:CYC:HMB1 | 1.87 | 1.03 |
| 3:JA:88:ILE:CD1 | 11:aA:512:TYR:CE1 | 2.40 | 1.03 |
| 4:MA:127:SER:O | 4:MA:130:SER:OG | 1.76 | 1.03 |
| 3:J3:84:ARG:CD | 11:a9:668:TYR:CG | 2.31 | 1.03 |
| 3:B4:120:LEU:CD1 | 4:M4:53:LEU:CA | 2.28 | 1.03 |
| 4:M3:127:SER:O | 4:M3:130:SER:OG | 1.76 | 1.03 |
| 5:N3:54:LEU:HD12 | 12:R3:201:CYC:C4B | 1.87 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:N4:111:ALA:HB3 | 5:Z4:34:LEU:HG | 1.33 | 1.03 |
| 3:Q4:120:LEU:CD1 | 5:Z4:40:SER:H | 1.71 | 1.03 |
| 8:W5:17:TYR:CE2 | 1:X5:44:ILE:HG22 | 1.88 | 1.03 |
| 10:j5:930:LEU:HB3 | 1:J7:33:THR:HG21 | 1.38 | 1.03 |
| 10:k5:934:ALA:HB3 | 1:D7:32:THR:CG2 | 1.84 | 1.03 |
| 10:k5:965:GLN:HG3 | 1:n7:69:GLY:O | 1.57 | 1.03 |
| 3:F6:85:ASP:OD2 | 12:F6:201:CYC:NA | 1.91 | 1.03 |
| 8:u7:29:PHE:CZ | 1:v7:31:PHE:CE1 | 2.47 | 1.03 |
| 2:X8:69:PRO:O | 2:S9:42:ARG:CD | 2.07 | 1.03 |
| 3:F8:109:CYS:CA | 4:M8:6:THR:CG2 | 2.35 | 1.03 |
| 4:M8:127:SER:CA | 12:M8:302:CYC:HMA2 | 1.60 | 1.03 |
| 4:M8:141:GLU:OE1 | 4:M8:144:ARG:HB2 | 1.57 | 1.03 |
| 12:M8:302:CYC:HAC2 | 3:S8:78:ARG:HG2 | 1.40 | 1.03 |
| 3:H1:77:ARG:NH1 | 12:H1:201:CYC:CGD | 2.21 | 1.03 |
| 3:HA:113:LEU:HD11 | 12:HA:202:CYC:CMB | 1.89 | 1.03 |
| 6:M2:127:SER:HA | 12:F2:201:CYC:O2A | 1.59 | 1.03 |
| 3:F4:107:ASP:CA | 4:M4:6:THR:O | 2.07 | 1.03 |
| 4:M4:217:VAL:CG2 | 5:Z4:30:PRO:HB3 | 1.89 | 1.03 |
| 8:K5:80:LEU:HD12 | 12:K5:201:CYC:CAD | 1.89 | 1.03 |
| 8:M5:19:SER:CB | 8:A5:6:LYS:HZ2 | 1.69 | 1.03 |
| 12:F5:201:CYC:HMA2 | 10:k5:591:ILE:CG2 | 1.88 | 1.03 |
| 8:e5:102:THR:HB | 8:e5:103:PRO:CD | 1.88 | 1.03 |
| 1:f5:30:TYR:OH | 10:j5:47:PHE:HZ | 1.35 | 1.03 |
| 10:k5:778:LYS:HZ1 | 12:F7:201:CYC:HBB2 | 1.24 | 1.03 |
| 10:k5:803:LYS:NZ | 9:z7:43:ARG:HH11 | 1.55 | 1.03 |
| 10:k5:820:HIS:ND1 | 10:k5:859:ILE:HD12 | 1.68 | 1.03 |
| 10:k5:1020:GLU:HG3 | 1:Z7:87:TYR:CZ | 1.94 | 1.03 |
| 10:k5:1153:VAL:HG22 | 1:p7:65:LEU:HD11 | 1.34 | 1.03 |
| 8:a7:63:PRO:HD2 | 11:a9:336:ILE:HG23 | 1.39 | 1.03 |
| 3:F9:68:ARG:NH1 | 3:Z9:68:ARG:CZ | 2.21 | 1.03 |
| 12:J9:202:CYC:HBA1 | 11:a9:511:LYS:HA | 1.06 | 1.03 |
| 11:aA:735:VAL:N | 12:aA:902:CYC:HBA2 | 1.72 | 1.03 |
| 3:TA:32:LYS:CD | 2:X4:57:GLN:NE2 | 2.21 | 1.02 |
| 12:R1:201:CYC:C4B | 5:N1:54:LEU:HD12 | 1.87 | 1.02 |
| 3:S4:113:LEU:O | 3:S4:116:THR:CG2 | 2.06 | 1.02 |
| 3:H4:84:ARG:CB | 11:aA:131:TYR:CZ | 2.42 | 1.02 |
| 12:J4:201:CYC:CMA | 11:aA:176:ASN:HD21 | 1.71 | 1.02 |
| 5:Z4:41:GLN:HG2 | 12:Z4:301:CYC:CMB | 1.84 | 1.02 |
| 1:D5:75:THR:HG21 | 8:E5:112:VAL:CG2 | 1.87 | 1.02 |
| 8:E5:80:LEU:HD12 | 12:E5:201:CYC:CAD | 1.89 | 1.02 |
| 1:H5:143:PRO:HG3 | 8:Q7:41:GLN:NE2 | 1.72 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:c5:9:VAL:HG11 | 10:j5:344:ARG:CZ | 1.89 | 1.02 |
| 1:f5:18:TYR:CD1 | 10:j5:165:ARG:CD | 2.42 | 1.02 |
| 1:f5:19:LEU:HD12 | 10:j5:172:LEU:CD1 | 1.88 | 1.02 |
| 1:P5:107:ARG:NH2 | 10:k5:619:GLU:OE1 | 1.92 | 1.02 |
| 12:R5:201:CYC:HMD1 | 12:R5:201:CYC:HC | 1.24 | 1.02 |
| 8:U5:76:LYS:CG | 8:U5:77:MET:CE | 2.36 | 1.02 |
| 8:W5:12:ASP:HA | 1:X5:94:TYR:HE2 | 1.20 | 1.02 |
| 8:a5:102:THR:HB | 8:a5:103:PRO:CD | 1.88 | 1.02 |
| 10:k5:974:LEU:HG | 1:p7:1:MET:H1 | 0.86 | 1.02 |
| 8:i7:20:PRO:HD2 | 8:s7:101:VAL:HG21 | 1.41 | 1.02 |
| 8:k7:68:PRO:HG2 | 11:a9:334:LYS:HD3 | 1.03 | 1.02 |
| 8:U7:102:THR:HB | 8:U7:103:PRO:CD | 1.88 | 1.02 |
| 3:B8:82:CYS:HA | 12:B8:202:CYC:C2C | 1.89 | 1.02 |
| 3:U8:114:LYS:NZ | 4:M8:13:LYS:HE3 | 1.70 | 1.02 |
| 4:M8:127:SER:O | 4:M8:130:SER:OG | 1.77 | 1.02 |
| 12:F1:201:CYC:CMA | 4:M1:36:TYR:O | 2.07 | 1.02 |
| 4:M9:127:SER:O | 4:M9:130:SER:OG | 1.76 | 1.02 |
| 4:M9:158:PHE:O | 3:V9:108:ARG:HG3 | 1.57 | 1.02 |
| 11:aA:448:ASN:OD1 | 11:aA:474:PHE:CE1 | 2.11 | 1.02 |
| 3:FA:151:GLY:N | 3:F9:150:ARG:HE | 1.57 | 1.02 |
| 2:SA:42:ARG:HE | 2:X4:69:PRO:CD | 1.73 | 1.02 |
| 3:B4:108:ARG:HA | 4:M4:61:ASN:HA | 1.42 | 1.02 |
| 2:U3:141:GLN:HA | 2:Q9:76:ASP:H | 1.21 | 1.02 |
| 3:B1:88:ILE:CG2 | 12:B1:202:CYC:HAB2 | 1.89 | 1.02 |
| 12:H4:201:CYC:HBB2 | 11:aA:259:ALA:HB2 | 1.36 | 1.02 |
| 4:M4:197:ASP:HB3 | 5:Z4:52:ARG:HG2 | 1.36 | 1.02 |
| 1:J5:73:TYR:O | 1:J5:77:ARG:CD | 2.07 | 1.02 |
| 1:f5:38:VAL:CG1 | 10:j5:40:VAL:CG1 | 2.36 | 1.02 |
| 8:W5:16:ARG:HB2 | 1:X5:90:ARG:NH1 | 1.68 | 1.02 |
| 10:j5:1049:PHE:CE1 | 10:j5:1065:HIS:CE1 | 2.47 | 1.02 |
| 10:k5:1049:PHE:CE1 | 10:k5:1065:HIS:CE1 | 2.47 | 1.02 |
| 12:E7:201:CYC:HMD1 | 12:E7:201:CYC:HC | 1.18 | 1.02 |
| 1:H7:68:PRO:HB2 | 1:J7:14:VAL:O | 1.56 | 1.02 |
| 8:i7:37:LEU:HD11 | 1:j7:31:PHE:CD2 | 1.95 | 1.02 |
| 3:B8:81:ALA:C | 12:B8:202:CYC:HMD3 | 1.83 | 1.02 |
| 8:o7:4:LEU:HD11 | 1:p7:30:TYR:CE2 | 1.94 | 1.02 |
| 8:o7:27:LYS:HE3 | 1:p7:35:ALA:HB1 | 1.09 | 1.02 |
| 1:v7:62:TYR:HB3 | 11:aA:601:ALA:HB1 | 1.40 | 1.02 |
| 3:O8:107:ASP:HB2 | 5:Z8:61:LYS:NZ | 1.74 | 1.02 |
| 2:P8:18:PHE:HA | 3:Q8:91:ARG:HH21 | 1.16 | 1.02 |
| 3:S8:113:LEU:O | 3:S8:116:THR:CG2 | 2.06 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:N9:53:LEU:HB3 | 12:T9:301:CYC:HBA2 | 1.04 | 1.02 |
| 3:F9:150:ARG:HH11 | 12:F9:302:CYC:C1C | 1.67 | 1.02 |
| 1:A:75:THR:HG21 | 10:k5:182:ASN:O | 1.58 | 1.02 |
| 12:Z:201:CYC:HMD1 | 12:Z:201:CYC:HC | 1.25 | 1.02 |
| 3:JA:70:GLY:CA | 11:aA:357:THR:O | 2.05 | 1.02 |
| 5:N3:1:MET:HE3 | 5:N3:1:MET:HA | 1.41 | 1.02 |
| 5:N3:22:LEU:HD21 | 5:N3:26:LEU:HD21 | 1.38 | 1.02 |
| 8:G5:61:ILE:CG2 | 8:o7:68:PRO:HG2 | 1.89 | 1.02 |
| 12:H5:201:CYC:HMD1 | 12:H5:201:CYC:HC | 1.25 | 1.02 |
| 12:J5:201:CYC:HMD1 | 12:J5:201:CYC:HC | 1.25 | 1.02 |
| 1:d5:28:LYS:NZ | 1:n7:143:PRO:HG2 | 1.67 | 1.02 |
| 1:X5:50:THR:CG2 | 8:a5:49:ARG:NH1 | 2.21 | 1.02 |
| 10:j5:989:THR:CG2 | 8:g7:106:GLU:OE2 | 2.07 | 1.02 |
| 10:j5:1118:THR:CG2 | 12:j5:1202:CYC:O2A | 2.07 | 1.02 |
| 10:k5:1045:TYR:OH | 10:k5:1062:LEU:CD2 | 2.08 | 1.02 |
| 3:F6:130:ALA:HB2 | 12:F6:201:CYC:HBC2 | 1.42 | 1.02 |
| 1:B7:68:PRO:HB2 | 1:D7:14:VAL:O | 1.55 | 1.02 |
| 8:m7:102:THR:HB | 8:m7:103:PRO:CD | 1.88 | 1.02 |
| 8:u7:4:LEU:HD11 | 1:v7:30:TYR:CE2 | 1.94 | 1.02 |
| 2:I8:115:GLU:OE1 | 11:a9:133:LEU:HD23 | 1.57 | 1.02 |
| 3:Q8:85:ASP:CG | 12:Z8:301:CYC:HBC1 | 1.76 | 1.02 |
| 3:L9:120:LEU:HD22 | 11:a9:538:ARG:HB2 | 1.42 | 1.02 |
| 4:M9:158:PHE:O | 3:V9:108:ARG:CG | 2.08 | 1.02 |
| 4:M9:274:VAL:HA | 3:V9:77:ARG:HG3 | 1.39 | 1.02 |
| 5:N9:70:ILE:HG22 | 3:T9:119:ALA:HB2 | 1.42 | 1.02 |
| 5:Z8:1:MET:HA | 5:Z8:1:MET:HE3 | 1.41 | 1.02 |
| 2:I9:37:SER:HA | 2:I9:97:LEU:HD21 | 1.41 | 1.02 |
| 11:a9:308:LEU:HD21 | 11:a9:315:LEU:HD12 | 1.40 | 1.02 |
| 11:a9:426:ARG:HH21 | 11:a9:496:ARG:HD3 | 1.15 | 1.02 |
| 11:aA:602:PRO:O | 11:aA:604:ALA:N | 1.91 | 1.02 |
| 11:aA:745:GLY:CA | 2:K1:15:GLN:HA | 1.89 | 1.02 |
| 4:M1:127:SER:O | 4:M1:130:SER:OG | 1.76 | 1.02 |
| 1:A:110:ASN:OD1 | 10:k5:462:TYR:CE1 | 2.13 | 1.02 |
| 3:FA:150:ARG:CA | 3:F9:150:ARG:HE | 1.72 | 1.02 |
| 2:Q1:14:SER:HB3 | 5:N1:62:ARG:HH21 | 0.89 | 1.02 |
| 3:J3:119:ALA:O | 11:a9:803:ASN:CA | 2.08 | 1.02 |
| 12:J3:202:CYC:HMA2 | 11:a9:666:ASN:HB2 | 1.40 | 1.02 |
| 6:M2:26:PHE:CE2 | 8:O5:90:ARG:NH2 | 2.26 | 1.02 |
| 12:M4:301:CYC:CBC | 3:Y4:82:CYS:SG | 2.46 | 1.02 |
| 8:A5:106:GLU:OE1 | 10:k5:557:VAL:O | 1.76 | 1.02 |
| 12:f5:201:CYC:HMD1 | 12:f5:201:CYC:HC | 1.25 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 6:M6:279:ASP:O | 8:Y7:76:LYS:NZ | 1.92 | 1.02 |
| 10:j5:136:VAL:CG1 | 10:j5:137:PRO:HD2 | 1.84 | 1.02 |
| 10:j5:386:ILE:HG23 | 10:j5:387:VAL:N | 1.65 | 1.02 |
| 10:j5:1146:THR:CA | 1:v7:77:ARG:NH2 | 2.20 | 1.02 |
| 10:k5:1054:SER:N | 1:l7:106:GLU:O | 1.92 | 1.02 |
| 1:T7:68:PRO:HB2 | 1:V7:14:VAL:O | 1.56 | 1.02 |
| 12:W7:201:CYC:HMD1 | 12:W7:201:CYC:HC | 1.18 | 1.02 |
| 12:D8:202:CYC:HBA2 | 4:M8:35:THR:CA | 1.89 | 1.02 |
| 12:U8:201:CYC:HBA2 | 4:M8:252:LEU:O | 1.56 | 1.02 |
| 2:X8:69:PRO:HD2 | 2:S9:42:ARG:HE | 1.22 | 1.02 |
| 3:O8:115:GLU:OE2 | 5:Z8:69:GLU:OE2 | 1.77 | 1.02 |
| 3:L9:14:LEU:CD1 | 11:a9:358:PRO:CG | 2.30 | 1.02 |
| 4:M9:258:LYS:HG2 | 3:V9:111:ASN:ND2 | 1.75 | 1.02 |
| 5:Z8:41:GLN:CG | 12:Z8:301:CYC:HBB2 | 1.85 | 1.02 |
| 5:N1:1:MET:HA | 5:N1:1:MET:HE3 | 1.41 | 1.02 |
| 5:N1:21:ALA:HB2 | 5:N1:68:LEU:HD11 | 1.42 | 1.02 |
| 12:HA:202:CYC:C4B | 11:aA:474:PHE:CZ | 2.43 | 1.02 |
| 3:JA:78:ARG:NH1 | 11:aA:359:ASP:HA | 1.74 | 1.02 |
| 12:H3:202:CYC:O2A | 11:a9:776:TYR:HD2 | 1.42 | 1.02 |
| 3:B4:85:ASP:N | 12:B4:202:CYC:HAC1 | 1.75 | 1.02 |
| 3:B4:120:LEU:HD21 | 4:M4:52:LEU:HB3 | 1.41 | 1.02 |
| 3:U4:120:LEU:HD12 | 4:M4:254:LEU:HG | 1.36 | 1.02 |
| 1:d5:28:LYS:HZ2 | 1:n7:143:PRO:HG2 | 0.88 | 1.02 |
| 8:S5:14:GLU:HG2 | 10:j5:538:PHE:CZ | 1.94 | 1.02 |
| 1:b5:30:TYR:CZ | 10:k5:47:PHE:CZ | 2.47 | 1.02 |
| 1:b5:114:GLU:CG | 10:k5:491:THR:OG1 | 2.07 | 1.02 |
| 6:M6:127:SER:HB2 | 3:F6:84:ARG:CZ | 1.81 | 1.02 |
| 6:M6:127:SER:O | 12:F6:201:CYC:CBA | 2.06 | 1.02 |
| 10:j5:190:LEU:CB | 10:j5:194:CYS:SG | 2.46 | 1.02 |
| 12:j5:1202:CYC:HMD1 | 12:j5:1202:CYC:HC | 1.25 | 1.02 |
| 10:k5:931:VAL:CG2 | 1:D7:29:ALA:C | 2.33 | 1.02 |
| 8:S7:49:ARG:HD2 | 11:aA:550:PHE:CD1 | 1.94 | 1.02 |
| 12:H7:201:CYC:HMD1 | 12:H7:201:CYC:HC | 1.25 | 1.02 |
| 8:i7:25:ARG:HE | 8:s7:3:VAL:HA | 1.25 | 1.02 |
| 8:i7:92:VAL:HG23 | 8:i7:156:LEU:CD1 | 1.88 | 1.02 |
| 8:u7:103:PRO:CG | 1:v7:9:ILE:HD13 | 1.90 | 1.02 |
| 5:N9:1:MET:HA | 5:N9:1:MET:HE3 | 1.41 | 1.02 |
| 5:Z8:37:HIS:NE2 | 12:Z8:301:CYC:C2A | 2.21 | 1.02 |
| 3:J9:78:ARG:NH1 | 11:a9:359:ASP:HA | 1.75 | 1.02 |
| 2:IA:25:GLN:HE21 | 2:IA:25:GLN:HA | 1.25 | 1.01 |
| 3:JA:111:ASN:N | 11:aA:518:ALA:HB3 | 1.73 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:J3:84:ARG:HD2 | 11:a9:668:TYR:CD1 | 1.71 | 1.01 |
| 12:F3:201:CYC:CMA | 4:M3:36:TYR:O | 2.07 | 1.01 |
| 3:H4:80:ALA:HB1 | 3:H4:84:ARG:HH12 | 1.25 | 1.01 |
| 3:H4:111:ASN:ND2 | 11:aA:291:TYR:OH | 1.93 | 1.01 |
| 12:B5:201:CYC:HMD1 | 12:B5:201:CYC:HC | 1.25 | 1.01 |
| 1:D5:73:TYR:O | 1:D5:77:ARG:CD | 2.07 | 1.01 |
| 1:Z5:110:ASN:HD21 | 10:k5:451:LYS:HB2 | 1.18 | 1.01 |
| 12:Z5:201:CYC:HMD1 | 12:Z5:201:CYC:HC | 1.25 | 1.01 |
| 10:j5:136:VAL:CG1 | 10:j5:137:PRO:HD3 | 1.86 | 1.01 |
| 10:j5:275:THR:HG21 | 10:j5:286:VAL:HG13 | 1.41 | 1.01 |
| 10:j5:804:GLU:OE1 | 9:w7:30:LYS:HE3 | 1.59 | 1.01 |
| 10:k5:951:MET:CE | 10:k5:955:LEU:HG | 1.88 | 1.01 |
| 10:k5:1023:SER:OG | 12:k5:1202:CYC:O2A | 1.75 | 1.01 |
| 12:R7:201:CYC:HMD1 | 12:R7:201:CYC:HC | 1.25 | 1.01 |
| 12:J7:201:CYC:HMD1 | 12:J7:201:CYC:HC | 1.25 | 1.01 |
| 8:i7:46:ALA:CB | 8:i7:140:LEU:HD12 | 1.90 | 1.01 |
| 12:c7:201:CYC:HMD1 | 12:c7:201:CYC:HC | 1.18 | 1.01 |
| 8:q7:66:VAL:CG1 | 11:aA:61:TYR:CE1 | 2.43 | 1.01 |
| 2:X8:69:PRO:CD | 2:S9:42:ARG:HE | 1.73 | 1.01 |
| 2:N8:111:ALA:C | 5:Z8:34:LEU:HA | 1.85 | 1.01 |
| 3:Q8:102:ALA:HB3 | 3:Q8:166:LYS:HE2 | 1.38 | 1.01 |
| 2:I9:25:GLN:HA | 2:I9:25:GLN:HE21 | 1.25 | 1.01 |
| 4:MA:158:PHE:O | 3:VA:108:ARG:HG3 | 1.57 | 1.01 |
| 3:D4:14:LEU:HD13 | 3:Y4:125:ARG:HD2 | 1.02 | 1.01 |
| 3:B1:88:ILE:CG2 | 12:B1:202:CYC:HMB2 | 1.89 | 1.01 |
| 3:S4:82:CYS:HA | 12:S4:202:CYC:CAC | 1.89 | 1.01 |
| 4:M4:82:ILE:HD11 | 12:M4:301:CYC:O2D | 0.85 | 1.01 |
| 2:N4:14:SER:HB2 | 5:Z4:62:ARG:HD2 | 1.41 | 1.01 |
| 3:O4:111:ASN:O | 5:Z4:67:ILE:CG2 | 2.07 | 1.01 |
| 8:A5:106:GLU:OE1 | 10:k5:557:VAL:HG13 | 1.61 | 1.01 |
| 12:B5:201:CYC:CBA | 9:z5:26:THR:CG2 | 2.38 | 1.01 |
| 12:F5:201:CYC:HMD1 | 12:F5:201:CYC:HC | 1.25 | 1.01 |
| 12:P5:201:CYC:HMD1 | 12:P5:201:CYC:HC | 1.25 | 1.01 |
| 8:U5:102:THR:HB | 8:U5:103:PRO:CD | 1.88 | 1.01 |
| 1:X5:65:LEU:CD1 | 10:j5:706:PRO:HG3 | 1.89 | 1.01 |
| 1:Z5:67:ARG:NH2 | 10:k5:705:THR:OG1 | 1.93 | 1.01 |
| 10:j5:741:GLN:HG3 | 1:J7:77:ARG:HH22 | 0.85 | 1.01 |
| 10:k5:136:VAL:CG1 | 10:k5:137:PRO:HD3 | 1.86 | 1.01 |
| 10:k5:138:PRO:HB3 | 10:k5:201:VAL:CG1 | 1.90 | 1.01 |
| 8:Q7:25:ARG:HB2 | 8:C7:25:ARG:NH2 | 1.72 | 1.01 |
| 1:B7:140:LEU:HG | 11:a9:561:ALA:HB2 | 1.39 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:h7:54:GLU:O | 1:h7:58:LYS:HG3 | 1.60 | 1.01 |
| 8:i7:96:ILE:N | 8:i7:152:TYR:CE2 | 2.28 | 1.01 |
| 8:k7:64:ASP:HB3 | 11:a9:69:ARG:HH22 | 1.25 | 1.01 |
| 1:b7:54:GLU:O | 1:b7:58:LYS:HG3 | 1.60 | 1.01 |
| 8:c7:8:ILE:HG23 | 1:d7:94:TYR:CD1 | 1.96 | 1.01 |
| 2:E8:15:GLN:HG2 | 11:a9:163:ASP:HB2 | 1.39 | 1.01 |
| 8:o7:103:PRO:CG | 1:p7:9:ILE:HD13 | 1.90 | 1.01 |
| 3:F8:107:ASP:HA | 4:M8:8:SER:H | 1.19 | 1.01 |
| 3:F8:112:GLY:C | 3:F8:114:LYS:H | 1.60 | 1.01 |
| 4:M8:144:ARG:CG | 4:M8:204:ILE:HG21 | 1.90 | 1.01 |
| 3:O8:107:ASP:CG | 5:Z8:66:ARG:CB | 2.33 | 1.01 |
| 11:aA:668:TYR:OH | 2:K1:115:GLU:CG | 2.07 | 1.01 |
| 4:M1:158:PHE:CD1 | 3:Z1:108:ARG:CZ | 2.39 | 1.01 |
| 4:M1:252:LEU:CD1 | 12:X1:201:CYC:O1D | 2.09 | 1.01 |
| 3:DA:68:ARG:NH2 | 3:XA:68:ARG:NH1 | 2.06 | 1.01 |
| 4:M3:245:ASP:HB3 | 3:X3:108:ARG:O | 1.60 | 1.01 |
| 3:F4:77:ARG:HD2 | 11:aA:146:ARG:NH1 | 1.74 | 1.01 |
| 3:F4:113:LEU:CB | 4:M4:5:THR:CG2 | 2.11 | 1.01 |
| 3:H4:80:ALA:HB1 | 3:H4:84:ARG:NH1 | 1.75 | 1.01 |
| 4:M4:210:ILE:HD11 | 5:Z4:26:LEU:HD22 | 1.37 | 1.01 |
| 2:N4:111:ALA:C | 5:Z4:34:LEU:CD1 | 2.31 | 1.01 |
| 8:M5:110:ILE:HD12 | 10:k5:533:LEU:CD1 | 1.89 | 1.01 |
| 8:G5:12:ASP:OD1 | 1:H5:91:TYR:CE1 | 2.13 | 1.01 |
| 8:G5:61:ILE:CD1 | 8:o7:68:PRO:HD2 | 1.90 | 1.01 |
| 8:G5:61:ILE:HG13 | 8:o7:68:PRO:HD2 | 1.03 | 1.01 |
| 1:f5:19:LEU:CD1 | 10:j5:172:LEU:HD13 | 1.82 | 1.01 |
| 1:R5:106:GLU:CG | 10:k5:504:ASP:O | 2.08 | 1.01 |
| 10:j5:75:ILE:HG22 | 10:j5:139:ASP:OD2 | 1.60 | 1.01 |
| 10:j5:283:ARG:HB2 | 10:j5:284:PRO:HD2 | 1.39 | 1.01 |
| 8:C7:102:THR:HB | 8:C7:103:PRO:CD | 1.88 | 1.01 |
| 2:X8:57:GLN:OE1 | 3:T9:32:LYS:CE | 2.08 | 1.01 |
| 3:L8:82:CYS:SG | 12:a9:901:CYC:C1C | 2.48 | 1.01 |
| 4:M8:233:GLU:HG3 | 3:Y8:112:GLY:HA3 | 1.37 | 1.01 |
| 3:Q8:87:GLU:CD | 5:Z8:31:TRP:HH2 | 1.67 | 1.01 |
| 5:Z8:21:ALA:HB2 | 5:Z8:68:LEU:HD11 | 1.42 | 1.01 |
| 5:Z8:22:LEU:HD21 | 5:Z8:26:LEU:HD21 | 1.38 | 1.01 |
| 3:B9:26:GLN:O | 3:B9:30:LEU:HD13 | 1.59 | 1.01 |
| 11:a9:476:ARG:HH12 | 11:a9:488:SER:HB2 | 1.23 | 1.01 |
| 11:aA:55:ASP:CB | 11:aA:612:TYR:CB | 2.22 | 1.01 |
| 3:JA:111:ASN:O | 11:aA:518:ALA:CB | 2.09 | 1.01 |
| 3:JA:111:ASN:C | 11:aA:518:ALA:HB3 | 1.85 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:MA:58:TYR:CD1 | 11:aA:496:ARG:NH2 | 2.28 | 1.01 |
| 2:QA:18:PHE:CZ | 3:RA:48:ALA:HB1 | 1.94 | 1.01 |
| 2:SA:42:ARG:HE | 2:X4:69:PRO:HD2 | 1.22 | 1.01 |
| 3:TA:32:LYS:CE | 2:X4:57:GLN:OE1 | 2.08 | 1.01 |
| 3:B4:82:CYS:CA | 12:B4:202:CYC:C1C | 2.37 | 1.01 |
| 3:F4:115:GLU:HG2 | 4:M4:3:VAL:CG2 | 1.90 | 1.01 |
| 12:L4:202:CYC:HBB2 | 11:aA:245:ALA:HB2 | 1.40 | 1.01 |
| 4:M4:127:SER:O | 4:M4:130:SER:OG | 1.77 | 1.01 |
| 4:M4:211:GLN:O | 5:Z4:28:HIS:CE1 | 2.14 | 1.01 |
| 3:Q4:124:THR:HB | 3:Q4:171:ILE:O | 1.60 | 1.01 |
| 5:Z4:1:MET:HA | 5:Z4:1:MET:HE3 | 1.41 | 1.01 |
| 8:G5:100:ASP:OD1 | 8:S5:20:PRO:CB | 2.07 | 1.01 |
| 1:T5:110:ASN:HD21 | 10:j5:692:LEU:HB2 | 1.21 | 1.01 |
| 12:X5:201:CYC:HMD1 | 12:X5:201:CYC:HC | 1.24 | 1.01 |
| 10:k5:1152:TYR:HD2 | 8:G7:68:PRO:HG3 | 0.84 | 1.01 |
| 12:F7:201:CYC:HMD1 | 12:F7:201:CYC:HC | 1.25 | 1.01 |
| 12:T7:201:CYC:HMD1 | 12:T7:201:CYC:HC | 1.25 | 1.01 |
| 8:c7:46:ALA:CB | 8:c7:140:LEU:HD12 | 1.90 | 1.01 |
| 4:M8:127:SER:HB3 | 12:M8:302:CYC:HMA3 | 1.02 | 1.01 |
| 4:M8:197:ASP:HB3 | 5:Z8:52:ARG:HG2 | 1.38 | 1.01 |
| 3:Q8:102:ALA:HB1 | 3:Q8:166:LYS:CE | 1.75 | 1.01 |
| 12:J9:202:CYC:CGA | 11:a9:511:LYS:CD | 2.39 | 1.01 |
| 11:aA:666:ASN:HB2 | 12:aA:901:CYC:HMA2 | 1.40 | 1.01 |
| 11:aA:776:TYR:N | 12:H1:201:CYC:CBA | 2.19 | 1.01 |
| 5:N1:22:LEU:HD21 | 5:N1:26:LEU:HD21 | 1.38 | 1.01 |
| 1:Z:110:ASN:OD1 | 10:j5:462:TYR:CZ | 2.12 | 1.01 |
| 2:EA:115:GLU:OE2 | 4:MA:33:LEU:CD2 | 2.09 | 1.01 |
| 5:NA:21:ALA:HB2 | 5:NA:68:LEU:HD11 | 1.42 | 1.01 |
| 3:J3:84:ARG:NH2 | 11:a9:670:LEU:HA | 1.76 | 1.01 |
| 3:L2:75:PRO:HG2 | 3:L2:78:ARG:CB | 1.90 | 1.01 |
| 2:A3:16:GLY:CA | 11:a9:677:GLN:NE2 | 2.22 | 1.01 |
| 3:B4:85:ASP:CB | 12:B4:202:CYC:C3C | 2.10 | 1.01 |
| 3:L3:84:ARG:CG | 11:a9:742:GLN:OE1 | 2.07 | 1.01 |
| 3:S4:120:LEU:HD22 | 12:S4:202:CYC:HBD1 | 1.03 | 1.01 |
| 10:j5:66:MET:HA | 10:j5:66:MET:HE3 | 1.39 | 1.01 |
| 10:j5:275:THR:HG21 | 10:j5:286:VAL:CG1 | 1.91 | 1.01 |
| 10:k5:192:LYS:HA | 10:k5:192:LYS:NZ | 1.76 | 1.01 |
| 10:k5:546:PHE:HE1 | 10:k5:561:GLU:CD | 1.68 | 1.01 |
| 12:k5:1203:CYC:HMD1 | 12:k5:1203:CYC:HC | 1.24 | 1.01 |
| 12:B7:201:CYC:HMD1 | 12:B7:201:CYC:HC | 1.25 | 1.01 |
| 2:X8:74:TYR:OH | 2:S9:35:THR:O | 1.79 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:L8:68:ARG:HB2 | 11:a9:82:GLN:H | 0.88 | 1.01 |
| 4:M8:127:SER:CB | 12:M8:302:CYC:HMA3 | 1.78 | 1.01 |
| 4:M9:58:TYR:CE2 | 11:a9:496:ARG:CZ | 2.44 | 1.01 |
| 2:K9:15:GLN:HB3 | 11:a9:393:ARG:HH12 | 1.16 | 1.01 |
| 11:a9:245:ALA:HB2 | 12:a9:901:CYC:C4B | 1.90 | 1.01 |
| 11:a9:275:THR:O | 11:a9:278:LEU:CD1 | 2.08 | 1.01 |
| 4:M1:245:ASP:HB3 | 3:X1:108:ARG:O | 1.60 | 1.01 |
| 3:HA:119:ALA:CA | 8:S7:49:ARG:HH12 | 1.73 | 1.00 |
| 4:MA:158:PHE:O | 3:VA:108:ARG:CG | 2.08 | 1.00 |
| 5:N3:21:ALA:HB2 | 5:N3:68:LEU:HD11 | 1.42 | 1.00 |
| 3:F4:108:ARG:CD | 4:M4:9:GLN:HG3 | 1.91 | 1.00 |
| 2:N4:112:GLY:N | 5:Z4:34:LEU:CB | 2.12 | 1.00 |
| 1:B5:14:VAL:HG12 | 10:k5:554:ASN:O | 1.58 | 1.00 |
| 1:B5:107:ARG:CZ | 9:z5:21:ARG:HD3 | 1.91 | 1.00 |
| 12:P7:201:CYC:HMD1 | 12:P7:201:CYC:HC | 1.25 | 1.00 |
| 1:R7:49:THR:CG2 | 8:C7:161:GLN:HG2 | 1.91 | 1.00 |
| 1:B7:136:VAL:CG1 | 11:a9:563:PHE:CE2 | 2.43 | 1.00 |
| 8:U7:52:LYS:HE3 | 11:a9:29:ARG:HH12 | 0.86 | 1.00 |
| 12:X7:201:CYC:HMD1 | 12:X7:201:CYC:HC | 1.24 | 1.00 |
| 8:a7:48:GLU:CA | 11:a9:318:TRP:CH2 | 2.41 | 1.00 |
| 8:c7:11:ALA:CB | 1:d7:94:TYR:CE1 | 2.43 | 1.00 |
| 8:c7:96:ILE:N | 8:c7:152:TYR:CE2 | 2.28 | 1.00 |
| 12:d7:201:CYC:HBB2 | 9:x7:42:GLN:OE1 | 1.61 | 1.00 |
| 8:o7:27:LYS:HD2 | 1:p7:35:ALA:CB | 1.91 | 1.00 |
| 8:u7:27:LYS:CD | 1:v7:35:ALA:CB | 2.40 | 1.00 |
| 8:u7:29:PHE:CZ | 1:v7:31:PHE:CZ | 2.50 | 1.00 |
| 4:M9:58:TYR:CD1 | 11:a9:496:ARG:NH2 | 2.28 | 1.00 |
| 3:J9:88:ILE:HD11 | 11:a9:512:TYR:CD1 | 1.96 | 1.00 |
| 2:K9:15:GLN:CB | 11:a9:393:ARG:HH11 | 1.66 | 1.00 |
| 11:aA:81:ASP:OD1 | 11:aA:81:ASP:O | 1.78 | 1.00 |
| 1:Z:161:SER:OG | 1:X5:14:VAL:HG21 | 1.59 | 1.00 |
| 3:LA:14:LEU:CD1 | 11:aA:358:PRO:CG | 2.31 | 1.00 |
| 4:MA:58:TYR:CE2 | 11:aA:496:ARG:CZ | 2.44 | 1.00 |
| 2:S1:16:GLY:HA2 | 5:N1:31:TRP:CD1 | 1.93 | 1.00 |
| 6:M2:39:ARG:NH1 | 8:O5:59:PHE:CD2 | 2.30 | 1.00 |
| 3:Z3:111:ASN:ND2 | 4:M3:258:LYS:NZ | 2.05 | 1.00 |
| 3:B4:108:ARG:O | 4:M4:61:ASN:HB3 | 1.60 | 1.00 |
| 3:L3:119:ALA:HB3 | 11:a9:813:PRO:HB3 | 1.38 | 1.00 |
| 3:B1:88:ILE:HG23 | 12:B1:202:CYC:HAB2 | 1.44 | 1.00 |
| 3:F4:115:GLU:C | 4:M4:3:VAL:HG11 | 1.87 | 1.00 |
| 2:I4:112:GLY:HA2 | 11:aA:133:LEU:HD21 | 1.44 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:Z4:21:ALA:HB2 | 5:Z4:68:LEU:HD11 | 1.42 | 1.00 |
| 8:A5:122:PRO:O | 12:A5:201:CYC:HMC3 | 1.61 | 1.00 |
| 8:Y5:9:VAL:HG11 | 10:k5:344:ARG:NH2 | 1.74 | 1.00 |
| 10:j5:138:PRO:HB3 | 10:j5:201:VAL:CG1 | 1.90 | 1.00 |
| 10:j5:192:LYS:HA | 10:j5:192:LYS:NZ | 1.76 | 1.00 |
| 10:k5:1025:LEU:HD23 | 10:k5:1030:ILE:HG23 | 1.43 | 1.00 |
| 12:j7:201:CYC:CBB | 9:y7:42:GLN:OE1 | 2.10 | 1.00 |
| 8:o7:27:LYS:CD | 1:p7:35:ALA:CB | 2.40 | 1.00 |
| 8:u7:27:LYS:HD2 | 1:v7:35:ALA:CB | 1.90 | 1.00 |
| 2:I8:112:GLY:HA2 | 11:a9:133:LEU:HD21 | 1.42 | 1.00 |
| 11:aA:312:ASP:O | 11:aA:315:LEU:N | 1.82 | 1.00 |
| 11:aA:667:THR:CG2 | 12:aA:901:CYC:CBA | 1.98 | 1.00 |
| 1:A:161:SER:CB | 1:R5:14:VAL:CB | 2.25 | 1.00 |
| 3:HA:113:LEU:CD2 | 12:HA:202:CYC:HMB1 | 1.90 | 1.00 |
| 3:JA:65:ASP:CB | 11:aA:354:VAL:CG2 | 2.39 | 1.00 |
| 3:LA:52:ILE:HD13 | 3:LA:87:GLU:CB | 1.85 | 1.00 |
| 5:NA:1:MET:HE3 | 5:NA:1:MET:HA | 1.41 | 1.00 |
| 3:J3:111:ASN:HD21 | 11:a9:631:GLY:CA | 1.75 | 1.00 |
| 3:B1:86:MET:CG | 12:B1:202:CYC:HBC1 | 1.92 | 1.00 |
| 4:M4:29:PRO:HG3 | 11:aA:226:PHE:HA | 1.43 | 1.00 |
| 4:M4:144:ARG:CG | 4:M4:204:ILE:HG21 | 1.90 | 1.00 |
| 8:K5:20:PRO:HG3 | 8:U5:151:PHE:O | 1.61 | 1.00 |
| 1:Z5:28:LYS:CD | 1:t7:143:PRO:HB3 | 1.90 | 1.00 |
| 3:L6:125:ARG:CD | 1:b7:69:GLY:HA3 | 1.84 | 1.00 |
| 10:j5:1081:VAL:HG11 | 12:r7:201:CYC:HMA2 | 1.41 | 1.00 |
| 10:k5:75:ILE:HG22 | 10:k5:139:ASP:OD2 | 1.60 | 1.00 |
| 10:k5:275:THR:HG21 | 10:k5:286:VAL:CG1 | 1.91 | 1.00 |
| 8:Q7:12:ASP:C | 9:z7:46:LYS:NZ | 2.18 | 1.00 |
| 1:f7:67:ARG:CD | 11:aA:311:LEU:CD2 | 2.29 | 1.00 |
| 8:o7:29:PHE:CZ | 1:p7:31:PHE:CZ | 2.49 | 1.00 |
| 3:F8:77:ARG:HD2 | 11:a9:146:ARG:NH1 | 1.76 | 1.00 |
| 3:F8:107:ASP:CA | 4:M8:6:THR:O | 2.09 | 1.00 |
| 3:F8:109:CYS:C | 4:M8:6:THR:CG2 | 2.34 | 1.00 |
| 3:L8:82:CYS:HB2 | 12:a9:901:CYC:CMD | 1.91 | 1.00 |
| 3:Q8:77:ARG:HA | 5:Z8:34:LEU:CB | 1.85 | 1.00 |
| 4:M9:158:PHE:O | 3:V9:108:ARG:HD3 | 1.59 | 1.00 |
| 3:Y8:87:GLU:CD | 3:Y8:91:ARG:NH2 | 2.17 | 1.00 |
| 3:F9:150:ARG:NH1 | 12:F9:302:CYC:OC | 1.93 | 1.00 |
| 3:J9:111:ASN:C | 11:a9:518:ALA:HB3 | 1.86 | 1.00 |
| 11:a9:81:ASP:OD1 | 11:a9:81:ASP:O | 1.78 | 1.00 |
| 11:aA:813:PRO:HB2 | 3:L1:119:ALA:HB2 | 1.03 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:A1:16:GLY:CA | 11:aA:677:GLN:NE2 | 2.24 | 1.00 |
| 4:M4:104:ALA:HB2 | 2:P4:14:SER:N | 1.76 | 1.00 |
| 3:Y4:89:ILE:CG2 | 3:Y4:92:TYR:CZ | 2.37 | 1.00 |
| 8:A5:103:PRO:HA | 10:k5:557:VAL:HG22 | 1.39 | 1.00 |
| 10:k5:929:PRO:HG2 | 1:D7:147:LYS:HG3 | 1.42 | 1.00 |
| 12:r7:201:CYC:HMD1 | 12:r7:201:CYC:HC | 1.24 | 1.00 |
| 3:H8:111:ASN:ND2 | 11:a9:291:TYR:OH | 1.93 | 1.00 |
| 3:H9:126:SER:HB3 | 12:H9:202:CYC:CMC | 1.91 | 1.00 |
| 2:G1:107:ASP:CA | 3:L1:77:ARG:NH2 | 2.25 | 1.00 |
| 11:a9:338:VAL:HG22 | 11:a9:340:PRO:HG3 | 1.42 | 1.00 |
| 3:HA:84:ARG:HA | 11:aA:478:HIS:NE2 | 1.71 | 1.00 |
| 4:MA:77:LEU:HD11 | 3:ZA:115:GLU:OE2 | 0.83 | 1.00 |
| 3:B4:86:MET:CA | 12:B4:202:CYC:HBC1 | 1.90 | 1.00 |
| 3:L4:71:GLY:N | 11:aA:82:GLN:CG | 2.24 | 1.00 |
| 3:Q4:102:ALA:CB | 3:Q4:166:LYS:CE | 2.32 | 1.00 |
| 1:R5:65:LEU:CD1 | 10:k5:706:PRO:HG3 | 1.92 | 1.00 |
| 8:W5:15:ALA:O | 1:X5:90:ARG:HD2 | 1.60 | 1.00 |
| 8:A7:56:ASP:OD1 | 11:aA:586:LEU:HD12 | 1.58 | 1.00 |
| 10:j5:1143:LEU:CD1 | 8:q7:106:GLU:HB2 | 1.92 | 1.00 |
| 10:k5:386:ILE:HG23 | 10:k5:387:VAL:H | 0.84 | 1.00 |
| 8:g7:48:GLU:CA | 11:aA:318:TRP:CH2 | 2.43 | 1.00 |
| 12:d7:201:CYC:C4B | 9:x7:38:PHE:CE1 | 2.44 | 1.00 |
| 8:q7:76:LYS:NZ | 11:aA:605:PRO:CB | 2.25 | 1.00 |
| 8:u7:23:LEU:HD22 | 1:v7:38:VAL:CB | 1.91 | 1.00 |
| 4:M9:33:LEU:CD2 | 2:E9:115:GLU:OE2 | 2.09 | 1.00 |
| 5:Z8:37:HIS:CE1 | 12:Z8:301:CYC:HB | 1.79 | 1.00 |
| 12:H9:202:CYC:C4B | 11:a9:474:PHE:CZ | 2.45 | 1.00 |
| 11:aA:803:ASN:CA | 3:J1:119:ALA:O | 2.07 | 1.00 |
| 11:aA:813:PRO:HB3 | 3:L1:119:ALA:HB3 | 1.40 | 1.00 |
| 3:S4:82:CYS:HA | 12:S4:202:CYC:HAC2 | 1.42 | 1.00 |
| 1:b5:18:TYR:CD1 | 10:k5:165:ARG:CD | 2.43 | 1.00 |
| 6:M6:271:VAL:HG11 | 1:d7:124:ALA:O | 1.61 | 1.00 |
| 12:k5:1204:CYC:HMD1 | 12:k5:1204:CYC:HC | 1.25 | 1.00 |
| 1:B7:140:LEU:CD1 | 11:a9:561:ALA:HB1 | 1.91 | 1.00 |
| 12:D7:201:CYC:HMD1 | 12:D7:201:CYC:HC | 1.25 | 1.00 |
| 12:V7:201:CYC:HMD1 | 12:V7:201:CYC:HC | 1.25 | 1.00 |
| 8:a7:52:LYS:HD2 | 11:a9:321:ALA:HB2 | 1.42 | 1.00 |
| 8:c7:15:ALA:CB | 1:d7:90:ARG:NH2 | 2.25 | 1.00 |
| 4:M8:214:GLY:N | 5:Z8:28:HIS:NE2 | 2.04 | 1.00 |
| 4:M9:38:PRO:O | 3:B9:116:THR:OG1 | 1.80 | 1.00 |
| 11:a9:275:THR:O | 11:a9:278:LEU:HD12 | 1.62 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:MA:1:MET:CG | 11:aA:422:SER:O | 2.10 | 1.00 |
| 4:MA:258:LYS:HG2 | 3:VA:111:ASN:ND2 | 1.75 | 1.00 |
| 5:NA:16:PHE:CZ | 3:TA:120:LEU:CD2 | 2.45 | 1.00 |
| 3:L3:119:ALA:HB2 | 11:a9:813:PRO:HB2 | 1.01 | 1.00 |
| 3:F4:109:CYS:N | 4:M4:6:THR:HG21 | 1.70 | 1.00 |
| 12:b5:201:CYC:HMD1 | 12:b5:201:CYC:HC | 1.25 | 1.00 |
| 10:k5:938:GLN:CD | 1:D7:28:LYS:CD | 2.33 | 1.00 |
| 8:i7:3:VAL:HG13 | 8:s7:25:ARG:HH22 | 1.25 | 1.00 |
| 8:a7:33:GLY:HA3 | 1:b7:31:PHE:CE2 | 1.97 | 1.00 |
| 8:u7:37:LEU:HD22 | 1:v7:24:LEU:HD22 | 1.00 | 1.00 |
| 11:aA:75:ALA:CB | 11:aA:81:ASP:CB | 2.19 | 1.00 |
| 4:M1:162:ASN:HB2 | 12:Z1:202:CYC:OB | 1.61 | 1.00 |
| 2:SA:39:GLU:HA | 2:X4:69:PRO:CB | 1.93 | 0.99 |
| 3:J3:84:ARG:CD | 11:a9:668:TYR:HB3 | 1.91 | 0.99 |
| 2:P4:19:LEU:CD2 | 3:Q4:95:TYR:CE1 | 2.43 | 0.99 |
| 8:M5:19:SER:HB3 | 8:A5:6:LYS:NZ | 1.76 | 0.99 |
| 8:M5:68:PRO:HB3 | 8:e5:59:PHE:HB2 | 1.43 | 0.99 |
| 8:A5:12:ASP:OD1 | 1:B5:91:TYR:CE1 | 2.13 | 0.99 |
| 1:d5:110:ASN:HD21 | 10:j5:451:LYS:HB2 | 1.27 | 0.99 |
| 8:U5:80:LEU:HG | 6:M6:28:ASN:HB2 | 1.37 | 0.99 |
| 12:V5:201:CYC:HMD1 | 12:V5:201:CYC:HC | 1.25 | 0.99 |
| 10:j5:1045:TYR:OH | 10:j5:1062:LEU:CD2 | 2.08 | 0.99 |
| 10:k5:136:VAL:CB | 10:k5:137:PRO:CD | 2.39 | 0.99 |
| 8:k7:76:LYS:HZ1 | 11:a9:605:PRO:CB | 1.75 | 0.99 |
| 8:c7:47:ARG:HD3 | 1:d7:18:TYR:CE1 | 1.96 | 0.99 |
| 3:B8:119:ALA:HB2 | 4:M8:69:ILE:CG2 | 1.92 | 0.99 |
| 12:D8:202:CYC:CBA | 4:M8:35:THR:CA | 2.39 | 0.99 |
| 12:D8:202:CYC:CGA | 4:M8:35:THR:HB | 1.91 | 0.99 |
| 3:F8:115:GLU:OE2 | 4:M8:3:VAL:CG2 | 2.09 | 0.99 |
| 3:Q8:72:ASN:ND2 | 12:Z8:301:CYC:HBD2 | 1.74 | 0.99 |
| 4:M9:1:MET:CG | 11:a9:422:SER:O | 2.10 | 0.99 |
| 5:N9:16:PHE:CZ | 3:T9:120:LEU:CD2 | 2.45 | 0.99 |
| 11:aA:631:GLY:CA | 3:J1:111:ASN:HD21 | 1.74 | 0.99 |
| 11:aA:742:GLN:OE1 | 3:L1:84:ARG:CG | 2.09 | 0.99 |
| 3:LA:120:LEU:HD22 | 11:aA:538:ARG:HB2 | 1.43 | 0.99 |
| 4:MA:158:PHE:O | 3:VA:108:ARG:HD3 | 1.59 | 0.99 |
| 10:k5:966:SER:HA | 1:p7:14:VAL:HG13 | 1.40 | 0.99 |
| 1:p7:140:LEU:HD12 | 11:a9:342:ARG:HD3 | 1.40 | 0.99 |
| 2:N8:115:GLU:HG3 | 5:Z8:32:PRO:HG2 | 1.00 | 0.99 |
| 12:L9:202:CYC:O1D | 11:a9:538:ARG:HB3 | 1.62 | 0.99 |
| 3:JA:88:ILE:HD11 | 11:aA:512:TYR:CD1 | 1.97 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:B4:119:ALA:HB2 | 4:M4:69:ILE:CG2 | 1.90 | 0.99 |
| 4:M4:217:VAL:CG2 | 5:Z4:30:PRO:CB | 2.40 | 0.99 |
| 1:T5:53:LYS:HZ2 | 8:U5:120:GLN:CG | 1.75 | 0.99 |
| 10:j5:1125:ARG:NH2 | 1:t7:114:GLU:CB | 2.25 | 0.99 |
| 10:k5:1151:GLN:O | 1:p7:122:PRO:HB2 | 1.62 | 0.99 |
| 3:B8:81:ALA:CA | 12:B8:202:CYC:HMD3 | 1.92 | 0.99 |
| 4:M8:214:GLY:CA | 5:Z8:28:HIS:CG | 2.44 | 0.99 |
| 2:N8:14:SER:CB | 5:Z8:62:ARG:CD | 2.34 | 0.99 |
| 2:K9:15:GLN:HB3 | 11:a9:393:ARG:NH1 | 1.68 | 0.99 |
| 11:aA:746:TYR:HB3 | 2:K1:14:SER:CB | 1.92 | 0.99 |
| 11:aA:798:SER:HB3 | 12:aA:901:CYC:HAA1 | 1.44 | 0.99 |
| 3:F4:109:CYS:N | 4:M4:6:THR:HG22 | 1.68 | 0.99 |
| 12:L5:201:CYC:HMD1 | 12:L5:201:CYC:HC | 1.25 | 0.99 |
| 8:Q5:15:ALA:O | 1:R5:90:ARG:HD2 | 1.60 | 0.99 |
| 4:M9:77:LEU:HD11 | 3:Z9:115:GLU:OE2 | 0.83 | 0.99 |
| 11:aA:275:THR:O | 11:aA:278:LEU:HD12 | 1.62 | 0.99 |
| 11:aA:476:ARG:HH12 | 11:aA:488:SER:HB2 | 1.23 | 0.99 |
| 2:IA:37:SER:HA | 2:IA:97:LEU:HD21 | 1.41 | 0.99 |
| 4:M3:252:LEU:CD1 | 12:X3:201:CYC:O1D | 2.09 | 0.99 |
| 3:B1:127:VAL:HA | 12:B1:202:CYC:HMC1 | 1.43 | 0.99 |
| 8:A5:121:THR:HG23 | 12:A5:201:CYC:NC | 1.78 | 0.99 |
| 1:f5:18:TYR:CD2 | 10:j5:165:ARG:HG3 | 1.97 | 0.99 |
| 8:i7:43:LEU:HD11 | 8:i7:141:LEU:HD11 | 1.45 | 0.99 |
| 8:k7:68:PRO:CG | 11:a9:334:LYS:HD3 | 1.91 | 0.99 |
| 12:p7:201:CYC:HMD1 | 12:p7:201:CYC:HC | 1.24 | 0.99 |
| 3:L8:68:ARG:HB3 | 11:a9:81:ASP:CA | 1.92 | 0.99 |
| 4:M8:138:SER:OG | 4:M8:215:GLU:OE2 | 1.79 | 0.99 |
| 3:Q8:82:CYS:HA | 12:Z8:301:CYC:HAC2 | 1.39 | 0.99 |
| 11:aA:631:GLY:C | 3:J1:111:ASN:HD21 | 1.69 | 0.99 |
| 11:aA:668:TYR:CE2 | 3:J1:80:ALA:HB1 | 1.97 | 0.99 |
| 2:G3:107:ASP:CA | 3:L3:77:ARG:NH2 | 2.24 | 0.99 |
| 3:U4:115:GLU:HB2 | 4:M4:74:LEU:CD1 | 1.72 | 0.99 |
| 3:F4:115:GLU:CB | 4:M4:3:VAL:CG1 | 2.40 | 0.99 |
| 1:L5:119:LEU:HD21 | 10:j5:546:PHE:HD2 | 1.24 | 0.99 |
| 8:O5:76:LYS:CG | 8:O5:77:MET:CE | 2.36 | 0.99 |
| 8:O5:151:PHE:HB3 | 8:E5:20:PRO:HB3 | 1.40 | 0.99 |
| 8:o7:23:LEU:HD22 | 1:p7:38:VAL:CB | 1.91 | 0.99 |
| 8:o7:23:LEU:CD2 | 1:p7:38:VAL:HG13 | 1.92 | 0.99 |
| 2:K9:25:GLN:O | 2:K9:26:ALA:C | 1.98 | 0.99 |
| 11:aA:275:THR:O | 11:aA:278:LEU:CD1 | 2.08 | 0.99 |
| 11:aA:476:ARG:HH12 | 11:aA:488:SER:CB | 1.71 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:F2:78:ARG:HD3 | 12:F2:201:CYC:CGD | 1.92 | 0.99 |
| 3:J3:111:ASN:HD21 | 11:a9:631:GLY:C | 1.70 | 0.99 |
| 3:H2:77:ARG:NH1 | 6:M2:117:MET:HE3 | 1.56 | 0.99 |
| 12:L4:202:CYC:C4B | 11:aA:239:TYR:CD1 | 2.45 | 0.99 |
| 2:N4:111:ALA:HB3 | 5:Z4:34:LEU:HD11 | 1.40 | 0.99 |
| 8:K5:24:ASP:OD2 | 8:U5:148:GLU:OE2 | 1.80 | 0.99 |
| 8:G5:121:THR:HG23 | 12:G5:201:CYC:NC | 1.78 | 0.99 |
| 12:R5:201:CYC:HBB2 | 10:k5:520:ARG:NE | 1.76 | 0.99 |
| 10:k5:1077:ILE:O | 12:k5:1203:CYC:HBA2 | 1.52 | 0.99 |
| 12:h7:201:CYC:HMD1 | 12:h7:201:CYC:HC | 1.25 | 0.99 |
| 12:f7:201:CYC:HMD1 | 12:f7:201:CYC:HC | 1.24 | 0.99 |
| 5:Z8:37:HIS:CE1 | 12:Z8:301:CYC:C3A | 2.44 | 0.99 |
| 3:J9:88:ILE:HD13 | 11:a9:512:TYR:CZ | 1.96 | 0.99 |
| 3:J9:111:ASN:O | 11:a9:518:ALA:CB | 2.10 | 0.99 |
| 5:NA:70:ILE:HG22 | 3:TA:119:ALA:HB2 | 1.42 | 0.99 |
| 2:SA:42:ARG:HD2 | 2:X4:69:PRO:O | 1.60 | 0.99 |
| 12:P1:201:CYC:HAA1 | 4:M1:134:ASN:CB | 1.93 | 0.99 |
| 12:Z3:201:CYC:OB | 4:M3:162:ASN:HB2 | 1.61 | 0.99 |
| 4:M3:113:ILE:CD1 | 4:M3:143:VAL:HG13 | 1.93 | 0.99 |
| 8:M5:110:ILE:HD11 | 10:k5:533:LEU:HD11 | 1.40 | 0.99 |
| 1:d5:83:ARG:NH1 | 10:j5:379:PHE:CE2 | 2.30 | 0.99 |
| 8:Q5:11:ALA:CB | 1:R5:94:TYR:CZ | 2.45 | 0.99 |
| 10:k5:1150:TYR:HE1 | 11:a9:38:VAL:HG22 | 1.07 | 0.99 |
| 1:p7:136:VAL:CG1 | 11:a9:342:ARG:HH12 | 1.74 | 0.99 |
| 8:u7:30:VAL:HA | 1:v7:31:PHE:CD1 | 1.97 | 0.99 |
| 2:N8:115:GLU:CD | 5:Z8:32:PRO:CD | 2.36 | 0.99 |
| 5:N9:1:MET:CG | 3:R9:119:ALA:HB3 | 1.87 | 0.99 |
| 11:a9:99:ALA:HB3 | 11:a9:100:PRO:HD2 | 1.44 | 0.99 |
| 12:A:201:CYC:HMD1 | 12:A:201:CYC:HC | 1.25 | 0.99 |
| 3:J3:14:LEU:HD21 | 11:a9:622:ALA:H | 1.19 | 0.99 |
| 4:M3:51:ARG:NH2 | 11:a9:694:ARG:HH12 | 1.55 | 0.99 |
| 4:M3:232:VAL:CG1 | 3:V3:111:ASN:O | 2.11 | 0.99 |
| 4:M4:138:SER:OG | 4:M4:215:GLU:OE2 | 1.79 | 0.99 |
| 8:W5:16:ARG:HA | 1:X5:90:ARG:HH11 | 0.91 | 0.99 |
| 1:X5:106:GLU:CG | 10:j5:504:ASP:O | 2.10 | 0.99 |
| 8:a5:29:PHE:CE1 | 8:a5:99:GLY:HA3 | 1.98 | 0.99 |
| 8:I7:161:GLN:HG2 | 1:X7:49:THR:HG21 | 1.43 | 0.99 |
| 12:N7:201:CYC:HMD1 | 12:N7:201:CYC:HC | 1.25 | 0.99 |
| 4:M8:92:GLU:HG2 | 4:M8:217:VAL:HG22 | 1.41 | 0.99 |
| 11:aA:338:VAL:HG22 | 11:aA:340:PRO:HG3 | 1.42 | 0.99 |
| 3:BA:26:GLN:O | 3:BA:30:LEU:HD13 | 1.59 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 12:JA:202:CYC:CGA | 11:aA:511:LYS:CD | 2.39 | 0.99 |
| 6:M2:39:ARG:NE | 8:O5:66:VAL:CG1 | 2.24 | 0.99 |
| 4:M4:141:GLU:OE2 | 4:M4:145:LEU:HG | 1.59 | 0.99 |
| 1:N5:53:LYS:HZ2 | 8:O5:120:GLN:CD | 1.70 | 0.99 |
| 8:Q5:12:ASP:HA | 1:R5:94:TYR:CE2 | 1.95 | 0.99 |
| 2:N8:115:GLU:CB | 5:Z8:32:PRO:CB | 2.35 | 0.99 |
| 3:Q8:102:ALA:HB1 | 3:Q8:166:LYS:CD | 1.92 | 0.99 |
| 3:J9:65:ASP:CB | 11:a9:354:VAL:CG2 | 2.39 | 0.99 |
| 3:J9:108:ARG:O | 11:a9:517:ALA:HA | 1.63 | 0.99 |
| 3:TA:21:GLU:HB3 | 2:R4:64:PRO:CG | 1.93 | 0.98 |
| 3:L2:65:ASP:CG | 1:h7:64:ASP:OD2 | 2.06 | 0.98 |
| 2:A4:63:PHE:O | 2:A4:66:LEU:HG | 1.63 | 0.98 |
| 2:N4:111:ALA:CB | 5:Z4:34:LEU:CD1 | 2.30 | 0.98 |
| 12:D5:201:CYC:HMD1 | 12:D5:201:CYC:HC | 1.25 | 0.98 |
| 8:U5:29:PHE:CE1 | 8:U5:99:GLY:HA3 | 1.98 | 0.98 |
| 6:M6:53:LEU:HD21 | 8:c7:80:LEU:HG | 1.41 | 0.98 |
| 8:i7:47:ARG:HD2 | 1:j7:18:TYR:CE1 | 1.96 | 0.98 |
| 8:u7:23:LEU:CD2 | 1:v7:38:VAL:HG13 | 1.92 | 0.98 |
| 11:a9:454:LEU:CD2 | 11:a9:535:ASP:OD2 | 2.11 | 0.98 |
| 2:K3:15:GLN:HA | 11:a9:745:GLY:CA | 1.91 | 0.98 |
| 3:F4:108:ARG:HH21 | 4:M4:9:GLN:HG2 | 1.02 | 0.98 |
| 12:N5:201:CYC:HMD1 | 12:N5:201:CYC:HC | 1.25 | 0.98 |
| 1:R5:65:LEU:HD12 | 10:k5:706:PRO:CG | 1.92 | 0.98 |
| 9:i5:6:LYS:HB3 | 9:i5:55:LYS:CA | 1.93 | 0.98 |
| 10:j5:362:LYS:CE | 10:j5:363:HIS:CD2 | 2.46 | 0.98 |
| 10:j5:386:ILE:HG23 | 10:j5:387:VAL:H | 0.84 | 0.98 |
| 10:j5:1155:ARG:HB3 | 10:j5:1155:ARG:HH21 | 1.26 | 0.98 |
| 10:k5:934:ALA:CB | 1:D7:32:THR:HG23 | 1.87 | 0.98 |
| 12:L7:201:CYC:HMD1 | 12:L7:201:CYC:HC | 1.24 | 0.98 |
| 8:g7:52:LYS:HD2 | 11:aA:321:ALA:HB2 | 1.43 | 0.98 |
| 2:A8:63:PHE:O | 2:A8:66:LEU:HG | 1.63 | 0.98 |
| 3:U8:112:GLY:HA2 | 4:M8:74:LEU:HD21 | 1.00 | 0.98 |
| 2:X8:108:TYR:CZ | 4:M8:273:ILE:HD12 | 1.98 | 0.98 |
| 12:H8:201:CYC:OB | 11:a9:129:ASN:ND2 | 1.95 | 0.98 |
| 2:N8:14:SER:HB3 | 5:Z8:62:ARG:HE | 1.22 | 0.98 |
| 3:L9:52:ILE:HD13 | 3:L9:87:GLU:HB2 | 0.99 | 0.98 |
| 3:JA:88:ILE:HD13 | 11:aA:512:TYR:CZ | 1.98 | 0.98 |
| 4:MA:274:VAL:C | 3:VA:77:ARG:NE | 2.22 | 0.98 |
| 5:N3:15:LEU:O | 5:N3:73:GLY:N | 1.96 | 0.98 |
| 5:N3:62:ARG:HH21 | 2:Q3:14:SER:CB | 1.72 | 0.98 |
| 3:L4:68:ARG:HB3 | 11:aA:81:ASP:HA | 1.41 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:G5:25:ARG:HH21 | 8:S5:25:ARG:HB3 | 1.28 | 0.98 |
| 12:T5:201:CYC:HMD1 | 12:T5:201:CYC:HC | 1.25 | 0.98 |
| 10:j5:1020:GLU:HG3 | 1:f7:87:TYR:CE1 | 1.98 | 0.98 |
| 10:j5:1025:LEU:HD22 | 10:j5:1035:PHE:HB2 | 1.45 | 0.98 |
| 10:k5:386:ILE:CD1 | 10:k5:395:SER:OG | 1.82 | 0.98 |
| 10:k5:1009:ALA:HB2 | 1:p7:87:TYR:CZ | 1.97 | 0.98 |
| 10:k5:1155:ARG:HB3 | 10:k5:1155:ARG:HH21 | 1.26 | 0.98 |
| 8:I7:29:PHE:CE1 | 8:I7:99:GLY:HA3 | 1.98 | 0.98 |
| 12:j7:201:CYC:HMD1 | 12:j7:201:CYC:HC | 1.25 | 0.98 |
| 8:m7:29:PHE:CE1 | 8:m7:99:GLY:HA3 | 1.98 | 0.98 |
| 8:q7:79:ALA:CB | 11:aA:53:VAL:HG21 | 1.93 | 0.98 |
| 2:N8:63:PHE:O | 2:N8:66:LEU:HG | 1.63 | 0.98 |
| 2:N8:111:ALA:HB3 | 5:Z8:34:LEU:HG | 1.42 | 0.98 |
| 5:N9:21:ALA:HB2 | 5:N9:68:LEU:HD11 | 1.42 | 0.98 |
| 2:A9:63:PHE:O | 2:A9:66:LEU:HG | 1.63 | 0.98 |
| 2:QA:116:VAL:HG23 | 3:TA:80:ALA:HB2 | 1.45 | 0.98 |
| 6:M2:127:SER:CB | 3:F2:84:ARG:NH1 | 2.18 | 0.98 |
| 3:F4:115:GLU:CG | 4:M4:3:VAL:CG2 | 2.42 | 0.98 |
| 8:G5:122:PRO:O | 12:G5:201:CYC:HMC3 | 1.61 | 0.98 |
| 8:I5:29:PHE:CE1 | 8:I5:99:GLY:HA3 | 1.98 | 0.98 |
| 10:k5:362:LYS:CE | 10:k5:363:HIS:CD2 | 2.46 | 0.98 |
| 3:F6:78:ARG:HD3 | 12:F6:201:CYC:O2D | 0.81 | 0.98 |
| 8:C7:29:PHE:CE1 | 8:C7:99:GLY:HA3 | 1.98 | 0.98 |
| 8:u7:23:LEU:CD1 | 1:v7:38:VAL:HG13 | 1.93 | 0.98 |
| 2:X8:68:GLN:HG2 | 3:T9:25:ASN:OD1 | 1.61 | 0.98 |
| 4:M8:235:PHE:CB | 12:M8:301:CYC:HAA1 | 1.93 | 0.98 |
| 12:M8:301:CYC:H3C | 3:Y8:127:VAL:HG22 | 0.98 | 0.98 |
| 12:Z8:301:CYC:HMD1 | 12:Z8:301:CYC:HC | 1.29 | 0.98 |
| 5:NA:15:LEU:O | 5:NA:73:GLY:N | 1.96 | 0.98 |
| 2:OA:63:PHE:O | 2:OA:66:LEU:HG | 1.63 | 0.98 |
| 4:M4:144:ARG:NH2 | 5:Z4:59:ARG:HH12 | 1.55 | 0.98 |
| 4:M4:210:ILE:CD1 | 5:Z4:26:LEU:HD22 | 1.92 | 0.98 |
| 1:Z5:110:ASN:ND2 | 10:k5:451:LYS:CB | 2.22 | 0.98 |
| 10:j5:586:LEU:CD1 | 10:j5:607:LEU:HD23 | 1.94 | 0.98 |
| 12:h7:201:CYC:HBB2 | 9:y7:21:ARG:CD | 1.93 | 0.98 |
| 8:u7:17:TYR:CE2 | 1:v7:93:THR:CB | 2.47 | 0.98 |
| 3:U8:114:LYS:CE | 4:M8:13:LYS:CE | 2.41 | 0.98 |
| 3:L8:71:GLY:HA3 | 11:a9:82:GLN:HE21 | 1.26 | 0.98 |
| 3:L8:86:MET:HG2 | 12:a9:901:CYC:HBC1 | 1.42 | 0.98 |
| 4:M8:215:GLU:CD | 5:Z8:27:ALA:CB | 2.29 | 0.98 |
| 4:M1:232:VAL:CG1 | 3:V1:111:ASN:O | 2.11 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:N1:15:LEU:O | 5:N1:73:GLY:N | 1.96 | 0.98 |
| 4:MA:273:ILE:HD13 | 3:VA:75:PRO:CD | 1.94 | 0.98 |
| 3:B4:68:ARG:HH22 | 3:U4:68:ARG:NH2 | 1.57 | 0.98 |
| 8:Q5:16:ARG:HA | 1:R5:90:ARG:HH11 | 0.91 | 0.98 |
| 10:k5:277:ILE:O | 10:k5:284:PRO:HA | 1.63 | 0.98 |
| 8:Q7:13:ALA:N | 9:z7:46:LYS:HZ3 | 1.62 | 0.98 |
| 8:g7:33:GLY:HA3 | 1:h7:31:PHE:CE2 | 1.97 | 0.98 |
| 2:X8:69:PRO:O | 2:S9:42:ARG:HD2 | 1.60 | 0.98 |
| 4:M8:139:VAL:HG23 | 4:M8:216:ASN:HA | 1.41 | 0.98 |
| 3:Q8:84:ARG:HH11 | 5:Z8:29:HIS:CD2 | 1.80 | 0.98 |
| 4:M9:274:VAL:HG11 | 2:W9:111:ALA:CB | 1.94 | 0.98 |
| 3:LA:14:LEU:HD11 | 11:aA:358:PRO:HG3 | 1.02 | 0.98 |
| 4:MA:113:ILE:CD1 | 4:MA:143:VAL:HG13 | 1.93 | 0.98 |
| 2:SA:35:THR:O | 2:X4:74:TYR:OH | 1.79 | 0.98 |
| 12:B3:202:CYC:HMD1 | 12:B3:202:CYC:HC | 1.28 | 0.98 |
| 3:H4:119:ALA:CB | 11:aA:266:ASN:HB2 | 1.93 | 0.98 |
| 4:M4:235:PHE:CB | 12:M4:301:CYC:HAA1 | 1.93 | 0.98 |
| 5:Z4:15:LEU:O | 5:Z4:73:GLY:N | 1.96 | 0.98 |
| 8:C5:29:PHE:CE1 | 8:C5:99:GLY:HA3 | 1.98 | 0.98 |
| 8:e5:29:PHE:CE1 | 8:e5:99:GLY:HA3 | 1.98 | 0.98 |
| 10:j5:277:ILE:O | 10:j5:284:PRO:HA | 1.63 | 0.98 |
| 10:k5:965:GLN:H | 1:n7:69:GLY:HA2 | 0.96 | 0.98 |
| 11:aA:308:LEU:HD21 | 11:aA:315:LEU:HD12 | 1.40 | 0.98 |
| 3:BA:116:THR:OG1 | 4:MA:38:PRO:O | 1.80 | 0.98 |
| 3:HA:126:SER:HB3 | 12:HA:202:CYC:HMC3 | 0.99 | 0.98 |
| 12:JA:202:CYC:HBA2 | 11:aA:511:LYS:HD3 | 1.44 | 0.98 |
| 3:S4:82:CYS:CA | 12:S4:202:CYC:HAC2 | 1.92 | 0.98 |
| 2:E4:1:MET:H3 | 4:M4:10:ARG:NH2 | 1.46 | 0.98 |
| 4:M4:104:ALA:CA | 2:P4:14:SER:CB | 2.27 | 0.98 |
| 4:M4:201:ASP:OD2 | 5:Z4:52:ARG:NH1 | 1.96 | 0.98 |
| 1:L5:82:ILE:CD1 | 8:G5:118:SER:HB2 | 1.93 | 0.98 |
| 1:b5:114:GLU:HB3 | 10:k5:491:THR:CG2 | 1.94 | 0.98 |
| 10:j5:965:GLN:CA | 1:t7:69:GLY:HA2 | 1.92 | 0.98 |
| 10:k5:929:PRO:CG | 1:D7:147:LYS:HE2 | 1.94 | 0.98 |
| 8:o7:30:VAL:HA | 1:p7:31:PHE:CD1 | 1.97 | 0.98 |
| 1:v7:62:TYR:CB | 11:aA:602:PRO:CD | 2.27 | 0.98 |
| 2:N8:112:GLY:N | 5:Z8:34:LEU:HA | 1.76 | 0.98 |
| 3:Q8:85:ASP:HB2 | 12:Z8:301:CYC:HBC1 | 0.99 | 0.98 |
| 4:MA:267:LEU:HD12 | 3:VA:119:ALA:O | 1.64 | 0.98 |
| 5:NA:62:ARG:NE | 2:SA:14:SER:HA | 1.78 | 0.98 |
| 3:H3:68:ARG:CD | 11:a9:615:ARG:O | 2.11 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:Q4:104:VAL:HG23 | 3:Q4:105:LEU:HD12 | 1.43 | 0.98 |
| 8:U5:29:PHE:HE1 | 8:U5:99:GLY:HA3 | 1.29 | 0.98 |
| 10:j5:542:GLN:HE21 | 10:j5:560:VAL:HG13 | 1.28 | 0.98 |
| 10:j5:974:LEU:CD2 | 1:v7:1:MET:N | 2.23 | 0.98 |
| 10:k5:275:THR:HG21 | 10:k5:286:VAL:HG13 | 1.41 | 0.98 |
| 10:k5:1034:GLU:OE1 | 10:k5:1037:ARG:NH2 | 1.96 | 0.98 |
| 12:k5:1202:CYC:HMD1 | 12:k5:1202:CYC:HC | 1.25 | 0.98 |
| 8:I7:161:GLN:CG | 1:X7:49:THR:CG2 | 2.42 | 0.98 |
| 8:o7:23:LEU:CD1 | 1:p7:38:VAL:HG13 | 1.93 | 0.98 |
| 8:s7:29:PHE:CE1 | 8:s7:99:GLY:HA3 | 1.98 | 0.98 |
| 3:L9:14:LEU:HD11 | 11:a9:358:PRO:HG3 | 1.01 | 0.98 |
| 5:N9:15:LEU:O | 5:N9:73:GLY:N | 1.96 | 0.98 |
| 12:LA:202:CYC:O1D | 11:aA:538:ARG:HB3 | 1.62 | 0.98 |
| 2:SA:42:ARG:NE | 2:X4:69:PRO:HD2 | 1.77 | 0.98 |
| 3:TA:25:ASN:OD1 | 2:X4:68:GLN:HG2 | 1.61 | 0.98 |
| 2:G3:111:ALA:HB3 | 3:L3:77:ARG:CG | 1.94 | 0.98 |
| 2:U3:47:ASN:HB2 | 2:Q9:74:TYR:OH | 1.57 | 0.98 |
| 12:H4:201:CYC:HBB3 | 11:aA:259:ALA:HA | 1.46 | 0.98 |
| 8:A5:118:SER:HB2 | 1:F5:82:ILE:CD1 | 1.93 | 0.98 |
| 1:R5:124:ALA:HB3 | 1:Z5:64:ASP:CG | 1.87 | 0.98 |
| 9:i5:14:LEU:HD12 | 9:i5:15:LYS:N | 1.78 | 0.98 |
| 10:j5:136:VAL:CB | 10:j5:137:PRO:CD | 2.39 | 0.98 |
| 10:j5:612:ILE:H | 10:j5:612:ILE:HD12 | 1.28 | 0.98 |
| 10:k5:974:LEU:CG | 1:p7:1:MET:H1 | 1.75 | 0.98 |
| 10:k5:978:LEU:HD22 | 1:p7:107:ARG:HH21 | 1.23 | 0.98 |
| 1:B7:54:GLU:OE2 | 11:a9:563:PHE:HB2 | 1.62 | 0.98 |
| 8:a7:29:PHE:CE1 | 8:a7:99:GLY:HA3 | 1.98 | 0.98 |
| 4:M9:263:PRO:C | 3:V9:119:ALA:HB1 | 1.89 | 0.98 |
| 11:aA:798:SER:HG | 12:aA:901:CYC:HMA1 | 1.16 | 0.98 |
| 4:M1:113:ILE:CD1 | 4:M1:143:VAL:HG13 | 1.93 | 0.98 |
| 5:NA:1:MET:CG | 3:RA:119:ALA:HB3 | 1.87 | 0.97 |
| 2:K3:14:SER:CB | 11:a9:746:TYR:HB3 | 1.92 | 0.97 |
| 6:M2:28:ASN:HB2 | 8:O5:80:LEU:CG | 1.92 | 0.97 |
| 6:M2:127:SER:CB | 3:F2:84:ARG:NH2 | 2.20 | 0.97 |
| 4:M3:51:ARG:NH2 | 11:a9:694:ARG:HH22 | 1.57 | 0.97 |
| 3:L4:68:ARG:HD2 | 11:aA:81:ASP:HA | 1.43 | 0.97 |
| 8:G5:6:LYS:NZ | 8:S5:21:GLY:H | 1.61 | 0.97 |
| 8:O7:29:PHE:HE1 | 8:O7:99:GLY:HA3 | 1.29 | 0.97 |
| 8:g7:29:PHE:CE1 | 8:g7:99:GLY:HA3 | 1.98 | 0.97 |
| 8:U7:29:PHE:CE1 | 8:U7:99:GLY:HA3 | 1.98 | 0.97 |
| 8:c7:43:LEU:HD11 | 8:c7:141:LEU:HD11 | 1.45 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:o7:17:TYR:CE2 | 1:p7:93:THR:CB | 2.47 | 0.97 |
| 3:H8:119:ALA:CB | 11:a9:266:ASN:HB2 | 1.94 | 0.97 |
| 4:M8:232:VAL:CG2 | 4:M8:235:PHE:HE2 | 1.76 | 0.97 |
| 3:L9:52:ILE:HD13 | 3:L9:87:GLU:CB | 1.85 | 0.97 |
| 4:M9:160:THR:N | 3:V9:108:ARG:HG2 | 1.78 | 0.97 |
| 3:L2:77:ARG:NH2 | 6:M2:70:GLU:OE2 | 1.93 | 0.97 |
| 3:B4:108:ARG:CA | 4:M4:61:ASN:HA | 1.93 | 0.97 |
| 3:H4:84:ARG:CD | 11:aA:131:TYR:CD1 | 2.27 | 0.97 |
| 8:G5:121:THR:HG23 | 12:G5:201:CYC:C4C | 1.94 | 0.97 |
| 12:X5:201:CYC:HBB2 | 10:j5:520:ARG:NE | 1.78 | 0.97 |
| 9:z5:14:LEU:HD12 | 9:z5:15:LYS:N | 1.78 | 0.97 |
| 10:k5:970:GLY:HA3 | 1:n7:77:ARG:HH21 | 1.28 | 0.97 |
| 10:k5:1009:ALA:CB | 1:p7:87:TYR:HE1 | 1.77 | 0.97 |
| 3:B8:107:ASP:O | 4:M8:61:ASN:HA | 1.63 | 0.97 |
| 3:B8:119:ALA:HB1 | 4:M8:52:LEU:HD11 | 1.40 | 0.97 |
| 8:o7:37:LEU:HD22 | 1:p7:24:LEU:HD22 | 1.00 | 0.97 |
| 3:F8:108:ARG:O | 4:M8:6:THR:HG21 | 1.64 | 0.97 |
| 4:M8:225:LYS:CE | 3:Y8:81:ALA:HB2 | 1.93 | 0.97 |
| 3:Q8:84:ARG:CD | 5:Z8:31:TRP:CD1 | 2.47 | 0.97 |
| 4:M9:267:LEU:HD12 | 3:V9:119:ALA:O | 1.64 | 0.97 |
| 11:aA:454:LEU:CD2 | 11:aA:535:ASP:OD2 | 2.11 | 0.97 |
| 11:aA:643:LEU:HD21 | 11:aA:689:VAL:CG2 | 1.94 | 0.97 |
| 1:A:131:GLN:CG | 1:R5:17:LYS:HZ3 | 1.51 | 0.97 |
| 2:G2:113:LEU:HA | 3:L2:76:ASN:HD21 | 1.09 | 0.97 |
| 2:A3:63:PHE:O | 2:A3:66:LEU:HG | 1.63 | 0.97 |
| 3:D4:14:LEU:HD13 | 3:Y4:125:ARG:CD | 1.92 | 0.97 |
| 3:F4:115:GLU:CG | 4:M4:3:VAL:HG11 | 1.88 | 0.97 |
| 8:O5:29:PHE:HE1 | 8:O5:99:GLY:HA3 | 1.29 | 0.97 |
| 10:k5:931:VAL:HG22 | 1:D7:30:TYR:N | 1.77 | 0.97 |
| 8:i7:36:ARG:NH2 | 8:i7:152:TYR:OH | 1.97 | 0.97 |
| 9:y7:3:ARG:NE | 9:y7:67:VAL:HG13 | 1.79 | 0.97 |
| 3:O8:104:VAL:O | 5:Z8:61:LYS:CE | 2.11 | 0.97 |
| 4:M9:273:ILE:HD13 | 3:V9:75:PRO:CD | 1.94 | 0.97 |
| 3:H9:59:LEU:HD21 | 12:H9:202:CYC:HBC2 | 1.46 | 0.97 |
| 12:J9:202:CYC:HBA2 | 11:a9:511:LYS:HD3 | 1.44 | 0.97 |
| 11:a9:283:GLN:CB | 11:a9:284:PRO:HD3 | 1.91 | 0.97 |
| 3:JA:108:ARG:O | 11:aA:517:ALA:HA | 1.64 | 0.97 |
| 4:MA:263:PRO:C | 3:VA:119:ALA:HB1 | 1.89 | 0.97 |
| 3:H4:84:ARG:CD | 11:aA:131:TYR:CE2 | 2.47 | 0.97 |
| 3:Q4:120:LEU:CD1 | 5:Z4:40:SER:N | 2.25 | 0.97 |
| 8:O5:29:PHE:CE1 | 8:O5:99:GLY:HA3 | 1.98 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 5:Z4:26:LEU:CD2 | 5:Z4:63:ASN:HB3 | 1.95 | 0.97 |
| 6:M6:271:VAL:HG21 | 1:d7:127:VAL:HB | 1.44 | 0.97 |
| 10:k5:1153:VAL:HG21 | 1:p7:125:ALA:CB | 1.88 | 0.97 |
| 9:x7:3:ARG:NE | 9:x7:67:VAL:HG13 | 1.79 | 0.97 |
| 2:R8:64:PRO:CG | 3:T9:21:GLU:HB3 | 1.93 | 0.97 |
| 5:Z8:15:LEU:O | 5:Z8:73:GLY:N | 1.96 | 0.97 |
| 3:J9:65:ASP:HB3 | 11:a9:354:VAL:HG22 | 1.46 | 0.97 |
| 11:aA:708:HIS:HA | 3:L1:108:ARG:HE | 1.28 | 0.97 |
| 2:QA:119:THR:CB | 3:TA:83:LEU:CD1 | 2.31 | 0.97 |
| 2:A1:63:PHE:O | 2:A1:66:LEU:HG | 1.63 | 0.97 |
| 4:M4:128:ALA:C | 4:M4:142:PHE:HZ | 1.69 | 0.97 |
| 4:M4:232:VAL:CG2 | 4:M4:235:PHE:HE2 | 1.76 | 0.97 |
| 1:N5:53:LYS:NZ | 8:O5:120:GLN:CG | 2.28 | 0.97 |
| 8:G5:126:VAL:CG2 | 12:G5:201:CYC:H3C | 1.93 | 0.97 |
| 10:j5:938:GLN:OE1 | 1:J7:28:LYS:HG2 | 1.63 | 0.97 |
| 10:k5:930:LEU:HD13 | 1:D7:33:THR:HB | 1.44 | 0.97 |
| 2:A6:63:PHE:O | 2:A6:66:LEU:HG | 1.63 | 0.97 |
| 8:O7:29:PHE:CE1 | 8:O7:99:GLY:HA3 | 1.98 | 0.97 |
| 12:d7:201:CYC:HMD1 | 12:d7:201:CYC:HC | 1.25 | 0.97 |
| 3:Q8:87:GLU:OE1 | 5:Z8:31:TRP:HH2 | 1.14 | 0.97 |
| 4:M9:65:ARG:HD2 | 3:F9:111:ASN:ND2 | 1.80 | 0.97 |
| 5:Z8:37:HIS:CD2 | 12:Z8:301:CYC:C1B | 2.47 | 0.97 |
| 2:G1:111:ALA:HB3 | 3:L1:77:ARG:CG | 1.94 | 0.97 |
| 11:a9:585:GLU:O | 11:a9:588:VAL:O | 1.81 | 0.97 |
| 4:MA:160:THR:N | 3:VA:108:ARG:HG2 | 1.78 | 0.97 |
| 2:O1:63:PHE:O | 2:O1:66:LEU:HG | 1.63 | 0.97 |
| 3:B4:85:ASP:CB | 12:B4:202:CYC:H3C | 1.94 | 0.97 |
| 3:U4:115:GLU:OE2 | 4:M4:70:SER:HB2 | 1.63 | 0.97 |
| 3:F4:107:ASP:CA | 4:M4:8:SER:N | 2.26 | 0.97 |
| 4:M4:144:ARG:HH22 | 5:Z4:59:ARG:HH12 | 1.03 | 0.97 |
| 4:M4:214:GLY:HA2 | 5:Z4:28:HIS:CD2 | 1.98 | 0.97 |
| 3:Q4:72:ASN:O | 12:Z4:301:CYC:CMD | 2.13 | 0.97 |
| 8:A5:126:VAL:CG2 | 12:A5:201:CYC:H3C | 1.93 | 0.97 |
| 10:j5:1074:GLN:OE1 | 1:r7:119:LEU:HD21 | 1.65 | 0.97 |
| 8:O7:25:ARG:HH21 | 8:E7:25:ARG:HB3 | 0.82 | 0.97 |
| 1:h7:75:THR:HG22 | 8:i7:115:MET:CE | 1.94 | 0.97 |
| 12:b7:201:CYC:HC | 12:b7:201:CYC:HMD1 | 1.25 | 0.97 |
| 12:v7:201:CYC:HMD1 | 12:v7:201:CYC:HC | 1.25 | 0.97 |
| 4:M8:113:ILE:CD1 | 4:M8:143:VAL:HG13 | 1.93 | 0.97 |
| 4:M8:160:THR:CG2 | 4:M8:257:GLN:CB | 2.42 | 0.97 |
| 4:M9:258:LYS:HG2 | 3:V9:111:ASN:HD21 | 1.27 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:N9:54:LEU:HD13 | 3:T9:84:ARG:NH2 | 1.80 | 0.97 |
| 2:O9:63:PHE:O | 2:O9:66:LEU:HG | 1.63 | 0.97 |
| 3:J9:116:THR:HG23 | 11:a9:521:PHE:CD2 | 2.00 | 0.97 |
| 11:a9:643:LEU:HD21 | 11:a9:689:VAL:CG2 | 1.95 | 0.97 |
| 11:aA:31:SER:OG | 11:aA:34:ILE:CB | 2.13 | 0.97 |
| 11:aA:707:PHE:HZ | 2:K1:13:ASP:OD2 | 1.33 | 0.97 |
| 4:M1:160:THR:CG2 | 4:M1:257:GLN:CB | 2.42 | 0.97 |
| 3:H3:78:ARG:CZ | 11:a9:623:ASP:HB2 | 1.95 | 0.97 |
| 3:J3:77:ARG:CG | 2:K3:111:ALA:HB3 | 1.94 | 0.97 |
| 5:N3:31:TRP:HB3 | 5:N3:32:PRO:HD2 | 1.47 | 0.97 |
| 12:B1:202:CYC:HMD1 | 12:B1:202:CYC:HC | 1.28 | 0.97 |
| 3:L4:68:ARG:HG3 | 11:aA:81:ASP:N | 1.78 | 0.97 |
| 8:O5:76:LYS:HD2 | 8:O5:77:MET:HE1 | 1.44 | 0.97 |
| 10:j5:743:VAL:HG12 | 12:J7:201:CYC:O2D | 1.64 | 0.97 |
| 10:j5:1025:LEU:HD23 | 10:j5:1030:ILE:HG23 | 1.43 | 0.97 |
| 10:j5:1034:GLU:OE1 | 10:j5:1037:ARG:NH2 | 1.96 | 0.97 |
| 8:g7:107:ILE:HG12 | 1:h7:13:ASP:OD2 | 1.63 | 0.97 |
| 8:i7:90:ARG:NH1 | 1:j7:13:ASP:OD1 | 1.97 | 0.97 |
| 8:c7:36:ARG:NH2 | 8:c7:152:TYR:OH | 1.97 | 0.97 |
| 8:o7:17:TYR:HE2 | 1:p7:93:THR:CB | 1.76 | 0.97 |
| 8:q7:75:GLU:C | 11:aA:53:VAL:HG11 | 1.88 | 0.97 |
| 3:F8:108:ARG:C | 4:M8:6:THR:CG2 | 2.34 | 0.97 |
| 3:L8:59:LEU:CD2 | 12:a9:901:CYC:HMC3 | 1.94 | 0.97 |
| 3:L8:113:LEU:CD2 | 12:a9:901:CYC:HMB3 | 1.95 | 0.97 |
| 3:O8:108:ARG:HB2 | 5:Z8:61:LYS:HD3 | 1.00 | 0.97 |
| 3:O8:111:ASN:OD1 | 5:Z8:68:LEU:CA | 2.12 | 0.97 |
| 4:M9:113:ILE:CD1 | 4:M9:143:VAL:HG13 | 1.93 | 0.97 |
| 11:aA:280:ASP:CG | 11:aA:281:PRO:HD3 | 1.88 | 0.97 |
| 11:aA:322:ALA:O | 11:aA:326:ILE:HG13 | 1.64 | 0.97 |
| 11:aA:666:ASN:CB | 12:aA:901:CYC:C4B | 2.41 | 0.97 |
| 5:N1:22:LEU:CD2 | 5:N1:26:LEU:CG | 2.38 | 0.97 |
| 3:FA:111:ASN:ND2 | 4:MA:65:ARG:HD2 | 1.80 | 0.97 |
| 3:HA:108:ARG:HH12 | 11:aA:448:ASN:HD21 | 1.13 | 0.97 |
| 4:MA:160:THR:CG2 | 4:MA:257:GLN:CB | 2.42 | 0.97 |
| 2:O3:63:PHE:O | 2:O3:66:LEU:HG | 1.63 | 0.97 |
| 1:d5:28:LYS:CE | 1:n7:143:PRO:CG | 2.42 | 0.97 |
| 8:Q5:17:TYR:CZ | 1:R5:44:ILE:HG22 | 1.98 | 0.97 |
| 1:b5:27:LEU:HD13 | 10:k5:172:LEU:HD22 | 1.47 | 0.97 |
| 1:b5:34:GLY:HA3 | 10:k5:47:PHE:HD2 | 1.28 | 0.97 |
| 10:j5:1016:LEU:CD1 | 10:j5:1017:ARG:N | 2.27 | 0.97 |
| 10:j5:1076:GLU:C | 10:j5:1078:SER:H | 1.51 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:H7:140:LEU:HD11 | 11:aA:561:ALA:HB1 | 1.01 | 0.97 |
| 8:i7:94:TYR:CE2 | 1:j7:9:ILE:CG2 | 2.47 | 0.97 |
| 2:X8:69:PRO:HD2 | 2:S9:42:ARG:NE | 1.77 | 0.97 |
| 4:M9:274:VAL:CG1 | 3:V9:77:ARG:NE | 2.27 | 0.97 |
| 5:N9:31:TRP:HB3 | 5:N9:32:PRO:HD2 | 1.47 | 0.97 |
| 1:A:110:ASN:CG | 10:k5:462:TYR:CZ | 2.42 | 0.97 |
| 12:LA:202:CYC:HBA2 | 11:aA:536:THR:HG21 | 1.46 | 0.97 |
| 4:MA:1:MET:CA | 11:aA:422:SER:O | 2.00 | 0.97 |
| 6:M2:34:ARG:HD2 | 8:O5:52:LYS:HB2 | 1.45 | 0.97 |
| 2:A4:60:TYR:HB3 | 2:A4:67:THR:HG23 | 1.47 | 0.97 |
| 3:B4:108:ARG:O | 12:B4:202:CYC:HBB2 | 1.63 | 0.97 |
| 4:M3:134:ASN:CB | 12:P3:201:CYC:HAA1 | 1.93 | 0.97 |
| 3:U4:108:ARG:HA | 4:M4:246:ALA:HB2 | 1.25 | 0.97 |
| 3:F4:84:ARG:HD3 | 11:aA:139:ILE:HG22 | 1.12 | 0.97 |
| 4:M4:136:SER:HB3 | 5:Z4:2:SER:HB2 | 1.47 | 0.97 |
| 12:O4:201:CYC:HMA2 | 5:Z4:53:LEU:HD13 | 1.44 | 0.97 |
| 10:k5:586:LEU:CD1 | 10:k5:607:LEU:HD23 | 1.94 | 0.97 |
| 8:a7:107:ILE:HG12 | 1:b7:13:ASP:OD2 | 1.63 | 0.97 |
| 3:U8:115:GLU:CB | 4:M8:74:LEU:HD11 | 1.69 | 0.97 |
| 2:X8:69:PRO:CB | 2:S9:39:GLU:HA | 1.93 | 0.97 |
| 3:F8:115:GLU:CG | 4:M8:3:VAL:HG13 | 1.95 | 0.97 |
| 11:a9:338:VAL:HG22 | 11:a9:340:PRO:CD | 1.95 | 0.97 |
| 11:aA:99:ALA:HB3 | 11:aA:100:PRO:HD2 | 1.44 | 0.97 |
| 3:LA:51:ILE:HG21 | 3:LA:90:LEU:HD12 | 1.47 | 0.97 |
| 4:M3:160:THR:CG2 | 4:M3:257:GLN:CB | 2.42 | 0.97 |
| 8:A5:12:ASP:OD1 | 1:B5:91:TYR:CZ | 2.18 | 0.97 |
| 1:T5:53:LYS:NZ | 8:U5:120:GLN:CG | 2.28 | 0.97 |
| 1:b5:5:ILE:CD1 | 10:k5:46:PHE:HZ | 1.77 | 0.97 |
| 10:j5:989:THR:HG22 | 8:g7:106:GLU:OE2 | 1.64 | 0.97 |
| 10:k5:612:ILE:H | 10:k5:612:ILE:HD12 | 1.28 | 0.97 |
| 10:k5:930:LEU:O | 1:D7:33:THR:HG21 | 1.62 | 0.97 |
| 10:k5:989:THR:CG2 | 8:a7:106:GLU:OE2 | 2.13 | 0.97 |
| 3:L9:38:LEU:HD22 | 2:K9:24:LEU:HD22 | 1.47 | 0.97 |
| 11:aA:338:VAL:HG22 | 11:aA:340:PRO:CD | 1.95 | 0.97 |
| 11:aA:615:ARG:O | 3:H1:68:ARG:CD | 2.13 | 0.97 |
| 2:A2:63:PHE:O | 2:A2:66:LEU:HG | 1.63 | 0.97 |
| 3:F4:107:ASP:CB | 4:M4:8:SER:N | 2.26 | 0.96 |
| 4:M4:104:ALA:HA | 2:P4:14:SER:HB3 | 1.43 | 0.96 |
| 2:N4:63:PHE:O | 2:N4:66:LEU:HG | 1.63 | 0.96 |
| 1:N5:53:LYS:HZ2 | 8:O5:120:GLN:HG3 | 1.27 | 0.96 |
| 8:M7:49:ARG:HH12 | 3:H9:119:ALA:CA | 1.77 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:W7:13:ALA:CA | 9:w7:46:LYS:NZ | 2.21 | 0.96 |
| 3:Q8:72:ASN:OD1 | 12:Z8:301:CYC:HMD1 | 1.63 | 0.96 |
| 11:a9:55:ASP:CB | 11:a9:612:TYR:CB | 2.22 | 0.96 |
| 2:EA:2:LYS:HZ1 | 2:IA:17:ARG:HH12 | 1.11 | 0.96 |
| 3:HA:84:ARG:NH2 | 11:aA:474:PHE:CE2 | 2.33 | 0.96 |
| 12:J3:202:CYC:CMA | 11:a9:798:SER:HG | 1.72 | 0.96 |
| 3:B3:88:ILE:HG21 | 12:B3:202:CYC:C2B | 1.93 | 0.96 |
| 5:N3:22:LEU:CD2 | 5:N3:26:LEU:CG | 2.38 | 0.96 |
| 8:M5:66:VAL:HG11 | 8:K7:68:PRO:HG3 | 0.99 | 0.96 |
| 8:G5:71:ASN:OD1 | 12:G5:201:CYC:HMD3 | 1.63 | 0.96 |
| 12:d5:201:CYC:HMD1 | 12:d5:201:CYC:HC | 1.25 | 0.96 |
| 1:T5:110:ASN:ND2 | 10:j5:692:LEU:CB | 2.02 | 0.96 |
| 10:k5:586:LEU:HD11 | 10:k5:607:LEU:HD23 | 1.47 | 0.96 |
| 10:k5:930:LEU:HB3 | 1:D7:33:THR:CG2 | 1.95 | 0.96 |
| 10:k5:974:LEU:HD23 | 1:p7:1:MET:H3 | 1.26 | 0.96 |
| 8:k7:66:VAL:HG12 | 11:a9:65:LEU:CD2 | 1.95 | 0.96 |
| 8:q7:79:ALA:HB2 | 11:aA:53:VAL:CG2 | 1.95 | 0.96 |
| 12:M8:302:CYC:HMC3 | 3:S8:72:ASN:HD21 | 0.90 | 0.96 |
| 4:M9:160:THR:CG2 | 4:M9:257:GLN:CB | 2.42 | 0.96 |
| 11:a9:92:LYS:HE3 | 11:a9:92:LYS:N | 1.80 | 0.96 |
| 11:a9:245:ALA:CB | 12:a9:901:CYC:CBB | 2.41 | 0.96 |
| 11:aA:668:TYR:HE2 | 11:aA:670:LEU:HD23 | 1.26 | 0.96 |
| 5:N1:31:TRP:HB3 | 5:N1:32:PRO:HD2 | 1.47 | 0.96 |
| 1:Z:161:SER:HB2 | 1:X5:14:VAL:HG21 | 1.19 | 0.96 |
| 3:FA:150:ARG:HA | 3:F9:150:ARG:HE | 1.13 | 0.96 |
| 5:NA:22:LEU:HD21 | 5:NA:26:LEU:HD11 | 1.47 | 0.96 |
| 5:NA:31:TRP:HB3 | 5:NA:32:PRO:HD2 | 1.47 | 0.96 |
| 2:O1:60:TYR:HB3 | 2:O1:67:THR:HG23 | 1.47 | 0.96 |
| 4:M4:205:ASP:HB3 | 5:Z4:59:ARG:NE | 1.79 | 0.96 |
| 8:G5:12:ASP:OD1 | 1:H5:91:TYR:CZ | 2.18 | 0.96 |
| 10:j5:631:HIS:CD2 | 10:j5:664:MET:HE1 | 2.01 | 0.96 |
| 10:k5:631:HIS:CD2 | 10:k5:664:MET:HE1 | 2.01 | 0.96 |
| 10:k5:1008:PHE:CZ | 1:p7:83:ARG:NH1 | 2.33 | 0.96 |
| 3:F6:82:CYS:HB2 | 12:F6:201:CYC:CMD | 1.95 | 0.96 |
| 8:i7:47:ARG:CG | 1:j7:18:TYR:CZ | 2.47 | 0.96 |
| 3:B8:68:ARG:HH22 | 3:U8:68:ARG:NH2 | 1.57 | 0.96 |
| 3:B8:116:THR:CG2 | 4:M8:53:LEU:HA | 1.94 | 0.96 |
| 8:o7:37:LEU:HD12 | 1:p7:28:LYS:HE3 | 1.45 | 0.96 |
| 8:u7:23:LEU:CD2 | 1:v7:38:VAL:HA | 1.95 | 0.96 |
| 2:N8:60:TYR:HB3 | 2:N8:67:THR:HG23 | 1.47 | 0.96 |
| 5:Z8:22:LEU:HD21 | 5:Z8:26:LEU:HD11 | 1.47 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:Z8:29:HIS:CD2 | 5:Z8:36:THR:HG23 | 2.00 | 0.96 |
| 1:A:161:SER:HB2 | 1:R5:14:VAL:HG21 | 1.38 | 0.96 |
| 3:J3:84:ARG:C | 11:a9:668:TYR:HH | 1.69 | 0.96 |
| 5:N3:22:LEU:HD21 | 5:N3:26:LEU:HD11 | 1.47 | 0.96 |
| 4:M4:27:HIS:O | 11:aA:227:GLY:HA3 | 1.65 | 0.96 |
| 4:M4:160:THR:CG2 | 4:M4:257:GLN:CB | 2.42 | 0.96 |
| 3:O4:95:TYR:CD2 | 3:O4:108:ARG:NH2 | 2.33 | 0.96 |
| 1:B5:143:PRO:HG3 | 8:W7:41:GLN:HE22 | 1.26 | 0.96 |
| 8:U5:76:LYS:CD | 8:U5:77:MET:HE2 | 1.91 | 0.96 |
| 8:W5:17:TYR:CZ | 1:X5:44:ILE:HG22 | 1.98 | 0.96 |
| 8:a5:29:PHE:HE1 | 8:a5:99:GLY:HA3 | 1.29 | 0.96 |
| 10:k5:1016:LEU:CD1 | 10:k5:1017:ARG:N | 2.27 | 0.96 |
| 3:B8:82:CYS:O | 12:B8:202:CYC:HAC2 | 1.62 | 0.96 |
| 4:M8:87:ILE:HD12 | 3:Y8:77:ARG:CG | 1.93 | 0.96 |
| 2:I9:31:PHE:CE2 | 3:J9:31:VAL:CA | 2.45 | 0.96 |
| 11:a9:379:LEU:HD13 | 11:a9:391:VAL:HG21 | 1.45 | 0.96 |
| 4:MA:162:ASN:N | 12:VA:201:CYC:HBB3 | 1.80 | 0.96 |
| 3:F4:108:ARG:CZ | 4:M4:9:GLN:HE21 | 1.77 | 0.96 |
| 1:N5:110:ASN:ND2 | 10:k5:692:LEU:O | 1.98 | 0.96 |
| 8:A5:71:ASN:OD1 | 12:A5:201:CYC:HMD3 | 1.63 | 0.96 |
| 8:W5:11:ALA:CB | 1:X5:94:TYR:CZ | 2.45 | 0.96 |
| 8:m7:102:THR:HB | 8:m7:103:PRO:HD3 | 1.48 | 0.96 |
| 8:u7:17:TYR:HE2 | 1:v7:93:THR:CB | 1.76 | 0.96 |
| 3:O8:95:TYR:CD2 | 3:O8:108:ARG:NH2 | 2.33 | 0.96 |
| 3:H9:123:PRO:HG2 | 12:H9:202:CYC:HMC3 | 1.46 | 0.96 |
| 11:aA:800:THR:HG22 | 12:aA:901:CYC:CAA | 1.92 | 0.96 |
| 3:D3:68:ARG:NH2 | 3:X3:68:ARG:NH2 | 2.14 | 0.96 |
| 2:O3:60:TYR:HB3 | 2:O3:67:THR:HG23 | 1.47 | 0.96 |
| 2:U3:141:GLN:O | 2:Q9:76:ASP:CA | 2.09 | 0.96 |
| 12:B1:202:CYC:CAA | 11:aA:684:ASN:CG | 2.38 | 0.96 |
| 4:M4:215:GLU:CD | 12:Z4:301:CYC:CAB | 2.39 | 0.96 |
| 12:J6:202:CYC:O2A | 6:M6:185:PHE:HD2 | 1.49 | 0.96 |
| 6:M6:118:GLU:OE1 | 2:C6:114:ARG:NH1 | 1.99 | 0.96 |
| 10:k5:1009:ALA:CB | 1:p7:87:TYR:CE1 | 2.48 | 0.96 |
| 8:O7:52:LYS:HE3 | 11:aA:29:ARG:HH12 | 0.81 | 0.96 |
| 8:i7:37:LEU:CD1 | 1:j7:31:PHE:CE2 | 2.47 | 0.96 |
| 8:i7:95:GLY:C | 8:i7:152:TYR:CE2 | 2.44 | 0.96 |
| 3:U8:120:LEU:HD21 | 12:U8:201:CYC:HBD1 | 0.99 | 0.96 |
| 12:O8:201:CYC:HBA2 | 5:Z8:50:LEU:HD13 | 1.45 | 0.96 |
| 4:M9:76:ALA:HB1 | 3:D9:112:GLY:H | 1.26 | 0.96 |
| 5:N9:3:VAL:HG11 | 3:R9:115:GLU:HB2 | 1.47 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 11:a9:280:ASP:CG | 11:a9:281:PRO:HD3 | 1.88 | 0.96 |
| 11:a9:312:ASP:CB | 11:a9:315:LEU:CD1 | 2.39 | 0.96 |
| 11:aA:107:ARG:HG3 | 11:aA:108:PRO:HD2 | 1.46 | 0.96 |
| 11:aA:800:THR:HG21 | 12:aA:901:CYC:HAA1 | 0.96 | 0.96 |
| 5:NA:53:LEU:CD1 | 12:TA:301:CYC:HAA1 | 1.96 | 0.96 |
| 3:J3:77:ARG:NH2 | 2:K3:107:ASP:CA | 2.25 | 0.96 |
| 3:Z3:108:ARG:CZ | 4:M3:158:PHE:CD1 | 2.39 | 0.96 |
| 3:L4:68:ARG:HB2 | 11:aA:82:GLN:H | 0.79 | 0.96 |
| 8:A5:122:PRO:HD2 | 12:A5:201:CYC:OC | 1.66 | 0.96 |
| 1:J5:39:ARG:O | 1:J5:41:ALA:N | 1.98 | 0.96 |
| 8:W5:12:ASP:HA | 1:X5:94:TYR:CE2 | 1.95 | 0.96 |
| 10:j5:1016:LEU:CD1 | 10:j5:1017:ARG:H | 1.79 | 0.96 |
| 8:I7:102:THR:HB | 8:I7:103:PRO:HD3 | 1.48 | 0.96 |
| 8:i7:101:VAL:HG11 | 8:i7:155:TYR:CE1 | 2.00 | 0.96 |
| 12:j7:201:CYC:HBB2 | 9:y7:42:GLN:OE1 | 1.65 | 0.96 |
| 2:N8:14:SER:CB | 5:Z8:62:ARG:CZ | 2.33 | 0.96 |
| 12:J9:202:CYC:NB | 11:a9:512:TYR:CB | 2.14 | 0.96 |
| 11:a9:107:ARG:HG3 | 11:a9:108:PRO:HD2 | 1.46 | 0.96 |
| 4:MA:274:VAL:HG11 | 2:WA:111:ALA:CB | 1.94 | 0.96 |
| 2:G2:16:GLY:HA3 | 6:M2:104:ARG:NH1 | 1.80 | 0.96 |
| 12:J2:202:CYC:O2A | 6:M2:185:PHE:HD2 | 1.49 | 0.96 |
| 3:H4:84:ARG:HD3 | 11:aA:131:TYR:CE2 | 2.00 | 0.96 |
| 8:C5:29:PHE:HE1 | 8:C5:99:GLY:HA3 | 1.29 | 0.96 |
| 1:f5:18:TYR:CE1 | 10:j5:165:ARG:CD | 2.48 | 0.96 |
| 9:z5:6:LYS:HB3 | 9:z5:55:LYS:CA | 1.93 | 0.96 |
| 10:j5:929:PRO:HG3 | 1:J7:147:LYS:HE2 | 1.46 | 0.96 |
| 10:j5:964:GLY:CA | 1:t7:69:GLY:HA3 | 1.96 | 0.96 |
| 2:A9:60:TYR:HB3 | 2:A9:67:THR:HG23 | 1.47 | 0.96 |
| 11:a9:322:ALA:O | 11:a9:326:ILE:HG13 | 1.65 | 0.96 |
| 11:aA:821:ARG:NH2 | 3:L1:120:LEU:O | 1.98 | 0.96 |
| 3:TA:32:LYS:HE3 | 2:X4:60:TYR:CE2 | 2.00 | 0.96 |
| 12:H4:201:CYC:OB | 11:aA:129:ASN:ND2 | 1.97 | 0.96 |
| 4:M4:210:ILE:HD13 | 5:Z4:26:LEU:CD2 | 1.96 | 0.96 |
| 4:M4:226:SER:OG | 3:Y4:88:ILE:CG2 | 2.14 | 0.96 |
| 1:D5:39:ARG:O | 1:D5:41:ALA:N | 1.98 | 0.96 |
| 8:U5:76:LYS:HD2 | 8:U5:77:MET:HE1 | 1.44 | 0.96 |
| 6:M6:127:SER:CB | 3:F6:84:ARG:NH1 | 2.18 | 0.96 |
| 10:j5:825:ASN:HB3 | 12:H7:201:CYC:OB | 1.65 | 0.96 |
| 10:j5:1118:THR:HA | 12:j5:1202:CYC:HBA1 | 1.46 | 0.96 |
| 10:k5:990:ARG:HH21 | 10:k5:1026:LYS:NZ | 1.62 | 0.96 |
| 8:Q7:25:ARG:HD3 | 8:C7:25:ARG:HH22 | 1.28 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:U7:102:THR:HB | 8:U7:103:PRO:HD3 | 1.48 | 0.96 |
| 8:c7:101:VAL:HG11 | 8:c7:155:TYR:CE1 | 2.00 | 0.96 |
| 3:O8:108:ARG:CA | 5:Z8:61:LYS:HD3 | 1.96 | 0.96 |
| 11:a9:681:LEU:HA | 11:a9:684:ASN:HD21 | 1.31 | 0.96 |
| 11:a9:818:ARG:HH11 | 11:a9:818:ARG:HG3 | 1.30 | 0.96 |
| 11:aA:92:LYS:HE3 | 11:aA:92:LYS:N | 1.80 | 0.96 |
| 5:N1:22:LEU:HD21 | 5:N1:26:LEU:HD11 | 1.47 | 0.96 |
| 3:JA:70:GLY:HA3 | 11:aA:356:ALA:HB1 | 1.46 | 0.96 |
| 3:JA:116:THR:HG23 | 11:aA:521:PHE:CD2 | 2.01 | 0.96 |
| 3:Q4:97:LEU:HA | 3:Q4:163:TYR:HE2 | 1.27 | 0.96 |
| 1:L5:75:THR:HB | 8:G5:112:VAL:HA | 1.48 | 0.96 |
| 8:M5:20:PRO:CB | 8:A5:100:ASP:OD1 | 2.14 | 0.96 |
| 8:C5:27:LYS:CA | 8:C5:30:VAL:HG22 | 1.95 | 0.96 |
| 12:F5:201:CYC:O2A | 10:k5:591:ILE:HG13 | 1.65 | 0.96 |
| 6:M6:104:ARG:NH1 | 2:G6:16:GLY:HA3 | 1.80 | 0.96 |
| 10:j5:889:LEU:HA | 12:J7:201:CYC:OB | 1.64 | 0.96 |
| 10:k5:386:ILE:HG21 | 10:k5:395:SER:H | 0.91 | 0.96 |
| 10:k5:978:LEU:CD1 | 1:p7:107:ARG:NH2 | 2.29 | 0.96 |
| 4:M9:162:ASN:N | 12:V9:201:CYC:HBB3 | 1.80 | 0.96 |
| 4:M9:273:ILE:HD11 | 3:V9:75:PRO:CD | 1.93 | 0.96 |
| 4:M9:274:VAL:HG12 | 3:V9:77:ARG:NE | 1.80 | 0.96 |
| 11:a9:67:GLN:O | 11:a9:68:THR:CG2 | 2.14 | 0.96 |
| 11:aA:643:LEU:HD12 | 11:aA:643:LEU:H | 1.31 | 0.96 |
| 11:aA:668:TYR:CE2 | 11:aA:670:LEU:HD23 | 2.00 | 0.96 |
| 11:aA:742:GLN:HG2 | 3:L1:88:ILE:HD12 | 0.99 | 0.96 |
| 2:I4:14:SER:HA | 11:aA:170:PHE:HZ | 1.29 | 0.95 |
| 1:d5:127:VAL:CG1 | 10:j5:698:GLY:CA | 2.43 | 0.95 |
| 8:S5:68:PRO:CB | 8:a5:59:PHE:CB | 2.40 | 0.95 |
| 8:g7:29:PHE:HE1 | 8:g7:99:GLY:HA3 | 1.29 | 0.95 |
| 8:i7:20:PRO:CD | 8:s7:155:TYR:CD1 | 2.49 | 0.95 |
| 8:c7:95:GLY:C | 8:c7:152:TYR:CE2 | 2.44 | 0.95 |
| 3:F8:115:GLU:C | 4:M8:3:VAL:HG11 | 1.91 | 0.95 |
| 2:K8:15:GLN:O | 11:a9:241:VAL:HG11 | 1.59 | 0.95 |
| 2:N8:115:GLU:HB2 | 5:Z8:32:PRO:CA | 1.96 | 0.95 |
| 2:N8:115:GLU:HB2 | 5:Z8:32:PRO:C | 1.90 | 0.95 |
| 5:N9:1:MET:CB | 5:N9:3:VAL:HG23 | 1.96 | 0.95 |
| 11:aA:312:ASP:CB | 11:aA:315:LEU:CD1 | 2.39 | 0.95 |
| 2:KA:24:LEU:HD22 | 3:LA:38:LEU:HD22 | 1.47 | 0.95 |
| 2:KA:25:GLN:O | 2:KA:26:ALA:C | 1.98 | 0.95 |
| 3:LA:52:ILE:HD13 | 3:LA:87:GLU:HB2 | 0.99 | 0.95 |
| 5:NA:54:LEU:HD13 | 3:TA:84:ARG:NH2 | 1.80 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:QA:33:ARG:HG2 | 2:UA:25:GLN:HG3 | 1.48 | 0.95 |
| 10:j5:990:ARG:HH21 | 10:j5:1026:LYS:NZ | 1.62 | 0.95 |
| 4:M9:188:LEU:HD22 | 12:V9:201:CYC:HB | 1.30 | 0.95 |
| 2:O9:60:TYR:HB3 | 2:O9:67:THR:HG23 | 1.47 | 0.95 |
| 11:aA:67:GLN:O | 11:aA:68:THR:HG22 | 1.66 | 0.95 |
| 11:aA:586:LEU:O | 11:aA:590:PRO:HG2 | 1.66 | 0.95 |
| 3:FA:151:GLY:H | 3:F9:150:ARG:CZ | 1.77 | 0.95 |
| 5:NA:3:VAL:HG11 | 3:RA:115:GLU:HB2 | 1.47 | 0.95 |
| 6:M2:57:GLU:OE1 | 8:i7:76:LYS:HE3 | 1.62 | 0.95 |
| 3:L3:120:LEU:O | 11:a9:821:ARG:NH2 | 1.99 | 0.95 |
| 2:N4:60:TYR:HB3 | 2:N4:67:THR:HG23 | 1.47 | 0.95 |
| 8:E5:80:LEU:HD12 | 12:E5:201:CYC:HAD2 | 1.44 | 0.95 |
| 1:b5:18:TYR:CE1 | 10:k5:165:ARG:HB2 | 2.00 | 0.95 |
| 10:k5:1055:SER:OG | 12:k5:1203:CYC:HBB2 | 0.78 | 0.95 |
| 8:i7:39:ILE:HD11 | 8:i7:148:GLU:CB | 1.95 | 0.95 |
| 8:o7:23:LEU:CD2 | 1:p7:38:VAL:HA | 1.95 | 0.95 |
| 11:a9:312:ASP:CA | 11:a9:315:LEU:H | 1.79 | 0.95 |
| 11:a9:636:ALA:O | 11:a9:774:PHE:HD2 | 1.49 | 0.95 |
| 4:MA:274:VAL:CB | 3:VA:77:ARG:HD3 | 1.97 | 0.95 |
| 1:N5:53:LYS:HZ2 | 8:O5:120:GLN:NE2 | 1.57 | 0.95 |
| 12:H5:201:CYC:HBB2 | 9:i5:21:ARG:HA | 1.47 | 0.95 |
| 12:P5:201:CYC:O2A | 10:k5:649:PHE:HD2 | 1.49 | 0.95 |
| 10:j5:1016:LEU:HD12 | 10:j5:1017:ARG:H | 1.15 | 0.95 |
| 8:C7:102:THR:HB | 8:C7:103:PRO:HD3 | 1.48 | 0.95 |
| 8:M7:45:GLU:OE2 | 3:H9:124:THR:OG1 | 1.84 | 0.95 |
| 1:X7:118:SER:O | 9:w7:61:GLN:CD | 2.10 | 0.95 |
| 8:q7:66:VAL:O | 11:aA:65:LEU:CD2 | 2.14 | 0.95 |
| 8:u7:23:LEU:CB | 1:v7:38:VAL:HG11 | 1.74 | 0.95 |
| 3:U8:115:GLU:OE1 | 4:M8:74:LEU:CD1 | 2.13 | 0.95 |
| 3:L8:59:LEU:HD21 | 12:a9:901:CYC:CMC | 1.94 | 0.95 |
| 4:M8:214:GLY:HA2 | 5:Z8:28:HIS:CE1 | 1.86 | 0.95 |
| 4:M8:267:LEU:O | 4:M8:269:SER:O | 1.83 | 0.95 |
| 3:Q8:89:ILE:CG2 | 3:Q8:92:TYR:CZ | 2.40 | 0.95 |
| 11:aA:67:GLN:O | 11:aA:68:THR:CG2 | 2.14 | 0.95 |
| 3:L2:77:ARG:HH12 | 6:M2:70:GLU:CD | 1.73 | 0.95 |
| 8:A5:121:THR:HG23 | 12:A5:201:CYC:C4C | 1.94 | 0.95 |
| 6:M6:62:ARG:NH2 | 1:b7:57:ALA:O | 1.69 | 0.95 |
| 10:j5:586:LEU:HD11 | 10:j5:607:LEU:HD23 | 1.48 | 0.95 |
| 10:j5:930:LEU:C | 1:J7:33:THR:HG21 | 1.89 | 0.95 |
| 10:k5:825:ASN:OD1 | 10:k5:854:LEU:CD1 | 2.14 | 0.95 |
| 12:B8:202:CYC:HMA1 | 4:M8:58:TYR:N | 1.81 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:o7:37:LEU:HD21 | 1:p7:24:LEU:HD22 | 1.48 | 0.95 |
| 3:U8:108:ARG:C | 4:M8:246:ALA:CB | 2.39 | 0.95 |
| 12:H8:201:CYC:HBB3 | 11:a9:259:ALA:HA | 1.47 | 0.95 |
| 4:M9:258:LYS:CG | 3:V9:111:ASN:HD21 | 1.80 | 0.95 |
| 5:N9:22:LEU:CD2 | 5:N9:26:LEU:CG | 2.38 | 0.95 |
| 11:a9:586:LEU:O | 11:a9:590:PRO:HG2 | 1.66 | 0.95 |
| 11:aA:585:GLU:O | 11:aA:588:VAL:O | 1.81 | 0.95 |
| 3:H1:81:ALA:HB3 | 12:H1:201:CYC:C2D | 1.95 | 0.95 |
| 3:FA:151:GLY:CA | 3:F9:150:ARG:NH2 | 2.30 | 0.95 |
| 4:M4:91:VAL:O | 4:M4:218:VAL:HG23 | 1.64 | 0.95 |
| 4:M4:205:ASP:OD2 | 5:Z4:59:ARG:HB3 | 1.67 | 0.95 |
| 5:Z4:1:MET:CB | 5:Z4:3:VAL:HG23 | 1.96 | 0.95 |
| 1:b5:6:THR:CG2 | 10:k5:19:THR:OG1 | 2.13 | 0.95 |
| 3:L6:125:ARG:HD3 | 1:b7:69:GLY:HA2 | 1.49 | 0.95 |
| 10:k5:136:VAL:HG12 | 10:k5:137:PRO:HD2 | 1.44 | 0.95 |
| 12:B8:202:CYC:HHA | 4:M8:54:ALA:HB2 | 1.49 | 0.95 |
| 2:X8:60:TYR:CE2 | 3:T9:32:LYS:HE3 | 2.00 | 0.95 |
| 2:X8:65:TYR:N | 3:T9:25:ASN:HB3 | 1.72 | 0.95 |
| 3:F8:107:ASP:O | 4:M8:6:THR:O | 1.83 | 0.95 |
| 2:I8:14:SER:HA | 11:a9:170:PHE:HZ | 1.30 | 0.95 |
| 4:M8:205:ASP:OD2 | 5:Z8:59:ARG:HG2 | 1.62 | 0.95 |
| 5:N9:66:ARG:NH1 | 3:T9:111:ASN:CG | 2.24 | 0.95 |
| 11:aA:800:THR:HG22 | 12:aA:901:CYC:HBA2 | 1.49 | 0.95 |
| 3:FA:150:ARG:HG2 | 3:F9:150:ARG:CA | 1.97 | 0.95 |
| 4:MA:258:LYS:HG2 | 3:VA:111:ASN:HD21 | 1.27 | 0.95 |
| 2:A3:60:TYR:HB3 | 2:A3:67:THR:HG23 | 1.47 | 0.95 |
| 3:F4:113:LEU:CA | 4:M4:5:THR:CG2 | 2.40 | 0.95 |
| 2:N4:112:GLY:CA | 5:Z4:34:LEU:N | 2.29 | 0.95 |
| 3:Y4:89:ILE:HG23 | 3:Y4:92:TYR:HH | 1.31 | 0.95 |
| 8:G5:6:LYS:NZ | 8:S5:19:SER:HB3 | 1.77 | 0.95 |
| 10:j5:978:LEU:CD1 | 1:v7:107:ARG:HH22 | 1.79 | 0.95 |
| 8:c7:39:ILE:HD11 | 8:c7:148:GLU:CB | 1.95 | 0.95 |
| 3:L8:82:CYS:SG | 12:a9:901:CYC:C2C | 2.53 | 0.95 |
| 5:N9:53:LEU:CD1 | 12:T9:301:CYC:HAA1 | 1.96 | 0.95 |
| 3:H9:84:ARG:NH2 | 11:a9:474:PHE:CE2 | 2.34 | 0.95 |
| 3:J9:116:THR:HG23 | 11:a9:521:PHE:CG | 2.00 | 0.95 |
| 11:aA:379:LEU:HD13 | 11:aA:391:VAL:HG21 | 1.45 | 0.95 |
| 5:N1:1:MET:CB | 5:N1:3:VAL:HG23 | 1.96 | 0.95 |
| 12:JA:202:CYC:HBA2 | 11:aA:510:PHE:O | 1.67 | 0.95 |
| 6:M2:26:PHE:CB | 8:O5:83:ARG:HD2 | 1.97 | 0.95 |
| 3:F4:113:LEU:N | 4:M4:5:THR:HG23 | 1.82 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 12:M4:301:CYC:C1C | 3:Y4:72:ASN:CG | 2.32 | 0.95 |
| 8:C5:102:THR:HB | 8:C5:103:PRO:HD3 | 1.48 | 0.95 |
| 8:G5:122:PRO:HD2 | 12:G5:201:CYC:OC | 1.66 | 0.95 |
| 10:j5:1153:VAL:CG2 | 1:v7:125:ALA:HB2 | 1.87 | 0.95 |
| 8:O7:22:GLU:HG2 | 8:O7:25:ARG:NH1 | 1.82 | 0.95 |
| 5:N9:54:LEU:CD1 | 12:T9:301:CYC:NB | 2.30 | 0.95 |
| 5:Z8:1:MET:CB | 5:Z8:3:VAL:HG23 | 1.96 | 0.95 |
| 11:a9:312:ASP:HA | 11:a9:315:LEU:H | 1.32 | 0.95 |
| 11:aA:312:ASP:CA | 11:aA:315:LEU:HB2 | 1.77 | 0.95 |
| 11:aA:803:ASN:HA | 3:J1:119:ALA:O | 1.67 | 0.95 |
| 1:Z:75:THR:HG21 | 10:j5:182:ASN:O | 1.67 | 0.95 |
| 5:NA:54:LEU:HD12 | 12:TA:301:CYC:HB | 1.12 | 0.95 |
| 2:A1:60:TYR:HB3 | 2:A1:67:THR:HG23 | 1.47 | 0.95 |
| 1:H5:14:VAL:HG12 | 10:j5:554:ASN:O | 1.63 | 0.95 |
| 1:Z5:67:ARG:CZ | 10:k5:705:THR:OG1 | 2.15 | 0.95 |
| 10:j5:741:GLN:CG | 1:J7:77:ARG:HH22 | 1.77 | 0.95 |
| 10:j5:1050:PHE:HZ | 1:r7:107:ARG:CZ | 1.79 | 0.95 |
| 10:j5:1119:LEU:CD2 | 1:t7:87:TYR:OH | 2.14 | 0.95 |
| 10:k5:1025:LEU:HD22 | 10:k5:1035:PHE:HB2 | 1.45 | 0.95 |
| 10:k5:1054:SER:HA | 1:l7:107:ARG:HA | 1.47 | 0.95 |
| 3:H8:84:ARG:CG | 11:a9:131:TYR:CZ | 2.50 | 0.95 |
| 11:a9:31:SER:OG | 11:a9:34:ILE:CB | 2.13 | 0.95 |
| 11:aA:601:ALA:O | 11:aA:604:ALA:CB | 2.15 | 0.95 |
| 11:aA:632:ILE:HG12 | 3:J1:107:ASP:CG | 1.91 | 0.95 |
| 2:AA:63:PHE:O | 2:AA:66:LEU:HG | 1.63 | 0.95 |
| 12:J3:202:CYC:HAA1 | 11:a9:798:SER:HB3 | 1.46 | 0.95 |
| 4:M4:205:ASP:OD2 | 5:Z4:59:ARG:CB | 2.15 | 0.95 |
| 6:M6:53:LEU:CD2 | 8:c7:80:LEU:CG | 2.40 | 0.95 |
| 10:k5:156:SER:OG | 12:k5:1201:CYC:C3C | 2.14 | 0.95 |
| 10:k5:357:LEU:HD22 | 10:k5:378:TYR:HB3 | 1.47 | 0.95 |
| 10:k5:825:ASN:HB3 | 12:B7:201:CYC:OB | 1.66 | 0.95 |
| 3:F8:91:ARG:HH22 | 11:a9:140:GLN:NE2 | 1.63 | 0.95 |
| 12:L9:202:CYC:HBA2 | 11:a9:536:THR:HG21 | 1.46 | 0.95 |
| 5:Z8:29:HIS:CD2 | 5:Z8:36:THR:CG2 | 2.49 | 0.95 |
| 11:a9:67:GLN:O | 11:a9:68:THR:HG22 | 1.66 | 0.95 |
| 11:aA:278:LEU:HD12 | 11:aA:278:LEU:H | 1.30 | 0.95 |
| 3:DA:112:GLY:H | 4:MA:76:ALA:HB1 | 1.26 | 0.94 |
| 5:NA:54:LEU:N | 12:TA:301:CYC:CBA | 2.30 | 0.94 |
| 12:B4:202:CYC:HMA1 | 4:M4:58:TYR:N | 1.80 | 0.94 |
| 4:M4:210:ILE:HD13 | 5:Z4:26:LEU:HD23 | 1.45 | 0.94 |
| 8:A5:122:PRO:HG2 | 12:A5:201:CYC:HMC2 | 1.48 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:d5:155:TYR:CE2 | 1:T5:113:LYS:NZ | 2.35 | 0.94 |
| 8:e5:29:PHE:HE1 | 8:e5:99:GLY:HA3 | 1.29 | 0.94 |
| 1:f5:18:TYR:CE2 | 10:j5:165:ARG:HA | 2.01 | 0.94 |
| 1:f5:19:LEU:HD11 | 10:j5:172:LEU:CD1 | 1.97 | 0.94 |
| 8:U5:83:ARG:HD2 | 6:M6:27:ALA:O | 1.64 | 0.94 |
| 10:j5:742:GLY:CA | 12:J7:201:CYC:CGD | 2.44 | 0.94 |
| 10:j5:1151:GLN:CA | 1:v7:122:PRO:HB3 | 1.97 | 0.94 |
| 8:O7:102:THR:HB | 8:O7:103:PRO:HD3 | 1.48 | 0.94 |
| 2:E8:1:MET:N | 4:M8:10:ARG:NH2 | 2.15 | 0.94 |
| 8:u7:17:TYR:HD2 | 1:v7:93:THR:HG21 | 1.25 | 0.94 |
| 3:L8:78:ARG:HD3 | 12:a9:901:CYC:O2D | 1.67 | 0.94 |
| 4:M8:215:GLU:CD | 5:Z8:27:ALA:HB2 | 1.51 | 0.94 |
| 12:M8:302:CYC:H2C | 3:S8:78:ARG:HD2 | 1.48 | 0.94 |
| 3:L9:52:ILE:HD11 | 3:L9:87:GLU:CG | 1.97 | 0.94 |
| 5:Z8:38:GLU:HB2 | 12:Z8:301:CYC:HMB2 | 0.96 | 0.94 |
| 5:Z8:41:GLN:HB2 | 12:Z8:301:CYC:CMB | 1.97 | 0.94 |
| 1:A:75:THR:OG1 | 10:k5:182:ASN:HA | 1.66 | 0.94 |
| 3:JA:116:THR:HG23 | 11:aA:521:PHE:CG | 2.02 | 0.94 |
| 2:K3:15:GLN:HA | 11:a9:745:GLY:HA3 | 0.95 | 0.94 |
| 1:N5:113:LYS:NZ | 1:Z5:155:TYR:HE2 | 1.40 | 0.94 |
| 12:B5:201:CYC:HBA2 | 9:z5:26:THR:CG2 | 1.95 | 0.94 |
| 1:H5:14:VAL:HG11 | 10:j5:554:ASN:O | 1.67 | 0.94 |
| 8:I5:27:LYS:CA | 8:I5:30:VAL:HG22 | 1.95 | 0.94 |
| 8:S5:110:ILE:CD1 | 10:j5:533:LEU:HD11 | 1.97 | 0.94 |
| 8:U5:59:PHE:HD2 | 6:M6:37:GLU:OE2 | 1.31 | 0.94 |
| 1:Z5:28:LYS:HD2 | 1:t7:143:PRO:CG | 1.86 | 0.94 |
| 10:k5:1016:LEU:CD1 | 10:k5:1017:ARG:H | 1.79 | 0.94 |
| 3:D1:68:ARG:NH2 | 3:X1:68:ARG:NH2 | 2.14 | 0.94 |
| 8:i7:96:ILE:HG13 | 8:i7:152:TYR:CD2 | 2.02 | 0.94 |
| 3:F8:115:GLU:CD | 4:M8:3:VAL:CG2 | 2.39 | 0.94 |
| 4:M8:190:ARG:NH1 | 4:M8:202:SER:HB2 | 1.82 | 0.94 |
| 4:M8:231:THR:CA | 12:M8:301:CYC:CBB | 2.46 | 0.94 |
| 11:aA:623:ASP:HB2 | 3:H1:78:ARG:CZ | 1.96 | 0.94 |
| 3:HA:78:ARG:HD3 | 12:HA:202:CYC:CGD | 1.97 | 0.94 |
| 3:JA:65:ASP:HB3 | 11:aA:354:VAL:HG22 | 1.46 | 0.94 |
| 3:F4:77:ARG:CD | 11:aA:146:ARG:HH12 | 1.79 | 0.94 |
| 4:M4:232:VAL:HG12 | 3:Y4:109:CYS:O | 1.66 | 0.94 |
| 8:O5:102:THR:HB | 8:O5:103:PRO:HD3 | 1.48 | 0.94 |
| 5:Z4:24:PRO:HG3 | 5:Z4:37:HIS:CD2 | 2.02 | 0.94 |
| 8:G5:6:LYS:HZ2 | 8:S5:21:GLY:H | 0.99 | 0.94 |
| 8:G5:100:ASP:CG | 8:S5:20:PRO:CB | 2.40 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:G5:121:THR:CG2 | 12:G5:201:CYC:C4C | 2.45 | 0.94 |
| 1:H5:107:ARG:CZ | 9:i5:21:ARG:HD3 | 1.97 | 0.94 |
| 1:P5:161:SER:OXT | 1:b5:110:ASN:OD1 | 1.85 | 0.94 |
| 1:T5:110:ASN:ND2 | 10:j5:692:LEU:C | 2.26 | 0.94 |
| 8:U5:59:PHE:CB | 6:M6:39:ARG:HD3 | 1.97 | 0.94 |
| 10:j5:642:ARG:HH11 | 10:j5:642:ARG:HG2 | 1.31 | 0.94 |
| 10:j5:929:PRO:HG2 | 1:J7:147:LYS:HE2 | 1.49 | 0.94 |
| 10:j5:1008:PHE:HE1 | 1:v7:87:TYR:CE2 | 1.41 | 0.94 |
| 10:k5:930:LEU:O | 1:D7:33:THR:CG2 | 2.15 | 0.94 |
| 3:L8:85:ASP:OD2 | 12:a9:901:CYC:NA | 2.01 | 0.94 |
| 3:L9:51:ILE:HG21 | 3:L9:90:LEU:HD12 | 1.47 | 0.94 |
| 5:N9:22:LEU:HD21 | 5:N9:26:LEU:HD11 | 1.47 | 0.94 |
| 11:a9:278:LEU:HD12 | 11:a9:278:LEU:H | 1.30 | 0.94 |
| 3:JA:120:LEU:O | 11:aA:361:ALA:HB2 | 1.67 | 0.94 |
| 4:MA:188:LEU:HD22 | 12:VA:201:CYC:HB | 1.30 | 0.94 |
| 4:MA:274:VAL:CB | 3:VA:77:ARG:CD | 2.44 | 0.94 |
| 5:NA:22:LEU:CD2 | 5:NA:26:LEU:CG | 2.38 | 0.94 |
| 12:F3:201:CYC:HMA1 | 4:M3:36:TYR:O | 1.65 | 0.94 |
| 3:B4:116:THR:N | 4:M4:56:MET:HG2 | 1.82 | 0.94 |
| 3:H4:84:ARG:HG2 | 11:aA:131:TYR:CE2 | 2.02 | 0.94 |
| 8:I5:102:THR:HB | 8:I5:103:PRO:HD3 | 1.48 | 0.94 |
| 8:e5:102:THR:HB | 8:e5:103:PRO:HD3 | 1.48 | 0.94 |
| 10:j5:1143:LEU:O | 1:r7:10:ASN:CG | 2.11 | 0.94 |
| 8:C7:29:PHE:HE1 | 8:C7:99:GLY:HA3 | 1.29 | 0.94 |
| 1:T7:106:GLU:HG3 | 9:w7:58:THR:CG2 | 1.96 | 0.94 |
| 8:o7:27:LYS:HE3 | 1:p7:35:ALA:CB | 1.87 | 0.94 |
| 3:H8:84:ARG:CG | 11:a9:131:TYR:CE2 | 2.49 | 0.94 |
| 3:H8:119:ALA:HB1 | 11:a9:266:ASN:CB | 1.97 | 0.94 |
| 4:M8:91:VAL:HG13 | 2:P8:14:SER:C | 1.91 | 0.94 |
| 3:J9:120:LEU:O | 11:a9:361:ALA:HB2 | 1.67 | 0.94 |
| 11:a9:426:ARG:HH21 | 11:a9:496:ARG:CD | 1.80 | 0.94 |
| 11:aA:786:GLU:OE1 | 3:H1:115:GLU:HB2 | 1.68 | 0.94 |
| 5:NA:61:LYS:HZ3 | 12:TA:301:CYC:HBB2 | 1.01 | 0.94 |
| 5:N3:54:LEU:HD12 | 12:R3:201:CYC:HB | 1.12 | 0.94 |
| 4:M4:205:ASP:CB | 5:Z4:59:ARG:HE | 1.81 | 0.94 |
| 8:A5:121:THR:CG2 | 12:A5:201:CYC:C4C | 2.45 | 0.94 |
| 1:T5:53:LYS:HZ1 | 8:U5:120:GLN:NE2 | 1.47 | 0.94 |
| 8:U5:78:THR:HG22 | 6:M6:35:GLY:HA2 | 1.48 | 0.94 |
| 10:k5:642:ARG:HH11 | 10:k5:642:ARG:HG2 | 1.31 | 0.94 |
| 10:k5:934:ALA:HB2 | 1:D7:32:THR:CG2 | 1.95 | 0.94 |
| 4:M9:51:ARG:HH21 | 11:a9:430:ARG:CD | 1.80 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:N9:54:LEU:HD12 | 12:T9:301:CYC:HB | 1.12 | 0.94 |
| 11:a9:476:ARG:HH11 | 11:a9:488:SER:CB | 1.69 | 0.94 |
| 1:A:73:TYR:CZ | 10:k5:162:TRP:CZ2 | 2.55 | 0.94 |
| 1:A:127:VAL:HG11 | 1:R5:15:GLN:CG | 1.96 | 0.94 |
| 3:FA:151:GLY:O | 3:F9:150:ARG:NH2 | 2.01 | 0.94 |
| 2:Q1:14:SER:CB | 5:N1:62:ARG:HH21 | 1.72 | 0.94 |
| 2:S1:16:GLY:HA3 | 5:N1:31:TRP:CD1 | 2.02 | 0.94 |
| 6:M2:118:GLU:OE1 | 2:C2:114:ARG:NH1 | 1.99 | 0.94 |
| 4:M4:235:PHE:CB | 12:M4:301:CYC:CAA | 2.46 | 0.94 |
| 8:S5:41:GLN:OE1 | 1:D7:143:PRO:CG | 2.14 | 0.94 |
| 10:j5:930:LEU:HB3 | 1:J7:33:THR:CG2 | 1.97 | 0.94 |
| 12:B8:202:CYC:HBB1 | 4:M8:61:ASN:HB2 | 1.49 | 0.94 |
| 2:N8:115:GLU:HB2 | 5:Z8:32:PRO:HB2 | 1.44 | 0.94 |
| 11:a9:56:ILE:CD1 | 11:a9:612:TYR:CE2 | 2.51 | 0.94 |
| 11:aA:93:LEU:CD2 | 11:aA:252:ARG:HH12 | 1.80 | 0.94 |
| 11:aA:818:ARG:HG3 | 11:aA:818:ARG:HH11 | 1.30 | 0.94 |
| 1:Z:131:GLN:CB | 1:X5:17:LYS:NZ | 2.31 | 0.94 |
| 2:AA:60:TYR:HB3 | 2:AA:67:THR:HG23 | 1.47 | 0.94 |
| 5:NA:66:ARG:NH1 | 3:TA:111:ASN:CG | 2.24 | 0.94 |
| 3:H3:78:ARG:HH12 | 11:a9:623:ASP:HA | 1.32 | 0.94 |
| 3:F4:107:ASP:HB3 | 4:M4:8:SER:OG | 0.77 | 0.94 |
| 8:G5:122:PRO:HG2 | 12:G5:201:CYC:HMC2 | 1.48 | 0.94 |
| 12:T5:201:CYC:CBB | 10:j5:482:GLN:NE2 | 2.31 | 0.94 |
| 12:M8:302:CYC:OC | 3:S8:78:ARG:NH1 | 2.00 | 0.94 |
| 2:N8:11:SER:HA | 5:Z8:62:ARG:NH2 | 1.82 | 0.94 |
| 3:H9:113:LEU:CD1 | 12:H9:202:CYC:CMB | 2.45 | 0.94 |
| 11:aA:275:THR:C | 11:aA:278:LEU:HD11 | 1.85 | 0.94 |
| 11:aA:312:ASP:CA | 11:aA:315:LEU:H | 1.79 | 0.94 |
| 11:aA:426:ARG:HH21 | 11:aA:496:ARG:CD | 1.80 | 0.94 |
| 11:aA:632:ILE:CG2 | 11:aA:634:ALA:N | 2.25 | 0.94 |
| 4:M1:190:ARG:NH1 | 4:M1:202:SER:HB2 | 1.82 | 0.94 |
| 1:Z:131:GLN:CB | 1:X5:17:LYS:HZ1 | 1.79 | 0.94 |
| 3:FA:36:LYS:CB | 3:FA:156:LEU:HD13 | 1.98 | 0.94 |
| 3:JA:120:LEU:O | 11:aA:361:ALA:CB | 2.16 | 0.94 |
| 2:KA:18:PHE:CE2 | 3:LA:48:ALA:HB1 | 2.02 | 0.94 |
| 4:MA:251:ASN:HD22 | 4:MA:251:ASN:H | 1.16 | 0.94 |
| 5:NA:1:MET:CB | 5:NA:3:VAL:HG23 | 1.96 | 0.94 |
| 5:N3:1:MET:CB | 5:N3:3:VAL:HG23 | 1.96 | 0.94 |
| 3:U4:120:LEU:HG | 4:M4:254:LEU:CD2 | 1.96 | 0.94 |
| 2:E4:1:MET:H2 | 4:M4:10:ARG:HH21 | 0.96 | 0.94 |
| 3:F4:88:ILE:HG12 | 11:aA:140:GLN:HE21 | 1.31 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:L4:71:GLY:CA | 11:aA:82:GLN:CG | 2.45 | 0.94 |
| 4:M4:217:VAL:HG22 | 5:Z4:30:PRO:HD3 | 1.44 | 0.94 |
| 12:O4:201:CYC:CMA | 5:Z4:53:LEU:CD1 | 2.46 | 0.94 |
| 8:A5:112:VAL:HA | 1:F5:75:THR:HB | 1.47 | 0.94 |
| 8:a5:102:THR:HB | 8:a5:103:PRO:HD3 | 1.48 | 0.94 |
| 1:b5:5:ILE:HD13 | 10:k5:46:PHE:CZ | 2.01 | 0.94 |
| 3:L6:125:ARG:HD2 | 1:b7:69:GLY:HA3 | 0.96 | 0.94 |
| 6:M6:117:MET:HE3 | 3:H6:77:ARG:NH1 | 1.56 | 0.94 |
| 10:j5:766:ALA:HB2 | 8:K7:14:GLU:OE2 | 1.65 | 0.94 |
| 10:j5:1025:LEU:HA | 10:j5:1030:ILE:HG22 | 1.49 | 0.94 |
| 10:j5:1025:LEU:HA | 10:j5:1030:ILE:CG2 | 1.98 | 0.94 |
| 10:k5:965:GLN:N | 1:n7:69:GLY:CA | 2.24 | 0.94 |
| 8:c7:96:ILE:HG13 | 8:c7:152:TYR:CD2 | 2.02 | 0.94 |
| 8:u7:27:LYS:HE3 | 1:v7:35:ALA:CB | 1.87 | 0.94 |
| 4:M8:140:ARG:NH2 | 5:Z8:26:LEU:HA | 1.83 | 0.94 |
| 4:M8:140:ARG:HD2 | 4:M8:214:GLY:O | 1.66 | 0.94 |
| 4:M8:144:ARG:CG | 4:M8:204:ILE:HD13 | 1.98 | 0.94 |
| 4:M8:235:PHE:CB | 12:M8:301:CYC:CAA | 2.46 | 0.94 |
| 12:M8:302:CYC:HBC1 | 3:S8:78:ARG:O | 1.68 | 0.94 |
| 2:N8:115:GLU:CD | 5:Z8:32:PRO:HG2 | 1.92 | 0.94 |
| 3:O8:111:ASN:O | 5:Z8:67:ILE:HG21 | 1.65 | 0.94 |
| 4:M9:163:ASN:HD21 | 12:V9:201:CYC:HMA1 | 1.25 | 0.94 |
| 5:Z8:37:HIS:CE1 | 12:Z8:301:CYC:CMA | 2.50 | 0.94 |
| 5:Z8:39:PRO:HG3 | 12:Z8:301:CYC:HHD | 1.48 | 0.94 |
| 3:J9:70:GLY:HA3 | 11:a9:356:ALA:HB1 | 1.47 | 0.94 |
| 3:J9:120:LEU:O | 11:a9:361:ALA:CB | 2.16 | 0.94 |
| 12:G1:201:CYC:HMD1 | 12:G1:201:CYC:HC | 1.33 | 0.94 |
| 11:a9:31:SER:HG | 11:a9:34:ILE:HB | 0.91 | 0.94 |
| 11:aA:668:TYR:HH | 2:K1:115:GLU:HG3 | 1.25 | 0.94 |
| 11:aA:694:ARG:HH22 | 4:M1:51:ARG:NH2 | 1.56 | 0.94 |
| 3:LA:52:ILE:HD11 | 3:LA:87:GLU:CG | 1.97 | 0.94 |
| 4:MA:158:PHE:O | 3:VA:108:ARG:CD | 2.15 | 0.94 |
| 2:OA:60:TYR:HB3 | 2:OA:67:THR:HG23 | 1.47 | 0.94 |
| 3:J3:107:ASP:CG | 11:a9:632:ILE:HG12 | 1.92 | 0.94 |
| 3:L2:65:ASP:OD2 | 1:h7:64:ASP:CG | 2.10 | 0.94 |
| 12:G4:201:CYC:HMD1 | 12:G4:201:CYC:HC | 1.33 | 0.94 |
| 3:O4:119:ALA:HB1 | 5:Z4:72:GLU:HB2 | 1.50 | 0.94 |
| 8:I5:37:LEU:HD21 | 1:J5:27:LEU:CD1 | 1.98 | 0.94 |
| 10:j5:825:ASN:OD1 | 10:j5:854:LEU:CD1 | 2.14 | 0.94 |
| 10:j5:1018:LEU:CD1 | 10:j5:1035:PHE:HZ | 1.61 | 0.94 |
| 10:k5:930:LEU:HB3 | 1:D7:33:THR:HG21 | 1.49 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:M8:301:CYC:C4B | 3:Y8:88:ILE:HG21 | 1.98 | 0.94 |
| 3:Q8:102:ALA:HB2 | 3:Q8:166:LYS:HZ1 | 1.28 | 0.94 |
| 11:a9:601:ALA:O | 11:a9:604:ALA:CB | 2.15 | 0.94 |
| 11:aA:694:ARG:HH12 | 4:M1:51:ARG:NH2 | 1.57 | 0.94 |
| 1:A:76:ARG:NH1 | 10:k5:262:TYR:CE2 | 2.35 | 0.94 |
| 4:MA:51:ARG:HH21 | 11:aA:430:ARG:CD | 1.79 | 0.94 |
| 3:B4:108:ARG:O | 4:M4:61:ASN:CB | 2.16 | 0.94 |
| 3:L3:88:ILE:HG13 | 11:a9:742:GLN:HE22 | 1.21 | 0.94 |
| 3:L3:111:ASN:O | 11:a9:711:SER:CB | 2.16 | 0.94 |
| 3:F4:107:ASP:C | 4:M4:6:THR:O | 2.10 | 0.94 |
| 3:H4:119:ALA:HB1 | 11:aA:266:ASN:CB | 1.96 | 0.94 |
| 3:Q4:97:LEU:HA | 3:Q4:163:TYR:CE2 | 2.03 | 0.94 |
| 8:G5:115:MET:HE1 | 12:G5:201:CYC:C1B | 1.97 | 0.94 |
| 8:S5:110:ILE:HD11 | 10:j5:533:LEU:HD11 | 1.48 | 0.94 |
| 8:U5:102:THR:HB | 8:U5:103:PRO:HD3 | 1.48 | 0.94 |
| 10:k5:929:PRO:HG2 | 1:D7:147:LYS:CG | 1.97 | 0.94 |
| 2:A6:60:TYR:HB3 | 2:A6:67:THR:HG23 | 1.47 | 0.94 |
| 8:q7:45:GLU:OE1 | 3:H1:125:ARG:CZ | 2.15 | 0.94 |
| 8:u7:90:ARG:CD | 1:v7:18:TYR:CD1 | 2.51 | 0.94 |
| 4:M8:139:VAL:CG2 | 4:M8:216:ASN:CA | 2.46 | 0.94 |
| 12:O8:201:CYC:HMA2 | 5:Z8:53:LEU:HD13 | 1.50 | 0.94 |
| 2:E9:2:LYS:HZ1 | 2:I9:17:ARG:HH12 | 1.08 | 0.94 |
| 3:HA:59:LEU:HD21 | 12:HA:202:CYC:HBC2 | 1.47 | 0.93 |
| 12:C4:201:CYC:HMD1 | 12:C4:201:CYC:HC | 1.33 | 0.93 |
| 12:W3:201:CYC:HMD1 | 12:W3:201:CYC:HC | 1.34 | 0.93 |
| 4:M4:197:ASP:HB3 | 5:Z4:52:ARG:CG | 1.97 | 0.93 |
| 3:Y4:88:ILE:HG22 | 3:Y4:91:ARG:HH22 | 1.30 | 0.93 |
| 10:j5:1064:LYS:HD2 | 10:j5:1065:HIS:CD2 | 2.03 | 0.93 |
| 10:k5:1015:TYR:OH | 8:k7:110:ILE:CG2 | 2.15 | 0.93 |
| 8:i7:104:ILE:HG21 | 8:i7:155:TYR:HE2 | 1.33 | 0.93 |
| 3:B8:119:ALA:HB2 | 4:M8:69:ILE:HG21 | 0.95 | 0.93 |
| 8:u7:37:LEU:HD21 | 1:v7:24:LEU:HD22 | 1.47 | 0.93 |
| 8:u7:37:LEU:HD12 | 1:v7:28:LYS:HE3 | 1.45 | 0.93 |
| 12:X8:201:CYC:HMD1 | 12:X8:201:CYC:HC | 1.33 | 0.93 |
| 2:N8:112:GLY:HA3 | 5:Z8:33:GLY:C | 1.93 | 0.93 |
| 5:N9:54:LEU:HD22 | 3:T9:84:ARG:NH1 | 1.83 | 0.93 |
| 2:A2:60:TYR:HB3 | 2:A2:67:THR:HG23 | 1.47 | 0.93 |
| 4:MA:258:LYS:CG | 3:VA:111:ASN:HD21 | 1.80 | 0.93 |
| 3:P1:115:GLU:CB | 5:N1:3:VAL:HG11 | 1.99 | 0.93 |
| 3:J3:84:ARG:HH22 | 11:a9:670:LEU:CA | 1.79 | 0.93 |
| 12:B1:202:CYC:HBA2 | 11:aA:684:ASN:CA | 1.97 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:A5:115:MET:HE1 | 12:A5:201:CYC:C1B | 1.97 | 0.93 |
| 8:U5:75:GLU:OE2 | 6:M6:32:MET:CE | 2.16 | 0.93 |
| 8:g7:63:PRO:HD2 | 11:aA:336:ILE:HG23 | 1.45 | 0.93 |
| 8:a7:29:PHE:HE1 | 8:a7:99:GLY:HA3 | 1.29 | 0.93 |
| 12:N8:201:CYC:HMD1 | 12:N8:201:CYC:HC | 1.34 | 0.93 |
| 3:L9:109:CYS:O | 11:a9:532:ALA:HB2 | 1.68 | 0.93 |
| 4:M9:158:PHE:O | 3:V9:108:ARG:CD | 2.15 | 0.93 |
| 5:Z8:22:LEU:CD2 | 5:Z8:26:LEU:CG | 2.38 | 0.93 |
| 11:a9:93:LEU:CD2 | 11:a9:252:ARG:HH12 | 1.80 | 0.93 |
| 11:aA:312:ASP:HA | 11:aA:315:LEU:H | 1.32 | 0.93 |
| 11:aA:348:GLN:HE21 | 11:aA:348:GLN:H | 0.94 | 0.93 |
| 11:aA:632:ILE:HG22 | 11:aA:634:ALA:H | 0.77 | 0.93 |
| 1:A:158:SER:HB3 | 1:R5:11:ASN:CG | 1.93 | 0.93 |
| 4:MA:190:ARG:NH1 | 4:MA:202:SER:HB2 | 1.82 | 0.93 |
| 2:G3:107:ASP:OD1 | 3:L3:77:ARG:NH2 | 2.02 | 0.93 |
| 12:A3:201:CYC:HMD1 | 12:A3:201:CYC:HC | 1.34 | 0.93 |
| 3:F3:119:ALA:CB | 4:M3:41:ASN:HD21 | 1.81 | 0.93 |
| 3:U4:120:LEU:HD22 | 3:U4:122:THR:OG1 | 1.69 | 0.93 |
| 3:L4:71:GLY:H | 11:aA:82:GLN:HG2 | 1.12 | 0.93 |
| 2:N4:14:SER:HB2 | 5:Z4:62:ARG:CD | 1.95 | 0.93 |
| 2:N4:112:GLY:N | 5:Z4:34:LEU:CA | 2.31 | 0.93 |
| 8:I5:29:PHE:HE1 | 8:I5:99:GLY:HA3 | 1.29 | 0.93 |
| 10:j5:779:ASP:OD2 | 12:L7:201:CYC:HMA2 | 1.68 | 0.93 |
| 10:k5:631:HIS:HD2 | 10:k5:664:MET:CE | 1.80 | 0.93 |
| 10:k5:1025:LEU:HA | 10:k5:1030:ILE:CG2 | 1.98 | 0.93 |
| 8:a7:63:PRO:HD2 | 11:a9:336:ILE:HG22 | 1.12 | 0.93 |
| 8:c7:12:ASP:N | 1:d7:94:TYR:OH | 2.00 | 0.93 |
| 1:d7:77:ARG:CZ | 9:x7:63:ALA:HB3 | 1.98 | 0.93 |
| 8:u7:27:LYS:CD | 1:v7:35:ALA:HA | 1.98 | 0.93 |
| 3:U8:114:LYS:CE | 4:M8:13:LYS:HZ1 | 1.74 | 0.93 |
| 4:M8:235:PHE:CB | 12:M8:301:CYC:C3A | 2.46 | 0.93 |
| 4:M9:190:ARG:NH1 | 4:M9:202:SER:HB2 | 1.82 | 0.93 |
| 12:O9:201:CYC:HMD1 | 12:O9:201:CYC:HC | 1.33 | 0.93 |
| 3:H9:108:ARG:HH12 | 11:a9:448:ASN:HD21 | 1.14 | 0.93 |
| 12:EA:201:CYC:HMD1 | 12:EA:201:CYC:HC | 1.34 | 0.93 |
| 4:MA:188:LEU:HG | 3:VA:84:ARG:CZ | 1.99 | 0.93 |
| 12:YA:201:CYC:HMD1 | 12:YA:201:CYC:HC | 1.34 | 0.93 |
| 4:M3:120:LEU:HD21 | 3:X3:84:ARG:CZ | 1.97 | 0.93 |
| 8:Q5:17:TYR:CB | 1:R5:45:SER:HB3 | 1.99 | 0.93 |
| 8:U5:75:GLU:HB2 | 6:M6:43:TRP:NE1 | 1.82 | 0.93 |
| 10:j5:729:ILE:CD1 | 1:J7:64:ASP:OD1 | 2.15 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:v7:136:VAL:HG13 | 11:aA:342:ARG:HH12 | 1.32 | 0.93 |
| 3:F8:109:CYS:O | 4:M8:5:THR:HG22 | 1.68 | 0.93 |
| 3:L8:68:ARG:HB3 | 11:a9:81:ASP:HA | 1.48 | 0.93 |
| 4:M8:57:THR:HA | 4:M8:60:LYS:HE3 | 1.50 | 0.93 |
| 12:U9:201:CYC:HMD1 | 12:U9:201:CYC:HC | 1.33 | 0.93 |
| 11:aA:56:ILE:CD1 | 11:aA:612:TYR:CE2 | 2.51 | 0.93 |
| 4:M1:251:ASN:HD22 | 4:M1:251:ASN:H | 1.16 | 0.93 |
| 4:M1:273:ILE:HG12 | 3:Z1:77:ARG:HH21 | 1.33 | 0.93 |
| 1:A:110:ASN:ND2 | 10:k5:462:TYR:OH | 1.96 | 0.93 |
| 3:FA:68:ARG:NH1 | 3:ZA:68:ARG:NH2 | 2.17 | 0.93 |
| 2:IA:31:PHE:CE2 | 3:JA:31:VAL:CA | 2.45 | 0.93 |
| 5:NA:54:LEU:CD1 | 12:TA:301:CYC:NB | 2.30 | 0.93 |
| 3:L3:119:ALA:O | 11:a9:817:LEU:HD11 | 1.67 | 0.93 |
| 4:M3:190:ARG:NH1 | 4:M3:202:SER:HB2 | 1.82 | 0.93 |
| 5:N3:31:TRP:CD1 | 2:S3:16:GLY:HA3 | 2.02 | 0.93 |
| 4:M4:100:SER:HB3 | 3:Q4:1:MET:HE3 | 0.95 | 0.93 |
| 4:M4:232:VAL:N | 12:M4:301:CYC:HBB3 | 1.84 | 0.93 |
| 12:R4:201:CYC:HMD1 | 12:R4:201:CYC:HC | 1.33 | 0.93 |
| 8:G5:103:PRO:HA | 10:j5:557:VAL:HG11 | 1.48 | 0.93 |
| 9:z5:14:LEU:HD12 | 9:z5:15:LYS:H | 1.33 | 0.93 |
| 10:k5:275:THR:CG2 | 10:k5:286:VAL:CG1 | 2.47 | 0.93 |
| 3:H8:81:ALA:HB2 | 3:H8:84:ARG:HH21 | 1.32 | 0.93 |
| 4:M8:268:ARG:C | 4:M8:269:SER:O | 1.90 | 0.93 |
| 3:J9:111:ASN:O | 11:a9:518:ALA:HB3 | 1.68 | 0.93 |
| 11:aA:93:LEU:HD23 | 11:aA:252:ARG:HH11 | 1.34 | 0.93 |
| 11:aA:326:ILE:O | 11:aA:329:ASN:O | 1.87 | 0.93 |
| 12:I1:201:CYC:HMD1 | 12:I1:201:CYC:HC | 1.33 | 0.93 |
| 4:M1:120:LEU:HD21 | 3:X1:84:ARG:CZ | 1.97 | 0.93 |
| 3:HA:82:CYS:SG | 12:HA:202:CYC:HAC2 | 2.08 | 0.93 |
| 3:LA:44:ILE:CG2 | 3:LA:90:LEU:HD21 | 1.98 | 0.93 |
| 4:MA:273:ILE:HD11 | 3:VA:75:PRO:CD | 1.93 | 0.93 |
| 12:QA:201:CYC:CGA | 3:TA:67:ILE:HG21 | 1.96 | 0.93 |
| 3:TA:25:ASN:HB3 | 2:X4:65:TYR:N | 1.72 | 0.93 |
| 12:WA:201:CYC:HMD1 | 12:WA:201:CYC:HC | 1.33 | 0.93 |
| 2:K4:15:GLN:O | 11:aA:241:VAL:HG11 | 1.57 | 0.93 |
| 4:M4:82:ILE:CD1 | 12:M4:301:CYC:O1D | 2.16 | 0.93 |
| 12:M4:301:CYC:HMC3 | 3:Y4:72:ASN:CB | 1.98 | 0.93 |
| 12:M4:301:CYC:C4B | 3:Y4:88:ILE:HD12 | 1.98 | 0.93 |
| 2:N4:111:ALA:CA | 5:Z4:34:LEU:HD12 | 1.98 | 0.93 |
| 8:W5:11:ALA:HB3 | 1:X5:94:TYR:CZ | 2.04 | 0.93 |
| 6:M6:104:ARG:NH1 | 2:G6:16:GLY:CA | 2.31 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 9:i5:18:ARG:CB | 9:i5:22:GLU:OE2 | 2.17 | 0.93 |
| 10:k5:36:ASN:HB2 | 10:k5:39:GLU:HB2 | 1.51 | 0.93 |
| 12:E1:201:CYC:HMD1 | 12:E1:201:CYC:HC | 1.34 | 0.93 |
| 2:A8:60:TYR:HB3 | 2:A8:67:THR:HG23 | 1.47 | 0.93 |
| 3:F8:77:ARG:CD | 11:a9:146:ARG:HH12 | 1.80 | 0.93 |
| 3:L9:44:ILE:CG2 | 3:L9:90:LEU:HD21 | 1.98 | 0.93 |
| 4:M9:188:LEU:HG | 3:V9:84:ARG:CZ | 1.99 | 0.93 |
| 5:Z8:37:HIS:CG | 12:Z8:301:CYC:C1B | 2.51 | 0.93 |
| 11:a9:710:THR:CG2 | 11:a9:807:GLN:HB3 | 1.99 | 0.93 |
| 11:aA:31:SER:HG | 11:aA:34:ILE:HB | 0.94 | 0.93 |
| 11:aA:800:THR:HG22 | 12:aA:901:CYC:CBA | 1.99 | 0.93 |
| 12:S1:201:CYC:HMD1 | 12:S1:201:CYC:HC | 1.34 | 0.93 |
| 12:I3:201:CYC:HMD1 | 12:I3:201:CYC:HC | 1.33 | 0.93 |
| 3:J3:119:ALA:O | 11:a9:803:ASN:HA | 1.66 | 0.93 |
| 12:H2:201:CYC:HBB2 | 6:M2:243:ALA:HB2 | 1.49 | 0.93 |
| 12:B3:202:CYC:CAA | 11:a9:684:ASN:CB | 2.42 | 0.93 |
| 12:A4:201:CYC:HMD1 | 12:A4:201:CYC:HC | 1.33 | 0.93 |
| 12:H4:201:CYC:HBB2 | 11:aA:259:ALA:CB | 1.99 | 0.93 |
| 4:M4:217:VAL:HG22 | 5:Z4:30:PRO:CB | 1.98 | 0.93 |
| 4:M4:217:VAL:CG2 | 5:Z4:30:PRO:CD | 2.46 | 0.93 |
| 1:f5:19:LEU:CD1 | 10:j5:172:LEU:HD11 | 1.99 | 0.93 |
| 1:b5:114:GLU:CB | 10:k5:491:THR:HG23 | 1.98 | 0.93 |
| 10:j5:289:SER:HB3 | 10:j5:292:GLU:OE2 | 1.69 | 0.93 |
| 10:j5:357:LEU:HD22 | 10:j5:378:TYR:HB3 | 1.47 | 0.93 |
| 10:k5:1055:SER:HG | 12:k5:1203:CYC:HBB2 | 1.32 | 0.93 |
| 10:k5:1064:LYS:HD2 | 10:k5:1065:HIS:CD2 | 2.03 | 0.93 |
| 8:I7:25:ARG:NH2 | 8:W7:25:ARG:HB2 | 1.81 | 0.93 |
| 3:O8:119:ALA:HB1 | 5:Z8:72:GLU:CG | 1.99 | 0.93 |
| 2:R8:64:PRO:HG2 | 3:T9:21:GLU:HB2 | 1.50 | 0.93 |
| 4:MA:274:VAL:HA | 3:VA:77:ARG:HG3 | 1.45 | 0.93 |
| 3:J3:120:LEU:HD21 | 11:a9:800:THR:HG21 | 0.93 | 0.93 |
| 3:B4:116:THR:CA | 4:M4:56:MET:HG2 | 1.98 | 0.93 |
| 8:G5:106:GLU:OE1 | 10:j5:557:VAL:HB | 1.67 | 0.93 |
| 1:f5:3:ASP:OD2 | 10:j5:21:MET:CB | 2.17 | 0.93 |
| 12:P5:201:CYC:HBB2 | 10:k5:623:VAL:HG21 | 1.48 | 0.93 |
| 6:M6:283:VAL:HG12 | 8:Y7:75:GLU:HB3 | 0.93 | 0.93 |
| 10:j5:322:LYS:HD2 | 10:j5:336:ARG:HH12 | 1.34 | 0.93 |
| 10:j5:1018:LEU:HD12 | 10:j5:1035:PHE:CZ | 2.01 | 0.93 |
| 10:k5:1046:ARG:NH2 | 8:k7:9:VAL:HG11 | 1.83 | 0.93 |
| 2:X8:74:TYR:OH | 2:S9:35:THR:C | 2.12 | 0.93 |
| 3:L8:68:ARG:HB2 | 11:a9:82:GLN:HB2 | 1.51 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:F1:201:CYC:HMA1 | 4:M1:36:TYR:O | 1.65 | 0.93 |
| 5:N9:54:LEU:N | 12:T9:301:CYC:CBA | 2.30 | 0.93 |
| 3:H9:113:LEU:HD21 | 12:H9:202:CYC:CMB | 1.99 | 0.93 |
| 3:J9:119:ALA:CA | 11:a9:365:LYS:HE2 | 1.99 | 0.93 |
| 12:A2:201:CYC:HMD1 | 12:A2:201:CYC:HC | 1.34 | 0.93 |
| 3:JA:65:ASP:CB | 11:aA:354:VAL:HG21 | 1.99 | 0.93 |
| 3:H3:115:GLU:HB2 | 11:a9:786:GLU:OE1 | 1.66 | 0.93 |
| 3:J3:77:ARG:NH2 | 2:K3:107:ASP:OD1 | 2.02 | 0.93 |
| 12:K3:201:CYC:HMD1 | 12:K3:201:CYC:HC | 1.34 | 0.93 |
| 12:B4:202:CYC:HHA | 4:M4:54:ALA:HB2 | 1.49 | 0.93 |
| 12:Q3:201:CYC:HMD1 | 12:Q3:201:CYC:HC | 1.34 | 0.93 |
| 2:N4:111:ALA:O | 5:Z4:34:LEU:CG | 2.14 | 0.93 |
| 8:U7:49:ARG:NH1 | 1:l7:114:GLU:OE2 | 2.02 | 0.93 |
| 8:o7:27:LYS:CD | 1:p7:35:ALA:HA | 1.99 | 0.93 |
| 3:L8:69:PRO:O | 11:a9:82:GLN:CB | 2.16 | 0.93 |
| 4:M8:128:ALA:CB | 4:M8:142:PHE:CE1 | 2.52 | 0.93 |
| 4:M8:205:ASP:HB2 | 5:Z8:59:ARG:HE | 1.30 | 0.93 |
| 4:M8:217:VAL:HG21 | 5:Z8:30:PRO:CG | 1.71 | 0.93 |
| 3:O8:107:ASP:CG | 5:Z8:66:ARG:CD | 2.37 | 0.93 |
| 3:L9:37:ARG:NH1 | 3:L9:97:LEU:O | 2.02 | 0.93 |
| 12:W9:201:CYC:HMD1 | 12:W9:201:CYC:HC | 1.33 | 0.93 |
| 11:a9:312:ASP:C | 11:a9:315:LEU:H | 1.74 | 0.93 |
| 11:aA:632:ILE:CG2 | 11:aA:634:ALA:HB2 | 1.98 | 0.93 |
| 12:KA:201:CYC:HMD1 | 12:KA:201:CYC:HC | 1.34 | 0.93 |
| 3:LA:37:ARG:NH1 | 3:LA:97:LEU:O | 2.02 | 0.93 |
| 3:LA:109:CYS:O | 11:aA:532:ALA:HB2 | 1.69 | 0.93 |
| 4:MA:274:VAL:CB | 3:VA:77:ARG:HG2 | 1.98 | 0.93 |
| 12:A1:201:CYC:HMD1 | 12:A1:201:CYC:HC | 1.34 | 0.93 |
| 12:O3:201:CYC:HMD1 | 12:O3:201:CYC:HC | 1.34 | 0.93 |
| 12:Y3:201:CYC:HMD1 | 12:Y3:201:CYC:HC | 1.33 | 0.93 |
| 3:L4:69:PRO:O | 11:aA:82:GLN:CB | 2.16 | 0.93 |
| 4:M4:94:TRP:CE3 | 3:Q4:88:ILE:HA | 2.04 | 0.93 |
| 4:M4:190:ARG:NH1 | 4:M4:202:SER:HB2 | 1.82 | 0.93 |
| 4:M4:226:SER:OG | 3:Y4:88:ILE:HG23 | 1.68 | 0.93 |
| 1:R5:124:ALA:CB | 1:Z5:64:ASP:OD1 | 2.16 | 0.93 |
| 8:U5:80:LEU:CG | 6:M6:28:ASN:HB2 | 1.81 | 0.93 |
| 6:M6:69:ALA:HB1 | 3:H6:10:VAL:HG13 | 1.50 | 0.93 |
| 10:j5:1047:LYS:O | 10:j5:1051:GLU:CB | 2.17 | 0.93 |
| 10:j5:1052:PRO:HB3 | 11:aA:32:ARG:NH2 | 1.83 | 0.93 |
| 10:k5:1018:LEU:CD1 | 10:k5:1035:PHE:HZ | 1.61 | 0.93 |
| 10:k5:1143:LEU:CG | 8:k7:106:GLU:OE1 | 2.16 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:I6:201:CYC:HMD1 | 12:I6:201:CYC:HC | 1.34 | 0.93 |
| 8:O7:22:GLU:O | 8:O7:25:ARG:HG3 | 1.69 | 0.93 |
| 8:o7:2:SER:HB3 | 1:p7:5:ILE:CG2 | 1.99 | 0.93 |
| 5:N9:50:LEU:CD2 | 12:T9:301:CYC:O1D | 2.17 | 0.93 |
| 3:H9:78:ARG:HD3 | 12:H9:202:CYC:CGD | 1.99 | 0.93 |
| 11:a9:476:ARG:HH12 | 11:a9:488:SER:CB | 1.71 | 0.93 |
| 11:a9:632:ILE:CG2 | 11:a9:634:ALA:HB2 | 1.98 | 0.93 |
| 4:M1:81:ASP:H | 3:X1:111:ASN:HD22 | 1.16 | 0.93 |
| 5:N1:34:LEU:CB | 3:T1:84:ARG:HD3 | 1.99 | 0.93 |
| 2:A3:16:GLY:HA2 | 11:a9:677:GLN:HE22 | 1.25 | 0.92 |
| 3:B3:82:CYS:HG | 12:B3:202:CYC:HAC2 | 1.29 | 0.92 |
| 3:Z3:120:LEU:HD21 | 4:M3:181:GLN:NE2 | 1.84 | 0.92 |
| 12:B4:202:CYC:HBB1 | 4:M4:61:ASN:HB2 | 1.49 | 0.92 |
| 12:V4:201:CYC:HMD1 | 12:V4:201:CYC:HC | 1.33 | 0.92 |
| 8:Q5:17:TYR:HB3 | 1:R5:45:SER:HB3 | 1.49 | 0.92 |
| 8:Q5:17:TYR:HD2 | 1:R5:93:THR:HG21 | 1.32 | 0.92 |
| 10:k5:362:LYS:HE2 | 10:k5:363:HIS:CD2 | 2.03 | 0.92 |
| 10:k5:929:PRO:HG3 | 1:D7:147:LYS:HE2 | 1.49 | 0.92 |
| 10:k5:974:LEU:CD1 | 1:p7:106:GLU:OE2 | 2.16 | 0.92 |
| 10:k5:1052:PRO:HB3 | 11:a9:32:ARG:NH2 | 1.82 | 0.92 |
| 8:g7:63:PRO:HD2 | 11:aA:336:ILE:HG22 | 1.12 | 0.92 |
| 8:a7:102:THR:HB | 8:a7:103:PRO:HD3 | 1.48 | 0.92 |
| 8:c7:16:ARG:N | 1:d7:90:ARG:HD2 | 1.82 | 0.92 |
| 8:q7:75:GLU:O | 11:aA:53:VAL:CG1 | 2.16 | 0.92 |
| 4:M8:223:GLY:O | 12:M8:301:CYC:CBA | 2.15 | 0.92 |
| 3:O8:119:ALA:C | 5:Z8:72:GLU:OE2 | 2.12 | 0.92 |
| 12:S9:201:CYC:HMD1 | 12:S9:201:CYC:HC | 1.33 | 0.92 |
| 11:a9:426:ARG:NH2 | 11:a9:496:ARG:HD3 | 1.84 | 0.92 |
| 11:aA:636:ALA:O | 11:aA:774:PHE:HD2 | 1.49 | 0.92 |
| 11:aA:709:CYS:O | 11:aA:807:GLN:HB2 | 1.70 | 0.92 |
| 11:aA:710:THR:CG2 | 11:aA:807:GLN:HB3 | 1.99 | 0.92 |
| 11:aA:817:LEU:HD11 | 3:L1:119:ALA:O | 1.68 | 0.92 |
| 12:GA:201:CYC:HMD1 | 12:GA:201:CYC:HC | 1.33 | 0.92 |
| 12:G3:201:CYC:HMD1 | 12:G3:201:CYC:HC | 1.33 | 0.92 |
| 5:N3:3:VAL:HG11 | 3:P3:115:GLU:CB | 1.99 | 0.92 |
| 3:F4:109:CYS:O | 4:M4:5:THR:HG22 | 1.68 | 0.92 |
| 12:I4:201:CYC:HMD1 | 12:I4:201:CYC:HC | 1.34 | 0.92 |
| 4:M4:92:GLU:OE1 | 5:Z4:30:PRO:HD3 | 1.66 | 0.92 |
| 8:G5:119:LEU:HD13 | 12:G5:201:CYC:C1A | 1.98 | 0.92 |
| 8:U5:48:GLU:HA | 6:M6:34:ARG:HH12 | 1.31 | 0.92 |
| 9:z5:18:ARG:CB | 9:z5:22:GLU:OE2 | 2.17 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:1006:ASP:OD1 | 10:j5:1065:HIS:NE2 | 2.01 | 0.92 |
| 10:k5:1151:GLN:HA | 1:p7:122:PRO:HB3 | 1.51 | 0.92 |
| 8:O7:52:LYS:CE | 11:aA:29:ARG:NH1 | 2.26 | 0.92 |
| 8:g7:102:THR:HB | 8:g7:103:PRO:HD3 | 1.48 | 0.92 |
| 8:i7:20:PRO:CD | 8:s7:101:VAL:HG21 | 1.99 | 0.92 |
| 12:b7:201:CYC:CBB | 9:x7:21:ARG:NE | 2.32 | 0.92 |
| 8:c7:104:ILE:HG21 | 8:c7:155:TYR:HE2 | 1.33 | 0.92 |
| 2:E8:15:GLN:CG | 11:a9:163:ASP:HB2 | 1.99 | 0.92 |
| 9:x7:3:ARG:CZ | 9:x7:67:VAL:HG13 | 1.98 | 0.92 |
| 2:N8:112:GLY:H | 5:Z8:34:LEU:CB | 1.82 | 0.92 |
| 4:M9:6:THR:HG22 | 3:D9:108:ARG:C | 1.95 | 0.92 |
| 3:H9:82:CYS:SG | 12:H9:202:CYC:HAC2 | 2.10 | 0.92 |
| 3:J9:111:ASN:O | 11:a9:518:ALA:CA | 2.17 | 0.92 |
| 11:aA:476:ARG:HH11 | 11:aA:488:SER:CB | 1.69 | 0.92 |
| 11:aA:776:TYR:CD1 | 12:H1:201:CYC:C4B | 2.51 | 0.92 |
| 5:N1:22:LEU:CD1 | 5:N1:26:LEU:CD2 | 2.47 | 0.92 |
| 3:FA:151:GLY:N | 3:F9:150:ARG:NH2 | 2.16 | 0.92 |
| 3:JA:111:ASN:O | 11:aA:518:ALA:HB3 | 1.67 | 0.92 |
| 4:MA:181:GLN:CD | 3:VA:120:LEU:HD21 | 1.94 | 0.92 |
| 1:R5:107:ARG:O | 10:k5:520:ARG:NH1 | 2.02 | 0.92 |
| 8:W5:17:TYR:HB3 | 1:X5:45:SER:HB3 | 1.49 | 0.92 |
| 10:j5:289:SER:CB | 10:j5:292:GLU:OE2 | 2.17 | 0.92 |
| 10:j5:825:ASN:HB2 | 12:H7:201:CYC:HBB2 | 1.51 | 0.92 |
| 10:k5:748:ARG:NE | 8:E7:106:GLU:OE2 | 2.03 | 0.92 |
| 12:A6:201:CYC:HMD1 | 12:A6:201:CYC:HC | 1.34 | 0.92 |
| 2:X8:65:TYR:N | 3:T9:25:ASN:CB | 2.32 | 0.92 |
| 3:Q8:77:ARG:CA | 5:Z8:34:LEU:HB3 | 1.98 | 0.92 |
| 4:M9:185:ALA:CA | 12:V9:201:CYC:CGA | 2.48 | 0.92 |
| 5:N9:1:MET:HG3 | 3:R9:119:ALA:CB | 1.90 | 0.92 |
| 5:N9:62:ARG:NE | 2:S9:14:SER:HA | 1.78 | 0.92 |
| 5:Z8:5:THR:O | 5:Z8:5:THR:HG23 | 1.67 | 0.92 |
| 5:Z8:22:LEU:HD13 | 5:Z8:26:LEU:CD2 | 1.99 | 0.92 |
| 5:Z8:31:TRP:HB3 | 5:Z8:32:PRO:HD2 | 1.50 | 0.92 |
| 3:H9:116:THR:CG2 | 11:a9:449:ASN:HD21 | 1.83 | 0.92 |
| 11:aA:54:ARG:NH1 | 11:aA:609:LEU:O | 2.03 | 0.92 |
| 3:DA:108:ARG:C | 4:MA:6:THR:HG22 | 1.95 | 0.92 |
| 3:JA:111:ASN:O | 11:aA:518:ALA:CA | 2.17 | 0.92 |
| 3:JA:119:ALA:HB1 | 11:aA:365:LYS:HE2 | 1.50 | 0.92 |
| 5:NA:54:LEU:HD22 | 3:TA:84:ARG:NH1 | 1.83 | 0.92 |
| 3:TA:21:GLU:HB2 | 2:R4:64:PRO:HG2 | 1.50 | 0.92 |
| 2:G2:16:GLY:CA | 6:M2:104:ARG:NH1 | 2.31 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 5:N3:22:LEU:HD13 | 5:N3:26:LEU:CD2 | 1.99 | 0.92 |
| 12:T4:201:CYC:HMD1 | 12:T4:201:CYC:HC | 1.33 | 0.92 |
| 3:F4:107:ASP:HA | 4:M4:6:THR:O | 1.66 | 0.92 |
| 4:M4:128:ALA:CB | 4:M4:142:PHE:CZ | 2.52 | 0.92 |
| 12:J5:201:CYC:HBB2 | 9:i5:42:GLN:NE2 | 1.84 | 0.92 |
| 1:Z5:83:ARG:HH12 | 10:k5:379:PHE:HE2 | 1.18 | 0.92 |
| 10:j5:1043:GLU:CG | 8:e7:14:GLU:OE2 | 2.17 | 0.92 |
| 10:j5:1150:TYR:CE2 | 1:v7:69:GLY:C | 2.42 | 0.92 |
| 10:k5:1006:ASP:OD1 | 10:k5:1065:HIS:NE2 | 2.01 | 0.92 |
| 12:B8:202:CYC:HBB2 | 4:M8:61:ASN:HB3 | 0.92 | 0.92 |
| 4:M8:104:ALA:HB3 | 2:P8:14:SER:CA | 1.96 | 0.92 |
| 3:L9:48:ALA:HB1 | 2:K9:18:PHE:CE2 | 2.02 | 0.92 |
| 11:aA:798:SER:HG | 12:aA:901:CYC:CMA | 1.73 | 0.92 |
| 12:JA:202:CYC:NB | 11:aA:512:TYR:CB | 2.14 | 0.92 |
| 5:NA:22:LEU:CD1 | 5:NA:26:LEU:CD2 | 2.47 | 0.92 |
| 4:M3:118:TYR:CD2 | 3:X3:84:ARG:NH2 | 2.38 | 0.92 |
| 4:M3:196:TYR:HB2 | 2:Y3:14:SER:O | 1.70 | 0.92 |
| 4:M3:251:ASN:HD22 | 4:M3:251:ASN:H | 1.16 | 0.92 |
| 5:N3:66:ARG:HH12 | 3:R3:111:ASN:HD21 | 1.14 | 0.92 |
| 2:E4:15:GLN:CG | 11:aA:163:ASP:HB2 | 1.99 | 0.92 |
| 12:L5:201:CYC:HMA1 | 12:L5:201:CYC:NB | 1.84 | 0.92 |
| 8:M5:20:PRO:HB2 | 8:A5:100:ASP:CG | 1.95 | 0.92 |
| 8:O5:76:LYS:O | 8:O5:79:ALA:N | 2.02 | 0.92 |
| 8:A5:119:LEU:HD13 | 12:A5:201:CYC:C1A | 1.98 | 0.92 |
| 8:e5:38:ARG:CZ | 1:R5:144:ASP:OD1 | 2.17 | 0.92 |
| 8:W5:17:TYR:CB | 1:X5:45:SER:HB3 | 1.99 | 0.92 |
| 10:k5:289:SER:CB | 10:k5:292:GLU:OE2 | 2.17 | 0.92 |
| 10:k5:1018:LEU:HD12 | 10:k5:1035:PHE:CZ | 2.01 | 0.92 |
| 8:o7:90:ARG:CD | 1:p7:18:TYR:CD1 | 2.51 | 0.92 |
| 3:L9:14:LEU:CD1 | 11:a9:358:PRO:HB3 | 1.93 | 0.92 |
| 4:M9:77:LEU:HD11 | 3:Z9:115:GLU:CD | 1.93 | 0.92 |
| 4:M9:274:VAL:CB | 3:V9:77:ARG:CG | 2.47 | 0.92 |
| 5:N9:22:LEU:CD1 | 5:N9:26:LEU:CD2 | 2.47 | 0.92 |
| 12:J9:202:CYC:HBA2 | 11:a9:510:PHE:O | 1.66 | 0.92 |
| 11:aA:798:SER:HB3 | 11:aA:800:THR:HG22 | 1.49 | 0.92 |
| 5:N1:22:LEU:HD13 | 5:N1:26:LEU:CD2 | 1.99 | 0.92 |
| 1:Z:161:SER:CB | 1:X5:14:VAL:HB | 1.99 | 0.92 |
| 12:AA:201:CYC:HMD1 | 12:AA:201:CYC:HC | 1.33 | 0.92 |
| 12:CA:201:CYC:HMD1 | 12:CA:201:CYC:HC | 1.34 | 0.92 |
| 3:HA:126:SER:HB3 | 12:HA:202:CYC:CMC | 1.87 | 0.92 |
| 3:JA:109:CYS:C | 11:aA:518:ALA:HB2 | 1.95 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:MA:77:LEU:HD11 | 3:ZA:115:GLU:CD | 1.93 | 0.92 |
| 6:M2:39:ARG:HE | 8:O5:66:VAL:HG11 | 1.13 | 0.92 |
| 3:B3:108:ARG:O | 4:M3:6:THR:CG2 | 2.18 | 0.92 |
| 8:Q5:11:ALA:HB3 | 1:R5:94:TYR:CZ | 2.04 | 0.92 |
| 8:U5:83:ARG:HB3 | 6:M6:26:PHE:CD1 | 2.02 | 0.92 |
| 8:W5:17:TYR:HD2 | 1:X5:93:THR:HG21 | 1.32 | 0.92 |
| 3:F6:82:CYS:SG | 12:F6:201:CYC:CAC | 2.57 | 0.92 |
| 12:E8:201:CYC:HMD1 | 12:E8:201:CYC:HC | 1.33 | 0.92 |
| 8:u7:5:THR:OG1 | 1:v7:6:THR:CG2 | 2.18 | 0.92 |
| 3:F8:115:GLU:HG2 | 4:M8:3:VAL:CG2 | 2.00 | 0.92 |
| 3:L8:71:GLY:H | 11:a9:82:GLN:CG | 1.77 | 0.92 |
| 3:O8:104:VAL:CA | 5:Z8:61:LYS:CE | 2.47 | 0.92 |
| 4:M9:157:PHE:C | 3:V9:108:ARG:HD2 | 1.95 | 0.92 |
| 12:Q9:201:CYC:HMD1 | 12:Q9:201:CYC:HC | 1.33 | 0.92 |
| 2:G1:107:ASP:OD1 | 3:L1:77:ARG:NH2 | 2.02 | 0.92 |
| 11:a9:275:THR:N | 11:a9:278:LEU:HD11 | 1.84 | 0.92 |
| 11:a9:632:ILE:CG2 | 11:a9:634:ALA:N | 2.25 | 0.92 |
| 12:E2:201:CYC:HMD1 | 12:E2:201:CYC:HC | 1.34 | 0.92 |
| 3:B4:85:ASP:HB2 | 12:B4:202:CYC:H3C | 1.50 | 0.92 |
| 3:F4:108:ARG:NH2 | 4:M4:9:GLN:CG | 2.20 | 0.92 |
| 1:B5:14:VAL:HG11 | 10:k5:554:ASN:C | 1.95 | 0.92 |
| 1:f5:18:TYR:OH | 10:j5:161:ASP:O | 1.87 | 0.92 |
| 1:V5:83:ARG:CZ | 10:j5:649:PHE:HE2 | 1.82 | 0.92 |
| 10:j5:275:THR:CG2 | 10:j5:286:VAL:CG1 | 2.47 | 0.92 |
| 10:j5:1118:THR:O | 12:j5:1202:CYC:CMA | 2.17 | 0.92 |
| 10:k5:1047:LYS:O | 10:k5:1051:GLU:CB | 2.17 | 0.92 |
| 8:c7:17:TYR:HE2 | 1:d7:93:THR:HG1 | 1.15 | 0.92 |
| 8:u7:37:LEU:HD22 | 1:v7:24:LEU:CG | 2.00 | 0.92 |
| 3:F9:68:ARG:NH1 | 3:Z9:68:ARG:NH2 | 2.17 | 0.92 |
| 11:a9:326:ILE:O | 11:a9:329:ASN:O | 1.87 | 0.92 |
| 11:a9:476:ARG:HH11 | 11:a9:488:SER:HB3 | 1.32 | 0.92 |
| 11:aA:742:GLN:HE22 | 3:L1:88:ILE:HG13 | 1.19 | 0.92 |
| 12:U1:201:CYC:HMD1 | 12:U1:201:CYC:HC | 1.33 | 0.92 |
| 2:A1:16:GLY:HA2 | 11:aA:677:GLN:HE22 | 1.27 | 0.92 |
| 3:J3:85:ASP:CA | 11:a9:668:TYR:OH | 2.16 | 0.92 |
| 4:M3:120:LEU:HD22 | 2:Y3:115:GLU:OE2 | 1.69 | 0.92 |
| 3:B1:88:ILE:CB | 12:B1:202:CYC:HMB2 | 2.00 | 0.92 |
| 8:C5:37:LEU:HD21 | 1:D5:27:LEU:CD1 | 1.98 | 0.92 |
| 6:M6:243:ALA:HB2 | 12:H6:201:CYC:HBB2 | 1.49 | 0.92 |
| 10:j5:20:VAL:O | 10:j5:24:THR:HG22 | 1.69 | 0.92 |
| 10:j5:971:VAL:N | 12:j5:1202:CYC:CGD | 2.27 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:k5:966:SER:N | 1:p7:14:VAL:CG1 | 2.32 | 0.92 |
| 10:k5:1015:TYR:OH | 8:k7:110:ILE:HG22 | 1.67 | 0.92 |
| 10:k5:1076:GLU:C | 10:k5:1078:SER:N | 2.27 | 0.92 |
| 8:i7:43:LEU:HD21 | 8:i7:149:ALA:HB1 | 1.52 | 0.92 |
| 3:U8:114:LYS:HZ3 | 4:M8:13:LYS:CE | 1.77 | 0.92 |
| 3:F8:88:ILE:HG12 | 11:a9:140:GLN:HE21 | 1.33 | 0.92 |
| 4:M8:128:ALA:C | 4:M8:142:PHE:CZ | 2.48 | 0.92 |
| 3:J9:88:ILE:CD1 | 11:a9:512:TYR:CZ | 2.51 | 0.92 |
| 12:Y9:201:CYC:HMD1 | 12:Y9:201:CYC:HC | 1.34 | 0.92 |
| 3:HA:116:THR:CG2 | 11:aA:449:ASN:HD21 | 1.83 | 0.92 |
| 3:JA:119:ALA:CA | 11:aA:365:LYS:HE2 | 1.99 | 0.92 |
| 4:MA:185:ALA:CA | 12:VA:201:CYC:CGA | 2.48 | 0.92 |
| 3:B3:127:VAL:HG22 | 12:B3:202:CYC:H3C | 1.52 | 0.92 |
| 3:F4:115:GLU:HG2 | 4:M4:3:VAL:CB | 1.99 | 0.92 |
| 4:M4:57:THR:HA | 4:M4:60:LYS:HE3 | 1.50 | 0.92 |
| 4:M4:144:ARG:CZ | 5:Z4:59:ARG:NH1 | 2.31 | 0.92 |
| 4:M4:217:VAL:CG2 | 5:Z4:30:PRO:N | 2.33 | 0.92 |
| 4:M4:223:GLY:O | 12:M4:301:CYC:CBA | 2.17 | 0.92 |
| 6:M6:45:ILE:CD1 | 8:c7:78:THR:HG22 | 2.00 | 0.92 |
| 10:j5:1118:THR:O | 12:j5:1202:CYC:HMA1 | 1.69 | 0.92 |
| 10:k5:190:LEU:HD21 | 12:k5:1201:CYC:ND | 1.85 | 0.92 |
| 8:c7:43:LEU:HD21 | 8:c7:149:ALA:HB1 | 1.52 | 0.92 |
| 12:d7:201:CYC:NB | 9:x7:38:PHE:HE1 | 1.67 | 0.92 |
| 1:f7:10:ASN:OD1 | 9:y7:64:ASN:ND2 | 2.03 | 0.92 |
| 8:s7:102:THR:HB | 8:s7:103:PRO:HD3 | 1.48 | 0.92 |
| 3:U8:115:GLU:CG | 4:M8:74:LEU:HD12 | 1.99 | 0.92 |
| 4:M8:91:VAL:HG22 | 2:P8:14:SER:C | 1.94 | 0.92 |
| 4:M8:128:ALA:C | 4:M8:142:PHE:HE1 | 1.72 | 0.92 |
| 12:M8:302:CYC:OC | 3:S8:78:ARG:CD | 1.91 | 0.92 |
| 5:N9:61:LYS:HZ3 | 12:T9:301:CYC:HBB2 | 1.05 | 0.92 |
| 11:aA:795:ASP:O | 12:aA:901:CYC:CBB | 2.17 | 0.92 |
| 4:MA:274:VAL:CA | 3:VA:77:ARG:CD | 2.29 | 0.92 |
| 5:NA:50:LEU:CD2 | 12:TA:301:CYC:O1D | 2.17 | 0.92 |
| 12:O1:201:CYC:HMD1 | 12:O1:201:CYC:HC | 1.34 | 0.92 |
| 3:H2:10:VAL:HG13 | 6:M2:69:ALA:HB1 | 1.50 | 0.92 |
| 6:M2:279:ASP:O | 8:e7:76:LYS:NZ | 2.03 | 0.92 |
| 3:Z3:77:ARG:HH21 | 4:M3:273:ILE:HG12 | 1.33 | 0.92 |
| 4:M4:93:LEU:C | 4:M4:216:ASN:HD21 | 1.78 | 0.92 |
| 12:N4:201:CYC:HMD1 | 12:N4:201:CYC:HC | 1.34 | 0.92 |
| 12:P4:201:CYC:HMD1 | 12:P4:201:CYC:HC | 1.33 | 0.92 |
| 1:f5:3:ASP:OD2 | 10:j5:21:MET:HB3 | 1.69 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:931:VAL:CG2 | 1:J7:29:ALA:O | 2.18 | 0.92 |
| 10:k5:20:VAL:O | 10:k5:24:THR:HG22 | 1.69 | 0.92 |
| 1:R7:77:ARG:NH2 | 9:z7:62:GLY:O | 2.01 | 0.92 |
| 12:B7:201:CYC:HMA1 | 12:B7:201:CYC:NB | 1.85 | 0.92 |
| 8:G7:86:ASP:HB2 | 11:a9:579:PHE:HZ | 1.34 | 0.92 |
| 12:L9:201:CYC:HAB2 | 2:K9:24:LEU:HB3 | 1.52 | 0.92 |
| 3:H9:126:SER:CB | 12:H9:202:CYC:HMC2 | 1.97 | 0.92 |
| 11:a9:54:ARG:NH1 | 11:a9:609:LEU:O | 2.03 | 0.92 |
| 11:a9:632:ILE:HG22 | 11:a9:634:ALA:H | 0.77 | 0.92 |
| 11:aA:283:GLN:CB | 11:aA:284:PRO:HD3 | 1.91 | 0.92 |
| 4:M1:196:TYR:HB2 | 2:Y1:14:SER:O | 1.70 | 0.92 |
| 12:Y1:201:CYC:HMD1 | 12:Y1:201:CYC:HC | 1.33 | 0.92 |
| 3:JA:88:ILE:CD1 | 11:aA:512:TYR:CZ | 2.53 | 0.91 |
| 3:H3:78:ARG:NH2 | 11:a9:623:ASP:HB2 | 1.84 | 0.91 |
| 6:M2:53:LEU:HD21 | 8:i7:80:LEU:HG | 1.51 | 0.91 |
| 3:B1:68:ARG:HH12 | 3:V1:68:ARG:HH12 | 1.13 | 0.91 |
| 4:M4:27:HIS:HD1 | 4:M4:35:THR:N | 1.59 | 0.91 |
| 3:Q4:4:ALA:HB2 | 3:Q4:99:ALA:O | 1.70 | 0.91 |
| 8:C5:110:ILE:HD12 | 9:z5:15:LYS:HB3 | 1.51 | 0.91 |
| 1:d5:67:ARG:CZ | 10:j5:705:THR:OG1 | 2.19 | 0.91 |
| 10:k5:970:GLY:H | 1:n7:77:ARG:NH2 | 1.66 | 0.91 |
| 8:k7:66:VAL:HG12 | 11:a9:65:LEU:HD21 | 1.49 | 0.91 |
| 8:U7:29:PHE:HE1 | 8:U7:99:GLY:HA3 | 1.29 | 0.91 |
| 8:q7:66:VAL:HG12 | 11:aA:65:LEU:CD2 | 2.00 | 0.91 |
| 12:I8:201:CYC:HMD1 | 12:I8:201:CYC:HC | 1.34 | 0.91 |
| 3:Y8:89:ILE:CA | 3:Y8:92:TYR:HE2 | 1.53 | 0.91 |
| 12:DA:201:CYC:HBA2 | 11:aA:420:ASN:HB2 | 1.52 | 0.91 |
| 4:MA:163:ASN:HD21 | 12:VA:201:CYC:HMA1 | 1.24 | 0.91 |
| 3:L4:68:ARG:CD | 11:aA:81:ASP:CA | 2.48 | 0.91 |
| 4:M4:208:GLU:OE1 | 4:M4:222:ARG:NH2 | 2.03 | 0.91 |
| 4:M4:232:VAL:HG23 | 4:M4:235:PHE:HE2 | 1.35 | 0.91 |
| 3:O4:107:ASP:CG | 5:Z4:66:ARG:HB3 | 1.94 | 0.91 |
| 12:O4:201:CYC:HBA2 | 5:Z4:50:LEU:HD13 | 1.52 | 0.91 |
| 1:R5:106:GLU:CD | 10:k5:504:ASP:O | 2.13 | 0.91 |
| 12:K6:201:CYC:HC | 12:K6:201:CYC:HMD1 | 1.34 | 0.91 |
| 6:M6:127:SER:CB | 3:F6:84:ARG:NH2 | 2.20 | 0.91 |
| 10:j5:386:ILE:CG2 | 10:j5:395:SER:H | 1.83 | 0.91 |
| 10:j5:1050:PHE:HE2 | 1:r7:107:ARG:HH22 | 0.96 | 0.91 |
| 10:j5:1151:GLN:HA | 1:v7:122:PRO:CB | 2.01 | 0.91 |
| 10:k5:1143:LEU:CD1 | 8:k7:103:PRO:HA | 1.99 | 0.91 |
| 12:E6:201:CYC:HMD1 | 12:E6:201:CYC:HC | 1.34 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 12:H7:201:CYC:HMA1 | 12:H7:201:CYC:NB | 1.85 | 0.91 |
| 8:i7:39:ILE:HD11 | 8:i7:148:GLU:CG | 2.00 | 0.91 |
| 8:u7:2:SER:HB3 | 1:v7:5:ILE:CG2 | 1.99 | 0.91 |
| 3:F8:115:GLU:CB | 4:M8:3:VAL:HG13 | 2.00 | 0.91 |
| 3:L8:82:CYS:HB2 | 12:a9:901:CYC:HMD3 | 0.96 | 0.91 |
| 12:R8:201:CYC:HMD1 | 12:R8:201:CYC:HC | 1.33 | 0.91 |
| 4:M9:81:ASP:H | 3:Z9:111:ASN:ND2 | 1.68 | 0.91 |
| 5:N9:54:LEU:CD2 | 3:T9:84:ARG:CD | 2.48 | 0.91 |
| 12:D9:201:CYC:HBA2 | 11:a9:420:ASN:HB2 | 1.52 | 0.91 |
| 11:a9:348:GLN:H | 11:a9:348:GLN:HE21 | 0.94 | 0.91 |
| 11:a9:709:CYS:O | 11:a9:807:GLN:HB2 | 1.70 | 0.91 |
| 11:aA:589:THR:N | 11:aA:590:PRO:HD3 | 1.80 | 0.91 |
| 11:aA:623:ASP:HA | 3:H1:78:ARG:HH12 | 1.34 | 0.91 |
| 4:M1:120:LEU:HD22 | 2:Y1:115:GLU:OE2 | 1.69 | 0.91 |
| 3:LA:14:LEU:CD2 | 11:aA:358:PRO:CB | 1.87 | 0.91 |
| 2:QA:33:ARG:CZ | 12:VA:202:CYC:HBB3 | 1.99 | 0.91 |
| 2:SA:35:THR:C | 2:X4:74:TYR:OH | 2.12 | 0.91 |
| 12:R1:201:CYC:HB | 5:N1:54:LEU:HD12 | 1.12 | 0.91 |
| 2:K2:14:SER:HA | 6:M2:226:ASN:HB2 | 1.52 | 0.91 |
| 5:N3:22:LEU:CD1 | 5:N3:26:LEU:CD2 | 2.47 | 0.91 |
| 5:N3:34:LEU:CB | 3:T3:84:ARG:HD3 | 1.99 | 0.91 |
| 3:H4:84:ARG:CG | 11:aA:131:TYR:CE2 | 2.53 | 0.91 |
| 8:M5:41:GLN:OE1 | 1:J7:143:PRO:CG | 2.17 | 0.91 |
| 8:U5:76:LYS:O | 8:U5:79:ALA:N | 2.02 | 0.91 |
| 10:j5:631:HIS:HD2 | 10:j5:664:MET:CE | 1.80 | 0.91 |
| 10:j5:1143:LEU:HD12 | 8:q7:106:GLU:CB | 1.89 | 0.91 |
| 10:k5:964:GLY:CA | 1:n7:69:GLY:HA3 | 1.99 | 0.91 |
| 8:c7:42:THR:CG2 | 8:c7:141:LEU:HD21 | 1.99 | 0.91 |
| 1:d7:77:ARG:HH22 | 9:x7:63:ALA:CB | 1.70 | 0.91 |
| 4:M9:208:GLU:OE1 | 4:M9:222:ARG:NH2 | 2.03 | 0.91 |
| 3:J9:65:ASP:CB | 11:a9:354:VAL:HG21 | 1.99 | 0.91 |
| 3:J9:65:ASP:HB3 | 11:a9:354:VAL:CG2 | 2.00 | 0.91 |
| 11:a9:275:THR:C | 11:a9:278:LEU:HD11 | 1.85 | 0.91 |
| 4:MA:185:ALA:HA | 12:VA:201:CYC:O2A | 1.71 | 0.91 |
| 3:R1:111:ASN:HD21 | 5:N1:66:ARG:HH12 | 1.14 | 0.91 |
| 12:J3:202:CYC:HMA1 | 11:a9:798:SER:HG | 1.12 | 0.91 |
| 3:H4:84:ARG:CG | 11:aA:131:TYR:CZ | 2.53 | 0.91 |
| 8:Y5:9:VAL:HG11 | 10:k5:344:ARG:CZ | 1.98 | 0.91 |
| 1:b5:18:TYR:CE1 | 10:k5:165:ARG:CD | 2.53 | 0.91 |
| 10:k5:289:SER:HB3 | 10:k5:292:GLU:OE2 | 1.69 | 0.91 |
| 8:i7:54:ALA:HB2 | 8:i7:133:MET:HG3 | 1.51 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:T7:106:GLU:CG | 9:w7:58:THR:CG2 | 2.47 | 0.91 |
| 8:o7:5:THR:OG1 | 1:p7:6:THR:CG2 | 2.18 | 0.91 |
| 3:F8:112:GLY:HA3 | 4:M8:4:LEU:HD12 | 1.51 | 0.91 |
| 3:O8:115:GLU:HB2 | 5:Z8:70:ILE:O | 1.70 | 0.91 |
| 5:Z8:22:LEU:CD1 | 5:Z8:26:LEU:CD2 | 2.47 | 0.91 |
| 5:Z8:37:HIS:ND1 | 12:Z8:301:CYC:NB | 2.16 | 0.91 |
| 12:G9:201:CYC:HMD1 | 12:G9:201:CYC:HC | 1.33 | 0.91 |
| 12:I9:201:CYC:HMD1 | 12:I9:201:CYC:HC | 1.33 | 0.91 |
| 3:J9:65:ASP:CB | 11:a9:354:VAL:HG22 | 2.01 | 0.91 |
| 11:a9:99:ALA:HB1 | 11:a9:100:PRO:CD | 1.99 | 0.91 |
| 1:A:161:SER:CB | 1:R5:14:VAL:HB | 1.91 | 0.91 |
| 5:NA:54:LEU:CD2 | 3:TA:84:ARG:CD | 2.48 | 0.91 |
| 12:B3:202:CYC:HAA1 | 11:a9:684:ASN:CB | 2.00 | 0.91 |
| 5:N3:39:PRO:HG3 | 3:T3:113:LEU:HD13 | 1.53 | 0.91 |
| 8:M5:110:ILE:CD1 | 10:k5:533:LEU:CD1 | 2.45 | 0.91 |
| 1:N5:110:ASN:ND2 | 10:k5:692:LEU:C | 2.28 | 0.91 |
| 1:D5:62:TYR:OH | 12:E5:201:CYC:O1D | 1.89 | 0.91 |
| 6:M6:271:VAL:HG21 | 1:d7:127:VAL:CB | 2.00 | 0.91 |
| 10:j5:362:LYS:HD3 | 10:j5:363:HIS:HD2 | 1.17 | 0.91 |
| 10:j5:362:LYS:HE2 | 10:j5:363:HIS:CD2 | 2.03 | 0.91 |
| 10:k5:934:ALA:HB2 | 1:D7:32:THR:HG23 | 1.52 | 0.91 |
| 8:I7:29:PHE:HE1 | 8:I7:99:GLY:HA3 | 1.29 | 0.91 |
| 8:o7:37:LEU:HD22 | 1:p7:24:LEU:CG | 2.00 | 0.91 |
| 1:p7:136:VAL:CG1 | 11:a9:342:ARG:NH1 | 2.30 | 0.91 |
| 8:q7:76:LYS:HZ2 | 11:aA:605:PRO:HB3 | 1.15 | 0.91 |
| 4:M8:140:ARG:HH22 | 4:M8:210:ILE:HG12 | 1.33 | 0.91 |
| 3:Q8:84:ARG:HG3 | 5:Z8:31:TRP:CD1 | 2.05 | 0.91 |
| 3:F1:119:ALA:CB | 4:M1:41:ASN:HD21 | 1.81 | 0.91 |
| 3:H9:113:LEU:HD21 | 12:H9:202:CYC:HMB1 | 1.51 | 0.91 |
| 5:N1:39:PRO:HG3 | 3:T1:113:LEU:HD13 | 1.53 | 0.91 |
| 3:HA:113:LEU:CD1 | 12:HA:202:CYC:CMB | 2.48 | 0.91 |
| 2:KA:24:LEU:HB3 | 12:LA:201:CYC:HAB2 | 1.52 | 0.91 |
| 12:UA:201:CYC:HMD1 | 12:UA:201:CYC:HC | 1.33 | 0.91 |
| 12:I2:201:CYC:HMD1 | 12:I2:201:CYC:HC | 1.34 | 0.91 |
| 4:M4:128:ALA:O | 4:M4:142:PHE:CE1 | 2.23 | 0.91 |
| 4:M4:210:ILE:CD1 | 5:Z4:26:LEU:CD2 | 2.49 | 0.91 |
| 3:Q4:102:ALA:HB2 | 3:Q4:166:LYS:HE2 | 0.93 | 0.91 |
| 2:K6:14:SER:HA | 6:M6:226:ASN:HB2 | 1.52 | 0.91 |
| 6:M6:277:GLY:C | 1:d7:62:TYR:O | 2.12 | 0.91 |
| 10:j5:1076:GLU:C | 10:j5:1078:SER:N | 2.27 | 0.91 |
| 12:j5:1202:CYC:HMA1 | 12:j5:1202:CYC:NB | 1.84 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:Q7:25:ARG:CD | 8:C7:25:ARG:NH2 | 2.34 | 0.91 |
| 8:c7:39:ILE:HD11 | 8:c7:148:GLU:CG | 2.01 | 0.91 |
| 12:B8:202:CYC:CMA | 4:M8:58:TYR:CB | 2.48 | 0.91 |
| 2:N8:115:GLU:CA | 5:Z8:32:PRO:HB2 | 2.00 | 0.91 |
| 3:Q8:120:LEU:HB3 | 5:Z8:39:PRO:O | 1.69 | 0.91 |
| 5:N9:22:LEU:HD13 | 5:N9:26:LEU:CD2 | 1.99 | 0.91 |
| 3:F9:68:ARG:NH1 | 3:Z9:68:ARG:HH22 | 1.69 | 0.91 |
| 11:aA:710:THR:CG2 | 11:aA:807:GLN:CB | 2.47 | 0.91 |
| 11:aA:711:SER:CB | 3:L1:111:ASN:O | 2.18 | 0.91 |
| 4:MA:81:ASP:H | 3:ZA:111:ASN:ND2 | 1.68 | 0.91 |
| 3:L2:77:ARG:HH12 | 6:M2:70:GLU:HG2 | 1.35 | 0.91 |
| 6:M2:39:ARG:HE | 8:O5:66:VAL:CG1 | 1.83 | 0.91 |
| 3:B4:116:THR:H | 4:M4:56:MET:HG2 | 1.35 | 0.91 |
| 4:M3:144:ARG:NH2 | 5:N3:52:ARG:NH2 | 2.19 | 0.91 |
| 4:M4:95:ALA:HB2 | 5:Z4:38:GLU:HB2 | 1.52 | 0.91 |
| 10:k5:989:THR:HG22 | 8:a7:106:GLU:OE2 | 1.70 | 0.91 |
| 8:K7:25:ARG:HE | 8:U7:25:ARG:NH2 | 1.68 | 0.91 |
| 8:u7:29:PHE:HE2 | 1:v7:31:PHE:CE1 | 1.85 | 0.91 |
| 9:y7:3:ARG:CZ | 9:y7:67:VAL:HG11 | 1.98 | 0.91 |
| 12:T8:201:CYC:HMD1 | 12:T8:201:CYC:HC | 1.33 | 0.91 |
| 12:M8:301:CYC:HMB2 | 3:Y8:89:ILE:HG13 | 1.53 | 0.91 |
| 4:M9:158:PHE:C | 3:V9:108:ARG:HG3 | 1.96 | 0.91 |
| 11:a9:643:LEU:H | 11:a9:643:LEU:HD12 | 1.31 | 0.91 |
| 3:H1:78:ARG:HA | 12:H1:201:CYC:HMD1 | 1.52 | 0.91 |
| 4:M1:118:TYR:OH | 3:X1:85:ASP:OD1 | 1.89 | 0.91 |
| 5:NA:22:LEU:HD13 | 5:NA:26:LEU:CD2 | 1.99 | 0.91 |
| 12:QA:201:CYC:HMD1 | 12:QA:201:CYC:HC | 1.33 | 0.91 |
| 12:C3:201:CYC:HMD1 | 12:C3:201:CYC:HC | 1.33 | 0.91 |
| 3:Z3:111:ASN:OD1 | 4:M3:258:LYS:NZ | 2.04 | 0.91 |
| 12:B4:202:CYC:CMA | 4:M4:58:TYR:CB | 2.48 | 0.91 |
| 4:M3:81:ASP:H | 3:X3:111:ASN:HD22 | 1.16 | 0.91 |
| 5:N3:74:GLU:HA | 3:P3:111:ASN:HD21 | 1.35 | 0.91 |
| 3:B1:108:ARG:O | 4:M1:6:THR:CG2 | 2.18 | 0.91 |
| 2:P4:19:LEU:HD21 | 3:Q4:95:TYR:CE1 | 2.04 | 0.91 |
| 12:P5:201:CYC:HBB2 | 10:k5:623:VAL:CG2 | 2.01 | 0.91 |
| 9:z5:11:ILE:HD12 | 9:z5:28:PHE:HE2 | 1.36 | 0.91 |
| 9:i5:11:ILE:HD12 | 9:i5:28:PHE:HE2 | 1.36 | 0.91 |
| 10:j5:190:LEU:HD21 | 12:j5:1201:CYC:ND | 1.86 | 0.91 |
| 10:j5:277:ILE:HG23 | 10:j5:284:PRO:HA | 1.53 | 0.91 |
| 10:j5:307:ARG:NH1 | 10:j5:346:GLU:OE1 | 2.04 | 0.91 |
| 10:j5:938:GLN:OE1 | 1:J7:28:LYS:HD2 | 1.65 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:j5:1008:PHE:CZ | 1:v7:87:TYR:CZ | 2.40 | 0.91 |
| 10:k5:388:ARG:HB3 | 10:k5:388:ARG:NH2 | 1.84 | 0.91 |
| 10:k5:1059:VAL:O | 10:k5:1063:THR:HG23 | 1.71 | 0.91 |
| 10:k5:1150:TYR:HE1 | 11:a9:38:VAL:CG2 | 1.84 | 0.91 |
| 1:T7:14:VAL:HG12 | 9:w7:64:ASN:ND2 | 1.84 | 0.91 |
| 3:O8:107:ASP:HA | 5:Z8:66:ARG:HB2 | 1.53 | 0.91 |
| 4:M9:53:LEU:CD1 | 12:F9:301:CYC:HB | 1.67 | 0.91 |
| 11:aA:99:ALA:HB1 | 11:aA:100:PRO:CD | 1.99 | 0.91 |
| 11:aA:426:ARG:NH2 | 11:aA:496:ARG:HD3 | 1.84 | 0.91 |
| 12:IA:201:CYC:HMD1 | 12:IA:201:CYC:HC | 1.33 | 0.91 |
| 12:J3:202:CYC:CBB | 11:a9:795:ASP:O | 2.19 | 0.91 |
| 5:Z4:31:TRP:HB3 | 5:Z4:32:PRO:HD2 | 1.50 | 0.91 |
| 1:B5:10:ASN:OD1 | 10:k5:557:VAL:CG2 | 2.19 | 0.91 |
| 1:J5:71:MEN:C | 1:J5:77:ARG:NH1 | 2.22 | 0.91 |
| 1:b5:3:ASP:OD2 | 10:k5:21:MET:HB2 | 1.68 | 0.91 |
| 10:j5:36:ASN:HB2 | 10:j5:39:GLU:HB2 | 1.51 | 0.91 |
| 10:j5:931:VAL:CG2 | 1:J7:29:ALA:C | 2.42 | 0.91 |
| 10:j5:1059:VAL:O | 10:j5:1063:THR:HG23 | 1.71 | 0.91 |
| 10:k5:362:LYS:HD3 | 10:k5:363:HIS:HD2 | 1.17 | 0.91 |
| 10:k5:1025:LEU:HA | 10:k5:1030:ILE:HG22 | 1.49 | 0.91 |
| 10:k5:1147:TYR:CE2 | 11:a9:39:PRO:HB3 | 2.05 | 0.91 |
| 12:G6:201:CYC:HMD1 | 12:G6:201:CYC:HC | 1.33 | 0.91 |
| 8:i7:94:TYR:CE2 | 1:j7:9:ILE:HG23 | 2.05 | 0.91 |
| 8:a7:10:ASN:HD22 | 8:o7:10:ASN:ND2 | 1.69 | 0.91 |
| 1:f7:10:ASN:CG | 9:y7:65:THR:OG1 | 2.13 | 0.91 |
| 3:B8:113:LEU:HB2 | 4:M8:60:LYS:HE2 | 1.53 | 0.91 |
| 12:K8:201:CYC:HMD1 | 12:K8:201:CYC:HC | 1.34 | 0.91 |
| 3:Q8:110:LEU:CD2 | 3:Q8:167:ALA:HA | 2.00 | 0.91 |
| 12:K9:201:CYC:HMD1 | 12:K9:201:CYC:HC | 1.34 | 0.91 |
| 3:JA:116:THR:OG1 | 11:aA:521:PHE:HB3 | 1.71 | 0.91 |
| 4:MA:159:CYS:CA | 3:VA:108:ARG:HG3 | 2.01 | 0.91 |
| 12:G2:201:CYC:HMD1 | 12:G2:201:CYC:HC | 1.33 | 0.91 |
| 12:K2:201:CYC:HMD1 | 12:K2:201:CYC:HC | 1.34 | 0.91 |
| 12:E3:201:CYC:HMD1 | 12:E3:201:CYC:HC | 1.33 | 0.91 |
| 3:B4:82:CYS:HA | 12:B4:202:CYC:NC | 1.86 | 0.91 |
| 12:S3:201:CYC:HMD1 | 12:S3:201:CYC:HC | 1.34 | 0.91 |
| 4:M4:144:ARG:CG | 4:M4:204:ILE:HD13 | 1.99 | 0.91 |
| 3:Y4:87:GLU:HG2 | 3:Y4:91:ARG:NH1 | 1.86 | 0.91 |
| 1:D5:71:MEN:C | 1:D5:77:ARG:NH1 | 2.22 | 0.91 |
| 12:P5:201:CYC:OB | 10:k5:623:VAL:HB | 1.70 | 0.91 |
| 10:j5:1118:THR:HG23 | 12:j5:1202:CYC:O2A | 1.71 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:k5:1016:LEU:HD12 | 10:k5:1017:ARG:H | 1.15 | 0.91 |
| 1:Z7:67:ARG:CD | 11:a9:311:LEU:CD2 | 2.34 | 0.91 |
| 9:x7:3:ARG:CZ | 9:x7:67:VAL:HG11 | 1.98 | 0.91 |
| 3:F8:107:ASP:CB | 4:M8:8:SER:H | 1.83 | 0.91 |
| 3:H8:81:ALA:HA | 3:H8:84:ARG:HE | 1.33 | 0.91 |
| 4:M8:215:GLU:OE1 | 5:Z8:27:ALA:CB | 2.19 | 0.91 |
| 4:M9:181:GLN:NE2 | 3:V9:120:LEU:CD2 | 2.34 | 0.91 |
| 4:M9:190:ARG:HH11 | 4:M9:202:SER:CB | 1.84 | 0.91 |
| 4:M9:263:PRO:CB | 3:V9:119:ALA:HB3 | 1.99 | 0.91 |
| 12:E9:201:CYC:HMD1 | 12:E9:201:CYC:HC | 1.34 | 0.91 |
| 11:a9:681:LEU:O | 11:a9:684:ASN:OD1 | 1.87 | 0.91 |
| 12:C2:201:CYC:HMD1 | 12:C2:201:CYC:HC | 1.34 | 0.91 |
| 3:FA:37:ARG:NH2 | 3:FA:159:GLU:OE1 | 2.04 | 0.90 |
| 3:JA:65:ASP:HB3 | 11:aA:354:VAL:CG2 | 2.00 | 0.90 |
| 4:M3:80:PRO:HA | 3:X3:111:ASN:HD21 | 1.36 | 0.90 |
| 2:U3:141:GLN:CA | 2:Q9:76:ASP:H | 1.82 | 0.90 |
| 10:j5:388:ARG:NH2 | 10:j5:388:ARG:HB3 | 1.84 | 0.90 |
| 8:a7:63:PRO:HD2 | 11:a9:336:ILE:HG21 | 0.93 | 0.90 |
| 8:o7:23:LEU:CB | 1:p7:38:VAL:HG11 | 1.74 | 0.90 |
| 12:H8:201:CYC:HBB2 | 11:a9:259:ALA:CB | 2.00 | 0.90 |
| 4:M8:128:ALA:O | 4:M8:142:PHE:HE1 | 1.43 | 0.90 |
| 4:M9:159:CYS:CA | 3:V9:108:ARG:HG3 | 2.01 | 0.90 |
| 12:J9:202:CYC:HB | 11:a9:512:TYR:HB2 | 1.09 | 0.90 |
| 11:a9:287:ALA:O | 11:a9:288:ARG:NE | 2.03 | 0.90 |
| 11:aA:275:THR:N | 11:aA:278:LEU:HD11 | 1.84 | 0.90 |
| 12:K1:201:CYC:HMD1 | 12:K1:201:CYC:HC | 1.34 | 0.90 |
| 12:JA:202:CYC:HB | 11:aA:512:TYR:HB2 | 1.08 | 0.90 |
| 4:MA:133:ARG:HB3 | 12:RA:201:CYC:HBA2 | 1.51 | 0.90 |
| 4:MA:208:GLU:OE1 | 4:MA:222:ARG:NH2 | 2.03 | 0.90 |
| 12:OA:201:CYC:HMD1 | 12:OA:201:CYC:HC | 1.33 | 0.90 |
| 12:QA:201:CYC:CBA | 3:TA:67:ILE:HG21 | 2.02 | 0.90 |
| 6:M2:37:GLU:OE2 | 6:M2:39:ARG:NH1 | 2.04 | 0.90 |
| 12:B4:202:CYC:HBB2 | 4:M4:61:ASN:HB3 | 0.92 | 0.90 |
| 12:U3:201:CYC:HMD1 | 12:U3:201:CYC:HC | 1.33 | 0.90 |
| 3:L4:88:ILE:CD1 | 11:aA:239:TYR:CE2 | 2.54 | 0.90 |
| 4:M4:141:GLU:O | 4:M4:145:LEU:N | 2.03 | 0.90 |
| 8:K5:23:LEU:HD13 | 8:U5:151:PHE:CE1 | 2.05 | 0.90 |
| 12:B5:201:CYC:HMA1 | 12:B5:201:CYC:NB | 1.85 | 0.90 |
| 1:d5:28:LYS:HD2 | 1:n7:143:PRO:HG3 | 0.94 | 0.90 |
| 10:j5:232:ARG:HB2 | 10:j5:232:ARG:CZ | 2.00 | 0.90 |
| 10:k5:1119:LEU:HD22 | 1:n7:87:TYR:OH | 1.70 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:B7:54:GLU:OE2 | 11:a9:563:PHE:CD2 | 2.23 | 0.90 |
| 1:j7:77:ARG:NH2 | 9:y7:63:ALA:CB | 2.34 | 0.90 |
| 8:c7:36:ARG:NH1 | 8:m7:24:ASP:OD2 | 2.03 | 0.90 |
| 8:o7:17:TYR:HD2 | 1:p7:93:THR:HG21 | 1.25 | 0.90 |
| 8:o7:29:PHE:CE2 | 1:p7:31:PHE:CZ | 2.60 | 0.90 |
| 12:V8:201:CYC:HC | 12:V8:201:CYC:HMD1 | 1.33 | 0.90 |
| 3:H8:81:ALA:CB | 3:H8:84:ARG:HH21 | 1.84 | 0.90 |
| 3:H8:84:ARG:CD | 11:a9:131:TYR:CD1 | 2.32 | 0.90 |
| 3:Q8:78:ARG:NH1 | 12:Z8:301:CYC:CGD | 2.34 | 0.90 |
| 12:A9:201:CYC:HMD1 | 12:A9:201:CYC:HC | 1.33 | 0.90 |
| 11:a9:249:GLU:C | 11:a9:285:VAL:HG21 | 1.95 | 0.90 |
| 11:a9:312:ASP:CA | 11:a9:315:LEU:HB2 | 1.77 | 0.90 |
| 11:a9:681:LEU:HA | 11:a9:684:ASN:ND2 | 1.85 | 0.90 |
| 11:aA:476:ARG:HH11 | 11:aA:488:SER:HB3 | 1.32 | 0.90 |
| 1:Z:73:TYR:CE1 | 10:j5:162:TRP:CH2 | 2.45 | 0.90 |
| 4:MA:157:PHE:C | 3:VA:108:ARG:HD2 | 1.95 | 0.90 |
| 4:MA:274:VAL:CG1 | 3:VA:77:ARG:NE | 2.33 | 0.90 |
| 3:J3:84:ARG:NH2 | 11:a9:670:LEU:CA | 2.34 | 0.90 |
| 6:M2:53:LEU:HD23 | 8:i7:80:LEU:HD23 | 1.53 | 0.90 |
| 3:B1:91:ARG:CZ | 11:aA:677:GLN:HE22 | 1.80 | 0.90 |
| 12:B1:202:CYC:HAA1 | 11:aA:684:ASN:CB | 2.01 | 0.90 |
| 4:M4:217:VAL:HG22 | 5:Z4:30:PRO:CG | 2.00 | 0.90 |
| 3:O4:107:ASP:HB3 | 5:Z4:66:ARG:HB3 | 0.91 | 0.90 |
| 12:X4:201:CYC:HMD1 | 12:X4:201:CYC:HC | 1.33 | 0.90 |
| 1:f5:1:MET:O | 10:j5:15:ARG:NH1 | 2.05 | 0.90 |
| 1:Z5:28:LYS:HD2 | 1:t7:143:PRO:HG3 | 0.92 | 0.90 |
| 12:C6:201:CYC:HMD1 | 12:C6:201:CYC:HC | 1.34 | 0.90 |
| 8:a7:107:ILE:HD13 | 1:b7:13:ASP:CG | 1.97 | 0.90 |
| 3:H8:111:ASN:OD1 | 11:a9:291:TYR:OH | 1.73 | 0.90 |
| 4:M8:251:ASN:H | 4:M8:251:ASN:HD22 | 1.16 | 0.90 |
| 12:P8:201:CYC:HMD1 | 12:P8:201:CYC:HC | 1.34 | 0.90 |
| 4:M9:133:ARG:HB3 | 12:R9:201:CYC:HBA2 | 1.51 | 0.90 |
| 3:H9:82:CYS:SG | 12:H9:202:CYC:CAC | 2.59 | 0.90 |
| 11:a9:377:VAL:O | 11:a9:391:VAL:HG22 | 1.71 | 0.90 |
| 4:M1:118:TYR:CD2 | 3:X1:84:ARG:NH2 | 2.38 | 0.90 |
| 4:M1:181:GLN:NE2 | 3:Z1:120:LEU:HD21 | 1.84 | 0.90 |
| 3:HA:119:ALA:HA | 8:S7:49:ARG:HH12 | 0.78 | 0.90 |
| 3:JA:114:LYS:HG2 | 8:S7:60:GLN:NE2 | 1.85 | 0.90 |
| 3:JA:119:ALA:CB | 11:aA:365:LYS:HE2 | 2.01 | 0.90 |
| 12:SA:201:CYC:HMD1 | 12:SA:201:CYC:HC | 1.33 | 0.90 |
| 3:J2:119:ALA:HB1 | 6:M2:260:THR:C | 1.95 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:D4:116:THR:OG1 | 4:M4:38:PRO:HB2 | 1.71 | 0.90 |
| 3:H4:111:ASN:OD1 | 11:aA:291:TYR:OH | 1.74 | 0.90 |
| 12:M4:301:CYC:NC | 3:Y4:72:ASN:OD1 | 2.04 | 0.90 |
| 3:O4:119:ALA:CB | 5:Z4:72:GLU:CG | 2.16 | 0.90 |
| 8:K5:80:LEU:HD12 | 12:K5:201:CYC:HAD2 | 1.44 | 0.90 |
| 10:j5:971:VAL:HG12 | 1:t7:76:ARG:HH12 | 1.33 | 0.90 |
| 10:k5:1050:PHE:HZ | 1:l7:107:ARG:NH1 | 1.30 | 0.90 |
| 8:K7:25:ARG:HB3 | 8:U7:25:ARG:HH21 | 1.33 | 0.90 |
| 12:g7:201:CYC:HMA1 | 12:g7:201:CYC:HB | 1.37 | 0.90 |
| 8:i7:112:VAL:HG13 | 8:i7:113:LYS:N | 1.85 | 0.90 |
| 12:C9:201:CYC:HMD1 | 12:C9:201:CYC:HC | 1.34 | 0.90 |
| 11:a9:280:ASP:CG | 11:a9:281:PRO:CD | 2.44 | 0.90 |
| 5:N1:34:LEU:HB2 | 3:T1:84:ARG:HD3 | 1.53 | 0.90 |
| 3:DA:115:GLU:CD | 4:MA:76:ALA:O | 2.15 | 0.90 |
| 3:P1:111:ASN:HD21 | 5:N1:74:GLU:HA | 1.35 | 0.90 |
| 4:M3:208:GLU:OE1 | 4:M3:222:ARG:NH2 | 2.03 | 0.90 |
| 1:B5:2:GLN:OE1 | 10:k5:551:MET:HE3 | 1.72 | 0.90 |
| 1:b5:34:GLY:HA3 | 10:k5:47:PHE:CD2 | 2.06 | 0.90 |
| 3:J6:119:ALA:HB1 | 6:M6:260:THR:C | 1.95 | 0.90 |
| 10:j5:964:GLY:HA2 | 1:t7:69:GLY:HA3 | 1.54 | 0.90 |
| 10:j5:1125:ARG:NH2 | 1:t7:114:GLU:HB3 | 1.85 | 0.90 |
| 10:j5:1147:TYR:CE2 | 11:aA:39:PRO:HB3 | 2.06 | 0.90 |
| 10:k5:277:ILE:HG23 | 10:k5:284:PRO:HA | 1.53 | 0.90 |
| 10:k5:307:ARG:NH1 | 10:k5:346:GLU:OE1 | 2.04 | 0.90 |
| 10:k5:322:LYS:HD2 | 10:k5:336:ARG:HH12 | 1.34 | 0.90 |
| 10:k5:1008:PHE:CE1 | 12:p7:201:CYC:C4B | 2.55 | 0.90 |
| 12:I7:201:CYC:HMA1 | 12:I7:201:CYC:HB | 1.37 | 0.90 |
| 8:i7:42:THR:CG2 | 8:i7:141:LEU:HD21 | 1.99 | 0.90 |
| 1:f7:67:ARG:CG | 11:aA:311:LEU:HD22 | 2.02 | 0.90 |
| 4:M8:98:ASP:C | 3:Q8:1:MET:HE1 | 1.97 | 0.90 |
| 4:M8:214:GLY:H | 5:Z8:28:HIS:CE1 | 1.85 | 0.90 |
| 2:N8:112:GLY:N | 5:Z8:34:LEU:N | 2.19 | 0.90 |
| 4:M9:181:GLN:CD | 3:V9:120:LEU:HD21 | 1.94 | 0.90 |
| 6:M2:57:GLU:OE2 | 8:i7:76:LYS:NZ | 2.04 | 0.90 |
| 12:B4:202:CYC:CBB | 4:M4:61:ASN:HB3 | 1.85 | 0.90 |
| 3:L3:77:ARG:HD3 | 11:a9:824:VAL:C | 1.97 | 0.90 |
| 4:M4:190:ARG:HH11 | 4:M4:202:SER:CB | 1.84 | 0.90 |
| 4:M4:228:SER:HB2 | 2:X4:16:GLY:HA2 | 0.92 | 0.90 |
| 10:j5:1043:GLU:HG2 | 8:e7:14:GLU:OE2 | 1.70 | 0.90 |
| 10:j5:1124:TYR:CZ | 1:t7:119:LEU:HD21 | 2.06 | 0.90 |
| 1:B7:140:LEU:CD1 | 11:a9:561:ALA:HA | 2.01 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:i7:92:VAL:HG23 | 8:i7:156:LEU:HD11 | 1.53 | 0.90 |
| 4:M8:208:GLU:OE1 | 4:M8:222:ARG:NH2 | 2.03 | 0.90 |
| 5:Z8:41:GLN:HB3 | 12:Z8:301:CYC:NB | 1.85 | 0.90 |
| 11:aA:249:GLU:C | 11:aA:285:VAL:HG21 | 1.95 | 0.90 |
| 11:aA:312:ASP:C | 11:aA:315:LEU:H | 1.74 | 0.90 |
| 11:aA:798:SER:OG | 12:aA:901:CYC:HAA1 | 1.72 | 0.90 |
| 2:QA:119:THR:HB | 3:TA:83:LEU:HD13 | 0.92 | 0.90 |
| 8:M5:41:GLN:CD | 1:J7:143:PRO:CG | 2.42 | 0.90 |
| 10:j5:931:VAL:HG22 | 1:J7:30:TYR:N | 1.86 | 0.90 |
| 10:k5:725:LEU:C | 10:k5:725:LEU:HD23 | 1.96 | 0.90 |
| 8:a7:52:LYS:CD | 11:a9:321:ALA:HB1 | 2.01 | 0.90 |
| 8:a7:161:GLN:CD | 1:p7:49:THR:HG22 | 1.96 | 0.90 |
| 4:M8:232:VAL:HG23 | 4:M8:235:PHE:HE2 | 1.35 | 0.90 |
| 3:O8:104:VAL:C | 5:Z8:61:LYS:HE2 | 1.96 | 0.90 |
| 4:M9:76:ALA:O | 3:D9:115:GLU:CD | 2.15 | 0.90 |
| 11:aA:106:LEU:HB2 | 11:aA:118:VAL:HG21 | 1.54 | 0.90 |
| 11:aA:287:ALA:O | 11:aA:288:ARG:NE | 2.03 | 0.90 |
| 11:aA:745:GLY:CA | 2:K1:15:GLN:CA | 2.49 | 0.90 |
| 3:F2:84:ARG:NH1 | 12:F2:201:CYC:O2A | 2.04 | 0.90 |
| 3:HA:82:CYS:SG | 12:HA:202:CYC:CAC | 2.60 | 0.90 |
| 2:QA:71:GLN:N | 2:QA:74:TYR:CD2 | 2.39 | 0.90 |
| 2:K3:112:GLY:HA3 | 11:a9:670:LEU:CD2 | 2.01 | 0.90 |
| 12:A5:201:CYC:HMA1 | 12:A5:201:CYC:HB | 1.37 | 0.90 |
| 12:c5:201:CYC:HB | 12:c5:201:CYC:HMA1 | 1.37 | 0.90 |
| 12:S5:201:CYC:HB | 12:S5:201:CYC:HMA1 | 1.37 | 0.90 |
| 10:k5:1153:VAL:CG2 | 1:p7:125:ALA:HB1 | 1.94 | 0.90 |
| 12:O7:201:CYC:HB | 12:O7:201:CYC:HMA1 | 1.37 | 0.90 |
| 12:C8:201:CYC:HMD1 | 12:C8:201:CYC:HC | 1.33 | 0.90 |
| 3:J9:109:CYS:C | 11:a9:518:ALA:HB2 | 1.95 | 0.90 |
| 11:aA:61:TYR:HD1 | 11:aA:65:LEU:HD22 | 1.35 | 0.90 |
| 11:aA:621:THR:HG23 | 3:J1:14:LEU:HD22 | 1.53 | 0.90 |
| 4:M1:208:GLU:OE1 | 4:M1:222:ARG:NH2 | 2.03 | 0.90 |
| 12:W1:201:CYC:HMD1 | 12:W1:201:CYC:HC | 1.34 | 0.90 |
| 3:HA:113:LEU:HD21 | 12:HA:202:CYC:CMB | 2.00 | 0.90 |
| 4:MA:181:GLN:NE2 | 3:VA:120:LEU:CD2 | 2.34 | 0.90 |
| 3:L2:65:ASP:OD1 | 1:h7:64:ASP:OD2 | 1.90 | 0.90 |
| 3:L3:119:ALA:HB1 | 11:a9:813:PRO:C | 1.96 | 0.90 |
| 3:B1:86:MET:HG3 | 12:B1:202:CYC:HBC1 | 1.53 | 0.90 |
| 2:E4:1:MET:CA | 4:M4:10:ARG:HH21 | 1.85 | 0.90 |
| 4:M4:56:MET:SD | 4:M4:66:VAL:HG21 | 2.11 | 0.90 |
| 4:M4:215:GLU:CD | 4:M4:215:GLU:O | 2.15 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:C5:27:LYS:HA | 8:C5:30:VAL:CG2 | 2.01 | 0.90 |
| 8:I5:27:LYS:HA | 8:I5:30:VAL:CG2 | 2.01 | 0.90 |
| 1:d5:110:ASN:ND2 | 10:j5:451:LYS:CB | 2.31 | 0.90 |
| 1:d5:110:ASN:O | 10:j5:352:ILE:CD1 | 2.20 | 0.90 |
| 1:f5:18:TYR:CE2 | 10:j5:165:ARG:CB | 2.55 | 0.90 |
| 12:P5:201:CYC:O2A | 10:k5:649:PHE:CD2 | 2.25 | 0.90 |
| 8:Q5:159:ALA:O | 8:Q5:160:MET:O | 1.90 | 0.90 |
| 10:k5:480:GLU:OE1 | 10:k5:689:GLY:HA3 | 1.72 | 0.90 |
| 10:k5:741:GLN:C | 1:D7:77:ARG:NH2 | 2.29 | 0.90 |
| 10:k5:971:VAL:H | 12:k5:1204:CYC:CGD | 1.81 | 0.90 |
| 8:Q7:19:SER:HB3 | 8:C7:6:LYS:HZ1 | 1.37 | 0.90 |
| 1:R7:118:SER:O | 9:z7:61:GLN:HG2 | 1.72 | 0.90 |
| 8:i7:3:VAL:HG11 | 8:s7:25:ARG:HH21 | 1.36 | 0.90 |
| 1:j7:77:ARG:HH22 | 9:y7:63:ALA:HB3 | 1.21 | 0.90 |
| 8:q7:76:LYS:HZ1 | 11:aA:605:PRO:CB | 1.82 | 0.90 |
| 3:J9:116:THR:OG1 | 11:a9:521:PHE:HB3 | 1.70 | 0.90 |
| 3:J9:119:ALA:CB | 11:a9:365:LYS:HE2 | 2.02 | 0.90 |
| 11:a9:312:ASP:HA | 11:a9:315:LEU:CA | 2.02 | 0.90 |
| 11:a9:589:THR:N | 11:a9:590:PRO:CD | 2.32 | 0.90 |
| 11:a9:635:VAL:HG11 | 11:a9:795:ASP:OD2 | 1.72 | 0.90 |
| 5:N1:22:LEU:CG | 5:N1:26:LEU:HD21 | 2.02 | 0.90 |
| 3:LA:52:ILE:CD1 | 3:LA:87:GLU:CA | 2.49 | 0.90 |
| 4:MA:192:GLN:HG2 | 3:VA:84:ARG:HG3 | 1.54 | 0.90 |
| 12:J3:202:CYC:C4B | 11:a9:666:ASN:CB | 2.42 | 0.90 |
| 3:L3:84:ARG:HH11 | 11:a9:739:ASP:HB2 | 1.37 | 0.90 |
| 4:M3:5:THR:O | 4:M3:6:THR:OG1 | 1.90 | 0.90 |
| 4:M3:118:TYR:OH | 3:X3:85:ASP:OD1 | 1.89 | 0.90 |
| 12:E4:201:CYC:HMD1 | 12:E4:201:CYC:HC | 1.33 | 0.90 |
| 12:K4:201:CYC:HMD1 | 12:K4:201:CYC:HC | 1.34 | 0.90 |
| 3:O4:111:ASN:O | 5:Z4:67:ILE:HG21 | 1.71 | 0.90 |
| 12:O4:201:CYC:HMA3 | 5:Z4:53:LEU:CD1 | 2.02 | 0.90 |
| 1:f5:19:LEU:HD12 | 10:j5:172:LEU:HD11 | 1.52 | 0.90 |
| 12:W5:201:CYC:HB | 12:W5:201:CYC:HMA1 | 1.37 | 0.90 |
| 10:k5:152:ARG:NH2 | 10:k5:193:SER:HB2 | 1.86 | 0.90 |
| 8:c7:112:VAL:HG13 | 8:c7:113:LYS:N | 1.85 | 0.90 |
| 12:d7:201:CYC:HBB1 | 9:x7:42:GLN:OE1 | 1.68 | 0.90 |
| 8:s7:29:PHE:HE1 | 8:s7:99:GLY:HA3 | 1.29 | 0.90 |
| 4:M8:99:VAL:HB | 3:Q8:1:MET:HE2 | 1.52 | 0.90 |
| 2:N8:115:GLU:CB | 5:Z8:32:PRO:HB2 | 2.00 | 0.90 |
| 5:Z8:41:GLN:HG3 | 12:Z8:301:CYC:C4B | 1.98 | 0.90 |
| 3:H9:78:ARG:HH11 | 12:H9:202:CYC:CGD | 1.84 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:a9:61:TYR:HD1 | 11:a9:65:LEU:HD22 | 1.35 | 0.90 |
| 11:aA:476:ARG:NH1 | 11:aA:488:SER:HB2 | 1.78 | 0.90 |
| 11:aA:738:LEU:HD13 | 12:aA:902:CYC:NB | 1.86 | 0.90 |
| 11:aA:745:GLY:HA3 | 2:K1:15:GLN:HA | 0.94 | 0.90 |
| 11:aA:813:PRO:C | 3:L1:119:ALA:HB1 | 1.97 | 0.90 |
| 3:FA:36:LYS:HB3 | 3:FA:156:LEU:CD1 | 2.02 | 0.89 |
| 3:FA:150:ARG:N | 3:F9:150:ARG:HG3 | 1.86 | 0.89 |
| 4:MA:190:ARG:HH11 | 4:MA:202:SER:CB | 1.84 | 0.89 |
| 5:NA:22:LEU:HD23 | 5:NA:26:LEU:HD11 | 0.89 | 0.89 |
| 12:QA:201:CYC:CBA | 3:TA:79:MET:HE3 | 2.02 | 0.89 |
| 2:K3:14:SER:HA | 11:a9:746:TYR:HB2 | 1.52 | 0.89 |
| 5:N3:54:LEU:HD11 | 12:R3:201:CYC:C4B | 2.00 | 0.89 |
| 3:H4:84:ARG:HD3 | 11:aA:131:TYR:CE1 | 2.06 | 0.89 |
| 4:M4:101:ASP:HA | 2:P4:13:ASP:HB3 | 0.90 | 0.89 |
| 8:W5:12:ASP:CB | 1:X5:94:TYR:HE2 | 1.80 | 0.89 |
| 1:b5:18:TYR:OH | 10:k5:161:ASP:O | 1.90 | 0.89 |
| 12:U7:201:CYC:HB | 12:U7:201:CYC:HMA1 | 1.37 | 0.89 |
| 12:u7:201:CYC:HB | 12:u7:201:CYC:HMA1 | 1.37 | 0.89 |
| 4:M8:5:THR:O | 4:M8:6:THR:OG1 | 1.90 | 0.89 |
| 11:aA:280:ASP:CG | 11:aA:281:PRO:CD | 2.44 | 0.89 |
| 11:aA:629:LYS:HA | 11:aA:629:LYS:NZ | 1.86 | 0.89 |
| 4:M1:144:ARG:NH2 | 5:N1:52:ARG:NH2 | 2.19 | 0.89 |
| 5:N1:22:LEU:HD23 | 5:N1:26:LEU:HD11 | 0.90 | 0.89 |
| 2:SA:35:THR:HG22 | 2:X4:74:TYR:CZ | 1.89 | 0.89 |
| 2:A4:33:ARG:NH2 | 2:K4:28:ASN:CG | 2.31 | 0.89 |
| 8:O5:76:LYS:CG | 8:O5:77:MET:N | 2.35 | 0.89 |
| 12:G5:201:CYC:HB | 12:G5:201:CYC:HMA1 | 1.37 | 0.89 |
| 2:X8:28:ASN:CG | 2:N8:33:ARG:NH2 | 2.30 | 0.89 |
| 2:N8:111:ALA:CB | 5:Z8:34:LEU:HG | 2.03 | 0.89 |
| 5:N9:53:LEU:HB3 | 12:T9:301:CYC:CAA | 2.02 | 0.89 |
| 2:O9:33:ARG:NH2 | 2:Y9:28:ASN:CG | 2.30 | 0.89 |
| 11:a9:312:ASP:HA | 11:a9:315:LEU:N | 1.87 | 0.89 |
| 11:aA:632:ILE:HG21 | 11:aA:634:ALA:HB2 | 1.55 | 0.89 |
| 12:QA:201:CYC:O2D | 3:TA:57:HIS:HD2 | 1.40 | 0.89 |
| 2:Q1:14:SER:HB2 | 5:N1:62:ARG:NH2 | 1.86 | 0.89 |
| 3:B3:68:ARG:HH12 | 3:V3:68:ARG:HH12 | 1.13 | 0.89 |
| 5:N3:62:ARG:NH2 | 2:Q3:14:SER:HB2 | 1.86 | 0.89 |
| 12:J4:202:CYC:HMD1 | 12:J4:202:CYC:NC | 1.88 | 0.89 |
| 8:G5:115:MET:CE | 12:G5:201:CYC:CHB | 2.50 | 0.89 |
| 1:J5:39:ARG:O | 1:J5:40:ALA:C | 2.14 | 0.89 |
| 8:U5:79:ALA:O | 6:M6:31:ASP:HB2 | 1.73 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:M6:65:VAL:HG12 | 1:b7:59:ALA:O | 1.71 | 0.89 |
| 10:j5:990:ARG:HE | 10:j5:1026:LYS:HZ3 | 1.19 | 0.89 |
| 10:k5:77:VAL:HG22 | 10:k5:141:GLU:HB3 | 1.54 | 0.89 |
| 8:c7:25:ARG:HH22 | 8:m7:6:LYS:HZ3 | 1.13 | 0.89 |
| 12:e7:201:CYC:HB | 12:e7:201:CYC:HMA1 | 1.37 | 0.89 |
| 12:A8:201:CYC:HMD1 | 12:A8:201:CYC:HC | 1.33 | 0.89 |
| 12:o7:201:CYC:HMA1 | 12:o7:201:CYC:HB | 1.37 | 0.89 |
| 12:F8:201:CYC:HMD1 | 12:F8:201:CYC:NC | 1.88 | 0.89 |
| 5:Z8:22:LEU:CG | 5:Z8:26:LEU:HD21 | 2.02 | 0.89 |
| 3:J9:119:ALA:HB1 | 11:a9:365:LYS:HE2 | 1.51 | 0.89 |
| 11:a9:710:THR:HG22 | 11:a9:807:GLN:HG3 | 1.40 | 0.89 |
| 1:Z:131:GLN:HG3 | 1:X5:17:LYS:HZ2 | 1.13 | 0.89 |
| 3:FA:68:ARG:NH1 | 3:ZA:68:ARG:HH22 | 1.69 | 0.89 |
| 4:MA:274:VAL:HG12 | 3:VA:77:ARG:NE | 1.87 | 0.89 |
| 4:M3:190:ARG:HH11 | 4:M3:202:SER:CB | 1.84 | 0.89 |
| 4:M4:5:THR:O | 4:M4:6:THR:OG1 | 1.90 | 0.89 |
| 8:e5:49:ARG:NH2 | 1:R5:50:THR:HG21 | 1.87 | 0.89 |
| 1:f5:18:TYR:OH | 10:j5:165:ARG:HB2 | 1.72 | 0.89 |
| 1:R5:106:GLU:HG3 | 10:k5:505:VAL:HA | 1.55 | 0.89 |
| 8:W5:159:ALA:O | 8:W5:160:MET:O | 1.90 | 0.89 |
| 10:j5:987:ASP:O | 1:h7:106:GLU:OE2 | 1.90 | 0.89 |
| 10:k5:742:GLY:CA | 12:D7:201:CYC:CGD | 2.50 | 0.89 |
| 10:k5:987:ASP:O | 1:b7:106:GLU:OE2 | 1.90 | 0.89 |
| 2:A6:63:PHE:CB | 2:A6:66:LEU:HD11 | 2.03 | 0.89 |
| 1:H7:136:VAL:CG1 | 11:aA:563:PHE:CZ | 2.55 | 0.89 |
| 8:g7:107:ILE:HD13 | 1:h7:13:ASP:CG | 1.97 | 0.89 |
| 12:a7:201:CYC:HB | 12:a7:201:CYC:HMA1 | 1.37 | 0.89 |
| 12:b7:201:CYC:HBB2 | 9:x7:21:ARG:HD3 | 1.54 | 0.89 |
| 8:m7:29:PHE:HE1 | 8:m7:99:GLY:HA3 | 1.29 | 0.89 |
| 12:s7:201:CYC:HMA1 | 12:s7:201:CYC:HB | 1.37 | 0.89 |
| 9:y7:3:ARG:CZ | 9:y7:67:VAL:HG13 | 1.98 | 0.89 |
| 12:G8:201:CYC:HMD1 | 12:G8:201:CYC:HC | 1.33 | 0.89 |
| 4:M8:141:GLU:HA | 4:M8:144:ARG:HE | 1.36 | 0.89 |
| 3:L9:112:GLY:C | 11:a9:532:ALA:HB3 | 1.98 | 0.89 |
| 11:a9:99:ALA:HB3 | 11:a9:100:PRO:CD | 1.99 | 0.89 |
| 2:IA:113:LEU:HD21 | 2:IA:161:LEU:CD2 | 2.02 | 0.89 |
| 12:QA:201:CYC:HBB2 | 3:TA:75:PRO:HA | 1.53 | 0.89 |
| 2:O1:33:ARG:NH2 | 2:Y1:28:ASN:CG | 2.31 | 0.89 |
| 2:O1:63:PHE:CB | 2:O1:66:LEU:HD11 | 2.03 | 0.89 |
| 4:M4:144:ARG:NE | 4:M4:204:ILE:HG21 | 1.74 | 0.89 |
| 3:Y4:88:ILE:CG2 | 3:Y4:91:ARG:NH2 | 2.34 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:Z5:67:ARG:HH12 | 10:k5:705:THR:HB | 1.35 | 0.89 |
| 10:k5:386:ILE:CG2 | 10:k5:395:SER:H | 1.83 | 0.89 |
| 10:k5:988:ALA:CA | 1:b7:106:GLU:OE2 | 2.19 | 0.89 |
| 12:B6:201:CYC:HMD1 | 12:B6:201:CYC:NC | 1.88 | 0.89 |
| 8:c7:12:ASP:HA | 1:d7:90:ARG:NH1 | 1.87 | 0.89 |
| 3:U8:115:GLU:HB3 | 4:M8:74:LEU:HD11 | 0.91 | 0.89 |
| 3:L8:113:LEU:HD21 | 12:a9:901:CYC:HMB3 | 1.51 | 0.89 |
| 4:M8:92:GLU:CG | 4:M8:217:VAL:HG22 | 2.02 | 0.89 |
| 4:M9:188:LEU:CD2 | 12:V9:201:CYC:HB | 1.85 | 0.89 |
| 4:M9:251:ASN:H | 4:M9:251:ASN:HD22 | 1.16 | 0.89 |
| 3:H1:109:CYS:HA | 12:H1:201:CYC:HBB1 | 1.53 | 0.89 |
| 4:M1:190:ARG:HH11 | 4:M1:202:SER:CB | 1.84 | 0.89 |
| 3:TA:25:ASN:CB | 2:X4:65:TYR:N | 2.32 | 0.89 |
| 12:XA:202:CYC:HMD1 | 12:XA:202:CYC:NC | 1.88 | 0.89 |
| 12:H2:201:CYC:HBB2 | 6:M2:243:ALA:CB | 2.03 | 0.89 |
| 3:F4:91:ARG:HH22 | 11:aA:140:GLN:NE2 | 1.65 | 0.89 |
| 2:P4:19:LEU:CD1 | 3:Q4:95:TYR:CE1 | 2.55 | 0.89 |
| 12:O5:201:CYC:HB | 12:O5:201:CYC:HMA1 | 1.37 | 0.89 |
| 8:A5:115:MET:CE | 12:A5:201:CYC:CHB | 2.50 | 0.89 |
| 1:d5:161:SER:CB | 10:j5:695:GLY:C | 2.44 | 0.89 |
| 2:K6:28:ASN:CG | 2:A6:33:ARG:NH2 | 2.31 | 0.89 |
| 6:M6:278:ARG:H | 1:d7:62:TYR:HB3 | 1.37 | 0.89 |
| 10:j5:152:ARG:NH2 | 10:j5:193:SER:HB2 | 1.87 | 0.89 |
| 10:j5:1020:GLU:N | 1:f7:87:TYR:OH | 2.06 | 0.89 |
| 12:B8:202:CYC:HMA2 | 4:M8:58:TYR:H | 0.72 | 0.89 |
| 3:F8:107:ASP:O | 4:M8:6:THR:HB | 1.73 | 0.89 |
| 3:H8:84:ARG:CD | 11:a9:131:TYR:CE2 | 2.55 | 0.89 |
| 2:E9:2:LYS:HZ3 | 2:I9:17:ARG:NH1 | 1.61 | 0.89 |
| 2:AA:63:PHE:CB | 2:AA:66:LEU:HD11 | 2.03 | 0.89 |
| 12:O1:201:CYC:HBB3 | 3:R1:74:TYR:CE1 | 2.07 | 0.89 |
| 12:Q1:201:CYC:HMD1 | 12:Q1:201:CYC:HC | 1.34 | 0.89 |
| 2:K3:28:ASN:CG | 2:A3:33:ARG:NH2 | 2.31 | 0.89 |
| 3:L2:77:ARG:NH1 | 6:M2:70:GLU:CD | 2.29 | 0.89 |
| 2:A4:63:PHE:CB | 2:A4:66:LEU:HD11 | 2.03 | 0.89 |
| 3:B4:82:CYS:SG | 12:B4:202:CYC:H2C | 2.11 | 0.89 |
| 3:S4:113:LEU:HD12 | 3:S4:116:THR:HG21 | 1.55 | 0.89 |
| 3:L4:68:ARG:CG | 11:aA:81:ASP:CA | 2.51 | 0.89 |
| 3:L4:68:ARG:CG | 11:aA:81:ASP:N | 2.36 | 0.89 |
| 4:M4:94:TRP:HB3 | 3:Q4:88:ILE:HD13 | 1.54 | 0.89 |
| 4:M4:144:ARG:HG2 | 4:M4:204:ILE:CD1 | 2.00 | 0.89 |
| 12:K5:201:CYC:O1D | 1:J5:62:TYR:OH | 1.89 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:C1:201:CYC:HMD1 | 12:C1:201:CYC:HC | 1.33 | 0.89 |
| 12:M7:201:CYC:HB | 12:M7:201:CYC:HMA1 | 1.37 | 0.89 |
| 8:c7:54:ALA:HB2 | 8:c7:133:MET:HG3 | 1.51 | 0.89 |
| 3:L8:116:THR:HG21 | 12:a9:901:CYC:CMA | 2.02 | 0.89 |
| 4:M8:95:ALA:HB2 | 5:Z8:38:GLU:HG3 | 1.53 | 0.89 |
| 12:M8:301:CYC:HMC1 | 3:Y8:127:VAL:HG23 | 1.54 | 0.89 |
| 12:L9:201:CYC:HMD1 | 12:L9:201:CYC:NC | 1.87 | 0.89 |
| 4:M9:274:VAL:C | 3:V9:77:ARG:NE | 2.29 | 0.89 |
| 12:B9:202:CYC:HMD1 | 12:B9:202:CYC:NC | 1.88 | 0.89 |
| 3:LA:112:GLY:C | 11:aA:532:ALA:HB3 | 1.98 | 0.89 |
| 5:NA:22:LEU:CG | 5:NA:26:LEU:HD21 | 2.02 | 0.89 |
| 2:QA:120:PHE:CE2 | 3:TA:79:MET:SD | 2.66 | 0.89 |
| 2:G2:113:LEU:CA | 3:L2:76:ASN:ND2 | 2.36 | 0.89 |
| 3:B4:85:ASP:C | 12:B4:202:CYC:CBC | 2.46 | 0.89 |
| 12:T3:302:CYC:HMD1 | 12:T3:302:CYC:NC | 1.88 | 0.89 |
| 2:N4:63:PHE:CB | 2:N4:66:LEU:HD11 | 2.03 | 0.89 |
| 3:Y4:89:ILE:CA | 3:Y4:92:TYR:HE2 | 1.53 | 0.89 |
| 8:G5:61:ILE:HD11 | 8:o7:67:SER:HB3 | 0.91 | 0.89 |
| 1:d5:110:ASN:HD21 | 10:j5:451:LYS:HB3 | 1.31 | 0.89 |
| 12:Q5:201:CYC:HMA1 | 12:Q5:201:CYC:HB | 1.37 | 0.89 |
| 8:U5:76:LYS:CG | 8:U5:77:MET:N | 2.35 | 0.89 |
| 10:j5:1150:TYR:HE2 | 1:v7:69:GLY:O | 1.30 | 0.89 |
| 10:k5:175:ASP:CB | 10:k5:176:PRO:CD | 1.97 | 0.89 |
| 10:k5:741:GLN:C | 1:D7:77:ARG:HH21 | 1.81 | 0.89 |
| 3:F6:82:CYS:SG | 12:F6:201:CYC:C4C | 2.61 | 0.89 |
| 8:i7:20:PRO:HD3 | 8:s7:155:TYR:CZ | 2.07 | 0.89 |
| 12:D8:202:CYC:CBA | 4:M8:35:THR:HA | 2.01 | 0.89 |
| 8:u7:29:PHE:CE2 | 1:v7:31:PHE:CZ | 2.60 | 0.89 |
| 8:u7:29:PHE:HE2 | 1:v7:5:ILE:HD11 | 1.38 | 0.89 |
| 12:M8:301:CYC:HMB2 | 3:Y8:89:ILE:CG1 | 2.03 | 0.89 |
| 4:M9:185:ALA:CB | 12:V9:201:CYC:CGA | 2.50 | 0.89 |
| 5:Z8:22:LEU:HD23 | 5:Z8:26:LEU:HD11 | 0.89 | 0.89 |
| 3:F9:153:CYS:HB3 | 12:F9:303:CYC:NC | 1.84 | 0.89 |
| 11:a9:339:GLU:N | 11:a9:340:PRO:HD3 | 1.87 | 0.89 |
| 11:aA:49:TRP:O | 11:aA:53:VAL:HG23 | 1.73 | 0.89 |
| 11:aA:312:ASP:HA | 11:aA:315:LEU:N | 1.87 | 0.89 |
| 11:aA:739:ASP:HB2 | 3:L1:84:ARG:HH11 | 1.38 | 0.89 |
| 12:JA:201:CYC:HMD1 | 12:JA:201:CYC:NC | 1.88 | 0.89 |
| 6:M2:28:ASN:CB | 8:O5:80:LEU:CG | 2.49 | 0.89 |
| 3:F4:115:GLU:C | 4:M4:3:VAL:CG1 | 2.46 | 0.89 |
| 10:j5:77:VAL:HG22 | 10:j5:141:GLU:HB3 | 1.54 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:480:GLU:OE1 | 10:j5:689:GLY:HA3 | 1.72 | 0.89 |
| 10:j5:974:LEU:CD1 | 1:v7:106:GLU:OE2 | 2.20 | 0.89 |
| 10:j5:1146:THR:HB | 1:v7:77:ARG:HH21 | 1.24 | 0.89 |
| 10:k5:1055:SER:HB2 | 12:k5:1203:CYC:CAB | 2.03 | 0.89 |
| 12:F6:202:CYC:HMD1 | 12:F6:202:CYC:NC | 1.88 | 0.89 |
| 8:i7:96:ILE:CA | 8:i7:152:TYR:CZ | 2.50 | 0.89 |
| 8:c7:39:ILE:CD1 | 8:c7:148:GLU:HG3 | 1.87 | 0.89 |
| 8:c7:92:VAL:HG23 | 8:c7:156:LEU:HD11 | 1.53 | 0.89 |
| 3:B8:68:ARG:CZ | 3:U8:68:ARG:NH2 | 2.34 | 0.89 |
| 8:u7:98:ALA:HB2 | 1:v7:9:ILE:HD11 | 1.53 | 0.89 |
| 4:M8:139:VAL:HG21 | 4:M8:216:ASN:C | 1.98 | 0.89 |
| 12:M8:301:CYC:HAB1 | 3:Y8:88:ILE:HG22 | 1.54 | 0.89 |
| 4:M9:162:ASN:H | 12:V9:201:CYC:CBB | 1.86 | 0.89 |
| 11:aA:621:THR:HG22 | 3:J1:14:LEU:HD21 | 1.54 | 0.89 |
| 2:GA:119:THR:HG21 | 3:LA:83:LEU:HD13 | 1.55 | 0.89 |
| 3:HA:108:ARG:NH1 | 11:aA:448:ASN:HD21 | 1.71 | 0.89 |
| 4:MA:211:GLN:O | 5:NA:28:HIS:NE2 | 2.06 | 0.89 |
| 12:R1:201:CYC:C4B | 5:N1:54:LEU:HD11 | 2.00 | 0.89 |
| 12:L3:202:CYC:NB | 11:a9:738:LEU:HD13 | 1.86 | 0.89 |
| 4:M4:228:SER:HB2 | 2:X4:16:GLY:HA3 | 1.54 | 0.89 |
| 1:T5:53:LYS:NZ | 8:U5:120:GLN:HG3 | 1.89 | 0.89 |
| 10:j5:725:LEU:HD23 | 10:j5:725:LEU:C | 1.96 | 0.89 |
| 10:j5:1008:PHE:HE1 | 1:v7:87:TYR:CD2 | 1.90 | 0.89 |
| 12:H6:202:CYC:HMD1 | 12:H6:202:CYC:NC | 1.88 | 0.89 |
| 12:k7:201:CYC:HMA1 | 12:k7:201:CYC:HB | 1.37 | 0.89 |
| 12:B8:201:CYC:HMD1 | 12:B8:201:CYC:NC | 1.88 | 0.89 |
| 3:Q8:127:VAL:HG21 | 12:Z8:301:CYC:CMC | 2.01 | 0.89 |
| 2:K9:15:GLN:C | 11:a9:393:ARG:HH11 | 1.70 | 0.89 |
| 4:M1:258:LYS:NZ | 3:Z1:111:ASN:CG | 2.32 | 0.89 |
| 12:V1:202:CYC:HMD1 | 12:V1:202:CYC:NC | 1.88 | 0.89 |
| 2:AA:114:ARG:HH12 | 11:aA:407:GLU:CD | 1.81 | 0.88 |
| 3:JA:65:ASP:CB | 11:aA:354:VAL:HG22 | 2.00 | 0.88 |
| 3:LA:111:ASN:O | 11:aA:532:ALA:HB3 | 1.73 | 0.88 |
| 2:OA:63:PHE:CB | 2:OA:66:LEU:HD11 | 2.03 | 0.88 |
| 12:ZA:201:CYC:HMD1 | 12:ZA:201:CYC:NC | 1.88 | 0.88 |
| 12:B4:201:CYC:HMD1 | 12:B4:201:CYC:NC | 1.88 | 0.88 |
| 2:N4:33:ARG:NH2 | 2:X4:28:ASN:CG | 2.30 | 0.88 |
| 5:Z4:24:PRO:CD | 12:Z4:301:CYC:O2A | 2.21 | 0.88 |
| 5:Z4:41:GLN:CB | 12:Z4:301:CYC:C3B | 2.50 | 0.88 |
| 1:X5:50:THR:HG21 | 8:a5:49:ARG:NH2 | 1.87 | 0.88 |
| 6:M6:53:LEU:HD23 | 8:c7:80:LEU:HD21 | 1.54 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 12:A7:201:CYC:HMA1 | 12:A7:201:CYC:HB | 1.37 | 0.88 |
| 10:k5:1020:GLU:HG3 | 1:Z7:87:TYR:CE1 | 2.07 | 0.88 |
| 12:Q7:201:CYC:HB | 12:Q7:201:CYC:HMA1 | 1.37 | 0.88 |
| 8:W7:13:ALA:HA | 9:w7:46:LYS:HZ2 | 0.74 | 0.88 |
| 12:B8:202:CYC:CBB | 4:M8:61:ASN:HB3 | 1.85 | 0.88 |
| 2:C8:13:ASP:OD2 | 11:a9:107:ARG:NH1 | 2.05 | 0.88 |
| 8:o7:103:PRO:HB3 | 1:p7:9:ILE:CG2 | 2.03 | 0.88 |
| 2:X8:57:GLN:NE2 | 3:T9:33:GLU:OE2 | 2.06 | 0.88 |
| 3:F8:112:GLY:C | 3:F8:114:LYS:N | 2.25 | 0.88 |
| 4:M8:215:GLU:CD | 4:M8:215:GLU:O | 2.15 | 0.88 |
| 5:N9:22:LEU:HD23 | 5:N9:26:LEU:HD11 | 0.89 | 0.88 |
| 11:a9:629:LYS:HA | 11:a9:629:LYS:NZ | 1.86 | 0.88 |
| 11:aA:75:ALA:CA | 11:aA:81:ASP:OD2 | 2.21 | 0.88 |
| 11:aA:377:VAL:O | 11:aA:391:VAL:HG22 | 1.71 | 0.88 |
| 11:aA:640:ALA:CB | 11:aA:767:THR:CG2 | 2.51 | 0.88 |
| 3:FA:111:ASN:HD21 | 4:MA:65:ARG:HD2 | 1.38 | 0.88 |
| 3:TA:33:GLU:OE2 | 2:X4:57:GLN:NE2 | 2.06 | 0.88 |
| 3:B4:82:CYS:HB2 | 12:B4:202:CYC:OC | 1.74 | 0.88 |
| 8:A5:115:MET:HE2 | 1:F5:75:THR:HG22 | 1.55 | 0.88 |
| 1:b5:30:TYR:CE2 | 10:k5:47:PHE:CZ | 2.61 | 0.88 |
| 10:k5:743:VAL:HG13 | 12:D7:201:CYC:O2D | 1.74 | 0.88 |
| 10:k5:1105:ILE:CD1 | 10:k5:1115:ARG:HH22 | 1.86 | 0.88 |
| 12:K7:201:CYC:HB | 12:K7:201:CYC:HMA1 | 1.37 | 0.88 |
| 8:i7:21:GLY:HA2 | 8:s7:100:ASP:HA | 1.53 | 0.88 |
| 8:k7:76:LYS:HZ3 | 11:a9:604:ALA:HB1 | 1.36 | 0.88 |
| 8:c7:121:THR:HG23 | 12:c7:201:CYC:HMC3 | 1.55 | 0.88 |
| 2:A8:33:ARG:NH2 | 2:K8:28:ASN:CG | 2.31 | 0.88 |
| 12:D8:202:CYC:CBA | 4:M8:35:THR:HB | 2.03 | 0.88 |
| 8:o7:18:LEU:CD2 | 1:p7:97:LEU:HD13 | 2.03 | 0.88 |
| 2:X8:57:GLN:CD | 3:T9:32:LYS:CE | 2.46 | 0.88 |
| 12:H8:202:CYC:HMD1 | 12:H8:202:CYC:NC | 1.88 | 0.88 |
| 12:L8:201:CYC:HMD1 | 12:L8:201:CYC:NC | 1.88 | 0.88 |
| 4:M9:51:ARG:HH21 | 11:a9:430:ARG:HD3 | 1.38 | 0.88 |
| 3:H9:66:LEU:CD2 | 12:H9:202:CYC:OC | 2.14 | 0.88 |
| 11:a9:640:ALA:CB | 11:a9:767:THR:CG2 | 2.51 | 0.88 |
| 11:a9:801:ASN:ND2 | 11:a9:801:ASN:O | 2.06 | 0.88 |
| 1:A:75:THR:CG2 | 10:k5:182:ASN:O | 2.22 | 0.88 |
| 4:MA:158:PHE:C | 3:VA:108:ARG:HG3 | 1.96 | 0.88 |
| 12:B3:201:CYC:HMD1 | 12:B3:201:CYC:NC | 1.88 | 0.88 |
| 12:B3:202:CYC:HBA2 | 11:a9:684:ASN:CA | 2.03 | 0.88 |
| 12:D3:201:CYC:HMD1 | 12:D3:201:CYC:NC | 1.88 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:O3:63:PHE:CB | 2:O3:66:LEU:HD11 | 2.03 | 0.88 |
| 2:P4:19:LEU:CD1 | 3:Q4:95:TYR:HE1 | 1.87 | 0.88 |
| 1:B5:76:ARG:HD2 | 9:z5:14:LEU:HB2 | 1.53 | 0.88 |
| 1:d5:28:LYS:HD3 | 1:n7:143:PRO:HB3 | 0.88 | 0.88 |
| 1:T5:87:TYR:CE2 | 10:j5:483:PHE:HE2 | 1.92 | 0.88 |
| 6:M6:65:VAL:CG1 | 1:b7:59:ALA:C | 2.46 | 0.88 |
| 12:C7:201:CYC:HB | 12:C7:201:CYC:HMA1 | 1.37 | 0.88 |
| 2:A8:63:PHE:CB | 2:A8:66:LEU:HD11 | 2.03 | 0.88 |
| 3:B8:116:THR:HG21 | 4:M8:53:LEU:HD12 | 1.55 | 0.88 |
| 8:o7:98:ALA:HB2 | 1:p7:9:ILE:HD11 | 1.53 | 0.88 |
| 4:M8:190:ARG:HH11 | 4:M8:202:SER:CB | 1.83 | 0.88 |
| 4:M8:231:THR:CA | 12:M8:301:CYC:HBB3 | 2.01 | 0.88 |
| 4:M8:235:PHE:HB3 | 12:M8:301:CYC:CMA | 2.01 | 0.88 |
| 2:N8:63:PHE:CB | 2:N8:66:LEU:HD11 | 2.03 | 0.88 |
| 3:Q8:117:TYR:HA | 3:Q8:120:LEU:CD2 | 2.03 | 0.88 |
| 3:L9:14:LEU:HD21 | 11:a9:358:PRO:N | 1.89 | 0.88 |
| 4:M9:184:ILE:HG22 | 12:V9:201:CYC:HBA2 | 1.56 | 0.88 |
| 4:M9:211:GLN:O | 5:N9:28:HIS:NE2 | 2.06 | 0.88 |
| 5:N9:3:VAL:HG11 | 3:R9:115:GLU:CB | 2.04 | 0.88 |
| 2:O9:63:PHE:CB | 2:O9:66:LEU:HD11 | 2.03 | 0.88 |
| 5:Z8:39:PRO:HG3 | 12:Z8:301:CYC:CHD | 2.04 | 0.88 |
| 11:aA:635:VAL:HG11 | 11:aA:795:ASP:OD2 | 1.72 | 0.88 |
| 11:aA:801:ASN:O | 11:aA:801:ASN:ND2 | 2.06 | 0.88 |
| 4:M1:118:TYR:HD2 | 3:X1:84:ARG:NH2 | 1.71 | 0.88 |
| 4:M1:258:LYS:NZ | 3:Z1:111:ASN:OD1 | 2.04 | 0.88 |
| 2:QA:119:THR:OG1 | 3:TA:83:LEU:HD13 | 1.73 | 0.88 |
| 3:L3:88:ILE:HG13 | 11:a9:742:GLN:HE21 | 1.34 | 0.88 |
| 3:F4:107:ASP:CB | 4:M4:8:SER:H | 1.86 | 0.88 |
| 12:M4:301:CYC:HAC2 | 3:Y4:82:CYS:HB2 | 1.54 | 0.88 |
| 2:P4:9:ILE:HD11 | 3:Q4:98:LEU:HD23 | 1.55 | 0.88 |
| 8:e5:49:ARG:CZ | 1:R5:50:THR:CG2 | 2.50 | 0.88 |
| 1:f5:5:ILE:CD1 | 10:j5:46:PHE:CZ | 2.56 | 0.88 |
| 1:f5:19:LEU:HD13 | 10:j5:172:LEU:HD13 | 1.56 | 0.88 |
| 10:j5:136:VAL:HG12 | 10:j5:137:PRO:HD2 | 1.44 | 0.88 |
| 10:j5:1150:TYR:HE1 | 11:aA:38:VAL:CG2 | 1.87 | 0.88 |
| 3:O8:95:TYR:HD2 | 3:O8:108:ARG:HH22 | 1.16 | 0.88 |
| 3:Q8:117:TYR:O | 3:Q8:120:LEU:HG | 1.71 | 0.88 |
| 3:S8:113:LEU:HD12 | 3:S8:116:THR:HG21 | 1.55 | 0.88 |
| 4:M9:36:TYR:O | 12:B9:201:CYC:CMA | 2.22 | 0.88 |
| 3:H9:117:TYR:CZ | 12:H9:202:CYC:HHB | 2.07 | 0.88 |
| 11:aA:795:ASP:O | 12:aA:901:CYC:HBB3 | 1.73 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M1:80:PRO:HA | 3:X1:111:ASN:HD21 | 1.36 | 0.88 |
| 2:A3:63:PHE:CB | 2:A3:66:LEU:HD11 | 2.03 | 0.88 |
| 3:D3:68:ARG:CZ | 3:X3:68:ARG:NH2 | 2.36 | 0.88 |
| 3:D4:116:THR:OG1 | 4:M4:38:PRO:CB | 2.22 | 0.88 |
| 4:M3:118:TYR:HD2 | 3:X3:84:ARG:NH2 | 1.71 | 0.88 |
| 2:N4:111:ALA:O | 5:Z4:34:LEU:CB | 2.05 | 0.88 |
| 10:j5:1125:ARG:HG2 | 1:t7:115:THR:OG1 | 1.73 | 0.88 |
| 3:D1:68:ARG:CZ | 3:X1:68:ARG:NH2 | 2.36 | 0.88 |
| 1:B7:140:LEU:CG | 11:a9:561:ALA:HB2 | 2.04 | 0.88 |
| 8:C7:17:TYR:CE2 | 1:D7:90:ARG:HA | 2.09 | 0.88 |
| 8:G7:86:ASP:HB2 | 11:a9:579:PHE:CZ | 2.07 | 0.88 |
| 1:N7:106:GLU:HG3 | 9:z7:58:THR:HG23 | 1.54 | 0.88 |
| 8:c7:50:ILE:HG22 | 8:c7:133:MET:HG2 | 1.56 | 0.88 |
| 8:u7:18:LEU:CD2 | 1:v7:97:LEU:HD13 | 2.03 | 0.88 |
| 11:aA:798:SER:OG | 12:aA:901:CYC:C3A | 2.20 | 0.88 |
| 12:HA:201:CYC:HMD1 | 12:HA:201:CYC:NC | 1.88 | 0.88 |
| 4:MA:51:ARG:HH21 | 11:aA:430:ARG:HD3 | 1.38 | 0.88 |
| 4:MA:185:ALA:CB | 12:VA:201:CYC:CGA | 2.50 | 0.88 |
| 5:NA:53:LEU:HB3 | 12:TA:301:CYC:CAA | 2.02 | 0.88 |
| 5:NA:72:GLU:HG3 | 3:TA:119:ALA:O | 1.73 | 0.88 |
| 12:H3:201:CYC:HMD1 | 12:H3:201:CYC:NC | 1.88 | 0.88 |
| 3:H2:77:ARG:HH11 | 6:M2:117:MET:HE3 | 0.71 | 0.88 |
| 2:K2:28:ASN:CG | 2:A2:33:ARG:NH2 | 2.31 | 0.88 |
| 12:L2:202:CYC:HMD1 | 12:L2:202:CYC:NC | 1.88 | 0.88 |
| 5:N3:22:LEU:CG | 5:N3:26:LEU:HD21 | 2.02 | 0.88 |
| 12:S4:201:CYC:HMD1 | 12:S4:201:CYC:NC | 1.88 | 0.88 |
| 2:N4:111:ALA:O | 5:Z4:34:LEU:HD13 | 1.72 | 0.88 |
| 12:B5:201:CYC:HBA1 | 9:z5:26:THR:HG21 | 1.56 | 0.88 |
| 1:D5:39:ARG:O | 1:D5:40:ALA:C | 2.14 | 0.88 |
| 8:Q5:12:ASP:CB | 1:R5:94:TYR:HE2 | 1.80 | 0.88 |
| 10:j5:449:ARG:HH21 | 10:j5:449:ARG:HG3 | 1.37 | 0.88 |
| 10:j5:1119:LEU:CD1 | 12:j5:1202:CYC:C4B | 2.51 | 0.88 |
| 10:j5:1124:TYR:CE2 | 1:t7:119:LEU:HD21 | 2.08 | 0.88 |
| 10:k5:476:ASN:ND2 | 10:k5:476:ASN:O | 2.07 | 0.88 |
| 12:G7:201:CYC:HB | 12:G7:201:CYC:HMA1 | 1.37 | 0.88 |
| 1:v7:62:TYR:CD1 | 11:aA:602:PRO:HD3 | 2.09 | 0.88 |
| 4:M8:136:SER:HB3 | 5:Z8:2:SER:HB2 | 1.53 | 0.88 |
| 2:A9:33:ARG:NH2 | 2:K9:28:ASN:CG | 2.31 | 0.88 |
| 11:a9:640:ALA:HB1 | 11:a9:767:THR:HG23 | 1.56 | 0.88 |
| 12:Z1:201:CYC:HMD1 | 12:Z1:201:CYC:NC | 1.88 | 0.88 |
| 1:Z:161:SER:OG | 1:X5:14:VAL:HG23 | 1.68 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:MA:5:THR:O | 4:MA:6:THR:OG1 | 1.90 | 0.88 |
| 2:OA:33:ARG:NH2 | 2:YA:28:ASN:CG | 2.30 | 0.88 |
| 3:TA:32:LYS:CE | 2:X4:57:GLN:CD | 2.46 | 0.88 |
| 3:B3:88:ILE:HD13 | 12:B3:202:CYC:C4B | 2.03 | 0.88 |
| 12:B4:202:CYC:HMA2 | 4:M4:58:TYR:H | 0.72 | 0.88 |
| 3:L3:104:VAL:CB | 3:L3:108:ARG:NH2 | 2.37 | 0.88 |
| 3:F4:91:ARG:HH22 | 11:aA:140:GLN:HE22 | 1.22 | 0.88 |
| 1:d5:161:SER:OG | 10:j5:696:ARG:HA | 1.71 | 0.88 |
| 10:k5:388:ARG:HB3 | 10:k5:388:ARG:CZ | 2.02 | 0.88 |
| 1:R7:49:THR:HG22 | 8:C7:161:GLN:CD | 1.98 | 0.88 |
| 8:i7:121:THR:HG23 | 12:i7:201:CYC:HMC3 | 1.55 | 0.88 |
| 8:m7:17:TYR:CE2 | 1:n7:90:ARG:HA | 2.09 | 0.88 |
| 4:M8:29:PRO:CB | 11:a9:225:VAL:O | 2.16 | 0.88 |
| 4:M9:5:THR:O | 4:M9:6:THR:OG1 | 1.90 | 0.88 |
| 2:A9:63:PHE:CB | 2:A9:66:LEU:HD11 | 2.03 | 0.88 |
| 2:I9:113:LEU:HD21 | 2:I9:161:LEU:CD2 | 2.02 | 0.88 |
| 11:aA:776:TYR:HE1 | 12:H1:201:CYC:OB | 1.44 | 0.88 |
| 12:X1:202:CYC:HMD1 | 12:X1:202:CYC:NC | 1.88 | 0.88 |
| 12:F2:202:CYC:HMD1 | 12:F2:202:CYC:NC | 1.88 | 0.88 |
| 3:DA:111:ASN:OD1 | 4:MA:76:ALA:HB3 | 1.73 | 0.88 |
| 3:HA:66:LEU:CD2 | 12:HA:202:CYC:OC | 2.15 | 0.88 |
| 12:PA:202:CYC:HMD1 | 12:PA:202:CYC:NC | 1.88 | 0.88 |
| 6:M2:26:PHE:HB2 | 8:O5:87:TYR:OH | 1.07 | 0.88 |
| 3:D4:14:LEU:HD11 | 3:Y4:125:ARG:NE | 1.88 | 0.88 |
| 12:T5:201:CYC:HBB1 | 10:j5:482:GLN:HE22 | 1.38 | 0.88 |
| 10:k5:232:ARG:CZ | 10:k5:232:ARG:HB2 | 2.00 | 0.88 |
| 10:k5:1153:VAL:HG23 | 1:p7:125:ALA:CB | 1.96 | 0.88 |
| 12:D6:202:CYC:HMD1 | 12:D6:202:CYC:NC | 1.88 | 0.88 |
| 8:g7:94:TYR:OH | 1:h7:17:LYS:O | 1.92 | 0.88 |
| 8:i7:96:ILE:N | 8:i7:152:TYR:CD2 | 2.42 | 0.88 |
| 8:U7:17:TYR:CE2 | 1:V7:90:ARG:HA | 2.09 | 0.88 |
| 3:B8:108:ARG:CA | 4:M8:61:ASN:HA | 2.04 | 0.88 |
| 3:B8:120:LEU:HD11 | 4:M8:53:LEU:CA | 2.04 | 0.88 |
| 3:U8:114:LYS:HZ1 | 4:M8:13:LYS:NZ | 1.69 | 0.88 |
| 4:M9:274:VAL:CB | 3:V9:77:ARG:CD | 2.51 | 0.88 |
| 12:H9:201:CYC:HMD1 | 12:H9:201:CYC:NC | 1.88 | 0.88 |
| 12:J9:202:CYC:HBA2 | 11:a9:511:LYS:CA | 2.00 | 0.88 |
| 12:T9:302:CYC:HMD1 | 12:T9:302:CYC:NC | 1.88 | 0.88 |
| 11:a9:75:ALA:CA | 11:a9:81:ASP:OD2 | 2.21 | 0.88 |
| 11:aA:670:LEU:CD2 | 2:K1:112:GLY:HA3 | 2.01 | 0.88 |
| 3:F2:78:ARG:CG | 12:F2:201:CYC:CGD | 2.52 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:MA:37:GLU:OE1 | 4:MA:40:GLN:CD | 2.17 | 0.88 |
| 2:G3:111:ALA:CB | 3:L3:77:ARG:HG2 | 2.04 | 0.88 |
| 3:B4:68:ARG:NH2 | 3:U4:68:ARG:HH22 | 1.65 | 0.88 |
| 2:O3:33:ARG:NH2 | 2:Y3:28:ASN:CG | 2.31 | 0.88 |
| 12:U4:202:CYC:HMD1 | 12:U4:202:CYC:NC | 1.88 | 0.88 |
| 12:L4:201:CYC:HMD1 | 12:L4:201:CYC:NC | 1.88 | 0.88 |
| 8:M5:90:ARG:HA | 1:N5:18:TYR:CE2 | 2.09 | 0.88 |
| 12:V5:201:CYC:HBB2 | 10:j5:623:VAL:HG21 | 1.56 | 0.88 |
| 10:k5:138:PRO:HB2 | 10:k5:201:VAL:HG11 | 1.55 | 0.88 |
| 10:k5:449:ARG:HH21 | 10:k5:449:ARG:HG3 | 1.37 | 0.88 |
| 10:k5:978:LEU:CD1 | 1:p7:107:ARG:HH22 | 1.86 | 0.88 |
| 10:k5:1146:THR:HB | 1:p7:77:ARG:HH22 | 1.33 | 0.88 |
| 1:H7:140:LEU:CG | 11:aA:561:ALA:HB2 | 2.03 | 0.88 |
| 8:c7:96:ILE:N | 8:c7:152:TYR:CD2 | 2.42 | 0.88 |
| 12:c7:201:CYC:HMA1 | 12:c7:201:CYC:HB | 1.37 | 0.88 |
| 12:q7:201:CYC:HB | 12:q7:201:CYC:HMA1 | 1.37 | 0.88 |
| 3:F8:91:ARG:HH22 | 11:a9:140:GLN:HE22 | 1.20 | 0.88 |
| 3:Q8:102:ALA:HB1 | 3:Q8:166:LYS:HD3 | 1.55 | 0.88 |
| 12:F1:202:CYC:HMD1 | 12:F1:202:CYC:NC | 1.88 | 0.88 |
| 3:L9:83:LEU:HD13 | 2:G9:119:THR:HG21 | 1.55 | 0.88 |
| 5:N9:16:PHE:CE1 | 3:T9:120:LEU:CD2 | 2.57 | 0.88 |
| 11:a9:95:ILE:CD1 | 11:a9:237:PHE:CD1 | 2.56 | 0.88 |
| 11:a9:632:ILE:HG21 | 11:a9:634:ALA:HB2 | 1.55 | 0.88 |
| 11:aA:95:ILE:CD1 | 11:aA:237:PHE:CD1 | 2.56 | 0.88 |
| 11:aA:312:ASP:HA | 11:aA:315:LEU:CA | 2.02 | 0.88 |
| 11:aA:623:ASP:CA | 3:H1:78:ARG:HH22 | 1.87 | 0.88 |
| 2:AA:33:ARG:NH2 | 2:KA:28:ASN:CG | 2.31 | 0.88 |
| 4:MA:188:LEU:CD2 | 12:VA:201:CYC:NB | 2.37 | 0.88 |
| 5:NA:3:VAL:HG11 | 3:RA:115:GLU:CB | 2.04 | 0.88 |
| 5:NA:16:PHE:CE1 | 3:TA:120:LEU:CD2 | 2.57 | 0.88 |
| 2:A1:33:ARG:NH2 | 2:K1:28:ASN:CG | 2.31 | 0.88 |
| 12:J3:202:CYC:HAA1 | 11:a9:798:SER:OG | 1.72 | 0.88 |
| 12:Z3:201:CYC:OB | 4:M3:162:ASN:CB | 2.22 | 0.88 |
| 4:M3:222:ARG:HG3 | 4:M3:222:ARG:HH11 | 1.38 | 0.88 |
| 12:B1:201:CYC:HMD1 | 12:B1:201:CYC:NC | 1.88 | 0.88 |
| 4:M4:104:ALA:HB3 | 2:P4:14:SER:N | 1.82 | 0.88 |
| 8:M5:94:TYR:OH | 1:N5:17:LYS:O | 1.91 | 0.88 |
| 5:Z4:25:THR:HG22 | 5:Z4:63:ASN:O | 1.73 | 0.88 |
| 1:P5:114:GLU:OE1 | 10:k5:496:GLU:CB | 2.22 | 0.88 |
| 8:S5:90:ARG:HA | 1:T5:18:TYR:CE2 | 2.09 | 0.88 |
| 12:Y5:201:CYC:HMA1 | 12:Y5:201:CYC:HB | 1.37 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 12:L6:202:CYC:HMD1 | 12:L6:202:CYC:NC | 1.88 | 0.88 |
| 1:Z7:53:LYS:HD3 | 8:a7:118:SER:O | 1.74 | 0.88 |
| 8:a7:94:TYR:OH | 1:b7:17:LYS:O | 1.92 | 0.88 |
| 2:N8:112:GLY:N | 5:Z8:34:LEU:H | 1.69 | 0.88 |
| 12:S8:201:CYC:HMD1 | 12:S8:201:CYC:NC | 1.88 | 0.88 |
| 3:L9:111:ASN:O | 11:a9:532:ALA:N | 2.07 | 0.88 |
| 4:M9:1:MET:CA | 11:a9:422:SER:O | 2.01 | 0.88 |
| 4:M9:1:MET:HG2 | 11:a9:422:SER:O | 1.72 | 0.88 |
| 2:G1:111:ALA:CB | 3:L1:77:ARG:HG2 | 2.04 | 0.88 |
| 11:a9:245:ALA:HB2 | 12:a9:901:CYC:C3B | 2.02 | 0.88 |
| 12:B2:201:CYC:HMD1 | 12:B2:201:CYC:NC | 1.88 | 0.88 |
| 4:MA:162:ASN:H | 12:VA:201:CYC:CBB | 1.86 | 0.87 |
| 4:MA:188:LEU:HD22 | 12:VA:201:CYC:NB | 1.88 | 0.87 |
| 2:QA:18:PHE:CZ | 3:RA:48:ALA:CB | 2.57 | 0.87 |
| 6:M2:28:ASN:CB | 8:O5:80:LEU:HD23 | 2.02 | 0.87 |
| 6:M2:53:LEU:HD23 | 8:i7:80:LEU:HG | 1.42 | 0.87 |
| 12:L3:201:CYC:HMD1 | 12:L3:201:CYC:NC | 1.88 | 0.87 |
| 5:N3:22:LEU:HD23 | 5:N3:26:LEU:HD11 | 0.90 | 0.87 |
| 5:N3:66:ARG:NH1 | 3:R3:111:ASN:ND2 | 2.22 | 0.87 |
| 1:F5:69:GLY:O | 10:k5:554:ASN:ND2 | 2.07 | 0.87 |
| 8:U5:87:TYR:CE2 | 6:M6:26:PHE:CD2 | 2.62 | 0.87 |
| 10:j5:939:GLN:O | 10:j5:943:THR:HG23 | 1.75 | 0.87 |
| 10:k5:931:VAL:HA | 1:D7:29:ALA:O | 1.73 | 0.87 |
| 10:k5:935:LEU:HD11 | 1:D7:25:ASP:O | 1.74 | 0.87 |
| 8:g7:25:ARG:HH21 | 8:u7:25:ARG:HH11 | 1.21 | 0.87 |
| 1:Z7:67:ARG:CG | 11:a9:311:LEU:HD22 | 2.04 | 0.87 |
| 3:L9:111:ASN:O | 11:a9:532:ALA:HB3 | 1.72 | 0.87 |
| 5:N9:22:LEU:CG | 5:N9:26:LEU:HD21 | 2.02 | 0.87 |
| 11:aA:746:TYR:HB2 | 2:K1:14:SER:HA | 1.53 | 0.87 |
| 3:JA:111:ASN:CA | 11:aA:518:ALA:HB3 | 2.05 | 0.87 |
| 4:MA:188:LEU:CD2 | 12:VA:201:CYC:HB | 1.86 | 0.87 |
| 5:NA:4:LEU:O | 3:RA:112:GLY:HA3 | 1.75 | 0.87 |
| 12:J3:201:CYC:HMD1 | 12:J3:201:CYC:NC | 1.88 | 0.87 |
| 2:C4:13:ASP:OD2 | 11:aA:107:ARG:NH1 | 2.06 | 0.87 |
| 12:D4:201:CYC:HMD1 | 12:D4:201:CYC:NC | 1.88 | 0.87 |
| 5:N3:34:LEU:HB2 | 3:T3:84:ARG:HD3 | 1.53 | 0.87 |
| 2:N4:14:SER:HB3 | 5:Z4:62:ARG:CD | 1.96 | 0.87 |
| 12:Q4:201:CYC:HMD1 | 12:Q4:201:CYC:NC | 1.88 | 0.87 |
| 6:M6:243:ALA:CB | 12:H6:201:CYC:HBB2 | 2.03 | 0.87 |
| 10:j5:820:HIS:HD1 | 10:j5:859:ILE:CD1 | 1.83 | 0.87 |
| 10:j5:1105:ILE:CD1 | 10:j5:1115:ARG:HH22 | 1.86 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:k5:1064:LYS:CD | 10:k5:1065:HIS:N | 2.38 | 0.87 |
| 10:k5:1118:THR:O | 12:k5:1204:CYC:CMA | 2.23 | 0.87 |
| 10:k5:1147:TYR:CE1 | 11:a9:35:ARG:CB | 2.58 | 0.87 |
| 8:g7:118:SER:O | 1:f7:53:LYS:HD3 | 1.74 | 0.87 |
| 12:W7:201:CYC:HB | 12:W7:201:CYC:HMA1 | 1.37 | 0.87 |
| 12:m7:201:CYC:HB | 12:m7:201:CYC:HMA1 | 1.37 | 0.87 |
| 2:X8:107:ASP:OD2 | 4:M8:273:ILE:HG22 | 1.74 | 0.87 |
| 2:A9:114:ARG:HH12 | 11:a9:407:GLU:CD | 1.81 | 0.87 |
| 3:H9:116:THR:HG21 | 12:H9:202:CYC:CMA | 2.04 | 0.87 |
| 11:a9:89:ALA:HA | 11:a9:92:LYS:HZ1 | 1.39 | 0.87 |
| 11:a9:338:VAL:HG22 | 11:a9:340:PRO:HD3 | 1.54 | 0.87 |
| 11:aA:371:VAL:HG11 | 11:aA:507:PHE:CD2 | 2.10 | 0.87 |
| 11:aA:640:ALA:HB1 | 11:aA:767:THR:HG23 | 1.55 | 0.87 |
| 4:M1:162:ASN:CB | 12:Z1:202:CYC:OB | 2.22 | 0.87 |
| 4:M1:258:LYS:HZ1 | 3:Z1:111:ASN:CG | 1.82 | 0.87 |
| 12:T1:302:CYC:HMD1 | 12:T1:302:CYC:NC | 1.88 | 0.87 |
| 1:Z:16:GLY:HA2 | 8:e5:90:ARG:NH1 | 1.89 | 0.87 |
| 3:F4:113:LEU:HB2 | 4:M4:5:THR:HG22 | 1.56 | 0.87 |
| 4:M4:104:ALA:HB3 | 2:P4:14:SER:HA | 1.48 | 0.87 |
| 2:N4:111:ALA:CA | 5:Z4:34:LEU:HG | 2.04 | 0.87 |
| 1:f5:6:THR:HG22 | 10:j5:19:THR:OG1 | 1.75 | 0.87 |
| 1:b5:18:TYR:CD2 | 10:k5:165:ARG:HG3 | 2.09 | 0.87 |
| 1:b5:38:VAL:HG13 | 10:k5:40:VAL:HG11 | 1.56 | 0.87 |
| 9:i5:14:LEU:HD12 | 9:i5:15:LYS:H | 1.33 | 0.87 |
| 10:j5:476:ASN:O | 10:j5:476:ASN:ND2 | 2.07 | 0.87 |
| 10:j5:1147:TYR:CE1 | 11:aA:35:ARG:CB | 2.56 | 0.87 |
| 10:k5:631:HIS:HD2 | 10:k5:664:MET:HE3 | 1.38 | 0.87 |
| 8:c7:39:ILE:HD13 | 8:c7:148:GLU:HB3 | 1.48 | 0.87 |
| 3:U8:114:LYS:CE | 4:M8:13:LYS:HE3 | 2.02 | 0.87 |
| 3:L8:82:CYS:HG | 12:a9:901:CYC:HAC2 | 1.02 | 0.87 |
| 12:R9:202:CYC:HMD1 | 12:R9:202:CYC:NC | 1.88 | 0.87 |
| 12:V9:202:CYC:HMD1 | 12:V9:202:CYC:NC | 1.88 | 0.87 |
| 12:Z9:201:CYC:HMD1 | 12:Z9:201:CYC:NC | 1.88 | 0.87 |
| 11:a9:99:ALA:CB | 11:a9:100:PRO:HD3 | 2.01 | 0.87 |
| 2:A2:63:PHE:CB | 2:A2:66:LEU:HD11 | 2.02 | 0.87 |
| 3:FA:36:LYS:CB | 3:FA:156:LEU:CD1 | 2.53 | 0.87 |
| 3:HA:107:ASP:HB3 | 11:aA:445:THR:HG22 | 1.54 | 0.87 |
| 2:QA:32:GLN:HG2 | 2:UA:28:ASN:HD21 | 1.39 | 0.87 |
| 3:J3:85:ASP:N | 11:a9:668:TYR:CZ | 2.38 | 0.87 |
| 3:L3:1:MET:HG3 | 3:L3:104:VAL:HG12 | 1.56 | 0.87 |
| 12:P3:202:CYC:HMD1 | 12:P3:202:CYC:NC | 1.88 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:U3:43:ALA:O | 2:U3:46:SER:O | 1.91 | 0.87 |
| 12:H4:202:CYC:HMD1 | 12:H4:202:CYC:NC | 1.88 | 0.87 |
| 4:M4:27:HIS:CD2 | 4:M4:34:ASP:OD1 | 2.27 | 0.87 |
| 3:Y4:109:CYS:SG | 3:Y4:110:LEU:HG | 2.15 | 0.87 |
| 12:Y4:201:CYC:HMD1 | 12:Y4:201:CYC:NC | 1.88 | 0.87 |
| 8:W5:16:ARG:HA | 1:X5:90:ARG:CZ | 2.04 | 0.87 |
| 10:k5:199:THR:HG22 | 12:k5:1201:CYC:CBC | 2.05 | 0.87 |
| 12:S7:201:CYC:HB | 12:S7:201:CYC:HMA1 | 1.37 | 0.87 |
| 3:L9:114:LYS:NZ | 3:L9:172:ALA:O | 2.07 | 0.87 |
| 4:M9:185:ALA:HA | 12:V9:201:CYC:O2A | 1.71 | 0.87 |
| 5:Z8:41:GLN:CG | 12:Z8:301:CYC:HBB3 | 2.02 | 0.87 |
| 3:H9:126:SER:HB3 | 12:H9:202:CYC:HMC2 | 1.54 | 0.87 |
| 11:aA:89:ALA:HA | 11:aA:92:LYS:HZ1 | 1.35 | 0.87 |
| 11:aA:338:VAL:CG2 | 11:aA:340:PRO:CG | 2.53 | 0.87 |
| 11:aA:339:GLU:N | 11:aA:340:PRO:HD3 | 1.87 | 0.87 |
| 1:Z:75:THR:OG1 | 10:j5:182:ASN:HA | 1.75 | 0.87 |
| 12:BA:201:CYC:CMA | 4:MA:36:TYR:O | 2.22 | 0.87 |
| 4:MA:263:PRO:CB | 3:VA:119:ALA:HB3 | 1.99 | 0.87 |
| 4:MA:274:VAL:CB | 3:VA:77:ARG:CG | 2.50 | 0.87 |
| 12:P1:202:CYC:HMD1 | 12:P1:202:CYC:NC | 1.88 | 0.87 |
| 12:J3:202:CYC:HB | 11:a9:666:ASN:HB3 | 1.40 | 0.87 |
| 3:B4:85:ASP:HB2 | 12:B4:202:CYC:CBC | 2.04 | 0.87 |
| 12:M4:301:CYC:HMC2 | 3:Y4:72:ASN:HB3 | 1.57 | 0.87 |
| 1:L5:75:THR:HG22 | 8:G5:115:MET:HE2 | 1.55 | 0.87 |
| 8:Q5:16:ARG:HA | 1:R5:90:ARG:CZ | 2.04 | 0.87 |
| 10:j5:990:ARG:NH2 | 10:j5:1026:LYS:HZ1 | 1.72 | 0.87 |
| 10:j5:1153:VAL:HG11 | 1:v7:59:ALA:O | 1.74 | 0.87 |
| 10:k5:924:ASP:CG | 1:D7:26:LYS:NZ | 2.32 | 0.87 |
| 10:k5:1074:GLN:OE1 | 1:l7:119:LEU:CD2 | 2.18 | 0.87 |
| 12:D1:201:CYC:HMD1 | 12:D1:201:CYC:NC | 1.88 | 0.87 |
| 1:H7:68:PRO:HB3 | 1:J7:14:VAL:O | 1.74 | 0.87 |
| 8:I7:17:TYR:CE2 | 1:J7:90:ARG:HA | 2.09 | 0.87 |
| 12:Y7:201:CYC:HB | 12:Y7:201:CYC:HMA1 | 1.37 | 0.87 |
| 3:B8:116:THR:CA | 4:M8:56:MET:HG3 | 1.94 | 0.87 |
| 12:M8:301:CYC:CAB | 3:Y8:88:ILE:HG22 | 2.04 | 0.87 |
| 4:M9:274:VAL:CA | 3:V9:77:ARG:CD | 2.37 | 0.87 |
| 3:Y8:89:ILE:CB | 3:Y8:92:TYR:CE2 | 2.58 | 0.87 |
| 11:a9:49:TRP:O | 11:a9:53:VAL:HG23 | 1.73 | 0.87 |
| 11:aA:338:VAL:HG22 | 11:aA:340:PRO:HD3 | 1.54 | 0.87 |
| 12:LA:201:CYC:HMD1 | 12:LA:201:CYC:NC | 1.87 | 0.87 |
| 4:MA:222:ARG:HG3 | 4:MA:222:ARG:HH11 | 1.38 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:R1:111:ASN:ND2 | 5:N1:66:ARG:NH1 | 2.22 | 0.87 |
| 3:B3:91:ARG:CZ | 11:a9:677:GLN:HE22 | 1.82 | 0.87 |
| 3:B3:115:GLU:OE2 | 4:M3:78:GLY:N | 2.07 | 0.87 |
| 12:V3:202:CYC:HMD1 | 12:V3:202:CYC:NC | 1.88 | 0.87 |
| 4:M4:104:ALA:C | 2:P4:14:SER:HB2 | 2.00 | 0.87 |
| 4:M4:217:VAL:CG2 | 5:Z4:30:PRO:CA | 2.52 | 0.87 |
| 12:M4:301:CYC:HAC1 | 3:Y4:82:CYS:SG | 2.12 | 0.87 |
| 12:d5:201:CYC:OB | 10:j5:353:ASN:HB2 | 1.74 | 0.87 |
| 12:U5:201:CYC:HMA1 | 12:U5:201:CYC:HB | 1.37 | 0.87 |
| 10:k5:971:VAL:N | 12:k5:1204:CYC:CGD | 2.34 | 0.87 |
| 10:k5:1054:SER:HA | 1:l7:107:ARG:C | 1.98 | 0.87 |
| 8:O7:17:TYR:CE2 | 1:P7:90:ARG:HA | 2.09 | 0.87 |
| 12:E7:201:CYC:HMA1 | 12:E7:201:CYC:HB | 1.37 | 0.87 |
| 8:o7:30:VAL:HB | 1:p7:31:PHE:O | 1.74 | 0.87 |
| 8:q7:49:ARG:CZ | 3:H1:62:GLU:OE1 | 2.22 | 0.87 |
| 8:u7:30:VAL:HB | 1:v7:31:PHE:O | 1.74 | 0.87 |
| 3:F8:115:GLU:HB3 | 4:M8:3:VAL:HG13 | 1.55 | 0.87 |
| 4:M9:76:ALA:HB3 | 3:D9:111:ASN:OD1 | 1.73 | 0.87 |
| 12:J9:202:CYC:HBB3 | 11:a9:516:GLN:CG | 2.05 | 0.87 |
| 11:a9:476:ARG:NH1 | 11:a9:488:SER:OG | 2.07 | 0.87 |
| 4:M1:5:THR:O | 4:M1:6:THR:OG1 | 1.90 | 0.87 |
| 1:A:73:TYR:CE1 | 10:k5:162:TRP:HZ2 | 1.58 | 0.87 |
| 2:A1:63:PHE:CB | 2:A1:66:LEU:HD11 | 2.03 | 0.87 |
| 3:Z3:111:ASN:CG | 4:M3:258:LYS:NZ | 2.32 | 0.87 |
| 12:B4:202:CYC:HBB2 | 4:M4:61:ASN:HB2 | 1.35 | 0.87 |
| 12:B1:202:CYC:CAA | 11:aA:684:ASN:CB | 2.46 | 0.87 |
| 4:M4:251:ASN:HD22 | 4:M4:251:ASN:H | 1.16 | 0.87 |
| 8:e5:45:GLU:OE1 | 1:R5:139:GLY:HA3 | 1.69 | 0.87 |
| 8:S5:94:TYR:OH | 1:T5:17:LYS:O | 1.91 | 0.87 |
| 8:Y5:114:GLU:OE1 | 10:k5:312:TYR:O | 1.93 | 0.87 |
| 1:b5:38:VAL:CG1 | 10:k5:40:VAL:HG11 | 2.04 | 0.87 |
| 10:j5:388:ARG:HB3 | 10:j5:388:ARG:CZ | 2.02 | 0.87 |
| 10:k5:547:ARG:O | 10:k5:547:ARG:NH2 | 2.07 | 0.87 |
| 8:g7:25:ARG:HE | 8:u7:25:ARG:NE | 1.71 | 0.87 |
| 8:i7:47:ARG:HD3 | 1:j7:18:TYR:CD2 | 2.08 | 0.87 |
| 8:s7:17:TYR:CE2 | 1:t7:90:ARG:HA | 2.09 | 0.87 |
| 3:F8:107:ASP:HA | 4:M8:6:THR:O | 1.74 | 0.87 |
| 4:M9:188:LEU:HD22 | 12:V9:201:CYC:NB | 1.88 | 0.87 |
| 4:M9:188:LEU:CD2 | 12:V9:201:CYC:NB | 2.37 | 0.87 |
| 5:N9:50:LEU:HD21 | 12:T9:301:CYC:O1D | 1.74 | 0.87 |
| 5:N9:72:GLU:HG3 | 3:T9:119:ALA:O | 1.73 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:aA:623:ASP:HB2 | 3:H1:78:ARG:NH2 | 1.85 | 0.87 |
| 12:DA:202:CYC:HMD1 | 12:DA:202:CYC:NC | 1.88 | 0.87 |
| 6:M2:278:ARG:HH21 | 1:j7:67:ARG:CZ | 1.58 | 0.87 |
| 1:f5:34:GLY:HA3 | 10:j5:47:PHE:CD2 | 2.09 | 0.87 |
| 6:M6:117:MET:HE3 | 3:H6:77:ARG:HH11 | 0.71 | 0.87 |
| 10:k5:939:GLN:O | 10:k5:943:THR:HG23 | 1.74 | 0.87 |
| 8:g7:52:LYS:CD | 11:aA:321:ALA:HB1 | 2.01 | 0.87 |
| 2:E8:1:MET:H2 | 4:M8:10:ARG:NH2 | 1.69 | 0.87 |
| 4:M9:222:ARG:HH11 | 4:M9:222:ARG:HG3 | 1.38 | 0.87 |
| 12:J9:202:CYC:HBB3 | 11:a9:516:GLN:HG3 | 1.56 | 0.87 |
| 11:aA:275:THR:C | 11:aA:278:LEU:HD12 | 1.99 | 0.87 |
| 11:aA:666:ASN:HB3 | 12:aA:901:CYC:HB | 1.39 | 0.87 |
| 12:H1:202:CYC:HMD1 | 12:H1:202:CYC:NC | 1.88 | 0.87 |
| 4:M1:188:LEU:CD2 | 12:Z1:202:CYC:HB | 1.88 | 0.87 |
| 4:M1:189:ASP:OD1 | 3:Z1:84:ARG:NH1 | 2.08 | 0.87 |
| 4:MA:274:VAL:HG12 | 3:VA:77:ARG:CD | 2.05 | 0.87 |
| 3:H3:78:ARG:HH22 | 11:a9:623:ASP:CA | 1.86 | 0.87 |
| 3:U4:115:GLU:HB2 | 4:M4:74:LEU:HD12 | 0.88 | 0.87 |
| 2:N4:112:GLY:CA | 5:Z4:34:LEU:CB | 2.51 | 0.87 |
| 8:K5:161:GLN:NE2 | 1:V5:49:THR:HG22 | 1.90 | 0.87 |
| 1:Z5:127:VAL:CG1 | 10:k5:698:GLY:N | 2.33 | 0.87 |
| 8:a5:35:ARG:HH22 | 8:a5:144:ASP:HB3 | 1.40 | 0.87 |
| 10:j5:357:LEU:HD11 | 10:j5:379:PHE:CA | 2.04 | 0.87 |
| 10:j5:1020:GLU:CG | 1:f7:87:TYR:CZ | 2.58 | 0.87 |
| 10:j5:1064:LYS:CD | 10:j5:1065:HIS:N | 2.38 | 0.87 |
| 10:k5:966:SER:N | 1:p7:14:VAL:HG11 | 1.87 | 0.87 |
| 12:D8:201:CYC:HMD1 | 12:D8:201:CYC:NC | 1.88 | 0.87 |
| 8:q7:45:GLU:CD | 3:H1:125:ARG:HH21 | 1.82 | 0.87 |
| 3:U8:108:ARG:O | 4:M8:246:ALA:CB | 2.22 | 0.87 |
| 3:F8:107:ASP:CB | 4:M8:8:SER:N | 2.37 | 0.87 |
| 3:O8:119:ALA:CB | 5:Z8:72:GLU:HG3 | 2.05 | 0.87 |
| 12:Q8:201:CYC:HMD1 | 12:Q8:201:CYC:NC | 1.88 | 0.87 |
| 5:N9:61:LYS:HZ2 | 12:T9:301:CYC:HBB2 | 1.38 | 0.87 |
| 3:HA:78:ARG:HH11 | 12:HA:202:CYC:CGD | 1.88 | 0.86 |
| 3:LA:114:LYS:NZ | 3:LA:172:ALA:O | 2.07 | 0.86 |
| 2:QA:71:GLN:N | 2:QA:74:TYR:HE2 | 1.67 | 0.86 |
| 3:J3:77:ARG:HE | 2:K3:111:ALA:CB | 1.88 | 0.86 |
| 3:L3:75:PRO:HD2 | 11:a9:823:ILE:HG13 | 1.57 | 0.86 |
| 3:L4:68:ARG:CB | 11:aA:81:ASP:CA | 2.53 | 0.86 |
| 3:L4:68:ARG:CD | 11:aA:81:ASP:N | 2.38 | 0.86 |
| 1:L5:75:THR:HG21 | 8:G5:112:VAL:HG23 | 1.57 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:e5:35:ARG:HH22 | 8:e5:144:ASP:HB3 | 1.40 | 0.86 |
| 10:j5:978:LEU:HD11 | 1:v7:107:ARG:HH22 | 1.37 | 0.86 |
| 1:H7:136:VAL:HA | 11:aA:563:PHE:CZ | 2.10 | 0.86 |
| 3:U8:114:LYS:HZ3 | 4:M8:13:LYS:HE3 | 1.31 | 0.86 |
| 3:J8:108:ARG:NH2 | 11:a9:171:ARG:CB | 2.37 | 0.86 |
| 4:M9:134:ASN:OD1 | 5:N9:1:MET:N | 2.08 | 0.86 |
| 3:H9:108:ARG:NH1 | 11:a9:448:ASN:HD21 | 1.72 | 0.86 |
| 11:aA:99:ALA:HB3 | 11:aA:100:PRO:CD | 1.99 | 0.86 |
| 11:aA:476:ARG:NH1 | 11:aA:488:SER:OG | 2.07 | 0.86 |
| 1:Z:122:PRO:CB | 1:V5:64:ASP:OD2 | 2.22 | 0.86 |
| 4:MA:1:MET:HG2 | 11:aA:422:SER:O | 1.73 | 0.86 |
| 4:MA:134:ASN:OD1 | 5:NA:1:MET:N | 2.08 | 0.86 |
| 2:K3:15:GLN:CA | 11:a9:745:GLY:CA | 2.50 | 0.86 |
| 3:H4:84:ARG:HE | 11:aA:131:TYR:HD2 | 1.22 | 0.86 |
| 4:M4:129:GLU:N | 4:M4:142:PHE:HZ | 1.71 | 0.86 |
| 10:j5:1005:LEU:HD13 | 10:j5:1016:LEU:HD21 | 1.57 | 0.86 |
| 10:k5:56:ILE:HG23 | 10:k5:57:VAL:N | 1.90 | 0.86 |
| 8:o7:29:PHE:HE2 | 1:p7:5:ILE:HD11 | 1.38 | 0.86 |
| 8:u7:5:THR:OG1 | 1:v7:3:ASP:OD2 | 1.93 | 0.86 |
| 5:Z8:41:GLN:CD | 12:Z8:301:CYC:HBB3 | 1.95 | 0.86 |
| 11:a9:338:VAL:CG2 | 11:a9:340:PRO:CG | 2.53 | 0.86 |
| 11:a9:589:THR:N | 11:a9:590:PRO:HD3 | 1.80 | 0.86 |
| 11:aA:589:THR:N | 11:aA:590:PRO:CD | 2.32 | 0.86 |
| 12:L1:201:CYC:HMD1 | 12:L1:201:CYC:NC | 1.88 | 0.86 |
| 4:M1:196:TYR:CB | 2:Y1:14:SER:O | 2.24 | 0.86 |
| 3:J3:14:LEU:HD21 | 11:a9:621:THR:HG22 | 1.54 | 0.86 |
| 12:B3:202:CYC:HBA1 | 11:a9:684:ASN:HB3 | 1.53 | 0.86 |
| 4:M3:196:TYR:CB | 2:Y3:14:SER:O | 2.24 | 0.86 |
| 3:B1:88:ILE:HB | 12:B1:202:CYC:HMB2 | 1.55 | 0.86 |
| 3:B1:115:GLU:OE2 | 4:M1:78:GLY:N | 2.07 | 0.86 |
| 8:O5:76:LYS:CD | 8:O5:77:MET:HE2 | 1.91 | 0.86 |
| 1:f5:18:TYR:CE2 | 10:j5:165:ARG:CA | 2.57 | 0.86 |
| 10:j5:1013:PRO:CB | 8:q7:114:GLU:OE2 | 2.23 | 0.86 |
| 10:k5:546:PHE:CE1 | 10:k5:561:GLU:CD | 2.53 | 0.86 |
| 10:k5:1009:ALA:HB2 | 1:p7:87:TYR:OH | 1.74 | 0.86 |
| 10:k5:1142:SER:O | 1:l7:10:ASN:ND2 | 2.08 | 0.86 |
| 12:J8:201:CYC:HMA1 | 11:a9:176:ASN:HD21 | 1.40 | 0.86 |
| 4:M8:217:VAL:HG23 | 5:Z8:30:PRO:HG3 | 1.53 | 0.86 |
| 4:M9:37:GLU:OE1 | 4:M9:40:GLN:CD | 2.17 | 0.86 |
| 4:M9:192:GLN:HG2 | 3:V9:84:ARG:HG3 | 1.54 | 0.86 |
| 5:N9:4:LEU:O | 3:R9:112:GLY:HA3 | 1.75 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:Z8:29:HIS:HD2 | 5:Z8:36:THR:CG2 | 1.87 | 0.86 |
| 11:a9:106:LEU:HB2 | 11:a9:118:VAL:HG21 | 1.54 | 0.86 |
| 3:H1:81:ALA:CB | 12:H1:201:CYC:C2D | 2.52 | 0.86 |
| 12:HA:202:CYC:OB | 11:aA:474:PHE:CE1 | 2.28 | 0.86 |
| 12:B4:202:CYC:HBD1 | 4:M4:53:LEU:HB3 | 1.58 | 0.86 |
| 3:J4:125:ARG:NH1 | 2:C2:69:PRO:HG2 | 1.89 | 0.86 |
| 10:k5:221:LYS:HZ3 | 10:k5:221:LYS:HB3 | 1.38 | 0.86 |
| 10:k5:1005:LEU:HD13 | 10:k5:1016:LEU:HD21 | 1.57 | 0.86 |
| 10:k5:1017:ARG:HB3 | 10:k5:1017:ARG:NH2 | 1.91 | 0.86 |
| 8:C7:35:ARG:HH22 | 8:C7:144:ASP:HB3 | 1.41 | 0.86 |
| 8:g7:25:ARG:NH2 | 8:u7:25:ARG:HH11 | 1.71 | 0.86 |
| 2:G1:111:ALA:CB | 3:L1:77:ARG:HE | 1.88 | 0.86 |
| 11:a9:639:GLN:NE2 | 11:a9:639:GLN:O | 2.08 | 0.86 |
| 11:aA:742:GLN:HE21 | 3:L1:88:ILE:HG13 | 1.36 | 0.86 |
| 3:J3:77:ARG:HG2 | 2:K3:111:ALA:CB | 2.04 | 0.86 |
| 12:J3:202:CYC:HBB3 | 11:a9:795:ASP:O | 1.75 | 0.86 |
| 3:Z3:84:ARG:NH1 | 4:M3:189:ASP:OD1 | 2.08 | 0.86 |
| 4:M3:113:ILE:HD11 | 4:M3:143:VAL:CG1 | 2.04 | 0.86 |
| 4:M4:92:GLU:OE1 | 4:M4:217:VAL:HA | 1.60 | 0.86 |
| 2:N4:14:SER:CB | 5:Z4:62:ARG:HD3 | 2.03 | 0.86 |
| 3:Q4:84:ARG:HD3 | 5:Z4:31:TRP:CD1 | 2.10 | 0.86 |
| 1:d5:110:ASN:O | 10:j5:352:ILE:HD12 | 1.74 | 0.86 |
| 10:k5:1153:VAL:CG2 | 1:p7:65:LEU:HD11 | 2.04 | 0.86 |
| 8:k7:79:ALA:CB | 11:a9:53:VAL:HG21 | 2.04 | 0.86 |
| 8:o7:23:LEU:CG | 1:p7:38:VAL:CG1 | 2.40 | 0.86 |
| 12:M8:301:CYC:HAC2 | 3:Y8:82:CYS:SG | 2.16 | 0.86 |
| 3:J3:14:LEU:HD22 | 11:a9:621:THR:HG23 | 1.54 | 0.86 |
| 3:J3:85:ASP:HA | 11:a9:668:TYR:OH | 1.72 | 0.86 |
| 6:M2:26:PHE:HB3 | 8:O5:83:ARG:CD | 2.04 | 0.86 |
| 3:F4:113:LEU:HB2 | 4:M4:5:THR:HG21 | 1.57 | 0.86 |
| 3:J4:108:ARG:NH2 | 11:aA:171:ARG:CB | 2.39 | 0.86 |
| 5:Z4:29:HIS:CE1 | 5:Z4:38:GLU:HB3 | 2.11 | 0.86 |
| 1:Z5:110:ASN:O | 10:k5:352:ILE:HD12 | 1.75 | 0.86 |
| 1:b5:1:MET:O | 10:k5:15:ARG:NH1 | 2.08 | 0.86 |
| 10:j5:547:ARG:O | 10:j5:547:ARG:NH2 | 2.07 | 0.86 |
| 10:j5:1019:SER:HG | 1:f7:87:TYR:HE1 | 1.21 | 0.86 |
| 8:i7:46:ALA:CB | 8:i7:140:LEU:CD1 | 2.52 | 0.86 |
| 8:c7:25:ARG:NH2 | 8:m7:6:LYS:NZ | 2.22 | 0.86 |
| 8:c7:46:ALA:CB | 8:c7:140:LEU:CD1 | 2.53 | 0.86 |
| 8:u7:90:ARG:CB | 1:v7:18:TYR:CZ | 2.59 | 0.86 |
| 2:N8:10:ALA:O | 5:Z8:62:ARG:NE | 2.07 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:N8:201:CYC:HB | 12:N8:201:CYC:HMA1 | 1.40 | 0.86 |
| 3:Q8:72:ASN:OD1 | 12:Z8:301:CYC:CMD | 2.24 | 0.86 |
| 3:J9:111:ASN:CA | 11:a9:518:ALA:HB3 | 2.05 | 0.86 |
| 11:a9:414:ALA:HB1 | 11:a9:428:PHE:HE1 | 1.40 | 0.86 |
| 2:GA:119:THR:HG21 | 3:LA:83:LEU:CD1 | 2.05 | 0.86 |
| 3:JA:114:LYS:CD | 8:S7:60:GLN:HE22 | 1.88 | 0.86 |
| 3:Q4:124:THR:CB | 3:Q4:171:ILE:O | 2.22 | 0.86 |
| 8:M5:38:ARG:HD3 | 1:J7:144:ASP:OD1 | 1.76 | 0.86 |
| 1:N5:113:LYS:NZ | 1:Z5:155:TYR:OH | 2.05 | 0.86 |
| 12:Z5:201:CYC:O2A | 10:k5:379:PHE:CD2 | 2.28 | 0.86 |
| 10:j5:778:LYS:NZ | 12:L7:201:CYC:HBB2 | 1.90 | 0.86 |
| 10:k5:357:LEU:HD11 | 10:k5:379:PHE:CA | 2.04 | 0.86 |
| 10:k5:1023:SER:HB3 | 12:k5:1202:CYC:CMA | 2.05 | 0.86 |
| 8:g7:10:ASN:ND2 | 8:u7:10:ASN:ND2 | 2.22 | 0.86 |
| 8:u7:23:LEU:CG | 1:v7:38:VAL:CG1 | 2.40 | 0.86 |
| 2:X8:108:TYR:CZ | 4:M8:273:ILE:CD1 | 2.57 | 0.86 |
| 4:M8:222:ARG:HH11 | 4:M8:222:ARG:HG3 | 1.38 | 0.86 |
| 3:J9:111:ASN:ND2 | 11:a9:519:ARG:HG2 | 1.90 | 0.86 |
| 11:aA:639:GLN:O | 11:aA:639:GLN:NE2 | 2.08 | 0.86 |
| 3:H1:109:CYS:HA | 12:H1:201:CYC:CBB | 2.06 | 0.86 |
| 3:LA:111:ASN:O | 11:aA:532:ALA:N | 2.08 | 0.86 |
| 3:J2:108:ARG:NH2 | 6:M2:155:ASN:HB3 | 1.91 | 0.86 |
| 6:M2:278:ARG:NH2 | 1:j7:67:ARG:CZ | 2.27 | 0.86 |
| 3:Q4:106:GLU:HA | 3:Q4:110:LEU:HB2 | 1.58 | 0.86 |
| 1:X5:110:ASN:OD1 | 10:j5:466:LEU:HB3 | 1.76 | 0.86 |
| 12:Z5:201:CYC:OB | 10:k5:353:ASN:HB2 | 1.73 | 0.86 |
| 10:k5:1008:PHE:CE1 | 1:p7:87:TYR:OH | 2.28 | 0.86 |
| 1:T7:68:PRO:HB3 | 1:V7:14:VAL:O | 1.74 | 0.86 |
| 8:c7:96:ILE:HG12 | 8:c7:152:TYR:CE1 | 2.11 | 0.86 |
| 1:d7:77:ARG:HH22 | 9:x7:63:ALA:HB3 | 0.84 | 0.86 |
| 3:L8:71:GLY:CA | 11:a9:82:GLN:CG | 2.54 | 0.86 |
| 4:M8:225:LYS:CA | 12:M8:301:CYC:CGA | 2.42 | 0.86 |
| 11:aA:351:THR:HB | 11:aA:352:PRO:HD2 | 0.86 | 0.86 |
| 1:A:16:GLY:HA2 | 8:a5:90:ARG:NH1 | 1.91 | 0.86 |
| 12:BA:202:CYC:HMD1 | 12:BA:202:CYC:NC | 1.88 | 0.86 |
| 3:HA:113:LEU:CD1 | 12:HA:202:CYC:HMB3 | 2.05 | 0.86 |
| 3:J2:120:LEU:HD21 | 6:M2:178:HIS:CE1 | 2.11 | 0.86 |
| 6:M2:127:SER:HB2 | 3:F2:84:ARG:HH22 | 1.39 | 0.86 |
| 3:U4:120:LEU:HD12 | 4:M4:254:LEU:CG | 1.94 | 0.86 |
| 3:Y4:89:ILE:CB | 3:Y4:92:TYR:CE2 | 2.58 | 0.86 |
| 3:Y4:106:GLU:HB2 | 3:Y4:166:LYS:HD3 | 1.57 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:B5:10:ASN:ND2 | 10:k5:557:VAL:HB | 1.90 | 0.86 |
| 10:j5:978:LEU:CD1 | 1:v7:107:ARG:NH2 | 2.38 | 0.86 |
| 10:k5:1151:GLN:O | 1:p7:122:PRO:CB | 2.24 | 0.86 |
| 8:Q7:12:ASP:C | 9:z7:46:LYS:HZ1 | 1.81 | 0.86 |
| 8:i7:94:TYR:CD2 | 1:j7:9:ILE:CG2 | 2.59 | 0.86 |
| 8:a7:35:ARG:HH22 | 8:a7:144:ASP:HB3 | 1.40 | 0.86 |
| 2:X8:67:THR:HB | 3:T9:28:THR:HG22 | 1.31 | 0.86 |
| 4:M8:214:GLY:HA3 | 5:Z8:28:HIS:CE1 | 2.10 | 0.86 |
| 3:L9:83:LEU:CD1 | 2:G9:119:THR:HG21 | 2.05 | 0.86 |
| 3:J9:65:ASP:HB2 | 11:a9:354:VAL:CG2 | 2.06 | 0.86 |
| 3:F2:82:CYS:HB2 | 12:F2:201:CYC:HMD3 | 1.55 | 0.86 |
| 1:Z:73:TYR:CE1 | 10:j5:162:TRP:HZ2 | 1.65 | 0.86 |
| 3:HA:117:TYR:CZ | 12:HA:202:CYC:HBB | 2.10 | 0.86 |
| 3:LA:14:LEU:HD21 | 11:aA:358:PRO:N | 1.90 | 0.86 |
| 3:LA:52:ILE:CD1 | 3:LA:87:GLU:HA | 2.06 | 0.86 |
| 4:MA:184:ILE:HG22 | 12:VA:201:CYC:HBA2 | 1.56 | 0.86 |
| 2:QA:67:THR:O | 2:U1:46:SER:CB | 2.24 | 0.86 |
| 2:QA:119:THR:HG21 | 3:TA:83:LEU:HD22 | 0.88 | 0.86 |
| 3:TA:28:THR:HG22 | 2:X4:67:THR:HB | 1.31 | 0.86 |
| 2:G3:111:ALA:CB | 3:L3:77:ARG:HE | 1.89 | 0.86 |
| 12:L3:202:CYC:HBA1 | 11:a9:738:LEU:HD12 | 1.58 | 0.86 |
| 3:F4:108:ARG:CZ | 4:M4:9:GLN:HG2 | 1.87 | 0.86 |
| 12:F5:201:CYC:HBA1 | 10:k5:591:ILE:HG23 | 1.56 | 0.86 |
| 1:Z5:110:ASN:O | 10:k5:352:ILE:CD1 | 2.24 | 0.86 |
| 10:j5:988:ALA:CA | 1:h7:106:GLU:OE2 | 2.24 | 0.86 |
| 10:j5:1043:GLU:CB | 8:e7:14:GLU:OE2 | 2.23 | 0.86 |
| 10:k5:199:THR:HG22 | 12:k5:1201:CYC:HBC2 | 1.58 | 0.86 |
| 3:D1:68:ARG:HH22 | 3:X1:68:ARG:NH1 | 1.74 | 0.86 |
| 12:d7:201:CYC:HMA2 | 9:x7:38:PHE:HD1 | 1.41 | 0.86 |
| 8:o7:5:THR:OG1 | 1:p7:3:ASP:OD2 | 1.93 | 0.86 |
| 1:r7:68:PRO:HB3 | 1:t7:14:VAL:O | 1.74 | 0.86 |
| 4:M9:65:ARG:HD2 | 3:F9:111:ASN:HD21 | 1.38 | 0.86 |
| 11:a9:371:VAL:HG11 | 11:a9:507:PHE:CD2 | 2.10 | 0.86 |
| 11:aA:578:MET:HE3 | 11:aA:582:MET:HE1 | 1.58 | 0.86 |
| 11:aA:710:THR:HG23 | 11:aA:807:GLN:HG3 | 1.58 | 0.86 |
| 12:JA:202:CYC:HBB3 | 11:aA:516:GLN:HG3 | 1.57 | 0.85 |
| 4:MA:58:TYR:CE2 | 11:aA:496:ARG:NH2 | 2.44 | 0.85 |
| 12:Z3:201:CYC:HB | 4:M3:188:LEU:CD2 | 1.88 | 0.85 |
| 3:B4:108:ARG:C | 4:M4:61:ASN:HA | 2.00 | 0.85 |
| 2:U3:46:SER:C | 2:Q9:74:TYR:CZ | 2.53 | 0.85 |
| 4:M4:128:ALA:CB | 4:M4:142:PHE:CE1 | 2.58 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M4:148:LYS:HZ2 | 5:Z4:52:ARG:CD | 1.88 | 0.85 |
| 8:W5:16:ARG:CB | 1:X5:90:ARG:HH11 | 1.81 | 0.85 |
| 1:b5:27:LEU:CD1 | 10:k5:172:LEU:HD22 | 2.06 | 0.85 |
| 8:i7:94:TYR:CD2 | 1:j7:9:ILE:HG21 | 2.11 | 0.85 |
| 1:l7:68:PRO:HB3 | 1:n7:14:VAL:O | 1.74 | 0.85 |
| 4:M8:104:ALA:HB3 | 2:P8:14:SER:N | 1.90 | 0.85 |
| 3:O8:95:TYR:CE2 | 3:O8:108:ARG:NH2 | 2.44 | 0.85 |
| 3:L9:52:ILE:CD1 | 3:L9:87:GLU:CA | 2.49 | 0.85 |
| 4:M9:274:VAL:HG21 | 2:W9:111:ALA:HB3 | 1.57 | 0.85 |
| 11:aA:414:ALA:HB1 | 11:aA:428:PHE:HE1 | 1.40 | 0.85 |
| 11:aA:776:TYR:HD1 | 12:H1:201:CYC:OB | 1.55 | 0.85 |
| 1:A:127:VAL:HG11 | 1:R5:15:GLN:HG2 | 1.55 | 0.85 |
| 3:DA:68:ARG:HH22 | 3:XA:68:ARG:HH12 | 0.88 | 0.85 |
| 5:NA:50:LEU:HD21 | 12:TA:301:CYC:O1D | 1.74 | 0.85 |
| 3:TA:32:LYS:HE2 | 2:X4:57:GLN:CD | 2.01 | 0.85 |
| 3:D3:68:ARG:HH22 | 3:X3:68:ARG:NH1 | 1.74 | 0.85 |
| 5:Z4:28:HIS:CB | 5:Z4:35:ASP:HA | 2.05 | 0.85 |
| 1:B5:107:ARG:NH2 | 10:k5:541:THR:OG1 | 2.09 | 0.85 |
| 12:B5:201:CYC:OB | 9:z5:23:LEU:N | 2.09 | 0.85 |
| 10:j5:138:PRO:HB2 | 10:j5:201:VAL:HG11 | 1.55 | 0.85 |
| 10:j5:298:ARG:HH21 | 10:j5:310:LYS:HD3 | 1.40 | 0.85 |
| 10:j5:631:HIS:HD2 | 10:j5:664:MET:HE3 | 1.38 | 0.85 |
| 10:k5:325:ASN:O | 10:k5:325:ASN:ND2 | 2.08 | 0.85 |
| 10:k5:1118:THR:OG1 | 12:k5:1204:CYC:O2A | 1.94 | 0.85 |
| 1:P7:14:VAL:O | 1:N7:68:PRO:HB3 | 1.74 | 0.85 |
| 3:L8:109:CYS:HA | 12:a9:901:CYC:CAB | 2.05 | 0.85 |
| 4:M8:144:ARG:HG2 | 4:M8:204:ILE:CD1 | 2.06 | 0.85 |
| 4:M8:223:GLY:C | 12:M8:301:CYC:HBA2 | 2.00 | 0.85 |
| 3:D9:68:ARG:HH22 | 3:X9:68:ARG:HH12 | 0.88 | 0.85 |
| 3:JA:65:ASP:HB2 | 11:aA:354:VAL:CG2 | 2.05 | 0.85 |
| 12:J3:202:CYC:C3A | 11:a9:798:SER:OG | 2.22 | 0.85 |
| 4:M3:118:TYR:HD2 | 3:X3:84:ARG:HH21 | 0.88 | 0.85 |
| 2:E4:1:MET:H3 | 4:M4:10:ARG:HH21 | 0.87 | 0.85 |
| 4:M4:222:ARG:HG3 | 4:M4:222:ARG:HH11 | 1.38 | 0.85 |
| 10:k5:298:ARG:HH21 | 10:k5:310:LYS:HD3 | 1.40 | 0.85 |
| 8:g7:63:PRO:HD2 | 11:aA:336:ILE:HG21 | 0.86 | 0.85 |
| 8:i7:50:ILE:HG22 | 8:i7:133:MET:HG2 | 1.56 | 0.85 |
| 12:B8:202:CYC:HBD1 | 4:M8:53:LEU:HB3 | 1.58 | 0.85 |
| 4:M9:163:ASN:HD21 | 12:V9:201:CYC:HMA3 | 1.42 | 0.85 |
| 4:MA:181:GLN:HE22 | 3:VA:120:LEU:HD21 | 1.39 | 0.85 |
| 3:H2:84:ARG:O | 3:H2:85:ASP:C | 2.11 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:M3:120:LEU:HD21 | 3:X3:84:ARG:HH11 | 1.40 | 0.85 |
| 5:N3:39:PRO:O | 3:T3:116:THR:OG1 | 1.95 | 0.85 |
| 12:B1:202:CYC:HBA2 | 11:aA:684:ASN:HB2 | 0.88 | 0.85 |
| 3:U4:115:GLU:CD | 4:M4:70:SER:HB2 | 2.00 | 0.85 |
| 8:O5:35:ARG:HH22 | 8:O5:144:ASP:HB3 | 1.40 | 0.85 |
| 8:c5:73:TYR:HE2 | 6:M6:9:ARG:NH1 | 1.72 | 0.85 |
| 1:d5:83:ARG:HH12 | 10:j5:379:PHE:HE2 | 1.21 | 0.85 |
| 8:U5:35:ARG:HH22 | 8:U5:144:ASP:HB3 | 1.40 | 0.85 |
| 10:j5:1123:ASN:O | 10:j5:1123:ASN:ND2 | 2.08 | 0.85 |
| 10:j5:1125:ARG:NH2 | 1:t7:114:GLU:HB2 | 1.90 | 0.85 |
| 1:v7:68:PRO:O | 11:aA:42:ARG:NE | 2.09 | 0.85 |
| 9:y7:3:ARG:NH2 | 9:y7:67:VAL:CG1 | 2.38 | 0.85 |
| 3:U8:114:LYS:HE2 | 4:M8:13:LYS:CE | 2.05 | 0.85 |
| 2:X8:67:THR:C | 3:T9:28:THR:CG2 | 2.46 | 0.85 |
| 4:M9:35:THR:HA | 12:B9:201:CYC:O2A | 1.77 | 0.85 |
| 2:E9:33:ARG:HG2 | 2:I9:25:GLN:NE2 | 1.92 | 0.85 |
| 3:H9:107:ASP:HB3 | 11:a9:445:THR:HG22 | 1.55 | 0.85 |
| 11:a9:523:GLN:NE2 | 11:a9:548:LEU:HD13 | 1.91 | 0.85 |
| 11:a9:578:MET:HE3 | 11:a9:582:MET:HE1 | 1.58 | 0.85 |
| 4:MA:274:VAL:HG21 | 2:WA:111:ALA:HB3 | 1.57 | 0.85 |
| 2:A1:34:ALA:HB3 | 3:B1:31:VAL:HG11 | 1.59 | 0.85 |
| 2:G3:111:ALA:HB3 | 3:L3:77:ARG:HE | 1.42 | 0.85 |
| 3:J3:77:ARG:HE | 2:K3:111:ALA:HB3 | 1.41 | 0.85 |
| 6:M2:39:ARG:NH2 | 8:O5:66:VAL:HG11 | 1.90 | 0.85 |
| 2:N4:112:GLY:HA3 | 5:Z4:34:LEU:HB2 | 1.56 | 0.85 |
| 3:O4:95:TYR:CE2 | 3:O4:108:ARG:NH2 | 2.44 | 0.85 |
| 8:K5:20:PRO:HB3 | 8:U5:151:PHE:HB3 | 1.58 | 0.85 |
| 8:c5:82:LEU:HD11 | 6:M6:15:ILE:HG13 | 1.57 | 0.85 |
| 12:T5:201:CYC:HBB2 | 10:j5:482:GLN:NE2 | 1.92 | 0.85 |
| 10:k5:1008:PHE:HZ | 1:p7:83:ARG:HH12 | 1.23 | 0.85 |
| 2:A8:65:TYR:O | 2:A8:71:GLN:HG3 | 1.77 | 0.85 |
| 2:X8:74:TYR:CZ | 2:S9:35:THR:HG22 | 1.89 | 0.85 |
| 3:Q8:72:ASN:CG | 12:Z8:301:CYC:HMD3 | 2.02 | 0.85 |
| 3:L9:48:ALA:CB | 2:K9:18:PHE:CZ | 2.60 | 0.85 |
| 4:M9:58:TYR:CE2 | 11:a9:496:ARG:NH2 | 2.43 | 0.85 |
| 4:M1:222:ARG:HG3 | 4:M1:222:ARG:HH11 | 1.38 | 0.85 |
| 1:R5:106:GLU:CG | 10:k5:505:VAL:HA | 2.05 | 0.85 |
| 10:j5:56:ILE:HG23 | 10:j5:57:VAL:N | 1.90 | 0.85 |
| 10:k5:1106:PHE:O | 10:k5:1110:ILE:HD12 | 1.76 | 0.85 |
| 8:U7:49:ARG:NH1 | 1:l7:114:GLU:CD | 2.34 | 0.85 |
| 2:X8:57:GLN:HA | 3:T9:32:LYS:HZ1 | 0.72 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:L8:113:LEU:HD22 | 12:a9:901:CYC:CMB | 2.07 | 0.85 |
| 2:N8:112:GLY:N | 5:Z8:34:LEU:CB | 2.39 | 0.85 |
| 4:M9:181:GLN:HE22 | 3:V9:120:LEU:HD21 | 1.39 | 0.85 |
| 3:F9:153:CYS:HB3 | 12:F9:303:CYC:C4C | 2.06 | 0.85 |
| 11:a9:476:ARG:NH1 | 11:a9:488:SER:HB2 | 1.78 | 0.85 |
| 11:aA:312:ASP:HB2 | 11:aA:315:LEU:HD13 | 1.57 | 0.85 |
| 5:NA:54:LEU:HD22 | 3:TA:84:ARG:CD | 2.07 | 0.85 |
| 2:QA:149:GLU:OE2 | 2:UA:21:ASN:ND2 | 2.10 | 0.85 |
| 2:A1:65:TYR:O | 2:A1:71:GLN:HG3 | 1.77 | 0.85 |
| 2:O3:34:ALA:HB3 | 3:P3:31:VAL:HG11 | 1.59 | 0.85 |
| 3:F4:113:LEU:H | 4:M4:5:THR:HA | 0.69 | 0.85 |
| 12:J4:201:CYC:HMA1 | 11:aA:176:ASN:HD21 | 1.40 | 0.85 |
| 2:N4:65:TYR:O | 2:N4:71:GLN:HG3 | 1.77 | 0.85 |
| 3:Q4:82:CYS:HA | 12:Z4:301:CYC:HAC2 | 1.58 | 0.85 |
| 8:A5:112:VAL:HG23 | 1:F5:75:THR:HG21 | 1.57 | 0.85 |
| 8:G5:119:LEU:HB3 | 12:G5:201:CYC:HBD1 | 1.58 | 0.85 |
| 12:J5:201:CYC:CBB | 9:i5:42:GLN:NE2 | 2.40 | 0.85 |
| 8:U5:79:ALA:HA | 6:M6:31:ASP:O | 1.76 | 0.85 |
| 1:Z5:67:ARG:NH1 | 10:k5:705:THR:HB | 1.92 | 0.85 |
| 10:j5:951:MET:HE1 | 10:j5:955:LEU:HG | 1.57 | 0.85 |
| 8:q7:64:ASP:HB3 | 11:aA:69:ARG:HH22 | 1.39 | 0.85 |
| 9:x7:3:ARG:NH2 | 9:x7:67:VAL:CG1 | 2.39 | 0.85 |
| 2:X8:107:ASP:HB3 | 4:M8:273:ILE:HG23 | 1.58 | 0.85 |
| 4:M8:235:PHE:HB3 | 12:M8:301:CYC:CAA | 2.05 | 0.85 |
| 3:Q8:120:LEU:HD12 | 3:Q8:122:THR:H | 1.07 | 0.85 |
| 4:M9:113:ILE:HD11 | 4:M9:143:VAL:CG1 | 2.04 | 0.85 |
| 5:N9:16:PHE:CZ | 3:T9:120:LEU:HD23 | 2.10 | 0.85 |
| 2:AA:65:TYR:O | 2:AA:71:GLN:HG3 | 1.77 | 0.85 |
| 4:MA:273:ILE:CD1 | 3:VA:75:PRO:HD3 | 2.01 | 0.85 |
| 12:QA:201:CYC:CAA | 3:TA:79:MET:HE3 | 2.07 | 0.85 |
| 8:C5:35:ARG:HH22 | 8:C5:144:ASP:HB3 | 1.41 | 0.85 |
| 8:G5:119:LEU:HD11 | 12:G5:201:CYC:C2A | 2.06 | 0.85 |
| 1:f5:19:LEU:HD13 | 10:j5:172:LEU:CD1 | 2.04 | 0.85 |
| 1:P5:114:GLU:HG2 | 10:k5:496:GLU:OE2 | 1.77 | 0.85 |
| 3:J6:119:ALA:HB1 | 6:M6:261:LYS:N | 1.92 | 0.85 |
| 10:j5:471:PRO:O | 10:j5:501:ILE:HG12 | 1.77 | 0.85 |
| 10:k5:66:MET:SD | 10:k5:66:MET:N | 2.50 | 0.85 |
| 10:k5:136:VAL:CB | 10:k5:137:PRO:HD2 | 2.04 | 0.85 |
| 10:k5:471:PRO:O | 10:k5:501:ILE:HG12 | 1.77 | 0.85 |
| 8:O7:35:ARG:HH22 | 8:O7:144:ASP:HB3 | 1.41 | 0.85 |
| 8:U7:35:ARG:HH22 | 8:U7:144:ASP:HB3 | 1.41 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:L8:120:LEU:O | 11:a9:90:GLN:NE2 | 2.09 | 0.85 |
| 4:M8:141:GLU:HB2 | 4:M8:144:ARG:NH2 | 1.91 | 0.85 |
| 4:M8:197:ASP:CG | 5:Z8:52:ARG:HG3 | 2.01 | 0.85 |
| 5:N9:61:LYS:CD | 3:T9:108:ARG:O | 2.20 | 0.85 |
| 11:aA:523:GLN:NE2 | 11:aA:548:LEU:HD13 | 1.91 | 0.85 |
| 11:aA:666:ASN:CB | 12:aA:901:CYC:NB | 2.38 | 0.85 |
| 11:aA:668:TYR:HE2 | 11:aA:670:LEU:CD2 | 1.89 | 0.85 |
| 6:M2:53:LEU:HD11 | 8:i7:76:LYS:HB2 | 1.59 | 0.85 |
| 3:L3:104:VAL:CG1 | 3:L3:108:ARG:HH22 | 1.89 | 0.85 |
| 2:U3:46:SER:O | 2:Q9:74:TYR:OH | 1.94 | 0.85 |
| 3:S4:108:ARG:O | 12:S4:202:CYC:HBB1 | 1.75 | 0.85 |
| 4:M4:144:ARG:CZ | 5:Z4:59:ARG:HH12 | 1.88 | 0.85 |
| 1:N5:83:ARG:HH12 | 10:k5:483:PHE:HZ | 0.87 | 0.85 |
| 9:i5:12:PRO:HD3 | 9:i5:49:GLY:HA2 | 1.59 | 0.85 |
| 10:j5:748:ARG:NE | 8:K7:106:GLU:OE2 | 2.08 | 0.85 |
| 10:k5:1056:PRO:HD2 | 10:k5:1057:LYS:N | 1.89 | 0.85 |
| 8:i7:96:ILE:HG12 | 8:i7:152:TYR:CE1 | 2.11 | 0.85 |
| 4:M8:230:GLN:CA | 12:M8:301:CYC:OB | 2.23 | 0.85 |
| 2:A9:65:TYR:O | 2:A9:71:GLN:HG3 | 1.77 | 0.85 |
| 4:M1:162:ASN:O | 4:M1:166:THR:HG23 | 1.77 | 0.85 |
| 3:HA:116:THR:HG21 | 12:HA:202:CYC:CMA | 2.06 | 0.85 |
| 5:NA:16:PHE:CZ | 3:TA:120:LEU:HD21 | 2.12 | 0.85 |
| 3:J3:84:ARG:NH2 | 11:a9:670:LEU:N | 2.23 | 0.85 |
| 2:A3:34:ALA:HB3 | 3:B3:31:VAL:HG11 | 1.59 | 0.85 |
| 4:M3:210:ILE:HD13 | 5:N3:59:ARG:HH11 | 1.42 | 0.85 |
| 1:N5:53:LYS:NZ | 8:O5:120:GLN:CD | 2.30 | 0.85 |
| 8:C5:27:LYS:O | 8:C5:30:VAL:N | 2.10 | 0.85 |
| 8:c5:9:VAL:HG13 | 10:j5:344:ARG:CZ | 2.03 | 0.85 |
| 10:j5:631:HIS:CD2 | 10:j5:664:MET:HE3 | 2.12 | 0.85 |
| 10:j5:822:ARG:HH11 | 10:j5:822:ARG:CB | 1.90 | 0.85 |
| 10:k5:822:ARG:HH11 | 10:k5:822:ARG:CB | 1.90 | 0.85 |
| 10:k5:1023:SER:CB | 12:k5:1202:CYC:HMA2 | 2.06 | 0.85 |
| 2:A6:65:TYR:O | 2:A6:71:GLN:HG3 | 1.77 | 0.85 |
| 8:I7:35:ARG:HH22 | 8:I7:144:ASP:HB3 | 1.41 | 0.85 |
| 8:I7:161:GLN:CG | 1:X7:49:THR:HG21 | 2.03 | 0.85 |
| 8:i7:39:ILE:HD13 | 8:i7:148:GLU:HB3 | 1.49 | 0.85 |
| 3:B8:68:ARG:NH1 | 3:U8:68:ARG:NH2 | 2.25 | 0.85 |
| 8:s7:35:ARG:HH22 | 8:s7:144:ASP:HB3 | 1.41 | 0.85 |
| 12:M8:302:CYC:HAC2 | 3:S8:78:ARG:HA | 1.59 | 0.85 |
| 2:N8:112:GLY:CA | 5:Z8:33:GLY:HA2 | 2.07 | 0.85 |
| 11:a9:351:THR:HB | 11:a9:352:PRO:HD2 | 0.86 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:a9:595:ARG:HG3 | 11:a9:596:THR:O | 1.77 | 0.85 |
| 11:aA:667:THR:HG22 | 12:aA:901:CYC:CGA | 2.05 | 0.85 |
| 5:N1:39:PRO:O | 3:T1:116:THR:OG1 | 1.95 | 0.85 |
| 5:NA:22:LEU:HD22 | 5:NA:26:LEU:HD13 | 1.59 | 0.84 |
| 2:SA:35:THR:HG23 | 2:X4:74:TYR:HE1 | 1.41 | 0.84 |
| 3:L2:77:ARG:NH1 | 6:M2:70:GLU:CG | 2.39 | 0.84 |
| 3:F4:108:ARG:CZ | 4:M4:9:GLN:NE2 | 2.39 | 0.84 |
| 4:M4:148:LYS:HD2 | 5:Z4:52:ARG:HE | 1.41 | 0.84 |
| 12:H5:201:CYC:HBA2 | 9:i5:26:THR:CG2 | 2.07 | 0.84 |
| 8:c5:114:GLU:OE1 | 10:j5:312:TYR:O | 1.94 | 0.84 |
| 1:f5:114:GLU:CB | 10:j5:491:THR:CG2 | 2.49 | 0.84 |
| 8:W5:17:TYR:HE2 | 1:X5:44:ILE:HG21 | 1.35 | 0.84 |
| 3:J6:120:LEU:HD21 | 6:M6:178:HIS:CE1 | 2.11 | 0.84 |
| 10:k5:951:MET:HE1 | 10:k5:955:LEU:HG | 1.57 | 0.84 |
| 3:U8:114:LYS:NZ | 4:M8:13:LYS:NZ | 2.16 | 0.84 |
| 3:L8:109:CYS:CA | 12:a9:901:CYC:HBB1 | 2.07 | 0.84 |
| 11:aA:312:ASP:CA | 11:aA:315:LEU:N | 2.40 | 0.84 |
| 11:aA:595:ARG:HG3 | 11:aA:596:THR:O | 1.77 | 0.84 |
| 11:aA:800:THR:OG1 | 3:J1:120:LEU:HD21 | 1.77 | 0.84 |
| 4:M1:120:LEU:HD21 | 3:X1:84:ARG:HH11 | 1.40 | 0.84 |
| 3:LA:14:LEU:CD1 | 11:aA:358:PRO:HB3 | 1.93 | 0.84 |
| 4:MA:133:ARG:HB3 | 12:RA:201:CYC:CBA | 2.07 | 0.84 |
| 4:MA:162:ASN:O | 4:MA:166:THR:HG23 | 1.77 | 0.84 |
| 2:O1:65:TYR:O | 2:O1:71:GLN:HG3 | 1.77 | 0.84 |
| 3:H2:77:ARG:HH12 | 6:M2:117:MET:CE | 1.89 | 0.84 |
| 2:A4:34:ALA:HB3 | 3:B4:31:VAL:HG11 | 1.59 | 0.84 |
| 3:B4:116:THR:OG1 | 4:M4:56:MET:CB | 2.12 | 0.84 |
| 5:N3:22:LEU:HD22 | 5:N3:26:LEU:HD13 | 1.59 | 0.84 |
| 2:O3:65:TYR:O | 2:O3:71:GLN:HG3 | 1.77 | 0.84 |
| 4:M4:217:VAL:CG1 | 5:Z4:30:PRO:HB3 | 2.07 | 0.84 |
| 2:N4:111:ALA:CA | 5:Z4:34:LEU:CG | 2.55 | 0.84 |
| 3:Y4:88:ILE:CG2 | 3:Y4:91:ARG:HH22 | 1.90 | 0.84 |
| 5:Z4:42:SER:CA | 12:Z4:301:CYC:CMA | 2.54 | 0.84 |
| 12:B5:201:CYC:CBB | 9:z5:21:ARG:HA | 2.06 | 0.84 |
| 1:H5:143:PRO:CG | 8:Q7:41:GLN:NE2 | 2.40 | 0.84 |
| 8:I5:27:LYS:O | 8:I5:30:VAL:N | 2.10 | 0.84 |
| 8:c5:9:VAL:HG13 | 10:j5:344:ARG:NH1 | 1.92 | 0.84 |
| 10:k5:194:CYS:HB2 | 12:k5:1201:CYC:CAC | 2.06 | 0.84 |
| 10:k5:988:ALA:CB | 1:b7:106:GLU:OE2 | 2.25 | 0.84 |
| 10:k5:1123:ASN:O | 10:k5:1123:ASN:ND2 | 2.08 | 0.84 |
| 3:F6:130:ALA:HB3 | 12:F6:201:CYC:CBC | 2.06 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:i7:39:ILE:CD1 | 8:i7:148:GLU:HG3 | 1.87 | 0.84 |
| 12:B8:202:CYC:HBB2 | 4:M8:61:ASN:HB2 | 1.36 | 0.84 |
| 8:o7:29:PHE:HE2 | 1:p7:31:PHE:CE1 | 1.85 | 0.84 |
| 3:F9:153:CYS:HB2 | 12:F9:303:CYC:HAC1 | 0.88 | 0.84 |
| 11:a9:710:THR:HG23 | 11:a9:807:GLN:HG3 | 1.58 | 0.84 |
| 11:aA:365:LYS:HZ2 | 11:aA:365:LYS:HB2 | 1.42 | 0.84 |
| 11:aA:631:GLY:C | 3:J1:111:ASN:ND2 | 2.35 | 0.84 |
| 11:aA:738:LEU:HD12 | 12:aA:902:CYC:HBA1 | 1.59 | 0.84 |
| 3:JA:111:ASN:ND2 | 11:aA:519:ARG:HG2 | 1.90 | 0.84 |
| 12:JA:202:CYC:HBB3 | 11:aA:516:GLN:CG | 2.06 | 0.84 |
| 2:KA:18:PHE:CZ | 3:LA:48:ALA:CB | 2.60 | 0.84 |
| 4:MA:274:VAL:C | 3:VA:77:ARG:HE | 1.80 | 0.84 |
| 3:L3:120:LEU:HD21 | 11:a9:731:GLN:CG | 2.06 | 0.84 |
| 3:F4:1:MET:C | 4:M4:10:ARG:O | 2.20 | 0.84 |
| 3:F4:88:ILE:HD11 | 11:aA:140:GLN:HG2 | 1.58 | 0.84 |
| 3:L4:68:ARG:HB2 | 11:aA:82:GLN:CB | 2.07 | 0.84 |
| 4:M4:27:HIS:CD2 | 4:M4:34:ASP:HA | 2.12 | 0.84 |
| 4:M4:82:ILE:HD13 | 12:M4:301:CYC:CGD | 2.05 | 0.84 |
| 3:Q4:85:ASP:HA | 3:Q4:88:ILE:HG13 | 1.59 | 0.84 |
| 8:A5:119:LEU:HB3 | 12:A5:201:CYC:HBD1 | 1.58 | 0.84 |
| 1:f5:110:ASN:OD1 | 1:V5:161:SER:OXT | 1.95 | 0.84 |
| 1:P5:118:SER:OG | 10:k5:498:ALA:HB1 | 1.75 | 0.84 |
| 8:U5:83:ARG:HG3 | 6:M6:31:ASP:HB2 | 1.58 | 0.84 |
| 10:j5:325:ASN:O | 10:j5:325:ASN:ND2 | 2.08 | 0.84 |
| 10:k5:1008:PHE:CD1 | 1:p7:87:TYR:CZ | 2.64 | 0.84 |
| 1:B7:68:PRO:HB3 | 1:D7:14:VAL:O | 1.74 | 0.84 |
| 8:u7:103:PRO:HB3 | 1:v7:9:ILE:CG2 | 2.03 | 0.84 |
| 2:A9:34:ALA:HB3 | 3:B9:31:VAL:HG11 | 1.59 | 0.84 |
| 11:a9:312:ASP:HB2 | 11:a9:315:LEU:HD13 | 1.57 | 0.84 |
| 11:aA:668:TYR:CD1 | 3:J1:84:ARG:HD3 | 2.12 | 0.84 |
| 3:FA:151:GLY:N | 3:F9:150:ARG:NE | 2.22 | 0.84 |
| 3:B1:88:ILE:CD1 | 12:B1:202:CYC:C2B | 2.54 | 0.84 |
| 2:E4:1:MET:H2 | 4:M4:10:ARG:NH2 | 1.56 | 0.84 |
| 2:P4:19:LEU:HG | 3:Q4:95:TYR:CZ | 2.12 | 0.84 |
| 8:M5:66:VAL:CG1 | 8:K7:68:PRO:CG | 2.51 | 0.84 |
| 8:I5:35:ARG:HH22 | 8:I5:144:ASP:HB3 | 1.41 | 0.84 |
| 3:J6:108:ARG:NH2 | 6:M6:155:ASN:HB3 | 1.91 | 0.84 |
| 9:z5:12:PRO:HD3 | 9:z5:49:GLY:HA2 | 1.59 | 0.84 |
| 10:k5:733:SER:HB3 | 1:J7:154:ASP:OD2 | 1.77 | 0.84 |
| 10:k5:974:LEU:CD2 | 1:p7:1:MET:N | 2.41 | 0.84 |
| 8:C7:15:ALA:HB1 | 1:D7:90:ARG:NH2 | 1.92 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:I7:15:ALA:HB1 | 1:J7:90:ARG:NH2 | 1.92 | 0.84 |
| 8:g7:63:PRO:CD | 11:aA:336:ILE:HG23 | 2.02 | 0.84 |
| 8:m7:15:ALA:HB1 | 1:n7:90:ARG:NH2 | 1.92 | 0.84 |
| 3:L8:65:ASP:C | 11:a9:82:GLN:NE2 | 2.33 | 0.84 |
| 3:L8:71:GLY:CA | 11:a9:82:GLN:NE2 | 2.40 | 0.84 |
| 4:M8:58:TYR:O | 4:M8:61:ASN:CG | 2.20 | 0.84 |
| 3:Q8:87:GLU:OE1 | 5:Z8:31:TRP:CZ3 | 2.30 | 0.84 |
| 5:N9:54:LEU:HD22 | 3:T9:84:ARG:CD | 2.07 | 0.84 |
| 11:aA:558:VAL:CG1 | 11:aA:560:SER:OG | 2.26 | 0.84 |
| 4:MA:163:ASN:ND2 | 12:VA:201:CYC:HMA3 | 1.92 | 0.84 |
| 5:NA:54:LEU:CD2 | 3:TA:84:ARG:HD2 | 2.06 | 0.84 |
| 12:J3:202:CYC:NB | 11:a9:666:ASN:CB | 2.39 | 0.84 |
| 2:A3:65:TYR:O | 2:A3:71:GLN:HG3 | 1.77 | 0.84 |
| 1:N5:53:LYS:NZ | 8:O5:120:GLN:HG3 | 1.88 | 0.84 |
| 8:A5:111:GLY:HA3 | 1:F5:76:ARG:HA | 1.60 | 0.84 |
| 1:R5:110:ASN:OD1 | 10:k5:466:LEU:HB3 | 1.76 | 0.84 |
| 8:S5:14:GLU:HG2 | 10:j5:538:PHE:HE2 | 1.38 | 0.84 |
| 10:j5:804:GLU:OE1 | 9:w7:30:LYS:CE | 2.26 | 0.84 |
| 10:j5:1017:ARG:HB3 | 10:j5:1017:ARG:NH2 | 1.91 | 0.84 |
| 10:j5:1024:LYS:CD | 10:j5:1038:ARG:HH12 | 1.91 | 0.84 |
| 10:k5:966:SER:CB | 1:p7:14:VAL:CG1 | 2.45 | 0.84 |
| 8:o7:90:ARG:CB | 1:p7:18:TYR:CZ | 2.59 | 0.84 |
| 1:p7:140:LEU:HD12 | 11:a9:342:ARG:CD | 1.99 | 0.84 |
| 3:F8:88:ILE:HD11 | 11:a9:140:GLN:HG2 | 1.59 | 0.84 |
| 3:Q8:89:ILE:CA | 3:Q8:92:TYR:HE2 | 1.57 | 0.84 |
| 4:M9:158:PHE:C | 3:V9:108:ARG:CG | 2.50 | 0.84 |
| 3:H9:120:LEU:CD1 | 12:H9:202:CYC:HAA1 | 1.96 | 0.84 |
| 11:aA:666:ASN:OD1 | 12:aA:901:CYC:OB | 1.93 | 0.84 |
| 5:NA:61:LYS:CD | 3:TA:108:ARG:O | 2.20 | 0.84 |
| 2:OA:25:GLN:CG | 2:YA:33:ARG:HG2 | 2.08 | 0.84 |
| 3:U4:120:LEU:HD11 | 12:U4:201:CYC:HBD1 | 0.87 | 0.84 |
| 4:M4:27:HIS:HE1 | 4:M4:35:THR:N | 1.43 | 0.84 |
| 8:K5:80:LEU:CD1 | 12:K5:201:CYC:CAD | 2.53 | 0.84 |
| 1:N5:110:ASN:OD1 | 10:k5:692:LEU:O | 1.95 | 0.84 |
| 8:A5:119:LEU:HD11 | 12:A5:201:CYC:C2A | 2.06 | 0.84 |
| 1:d5:67:ARG:NH2 | 10:j5:705:THR:OG1 | 2.10 | 0.84 |
| 1:b5:38:VAL:HG11 | 10:k5:40:VAL:HG12 | 1.60 | 0.84 |
| 10:j5:136:VAL:CB | 10:j5:137:PRO:HD2 | 2.04 | 0.84 |
| 10:j5:793:SER:CB | 12:T7:201:CYC:O2A | 2.25 | 0.84 |
| 10:j5:978:LEU:CG | 1:v7:107:ARG:NH2 | 2.40 | 0.84 |
| 10:j5:1054:SER:OG | 1:r7:110:ASN:HB3 | 1.76 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:k5:1118:THR:HG22 | 12:k5:1204:CYC:HMA2 | 1.59 | 0.84 |
| 10:k5:1146:THR:HB | 1:p7:77:ARG:HH21 | 1.40 | 0.84 |
| 2:A6:34:ALA:HB3 | 3:B6:31:VAL:HG11 | 1.59 | 0.84 |
| 8:u7:23:LEU:CD2 | 1:v7:38:VAL:HG22 | 2.08 | 0.84 |
| 4:M8:162:ASN:O | 4:M8:166:THR:HG23 | 1.77 | 0.84 |
| 3:Q8:89:ILE:CB | 3:Q8:92:TYR:CE2 | 2.60 | 0.84 |
| 2:O9:65:TYR:O | 2:O9:71:GLN:HG3 | 1.77 | 0.84 |
| 12:J9:202:CYC:HB | 11:a9:512:TYR:CB | 1.82 | 0.84 |
| 11:a9:95:ILE:HG22 | 11:a9:99:ALA:N | 1.93 | 0.84 |
| 11:a9:632:ILE:CG2 | 11:a9:634:ALA:CB | 2.55 | 0.84 |
| 11:aA:476:ARG:NH1 | 11:aA:488:SER:HB3 | 1.86 | 0.84 |
| 3:FA:150:ARG:C | 3:F9:150:ARG:HE | 1.86 | 0.84 |
| 4:MA:163:ASN:HD21 | 12:VA:201:CYC:HMA3 | 1.42 | 0.84 |
| 2:QA:33:ARG:NH1 | 12:VA:202:CYC:C4B | 2.41 | 0.84 |
| 3:TA:28:THR:CG2 | 2:X4:67:THR:C | 2.46 | 0.84 |
| 12:B3:202:CYC:HAA1 | 11:a9:684:ASN:HB2 | 1.59 | 0.84 |
| 3:Z3:111:ASN:CG | 4:M3:258:LYS:HZ1 | 1.84 | 0.84 |
| 4:M3:162:ASN:O | 4:M3:166:THR:HG23 | 1.77 | 0.84 |
| 2:N4:34:ALA:HB3 | 3:O4:31:VAL:HG11 | 1.59 | 0.84 |
| 5:Z4:41:GLN:HG3 | 12:Z4:301:CYC:C3B | 2.07 | 0.84 |
| 8:U5:84:ASP:OD1 | 6:M6:26:PHE:CZ | 2.31 | 0.84 |
| 8:W5:15:ALA:C | 1:X5:90:ARG:HD2 | 1.96 | 0.84 |
| 10:j5:1008:PHE:CD1 | 12:v7:201:CYC:CBB | 2.60 | 0.84 |
| 10:j5:1151:GLN:O | 1:v7:122:PRO:CB | 2.26 | 0.84 |
| 8:o7:90:ARG:CA | 1:p7:18:TYR:CE2 | 2.61 | 0.84 |
| 3:H9:120:LEU:HD13 | 12:H9:202:CYC:C2A | 2.08 | 0.84 |
| 2:I9:98:VAL:HG21 | 3:J9:19:LEU:HD11 | 1.60 | 0.84 |
| 11:aA:588:VAL:O | 11:aA:590:PRO:HD3 | 1.77 | 0.84 |
| 2:EA:33:ARG:HG2 | 2:IA:25:GLN:NE2 | 1.92 | 0.84 |
| 3:HA:125:ARG:HE | 8:S7:41:GLN:HE21 | 1.25 | 0.84 |
| 3:LA:77:ARG:CZ | 11:aA:538:ARG:HH21 | 1.91 | 0.84 |
| 2:OA:65:TYR:O | 2:OA:71:GLN:HG3 | 1.77 | 0.84 |
| 2:G3:111:ALA:HB3 | 3:L3:77:ARG:HG2 | 1.59 | 0.84 |
| 3:L4:68:ARG:HB3 | 11:aA:81:ASP:C | 2.02 | 0.84 |
| 4:M4:205:ASP:HB2 | 5:Z4:63:ASN:ND2 | 1.93 | 0.84 |
| 12:M4:301:CYC:CAC | 3:Y4:82:CYS:HB2 | 2.07 | 0.84 |
| 10:j5:971:VAL:HG13 | 1:t7:76:ARG:NH1 | 1.91 | 0.84 |
| 10:j5:1053:TYR:HB2 | 10:j5:1058:VAL:CG2 | 2.07 | 0.84 |
| 8:i7:25:ARG:NH2 | 8:s7:6:LYS:N | 2.26 | 0.84 |
| 8:i7:39:ILE:HD12 | 8:i7:148:GLU:HG2 | 1.59 | 0.84 |
| 8:k7:75:GLU:O | 11:a9:53:VAL:HG11 | 1.77 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:a7:161:GLN:HG2 | 1:p7:49:THR:HG21 | 1.57 | 0.84 |
| 2:E8:1:MET:H2 | 4:M8:10:ARG:HH21 | 0.87 | 0.84 |
| 8:m7:35:ARG:HH22 | 8:m7:144:ASP:HB3 | 1.41 | 0.84 |
| 8:q7:45:GLU:CD | 3:H1:125:ARG:NH2 | 2.35 | 0.84 |
| 9:y7:23:LEU:O | 9:y7:23:LEU:HD12 | 1.78 | 0.84 |
| 4:M8:104:ALA:C | 2:P8:14:SER:HB2 | 2.02 | 0.84 |
| 4:M8:190:ARG:NH1 | 4:M8:202:SER:OG | 2.11 | 0.84 |
| 4:M9:134:ASN:ND2 | 5:N9:1:MET:H1 | 1.76 | 0.84 |
| 2:E9:2:LYS:HZ3 | 2:I9:17:ARG:HH12 | 0.84 | 0.84 |
| 11:aA:508:ARG:O | 11:aA:513:GLN:NE2 | 2.10 | 0.84 |
| 2:EA:152:ALA:HB1 | 2:IA:21:ASN:HD21 | 1.42 | 0.84 |
| 3:Z3:84:ARG:HG3 | 4:M3:192:GLN:HG2 | 1.60 | 0.84 |
| 3:S4:82:CYS:SG | 12:S4:202:CYC:CBC | 2.66 | 0.84 |
| 4:M4:197:ASP:O | 5:Z4:52:ARG:NH1 | 2.10 | 0.84 |
| 3:O4:95:TYR:HD2 | 3:O4:108:ARG:HH22 | 1.17 | 0.84 |
| 8:e5:45:GLU:CD | 1:R5:139:GLY:HA2 | 2.03 | 0.84 |
| 1:T5:110:ASN:HD21 | 10:j5:692:LEU:HB3 | 0.83 | 0.84 |
| 1:Z5:28:LYS:CE | 1:t7:143:PRO:HG2 | 1.97 | 0.84 |
| 10:j5:193:SER:OG | 12:j5:1201:CYC:O2D | 1.96 | 0.84 |
| 10:j5:1125:ARG:CZ | 1:t7:114:GLU:HB3 | 2.05 | 0.84 |
| 8:i7:20:PRO:HG2 | 8:s7:155:TYR:CD2 | 2.11 | 0.84 |
| 3:B8:68:ARG:NH2 | 3:U8:68:ARG:HH22 | 1.65 | 0.84 |
| 8:o7:23:LEU:CD2 | 1:p7:38:VAL:HG22 | 2.08 | 0.84 |
| 1:p7:62:TYR:HB3 | 11:a9:601:ALA:HB1 | 1.59 | 0.84 |
| 2:N8:60:TYR:CG | 2:N8:67:THR:HG23 | 2.13 | 0.84 |
| 2:N8:65:TYR:O | 2:N8:71:GLN:HG3 | 1.77 | 0.84 |
| 2:N8:112:GLY:N | 5:Z8:34:LEU:HB2 | 1.91 | 0.84 |
| 5:Z8:38:GLU:CA | 12:Z8:301:CYC:HMB2 | 2.06 | 0.84 |
| 3:H9:107:ASP:HB3 | 11:a9:445:THR:CG2 | 2.07 | 0.84 |
| 11:a9:588:VAL:O | 11:a9:590:PRO:HD3 | 1.77 | 0.84 |
| 11:aA:632:ILE:CG2 | 11:aA:634:ALA:CB | 2.55 | 0.84 |
| 2:AA:34:ALA:HB3 | 3:BA:31:VAL:HG11 | 1.59 | 0.84 |
| 4:MA:274:VAL:CA | 3:VA:77:ARG:NE | 2.41 | 0.84 |
| 2:QA:162:SER:C | 2:WA:118:ARG:CD | 2.51 | 0.84 |
| 2:O1:25:GLN:CG | 2:Y1:33:ARG:HG2 | 2.08 | 0.84 |
| 3:J2:119:ALA:HB1 | 6:M2:261:LYS:N | 1.92 | 0.84 |
| 4:M4:104:ALA:CB | 2:P4:14:SER:H | 1.86 | 0.84 |
| 10:j5:74:ARG:HD3 | 10:j5:205:GLU:HG3 | 1.59 | 0.84 |
| 10:j5:1023:SER:HB3 | 12:f7:201:CYC:CMA | 2.08 | 0.84 |
| 10:j5:1119:LEU:CD2 | 1:t7:87:TYR:CZ | 2.60 | 0.84 |
| 10:j5:1124:TYR:OH | 1:t7:119:LEU:HD21 | 1.78 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:i7:46:ALA:HB1 | 8:i7:140:LEU:CD1 | 2.08 | 0.84 |
| 8:a7:37:LEU:HD13 | 1:b7:24:LEU:HD21 | 1.59 | 0.84 |
| 8:u7:23:LEU:O | 1:v7:38:VAL:HG21 | 1.78 | 0.84 |
| 3:H8:84:ARG:HD2 | 11:a9:131:TYR:CE1 | 2.12 | 0.84 |
| 3:L9:52:ILE:CD1 | 3:L9:87:GLU:HA | 2.06 | 0.84 |
| 4:M9:133:ARG:HB3 | 12:R9:201:CYC:CBA | 2.07 | 0.84 |
| 11:aA:448:ASN:OD1 | 11:aA:474:PHE:HE1 | 1.60 | 0.84 |
| 4:M1:118:TYR:HD2 | 3:X1:84:ARG:HH21 | 0.88 | 0.84 |
| 3:LA:44:ILE:HG23 | 3:LA:90:LEU:HD21 | 1.60 | 0.83 |
| 12:J3:202:CYC:CGA | 11:a9:667:THR:HG22 | 2.07 | 0.83 |
| 4:M4:91:VAL:HG22 | 2:P4:15:GLN:HA | 1.60 | 0.83 |
| 4:M4:100:SER:OG | 2:P4:9:ILE:HG22 | 1.77 | 0.83 |
| 12:B5:201:CYC:HBB2 | 9:z5:21:ARG:HG3 | 1.57 | 0.83 |
| 1:P5:114:GLU:HG2 | 10:k5:496:GLU:CB | 2.06 | 0.83 |
| 1:V5:83:ARG:CZ | 10:j5:649:PHE:CE2 | 2.60 | 0.83 |
| 10:j5:663:ALA:O | 10:j5:664:MET:C | 2.05 | 0.83 |
| 10:j5:822:ARG:HG3 | 1:H7:106:GLU:OE2 | 1.77 | 0.83 |
| 10:j5:868:ASP:O | 9:w7:43:ARG:NE | 2.11 | 0.83 |
| 10:k5:246:VAL:CG2 | 10:k5:257:THR:HG22 | 2.08 | 0.83 |
| 10:k5:1020:GLU:N | 1:Z7:87:TYR:OH | 2.10 | 0.83 |
| 10:k5:1053:TYR:HB2 | 10:k5:1058:VAL:CG2 | 2.07 | 0.83 |
| 1:B7:54:GLU:CD | 11:a9:563:PHE:CD2 | 2.56 | 0.83 |
| 8:g7:35:ARG:HH22 | 8:g7:144:ASP:HB3 | 1.40 | 0.83 |
| 8:a7:52:LYS:CD | 11:a9:321:ALA:CB | 2.48 | 0.83 |
| 2:X8:57:GLN:HE22 | 3:T9:32:LYS:CG | 1.91 | 0.83 |
| 4:M8:207:ASP:O | 4:M8:210:ILE:O | 1.96 | 0.83 |
| 2:A9:60:TYR:CG | 2:A9:67:THR:HG23 | 2.13 | 0.83 |
| 11:aA:731:GLN:CG | 3:L1:120:LEU:HD21 | 2.07 | 0.83 |
| 12:BA:201:CYC:O2A | 4:MA:35:THR:HA | 1.77 | 0.83 |
| 3:FA:145:PRO:HG3 | 12:F9:302:CYC:CMC | 2.06 | 0.83 |
| 3:HA:107:ASP:HB3 | 11:aA:445:THR:CG2 | 2.07 | 0.83 |
| 2:A1:25:GLN:CG | 2:K1:33:ARG:HG2 | 2.08 | 0.83 |
| 3:S4:120:LEU:HD11 | 12:S4:202:CYC:CHA | 2.07 | 0.83 |
| 3:L4:68:ARG:CD | 11:aA:81:ASP:HA | 2.08 | 0.83 |
| 1:D5:3:ASP:N | 1:D5:3:ASP:OD1 | 2.09 | 0.83 |
| 6:M6:127:SER:HB2 | 3:F6:84:ARG:HH22 | 1.39 | 0.83 |
| 10:j5:66:MET:SD | 10:j5:66:MET:N | 2.50 | 0.83 |
| 10:j5:1016:LEU:HB2 | 10:j5:1044:ASN:ND2 | 1.93 | 0.83 |
| 2:A8:25:GLN:CG | 2:K8:33:ARG:HG2 | 2.08 | 0.83 |
| 8:s7:15:ALA:HB1 | 1:t7:90:ARG:NH2 | 1.92 | 0.83 |
| 3:L8:113:LEU:HD11 | 12:a9:901:CYC:HBB | 1.60 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:N8:115:GLU:HG3 | 5:Z8:32:PRO:HG3 | 1.57 | 0.83 |
| 2:O9:60:TYR:CG | 2:O9:67:THR:HG23 | 2.13 | 0.83 |
| 11:aA:798:SER:CA | 11:aA:800:THR:HG23 | 2.08 | 0.83 |
| 5:N1:1:MET:C | 5:N1:3:VAL:H | 1.86 | 0.83 |
| 2:A2:65:TYR:O | 2:A2:71:GLN:HG3 | 1.77 | 0.83 |
| 5:NA:61:LYS:HZ2 | 12:TA:301:CYC:HBB2 | 1.42 | 0.83 |
| 2:OA:60:TYR:CG | 2:OA:67:THR:HG23 | 2.13 | 0.83 |
| 12:H3:202:CYC:O2A | 11:a9:776:TYR:CE2 | 2.31 | 0.83 |
| 3:Z3:116:THR:OG1 | 4:M3:259:ARG:NH1 | 2.12 | 0.83 |
| 4:M4:58:TYR:O | 4:M4:61:ASN:CG | 2.21 | 0.83 |
| 4:M4:138:SER:OG | 12:Z4:301:CYC:HBB1 | 1.77 | 0.83 |
| 10:j5:209:ASN:ND2 | 10:j5:209:ASN:O | 2.10 | 0.83 |
| 10:j5:286:VAL:HG21 | 10:j5:324:LYS:O | 1.78 | 0.83 |
| 8:Q7:19:SER:HB3 | 8:C7:6:LYS:NZ | 1.93 | 0.83 |
| 8:c7:15:ALA:C | 1:d7:90:ARG:HE | 1.79 | 0.83 |
| 8:c7:46:ALA:HB1 | 8:c7:140:LEU:CD1 | 2.08 | 0.83 |
| 8:o7:37:LEU:HD12 | 1:p7:28:LYS:CE | 2.08 | 0.83 |
| 9:x7:23:LEU:HD12 | 9:x7:23:LEU:O | 1.78 | 0.83 |
| 2:X8:33:ARG:HG2 | 2:N8:25:GLN:CG | 2.08 | 0.83 |
| 3:Q8:92:TYR:CZ | 3:Q8:109:CYS:SG | 2.71 | 0.83 |
| 3:Y8:89:ILE:HG23 | 3:Y8:92:TYR:HH | 1.06 | 0.83 |
| 2:A9:25:GLN:CG | 2:K9:33:ARG:HG2 | 2.08 | 0.83 |
| 2:G1:111:ALA:HB3 | 3:L1:77:ARG:HG2 | 1.59 | 0.83 |
| 11:a9:508:ARG:O | 11:a9:513:GLN:NE2 | 2.10 | 0.83 |
| 11:aA:249:GLU:O | 11:aA:285:VAL:CG2 | 2.25 | 0.83 |
| 2:A4:65:TYR:O | 2:A4:71:GLN:HG3 | 1.77 | 0.83 |
| 8:G5:107:ILE:HD13 | 1:H5:13:ASP:CG | 2.03 | 0.83 |
| 12:V5:201:CYC:O2A | 10:j5:649:PHE:HD2 | 1.60 | 0.83 |
| 3:J6:108:ARG:NH2 | 6:M6:155:ASN:CB | 2.42 | 0.83 |
| 10:k5:209:ASN:O | 10:k5:209:ASN:ND2 | 2.10 | 0.83 |
| 10:k5:761:ARG:O | 10:k5:761:ARG:HD2 | 1.79 | 0.83 |
| 10:k5:1053:TYR:C | 1:l7:106:GLU:O | 2.21 | 0.83 |
| 2:A6:60:TYR:CG | 2:A6:67:THR:HG23 | 2.13 | 0.83 |
| 8:O7:15:ALA:HB1 | 1:P7:90:ARG:NH2 | 1.92 | 0.83 |
| 12:b7:201:CYC:HBB2 | 9:x7:21:ARG:NE | 1.93 | 0.83 |
| 9:y7:3:ARG:NH2 | 9:y7:67:VAL:HG12 | 1.92 | 0.83 |
| 3:O8:115:GLU:CB | 5:Z8:70:ILE:O | 2.25 | 0.83 |
| 3:Q8:120:LEU:HD11 | 3:Q8:122:THR:N | 1.78 | 0.83 |
| 4:M9:160:THR:O | 3:V9:108:ARG:HG2 | 1.78 | 0.83 |
| 5:N9:16:PHE:CZ | 3:T9:120:LEU:HD21 | 2.12 | 0.83 |
| 11:a9:287:ALA:C | 11:a9:289:THR:N | 2.32 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:a9:710:THR:CG2 | 11:a9:807:GLN:CB | 2.47 | 0.83 |
| 11:aA:823:ILE:HG13 | 3:L1:75:PRO:HD2 | 1.59 | 0.83 |
| 2:AA:60:TYR:CG | 2:AA:67:THR:HG23 | 2.13 | 0.83 |
| 3:FA:68:ARG:CZ | 3:ZA:68:ARG:NH1 | 2.41 | 0.83 |
| 12:FA:301:CYC:HB | 4:MA:53:LEU:CD1 | 1.67 | 0.83 |
| 12:FA:301:CYC:HB | 4:MA:53:LEU:HD13 | 0.76 | 0.83 |
| 3:TA:32:LYS:CG | 2:X4:57:GLN:HE22 | 1.91 | 0.83 |
| 12:R1:201:CYC:HBB2 | 5:N1:61:LYS:NZ | 1.94 | 0.83 |
| 6:M2:28:ASN:CA | 8:O5:80:LEU:HD23 | 2.09 | 0.83 |
| 4:M3:190:ARG:NH1 | 4:M3:202:SER:OG | 2.11 | 0.83 |
| 3:H4:80:ALA:CB | 3:H4:84:ARG:NH1 | 2.34 | 0.83 |
| 8:S5:41:GLN:CD | 1:D7:143:PRO:CG | 2.50 | 0.83 |
| 6:M6:118:GLU:OE2 | 2:I6:118:ARG:NH2 | 2.11 | 0.83 |
| 10:j5:238:ARG:HH11 | 10:j5:238:ARG:HG3 | 1.42 | 0.83 |
| 10:j5:934:ALA:HB2 | 1:J7:32:THR:CG2 | 2.06 | 0.83 |
| 10:k5:1052:PRO:CA | 1:l7:106:GLU:OE2 | 2.26 | 0.83 |
| 10:k5:1125:ARG:CZ | 1:n7:114:GLU:HB3 | 2.08 | 0.83 |
| 8:i7:92:VAL:HG13 | 8:i7:152:TYR:HB3 | 1.60 | 0.83 |
| 8:U7:15:ALA:HB1 | 1:V7:90:ARG:NH2 | 1.92 | 0.83 |
| 1:X7:118:SER:O | 9:w7:61:GLN:NE2 | 2.11 | 0.83 |
| 8:c7:92:VAL:HG13 | 8:c7:152:TYR:HB3 | 1.60 | 0.83 |
| 8:c7:96:ILE:CA | 8:c7:152:TYR:CZ | 2.50 | 0.83 |
| 3:F8:111:ASN:HB3 | 4:M8:6:THR:HA | 1.60 | 0.83 |
| 11:a9:107:ARG:CG | 11:a9:108:PRO:CD | 2.52 | 0.83 |
| 11:a9:476:ARG:NH1 | 11:a9:488:SER:HB3 | 1.86 | 0.83 |
| 11:aA:91:THR:CG2 | 11:aA:96:THR:HA | 2.08 | 0.83 |
| 2:A2:34:ALA:HB3 | 3:B2:31:VAL:HG11 | 1.59 | 0.83 |
| 3:FA:151:GLY:H | 3:F9:150:ARG:HE | 1.14 | 0.83 |
| 5:NA:16:PHE:CZ | 3:TA:120:LEU:HD23 | 2.10 | 0.83 |
| 6:M2:26:PHE:HB2 | 8:O5:87:TYR:HH | 1.42 | 0.83 |
| 2:A4:60:TYR:CG | 2:A4:67:THR:HG23 | 2.13 | 0.83 |
| 5:N3:3:VAL:HG11 | 3:P3:115:GLU:HB3 | 1.61 | 0.83 |
| 5:N3:54:LEU:CD1 | 12:R3:201:CYC:HB | 1.81 | 0.83 |
| 1:L5:76:ARG:HA | 8:G5:111:GLY:HA3 | 1.60 | 0.83 |
| 1:f5:19:LEU:CD1 | 10:j5:172:LEU:HD12 | 2.08 | 0.83 |
| 8:Q5:17:TYR:HE2 | 1:R5:44:ILE:HG21 | 1.35 | 0.83 |
| 10:j5:246:VAL:CG2 | 10:j5:257:THR:HG22 | 2.08 | 0.83 |
| 10:k5:978:LEU:HD21 | 1:p7:107:ARG:NE | 1.93 | 0.83 |
| 8:c7:18:LEU:HD22 | 1:d7:97:LEU:CD1 | 2.07 | 0.83 |
| 2:X8:67:THR:O | 3:T9:28:THR:HG21 | 1.78 | 0.83 |
| 3:B9:27:LEU:HA | 3:B9:30:LEU:HD13 | 1.61 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:a9:93:LEU:HD23 | 11:a9:252:ARG:HH11 | 1.34 | 0.83 |
| 11:aA:596:THR:HB | 11:aA:597:THR:HG23 | 1.58 | 0.83 |
| 3:JA:114:LYS:CD | 8:S7:60:GLN:NE2 | 2.42 | 0.83 |
| 2:QA:162:SER:O | 2:WA:118:ARG:HD3 | 1.78 | 0.83 |
| 12:QA:201:CYC:HBB2 | 3:TA:75:PRO:HB3 | 1.32 | 0.83 |
| 2:A1:60:TYR:CG | 2:A1:67:THR:HG23 | 2.13 | 0.83 |
| 3:J3:120:LEU:CD2 | 11:a9:800:THR:CG2 | 2.45 | 0.83 |
| 2:K3:33:ARG:HG2 | 2:A3:25:GLN:CG | 2.08 | 0.83 |
| 2:K2:33:ARG:HG2 | 2:A2:25:GLN:CG | 2.08 | 0.83 |
| 5:N3:61:LYS:NZ | 12:R3:201:CYC:HBB2 | 1.94 | 0.83 |
| 2:O3:25:GLN:CG | 2:Y3:33:ARG:HG2 | 2.08 | 0.83 |
| 3:B1:88:ILE:HG21 | 12:B1:202:CYC:C3B | 2.07 | 0.83 |
| 3:L4:71:GLY:H | 11:aA:82:GLN:CG | 1.86 | 0.83 |
| 12:L4:202:CYC:OB | 11:aA:239:TYR:CE1 | 2.32 | 0.83 |
| 4:M4:101:ASP:HA | 2:P4:13:ASP:CG | 2.03 | 0.83 |
| 4:M4:190:ARG:NH1 | 4:M4:202:SER:OG | 2.11 | 0.83 |
| 1:b5:18:TYR:CG | 10:k5:165:ARG:HG3 | 2.13 | 0.83 |
| 8:c7:12:ASP:HB2 | 1:d7:94:TYR:CE2 | 2.13 | 0.83 |
| 8:o7:23:LEU:HD23 | 1:p7:38:VAL:HG22 | 1.59 | 0.83 |
| 8:u7:37:LEU:HD12 | 1:v7:28:LYS:CE | 2.08 | 0.83 |
| 9:x7:3:ARG:NH2 | 9:x7:67:VAL:HG12 | 1.92 | 0.83 |
| 3:F8:115:GLU:CG | 4:M8:3:VAL:CG2 | 2.57 | 0.83 |
| 3:L8:68:ARG:HB3 | 11:a9:81:ASP:C | 2.03 | 0.83 |
| 4:M9:162:ASN:O | 4:M9:166:THR:HG23 | 1.77 | 0.83 |
| 3:D9:68:ARG:HH22 | 3:X9:68:ARG:CZ | 1.90 | 0.83 |
| 11:a9:249:GLU:O | 11:a9:285:VAL:CG2 | 2.25 | 0.83 |
| 3:DA:68:ARG:HH22 | 3:XA:68:ARG:CZ | 1.90 | 0.83 |
| 12:QA:201:CYC:HBB1 | 3:TA:75:PRO:HB3 | 1.59 | 0.83 |
| 2:O1:60:TYR:CG | 2:O1:67:THR:HG23 | 2.13 | 0.83 |
| 5:N3:1:MET:C | 5:N3:3:VAL:H | 1.86 | 0.83 |
| 4:M4:148:LYS:HE3 | 4:M4:197:ASP:OD2 | 1.79 | 0.83 |
| 4:M4:232:VAL:O | 4:M4:235:PHE:HE2 | 1.62 | 0.83 |
| 8:A5:107:ILE:HD13 | 1:B5:13:ASP:CG | 2.04 | 0.83 |
| 1:f5:17:LYS:O | 10:j5:169:TYR:OH | 1.95 | 0.83 |
| 8:W5:12:ASP:HB2 | 1:X5:94:TYR:CD2 | 2.14 | 0.83 |
| 1:X5:143:PRO:HB2 | 8:a5:38:ARG:NH1 | 1.94 | 0.83 |
| 10:j5:971:VAL:H | 12:j5:1202:CYC:CGD | 1.89 | 0.83 |
| 10:k5:362:LYS:CE | 10:k5:363:HIS:NE2 | 2.42 | 0.83 |
| 10:k5:951:MET:HE3 | 10:k5:951:MET:O | 1.79 | 0.83 |
| 10:k5:964:GLY:HA2 | 1:n7:69:GLY:HA3 | 1.58 | 0.83 |
| 10:k5:988:ALA:HA | 1:b7:106:GLU:OE2 | 1.79 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:k5:990:ARG:NH2 | 10:k5:1026:LYS:HZ1 | 1.74 | 0.83 |
| 10:k5:1008:PHE:HE1 | 1:p7:87:TYR:CD2 | 1.96 | 0.83 |
| 8:g7:37:LEU:HD13 | 1:h7:24:LEU:HD21 | 1.59 | 0.83 |
| 8:i7:20:PRO:CD | 8:s7:155:TYR:CZ | 2.61 | 0.83 |
| 1:T7:68:PRO:HB3 | 1:V7:14:VAL:C | 2.04 | 0.83 |
| 12:B8:202:CYC:CHA | 4:M8:54:ALA:N | 2.41 | 0.83 |
| 8:o7:23:LEU:O | 1:p7:38:VAL:HG21 | 1.78 | 0.83 |
| 1:r7:68:PRO:HB3 | 1:t7:14:VAL:C | 2.04 | 0.83 |
| 3:L8:68:ARG:O | 3:L8:69:PRO:O | 1.97 | 0.83 |
| 4:M9:160:THR:CG2 | 4:M9:257:GLN:HB3 | 2.09 | 0.83 |
| 3:F9:68:ARG:CZ | 3:Z9:68:ARG:NH1 | 2.41 | 0.83 |
| 11:a9:644:ARG:O | 11:a9:645:PRO:C | 2.22 | 0.83 |
| 11:aA:308:LEU:HD21 | 11:aA:315:LEU:CD1 | 2.09 | 0.83 |
| 2:A2:60:TYR:CG | 2:A2:67:THR:HG23 | 2.13 | 0.83 |
| 3:HA:113:LEU:HD21 | 12:HA:202:CYC:HMB1 | 1.56 | 0.83 |
| 3:J3:77:ARG:NE | 2:K3:107:ASP:HA | 1.94 | 0.83 |
| 3:L4:120:LEU:O | 11:aA:90:GLN:NE2 | 2.11 | 0.83 |
| 4:M4:128:ALA:C | 4:M4:142:PHE:CE1 | 2.57 | 0.83 |
| 5:Z4:22:LEU:HD13 | 12:Z4:301:CYC:OB | 1.78 | 0.83 |
| 5:Z4:41:GLN:HB2 | 12:Z4:301:CYC:CHB | 2.08 | 0.83 |
| 8:A5:119:LEU:CD1 | 12:A5:201:CYC:C1A | 2.57 | 0.83 |
| 8:G5:107:ILE:CG1 | 1:H5:13:ASP:OD2 | 2.27 | 0.83 |
| 8:Q5:8:ILE:HG23 | 1:R5:94:TYR:CD1 | 2.14 | 0.83 |
| 8:Q5:12:ASP:HB2 | 1:R5:94:TYR:CD2 | 2.14 | 0.83 |
| 2:K6:33:ARG:HG2 | 2:A6:25:GLN:CG | 2.08 | 0.83 |
| 10:j5:1054:SER:HA | 1:r7:107:ARG:HA | 1.61 | 0.83 |
| 10:k5:74:ARG:HD3 | 10:k5:205:GLU:HG3 | 1.59 | 0.83 |
| 10:k5:930:LEU:HB3 | 1:D7:33:THR:CB | 2.09 | 0.83 |
| 10:k5:1146:THR:CB | 1:p7:77:ARG:HH22 | 1.85 | 0.83 |
| 8:I7:29:PHE:HZ | 8:I7:98:ALA:O | 1.62 | 0.83 |
| 8:c7:20:PRO:HG2 | 8:m7:155:TYR:HB3 | 1.60 | 0.83 |
| 12:B8:202:CYC:HMA3 | 4:M8:58:TYR:HB2 | 1.60 | 0.83 |
| 3:L8:109:CYS:CA | 12:a9:901:CYC:CBB | 2.54 | 0.83 |
| 3:Q8:78:ARG:HH11 | 12:Z8:301:CYC:HAD1 | 1.42 | 0.83 |
| 4:M9:190:ARG:NH1 | 4:M9:202:SER:OG | 2.11 | 0.83 |
| 11:a9:365:LYS:HB2 | 11:a9:365:LYS:HZ2 | 1.41 | 0.83 |
| 11:a9:371:VAL:HG13 | 11:a9:507:PHE:HB2 | 1.60 | 0.83 |
| 11:a9:581:ARG:HG3 | 11:a9:581:ARG:HH11 | 1.43 | 0.83 |
| 2:OA:34:ALA:HB3 | 3:PA:31:VAL:HG11 | 1.59 | 0.83 |
| 3:TA:24:LEU:HD22 | 2:X4:68:GLN:HE21 | 1.44 | 0.83 |
| 3:B4:68:ARG:CZ | 3:U4:68:ARG:NH2 | 2.34 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M4:162:ASN:O | 4:M4:166:THR:HG23 | 1.77 | 0.83 |
| 4:M4:217:VAL:HG21 | 5:Z4:30:PRO:CB | 2.06 | 0.83 |
| 4:M4:273:ILE:CD1 | 2:X4:108:TYR:CZ | 2.61 | 0.83 |
| 2:N4:25:GLN:CG | 2:X4:33:ARG:HG2 | 2.08 | 0.83 |
| 8:M5:140:LEU:HD22 | 1:J7:140:LEU:HG | 1.59 | 0.83 |
| 8:C5:29:PHE:HZ | 8:C5:98:ALA:O | 1.62 | 0.83 |
| 10:j5:733:SER:HB3 | 1:D7:154:ASP:OD2 | 1.79 | 0.83 |
| 10:k5:934:ALA:HB3 | 1:D7:32:THR:HG21 | 1.42 | 0.83 |
| 1:B7:68:PRO:HB3 | 1:D7:14:VAL:C | 2.04 | 0.83 |
| 1:b7:75:THR:HG22 | 8:c7:115:MET:HE2 | 1.60 | 0.83 |
| 11:a9:596:THR:HB | 11:a9:597:THR:HG23 | 1.58 | 0.83 |
| 11:aA:803:ASN:HB3 | 3:J1:119:ALA:O | 1.78 | 0.83 |
| 4:M1:81:ASP:N | 3:X1:111:ASN:ND2 | 2.26 | 0.83 |
| 4:M1:210:ILE:HD13 | 5:N1:59:ARG:HH11 | 1.42 | 0.83 |
| 3:FA:37:ARG:HH22 | 3:FA:159:GLU:CD | 1.87 | 0.82 |
| 2:QA:84:ARG:HH12 | 3:TA:67:ILE:HD12 | 1.44 | 0.82 |
| 2:O1:34:ALA:HB3 | 3:P1:31:VAL:HG11 | 1.59 | 0.82 |
| 3:L2:77:ARG:CZ | 6:M2:70:GLU:CD | 2.50 | 0.82 |
| 6:M2:278:ARG:NH2 | 1:j7:64:ASP:OD1 | 2.12 | 0.82 |
| 3:B4:86:MET:H | 12:B4:202:CYC:HBC1 | 1.01 | 0.82 |
| 1:H5:143:PRO:CG | 8:Q7:41:GLN:HE22 | 1.91 | 0.82 |
| 1:f5:114:GLU:CB | 10:j5:491:THR:OG1 | 2.27 | 0.82 |
| 1:f5:161:SER:O | 1:V5:101:PRO:HG2 | 1.77 | 0.82 |
| 1:P5:114:GLU:CG | 10:k5:496:GLU:OE2 | 2.26 | 0.82 |
| 1:V5:114:GLU:OE1 | 10:j5:496:GLU:HG3 | 1.79 | 0.82 |
| 10:j5:362:LYS:CE | 10:j5:363:HIS:NE2 | 2.42 | 0.82 |
| 10:j5:800:THR:HA | 9:w7:30:LYS:HB2 | 1.61 | 0.82 |
| 10:j5:1009:ALA:HB2 | 1:v7:87:TYR:CZ | 2.14 | 0.82 |
| 10:k5:663:ALA:O | 10:k5:664:MET:C | 2.05 | 0.82 |
| 10:k5:990:ARG:NE | 10:k5:1026:LYS:HZ1 | 1.77 | 0.82 |
| 1:d7:87:TYR:OH | 9:x7:38:PHE:HE2 | 1.56 | 0.82 |
| 4:M8:214:GLY:CA | 5:Z8:28:HIS:ND1 | 2.41 | 0.82 |
| 3:F1:111:ASN:O | 4:M1:39:SER:HB3 | 1.79 | 0.82 |
| 12:L9:201:CYC:CAB | 2:K9:24:LEU:HB3 | 2.09 | 0.82 |
| 3:H9:117:TYR:CE1 | 12:H9:202:CYC:CHB | 2.62 | 0.82 |
| 11:a9:312:ASP:CA | 11:a9:315:LEU:N | 2.40 | 0.82 |
| 11:aA:594:ARG:HH11 | 11:aA:594:ARG:HG3 | 1.44 | 0.82 |
| 4:M1:259:ARG:NH1 | 3:Z1:116:THR:OG1 | 2.12 | 0.82 |
| 5:N1:22:LEU:HD22 | 5:N1:26:LEU:HD13 | 1.59 | 0.82 |
| 2:A2:60:TYR:CB | 2:A2:67:THR:HG23 | 2.09 | 0.82 |
| 5:NA:1:MET:C | 5:NA:3:VAL:H | 1.86 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 12:J3:202:CYC:OB | 11:a9:666:ASN:OD1 | 1.95 | 0.82 |
| 2:I2:118:ARG:NH2 | 6:M2:118:GLU:OE2 | 2.11 | 0.82 |
| 6:M2:57:GLU:OE1 | 8:i7:76:LYS:CD | 2.26 | 0.82 |
| 2:A3:60:TYR:CG | 2:A3:67:THR:HG23 | 2.13 | 0.82 |
| 2:A4:25:GLN:CG | 2:K4:33:ARG:HG2 | 2.08 | 0.82 |
| 3:B4:108:ARG:CA | 4:M4:61:ASN:CA | 2.55 | 0.82 |
| 3:L3:1:MET:HG3 | 3:L3:104:VAL:CG1 | 2.09 | 0.82 |
| 4:M4:27:HIS:ND1 | 4:M4:34:ASP:HA | 1.87 | 0.82 |
| 4:M4:98:ASP:HB3 | 3:Q4:92:TYR:HB2 | 1.59 | 0.82 |
| 8:K5:20:PRO:HD3 | 8:U5:155:TYR:HB2 | 1.59 | 0.82 |
| 3:Y4:87:GLU:CG | 3:Y4:91:ARG:NH1 | 2.42 | 0.82 |
| 8:G5:6:LYS:NZ | 8:S5:21:GLY:N | 2.27 | 0.82 |
| 8:U5:83:ARG:HB2 | 6:M6:26:PHE:CE1 | 2.12 | 0.82 |
| 10:j5:761:ARG:O | 10:j5:761:ARG:HD2 | 1.79 | 0.82 |
| 10:j5:931:VAL:CG2 | 1:J7:30:TYR:HA | 2.09 | 0.82 |
| 10:k5:1024:LYS:CD | 10:k5:1038:ARG:HH12 | 1.91 | 0.82 |
| 8:u7:90:ARG:CA | 1:v7:18:TYR:CE2 | 2.61 | 0.82 |
| 4:M9:160:THR:CG2 | 4:M9:257:GLN:HB2 | 2.07 | 0.82 |
| 4:M9:163:ASN:ND2 | 12:V9:201:CYC:HMA3 | 1.92 | 0.82 |
| 5:N9:54:LEU:CD2 | 3:T9:84:ARG:HD2 | 2.06 | 0.82 |
| 2:O9:25:GLN:CG | 2:Y9:33:ARG:HG2 | 2.08 | 0.82 |
| 2:A9:63:PHE:CB | 2:A9:66:LEU:CD1 | 2.56 | 0.82 |
| 11:aA:95:ILE:HG22 | 11:aA:99:ALA:N | 1.93 | 0.82 |
| 3:BA:111:ASN:O | 4:MA:39:SER:HB3 | 1.79 | 0.82 |
| 4:MA:158:PHE:CA | 3:VA:108:ARG:CD | 2.56 | 0.82 |
| 2:OA:63:PHE:CB | 2:OA:66:LEU:CD1 | 2.56 | 0.82 |
| 3:TA:28:THR:HG21 | 2:X4:67:THR:O | 1.78 | 0.82 |
| 3:VA:108:ARG:CZ | 3:VA:108:ARG:HB3 | 2.09 | 0.82 |
| 3:H3:62:GLU:OE1 | 8:k7:49:ARG:NH1 | 2.11 | 0.82 |
| 3:L2:75:PRO:HG2 | 3:L2:78:ARG:H | 1.44 | 0.82 |
| 3:L3:119:ALA:CB | 11:a9:813:PRO:C | 2.52 | 0.82 |
| 4:M3:160:THR:CG2 | 4:M3:257:GLN:HB3 | 2.09 | 0.82 |
| 2:N4:60:TYR:CG | 2:N4:67:THR:HG23 | 2.13 | 0.82 |
| 1:b5:34:GLY:CA | 10:k5:47:PHE:HD2 | 1.91 | 0.82 |
| 10:k5:978:LEU:HD11 | 1:p7:107:ARG:NH2 | 1.94 | 0.82 |
| 10:k5:1050:PHE:CZ | 1:l7:107:ARG:NH1 | 2.17 | 0.82 |
| 1:P7:14:VAL:C | 1:N7:68:PRO:HB3 | 2.04 | 0.82 |
| 8:I7:161:GLN:CG | 1:X7:49:THR:HG22 | 2.05 | 0.82 |
| 8:U7:22:GLU:C | 8:U7:24:ASP:H | 1.87 | 0.82 |
| 8:a7:22:GLU:HG2 | 8:a7:25:ARG:NH1 | 1.94 | 0.82 |
| 2:X8:57:GLN:CD | 3:T9:32:LYS:HE2 | 2.01 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:Q8:117:TYR:CE1 | 5:Z8:39:PRO:HG2 | 2.14 | 0.82 |
| 11:a9:823:ILE:C | 11:a9:824:VAL:OXT | 2.14 | 0.82 |
| 11:aA:813:PRO:C | 3:L1:119:ALA:CB | 2.52 | 0.82 |
| 3:H1:81:ALA:HB1 | 12:H1:201:CYC:C3D | 2.10 | 0.82 |
| 2:IA:1:MET:CE | 2:IA:108:TYR:HE1 | 1.92 | 0.82 |
| 4:MA:113:ILE:HD11 | 4:MA:143:VAL:CG1 | 2.05 | 0.82 |
| 4:MA:190:ARG:NH1 | 4:MA:202:SER:OG | 2.11 | 0.82 |
| 4:M4:201:ASP:CB | 5:Z4:59:ARG:HD2 | 2.09 | 0.82 |
| 8:M5:19:SER:HG | 8:A5:6:LYS:HZ2 | 1.25 | 0.82 |
| 8:W5:8:ILE:HG23 | 1:X5:94:TYR:CD1 | 2.14 | 0.82 |
| 10:j5:1024:LYS:HD3 | 10:j5:1038:ARG:HH12 | 1.44 | 0.82 |
| 10:k5:971:VAL:HG12 | 12:k5:1204:CYC:O1D | 1.61 | 0.82 |
| 8:c7:101:VAL:HG11 | 8:c7:155:TYR:CZ | 2.13 | 0.82 |
| 9:y7:9:ALA:CB | 9:y7:44:ILE:CD1 | 2.58 | 0.82 |
| 2:N8:60:TYR:CB | 2:N8:67:THR:HG23 | 2.10 | 0.82 |
| 4:M9:36:TYR:O | 12:B9:201:CYC:HMA1 | 1.79 | 0.82 |
| 4:M9:58:TYR:CE2 | 11:a9:496:ARG:NH1 | 2.47 | 0.82 |
| 2:O9:34:ALA:HB3 | 3:P9:31:VAL:HG11 | 1.59 | 0.82 |
| 2:K9:17:ARG:NH1 | 2:K9:17:ARG:HB3 | 1.95 | 0.82 |
| 11:aA:107:ARG:CG | 11:aA:108:PRO:CD | 2.52 | 0.82 |
| 4:M1:190:ARG:NH1 | 4:M1:202:SER:OG | 2.11 | 0.82 |
| 2:AA:25:GLN:CG | 2:KA:33:ARG:HG2 | 2.08 | 0.82 |
| 2:AA:60:TYR:CB | 2:AA:67:THR:HG23 | 2.09 | 0.82 |
| 3:BA:26:GLN:O | 3:BA:30:LEU:HD12 | 1.80 | 0.82 |
| 2:IA:98:VAL:HG21 | 3:JA:19:LEU:HD11 | 1.60 | 0.82 |
| 2:KA:17:ARG:HB3 | 2:KA:17:ARG:NH1 | 1.95 | 0.82 |
| 2:G3:107:ASP:HA | 3:L3:77:ARG:NE | 1.94 | 0.82 |
| 3:J2:108:ARG:NH2 | 6:M2:155:ASN:CB | 2.42 | 0.82 |
| 12:B4:202:CYC:HMA3 | 4:M4:58:TYR:HB2 | 1.60 | 0.82 |
| 2:O3:60:TYR:CB | 2:O3:67:THR:HG23 | 2.10 | 0.82 |
| 3:O4:119:ALA:CB | 5:Z4:72:GLU:CB | 2.52 | 0.82 |
| 8:I5:25:ARG:HD3 | 8:I5:25:ARG:C | 2.05 | 0.82 |
| 8:Y5:9:VAL:HG13 | 10:k5:344:ARG:CZ | 2.07 | 0.82 |
| 1:b5:18:TYR:CZ | 10:k5:165:ARG:CA | 2.62 | 0.82 |
| 10:j5:1008:PHE:CD1 | 12:v7:201:CYC:HBB3 | 2.13 | 0.82 |
| 10:j5:1064:LYS:HD2 | 10:j5:1065:HIS:N | 1.95 | 0.82 |
| 10:k5:286:VAL:HG21 | 10:k5:324:LYS:O | 1.78 | 0.82 |
| 8:i7:101:VAL:HG11 | 8:i7:155:TYR:CZ | 2.13 | 0.82 |
| 8:c7:112:VAL:CG1 | 8:c7:113:LYS:N | 2.41 | 0.82 |
| 2:A8:60:TYR:CG | 2:A8:67:THR:HG23 | 2.13 | 0.82 |
| 8:u7:17:TYR:CZ | 1:v7:90:ARG:HA | 2.14 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 4:M8:214:GLY:HA3 | 5:Z8:28:HIS:CG | 2.13 | 0.82 |
| 2:E9:152:ALA:HB1 | 2:I9:21:ASN:HD21 | 1.42 | 0.82 |
| 3:H9:78:ARG:HG2 | 12:H9:202:CYC:HAD1 | 1.62 | 0.82 |
| 11:a9:360:ALA:HA | 11:a9:363:GLN:CD | 2.04 | 0.82 |
| 11:a9:377:VAL:HG11 | 11:a9:390:ALA:HB1 | 1.60 | 0.82 |
| 11:aA:643:LEU:CD1 | 11:aA:766:ASN:HB3 | 2.09 | 0.82 |
| 4:MA:29:PRO:CD | 11:aA:378:GLU:OE1 | 2.26 | 0.82 |
| 4:MA:159:CYS:HA | 3:VA:108:ARG:HG3 | 1.61 | 0.82 |
| 4:MA:160:THR:O | 3:VA:108:ARG:HG2 | 1.78 | 0.82 |
| 4:MA:263:PRO:C | 3:VA:119:ALA:CB | 2.53 | 0.82 |
| 2:QA:116:VAL:CG2 | 3:TA:80:ALA:N | 2.43 | 0.82 |
| 3:J3:77:ARG:HG2 | 2:K3:111:ALA:HB3 | 1.59 | 0.82 |
| 2:O3:60:TYR:CG | 2:O3:67:THR:HG23 | 2.13 | 0.82 |
| 4:M4:160:THR:CG2 | 4:M4:257:GLN:HB3 | 2.09 | 0.82 |
| 3:O4:115:GLU:OE2 | 5:Z4:69:GLU:OE2 | 1.98 | 0.82 |
| 8:A5:107:ILE:CG1 | 1:B5:13:ASP:OD2 | 2.27 | 0.82 |
| 8:e5:29:PHE:HZ | 8:e5:98:ALA:O | 1.62 | 0.82 |
| 10:j5:1008:PHE:HZ | 1:v7:87:TYR:HE2 | 0.87 | 0.82 |
| 10:j5:1049:PHE:CZ | 10:j5:1065:HIS:CE1 | 2.68 | 0.82 |
| 10:k5:238:ARG:HG3 | 10:k5:238:ARG:HH11 | 1.42 | 0.82 |
| 12:B8:202:CYC:HBB3 | 4:M8:61:ASN:HD22 | 1.43 | 0.82 |
| 8:o7:17:TYR:CZ | 1:p7:90:ARG:HA | 2.14 | 0.82 |
| 3:F8:91:ARG:NH2 | 11:a9:140:GLN:HE22 | 1.73 | 0.82 |
| 4:M8:230:GLN:HB3 | 12:M8:301:CYC:C4B | 2.06 | 0.82 |
| 2:N8:115:GLU:CD | 5:Z8:32:PRO:CG | 2.50 | 0.82 |
| 3:O8:104:VAL:CA | 5:Z8:61:LYS:NZ | 2.40 | 0.82 |
| 3:Q8:110:LEU:HB3 | 3:Q8:170:SER:OG | 1.80 | 0.82 |
| 3:L9:77:ARG:CZ | 11:a9:538:ARG:HH21 | 1.91 | 0.82 |
| 4:M9:29:PRO:CD | 11:a9:378:GLU:OE1 | 2.26 | 0.82 |
| 12:H9:202:CYC:OB | 11:a9:474:PHE:CE1 | 2.32 | 0.82 |
| 1:A:110:ASN:OD1 | 10:k5:462:TYR:CZ | 2.32 | 0.82 |
| 3:FA:150:ARG:HA | 3:F9:150:ARG:HG3 | 1.52 | 0.82 |
| 6:M2:65:VAL:HG12 | 1:h7:59:ALA:O | 1.78 | 0.82 |
| 3:F4:106:GLU:O | 4:M4:6:THR:C | 2.23 | 0.82 |
| 3:L4:63:GLN:O | 3:L4:65:ASP:O | 1.96 | 0.82 |
| 3:L4:68:ARG:CB | 11:aA:81:ASP:HA | 2.10 | 0.82 |
| 8:Q5:15:ALA:C | 1:R5:90:ARG:HD2 | 1.97 | 0.82 |
| 1:T5:83:ARG:NH1 | 10:j5:483:PHE:CE1 | 2.47 | 0.82 |
| 10:k5:1016:LEU:HD12 | 10:k5:1017:ARG:CA | 2.10 | 0.82 |
| 10:k5:1053:TYR:HB2 | 10:k5:1058:VAL:HG23 | 1.60 | 0.82 |
| 8:Q7:13:ALA:N | 9:z7:46:LYS:NZ | 2.24 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:H7:68:PRO:HB3 | 1:J7:14:VAL:C | 2.04 | 0.82 |
| 1:H7:136:VAL:CG1 | 11:aA:563:PHE:CE2 | 2.56 | 0.82 |
| 2:A8:34:ALA:HB3 | 3:B8:31:VAL:HG11 | 1.59 | 0.82 |
| 12:M8:302:CYC:HMD3 | 3:S8:77:ARG:CZ | 2.09 | 0.82 |
| 2:N8:34:ALA:HB3 | 3:O8:31:VAL:HG11 | 1.59 | 0.82 |
| 5:N9:1:MET:C | 5:N9:3:VAL:H | 1.86 | 0.82 |
| 2:I9:1:MET:CE | 2:I9:108:TYR:HE1 | 1.92 | 0.82 |
| 4:MA:58:TYR:CE2 | 11:aA:496:ARG:NH1 | 2.47 | 0.82 |
| 4:MA:205:ASP:OD2 | 5:NA:52:ARG:NH1 | 2.13 | 0.82 |
| 12:B4:202:CYC:CBB | 4:M4:61:ASN:CG | 2.53 | 0.82 |
| 8:M5:110:ILE:HD12 | 10:k5:533:LEU:HD12 | 1.61 | 0.82 |
| 8:G5:119:LEU:CD1 | 12:G5:201:CYC:C1A | 2.57 | 0.82 |
| 1:Z5:67:ARG:NH1 | 10:k5:705:THR:CB | 2.42 | 0.82 |
| 10:j5:951:MET:HE3 | 10:j5:951:MET:O | 1.79 | 0.82 |
| 10:j5:1008:PHE:CE1 | 12:v7:201:CYC:C4B | 2.63 | 0.82 |
| 10:k5:542:GLN:HE21 | 10:k5:560:VAL:HG12 | 1.42 | 0.82 |
| 10:k5:1077:ILE:C | 12:k5:1203:CYC:CBA | 2.39 | 0.82 |
| 1:R7:49:THR:HG21 | 8:C7:161:GLN:CG | 2.10 | 0.82 |
| 8:a7:10:ASN:ND2 | 8:o7:10:ASN:ND2 | 2.28 | 0.82 |
| 1:v7:62:TYR:HB3 | 11:aA:602:PRO:CD | 2.00 | 0.82 |
| 4:M8:148:LYS:HE3 | 4:M8:197:ASP:OD2 | 1.79 | 0.82 |
| 12:O8:201:CYC:CBA | 5:Z8:50:LEU:HD13 | 2.10 | 0.82 |
| 2:G1:111:ALA:HB3 | 3:L1:77:ARG:HE | 1.41 | 0.82 |
| 2:O1:60:TYR:CB | 2:O1:67:THR:HG23 | 2.10 | 0.82 |
| 3:J3:119:ALA:O | 11:a9:803:ASN:HB3 | 1.79 | 0.82 |
| 6:M2:57:GLU:CD | 8:i7:76:LYS:NZ | 2.37 | 0.82 |
| 3:B4:68:ARG:NH1 | 3:U4:68:ARG:NH2 | 2.25 | 0.82 |
| 1:N5:110:ASN:CG | 10:k5:692:LEU:HB3 | 2.04 | 0.82 |
| 1:d5:67:ARG:NH1 | 10:j5:705:THR:OG1 | 2.12 | 0.82 |
| 1:f5:5:ILE:HD12 | 10:j5:46:PHE:CZ | 2.15 | 0.82 |
| 10:j5:1153:VAL:HG21 | 1:v7:125:ALA:CB | 1.94 | 0.82 |
| 3:D1:68:ARG:NH1 | 3:X1:68:ARG:NH2 | 2.27 | 0.82 |
| 8:C7:9:VAL:HG22 | 1:D7:107:ARG:HH22 | 1.45 | 0.82 |
| 8:i7:25:ARG:NH2 | 8:s7:3:VAL:O | 2.13 | 0.82 |
| 8:o7:90:ARG:CD | 1:p7:18:TYR:CE1 | 2.60 | 0.82 |
| 4:M9:39:SER:HB3 | 3:B9:111:ASN:O | 1.79 | 0.82 |
| 4:M1:113:ILE:HD11 | 4:M1:143:VAL:CG1 | 2.04 | 0.82 |
| 3:L2:75:PRO:CG | 3:L2:78:ARG:CB | 2.52 | 0.82 |
| 3:B1:111:ASN:O | 4:M1:6:THR:N | 2.13 | 0.82 |
| 4:M4:273:ILE:HD12 | 2:X4:108:TYR:OH | 1.78 | 0.82 |
| 2:P4:12:ALA:CB | 3:Q4:95:TYR:OH | 2.28 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:A5:103:PRO:HA | 10:k5:557:VAL:CG2 | 2.09 | 0.82 |
| 1:T5:53:LYS:HZ2 | 8:U5:120:GLN:HG3 | 1.44 | 0.82 |
| 8:U5:29:PHE:HE1 | 8:U5:99:GLY:CA | 1.93 | 0.82 |
| 10:j5:741:GLN:C | 1:J7:77:ARG:HH21 | 1.88 | 0.82 |
| 10:j5:930:LEU:O | 1:J7:33:THR:HG21 | 1.79 | 0.82 |
| 10:k5:931:VAL:CG1 | 1:D7:29:ALA:HB1 | 2.07 | 0.82 |
| 10:k5:1015:TYR:C | 10:k5:1017:ARG:HG2 | 2.02 | 0.82 |
| 3:F6:78:ARG:CD | 12:F6:201:CYC:CGD | 2.46 | 0.82 |
| 8:Q7:13:ALA:HA | 9:z7:46:LYS:CE | 2.09 | 0.82 |
| 8:a7:63:PRO:CD | 11:a9:336:ILE:HG23 | 2.00 | 0.82 |
| 3:B8:120:LEU:CD1 | 4:M8:53:LEU:CB | 2.48 | 0.82 |
| 12:B8:202:CYC:CBB | 4:M8:61:ASN:CG | 2.53 | 0.82 |
| 8:o7:27:LYS:HE2 | 1:p7:35:ALA:CB | 1.95 | 0.82 |
| 8:o7:80:LEU:HD12 | 12:o7:201:CYC:CAD | 2.10 | 0.82 |
| 4:M8:91:VAL:HA | 2:P8:15:GLN:HA | 1.60 | 0.82 |
| 4:M9:273:ILE:CD1 | 3:V9:75:PRO:CG | 2.57 | 0.82 |
| 5:N9:54:LEU:HB2 | 12:T9:301:CYC:O2A | 1.80 | 0.82 |
| 11:a9:308:LEU:HD21 | 11:a9:315:LEU:CD1 | 2.09 | 0.82 |
| 11:aA:360:ALA:HA | 11:aA:363:GLN:CD | 2.04 | 0.82 |
| 4:MA:134:ASN:ND2 | 5:NA:1:MET:H1 | 1.77 | 0.81 |
| 3:B1:84:ARG:CD | 11:aA:680:SER:OG | 2.27 | 0.81 |
| 10:j5:931:VAL:HG13 | 1:J7:29:ALA:HB3 | 1.62 | 0.81 |
| 10:j5:1008:PHE:CE1 | 1:v7:87:TYR:OH | 2.33 | 0.81 |
| 10:k5:1054:SER:HA | 1:l7:107:ARG:CA | 2.10 | 0.81 |
| 10:k5:1064:LYS:HD2 | 10:k5:1065:HIS:N | 1.95 | 0.81 |
| 8:U7:29:PHE:HE1 | 8:U7:99:GLY:CA | 1.93 | 0.81 |
| 8:a7:29:PHE:HE1 | 8:a7:99:GLY:CA | 1.93 | 0.81 |
| 8:c7:39:ILE:HD12 | 8:c7:148:GLU:HG2 | 1.59 | 0.81 |
| 2:A8:60:TYR:CB | 2:A8:67:THR:HG23 | 2.10 | 0.81 |
| 12:B8:202:CYC:HMA1 | 4:M8:58:TYR:HB2 | 1.62 | 0.81 |
| 2:X8:68:GLN:HG3 | 3:T9:25:ASN:OD1 | 1.79 | 0.81 |
| 5:Z8:27:ALA:CB | 12:Z8:301:CYC:HAB1 | 2.09 | 0.81 |
| 11:aA:371:VAL:HG13 | 11:aA:507:PHE:HB2 | 1.60 | 0.81 |
| 11:aA:746:TYR:CB | 2:K1:14:SER:CB | 2.55 | 0.81 |
| 4:M1:192:GLN:HG2 | 3:Z1:84:ARG:HG3 | 1.60 | 0.81 |
| 12:BA:201:CYC:HMA1 | 4:MA:36:TYR:O | 1.79 | 0.81 |
| 2:IA:16:GLY:HA2 | 3:JA:91:ARG:HH11 | 1.43 | 0.81 |
| 3:H3:62:GLU:HB3 | 8:k7:49:ARG:NH1 | 1.94 | 0.81 |
| 6:M2:45:ILE:CD1 | 8:i7:78:THR:HG22 | 2.10 | 0.81 |
| 3:B3:111:ASN:O | 4:M3:6:THR:N | 2.13 | 0.81 |
| 4:M3:81:ASP:N | 3:X3:111:ASN:ND2 | 2.26 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:N3:31:TRP:HD1 | 2:S3:16:GLY:CA | 1.89 | 0.81 |
| 3:H4:119:ALA:CA | 11:aA:266:ASN:HB2 | 2.09 | 0.81 |
| 3:L4:68:ARG:O | 3:L4:69:PRO:O | 1.98 | 0.81 |
| 4:M4:100:SER:CB | 3:Q4:1:MET:CE | 2.50 | 0.81 |
| 4:M4:144:ARG:NH1 | 5:Z4:59:ARG:HH22 | 1.78 | 0.81 |
| 1:Z5:64:ASP:CB | 10:k5:705:THR:HG23 | 2.01 | 0.81 |
| 8:a5:29:PHE:HE1 | 8:a5:99:GLY:CA | 1.93 | 0.81 |
| 10:k5:931:VAL:CG2 | 1:D7:30:TYR:CA | 2.57 | 0.81 |
| 1:d7:87:TYR:CE2 | 9:x7:38:PHE:CE1 | 2.67 | 0.81 |
| 8:s7:29:PHE:HE1 | 8:s7:99:GLY:CA | 1.93 | 0.81 |
| 8:u7:23:LEU:HD23 | 1:v7:38:VAL:HG22 | 1.59 | 0.81 |
| 9:x7:9:ALA:CB | 9:x7:44:ILE:CD1 | 2.58 | 0.81 |
| 2:X8:69:PRO:HB3 | 2:S9:39:GLU:HA | 1.62 | 0.81 |
| 3:H8:84:ARG:HD2 | 11:a9:131:TYR:CE2 | 2.14 | 0.81 |
| 4:M9:205:ASP:OD2 | 5:N9:52:ARG:NH1 | 2.13 | 0.81 |
| 2:O9:60:TYR:CB | 2:O9:67:THR:HG23 | 2.09 | 0.81 |
| 5:Z8:1:MET:C | 5:Z8:3:VAL:H | 1.86 | 0.81 |
| 2:G1:107:ASP:HA | 3:L1:77:ARG:NE | 1.94 | 0.81 |
| 3:FA:151:GLY:C | 3:F9:150:ARG:HH21 | 1.77 | 0.81 |
| 12:QA:201:CYC:HMA1 | 3:TA:79:MET:HG2 | 1.61 | 0.81 |
| 2:A1:60:TYR:CB | 2:A1:67:THR:HG23 | 2.10 | 0.81 |
| 3:B3:84:ARG:CD | 11:a9:680:SER:OG | 2.29 | 0.81 |
| 3:D3:68:ARG:NH1 | 3:X3:68:ARG:NH2 | 2.27 | 0.81 |
| 3:F3:111:ASN:O | 4:M3:39:SER:HB3 | 1.79 | 0.81 |
| 3:B4:85:ASP:CA | 12:B4:202:CYC:CAC | 2.42 | 0.81 |
| 3:L3:84:ARG:HD2 | 11:a9:739:ASP:HA | 1.62 | 0.81 |
| 4:M4:217:VAL:HG21 | 5:Z4:30:PRO:HA | 1.62 | 0.81 |
| 2:N4:112:GLY:HA3 | 5:Z4:34:LEU:CB | 2.10 | 0.81 |
| 3:Q4:85:ASP:HB2 | 12:Z4:301:CYC:CBC | 2.10 | 0.81 |
| 5:Z4:44:TYR:HE2 | 5:Z4:46:THR:OG1 | 1.58 | 0.81 |
| 8:G5:61:ILE:HG21 | 8:o7:68:PRO:CG | 2.10 | 0.81 |
| 8:I5:29:PHE:HE1 | 8:I5:99:GLY:CA | 1.93 | 0.81 |
| 1:J5:87:TYR:CE2 | 9:i5:38:PHE:CE2 | 2.62 | 0.81 |
| 12:d5:201:CYC:O2A | 10:j5:379:PHE:CD2 | 2.33 | 0.81 |
| 12:P5:201:CYC:CBB | 10:k5:623:VAL:HG21 | 2.10 | 0.81 |
| 8:Y5:9:VAL:HG13 | 10:k5:344:ARG:NH1 | 1.95 | 0.81 |
| 1:b5:38:VAL:CG1 | 10:k5:40:VAL:HG12 | 2.10 | 0.81 |
| 1:b5:38:VAL:HG11 | 10:k5:40:VAL:CG1 | 2.08 | 0.81 |
| 6:M6:65:VAL:CG1 | 1:b7:59:ALA:O | 2.28 | 0.81 |
| 10:k5:1024:LYS:HD3 | 10:k5:1038:ARG:HH12 | 1.44 | 0.81 |
| 10:k5:1025:LEU:HD23 | 10:k5:1030:ILE:HG21 | 1.62 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:F6:126:SER:C | 12:F6:201:CYC:CMC | 2.54 | 0.81 |
| 8:I7:9:VAL:HG22 | 1:J7:107:ARG:HH22 | 1.44 | 0.81 |
| 8:i7:112:VAL:CG1 | 8:i7:113:LYS:N | 2.41 | 0.81 |
| 8:c7:15:ALA:CB | 1:d7:90:ARG:HH21 | 1.89 | 0.81 |
| 2:A8:63:PHE:CB | 2:A8:66:LEU:CD1 | 2.55 | 0.81 |
| 3:F8:115:GLU:C | 4:M8:3:VAL:CG1 | 2.53 | 0.81 |
| 3:L8:69:PRO:O | 3:L8:71:GLY:N | 2.13 | 0.81 |
| 4:M8:130:SER:HB3 | 12:M8:302:CYC:HAA1 | 1.63 | 0.81 |
| 3:Q8:117:TYR:CD1 | 3:Q8:120:LEU:HD21 | 2.14 | 0.81 |
| 4:M9:274:VAL:HG21 | 2:W9:111:ALA:CB | 2.10 | 0.81 |
| 5:N9:6:GLY:C | 3:R9:107:ASP:O | 2.24 | 0.81 |
| 3:Y8:113:LEU:HD22 | 3:Y8:171:ILE:HG12 | 1.61 | 0.81 |
| 3:F9:153:CYS:CB | 12:F9:303:CYC:CAC | 2.31 | 0.81 |
| 3:H9:113:LEU:CD1 | 12:H9:202:CYC:HMB3 | 2.05 | 0.81 |
| 11:a9:91:THR:CG2 | 11:a9:96:THR:HA | 2.08 | 0.81 |
| 11:a9:312:ASP:CA | 11:a9:315:LEU:CA | 2.58 | 0.81 |
| 11:a9:714:ARG:HD3 | 11:a9:809:ARG:HA | 1.62 | 0.81 |
| 11:aA:48:LEU:O | 11:aA:48:LEU:HD12 | 1.80 | 0.81 |
| 11:aA:708:HIS:HA | 3:L1:108:ARG:NE | 1.94 | 0.81 |
| 11:aA:714:ARG:HD3 | 11:aA:809:ARG:HA | 1.62 | 0.81 |
| 4:MA:188:LEU:O | 4:MA:188:LEU:HD12 | 1.80 | 0.81 |
| 2:OA:60:TYR:CB | 2:OA:67:THR:HG23 | 2.09 | 0.81 |
| 3:J3:111:ASN:ND2 | 11:a9:631:GLY:C | 2.36 | 0.81 |
| 3:J3:121:GLY:HA2 | 11:a9:804:ARG:NH2 | 1.96 | 0.81 |
| 6:M2:53:LEU:HD23 | 8:i7:80:LEU:HD21 | 1.58 | 0.81 |
| 1:N5:113:LYS:HZ2 | 1:Z5:155:TYR:HE2 | 1.29 | 0.81 |
| 3:Y4:80:ALA:O | 3:Y4:84:ARG:HG3 | 1.80 | 0.81 |
| 8:A5:122:PRO:CD | 12:A5:201:CYC:OC | 2.27 | 0.81 |
| 1:b5:18:TYR:OH | 10:k5:165:ARG:HB2 | 1.80 | 0.81 |
| 3:L6:77:ARG:HH21 | 6:M6:70:GLU:HG2 | 1.44 | 0.81 |
| 6:M6:283:VAL:HG11 | 8:Y7:75:GLU:HB3 | 1.62 | 0.81 |
| 10:j5:1015:TYR:C | 10:j5:1017:ARG:HG2 | 2.02 | 0.81 |
| 10:j5:1147:TYR:CE1 | 11:aA:35:ARG:HB3 | 2.16 | 0.81 |
| 10:k5:385:PRO:O | 10:k5:387:VAL:N | 2.14 | 0.81 |
| 10:k5:386:ILE:CG2 | 10:k5:395:SER:C | 2.52 | 0.81 |
| 10:k5:1043:GLU:HG2 | 8:Y7:14:GLU:OE2 | 1.81 | 0.81 |
| 10:k5:1153:VAL:HG22 | 1:p7:65:LEU:CD1 | 2.10 | 0.81 |
| 8:i7:47:ARG:NE | 1:j7:18:TYR:CD2 | 2.49 | 0.81 |
| 2:E1:114:ARG:NH1 | 11:aA:671:GLU:OE2 | 2.13 | 0.81 |
| 12:B8:202:CYC:HMA1 | 4:M8:58:TYR:CA | 2.10 | 0.81 |
| 1:l7:68:PRO:HB3 | 1:n7:14:VAL:C | 2.04 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:q7:76:LYS:HZ1 | 11:aA:605:PRO:HB3 | 0.99 | 0.81 |
| 2:X8:68:GLN:HG3 | 3:T9:24:LEU:HB3 | 1.62 | 0.81 |
| 3:L8:86:MET:HG3 | 12:a9:901:CYC:HBC1 | 1.60 | 0.81 |
| 4:M8:127:SER:N | 12:M8:302:CYC:CMA | 2.22 | 0.81 |
| 3:Q8:80:ALA:HB1 | 5:Z8:33:GLY:HA3 | 1.63 | 0.81 |
| 3:L9:44:ILE:HG23 | 3:L9:90:LEU:HD21 | 1.60 | 0.81 |
| 5:Z8:22:LEU:HD13 | 5:Z8:26:LEU:HD22 | 1.63 | 0.81 |
| 2:A9:60:TYR:CB | 2:A9:67:THR:HG23 | 2.09 | 0.81 |
| 11:a9:48:LEU:HD12 | 11:a9:48:LEU:O | 1.80 | 0.81 |
| 11:a9:448:ASN:OD1 | 11:a9:474:PHE:HE1 | 1.60 | 0.81 |
| 4:M1:188:LEU:O | 4:M1:188:LEU:HD12 | 1.80 | 0.81 |
| 2:A2:63:PHE:CB | 2:A2:66:LEU:CD1 | 2.55 | 0.81 |
| 2:KA:24:LEU:HB3 | 12:LA:201:CYC:CAB | 2.09 | 0.81 |
| 4:MA:160:THR:CG2 | 4:MA:257:GLN:HB3 | 2.09 | 0.81 |
| 2:QA:116:VAL:HA | 3:TA:83:LEU:HD12 | 1.62 | 0.81 |
| 2:QA:116:VAL:HG13 | 3:TA:79:MET:HG3 | 1.62 | 0.81 |
| 3:P1:115:GLU:HB3 | 5:N1:3:VAL:HG11 | 1.61 | 0.81 |
| 12:B4:202:CYC:CBB | 4:M4:61:ASN:ND2 | 2.44 | 0.81 |
| 3:B1:82:CYS:HA | 12:B1:202:CYC:CHD | 2.10 | 0.81 |
| 3:U4:120:LEU:CG | 4:M4:254:LEU:HD21 | 2.10 | 0.81 |
| 4:M4:95:ALA:HA | 5:Z4:38:GLU:HG3 | 1.63 | 0.81 |
| 12:H5:201:CYC:CBA | 9:i5:26:THR:CG2 | 2.57 | 0.81 |
| 10:j5:283:ARG:CB | 10:j5:284:PRO:HD2 | 2.10 | 0.81 |
| 10:j5:1018:LEU:HD12 | 10:j5:1035:PHE:HZ | 1.36 | 0.81 |
| 10:k5:1049:PHE:CZ | 10:k5:1065:HIS:CE1 | 2.68 | 0.81 |
| 10:k5:1147:TYR:CE1 | 11:a9:35:ARG:HB3 | 2.16 | 0.81 |
| 8:O7:44:THR:HG1 | 1:P7:18:TYR:HD2 | 1.25 | 0.81 |
| 8:g7:63:PRO:CD | 11:aA:336:ILE:HG21 | 1.81 | 0.81 |
| 1:Z7:67:ARG:HD3 | 11:a9:311:LEU:HD22 | 0.81 | 0.81 |
| 8:a7:90:ARG:NH1 | 1:b7:16:GLY:HA2 | 1.96 | 0.81 |
| 8:c7:8:ILE:HG21 | 1:d7:94:TYR:HB3 | 1.63 | 0.81 |
| 8:c7:39:ILE:HD11 | 8:c7:148:GLU:HG2 | 1.60 | 0.81 |
| 8:c7:49:ARG:CZ | 8:c7:140:LEU:HD21 | 2.11 | 0.81 |
| 8:u7:23:LEU:HB3 | 1:v7:38:VAL:HG11 | 0.82 | 0.81 |
| 8:u7:80:LEU:HD12 | 12:u7:201:CYC:CAD | 2.10 | 0.81 |
| 3:U8:120:LEU:HD21 | 12:U8:201:CYC:HBD2 | 1.63 | 0.81 |
| 5:Z8:38:GLU:N | 12:Z8:301:CYC:HMB2 | 1.95 | 0.81 |
| 11:a9:643:LEU:HD11 | 11:a9:689:VAL:CG2 | 2.10 | 0.81 |
| 11:aA:348:GLN:H | 11:aA:348:GLN:NE2 | 1.76 | 0.81 |
| 11:aA:377:VAL:HG11 | 11:aA:390:ALA:HB1 | 1.60 | 0.81 |
| 3:FA:145:PRO:HG3 | 12:F9:302:CYC:HMC2 | 1.62 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:FA:151:GLY:H | 3:F9:150:ARG:NH2 | 1.76 | 0.81 |
| 5:NA:61:LYS:HZ3 | 12:TA:301:CYC:CBB | 1.88 | 0.81 |
| 2:A3:60:TYR:CB | 2:A3:67:THR:HG23 | 2.09 | 0.81 |
| 3:B1:88:ILE:HG22 | 12:B1:202:CYC:HMB1 | 1.61 | 0.81 |
| 8:M5:68:PRO:HB3 | 8:e5:59:PHE:CB | 2.11 | 0.81 |
| 8:G5:6:LYS:HZ2 | 8:S5:21:GLY:N | 1.76 | 0.81 |
| 8:S5:68:PRO:CG | 8:a5:59:PHE:HB3 | 2.11 | 0.81 |
| 10:j5:277:ILE:HG23 | 10:j5:284:PRO:CA | 2.11 | 0.81 |
| 10:j5:931:VAL:O | 1:J7:29:ALA:HB1 | 1.80 | 0.81 |
| 10:k5:148:TYR:O | 10:k5:152:ARG:CG | 2.28 | 0.81 |
| 10:k5:1016:LEU:HB2 | 10:k5:1044:ASN:ND2 | 1.94 | 0.81 |
| 8:O7:25:ARG:NH2 | 8:E7:25:ARG:HB2 | 1.93 | 0.81 |
| 1:D7:76:ARG:HD3 | 8:E7:110:ILE:HD11 | 1.62 | 0.81 |
| 8:g7:25:ARG:HH21 | 8:u7:25:ARG:NE | 1.78 | 0.81 |
| 8:U7:9:VAL:HG22 | 1:V7:107:ARG:HH22 | 1.44 | 0.81 |
| 8:c7:11:ALA:HB3 | 1:d7:94:TYR:CZ | 2.15 | 0.81 |
| 4:M8:235:PHE:HB2 | 12:M8:301:CYC:CAA | 2.11 | 0.81 |
| 5:N9:7:ASP:H | 3:R9:108:ARG:HA | 1.46 | 0.81 |
| 3:J9:88:ILE:CD1 | 11:a9:512:TYR:CD1 | 2.62 | 0.81 |
| 11:a9:643:LEU:CD1 | 11:a9:766:ASN:HB3 | 2.11 | 0.81 |
| 11:aA:275:THR:HA | 11:aA:278:LEU:HD11 | 0.86 | 0.81 |
| 5:N1:1:MET:HA | 5:N1:1:MET:CE | 2.10 | 0.81 |
| 12:B4:202:CYC:HMA1 | 4:M4:58:TYR:CA | 2.10 | 0.81 |
| 3:L4:69:PRO:O | 3:L4:71:GLY:N | 2.13 | 0.81 |
| 8:G5:122:PRO:CD | 12:G5:201:CYC:OC | 2.27 | 0.81 |
| 8:U5:75:GLU:HG3 | 6:M6:36:ILE:CG1 | 2.10 | 0.81 |
| 8:U5:83:ARG:C | 6:M6:26:PHE:HE1 | 1.88 | 0.81 |
| 6:M6:117:MET:CE | 3:H6:77:ARG:HH12 | 1.89 | 0.81 |
| 10:k5:388:ARG:CD | 10:k5:393:MET:H | 1.93 | 0.81 |
| 10:k5:990:ARG:HE | 10:k5:1026:LYS:HZ3 | 1.23 | 0.81 |
| 8:I7:25:ARG:NH2 | 8:W7:25:ARG:NE | 2.28 | 0.81 |
| 8:c7:16:ARG:HA | 1:d7:90:ARG:HD3 | 1.60 | 0.81 |
| 3:B8:81:ALA:CA | 12:B8:202:CYC:CMD | 2.56 | 0.81 |
| 9:y7:4:TYR:HB2 | 9:y7:58:THR:HG1 | 1.46 | 0.81 |
| 4:M8:87:ILE:HD12 | 3:Y8:77:ARG:HG3 | 1.49 | 0.81 |
| 4:M8:113:ILE:HD11 | 4:M8:143:VAL:CG1 | 2.04 | 0.81 |
| 5:N9:22:LEU:HD13 | 5:N9:26:LEU:HD22 | 1.63 | 0.81 |
| 3:H9:72:ASN:OD1 | 12:H9:202:CYC:C2D | 2.29 | 0.81 |
| 3:J9:108:ARG:O | 11:a9:517:ALA:CA | 2.29 | 0.81 |
| 11:a9:31:SER:HG | 11:a9:34:ILE:CB | 1.86 | 0.81 |
| 11:a9:330:ASP:OD1 | 11:a9:330:ASP:N | 2.13 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 11:a9:636:ALA:O | 11:a9:774:PHE:CD2 | 2.33 | 0.81 |
| 11:aA:803:ASN:CB | 3:J1:119:ALA:O | 2.29 | 0.81 |
| 2:KA:18:PHE:CE2 | 3:LA:48:ALA:HB2 | 2.16 | 0.81 |
| 5:NA:7:ASP:H | 3:RA:108:ARG:HA | 1.46 | 0.81 |
| 2:QA:120:PHE:HE2 | 3:TA:79:MET:SD | 2.03 | 0.81 |
| 3:R1:116:THR:HA | 5:N1:70:ILE:HG21 | 1.62 | 0.81 |
| 2:A4:60:TYR:CB | 2:A4:67:THR:HG23 | 2.10 | 0.81 |
| 3:S4:82:CYS:SG | 12:S4:202:CYC:HAC2 | 2.19 | 0.81 |
| 3:U4:108:ARG:O | 4:M4:246:ALA:HB1 | 1.80 | 0.81 |
| 3:F4:84:ARG:HD3 | 11:aA:139:ILE:HG21 | 1.63 | 0.81 |
| 2:N4:60:TYR:CB | 2:N4:67:THR:HG23 | 2.10 | 0.81 |
| 8:K5:17:TYR:HB3 | 1:L5:45:SER:HB3 | 1.62 | 0.81 |
| 8:C5:25:ARG:HD3 | 8:C5:25:ARG:C | 2.05 | 0.81 |
| 10:j5:990:ARG:NE | 10:j5:1026:LYS:NZ | 2.28 | 0.81 |
| 10:j5:1008:PHE:CZ | 1:v7:87:TYR:OH | 2.32 | 0.81 |
| 10:k5:388:ARG:HG2 | 10:k5:394:PRO:HG3 | 1.63 | 0.81 |
| 8:C7:29:PHE:HE1 | 8:C7:99:GLY:CA | 1.93 | 0.81 |
| 4:M8:188:LEU:HD12 | 4:M8:188:LEU:O | 1.80 | 0.81 |
| 3:Q8:120:LEU:CD1 | 3:Q8:122:THR:CA | 2.46 | 0.81 |
| 3:V9:108:ARG:HB3 | 3:V9:108:ARG:CZ | 2.09 | 0.81 |
| 11:a9:594:ARG:HG3 | 11:a9:594:ARG:HH11 | 1.44 | 0.81 |
| 11:aA:644:ARG:O | 11:aA:645:PRO:C | 2.22 | 0.81 |
| 11:aA:668:TYR:HD1 | 3:J1:84:ARG:HD3 | 1.45 | 0.81 |
| 11:aA:804:ARG:NH2 | 3:J1:121:GLY:HA2 | 1.95 | 0.81 |
| 3:JA:114:LYS:HD3 | 8:S7:60:GLN:HE22 | 1.44 | 0.81 |
| 3:J3:14:LEU:HD13 | 11:a9:621:THR:HG21 | 0.83 | 0.81 |
| 3:J3:80:ALA:O | 3:J3:84:ARG:HG3 | 1.80 | 0.81 |
| 3:D3:68:ARG:NH2 | 3:X3:68:ARG:CZ | 2.44 | 0.81 |
| 3:H4:111:ASN:CG | 11:aA:291:TYR:CZ | 2.58 | 0.81 |
| 4:M4:104:ALA:C | 2:P4:14:SER:CB | 2.53 | 0.81 |
| 3:Q4:124:THR:CG2 | 3:Q4:171:ILE:O | 2.29 | 0.81 |
| 8:O5:29:PHE:HE1 | 8:O5:99:GLY:CA | 1.93 | 0.81 |
| 5:Z4:1:MET:C | 5:Z4:3:VAL:H | 1.86 | 0.81 |
| 1:H5:76:ARG:HD2 | 9:i5:14:LEU:O | 1.81 | 0.81 |
| 1:V5:87:TYR:HE2 | 10:j5:649:PHE:HZ | 1.25 | 0.81 |
| 10:j5:1053:TYR:HB2 | 10:j5:1058:VAL:HG23 | 1.60 | 0.81 |
| 10:k5:1049:PHE:CZ | 10:k5:1065:HIS:HE1 | 1.99 | 0.81 |
| 8:a7:33:GLY:HA3 | 1:b7:31:PHE:CZ | 2.16 | 0.81 |
| 8:o7:58:LEU:HD12 | 8:o7:58:LEU:O | 1.79 | 0.81 |
| 2:X8:108:TYR:OH | 4:M8:273:ILE:HD12 | 1.81 | 0.81 |
| 4:M9:81:ASP:H | 3:Z9:111:ASN:HD22 | 1.28 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M9:188:LEU:HD12 | 4:M9:188:LEU:O | 1.80 | 0.81 |
| 5:N9:22:LEU:HD22 | 5:N9:26:LEU:HD13 | 1.59 | 0.81 |
| 11:aA:75:ALA:CB | 11:aA:81:ASP:OD2 | 2.29 | 0.81 |
| 11:aA:581:ARG:HH11 | 11:aA:581:ARG:HG3 | 1.43 | 0.81 |
| 11:aA:666:ASN:HB2 | 12:aA:901:CYC:CMA | 2.11 | 0.81 |
| 12:HA:202:CYC:NB | 11:aA:474:PHE:CE2 | 2.49 | 0.81 |
| 3:JA:108:ARG:HA | 11:aA:517:ALA:HA | 1.63 | 0.81 |
| 4:MA:274:VAL:HG21 | 2:WA:111:ALA:CB | 2.10 | 0.81 |
| 2:QA:33:ARG:HG2 | 2:UA:25:GLN:CG | 2.11 | 0.81 |
| 6:M2:28:ASN:CB | 8:O5:80:LEU:HG | 2.07 | 0.81 |
| 3:O4:95:TYR:HD2 | 3:O4:108:ARG:NH2 | 1.75 | 0.81 |
| 8:O5:29:PHE:HZ | 8:O5:98:ALA:O | 1.62 | 0.81 |
| 8:U5:35:ARG:NH2 | 8:U5:144:ASP:HB3 | 1.96 | 0.81 |
| 8:a5:29:PHE:HZ | 8:a5:98:ALA:O | 1.62 | 0.81 |
| 10:j5:190:LEU:C | 10:j5:194:CYS:HG | 1.87 | 0.81 |
| 10:j5:221:LYS:HZ3 | 10:j5:221:LYS:HB3 | 1.44 | 0.81 |
| 10:j5:385:PRO:O | 10:j5:387:VAL:N | 2.13 | 0.81 |
| 10:j5:388:ARG:HG2 | 10:j5:394:PRO:HG3 | 1.63 | 0.81 |
| 8:O7:9:VAL:HG22 | 1:P7:107:ARG:HH22 | 1.44 | 0.81 |
| 8:i7:94:TYR:CZ | 1:j7:9:ILE:CG2 | 2.58 | 0.81 |
| 8:W7:12:ASP:O | 9:w7:46:LYS:NZ | 2.12 | 0.81 |
| 8:c7:15:ALA:HB1 | 1:d7:90:ARG:HH21 | 1.44 | 0.81 |
| 8:o7:29:PHE:CZ | 1:p7:31:PHE:HZ | 1.99 | 0.81 |
| 8:u7:58:LEU:O | 8:u7:58:LEU:HD12 | 1.79 | 0.81 |
| 4:M9:185:ALA:HA | 12:V9:201:CYC:CBA | 2.11 | 0.81 |
| 4:M9:263:PRO:C | 3:V9:119:ALA:CB | 2.53 | 0.81 |
| 2:EA:2:LYS:HZ3 | 2:IA:17:ARG:NH1 | 1.59 | 0.80 |
| 3:FA:150:ARG:CG | 3:F9:150:ARG:HA | 2.11 | 0.80 |
| 4:MA:81:ASP:H | 3:ZA:111:ASN:HD22 | 1.28 | 0.80 |
| 5:NA:22:LEU:HD13 | 5:NA:26:LEU:HD22 | 1.63 | 0.80 |
| 3:TA:32:LYS:HZ1 | 2:X4:57:GLN:HA | 0.66 | 0.80 |
| 3:O4:107:ASP:OD2 | 5:Z4:66:ARG:HD2 | 1.80 | 0.80 |
| 8:E5:161:GLN:NE2 | 1:P5:49:THR:HG22 | 1.96 | 0.80 |
| 1:R5:107:ARG:HB3 | 10:k5:520:ARG:HH22 | 1.47 | 0.80 |
| 1:T5:14:VAL:O | 1:X5:68:PRO:HB3 | 1.81 | 0.80 |
| 6:M6:273:PHE:CE1 | 1:d7:128:GLY:HA2 | 2.16 | 0.80 |
| 10:k5:277:ILE:HG23 | 10:k5:284:PRO:CA | 2.11 | 0.80 |
| 10:k5:990:ARG:NE | 10:k5:1026:LYS:NZ | 2.28 | 0.80 |
| 8:O7:29:PHE:HE1 | 8:O7:99:GLY:CA | 1.93 | 0.80 |
| 1:B7:136:VAL:HA | 11:a9:563:PHE:CZ | 2.15 | 0.80 |
| 8:I7:29:PHE:HE1 | 8:I7:99:GLY:CA | 1.93 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:g7:22:GLU:HG2 | 8:g7:25:ARG:NH1 | 1.94 | 0.80 |
| 8:c7:50:ILE:CD1 | 8:c7:137:ALA:HB2 | 2.11 | 0.80 |
| 8:o7:18:LEU:CD1 | 1:p7:97:LEU:CD1 | 2.58 | 0.80 |
| 3:H8:119:ALA:CA | 11:a9:266:ASN:HB2 | 2.09 | 0.80 |
| 2:I8:112:GLY:CA | 11:a9:133:LEU:HD21 | 2.10 | 0.80 |
| 4:M8:160:THR:CG2 | 4:M8:257:GLN:HB3 | 2.09 | 0.80 |
| 3:Q8:84:ARG:NH1 | 5:Z8:29:HIS:CD2 | 2.48 | 0.80 |
| 12:L9:202:CYC:O2A | 11:a9:404:TYR:CB | 2.29 | 0.80 |
| 5:Z8:41:GLN:CB | 12:Z8:301:CYC:C4B | 2.55 | 0.80 |
| 3:X1:80:ALA:O | 3:X1:84:ARG:HG3 | 1.81 | 0.80 |
| 3:BA:27:LEU:HA | 3:BA:30:LEU:HD13 | 1.61 | 0.80 |
| 5:NA:6:GLY:C | 3:RA:107:ASP:O | 2.24 | 0.80 |
| 3:B3:88:ILE:HG21 | 12:B3:202:CYC:HAB2 | 1.28 | 0.80 |
| 3:B3:88:ILE:HG23 | 12:B3:202:CYC:CAB | 1.97 | 0.80 |
| 2:E3:114:ARG:NH1 | 11:a9:671:GLU:OE2 | 2.14 | 0.80 |
| 4:M4:82:ILE:HD13 | 12:M4:301:CYC:O1D | 1.80 | 0.80 |
| 3:Q4:120:LEU:HD21 | 5:Z4:42:SER:HB2 | 0.82 | 0.80 |
| 12:B5:201:CYC:HBB2 | 9:z5:21:ARG:CA | 2.10 | 0.80 |
| 1:P5:87:TYR:HE2 | 10:k5:649:PHE:HZ | 1.26 | 0.80 |
| 1:T5:110:ASN:ND2 | 10:j5:692:LEU:O | 2.13 | 0.80 |
| 8:W5:4:LEU:CD2 | 8:W5:26:ILE:HD13 | 2.12 | 0.80 |
| 1:X5:63:SER:OG | 10:j5:706:PRO:CA | 2.24 | 0.80 |
| 9:z5:23:LEU:C | 9:z5:25:ASN:N | 2.30 | 0.80 |
| 10:j5:1119:LEU:HD21 | 1:t7:87:TYR:CE1 | 2.15 | 0.80 |
| 8:C7:29:PHE:HZ | 8:C7:98:ALA:O | 1.62 | 0.80 |
| 8:i7:50:ILE:CD1 | 8:i7:137:ALA:HB2 | 2.11 | 0.80 |
| 8:o7:4:LEU:CD2 | 8:o7:26:ILE:HD13 | 2.12 | 0.80 |
| 8:o7:23:LEU:HB3 | 1:p7:38:VAL:HG11 | 0.82 | 0.80 |
| 8:s7:35:ARG:NH2 | 8:s7:144:ASP:HB3 | 1.97 | 0.80 |
| 8:u7:17:TYR:CD2 | 1:v7:93:THR:CG2 | 2.64 | 0.80 |
| 2:X8:69:PRO:C | 2:S9:42:ARG:HD2 | 2.06 | 0.80 |
| 3:O8:108:ARG:N | 5:Z8:61:LYS:HD3 | 1.95 | 0.80 |
| 11:a9:348:GLN:H | 11:a9:348:GLN:NE2 | 1.76 | 0.80 |
| 12:JA:202:CYC:HB | 11:aA:512:TYR:CB | 1.82 | 0.80 |
| 4:MA:58:TYR:CZ | 11:aA:496:ARG:CZ | 2.64 | 0.80 |
| 3:B3:88:ILE:HG21 | 12:B3:202:CYC:CMB | 2.10 | 0.80 |
| 3:B4:107:ASP:O | 4:M4:61:ASN:O | 1.97 | 0.80 |
| 2:O3:63:PHE:CB | 2:O3:66:LEU:CD1 | 2.56 | 0.80 |
| 3:Q4:96:ALA:C | 3:Q4:98:LEU:H | 1.89 | 0.80 |
| 3:Y4:87:GLU:CG | 3:Y4:91:ARG:HH11 | 1.93 | 0.80 |
| 10:j5:1023:SER:CB | 12:f7:201:CYC:HMA2 | 2.10 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:j5:1025:LEU:HD23 | 10:j5:1030:ILE:HG21 | 1.62 | 0.80 |
| 10:k5:283:ARG:CB | 10:k5:284:PRO:HD2 | 2.10 | 0.80 |
| 2:A6:60:TYR:CB | 2:A6:67:THR:HG23 | 2.09 | 0.80 |
| 8:I7:35:ARG:NH2 | 8:I7:144:ASP:HB3 | 1.96 | 0.80 |
| 8:g7:35:ARG:NH2 | 8:g7:144:ASP:HB3 | 1.96 | 0.80 |
| 1:j7:77:ARG:CZ | 9:y7:63:ALA:HB3 | 2.12 | 0.80 |
| 1:Z7:10:ASN:ND2 | 9:x7:65:THR:O | 2.14 | 0.80 |
| 2:X8:57:GLN:HE22 | 3:T9:32:LYS:CD | 1.95 | 0.80 |
| 3:F9:36:LYS:HB3 | 3:F9:156:LEU:HD13 | 1.62 | 0.80 |
| 2:K9:15:GLN:CG | 11:a9:393:ARG:NH1 | 2.42 | 0.80 |
| 11:aA:312:ASP:CA | 11:aA:315:LEU:CA | 2.58 | 0.80 |
| 11:aA:348:GLN:HE21 | 11:aA:348:GLN:N | 1.78 | 0.80 |
| 4:M1:160:THR:CG2 | 4:M1:257:GLN:HB3 | 2.09 | 0.80 |
| 1:Z:158:SER:HB2 | 1:X5:11:ASN:ND2 | 1.92 | 0.80 |
| 3:LA:14:LEU:CG | 11:aA:358:PRO:HB2 | 2.12 | 0.80 |
| 5:NA:54:LEU:HB2 | 12:TA:301:CYC:O2A | 1.80 | 0.80 |
| 12:J3:202:CYC:CGA | 11:a9:667:THR:CG2 | 2.59 | 0.80 |
| 2:E4:15:GLN:CG | 11:aA:163:ASP:CB | 2.59 | 0.80 |
| 2:I4:112:GLY:CA | 11:aA:133:LEU:HD21 | 2.12 | 0.80 |
| 4:M4:104:ALA:O | 2:P4:14:SER:HB2 | 1.80 | 0.80 |
| 4:M4:148:LYS:NZ | 5:Z4:52:ARG:HD2 | 1.95 | 0.80 |
| 5:Z4:29:HIS:HE2 | 5:Z4:37:HIS:C | 1.89 | 0.80 |
| 8:E5:17:TYR:HB3 | 1:F5:45:SER:HB3 | 1.62 | 0.80 |
| 8:a5:35:ARG:NH2 | 8:a5:144:ASP:HB3 | 1.96 | 0.80 |
| 6:M6:53:LEU:CD2 | 8:c7:80:LEU:HD23 | 2.06 | 0.80 |
| 6:M6:66:GLY:HA2 | 1:b7:125:ALA:HA | 1.64 | 0.80 |
| 10:j5:988:ALA:CB | 1:h7:106:GLU:OE2 | 2.27 | 0.80 |
| 10:k5:547:ARG:O | 10:k5:547:ARG:HD2 | 1.82 | 0.80 |
| 1:B7:54:GLU:OE2 | 11:a9:563:PHE:HD2 | 1.62 | 0.80 |
| 8:K7:25:ARG:NE | 8:U7:25:ARG:NH2 | 2.29 | 0.80 |
| 8:c7:104:ILE:HG21 | 8:c7:155:TYR:CE2 | 2.17 | 0.80 |
| 12:D8:202:CYC:O2A | 4:M8:35:THR:CB | 2.28 | 0.80 |
| 4:M9:58:TYR:CZ | 11:a9:496:ARG:CZ | 2.64 | 0.80 |
| 3:J9:108:ARG:HA | 11:a9:517:ALA:HA | 1.63 | 0.80 |
| 11:a9:312:ASP:HB3 | 11:a9:315:LEU:HD12 | 1.64 | 0.80 |
| 11:a9:585:GLU:CA | 11:a9:588:VAL:O | 2.30 | 0.80 |
| 12:LA:202:CYC:O2A | 11:aA:404:TYR:CB | 2.29 | 0.80 |
| 4:MA:185:ALA:HA | 12:VA:201:CYC:CBA | 2.11 | 0.80 |
| 5:NA:66:ARG:HH12 | 3:TA:111:ASN:ND2 | 1.79 | 0.80 |
| 2:QA:108:TYR:O | 3:TA:75:PRO:HB2 | 1.82 | 0.80 |
| 2:QA:162:SER:O | 2:WA:118:ARG:CD | 2.29 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:j5:619:GLU:CB | 10:j5:620:PRO:CD | 2.60 | 0.80 |
| 10:k5:549:LYS:N | 10:k5:549:LYS:HD2 | 1.97 | 0.80 |
| 10:k5:1074:GLN:CD | 1:l7:119:LEU:CD2 | 2.55 | 0.80 |
| 10:k5:1081:VAL:CG1 | 12:k5:1203:CYC:HMA2 | 2.11 | 0.80 |
| 8:W7:4:LEU:CD2 | 8:W7:26:ILE:HD13 | 2.12 | 0.80 |
| 8:m7:35:ARG:NH2 | 8:m7:144:ASP:HB3 | 1.97 | 0.80 |
| 3:Y8:80:ALA:O | 3:Y8:84:ARG:HG3 | 1.80 | 0.80 |
| 11:a9:75:ALA:CB | 11:a9:81:ASP:OD2 | 2.29 | 0.80 |
| 11:a9:245:ALA:CB | 12:a9:901:CYC:C4B | 2.60 | 0.80 |
| 11:a9:377:VAL:HG11 | 11:a9:390:ALA:CB | 2.11 | 0.80 |
| 11:a9:403:THR:HG22 | 11:a9:536:THR:HG21 | 1.59 | 0.80 |
| 11:aA:636:ALA:O | 11:aA:774:PHE:CD2 | 2.33 | 0.80 |
| 4:M4:197:ASP:CB | 5:Z4:52:ARG:CG | 2.58 | 0.80 |
| 2:N4:14:SER:HA | 5:Z4:62:ARG:HD3 | 1.64 | 0.80 |
| 8:C5:29:PHE:HE1 | 8:C5:99:GLY:CA | 1.93 | 0.80 |
| 8:G5:25:ARG:NH2 | 8:S5:25:ARG:HB3 | 1.95 | 0.80 |
| 8:e5:38:ARG:HG2 | 1:R5:143:PRO:HG2 | 1.64 | 0.80 |
| 3:F6:59:LEU:CD2 | 12:F6:201:CYC:H2C | 2.11 | 0.80 |
| 8:E7:4:LEU:CD2 | 8:E7:26:ILE:HD13 | 2.12 | 0.80 |
| 8:i7:49:ARG:CZ | 8:i7:140:LEU:HD21 | 2.11 | 0.80 |
| 8:c7:4:LEU:CD2 | 8:c7:26:ILE:HD13 | 2.12 | 0.80 |
| 8:c7:15:ALA:CA | 1:d7:90:ARG:HH21 | 1.93 | 0.80 |
| 8:m7:9:VAL:HG22 | 1:n7:107:ARG:HH22 | 1.44 | 0.80 |
| 8:u7:90:ARG:CD | 1:v7:18:TYR:CE1 | 2.60 | 0.80 |
| 3:U8:115:GLU:HB2 | 4:M8:74:LEU:HD12 | 0.81 | 0.80 |
| 3:L8:113:LEU:HD11 | 12:a9:901:CYC:CHB | 2.10 | 0.80 |
| 4:M8:141:GLU:O | 4:M8:145:LEU:N | 2.13 | 0.80 |
| 3:O8:107:ASP:HB2 | 5:Z8:61:LYS:HZ2 | 1.43 | 0.80 |
| 3:H9:84:ARG:CA | 11:a9:478:HIS:NE2 | 2.28 | 0.80 |
| 3:TA:24:LEU:HB3 | 2:X4:68:GLN:HG3 | 1.62 | 0.80 |
| 3:R1:111:ASN:HD21 | 5:N1:66:ARG:HH11 | 1.30 | 0.80 |
| 12:B4:202:CYC:HMA1 | 4:M4:58:TYR:HB2 | 1.62 | 0.80 |
| 4:M4:27:HIS:NE2 | 4:M4:34:ASP:CA | 2.16 | 0.80 |
| 2:N4:115:GLU:OE1 | 5:Z4:33:GLY:HA3 | 1.82 | 0.80 |
| 1:P5:114:GLU:CD | 10:k5:496:GLU:HB2 | 2.06 | 0.80 |
| 10:j5:148:TYR:O | 10:j5:152:ARG:CG | 2.28 | 0.80 |
| 10:j5:968:GLU:OE1 | 1:v7:10:ASN:ND2 | 2.15 | 0.80 |
| 10:j5:990:ARG:HH21 | 10:j5:1026:LYS:HZ1 | 1.27 | 0.80 |
| 10:j5:1049:PHE:CZ | 10:j5:1065:HIS:HE1 | 1.99 | 0.80 |
| 10:k5:221:LYS:HE2 | 10:k5:221:LYS:HA | 1.64 | 0.80 |
| 8:C7:44:THR:HG1 | 1:D7:18:TYR:HD2 | 1.30 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:K7:25:ARG:NE | 8:U7:25:ARG:HH22 | 1.80 | 0.80 |
| 8:g7:90:ARG:NH1 | 1:h7:16:GLY:HA2 | 1.96 | 0.80 |
| 8:q7:66:VAL:HG12 | 11:aA:65:LEU:HD22 | 1.64 | 0.80 |
| 8:s7:9:VAL:HG22 | 1:t7:107:ARG:HH22 | 1.44 | 0.80 |
| 8:u7:4:LEU:HD11 | 1:v7:30:TYR:CZ | 2.17 | 0.80 |
| 8:u7:18:LEU:CD1 | 1:v7:97:LEU:CD1 | 2.58 | 0.80 |
| 3:L8:71:GLY:H | 11:a9:82:GLN:HG2 | 0.98 | 0.80 |
| 4:M9:158:PHE:CA | 3:V9:108:ARG:CD | 2.56 | 0.80 |
| 4:MA:158:PHE:C | 3:VA:108:ARG:CG | 2.50 | 0.80 |
| 3:B3:84:ARG:HD2 | 11:a9:680:SER:OG | 1.82 | 0.80 |
| 12:B4:202:CYC:CHA | 4:M4:54:ALA:N | 2.41 | 0.80 |
| 3:L3:119:ALA:CB | 11:a9:813:PRO:HB2 | 1.92 | 0.80 |
| 4:M4:26:SER:CB | 11:aA:228:GLU:CD | 2.55 | 0.80 |
| 4:M4:94:TRP:CD2 | 3:Q4:88:ILE:HG12 | 2.16 | 0.80 |
| 4:M4:144:ARG:HH22 | 5:Z4:59:ARG:HH11 | 1.28 | 0.80 |
| 4:M4:228:SER:CB | 2:X4:16:GLY:C | 2.54 | 0.80 |
| 2:N4:63:PHE:CB | 2:N4:66:LEU:CD1 | 2.55 | 0.80 |
| 5:Z4:41:GLN:HG2 | 12:Z4:301:CYC:HMB3 | 1.63 | 0.80 |
| 8:e5:29:PHE:HE1 | 8:e5:99:GLY:CA | 1.93 | 0.80 |
| 8:Q5:4:LEU:CD2 | 8:Q5:26:ILE:HD13 | 2.12 | 0.80 |
| 10:j5:194:CYS:HB2 | 12:j5:1201:CYC:CAC | 2.12 | 0.80 |
| 10:j5:1143:LEU:HD13 | 8:q7:103:PRO:HA | 1.63 | 0.80 |
| 10:j5:1146:THR:HB | 1:v7:77:ARG:CZ | 2.12 | 0.80 |
| 10:k5:1043:GLU:CB | 8:Y7:14:GLU:OE2 | 2.30 | 0.80 |
| 8:g7:37:LEU:HD13 | 1:h7:24:LEU:CD2 | 2.12 | 0.80 |
| 8:m7:29:PHE:HE1 | 8:m7:99:GLY:CA | 1.93 | 0.80 |
| 8:m7:29:PHE:HZ | 8:m7:98:ALA:O | 1.62 | 0.80 |
| 1:v7:136:VAL:HG13 | 11:aA:342:ARG:NH1 | 1.96 | 0.80 |
| 2:X8:68:GLN:HE21 | 3:T9:24:LEU:HD22 | 1.44 | 0.80 |
| 3:J8:108:ARG:HH22 | 11:a9:171:ARG:HB3 | 1.46 | 0.80 |
| 4:M8:140:ARG:CD | 4:M8:215:GLU:HA | 2.12 | 0.80 |
| 12:M8:301:CYC:OC | 3:Y8:72:ASN:HB3 | 1.81 | 0.80 |
| 12:M8:302:CYC:C1C | 3:S8:78:ARG:HH11 | 1.94 | 0.80 |
| 12:M8:302:CYC:CAC | 3:S8:78:ARG:HG2 | 2.12 | 0.80 |
| 2:I9:16:GLY:HA2 | 3:J9:91:ARG:HH11 | 1.43 | 0.80 |
| 11:aA:776:TYR:HB2 | 12:H1:201:CYC:HMA2 | 1.63 | 0.80 |
| 3:H1:108:ARG:O | 12:H1:201:CYC:HBB1 | 1.80 | 0.80 |
| 4:MA:273:ILE:CD1 | 3:VA:75:PRO:CG | 2.57 | 0.80 |
| 3:TA:25:ASN:OD1 | 2:X4:68:GLN:HG3 | 1.79 | 0.80 |
| 3:B4:86:MET:HG3 | 12:B4:202:CYC:HBC2 | 1.64 | 0.80 |
| 3:B4:108:ARG:HA | 4:M4:61:ASN:C | 2.06 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:B4:113:LEU:HD13 | 4:M4:60:LYS:HE2 | 1.62 | 0.80 |
| 12:B4:202:CYC:HBB3 | 4:M4:61:ASN:HD22 | 1.43 | 0.80 |
| 5:N3:66:ARG:HB2 | 5:N3:66:ARG:HH11 | 1.46 | 0.80 |
| 3:U4:115:GLU:HG3 | 4:M4:71:PRO:HD2 | 1.64 | 0.80 |
| 12:M4:301:CYC:HMB2 | 3:Y4:89:ILE:CD1 | 2.11 | 0.80 |
| 12:O4:201:CYC:HMA2 | 5:Z4:53:LEU:CD1 | 2.10 | 0.80 |
| 1:B5:143:PRO:CG | 8:W7:41:GLN:NE2 | 2.44 | 0.80 |
| 8:I5:35:ARG:NH2 | 8:I5:144:ASP:HB3 | 1.96 | 0.80 |
| 8:U5:84:ASP:OD1 | 6:M6:26:PHE:HZ | 1.64 | 0.80 |
| 10:j5:549:LYS:HD2 | 10:j5:549:LYS:N | 1.97 | 0.80 |
| 10:j5:1016:LEU:HD12 | 10:j5:1017:ARG:CA | 2.10 | 0.80 |
| 10:k5:1043:GLU:CG | 8:Y7:14:GLU:OE2 | 2.30 | 0.80 |
| 8:g7:33:GLY:HA3 | 1:h7:31:PHE:CZ | 2.16 | 0.80 |
| 8:i7:104:ILE:HG21 | 8:i7:155:TYR:CE2 | 2.17 | 0.80 |
| 9:x7:4:TYR:HB2 | 9:x7:58:THR:HG1 | 1.46 | 0.80 |
| 3:F8:84:ARG:HD2 | 11:a9:139:ILE:CG2 | 2.00 | 0.80 |
| 4:M8:50:ASP:OD1 | 4:M8:50:ASP:N | 2.15 | 0.80 |
| 4:M9:28:HIS:HA | 11:a9:378:GLU:OE2 | 1.81 | 0.80 |
| 11:a9:776:TYR:O | 11:a9:776:TYR:CD1 | 2.34 | 0.80 |
| 11:aA:585:GLU:CA | 11:aA:588:VAL:O | 2.30 | 0.80 |
| 3:HA:78:ARG:HG2 | 12:HA:202:CYC:HAD1 | 1.64 | 0.80 |
| 6:M2:62:ARG:HH22 | 1:h7:58:LYS:HA | 1.44 | 0.80 |
| 4:M3:160:THR:CG2 | 4:M3:257:GLN:HB2 | 2.07 | 0.80 |
| 4:M3:188:LEU:O | 4:M3:188:LEU:HD12 | 1.80 | 0.80 |
| 4:M4:188:LEU:O | 4:M4:188:LEU:HD12 | 1.80 | 0.80 |
| 3:Q4:120:LEU:HD23 | 5:Z4:42:SER:CB | 2.11 | 0.80 |
| 8:M5:90:ARG:HB2 | 1:N5:18:TYR:CE1 | 2.17 | 0.80 |
| 8:A5:49:ARG:HH21 | 8:A5:140:LEU:HD22 | 1.46 | 0.80 |
| 6:M6:267:THR:HG21 | 1:d7:161:SER:OXT | 1.82 | 0.80 |
| 10:j5:186:LEU:O | 10:j5:186:LEU:HD12 | 1.82 | 0.80 |
| 1:P7:76:ARG:N | 8:Q7:110:ILE:O | 2.15 | 0.80 |
| 1:J7:76:ARG:HD3 | 8:K7:110:ILE:HD11 | 1.62 | 0.80 |
| 8:g7:29:PHE:HE1 | 8:g7:99:GLY:CA | 1.93 | 0.80 |
| 8:g7:56:ASP:OD1 | 11:aA:325:LEU:HD13 | 1.81 | 0.80 |
| 8:a7:35:ARG:NH2 | 8:a7:144:ASP:HB3 | 1.96 | 0.80 |
| 8:c7:95:GLY:C | 8:c7:152:TYR:HE2 | 1.87 | 0.80 |
| 11:a9:714:ARG:HB2 | 11:a9:808:LEU:O | 1.82 | 0.80 |
| 3:FA:125:ARG:HD2 | 3:VA:14:LEU:CD1 | 2.12 | 0.79 |
| 4:MA:50:ASP:N | 4:MA:50:ASP:OD1 | 2.15 | 0.79 |
| 2:S1:16:GLY:CA | 5:N1:31:TRP:HD1 | 1.89 | 0.79 |
| 12:D4:202:CYC:O2A | 4:M4:35:THR:HB | 1.78 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:N3:70:ILE:HG21 | 3:R3:116:THR:HA | 1.62 | 0.79 |
| 2:N4:111:ALA:CA | 5:Z4:34:LEU:CD1 | 2.59 | 0.79 |
| 8:K5:23:LEU:HD13 | 8:U5:151:PHE:HE1 | 1.42 | 0.79 |
| 3:Y4:105:LEU:HD13 | 3:Y4:163:TYR:HB3 | 1.63 | 0.79 |
| 8:E5:4:LEU:CD2 | 8:E5:26:ILE:HD13 | 2.12 | 0.79 |
| 10:j5:1008:PHE:CD1 | 1:v7:87:TYR:CZ | 2.67 | 0.79 |
| 10:j5:1147:TYR:CE1 | 11:aA:35:ARG:HB2 | 2.17 | 0.79 |
| 10:k5:186:LEU:O | 10:k5:186:LEU:HD12 | 1.82 | 0.79 |
| 3:H6:84:ARG:O | 3:H6:85:ASP:C | 2.11 | 0.79 |
| 8:i7:25:ARG:HH12 | 8:s7:6:LYS:CB | 1.93 | 0.79 |
| 8:a7:29:PHE:HZ | 8:a7:98:ALA:O | 1.62 | 0.79 |
| 8:a7:37:LEU:HD13 | 1:b7:24:LEU:CD2 | 2.12 | 0.79 |
| 12:b7:201:CYC:OB | 9:x7:21:ARG:O | 2.00 | 0.79 |
| 8:u7:4:LEU:CD2 | 8:u7:26:ILE:HD13 | 2.12 | 0.79 |
| 3:L8:71:GLY:HA3 | 11:a9:82:GLN:NE2 | 1.97 | 0.79 |
| 4:M8:214:GLY:HA3 | 5:Z8:28:HIS:ND1 | 1.97 | 0.79 |
| 3:F9:125:ARG:HD2 | 3:V9:14:LEU:CD1 | 2.12 | 0.79 |
| 11:aA:312:ASP:HB3 | 11:aA:315:LEU:HD12 | 1.64 | 0.79 |
| 11:aA:739:ASP:HA | 3:L1:84:ARG:HD2 | 1.64 | 0.79 |
| 2:EA:2:LYS:HZ3 | 2:IA:17:ARG:HH12 | 0.81 | 0.79 |
| 3:JA:88:ILE:HD13 | 11:aA:512:TYR:CD2 | 2.17 | 0.79 |
| 2:G2:107:ASP:O | 3:L2:77:ARG:NH2 | 2.15 | 0.79 |
| 3:F3:84:ARG:NH1 | 4:M3:35:THR:HB | 1.97 | 0.79 |
| 3:Q4:104:VAL:CG2 | 3:Q4:105:LEU:CD1 | 2.59 | 0.79 |
| 8:K5:47:ARG:HD3 | 1:L5:18:TYR:CZ | 2.17 | 0.79 |
| 8:U5:23:LEU:HD22 | 1:V5:38:VAL:HG13 | 1.64 | 0.79 |
| 10:j5:1119:LEU:CD1 | 1:t7:87:TYR:CZ | 2.64 | 0.79 |
| 8:Q7:4:LEU:CD2 | 8:Q7:26:ILE:HD13 | 2.12 | 0.79 |
| 8:q7:120:GLN:HG3 | 1:v7:53:LYS:HZ1 | 1.46 | 0.79 |
| 8:u7:29:PHE:CZ | 1:v7:31:PHE:HZ | 1.99 | 0.79 |
| 2:N8:63:PHE:CB | 2:N8:66:LEU:CD1 | 2.55 | 0.79 |
| 3:L9:48:ALA:HB2 | 2:K9:18:PHE:CE2 | 2.16 | 0.79 |
| 3:L9:51:ILE:CG2 | 3:L9:90:LEU:CD1 | 2.61 | 0.79 |
| 4:M9:274:VAL:CB | 3:V9:77:ARG:HD3 | 2.12 | 0.79 |
| 5:N9:61:LYS:HZ3 | 12:T9:301:CYC:CBB | 1.92 | 0.79 |
| 11:aA:308:LEU:CD2 | 11:aA:315:LEU:HD12 | 2.12 | 0.79 |
| 11:aA:312:ASP:OD1 | 11:aA:316:GLY:N | 2.14 | 0.79 |
| 11:aA:403:THR:HG22 | 11:aA:536:THR:HG21 | 1.59 | 0.79 |
| 3:J3:116:THR:OG1 | 11:a9:797:ASP:HA | 1.82 | 0.79 |
| 8:O5:35:ARG:NH2 | 8:O5:144:ASP:HB3 | 1.96 | 0.79 |
| 8:A5:118:SER:HB2 | 1:F5:82:ILE:HD11 | 1.65 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:f5:27:LEU:HD13 | 10:j5:172:LEU:HD22 | 1.63 | 0.79 |
| 1:f5:34:GLY:HA3 | 10:j5:47:PHE:HD2 | 1.44 | 0.79 |
| 10:j5:386:ILE:CG2 | 10:j5:395:SER:C | 2.52 | 0.79 |
| 10:k5:586:LEU:CD1 | 10:k5:607:LEU:CD2 | 2.60 | 0.79 |
| 10:k5:1118:THR:CG2 | 12:k5:1204:CYC:HMA2 | 2.12 | 0.79 |
| 8:U7:35:ARG:NH2 | 8:U7:144:ASP:HB3 | 1.97 | 0.79 |
| 3:L8:86:MET:CG | 12:a9:901:CYC:CBC | 2.57 | 0.79 |
| 4:M8:104:ALA:C | 2:P8:14:SER:CB | 2.54 | 0.79 |
| 12:N8:201:CYC:HMA1 | 12:N8:201:CYC:NB | 1.96 | 0.79 |
| 3:Y8:102:ALA:HB1 | 3:Y8:106:GLU:H | 1.44 | 0.79 |
| 3:H9:72:ASN:HD21 | 12:H9:202:CYC:HBD2 | 1.48 | 0.79 |
| 11:aA:377:VAL:HG11 | 11:aA:390:ALA:CB | 2.11 | 0.79 |
| 11:aA:714:ARG:HB2 | 11:aA:808:LEU:O | 1.82 | 0.79 |
| 3:H1:81:ALA:HB3 | 12:H1:201:CYC:CMD | 2.10 | 0.79 |
| 3:FA:125:ARG:HD2 | 3:VA:14:LEU:HD13 | 1.64 | 0.79 |
| 5:NA:66:ARG:HB2 | 3:TA:111:ASN:HD22 | 1.45 | 0.79 |
| 2:SA:42:ARG:HD2 | 2:X4:69:PRO:C | 2.06 | 0.79 |
| 12:F3:201:CYC:HMA3 | 4:M3:36:TYR:O | 1.81 | 0.79 |
| 3:B4:85:ASP:CB | 12:B4:202:CYC:CBC | 2.61 | 0.79 |
| 4:M4:144:ARG:NH1 | 5:Z4:59:ARG:HH12 | 1.80 | 0.79 |
| 4:M4:227:GLN:O | 3:Y4:91:ARG:NH2 | 2.15 | 0.79 |
| 8:K5:4:LEU:CD2 | 8:K5:26:ILE:HD13 | 2.12 | 0.79 |
| 1:N5:110:ASN:HD21 | 10:k5:692:LEU:C | 1.89 | 0.79 |
| 8:C5:98:ALA:HA | 1:D5:5:ILE:HG21 | 1.65 | 0.79 |
| 10:j5:275:THR:HG23 | 10:j5:286:VAL:HG13 | 1.64 | 0.79 |
| 10:j5:978:LEU:HD11 | 1:v7:107:ARG:NH2 | 1.98 | 0.79 |
| 10:k5:1023:SER:CB | 12:k5:1202:CYC:HBA1 | 2.12 | 0.79 |
| 8:O7:35:ARG:NH2 | 8:O7:144:ASP:HB3 | 1.97 | 0.79 |
| 8:Q7:13:ALA:HA | 9:z7:46:LYS:CD | 2.13 | 0.79 |
| 8:C7:29:PHE:CE1 | 8:C7:98:ALA:C | 2.61 | 0.79 |
| 1:J7:75:THR:O | 8:K7:111:GLY:HA3 | 1.82 | 0.79 |
| 8:g7:10:ASN:HD22 | 8:u7:10:ASN:HD21 | 1.30 | 0.79 |
| 8:g7:52:LYS:CD | 11:aA:321:ALA:CB | 2.50 | 0.79 |
| 1:V7:76:ARG:N | 8:W7:110:ILE:O | 2.15 | 0.79 |
| 8:c7:16:ARG:CA | 1:d7:90:ARG:HD2 | 2.05 | 0.79 |
| 2:E8:15:GLN:CG | 11:a9:163:ASP:CB | 2.60 | 0.79 |
| 4:M8:226:SER:OG | 3:Y8:88:ILE:HG12 | 1.82 | 0.79 |
| 12:M8:301:CYC:HBC3 | 3:Y8:127:VAL:HA | 1.65 | 0.79 |
| 3:Q8:77:ARG:H | 5:Z8:34:LEU:HD13 | 1.47 | 0.79 |
| 3:Q8:87:GLU:O | 3:Q8:91:ARG:HG2 | 1.81 | 0.79 |
| 5:N1:36:THR:HG1 | 12:T1:301:CYC:C4B | 1.94 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:Z:127:VAL:CG1 | 1:X5:15:GLN:HG2 | 2.08 | 0.79 |
| 1:Z:158:SER:CB | 1:X5:11:ASN:HD22 | 1.96 | 0.79 |
| 4:MA:28:HIS:HA | 11:aA:378:GLU:OE2 | 1.81 | 0.79 |
| 4:MA:274:VAL:HG12 | 3:VA:77:ARG:HE | 1.47 | 0.79 |
| 4:M4:232:VAL:HA | 12:M4:301:CYC:C4B | 2.12 | 0.79 |
| 2:P4:19:LEU:HD11 | 3:Q4:95:TYR:CE1 | 2.18 | 0.79 |
| 1:d5:124:ALA:HB1 | 10:j5:699:SER:HB3 | 1.63 | 0.79 |
| 8:U5:75:GLU:CG | 6:M6:36:ILE:HG13 | 2.06 | 0.79 |
| 8:A7:86:ASP:HB2 | 11:aA:579:PHE:HZ | 1.48 | 0.79 |
| 10:k5:1008:PHE:HZ | 1:p7:83:ARG:NH1 | 1.75 | 0.79 |
| 10:k5:1146:THR:CA | 1:p7:77:ARG:HH22 | 1.94 | 0.79 |
| 8:c7:25:ARG:HH22 | 8:m7:6:LYS:CE | 1.96 | 0.79 |
| 8:o7:4:LEU:HD11 | 1:p7:30:TYR:CZ | 2.17 | 0.79 |
| 11:a9:290:ASP:O | 11:a9:291:TYR:CG | 2.36 | 0.79 |
| 11:a9:531:ASP:OD1 | 11:a9:531:ASP:N | 2.13 | 0.79 |
| 4:M1:98:ASP:OD1 | 3:T1:1:MET:N | 2.16 | 0.79 |
| 5:N1:37:HIS:O | 12:T1:301:CYC:HMA1 | 1.82 | 0.79 |
| 3:HA:84:ARG:CA | 11:aA:478:HIS:NE2 | 2.28 | 0.79 |
| 4:MA:158:PHE:CZ | 2:UA:10:ALA:HB1 | 2.18 | 0.79 |
| 2:QA:116:VAL:HG13 | 3:TA:79:MET:CG | 2.11 | 0.79 |
| 3:TA:32:LYS:HD3 | 2:X4:57:GLN:CD | 2.08 | 0.79 |
| 3:TA:32:LYS:CD | 2:X4:57:GLN:HE22 | 1.95 | 0.79 |
| 3:B3:108:ARG:C | 4:M3:6:THR:HG22 | 2.08 | 0.79 |
| 3:D4:150:ARG:CZ | 2:C1:140:SER:O | 2.31 | 0.79 |
| 5:N3:22:LEU:HD13 | 5:N3:26:LEU:HD22 | 1.63 | 0.79 |
| 3:X3:80:ALA:O | 3:X3:84:ARG:HG3 | 1.81 | 0.79 |
| 3:U4:115:GLU:OE1 | 4:M4:74:LEU:HD13 | 1.82 | 0.79 |
| 1:B5:107:ARG:NE | 9:z5:21:ARG:HD3 | 1.96 | 0.79 |
| 8:E5:47:ARG:HD3 | 1:F5:18:TYR:CZ | 2.17 | 0.79 |
| 1:J5:87:TYR:HE2 | 9:i5:38:PHE:CE2 | 2.00 | 0.79 |
| 8:e5:35:ARG:NH2 | 8:e5:144:ASP:HB3 | 1.96 | 0.79 |
| 10:j5:388:ARG:CD | 10:j5:393:MET:H | 1.93 | 0.79 |
| 10:j5:586:LEU:CD1 | 10:j5:607:LEU:CD2 | 2.60 | 0.79 |
| 10:j5:1064:LYS:HA | 10:j5:1069:ARG:H | 1.47 | 0.79 |
| 10:k5:1064:LYS:O | 10:k5:1068:GLY:N | 2.15 | 0.79 |
| 10:k5:1067:LEU:CD1 | 10:k5:1101:GLU:CG | 2.61 | 0.79 |
| 2:A6:63:PHE:CB | 2:A6:66:LEU:CD1 | 2.55 | 0.79 |
| 8:i7:39:ILE:HD11 | 8:i7:148:GLU:HG2 | 1.60 | 0.79 |
| 8:c7:15:ALA:HA | 1:d7:90:ARG:HH22 | 1.40 | 0.79 |
| 8:s7:29:PHE:CE1 | 8:s7:98:ALA:C | 2.61 | 0.79 |
| 3:U8:114:LYS:HZ3 | 4:M8:13:LYS:CD | 1.88 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:F8:107:ASP:CA | 4:M8:8:SER:N | 2.43 | 0.79 |
| 4:M9:158:PHE:CZ | 2:U9:10:ALA:HB1 | 2.18 | 0.79 |
| 3:B9:26:GLN:O | 3:B9:30:LEU:HD12 | 1.80 | 0.79 |
| 3:H9:116:THR:CG2 | 12:H9:202:CYC:HMA3 | 2.10 | 0.79 |
| 12:H9:202:CYC:NB | 11:a9:474:PHE:CE2 | 2.51 | 0.79 |
| 11:aA:621:THR:HG21 | 3:J1:14:LEU:HD13 | 0.81 | 0.79 |
| 3:HA:59:LEU:CD2 | 12:HA:202:CYC:HBC2 | 2.12 | 0.79 |
| 2:IA:16:GLY:HA3 | 11:aA:514:VAL:HG11 | 1.65 | 0.79 |
| 3:JA:88:ILE:CD1 | 11:aA:512:TYR:CD1 | 2.62 | 0.79 |
| 12:JA:202:CYC:HBA2 | 11:aA:511:LYS:CA | 2.01 | 0.79 |
| 5:NA:66:ARG:CB | 3:TA:111:ASN:ND2 | 2.45 | 0.79 |
| 2:O1:63:PHE:CB | 2:O1:66:LEU:CD1 | 2.56 | 0.79 |
| 3:B1:84:ARG:HD2 | 11:aA:680:SER:OG | 1.81 | 0.79 |
| 4:M4:50:ASP:OD1 | 4:M4:50:ASP:N | 2.15 | 0.79 |
| 8:I5:98:ALA:HA | 1:J5:5:ILE:HG21 | 1.65 | 0.79 |
| 8:S5:110:ILE:CD1 | 10:j5:533:LEU:CD1 | 2.60 | 0.79 |
| 6:M6:104:ARG:CZ | 2:G6:16:GLY:HA3 | 2.13 | 0.79 |
| 8:k7:66:VAL:HG11 | 11:a9:61:TYR:CE1 | 2.17 | 0.79 |
| 4:M8:97:ALA:HB1 | 4:M8:101:ASP:HB3 | 1.64 | 0.79 |
| 3:F9:125:ARG:HD2 | 3:V9:14:LEU:HD13 | 1.64 | 0.79 |
| 3:J9:88:ILE:HD13 | 11:a9:512:TYR:CD2 | 2.17 | 0.79 |
| 11:aA:643:LEU:HD11 | 11:aA:689:VAL:CG2 | 2.11 | 0.79 |
| 1:Z:73:TYR:CZ | 10:j5:162:TRP:CZ2 | 2.70 | 0.79 |
| 3:O4:115:GLU:HB3 | 5:Z4:70:ILE:O | 1.81 | 0.79 |
| 1:N5:14:VAL:O | 1:R5:68:PRO:HB3 | 1.81 | 0.79 |
| 3:Y4:85:ASP:HA | 3:Y4:88:ILE:HG12 | 1.64 | 0.79 |
| 8:C5:35:ARG:NH2 | 8:C5:144:ASP:HB3 | 1.96 | 0.79 |
| 1:f5:5:ILE:CD1 | 10:j5:46:PHE:HZ | 1.95 | 0.79 |
| 10:k5:246:VAL:HG22 | 10:k5:257:THR:HG22 | 1.65 | 0.79 |
| 10:k5:971:VAL:CG1 | 1:n7:76:ARG:NH1 | 2.46 | 0.79 |
| 10:k5:1019:SER:OG | 1:Z7:87:TYR:HE1 | 1.65 | 0.79 |
| 1:V7:75:THR:O | 8:W7:111:GLY:HA3 | 1.82 | 0.79 |
| 3:B8:119:ALA:HB3 | 4:M8:52:LEU:HD11 | 1.64 | 0.79 |
| 3:F8:113:LEU:HA | 4:M8:5:THR:HG23 | 1.63 | 0.79 |
| 3:Q8:117:TYR:HA | 3:Q8:120:LEU:HD21 | 1.64 | 0.79 |
| 3:Q8:120:LEU:HD11 | 3:Q8:122:THR:OG1 | 1.69 | 0.79 |
| 11:a9:312:ASP:OD1 | 11:a9:316:GLY:N | 2.14 | 0.79 |
| 11:aA:106:LEU:O | 11:aA:106:LEU:HD23 | 1.83 | 0.79 |
| 11:aA:804:ARG:HH21 | 3:J1:121:GLY:HA2 | 1.47 | 0.79 |
| 3:JA:111:ASN:C | 11:aA:518:ALA:CB | 2.55 | 0.79 |
| 12:F3:201:CYC:HAA1 | 4:M3:36:TYR:CZ | 2.18 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 12:Z3:202:CYC:OB | 2:O3:33:ARG:CZ | 2.31 | 0.79 |
| 5:N3:66:ARG:HH11 | 3:R3:111:ASN:HD21 | 1.30 | 0.79 |
| 3:L4:88:ILE:HD11 | 11:aA:239:TYR:CD2 | 2.17 | 0.79 |
| 4:M4:100:SER:CA | 3:Q4:1:MET:CE | 2.60 | 0.79 |
| 4:M4:225:LYS:HE3 | 3:Y4:81:ALA:CB | 2.09 | 0.79 |
| 4:M4:273:ILE:CG2 | 2:X4:107:ASP:HB3 | 2.12 | 0.79 |
| 2:N4:112:GLY:HA2 | 5:Z4:34:LEU:H | 1.43 | 0.79 |
| 1:d5:161:SER:HB2 | 10:j5:695:GLY:C | 2.08 | 0.79 |
| 8:U5:29:PHE:CE1 | 8:U5:98:ALA:C | 2.61 | 0.79 |
| 1:Z5:127:VAL:HG12 | 10:k5:698:GLY:HA3 | 1.64 | 0.79 |
| 9:i5:23:LEU:C | 9:i5:25:ASN:N | 2.30 | 0.79 |
| 10:k5:990:ARG:HE | 10:k5:1026:LYS:HZ1 | 1.30 | 0.79 |
| 10:k5:1018:LEU:HD12 | 10:k5:1035:PHE:HZ | 1.36 | 0.79 |
| 12:h7:201:CYC:CBB | 9:y7:21:ARG:NE | 2.46 | 0.79 |
| 8:U7:29:PHE:HZ | 8:U7:98:ALA:O | 1.62 | 0.79 |
| 3:B8:120:LEU:HD11 | 4:M8:53:LEU:N | 1.98 | 0.79 |
| 3:L8:120:LEU:HD11 | 12:a9:901:CYC:CAA | 2.12 | 0.79 |
| 3:O8:119:ALA:HB1 | 5:Z8:72:GLU:HG3 | 1.63 | 0.79 |
| 12:F1:201:CYC:HMA3 | 4:M1:36:TYR:O | 1.81 | 0.79 |
| 2:O9:25:GLN:HG2 | 2:Y9:33:ARG:HG2 | 1.65 | 0.79 |
| 3:H9:59:LEU:CD2 | 12:H9:202:CYC:HBC2 | 2.12 | 0.79 |
| 11:a9:350:LEU:HD12 | 11:a9:350:LEU:N | 1.97 | 0.79 |
| 11:aA:55:ASP:HB3 | 11:aA:612:TYR:HB2 | 0.79 | 0.79 |
| 11:aA:632:ILE:HG21 | 11:aA:634:ALA:CB | 2.13 | 0.79 |
| 5:N1:66:ARG:HH11 | 5:N1:66:ARG:HB2 | 1.46 | 0.79 |
| 3:JA:108:ARG:O | 11:aA:517:ALA:CA | 2.30 | 0.79 |
| 12:J3:202:CYC:CMA | 11:a9:666:ASN:HB2 | 2.11 | 0.79 |
| 2:K3:14:SER:CB | 11:a9:746:TYR:CB | 2.56 | 0.79 |
| 5:N3:37:HIS:O | 12:T3:301:CYC:HMA1 | 1.82 | 0.79 |
| 12:B5:201:CYC:HBA1 | 9:z5:26:THR:CG2 | 2.11 | 0.79 |
| 12:B5:201:CYC:CAA | 9:z5:26:THR:HG21 | 2.12 | 0.79 |
| 8:G5:122:PRO:HD2 | 12:G5:201:CYC:C1C | 2.13 | 0.79 |
| 8:I5:25:ARG:HD3 | 8:I5:25:ARG:O | 1.81 | 0.79 |
| 8:Q5:12:ASP:N | 1:R5:94:TYR:CE2 | 2.38 | 0.79 |
| 8:S5:90:ARG:HB2 | 1:T5:18:TYR:CE1 | 2.17 | 0.79 |
| 8:a5:29:PHE:CE1 | 8:a5:98:ALA:C | 2.61 | 0.79 |
| 10:j5:1005:LEU:HD13 | 10:j5:1016:LEU:CD2 | 2.13 | 0.79 |
| 10:j5:1064:LYS:O | 10:j5:1068:GLY:N | 2.15 | 0.79 |
| 10:k5:825:ASN:HB2 | 12:B7:201:CYC:HBB2 | 1.64 | 0.79 |
| 10:k5:1013:PRO:HB2 | 8:k7:114:GLU:OE2 | 1.80 | 0.79 |
| 10:k5:1064:LYS:HA | 10:k5:1069:ARG:H | 1.47 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:O7:29:PHE:CE1 | 8:O7:98:ALA:C | 2.61 | 0.79 |
| 8:C7:35:ARG:NH2 | 8:C7:144:ASP:HB3 | 1.97 | 0.79 |
| 8:K7:4:LEU:CD2 | 8:K7:26:ILE:HD13 | 2.12 | 0.79 |
| 8:i7:47:ARG:NE | 1:j7:18:TYR:CE2 | 2.51 | 0.79 |
| 8:c7:11:ALA:CB | 1:d7:94:TYR:HE1 | 1.93 | 0.79 |
| 8:o7:17:TYR:CD2 | 1:p7:93:THR:CG2 | 2.64 | 0.79 |
| 2:X8:33:ARG:HG2 | 2:N8:25:GLN:HG2 | 1.65 | 0.79 |
| 4:M9:184:ILE:HG22 | 12:V9:201:CYC:CBA | 2.13 | 0.79 |
| 5:Z8:41:GLN:HG2 | 12:Z8:301:CYC:HBB3 | 1.60 | 0.79 |
| 11:a9:55:ASP:HB3 | 11:a9:612:TYR:HB2 | 0.79 | 0.79 |
| 11:a9:106:LEU:O | 11:a9:106:LEU:HD23 | 1.83 | 0.79 |
| 3:HA:120:LEU:HD13 | 12:HA:202:CYC:C2A | 2.13 | 0.78 |
| 3:H3:78:ARG:HH22 | 11:a9:623:ASP:HB3 | 1.33 | 0.78 |
| 3:B3:111:ASN:ND2 | 4:M3:7:SER:OG | 2.16 | 0.78 |
| 3:H4:80:ALA:O | 3:H4:84:ARG:HG3 | 1.83 | 0.78 |
| 3:J4:108:ARG:HH22 | 11:aA:171:ARG:HB3 | 1.47 | 0.78 |
| 4:M4:134:ASN:OD1 | 5:Z4:1:MET:CE | 2.30 | 0.78 |
| 12:M4:301:CYC:CAC | 3:Y4:82:CYS:CB | 2.60 | 0.78 |
| 2:N4:14:SER:CA | 5:Z4:62:ARG:HD3 | 2.13 | 0.78 |
| 8:e5:29:PHE:CE1 | 8:e5:98:ALA:C | 2.61 | 0.78 |
| 10:k5:929:PRO:HG3 | 1:D7:147:LYS:CE | 2.13 | 0.78 |
| 8:i7:47:ARG:CG | 1:j7:18:TYR:OH | 2.31 | 0.78 |
| 3:H8:84:ARG:HG2 | 11:a9:131:TYR:CZ | 2.16 | 0.78 |
| 3:Q8:72:ASN:CG | 12:Z8:301:CYC:CMD | 2.55 | 0.78 |
| 3:Q8:72:ASN:O | 12:Z8:301:CYC:CMD | 2.30 | 0.78 |
| 2:O9:33:ARG:CZ | 12:Z9:201:CYC:OB | 2.31 | 0.78 |
| 5:Z8:66:ARG:HB2 | 5:Z8:66:ARG:HH11 | 1.46 | 0.78 |
| 2:I9:9:ILE:CD1 | 3:J9:99:ALA:HB2 | 2.13 | 0.78 |
| 2:I9:37:SER:HB3 | 2:I9:97:LEU:HD13 | 1.64 | 0.78 |
| 11:a9:585:GLU:N | 11:a9:585:GLU:OE1 | 2.17 | 0.78 |
| 5:N1:24:PRO:HG2 | 5:N1:35:ASP:O | 1.83 | 0.78 |
| 5:NA:54:LEU:CB | 12:TA:301:CYC:O2A | 2.31 | 0.78 |
| 3:P1:115:GLU:HB2 | 5:N1:3:VAL:HG11 | 1.63 | 0.78 |
| 2:A3:63:PHE:CB | 2:A3:66:LEU:CD1 | 2.56 | 0.78 |
| 5:N3:3:VAL:HG11 | 3:P3:115:GLU:HB2 | 1.63 | 0.78 |
| 3:B1:85:ASP:OD2 | 12:B1:202:CYC:ND | 2.11 | 0.78 |
| 12:L4:202:CYC:HAB1 | 11:aA:239:TYR:CE1 | 2.18 | 0.78 |
| 4:M4:197:ASP:CG | 5:Z4:52:ARG:HG3 | 2.08 | 0.78 |
| 8:M5:25:ARG:HE | 8:A5:25:ARG:NH2 | 1.81 | 0.78 |
| 8:C5:27:LYS:C | 8:C5:29:PHE:N | 2.40 | 0.78 |
| 8:I5:27:LYS:C | 8:I5:29:PHE:N | 2.40 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:d5:155:TYR:CZ | 1:T5:113:LYS:NZ | 2.52 | 0.78 |
| 8:U5:59:PHE:HB3 | 6:M6:39:ARG:CD | 2.12 | 0.78 |
| 10:j5:221:LYS:HE2 | 10:j5:221:LYS:HA | 1.64 | 0.78 |
| 10:j5:990:ARG:NE | 10:j5:1026:LYS:HZ1 | 1.81 | 0.78 |
| 10:k5:931:VAL:HG23 | 1:D7:30:TYR:HA | 1.65 | 0.78 |
| 8:i7:4:LEU:CD2 | 8:i7:26:ILE:HD13 | 2.12 | 0.78 |
| 8:i7:95:GLY:C | 8:i7:152:TYR:HE2 | 1.87 | 0.78 |
| 2:A8:25:GLN:HG2 | 2:K8:33:ARG:HG2 | 1.66 | 0.78 |
| 3:B8:107:ASP:O | 4:M8:61:ASN:CA | 2.32 | 0.78 |
| 12:B8:202:CYC:CBB | 4:M8:61:ASN:ND2 | 2.44 | 0.78 |
| 2:X8:57:GLN:HE22 | 3:T9:32:LYS:HD3 | 1.48 | 0.78 |
| 3:L8:82:CYS:HA | 12:a9:901:CYC:CHD | 2.13 | 0.78 |
| 3:O8:104:VAL:CA | 5:Z8:61:LYS:HZ1 | 1.93 | 0.78 |
| 4:M9:159:CYS:HA | 3:V9:108:ARG:HG3 | 1.61 | 0.78 |
| 5:N9:66:ARG:HB2 | 3:T9:111:ASN:HD22 | 1.45 | 0.78 |
| 5:N9:66:ARG:HH12 | 3:T9:111:ASN:ND2 | 1.79 | 0.78 |
| 3:B9:107:ASP:CA | 11:a9:382:ASN:ND2 | 2.45 | 0.78 |
| 2:I9:16:GLY:HA3 | 11:a9:514:VAL:HG11 | 1.64 | 0.78 |
| 11:aA:742:GLN:OE1 | 3:L1:88:ILE:CG1 | 2.30 | 0.78 |
| 2:AA:63:PHE:CB | 2:AA:66:LEU:CD1 | 2.56 | 0.78 |
| 3:HA:125:ARG:HE | 8:S7:41:GLN:NE2 | 1.80 | 0.78 |
| 3:J3:119:ALA:O | 11:a9:803:ASN:CB | 2.30 | 0.78 |
| 5:N3:36:THR:HG1 | 12:T3:301:CYC:C4B | 1.96 | 0.78 |
| 5:Z4:38:GLU:O | 12:Z4:301:CYC:HMB3 | 1.84 | 0.78 |
| 8:C5:29:PHE:CE1 | 8:C5:98:ALA:C | 2.61 | 0.78 |
| 8:U5:76:LYS:O | 8:U5:78:THR:N | 2.17 | 0.78 |
| 10:j5:246:VAL:HG22 | 10:j5:257:THR:HG22 | 1.65 | 0.78 |
| 10:j5:1118:THR:HG21 | 1:t7:83:ARG:NH1 | 1.97 | 0.78 |
| 10:k5:56:ILE:CG2 | 10:k5:57:VAL:N | 2.46 | 0.78 |
| 10:k5:778:LYS:CE | 12:F7:201:CYC:HBB2 | 2.13 | 0.78 |
| 3:D1:68:ARG:NH2 | 3:X1:68:ARG:CZ | 2.44 | 0.78 |
| 1:P7:75:THR:O | 8:Q7:111:GLY:HA3 | 1.82 | 0.78 |
| 8:S7:64:ASP:HA | 8:S7:67:SER:OG | 1.84 | 0.78 |
| 8:g7:29:PHE:CE1 | 8:g7:98:ALA:C | 2.61 | 0.78 |
| 3:O8:107:ASP:HB2 | 5:Z8:61:LYS:HZ3 | 1.45 | 0.78 |
| 3:L9:120:LEU:CD2 | 11:a9:538:ARG:HB2 | 2.13 | 0.78 |
| 3:F9:36:LYS:HB3 | 3:F9:156:LEU:CD1 | 2.13 | 0.78 |
| 11:a9:338:VAL:C | 11:a9:340:PRO:HD3 | 2.08 | 0.78 |
| 1:Z:18:TYR:CE2 | 8:e5:90:ARG:HA | 2.18 | 0.78 |
| 1:Z:127:VAL:CG1 | 1:X5:15:GLN:OE1 | 2.32 | 0.78 |
| 4:MA:192:GLN:NE2 | 3:VA:87:GLU:OE1 | 2.17 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:QA:33:ARG:CB | 2:UA:25:GLN:HG2 | 2.12 | 0.78 |
| 2:SA:42:ARG:HD3 | 2:X4:69:PRO:O | 1.83 | 0.78 |
| 5:N3:24:PRO:HG2 | 5:N3:35:ASP:O | 1.83 | 0.78 |
| 2:O3:25:GLN:HG2 | 2:Y3:33:ARG:HG2 | 1.65 | 0.78 |
| 12:H4:201:CYC:CBB | 11:aA:259:ALA:HA | 2.13 | 0.78 |
| 2:N4:25:GLN:HG2 | 2:X4:33:ARG:HG2 | 1.65 | 0.78 |
| 3:Q4:85:ASP:HB2 | 12:Z4:301:CYC:HBC3 | 1.65 | 0.78 |
| 8:U5:83:ARG:CA | 6:M6:26:PHE:HE1 | 1.96 | 0.78 |
| 10:k5:748:ARG:HE | 8:E7:106:GLU:CD | 1.91 | 0.78 |
| 8:i7:42:THR:HG22 | 8:i7:141:LEU:CD2 | 2.13 | 0.78 |
| 8:c7:101:VAL:CG1 | 8:c7:155:TYR:CZ | 2.67 | 0.78 |
| 1:f7:67:ARG:HH12 | 11:aA:307:ARG:HG2 | 1.48 | 0.78 |
| 3:F1:84:ARG:NH1 | 4:M1:35:THR:HB | 1.97 | 0.78 |
| 12:L9:201:CYC:OB | 2:A9:33:ARG:CZ | 2.32 | 0.78 |
| 3:F9:143:ASN:HA | 12:F9:303:CYC:HMC3 | 1.65 | 0.78 |
| 3:J9:111:ASN:C | 11:a9:518:ALA:CB | 2.55 | 0.78 |
| 11:aA:797:ASP:HA | 3:J1:116:THR:OG1 | 1.82 | 0.78 |
| 4:M1:274:VAL:HG13 | 3:Z1:77:ARG:HG3 | 1.65 | 0.78 |
| 5:N1:22:LEU:HD13 | 5:N1:26:LEU:HD22 | 1.63 | 0.78 |
| 1:A:73:TYR:OH | 10:k5:162:TRP:NE1 | 2.17 | 0.78 |
| 3:HA:117:TYR:CE1 | 12:HA:202:CYC:CHB | 2.67 | 0.78 |
| 2:IA:9:ILE:CD1 | 3:JA:99:ALA:HB2 | 2.13 | 0.78 |
| 3:JA:114:LYS:CG | 8:S7:60:GLN:HE22 | 1.97 | 0.78 |
| 2:KA:18:PHE:CZ | 3:LA:48:ALA:HB2 | 2.18 | 0.78 |
| 5:NA:24:PRO:HG2 | 5:NA:35:ASP:O | 1.83 | 0.78 |
| 2:N4:112:GLY:HA2 | 5:Z4:33:GLY:HA2 | 1.66 | 0.78 |
| 8:O5:29:PHE:CE1 | 8:O5:98:ALA:C | 2.61 | 0.78 |
| 1:H5:14:VAL:HG11 | 10:j5:554:ASN:C | 2.09 | 0.78 |
| 8:S5:107:ILE:HG12 | 1:T5:13:ASP:OD2 | 1.83 | 0.78 |
| 1:Z5:161:SER:CB | 10:k5:695:GLY:C | 2.55 | 0.78 |
| 10:j5:547:ARG:O | 10:j5:547:ARG:HD2 | 1.82 | 0.78 |
| 10:k5:631:HIS:CD2 | 10:k5:664:MET:HE3 | 2.12 | 0.78 |
| 10:k5:931:VAL:HG13 | 1:D7:29:ALA:HB3 | 1.65 | 0.78 |
| 1:d7:87:TYR:HE2 | 9:x7:38:PHE:CE1 | 2.01 | 0.78 |
| 1:d7:87:TYR:HE2 | 9:x7:38:PHE:CZ | 2.02 | 0.78 |
| 3:L8:71:GLY:CA | 11:a9:82:GLN:HE21 | 1.96 | 0.78 |
| 4:M8:87:ILE:CD1 | 3:Y8:77:ARG:HG2 | 2.13 | 0.78 |
| 3:D9:14:LEU:HD11 | 3:Z9:125:ARG:HD2 | 1.65 | 0.78 |
| 12:Y9:201:CYC:HC | 12:Y9:201:CYC:CMD | 1.97 | 0.78 |
| 11:aA:287:ALA:C | 11:aA:289:THR:N | 2.32 | 0.78 |
| 11:aA:585:GLU:N | 11:aA:585:GLU:OE1 | 2.17 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:FA:36:LYS:HB2 | 3:FA:156:LEU:HD11 | 1.64 | 0.78 |
| 4:MA:184:ILE:HG22 | 12:VA:201:CYC:CBA | 2.13 | 0.78 |
| 12:C3:201:CYC:HC | 12:C3:201:CYC:CMD | 1.97 | 0.78 |
| 12:Q3:201:CYC:HC | 12:Q3:201:CYC:CMD | 1.97 | 0.78 |
| 12:M4:301:CYC:HAC2 | 3:Y4:82:CYS:CB | 2.13 | 0.78 |
| 8:C5:25:ARG:HD3 | 8:C5:25:ARG:O | 1.82 | 0.78 |
| 12:C1:201:CYC:HC | 12:C1:201:CYC:CMD | 1.97 | 0.78 |
| 10:j5:741:GLN:C | 1:J7:77:ARG:NH2 | 2.40 | 0.78 |
| 10:j5:951:MET:HE1 | 10:j5:955:LEU:CG | 2.14 | 0.78 |
| 10:k5:1005:LEU:HD13 | 10:k5:1016:LEU:CD2 | 2.13 | 0.78 |
| 10:k5:1020:GLU:CG | 1:Z7:87:TYR:CZ | 2.66 | 0.78 |
| 8:O7:12:ASP:OD1 | 1:P7:91:TYR:OH | 2.02 | 0.78 |
| 1:D7:75:THR:O | 8:E7:111:GLY:HA3 | 1.82 | 0.78 |
| 8:G7:64:ASP:HA | 8:G7:67:SER:OG | 1.84 | 0.78 |
| 8:e7:64:ASP:HA | 8:e7:67:SER:OG | 1.83 | 0.78 |
| 8:q7:64:ASP:HA | 8:q7:67:SER:OG | 1.84 | 0.78 |
| 3:U8:114:LYS:CE | 4:M8:13:LYS:HZ2 | 1.94 | 0.78 |
| 12:F1:201:CYC:HAA1 | 4:M1:36:TYR:CZ | 2.18 | 0.78 |
| 5:N9:24:PRO:HG2 | 5:N9:35:ASP:O | 1.83 | 0.78 |
| 5:N9:54:LEU:CB | 12:T9:301:CYC:O2A | 2.31 | 0.78 |
| 5:Z8:37:HIS:CD2 | 12:Z8:301:CYC:NB | 2.51 | 0.78 |
| 2:E9:2:LYS:HZ1 | 2:I9:17:ARG:NH1 | 1.68 | 0.78 |
| 11:a9:348:GLN:HE21 | 11:a9:348:GLN:N | 1.78 | 0.78 |
| 11:aA:350:LEU:HD12 | 11:aA:350:LEU:N | 1.97 | 0.78 |
| 11:aA:621:THR:CG2 | 3:J1:14:LEU:CG | 2.38 | 0.78 |
| 4:M1:1:MET:HB3 | 4:M1:44:SER:O | 1.84 | 0.78 |
| 1:Z:75:THR:CG2 | 10:j5:182:ASN:O | 2.32 | 0.78 |
| 3:HA:111:ASN:O | 11:aA:447:SER:HB3 | 1.83 | 0.78 |
| 2:E3:13:ASP:OD1 | 11:a9:644:ARG:NH1 | 2.17 | 0.78 |
| 3:L3:1:MET:HE2 | 3:L3:108:ARG:NH1 | 1.98 | 0.78 |
| 4:M3:50:ASP:OD1 | 4:M3:50:ASP:N | 2.15 | 0.78 |
| 2:U3:46:SER:OG | 2:Q9:74:TYR:CE1 | 2.37 | 0.78 |
| 3:B1:108:ARG:C | 4:M1:6:THR:HG22 | 2.08 | 0.78 |
| 3:U4:112:GLY:CA | 4:M4:74:LEU:CD2 | 2.33 | 0.78 |
| 3:F4:108:ARG:NH1 | 4:M4:9:GLN:HE21 | 1.80 | 0.78 |
| 4:M4:27:HIS:O | 11:aA:227:GLY:CA | 2.30 | 0.78 |
| 4:M4:215:GLU:N | 5:Z4:28:HIS:N | 2.32 | 0.78 |
| 8:M5:107:ILE:HG12 | 1:N5:13:ASP:OD2 | 1.83 | 0.78 |
| 8:A5:122:PRO:HD2 | 12:A5:201:CYC:C1C | 2.13 | 0.78 |
| 6:M6:50:LEU:HD22 | 8:c7:83:ARG:HB2 | 1.66 | 0.78 |
| 6:M6:104:ARG:CZ | 2:G6:16:GLY:CA | 2.61 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:j5:136:VAL:HB | 10:j5:137:PRO:CD | 2.14 | 0.78 |
| 10:j5:978:LEU:HD22 | 1:v7:107:ARG:NH2 | 1.96 | 0.78 |
| 10:k5:1125:ARG:NH2 | 1:n7:114:GLU:CB | 2.46 | 0.78 |
| 8:i7:20:PRO:CG | 8:s7:155:TYR:CE2 | 2.67 | 0.78 |
| 8:i7:124:PRO:O | 8:i7:125:ALA:C | 2.13 | 0.78 |
| 8:c7:11:ALA:CB | 1:d7:94:TYR:CZ | 2.67 | 0.78 |
| 3:B8:120:LEU:HD21 | 4:M8:52:LEU:HB3 | 1.64 | 0.78 |
| 8:u7:17:TYR:HD2 | 1:v7:93:THR:CG2 | 1.96 | 0.78 |
| 2:X8:57:GLN:CD | 3:T9:32:LYS:HD3 | 2.08 | 0.78 |
| 3:F8:107:ASP:CB | 4:M8:8:SER:C | 2.25 | 0.78 |
| 3:H8:111:ASN:CG | 11:a9:291:TYR:CZ | 2.58 | 0.78 |
| 3:Q8:84:ARG:CG | 5:Z8:31:TRP:CD1 | 2.64 | 0.78 |
| 3:L9:14:LEU:CG | 11:a9:358:PRO:HB2 | 2.10 | 0.78 |
| 5:N9:66:ARG:CB | 3:T9:111:ASN:ND2 | 2.45 | 0.78 |
| 11:a9:56:ILE:HD11 | 11:a9:612:TYR:HE2 | 1.40 | 0.78 |
| 3:BA:107:ASP:CA | 11:aA:382:ASN:ND2 | 2.46 | 0.78 |
| 2:K2:33:ARG:HG2 | 2:A2:25:GLN:HG2 | 1.66 | 0.78 |
| 3:L2:75:PRO:HG2 | 3:L2:78:ARG:N | 1.99 | 0.78 |
| 6:M2:50:LEU:HD23 | 8:i7:79:ALA:HB1 | 1.66 | 0.78 |
| 6:M2:62:ARG:NH2 | 1:h7:57:ALA:O | 2.16 | 0.78 |
| 12:C4:201:CYC:HC | 12:C4:201:CYC:CMD | 1.97 | 0.78 |
| 12:Y3:201:CYC:HC | 12:Y3:201:CYC:CMD | 1.97 | 0.78 |
| 12:V4:201:CYC:HC | 12:V4:201:CYC:CMD | 1.97 | 0.78 |
| 3:O4:104:VAL:HG23 | 5:Z4:61:LYS:HE2 | 1.66 | 0.78 |
| 3:Q4:7:LYS:HE3 | 3:Q4:101:ASP:OD1 | 1.83 | 0.78 |
| 8:S5:64:ASP:HA | 8:S5:67:SER:OG | 1.83 | 0.78 |
| 12:T5:201:CYC:OB | 10:j5:482:GLN:HB2 | 1.83 | 0.78 |
| 10:k5:1023:SER:HB3 | 12:k5:1202:CYC:HBA1 | 1.66 | 0.78 |
| 10:k5:1052:PRO:HA | 1:l7:106:GLU:HG2 | 1.66 | 0.78 |
| 10:k5:1147:TYR:CD2 | 11:a9:39:PRO:HB3 | 2.19 | 0.78 |
| 10:k5:1150:TYR:HE2 | 1:p7:69:GLY:O | 1.44 | 0.78 |
| 3:F6:126:SER:HB3 | 12:F6:201:CYC:HMC1 | 1.64 | 0.78 |
| 1:R7:49:THR:CG2 | 8:C7:161:GLN:CG | 2.62 | 0.78 |
| 8:i7:101:VAL:CG1 | 8:i7:155:TYR:CZ | 2.67 | 0.78 |
| 1:T7:106:GLU:HG2 | 9:w7:58:THR:HG23 | 1.65 | 0.78 |
| 8:Y7:64:ASP:HA | 8:Y7:67:SER:OG | 1.83 | 0.78 |
| 12:E8:201:CYC:HC | 12:E8:201:CYC:CMD | 1.97 | 0.78 |
| 4:M8:1:MET:HB3 | 4:M8:44:SER:O | 1.84 | 0.78 |
| 4:M8:215:GLU:OE1 | 5:Z8:27:ALA:HB1 | 1.83 | 0.78 |
| 12:E9:201:CYC:HC | 12:E9:201:CYC:CMD | 1.97 | 0.78 |
| 11:a9:89:ALA:HA | 11:a9:92:LYS:NZ | 1.98 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:aA:615:ARG:HB3 | 11:aA:615:ARG:HH11 | 1.48 | 0.78 |
| 3:HA:84:ARG:NH2 | 11:aA:474:PHE:CD2 | 2.52 | 0.78 |
| 3:HA:113:LEU:CD2 | 12:HA:202:CYC:CMB | 2.59 | 0.78 |
| 2:QA:33:ARG:CZ | 12:VA:202:CYC:CBB | 2.61 | 0.78 |
| 2:QA:116:VAL:HG22 | 3:TA:80:ALA:N | 1.98 | 0.78 |
| 12:UA:201:CYC:HC | 12:UA:201:CYC:CMD | 1.97 | 0.78 |
| 2:A1:33:ARG:CZ | 12:L1:201:CYC:OB | 2.32 | 0.78 |
| 2:G2:16:GLY:HA3 | 6:M2:104:ARG:CZ | 2.13 | 0.78 |
| 6:M2:28:ASN:HA | 8:O5:80:LEU:HD23 | 1.64 | 0.78 |
| 3:U4:112:GLY:HA2 | 4:M4:74:LEU:HD21 | 0.78 | 0.78 |
| 3:F4:109:CYS:O | 4:M4:5:THR:CG2 | 2.31 | 0.78 |
| 3:O4:107:ASP:CG | 5:Z4:66:ARG:CB | 2.57 | 0.78 |
| 3:O4:107:ASP:HA | 3:O4:111:ASN:ND2 | 1.99 | 0.78 |
| 12:P4:201:CYC:HC | 12:P4:201:CYC:CMD | 1.97 | 0.78 |
| 3:Q4:59:LEU:HD22 | 3:Q4:130:ALA:HB2 | 1.66 | 0.78 |
| 8:M5:90:ARG:HD2 | 1:N5:17:LYS:C | 2.09 | 0.78 |
| 8:I5:29:PHE:CE1 | 8:I5:98:ALA:C | 2.61 | 0.78 |
| 9:z5:22:GLU:O | 9:z5:25:ASN:N | 2.16 | 0.78 |
| 10:k5:619:GLU:CB | 10:k5:620:PRO:CD | 2.59 | 0.78 |
| 10:k5:743:VAL:CA | 12:D7:201:CYC:O2D | 2.32 | 0.78 |
| 3:F8:84:ARG:HD3 | 11:a9:139:ILE:HG21 | 1.65 | 0.78 |
| 3:F8:115:GLU:CG | 4:M8:3:VAL:HG11 | 2.04 | 0.78 |
| 3:O8:95:TYR:HD2 | 3:O8:108:ARG:NH2 | 1.75 | 0.78 |
| 3:L9:48:ALA:HB1 | 2:K9:18:PHE:CZ | 2.19 | 0.78 |
| 4:M9:192:GLN:NE2 | 3:V9:87:GLU:OE1 | 2.17 | 0.78 |
| 12:C9:201:CYC:HC | 12:C9:201:CYC:CMD | 1.97 | 0.78 |
| 3:H9:111:ASN:O | 11:a9:447:SER:HB3 | 1.83 | 0.78 |
| 11:aA:56:ILE:HD11 | 11:aA:612:TYR:HE2 | 1.40 | 0.78 |
| 11:aA:742:GLN:CD | 3:L1:88:ILE:HG12 | 2.04 | 0.78 |
| 3:F2:78:ARG:CD | 12:F2:201:CYC:CGD | 2.56 | 0.78 |
| 12:GA:201:CYC:HC | 12:GA:201:CYC:CMD | 1.97 | 0.78 |
| 2:IA:37:SER:HB3 | 2:IA:97:LEU:HD13 | 1.64 | 0.78 |
| 3:LA:51:ILE:CG2 | 3:LA:90:LEU:CD1 | 2.61 | 0.78 |
| 4:MA:1:MET:HB3 | 4:MA:44:SER:O | 1.84 | 0.78 |
| 2:SA:39:GLU:HA | 2:X4:69:PRO:HB3 | 1.62 | 0.78 |
| 12:K3:201:CYC:HC | 12:K3:201:CYC:CMD | 1.97 | 0.78 |
| 12:K2:201:CYC:HC | 12:K2:201:CYC:CMD | 1.97 | 0.78 |
| 12:S3:201:CYC:HC | 12:S3:201:CYC:CMD | 1.97 | 0.78 |
| 3:F4:84:ARG:CD | 11:aA:139:ILE:HG21 | 2.14 | 0.78 |
| 3:L4:68:ARG:CB | 11:aA:81:ASP:C | 2.57 | 0.78 |
| 4:M4:29:PRO:CG | 11:aA:226:PHE:CA | 2.49 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:M4:95:ALA:H | 3:Q4:88:ILE:HD13 | 1.49 | 0.78 |
| 3:O4:107:ASP:OD1 | 5:Z4:66:ARG:NH1 | 2.16 | 0.78 |
| 3:O4:119:ALA:HB2 | 5:Z4:72:GLU:H | 1.48 | 0.78 |
| 8:A5:106:GLU:CD | 10:k5:557:VAL:O | 2.27 | 0.78 |
| 1:B5:14:VAL:HG11 | 10:k5:555:ALA:HA | 1.66 | 0.78 |
| 8:e5:49:ARG:NH1 | 1:R5:50:THR:CG2 | 2.46 | 0.78 |
| 6:M6:283:VAL:CG1 | 8:Y7:75:GLU:CB | 2.42 | 0.78 |
| 8:A7:64:ASP:HA | 8:A7:67:SER:OG | 1.84 | 0.78 |
| 10:j5:230:VAL:O | 10:j5:234:LEU:CG | 2.31 | 0.78 |
| 10:j5:929:PRO:CG | 1:J7:147:LYS:CE | 2.60 | 0.78 |
| 10:j5:974:LEU:HG | 1:v7:1:MET:H3 | 1.02 | 0.78 |
| 10:j5:1118:THR:CB | 12:j5:1202:CYC:O2A | 2.32 | 0.78 |
| 1:N7:106:GLU:CG | 9:z7:58:THR:HG23 | 2.14 | 0.78 |
| 8:a7:56:ASP:OD1 | 11:a9:325:LEU:HD13 | 1.84 | 0.78 |
| 8:c7:17:TYR:HB3 | 1:d7:45:SER:HB3 | 1.64 | 0.78 |
| 2:A8:33:ARG:CZ | 12:L8:201:CYC:OB | 2.31 | 0.78 |
| 8:o7:97:VAL:CG2 | 1:p7:19:LEU:HD13 | 2.04 | 0.78 |
| 1:v7:68:PRO:O | 11:aA:42:ARG:CZ | 2.32 | 0.78 |
| 9:y7:3:ARG:NE | 9:y7:67:VAL:CG1 | 2.42 | 0.78 |
| 12:X8:201:CYC:HC | 12:X8:201:CYC:CMD | 1.97 | 0.78 |
| 12:H8:201:CYC:CBB | 11:a9:259:ALA:HA | 2.14 | 0.78 |
| 5:Z8:24:PRO:HG2 | 5:Z8:35:ASP:O | 1.83 | 0.78 |
| 12:S9:201:CYC:HC | 12:S9:201:CYC:CMD | 1.97 | 0.78 |
| 11:a9:308:LEU:CD2 | 11:a9:315:LEU:HD12 | 2.12 | 0.78 |
| 11:aA:89:ALA:HA | 11:aA:92:LYS:NZ | 1.98 | 0.78 |
| 12:AA:201:CYC:HC | 12:AA:201:CYC:CMD | 1.97 | 0.77 |
| 4:MA:29:PRO:HD3 | 11:aA:378:GLU:OE1 | 1.82 | 0.77 |
| 3:J3:84:ARG:HD3 | 11:a9:668:TYR:HD1 | 0.61 | 0.77 |
| 12:I2:201:CYC:HC | 12:I2:201:CYC:CMD | 1.97 | 0.77 |
| 4:M4:141:GLU:CD | 4:M4:145:LEU:HG | 2.09 | 0.77 |
| 2:N4:13:ASP:CG | 3:O4:108:ARG:CZ | 2.57 | 0.77 |
| 3:Q4:85:ASP:HA | 3:Q4:88:ILE:CG1 | 2.14 | 0.77 |
| 1:L5:82:ILE:HD11 | 8:G5:118:SER:HB2 | 1.65 | 0.77 |
| 12:F5:201:CYC:HMA2 | 10:k5:591:ILE:HG21 | 1.65 | 0.77 |
| 8:Y5:64:ASP:HA | 8:Y5:67:SER:OG | 1.83 | 0.77 |
| 8:A7:120:GLN:HG3 | 1:F7:53:LYS:HZ1 | 1.48 | 0.77 |
| 10:j5:929:PRO:HG2 | 1:J7:147:LYS:HG3 | 1.63 | 0.77 |
| 10:j5:1119:LEU:HD11 | 1:t7:87:TYR:CE2 | 2.19 | 0.77 |
| 8:I7:25:ARG:HH21 | 8:W7:25:ARG:CG | 1.96 | 0.77 |
| 8:M7:64:ASP:HA | 8:M7:67:SER:OG | 1.83 | 0.77 |
| 8:a7:29:PHE:CE1 | 8:a7:98:ALA:C | 2.61 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:c7:2:SER:OG | 1:d7:3:ASP:OD2 | 2.01 | 0.77 |
| 8:m7:29:PHE:CE1 | 8:m7:98:ALA:C | 2.61 | 0.77 |
| 8:o7:17:TYR:CE2 | 1:p7:93:THR:HB | 2.18 | 0.77 |
| 8:q7:45:GLU:OE1 | 3:H1:125:ARG:NE | 2.16 | 0.77 |
| 3:F8:115:GLU:CB | 4:M8:3:VAL:CG1 | 2.61 | 0.77 |
| 11:a9:632:ILE:HG21 | 11:a9:634:ALA:CB | 2.13 | 0.77 |
| 11:aA:290:ASP:O | 11:aA:291:TYR:CG | 2.36 | 0.77 |
| 12:K1:201:CYC:HC | 12:K1:201:CYC:CMD | 1.97 | 0.77 |
| 3:DA:14:LEU:HD11 | 3:ZA:125:ARG:HD2 | 1.65 | 0.77 |
| 4:MA:158:PHE:HA | 3:VA:108:ARG:CD | 2.14 | 0.77 |
| 2:O1:25:GLN:HG2 | 2:Y1:33:ARG:HG2 | 1.65 | 0.77 |
| 2:O1:33:ARG:CZ | 12:Z1:201:CYC:OB | 2.31 | 0.77 |
| 2:K3:33:ARG:HG2 | 2:A3:25:GLN:HG2 | 1.65 | 0.77 |
| 2:G2:16:GLY:CA | 6:M2:104:ARG:CZ | 2.61 | 0.77 |
| 12:A3:201:CYC:HC | 12:A3:201:CYC:CMD | 1.97 | 0.77 |
| 3:F4:113:LEU:HA | 4:M4:5:THR:HG23 | 1.61 | 0.77 |
| 2:N4:33:ARG:CZ | 12:Y4:201:CYC:OB | 2.32 | 0.77 |
| 3:Y4:88:ILE:HG22 | 3:Y4:91:ARG:HH21 | 1.48 | 0.77 |
| 8:A5:110:ILE:HG13 | 1:F5:76:ARG:HD3 | 1.66 | 0.77 |
| 8:c5:64:ASP:HA | 8:c5:67:SER:OG | 1.83 | 0.77 |
| 12:T5:201:CYC:O2A | 10:j5:483:PHE:HE1 | 1.68 | 0.77 |
| 8:U5:83:ARG:C | 6:M6:26:PHE:CE1 | 2.63 | 0.77 |
| 10:j5:192:LYS:HA | 10:j5:192:LYS:HZ2 | 1.48 | 0.77 |
| 10:j5:1019:SER:OG | 1:f7:87:TYR:HE1 | 1.66 | 0.77 |
| 10:j5:1056:PRO:HD2 | 10:j5:1057:LYS:N | 1.89 | 0.77 |
| 10:k5:136:VAL:HB | 10:k5:137:PRO:CD | 2.14 | 0.77 |
| 10:k5:230:VAL:O | 10:k5:234:LEU:CG | 2.31 | 0.77 |
| 10:k5:951:MET:HE1 | 10:k5:955:LEU:CG | 2.14 | 0.77 |
| 10:k5:990:ARG:CZ | 10:k5:1026:LYS:HZ1 | 1.97 | 0.77 |
| 10:k5:1015:TYR:O | 10:k5:1016:LEU:C | 2.27 | 0.77 |
| 12:E6:201:CYC:HC | 12:E6:201:CYC:CMD | 1.97 | 0.77 |
| 12:G6:201:CYC:HC | 12:G6:201:CYC:CMD | 1.97 | 0.77 |
| 8:I7:12:ASP:OD1 | 1:J7:91:TYR:OH | 2.02 | 0.77 |
| 8:i7:47:ARG:CD | 1:j7:18:TYR:CD2 | 2.67 | 0.77 |
| 8:U7:29:PHE:CE1 | 8:U7:98:ALA:C | 2.61 | 0.77 |
| 12:E1:201:CYC:HC | 12:E1:201:CYC:CMD | 1.97 | 0.77 |
| 12:B8:202:CYC:CMA | 4:M8:58:TYR:CA | 2.63 | 0.77 |
| 2:X8:69:PRO:O | 2:S9:42:ARG:HD3 | 1.83 | 0.77 |
| 3:H8:119:ALA:HB1 | 11:a9:266:ASN:ND2 | 1.98 | 0.77 |
| 2:N8:115:GLU:CB | 5:Z8:33:GLY:N | 2.47 | 0.77 |
| 3:Q8:78:ARG:HD3 | 12:Z8:301:CYC:HAD1 | 0.88 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:S8:113:LEU:C | 3:S8:116:THR:HG22 | 2.08 | 0.77 |
| 4:M9:274:VAL:CA | 3:V9:77:ARG:NE | 2.47 | 0.77 |
| 2:AA:25:GLN:HG2 | 2:KA:33:ARG:HG2 | 1.66 | 0.77 |
| 3:JA:111:ASN:N | 11:aA:518:ALA:CB | 2.48 | 0.77 |
| 12:QA:201:CYC:HAA1 | 3:TA:79:MET:HE3 | 1.64 | 0.77 |
| 2:K3:13:ASP:OD2 | 11:a9:707:PHE:CE2 | 2.37 | 0.77 |
| 2:A3:33:ARG:CZ | 12:L3:201:CYC:OB | 2.32 | 0.77 |
| 2:C3:140:SER:O | 3:D8:150:ARG:CZ | 2.31 | 0.77 |
| 12:B4:202:CYC:CMA | 4:M4:58:TYR:CA | 2.63 | 0.77 |
| 4:M3:1:MET:HB3 | 4:M3:44:SER:O | 1.84 | 0.77 |
| 4:M3:80:PRO:HA | 3:X3:111:ASN:ND2 | 2.00 | 0.77 |
| 12:O3:201:CYC:HC | 12:O3:201:CYC:CMD | 1.97 | 0.77 |
| 1:P5:114:GLU:CD | 10:k5:496:GLU:CG | 2.49 | 0.77 |
| 10:k5:388:ARG:HD3 | 10:k5:393:MET:H | 1.49 | 0.77 |
| 12:K8:201:CYC:HC | 12:K8:201:CYC:CMD | 1.97 | 0.77 |
| 4:M8:270:GLY:H | 3:Y8:108:ARG:HA | 1.49 | 0.77 |
| 3:O8:111:ASN:ND2 | 5:Z8:68:LEU:CD2 | 2.47 | 0.77 |
| 4:M9:1:MET:HB3 | 4:M9:44:SER:O | 1.84 | 0.77 |
| 4:M9:58:TYR:CE1 | 11:a9:496:ARG:NH2 | 2.52 | 0.77 |
| 11:aA:338:VAL:C | 11:aA:340:PRO:HD3 | 2.08 | 0.77 |
| 11:aA:643:LEU:CD2 | 11:aA:689:VAL:HG23 | 2.14 | 0.77 |
| 11:aA:667:THR:CG2 | 12:aA:901:CYC:CGA | 2.57 | 0.77 |
| 11:aA:735:VAL:N | 12:aA:902:CYC:CBA | 2.39 | 0.77 |
| 12:Y1:201:CYC:HC | 12:Y1:201:CYC:CMD | 1.97 | 0.77 |
| 12:C2:201:CYC:HC | 12:C2:201:CYC:CMD | 1.97 | 0.77 |
| 6:M2:57:GLU:CD | 8:i7:76:LYS:HZ1 | 1.92 | 0.77 |
| 7:N2:49:LEU:HD12 | 3:B2:84:ARG:CZ | 2.14 | 0.77 |
| 2:A4:33:ARG:CZ | 12:L4:201:CYC:OB | 2.31 | 0.77 |
| 3:B4:86:MET:HG3 | 12:B4:202:CYC:CBC | 2.14 | 0.77 |
| 5:N3:34:LEU:HB3 | 3:T3:84:ARG:HH11 | 1.49 | 0.77 |
| 3:F4:115:GLU:HG2 | 4:M4:3:VAL:HG21 | 1.64 | 0.77 |
| 4:M4:129:GLU:N | 4:M4:142:PHE:CZ | 2.50 | 0.77 |
| 4:M4:232:VAL:HG23 | 4:M4:235:PHE:CE2 | 2.19 | 0.77 |
| 1:L5:76:ARG:HD3 | 8:G5:110:ILE:HG13 | 1.66 | 0.77 |
| 8:O5:76:LYS:O | 8:O5:78:THR:N | 2.17 | 0.77 |
| 8:G5:134:LYS:HE2 | 8:o7:75:GLU:OE2 | 1.84 | 0.77 |
| 1:R5:106:GLU:HG3 | 10:k5:505:VAL:CA | 2.15 | 0.77 |
| 1:X5:144:ASP:HB3 | 8:a5:38:ARG:HH21 | 1.44 | 0.77 |
| 8:A7:56:ASP:CG | 11:aA:586:LEU:HD11 | 2.08 | 0.77 |
| 9:z5:8:THR:CG2 | 9:z5:52:LEU:HB2 | 2.14 | 0.77 |
| 10:j5:388:ARG:HD3 | 10:j5:393:MET:H | 1.49 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:j5:1024:LYS:O | 10:j5:1030:ILE:HG22 | 1.84 | 0.77 |
| 10:k5:931:VAL:O | 1:D7:29:ALA:HB1 | 1.83 | 0.77 |
| 10:k5:1024:LYS:O | 10:k5:1030:ILE:HG22 | 1.84 | 0.77 |
| 8:k7:64:ASP:HA | 8:k7:67:SER:OG | 1.83 | 0.77 |
| 2:E1:13:ASP:OD1 | 11:aA:644:ARG:NH1 | 2.16 | 0.77 |
| 3:H8:119:ALA:CB | 11:a9:266:ASN:CG | 2.58 | 0.77 |
| 3:T1:59:LEU:HD22 | 3:T1:130:ALA:HB2 | 1.67 | 0.77 |
| 12:HA:202:CYC:OB | 11:aA:474:PHE:CZ | 2.37 | 0.77 |
| 5:NA:66:ARG:HH12 | 3:TA:111:ASN:CG | 1.92 | 0.77 |
| 3:S4:113:LEU:C | 3:S4:116:THR:HG22 | 2.08 | 0.77 |
| 12:E4:201:CYC:HC | 12:E4:201:CYC:CMD | 1.97 | 0.77 |
| 4:M4:1:MET:HB3 | 4:M4:44:SER:O | 1.84 | 0.77 |
| 8:U5:79:ALA:CB | 6:M6:32:MET:CA | 2.63 | 0.77 |
| 9:z5:6:LYS:CB | 9:z5:55:LYS:HB3 | 2.15 | 0.77 |
| 9:i5:22:GLU:O | 9:i5:25:ASN:N | 2.16 | 0.77 |
| 10:j5:586:LEU:HD11 | 10:j5:607:LEU:CD2 | 2.14 | 0.77 |
| 10:k5:190:LEU:HB3 | 10:k5:194:CYS:HG | 1.47 | 0.77 |
| 8:I7:29:PHE:CE1 | 8:I7:98:ALA:C | 2.61 | 0.77 |
| 8:W7:13:ALA:HA | 9:w7:46:LYS:CE | 2.15 | 0.77 |
| 8:c7:44:THR:HG23 | 1:d7:18:TYR:CD2 | 2.20 | 0.77 |
| 12:A8:201:CYC:HC | 12:A8:201:CYC:CMD | 1.97 | 0.77 |
| 3:B8:120:LEU:HG | 4:M8:52:LEU:HD13 | 1.64 | 0.77 |
| 8:s7:12:ASP:OD1 | 1:t7:91:TYR:OH | 2.02 | 0.77 |
| 8:s7:29:PHE:HZ | 8:s7:98:ALA:O | 1.62 | 0.77 |
| 3:U8:59:LEU:HD22 | 3:U8:130:ALA:HB2 | 1.67 | 0.77 |
| 2:X8:107:ASP:HB3 | 4:M8:273:ILE:CG2 | 2.13 | 0.77 |
| 12:M8:302:CYC:HAC2 | 3:S8:78:ARG:CG | 2.14 | 0.77 |
| 12:N8:201:CYC:HC | 12:N8:201:CYC:CMD | 1.97 | 0.77 |
| 5:Z8:29:HIS:HE1 | 5:Z8:31:TRP:HB2 | 1.43 | 0.77 |
| 3:H9:84:ARG:NH2 | 11:a9:474:PHE:CD2 | 2.53 | 0.77 |
| 12:I9:201:CYC:HC | 12:I9:201:CYC:CMD | 1.97 | 0.77 |
| 11:aA:531:ASP:OD1 | 11:aA:531:ASP:N | 2.13 | 0.77 |
| 3:H1:81:ALA:CB | 12:H1:201:CYC:C3D | 2.63 | 0.77 |
| 12:E2:201:CYC:HC | 12:E2:201:CYC:CMD | 1.97 | 0.77 |
| 3:HA:72:ASN:OD1 | 12:HA:202:CYC:C2D | 2.32 | 0.77 |
| 12:OA:201:CYC:HC | 12:OA:201:CYC:CMD | 1.97 | 0.77 |
| 3:VA:59:LEU:HD22 | 3:VA:130:ALA:HB2 | 1.67 | 0.77 |
| 12:Q1:201:CYC:HC | 12:Q1:201:CYC:CMD | 1.97 | 0.77 |
| 12:I3:201:CYC:HC | 12:I3:201:CYC:CMD | 1.97 | 0.77 |
| 3:H2:77:ARG:HD2 | 6:M2:117:MET:HE3 | 1.67 | 0.77 |
| 2:A4:63:PHE:CB | 2:A4:66:LEU:CD1 | 2.55 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:B4:82:CYS:CB | 12:B4:202:CYC:C1C | 2.62 | 0.77 |
| 12:U3:201:CYC:HC | 12:U3:201:CYC:CMD | 1.97 | 0.77 |
| 3:H4:59:LEU:HD22 | 3:H4:130:ALA:HB2 | 1.67 | 0.77 |
| 4:M4:128:ALA:HB1 | 4:M4:142:PHE:CZ | 2.19 | 0.77 |
| 12:N4:201:CYC:HC | 12:N4:201:CYC:CMD | 1.97 | 0.77 |
| 10:k5:275:THR:HG23 | 10:k5:286:VAL:HG13 | 1.64 | 0.77 |
| 10:k5:1017:ARG:HH21 | 10:k5:1017:ARG:CB | 1.98 | 0.77 |
| 1:H7:54:GLU:OE2 | 11:aA:563:PHE:HB2 | 1.84 | 0.77 |
| 8:g7:25:ARG:CZ | 8:u7:25:ARG:CZ | 2.62 | 0.77 |
| 8:i7:25:ARG:HH22 | 8:s7:6:LYS:H | 1.31 | 0.77 |
| 8:U7:60:GLN:NE2 | 1:p7:117:ASN:OD1 | 2.17 | 0.77 |
| 1:Z7:67:ARG:HH12 | 11:a9:307:ARG:HG2 | 1.48 | 0.77 |
| 8:a7:25:ARG:NE | 8:o7:25:ARG:NE | 2.28 | 0.77 |
| 3:H8:59:LEU:HD22 | 3:H8:130:ALA:HB2 | 1.67 | 0.77 |
| 12:P8:201:CYC:HC | 12:P8:201:CYC:CMD | 1.97 | 0.77 |
| 3:L9:48:ALA:HB2 | 2:K9:18:PHE:CZ | 2.18 | 0.77 |
| 3:L9:97:LEU:O | 3:L9:97:LEU:HD12 | 1.84 | 0.77 |
| 3:H9:113:LEU:CD2 | 12:H9:202:CYC:CMB | 2.58 | 0.77 |
| 3:J9:111:ASN:N | 11:a9:518:ALA:CB | 2.48 | 0.77 |
| 11:aA:338:VAL:CG2 | 11:aA:340:PRO:HG3 | 2.15 | 0.77 |
| 12:I1:201:CYC:HC | 12:I1:201:CYC:CMD | 1.97 | 0.77 |
| 2:AA:33:ARG:CZ | 12:LA:201:CYC:OB | 2.31 | 0.77 |
| 3:FA:150:ARG:CA | 3:F9:150:ARG:HG2 | 2.07 | 0.77 |
| 2:OA:25:GLN:HG2 | 2:YA:33:ARG:HG2 | 1.65 | 0.77 |
| 2:OA:33:ARG:CZ | 12:ZA:201:CYC:OB | 2.31 | 0.77 |
| 3:TA:32:LYS:CD | 2:X4:57:GLN:CD | 2.58 | 0.77 |
| 12:O1:201:CYC:HC | 12:O1:201:CYC:CMD | 1.97 | 0.77 |
| 3:F4:108:ARG:C | 4:M4:6:THR:CG2 | 2.47 | 0.77 |
| 4:M4:205:ASP:CG | 5:Z4:62:ARG:HH21 | 1.92 | 0.77 |
| 5:Z4:1:MET:HA | 5:Z4:1:MET:CE | 2.10 | 0.77 |
| 12:K6:201:CYC:HC | 12:K6:201:CYC:CMD | 1.97 | 0.77 |
| 6:M6:50:LEU:HD21 | 8:c7:79:ALA:O | 1.82 | 0.77 |
| 9:i5:8:THR:CG2 | 9:i5:52:LEU:HB2 | 2.14 | 0.77 |
| 10:k5:729:ILE:CD1 | 1:D7:64:ASP:OD1 | 2.32 | 0.77 |
| 8:g7:10:ASN:HD22 | 8:u7:10:ASN:ND2 | 1.80 | 0.77 |
| 8:g7:29:PHE:HZ | 8:g7:98:ALA:O | 1.62 | 0.77 |
| 8:c7:112:VAL:CG1 | 8:c7:113:LYS:H | 1.98 | 0.77 |
| 8:u7:37:LEU:HD13 | 1:v7:24:LEU:HB3 | 1.67 | 0.77 |
| 3:L8:113:LEU:CD2 | 12:a9:901:CYC:CMB | 2.63 | 0.77 |
| 4:M8:224:PHE:O | 12:M8:301:CYC:O1A | 2.02 | 0.77 |
| 3:J9:70:GLY:HA2 | 11:a9:357:THR:C | 2.09 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:a9:818:ARG:HG3 | 11:a9:818:ARG:NH1 | 1.94 | 0.77 |
| 12:U1:201:CYC:HC | 12:U1:201:CYC:CMD | 1.97 | 0.77 |
| 3:HA:78:ARG:HD3 | 12:HA:202:CYC:O2D | 1.84 | 0.77 |
| 2:SA:38:MET:O | 2:X4:69:PRO:CG | 2.23 | 0.77 |
| 2:A1:63:PHE:CB | 2:A1:66:LEU:CD1 | 2.56 | 0.77 |
| 3:J3:121:GLY:HA2 | 11:a9:804:ARG:HH21 | 1.49 | 0.77 |
| 2:G2:116:VAL:HG21 | 3:L2:76:ASN:OD1 | 1.85 | 0.77 |
| 12:G2:201:CYC:HC | 12:G2:201:CYC:CMD | 1.97 | 0.77 |
| 3:Z3:77:ARG:HG3 | 4:M3:274:VAL:HG13 | 1.65 | 0.77 |
| 4:M4:232:VAL:CG2 | 4:M4:235:PHE:CE2 | 2.66 | 0.77 |
| 12:M4:301:CYC:HMC2 | 3:Y4:66:LEU:HD22 | 1.67 | 0.77 |
| 12:X4:201:CYC:HC | 12:X4:201:CYC:CMD | 1.97 | 0.77 |
| 8:E5:80:LEU:CD1 | 12:E5:201:CYC:CAD | 2.53 | 0.77 |
| 8:G5:107:ILE:CD1 | 1:H5:13:ASP:CG | 2.57 | 0.77 |
| 8:W5:16:ARG:HB2 | 1:X5:90:ARG:HH12 | 1.47 | 0.77 |
| 1:b5:18:TYR:HE2 | 10:k5:165:ARG:HA | 1.50 | 0.77 |
| 10:j5:1050:PHE:HZ | 1:r7:107:ARG:NH1 | 1.82 | 0.77 |
| 8:U7:12:ASP:OD1 | 1:V7:91:TYR:OH | 2.02 | 0.77 |
| 3:U8:115:GLU:OE2 | 4:M8:70:SER:HB2 | 1.83 | 0.77 |
| 12:G8:201:CYC:HC | 12:G8:201:CYC:CMD | 1.97 | 0.77 |
| 4:M8:56:MET:HE1 | 4:M8:66:VAL:HG22 | 1.66 | 0.77 |
| 2:N8:13:ASP:CG | 3:O8:108:ARG:CZ | 2.57 | 0.77 |
| 2:N8:33:ARG:CZ | 12:Y8:201:CYC:OB | 2.32 | 0.77 |
| 3:S8:59:LEU:HD22 | 3:S8:130:ALA:HB2 | 1.67 | 0.77 |
| 1:A:158:SER:HB2 | 1:R5:11:ASN:HD22 | 1.46 | 0.77 |
| 3:JA:114:LYS:CG | 8:S7:60:GLN:NE2 | 2.48 | 0.77 |
| 3:TA:59:LEU:HD22 | 3:TA:130:ALA:HB2 | 1.67 | 0.77 |
| 3:B3:84:ARG:NH1 | 12:B3:202:CYC:O2A | 2.17 | 0.77 |
| 3:F4:91:ARG:NH2 | 11:aA:140:GLN:HE22 | 1.74 | 0.77 |
| 12:K4:201:CYC:HC | 12:K4:201:CYC:CMD | 1.97 | 0.77 |
| 2:N4:111:ALA:HB1 | 5:Z4:34:LEU:HG | 0.77 | 0.77 |
| 1:L5:68:PRO:C | 1:H5:14:VAL:O | 2.28 | 0.77 |
| 8:M5:64:ASP:HA | 8:M5:67:SER:OG | 1.83 | 0.77 |
| 8:G5:49:ARG:HH21 | 8:G5:140:LEU:HD22 | 1.46 | 0.77 |
| 8:S5:90:ARG:HD2 | 1:T5:17:LYS:C | 2.09 | 0.77 |
| 8:W5:12:ASP:N | 1:X5:94:TYR:CE2 | 2.38 | 0.77 |
| 3:J6:59:LEU:HD22 | 3:J6:130:ALA:HB2 | 1.67 | 0.77 |
| 12:L6:202:CYC:OB | 2:A6:33:ARG:CZ | 2.32 | 0.77 |
| 10:j5:56:ILE:CG2 | 10:j5:57:VAL:N | 2.46 | 0.77 |
| 10:j5:990:ARG:CZ | 10:j5:1026:LYS:HZ1 | 1.98 | 0.77 |
| 10:k5:586:LEU:HD11 | 10:k5:607:LEU:CD2 | 2.15 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:k5:1119:LEU:HD11 | 12:k5:1204:CYC:CBB | 2.14 | 0.77 |
| 8:O7:49:ARG:HH11 | 1:r7:114:GLU:CD | 1.89 | 0.77 |
| 1:h7:66:THR:OG1 | 12:i7:201:CYC:O2A | 2.02 | 0.77 |
| 8:i7:47:ARG:HG3 | 1:j7:18:TYR:OH | 1.83 | 0.77 |
| 8:m7:12:ASP:OD1 | 1:n7:91:TYR:OH | 2.02 | 0.77 |
| 3:J8:59:LEU:HD22 | 3:J8:130:ALA:HB2 | 1.67 | 0.77 |
| 3:L8:59:LEU:HD22 | 3:L8:130:ALA:HB2 | 1.67 | 0.77 |
| 3:L9:14:LEU:HG | 11:a9:358:PRO:CB | 2.14 | 0.77 |
| 3:L9:113:LEU:N | 11:a9:532:ALA:HB3 | 1.99 | 0.77 |
| 3:J9:59:LEU:HD22 | 3:J9:130:ALA:HB2 | 1.67 | 0.77 |
| 4:MA:58:TYR:CE1 | 11:aA:496:ARG:NH2 | 2.53 | 0.77 |
| 3:TA:28:THR:CG2 | 2:X4:67:THR:O | 2.33 | 0.77 |
| 3:L2:70:GLY:CA | 6:M2:67:GLY:HA2 | 2.15 | 0.77 |
| 3:B3:59:LEU:HD22 | 3:B3:130:ALA:HB2 | 1.67 | 0.77 |
| 3:F4:88:ILE:CD1 | 11:aA:140:GLN:HG2 | 2.15 | 0.77 |
| 4:M4:56:MET:SD | 4:M4:66:VAL:CG2 | 2.73 | 0.77 |
| 3:O4:59:LEU:HD22 | 3:O4:130:ALA:HB2 | 1.67 | 0.77 |
| 3:O4:111:ASN:HB2 | 5:Z4:67:ILE:HB | 1.66 | 0.77 |
| 2:P4:12:ALA:HB1 | 3:Q4:95:TYR:OH | 1.85 | 0.77 |
| 12:R4:201:CYC:HC | 12:R4:201:CYC:CMD | 1.97 | 0.77 |
| 1:f5:114:GLU:HB3 | 10:j5:491:THR:CB | 2.15 | 0.77 |
| 10:j5:1017:ARG:HH21 | 10:j5:1017:ARG:CB | 1.98 | 0.77 |
| 10:k5:136:VAL:HB | 10:k5:137:PRO:HD2 | 1.67 | 0.77 |
| 12:I6:201:CYC:HC | 12:I6:201:CYC:CMD | 1.97 | 0.77 |
| 1:H7:136:VAL:HA | 11:aA:563:PHE:HZ | 1.49 | 0.77 |
| 8:c7:124:PRO:O | 8:c7:125:ALA:C | 2.13 | 0.77 |
| 12:V8:201:CYC:HC | 12:V8:201:CYC:CMD | 1.97 | 0.77 |
| 3:L8:68:ARG:CB | 11:a9:81:ASP:HA | 2.09 | 0.77 |
| 4:M8:217:VAL:HG21 | 5:Z8:30:PRO:HG3 | 0.77 | 0.77 |
| 4:M9:160:THR:N | 3:V9:108:ARG:CG | 2.48 | 0.77 |
| 3:B9:59:LEU:HD22 | 3:B9:130:ALA:HB2 | 1.67 | 0.77 |
| 12:W9:201:CYC:HC | 12:W9:201:CYC:CMD | 1.97 | 0.77 |
| 11:aA:710:THR:HG22 | 11:aA:807:GLN:HG3 | 1.40 | 0.77 |
| 3:HA:59:LEU:HD22 | 3:HA:130:ALA:HB2 | 1.67 | 0.76 |
| 3:HA:108:ARG:NH1 | 11:aA:448:ASN:ND2 | 2.32 | 0.76 |
| 3:LA:113:LEU:N | 11:aA:532:ALA:HB3 | 2.00 | 0.76 |
| 12:SA:201:CYC:HC | 12:SA:201:CYC:CMD | 1.97 | 0.76 |
| 3:J3:84:ARG:CZ | 11:a9:669:ILE:O | 2.32 | 0.76 |
| 12:J3:202:CYC:HMA2 | 11:a9:666:ASN:CB | 2.15 | 0.76 |
| 3:H2:59:LEU:HD22 | 3:H2:130:ALA:HB2 | 1.67 | 0.76 |
| 3:B3:88:ILE:CG2 | 12:B3:202:CYC:CMB | 2.62 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:A4:25:GLN:HG2 | 2:K4:33:ARG:HG2 | 1.66 | 0.76 |
| 3:D4:59:LEU:HD22 | 3:D4:130:ALA:HB2 | 1.67 | 0.76 |
| 4:M3:98:ASP:OD1 | 3:T3:1:MET:N | 2.16 | 0.76 |
| 12:N5:201:CYC:O2A | 10:k5:483:PHE:HE1 | 1.68 | 0.76 |
| 8:S5:66:VAL:CG1 | 8:E7:68:PRO:HG3 | 2.13 | 0.76 |
| 10:j5:990:ARG:HH11 | 10:j5:990:ARG:HG2 | 1.50 | 0.76 |
| 10:j5:1009:ALA:CB | 1:v7:87:TYR:CE1 | 2.44 | 0.76 |
| 10:j5:1023:SER:CB | 12:f7:201:CYC:HBA1 | 2.15 | 0.76 |
| 10:j5:1077:ILE:C | 12:r7:201:CYC:HBA2 | 2.11 | 0.76 |
| 10:k5:385:PRO:O | 10:k5:386:ILE:C | 2.23 | 0.76 |
| 3:F6:59:LEU:HD22 | 3:F6:130:ALA:HB2 | 1.67 | 0.76 |
| 3:F6:130:ALA:HB1 | 12:F6:201:CYC:CBC | 2.15 | 0.76 |
| 3:H6:59:LEU:HD22 | 3:H6:130:ALA:HB2 | 1.67 | 0.76 |
| 8:g7:90:ARG:HD2 | 1:h7:17:LYS:C | 2.10 | 0.76 |
| 12:C8:201:CYC:HC | 12:C8:201:CYC:CMD | 1.97 | 0.76 |
| 8:o7:17:TYR:HD2 | 1:p7:93:THR:CG2 | 1.97 | 0.76 |
| 1:v7:136:VAL:CG1 | 11:aA:342:ARG:HH12 | 1.97 | 0.76 |
| 2:T8:111:ALA:HB1 | 4:M8:87:ILE:HG21 | 1.67 | 0.76 |
| 11:a9:643:LEU:CD2 | 11:a9:689:VAL:HG23 | 2.15 | 0.76 |
| 11:aA:795:ASP:HB3 | 3:J1:108:ARG:O | 1.85 | 0.76 |
| 3:H1:78:ARG:O | 12:H1:201:CYC:HMD3 | 1.85 | 0.76 |
| 5:N1:34:LEU:HB3 | 3:T1:84:ARG:HH11 | 1.49 | 0.76 |
| 1:Z:13:ASP:CG | 8:e5:107:ILE:HD13 | 2.09 | 0.76 |
| 1:Z:118:SER:OG | 10:j5:9:SER:HB2 | 1.85 | 0.76 |
| 2:QA:70:GLY:C | 2:QA:74:TYR:CE2 | 2.62 | 0.76 |
| 3:P1:59:LEU:HD22 | 3:P1:130:ALA:HB2 | 1.67 | 0.76 |
| 3:L2:59:LEU:HD22 | 3:L2:130:ALA:HB2 | 1.67 | 0.76 |
| 12:Z3:202:CYC:HC | 12:Z3:202:CYC:CMD | 1.99 | 0.76 |
| 3:V3:59:LEU:HD22 | 3:V3:130:ALA:HB2 | 1.67 | 0.76 |
| 12:G4:201:CYC:HC | 12:G4:201:CYC:CMD | 1.97 | 0.76 |
| 4:M4:93:LEU:O | 4:M4:216:ASN:ND2 | 2.18 | 0.76 |
| 3:Y4:124:THR:CB | 3:Y4:172:ALA:HA | 2.14 | 0.76 |
| 5:Z4:28:HIS:HB3 | 5:Z4:35:ASP:HA | 1.66 | 0.76 |
| 8:A5:107:ILE:CD1 | 1:B5:13:ASP:CG | 2.58 | 0.76 |
| 8:S5:110:ILE:HD12 | 10:j5:533:LEU:CD1 | 2.15 | 0.76 |
| 1:T5:110:ASN:CG | 10:j5:692:LEU:C | 2.53 | 0.76 |
| 7:N6:49:LEU:HD12 | 3:B6:84:ARG:CZ | 2.14 | 0.76 |
| 10:k5:192:LYS:HA | 10:k5:192:LYS:HZ2 | 1.48 | 0.76 |
| 12:k5:1204:CYC:CMA | 12:k5:1204:CYC:HB | 1.99 | 0.76 |
| 8:c7:17:TYR:CE2 | 1:d7:44:ILE:HG22 | 2.19 | 0.76 |
| 8:o7:30:VAL:HA | 1:p7:31:PHE:HD1 | 1.50 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:U8:202:CYC:CMD | 12:U8:202:CYC:HC | 1.99 | 0.76 |
| 3:F8:59:LEU:HD22 | 3:F8:130:ALA:HB2 | 1.67 | 0.76 |
| 4:M8:197:ASP:O | 5:Z8:52:ARG:NH1 | 2.16 | 0.76 |
| 3:Q8:72:ASN:ND2 | 12:Z8:301:CYC:HMD3 | 1.99 | 0.76 |
| 3:Q8:77:ARG:N | 5:Z8:34:LEU:HD13 | 1.98 | 0.76 |
| 3:Q8:117:TYR:HE1 | 5:Z8:39:PRO:HG2 | 1.47 | 0.76 |
| 12:Q9:201:CYC:HC | 12:Q9:201:CYC:CMD | 1.97 | 0.76 |
| 12:G1:201:CYC:HC | 12:G1:201:CYC:CMD | 1.97 | 0.76 |
| 11:a9:615:ARG:HH11 | 11:a9:615:ARG:HB3 | 1.48 | 0.76 |
| 11:aA:711:SER:HB3 | 3:L1:111:ASN:HB3 | 1.65 | 0.76 |
| 12:W1:201:CYC:HC | 12:W1:201:CYC:CMD | 1.97 | 0.76 |
| 3:X1:59:LEU:HD22 | 3:X1:130:ALA:HB2 | 1.67 | 0.76 |
| 3:LA:97:LEU:O | 3:LA:97:LEU:HD12 | 1.84 | 0.76 |
| 12:YA:201:CYC:HC | 12:YA:201:CYC:CMD | 1.97 | 0.76 |
| 4:M4:232:VAL:N | 12:M4:301:CYC:CBB | 2.48 | 0.76 |
| 4:M4:273:ILE:HG23 | 2:X4:107:ASP:HB3 | 1.68 | 0.76 |
| 8:K5:24:ASP:OD1 | 8:U5:148:GLU:OE1 | 2.02 | 0.76 |
| 12:N5:201:CYC:CMA | 12:N5:201:CYC:HB | 1.99 | 0.76 |
| 5:Z4:22:LEU:HD12 | 5:Z4:22:LEU:O | 1.86 | 0.76 |
| 1:d5:67:ARG:NH1 | 10:j5:705:THR:CB | 2.47 | 0.76 |
| 8:Q5:16:ARG:CB | 1:R5:90:ARG:HH11 | 1.81 | 0.76 |
| 3:L6:59:LEU:HD22 | 3:L6:130:ALA:HB2 | 1.67 | 0.76 |
| 10:j5:320:GLU:HA | 10:j5:333:PHE:HE1 | 1.50 | 0.76 |
| 10:j5:875:LEU:HD21 | 10:j5:885:GLN:HE22 | 1.50 | 0.76 |
| 12:j7:201:CYC:CMA | 12:j7:201:CYC:HB | 1.99 | 0.76 |
| 8:c7:20:PRO:HG3 | 8:m7:155:TYR:CB | 1.97 | 0.76 |
| 8:o7:23:LEU:HD22 | 1:p7:38:VAL:CG1 | 2.15 | 0.76 |
| 8:u7:17:TYR:CE2 | 1:v7:93:THR:HB | 2.18 | 0.76 |
| 1:v7:68:PRO:HB2 | 11:aA:42:ARG:HD3 | 1.67 | 0.76 |
| 3:U8:111:ASN:OD1 | 4:M8:77:LEU:CD1 | 2.32 | 0.76 |
| 3:U8:114:LYS:HZ1 | 4:M8:13:LYS:HZ2 | 1.32 | 0.76 |
| 2:X8:60:TYR:CB | 3:T9:32:LYS:HZ2 | 1.99 | 0.76 |
| 3:L8:68:ARG:HB2 | 11:a9:82:GLN:CB | 2.15 | 0.76 |
| 4:M8:197:ASP:O | 5:Z8:52:ARG:NH2 | 2.17 | 0.76 |
| 12:M8:301:CYC:OC | 3:Y8:72:ASN:OD1 | 2.03 | 0.76 |
| 3:Q8:127:VAL:HG21 | 12:Z8:301:CYC:HMC2 | 1.65 | 0.76 |
| 12:O9:201:CYC:HC | 12:O9:201:CYC:CMD | 1.97 | 0.76 |
| 3:Y8:59:LEU:HD22 | 3:Y8:130:ALA:HB2 | 1.67 | 0.76 |
| 3:V9:59:LEU:HD22 | 3:V9:130:ALA:HB2 | 1.67 | 0.76 |
| 4:M1:118:TYR:CD2 | 3:X1:84:ARG:NE | 2.54 | 0.76 |
| 12:T1:301:CYC:HMA1 | 12:T1:301:CYC:HB | 1.51 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:D2:202:CYC:CMD | 12:D2:202:CYC:HC | 1.99 | 0.76 |
| 12:EA:201:CYC:HC | 12:EA:201:CYC:CMD | 1.97 | 0.76 |
| 5:NA:7:ASP:N | 3:RA:107:ASP:O | 2.19 | 0.76 |
| 12:QA:201:CYC:CBB | 3:TA:75:PRO:HB2 | 2.12 | 0.76 |
| 12:WA:201:CYC:HC | 12:WA:201:CYC:CMD | 1.97 | 0.76 |
| 12:L2:202:CYC:OB | 2:A2:33:ARG:CZ | 2.32 | 0.76 |
| 3:Z3:59:LEU:HD22 | 3:Z3:130:ALA:HB2 | 1.67 | 0.76 |
| 12:B4:202:CYC:HMA1 | 12:B4:202:CYC:HB | 1.51 | 0.76 |
| 3:S4:59:LEU:HD22 | 3:S4:130:ALA:HB2 | 1.67 | 0.76 |
| 3:U4:108:ARG:HB3 | 4:M4:246:ALA:HB2 | 1.63 | 0.76 |
| 1:N5:110:ASN:HD21 | 10:k5:692:LEU:HB3 | 0.61 | 0.76 |
| 5:Z4:14:LYS:HE2 | 5:Z4:50:LEU:HD23 | 1.67 | 0.76 |
| 8:G5:61:ILE:CD1 | 8:o7:68:PRO:CD | 2.64 | 0.76 |
| 8:U5:75:GLU:OE1 | 6:M6:43:TRP:HZ2 | 1.64 | 0.76 |
| 12:X5:201:CYC:HBB2 | 10:j5:520:ARG:CD | 2.14 | 0.76 |
| 1:Z5:67:ARG:NH1 | 10:k5:705:THR:OG1 | 2.18 | 0.76 |
| 1:b5:5:ILE:HD13 | 10:k5:46:PHE:HZ | 1.41 | 0.76 |
| 10:j5:66:MET:HA | 10:j5:66:MET:CE | 2.16 | 0.76 |
| 10:j5:929:PRO:HG3 | 1:J7:147:LYS:CE | 2.14 | 0.76 |
| 10:k5:990:ARG:HH11 | 10:k5:990:ARG:HG2 | 1.50 | 0.76 |
| 12:A6:201:CYC:HC | 12:A6:201:CYC:CMD | 1.97 | 0.76 |
| 3:D1:59:LEU:HD22 | 3:D1:130:ALA:HB2 | 1.67 | 0.76 |
| 8:S7:25:ARG:CZ | 8:G7:25:ARG:CZ | 2.63 | 0.76 |
| 12:X7:201:CYC:CMA | 12:X7:201:CYC:HB | 1.99 | 0.76 |
| 8:a7:90:ARG:HD2 | 1:b7:17:LYS:C | 2.10 | 0.76 |
| 8:a7:107:ILE:CD1 | 1:b7:13:ASP:CG | 2.57 | 0.76 |
| 8:c7:11:ALA:HB1 | 1:d7:94:TYR:CE1 | 2.19 | 0.76 |
| 12:p7:201:CYC:CMA | 12:p7:201:CYC:HB | 1.99 | 0.76 |
| 8:q7:64:ASP:HB3 | 11:aA:69:ARG:NH2 | 1.99 | 0.76 |
| 12:I8:201:CYC:HC | 12:I8:201:CYC:CMD | 1.97 | 0.76 |
| 3:L8:85:ASP:OD2 | 12:a9:901:CYC:ND | 2.18 | 0.76 |
| 4:M9:50:ASP:OD1 | 4:M9:50:ASP:N | 2.15 | 0.76 |
| 4:M9:190:ARG:HH12 | 4:M9:202:SER:CB | 1.98 | 0.76 |
| 5:N9:22:LEU:HD12 | 5:N9:22:LEU:O | 1.86 | 0.76 |
| 12:A9:201:CYC:HC | 12:A9:201:CYC:CMD | 1.97 | 0.76 |
| 3:F9:148:VAL:O | 3:F9:149:THR:C | 2.27 | 0.76 |
| 12:F9:303:CYC:CMD | 12:F9:303:CYC:HC | 1.98 | 0.76 |
| 3:H9:59:LEU:HD22 | 3:H9:130:ALA:HB2 | 1.67 | 0.76 |
| 11:a9:239:TYR:OH | 12:a9:901:CYC:NB | 2.16 | 0.76 |
| 11:a9:350:LEU:HD12 | 11:a9:350:LEU:H | 1.50 | 0.76 |
| 11:aA:803:ASN:HB3 | 3:J1:119:ALA:C | 2.11 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:A:201:CYC:CMA | 12:A:201:CYC:HB | 1.99 | 0.76 |
| 3:BA:59:LEU:HD22 | 3:BA:130:ALA:HB2 | 1.67 | 0.76 |
| 12:CA:201:CYC:HC | 12:CA:201:CYC:CMD | 1.97 | 0.76 |
| 12:IA:201:CYC:HC | 12:IA:201:CYC:CMD | 1.97 | 0.76 |
| 3:LA:120:LEU:CD2 | 11:aA:538:ARG:HB2 | 2.15 | 0.76 |
| 5:NA:54:LEU:HD21 | 3:TA:84:ARG:HD2 | 1.67 | 0.76 |
| 2:A1:25:GLN:HG2 | 2:K1:33:ARG:HG2 | 1.65 | 0.76 |
| 2:K3:15:GLN:C | 11:a9:745:GLY:CA | 2.58 | 0.76 |
| 6:M2:62:ARG:HH22 | 1:h7:57:ALA:C | 1.93 | 0.76 |
| 3:X3:59:LEU:HD22 | 3:X3:130:ALA:HB2 | 1.67 | 0.76 |
| 3:B1:111:ASN:ND2 | 4:M1:7:SER:OG | 2.16 | 0.76 |
| 3:F4:107:ASP:CB | 4:M4:8:SER:CB | 2.24 | 0.76 |
| 3:Q4:104:VAL:HG22 | 3:Q4:105:LEU:HD12 | 1.64 | 0.76 |
| 12:L5:201:CYC:O2A | 10:j5:591:ILE:HG13 | 1.86 | 0.76 |
| 1:B5:14:VAL:O | 1:F5:68:PRO:C | 2.28 | 0.76 |
| 1:d5:67:ARG:HH12 | 10:j5:705:THR:HB | 1.50 | 0.76 |
| 10:j5:275:THR:CG2 | 10:j5:286:VAL:O | 2.33 | 0.76 |
| 10:j5:631:HIS:CG | 10:j5:664:MET:HE1 | 2.21 | 0.76 |
| 10:j5:1015:TYR:O | 10:j5:1016:LEU:C | 2.27 | 0.76 |
| 10:k5:1070:ALA:HB1 | 10:k5:1071:PRO:HD3 | 1.67 | 0.76 |
| 1:N7:14:VAL:HG12 | 9:z7:64:ASN:ND2 | 2.00 | 0.76 |
| 8:g7:107:ILE:CD1 | 1:h7:13:ASP:CG | 2.57 | 0.76 |
| 12:h7:201:CYC:CMA | 12:h7:201:CYC:HB | 1.99 | 0.76 |
| 1:T7:106:GLU:HG2 | 9:w7:58:THR:CG2 | 2.15 | 0.76 |
| 12:T8:201:CYC:HC | 12:T8:201:CYC:CMD | 1.97 | 0.76 |
| 2:X8:16:GLY:C | 4:M8:228:SER:CB | 2.58 | 0.76 |
| 2:X8:67:THR:O | 3:T9:28:THR:CG2 | 2.33 | 0.76 |
| 12:R8:201:CYC:HC | 12:R8:201:CYC:CMD | 1.97 | 0.76 |
| 12:F9:302:CYC:HC | 12:F9:302:CYC:CMD | 1.98 | 0.76 |
| 11:a9:338:VAL:CG2 | 11:a9:340:PRO:HG3 | 2.15 | 0.76 |
| 11:aA:632:ILE:N | 3:J1:111:ASN:ND2 | 2.34 | 0.76 |
| 3:L1:59:LEU:HD22 | 3:L1:130:ALA:HB2 | 1.67 | 0.76 |
| 5:N1:36:THR:OG1 | 12:T1:301:CYC:C4B | 2.33 | 0.76 |
| 12:A2:201:CYC:HC | 12:A2:201:CYC:CMD | 1.97 | 0.76 |
| 3:JA:59:LEU:HD22 | 3:JA:130:ALA:HB2 | 1.67 | 0.76 |
| 3:ZA:59:LEU:HD22 | 3:ZA:130:ALA:HB2 | 1.67 | 0.76 |
| 12:R1:202:CYC:HC | 12:R1:202:CYC:CMD | 1.99 | 0.76 |
| 3:B3:112:GLY:N | 4:M3:76:ALA:HB1 | 2.01 | 0.76 |
| 12:E3:201:CYC:HC | 12:E3:201:CYC:CMD | 1.97 | 0.76 |
| 12:A4:201:CYC:HC | 12:A4:201:CYC:CMD | 1.97 | 0.76 |
| 3:L3:104:VAL:HB | 3:L3:108:ARG:HH22 | 1.50 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:W3:201:CYC:HC | 12:W3:201:CYC:CMD | 1.97 | 0.76 |
| 3:B1:112:GLY:N | 4:M1:76:ALA:HB1 | 2.01 | 0.76 |
| 3:L4:59:LEU:HD22 | 3:L4:130:ALA:HB2 | 1.67 | 0.76 |
| 4:M4:87:ILE:HD12 | 3:Y4:77:ARG:CG | 2.13 | 0.76 |
| 5:Z4:41:GLN:OE1 | 12:Z4:301:CYC:HBB2 | 1.85 | 0.76 |
| 1:J5:3:ASP:OD1 | 1:J5:3:ASP:N | 2.10 | 0.76 |
| 1:d5:127:VAL:HG11 | 10:j5:697:PHE:C | 2.10 | 0.76 |
| 12:P5:201:CYC:HB | 12:P5:201:CYC:CMA | 1.99 | 0.76 |
| 2:K6:33:ARG:HG2 | 2:A6:25:GLN:HG2 | 1.66 | 0.76 |
| 6:M6:66:GLY:CA | 1:b7:125:ALA:HA | 2.16 | 0.76 |
| 10:k5:875:LEU:HD21 | 10:k5:885:GLN:HE22 | 1.50 | 0.76 |
| 10:k5:888:THR:HG21 | 1:D7:83:ARG:NH1 | 1.99 | 0.76 |
| 12:C6:201:CYC:HC | 12:C6:201:CYC:CMD | 1.97 | 0.76 |
| 3:F6:78:ARG:HG2 | 12:F6:201:CYC:CGD | 2.16 | 0.76 |
| 8:C7:102:THR:CB | 8:C7:103:PRO:CD | 2.64 | 0.76 |
| 8:a7:90:ARG:CZ | 1:b7:16:GLY:HA2 | 2.16 | 0.76 |
| 8:s7:102:THR:CB | 8:s7:103:PRO:CD | 2.64 | 0.76 |
| 4:M8:205:ASP:OD2 | 5:Z8:59:ARG:CB | 2.34 | 0.76 |
| 3:O8:59:LEU:HD22 | 3:O8:130:ALA:HB2 | 1.67 | 0.76 |
| 3:L9:52:ILE:CD1 | 3:L9:87:GLU:CG | 2.61 | 0.76 |
| 4:M9:29:PRO:HD3 | 11:a9:378:GLU:OE1 | 1.83 | 0.76 |
| 5:N9:54:LEU:HA | 12:T9:301:CYC:HMA2 | 1.68 | 0.76 |
| 3:X9:59:LEU:HD22 | 3:X9:130:ALA:HB2 | 1.67 | 0.76 |
| 3:H1:59:LEU:HD22 | 3:H1:130:ALA:HB2 | 1.67 | 0.76 |
| 12:J1:201:CYC:CMD | 12:J1:201:CYC:HC | 1.99 | 0.76 |
| 3:TA:25:ASN:HB3 | 2:X4:64:PRO:O | 1.85 | 0.76 |
| 3:T3:59:LEU:HD22 | 3:T3:130:ALA:HB2 | 1.67 | 0.76 |
| 3:S4:82:CYS:HA | 12:S4:202:CYC:HAC1 | 1.65 | 0.76 |
| 4:M4:269:SER:O | 3:Y4:108:ARG:HA | 1.85 | 0.76 |
| 12:d5:201:CYC:HB | 12:d5:201:CYC:CMA | 1.99 | 0.76 |
| 1:R5:86:ASP:CG | 1:R5:90:ARG:HE | 1.94 | 0.76 |
| 12:Z5:201:CYC:CMA | 12:Z5:201:CYC:HB | 1.99 | 0.76 |
| 3:L6:70:GLY:CA | 6:M6:67:GLY:HA2 | 2.15 | 0.76 |
| 10:j5:743:VAL:HG13 | 12:J7:201:CYC:O2D | 1.86 | 0.76 |
| 8:k7:76:LYS:NZ | 11:a9:604:ALA:HB1 | 2.01 | 0.76 |
| 12:f7:201:CYC:CMA | 12:f7:201:CYC:HB | 1.99 | 0.76 |
| 12:B8:202:CYC:HMA1 | 12:B8:202:CYC:HB | 1.50 | 0.76 |
| 8:o7:97:VAL:HG22 | 1:p7:19:LEU:CD1 | 2.15 | 0.76 |
| 3:L8:68:ARG:CB | 11:a9:81:ASP:C | 2.58 | 0.76 |
| 4:M8:140:ARG:NE | 4:M8:209:TYR:CE1 | 2.53 | 0.76 |
| 12:M8:301:CYC:C3B | 3:Y8:88:ILE:CG2 | 2.64 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:M8:302:CYC:C2C | 3:S8:78:ARG:HD2 | 2.06 | 0.76 |
| 3:L9:59:LEU:HD22 | 3:L9:130:ALA:HB2 | 1.67 | 0.76 |
| 3:F9:59:LEU:HD22 | 3:F9:130:ALA:HB2 | 1.67 | 0.76 |
| 12:G9:201:CYC:HC | 12:G9:201:CYC:CMD | 1.97 | 0.76 |
| 3:H9:120:LEU:HD13 | 12:H9:202:CYC:CAA | 2.14 | 0.76 |
| 12:J9:201:CYC:HC | 12:J9:201:CYC:CMD | 1.98 | 0.76 |
| 11:a9:418:LEU:HD13 | 11:a9:428:PHE:HB2 | 1.68 | 0.76 |
| 11:aA:775:LYS:CA | 12:H1:201:CYC:HBA2 | 2.13 | 0.76 |
| 3:Z1:59:LEU:HD22 | 3:Z1:130:ALA:HB2 | 1.67 | 0.76 |
| 12:Z:201:CYC:HB | 12:Z:201:CYC:CMA | 1.99 | 0.76 |
| 3:DA:111:ASN:O | 4:MA:6:THR:N | 2.18 | 0.76 |
| 3:LA:59:LEU:HD22 | 3:LA:130:ALA:HB2 | 1.67 | 0.76 |
| 4:MA:160:THR:N | 3:VA:108:ARG:CG | 2.48 | 0.76 |
| 12:QA:201:CYC:HC | 12:QA:201:CYC:CMD | 1.97 | 0.76 |
| 12:H2:202:CYC:CMD | 12:H2:202:CYC:HC | 1.99 | 0.76 |
| 12:J2:201:CYC:CMD | 12:J2:201:CYC:HC | 1.98 | 0.76 |
| 6:M2:62:ARG:HH22 | 1:h7:58:LYS:CA | 1.92 | 0.76 |
| 12:F3:202:CYC:HC | 12:F3:202:CYC:CMD | 1.99 | 0.76 |
| 3:L3:59:LEU:HD22 | 3:L3:130:ALA:HB2 | 1.67 | 0.76 |
| 3:R3:59:LEU:HD22 | 3:R3:130:ALA:HB2 | 1.67 | 0.76 |
| 12:W4:202:CYC:CMD | 12:W4:202:CYC:HC | 1.99 | 0.76 |
| 3:F4:59:LEU:HD22 | 3:F4:130:ALA:HB2 | 1.67 | 0.76 |
| 4:M4:205:ASP:CG | 5:Z4:62:ARG:NH2 | 2.44 | 0.76 |
| 3:Q4:77:ARG:HA | 5:Z4:34:LEU:CB | 2.01 | 0.76 |
| 8:K5:20:PRO:CD | 8:U5:155:TYR:HB2 | 2.14 | 0.76 |
| 8:Q5:16:ARG:HB2 | 1:R5:90:ARG:HH12 | 1.47 | 0.76 |
| 1:b5:18:TYR:CE2 | 10:k5:165:ARG:CB | 2.66 | 0.76 |
| 6:M6:45:ILE:CD1 | 8:c7:78:THR:CG2 | 2.64 | 0.76 |
| 10:j5:199:THR:HG22 | 12:j5:1201:CYC:CBC | 2.16 | 0.76 |
| 10:j5:931:VAL:HA | 1:J7:29:ALA:O | 1.85 | 0.76 |
| 10:k5:988:ALA:HB2 | 1:b7:106:GLU:OE2 | 1.86 | 0.76 |
| 10:k5:1147:TYR:CE1 | 11:a9:35:ARG:HB2 | 2.21 | 0.76 |
| 3:B6:59:LEU:HD22 | 3:B6:130:ALA:HB2 | 1.67 | 0.76 |
| 8:O7:22:GLU:O | 8:O7:25:ARG:CG | 2.33 | 0.76 |
| 12:F7:201:CYC:CMA | 12:F7:201:CYC:HB | 1.98 | 0.76 |
| 8:M7:41:GLN:HE21 | 3:H9:125:ARG:HE | 1.34 | 0.76 |
| 12:V7:201:CYC:CMA | 12:V7:201:CYC:HB | 1.99 | 0.76 |
| 8:u7:97:VAL:HG22 | 1:v7:19:LEU:CD1 | 2.16 | 0.76 |
| 3:W8:59:LEU:HD22 | 3:W8:130:ALA:HB2 | 1.67 | 0.76 |
| 4:M8:100:SER:H | 3:Q8:1:MET:HE2 | 1.49 | 0.76 |
| 12:O8:202:CYC:HC | 12:O8:202:CYC:CMD | 1.99 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:Q8:78:ARG:HH11 | 12:Z8:301:CYC:HAD2 | 1.49 | 0.76 |
| 12:F1:201:CYC:HMA1 | 12:F1:201:CYC:HB | 1.51 | 0.76 |
| 4:M9:6:THR:N | 3:D9:111:ASN:O | 2.18 | 0.76 |
| 5:Z8:37:HIS:CD2 | 12:Z8:301:CYC:NA | 2.54 | 0.76 |
| 12:Z8:301:CYC:HMA1 | 12:Z8:301:CYC:HB | 1.50 | 0.76 |
| 2:A9:25:GLN:HG2 | 2:K9:33:ARG:HG2 | 1.66 | 0.76 |
| 12:H9:202:CYC:OB | 11:a9:474:PHE:CZ | 2.37 | 0.76 |
| 12:J9:202:CYC:CGA | 11:a9:511:LYS:HA | 2.16 | 0.76 |
| 12:K9:201:CYC:HC | 12:K9:201:CYC:CMD | 1.97 | 0.76 |
| 11:aA:594:ARG:HG3 | 11:aA:594:ARG:NH1 | 2.01 | 0.76 |
| 4:M1:160:THR:CG2 | 4:M1:257:GLN:HB2 | 2.07 | 0.76 |
| 3:D2:59:LEU:HD22 | 3:D2:130:ALA:HB2 | 1.67 | 0.76 |
| 1:Z:17:LYS:O | 8:e5:94:TYR:OH | 2.03 | 0.76 |
| 12:BA:201:CYC:HMA1 | 12:BA:201:CYC:HB | 1.51 | 0.76 |
| 3:HA:72:ASN:HD21 | 12:HA:202:CYC:HBD2 | 1.49 | 0.76 |
| 3:JA:108:ARG:O | 11:aA:518:ALA:N | 2.18 | 0.76 |
| 12:KA:201:CYC:HC | 12:KA:201:CYC:CMD | 1.97 | 0.76 |
| 4:MA:158:PHE:CE1 | 2:UA:10:ALA:HA | 2.21 | 0.76 |
| 6:M2:127:SER:HB2 | 3:F2:84:ARG:CZ | 1.81 | 0.76 |
| 12:T3:301:CYC:HMA1 | 12:T3:301:CYC:HB | 1.51 | 0.76 |
| 12:I4:201:CYC:HC | 12:I4:201:CYC:CMD | 1.97 | 0.76 |
| 3:O4:107:ASP:HA | 5:Z4:66:ARG:HB2 | 1.66 | 0.76 |
| 12:O4:202:CYC:CMD | 12:O4:202:CYC:HC | 1.99 | 0.76 |
| 12:H5:201:CYC:HB | 12:H5:201:CYC:CMA | 1.99 | 0.76 |
| 12:X5:201:CYC:HB | 12:X5:201:CYC:CMA | 1.99 | 0.76 |
| 8:Y5:120:GLN:HG3 | 1:b5:53:LYS:HZ1 | 1.51 | 0.76 |
| 10:k5:1152:TYR:HE2 | 8:G7:68:PRO:HG2 | 0.93 | 0.76 |
| 12:R7:201:CYC:CMA | 12:R7:201:CYC:HB | 1.99 | 0.76 |
| 12:N7:201:CYC:CMA | 12:N7:201:CYC:HB | 1.99 | 0.76 |
| 8:a7:25:ARG:NE | 8:o7:25:ARG:NH2 | 2.32 | 0.76 |
| 8:c7:92:VAL:HG13 | 8:c7:152:TYR:CB | 2.16 | 0.76 |
| 12:J8:202:CYC:CMD | 12:J8:202:CYC:HC | 1.99 | 0.76 |
| 4:M8:232:VAL:CG2 | 4:M8:235:PHE:CE2 | 2.67 | 0.76 |
| 5:N9:7:ASP:N | 3:R9:107:ASP:O | 2.19 | 0.76 |
| 5:N9:54:LEU:HD21 | 3:T9:84:ARG:HD2 | 1.67 | 0.76 |
| 3:J9:108:ARG:O | 11:a9:518:ALA:N | 2.18 | 0.76 |
| 11:a9:640:ALA:HB1 | 11:a9:767:THR:HG22 | 1.68 | 0.76 |
| 11:aA:745:GLY:CA | 2:K1:15:GLN:C | 2.58 | 0.76 |
| 11:aA:787:ARG:HH22 | 11:aA:819:SER:HB3 | 1.51 | 0.76 |
| 12:QA:201:CYC:CBA | 3:TA:79:MET:CE | 2.63 | 0.76 |
| 12:A1:201:CYC:HC | 12:A1:201:CYC:CMD | 1.97 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:G3:201:CYC:HC | 12:G3:201:CYC:CMD | 1.97 | 0.76 |
| 5:N3:36:THR:OG1 | 12:T3:301:CYC:C4B | 2.33 | 0.76 |
| 3:B1:107:ASP:O | 4:M1:7:SER:N | 2.19 | 0.76 |
| 12:B1:202:CYC:HB | 12:B1:202:CYC:HMA1 | 1.51 | 0.76 |
| 3:S4:120:LEU:HD22 | 12:S4:202:CYC:CGD | 2.16 | 0.76 |
| 12:T4:201:CYC:HC | 12:T4:201:CYC:CMD | 1.97 | 0.76 |
| 3:H4:80:ALA:HB3 | 3:H4:84:ARG:HH12 | 1.50 | 0.76 |
| 3:H4:119:ALA:CB | 11:aA:266:ASN:CG | 2.58 | 0.76 |
| 3:L4:115:GLU:HG2 | 11:aA:295:ARG:HH21 | 1.48 | 0.76 |
| 12:O4:201:CYC:HB | 12:O4:201:CYC:HMA1 | 1.51 | 0.76 |
| 8:K5:131:ARG:HG2 | 8:K5:157:VAL:HG21 | 1.68 | 0.76 |
| 8:C5:110:ILE:HD12 | 9:z5:15:LYS:CB | 2.15 | 0.76 |
| 12:F5:201:CYC:CMA | 12:F5:201:CYC:HB | 1.99 | 0.76 |
| 10:j5:136:VAL:HB | 10:j5:137:PRO:HD2 | 1.67 | 0.76 |
| 10:j5:793:SER:HB3 | 12:T7:201:CYC:CGA | 2.15 | 0.76 |
| 12:k5:1202:CYC:CMA | 12:k5:1202:CYC:HB | 1.98 | 0.76 |
| 12:D7:201:CYC:HB | 12:D7:201:CYC:CMA | 1.99 | 0.76 |
| 12:T7:201:CYC:HB | 12:T7:201:CYC:CMA | 1.99 | 0.76 |
| 8:c7:42:THR:HG22 | 8:c7:141:LEU:HD21 | 1.68 | 0.76 |
| 3:D8:59:LEU:HD22 | 3:D8:130:ALA:HB2 | 1.67 | 0.76 |
| 2:X8:67:THR:HB | 3:T9:28:THR:HG23 | 1.66 | 0.76 |
| 4:M8:190:ARG:HH12 | 4:M8:202:SER:CB | 1.98 | 0.76 |
| 3:F1:84:ARG:CZ | 4:M1:35:THR:HB | 2.16 | 0.76 |
| 11:a9:61:TYR:CD1 | 11:a9:65:LEU:HD22 | 2.20 | 0.76 |
| 11:aA:98:ILE:HD12 | 11:aA:101:ASP:CB | 2.15 | 0.76 |
| 11:aA:817:LEU:HD11 | 3:L1:119:ALA:C | 2.11 | 0.76 |
| 3:V1:59:LEU:HD22 | 3:V1:130:ALA:HB2 | 1.67 | 0.76 |
| 5:NA:14:LYS:HE2 | 5:NA:50:LEU:HD23 | 1.67 | 0.75 |
| 3:RA:59:LEU:HD22 | 3:RA:130:ALA:HB2 | 1.67 | 0.75 |
| 3:XA:59:LEU:HD22 | 3:XA:130:ALA:HB2 | 1.67 | 0.75 |
| 3:R1:59:LEU:HD22 | 3:R1:130:ALA:HB2 | 1.67 | 0.75 |
| 12:S1:201:CYC:HC | 12:S1:201:CYC:CMD | 1.97 | 0.75 |
| 3:L2:70:GLY:HA2 | 6:M2:67:GLY:HA2 | 1.68 | 0.75 |
| 12:Z3:201:CYC:HMA2 | 4:M3:188:LEU:CD2 | 2.16 | 0.75 |
| 3:B4:82:CYS:CA | 12:B4:202:CYC:C2C | 2.63 | 0.75 |
| 3:B4:116:THR:N | 4:M4:56:MET:HE3 | 2.01 | 0.75 |
| 12:R3:202:CYC:HC | 12:R3:202:CYC:CMD | 1.99 | 0.75 |
| 3:U4:115:GLU:CG | 4:M4:74:LEU:HD12 | 2.15 | 0.75 |
| 4:M4:51:ARG:HH11 | 4:M4:51:ARG:HB3 | 1.51 | 0.75 |
| 8:I5:110:ILE:HD12 | 9:i5:15:LYS:HB3 | 1.68 | 0.75 |
| 8:U5:83:ARG:CG | 6:M6:31:ASP:CG | 2.51 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:j5:1013:PRO:HB2 | 8:q7:114:GLU:OE2 | 1.86 | 0.75 |
| 10:j5:1056:PRO:CD | 10:j5:1057:LYS:H | 1.97 | 0.75 |
| 10:k5:841:VAL:CG1 | 10:k5:846:GLU:OE1 | 2.33 | 0.75 |
| 10:k5:1046:ARG:HH21 | 8:k7:9:VAL:HG11 | 1.50 | 0.75 |
| 10:k5:1078:SER:HA | 12:k5:1203:CYC:CGA | 2.16 | 0.75 |
| 10:k5:1143:LEU:HA | 1:l7:10:ASN:ND2 | 2.00 | 0.75 |
| 12:k5:1203:CYC:HB | 12:k5:1203:CYC:CMA | 1.99 | 0.75 |
| 8:Q7:13:ALA:HA | 9:z7:46:LYS:HZ3 | 0.60 | 0.75 |
| 8:g7:90:ARG:CZ | 1:h7:16:GLY:HA2 | 2.16 | 0.75 |
| 8:U7:29:PHE:HE1 | 8:U7:98:ALA:O | 1.68 | 0.75 |
| 8:a7:61:ILE:O | 11:a9:336:ILE:HB | 1.85 | 0.75 |
| 12:b7:201:CYC:CMA | 12:b7:201:CYC:HB | 1.99 | 0.75 |
| 8:o7:37:LEU:HD13 | 1:p7:24:LEU:HB3 | 1.67 | 0.75 |
| 8:q7:68:PRO:HG2 | 11:aA:334:LYS:CD | 2.06 | 0.75 |
| 8:u7:36:ARG:HH21 | 8:u7:36:ARG:HG2 | 1.50 | 0.75 |
| 2:X8:57:GLN:CA | 3:T9:32:LYS:NZ | 2.28 | 0.75 |
| 3:Q8:59:LEU:HD22 | 3:Q8:130:ALA:HB2 | 1.67 | 0.75 |
| 12:P9:202:CYC:HC | 12:P9:202:CYC:CMD | 1.98 | 0.75 |
| 12:U9:201:CYC:HC | 12:U9:201:CYC:CMD | 1.97 | 0.75 |
| 11:aA:670:LEU:HD21 | 2:K1:112:GLY:CA | 2.15 | 0.75 |
| 5:N1:22:LEU:O | 5:N1:22:LEU:HD12 | 1.86 | 0.75 |
| 2:U1:47:ASN:O | 2:U1:51:LEU:HG | 1.86 | 0.75 |
| 3:FA:59:LEU:HD22 | 3:FA:130:ALA:HB2 | 1.67 | 0.75 |
| 4:MA:51:ARG:HH11 | 4:MA:51:ARG:HB3 | 1.51 | 0.75 |
| 12:R1:201:CYC:HBB2 | 5:N1:61:LYS:HZ2 | 1.49 | 0.75 |
| 3:L3:111:ASN:HB3 | 11:a9:711:SER:HB3 | 1.66 | 0.75 |
| 3:F4:107:ASP:C | 4:M4:6:THR:HB | 2.12 | 0.75 |
| 8:I5:35:ARG:HH22 | 8:I5:144:ASP:CB | 1.99 | 0.75 |
| 8:e5:102:THR:CB | 8:e5:103:PRO:CD | 2.64 | 0.75 |
| 1:R5:106:GLU:CG | 10:k5:504:ASP:C | 2.59 | 0.75 |
| 12:J6:201:CYC:HC | 12:J6:201:CYC:CMD | 1.98 | 0.75 |
| 10:j5:1013:PRO:HB3 | 8:q7:114:GLU:OE2 | 1.84 | 0.75 |
| 10:j5:1041:ARG:NH2 | 10:j5:1094:ASP:OD2 | 2.19 | 0.75 |
| 10:j5:1146:THR:N | 1:v7:77:ARG:NH2 | 2.29 | 0.75 |
| 10:k5:386:ILE:HD13 | 10:k5:395:SER:HG | 1.50 | 0.75 |
| 10:k5:966:SER:HA | 1:p7:14:VAL:HG12 | 0.76 | 0.75 |
| 8:C7:12:ASP:OD1 | 1:D7:91:TYR:OH | 2.02 | 0.75 |
| 12:J7:201:CYC:CMA | 12:J7:201:CYC:HB | 1.99 | 0.75 |
| 8:i7:42:THR:HG22 | 8:i7:141:LEU:HD21 | 1.68 | 0.75 |
| 8:o7:36:ARG:HG2 | 8:o7:36:ARG:HH21 | 1.51 | 0.75 |
| 8:u7:23:LEU:HD22 | 1:v7:38:VAL:CG1 | 2.15 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:u7:23:LEU:HD13 | 1:v7:38:VAL:CG1 | 2.16 | 0.75 |
| 8:u7:27:LYS:CD | 1:v7:35:ALA:CA | 2.58 | 0.75 |
| 3:F8:113:LEU:CA | 4:M8:5:THR:HG23 | 2.17 | 0.75 |
| 3:H9:82:CYS:SG | 12:H9:202:CYC:HAC1 | 2.26 | 0.75 |
| 3:H9:108:ARG:NH1 | 11:a9:448:ASN:ND2 | 2.33 | 0.75 |
| 3:R9:59:LEU:HD22 | 3:R9:130:ALA:HB2 | 1.67 | 0.75 |
| 3:T9:59:LEU:HD22 | 3:T9:130:ALA:HB2 | 1.67 | 0.75 |
| 11:aA:707:PHE:CE2 | 2:K1:13:ASP:OD2 | 2.39 | 0.75 |
| 4:M1:273:ILE:HG23 | 3:Z1:77:ARG:HE | 1.51 | 0.75 |
| 5:N1:22:LEU:HD23 | 5:N1:26:LEU:CD1 | 1.83 | 0.75 |
| 1:Z:131:GLN:CG | 1:X5:17:LYS:HZ3 | 1.95 | 0.75 |
| 3:H3:59:LEU:HD22 | 3:H3:130:ALA:HB2 | 1.67 | 0.75 |
| 3:F3:59:LEU:HD22 | 3:F3:130:ALA:HB2 | 1.67 | 0.75 |
| 3:F3:84:ARG:CZ | 4:M3:35:THR:HB | 2.16 | 0.75 |
| 4:M3:190:ARG:HH12 | 4:M3:202:SER:CB | 1.98 | 0.75 |
| 3:H4:119:ALA:CB | 11:aA:266:ASN:CB | 2.59 | 0.75 |
| 8:C5:29:PHE:HE1 | 8:C5:98:ALA:O | 1.69 | 0.75 |
| 1:H5:14:VAL:HG11 | 10:j5:555:ALA:HA | 1.68 | 0.75 |
| 1:f5:114:GLU:HB3 | 10:j5:491:THR:OG1 | 1.86 | 0.75 |
| 12:f5:201:CYC:CMA | 12:f5:201:CYC:HB | 1.99 | 0.75 |
| 12:T5:201:CYC:HB | 12:T5:201:CYC:CMA | 1.99 | 0.75 |
| 1:X5:65:LEU:CD1 | 10:j5:706:PRO:CG | 2.59 | 0.75 |
| 1:X5:144:ASP:OD1 | 1:X5:145:ALA:N | 2.19 | 0.75 |
| 6:M6:267:THR:CG2 | 1:d7:161:SER:OXT | 2.34 | 0.75 |
| 10:j5:741:GLN:CG | 1:J7:77:ARG:NH2 | 2.39 | 0.75 |
| 10:j5:1055:SER:CB | 12:r7:201:CYC:HBB2 | 2.17 | 0.75 |
| 10:j5:1067:LEU:CD1 | 10:j5:1101:GLU:CG | 2.61 | 0.75 |
| 10:j5:1118:THR:CA | 12:j5:1202:CYC:HBA1 | 2.15 | 0.75 |
| 10:k5:631:HIS:CG | 10:k5:664:MET:HE1 | 2.21 | 0.75 |
| 12:L7:201:CYC:HB | 12:L7:201:CYC:CMA | 1.98 | 0.75 |
| 8:U7:35:ARG:HH22 | 8:U7:144:ASP:CB | 2.00 | 0.75 |
| 12:r7:201:CYC:HB | 12:r7:201:CYC:CMA | 1.99 | 0.75 |
| 8:u7:27:LYS:HE2 | 1:v7:35:ALA:CB | 1.95 | 0.75 |
| 3:F8:115:GLU:HG2 | 4:M8:3:VAL:CB | 2.16 | 0.75 |
| 3:B9:107:ASP:CG | 11:a9:382:ASN:HD22 | 1.94 | 0.75 |
| 12:D9:202:CYC:HC | 12:D9:202:CYC:CMD | 1.99 | 0.75 |
| 12:X9:202:CYC:HC | 12:X9:202:CYC:CMD | 1.98 | 0.75 |
| 3:F2:59:LEU:HD22 | 3:F2:130:ALA:HB2 | 1.67 | 0.75 |
| 3:HA:120:LEU:HD13 | 12:HA:202:CYC:CAA | 2.17 | 0.75 |
| 5:NA:54:LEU:HA | 12:TA:301:CYC:HMA2 | 1.68 | 0.75 |
| 3:B4:110:LEU:HA | 3:B4:113:LEU:HB2 | 1.69 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:N3:22:LEU:O | 5:N3:22:LEU:HD12 | 1.86 | 0.75 |
| 12:X3:202:CYC:HC | 12:X3:202:CYC:CMD | 1.98 | 0.75 |
| 8:A5:115:MET:CE | 12:A5:201:CYC:C1B | 2.65 | 0.75 |
| 12:D5:201:CYC:CMA | 12:D5:201:CYC:HB | 1.99 | 0.75 |
| 1:T5:87:TYR:CE2 | 10:j5:483:PHE:CE2 | 2.74 | 0.75 |
| 8:U5:35:ARG:HH22 | 8:U5:144:ASP:CB | 1.99 | 0.75 |
| 10:j5:935:LEU:HD11 | 1:J7:25:ASP:O | 1.85 | 0.75 |
| 10:k5:275:THR:CG2 | 10:k5:286:VAL:O | 2.33 | 0.75 |
| 10:k5:306:GLU:OE2 | 10:k5:362:LYS:NZ | 2.19 | 0.75 |
| 12:h7:201:CYC:HBB2 | 9:y7:21:ARG:HD3 | 1.66 | 0.75 |
| 3:L8:71:GLY:HA2 | 11:a9:82:GLN:NE2 | 2.02 | 0.75 |
| 3:L8:78:ARG:HH22 | 11:a9:88:ALA:H | 1.33 | 0.75 |
| 4:M8:140:ARG:HD2 | 4:M8:215:GLU:HA | 1.67 | 0.75 |
| 4:M8:201:ASP:N | 5:Z8:52:ARG:HH22 | 1.83 | 0.75 |
| 5:N9:66:ARG:HH12 | 3:T9:111:ASN:CG | 1.92 | 0.75 |
| 12:Y8:201:CYC:HC | 12:Y8:201:CYC:CMD | 1.99 | 0.75 |
| 11:a9:787:ARG:HH22 | 11:a9:819:SER:HB3 | 1.51 | 0.75 |
| 4:M1:190:ARG:HH12 | 4:M1:202:SER:CB | 1.98 | 0.75 |
| 2:IA:25:GLN:HA | 2:IA:25:GLN:NE2 | 2.01 | 0.75 |
| 5:NA:22:LEU:O | 5:NA:22:LEU:HD12 | 1.86 | 0.75 |
| 5:NA:54:LEU:H | 12:TA:301:CYC:CBA | 1.99 | 0.75 |
| 12:RA:202:CYC:HC | 12:RA:202:CYC:CMD | 1.99 | 0.75 |
| 12:TA:302:CYC:HC | 12:TA:302:CYC:CMD | 1.98 | 0.75 |
| 3:J3:84:ARG:NH1 | 11:a9:668:TYR:HB3 | 2.02 | 0.75 |
| 5:N3:14:LYS:HE2 | 5:N3:50:LEU:HD23 | 1.67 | 0.75 |
| 3:B1:111:ASN:OD1 | 4:M1:76:ALA:HB3 | 1.87 | 0.75 |
| 12:F4:201:CYC:HC | 12:F4:201:CYC:CMD | 1.98 | 0.75 |
| 4:M4:190:ARG:HH12 | 4:M4:202:SER:CB | 1.98 | 0.75 |
| 3:Y4:113:LEU:CD1 | 3:Y4:171:ILE:HG23 | 2.17 | 0.75 |
| 1:B5:76:ARG:CD | 9:z5:14:LEU:HB2 | 2.16 | 0.75 |
| 8:E5:4:LEU:HD23 | 8:E5:26:ILE:HD13 | 1.69 | 0.75 |
| 8:G5:115:MET:CE | 12:G5:201:CYC:C1B | 2.65 | 0.75 |
| 12:V5:201:CYC:CBB | 10:j5:623:VAL:HG21 | 2.15 | 0.75 |
| 8:W5:4:LEU:HD23 | 8:W5:26:ILE:HD13 | 1.69 | 0.75 |
| 8:a5:35:ARG:HH22 | 8:a5:144:ASP:CB | 1.99 | 0.75 |
| 12:b5:201:CYC:CMA | 12:b5:201:CYC:HB | 1.99 | 0.75 |
| 10:k5:1118:THR:HG23 | 12:k5:1204:CYC:HBA1 | 1.68 | 0.75 |
| 8:c7:89:LEU:CD1 | 8:c7:153:PHE:CZ | 2.70 | 0.75 |
| 12:d7:201:CYC:CMA | 12:d7:201:CYC:HB | 1.99 | 0.75 |
| 12:v7:201:CYC:HB | 12:v7:201:CYC:CMA | 1.99 | 0.75 |
| 9:y7:3:ARG:CZ | 9:y7:67:VAL:HG12 | 2.15 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:W8:202:CYC:HC | 12:W8:202:CYC:CMD | 1.99 | 0.75 |
| 4:M8:232:VAL:HG23 | 4:M8:235:PHE:CE2 | 2.19 | 0.75 |
| 12:Z9:202:CYC:HMA1 | 12:Z9:202:CYC:HB | 1.51 | 0.75 |
| 12:JA:202:CYC:HB | 12:JA:202:CYC:HMA1 | 1.51 | 0.75 |
| 4:MA:274:VAL:HA | 3:VA:77:ARG:NE | 2.02 | 0.75 |
| 12:RA:201:CYC:HMA1 | 12:RA:201:CYC:HB | 1.51 | 0.75 |
| 3:J3:119:ALA:C | 11:a9:803:ASN:HB3 | 2.12 | 0.75 |
| 3:B1:59:LEU:HD22 | 3:B1:130:ALA:HB2 | 1.67 | 0.75 |
| 3:U4:59:LEU:HD22 | 3:U4:130:ALA:HB2 | 1.67 | 0.75 |
| 8:K5:4:LEU:HD23 | 8:K5:26:ILE:HD13 | 1.69 | 0.75 |
| 8:G5:126:VAL:HA | 12:G5:201:CYC:HBC3 | 1.69 | 0.75 |
| 12:V5:201:CYC:CMA | 12:V5:201:CYC:HB | 1.99 | 0.75 |
| 1:Z5:161:SER:OG | 10:k5:696:ARG:HA | 1.85 | 0.75 |
| 3:L6:65:ASP:OD2 | 1:b7:64:ASP:CG | 2.29 | 0.75 |
| 6:M6:117:MET:HE3 | 3:H6:77:ARG:HD2 | 1.67 | 0.75 |
| 10:j5:929:PRO:HG2 | 1:J7:147:LYS:CG | 2.17 | 0.75 |
| 10:j5:965:GLN:HB3 | 10:j5:969:VAL:HG11 | 1.69 | 0.75 |
| 8:M7:49:ARG:HD2 | 11:a9:550:PHE:HE1 | 1.45 | 0.75 |
| 8:M7:60:GLN:HE22 | 3:J9:114:LYS:HD3 | 1.52 | 0.75 |
| 8:g7:61:ILE:O | 11:aA:336:ILE:HB | 1.87 | 0.75 |
| 8:i7:92:VAL:HG13 | 8:i7:152:TYR:CB | 2.16 | 0.75 |
| 2:E8:15:GLN:HG2 | 11:a9:163:ASP:CB | 2.16 | 0.75 |
| 8:o7:47:ARG:HG2 | 8:o7:47:ARG:HH21 | 1.51 | 0.75 |
| 3:F8:88:ILE:CD1 | 11:a9:140:GLN:HG2 | 2.15 | 0.75 |
| 2:N8:11:SER:CA | 5:Z8:62:ARG:HH21 | 1.97 | 0.75 |
| 4:M9:158:PHE:CE1 | 2:U9:10:ALA:HA | 2.21 | 0.75 |
| 12:J9:202:CYC:HB | 12:J9:202:CYC:HMA1 | 1.51 | 0.75 |
| 12:R9:201:CYC:HB | 12:R9:201:CYC:HMA1 | 1.51 | 0.75 |
| 11:a9:389:GLN:HA | 11:a9:389:GLN:NE2 | 2.01 | 0.75 |
| 11:aA:95:ILE:CD1 | 11:aA:237:PHE:CZ | 2.70 | 0.75 |
| 11:aA:312:ASP:CB | 11:aA:315:LEU:HD12 | 2.16 | 0.75 |
| 11:aA:330:ASP:OD1 | 11:aA:330:ASP:N | 2.13 | 0.75 |
| 11:aA:350:LEU:HD12 | 11:aA:350:LEU:H | 1.50 | 0.75 |
| 11:aA:418:LEU:HD13 | 11:aA:428:PHE:HB2 | 1.68 | 0.75 |
| 4:M1:188:LEU:CD2 | 12:Z1:202:CYC:HMA2 | 2.16 | 0.75 |
| 12:ZA:202:CYC:HB | 12:ZA:202:CYC:HMA1 | 1.51 | 0.75 |
| 12:R1:201:CYC:HB | 5:N1:54:LEU:CD1 | 1.81 | 0.75 |
| 3:J3:108:ARG:O | 11:a9:795:ASP:HB3 | 1.87 | 0.75 |
| 3:B4:120:LEU:CD1 | 4:M4:53:LEU:N | 2.44 | 0.75 |
| 3:J4:59:LEU:HD22 | 3:J4:130:ALA:HB2 | 1.67 | 0.75 |
| 4:M4:197:ASP:O | 5:Z4:52:ARG:CZ | 2.34 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:O4:116:THR:N | 5:Z4:70:ILE:HG22 | 2.00 | 0.75 |
| 8:K5:112:VAL:HA | 1:J5:75:THR:HB | 1.69 | 0.75 |
| 12:J5:201:CYC:CMA | 12:J5:201:CYC:HB | 1.99 | 0.75 |
| 10:j5:1023:SER:HB3 | 12:f7:201:CYC:HBA1 | 1.67 | 0.75 |
| 10:k5:965:GLN:HB3 | 10:k5:969:VAL:HG11 | 1.68 | 0.75 |
| 8:Q7:12:ASP:C | 9:z7:46:LYS:CE | 2.59 | 0.75 |
| 5:N9:14:LYS:HE2 | 5:N9:50:LEU:HD23 | 1.67 | 0.75 |
| 12:P9:201:CYC:HMA1 | 12:P9:201:CYC:HB | 1.51 | 0.75 |
| 2:G1:111:ALA:HB3 | 3:L1:77:ARG:NE | 2.01 | 0.75 |
| 11:aA:631:GLY:CA | 3:J1:111:ASN:ND2 | 2.49 | 0.75 |
| 1:A:127:VAL:CG1 | 1:R5:15:GLN:OE1 | 2.35 | 0.75 |
| 3:DA:59:LEU:HD22 | 3:DA:130:ALA:HB2 | 1.67 | 0.75 |
| 3:HA:116:THR:CG2 | 12:HA:202:CYC:HMA3 | 2.15 | 0.75 |
| 12:PA:201:CYC:HB | 12:PA:201:CYC:HMA1 | 1.51 | 0.75 |
| 3:J2:59:LEU:HD22 | 3:J2:130:ALA:HB2 | 1.67 | 0.75 |
| 3:B3:107:ASP:O | 4:M3:7:SER:N | 2.19 | 0.75 |
| 3:D3:59:LEU:HD22 | 3:D3:130:ALA:HB2 | 1.67 | 0.75 |
| 3:B4:86:MET:H | 12:B4:202:CYC:CBC | 1.80 | 0.75 |
| 3:B1:82:CYS:SG | 12:B1:202:CYC:C3C | 2.75 | 0.75 |
| 4:M4:58:TYR:O | 4:M4:61:ASN:ND2 | 2.20 | 0.75 |
| 12:M4:301:CYC:HB | 12:M4:301:CYC:HMA1 | 1.51 | 0.75 |
| 1:L5:69:GLY:O | 10:j5:554:ASN:ND2 | 2.19 | 0.75 |
| 8:M5:68:PRO:CB | 8:e5:59:PHE:HB2 | 2.17 | 0.75 |
| 8:A5:126:VAL:HA | 12:A5:201:CYC:HBC3 | 1.68 | 0.75 |
| 1:X5:86:ASP:CG | 1:X5:90:ARG:HE | 1.94 | 0.75 |
| 10:j5:388:ARG:HH21 | 10:j5:392:SER:HA | 1.51 | 0.75 |
| 10:k5:388:ARG:HH21 | 10:k5:392:SER:HA | 1.51 | 0.75 |
| 10:k5:449:ARG:HG3 | 10:k5:449:ARG:NH2 | 1.98 | 0.75 |
| 10:k5:970:GLY:N | 1:n7:77:ARG:HH22 | 1.84 | 0.75 |
| 8:S7:106:GLU:OE2 | 9:w7:68:GLY:HA3 | 1.86 | 0.75 |
| 3:O8:111:ASN:O | 5:Z8:67:ILE:HG22 | 1.84 | 0.75 |
| 3:P9:59:LEU:HD22 | 3:P9:130:ALA:HB2 | 1.67 | 0.75 |
| 5:Z8:14:LYS:HE2 | 5:Z8:50:LEU:HD23 | 1.67 | 0.75 |
| 5:Z8:22:LEU:HD22 | 5:Z8:26:LEU:HD13 | 1.59 | 0.75 |
| 5:Z8:22:LEU:HD12 | 5:Z8:22:LEU:O | 1.85 | 0.75 |
| 3:D9:59:LEU:HD22 | 3:D9:130:ALA:HB2 | 1.67 | 0.75 |
| 2:I9:31:PHE:HE2 | 3:J9:31:VAL:HA | 1.48 | 0.75 |
| 11:aA:508:ARG:HB2 | 11:aA:513:GLN:NE2 | 2.02 | 0.75 |
| 11:aA:666:ASN:CB | 12:aA:901:CYC:HMA2 | 2.15 | 0.75 |
| 3:J1:59:LEU:HD22 | 3:J1:130:ALA:HB2 | 1.67 | 0.75 |
| 3:HA:113:LEU:HD22 | 12:HA:202:CYC:HMB1 | 1.68 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:KA:18:PHE:CZ | 3:LA:48:ALA:HB1 | 2.19 | 0.75 |
| 2:G2:16:GLY:HA3 | 6:M2:104:ARG:HH11 | 1.51 | 0.75 |
| 3:Z3:120:LEU:HD21 | 4:M3:181:GLN:HE22 | 1.52 | 0.75 |
| 3:B4:59:LEU:HD22 | 3:B4:130:ALA:HB2 | 1.67 | 0.75 |
| 3:L4:68:ARG:HD2 | 11:aA:81:ASP:N | 2.00 | 0.75 |
| 3:L4:78:ARG:HH22 | 11:aA:88:ALA:H | 1.34 | 0.75 |
| 1:d5:67:ARG:NH1 | 10:j5:705:THR:HB | 2.00 | 0.75 |
| 8:A7:51:VAL:HG11 | 11:aA:579:PHE:HE1 | 1.52 | 0.75 |
| 9:i5:22:GLU:C | 9:i5:25:ASN:N | 2.43 | 0.75 |
| 10:j5:934:ALA:CB | 1:J7:32:THR:HG23 | 2.15 | 0.75 |
| 8:i7:47:ARG:NH1 | 1:j7:18:TYR:CD1 | 2.54 | 0.75 |
| 1:T7:110:ASN:HD21 | 9:w7:57:PHE:HA | 1.51 | 0.75 |
| 8:a7:35:ARG:HH22 | 8:a7:144:ASP:CB | 1.99 | 0.75 |
| 8:c7:39:ILE:HD12 | 8:c7:148:GLU:CG | 2.09 | 0.75 |
| 8:o7:16:ARG:O | 1:p7:94:TYR:HE1 | 1.70 | 0.75 |
| 8:u7:4:LEU:HD23 | 8:u7:26:ILE:HD13 | 1.69 | 0.75 |
| 4:M8:58:TYR:O | 4:M8:61:ASN:ND2 | 2.19 | 0.75 |
| 3:F1:59:LEU:HD22 | 3:F1:130:ALA:HB2 | 1.67 | 0.75 |
| 3:F9:150:ARG:CZ | 12:F9:302:CYC:C1C | 2.62 | 0.75 |
| 11:aA:274:LEU:C | 11:aA:278:LEU:HD11 | 2.12 | 0.75 |
| 3:LA:14:LEU:HG | 11:aA:358:PRO:CB | 2.15 | 0.74 |
| 3:J3:59:LEU:HD22 | 3:J3:130:ALA:HB2 | 1.67 | 0.74 |
| 3:J3:77:ARG:NE | 2:K3:111:ALA:HB3 | 2.01 | 0.74 |
| 4:M3:118:TYR:CD2 | 3:X3:84:ARG:NE | 2.54 | 0.74 |
| 4:M4:197:ASP:CG | 5:Z4:52:ARG:NE | 2.45 | 0.74 |
| 8:O5:35:ARG:HH22 | 8:O5:144:ASP:CB | 1.99 | 0.74 |
| 8:e5:35:ARG:HH22 | 8:e5:144:ASP:CB | 1.99 | 0.74 |
| 8:a5:29:PHE:HE1 | 8:a5:98:ALA:O | 1.68 | 0.74 |
| 10:j5:930:LEU:CB | 1:J7:33:THR:HG21 | 2.16 | 0.74 |
| 10:j5:934:ALA:HB3 | 1:J7:32:THR:CG2 | 2.14 | 0.74 |
| 10:j5:988:ALA:HA | 1:h7:106:GLU:OE2 | 1.85 | 0.74 |
| 10:k5:503:LYS:HG2 | 10:k5:503:LYS:O | 1.87 | 0.74 |
| 10:k5:803:LYS:HZ2 | 9:z7:43:ARG:HH11 | 1.33 | 0.74 |
| 10:k5:929:PRO:HG2 | 1:D7:147:LYS:HE2 | 1.66 | 0.74 |
| 10:k5:951:MET:CE | 10:k5:955:LEU:CG | 2.65 | 0.74 |
| 10:k5:1041:ARG:NH2 | 10:k5:1094:ASP:OD2 | 2.19 | 0.74 |
| 8:Q7:25:ARG:CG | 8:C7:25:ARG:NH2 | 2.49 | 0.74 |
| 8:S7:25:ARG:NE | 8:G7:25:ARG:NE | 2.35 | 0.74 |
| 1:B7:140:LEU:CD1 | 11:a9:561:ALA:CA | 2.65 | 0.74 |
| 1:B7:140:LEU:CG | 11:a9:561:ALA:CB | 2.65 | 0.74 |
| 8:I7:35:ARG:HH22 | 8:I7:144:ASP:CB | 1.99 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:i7:25:ARG:NH1 | 8:s7:6:LYS:C | 2.44 | 0.74 |
| 8:o7:23:LEU:HD13 | 1:p7:38:VAL:CG1 | 2.16 | 0.74 |
| 8:q7:66:VAL:HG12 | 11:aA:65:LEU:HD21 | 1.66 | 0.74 |
| 2:X8:57:GLN:CD | 3:T9:32:LYS:CD | 2.58 | 0.74 |
| 3:F8:84:ARG:CD | 11:a9:139:ILE:HG21 | 2.15 | 0.74 |
| 4:M8:77:LEU:HD12 | 4:M8:77:LEU:O | 1.87 | 0.74 |
| 4:M8:160:THR:CG2 | 4:M8:257:GLN:HB2 | 2.08 | 0.74 |
| 4:M8:232:VAL:O | 4:M8:235:PHE:HE2 | 1.62 | 0.74 |
| 4:M9:146:LEU:N | 4:M9:146:LEU:HD23 | 2.02 | 0.74 |
| 3:Y8:113:LEU:CD2 | 3:Y8:171:ILE:HG12 | 2.17 | 0.74 |
| 3:BA:107:ASP:CG | 11:aA:382:ASN:HD22 | 1.95 | 0.74 |
| 4:MA:134:ASN:HB2 | 12:RA:201:CYC:CAA | 2.15 | 0.74 |
| 4:MA:146:LEU:HD23 | 4:MA:146:LEU:N | 2.02 | 0.74 |
| 2:OA:33:ARG:NE | 2:YA:28:ASN:ND2 | 2.35 | 0.74 |
| 12:VA:202:CYC:HC | 12:VA:202:CYC:CMD | 1.99 | 0.74 |
| 3:H2:77:ARG:NH1 | 6:M2:117:MET:HE1 | 1.97 | 0.74 |
| 6:M2:45:ILE:CD1 | 8:i7:78:THR:CG2 | 2.65 | 0.74 |
| 3:L3:119:ALA:CB | 11:a9:813:PRO:CA | 2.65 | 0.74 |
| 4:M3:51:ARG:HH11 | 4:M3:51:ARG:CB | 2.00 | 0.74 |
| 5:Z4:38:GLU:H | 12:Z4:301:CYC:HMB2 | 1.52 | 0.74 |
| 1:b5:30:TYR:HE2 | 10:k5:47:PHE:CE1 | 2.05 | 0.74 |
| 10:j5:902:ASN:O | 10:j5:902:ASN:ND2 | 2.16 | 0.74 |
| 10:k5:742:GLY:C | 12:D7:201:CYC:CGD | 2.59 | 0.74 |
| 3:D1:68:ARG:HH22 | 3:X1:68:ARG:NH2 | 1.82 | 0.74 |
| 12:P7:201:CYC:HB | 12:P7:201:CYC:CMA | 1.99 | 0.74 |
| 8:i7:112:VAL:CG1 | 8:i7:113:LYS:H | 1.98 | 0.74 |
| 8:i7:131:ARG:O | 8:i7:131:ARG:HG3 | 1.87 | 0.74 |
| 3:B8:59:LEU:HD22 | 3:B8:130:ALA:HB2 | 1.67 | 0.74 |
| 8:s7:35:ARG:HH22 | 8:s7:144:ASP:CB | 2.00 | 0.74 |
| 2:X8:64:PRO:O | 3:T9:25:ASN:HB3 | 1.85 | 0.74 |
| 4:M8:140:ARG:HH21 | 5:Z8:26:LEU:HA | 1.51 | 0.74 |
| 3:O8:107:ASP:CA | 5:Z8:66:ARG:CB | 2.65 | 0.74 |
| 12:L9:202:CYC:HMA1 | 11:a9:534:SER:CB | 2.17 | 0.74 |
| 4:M9:51:ARG:HH11 | 4:M9:51:ARG:HB3 | 1.51 | 0.74 |
| 4:M9:273:ILE:CD1 | 3:V9:75:PRO:HD3 | 2.01 | 0.74 |
| 2:I9:25:GLN:HA | 2:I9:25:GLN:NE2 | 2.01 | 0.74 |
| 11:a9:275:THR:C | 11:a9:278:LEU:HD12 | 1.99 | 0.74 |
| 12:HA:202:CYC:NB | 11:aA:474:PHE:CZ | 2.53 | 0.74 |
| 5:NA:1:MET:HA | 5:NA:1:MET:CE | 2.10 | 0.74 |
| 2:QA:162:SER:C | 2:WA:118:ARG:HD2 | 2.11 | 0.74 |
| 12:B3:202:CYC:HBA2 | 11:a9:684:ASN:HB3 | 0.74 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 3:P3:59:LEU:HD22 | 3:P3:130:ALA:HB2 | 1.67 | 0.74 |
| 3:U4:108:ARG:CG | 4:M4:246:ALA:HB2 | 2.17 | 0.74 |
| 3:W4:59:LEU:HD22 | 3:W4:130:ALA:HB2 | 1.67 | 0.74 |
| 4:M4:205:ASP:HB2 | 5:Z4:63:ASN:HD21 | 1.49 | 0.74 |
| 8:O5:29:PHE:HE1 | 8:O5:98:ALA:O | 1.68 | 0.74 |
| 8:e5:38:ARG:NH2 | 1:R5:144:ASP:CG | 2.43 | 0.74 |
| 3:L6:70:GLY:HA2 | 6:M6:67:GLY:HA2 | 1.68 | 0.74 |
| 10:j5:995:VAL:HG21 | 8:u7:14:GLU:OE2 | 1.87 | 0.74 |
| 10:k5:501:ILE:H | 10:k5:501:ILE:HD12 | 1.52 | 0.74 |
| 10:k5:1077:ILE:HG22 | 12:k5:1203:CYC:HAA1 | 1.69 | 0.74 |
| 1:P7:76:ARG:HB2 | 8:Q7:110:ILE:HG13 | 1.70 | 0.74 |
| 8:C7:35:ARG:HH22 | 8:C7:144:ASP:CB | 1.99 | 0.74 |
| 8:i7:39:ILE:HD12 | 8:i7:148:GLU:CG | 2.09 | 0.74 |
| 8:i7:47:ARG:CZ | 1:j7:18:TYR:CG | 2.70 | 0.74 |
| 8:W7:4:LEU:HD23 | 8:W7:26:ILE:HD13 | 1.69 | 0.74 |
| 4:M8:51:ARG:HH11 | 4:M8:51:ARG:CB | 2.00 | 0.74 |
| 3:L9:112:GLY:CA | 11:a9:532:ALA:HB3 | 2.16 | 0.74 |
| 5:N9:4:LEU:HD11 | 3:R9:111:ASN:ND2 | 2.02 | 0.74 |
| 5:N9:20:ILE:HG21 | 5:N9:60:ILE:HD13 | 1.69 | 0.74 |
| 5:N9:70:ILE:HG21 | 3:T9:116:THR:CA | 2.15 | 0.74 |
| 5:Z8:41:GLN:HB3 | 12:Z8:301:CYC:CHB | 2.11 | 0.74 |
| 3:Z9:59:LEU:HD22 | 3:Z9:130:ALA:HB2 | 1.67 | 0.74 |
| 11:a9:316:GLY:HA2 | 11:a9:319:LEU:HB2 | 1.68 | 0.74 |
| 2:AA:33:ARG:NE | 2:KA:28:ASN:ND2 | 2.36 | 0.74 |
| 5:NA:4:LEU:HD11 | 3:RA:111:ASN:ND2 | 2.02 | 0.74 |
| 5:NA:70:ILE:CG2 | 3:TA:119:ALA:CB | 2.65 | 0.74 |
| 2:A1:33:ARG:NE | 2:K1:28:ASN:ND2 | 2.36 | 0.74 |
| 12:Z3:201:CYC:HB | 4:M3:188:LEU:HD21 | 1.52 | 0.74 |
| 12:H4:201:CYC:HMA1 | 11:aA:261:SER:HB3 | 1.69 | 0.74 |
| 1:B5:14:VAL:O | 1:F5:69:GLY:N | 2.21 | 0.74 |
| 12:D5:201:CYC:HBB2 | 9:z5:42:GLN:NE2 | 2.02 | 0.74 |
| 8:I5:29:PHE:HZ | 8:I5:98:ALA:O | 1.62 | 0.74 |
| 8:Q5:4:LEU:HD23 | 8:Q5:26:ILE:HD13 | 1.69 | 0.74 |
| 12:R5:201:CYC:CMA | 12:R5:201:CYC:HB | 1.99 | 0.74 |
| 1:Z5:67:ARG:HH12 | 10:k5:705:THR:CB | 1.98 | 0.74 |
| 10:j5:283:ARG:HB2 | 10:j5:284:PRO:CD | 2.18 | 0.74 |
| 10:k5:283:ARG:HD3 | 10:k5:283:ARG:N | 2.02 | 0.74 |
| 10:k5:1054:SER:CA | 1:l7:107:ARG:HA | 2.17 | 0.74 |
| 8:G7:120:GLN:HG3 | 1:L7:53:LYS:HZ1 | 1.52 | 0.74 |
| 2:A8:33:ARG:NE | 2:K8:28:ASN:ND2 | 2.35 | 0.74 |
| 8:u7:5:THR:CB | 1:v7:6:THR:HG21 | 2.18 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:u7:47:ARG:HG2 | 8:u7:47:ARG:HH21 | 1.51 | 0.74 |
| 2:X8:60:TYR:HB2 | 3:T9:32:LYS:HZ2 | 1.52 | 0.74 |
| 4:M9:77:LEU:O | 4:M9:77:LEU:HD12 | 1.87 | 0.74 |
| 4:M9:263:PRO:CB | 3:V9:119:ALA:HB2 | 2.10 | 0.74 |
| 3:H9:116:THR:CG2 | 12:H9:202:CYC:CMA | 2.66 | 0.74 |
| 11:a9:95:ILE:CD1 | 11:a9:237:PHE:CZ | 2.70 | 0.74 |
| 11:aA:632:ILE:CG1 | 3:J1:107:ASP:OD1 | 2.34 | 0.74 |
| 4:M1:80:PRO:HA | 3:X1:111:ASN:ND2 | 2.00 | 0.74 |
| 5:N1:14:LYS:HE2 | 5:N1:50:LEU:HD23 | 1.67 | 0.74 |
| 4:MA:190:ARG:HH12 | 4:MA:202:SER:CB | 1.98 | 0.74 |
| 2:QA:91:ARG:NH2 | 3:TA:74:TYR:OH | 2.19 | 0.74 |
| 3:J3:111:ASN:ND2 | 11:a9:632:ILE:N | 2.34 | 0.74 |
| 4:M3:51:ARG:HH11 | 4:M3:51:ARG:HB3 | 1.51 | 0.74 |
| 4:M3:246:ALA:HA | 12:X3:201:CYC:HBB2 | 1.69 | 0.74 |
| 2:E4:1:MET:C | 4:M4:10:ARG:NH2 | 2.45 | 0.74 |
| 4:M4:51:ARG:HH11 | 4:M4:51:ARG:CB | 2.01 | 0.74 |
| 4:M4:92:GLU:OE1 | 4:M4:217:VAL:CG2 | 2.16 | 0.74 |
| 5:Z4:23:SER:OG | 5:Z4:25:THR:HB | 1.88 | 0.74 |
| 8:A5:122:PRO:CG | 12:A5:201:CYC:OC | 2.36 | 0.74 |
| 1:B5:83:ARG:HD2 | 9:z5:18:ARG:O | 1.87 | 0.74 |
| 1:f5:34:GLY:CA | 10:j5:47:PHE:CD2 | 2.71 | 0.74 |
| 1:R5:86:ASP:OD2 | 1:R5:90:ARG:NE | 2.19 | 0.74 |
| 1:Z5:64:ASP:CB | 10:k5:705:THR:CG2 | 2.63 | 0.74 |
| 9:i5:6:LYS:CB | 9:i5:55:LYS:HB3 | 2.15 | 0.74 |
| 10:j5:1054:SER:C | 10:j5:1056:PRO:HD3 | 2.13 | 0.74 |
| 10:k5:1019:SER:HG | 1:Z7:87:TYR:HE1 | 1.34 | 0.74 |
| 10:k5:1143:LEU:HD12 | 8:k7:106:GLU:HB2 | 1.70 | 0.74 |
| 8:i7:89:LEU:CD1 | 8:i7:153:PHE:CZ | 2.70 | 0.74 |
| 4:M8:101:ASP:HA | 2:P8:13:ASP:CB | 2.14 | 0.74 |
| 12:M8:302:CYC:C2C | 3:S8:78:ARG:CG | 2.65 | 0.74 |
| 11:a9:602:PRO:C | 11:a9:604:ALA:N | 2.41 | 0.74 |
| 11:aA:798:SER:OG | 12:aA:901:CYC:CAA | 2.35 | 0.74 |
| 3:J3:84:ARG:HH21 | 11:a9:670:LEU:HA | 1.51 | 0.74 |
| 6:M2:32:MET:HA | 8:O5:79:ALA:HB2 | 1.68 | 0.74 |
| 12:B3:202:CYC:HBA1 | 11:a9:684:ASN:HD22 | 1.53 | 0.74 |
| 3:B4:120:LEU:HD21 | 4:M4:52:LEU:CB | 2.16 | 0.74 |
| 12:B4:202:CYC:HBB3 | 4:M4:61:ASN:CG | 2.13 | 0.74 |
| 4:M3:77:LEU:HD12 | 4:M3:77:LEU:O | 1.87 | 0.74 |
| 2:O3:33:ARG:NE | 2:Y3:28:ASN:ND2 | 2.36 | 0.74 |
| 3:U4:115:GLU:OE1 | 4:M4:74:LEU:CD1 | 2.35 | 0.74 |
| 4:M4:29:PRO:CG | 11:aA:226:PHE:C | 2.49 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:E5:131:ARG:HG2 | 8:E5:157:VAL:HG21 | 1.68 | 0.74 |
| 8:G5:121:THR:HG21 | 12:G5:201:CYC:CHD | 2.18 | 0.74 |
| 1:f5:18:TYR:CE2 | 10:j5:165:ARG:HG3 | 2.23 | 0.74 |
| 10:k5:194:CYS:HB2 | 12:k5:1201:CYC:HAC1 | 1.70 | 0.74 |
| 3:D6:59:LEU:HD22 | 3:D6:130:ALA:HB2 | 1.67 | 0.74 |
| 3:F6:127:VAL:N | 12:F6:201:CYC:HMC2 | 2.03 | 0.74 |
| 8:g7:37:LEU:HD22 | 1:h7:24:LEU:HD21 | 1.70 | 0.74 |
| 12:j7:201:CYC:NB | 9:y7:38:PHE:CE1 | 2.55 | 0.74 |
| 3:B8:120:LEU:CD2 | 4:M8:49:LEU:O | 2.36 | 0.74 |
| 2:X8:69:PRO:CG | 2:S9:38:MET:O | 2.23 | 0.74 |
| 4:M8:27:HIS:O | 11:a9:227:GLY:HA3 | 1.87 | 0.74 |
| 4:M8:51:ARG:HH11 | 4:M8:51:ARG:HB3 | 1.51 | 0.74 |
| 4:M9:53:LEU:HD13 | 12:F9:301:CYC:HB | 0.76 | 0.74 |
| 5:N9:22:LEU:HD23 | 5:N9:26:LEU:CD1 | 1.83 | 0.74 |
| 11:aA:389:GLN:HA | 11:aA:389:GLN:NE2 | 2.01 | 0.74 |
| 4:M1:50:ASP:OD1 | 4:M1:50:ASP:N | 2.15 | 0.74 |
| 3:F2:78:ARG:CG | 12:F2:201:CYC:O2D | 2.36 | 0.74 |
| 5:Z4:37:HIS:HB2 | 12:Z4:301:CYC:C1B | 2.18 | 0.74 |
| 1:P5:114:GLU:CD | 10:k5:496:GLU:CB | 2.61 | 0.74 |
| 1:V5:114:GLU:HG2 | 10:j5:496:GLU:OE2 | 1.86 | 0.74 |
| 8:W5:130:VAL:HG21 | 8:W5:160:MET:HE3 | 1.69 | 0.74 |
| 10:j5:1070:ALA:HB1 | 10:j5:1071:PRO:HD3 | 1.67 | 0.74 |
| 10:k5:193:SER:OG | 12:k5:1201:CYC:O2D | 2.05 | 0.74 |
| 3:F6:59:LEU:HD21 | 12:F6:201:CYC:H2C | 1.70 | 0.74 |
| 8:g7:102:THR:CB | 8:g7:103:PRO:CD | 2.64 | 0.74 |
| 8:k7:76:LYS:HZ1 | 11:a9:605:PRO:HB3 | 0.78 | 0.74 |
| 8:u7:49:ARG:O | 8:u7:49:ARG:HG2 | 1.87 | 0.74 |
| 3:U8:108:ARG:HA | 4:M8:246:ALA:HB2 | 0.95 | 0.74 |
| 4:M9:51:ARG:HH11 | 4:M9:51:ARG:CB | 2.01 | 0.74 |
| 5:N9:70:ILE:CG2 | 3:T9:119:ALA:CB | 2.65 | 0.74 |
| 12:B9:201:CYC:HMA1 | 12:B9:201:CYC:HB | 1.51 | 0.74 |
| 3:H9:116:THR:CB | 11:a9:449:ASN:HD21 | 2.01 | 0.74 |
| 5:N1:20:ILE:HG21 | 5:N1:60:ILE:HD13 | 1.69 | 0.74 |
| 3:DA:111:ASN:OD1 | 4:MA:76:ALA:CB | 2.36 | 0.74 |
| 3:HA:116:THR:CB | 11:aA:449:ASN:HD21 | 2.01 | 0.74 |
| 12:LA:202:CYC:HMA1 | 11:aA:534:SER:CB | 2.17 | 0.74 |
| 4:MA:77:LEU:HD12 | 4:MA:77:LEU:O | 1.87 | 0.74 |
| 2:QA:67:THR:O | 2:U1:46:SER:OG | 2.06 | 0.74 |
| 3:J3:111:ASN:ND2 | 11:a9:631:GLY:CA | 2.51 | 0.74 |
| 6:M2:39:ARG:CZ | 8:O5:66:VAL:CG1 | 2.62 | 0.74 |
| 3:L3:119:ALA:C | 11:a9:817:LEU:HD11 | 2.11 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:N3:61:LYS:HZ2 | 12:R3:201:CYC:HBB2 | 1.51 | 0.74 |
| 4:M4:160:THR:CG2 | 4:M4:257:GLN:HB2 | 2.07 | 0.74 |
| 12:M4:301:CYC:HAC2 | 3:Y4:82:CYS:SG | 2.27 | 0.74 |
| 8:A5:49:ARG:HH21 | 8:A5:140:LEU:CD2 | 2.00 | 0.74 |
| 1:f5:34:GLY:CA | 10:j5:47:PHE:HD2 | 2.01 | 0.74 |
| 10:j5:362:LYS:CE | 10:j5:363:HIS:HE2 | 1.99 | 0.74 |
| 10:j5:841:VAL:CG1 | 10:j5:846:GLU:OE1 | 2.33 | 0.74 |
| 10:j5:988:ALA:HB2 | 1:h7:106:GLU:OE2 | 1.85 | 0.74 |
| 10:k5:1054:SER:C | 10:k5:1056:PRO:HD3 | 2.13 | 0.74 |
| 8:O7:161:GLN:HG2 | 1:F7:49:THR:HG21 | 1.70 | 0.74 |
| 1:H7:140:LEU:CD1 | 11:aA:561:ALA:HA | 2.16 | 0.74 |
| 8:g7:35:ARG:HH22 | 8:g7:144:ASP:CB | 2.00 | 0.74 |
| 8:i7:4:LEU:HD23 | 8:i7:26:ILE:HD13 | 1.68 | 0.74 |
| 8:c7:131:ARG:O | 8:c7:131:ARG:HG3 | 1.87 | 0.74 |
| 9:w7:35:GLU:N | 9:w7:35:GLU:OE1 | 2.20 | 0.74 |
| 4:M8:140:ARG:NE | 4:M8:209:TYR:HE1 | 1.85 | 0.74 |
| 4:M8:230:GLN:NE2 | 12:M8:301:CYC:HMA2 | 2.02 | 0.74 |
| 11:a9:454:LEU:HD23 | 11:a9:535:ASP:OD2 | 1.88 | 0.74 |
| 11:aA:32:ARG:HH11 | 11:aA:32:ARG:HG3 | 1.53 | 0.74 |
| 11:aA:377:VAL:CG1 | 11:aA:390:ALA:HB1 | 2.17 | 0.74 |
| 11:aA:746:TYR:HB2 | 2:K1:14:SER:CA | 2.18 | 0.74 |
| 4:M1:51:ARG:HH11 | 4:M1:51:ARG:CB | 2.00 | 0.74 |
| 2:EA:33:ARG:CG | 2:IA:25:GLN:OE1 | 2.33 | 0.74 |
| 2:G3:111:ALA:HB3 | 3:L3:77:ARG:NE | 2.01 | 0.74 |
| 4:M4:222:ARG:HG3 | 4:M4:222:ARG:NH1 | 2.01 | 0.74 |
| 2:P4:19:LEU:HD11 | 3:Q4:95:TYR:CD1 | 2.22 | 0.74 |
| 1:L5:79:ALA:CB | 8:G5:114:GLU:HB2 | 2.18 | 0.74 |
| 1:D5:87:TYR:CE2 | 9:z5:38:PHE:CE2 | 2.73 | 0.74 |
| 9:z5:11:ILE:CD1 | 9:z5:28:PHE:HE2 | 2.01 | 0.74 |
| 9:i5:2:SER:N | 9:i5:67:VAL:O | 2.21 | 0.74 |
| 10:k5:970:GLY:CA | 1:n7:77:ARG:NH2 | 2.42 | 0.74 |
| 8:o7:49:ARG:HG2 | 8:o7:49:ARG:O | 1.87 | 0.74 |
| 3:H8:119:ALA:C | 11:a9:266:ASN:CG | 2.55 | 0.74 |
| 3:H8:119:ALA:HB1 | 11:a9:266:ASN:CG | 2.12 | 0.74 |
| 5:N9:1:MET:HA | 5:N9:1:MET:CE | 2.10 | 0.74 |
| 5:N9:61:LYS:NZ | 12:T9:301:CYC:CBB | 2.41 | 0.74 |
| 3:H9:120:LEU:CD1 | 12:H9:202:CYC:HAA2 | 2.18 | 0.74 |
| 11:aA:31:SER:HG | 11:aA:34:ILE:CB | 1.89 | 0.74 |
| 11:aA:640:ALA:HB1 | 11:aA:767:THR:HG22 | 1.68 | 0.74 |
| 3:H1:82:CYS:HB2 | 12:H1:201:CYC:C4C | 2.18 | 0.74 |
| 4:MA:51:ARG:HH11 | 4:MA:51:ARG:CB | 2.01 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:QA:81:LYS:NZ | 3:TA:67:ILE:CD1 | 2.51 | 0.74 |
| 2:QA:116:VAL:HG23 | 3:TA:80:ALA:CB | 2.18 | 0.74 |
| 3:L3:104:VAL:CB | 3:L3:108:ARG:HH22 | 2.00 | 0.74 |
| 3:L3:104:VAL:HG12 | 3:L3:108:ARG:HH12 | 1.52 | 0.74 |
| 3:H4:84:ARG:NE | 11:aA:131:TYR:CG | 2.40 | 0.74 |
| 4:M4:226:SER:HG | 3:Y4:88:ILE:HG23 | 1.52 | 0.74 |
| 5:Z4:4:LEU:O | 5:Z4:4:LEU:HG | 1.88 | 0.74 |
| 1:D5:75:THR:HB | 8:E5:112:VAL:HA | 1.68 | 0.74 |
| 8:G5:49:ARG:HH21 | 8:G5:140:LEU:CD2 | 2.00 | 0.74 |
| 1:J5:87:TYR:HE2 | 9:i5:38:PHE:HE2 | 1.34 | 0.74 |
| 10:k5:963:ASP:OD1 | 10:k5:963:ASP:N | 2.20 | 0.74 |
| 8:O7:35:ARG:HH22 | 8:O7:144:ASP:CB | 2.00 | 0.74 |
| 8:Q7:19:SER:CB | 8:C7:6:LYS:HZ1 | 2.00 | 0.74 |
| 1:h7:75:THR:CG2 | 8:i7:115:MET:HE2 | 2.17 | 0.74 |
| 8:i7:95:GLY:O | 8:i7:152:TYR:HE2 | 1.71 | 0.74 |
| 8:m7:35:ARG:HH22 | 8:m7:144:ASP:CB | 1.99 | 0.74 |
| 8:o7:5:THR:CB | 1:p7:6:THR:HG21 | 2.18 | 0.74 |
| 9:z7:32:VAL:HG13 | 9:z7:37:TRP:HB2 | 1.69 | 0.74 |
| 4:M8:129:GLU:N | 4:M8:142:PHE:CZ | 2.56 | 0.74 |
| 12:O8:201:CYC:CMA | 5:Z8:53:LEU:CD1 | 2.36 | 0.74 |
| 12:O8:201:CYC:HMA1 | 5:Z8:53:LEU:HD12 | 1.70 | 0.74 |
| 4:M9:134:ASN:HB2 | 12:R9:201:CYC:CAA | 2.15 | 0.74 |
| 11:a9:98:ILE:HD12 | 11:a9:101:ASP:CB | 2.15 | 0.74 |
| 11:a9:508:ARG:HB2 | 11:a9:513:GLN:NE2 | 2.02 | 0.74 |
| 11:aA:668:TYR:HB2 | 3:J1:84:ARG:HD3 | 1.68 | 0.74 |
| 4:M1:188:LEU:HD21 | 12:Z1:202:CYC:HB | 1.52 | 0.74 |
| 4:M1:246:ALA:HA | 12:X1:201:CYC:HBB2 | 1.69 | 0.74 |
| 2:IA:31:PHE:HE2 | 3:JA:31:VAL:HA | 1.48 | 0.73 |
| 3:PA:59:LEU:HD22 | 3:PA:130:ALA:HB2 | 1.67 | 0.73 |
| 3:F4:108:ARG:O | 4:M4:6:THR:HG21 | 1.87 | 0.73 |
| 4:M4:77:LEU:HD12 | 4:M4:77:LEU:O | 1.87 | 0.73 |
| 4:M4:144:ARG:NH1 | 5:Z4:59:ARG:NH2 | 2.36 | 0.73 |
| 2:N4:33:ARG:NE | 2:X4:28:ASN:ND2 | 2.35 | 0.73 |
| 3:Q4:77:ARG:N | 5:Z4:34:LEU:HD13 | 2.03 | 0.73 |
| 8:C5:35:ARG:HH22 | 8:C5:144:ASP:CB | 2.00 | 0.73 |
| 1:f5:19:LEU:HD11 | 10:j5:172:LEU:HD13 | 1.62 | 0.73 |
| 8:U5:29:PHE:HZ | 8:U5:98:ALA:O | 1.62 | 0.73 |
| 1:Z5:28:LYS:HZ1 | 1:t7:143:PRO:HG2 | 0.91 | 0.73 |
| 3:J6:108:ARG:HH21 | 6:M6:155:ASN:HB3 | 1.51 | 0.73 |
| 9:z5:2:SER:N | 9:z5:67:VAL:O | 2.21 | 0.73 |
| 9:i5:11:ILE:CD1 | 9:i5:28:PHE:HE2 | 2.01 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:W7:13:ALA:HA | 9:w7:46:LYS:CD | 2.17 | 0.73 |
| 8:c7:8:ILE:HG23 | 1:d7:94:TYR:CG | 2.23 | 0.73 |
| 8:c7:95:GLY:O | 8:c7:152:TYR:HE2 | 1.71 | 0.73 |
| 2:E8:15:GLN:HG3 | 11:a9:163:ASP:OD2 | 1.88 | 0.73 |
| 8:o7:23:LEU:CD2 | 1:p7:38:VAL:CG1 | 2.66 | 0.73 |
| 9:z7:35:GLU:N | 9:z7:35:GLU:OE1 | 2.20 | 0.73 |
| 4:M8:99:VAL:HG22 | 3:Q8:108:ARG:NH1 | 2.03 | 0.73 |
| 2:O9:63:PHE:CB | 2:O9:66:LEU:CD1 | 2.56 | 0.73 |
| 12:D9:201:CYC:HMA1 | 12:D9:201:CYC:HB | 1.51 | 0.73 |
| 11:a9:331:TYR:CA | 11:a9:333:GLN:NE2 | 2.50 | 0.73 |
| 3:B2:59:LEU:HD22 | 3:B2:130:ALA:HB2 | 1.67 | 0.73 |
| 12:DA:201:CYC:HB | 12:DA:201:CYC:HMA1 | 1.51 | 0.73 |
| 3:LA:112:GLY:CA | 11:aA:532:ALA:HB3 | 2.17 | 0.73 |
| 12:LA:202:CYC:O1D | 11:aA:538:ARG:CB | 2.35 | 0.73 |
| 6:M2:39:ARG:HD3 | 8:O5:59:PHE:HB3 | 1.69 | 0.73 |
| 6:M2:50:LEU:CD2 | 8:i7:79:ALA:C | 2.61 | 0.73 |
| 12:F3:201:CYC:HMA1 | 12:F3:201:CYC:HB | 1.51 | 0.73 |
| 3:Z3:77:ARG:HE | 4:M3:273:ILE:HG23 | 1.51 | 0.73 |
| 4:M3:130:SER:HA | 12:P3:201:CYC:O2A | 1.87 | 0.73 |
| 3:F4:107:ASP:O | 4:M4:6:THR:HB | 1.88 | 0.73 |
| 4:M4:232:VAL:CG1 | 3:Y4:109:CYS:O | 2.35 | 0.73 |
| 8:Q5:130:VAL:HG21 | 8:Q5:160:MET:HE3 | 1.69 | 0.73 |
| 10:j5:199:THR:HG22 | 12:j5:1201:CYC:HBC2 | 1.70 | 0.73 |
| 10:j5:778:LYS:HZ1 | 12:L7:201:CYC:HBB2 | 1.51 | 0.73 |
| 10:j5:1118:THR:HG23 | 12:j5:1202:CYC:CGA | 2.18 | 0.73 |
| 8:Q7:4:LEU:HD23 | 8:Q7:26:ILE:HD13 | 1.69 | 0.73 |
| 8:S7:4:LEU:HD23 | 8:S7:26:ILE:HD13 | 1.71 | 0.73 |
| 8:a7:37:LEU:HD22 | 1:b7:24:LEU:HD21 | 1.70 | 0.73 |
| 12:B8:202:CYC:HMB3 | 4:M8:57:THR:CG2 | 2.18 | 0.73 |
| 8:o7:103:PRO:HB2 | 1:p7:9:ILE:HG21 | 1.70 | 0.73 |
| 8:q7:75:GLU:HB3 | 11:aA:53:VAL:HG12 | 1.70 | 0.73 |
| 3:H8:111:ASN:OD1 | 11:a9:291:TYR:CZ | 2.41 | 0.73 |
| 3:H8:119:ALA:C | 11:a9:266:ASN:HB2 | 2.13 | 0.73 |
| 4:M8:139:VAL:HG21 | 4:M8:216:ASN:CA | 2.15 | 0.73 |
| 11:a9:377:VAL:CG1 | 11:a9:390:ALA:HB1 | 2.17 | 0.73 |
| 11:aA:670:LEU:HD21 | 3:J1:80:ALA:CB | 2.17 | 0.73 |
| 4:M1:51:ARG:HH11 | 4:M1:51:ARG:HB3 | 1.51 | 0.73 |
| 4:M1:146:LEU:HD23 | 4:M1:146:LEU:N | 2.02 | 0.73 |
| 1:A:131:GLN:CD | 1:R5:17:LYS:NZ | 2.46 | 0.73 |
| 12:P1:201:CYC:O2A | 4:M1:130:SER:HA | 1.87 | 0.73 |
| 3:J3:80:ALA:CB | 11:a9:670:LEU:HD21 | 2.18 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:K3:28:ASN:ND2 | 2:A3:33:ARG:NE | 2.36 | 0.73 |
| 3:B3:111:ASN:OD1 | 4:M3:76:ALA:HB3 | 1.87 | 0.73 |
| 12:B4:202:CYC:HHA | 4:M4:54:ALA:N | 2.04 | 0.73 |
| 3:B1:88:ILE:HG21 | 12:B1:202:CYC:HAB2 | 1.66 | 0.73 |
| 3:B1:88:ILE:HG21 | 12:B1:202:CYC:CAB | 2.18 | 0.73 |
| 3:F4:109:CYS:CA | 4:M4:6:THR:HG21 | 2.12 | 0.73 |
| 3:H4:119:ALA:C | 11:aA:266:ASN:CG | 2.56 | 0.73 |
| 5:Z4:24:PRO:HG3 | 12:Z4:301:CYC:O2A | 1.87 | 0.73 |
| 1:F5:119:LEU:CD2 | 10:k5:546:PHE:CD2 | 2.71 | 0.73 |
| 8:A7:86:ASP:HB2 | 11:aA:579:PHE:CZ | 2.23 | 0.73 |
| 8:G7:4:LEU:HD23 | 8:G7:26:ILE:HD13 | 1.71 | 0.73 |
| 8:g7:56:ASP:OD1 | 11:aA:325:LEU:CD1 | 2.35 | 0.73 |
| 8:o7:30:VAL:HG12 | 1:p7:31:PHE:HD1 | 1.53 | 0.73 |
| 4:M8:126:THR:CA | 12:M8:302:CYC:O2A | 2.36 | 0.73 |
| 4:M8:205:ASP:OD2 | 5:Z8:59:ARG:CD | 2.35 | 0.73 |
| 4:M9:274:VAL:CG2 | 2:W9:111:ALA:HB3 | 2.18 | 0.73 |
| 2:O9:33:ARG:NE | 2:Y9:28:ASN:ND2 | 2.35 | 0.73 |
| 11:a9:32:ARG:HG3 | 11:a9:32:ARG:HH11 | 1.53 | 0.73 |
| 11:aA:602:PRO:C | 11:aA:604:ALA:N | 2.41 | 0.73 |
| 11:aA:667:THR:HG22 | 11:aA:800:THR:HG22 | 1.69 | 0.73 |
| 2:AA:59:VAL:O | 2:AA:66:LEU:HD12 | 1.88 | 0.73 |
| 3:LA:52:ILE:CD1 | 3:LA:87:GLU:CG | 2.61 | 0.73 |
| 3:LA:97:LEU:HD12 | 3:LA:97:LEU:C | 2.13 | 0.73 |
| 2:A3:59:VAL:O | 2:A3:66:LEU:HD12 | 1.88 | 0.73 |
| 3:Z3:111:ASN:HD21 | 4:M3:258:LYS:HZ2 | 0.75 | 0.73 |
| 3:L3:120:LEU:HD21 | 11:a9:731:GLN:HG2 | 1.70 | 0.73 |
| 2:N4:112:GLY:N | 5:Z4:34:LEU:N | 2.37 | 0.73 |
| 10:j5:320:GLU:HA | 10:j5:333:PHE:CE1 | 2.24 | 0.73 |
| 8:c7:4:LEU:HD23 | 8:c7:26:ILE:HD13 | 1.69 | 0.73 |
| 8:o7:27:LYS:CD | 1:p7:35:ALA:CA | 2.58 | 0.73 |
| 8:u7:30:VAL:HG12 | 1:v7:31:PHE:HD1 | 1.53 | 0.73 |
| 9:w7:32:VAL:HG13 | 9:w7:37:TRP:HB2 | 1.69 | 0.73 |
| 2:X8:108:TYR:CE1 | 4:M8:273:ILE:HD12 | 2.22 | 0.73 |
| 3:F8:107:ASP:HA | 4:M8:8:SER:N | 1.99 | 0.73 |
| 12:M8:302:CYC:C1C | 3:S8:78:ARG:CG | 2.66 | 0.73 |
| 3:S8:116:THR:HG23 | 3:S8:117:TYR:N | 2.04 | 0.73 |
| 12:L9:202:CYC:O1D | 11:a9:538:ARG:CB | 2.36 | 0.73 |
| 3:Y8:89:ILE:CG2 | 3:Y8:92:TYR:HH | 1.76 | 0.73 |
| 2:A9:59:VAL:O | 2:A9:66:LEU:HD12 | 1.88 | 0.73 |
| 11:a9:95:ILE:HD11 | 11:a9:237:PHE:CZ | 2.24 | 0.73 |
| 11:a9:274:LEU:C | 11:a9:278:LEU:HD11 | 2.12 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 11:a9:710:THR:CB | 11:a9:807:GLN:HB3 | 2.18 | 0.73 |
| 3:HA:82:CYS:SG | 12:HA:202:CYC:HAC1 | 2.27 | 0.73 |
| 2:A4:33:ARG:NE | 2:K4:28:ASN:ND2 | 2.35 | 0.73 |
| 3:H4:111:ASN:OD1 | 11:aA:291:TYR:CZ | 2.41 | 0.73 |
| 4:M4:95:ALA:O | 3:Q4:88:ILE:HG21 | 1.89 | 0.73 |
| 12:R5:201:CYC:HBB2 | 10:k5:520:ARG:CG | 2.19 | 0.73 |
| 10:j5:501:ILE:H | 10:j5:501:ILE:HD12 | 1.52 | 0.73 |
| 10:j5:1077:ILE:O | 12:r7:201:CYC:CBA | 2.36 | 0.73 |
| 10:k5:370:GLU:N | 10:k5:374:GLU:OE1 | 2.21 | 0.73 |
| 8:k7:4:LEU:HD23 | 8:k7:26:ILE:HD13 | 1.71 | 0.73 |
| 8:k7:90:ARG:HD3 | 1:l7:18:TYR:CD1 | 2.24 | 0.73 |
| 8:c7:8:ILE:CG2 | 1:d7:94:TYR:CG | 2.72 | 0.73 |
| 12:D8:202:CYC:CGA | 4:M8:35:THR:CB | 2.55 | 0.73 |
| 9:w7:23:LEU:HD12 | 9:w7:23:LEU:O | 1.89 | 0.73 |
| 3:H8:119:ALA:CA | 11:a9:266:ASN:CB | 2.66 | 0.73 |
| 2:O9:59:VAL:O | 2:O9:66:LEU:HD12 | 1.89 | 0.73 |
| 5:Z8:5:THR:O | 5:Z8:5:THR:CG2 | 2.37 | 0.73 |
| 5:Z8:20:ILE:HG21 | 5:Z8:60:ILE:HD13 | 1.69 | 0.73 |
| 11:aA:731:GLN:HG2 | 3:L1:120:LEU:HD21 | 1.70 | 0.73 |
| 4:M1:77:LEU:HD12 | 4:M1:77:LEU:O | 1.87 | 0.73 |
| 1:A:18:TYR:CE2 | 8:a5:90:ARG:HA | 2.23 | 0.73 |
| 4:MA:274:VAL:CG2 | 2:WA:111:ALA:HB3 | 2.18 | 0.73 |
| 12:J3:202:CYC:CAA | 11:a9:798:SER:OG | 2.36 | 0.73 |
| 2:K3:14:SER:CA | 11:a9:746:TYR:HB2 | 2.17 | 0.73 |
| 2:C3:140:SER:HB2 | 3:D8:150:ARG:NH1 | 2.03 | 0.73 |
| 12:Z3:201:CYC:NB | 4:M3:188:LEU:HD21 | 2.04 | 0.73 |
| 3:B4:120:LEU:HD11 | 4:M4:53:LEU:HA | 1.62 | 0.73 |
| 3:L3:119:ALA:C | 11:a9:817:LEU:CD1 | 2.60 | 0.73 |
| 2:O3:59:VAL:O | 2:O3:66:LEU:HD12 | 1.89 | 0.73 |
| 2:U3:47:ASN:CB | 2:Q9:74:TYR:OH | 2.34 | 0.73 |
| 3:H4:119:ALA:HB1 | 11:aA:266:ASN:CG | 2.13 | 0.73 |
| 3:H4:119:ALA:CA | 11:aA:266:ASN:CB | 2.65 | 0.73 |
| 4:M4:94:TRP:CZ3 | 3:Q4:88:ILE:HA | 2.23 | 0.73 |
| 1:L5:69:GLY:N | 1:H5:14:VAL:O | 2.21 | 0.73 |
| 1:B5:87:TYR:CE1 | 9:z5:20:GLY:HA2 | 2.23 | 0.73 |
| 9:z5:22:GLU:C | 9:z5:25:ASN:N | 2.43 | 0.73 |
| 10:j5:283:ARG:N | 10:j5:283:ARG:HD3 | 2.01 | 0.73 |
| 10:j5:1147:TYR:CD2 | 11:aA:39:PRO:HB3 | 2.23 | 0.73 |
| 10:k5:194:CYS:HB2 | 12:k5:1201:CYC:HAC2 | 1.71 | 0.73 |
| 10:k5:283:ARG:HB2 | 10:k5:284:PRO:CD | 2.18 | 0.73 |
| 10:k5:320:GLU:HA | 10:k5:333:PHE:HE1 | 1.50 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:i7:114:GLU:N | 8:i7:114:GLU:OE1 | 2.22 | 0.73 |
| 8:k7:52:LYS:HE3 | 11:a9:56:ILE:HG21 | 1.69 | 0.73 |
| 1:Z7:67:ARG:HH12 | 11:a9:307:ARG:CG | 2.01 | 0.73 |
| 8:a7:63:PRO:HG2 | 11:a9:334:LYS:HA | 1.68 | 0.73 |
| 1:f7:67:ARG:HH11 | 11:aA:311:LEU:HD13 | 1.53 | 0.73 |
| 8:o7:4:LEU:HD23 | 8:o7:26:ILE:HD13 | 1.69 | 0.73 |
| 2:X8:57:GLN:O | 3:T9:32:LYS:NZ | 2.22 | 0.73 |
| 4:M8:29:PRO:HG3 | 11:a9:226:PHE:C | 2.13 | 0.73 |
| 4:M8:140:ARG:NH2 | 4:M8:210:ILE:HG12 | 2.02 | 0.73 |
| 4:M8:146:LEU:HD23 | 4:M8:146:LEU:N | 2.02 | 0.73 |
| 4:M8:205:ASP:CG | 5:Z8:59:ARG:HE | 1.96 | 0.73 |
| 2:P8:18:PHE:H | 3:Q8:91:ARG:NH2 | 1.85 | 0.73 |
| 4:M9:76:ALA:CB | 3:D9:111:ASN:OD1 | 2.36 | 0.73 |
| 11:aA:61:TYR:CD1 | 11:aA:65:LEU:HD22 | 2.20 | 0.73 |
| 11:aA:316:GLY:HA2 | 11:aA:319:LEU:HB2 | 1.68 | 0.73 |
| 11:aA:371:VAL:CG1 | 11:aA:507:PHE:HB2 | 2.18 | 0.73 |
| 11:aA:414:ALA:HB1 | 11:aA:428:PHE:CE1 | 2.23 | 0.73 |
| 2:EA:152:ALA:HB1 | 2:IA:21:ASN:ND2 | 2.02 | 0.73 |
| 12:QA:201:CYC:O2D | 3:TA:57:HIS:NE2 | 2.21 | 0.73 |
| 3:B1:88:ILE:HD13 | 12:B1:202:CYC:C4B | 2.17 | 0.73 |
| 3:H4:84:ARG:HD2 | 11:aA:131:TYR:CG | 2.14 | 0.73 |
| 8:A5:121:THR:HG21 | 12:A5:201:CYC:CHD | 2.18 | 0.73 |
| 8:G5:64:ASP:OD2 | 8:U5:69:GLY:C | 2.31 | 0.73 |
| 8:G5:161:GLN:CD | 1:T5:49:THR:HG22 | 2.14 | 0.73 |
| 1:d5:53:LYS:CD | 8:e5:118:SER:O | 2.34 | 0.73 |
| 8:U5:87:TYR:CE2 | 6:M6:26:PHE:CG | 2.68 | 0.73 |
| 2:K6:28:ASN:ND2 | 2:A6:33:ARG:NE | 2.36 | 0.73 |
| 6:M6:271:VAL:CG2 | 1:d7:127:VAL:HG11 | 2.18 | 0.73 |
| 10:j5:1043:GLU:OE1 | 8:e7:14:GLU:HG2 | 1.88 | 0.73 |
| 10:j5:1119:LEU:HD13 | 1:t7:87:TYR:OH | 1.89 | 0.73 |
| 10:j5:1144:SER:HB3 | 1:r7:13:ASP:OD2 | 1.88 | 0.73 |
| 8:S7:90:ARG:HD3 | 1:T7:18:TYR:CD1 | 2.24 | 0.73 |
| 8:I7:25:ARG:NH2 | 8:W7:25:ARG:HB3 | 1.90 | 0.73 |
| 8:i7:94:TYR:CG | 1:j7:9:ILE:HG21 | 2.22 | 0.73 |
| 8:u7:16:ARG:O | 1:v7:94:TYR:HE1 | 1.70 | 0.73 |
| 8:u7:30:VAL:HA | 1:v7:31:PHE:HD1 | 1.50 | 0.73 |
| 2:X8:28:ASN:ND2 | 2:N8:33:ARG:NE | 2.35 | 0.73 |
| 3:F8:1:MET:N | 4:M8:10:ARG:HB3 | 2.03 | 0.73 |
| 3:L9:77:ARG:CZ | 11:a9:538:ARG:NH2 | 2.52 | 0.73 |
| 2:E9:152:ALA:HB1 | 2:I9:21:ASN:ND2 | 2.02 | 0.73 |
| 11:a9:439:ARG:HG3 | 11:a9:439:ARG:HH11 | 1.54 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 11:aA:454:LEU:HD23 | 11:aA:535:ASP:OD2 | 1.88 | 0.73 |
| 11:aA:813:PRO:CA | 3:L1:119:ALA:CB | 2.67 | 0.73 |
| 3:LA:115:GLU:N | 3:LA:115:GLU:OE1 | 2.22 | 0.73 |
| 2:QA:76:ASP:H | 2:U1:141:GLN:HA | 1.53 | 0.73 |
| 2:O1:33:ARG:NE | 2:Y1:28:ASN:ND2 | 2.36 | 0.73 |
| 2:O1:59:VAL:O | 2:O1:66:LEU:HD12 | 1.89 | 0.73 |
| 2:O1:63:PHE:HB2 | 2:O1:66:LEU:HD12 | 1.70 | 0.73 |
| 3:J2:108:ARG:HH21 | 6:M2:155:ASN:HB3 | 1.51 | 0.73 |
| 6:M2:37:GLU:OE2 | 8:O5:59:PHE:CE2 | 2.41 | 0.73 |
| 6:M2:57:GLU:OE1 | 8:i7:76:LYS:HD2 | 1.87 | 0.73 |
| 6:M2:128:LEU:HG | 12:F2:201:CYC:OB | 1.89 | 0.73 |
| 3:B4:68:ARG:HH12 | 3:U4:68:ARG:HH22 | 1.37 | 0.73 |
| 3:B4:108:ARG:C | 4:M4:61:ASN:CA | 2.62 | 0.73 |
| 4:M3:146:LEU:HD23 | 4:M3:146:LEU:N | 2.02 | 0.73 |
| 4:M3:269:SER:HA | 3:V3:111:ASN:HD22 | 1.54 | 0.73 |
| 5:N3:39:PRO:CB | 3:T3:113:LEU:HA | 2.15 | 0.73 |
| 3:H4:119:ALA:HB3 | 11:aA:266:ASN:HD22 | 0.56 | 0.73 |
| 5:Z4:1:MET:HE3 | 5:Z4:1:MET:CA | 2.17 | 0.73 |
| 8:A5:118:SER:CB | 1:F5:82:ILE:CD1 | 2.67 | 0.73 |
| 1:b5:5:ILE:HD12 | 10:k5:46:PHE:HE1 | 1.52 | 0.73 |
| 10:j5:722:ILE:HD11 | 8:K7:82:LEU:HD12 | 1.71 | 0.73 |
| 10:j5:868:ASP:C | 9:w7:43:ARG:CD | 2.61 | 0.73 |
| 10:k5:74:ARG:O | 10:k5:74:ARG:HG3 | 1.89 | 0.73 |
| 10:k5:902:ASN:O | 10:k5:902:ASN:ND2 | 2.16 | 0.73 |
| 10:k5:1119:LEU:HD11 | 12:k5:1204:CYC:HBB3 | 1.69 | 0.73 |
| 8:E7:4:LEU:HD23 | 8:E7:26:ILE:HD13 | 1.69 | 0.73 |
| 8:G7:90:ARG:HD3 | 1:H7:18:TYR:CD1 | 2.24 | 0.73 |
| 8:s7:29:PHE:HE1 | 8:s7:98:ALA:O | 1.69 | 0.73 |
| 9:z7:23:LEU:O | 9:z7:23:LEU:HD12 | 1.89 | 0.73 |
| 12:H8:201:CYC:HMA1 | 11:a9:261:SER:HB3 | 1.70 | 0.73 |
| 3:O8:107:ASP:CA | 5:Z8:66:ARG:HB2 | 2.19 | 0.73 |
| 4:M9:133:ARG:HD2 | 12:R9:201:CYC:CGA | 2.19 | 0.73 |
| 5:N9:70:ILE:CG2 | 3:T9:119:ALA:HB3 | 2.19 | 0.73 |
| 5:Z8:1:MET:HE3 | 5:Z8:1:MET:CA | 2.17 | 0.73 |
| 5:Z8:50:LEU:C | 5:Z8:50:LEU:HD12 | 2.14 | 0.73 |
| 2:K9:12:ALA:O | 2:K9:16:GLY:N | 2.22 | 0.73 |
| 11:aA:107:ARG:HG3 | 11:aA:108:PRO:CD | 2.18 | 0.73 |
| 5:N1:50:LEU:C | 5:N1:50:LEU:HD12 | 2.14 | 0.73 |
| 2:A2:59:VAL:O | 2:A2:66:LEU:HD12 | 1.89 | 0.73 |
| 1:A:31:PHE:HE2 | 8:a5:37:LEU:HD11 | 1.54 | 0.73 |
| 3:J3:107:ASP:OD1 | 11:a9:632:ILE:CG1 | 2.36 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:F4:115:GLU:CG | 4:M4:3:VAL:HG21 | 2.16 | 0.73 |
| 4:M4:146:LEU:HD23 | 4:M4:146:LEU:N | 2.02 | 0.73 |
| 8:E5:77:MET:O | 12:E5:201:CYC:HMD1 | 1.89 | 0.73 |
| 8:G5:126:VAL:HG22 | 12:G5:201:CYC:C3C | 2.12 | 0.73 |
| 8:c5:90:ARG:HD3 | 1:d5:18:TYR:CD1 | 2.24 | 0.73 |
| 1:f5:6:THR:CG2 | 10:j5:19:THR:OG1 | 2.36 | 0.73 |
| 8:Q5:18:LEU:HD22 | 1:R5:97:LEU:CD1 | 2.19 | 0.73 |
| 8:S5:4:LEU:HD23 | 8:S5:26:ILE:HD13 | 1.71 | 0.73 |
| 10:j5:306:GLU:OE2 | 10:j5:362:LYS:NZ | 2.19 | 0.73 |
| 10:j5:385:PRO:O | 10:j5:386:ILE:C | 2.23 | 0.73 |
| 10:j5:1015:TYR:CE2 | 10:j5:1048:ARG:NH2 | 2.57 | 0.73 |
| 8:M7:4:LEU:HD23 | 8:M7:26:ILE:HD13 | 1.71 | 0.73 |
| 8:q7:4:LEU:HD23 | 8:q7:26:ILE:HD13 | 1.71 | 0.73 |
| 3:U8:120:LEU:HD11 | 12:U8:201:CYC:CGD | 2.19 | 0.73 |
| 4:M8:231:THR:CA | 12:M8:301:CYC:HBB2 | 2.18 | 0.73 |
| 2:N8:60:TYR:HB3 | 2:N8:67:THR:CG2 | 2.19 | 0.73 |
| 2:A9:33:ARG:NE | 2:K9:28:ASN:ND2 | 2.36 | 0.73 |
| 11:aA:331:TYR:CA | 11:aA:333:GLN:NE2 | 2.50 | 0.73 |
| 11:aA:629:LYS:HA | 11:aA:629:LYS:CE | 2.19 | 0.73 |
| 1:Z:16:GLY:HA2 | 8:e5:90:ARG:CZ | 2.19 | 0.73 |
| 3:HA:120:LEU:CD1 | 12:HA:202:CYC:HAA1 | 1.99 | 0.73 |
| 3:JA:70:GLY:HA2 | 11:aA:357:THR:C | 2.10 | 0.73 |
| 3:D4:150:ARG:NH1 | 2:C1:140:SER:HB2 | 2.03 | 0.73 |
| 4:M4:29:PRO:HG3 | 11:aA:226:PHE:O | 1.88 | 0.73 |
| 4:M4:144:ARG:CZ | 4:M4:204:ILE:HG22 | 2.19 | 0.73 |
| 8:S5:107:ILE:HD13 | 1:T5:13:ASP:CG | 2.14 | 0.73 |
| 10:j5:449:ARG:HG3 | 10:j5:449:ARG:NH2 | 1.98 | 0.73 |
| 10:k5:195:SER:O | 10:k5:199:THR:HG23 | 1.89 | 0.73 |
| 10:k5:930:LEU:CB | 1:D7:33:THR:HG21 | 2.18 | 0.73 |
| 10:k5:990:ARG:NH2 | 10:k5:1026:LYS:NZ | 2.31 | 0.73 |
| 2:A6:59:VAL:O | 2:A6:66:LEU:HD12 | 1.89 | 0.73 |
| 8:k7:66:VAL:O | 11:a9:65:LEU:HD21 | 1.89 | 0.73 |
| 1:V7:76:ARG:HB2 | 8:W7:110:ILE:HG13 | 1.70 | 0.73 |
| 2:A8:60:TYR:HB3 | 2:A8:67:THR:CG2 | 2.19 | 0.73 |
| 3:B8:82:CYS:HA | 12:B8:202:CYC:OC | 1.86 | 0.73 |
| 4:M8:226:SER:OG | 3:Y8:88:ILE:CG1 | 2.36 | 0.73 |
| 2:A9:60:TYR:HB3 | 2:A9:67:THR:CG2 | 2.19 | 0.73 |
| 3:J9:109:CYS:O | 11:a9:518:ALA:CB | 2.33 | 0.73 |
| 11:a9:414:ALA:HB1 | 11:a9:428:PHE:CE1 | 2.23 | 0.73 |
| 2:A2:60:TYR:HB3 | 2:A2:67:THR:CG2 | 2.19 | 0.73 |
| 3:FA:36:LYS:C | 3:FA:156:LEU:HD21 | 2.14 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:FA:148:VAL:HG11 | 12:F9:302:CYC:CHD | 2.19 | 0.72 |
| 3:LA:120:LEU:HD23 | 11:aA:539:GLY:N | 2.04 | 0.72 |
| 4:MA:274:VAL:H | 3:VA:77:ARG:HG2 | 1.49 | 0.72 |
| 3:L2:75:PRO:HD2 | 3:L2:78:ARG:CB | 2.15 | 0.72 |
| 2:A4:63:PHE:HB2 | 2:A4:66:LEU:HD12 | 1.70 | 0.72 |
| 3:F4:109:CYS:C | 4:M4:6:THR:HG23 | 2.11 | 0.72 |
| 4:M4:27:HIS:HE1 | 4:M4:34:ASP:CA | 1.80 | 0.72 |
| 4:M4:29:PRO:HB2 | 11:aA:225:VAL:O | 1.84 | 0.72 |
| 4:M4:104:ALA:HB2 | 2:P4:14:SER:H | 1.50 | 0.72 |
| 5:Z4:50:LEU:C | 5:Z4:50:LEU:HD12 | 2.14 | 0.72 |
| 6:M6:273:PHE:HE1 | 1:d7:128:GLY:HA2 | 1.53 | 0.72 |
| 10:j5:1077:ILE:O | 12:r7:201:CYC:HBA2 | 1.88 | 0.72 |
| 10:k5:320:GLU:HA | 10:k5:333:PHE:CE1 | 2.24 | 0.72 |
| 10:k5:387:VAL:O | 10:k5:394:PRO:CB | 2.37 | 0.72 |
| 10:k5:990:ARG:HH21 | 10:k5:1026:LYS:HZ2 | 1.37 | 0.72 |
| 1:B7:136:VAL:HA | 11:a9:563:PHE:HZ | 1.53 | 0.72 |
| 12:B8:202:CYC:HMA1 | 12:B8:202:CYC:NB | 2.05 | 0.72 |
| 8:m7:29:PHE:HE1 | 8:m7:98:ALA:O | 1.69 | 0.72 |
| 4:M8:104:ALA:CB | 2:P8:14:SER:H | 1.98 | 0.72 |
| 3:L9:115:GLU:N | 3:L9:115:GLU:OE1 | 2.22 | 0.72 |
| 11:a9:48:LEU:HD12 | 11:a9:48:LEU:C | 2.14 | 0.72 |
| 11:a9:371:VAL:CG1 | 11:a9:507:PHE:HB2 | 2.18 | 0.72 |
| 11:a9:594:ARG:HG3 | 11:a9:594:ARG:NH1 | 2.01 | 0.72 |
| 11:aA:95:ILE:HD11 | 11:aA:237:PHE:CZ | 2.24 | 0.72 |
| 11:aA:817:LEU:CD1 | 3:L1:119:ALA:C | 2.60 | 0.72 |
| 2:GA:14:SER:O | 11:aA:482:TYR:HB3 | 1.89 | 0.72 |
| 5:NA:50:LEU:C | 5:NA:50:LEU:HD12 | 2.14 | 0.72 |
| 5:NA:61:LYS:NZ | 12:TA:301:CYC:CBB | 2.41 | 0.72 |
| 5:NA:70:ILE:CG2 | 3:TA:119:ALA:HB3 | 2.19 | 0.72 |
| 2:T4:111:ALA:HB1 | 4:M4:87:ILE:HG21 | 1.70 | 0.72 |
| 3:Q4:120:LEU:HD23 | 5:Z4:42:SER:HB2 | 1.60 | 0.72 |
| 1:L5:82:ILE:CD1 | 8:G5:118:SER:CB | 2.67 | 0.72 |
| 1:N5:87:TYR:OH | 10:k5:483:PHE:CE2 | 2.41 | 0.72 |
| 8:A5:106:GLU:OE2 | 10:k5:559:THR:HA | 1.88 | 0.72 |
| 8:G5:4:LEU:HD23 | 8:G5:26:ILE:HD13 | 1.71 | 0.72 |
| 8:U5:75:GLU:HB2 | 6:M6:43:TRP:HE1 | 1.50 | 0.72 |
| 8:Y5:4:LEU:HD23 | 8:Y5:26:ILE:HD13 | 1.71 | 0.72 |
| 8:Y5:90:ARG:HD3 | 1:Z5:18:TYR:CD1 | 2.24 | 0.72 |
| 1:b5:34:GLY:CA | 10:k5:47:PHE:CD2 | 2.69 | 0.72 |
| 6:M6:104:ARG:HD3 | 2:G6:15:GLN:HA | 1.72 | 0.72 |
| 6:M6:271:VAL:HG23 | 1:d7:127:VAL:HG11 | 1.71 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:289:SER:HB3 | 10:j5:292:GLU:CD | 2.14 | 0.72 |
| 10:k5:1015:TYR:CE2 | 10:k5:1048:ARG:NH2 | 2.57 | 0.72 |
| 8:O7:12:ASP:OD1 | 1:P7:91:TYR:CZ | 2.43 | 0.72 |
| 4:M8:200:ILE:HB | 5:Z8:52:ARG:NH2 | 2.03 | 0.72 |
| 12:M8:302:CYC:OC | 3:S8:78:ARG:CZ | 2.37 | 0.72 |
| 2:N8:115:GLU:OE1 | 5:Z8:32:PRO:HD2 | 1.87 | 0.72 |
| 3:Q8:84:ARG:CD | 5:Z8:31:TRP:NE1 | 2.51 | 0.72 |
| 2:O9:60:TYR:HB3 | 2:O9:67:THR:CG2 | 2.19 | 0.72 |
| 12:H9:202:CYC:NB | 11:a9:474:PHE:CZ | 2.57 | 0.72 |
| 11:a9:312:ASP:CB | 11:a9:315:LEU:HD12 | 2.16 | 0.72 |
| 11:aA:668:TYR:CB | 3:J1:84:ARG:HD3 | 2.19 | 0.72 |
| 11:aA:800:THR:HG22 | 12:aA:901:CYC:HAA1 | 1.52 | 0.72 |
| 4:M1:269:SER:HA | 3:V1:111:ASN:HD22 | 1.54 | 0.72 |
| 3:FA:68:ARG:CZ | 3:ZA:68:ARG:HH12 | 1.95 | 0.72 |
| 4:MA:172:HIS:HE1 | 4:MA:249:ASP:OD2 | 1.73 | 0.72 |
| 3:TA:32:LYS:NZ | 2:X4:57:GLN:O | 2.22 | 0.72 |
| 2:A1:59:VAL:O | 2:A1:66:LEU:HD12 | 1.88 | 0.72 |
| 2:A1:60:TYR:HB3 | 2:A1:67:THR:CG2 | 2.19 | 0.72 |
| 6:M2:164:GLU:OE1 | 6:M2:258:VAL:HG22 | 1.89 | 0.72 |
| 3:B1:84:ARG:NH1 | 12:B1:202:CYC:O2A | 2.22 | 0.72 |
| 12:H4:201:CYC:OB | 11:aA:129:ASN:HB3 | 1.89 | 0.72 |
| 3:L4:68:ARG:HH11 | 11:aA:75:ALA:HB3 | 1.51 | 0.72 |
| 1:L5:106:GLU:HG3 | 9:i5:58:THR:CG2 | 2.19 | 0.72 |
| 8:G5:122:PRO:CG | 12:G5:201:CYC:OC | 2.36 | 0.72 |
| 1:d5:28:LYS:CE | 1:n7:143:PRO:HB2 | 2.07 | 0.72 |
| 8:W5:18:LEU:HD22 | 1:X5:97:LEU:CD1 | 2.19 | 0.72 |
| 8:A7:90:ARG:HD3 | 1:B7:18:TYR:CD1 | 2.24 | 0.72 |
| 10:j5:503:LYS:O | 10:j5:503:LYS:HG2 | 1.87 | 0.72 |
| 10:k5:1034:GLU:CD | 10:k5:1037:ARG:NH2 | 2.48 | 0.72 |
| 8:S7:120:GLN:HG3 | 1:X7:53:LYS:HZ1 | 1.54 | 0.72 |
| 8:K7:4:LEU:HD23 | 8:K7:26:ILE:HD13 | 1.69 | 0.72 |
| 8:M7:90:ARG:HD3 | 1:N7:18:TYR:CD1 | 2.24 | 0.72 |
| 8:i7:131:ARG:HH11 | 8:i7:131:ARG:CG | 2.03 | 0.72 |
| 8:a7:33:GLY:CA | 1:b7:31:PHE:CE2 | 2.71 | 0.72 |
| 8:s7:12:ASP:OD1 | 1:t7:91:TYR:CZ | 2.43 | 0.72 |
| 3:L9:120:LEU:HD23 | 11:a9:539:GLY:N | 2.04 | 0.72 |
| 3:H9:113:LEU:HD22 | 12:H9:202:CYC:HMB1 | 1.69 | 0.72 |
| 5:N1:1:MET:HE3 | 5:N1:1:MET:CA | 2.17 | 0.72 |
| 2:AA:60:TYR:HB3 | 2:AA:67:THR:CG2 | 2.19 | 0.72 |
| 3:HA:120:LEU:CD1 | 12:HA:202:CYC:HAA2 | 2.19 | 0.72 |
| 4:MA:81:ASP:N | 3:ZA:111:ASN:ND2 | 2.37 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:NA:4:LEU:O | 5:NA:4:LEU:HG | 1.88 | 0.72 |
| 2:OA:60:TYR:OH | 2:OA:79:GLN:HG2 | 1.90 | 0.72 |
| 2:O1:60:TYR:HB3 | 2:O1:67:THR:CG2 | 2.19 | 0.72 |
| 2:K2:28:ASN:ND2 | 2:A2:33:ARG:NE | 2.36 | 0.72 |
| 6:M2:34:ARG:HG2 | 8:O5:52:LYS:HD2 | 1.70 | 0.72 |
| 7:N2:1:MET:H1 | 7:N2:1:MET:HE2 | 1.54 | 0.72 |
| 3:B1:91:ARG:NH2 | 11:aA:677:GLN:CD | 2.47 | 0.72 |
| 3:F4:88:ILE:HG12 | 11:aA:140:GLN:NE2 | 2.03 | 0.72 |
| 4:M4:27:HIS:ND1 | 4:M4:34:ASP:CA | 2.47 | 0.72 |
| 12:O4:201:CYC:HMA1 | 12:O4:201:CYC:NB | 2.05 | 0.72 |
| 8:M5:107:ILE:HD13 | 1:N5:13:ASP:CG | 2.14 | 0.72 |
| 5:Z4:39:PRO:CD | 12:Z4:301:CYC:HHD | 2.19 | 0.72 |
| 5:Z4:39:PRO:HD3 | 12:Z4:301:CYC:HHD | 1.71 | 0.72 |
| 8:A5:115:MET:HE1 | 12:A5:201:CYC:C2B | 2.19 | 0.72 |
| 8:A5:121:THR:HG21 | 12:A5:201:CYC:C4C | 2.20 | 0.72 |
| 1:T5:110:ASN:HD21 | 10:j5:692:LEU:C | 1.94 | 0.72 |
| 10:j5:275:THR:HG21 | 10:j5:286:VAL:O | 1.89 | 0.72 |
| 10:j5:990:ARG:NH2 | 10:j5:1026:LYS:NZ | 2.31 | 0.72 |
| 10:k5:275:THR:HG21 | 10:k5:286:VAL:O | 1.89 | 0.72 |
| 10:k5:929:PRO:CG | 1:D7:147:LYS:CE | 2.65 | 0.72 |
| 10:k5:1052:PRO:HA | 1:l7:106:GLU:CG | 2.20 | 0.72 |
| 8:c7:114:GLU:N | 8:c7:114:GLU:OE1 | 2.22 | 0.72 |
| 8:e7:4:LEU:HD23 | 8:e7:26:ILE:HD13 | 1.71 | 0.72 |
| 2:A8:59:VAL:O | 2:A8:66:LEU:HD12 | 1.89 | 0.72 |
| 2:A8:60:TYR:OH | 2:A8:79:GLN:HG2 | 1.90 | 0.72 |
| 8:m7:12:ASP:OD1 | 1:n7:91:TYR:CZ | 2.43 | 0.72 |
| 1:v7:62:TYR:CB | 11:aA:601:ALA:HB1 | 2.19 | 0.72 |
| 3:H8:81:ALA:HB2 | 3:H8:84:ARG:NH2 | 2.03 | 0.72 |
| 12:N8:201:CYC:HBB2 | 3:Q8:75:PRO:HB2 | 1.69 | 0.72 |
| 11:aA:710:THR:CB | 11:aA:807:GLN:HB3 | 2.18 | 0.72 |
| 4:M1:163:ASN:HD21 | 12:Z1:202:CYC:HMA1 | 1.54 | 0.72 |
| 2:AA:60:TYR:OH | 2:AA:79:GLN:HG2 | 1.90 | 0.72 |
| 3:FA:68:ARG:CZ | 3:ZA:68:ARG:NH2 | 2.53 | 0.72 |
| 4:MA:58:TYR:CZ | 11:aA:496:ARG:NH2 | 2.58 | 0.72 |
| 4:MA:133:ARG:HD2 | 12:RA:201:CYC:CGA | 2.19 | 0.72 |
| 4:MA:160:THR:HG21 | 4:MA:257:GLN:HB3 | 1.72 | 0.72 |
| 6:M2:26:PHE:HZ | 8:O5:90:ARG:HE | 1.36 | 0.72 |
| 2:A3:60:TYR:HB3 | 2:A3:67:THR:CG2 | 2.19 | 0.72 |
| 3:O4:88:ILE:HD11 | 5:Z4:54:LEU:HD11 | 1.71 | 0.72 |
| 8:M5:90:ARG:NH1 | 1:N5:16:GLY:HA2 | 2.05 | 0.72 |
| 8:U5:102:THR:CB | 8:U5:103:PRO:CD | 2.64 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:X5:144:ASP:CB | 8:a5:38:ARG:NH2 | 2.51 | 0.72 |
| 6:M6:67:GLY:HA3 | 3:H6:14:LEU:HD22 | 1.71 | 0.72 |
| 6:M6:117:MET:HE1 | 3:H6:77:ARG:NH1 | 1.97 | 0.72 |
| 10:j5:192:LYS:HA | 10:j5:192:LYS:CE | 2.19 | 0.72 |
| 10:k5:66:MET:HA | 10:k5:66:MET:CE | 2.16 | 0.72 |
| 8:U7:52:LYS:CE | 11:a9:29:ARG:NH1 | 2.37 | 0.72 |
| 3:U8:115:GLU:HB2 | 4:M8:74:LEU:CG | 2.17 | 0.72 |
| 2:N8:59:VAL:O | 2:N8:66:LEU:HD12 | 1.88 | 0.72 |
| 3:Q8:84:ARG:HD2 | 5:Z8:31:TRP:CD1 | 2.24 | 0.72 |
| 5:N9:54:LEU:HD13 | 3:T9:84:ARG:HH21 | 1.53 | 0.72 |
| 5:Z8:22:LEU:HD11 | 5:Z8:26:LEU:HD21 | 1.71 | 0.72 |
| 12:D9:201:CYC:CBA | 11:a9:420:ASN:HB2 | 2.19 | 0.72 |
| 11:a9:426:ARG:HD2 | 11:a9:490:ILE:CG2 | 2.20 | 0.72 |
| 4:M1:172:HIS:HE1 | 4:M1:249:ASP:OD2 | 1.73 | 0.72 |
| 4:M1:181:GLN:HE22 | 3:Z1:120:LEU:HD21 | 1.52 | 0.72 |
| 2:A2:60:TYR:OH | 2:A2:79:GLN:HG2 | 1.90 | 0.72 |
| 2:OA:60:TYR:HB3 | 2:OA:67:THR:CG2 | 2.19 | 0.72 |
| 3:J3:87:GLU:O | 3:J3:91:ARG:HG3 | 1.90 | 0.72 |
| 12:Z3:201:CYC:HMA1 | 4:M3:163:ASN:HD21 | 1.54 | 0.72 |
| 3:B1:115:GLU:CD | 4:M1:76:ALA:O | 2.33 | 0.72 |
| 12:S4:201:CYC:HC | 12:S4:201:CYC:CMD | 1.98 | 0.72 |
| 3:F4:84:ARG:HD2 | 11:aA:139:ILE:CG2 | 2.00 | 0.72 |
| 5:Z4:20:ILE:HG21 | 5:Z4:60:ILE:HD13 | 1.69 | 0.72 |
| 8:A5:115:MET:HE1 | 12:A5:201:CYC:CHB | 2.18 | 0.72 |
| 1:P5:105:ASP:OD2 | 1:b5:113:LYS:HE2 | 1.89 | 0.72 |
| 8:A7:4:LEU:HD23 | 8:A7:26:ILE:HD13 | 1.71 | 0.72 |
| 10:j5:203:LEU:HA | 10:j5:206:MET:HE3 | 1.72 | 0.72 |
| 10:j5:1119:LEU:HD22 | 1:t7:87:TYR:CZ | 2.24 | 0.72 |
| 10:k5:192:LYS:HA | 10:k5:192:LYS:CE | 2.19 | 0.72 |
| 1:B7:54:GLU:OE2 | 11:a9:563:PHE:CB | 2.37 | 0.72 |
| 8:C7:12:ASP:OD1 | 1:D7:91:TYR:CZ | 2.42 | 0.72 |
| 3:L8:86:MET:SD | 12:a9:901:CYC:HBC1 | 2.28 | 0.72 |
| 4:M9:172:HIS:HE1 | 4:M9:249:ASP:OD2 | 1.73 | 0.72 |
| 3:J9:87:GLU:O | 3:J9:91:ARG:HG3 | 1.90 | 0.72 |
| 11:a9:275:THR:HA | 11:a9:278:LEU:HD11 | 0.86 | 0.72 |
| 11:a9:629:LYS:HA | 11:a9:629:LYS:CE | 2.19 | 0.72 |
| 3:FA:37:ARG:CZ | 3:FA:159:GLU:OE1 | 2.37 | 0.72 |
| 4:MA:4:LEU:O | 4:MA:4:LEU:HD12 | 1.90 | 0.72 |
| 5:NA:1:MET:HB3 | 5:NA:3:VAL:CG2 | 2.15 | 0.72 |
| 12:R1:201:CYC:OB | 5:N1:54:LEU:CD1 | 2.37 | 0.72 |
| 2:A1:60:TYR:OH | 2:A1:79:GLN:HG2 | 1.90 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:I3:15:GLN:HG2 | 11:a9:654:ALA:HB2 | 1.70 | 0.72 |
| 2:A4:59:VAL:O | 2:A4:66:LEU:HD12 | 1.89 | 0.72 |
| 3:H4:119:ALA:C | 11:aA:266:ASN:HB2 | 2.12 | 0.72 |
| 3:H4:119:ALA:HB1 | 11:aA:266:ASN:ND2 | 1.99 | 0.72 |
| 12:H4:201:CYC:HBB3 | 11:aA:259:ALA:CA | 2.20 | 0.72 |
| 2:N4:59:VAL:O | 2:N4:66:LEU:HD12 | 1.89 | 0.72 |
| 1:B5:10:ASN:CG | 10:k5:557:VAL:CB | 2.41 | 0.72 |
| 8:G5:121:THR:HG21 | 12:G5:201:CYC:C4C | 2.20 | 0.72 |
| 1:J5:71:MEN:HA | 1:J5:77:ARG:HH12 | 0.89 | 0.72 |
| 1:V5:68:PRO:HB3 | 1:X5:13:ASP:O | 1.89 | 0.72 |
| 1:X5:86:ASP:OD2 | 1:X5:90:ARG:NE | 2.19 | 0.72 |
| 6:M6:283:VAL:HG12 | 8:Y7:75:GLU:CG | 2.18 | 0.72 |
| 10:j5:370:GLU:N | 10:j5:374:GLU:OE1 | 2.21 | 0.72 |
| 10:j5:387:VAL:O | 10:j5:394:PRO:CB | 2.37 | 0.72 |
| 8:g7:29:PHE:HE1 | 8:g7:98:ALA:O | 1.69 | 0.72 |
| 8:i7:124:PRO:O | 8:i7:125:ALA:O | 2.07 | 0.72 |
| 8:k7:76:LYS:HZ3 | 11:a9:604:ALA:CB | 2.02 | 0.72 |
| 8:a7:48:GLU:HA | 11:a9:318:TRP:CZ3 | 2.19 | 0.72 |
| 8:a7:56:ASP:OD1 | 11:a9:325:LEU:CD1 | 2.37 | 0.72 |
| 3:H8:119:ALA:HB3 | 11:a9:266:ASN:HD22 | 0.56 | 0.72 |
| 4:M8:15:PHE:HD1 | 4:M8:71:PRO:HA | 1.55 | 0.72 |
| 12:O8:201:CYC:CGA | 5:Z8:50:LEU:HD13 | 2.19 | 0.72 |
| 4:M9:58:TYR:CZ | 11:a9:496:ARG:NH2 | 2.57 | 0.72 |
| 5:N9:22:LEU:HD11 | 5:N9:26:LEU:HD21 | 1.71 | 0.72 |
| 5:N9:54:LEU:H | 12:T9:301:CYC:CBA | 1.99 | 0.72 |
| 3:J9:68:ARG:HD2 | 11:a9:353:ALA:HB1 | 1.71 | 0.72 |
| 4:M1:268:ARG:C | 3:V1:111:ASN:ND2 | 2.48 | 0.72 |
| 4:MA:15:PHE:HD1 | 4:MA:71:PRO:HA | 1.54 | 0.72 |
| 12:RA:201:CYC:HMA1 | 12:RA:201:CYC:NB | 2.05 | 0.72 |
| 3:XA:87:GLU:O | 3:XA:91:ARG:HG3 | 1.90 | 0.72 |
| 2:A3:60:TYR:OH | 2:A3:79:GLN:HG2 | 1.90 | 0.72 |
| 3:L3:111:ASN:O | 11:a9:711:SER:HB3 | 1.89 | 0.72 |
| 5:N3:1:MET:HA | 5:N3:1:MET:CE | 2.10 | 0.72 |
| 8:K5:77:MET:O | 12:K5:201:CYC:CMD | 2.37 | 0.72 |
| 1:N5:53:LYS:CE | 8:O5:120:GLN:HE21 | 2.01 | 0.72 |
| 1:D5:74:THR:HG1 | 1:D5:77:ARG:HD3 | 1.55 | 0.72 |
| 1:X5:143:PRO:HG2 | 8:a5:38:ARG:HE | 1.54 | 0.72 |
| 1:b5:114:GLU:CB | 10:k5:491:THR:CG2 | 2.64 | 0.72 |
| 10:j5:1153:VAL:HG22 | 1:v7:65:LEU:CD1 | 2.19 | 0.72 |
| 8:Q7:25:ARG:HB3 | 8:C7:25:ARG:HH21 | 0.57 | 0.72 |
| 8:I7:12:ASP:OD1 | 1:J7:91:TYR:CZ | 2.42 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:i7:37:LEU:HD11 | 1:j7:31:PHE:CZ | 2.25 | 0.72 |
| 8:a7:19:SER:HB2 | 8:a7:20:PRO:CD | 2.20 | 0.72 |
| 8:a7:19:SER:HB2 | 8:a7:20:PRO:HD3 | 1.71 | 0.72 |
| 8:c7:16:ARG:H | 1:d7:90:ARG:HD2 | 1.55 | 0.72 |
| 3:B8:82:CYS:HA | 12:B8:202:CYC:NC | 2.04 | 0.72 |
| 12:F1:202:CYC:HC | 12:F1:202:CYC:CMD | 1.99 | 0.72 |
| 3:L9:45:THR:HG23 | 2:K9:18:PHE:HB3 | 1.72 | 0.72 |
| 4:M9:77:LEU:CG | 3:Z9:115:GLU:OE2 | 2.37 | 0.72 |
| 2:O9:63:PHE:HB2 | 2:O9:66:LEU:HD12 | 1.70 | 0.72 |
| 12:P9:201:CYC:HMA1 | 12:P9:201:CYC:NB | 2.05 | 0.72 |
| 2:G9:14:SER:O | 11:a9:482:TYR:HB3 | 1.90 | 0.72 |
| 12:J9:202:CYC:NB | 12:J9:202:CYC:HMA1 | 2.05 | 0.72 |
| 12:R9:201:CYC:HMA1 | 12:R9:201:CYC:NB | 2.05 | 0.72 |
| 11:aA:668:TYR:CE2 | 3:J1:80:ALA:CB | 2.71 | 0.72 |
| 11:aA:818:ARG:HG3 | 11:aA:818:ARG:NH1 | 1.94 | 0.72 |
| 3:FA:150:ARG:CB | 3:F9:150:ARG:CG | 2.48 | 0.72 |
| 4:MA:77:LEU:CG | 3:ZA:115:GLU:OE2 | 2.37 | 0.72 |
| 2:K3:13:ASP:CG | 11:a9:707:PHE:HZ | 1.98 | 0.72 |
| 2:A4:60:TYR:OH | 2:A4:79:GLN:HG2 | 1.90 | 0.72 |
| 4:M3:268:ARG:C | 3:V3:111:ASN:ND2 | 2.48 | 0.72 |
| 5:N3:1:MET:HB3 | 5:N3:3:VAL:CG2 | 2.15 | 0.72 |
| 4:M4:176:ARG:HH11 | 4:M4:176:ARG:CG | 2.03 | 0.72 |
| 1:D5:71:MEN:HA | 1:D5:77:ARG:HH12 | 0.89 | 0.72 |
| 1:P5:118:SER:OG | 10:k5:498:ALA:CB | 2.38 | 0.72 |
| 10:j5:1119:LEU:CD1 | 1:t7:87:TYR:CE2 | 2.72 | 0.72 |
| 10:k5:971:VAL:HG12 | 1:n7:76:ARG:HH12 | 1.52 | 0.72 |
| 10:k5:1054:SER:HB2 | 10:k5:1056:PRO:HD3 | 1.72 | 0.72 |
| 8:i7:25:ARG:NE | 8:s7:3:VAL:HA | 2.04 | 0.72 |
| 1:T7:110:ASN:ND2 | 9:w7:57:PHE:CG | 2.57 | 0.72 |
| 1:Z7:67:ARG:CZ | 11:a9:307:ARG:HB3 | 2.17 | 0.72 |
| 1:f7:64:ASP:OD2 | 11:aA:307:ARG:CZ | 2.37 | 0.72 |
| 3:B8:108:ARG:HA | 4:M8:61:ASN:CB | 2.19 | 0.72 |
| 3:D8:116:THR:OG1 | 4:M8:38:PRO:CB | 2.37 | 0.72 |
| 8:o7:2:SER:HB3 | 1:p7:5:ILE:HB | 1.72 | 0.72 |
| 4:M8:92:GLU:CD | 4:M8:217:VAL:HG22 | 2.07 | 0.72 |
| 4:M9:15:PHE:HD1 | 4:M9:71:PRO:HA | 1.54 | 0.72 |
| 12:Z8:301:CYC:NB | 12:Z8:301:CYC:HMA1 | 2.05 | 0.72 |
| 2:I9:37:SER:CA | 2:I9:97:LEU:HD11 | 2.18 | 0.72 |
| 12:Z9:202:CYC:HMA1 | 12:Z9:202:CYC:NB | 2.05 | 0.72 |
| 11:a9:54:ARG:HD2 | 11:a9:610:ALA:HB2 | 1.72 | 0.72 |
| 11:aA:48:LEU:HD12 | 11:aA:48:LEU:C | 2.14 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 5:NA:20:ILE:HG21 | 5:NA:60:ILE:HD13 | 1.69 | 0.72 |
| 4:M3:160:THR:HG21 | 4:M3:257:GLN:HB3 | 1.72 | 0.72 |
| 5:N3:50:LEU:C | 5:N3:50:LEU:HD12 | 2.14 | 0.72 |
| 2:U3:43:ALA:HA | 2:Q9:74:TYR:CD1 | 2.17 | 0.72 |
| 3:X3:87:GLU:O | 3:X3:91:ARG:HG3 | 1.90 | 0.72 |
| 12:B5:201:CYC:C4B | 9:z5:23:LEU:HB2 | 2.20 | 0.72 |
| 1:D5:118:SER:HB3 | 9:z5:56:LEU:HD11 | 1.70 | 0.72 |
| 8:G5:115:MET:HE1 | 12:G5:201:CYC:C2B | 2.20 | 0.72 |
| 1:P5:114:GLU:OE1 | 10:k5:496:GLU:CA | 2.38 | 0.72 |
| 10:j5:963:ASP:OD1 | 10:j5:963:ASP:N | 2.20 | 0.72 |
| 10:j5:1018:LEU:HD13 | 10:j5:1035:PHE:HE2 | 1.53 | 0.72 |
| 10:k5:203:LEU:HA | 10:k5:206:MET:HE3 | 1.72 | 0.72 |
| 10:k5:289:SER:HB3 | 10:k5:292:GLU:CD | 2.14 | 0.72 |
| 10:k5:793:SER:HB3 | 12:N7:201:CYC:O2A | 1.88 | 0.72 |
| 2:A6:60:TYR:HB3 | 2:A6:67:THR:CG2 | 2.19 | 0.72 |
| 1:B7:136:VAL:HG13 | 11:a9:563:PHE:HZ | 1.45 | 0.72 |
| 8:g7:33:GLY:CA | 1:h7:31:PHE:CE2 | 2.71 | 0.72 |
| 8:i7:37:LEU:HD21 | 1:j7:31:PHE:CZ | 2.24 | 0.72 |
| 1:T7:14:VAL:CG1 | 9:w7:64:ASN:ND2 | 2.53 | 0.72 |
| 8:c7:39:ILE:HD11 | 8:c7:148:GLU:HB3 | 1.59 | 0.72 |
| 8:q7:90:ARG:HD3 | 1:r7:18:TYR:CD1 | 2.24 | 0.72 |
| 8:u7:27:LYS:HD2 | 1:v7:35:ALA:HB2 | 1.70 | 0.72 |
| 4:M8:4:LEU:HD12 | 4:M8:4:LEU:O | 1.90 | 0.72 |
| 4:M8:172:HIS:HE1 | 4:M8:249:ASP:OD2 | 1.72 | 0.72 |
| 12:M8:302:CYC:H2C | 3:S8:78:ARG:CG | 2.19 | 0.72 |
| 5:N9:50:LEU:C | 5:N9:50:LEU:HD12 | 2.14 | 0.72 |
| 5:N9:70:ILE:HG22 | 3:T9:119:ALA:HB3 | 1.71 | 0.72 |
| 3:J9:68:ARG:HD2 | 11:a9:353:ALA:CB | 2.20 | 0.72 |
| 11:a9:598:SER:HB3 | 11:a9:599:PRO:CG | 2.20 | 0.72 |
| 11:a9:601:ALA:HB1 | 11:a9:602:PRO:HD2 | 1.72 | 0.72 |
| 4:M1:15:PHE:HD1 | 4:M1:71:PRO:HA | 1.54 | 0.72 |
| 3:HA:117:TYR:HE1 | 12:HA:202:CYC:NA | 1.88 | 0.71 |
| 3:JA:87:GLU:O | 3:JA:91:ARG:HG3 | 1.90 | 0.71 |
| 3:LA:77:ARG:CZ | 11:aA:538:ARG:NH2 | 2.52 | 0.71 |
| 5:NA:22:LEU:HD23 | 5:NA:26:LEU:CD1 | 1.83 | 0.71 |
| 4:M3:4:LEU:O | 4:M3:4:LEU:HD12 | 1.90 | 0.71 |
| 4:M3:210:ILE:HD13 | 5:N3:59:ARG:NH1 | 2.05 | 0.71 |
| 5:N3:4:LEU:O | 5:N3:4:LEU:HG | 1.88 | 0.71 |
| 8:K5:111:GLY:O | 1:J5:75:THR:HB | 1.90 | 0.71 |
| 12:L5:201:CYC:HBB2 | 10:j5:588:VAL:HG21 | 1.70 | 0.71 |
| 8:E5:77:MET:O | 12:E5:201:CYC:CMD | 2.37 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:c5:4:LEU:HD23 | 8:c5:26:ILE:HD13 | 1.71 | 0.71 |
| 10:j5:188:GLU:N | 10:j5:188:GLU:OE1 | 2.23 | 0.71 |
| 10:j5:195:SER:O | 10:j5:199:THR:HG23 | 1.89 | 0.71 |
| 10:k5:743:VAL:CG1 | 12:D7:201:CYC:CGD | 2.66 | 0.71 |
| 10:k5:1050:PHE:HD2 | 10:k5:1058:VAL:HG11 | 1.55 | 0.71 |
| 8:i7:25:ARG:HH12 | 8:s7:7:ALA:N | 1.88 | 0.71 |
| 8:U7:12:ASP:OD1 | 1:V7:91:TYR:CZ | 2.43 | 0.71 |
| 8:a7:161:GLN:CD | 1:p7:49:THR:CG2 | 2.63 | 0.71 |
| 1:f7:67:ARG:HD3 | 11:aA:311:LEU:HD22 | 0.73 | 0.71 |
| 3:B8:109:CYS:HA | 4:M8:60:LYS:NZ | 2.05 | 0.71 |
| 8:o7:27:LYS:HD2 | 1:p7:35:ALA:HB2 | 1.70 | 0.71 |
| 8:u7:2:SER:HB3 | 1:v7:5:ILE:HB | 1.72 | 0.71 |
| 3:F8:88:ILE:HG12 | 11:a9:140:GLN:NE2 | 2.04 | 0.71 |
| 3:Q8:110:LEU:HD22 | 3:Q8:170:SER:CB | 2.18 | 0.71 |
| 3:F9:68:ARG:CZ | 3:Z9:68:ARG:NH2 | 2.53 | 0.71 |
| 3:H9:78:ARG:HD3 | 12:H9:202:CYC:O2D | 1.88 | 0.71 |
| 3:H9:113:LEU:CD1 | 12:H9:202:CYC:C2B | 2.67 | 0.71 |
| 11:aA:439:ARG:HH11 | 11:aA:439:ARG:HG3 | 1.54 | 0.71 |
| 3:FA:149:THR:O | 12:F9:302:CYC:HMD2 | 1.89 | 0.71 |
| 2:KA:12:ALA:O | 2:KA:16:GLY:N | 2.22 | 0.71 |
| 4:MA:176:ARG:HH11 | 4:MA:176:ARG:CG | 2.03 | 0.71 |
| 5:NA:61:LYS:HD2 | 12:TA:301:CYC:CBB | 2.20 | 0.71 |
| 12:PA:201:CYC:HMA1 | 12:PA:201:CYC:NB | 2.05 | 0.71 |
| 2:O1:60:TYR:OH | 2:O1:79:GLN:HG2 | 1.90 | 0.71 |
| 3:B3:115:GLU:CD | 4:M3:76:ALA:O | 2.33 | 0.71 |
| 3:B4:82:CYS:O | 12:B4:202:CYC:CBC | 2.37 | 0.71 |
| 3:L3:120:LEU:CD2 | 11:a9:731:GLN:HG2 | 2.19 | 0.71 |
| 2:O3:60:TYR:OH | 2:O3:79:GLN:HG2 | 1.90 | 0.71 |
| 2:U3:141:GLN:C | 2:Q9:76:ASP:H | 1.98 | 0.71 |
| 8:K5:77:MET:O | 12:K5:201:CYC:HMD1 | 1.89 | 0.71 |
| 8:A5:4:LEU:HD23 | 8:A5:26:ILE:HD13 | 1.71 | 0.71 |
| 1:H5:2:GLN:OE1 | 10:j5:551:MET:HE3 | 1.89 | 0.71 |
| 8:I5:91:LEU:O | 8:I5:104:ILE:CD1 | 2.38 | 0.71 |
| 1:V5:114:GLU:CB | 10:j5:496:GLU:HG3 | 2.19 | 0.71 |
| 6:M6:164:GLU:OE1 | 6:M6:258:VAL:HG22 | 1.89 | 0.71 |
| 10:j5:1034:GLU:CD | 10:j5:1037:ARG:NH2 | 2.48 | 0.71 |
| 10:k5:362:LYS:CE | 10:k5:363:HIS:HE2 | 1.99 | 0.71 |
| 8:c7:131:ARG:HH11 | 8:c7:131:ARG:CG | 2.03 | 0.71 |
| 3:B8:68:ARG:HH12 | 3:U8:68:ARG:NH2 | 1.88 | 0.71 |
| 3:F8:107:ASP:C | 4:M8:6:THR:HB | 2.14 | 0.71 |
| 3:F8:115:GLU:HG2 | 4:M8:3:VAL:HG21 | 1.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:M8:21:LEU:O | 4:M8:21:LEU:HD12 | 1.90 | 0.71 |
| 3:O8:119:ALA:HB2 | 5:Z8:72:GLU:H | 1.55 | 0.71 |
| 12:F1:201:CYC:HMA1 | 12:F1:201:CYC:NB | 2.05 | 0.71 |
| 5:N9:61:LYS:HD2 | 12:T9:301:CYC:CBB | 2.20 | 0.71 |
| 2:E9:33:ARG:HD3 | 2:I9:25:GLN:HE22 | 1.55 | 0.71 |
| 11:aA:598:SER:HB3 | 11:aA:599:PRO:CG | 2.20 | 0.71 |
| 11:aA:601:ALA:HB1 | 11:aA:602:PRO:HD2 | 1.72 | 0.71 |
| 4:M1:263:PRO:CB | 3:Z1:119:ALA:CB | 2.61 | 0.71 |
| 5:N1:22:LEU:HD11 | 5:N1:26:LEU:HD21 | 1.71 | 0.71 |
| 12:F3:201:CYC:HMA1 | 12:F3:201:CYC:NB | 2.05 | 0.71 |
| 4:M3:172:HIS:HE1 | 4:M3:249:ASP:OD2 | 1.73 | 0.71 |
| 2:O3:60:TYR:HB3 | 2:O3:67:THR:CG2 | 2.19 | 0.71 |
| 12:B1:202:CYC:HMA1 | 12:B1:202:CYC:NB | 2.05 | 0.71 |
| 4:M4:4:LEU:O | 4:M4:4:LEU:HD12 | 1.90 | 0.71 |
| 4:M4:144:ARG:NH1 | 5:Z4:59:ARG:NH1 | 2.38 | 0.71 |
| 3:O4:107:ASP:HA | 5:Z4:66:ARG:NH1 | 2.06 | 0.71 |
| 8:M5:4:LEU:HD23 | 8:M5:26:ILE:HD13 | 1.71 | 0.71 |
| 8:G5:119:LEU:CD1 | 12:G5:201:CYC:C2A | 2.67 | 0.71 |
| 3:J6:87:GLU:O | 3:J6:91:ARG:HG3 | 1.90 | 0.71 |
| 9:i5:6:LYS:HB2 | 9:i5:55:LYS:CB | 2.17 | 0.71 |
| 10:j5:951:MET:CE | 10:j5:955:LEU:CG | 2.65 | 0.71 |
| 10:j5:1050:PHE:HD2 | 10:j5:1058:VAL:HG11 | 1.55 | 0.71 |
| 10:k5:147:ARG:O | 10:k5:147:ARG:HD3 | 1.90 | 0.71 |
| 10:k5:642:ARG:HG2 | 10:k5:642:ARG:NH1 | 2.02 | 0.71 |
| 10:k5:1053:TYR:O | 1:l7:107:ARG:HD2 | 1.90 | 0.71 |
| 10:k5:1056:PRO:CD | 10:k5:1057:LYS:H | 1.97 | 0.71 |
| 10:k5:1118:THR:CG2 | 12:k5:1204:CYC:O2A | 2.38 | 0.71 |
| 12:D6:202:CYC:HC | 12:D6:202:CYC:CMD | 1.99 | 0.71 |
| 1:H7:140:LEU:HD12 | 11:aA:561:ALA:CA | 2.18 | 0.71 |
| 8:I7:44:THR:HG1 | 1:J7:18:TYR:HD2 | 1.39 | 0.71 |
| 8:i7:89:LEU:HD13 | 8:i7:153:PHE:CZ | 2.25 | 0.71 |
| 8:Y7:4:LEU:HD23 | 8:Y7:26:ILE:HD13 | 1.71 | 0.71 |
| 1:f7:10:ASN:CG | 9:y7:65:THR:HG1 | 1.96 | 0.71 |
| 2:A8:63:PHE:HB2 | 2:A8:66:LEU:HD12 | 1.70 | 0.71 |
| 12:B8:202:CYC:HBB3 | 4:M8:61:ASN:CG | 2.13 | 0.71 |
| 4:M9:7:SER:OG | 3:D9:111:ASN:ND2 | 2.23 | 0.71 |
| 2:O9:60:TYR:OH | 2:O9:79:GLN:HG2 | 1.90 | 0.71 |
| 2:O9:63:PHE:O | 2:O9:66:LEU:CG | 2.39 | 0.71 |
| 3:X9:87:GLU:O | 3:X9:91:ARG:HG3 | 1.90 | 0.71 |
| 11:a9:61:TYR:HA | 11:a9:65:LEU:HB2 | 1.72 | 0.71 |
| 11:a9:290:ASP:C | 11:a9:291:TYR:CD1 | 2.68 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 11:aA:731:GLN:HG2 | 3:L1:120:LEU:CD2 | 2.20 | 0.71 |
| 4:M1:188:LEU:HD21 | 12:Z1:202:CYC:NB | 2.04 | 0.71 |
| 2:AA:63:PHE:HB2 | 2:AA:66:LEU:HD12 | 1.70 | 0.71 |
| 3:FA:150:ARG:HG2 | 3:F9:150:ARG:HA | 1.71 | 0.71 |
| 2:G3:111:ALA:CB | 3:L3:77:ARG:NE | 2.53 | 0.71 |
| 2:A4:60:TYR:HB3 | 2:A4:67:THR:CG2 | 2.19 | 0.71 |
| 12:L3:202:CYC:HB | 11:a9:738:LEU:CD1 | 1.95 | 0.71 |
| 4:M3:21:LEU:HD12 | 4:M3:21:LEU:O | 1.90 | 0.71 |
| 3:B1:88:ILE:CG2 | 12:B1:202:CYC:CAB | 2.67 | 0.71 |
| 3:U4:112:GLY:C | 4:M4:74:LEU:HD21 | 2.15 | 0.71 |
| 12:L4:202:CYC:HBB2 | 11:aA:245:ALA:CB | 2.20 | 0.71 |
| 8:K5:131:ARG:CG | 8:K5:157:VAL:HG21 | 2.21 | 0.71 |
| 8:K5:152:TYR:CE2 | 8:U5:20:PRO:HB3 | 2.26 | 0.71 |
| 8:I5:102:THR:CB | 8:I5:103:PRO:CD | 2.64 | 0.71 |
| 1:P5:68:PRO:HB3 | 1:R5:13:ASP:O | 1.89 | 0.71 |
| 8:a5:91:LEU:O | 8:a5:104:ILE:CD1 | 2.38 | 0.71 |
| 10:j5:930:LEU:O | 1:J7:33:THR:CG2 | 2.38 | 0.71 |
| 10:j5:1024:LYS:C | 10:j5:1030:ILE:HG22 | 2.16 | 0.71 |
| 10:j5:1053:TYR:CB | 10:j5:1058:VAL:HG23 | 2.20 | 0.71 |
| 8:O7:6:LYS:NZ | 8:E7:21:GLY:HA3 | 2.05 | 0.71 |
| 8:i7:25:ARG:NH2 | 8:s7:6:LYS:H | 1.85 | 0.71 |
| 8:a7:91:LEU:O | 8:a7:104:ILE:CD1 | 2.39 | 0.71 |
| 8:c7:124:PRO:O | 8:c7:125:ALA:O | 2.07 | 0.71 |
| 8:m7:91:LEU:O | 8:m7:104:ILE:CD1 | 2.39 | 0.71 |
| 8:u7:23:LEU:CD1 | 1:v7:38:VAL:CG1 | 2.67 | 0.71 |
| 1:v7:62:TYR:HB3 | 11:aA:601:ALA:CB | 2.19 | 0.71 |
| 12:H8:201:CYC:OB | 11:a9:129:ASN:HB3 | 1.90 | 0.71 |
| 3:J8:87:GLU:O | 3:J8:91:ARG:HG3 | 1.90 | 0.71 |
| 2:N8:60:TYR:OH | 2:N8:79:GLN:HG2 | 1.90 | 0.71 |
| 4:M9:160:THR:HG21 | 4:M9:257:GLN:HB3 | 1.72 | 0.71 |
| 2:I9:41:ALA:HB2 | 2:I9:97:LEU:HD12 | 1.73 | 0.71 |
| 11:aA:351:THR:CB | 11:aA:352:PRO:CD | 2.33 | 0.71 |
| 11:aA:426:ARG:HD2 | 11:aA:490:ILE:CG2 | 2.20 | 0.71 |
| 12:Z1:201:CYC:HC | 12:Z1:201:CYC:CMD | 1.99 | 0.71 |
| 3:DA:111:ASN:ND2 | 4:MA:7:SER:OG | 2.23 | 0.71 |
| 3:LA:52:ILE:HD11 | 3:LA:87:GLU:HG2 | 1.71 | 0.71 |
| 2:QA:68:GLN:NE2 | 2:U1:45:THR:O | 2.18 | 0.71 |
| 3:TA:32:LYS:NZ | 2:X4:60:TYR:HB2 | 2.05 | 0.71 |
| 3:B4:108:ARG:O | 12:B4:202:CYC:CBB | 2.39 | 0.71 |
| 4:M4:15:PHE:HD1 | 4:M4:71:PRO:HA | 1.54 | 0.71 |
| 5:Z4:38:GLU:HG2 | 12:Z4:301:CYC:CMB | 2.21 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:D5:75:THR:HB | 8:E5:111:GLY:O | 1.90 | 0.71 |
| 1:J5:74:THR:OG1 | 1:J5:77:ARG:HD3 | 1.91 | 0.71 |
| 1:d5:127:VAL:CB | 10:j5:698:GLY:HA3 | 2.20 | 0.71 |
| 8:U5:91:LEU:O | 8:U5:104:ILE:CD1 | 2.39 | 0.71 |
| 1:X5:107:ARG:O | 10:j5:520:ARG:NH1 | 2.23 | 0.71 |
| 6:M6:281:ASP:OD1 | 8:Y7:76:LYS:HB3 | 1.89 | 0.71 |
| 10:j5:74:ARG:O | 10:j5:74:ARG:HG3 | 1.89 | 0.71 |
| 10:j5:547:ARG:HD2 | 10:j5:547:ARG:C | 2.16 | 0.71 |
| 10:j5:742:GLY:HA2 | 12:J7:201:CYC:O1D | 1.91 | 0.71 |
| 10:k5:755:GLN:O | 10:k5:755:GLN:HG3 | 1.90 | 0.71 |
| 10:k5:938:GLN:NE2 | 1:D7:28:LYS:HD2 | 2.04 | 0.71 |
| 10:k5:978:LEU:CG | 1:p7:107:ARG:NH2 | 2.54 | 0.71 |
| 8:O7:91:LEU:O | 8:O7:104:ILE:CD1 | 2.39 | 0.71 |
| 4:M8:232:VAL:HG22 | 4:M8:235:PHE:HE2 | 1.54 | 0.71 |
| 2:N8:112:GLY:HA3 | 5:Z8:33:GLY:CA | 2.21 | 0.71 |
| 2:N8:112:GLY:HA3 | 5:Z8:33:GLY:HA2 | 1.70 | 0.71 |
| 4:M9:81:ASP:N | 3:Z9:111:ASN:ND2 | 2.37 | 0.71 |
| 4:M9:158:PHE:HA | 3:V9:108:ARG:CD | 2.14 | 0.71 |
| 4:M9:273:ILE:HD13 | 3:V9:75:PRO:HG3 | 1.73 | 0.71 |
| 11:aA:61:TYR:HA | 11:aA:65:LEU:HB2 | 1.72 | 0.71 |
| 3:X1:87:GLU:O | 3:X1:91:ARG:HG3 | 1.90 | 0.71 |
| 12:DA:201:CYC:HMA1 | 12:DA:201:CYC:NB | 2.05 | 0.71 |
| 12:JA:202:CYC:CGA | 11:aA:511:LYS:HA | 2.17 | 0.71 |
| 2:OA:63:PHE:HB2 | 2:OA:66:LEU:HD12 | 1.70 | 0.71 |
| 3:TA:29:ASN:ND2 | 2:X4:61:ASN:OD1 | 2.20 | 0.71 |
| 12:ZA:202:CYC:HMA1 | 12:ZA:202:CYC:NB | 2.05 | 0.71 |
| 4:M3:222:ARG:HG3 | 4:M3:222:ARG:NH1 | 2.01 | 0.71 |
| 5:N3:20:ILE:HG21 | 5:N3:60:ILE:HD13 | 1.69 | 0.71 |
| 2:E4:15:GLN:HG3 | 11:aA:163:ASP:OD2 | 1.89 | 0.71 |
| 4:M4:21:LEU:O | 4:M4:36:TYR:CE2 | 2.44 | 0.71 |
| 4:M4:230:GLN:CG | 12:M4:301:CYC:OB | 2.33 | 0.71 |
| 4:M4:232:VAL:HB | 12:M4:301:CYC:CBB | 2.09 | 0.71 |
| 8:A5:114:GLU:HB2 | 1:F5:79:ALA:CB | 2.18 | 0.71 |
| 8:Q5:156:LEU:O | 8:Q5:160:MET:HG2 | 1.90 | 0.71 |
| 1:R5:124:ALA:HB3 | 1:Z5:64:ASP:OD2 | 1.89 | 0.71 |
| 10:j5:1008:PHE:HD1 | 12:v7:201:CYC:CBB | 2.02 | 0.71 |
| 10:j5:1064:LYS:HG3 | 10:j5:1065:HIS:H | 1.55 | 0.71 |
| 10:k5:1143:LEU:HD23 | 1:l7:10:ASN:OD1 | 1.90 | 0.71 |
| 8:O7:29:PHE:HZ | 8:O7:98:ALA:O | 1.62 | 0.71 |
| 12:P7:201:CYC:HBB2 | 9:z7:21:ARG:HG2 | 1.73 | 0.71 |
| 1:B7:140:LEU:HG | 11:a9:561:ALA:CB | 2.17 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:I7:91:LEU:O | 8:I7:104:ILE:CD1 | 2.39 | 0.71 |
| 8:k7:120:GLN:HG3 | 1:p7:53:LYS:HZ1 | 1.56 | 0.71 |
| 12:d7:201:CYC:NB | 9:x7:38:PHE:CD1 | 2.59 | 0.71 |
| 3:B8:105:LEU:HD12 | 3:B8:109:CYS:HB3 | 1.71 | 0.71 |
| 8:u7:103:PRO:CB | 1:v7:9:ILE:HD13 | 2.21 | 0.71 |
| 9:y7:35:GLU:N | 9:y7:35:GLU:OE1 | 2.23 | 0.71 |
| 9:y7:60:VAL:HG23 | 9:y7:62:GLY:H | 1.56 | 0.71 |
| 2:X8:60:TYR:HB2 | 3:T9:32:LYS:NZ | 2.05 | 0.71 |
| 3:Q8:84:ARG:HD3 | 5:Z8:31:TRP:CD1 | 2.25 | 0.71 |
| 4:M9:134:ASN:HD21 | 5:N9:1:MET:H1 | 1.39 | 0.71 |
| 12:B9:201:CYC:HMA1 | 12:B9:201:CYC:NB | 2.05 | 0.71 |
| 2:E9:33:ARG:CG | 2:I9:25:GLN:OE1 | 2.33 | 0.71 |
| 3:H9:113:LEU:HD11 | 12:H9:202:CYC:C2B | 2.19 | 0.71 |
| 3:H1:77:ARG:NH1 | 12:H1:201:CYC:O2D | 2.21 | 0.71 |
| 4:M1:21:LEU:O | 4:M1:36:TYR:CE2 | 2.44 | 0.71 |
| 1:A:76:ARG:HH21 | 10:k5:16:LEU:CD1 | 2.04 | 0.71 |
| 1:A:131:GLN:CB | 1:R5:17:LYS:NZ | 2.52 | 0.71 |
| 2:EA:33:ARG:HD3 | 2:IA:25:GLN:HE22 | 1.55 | 0.71 |
| 3:JA:68:ARG:HD2 | 11:aA:353:ALA:CB | 2.21 | 0.71 |
| 4:M3:233:GLU:OE1 | 4:M3:237:ARG:NH2 | 2.24 | 0.71 |
| 3:J4:87:GLU:O | 3:J4:91:ARG:HG3 | 1.90 | 0.71 |
| 4:M4:21:LEU:O | 4:M4:21:LEU:HD12 | 1.90 | 0.71 |
| 2:N4:60:TYR:OH | 2:N4:79:GLN:HG2 | 1.90 | 0.71 |
| 12:O4:201:CYC:CBA | 5:Z4:50:LEU:HD13 | 2.19 | 0.71 |
| 8:A5:119:LEU:CD1 | 12:A5:201:CYC:C2A | 2.67 | 0.71 |
| 8:C5:102:THR:CB | 8:C5:103:PRO:CD | 2.64 | 0.71 |
| 1:J5:83:ARG:NH1 | 9:i5:38:PHE:CE2 | 2.58 | 0.71 |
| 8:i7:20:PRO:HG2 | 8:s7:155:TYR:CE2 | 2.25 | 0.71 |
| 8:i7:49:ARG:CZ | 8:i7:140:LEU:CD2 | 2.69 | 0.71 |
| 2:X8:61:ASN:OD1 | 3:T9:29:ASN:ND2 | 2.20 | 0.71 |
| 3:F8:109:CYS:O | 4:M8:5:THR:CG2 | 2.38 | 0.71 |
| 2:A9:60:TYR:OH | 2:A9:79:GLN:HG2 | 1.90 | 0.71 |
| 2:G1:111:ALA:CB | 3:L1:77:ARG:NE | 2.53 | 0.71 |
| 11:a9:776:TYR:O | 11:a9:776:TYR:CG | 2.42 | 0.71 |
| 4:M1:4:LEU:O | 4:M1:4:LEU:HD12 | 1.90 | 0.71 |
| 4:M1:21:LEU:O | 4:M1:21:LEU:HD12 | 1.90 | 0.71 |
| 4:M1:160:THR:HG21 | 4:M1:257:GLN:HB3 | 1.72 | 0.71 |
| 12:T1:301:CYC:NB | 12:T1:301:CYC:HMA1 | 2.05 | 0.71 |
| 4:MA:1:MET:HA | 11:aA:422:SER:O | 1.91 | 0.71 |
| 4:MA:21:LEU:O | 4:MA:36:TYR:CE2 | 2.44 | 0.71 |
| 3:J3:84:ARG:HH11 | 11:a9:668:TYR:HB3 | 1.55 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:G2:15:GLN:HA | 6:M2:104:ARG:HD3 | 1.71 | 0.71 |
| 3:H2:14:LEU:HD22 | 6:M2:67:GLY:HA3 | 1.71 | 0.71 |
| 2:A4:63:PHE:O | 2:A4:66:LEU:CG | 2.39 | 0.71 |
| 3:B4:119:ALA:C | 4:M4:52:LEU:CD1 | 2.64 | 0.71 |
| 12:B4:202:CYC:HMA1 | 12:B4:202:CYC:NB | 2.05 | 0.71 |
| 4:M3:15:PHE:HD1 | 4:M3:71:PRO:HA | 1.54 | 0.71 |
| 4:M3:176:ARG:HH11 | 4:M3:176:ARG:CG | 2.03 | 0.71 |
| 2:O3:63:PHE:HB2 | 2:O3:66:LEU:HD12 | 1.70 | 0.71 |
| 3:S4:116:THR:HG23 | 3:S4:117:TYR:N | 2.04 | 0.71 |
| 12:M4:301:CYC:HMA1 | 12:M4:301:CYC:NB | 2.05 | 0.71 |
| 8:E5:131:ARG:CG | 8:E5:157:VAL:HG21 | 2.21 | 0.71 |
| 8:S5:14:GLU:CG | 10:j5:538:PHE:CE2 | 2.70 | 0.71 |
| 6:M6:104:ARG:HH11 | 2:G6:16:GLY:HA3 | 1.51 | 0.71 |
| 3:F6:126:SER:O | 12:F6:201:CYC:HMC3 | 1.91 | 0.71 |
| 8:O7:25:ARG:HH22 | 8:E7:25:ARG:CD | 2.02 | 0.71 |
| 8:S7:100:ASP:OD1 | 8:G7:19:SER:OG | 2.07 | 0.71 |
| 8:I7:25:ARG:NH2 | 8:W7:25:ARG:CG | 2.53 | 0.71 |
| 8:i7:121:THR:CG2 | 12:i7:201:CYC:HMC3 | 2.21 | 0.71 |
| 8:W7:13:ALA:HA | 9:w7:46:LYS:HD3 | 1.71 | 0.71 |
| 8:c7:104:ILE:CG2 | 8:c7:155:TYR:HE2 | 2.04 | 0.71 |
| 8:s7:91:LEU:HB3 | 8:s7:104:ILE:HG23 | 1.73 | 0.71 |
| 9:y7:9:ALA:CB | 9:y7:44:ILE:HD13 | 2.20 | 0.71 |
| 3:Q8:89:ILE:HG12 | 3:Q8:92:TYR:OH | 1.90 | 0.71 |
| 3:L9:113:LEU:N | 11:a9:532:ALA:CB | 2.54 | 0.71 |
| 4:M9:21:LEU:O | 4:M9:21:LEU:HD12 | 1.90 | 0.71 |
| 4:M9:21:LEU:O | 4:M9:36:TYR:CE2 | 2.44 | 0.71 |
| 4:M9:273:ILE:CD1 | 3:V9:75:PRO:HG3 | 2.21 | 0.71 |
| 5:Z8:1:MET:HA | 5:Z8:1:MET:CE | 2.10 | 0.71 |
| 5:Z8:26:LEU:CD2 | 12:Z8:301:CYC:OB | 2.38 | 0.71 |
| 11:a9:107:ARG:HG3 | 11:a9:108:PRO:CD | 2.18 | 0.71 |
| 1:Z:158:SER:HB3 | 1:X5:11:ASN:HD21 | 0.75 | 0.71 |
| 2:IA:41:ALA:HB2 | 2:IA:97:LEU:HD12 | 1.72 | 0.71 |
| 12:ZA:201:CYC:HC | 12:ZA:201:CYC:CMD | 1.98 | 0.71 |
| 3:J3:14:LEU:CG | 11:a9:621:THR:CG2 | 2.40 | 0.71 |
| 3:L2:75:PRO:HG3 | 3:L2:78:ARG:HG3 | 1.73 | 0.71 |
| 6:M2:39:ARG:NH1 | 8:O5:59:PHE:CE2 | 2.58 | 0.71 |
| 3:B3:91:ARG:NH2 | 11:a9:677:GLN:CD | 2.49 | 0.71 |
| 3:W4:87:GLU:O | 3:W4:91:ARG:HG3 | 1.90 | 0.71 |
| 2:N4:13:ASP:CB | 3:O4:108:ARG:NH1 | 2.53 | 0.71 |
| 8:A5:126:VAL:HG22 | 12:A5:201:CYC:C3C | 2.12 | 0.71 |
| 1:D5:74:THR:OG1 | 1:D5:77:ARG:HD3 | 1.91 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:P5:114:GLU:OE1 | 10:k5:496:GLU:HB2 | 1.89 | 0.71 |
| 8:W5:156:LEU:O | 8:W5:160:MET:HG2 | 1.90 | 0.71 |
| 10:j5:755:GLN:O | 10:j5:755:GLN:HG3 | 1.90 | 0.71 |
| 10:j5:974:LEU:CG | 1:v7:1:MET:H1 | 1.77 | 0.71 |
| 10:j5:1019:SER:O | 10:j5:1020:GLU:HB2 | 1.90 | 0.71 |
| 10:j5:1143:LEU:O | 1:r7:10:ASN:OD1 | 2.09 | 0.71 |
| 1:d7:48:ALA:HB3 | 8:m7:161:GLN:OE1 | 1.91 | 0.71 |
| 8:o7:47:ARG:HH21 | 8:o7:47:ARG:CG | 2.04 | 0.71 |
| 8:u7:47:ARG:HH21 | 8:u7:47:ARG:CG | 2.04 | 0.71 |
| 8:u7:121:THR:HG23 | 12:u7:201:CYC:CMC | 2.14 | 0.71 |
| 4:M8:21:LEU:O | 4:M8:36:TYR:CE2 | 2.44 | 0.71 |
| 3:Q8:110:LEU:HD21 | 3:Q8:167:ALA:CA | 2.13 | 0.71 |
| 3:L9:97:LEU:HD12 | 3:L9:97:LEU:C | 2.13 | 0.71 |
| 3:L9:111:ASN:O | 11:a9:532:ALA:HB2 | 1.91 | 0.71 |
| 4:M9:274:VAL:CA | 3:V9:77:ARG:HE | 2.04 | 0.71 |
| 12:V1:202:CYC:HC | 12:V1:202:CYC:CMD | 1.99 | 0.71 |
| 2:EA:33:ARG:CD | 2:IA:25:GLN:HE22 | 2.04 | 0.71 |
| 3:FA:36:LYS:HB2 | 3:FA:156:LEU:CD1 | 2.20 | 0.71 |
| 2:O1:63:PHE:O | 2:O1:66:LEU:CG | 2.39 | 0.71 |
| 2:A1:63:PHE:HB2 | 2:A1:66:LEU:HD12 | 1.70 | 0.71 |
| 2:C3:140:SER:CB | 3:D8:150:ARG:NH1 | 2.54 | 0.71 |
| 4:M3:246:ALA:HA | 12:X3:201:CYC:CBB | 2.21 | 0.71 |
| 3:S4:120:LEU:CD1 | 12:S4:202:CYC:CHA | 2.68 | 0.71 |
| 3:F4:108:ARG:CZ | 4:M4:9:GLN:CD | 2.62 | 0.71 |
| 4:M4:197:ASP:OD1 | 5:Z4:52:ARG:CZ | 2.38 | 0.71 |
| 4:M4:233:GLU:OE1 | 4:M4:237:ARG:NH2 | 2.24 | 0.71 |
| 8:C5:91:LEU:O | 8:C5:104:ILE:CD1 | 2.38 | 0.71 |
| 8:I5:29:PHE:HE1 | 8:I5:98:ALA:O | 1.69 | 0.71 |
| 8:e5:91:LEU:O | 8:e5:104:ILE:CD1 | 2.39 | 0.71 |
| 1:f5:114:GLU:CA | 10:j5:491:THR:HG23 | 2.20 | 0.71 |
| 1:V5:114:GLU:OE1 | 10:j5:496:GLU:CB | 2.39 | 0.71 |
| 1:X5:106:GLU:CG | 10:j5:504:ASP:C | 2.63 | 0.71 |
| 7:N6:49:LEU:HG | 12:N6:101:CYC:NB | 2.05 | 0.71 |
| 10:k5:246:VAL:HG22 | 10:k5:257:THR:CG2 | 2.21 | 0.71 |
| 3:F6:84:ARG:NH1 | 12:F6:201:CYC:O2A | 2.23 | 0.71 |
| 8:Q7:13:ALA:C | 9:z7:46:LYS:HZ3 | 1.96 | 0.71 |
| 8:g7:19:SER:HB2 | 8:g7:20:PRO:HD3 | 1.72 | 0.71 |
| 8:i7:47:ARG:CB | 1:j7:18:TYR:CE2 | 2.74 | 0.71 |
| 8:a7:107:ILE:CG1 | 1:b7:13:ASP:OD2 | 2.38 | 0.71 |
| 8:c7:121:THR:CG2 | 12:c7:201:CYC:HMC3 | 2.21 | 0.71 |
| 3:B8:68:ARG:HH12 | 3:U8:68:ARG:HH22 | 1.37 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:W8:87:GLU:O | 3:W8:91:ARG:HG3 | 1.90 | 0.71 |
| 4:M8:235:PHE:HB2 | 12:M8:301:CYC:HAA1 | 1.71 | 0.71 |
| 3:L9:82:CYS:O | 3:L9:85:ASP:HB2 | 1.91 | 0.71 |
| 4:M9:4:LEU:HD12 | 4:M9:4:LEU:O | 1.90 | 0.71 |
| 11:a9:629:LYS:O | 11:a9:629:LYS:HD3 | 1.91 | 0.71 |
| 11:aA:290:ASP:C | 11:aA:291:TYR:CD1 | 2.68 | 0.71 |
| 4:M1:210:ILE:HD13 | 5:N1:59:ARG:NH1 | 2.05 | 0.71 |
| 4:M1:233:GLU:OE1 | 4:M1:237:ARG:NH2 | 2.24 | 0.71 |
| 4:M1:246:ALA:HA | 12:X1:201:CYC:CBB | 2.21 | 0.71 |
| 4:M1:258:LYS:HZ2 | 3:Z1:111:ASN:HD21 | 0.74 | 0.71 |
| 3:F2:82:CYS:SG | 12:F2:201:CYC:C4C | 2.79 | 0.71 |
| 2:IA:37:SER:CA | 2:IA:97:LEU:HD11 | 2.18 | 0.70 |
| 4:MA:233:GLU:OE1 | 4:MA:237:ARG:NH2 | 2.24 | 0.70 |
| 5:NA:54:LEU:HD13 | 3:TA:84:ARG:HH21 | 1.53 | 0.70 |
| 2:OA:59:VAL:O | 2:OA:66:LEU:HD12 | 1.89 | 0.70 |
| 5:N3:34:LEU:C | 3:T3:84:ARG:HH11 | 1.98 | 0.70 |
| 5:N3:54:LEU:CD1 | 12:R3:201:CYC:OB | 2.37 | 0.70 |
| 3:B1:84:ARG:CZ | 11:aA:680:SER:HB3 | 2.20 | 0.70 |
| 3:S4:113:LEU:HD12 | 3:S4:116:THR:CG2 | 2.20 | 0.70 |
| 3:F4:113:LEU:N | 4:M4:5:THR:CA | 2.33 | 0.70 |
| 4:M4:144:ARG:HH12 | 5:Z4:59:ARG:HH12 | 1.38 | 0.70 |
| 4:M4:217:VAL:HG21 | 5:Z4:30:PRO:HB3 | 1.67 | 0.70 |
| 1:B5:87:TYR:HE1 | 9:z5:20:GLY:HA2 | 1.55 | 0.70 |
| 1:P5:114:GLU:OE1 | 10:k5:496:GLU:HA | 1.91 | 0.70 |
| 12:W5:201:CYC:HMD1 | 12:W5:201:CYC:NC | 2.02 | 0.70 |
| 9:z5:6:LYS:HB2 | 9:z5:55:LYS:CB | 2.17 | 0.70 |
| 10:j5:825:ASN:CB | 12:H7:201:CYC:HBB2 | 2.21 | 0.70 |
| 10:j5:974:LEU:HG | 1:v7:1:MET:H1 | 0.88 | 0.70 |
| 10:k5:951:MET:HE3 | 10:k5:955:LEU:HG | 1.73 | 0.70 |
| 2:A6:60:TYR:OH | 2:A6:79:GLN:HG2 | 1.90 | 0.70 |
| 8:U7:102:THR:CB | 8:U7:103:PRO:CD | 2.64 | 0.70 |
| 8:u7:23:LEU:CD2 | 1:v7:38:VAL:CG1 | 2.66 | 0.70 |
| 3:L8:120:LEU:HD11 | 12:a9:901:CYC:HAA1 | 1.72 | 0.70 |
| 4:M8:144:ARG:HG3 | 4:M8:204:ILE:HG21 | 1.72 | 0.70 |
| 4:M9:176:ARG:CG | 4:M9:176:ARG:HH11 | 2.03 | 0.70 |
| 4:M9:233:GLU:OE1 | 4:M9:237:ARG:NH2 | 2.24 | 0.70 |
| 11:aA:654:ALA:HB2 | 2:I1:15:GLN:HG2 | 1.70 | 0.70 |
| 11:aA:802:ARG:HG3 | 12:aA:901:CYC:O1D | 1.91 | 0.70 |
| 5:N1:34:LEU:C | 3:T1:84:ARG:HH11 | 1.98 | 0.70 |
| 3:B4:120:LEU:HG | 4:M4:52:LEU:HD13 | 1.72 | 0.70 |
| 4:M3:21:LEU:O | 4:M3:36:TYR:CE2 | 2.44 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:M4:160:THR:HG21 | 4:M4:257:GLN:HB3 | 1.72 | 0.70 |
| 5:Z4:29:HIS:HE1 | 5:Z4:38:GLU:HB3 | 1.52 | 0.70 |
| 8:G5:64:ASP:OD2 | 8:U5:69:GLY:O | 2.09 | 0.70 |
| 8:I5:91:LEU:HB3 | 8:I5:104:ILE:HG23 | 1.73 | 0.70 |
| 12:R5:201:CYC:HBB2 | 10:k5:520:ARG:CD | 2.20 | 0.70 |
| 8:U5:75:GLU:HG2 | 6:M6:32:MET:SD | 2.30 | 0.70 |
| 12:V5:201:CYC:HBB2 | 10:j5:623:VAL:CG2 | 2.21 | 0.70 |
| 6:M6:50:LEU:CD2 | 8:c7:79:ALA:C | 2.64 | 0.70 |
| 10:j5:725:LEU:HD23 | 10:j5:725:LEU:O | 1.91 | 0.70 |
| 10:j5:1054:SER:HB2 | 10:j5:1056:PRO:HD3 | 1.71 | 0.70 |
| 10:k5:188:GLU:N | 10:k5:188:GLU:OE1 | 2.23 | 0.70 |
| 10:k5:235:ASP:OD1 | 10:k5:235:ASP:N | 2.22 | 0.70 |
| 10:k5:930:LEU:HB3 | 1:D7:33:THR:HB | 1.72 | 0.70 |
| 1:H7:54:GLU:OE2 | 11:aA:563:PHE:CD2 | 2.44 | 0.70 |
| 8:g7:91:LEU:O | 8:g7:104:ILE:CD1 | 2.39 | 0.70 |
| 8:g7:107:ILE:CG1 | 1:h7:13:ASP:OD2 | 2.38 | 0.70 |
| 12:i7:201:CYC:HMD1 | 12:i7:201:CYC:NC | 2.02 | 0.70 |
| 9:x7:3:ARG:NE | 9:x7:67:VAL:CG1 | 2.42 | 0.70 |
| 2:A9:101:GLY:HA2 | 2:K9:22:THR:OG1 | 1.91 | 0.70 |
| 11:a9:102:GLN:OE1 | 11:a9:103:GLY:N | 2.24 | 0.70 |
| 3:J1:87:GLU:O | 3:J1:91:ARG:HG3 | 1.90 | 0.70 |
| 5:N1:39:PRO:CB | 3:T1:113:LEU:HA | 2.15 | 0.70 |
| 3:F2:72:ASN:O | 12:F2:201:CYC:HMD2 | 1.91 | 0.70 |
| 2:AA:101:GLY:HA2 | 2:KA:22:THR:OG1 | 1.91 | 0.70 |
| 3:JA:68:ARG:HD2 | 11:aA:353:ALA:HB1 | 1.72 | 0.70 |
| 4:MA:21:LEU:O | 4:MA:21:LEU:HD12 | 1.90 | 0.70 |
| 2:QA:101:GLY:HA2 | 2:UA:22:THR:OG1 | 1.90 | 0.70 |
| 12:QA:201:CYC:CBA | 3:TA:67:ILE:CG2 | 2.69 | 0.70 |
| 12:P1:201:CYC:CBA | 4:M1:134:ASN:HB2 | 2.20 | 0.70 |
| 3:H3:115:GLU:CB | 11:a9:786:GLU:OE1 | 2.40 | 0.70 |
| 2:N4:63:PHE:O | 2:N4:66:LEU:CG | 2.39 | 0.70 |
| 1:B5:76:ARG:HD2 | 9:z5:14:LEU:O | 1.91 | 0.70 |
| 8:e5:45:GLU:OE1 | 1:R5:139:GLY:C | 2.34 | 0.70 |
| 1:f5:18:TYR:CE2 | 10:j5:165:ARG:CG | 2.74 | 0.70 |
| 8:S5:14:GLU:CG | 10:j5:538:PHE:HE2 | 2.04 | 0.70 |
| 8:S5:106:GLU:HG2 | 10:j5:533:LEU:HD21 | 1.71 | 0.70 |
| 12:T5:201:CYC:HBB1 | 10:j5:482:GLN:NE2 | 2.02 | 0.70 |
| 10:j5:388:ARG:HA | 10:j5:394:PRO:HG3 | 1.72 | 0.70 |
| 10:k5:974:LEU:HD12 | 1:p7:106:GLU:CD | 2.15 | 0.70 |
| 10:k5:1053:TYR:CB | 10:k5:1058:VAL:HG23 | 2.20 | 0.70 |
| 10:k5:1150:TYR:CE2 | 1:p7:69:GLY:C | 2.53 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:O7:29:PHE:HE1 | 8:O7:98:ALA:O | 1.69 | 0.70 |
| 8:I7:6:LYS:NZ | 8:W7:19:SER:HB3 | 2.06 | 0.70 |
| 8:g7:91:LEU:HB3 | 8:g7:104:ILE:HG23 | 1.73 | 0.70 |
| 1:h7:46:SER:HB2 | 8:u7:157:VAL:HG12 | 1.72 | 0.70 |
| 8:c7:89:LEU:HD13 | 8:c7:153:PHE:CZ | 2.25 | 0.70 |
| 8:m7:44:THR:HG1 | 1:n7:18:TYR:HD2 | 1.38 | 0.70 |
| 9:x7:35:GLU:N | 9:x7:35:GLU:OE1 | 2.23 | 0.70 |
| 2:N8:63:PHE:O | 2:N8:66:LEU:CG | 2.39 | 0.70 |
| 12:D9:201:CYC:HMA1 | 12:D9:201:CYC:NB | 2.05 | 0.70 |
| 3:H9:84:ARG:HH11 | 11:a9:475:ASN:HA | 1.56 | 0.70 |
| 11:aA:629:LYS:HD3 | 11:aA:629:LYS:O | 1.91 | 0.70 |
| 4:M1:245:ASP:HB3 | 3:X1:108:ARG:C | 2.15 | 0.70 |
| 5:N1:14:LYS:HD3 | 5:N1:14:LYS:H | 1.57 | 0.70 |
| 12:F2:202:CYC:HC | 12:F2:202:CYC:CMD | 1.98 | 0.70 |
| 3:J3:109:CYS:O | 11:a9:796:ALA:HB2 | 1.92 | 0.70 |
| 3:B4:82:CYS:HA | 12:B4:202:CYC:C3C | 2.21 | 0.70 |
| 3:B4:116:THR:HG23 | 3:B4:117:TYR:N | 2.04 | 0.70 |
| 3:B4:119:ALA:CB | 4:M4:52:LEU:CD1 | 2.64 | 0.70 |
| 4:M3:248:SER:OG | 12:X3:201:CYC:HMA1 | 1.91 | 0.70 |
| 12:T3:301:CYC:NB | 12:T3:301:CYC:HMA1 | 2.05 | 0.70 |
| 4:M4:172:HIS:HE1 | 4:M4:249:ASP:OD2 | 1.73 | 0.70 |
| 4:M4:214:GLY:CA | 5:Z4:28:HIS:CG | 2.74 | 0.70 |
| 4:M4:232:VAL:HG22 | 4:M4:235:PHE:HE2 | 1.54 | 0.70 |
| 8:C5:37:LEU:CD2 | 1:D5:27:LEU:CD1 | 2.69 | 0.70 |
| 1:D5:39:ARG:O | 1:D5:42:ALA:N | 2.24 | 0.70 |
| 8:G5:115:MET:HE1 | 12:G5:201:CYC:CHB | 2.18 | 0.70 |
| 1:V5:87:TYR:HE2 | 10:j5:649:PHE:CZ | 2.07 | 0.70 |
| 9:i5:9:ALA:HA | 9:i5:50:LYS:O | 1.92 | 0.70 |
| 10:j5:18:ARG:NH1 | 10:j5:268:SER:HB3 | 2.06 | 0.70 |
| 10:j5:820:HIS:HE1 | 10:j5:859:ILE:CD1 | 1.95 | 0.70 |
| 10:j5:869:GLY:O | 9:w7:43:ARG:NH1 | 2.24 | 0.70 |
| 10:j5:1008:PHE:CZ | 12:v7:201:CYC:C4B | 2.74 | 0.70 |
| 10:j5:1119:LEU:HD11 | 1:t7:87:TYR:CZ | 2.26 | 0.70 |
| 10:k5:1024:LYS:C | 10:k5:1030:ILE:HG22 | 2.16 | 0.70 |
| 10:k5:1064:LYS:CG | 10:k5:1065:HIS:N | 2.55 | 0.70 |
| 8:i7:20:PRO:HG3 | 8:s7:155:TYR:CB | 2.22 | 0.70 |
| 3:O8:104:VAL:HA | 5:Z8:61:LYS:HE3 | 1.71 | 0.70 |
| 4:M9:51:ARG:NH2 | 11:a9:430:ARG:CD | 2.55 | 0.70 |
| 4:M9:189:ASP:CG | 3:V9:84:ARG:HH11 | 1.98 | 0.70 |
| 5:Z8:1:MET:HB3 | 5:Z8:3:VAL:CG2 | 2.15 | 0.70 |
| 11:aA:54:ARG:HD2 | 11:aA:610:ALA:HB2 | 1.72 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 12:X1:202:CYC:HC | 12:X1:202:CYC:CMD | 1.98 | 0.70 |
| 3:HA:116:THR:CG2 | 12:HA:202:CYC:CMA | 2.69 | 0.70 |
| 3:JA:109:CYS:O | 11:aA:518:ALA:CB | 2.34 | 0.70 |
| 2:KA:18:PHE:HB3 | 3:LA:45:THR:HG23 | 1.72 | 0.70 |
| 5:NA:1:MET:HE3 | 5:NA:1:MET:CA | 2.17 | 0.70 |
| 7:N2:2:TYR:H | 7:N2:2:TYR:HD1 | 1.39 | 0.70 |
| 4:M3:245:ASP:HB3 | 3:X3:108:ARG:C | 2.15 | 0.70 |
| 4:M4:94:TRP:HB3 | 3:Q4:88:ILE:CD1 | 2.20 | 0.70 |
| 4:M4:100:SER:C | 2:P4:13:ASP:OD2 | 2.33 | 0.70 |
| 4:M4:101:ASP:CA | 2:P4:13:ASP:CB | 2.53 | 0.70 |
| 3:Q4:77:ARG:HH12 | 5:Z4:37:HIS:CE1 | 2.09 | 0.70 |
| 3:Q4:104:VAL:HG22 | 3:Q4:105:LEU:CD1 | 2.20 | 0.70 |
| 8:O5:91:LEU:O | 8:O5:104:ILE:CD1 | 2.39 | 0.70 |
| 8:I5:37:LEU:CD2 | 1:J5:27:LEU:CD1 | 2.69 | 0.70 |
| 8:e5:29:PHE:HE1 | 8:e5:98:ALA:O | 1.69 | 0.70 |
| 1:V5:118:SER:OG | 10:j5:498:ALA:HB1 | 1.90 | 0.70 |
| 6:M6:278:ARG:HH22 | 1:d7:64:ASP:CG | 1.99 | 0.70 |
| 9:z5:15:LYS:HD2 | 9:z5:15:LYS:C | 2.17 | 0.70 |
| 10:j5:1025:LEU:CA | 10:j5:1030:ILE:HG22 | 2.22 | 0.70 |
| 10:k5:274:MET:CE | 10:k5:323:VAL:O | 2.39 | 0.70 |
| 2:A6:63:PHE:O | 2:A6:66:LEU:CG | 2.39 | 0.70 |
| 8:i7:104:ILE:CG2 | 8:i7:155:TYR:HE2 | 2.04 | 0.70 |
| 8:k7:66:VAL:CG1 | 11:a9:65:LEU:HD21 | 2.21 | 0.70 |
| 8:U7:44:THR:HG1 | 1:V7:18:TYR:HD2 | 1.40 | 0.70 |
| 1:b7:76:ARG:N | 8:c7:110:ILE:O | 2.25 | 0.70 |
| 8:c7:20:PRO:CD | 8:m7:155:TYR:CB | 2.56 | 0.70 |
| 8:o7:103:PRO:CB | 1:p7:9:ILE:HD13 | 2.21 | 0.70 |
| 8:s7:91:LEU:O | 8:s7:104:ILE:CD1 | 2.39 | 0.70 |
| 1:v7:62:TYR:HB2 | 11:aA:602:PRO:HD2 | 1.63 | 0.70 |
| 9:x7:9:ALA:CB | 9:x7:44:ILE:HD13 | 2.20 | 0.70 |
| 4:M8:104:ALA:CB | 2:P8:10:ALA:O | 2.32 | 0.70 |
| 4:M8:127:SER:CB | 12:M8:302:CYC:HMA2 | 1.97 | 0.70 |
| 4:M9:1:MET:SD | 11:a9:422:SER:O | 2.49 | 0.70 |
| 4:M9:162:ASN:HB2 | 12:V9:201:CYC:HBB3 | 1.74 | 0.70 |
| 5:Z8:14:LYS:HD3 | 5:Z8:14:LYS:H | 1.57 | 0.70 |
| 11:a9:426:ARG:O | 11:a9:426:ARG:HG3 | 1.91 | 0.70 |
| 11:aA:339:GLU:N | 11:aA:340:PRO:CD | 2.55 | 0.70 |
| 3:F2:82:CYS:HG | 12:F2:201:CYC:HAC2 | 1.53 | 0.70 |
| 1:Z:13:ASP:OD2 | 8:e5:107:ILE:HG12 | 1.90 | 0.70 |
| 4:MA:162:ASN:HB2 | 12:VA:201:CYC:HBB3 | 1.74 | 0.70 |
| 3:D3:68:ARG:HH12 | 3:X3:68:ARG:NH1 | 1.90 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 3:B1:68:ARG:HH12 | 3:V1:68:ARG:NH1 | 1.88 | 0.70 |
| 2:I4:115:GLU:OE1 | 11:aA:133:LEU:CD2 | 2.38 | 0.70 |
| 4:M4:61:ASN:OD1 | 4:M4:62:LYS:CG | 2.40 | 0.70 |
| 4:M4:144:ARG:HG2 | 4:M4:204:ILE:HG21 | 1.72 | 0.70 |
| 5:Z4:41:GLN:HB3 | 12:Z4:301:CYC:C3B | 2.20 | 0.70 |
| 8:a5:91:LEU:HB3 | 8:a5:104:ILE:HG23 | 1.73 | 0.70 |
| 8:c7:42:THR:HG22 | 8:c7:141:LEU:CD2 | 2.13 | 0.70 |
| 3:L8:71:GLY:HA2 | 11:a9:82:GLN:CD | 2.17 | 0.70 |
| 2:N8:115:GLU:CB | 5:Z8:32:PRO:C | 2.63 | 0.70 |
| 3:L9:14:LEU:HG | 11:a9:358:PRO:HB2 | 1.74 | 0.70 |
| 4:M9:271:ARG:NH2 | 12:V9:201:CYC:O2D | 2.24 | 0.70 |
| 5:N9:4:LEU:O | 5:N9:4:LEU:HG | 1.88 | 0.70 |
| 5:Z8:41:GLN:HB3 | 12:Z8:301:CYC:C4B | 2.17 | 0.70 |
| 11:aA:30:MET:HE3 | 11:aA:35:ARG:HD3 | 1.72 | 0.70 |
| 11:aA:803:ASN:HA | 3:J1:120:LEU:HA | 1.73 | 0.70 |
| 12:H1:202:CYC:HC | 12:H1:202:CYC:CMD | 1.99 | 0.70 |
| 1:Z:17:LYS:C | 8:e5:90:ARG:HD2 | 2.17 | 0.70 |
| 2:EA:2:LYS:HZ1 | 2:IA:17:ARG:NH1 | 1.70 | 0.70 |
| 5:NA:66:ARG:CB | 3:TA:111:ASN:HD22 | 2.04 | 0.70 |
| 2:QA:76:ASP:HB2 | 2:U1:140:SER:O | 1.89 | 0.70 |
| 2:QA:119:THR:CG2 | 3:TA:83:LEU:HD13 | 2.21 | 0.70 |
| 2:K3:112:GLY:CA | 11:a9:670:LEU:HD21 | 2.16 | 0.70 |
| 4:M3:148:LYS:CD | 4:M3:197:ASP:OD1 | 2.37 | 0.70 |
| 5:N3:22:LEU:HD21 | 5:N3:26:LEU:CD2 | 2.08 | 0.70 |
| 2:O3:63:PHE:O | 2:O3:66:LEU:CG | 2.39 | 0.70 |
| 3:Q4:104:VAL:HG23 | 3:Q4:105:LEU:CD1 | 2.20 | 0.70 |
| 3:Q4:124:THR:HB | 3:Q4:171:ILE:C | 2.16 | 0.70 |
| 12:V5:201:CYC:OB | 10:j5:623:VAL:HB | 1.91 | 0.70 |
| 10:j5:194:CYS:HB2 | 12:j5:1201:CYC:HAC2 | 1.71 | 0.70 |
| 10:j5:1153:VAL:CG2 | 1:v7:125:ALA:CA | 2.68 | 0.70 |
| 10:j5:1153:VAL:HG23 | 1:v7:125:ALA:CA | 2.21 | 0.70 |
| 8:C7:91:LEU:O | 8:C7:104:ILE:CD1 | 2.39 | 0.70 |
| 8:c7:50:ILE:HG12 | 8:c7:137:ALA:HB2 | 1.74 | 0.70 |
| 9:x7:60:VAL:HG23 | 9:x7:62:GLY:H | 1.56 | 0.70 |
| 4:M8:176:ARG:CG | 4:M8:176:ARG:HH11 | 2.03 | 0.70 |
| 4:M8:232:VAL:O | 4:M8:235:PHE:HD2 | 1.69 | 0.70 |
| 3:S8:113:LEU:HD12 | 3:S8:116:THR:CG2 | 2.20 | 0.70 |
| 4:M9:273:ILE:CD1 | 3:V9:75:PRO:HD2 | 2.20 | 0.70 |
| 2:E9:33:ARG:CD | 2:I9:25:GLN:HE22 | 2.04 | 0.70 |
| 1:A:73:TYR:CE1 | 10:k5:162:TRP:CE2 | 2.73 | 0.70 |
| 3:JA:108:ARG:C | 11:aA:517:ALA:HA | 2.17 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:SA:39:GLU:HA | 2:X4:69:PRO:HB2 | 1.73 | 0.70 |
| 3:J3:77:ARG:NE | 2:K3:111:ALA:CB | 2.53 | 0.70 |
| 3:H2:88:ILE:HD11 | 6:M2:115:TYR:OH | 1.92 | 0.70 |
| 6:M2:130:ARG:HB3 | 12:F2:201:CYC:HBA2 | 1.74 | 0.70 |
| 3:L3:120:LEU:HA | 11:a9:817:LEU:HD11 | 1.74 | 0.70 |
| 12:T3:302:CYC:HC | 12:T3:302:CYC:CMD | 1.99 | 0.70 |
| 2:N4:60:TYR:HB3 | 2:N4:67:THR:CG2 | 2.19 | 0.70 |
| 6:M6:251:LYS:HZ1 | 3:H6:121:GLY:HA3 | 1.56 | 0.70 |
| 10:j5:742:GLY:C | 12:J7:201:CYC:CGD | 2.65 | 0.70 |
| 10:j5:974:LEU:HD23 | 1:v7:1:MET:N | 2.07 | 0.70 |
| 10:k5:778:LYS:NZ | 12:F7:201:CYC:OB | 2.24 | 0.70 |
| 10:k5:964:GLY:CA | 1:n7:69:GLY:CA | 2.70 | 0.70 |
| 10:k5:1008:PHE:CD1 | 12:p7:201:CYC:OB | 2.45 | 0.70 |
| 3:D1:68:ARG:HH12 | 3:X1:68:ARG:NH1 | 1.90 | 0.70 |
| 8:U7:91:LEU:O | 8:U7:104:ILE:CD1 | 2.39 | 0.70 |
| 8:c7:49:ARG:CZ | 8:c7:140:LEU:CD2 | 2.69 | 0.70 |
| 8:c7:50:ILE:HD13 | 8:c7:137:ALA:HB2 | 1.73 | 0.70 |
| 12:D8:201:CYC:HC | 12:D8:201:CYC:CMD | 1.99 | 0.70 |
| 8:m7:91:LEU:HB3 | 8:m7:104:ILE:HG23 | 1.73 | 0.70 |
| 8:m7:102:THR:CB | 8:m7:103:PRO:CD | 2.64 | 0.70 |
| 8:u7:37:LEU:HD11 | 1:v7:24:LEU:O | 1.92 | 0.70 |
| 3:U8:114:LYS:HZ3 | 4:M8:13:LYS:HD3 | 1.50 | 0.70 |
| 12:F8:201:CYC:HC | 12:F8:201:CYC:CMD | 1.98 | 0.70 |
| 3:O8:119:ALA:CB | 5:Z8:72:GLU:H | 2.04 | 0.70 |
| 2:A9:63:PHE:HB2 | 2:A9:66:LEU:HD12 | 1.70 | 0.70 |
| 12:J9:202:CYC:HBA1 | 11:a9:511:LYS:C | 2.17 | 0.70 |
| 11:aA:813:PRO:HB2 | 3:L1:119:ALA:CB | 1.93 | 0.70 |
| 4:M1:176:ARG:HH11 | 4:M1:176:ARG:CG | 2.03 | 0.70 |
| 2:AA:63:PHE:O | 2:AA:66:LEU:CG | 2.39 | 0.70 |
| 12:BA:201:CYC:HMA1 | 12:BA:201:CYC:NB | 2.05 | 0.70 |
| 12:JA:202:CYC:NB | 12:JA:202:CYC:HMA1 | 2.05 | 0.70 |
| 3:LA:113:LEU:N | 11:aA:532:ALA:CB | 2.54 | 0.70 |
| 4:MA:189:ASP:CG | 3:VA:84:ARG:HH11 | 1.98 | 0.70 |
| 8:S5:90:ARG:NH1 | 1:T5:16:GLY:HA2 | 2.05 | 0.70 |
| 8:W5:17:TYR:CD2 | 1:X5:93:THR:HG21 | 2.22 | 0.70 |
| 9:z5:9:ALA:HA | 9:z5:50:LYS:O | 1.92 | 0.70 |
| 10:j5:19:THR:OG1 | 10:j5:19:THR:O | 2.04 | 0.70 |
| 10:j5:1008:PHE:CD1 | 12:v7:201:CYC:HBB2 | 2.27 | 0.70 |
| 10:k5:63:ASN:OD1 | 10:k5:63:ASN:N | 2.22 | 0.70 |
| 10:k5:743:VAL:N | 12:D7:201:CYC:CGD | 2.53 | 0.70 |
| 8:C7:91:LEU:HB3 | 8:C7:104:ILE:HG23 | 1.73 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:i7:50:ILE:HG12 | 8:i7:137:ALA:HB2 | 1.74 | 0.70 |
| 3:B8:107:ASP:O | 4:M8:60:LYS:O | 2.10 | 0.70 |
| 8:u7:17:TYR:HE2 | 1:v7:93:THR:HG1 | 0.70 | 0.70 |
| 3:H8:80:ALA:O | 3:H8:84:ARG:HG3 | 1.91 | 0.70 |
| 3:H8:81:ALA:CA | 3:H8:84:ARG:HH21 | 2.04 | 0.70 |
| 4:M8:144:ARG:CD | 4:M8:204:ILE:HG21 | 2.22 | 0.70 |
| 12:M8:301:CYC:C3B | 3:Y8:88:ILE:HG22 | 2.21 | 0.70 |
| 4:M9:78:GLY:CA | 3:D9:115:GLU:OE2 | 2.40 | 0.70 |
| 3:D9:68:ARG:CZ | 3:X9:68:ARG:HH12 | 2.04 | 0.70 |
| 3:J9:20:SER:C | 3:J9:22:GLN:N | 2.46 | 0.70 |
| 3:J9:78:ARG:CZ | 11:a9:359:ASP:HA | 2.15 | 0.70 |
| 11:aA:102:GLN:OE1 | 11:aA:103:GLY:N | 2.24 | 0.70 |
| 11:aA:376:ALA:HB1 | 11:aA:504:VAL:HB | 1.73 | 0.70 |
| 4:M1:248:SER:OG | 12:X1:201:CYC:HMA1 | 1.91 | 0.70 |
| 5:N1:33:GLY:C | 3:T1:84:ARG:CD | 2.65 | 0.70 |
| 3:HA:84:ARG:HH11 | 11:aA:475:ASN:HA | 1.56 | 0.70 |
| 4:MA:271:ARG:NH2 | 12:VA:201:CYC:O2D | 2.24 | 0.70 |
| 3:L3:75:PRO:HG2 | 11:a9:823:ILE:HD11 | 1.73 | 0.70 |
| 8:K5:17:TYR:OH | 1:L5:89:LEU:HG | 1.92 | 0.70 |
| 1:N5:14:VAL:O | 1:R5:68:PRO:CB | 2.38 | 0.70 |
| 1:N5:110:ASN:HD21 | 10:k5:692:LEU:CA | 2.04 | 0.70 |
| 1:H5:107:ARG:NH2 | 10:j5:541:THR:OG1 | 2.24 | 0.70 |
| 1:T5:14:VAL:O | 1:X5:68:PRO:CB | 2.38 | 0.70 |
| 8:U5:91:LEU:HB3 | 8:U5:104:ILE:HG23 | 1.73 | 0.70 |
| 12:V5:201:CYC:O2A | 10:j5:649:PHE:CD2 | 2.43 | 0.70 |
| 1:Z5:53:LYS:CD | 8:a5:118:SER:O | 2.34 | 0.70 |
| 1:Z5:127:VAL:CB | 10:k5:698:GLY:HA3 | 2.21 | 0.70 |
| 1:b5:18:TYR:CE1 | 10:k5:165:ARG:CG | 2.75 | 0.70 |
| 10:j5:235:ASP:OD1 | 10:j5:235:ASP:N | 2.22 | 0.70 |
| 8:Q7:25:ARG:NE | 8:C7:25:ARG:NH2 | 2.40 | 0.70 |
| 8:i7:25:ARG:NH2 | 8:s7:6:LYS:CA | 2.36 | 0.70 |
| 8:k7:76:LYS:NZ | 11:a9:605:PRO:CB | 2.43 | 0.70 |
| 8:U7:91:LEU:HB3 | 8:U7:104:ILE:HG23 | 1.73 | 0.70 |
| 8:c7:94:TYR:CG | 1:d7:9:ILE:HG23 | 2.27 | 0.70 |
| 8:o7:29:PHE:CE2 | 1:p7:5:ILE:HD11 | 2.25 | 0.70 |
| 8:u7:23:LEU:HD22 | 1:v7:38:VAL:HG13 | 1.72 | 0.70 |
| 2:A9:63:PHE:O | 2:A9:66:LEU:CG | 2.39 | 0.70 |
| 3:H9:117:TYR:HE1 | 12:H9:202:CYC:NA | 1.90 | 0.70 |
| 2:I9:37:SER:CA | 2:I9:97:LEU:HD21 | 2.20 | 0.70 |
| 11:aA:278:LEU:HD12 | 11:aA:278:LEU:N | 2.07 | 0.70 |
| 11:aA:796:ALA:HB2 | 3:J1:109:CYS:O | 1.90 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 5:N1:31:TRP:HZ2 | 3:T1:92:TYR:HH | 1.35 | 0.70 |
| 3:DA:68:ARG:CZ | 3:XA:68:ARG:HH12 | 2.04 | 0.69 |
| 5:NA:54:LEU:CA | 12:TA:301:CYC:HBA1 | 2.22 | 0.69 |
| 3:J2:87:GLU:O | 3:J2:91:ARG:HG3 | 1.90 | 0.69 |
| 12:B4:201:CYC:HC | 12:B4:201:CYC:CMD | 1.99 | 0.69 |
| 3:U4:112:GLY:N | 4:M4:74:LEU:HD21 | 2.07 | 0.69 |
| 3:U4:120:LEU:HD21 | 12:U4:201:CYC:HBD2 | 1.72 | 0.69 |
| 5:Z4:1:MET:HB3 | 5:Z4:3:VAL:CG2 | 2.15 | 0.69 |
| 8:S5:90:ARG:HD3 | 1:T5:18:TYR:CD1 | 2.27 | 0.69 |
| 9:i5:16:ARG:HE | 9:i5:16:ARG:C | 1.99 | 0.69 |
| 10:j5:147:ARG:HD3 | 10:j5:147:ARG:O | 1.91 | 0.69 |
| 10:j5:1064:LYS:CG | 10:j5:1065:HIS:N | 2.55 | 0.69 |
| 10:k5:18:ARG:NH1 | 10:k5:268:SER:HB3 | 2.06 | 0.69 |
| 10:k5:1069:ARG:NH1 | 10:k5:1069:ARG:HG3 | 2.07 | 0.69 |
| 1:H7:140:LEU:CG | 11:aA:561:ALA:CB | 2.67 | 0.69 |
| 1:h7:37:ARG:NH1 | 1:h7:96:MET:O | 2.26 | 0.69 |
| 8:i7:131:ARG:HH11 | 8:i7:131:ARG:HG2 | 1.57 | 0.69 |
| 12:j7:201:CYC:HBB1 | 9:y7:42:GLN:OE1 | 1.90 | 0.69 |
| 2:A8:63:PHE:O | 2:A8:66:LEU:CG | 2.39 | 0.69 |
| 1:v7:139:GLY:C | 11:aA:342:ARG:HD2 | 2.16 | 0.69 |
| 4:M8:233:GLU:OE1 | 4:M8:237:ARG:NH2 | 2.24 | 0.69 |
| 5:Z8:4:LEU:O | 5:Z8:4:LEU:HG | 1.88 | 0.69 |
| 3:J9:108:ARG:O | 11:a9:517:ALA:C | 2.36 | 0.69 |
| 11:a9:403:THR:CG2 | 11:a9:536:THR:HG23 | 1.95 | 0.69 |
| 11:aA:283:GLN:HB3 | 11:aA:284:PRO:HD2 | 0.70 | 0.69 |
| 11:aA:798:SER:OG | 12:aA:901:CYC:C2A | 2.40 | 0.69 |
| 5:N1:1:MET:HB3 | 5:N1:3:VAL:CG2 | 2.15 | 0.69 |
| 12:DA:201:CYC:CBA | 11:aA:420:ASN:HB2 | 2.19 | 0.69 |
| 3:LA:82:CYS:O | 3:LA:85:ASP:HB2 | 1.91 | 0.69 |
| 4:MA:1:MET:CB | 11:aA:422:SER:O | 2.40 | 0.69 |
| 4:MA:273:ILE:CD1 | 3:VA:75:PRO:HG3 | 2.21 | 0.69 |
| 2:I2:14:SER:O | 6:M2:193:TYR:HB3 | 1.92 | 0.69 |
| 7:N2:49:LEU:HG | 12:N2:101:CYC:NB | 2.05 | 0.69 |
| 2:A3:63:PHE:HB2 | 2:A3:66:LEU:HD12 | 1.70 | 0.69 |
| 3:D4:150:ARG:NH1 | 2:C1:140:SER:CB | 2.54 | 0.69 |
| 4:M4:233:GLU:HG3 | 3:Y4:112:GLY:HA3 | 1.74 | 0.69 |
| 8:E5:17:TYR:OH | 1:F5:89:LEU:HG | 1.92 | 0.69 |
| 10:j5:1119:LEU:HD21 | 1:t7:87:TYR:CZ | 2.26 | 0.69 |
| 10:k5:546:PHE:CE1 | 10:k5:561:GLU:OE1 | 2.44 | 0.69 |
| 10:k5:631:HIS:CB | 10:k5:664:MET:HE1 | 2.22 | 0.69 |
| 10:k5:1008:PHE:CD1 | 12:p7:201:CYC:C4B | 2.74 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:k5:1019:SER:O | 10:k5:1020:GLU:HB2 | 1.90 | 0.69 |
| 10:k5:1055:SER:CB | 12:k5:1203:CYC:CAB | 2.70 | 0.69 |
| 10:k5:1064:LYS:HG3 | 10:k5:1065:HIS:H | 1.54 | 0.69 |
| 8:c7:12:ASP:OD2 | 1:d7:91:TYR:CE1 | 2.35 | 0.69 |
| 2:N8:13:ASP:CB | 3:O8:108:ARG:NH1 | 2.53 | 0.69 |
| 3:Q8:82:CYS:HA | 12:Z8:301:CYC:CAC | 2.20 | 0.69 |
| 4:M9:274:VAL:HA | 3:V9:77:ARG:NE | 2.07 | 0.69 |
| 5:N9:1:MET:HE3 | 5:N9:1:MET:CA | 2.17 | 0.69 |
| 11:a9:586:LEU:N | 11:a9:586:LEU:HD22 | 2.05 | 0.69 |
| 11:a9:598:SER:HB3 | 11:a9:599:PRO:CB | 2.22 | 0.69 |
| 3:FA:150:ARG:HG3 | 3:F9:150:ARG:HA | 1.73 | 0.69 |
| 12:HA:201:CYC:HC | 12:HA:201:CYC:CMD | 1.98 | 0.69 |
| 12:LA:201:CYC:HC | 12:LA:201:CYC:CMD | 1.98 | 0.69 |
| 7:N2:20:VAL:HG21 | 7:N2:39:TYR:CZ | 2.27 | 0.69 |
| 3:L3:88:ILE:HG12 | 11:a9:742:GLN:OE1 | 1.90 | 0.69 |
| 4:M3:134:ASN:HB2 | 12:P3:201:CYC:CBA | 2.20 | 0.69 |
| 4:M3:205:ASP:OD2 | 5:N3:52:ARG:CZ | 2.40 | 0.69 |
| 5:N3:1:MET:C | 5:N3:3:VAL:N | 2.50 | 0.69 |
| 5:N3:14:LYS:HD3 | 5:N3:14:LYS:H | 1.57 | 0.69 |
| 3:H4:84:ARG:HD3 | 11:aA:131:TYR:CZ | 2.27 | 0.69 |
| 4:M4:144:ARG:CD | 4:M4:204:ILE:HG21 | 2.22 | 0.69 |
| 3:O4:107:ASP:CA | 5:Z4:66:ARG:HB2 | 2.22 | 0.69 |
| 8:O5:91:LEU:HB3 | 8:O5:104:ILE:HG23 | 1.73 | 0.69 |
| 1:f5:30:TYR:CZ | 10:j5:47:PHE:CZ | 2.80 | 0.69 |
| 8:U5:79:ALA:HB1 | 6:M6:32:MET:HA | 1.71 | 0.69 |
| 1:V5:114:GLU:CD | 10:j5:496:GLU:CG | 2.55 | 0.69 |
| 1:X5:106:GLU:CD | 10:j5:504:ASP:O | 2.34 | 0.69 |
| 9:z5:14:LEU:CD1 | 9:z5:15:LYS:N | 2.54 | 0.69 |
| 9:z5:16:ARG:C | 9:z5:16:ARG:HE | 1.99 | 0.69 |
| 10:j5:501:ILE:HD12 | 10:j5:501:ILE:N | 2.07 | 0.69 |
| 10:j5:951:MET:HE3 | 10:j5:955:LEU:HG | 1.73 | 0.69 |
| 10:k5:974:LEU:HD23 | 1:p7:1:MET:N | 2.02 | 0.69 |
| 10:k5:1025:LEU:CA | 10:k5:1030:ILE:HG22 | 2.21 | 0.69 |
| 8:O7:22:GLU:HG2 | 8:O7:25:ARG:HH11 | 1.57 | 0.69 |
| 8:i7:21:GLY:CA | 8:s7:101:VAL:HG22 | 2.22 | 0.69 |
| 8:U7:60:GLN:OE1 | 1:p7:117:ASN:CG | 2.34 | 0.69 |
| 12:d7:201:CYC:HBB2 | 9:x7:42:GLN:CD | 2.16 | 0.69 |
| 8:o7:17:TYR:HE2 | 1:p7:93:THR:HG1 | 0.70 | 0.69 |
| 8:u7:2:SER:HB3 | 1:v7:5:ILE:CB | 2.22 | 0.69 |
| 8:u7:29:PHE:CE2 | 1:v7:5:ILE:HD11 | 2.25 | 0.69 |
| 3:L8:113:LEU:HD22 | 12:a9:901:CYC:HMB1 | 1.74 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:N9:61:LYS:HD3 | 3:T9:108:ARG:C | 2.14 | 0.69 |
| 3:Y8:102:ALA:HB1 | 3:Y8:105:LEU:HB3 | 1.73 | 0.69 |
| 3:J9:108:ARG:C | 11:a9:517:ALA:HA | 2.16 | 0.69 |
| 11:aA:598:SER:HB3 | 11:aA:599:PRO:CB | 2.22 | 0.69 |
| 11:aA:623:ASP:HA | 3:H1:78:ARG:NH1 | 2.08 | 0.69 |
| 11:aA:643:LEU:HD12 | 11:aA:766:ASN:HB3 | 1.74 | 0.69 |
| 11:aA:738:LEU:CD1 | 12:aA:902:CYC:HB | 1.95 | 0.69 |
| 5:N1:33:GLY:C | 3:T1:84:ARG:HD2 | 2.17 | 0.69 |
| 1:Z:18:TYR:CE1 | 8:e5:90:ARG:HB2 | 2.27 | 0.69 |
| 3:JA:108:ARG:O | 11:aA:517:ALA:C | 2.36 | 0.69 |
| 3:JA:108:ARG:CA | 11:aA:517:ALA:HA | 2.23 | 0.69 |
| 4:MA:1:MET:SD | 11:aA:422:SER:O | 2.49 | 0.69 |
| 3:J3:84:ARG:CD | 11:a9:668:TYR:CB | 2.46 | 0.69 |
| 12:L2:202:CYC:HC | 12:L2:202:CYC:CMD | 1.98 | 0.69 |
| 3:H4:111:ASN:OD1 | 11:aA:291:TYR:CE1 | 2.44 | 0.69 |
| 12:H4:201:CYC:HMA1 | 11:aA:261:SER:CB | 2.22 | 0.69 |
| 4:M4:27:HIS:HE1 | 4:M4:34:ASP:C | 1.71 | 0.69 |
| 3:Q4:84:ARG:CZ | 5:Z4:31:TRP:HB2 | 2.21 | 0.69 |
| 8:W5:16:ARG:HA | 1:X5:90:ARG:NE | 2.07 | 0.69 |
| 7:N6:20:VAL:HG21 | 7:N6:39:TYR:CZ | 2.27 | 0.69 |
| 10:j5:1118:THR:O | 12:j5:1202:CYC:HMA3 | 1.90 | 0.69 |
| 10:k5:1143:LEU:HD12 | 8:k7:106:GLU:CD | 2.16 | 0.69 |
| 3:F6:84:ARG:HH22 | 12:F6:201:CYC:CGA | 2.04 | 0.69 |
| 8:c7:92:VAL:CG2 | 8:c7:156:LEU:CD1 | 2.69 | 0.69 |
| 1:f7:67:ARG:HH12 | 11:aA:307:ARG:CG | 2.05 | 0.69 |
| 8:u7:37:LEU:CD1 | 1:v7:28:LYS:HE3 | 2.22 | 0.69 |
| 3:H8:111:ASN:OD1 | 11:a9:291:TYR:CE1 | 2.45 | 0.69 |
| 4:M8:99:VAL:HA | 3:Q8:108:ARG:NH1 | 2.07 | 0.69 |
| 4:M8:217:VAL:HG23 | 5:Z8:30:PRO:CG | 2.14 | 0.69 |
| 3:O8:112:GLY:HA3 | 5:Z8:69:GLU:C | 2.18 | 0.69 |
| 3:Q8:89:ILE:HA | 3:Q8:92:TYR:HE2 | 0.88 | 0.69 |
| 3:L9:77:ARG:NH1 | 11:a9:538:ARG:NH2 | 2.40 | 0.69 |
| 4:M9:134:ASN:CG | 5:N9:1:MET:N | 2.50 | 0.69 |
| 5:N9:14:LYS:CE | 5:N9:50:LEU:HD23 | 2.23 | 0.69 |
| 5:Z8:42:SER:N | 12:Z8:301:CYC:HMA2 | 2.08 | 0.69 |
| 11:a9:239:TYR:CD1 | 12:a9:901:CYC:O2A | 2.45 | 0.69 |
| 11:a9:776:TYR:CD1 | 11:a9:776:TYR:C | 2.70 | 0.69 |
| 11:aA:308:LEU:O | 11:aA:308:LEU:HD23 | 1.92 | 0.69 |
| 11:aA:711:SER:HB3 | 3:L1:111:ASN:O | 1.91 | 0.69 |
| 11:aA:776:TYR:CE1 | 12:H1:201:CYC:C4B | 2.72 | 0.69 |
| 2:A2:60:TYR:CE2 | 2:A2:79:GLN:NE2 | 2.61 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:H3:62:GLU:OE1 | 8:k7:49:ARG:NH2 | 2.25 | 0.69 |
| 6:M2:57:GLU:CD | 8:i7:76:LYS:CE | 2.65 | 0.69 |
| 2:A3:60:TYR:CE2 | 2:A3:79:GLN:NE2 | 2.61 | 0.69 |
| 3:D3:68:ARG:HH22 | 3:X3:68:ARG:NH2 | 1.82 | 0.69 |
| 12:L3:202:CYC:CBA | 11:a9:735:VAL:N | 2.37 | 0.69 |
| 12:J4:202:CYC:HC | 12:J4:202:CYC:CMD | 1.99 | 0.69 |
| 1:V5:87:TYR:CE2 | 10:j5:649:PHE:HZ | 2.09 | 0.69 |
| 10:j5:274:MET:CE | 10:j5:323:VAL:O | 2.39 | 0.69 |
| 10:j5:1119:LEU:CD1 | 12:j5:1202:CYC:OB | 2.33 | 0.69 |
| 10:k5:175:ASP:HB2 | 10:k5:176:PRO:CG | 2.18 | 0.69 |
| 8:i7:24:ASP:CB | 8:s7:99:GLY:O | 2.40 | 0.69 |
| 8:U7:22:GLU:C | 8:U7:24:ASP:N | 2.47 | 0.69 |
| 8:a7:22:GLU:HG2 | 8:a7:25:ARG:HH12 | 1.57 | 0.69 |
| 2:A8:60:TYR:CE2 | 2:A8:79:GLN:NE2 | 2.61 | 0.69 |
| 3:L8:108:ARG:C | 12:a9:901:CYC:HBB1 | 2.16 | 0.69 |
| 5:N9:66:ARG:CB | 3:T9:111:ASN:HD22 | 2.04 | 0.69 |
| 11:a9:339:GLU:N | 11:a9:340:PRO:CD | 2.55 | 0.69 |
| 5:N1:14:LYS:CE | 5:N1:50:LEU:HD23 | 2.23 | 0.69 |
| 5:N1:34:LEU:HB3 | 3:T1:84:ARG:NH1 | 2.08 | 0.69 |
| 1:Z:18:TYR:OH | 8:e5:89:LEU:HB3 | 1.92 | 0.69 |
| 4:MA:51:ARG:NH2 | 11:aA:430:ARG:CD | 2.54 | 0.69 |
| 2:A4:60:TYR:CE2 | 2:A4:79:GLN:NE2 | 2.61 | 0.69 |
| 12:B4:202:CYC:HMA1 | 4:M4:58:TYR:CB | 2.19 | 0.69 |
| 5:N3:33:GLY:C | 3:T3:84:ARG:CD | 2.65 | 0.69 |
| 4:M4:138:SER:HB3 | 12:Z4:301:CYC:CAB | 2.22 | 0.69 |
| 4:M4:226:SER:OG | 3:Y4:88:ILE:HG21 | 1.90 | 0.69 |
| 3:Q4:72:ASN:OD1 | 12:Z4:301:CYC:CMD | 2.33 | 0.69 |
| 1:L5:76:ARG:HB2 | 8:G5:110:ILE:O | 1.93 | 0.69 |
| 12:R5:201:CYC:CBB | 10:k5:520:ARG:NE | 2.53 | 0.69 |
| 8:W5:47:ARG:HD3 | 1:X5:18:TYR:OH | 1.93 | 0.69 |
| 6:M6:278:ARG:N | 1:d7:62:TYR:O | 2.26 | 0.69 |
| 9:z5:56:LEU:HD12 | 9:z5:56:LEU:N | 2.08 | 0.69 |
| 9:i5:15:LYS:C | 9:i5:15:LYS:HD2 | 2.17 | 0.69 |
| 10:k5:388:ARG:HA | 10:k5:394:PRO:HG3 | 1.72 | 0.69 |
| 8:I7:91:LEU:HB3 | 8:I7:104:ILE:HG23 | 1.73 | 0.69 |
| 8:g7:19:SER:HB2 | 8:g7:20:PRO:CD | 2.20 | 0.69 |
| 12:h7:201:CYC:OB | 9:y7:21:ARG:O | 2.10 | 0.69 |
| 8:o7:2:SER:HB3 | 1:p7:5:ILE:CB | 2.22 | 0.69 |
| 8:u7:30:VAL:HB | 1:v7:31:PHE:C | 2.18 | 0.69 |
| 12:J8:201:CYC:HMA3 | 11:a9:176:ASN:HD21 | 1.58 | 0.69 |
| 4:M8:61:ASN:OD1 | 4:M8:62:LYS:CG | 2.40 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:Z8:38:GLU:H | 12:Z8:301:CYC:HMB2 | 1.58 | 0.69 |
| 11:a9:32:ARG:HG3 | 11:a9:32:ARG:NH1 | 2.06 | 0.69 |
| 11:a9:732:SER:CB | 11:a9:824:VAL:HG21 | 2.23 | 0.69 |
| 11:aA:817:LEU:HD11 | 3:L1:120:LEU:HA | 1.75 | 0.69 |
| 4:M1:94:TRP:CH2 | 5:N1:29:HIS:CE1 | 2.81 | 0.69 |
| 1:Z:13:ASP:OD1 | 8:e5:107:ILE:HD13 | 1.93 | 0.69 |
| 3:LA:107:ASP:O | 3:LA:111:ASN:ND2 | 2.23 | 0.69 |
| 5:NA:14:LYS:CE | 5:NA:50:LEU:HD23 | 2.23 | 0.69 |
| 2:OA:63:PHE:O | 2:OA:66:LEU:CG | 2.39 | 0.69 |
| 2:QA:68:GLN:CB | 2:QA:69:PRO:CD | 2.71 | 0.69 |
| 2:QA:68:GLN:CG | 2:QA:69:PRO:HD3 | 2.22 | 0.69 |
| 2:O1:60:TYR:CE2 | 2:O1:79:GLN:NE2 | 2.61 | 0.69 |
| 3:H3:78:ARG:NH1 | 11:a9:623:ASP:HA | 2.06 | 0.69 |
| 3:H3:84:ARG:HD2 | 11:a9:776:TYR:CE1 | 2.27 | 0.69 |
| 3:L3:119:ALA:HB1 | 11:a9:813:PRO:O | 1.92 | 0.69 |
| 4:M3:94:TRP:CH2 | 5:N3:29:HIS:CE1 | 2.81 | 0.69 |
| 2:O3:60:TYR:CE2 | 2:O3:79:GLN:NE2 | 2.61 | 0.69 |
| 8:M5:21:GLY:H | 8:A5:6:LYS:HZ3 | 1.40 | 0.69 |
| 8:C5:91:LEU:HB3 | 8:C5:104:ILE:HG23 | 1.73 | 0.69 |
| 1:T5:53:LYS:CE | 8:U5:120:GLN:HE21 | 2.01 | 0.69 |
| 6:M6:115:TYR:OH | 3:H6:88:ILE:HD11 | 1.91 | 0.69 |
| 6:M6:127:SER:HA | 12:F6:201:CYC:O2A | 1.92 | 0.69 |
| 10:k5:725:LEU:HD23 | 10:k5:725:LEU:O | 1.91 | 0.69 |
| 10:k5:1143:LEU:CD2 | 1:l7:10:ASN:OD1 | 2.41 | 0.69 |
| 8:O7:91:LEU:HB3 | 8:O7:104:ILE:HG23 | 1.73 | 0.69 |
| 12:h7:201:CYC:HBB2 | 9:y7:21:ARG:NE | 2.05 | 0.69 |
| 8:c7:131:ARG:HH11 | 8:c7:131:ARG:HG2 | 1.57 | 0.69 |
| 12:B8:202:CYC:CBB | 4:M8:61:ASN:HD22 | 2.04 | 0.69 |
| 8:o7:37:LEU:HD11 | 1:p7:24:LEU:O | 1.92 | 0.69 |
| 8:s7:44:THR:HG1 | 1:t7:18:TYR:HD2 | 1.40 | 0.69 |
| 2:X8:68:GLN:CD | 3:T9:24:LEU:O | 2.36 | 0.69 |
| 2:N8:115:GLU:OE1 | 5:Z8:31:TRP:HB3 | 1.93 | 0.69 |
| 5:N9:1:MET:HB3 | 5:N9:3:VAL:CG2 | 2.15 | 0.69 |
| 5:N9:50:LEU:HD22 | 12:T9:301:CYC:O1D | 1.93 | 0.69 |
| 11:a9:30:MET:HE3 | 11:a9:35:ARG:HD3 | 1.72 | 0.69 |
| 11:aA:670:LEU:HD21 | 2:K1:112:GLY:HA3 | 1.74 | 0.69 |
| 4:M1:71:PRO:HG2 | 4:M1:74:LEU:HB2 | 1.75 | 0.69 |
| 3:JA:108:ARG:NH2 | 11:aA:515:GLY:O | 2.25 | 0.69 |
| 3:LA:77:ARG:NH1 | 11:aA:538:ARG:NH2 | 2.41 | 0.69 |
| 4:MA:185:ALA:CB | 12:VA:201:CYC:O1A | 2.40 | 0.69 |
| 5:NA:23:SER:O | 5:NA:25:THR:N | 2.26 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:OA:38:MET:HE1 | 3:PA:28:THR:OG1 | 1.93 | 0.69 |
| 2:A1:60:TYR:CE2 | 2:A1:79:GLN:NE2 | 2.61 | 0.69 |
| 2:A1:63:PHE:O | 2:A1:66:LEU:CG | 2.39 | 0.69 |
| 3:B4:68:ARG:HH12 | 3:U4:68:ARG:NH2 | 1.88 | 0.69 |
| 2:E4:1:MET:H2 | 4:M4:10:ARG:CZ | 2.06 | 0.69 |
| 4:M4:27:HIS:CE1 | 4:M4:34:ASP:N | 2.59 | 0.69 |
| 4:M4:27:HIS:CD2 | 4:M4:34:ASP:CG | 2.71 | 0.69 |
| 4:M4:228:SER:HA | 3:Y4:91:ARG:HH21 | 1.58 | 0.69 |
| 3:Q4:85:ASP:CB | 3:Q4:88:ILE:HD12 | 2.21 | 0.69 |
| 8:K5:17:TYR:CB | 1:L5:45:SER:HB3 | 2.23 | 0.69 |
| 8:M5:90:ARG:HD3 | 1:N5:18:TYR:CD1 | 2.27 | 0.69 |
| 3:Y4:89:ILE:HG12 | 3:Y4:92:TYR:OH | 1.92 | 0.69 |
| 8:e5:91:LEU:HB3 | 8:e5:104:ILE:HG23 | 1.73 | 0.69 |
| 8:Q5:17:TYR:CD2 | 1:R5:93:THR:HG21 | 2.22 | 0.69 |
| 8:Q5:47:ARG:HD3 | 1:R5:18:TYR:OH | 1.93 | 0.69 |
| 12:Q5:201:CYC:HMD1 | 12:Q5:201:CYC:NC | 2.02 | 0.69 |
| 8:S5:89:LEU:HB3 | 1:T5:18:TYR:OH | 1.93 | 0.69 |
| 8:W5:159:ALA:O | 8:W5:160:MET:C | 2.34 | 0.69 |
| 8:a5:29:PHE:HE1 | 8:a5:98:ALA:C | 2.01 | 0.69 |
| 10:j5:246:VAL:HG22 | 10:j5:257:THR:CG2 | 2.21 | 0.69 |
| 10:j5:826:THR:HG21 | 12:H7:201:CYC:HMA2 | 1.75 | 0.69 |
| 10:j5:1016:LEU:HB2 | 10:j5:1044:ASN:HD22 | 1.58 | 0.69 |
| 2:A6:38:MET:HE1 | 3:B6:28:THR:OG1 | 1.93 | 0.69 |
| 8:O7:21:GLY:O | 8:O7:24:ASP:N | 2.25 | 0.69 |
| 8:Q7:12:ASP:C | 9:z7:46:LYS:HE2 | 2.17 | 0.69 |
| 8:Q7:13:ALA:HA | 9:z7:46:LYS:HZ2 | 1.52 | 0.69 |
| 8:Q7:13:ALA:C | 9:z7:46:LYS:NZ | 2.50 | 0.69 |
| 8:S7:49:ARG:HD2 | 11:aA:550:PHE:HE1 | 1.48 | 0.69 |
| 8:i7:50:ILE:HD13 | 8:i7:137:ALA:HB2 | 1.73 | 0.69 |
| 8:a7:91:LEU:HB3 | 8:a7:104:ILE:HG23 | 1.73 | 0.69 |
| 8:c7:11:ALA:CB | 1:d7:94:TYR:OH | 2.41 | 0.69 |
| 8:o7:30:VAL:HB | 1:p7:31:PHE:C | 2.18 | 0.69 |
| 3:U8:108:ARG:HB3 | 4:M8:246:ALA:HB2 | 1.69 | 0.69 |
| 4:M8:92:GLU:OE2 | 4:M8:217:VAL:CG2 | 2.38 | 0.69 |
| 4:M8:127:SER:CB | 12:M8:302:CYC:HMA1 | 1.97 | 0.69 |
| 4:M8:160:THR:HG21 | 4:M8:257:GLN:HB3 | 1.72 | 0.69 |
| 3:L9:52:ILE:HD11 | 3:L9:87:GLU:HG2 | 1.71 | 0.69 |
| 3:L9:107:ASP:O | 3:L9:111:ASN:ND2 | 2.23 | 0.69 |
| 5:Z8:14:LYS:CE | 5:Z8:50:LEU:HD23 | 2.23 | 0.69 |
| 3:J9:120:LEU:O | 11:a9:361:ALA:HB1 | 1.91 | 0.69 |
| 11:aA:32:ARG:HG3 | 11:aA:32:ARG:NH1 | 2.06 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:aA:642:GLU:HB2 | 11:aA:766:ASN:O | 1.93 | 0.69 |
| 11:aA:707:PHE:HZ | 2:K1:13:ASP:CG | 1.99 | 0.69 |
| 4:M1:19:MET:HE2 | 4:M1:59:ILE:HD11 | 1.75 | 0.69 |
| 4:M1:205:ASP:OD2 | 5:N1:52:ARG:CZ | 2.40 | 0.69 |
| 2:AA:38:MET:HE1 | 3:BA:28:THR:OG1 | 1.93 | 0.69 |
| 3:DA:115:GLU:OE2 | 4:MA:78:GLY:CA | 2.40 | 0.69 |
| 4:MA:71:PRO:HG2 | 4:MA:74:LEU:HB2 | 1.75 | 0.69 |
| 5:NA:22:LEU:HD11 | 5:NA:26:LEU:HD21 | 1.71 | 0.69 |
| 12:QA:201:CYC:HBB2 | 3:TA:75:PRO:HB2 | 1.60 | 0.69 |
| 3:TA:24:LEU:O | 2:X4:68:GLN:OE1 | 2.10 | 0.69 |
| 3:TA:24:LEU:O | 2:X4:68:GLN:CD | 2.36 | 0.69 |
| 2:E4:15:GLN:HG2 | 11:aA:163:ASP:CB | 2.15 | 0.69 |
| 2:N4:60:TYR:CE2 | 2:N4:79:GLN:NE2 | 2.61 | 0.69 |
| 1:D5:62:TYR:CE1 | 12:E5:201:CYC:O1D | 2.46 | 0.69 |
| 12:Z5:201:CYC:O2A | 10:k5:379:PHE:HD2 | 1.73 | 0.69 |
| 10:j5:175:ASP:HB2 | 10:j5:176:PRO:CG | 2.18 | 0.69 |
| 12:H6:202:CYC:HC | 12:H6:202:CYC:CMD | 1.99 | 0.69 |
| 8:Q7:12:ASP:O | 9:z7:46:LYS:CE | 2.41 | 0.69 |
| 8:C7:29:PHE:HE1 | 8:C7:98:ALA:O | 1.68 | 0.69 |
| 3:B8:120:LEU:HD12 | 4:M8:53:LEU:HB2 | 1.69 | 0.69 |
| 12:H8:201:CYC:HMA1 | 11:a9:261:SER:CB | 2.23 | 0.69 |
| 5:N9:54:LEU:CA | 12:T9:301:CYC:HBA1 | 2.22 | 0.69 |
| 5:Z8:23:SER:O | 5:Z8:25:THR:N | 2.26 | 0.69 |
| 2:A9:60:TYR:CE2 | 2:A9:79:GLN:NE2 | 2.61 | 0.69 |
| 3:D9:14:LEU:CD1 | 3:Z9:125:ARG:HD2 | 2.22 | 0.69 |
| 11:aA:795:ASP:O | 12:aA:901:CYC:HBB2 | 1.92 | 0.69 |
| 2:AA:33:ARG:NE | 2:KA:28:ASN:HD21 | 1.91 | 0.69 |
| 3:HA:113:LEU:CD1 | 12:HA:202:CYC:C2B | 2.71 | 0.69 |
| 5:NA:31:TRP:HB3 | 5:NA:32:PRO:CD | 2.23 | 0.69 |
| 2:QA:68:GLN:HB3 | 2:QA:69:PRO:CD | 2.23 | 0.69 |
| 12:P1:201:CYC:HBA1 | 4:M1:130:SER:O | 1.93 | 0.69 |
| 3:J3:84:ARG:O | 11:a9:668:TYR:OH | 1.97 | 0.69 |
| 3:L3:1:MET:CE | 11:a9:708:HIS:CE1 | 2.76 | 0.69 |
| 4:M3:130:SER:O | 12:P3:201:CYC:HBA1 | 1.93 | 0.69 |
| 3:F4:112:GLY:O | 3:F4:114:LYS:N | 2.21 | 0.69 |
| 8:S5:41:GLN:NE2 | 1:D7:143:PRO:HD3 | 2.08 | 0.69 |
| 1:Z5:110:ASN:HD22 | 10:k5:451:LYS:HB3 | 1.56 | 0.69 |
| 3:J6:108:ARG:NH2 | 6:M6:155:ASN:CG | 2.51 | 0.69 |
| 6:M6:193:TYR:HB3 | 2:I6:14:SER:O | 1.92 | 0.69 |
| 10:j5:974:LEU:HD12 | 1:v7:106:GLU:CD | 2.17 | 0.69 |
| 10:k5:938:GLN:OE1 | 1:D7:28:LYS:HD3 | 1.90 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:o7:37:LEU:CD1 | 1:p7:28:LYS:HE3 | 2.22 | 0.69 |
| 3:Y8:89:ILE:HG12 | 3:Y8:92:TYR:OH | 1.92 | 0.69 |
| 2:A2:63:PHE:O | 2:A2:66:LEU:CG | 2.38 | 0.69 |
| 1:A:73:TYR:CZ | 10:k5:162:TRP:HZ2 | 2.05 | 0.68 |
| 2:AA:60:TYR:CE2 | 2:AA:79:GLN:NE2 | 2.61 | 0.68 |
| 2:IA:97:LEU:HD13 | 2:IA:97:LEU:C | 2.18 | 0.68 |
| 4:MA:134:ASN:CG | 5:NA:1:MET:N | 2.50 | 0.68 |
| 2:O1:38:MET:HE1 | 3:P1:28:THR:OG1 | 1.93 | 0.68 |
| 2:A1:38:MET:HE1 | 3:B1:28:THR:OG1 | 1.93 | 0.68 |
| 2:A3:38:MET:HE1 | 3:B3:28:THR:OG1 | 1.93 | 0.68 |
| 3:B3:120:LEU:HD13 | 12:B3:202:CYC:HBD1 | 1.75 | 0.68 |
| 4:M3:160:THR:HG22 | 4:M3:257:GLN:HB3 | 1.73 | 0.68 |
| 3:U4:120:LEU:O | 3:U4:120:LEU:HD23 | 1.93 | 0.68 |
| 4:M4:92:GLU:OE2 | 5:Z4:30:PRO:HB3 | 1.82 | 0.68 |
| 4:M4:104:ALA:HB2 | 2:P4:10:ALA:O | 1.94 | 0.68 |
| 3:Q4:93:VAL:HG13 | 3:Q4:163:TYR:HB2 | 1.75 | 0.68 |
| 5:Z4:14:LYS:HD3 | 5:Z4:14:LYS:H | 1.57 | 0.68 |
| 1:F5:69:GLY:C | 10:k5:554:ASN:HD22 | 2.01 | 0.68 |
| 8:e5:91:LEU:O | 8:e5:104:ILE:HD11 | 1.93 | 0.68 |
| 8:S5:68:PRO:CB | 8:a5:59:PHE:HB3 | 2.21 | 0.68 |
| 8:a5:102:THR:CB | 8:a5:103:PRO:CD | 2.64 | 0.68 |
| 10:j5:990:ARG:HH21 | 10:j5:1026:LYS:HZ2 | 1.40 | 0.68 |
| 10:k5:774:GLN:HA | 10:k5:774:GLN:NE2 | 2.07 | 0.68 |
| 1:j7:87:TYR:HE2 | 9:y7:38:PHE:CE1 | 2.11 | 0.68 |
| 12:H8:201:CYC:HBB3 | 11:a9:259:ALA:CA | 2.21 | 0.68 |
| 12:L8:201:CYC:HC | 12:L8:201:CYC:CMD | 1.99 | 0.68 |
| 4:M9:222:ARG:HG3 | 4:M9:222:ARG:NH1 | 2.01 | 0.68 |
| 2:O9:60:TYR:CE2 | 2:O9:79:GLN:NE2 | 2.61 | 0.68 |
| 5:Z8:38:GLU:CB | 12:Z8:301:CYC:HMB3 | 2.01 | 0.68 |
| 2:A9:33:ARG:NE | 2:K9:28:ASN:HD21 | 1.91 | 0.68 |
| 11:a9:376:ALA:CB | 11:a9:504:VAL:O | 2.42 | 0.68 |
| 11:aA:376:ALA:CB | 11:aA:504:VAL:O | 2.42 | 0.68 |
| 5:N1:23:SER:O | 5:N1:25:THR:N | 2.26 | 0.68 |
| 1:A:13:ASP:CG | 8:a5:107:ILE:HD13 | 2.18 | 0.68 |
| 1:Z:127:VAL:HG11 | 1:X5:15:GLN:CD | 2.19 | 0.68 |
| 3:DA:14:LEU:CD1 | 3:ZA:125:ARG:HD2 | 2.22 | 0.68 |
| 3:JA:120:LEU:O | 11:aA:361:ALA:HB1 | 1.92 | 0.68 |
| 2:O1:33:ARG:NE | 2:Y1:28:ASN:HD21 | 1.91 | 0.68 |
| 2:A1:33:ARG:NE | 2:K1:28:ASN:HD21 | 1.91 | 0.68 |
| 2:K2:28:ASN:HD21 | 2:A2:33:ARG:NE | 1.91 | 0.68 |
| 2:A4:38:MET:HE1 | 3:B4:28:THR:OG1 | 1.93 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:B4:120:LEU:CD2 | 4:M4:49:LEU:O | 2.40 | 0.68 |
| 4:M3:19:MET:HE2 | 4:M3:59:ILE:HD11 | 1.75 | 0.68 |
| 5:N3:31:TRP:NE1 | 2:S3:13:ASP:O | 2.23 | 0.68 |
| 12:H4:201:CYC:CBB | 11:aA:259:ALA:CA | 2.70 | 0.68 |
| 8:O5:91:LEU:O | 8:O5:104:ILE:HD11 | 1.94 | 0.68 |
| 3:Y4:2:GLN:HB2 | 3:Y4:103:SER:CB | 2.23 | 0.68 |
| 5:Z4:14:LYS:CE | 5:Z4:50:LEU:HD23 | 2.23 | 0.68 |
| 5:Z4:29:HIS:HB3 | 5:Z4:31:TRP:HD1 | 1.57 | 0.68 |
| 8:G5:126:VAL:HA | 12:G5:201:CYC:CBC | 2.23 | 0.68 |
| 8:Q5:63:PRO:O | 8:Q5:65:VAL:N | 2.26 | 0.68 |
| 2:A6:60:TYR:CE2 | 2:A6:79:GLN:NE2 | 2.61 | 0.68 |
| 12:B6:201:CYC:HC | 12:B6:201:CYC:CMD | 1.99 | 0.68 |
| 12:i7:201:CYC:HB | 12:i7:201:CYC:HMA3 | 1.59 | 0.68 |
| 1:b7:37:ARG:NH1 | 1:b7:96:MET:O | 2.26 | 0.68 |
| 8:c7:50:ILE:CG1 | 8:c7:137:ALA:HB2 | 2.24 | 0.68 |
| 2:A8:33:ARG:NE | 2:K8:28:ASN:HD21 | 1.91 | 0.68 |
| 8:m7:91:LEU:O | 8:m7:104:ILE:HD11 | 1.94 | 0.68 |
| 8:q7:75:GLU:HB3 | 11:aA:53:VAL:CG1 | 2.23 | 0.68 |
| 8:u7:63:PRO:O | 8:u7:65:VAL:N | 2.27 | 0.68 |
| 2:N8:60:TYR:CE2 | 2:N8:79:GLN:NE2 | 2.61 | 0.68 |
| 3:O8:104:VAL:CG2 | 5:Z8:61:LYS:CE | 2.67 | 0.68 |
| 4:M9:1:MET:CB | 11:a9:422:SER:O | 2.40 | 0.68 |
| 11:a9:30:MET:HE3 | 11:a9:35:ARG:HA | 1.76 | 0.68 |
| 11:a9:308:LEU:O | 11:a9:308:LEU:HD23 | 1.92 | 0.68 |
| 11:a9:376:ALA:HB1 | 11:a9:504:VAL:HB | 1.73 | 0.68 |
| 11:aA:249:GLU:C | 11:aA:285:VAL:CG2 | 2.66 | 0.68 |
| 11:aA:643:LEU:CD1 | 11:aA:766:ASN:CB | 2.71 | 0.68 |
| 11:aA:671:GLU:HG3 | 2:K1:115:GLU:OE2 | 1.93 | 0.68 |
| 4:M1:260:ARG:NH1 | 4:M1:260:ARG:HG3 | 2.09 | 0.68 |
| 12:JA:202:CYC:HBA1 | 11:aA:511:LYS:C | 2.18 | 0.68 |
| 4:MA:19:MET:HE2 | 4:MA:59:ILE:HD11 | 1.75 | 0.68 |
| 5:NA:14:LYS:HD3 | 5:NA:14:LYS:H | 1.57 | 0.68 |
| 3:B3:84:ARG:CZ | 11:a9:680:SER:HB3 | 2.22 | 0.68 |
| 4:M3:71:PRO:HG2 | 4:M3:74:LEU:HB2 | 1.75 | 0.68 |
| 2:U3:142:LEU:O | 2:Q9:76:ASP:OD2 | 2.00 | 0.68 |
| 4:M4:128:ALA:HB3 | 4:M4:142:PHE:CZ | 2.28 | 0.68 |
| 3:Q4:72:ASN:O | 12:Z4:301:CYC:HMD3 | 1.91 | 0.68 |
| 8:O5:75:GLU:OE2 | 8:i7:56:ASP:OD2 | 2.12 | 0.68 |
| 8:G5:100:ASP:OD2 | 8:S5:20:PRO:CB | 2.35 | 0.68 |
| 8:I5:91:LEU:O | 8:I5:104:ILE:HD11 | 1.93 | 0.68 |
| 1:J5:39:ARG:O | 1:J5:42:ALA:N | 2.24 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:j5:1008:PHE:CE1 | 12:v7:201:CYC:HBB3 | 2.28 | 0.68 |
| 10:j5:1069:ARG:NH1 | 10:j5:1069:ARG:HG3 | 2.07 | 0.68 |
| 10:j5:1089:LEU:HD22 | 10:j5:1089:LEU:O | 1.94 | 0.68 |
| 1:P7:53:LYS:NZ | 8:Q7:120:GLN:OE1 | 2.26 | 0.68 |
| 1:D7:53:LYS:NZ | 8:E7:120:GLN:OE1 | 2.26 | 0.68 |
| 8:E7:63:PRO:O | 8:E7:65:VAL:N | 2.27 | 0.68 |
| 12:E7:201:CYC:HMD1 | 12:E7:201:CYC:NC | 2.02 | 0.68 |
| 8:g7:91:LEU:O | 8:g7:104:ILE:HD11 | 1.93 | 0.68 |
| 8:i7:96:ILE:HG13 | 8:i7:152:TYR:CB | 2.23 | 0.68 |
| 8:W7:63:PRO:O | 8:W7:65:VAL:N | 2.27 | 0.68 |
| 8:a7:90:ARG:HA | 1:b7:18:TYR:CE2 | 2.29 | 0.68 |
| 8:a7:91:LEU:O | 8:a7:104:ILE:HD11 | 1.94 | 0.68 |
| 8:c7:23:LEU:HD13 | 1:d7:42:ALA:HB2 | 1.75 | 0.68 |
| 3:B8:120:LEU:HD23 | 4:M8:49:LEU:HD12 | 1.73 | 0.68 |
| 8:o7:34:GLU:HA | 1:p7:28:LYS:HE2 | 1.75 | 0.68 |
| 4:M8:127:SER:H | 12:M8:302:CYC:HMA2 | 1.56 | 0.68 |
| 3:Q8:120:LEU:HD12 | 3:Q8:120:LEU:C | 2.19 | 0.68 |
| 3:L9:108:ARG:HA | 11:a9:531:ASP:HB2 | 1.75 | 0.68 |
| 12:L9:201:CYC:HC | 12:L9:201:CYC:CMD | 1.98 | 0.68 |
| 4:M9:185:ALA:CB | 12:V9:201:CYC:O1A | 2.40 | 0.68 |
| 2:S9:42:ARG:NH2 | 3:T9:24:LEU:HB3 | 2.07 | 0.68 |
| 11:a9:714:ARG:CG | 11:a9:808:LEU:O | 2.42 | 0.68 |
| 11:aA:360:ALA:O | 11:aA:364:THR:HG23 | 1.93 | 0.68 |
| 11:aA:714:ARG:CG | 11:aA:808:LEU:O | 2.42 | 0.68 |
| 11:aA:742:GLN:OE1 | 3:L1:88:ILE:HG12 | 1.90 | 0.68 |
| 2:IA:1:MET:HE2 | 2:IA:108:TYR:HE1 | 1.57 | 0.68 |
| 3:LA:90:LEU:HD23 | 3:LA:90:LEU:C | 2.18 | 0.68 |
| 5:NA:1:MET:HG3 | 3:RA:119:ALA:CB | 1.90 | 0.68 |
| 5:NA:7:ASP:N | 3:RA:108:ARG:HA | 2.09 | 0.68 |
| 5:NA:61:LYS:HD3 | 3:TA:108:ARG:C | 2.14 | 0.68 |
| 3:L3:84:ARG:NH1 | 11:a9:739:ASP:HB2 | 2.08 | 0.68 |
| 5:N3:14:LYS:CE | 5:N3:50:LEU:HD23 | 2.23 | 0.68 |
| 2:U3:141:GLN:C | 2:Q9:76:ASP:N | 2.51 | 0.68 |
| 12:M4:301:CYC:HMB1 | 3:Y4:89:ILE:HD11 | 1.76 | 0.68 |
| 8:I5:110:ILE:HD12 | 9:i5:15:LYS:CB | 2.24 | 0.68 |
| 8:c5:120:GLN:HG3 | 1:f5:53:LYS:NZ | 2.09 | 0.68 |
| 8:U5:91:LEU:O | 8:U5:104:ILE:HD11 | 1.94 | 0.68 |
| 10:j5:844:GLN:NE2 | 10:j5:916:PHE:H | 1.91 | 0.68 |
| 10:k5:1089:LEU:HD22 | 10:k5:1089:LEU:O | 1.93 | 0.68 |
| 3:F6:126:SER:CB | 12:F6:201:CYC:HMC1 | 2.23 | 0.68 |
| 8:K7:63:PRO:O | 8:K7:65:VAL:N | 2.27 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:B8:120:LEU:CD2 | 4:M8:52:LEU:HB3 | 2.22 | 0.68 |
| 9:x7:3:ARG:CZ | 9:x7:67:VAL:HG12 | 2.15 | 0.68 |
| 12:Q8:201:CYC:HC | 12:Q8:201:CYC:CMD | 1.99 | 0.68 |
| 3:Y8:87:GLU:O | 3:Y8:91:ARG:HG3 | 1.94 | 0.68 |
| 5:Z8:39:PRO:HA | 12:Z8:301:CYC:NA | 2.09 | 0.68 |
| 2:A9:38:MET:HE1 | 3:B9:28:THR:OG1 | 1.93 | 0.68 |
| 12:T9:302:CYC:HC | 12:T9:302:CYC:CMD | 1.98 | 0.68 |
| 11:a9:360:ALA:O | 11:a9:364:THR:HG23 | 1.93 | 0.68 |
| 11:aA:415:GLU:CD | 11:aA:415:GLU:H | 2.00 | 0.68 |
| 3:LA:111:ASN:O | 11:aA:532:ALA:HB2 | 1.91 | 0.68 |
| 4:MA:273:ILE:CD1 | 3:VA:75:PRO:HD2 | 2.20 | 0.68 |
| 3:H2:120:LEU:O | 6:M2:251:LYS:NZ | 2.27 | 0.68 |
| 6:M2:34:ARG:CG | 8:O5:52:LYS:HD2 | 2.23 | 0.68 |
| 3:B4:112:GLY:C | 3:B4:114:LYS:H | 2.02 | 0.68 |
| 3:F4:109:CYS:O | 4:M4:6:THR:HG23 | 1.93 | 0.68 |
| 1:N5:107:ARG:NH1 | 10:k5:482:GLN:OE1 | 2.27 | 0.68 |
| 12:I5:201:CYC:HB | 12:I5:201:CYC:HMA3 | 1.59 | 0.68 |
| 12:d5:201:CYC:NB | 10:j5:379:PHE:CZ | 2.60 | 0.68 |
| 1:T5:53:LYS:NZ | 8:U5:120:GLN:CD | 2.30 | 0.68 |
| 8:U5:29:PHE:HE1 | 8:U5:98:ALA:C | 2.01 | 0.68 |
| 6:M6:251:LYS:NZ | 3:H6:120:LEU:O | 2.27 | 0.68 |
| 8:A7:120:GLN:HG3 | 1:F7:53:LYS:NZ | 2.09 | 0.68 |
| 9:i5:56:LEU:HD12 | 9:i5:56:LEU:N | 2.08 | 0.68 |
| 10:j5:631:HIS:CB | 10:j5:664:MET:HE1 | 2.22 | 0.68 |
| 10:k5:743:VAL:HG13 | 12:D7:201:CYC:CGD | 2.24 | 0.68 |
| 10:k5:964:GLY:C | 1:n7:69:GLY:HA2 | 2.16 | 0.68 |
| 12:D1:201:CYC:HC | 12:D1:201:CYC:CMD | 1.99 | 0.68 |
| 8:Q7:63:PRO:O | 8:Q7:65:VAL:N | 2.26 | 0.68 |
| 3:B8:82:CYS:HB2 | 12:B8:202:CYC:OC | 1.94 | 0.68 |
| 12:B8:202:CYC:CHA | 4:M8:54:ALA:HB2 | 2.24 | 0.68 |
| 9:y7:9:ALA:HB1 | 9:y7:44:ILE:HD13 | 1.75 | 0.68 |
| 4:M8:198:ALA:HB2 | 5:Z8:55:PRO:HG2 | 1.74 | 0.68 |
| 4:M8:230:GLN:CG | 12:M8:301:CYC:OB | 2.40 | 0.68 |
| 4:M8:260:ARG:NH1 | 4:M8:260:ARG:HG3 | 2.09 | 0.68 |
| 12:M8:301:CYC:HAB2 | 3:Y8:92:TYR:CD2 | 2.28 | 0.68 |
| 2:N8:63:PHE:HB2 | 2:N8:66:LEU:HD12 | 1.70 | 0.68 |
| 12:S8:201:CYC:HC | 12:S8:201:CYC:CMD | 1.98 | 0.68 |
| 3:L9:84:ARG:NH2 | 11:a9:406:LEU:HA | 2.08 | 0.68 |
| 3:L9:90:LEU:HD23 | 3:L9:90:LEU:C | 2.19 | 0.68 |
| 2:I9:97:LEU:HD13 | 2:I9:97:LEU:C | 2.18 | 0.68 |
| 11:a9:598:SER:HB3 | 11:a9:599:PRO:CD | 2.24 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:a9:642:GLU:HB2 | 11:a9:766:ASN:O | 1.93 | 0.68 |
| 3:FA:150:ARG:CD | 3:F9:150:ARG:CG | 2.56 | 0.68 |
| 2:QA:68:GLN:HG3 | 2:QA:69:PRO:HD3 | 1.74 | 0.68 |
| 12:QA:201:CYC:HBA1 | 3:TA:67:ILE:CG2 | 2.23 | 0.68 |
| 12:F3:201:CYC:HBA2 | 4:M3:36:TYR:CE2 | 2.29 | 0.68 |
| 5:N3:34:LEU:HB3 | 3:T3:84:ARG:NH1 | 2.08 | 0.68 |
| 3:L4:71:GLY:HA2 | 11:aA:82:GLN:HG2 | 1.72 | 0.68 |
| 4:M4:214:GLY:HA3 | 5:Z4:28:HIS:CG | 2.28 | 0.68 |
| 12:K5:201:CYC:O1D | 1:J5:62:TYR:CE1 | 2.46 | 0.68 |
| 8:A5:126:VAL:HA | 12:A5:201:CYC:CBC | 2.23 | 0.68 |
| 9:i5:14:LEU:CD1 | 9:i5:15:LYS:N | 2.54 | 0.68 |
| 10:j5:820:HIS:HD1 | 10:j5:859:ILE:HD12 | 1.45 | 0.68 |
| 10:j5:931:VAL:CG1 | 1:J7:29:ALA:HB1 | 2.17 | 0.68 |
| 10:j5:931:VAL:HG23 | 1:J7:30:TYR:HA | 1.75 | 0.68 |
| 10:k5:501:ILE:HD12 | 10:k5:501:ILE:N | 2.06 | 0.68 |
| 10:k5:1052:PRO:HA | 1:l7:106:GLU:OE2 | 1.92 | 0.68 |
| 8:i7:25:ARG:NH1 | 8:s7:7:ALA:N | 2.40 | 0.68 |
| 8:i7:47:ARG:CD | 1:j7:18:TYR:CD1 | 2.77 | 0.68 |
| 8:i7:90:ARG:HH12 | 1:j7:13:ASP:CG | 2.00 | 0.68 |
| 1:V7:53:LYS:NZ | 8:W7:120:GLN:OE1 | 2.26 | 0.68 |
| 8:a7:29:PHE:HE1 | 8:a7:98:ALA:C | 2.02 | 0.68 |
| 8:c7:63:PRO:O | 8:c7:65:VAL:N | 2.27 | 0.68 |
| 3:B8:92:TYR:OH | 12:B8:202:CYC:HAB2 | 1.94 | 0.68 |
| 3:D8:116:THR:OG1 | 4:M8:38:PRO:CA | 2.42 | 0.68 |
| 4:M8:91:VAL:HG22 | 2:P8:15:GLN:HA | 1.75 | 0.68 |
| 4:M8:104:ALA:CA | 2:P8:14:SER:CB | 2.43 | 0.68 |
| 4:M9:71:PRO:HG2 | 4:M9:74:LEU:HB2 | 1.75 | 0.68 |
| 5:N9:14:LYS:HD3 | 5:N9:14:LYS:H | 1.57 | 0.68 |
| 5:Z8:37:HIS:CE1 | 12:Z8:301:CYC:NB | 2.56 | 0.68 |
| 5:Z8:41:GLN:C | 12:Z8:301:CYC:CMA | 2.66 | 0.68 |
| 11:aA:439:ARG:HG3 | 11:aA:439:ARG:NH1 | 2.08 | 0.68 |
| 11:aA:586:LEU:HD22 | 11:aA:586:LEU:N | 2.05 | 0.68 |
| 11:aA:823:ILE:HD11 | 3:L1:75:PRO:HG2 | 1.74 | 0.68 |
| 1:Z:158:SER:HB3 | 1:X5:11:ASN:CG | 2.12 | 0.68 |
| 2:OA:60:TYR:CE2 | 2:OA:79:GLN:NE2 | 2.61 | 0.68 |
| 3:J2:108:ARG:NH2 | 6:M2:155:ASN:CG | 2.51 | 0.68 |
| 12:K5:201:CYC:HB | 12:K5:201:CYC:HMA3 | 1.58 | 0.68 |
| 8:O5:24:ASP:O | 8:O5:27:LYS:N | 2.26 | 0.68 |
| 8:G5:25:ARG:HH21 | 8:S5:25:ARG:CB | 2.04 | 0.68 |
| 1:d5:67:ARG:HH12 | 10:j5:705:THR:CB | 2.07 | 0.68 |
| 12:a5:201:CYC:HB | 12:a5:201:CYC:HMA3 | 1.59 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:586:LEU:HD12 | 10:j5:607:LEU:CD2 | 2.23 | 0.68 |
| 10:j5:878:GLU:HG3 | 9:w7:28:PHE:CE2 | 2.27 | 0.68 |
| 8:O7:29:PHE:HE1 | 8:O7:98:ALA:C | 2.01 | 0.68 |
| 8:i7:94:TYR:CD1 | 1:j7:9:ILE:HG23 | 2.29 | 0.68 |
| 3:B8:119:ALA:O | 4:M8:15:PHE:CE2 | 2.47 | 0.68 |
| 8:s7:91:LEU:O | 8:s7:104:ILE:HD11 | 1.94 | 0.68 |
| 9:x7:3:ARG:HG2 | 9:x7:59:GLY:HA3 | 1.76 | 0.68 |
| 2:X8:28:ASN:HD21 | 2:N8:33:ARG:NE | 1.91 | 0.68 |
| 3:H9:72:ASN:ND2 | 12:H9:202:CYC:HBD2 | 2.09 | 0.68 |
| 2:I9:9:ILE:HD11 | 3:J9:99:ALA:HB2 | 1.74 | 0.68 |
| 2:A2:63:PHE:HB2 | 2:A2:66:LEU:HD12 | 1.70 | 0.68 |
| 3:F2:127:VAL:HG22 | 12:F2:201:CYC:H3C | 1.74 | 0.68 |
| 3:LA:93:VAL:HG11 | 3:LA:164:PHE:CE2 | 2.29 | 0.68 |
| 4:MA:267:LEU:CD1 | 3:VA:119:ALA:O | 2.40 | 0.68 |
| 2:O1:65:TYR:CE1 | 2:U1:65:TYR:CE1 | 2.82 | 0.68 |
| 3:L2:65:ASP:OD2 | 1:h7:64:ASP:CB | 2.42 | 0.68 |
| 6:M2:39:ARG:HH11 | 8:O5:59:PHE:HD2 | 1.40 | 0.68 |
| 3:H4:84:ARG:CD | 11:aA:131:TYR:CB | 2.71 | 0.68 |
| 4:M4:86:ALA:HB3 | 3:Y4:77:ARG:HD2 | 1.75 | 0.68 |
| 4:M4:160:THR:HG22 | 4:M4:257:GLN:HB3 | 1.73 | 0.68 |
| 2:N4:38:MET:HE1 | 3:O4:28:THR:OG1 | 1.93 | 0.68 |
| 1:L5:75:THR:HB | 8:G5:112:VAL:CA | 2.23 | 0.68 |
| 12:L5:201:CYC:HBA1 | 10:j5:591:ILE:HG23 | 1.75 | 0.68 |
| 12:B5:201:CYC:HBB2 | 9:z5:21:ARG:CG | 2.23 | 0.68 |
| 8:G5:71:ASN:OD1 | 12:G5:201:CYC:C2D | 2.41 | 0.68 |
| 8:Q5:23:LEU:CD1 | 1:R5:42:ALA:HB2 | 2.24 | 0.68 |
| 1:T5:87:TYR:OH | 10:j5:483:PHE:CE2 | 2.45 | 0.68 |
| 8:U5:75:GLU:CG | 6:M6:36:ILE:CG1 | 2.71 | 0.68 |
| 10:j5:63:ASN:OD1 | 10:j5:63:ASN:N | 2.22 | 0.68 |
| 10:k5:385:PRO:O | 10:k5:386:ILE:HG22 | 1.94 | 0.68 |
| 10:k5:586:LEU:HD12 | 10:k5:607:LEU:CD2 | 2.23 | 0.68 |
| 10:k5:1052:PRO:HA | 1:l7:106:GLU:CD | 2.19 | 0.68 |
| 8:O7:60:GLN:NE2 | 1:v7:117:ASN:OD1 | 2.11 | 0.68 |
| 8:Q7:12:ASP:CG | 9:z7:46:LYS:HE2 | 2.19 | 0.68 |
| 8:I7:102:THR:HB | 8:I7:103:PRO:HD2 | 1.76 | 0.68 |
| 8:W7:126:VAL:CG2 | 12:W7:201:CYC:CMC | 2.72 | 0.68 |
| 3:B8:106:GLU:HA | 3:B8:110:LEU:HB2 | 1.76 | 0.68 |
| 8:u7:5:THR:HG1 | 1:v7:3:ASP:CG | 1.99 | 0.68 |
| 8:u7:23:LEU:HD13 | 1:v7:38:VAL:HG13 | 1.73 | 0.68 |
| 3:H8:119:ALA:CB | 11:a9:266:ASN:CB | 2.60 | 0.68 |
| 4:M8:129:GLU:N | 4:M8:142:PHE:HZ | 1.89 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:O8:104:VAL:C | 5:Z8:61:LYS:CE | 2.60 | 0.68 |
| 3:Q8:84:ARG:HH11 | 5:Z8:29:HIS:CG | 2.11 | 0.68 |
| 3:L9:120:LEU:HA | 11:a9:539:GLY:CA | 2.23 | 0.68 |
| 4:M9:148:LYS:CD | 4:M9:197:ASP:OD1 | 2.37 | 0.68 |
| 5:Z8:26:LEU:HD21 | 12:Z8:301:CYC:OB | 1.93 | 0.68 |
| 3:H9:120:LEU:HD13 | 12:H9:202:CYC:C1A | 2.24 | 0.68 |
| 2:I9:1:MET:HE1 | 2:I9:108:TYR:HE1 | 1.59 | 0.68 |
| 2:K9:15:GLN:HA | 11:a9:393:ARG:CD | 2.23 | 0.68 |
| 11:a9:622:ALA:HB3 | 11:a9:625:ASP:HB2 | 1.76 | 0.68 |
| 11:aA:666:ASN:CB | 12:aA:901:CYC:HB | 2.01 | 0.68 |
| 3:LA:108:ARG:HA | 11:aA:531:ASP:HB2 | 1.76 | 0.68 |
| 4:MA:132:LEU:CD1 | 4:MA:142:PHE:HB2 | 2.24 | 0.68 |
| 12:R1:201:CYC:OB | 5:N1:54:LEU:HD12 | 1.94 | 0.68 |
| 3:L3:1:MET:CG | 3:L3:104:VAL:CG1 | 2.72 | 0.68 |
| 3:H4:14:LEU:CD2 | 11:aA:85:ALA:HA | 2.21 | 0.68 |
| 4:M4:141:GLU:HG3 | 4:M4:145:LEU:HD12 | 1.75 | 0.68 |
| 8:K5:63:PRO:O | 8:K5:65:VAL:N | 2.27 | 0.68 |
| 8:O5:102:THR:CB | 8:O5:103:PRO:CD | 2.64 | 0.68 |
| 1:B5:14:VAL:HG11 | 10:k5:555:ALA:CA | 2.24 | 0.68 |
| 8:E5:17:TYR:CB | 1:F5:45:SER:HB3 | 2.23 | 0.68 |
| 12:e5:201:CYC:HB | 12:e5:201:CYC:HMA3 | 1.59 | 0.68 |
| 1:f5:5:ILE:HD12 | 10:j5:46:PHE:CE1 | 2.29 | 0.68 |
| 8:U5:102:THR:HB | 8:U5:103:PRO:HD2 | 1.76 | 0.68 |
| 8:W5:23:LEU:CD1 | 1:X5:42:ALA:HB2 | 2.24 | 0.68 |
| 6:M6:65:VAL:CB | 1:b7:59:ALA:O | 2.42 | 0.68 |
| 9:z5:18:ARG:HD3 | 9:z5:18:ARG:N | 2.09 | 0.68 |
| 10:k5:1008:PHE:CZ | 12:p7:201:CYC:NB | 2.62 | 0.68 |
| 8:Q7:25:ARG:NE | 8:C7:25:ARG:HH22 | 1.92 | 0.68 |
| 8:i7:24:ASP:HB3 | 8:s7:99:GLY:O | 1.94 | 0.68 |
| 8:U7:91:LEU:O | 8:U7:104:ILE:HD11 | 1.94 | 0.68 |
| 8:m7:27:LYS:O | 8:m7:30:VAL:CG2 | 2.42 | 0.68 |
| 8:q7:68:PRO:HB2 | 11:aA:334:LYS:HZ2 | 1.59 | 0.68 |
| 2:X8:68:GLN:OE1 | 3:T9:24:LEU:O | 2.10 | 0.68 |
| 12:M8:301:CYC:HAB1 | 3:Y8:88:ILE:CG2 | 2.24 | 0.68 |
| 12:M8:301:CYC:C3B | 3:Y8:88:ILE:HG21 | 2.24 | 0.68 |
| 4:M9:1:MET:HA | 11:a9:422:SER:O | 1.92 | 0.68 |
| 2:O9:65:TYR:CE1 | 2:U9:65:TYR:CE1 | 2.82 | 0.68 |
| 3:J9:108:ARG:CA | 11:a9:517:ALA:HA | 2.23 | 0.68 |
| 11:a9:339:GLU:N | 11:a9:339:GLU:OE2 | 2.27 | 0.68 |
| 11:a9:415:GLU:CD | 11:a9:415:GLU:H | 2.00 | 0.68 |
| 11:a9:574:ASP:OD1 | 11:a9:574:ASP:N | 2.27 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:a9:643:LEU:HD11 | 11:a9:689:VAL:HG23 | 1.75 | 0.68 |
| 11:aA:377:VAL:CG1 | 11:aA:390:ALA:CB | 2.71 | 0.68 |
| 11:aA:643:LEU:HD11 | 11:aA:689:VAL:HG21 | 1.76 | 0.68 |
| 3:FA:37:ARG:N | 3:FA:156:LEU:HD21 | 2.09 | 0.68 |
| 12:J3:202:CYC:C2A | 11:a9:798:SER:OG | 2.42 | 0.68 |
| 2:K3:28:ASN:HD21 | 2:A3:33:ARG:NE | 1.91 | 0.68 |
| 3:B4:115:GLU:C | 4:M4:56:MET:HE3 | 2.19 | 0.68 |
| 4:M3:132:LEU:CD1 | 4:M3:142:PHE:HB2 | 2.24 | 0.68 |
| 2:O3:33:ARG:NE | 2:Y3:28:ASN:HD21 | 1.91 | 0.68 |
| 3:S4:82:CYS:SG | 12:S4:202:CYC:HBC2 | 2.34 | 0.68 |
| 4:M4:86:ALA:CB | 3:Y4:77:ARG:NH1 | 2.57 | 0.68 |
| 8:O5:29:PHE:HE1 | 8:O5:98:ALA:C | 2.01 | 0.68 |
| 5:Z4:20:ILE:HD11 | 5:Z4:22:LEU:HB3 | 1.76 | 0.68 |
| 8:A5:71:ASN:OD1 | 12:A5:201:CYC:C2D | 2.41 | 0.68 |
| 1:f5:3:ASP:OD2 | 10:j5:21:MET:HB2 | 1.93 | 0.68 |
| 10:j5:965:GLN:H | 1:t7:69:GLY:C | 2.01 | 0.68 |
| 10:k5:238:ARG:HH11 | 10:k5:238:ARG:CG | 2.07 | 0.68 |
| 10:k5:386:ILE:CG2 | 10:k5:395:SER:N | 2.37 | 0.68 |
| 1:D7:75:THR:HB | 8:E7:112:VAL:N | 2.09 | 0.68 |
| 8:i7:50:ILE:HA | 8:i7:136:VAL:HG11 | 1.76 | 0.68 |
| 8:i7:54:ALA:HB2 | 8:i7:133:MET:HA | 1.76 | 0.68 |
| 8:i7:63:PRO:O | 8:i7:65:VAL:N | 2.27 | 0.68 |
| 2:A8:65:TYR:CE1 | 2:G8:65:TYR:CE1 | 2.82 | 0.68 |
| 8:s7:29:PHE:HE1 | 8:s7:98:ALA:C | 2.01 | 0.68 |
| 2:X8:69:PRO:CG | 2:S9:39:GLU:N | 2.57 | 0.68 |
| 4:M8:140:ARG:O | 4:M8:143:VAL:HB | 1.93 | 0.68 |
| 4:M8:179:TYR:CE1 | 4:M8:230:GLN:HG3 | 2.29 | 0.68 |
| 3:O8:119:ALA:HB3 | 5:Z8:72:GLU:HG3 | 1.76 | 0.68 |
| 3:F9:68:ARG:CZ | 3:Z9:68:ARG:CZ | 2.72 | 0.68 |
| 12:V9:202:CYC:HC | 12:V9:202:CYC:CMD | 1.99 | 0.68 |
| 11:aA:703:LYS:O | 11:aA:708:HIS:CD2 | 2.46 | 0.68 |
| 11:aA:813:PRO:O | 3:L1:119:ALA:HB1 | 1.93 | 0.68 |
| 3:JA:114:LYS:HD3 | 8:S7:60:GLN:NE2 | 2.09 | 0.67 |
| 3:TA:32:LYS:HD3 | 2:X4:57:GLN:HE22 | 1.48 | 0.67 |
| 2:A1:16:GLY:HA2 | 11:aA:677:GLN:CD | 2.18 | 0.67 |
| 2:G2:65:TYR:CE1 | 2:A2:65:TYR:CE1 | 2.82 | 0.67 |
| 3:B4:82:CYS:HA | 12:B4:202:CYC:C4C | 2.25 | 0.67 |
| 2:O3:65:TYR:CE1 | 2:U3:65:TYR:CE1 | 2.82 | 0.67 |
| 3:L4:88:ILE:CD1 | 11:aA:239:TYR:CZ | 2.76 | 0.67 |
| 8:K5:80:LEU:HD13 | 12:K5:201:CYC:HAD2 | 1.76 | 0.67 |
| 12:d5:201:CYC:O2A | 10:j5:379:PHE:HD2 | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:W5:63:PRO:O | 8:W5:65:VAL:N | 2.26 | 0.67 |
| 10:k5:931:VAL:CG2 | 1:D7:30:TYR:N | 2.52 | 0.67 |
| 10:k5:1150:TYR:OH | 11:a9:39:PRO:HD3 | 1.93 | 0.67 |
| 2:A6:65:TYR:CE1 | 2:G6:65:TYR:CE1 | 2.82 | 0.67 |
| 8:S7:120:GLN:HG3 | 1:X7:53:LYS:NZ | 2.09 | 0.67 |
| 8:C7:27:LYS:O | 8:C7:30:VAL:CG2 | 2.42 | 0.67 |
| 8:g7:90:ARG:HA | 1:h7:18:TYR:CE2 | 2.29 | 0.67 |
| 1:b7:76:ARG:HB2 | 8:c7:110:ILE:HG13 | 1.75 | 0.67 |
| 8:c7:16:ARG:O | 1:d7:90:ARG:CD | 2.31 | 0.67 |
| 2:T8:65:TYR:CE1 | 2:N8:65:TYR:CE1 | 2.82 | 0.67 |
| 3:Q8:84:ARG:NH1 | 5:Z8:29:HIS:HD2 | 1.89 | 0.67 |
| 4:M9:267:LEU:CD1 | 3:V9:119:ALA:O | 2.40 | 0.67 |
| 5:Z8:20:ILE:HD11 | 5:Z8:22:LEU:HB3 | 1.76 | 0.67 |
| 11:a9:283:GLN:HB3 | 11:a9:284:PRO:HD2 | 0.70 | 0.67 |
| 11:aA:574:ASP:OD1 | 11:aA:574:ASP:N | 2.27 | 0.67 |
| 11:aA:786:GLU:OE1 | 3:H1:115:GLU:CB | 2.40 | 0.67 |
| 5:N1:20:ILE:HD11 | 5:N1:22:LEU:HB3 | 1.77 | 0.67 |
| 1:Z:13:ASP:CG | 8:e5:107:ILE:CD1 | 2.67 | 0.67 |
| 2:SA:42:ARG:NE | 2:X4:69:PRO:CD | 2.46 | 0.67 |
| 2:A1:65:TYR:CE1 | 2:G1:65:TYR:CE1 | 2.82 | 0.67 |
| 12:J3:201:CYC:HC | 12:J3:201:CYC:CMD | 1.99 | 0.67 |
| 6:M2:131:ASN:HB2 | 12:F2:201:CYC:HMA1 | 1.77 | 0.67 |
| 2:A3:16:GLY:HA2 | 11:a9:677:GLN:CD | 2.18 | 0.67 |
| 3:B3:127:VAL:CA | 12:B3:202:CYC:HMC1 | 2.24 | 0.67 |
| 3:B4:85:ASP:H | 12:B4:202:CYC:HAC1 | 1.57 | 0.67 |
| 3:B4:116:THR:CB | 4:M4:56:MET:HB2 | 2.15 | 0.67 |
| 3:D4:107:ASP:HB3 | 11:aA:109:ASN:HB3 | 1.76 | 0.67 |
| 5:N3:33:GLY:C | 3:T3:84:ARG:HD2 | 2.17 | 0.67 |
| 3:S4:82:CYS:SG | 12:S4:202:CYC:CAC | 2.82 | 0.67 |
| 1:L5:10:ASN:HB2 | 9:i5:65:THR:OG1 | 1.94 | 0.67 |
| 12:Y4:201:CYC:HC | 12:Y4:201:CYC:CMD | 1.99 | 0.67 |
| 5:Z4:22:LEU:O | 12:Z4:301:CYC:HMA2 | 1.94 | 0.67 |
| 8:A5:110:ILE:O | 1:F5:76:ARG:HB2 | 1.93 | 0.67 |
| 8:A5:115:MET:HE1 | 1:F5:75:THR:HG22 | 1.76 | 0.67 |
| 8:U5:27:LYS:O | 8:U5:30:VAL:CG2 | 2.42 | 0.67 |
| 8:U5:79:ALA:HB1 | 6:M6:32:MET:CA | 2.24 | 0.67 |
| 8:W5:126:VAL:CG2 | 12:W5:201:CYC:CMC | 2.72 | 0.67 |
| 10:j5:238:ARG:HH11 | 10:j5:238:ARG:CG | 2.07 | 0.67 |
| 10:j5:1102:TYR:O | 10:j5:1106:PHE:O | 2.12 | 0.67 |
| 10:k5:959:PHE:CD2 | 1:n7:67:ARG:NH1 | 2.63 | 0.67 |
| 10:k5:987:ASP:O | 1:b7:106:GLU:CD | 2.38 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:k5:1125:ARG:HG2 | 1:n7:115:THR:OG1 | 1.93 | 0.67 |
| 8:G7:120:GLN:HG3 | 1:L7:53:LYS:NZ | 2.09 | 0.67 |
| 8:k7:120:GLN:HG3 | 1:p7:53:LYS:NZ | 2.09 | 0.67 |
| 1:Z7:67:ARG:HH11 | 11:a9:311:LEU:HD13 | 1.59 | 0.67 |
| 3:B8:92:TYR:OH | 12:B8:202:CYC:CAB | 2.42 | 0.67 |
| 8:o7:63:PRO:O | 8:o7:65:VAL:N | 2.27 | 0.67 |
| 1:v7:139:GLY:C | 11:aA:342:ARG:CD | 2.67 | 0.67 |
| 12:H8:201:CYC:CBB | 11:a9:259:ALA:CA | 2.72 | 0.67 |
| 12:K8:201:CYC:HMD1 | 12:K8:201:CYC:NC | 2.09 | 0.67 |
| 3:L9:56:ALA:HA | 3:L9:86:MET:HE1 | 1.76 | 0.67 |
| 3:Y8:104:VAL:HA | 3:Y8:108:ARG:HB2 | 1.75 | 0.67 |
| 3:J9:108:ARG:NH2 | 11:a9:515:GLY:O | 2.27 | 0.67 |
| 5:NA:20:ILE:HD11 | 5:NA:22:LEU:HB3 | 1.77 | 0.67 |
| 2:QA:25:GLN:HB3 | 2:UA:4:VAL:HG21 | 1.76 | 0.67 |
| 2:QA:162:SER:C | 2:WA:118:ARG:HD3 | 2.18 | 0.67 |
| 2:A3:63:PHE:O | 2:A3:66:LEU:CG | 2.39 | 0.67 |
| 3:D3:111:ASN:ND2 | 4:M3:65:ARG:HD2 | 2.10 | 0.67 |
| 2:A4:65:TYR:CE1 | 2:G4:65:TYR:CE1 | 2.82 | 0.67 |
| 5:N3:22:LEU:HD23 | 5:N3:26:LEU:CD1 | 1.83 | 0.67 |
| 5:N3:22:LEU:HD11 | 5:N3:26:LEU:HD21 | 1.71 | 0.67 |
| 5:N3:23:SER:O | 5:N3:25:THR:N | 2.26 | 0.67 |
| 4:M4:215:GLU:H | 5:Z4:28:HIS:N | 1.92 | 0.67 |
| 12:M4:301:CYC:HAC1 | 3:Y4:82:CYS:CB | 2.23 | 0.67 |
| 3:O4:120:LEU:CD2 | 5:Z4:14:LYS:NZ | 2.57 | 0.67 |
| 8:E5:63:PRO:O | 8:E5:65:VAL:N | 2.27 | 0.67 |
| 1:J5:74:THR:HG1 | 1:J5:77:ARG:HD3 | 1.59 | 0.67 |
| 1:P5:114:GLU:OE1 | 10:k5:496:GLU:HG3 | 1.94 | 0.67 |
| 8:S5:14:GLU:OE2 | 10:j5:538:PHE:HE2 | 1.77 | 0.67 |
| 1:b5:114:GLU:CB | 10:k5:491:THR:OG1 | 2.41 | 0.67 |
| 6:M6:104:ARG:CZ | 2:G6:16:GLY:N | 2.57 | 0.67 |
| 9:i5:18:ARG:HD3 | 9:i5:18:ARG:N | 2.09 | 0.67 |
| 10:k5:17:PHE:HD1 | 10:k5:19:THR:HG22 | 1.60 | 0.67 |
| 10:k5:642:ARG:HH11 | 10:k5:642:ARG:CG | 2.07 | 0.67 |
| 10:k5:1125:ARG:NH2 | 1:n7:114:GLU:HB3 | 2.07 | 0.67 |
| 8:O7:27:LYS:O | 8:O7:30:VAL:CG2 | 2.42 | 0.67 |
| 8:Q7:126:VAL:CG2 | 12:Q7:201:CYC:CMC | 2.72 | 0.67 |
| 8:C7:29:PHE:HE1 | 8:C7:98:ALA:C | 2.01 | 0.67 |
| 8:s7:27:LYS:O | 8:s7:30:VAL:CG2 | 2.42 | 0.67 |
| 8:u7:34:GLU:HA | 1:v7:28:LYS:HE2 | 1.75 | 0.67 |
| 8:u7:72:ALA:HB2 | 12:u7:201:CYC:C1C | 2.25 | 0.67 |
| 4:M8:144:ARG:HG2 | 4:M8:204:ILE:HG21 | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:L9:51:ILE:CG2 | 3:L9:90:LEU:HD12 | 2.24 | 0.67 |
| 11:a9:30:MET:CG | 11:a9:34:ILE:O | 2.43 | 0.67 |
| 11:a9:439:ARG:HG3 | 11:a9:439:ARG:NH1 | 2.08 | 0.67 |
| 11:a9:584:ARG:O | 11:a9:588:VAL:O | 2.12 | 0.67 |
| 11:aA:714:ARG:CB | 11:aA:808:LEU:O | 2.41 | 0.67 |
| 11:aA:739:ASP:HB2 | 3:L1:84:ARG:NH1 | 2.09 | 0.67 |
| 1:A:16:GLY:HA2 | 8:a5:90:ARG:CZ | 2.24 | 0.67 |
| 5:NA:70:ILE:HG21 | 3:TA:116:THR:CA | 2.15 | 0.67 |
| 12:R1:201:CYC:CBB | 5:N1:61:LYS:HZ2 | 2.06 | 0.67 |
| 3:B3:84:ARG:HH22 | 12:B3:202:CYC:CGA | 2.07 | 0.67 |
| 2:A4:33:ARG:NE | 2:K4:28:ASN:HD21 | 1.91 | 0.67 |
| 12:B4:202:CYC:CBB | 4:M4:61:ASN:HD22 | 2.04 | 0.67 |
| 4:M3:268:ARG:C | 3:V3:111:ASN:HD21 | 2.03 | 0.67 |
| 12:P3:202:CYC:HC | 12:P3:202:CYC:CMD | 1.99 | 0.67 |
| 3:H4:14:LEU:HD13 | 11:aA:85:ALA:HB1 | 1.76 | 0.67 |
| 12:L4:201:CYC:HC | 12:L4:201:CYC:CMD | 1.99 | 0.67 |
| 12:M5:201:CYC:HB | 12:M5:201:CYC:HMA3 | 1.59 | 0.67 |
| 8:O5:27:LYS:O | 8:O5:30:VAL:CG2 | 2.42 | 0.67 |
| 8:C5:91:LEU:O | 8:C5:104:ILE:HD11 | 1.93 | 0.67 |
| 8:G5:100:ASP:CG | 8:S5:20:PRO:HG2 | 2.20 | 0.67 |
| 1:V5:87:TYR:OH | 10:j5:653:SER:HB3 | 1.94 | 0.67 |
| 6:M6:62:ARG:CZ | 1:b7:57:ALA:O | 2.40 | 0.67 |
| 10:j5:17:PHE:CD1 | 10:j5:19:THR:HG22 | 2.29 | 0.67 |
| 10:j5:732:ARG:NE | 1:J7:69:GLY:HA3 | 2.10 | 0.67 |
| 10:j5:930:LEU:HB3 | 1:J7:33:THR:CB | 2.24 | 0.67 |
| 10:j5:1060:GLU:O | 10:j5:1063:THR:OG1 | 2.11 | 0.67 |
| 10:k5:542:GLN:NE2 | 10:k5:560:VAL:O | 2.26 | 0.67 |
| 10:k5:965:GLN:CG | 1:n7:69:GLY:O | 2.38 | 0.67 |
| 10:k5:966:SER:N | 1:p7:14:VAL:HG12 | 2.03 | 0.67 |
| 10:k5:1143:LEU:HG | 8:k7:106:GLU:OE1 | 1.93 | 0.67 |
| 10:k5:1147:TYR:CD1 | 11:a9:35:ARG:HB2 | 2.30 | 0.67 |
| 8:I7:91:LEU:O | 8:I7:104:ILE:HD11 | 1.94 | 0.67 |
| 8:g7:27:LYS:O | 8:g7:30:VAL:CG2 | 2.42 | 0.67 |
| 8:g7:63:PRO:HG2 | 11:aA:334:LYS:HA | 1.75 | 0.67 |
| 8:i7:47:ARG:NH1 | 1:j7:18:TYR:CG | 2.62 | 0.67 |
| 8:i7:50:ILE:CG1 | 8:i7:137:ALA:HB2 | 2.24 | 0.67 |
| 8:k7:68:PRO:HB2 | 11:a9:334:LYS:HZ3 | 1.60 | 0.67 |
| 8:a7:27:LYS:O | 8:a7:30:VAL:CG2 | 2.42 | 0.67 |
| 8:a7:161:GLN:CG | 1:p7:49:THR:HG21 | 2.23 | 0.67 |
| 8:c7:17:TYR:CE2 | 1:d7:44:ILE:CG2 | 2.77 | 0.67 |
| 8:c7:89:LEU:CD1 | 8:c7:153:PHE:HZ | 2.07 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:B8:202:CYC:HHA | 4:M8:54:ALA:N | 2.04 | 0.67 |
| 8:o7:23:LEU:CD1 | 1:p7:38:VAL:CG1 | 2.67 | 0.67 |
| 2:X8:69:PRO:CD | 2:S9:42:ARG:NE | 2.46 | 0.67 |
| 3:L8:109:CYS:O | 12:a9:901:CYC:HBB2 | 1.94 | 0.67 |
| 3:L8:120:LEU:HD11 | 12:a9:901:CYC:HAA2 | 1.77 | 0.67 |
| 4:M8:235:PHE:HB3 | 12:M8:301:CYC:HMA1 | 1.76 | 0.67 |
| 2:N8:38:MET:HE1 | 3:O8:28:THR:OG1 | 1.93 | 0.67 |
| 4:M9:132:LEU:CD1 | 4:M9:142:PHE:HB2 | 2.24 | 0.67 |
| 4:M9:260:ARG:NH1 | 4:M9:260:ARG:HG3 | 2.09 | 0.67 |
| 2:I9:1:MET:HE2 | 2:I9:108:TYR:HE1 | 1.57 | 0.67 |
| 11:a9:714:ARG:CB | 11:a9:808:LEU:O | 2.41 | 0.67 |
| 3:F2:82:CYS:HA | 12:F2:201:CYC:CHD | 2.25 | 0.67 |
| 12:QA:201:CYC:HMA1 | 3:TA:79:MET:CG | 2.24 | 0.67 |
| 2:SA:42:ARG:NH2 | 3:TA:24:LEU:HB3 | 2.07 | 0.67 |
| 3:TA:32:LYS:HZ2 | 2:X4:60:TYR:CB | 2.06 | 0.67 |
| 12:UA:201:CYC:HMD1 | 12:UA:201:CYC:NC | 2.09 | 0.67 |
| 12:B4:202:CYC:CHA | 4:M4:54:ALA:CB | 2.69 | 0.67 |
| 3:D4:77:ARG:HD2 | 4:M4:33:LEU:HD11 | 1.76 | 0.67 |
| 4:M3:245:ASP:CB | 3:X3:108:ARG:O | 2.41 | 0.67 |
| 4:M4:217:VAL:CG2 | 5:Z4:30:PRO:HD3 | 2.09 | 0.67 |
| 8:M5:110:ILE:HD12 | 10:k5:533:LEU:HD11 | 1.52 | 0.67 |
| 8:e5:27:LYS:O | 8:e5:30:VAL:CG2 | 2.43 | 0.67 |
| 1:f5:18:TYR:HE2 | 10:j5:165:ARG:HA | 1.59 | 0.67 |
| 8:a5:91:LEU:O | 8:a5:104:ILE:HD11 | 1.94 | 0.67 |
| 10:j5:17:PHE:HD1 | 10:j5:19:THR:HG22 | 1.60 | 0.67 |
| 10:j5:385:PRO:O | 10:j5:386:ILE:HG22 | 1.94 | 0.67 |
| 10:j5:542:GLN:O | 10:j5:544:VAL:N | 2.28 | 0.67 |
| 10:j5:774:GLN:HA | 10:j5:774:GLN:NE2 | 2.07 | 0.67 |
| 8:O7:25:ARG:HH22 | 8:E7:25:ARG:HD3 | 1.57 | 0.67 |
| 8:E7:126:VAL:CG2 | 12:E7:201:CYC:CMC | 2.72 | 0.67 |
| 3:D8:107:ASP:HB3 | 11:a9:109:ASN:HB3 | 1.77 | 0.67 |
| 3:F8:115:GLU:O | 4:M8:3:VAL:HG11 | 1.94 | 0.67 |
| 12:G8:201:CYC:HMD1 | 12:G8:201:CYC:NC | 2.09 | 0.67 |
| 4:M8:19:MET:HE2 | 4:M8:59:ILE:HD11 | 1.75 | 0.67 |
| 4:M8:71:PRO:HG2 | 4:M8:74:LEU:HB2 | 1.75 | 0.67 |
| 4:M8:210:ILE:CD1 | 5:Z8:25:THR:O | 2.43 | 0.67 |
| 4:M9:8:SER:O | 3:D9:108:ARG:HG2 | 1.94 | 0.67 |
| 4:M9:134:ASN:ND2 | 5:N9:1:MET:N | 2.43 | 0.67 |
| 5:N9:20:ILE:HD11 | 5:N9:22:LEU:HB3 | 1.76 | 0.67 |
| 3:H9:92:TYR:OH | 3:H9:108:ARG:NE | 2.28 | 0.67 |
| 11:a9:377:VAL:CG1 | 11:a9:390:ALA:CB | 2.71 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:aA:708:HIS:CA | 3:L1:108:ARG:HH21 | 2.08 | 0.67 |
| 12:B2:201:CYC:HC | 12:B2:201:CYC:CMD | 1.99 | 0.67 |
| 3:FA:37:ARG:HA | 3:FA:156:LEU:HD21 | 1.77 | 0.67 |
| 2:SA:38:MET:HE2 | 2:X4:69:PRO:HD3 | 1.76 | 0.67 |
| 3:L2:65:ASP:OD2 | 1:h7:64:ASP:HB2 | 1.95 | 0.67 |
| 3:L3:1:MET:SD | 3:L3:104:VAL:HG11 | 2.34 | 0.67 |
| 4:M3:164:ARG:HD3 | 4:M3:259:ARG:N | 2.10 | 0.67 |
| 5:N3:54:LEU:HD12 | 12:R3:201:CYC:OB | 1.94 | 0.67 |
| 4:M4:197:ASP:CG | 5:Z4:52:ARG:CG | 2.68 | 0.67 |
| 5:Z4:27:ALA:O | 5:Z4:28:HIS:CD2 | 2.48 | 0.67 |
| 8:C5:27:LYS:O | 8:C5:29:PHE:CA | 2.42 | 0.67 |
| 1:P5:87:TYR:CE2 | 10:k5:649:PHE:HZ | 2.11 | 0.67 |
| 8:Q5:16:ARG:HA | 1:R5:90:ARG:NE | 2.07 | 0.67 |
| 1:T5:53:LYS:HZ1 | 8:U5:120:GLN:HE21 | 0.67 | 0.67 |
| 1:V5:87:TYR:CE2 | 10:j5:649:PHE:CZ | 2.83 | 0.67 |
| 8:Y5:120:GLN:HG3 | 1:b5:53:LYS:NZ | 2.09 | 0.67 |
| 3:J6:88:ILE:HD11 | 6:M6:185:PHE:CE1 | 2.30 | 0.67 |
| 2:K6:28:ASN:HD21 | 2:A6:33:ARG:NE | 1.91 | 0.67 |
| 10:j5:971:VAL:N | 12:j5:1202:CYC:O1D | 2.15 | 0.67 |
| 10:k5:1060:GLU:O | 10:k5:1063:THR:OG1 | 2.11 | 0.67 |
| 1:J7:53:LYS:NZ | 8:K7:120:GLN:OE1 | 2.26 | 0.67 |
| 8:c7:16:ARG:N | 1:d7:90:ARG:CZ | 2.52 | 0.67 |
| 8:u7:29:PHE:CD2 | 1:v7:31:PHE:CE1 | 2.58 | 0.67 |
| 3:F8:112:GLY:O | 3:F8:114:LYS:N | 2.26 | 0.67 |
| 3:F8:120:LEU:HD11 | 11:a9:147:ASN:ND2 | 2.10 | 0.67 |
| 2:I8:115:GLU:OE1 | 11:a9:133:LEU:CD2 | 2.39 | 0.67 |
| 4:M8:86:ALA:HB1 | 3:Y8:77:ARG:NH1 | 2.09 | 0.67 |
| 4:M8:164:ARG:HD3 | 4:M8:259:ARG:N | 2.10 | 0.67 |
| 2:P8:18:PHE:N | 3:Q8:91:ARG:HH21 | 1.69 | 0.67 |
| 12:F1:201:CYC:O2A | 4:M1:35:THR:CA | 2.40 | 0.67 |
| 4:M9:19:MET:HE2 | 4:M9:59:ILE:HD11 | 1.75 | 0.67 |
| 4:M9:164:ARG:HD3 | 4:M9:259:ARG:N | 2.10 | 0.67 |
| 2:O9:38:MET:HE1 | 3:P9:28:THR:OG1 | 1.93 | 0.67 |
| 3:Y8:89:ILE:HA | 3:Y8:92:TYR:HE2 | 0.84 | 0.67 |
| 3:Y8:89:ILE:CB | 3:Y8:92:TYR:CZ | 2.78 | 0.67 |
| 2:K9:15:GLN:O | 11:a9:393:ARG:CZ | 2.42 | 0.67 |
| 11:aA:598:SER:HB3 | 11:aA:599:PRO:CD | 2.24 | 0.67 |
| 4:M1:222:ARG:HG3 | 4:M1:222:ARG:NH1 | 2.01 | 0.67 |
| 2:U1:43:ALA:O | 2:U1:47:ASN:ND2 | 2.27 | 0.67 |
| 2:A2:38:MET:HE1 | 3:B2:28:THR:OG1 | 1.93 | 0.67 |
| 12:AA:201:CYC:HMD1 | 12:AA:201:CYC:NC | 2.10 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:FA:37:ARG:NH1 | 3:FA:159:GLU:OE1 | 2.27 | 0.67 |
| 2:KA:15:GLN:HA | 11:aA:393:ARG:CD | 2.25 | 0.67 |
| 3:LA:84:ARG:NH2 | 11:aA:406:LEU:HA | 2.09 | 0.67 |
| 4:MA:134:ASN:HD21 | 5:NA:1:MET:H1 | 1.42 | 0.67 |
| 12:QA:201:CYC:HMD1 | 12:QA:201:CYC:NC | 2.09 | 0.67 |
| 3:J3:120:LEU:HA | 11:a9:803:ASN:HA | 1.75 | 0.67 |
| 12:G2:201:CYC:HMD1 | 12:G2:201:CYC:NC | 2.09 | 0.67 |
| 3:B3:68:ARG:HH12 | 3:V3:68:ARG:NH1 | 1.88 | 0.67 |
| 12:B1:202:CYC:HAA1 | 11:aA:684:ASN:ND2 | 2.07 | 0.67 |
| 3:O4:107:ASP:OD1 | 5:Z4:66:ARG:CZ | 2.43 | 0.67 |
| 3:O4:119:ALA:CB | 5:Z4:72:GLU:HB2 | 2.23 | 0.67 |
| 3:Q4:96:ALA:C | 3:Q4:98:LEU:N | 2.53 | 0.67 |
| 8:K5:20:PRO:HG2 | 8:U5:152:TYR:HA | 1.75 | 0.67 |
| 8:M5:89:LEU:HB3 | 1:N5:18:TYR:OH | 1.93 | 0.67 |
| 8:E5:80:LEU:HD13 | 12:E5:201:CYC:HAD2 | 1.76 | 0.67 |
| 8:Q5:126:VAL:CG2 | 12:Q5:201:CYC:CMC | 2.72 | 0.67 |
| 8:U5:75:GLU:CG | 6:M6:32:MET:HE1 | 2.24 | 0.67 |
| 8:a5:27:LYS:O | 8:a5:30:VAL:CG2 | 2.42 | 0.67 |
| 10:j5:1125:ARG:CZ | 1:t7:114:GLU:CB | 2.70 | 0.67 |
| 10:k5:844:GLN:NE2 | 10:k5:916:PHE:H | 1.92 | 0.67 |
| 10:k5:978:LEU:HD11 | 1:p7:107:ARG:HH22 | 1.57 | 0.67 |
| 10:k5:1147:TYR:HE1 | 11:a9:35:ARG:HB3 | 1.60 | 0.67 |
| 3:D1:68:ARG:HH12 | 3:X1:68:ARG:HH12 | 1.43 | 0.67 |
| 8:g7:22:GLU:HG2 | 8:g7:25:ARG:HH12 | 1.57 | 0.67 |
| 12:j7:201:CYC:C4B | 9:y7:38:PHE:CE1 | 2.78 | 0.67 |
| 8:U7:27:LYS:O | 8:U7:30:VAL:CG2 | 2.42 | 0.67 |
| 1:V7:75:THR:HB | 8:W7:112:VAL:N | 2.09 | 0.67 |
| 8:c7:92:VAL:HG23 | 8:c7:156:LEU:HD12 | 1.75 | 0.67 |
| 1:n7:75:THR:HB | 8:o7:111:GLY:C | 2.20 | 0.67 |
| 1:t7:75:THR:HB | 8:u7:111:GLY:C | 2.20 | 0.67 |
| 3:F8:108:ARG:HG2 | 4:M8:9:GLN:HG2 | 1.75 | 0.67 |
| 3:L8:84:ARG:HH22 | 12:a9:901:CYC:CGA | 2.07 | 0.67 |
| 4:M8:235:PHE:HB2 | 12:M8:301:CYC:C2A | 2.23 | 0.67 |
| 12:F1:201:CYC:HBA2 | 4:M1:36:TYR:CE2 | 2.29 | 0.67 |
| 3:L9:93:VAL:HG11 | 3:L9:164:PHE:CE2 | 2.29 | 0.67 |
| 4:M9:232:VAL:HG11 | 3:X9:111:ASN:N | 2.10 | 0.67 |
| 2:O9:33:ARG:NE | 2:Y9:28:ASN:HD21 | 1.91 | 0.67 |
| 12:H9:201:CYC:HC | 12:H9:201:CYC:CMD | 1.98 | 0.67 |
| 11:aA:735:VAL:O | 12:aA:902:CYC:O2A | 2.13 | 0.67 |
| 2:OA:33:ARG:NE | 2:YA:28:ASN:HD21 | 1.92 | 0.67 |
| 2:QA:68:GLN:HB3 | 2:QA:69:PRO:HD2 | 1.75 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:SA:42:ARG:HE | 2:X4:69:PRO:N | 1.93 | 0.67 |
| 2:G2:16:GLY:N | 6:M2:104:ARG:CZ | 2.57 | 0.67 |
| 3:H2:120:LEU:HA | 6:M2:250:GLY:HA2 | 1.77 | 0.67 |
| 3:L4:70:GLY:O | 3:L4:71:GLY:C | 2.38 | 0.67 |
| 8:U5:76:LYS:CG | 8:U5:77:MET:HE3 | 2.24 | 0.67 |
| 10:j5:793:SER:HB3 | 12:T7:201:CYC:HBA1 | 1.77 | 0.67 |
| 10:j5:816:ARG:HG2 | 10:j5:816:ARG:O | 1.95 | 0.67 |
| 10:j5:822:ARG:HB2 | 10:j5:822:ARG:NH1 | 2.04 | 0.67 |
| 10:j5:822:ARG:CG | 1:H7:106:GLU:OE2 | 2.43 | 0.67 |
| 10:j5:1145:PRO:HG2 | 1:r7:14:VAL:HG11 | 1.75 | 0.67 |
| 10:j5:1153:VAL:HG22 | 1:v7:125:ALA:CB | 2.23 | 0.67 |
| 12:A6:201:CYC:HMD1 | 12:A6:201:CYC:NC | 2.10 | 0.67 |
| 3:F6:78:ARG:CG | 12:F6:201:CYC:CGD | 2.73 | 0.67 |
| 1:R7:53:LYS:NZ | 8:M7:120:GLN:HG3 | 2.09 | 0.67 |
| 8:K7:126:VAL:CG2 | 12:K7:201:CYC:CMC | 2.72 | 0.67 |
| 8:k7:66:VAL:CG1 | 11:a9:65:LEU:CD2 | 2.72 | 0.67 |
| 8:a7:25:ARG:HE | 8:o7:25:ARG:NH2 | 1.92 | 0.67 |
| 1:b7:75:THR:HB | 8:c7:112:VAL:N | 2.09 | 0.67 |
| 9:x7:9:ALA:HB1 | 9:x7:44:ILE:HD13 | 1.75 | 0.67 |
| 2:X8:69:PRO:HD3 | 2:S9:38:MET:HE2 | 1.76 | 0.67 |
| 4:M8:222:ARG:HG3 | 4:M8:222:ARG:NH1 | 2.01 | 0.67 |
| 2:N8:107:ASP:O | 5:Z8:34:LEU:HD11 | 1.94 | 0.67 |
| 4:M9:274:VAL:OXT | 3:V9:77:ARG:CZ | 2.42 | 0.67 |
| 12:Z9:201:CYC:HC | 12:Z9:201:CYC:CMD | 1.98 | 0.67 |
| 11:aA:95:ILE:HG22 | 11:aA:99:ALA:H | 1.60 | 0.67 |
| 11:aA:796:ALA:HB1 | 3:J1:113:LEU:HD13 | 1.75 | 0.67 |
| 12:K1:201:CYC:HMD1 | 12:K1:201:CYC:NC | 2.10 | 0.67 |
| 5:N1:4:LEU:O | 5:N1:4:LEU:HG | 1.88 | 0.67 |
| 3:F2:82:CYS:SG | 12:F2:201:CYC:C3C | 2.83 | 0.67 |
| 4:MA:164:ARG:HD3 | 4:MA:259:ARG:N | 2.10 | 0.67 |
| 2:S1:16:GLY:N | 5:N1:31:TRP:HD1 | 1.92 | 0.67 |
| 4:M3:17:VAL:O | 4:M3:44:SER:HA | 1.95 | 0.67 |
| 5:N3:29:HIS:CD2 | 12:T3:301:CYC:OB | 2.48 | 0.67 |
| 2:O3:38:MET:HE1 | 3:P3:28:THR:OG1 | 1.93 | 0.67 |
| 2:T4:65:TYR:CE1 | 2:N4:65:TYR:CE1 | 2.82 | 0.67 |
| 4:M4:17:VAL:O | 4:M4:44:SER:HA | 1.95 | 0.67 |
| 4:M4:164:ARG:HD3 | 4:M4:259:ARG:N | 2.10 | 0.67 |
| 8:K5:72:ALA:HB2 | 12:K5:201:CYC:C1C | 2.25 | 0.67 |
| 12:E5:201:CYC:HB | 12:E5:201:CYC:HMA3 | 1.58 | 0.67 |
| 12:H5:201:CYC:HBB2 | 9:i5:21:ARG:HG3 | 1.77 | 0.67 |
| 1:d5:161:SER:OG | 10:j5:695:GLY:O | 2.13 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:U5:80:LEU:CG | 6:M6:28:ASN:CB | 2.52 | 0.67 |
| 1:V5:114:GLU:CG | 10:j5:496:GLU:OE2 | 2.42 | 0.67 |
| 12:Z5:201:CYC:NB | 10:k5:379:PHE:CZ | 2.62 | 0.67 |
| 6:M6:45:ILE:HD12 | 8:c7:78:THR:HG22 | 1.74 | 0.67 |
| 6:M6:276:PRO:O | 1:d7:62:TYR:O | 2.11 | 0.67 |
| 10:k5:542:GLN:O | 10:k5:544:VAL:N | 2.28 | 0.67 |
| 10:k5:1008:PHE:HZ | 1:p7:87:TYR:HE2 | 1.34 | 0.67 |
| 8:O7:91:LEU:O | 8:O7:104:ILE:HD11 | 1.94 | 0.67 |
| 8:C7:91:LEU:O | 8:C7:104:ILE:HD11 | 1.94 | 0.67 |
| 1:h7:75:THR:HG21 | 8:i7:112:VAL:HG23 | 1.77 | 0.67 |
| 8:i7:20:PRO:CD | 8:s7:155:TYR:CG | 2.76 | 0.67 |
| 8:u7:18:LEU:HD22 | 1:v7:97:LEU:CD1 | 2.20 | 0.67 |
| 4:M8:128:ALA:CA | 4:M8:142:PHE:HE1 | 2.08 | 0.67 |
| 12:B9:202:CYC:HC | 12:B9:202:CYC:CMD | 1.99 | 0.67 |
| 11:a9:239:TYR:HD1 | 12:a9:901:CYC:O2A | 1.76 | 0.67 |
| 11:a9:325:LEU:HD23 | 11:a9:325:LEU:H | 1.60 | 0.67 |
| 11:aA:643:LEU:HD13 | 11:aA:766:ASN:CB | 2.25 | 0.67 |
| 4:M1:268:ARG:C | 3:V1:111:ASN:HD21 | 2.03 | 0.67 |
| 5:N1:34:LEU:CA | 3:T1:84:ARG:HD3 | 2.25 | 0.67 |
| 1:Z:16:GLY:CA | 8:e5:90:ARG:CZ | 2.73 | 0.67 |
| 2:AA:65:TYR:CE1 | 2:GA:65:TYR:CE1 | 2.82 | 0.67 |
| 2:IA:9:ILE:HD11 | 3:JA:99:ALA:HB2 | 1.74 | 0.67 |
| 4:MA:160:THR:H | 3:VA:108:ARG:HG2 | 1.59 | 0.67 |
| 4:MA:273:ILE:HD13 | 3:VA:75:PRO:HD2 | 1.77 | 0.67 |
| 2:OA:65:TYR:CE1 | 2:UA:65:TYR:CE1 | 2.82 | 0.67 |
| 12:O1:201:CYC:HMD1 | 12:O1:201:CYC:NC | 2.10 | 0.67 |
| 2:I2:80:ALA:HB2 | 11:aA:297:ASP:OD2 | 1.94 | 0.67 |
| 12:C3:201:CYC:HMD1 | 12:C3:201:CYC:NC | 2.09 | 0.67 |
| 12:L3:202:CYC:O2A | 11:a9:735:VAL:O | 2.11 | 0.67 |
| 5:N3:20:ILE:HD11 | 5:N3:22:LEU:HB3 | 1.77 | 0.67 |
| 4:M4:19:MET:HE2 | 4:M4:59:ILE:HD11 | 1.75 | 0.67 |
| 8:K5:20:PRO:HB3 | 8:U5:151:PHE:CB | 2.25 | 0.67 |
| 1:B5:14:VAL:CG1 | 10:k5:555:ALA:HA | 2.24 | 0.67 |
| 8:C5:29:PHE:HE1 | 8:C5:98:ALA:C | 2.01 | 0.67 |
| 8:G5:25:ARG:HH22 | 8:S5:25:ARG:HE | 1.43 | 0.67 |
| 8:I5:29:PHE:HE1 | 8:I5:98:ALA:C | 2.01 | 0.67 |
| 12:K7:201:CYC:HMD1 | 12:K7:201:CYC:NC | 2.02 | 0.67 |
| 8:u7:39:ILE:CD1 | 8:u7:145:ASP:HB3 | 2.24 | 0.67 |
| 8:u7:103:PRO:HB2 | 1:v7:9:ILE:HG21 | 1.70 | 0.67 |
| 9:y7:3:ARG:HG2 | 9:y7:59:GLY:HA3 | 1.76 | 0.67 |
| 3:O8:112:GLY:HA2 | 5:Z8:69:GLU:HA | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:L9:38:LEU:CD2 | 2:K9:24:LEU:HD22 | 2.25 | 0.67 |
| 5:N9:7:ASP:N | 3:R9:108:ARG:HA | 2.09 | 0.67 |
| 12:A9:201:CYC:HMD1 | 12:A9:201:CYC:NC | 2.10 | 0.67 |
| 11:a9:599:PRO:O | 11:a9:600:THR:HB | 1.94 | 0.67 |
| 11:a9:643:LEU:HD11 | 11:a9:689:VAL:HG21 | 1.75 | 0.67 |
| 11:aA:298:ILE:O | 11:aA:299:PRO:C | 2.38 | 0.67 |
| 11:aA:365:LYS:NZ | 11:aA:365:LYS:HB2 | 2.10 | 0.67 |
| 5:N1:22:LEU:HD21 | 5:N1:26:LEU:CD2 | 2.08 | 0.67 |
| 5:N1:31:TRP:HB3 | 5:N1:32:PRO:CD | 2.23 | 0.67 |
| 3:FA:43:ALA:CB | 3:FA:142:VAL:HG22 | 2.26 | 0.66 |
| 2:IA:37:SER:O | 2:IA:97:LEU:CG | 2.43 | 0.66 |
| 12:QA:201:CYC:HBA1 | 3:TA:79:MET:HE3 | 1.77 | 0.66 |
| 3:J2:88:ILE:HD11 | 6:M2:185:PHE:CE1 | 2.30 | 0.66 |
| 3:B3:88:ILE:HD13 | 12:B3:202:CYC:C2B | 2.24 | 0.66 |
| 3:L3:111:ASN:O | 11:a9:711:SER:HB2 | 1.94 | 0.66 |
| 12:L3:201:CYC:HC | 12:L3:201:CYC:CMD | 1.99 | 0.66 |
| 4:M3:134:ASN:OD1 | 5:N3:1:MET:N | 2.29 | 0.66 |
| 12:U3:201:CYC:HMD1 | 12:U3:201:CYC:NC | 2.09 | 0.66 |
| 3:L4:68:ARG:CB | 11:aA:82:GLN:HB2 | 2.18 | 0.66 |
| 4:M4:87:ILE:HD13 | 3:Y4:77:ARG:HG3 | 0.72 | 0.66 |
| 10:k5:929:PRO:CG | 1:D7:147:LYS:CG | 2.70 | 0.66 |
| 1:P7:75:THR:HB | 8:Q7:112:VAL:N | 2.09 | 0.66 |
| 8:I7:27:LYS:O | 8:I7:30:VAL:CG2 | 2.42 | 0.66 |
| 8:g7:90:ARG:CZ | 1:h7:16:GLY:CA | 2.73 | 0.66 |
| 1:h7:46:SER:HB2 | 8:u7:157:VAL:CG1 | 2.24 | 0.66 |
| 8:i7:37:LEU:HD21 | 1:j7:31:PHE:CE2 | 2.30 | 0.66 |
| 12:W7:201:CYC:HMD1 | 12:W7:201:CYC:NC | 2.02 | 0.66 |
| 8:o7:72:ALA:HB2 | 12:o7:201:CYC:C1C | 2.25 | 0.66 |
| 2:N8:115:GLU:HB2 | 5:Z8:33:GLY:N | 2.08 | 0.66 |
| 12:Q9:201:CYC:HMD1 | 12:Q9:201:CYC:NC | 2.09 | 0.66 |
| 2:A9:65:TYR:CE1 | 2:G9:65:TYR:CE1 | 2.82 | 0.66 |
| 12:U9:201:CYC:HMD1 | 12:U9:201:CYC:NC | 2.09 | 0.66 |
| 11:a9:95:ILE:HG22 | 11:a9:99:ALA:H | 1.60 | 0.66 |
| 11:a9:643:LEU:CD1 | 11:a9:766:ASN:CB | 2.73 | 0.66 |
| 11:aA:802:ARG:HB2 | 3:J1:120:LEU:CD2 | 2.24 | 0.66 |
| 12:L1:201:CYC:HC | 12:L1:201:CYC:CMD | 1.99 | 0.66 |
| 1:A:73:TYR:CD1 | 10:k5:162:TRP:CH2 | 2.83 | 0.66 |
| 4:MA:232:VAL:HG11 | 3:XA:111:ASN:N | 2.10 | 0.66 |
| 3:H3:125:ARG:NE | 8:k7:45:GLU:OE1 | 2.27 | 0.66 |
| 3:J3:113:LEU:HD13 | 11:a9:796:ALA:HB1 | 1.76 | 0.66 |
| 12:B3:201:CYC:HC | 12:B3:201:CYC:CMD | 1.99 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 5:N3:34:LEU:CA | 3:T3:84:ARG:HD3 | 2.25 | 0.66 |
| 3:U4:115:GLU:OE2 | 4:M4:70:SER:CB | 2.42 | 0.66 |
| 3:F4:113:LEU:N | 4:M4:5:THR:CG2 | 2.54 | 0.66 |
| 4:M4:71:PRO:HG2 | 4:M4:74:LEU:HB2 | 1.75 | 0.66 |
| 12:P4:201:CYC:HMD1 | 12:P4:201:CYC:NC | 2.09 | 0.66 |
| 8:K5:152:TYR:CZ | 8:U5:20:PRO:HB3 | 2.30 | 0.66 |
| 8:O5:102:THR:HB | 8:O5:103:PRO:HD2 | 1.76 | 0.66 |
| 12:C1:201:CYC:HMD1 | 12:C1:201:CYC:NC | 2.09 | 0.66 |
| 1:f5:161:SER:OXT | 1:V5:101:PRO:HG3 | 1.94 | 0.66 |
| 10:j5:929:PRO:HG2 | 1:J7:147:LYS:CE | 2.24 | 0.66 |
| 10:j5:934:ALA:HB2 | 1:J7:32:THR:HG23 | 1.75 | 0.66 |
| 10:k5:733:SER:CB | 1:J7:154:ASP:OD2 | 2.42 | 0.66 |
| 10:k5:1016:LEU:HB2 | 10:k5:1044:ASN:HD22 | 1.58 | 0.66 |
| 3:D1:111:ASN:ND2 | 4:M1:65:ARG:HD2 | 2.10 | 0.66 |
| 8:O7:102:THR:CB | 8:O7:103:PRO:CD | 2.64 | 0.66 |
| 8:g7:151:PHE:HZ | 1:v7:39:ARG:HG2 | 1.59 | 0.66 |
| 12:b7:201:CYC:HBB1 | 9:x7:21:ARG:NE | 2.10 | 0.66 |
| 2:A8:38:MET:HE1 | 3:B8:28:THR:OG1 | 1.93 | 0.66 |
| 12:A8:201:CYC:HMD1 | 12:A8:201:CYC:NC | 2.09 | 0.66 |
| 8:o7:39:ILE:CD1 | 8:o7:145:ASP:HB3 | 2.25 | 0.66 |
| 8:q7:49:ARG:NH1 | 3:H1:62:GLU:OE1 | 2.27 | 0.66 |
| 4:M8:29:PRO:HB3 | 11:a9:225:VAL:C | 2.16 | 0.66 |
| 11:a9:249:GLU:C | 11:a9:285:VAL:CG2 | 2.66 | 0.66 |
| 11:aA:643:LEU:HD11 | 11:aA:689:VAL:HG23 | 1.75 | 0.66 |
| 4:M1:17:VAL:O | 4:M1:44:SER:HA | 1.95 | 0.66 |
| 4:M1:118:TYR:CG | 3:X1:84:ARG:NE | 2.63 | 0.66 |
| 3:DA:108:ARG:HG2 | 4:MA:8:SER:O | 1.94 | 0.66 |
| 3:HA:92:TYR:OH | 3:HA:108:ARG:NE | 2.28 | 0.66 |
| 4:MA:260:ARG:NH1 | 4:MA:260:ARG:HG3 | 2.09 | 0.66 |
| 2:G3:65:TYR:CE1 | 2:A3:65:TYR:CE1 | 2.82 | 0.66 |
| 12:Z3:201:CYC:HMA2 | 4:M3:188:LEU:HD22 | 1.76 | 0.66 |
| 3:B4:120:LEU:CG | 4:M4:52:LEU:HB3 | 2.24 | 0.66 |
| 5:N3:31:TRP:HD1 | 2:S3:16:GLY:N | 1.93 | 0.66 |
| 12:W3:201:CYC:HMD1 | 12:W3:201:CYC:NC | 2.09 | 0.66 |
| 12:T4:201:CYC:HMD1 | 12:T4:201:CYC:NC | 2.09 | 0.66 |
| 4:M4:215:GLU:CG | 12:Z4:301:CYC:HAB1 | 2.24 | 0.66 |
| 12:K5:201:CYC:O2A | 1:J5:62:TYR:N | 2.26 | 0.66 |
| 1:L5:75:THR:HG22 | 8:G5:115:MET:HE1 | 1.76 | 0.66 |
| 8:G5:103:PRO:HA | 10:j5:557:VAL:CG1 | 2.22 | 0.66 |
| 10:k5:1056:PRO:CD | 10:k5:1057:LYS:N | 2.57 | 0.66 |
| 3:F6:82:CYS:HG | 12:F6:201:CYC:HAC2 | 1.60 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:S7:19:SER:OG | 8:G7:100:ASP:OD1 | 2.13 | 0.66 |
| 8:S7:66:VAL:HG12 | 8:S7:66:VAL:O | 1.96 | 0.66 |
| 8:i7:92:VAL:HG23 | 8:i7:156:LEU:HD12 | 1.75 | 0.66 |
| 8:W7:66:VAL:HG12 | 8:W7:66:VAL:O | 1.96 | 0.66 |
| 8:c7:50:ILE:HA | 8:c7:136:VAL:HG11 | 1.77 | 0.66 |
| 2:E8:15:GLN:HG3 | 11:a9:163:ASP:CB | 2.24 | 0.66 |
| 12:E8:201:CYC:HMD1 | 12:E8:201:CYC:NC | 2.09 | 0.66 |
| 2:X8:69:PRO:HB2 | 2:S9:39:GLU:HA | 1.73 | 0.66 |
| 4:M8:29:PRO:HG3 | 11:a9:226:PHE:HA | 1.75 | 0.66 |
| 5:N9:31:TRP:HB3 | 5:N9:32:PRO:CD | 2.23 | 0.66 |
| 11:aA:30:MET:HE3 | 11:aA:35:ARG:HA | 1.76 | 0.66 |
| 11:aA:339:GLU:N | 11:aA:339:GLU:OE2 | 2.27 | 0.66 |
| 11:aA:523:GLN:HE21 | 11:aA:548:LEU:HD13 | 1.60 | 0.66 |
| 11:aA:746:TYR:CB | 2:K1:14:SER:CA | 2.74 | 0.66 |
| 4:M1:164:ARG:HD3 | 4:M1:259:ARG:N | 2.10 | 0.66 |
| 2:EA:33:ARG:CG | 2:IA:25:GLN:NE2 | 2.58 | 0.66 |
| 2:IA:37:SER:CA | 2:IA:97:LEU:HD21 | 2.20 | 0.66 |
| 3:LA:120:LEU:HA | 11:aA:539:GLY:CA | 2.25 | 0.66 |
| 4:MA:17:VAL:O | 4:MA:44:SER:HA | 1.95 | 0.66 |
| 4:MA:58:TYR:CD2 | 11:aA:496:ARG:CZ | 2.72 | 0.66 |
| 5:NA:54:LEU:HD21 | 3:TA:84:ARG:CD | 2.24 | 0.66 |
| 2:SA:39:GLU:N | 2:X4:69:PRO:CG | 2.57 | 0.66 |
| 3:J3:84:ARG:HH11 | 11:a9:668:TYR:CB | 1.91 | 0.66 |
| 4:M4:215:GLU:N | 5:Z4:27:ALA:CA | 2.54 | 0.66 |
| 3:Q4:96:ALA:O | 3:Q4:98:LEU:N | 2.25 | 0.66 |
| 8:A5:112:VAL:CA | 1:F5:75:THR:HB | 2.23 | 0.66 |
| 12:C5:201:CYC:HB | 12:C5:201:CYC:HMA3 | 1.59 | 0.66 |
| 8:I5:27:LYS:O | 8:I5:29:PHE:CA | 2.42 | 0.66 |
| 8:e5:102:THR:HB | 8:e5:103:PRO:HD2 | 1.76 | 0.66 |
| 12:T5:201:CYC:HBB2 | 10:j5:482:GLN:CD | 2.20 | 0.66 |
| 10:j5:1147:TYR:CD1 | 11:aA:35:ARG:HB2 | 2.29 | 0.66 |
| 10:k5:803:LYS:HZ1 | 9:z7:43:ARG:HH11 | 1.41 | 0.66 |
| 10:k5:978:LEU:HD13 | 1:p7:107:ARG:HH22 | 1.60 | 0.66 |
| 10:k5:1118:THR:HG23 | 12:k5:1204:CYC:CBA | 2.25 | 0.66 |
| 8:g7:63:PRO:CG | 11:aA:336:ILE:CG2 | 2.73 | 0.66 |
| 1:h7:75:THR:HB | 8:i7:112:VAL:HA | 1.77 | 0.66 |
| 8:i7:89:LEU:CD1 | 8:i7:153:PHE:HZ | 2.07 | 0.66 |
| 8:c7:43:LEU:CD1 | 8:c7:141:LEU:HD21 | 2.26 | 0.66 |
| 8:c7:94:TYR:CD2 | 1:d7:9:ILE:HG23 | 2.29 | 0.66 |
| 3:U8:115:GLU:HG3 | 4:M8:71:PRO:HD2 | 1.77 | 0.66 |
| 12:M8:302:CYC:HAC2 | 3:S8:78:ARG:CA | 2.25 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:O8:115:GLU:CD | 5:Z8:69:GLU:OE2 | 2.37 | 0.66 |
| 3:Q8:120:LEU:CD1 | 3:Q8:122:THR:HB | 2.02 | 0.66 |
| 11:a9:338:VAL:CG2 | 11:a9:340:PRO:HD3 | 2.25 | 0.66 |
| 11:a9:643:LEU:HD12 | 11:a9:766:ASN:HB3 | 1.76 | 0.66 |
| 11:aA:30:MET:CG | 11:aA:34:ILE:O | 2.43 | 0.66 |
| 11:aA:377:VAL:O | 11:aA:391:VAL:CG2 | 2.44 | 0.66 |
| 11:aA:599:PRO:O | 11:aA:600:THR:HB | 1.94 | 0.66 |
| 11:aA:644:ARG:O | 11:aA:645:PRO:O | 2.13 | 0.66 |
| 4:M1:132:LEU:CD1 | 4:M1:142:PHE:HB2 | 2.24 | 0.66 |
| 12:Q1:201:CYC:HMD1 | 12:Q1:201:CYC:NC | 2.10 | 0.66 |
| 2:K3:14:SER:CA | 11:a9:746:TYR:CB | 2.73 | 0.66 |
| 6:M2:276:PRO:O | 1:j7:63:SER:CA | 2.34 | 0.66 |
| 7:N2:53:GLN:O | 7:N2:57:ASN:HB2 | 1.96 | 0.66 |
| 2:E4:15:GLN:HG3 | 11:aA:163:ASP:CB | 2.24 | 0.66 |
| 3:F4:115:GLU:O | 4:M4:3:VAL:HG11 | 1.95 | 0.66 |
| 4:M4:144:ARG:HH12 | 5:Z4:59:ARG:HH22 | 1.42 | 0.66 |
| 4:M4:235:PHE:CZ | 3:Y4:113:LEU:HD22 | 2.30 | 0.66 |
| 1:d5:161:SER:OG | 10:j5:696:ARG:CA | 2.44 | 0.66 |
| 8:Q5:159:ALA:O | 8:Q5:160:MET:C | 2.34 | 0.66 |
| 8:S5:66:VAL:O | 8:S5:66:VAL:HG12 | 1.96 | 0.66 |
| 3:J6:84:ARG:CD | 6:M6:185:PHE:CZ | 2.58 | 0.66 |
| 2:A6:63:PHE:HB2 | 2:A6:66:LEU:HD12 | 1.70 | 0.66 |
| 8:a7:90:ARG:CZ | 1:b7:16:GLY:CA | 2.73 | 0.66 |
| 1:d7:110:ASN:ND2 | 9:x7:51:VAL:H | 1.94 | 0.66 |
| 3:H8:81:ALA:HA | 3:H8:84:ARG:NE | 2.06 | 0.66 |
| 12:R8:201:CYC:HMD1 | 12:R8:201:CYC:NC | 2.10 | 0.66 |
| 5:Z8:42:SER:HA | 12:Z8:301:CYC:C3A | 2.26 | 0.66 |
| 11:a9:92:LYS:HE3 | 11:a9:92:LYS:CA | 2.26 | 0.66 |
| 11:aA:462:ARG:CG | 11:aA:462:ARG:HH11 | 2.09 | 0.66 |
| 11:aA:622:ALA:HB3 | 11:aA:625:ASP:HB2 | 1.76 | 0.66 |
| 1:A:13:ASP:OD1 | 8:a5:107:ILE:HD13 | 1.96 | 0.66 |
| 3:HA:72:ASN:ND2 | 12:HA:202:CYC:HBD2 | 2.09 | 0.66 |
| 7:N2:48:LEU:HD23 | 12:N2:101:CYC:HAA1 | 1.77 | 0.66 |
| 2:A3:60:TYR:CG | 2:A3:67:THR:CG2 | 2.79 | 0.66 |
| 12:B3:202:CYC:CMA | 11:a9:684:ASN:HD22 | 2.09 | 0.66 |
| 12:F3:201:CYC:O2A | 4:M3:35:THR:CA | 2.40 | 0.66 |
| 4:M3:120:LEU:CD2 | 3:X3:84:ARG:HH11 | 2.00 | 0.66 |
| 5:N3:31:TRP:HB3 | 5:N3:32:PRO:CD | 2.23 | 0.66 |
| 3:B1:88:ILE:CD1 | 12:B1:202:CYC:C3B | 2.58 | 0.66 |
| 12:V4:201:CYC:HMD1 | 12:V4:201:CYC:NC | 2.09 | 0.66 |
| 12:N4:201:CYC:HMD1 | 12:N4:201:CYC:NC | 2.09 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:Q4:4:ALA:CB | 3:Q4:99:ALA:O | 2.43 | 0.66 |
| 3:Q4:124:THR:HG21 | 3:Q4:171:ILE:O | 1.96 | 0.66 |
| 8:C5:6:LYS:O | 8:C5:6:LYS:HE2 | 1.95 | 0.66 |
| 8:E5:109:ILE:HD12 | 8:E5:109:ILE:O | 1.96 | 0.66 |
| 1:R5:120:GLY:O | 10:k5:703:LEU:HD11 | 1.96 | 0.66 |
| 1:X5:144:ASP:HB3 | 8:a5:38:ARG:HH22 | 1.57 | 0.66 |
| 7:N6:1:MET:H1 | 7:N6:1:MET:HE2 | 1.60 | 0.66 |
| 7:N6:53:GLN:O | 7:N6:57:ASN:HB2 | 1.96 | 0.66 |
| 10:j5:178:ILE:O | 10:j5:178:ILE:HG12 | 1.94 | 0.66 |
| 10:j5:277:ILE:HG23 | 10:j5:284:PRO:N | 2.11 | 0.66 |
| 10:k5:261:ILE:O | 10:k5:261:ILE:HG13 | 1.96 | 0.66 |
| 10:k5:816:ARG:HG2 | 10:k5:816:ARG:O | 1.95 | 0.66 |
| 8:K7:66:VAL:O | 8:K7:66:VAL:HG12 | 1.96 | 0.66 |
| 8:k7:78:THR:HG21 | 11:a9:61:TYR:OH | 1.95 | 0.66 |
| 12:X8:201:CYC:HMD1 | 12:X8:201:CYC:NC | 2.09 | 0.66 |
| 4:M9:252:LEU:HD13 | 12:Z9:202:CYC:O1D | 1.95 | 0.66 |
| 11:a9:89:ALA:HB1 | 11:a9:92:LYS:HZ2 | 1.59 | 0.66 |
| 11:a9:312:ASP:C | 11:a9:314:SER:N | 2.45 | 0.66 |
| 11:a9:595:ARG:HG3 | 11:a9:596:THR:N | 2.11 | 0.66 |
| 11:aA:38:VAL:HG12 | 11:aA:39:PRO:HD2 | 1.78 | 0.66 |
| 11:aA:92:LYS:HE3 | 11:aA:92:LYS:CA | 2.26 | 0.66 |
| 11:aA:106:LEU:HD23 | 11:aA:106:LEU:C | 2.21 | 0.66 |
| 11:aA:584:ARG:O | 11:aA:588:VAL:O | 2.12 | 0.66 |
| 5:N1:29:HIS:CD2 | 12:T1:301:CYC:OB | 2.48 | 0.66 |
| 12:C2:201:CYC:HMD1 | 12:C2:201:CYC:NC | 2.10 | 0.66 |
| 4:MA:252:LEU:HD13 | 12:ZA:202:CYC:O1D | 1.95 | 0.66 |
| 5:NA:50:LEU:HD22 | 12:TA:301:CYC:O1D | 1.93 | 0.66 |
| 6:M2:278:ARG:NH2 | 1:j7:67:ARG:NH1 | 2.43 | 0.66 |
| 3:L3:1:MET:SD | 3:L3:104:VAL:CG1 | 2.84 | 0.66 |
| 4:M3:246:ALA:CA | 12:X3:201:CYC:HBB2 | 2.26 | 0.66 |
| 5:N3:37:HIS:CD2 | 12:T3:301:CYC:CMA | 2.79 | 0.66 |
| 3:H4:84:ARG:CD | 11:aA:131:TYR:CE1 | 2.73 | 0.66 |
| 4:M4:215:GLU:OE2 | 12:Z4:301:CYC:CAB | 2.43 | 0.66 |
| 2:N4:112:GLY:CA | 5:Z4:34:LEU:H | 2.01 | 0.66 |
| 3:Q4:7:LYS:HD2 | 3:Q4:101:ASP:CG | 2.21 | 0.66 |
| 5:Z4:41:GLN:HG2 | 12:Z4:301:CYC:HMB1 | 1.56 | 0.66 |
| 1:D5:87:TYR:HE2 | 9:z5:38:PHE:CE2 | 2.14 | 0.66 |
| 8:E5:66:VAL:HG12 | 8:E5:66:VAL:O | 1.96 | 0.66 |
| 8:W5:66:VAL:O | 8:W5:66:VAL:HG12 | 1.96 | 0.66 |
| 9:z5:56:LEU:HD12 | 9:z5:56:LEU:H | 1.61 | 0.66 |
| 10:k5:17:PHE:CD1 | 10:k5:19:THR:HG22 | 2.29 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:k5:362:LYS:CD | 10:k5:363:HIS:HD2 | 1.82 | 0.66 |
| 10:k5:741:GLN:CG | 1:D7:77:ARG:HH22 | 1.97 | 0.66 |
| 10:k5:934:ALA:HB3 | 1:D7:32:THR:HG22 | 1.77 | 0.66 |
| 10:k5:1005:LEU:CD1 | 10:k5:1016:LEU:HD21 | 2.26 | 0.66 |
| 10:k5:1125:ARG:CZ | 1:n7:114:GLU:CB | 2.74 | 0.66 |
| 3:D1:68:ARG:NH1 | 3:X1:68:ARG:HH12 | 1.94 | 0.66 |
| 8:i7:66:VAL:O | 8:i7:66:VAL:HG12 | 1.96 | 0.66 |
| 8:a7:37:LEU:HD21 | 1:b7:27:LEU:HD12 | 1.77 | 0.66 |
| 8:o7:30:VAL:HG12 | 1:p7:31:PHE:CD1 | 2.31 | 0.66 |
| 8:q7:76:LYS:HZ3 | 11:aA:604:ALA:HB1 | 1.61 | 0.66 |
| 8:u7:23:LEU:HA | 1:v7:38:VAL:CG2 | 2.25 | 0.66 |
| 4:M9:29:PRO:HD2 | 11:a9:378:GLU:OE1 | 1.95 | 0.66 |
| 4:M9:273:ILE:HD13 | 3:V9:75:PRO:HD2 | 1.77 | 0.66 |
| 5:N9:23:SER:O | 5:N9:25:THR:N | 2.26 | 0.66 |
| 5:Z8:21:ALA:CB | 5:Z8:68:LEU:HD11 | 2.23 | 0.66 |
| 2:E9:33:ARG:CG | 2:I9:25:GLN:NE2 | 2.58 | 0.66 |
| 11:a9:38:VAL:HG12 | 11:a9:39:PRO:HD2 | 1.78 | 0.66 |
| 11:a9:462:ARG:HH11 | 11:a9:462:ARG:CG | 2.09 | 0.66 |
| 11:a9:629:LYS:HA | 11:a9:629:LYS:HZ3 | 1.59 | 0.66 |
| 11:aA:524:MET:O | 11:aA:524:MET:HG3 | 1.95 | 0.66 |
| 11:aA:595:ARG:HG3 | 11:aA:596:THR:N | 2.11 | 0.66 |
| 4:M1:134:ASN:OD1 | 5:N1:1:MET:N | 2.29 | 0.66 |
| 2:AA:60:TYR:CG | 2:AA:67:THR:CG2 | 2.79 | 0.66 |
| 2:QA:120:PHE:CD2 | 3:TA:83:LEU:HD11 | 2.29 | 0.66 |
| 3:L2:75:PRO:CG | 3:L2:78:ARG:HG3 | 2.25 | 0.66 |
| 6:M2:28:ASN:CA | 8:O5:80:LEU:CD2 | 2.69 | 0.66 |
| 7:N2:49:LEU:HD11 | 3:B2:88:ILE:HD11 | 1.77 | 0.66 |
| 12:B1:202:CYC:HBA2 | 11:aA:684:ASN:N | 2.09 | 0.66 |
| 2:G4:53:LYS:HE3 | 11:aA:71:ILE:HG23 | 1.77 | 0.66 |
| 4:M4:260:ARG:NH1 | 4:M4:260:ARG:HG3 | 2.09 | 0.66 |
| 3:O4:120:LEU:CD2 | 5:Z4:14:LYS:HZ2 | 2.09 | 0.66 |
| 3:Q4:72:ASN:ND2 | 12:Z4:301:CYC:HMD2 | 2.10 | 0.66 |
| 3:Y4:89:ILE:CB | 3:Y4:92:TYR:CZ | 2.78 | 0.66 |
| 3:Y4:110:LEU:CD2 | 3:Y4:167:ALA:HA | 2.26 | 0.66 |
| 1:B5:2:GLN:OE1 | 10:k5:551:MET:CE | 2.44 | 0.66 |
| 8:I5:6:LYS:HE2 | 8:I5:6:LYS:O | 1.95 | 0.66 |
| 8:U5:66:VAL:HG12 | 8:U5:66:VAL:O | 1.96 | 0.66 |
| 6:M6:278:ARG:H | 1:d7:62:TYR:CB | 2.09 | 0.66 |
| 10:j5:298:ARG:NH2 | 10:j5:310:LYS:HD3 | 2.09 | 0.66 |
| 10:j5:1064:LYS:CD | 10:j5:1065:HIS:CD2 | 2.77 | 0.66 |
| 12:G6:201:CYC:HMD1 | 12:G6:201:CYC:NC | 2.09 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:k7:66:VAL:HG12 | 8:k7:66:VAL:O | 1.95 | 0.66 |
| 8:c7:12:ASP:N | 1:d7:94:TYR:CZ | 2.62 | 0.66 |
| 8:c7:66:VAL:HG12 | 8:c7:66:VAL:O | 1.96 | 0.66 |
| 12:V8:201:CYC:HMD1 | 12:V8:201:CYC:NC | 2.09 | 0.66 |
| 3:H8:14:LEU:CD2 | 11:a9:85:ALA:HA | 2.21 | 0.66 |
| 4:M8:205:ASP:HB3 | 5:Z8:59:ARG:NH1 | 2.10 | 0.66 |
| 5:N9:20:ILE:HG21 | 5:N9:60:ILE:CD1 | 2.26 | 0.66 |
| 12:E9:201:CYC:HMD1 | 12:E9:201:CYC:NC | 2.10 | 0.66 |
| 11:a9:56:ILE:HG22 | 11:a9:56:ILE:O | 1.96 | 0.66 |
| 11:a9:360:ALA:HA | 11:a9:363:GLN:NE2 | 2.11 | 0.66 |
| 12:T1:302:CYC:HC | 12:T1:302:CYC:CMD | 1.99 | 0.66 |
| 3:LA:56:ALA:HA | 3:LA:86:MET:HE1 | 1.76 | 0.66 |
| 4:MA:134:ASN:ND2 | 5:NA:1:MET:N | 2.43 | 0.66 |
| 5:NA:20:ILE:HG21 | 5:NA:60:ILE:CD1 | 2.26 | 0.66 |
| 2:OA:33:ARG:HE | 2:YA:28:ASN:HD21 | 1.44 | 0.66 |
| 12:SA:201:CYC:HMD1 | 12:SA:201:CYC:NC | 2.09 | 0.66 |
| 3:TA:28:THR:HG23 | 2:X4:67:THR:HB | 1.66 | 0.66 |
| 3:D3:68:ARG:HH12 | 3:X3:68:ARG:HH12 | 1.43 | 0.66 |
| 3:L3:111:ASN:ND2 | 11:a9:807:GLN:O | 2.28 | 0.66 |
| 5:N3:20:ILE:HD13 | 5:N3:60:ILE:HD13 | 1.78 | 0.66 |
| 3:F4:115:GLU:HB3 | 4:M4:3:VAL:CG1 | 2.14 | 0.66 |
| 12:H4:202:CYC:HC | 12:H4:202:CYC:CMD | 1.99 | 0.66 |
| 3:O4:107:ASP:OD1 | 5:Z4:66:ARG:NE | 2.28 | 0.66 |
| 3:Y4:88:ILE:HA | 3:Y4:91:ARG:CZ | 2.25 | 0.66 |
| 8:G5:61:ILE:CG1 | 8:o7:67:SER:HB3 | 2.25 | 0.66 |
| 1:f5:18:TYR:CG | 10:j5:165:ARG:HD3 | 2.26 | 0.66 |
| 1:f5:18:TYR:CG | 10:j5:165:ARG:HG3 | 2.31 | 0.66 |
| 8:Y5:66:VAL:HG12 | 8:Y5:66:VAL:O | 1.96 | 0.66 |
| 1:Z5:127:VAL:HG11 | 10:k5:697:PHE:C | 2.17 | 0.66 |
| 7:N6:2:TYR:HD1 | 7:N6:2:TYR:H | 1.39 | 0.66 |
| 10:j5:879:ASP:OD1 | 9:w7:25:ASN:ND2 | 2.29 | 0.66 |
| 1:f7:67:ARG:CZ | 11:aA:307:ARG:HB3 | 2.23 | 0.66 |
| 2:A8:33:ARG:HE | 2:K8:28:ASN:HD21 | 1.44 | 0.66 |
| 8:s7:66:VAL:HG12 | 8:s7:66:VAL:O | 1.96 | 0.66 |
| 8:u7:2:SER:CB | 1:v7:5:ILE:HB | 2.26 | 0.66 |
| 2:G8:53:LYS:HE3 | 11:a9:71:ILE:HG23 | 1.78 | 0.66 |
| 12:H8:202:CYC:HC | 12:H8:202:CYC:CMD | 1.99 | 0.66 |
| 4:M8:128:ALA:CB | 4:M8:142:PHE:CZ | 2.78 | 0.66 |
| 4:M8:217:VAL:CG2 | 5:Z8:30:PRO:CD | 2.71 | 0.66 |
| 4:M9:17:VAL:O | 4:M9:44:SER:HA | 1.95 | 0.66 |
| 12:J9:202:CYC:CGA | 11:a9:511:LYS:HD2 | 2.26 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:aA:360:ALA:HA | 11:aA:363:GLN:OE1 | 1.96 | 0.66 |
| 11:aA:448:ASN:OD1 | 11:aA:474:PHE:CD1 | 2.49 | 0.66 |
| 11:aA:639:GLN:HE21 | 11:aA:639:GLN:C | 2.04 | 0.66 |
| 5:NA:70:ILE:HG22 | 3:TA:119:ALA:HB3 | 1.71 | 0.66 |
| 2:S1:16:GLY:N | 5:N1:31:TRP:CD1 | 2.64 | 0.66 |
| 3:D4:150:ARG:HG3 | 2:C1:140:SER:CB | 2.10 | 0.66 |
| 2:O3:60:TYR:CG | 2:O3:67:THR:CG2 | 2.79 | 0.66 |
| 3:O4:104:VAL:CG2 | 5:Z4:61:LYS:HE2 | 2.26 | 0.66 |
| 8:A5:121:THR:HG23 | 12:A5:201:CYC:C1C | 2.25 | 0.66 |
| 8:E5:23:LEU:HD13 | 1:F5:42:ALA:HB2 | 1.78 | 0.66 |
| 1:H5:107:ARG:NE | 9:i5:21:ARG:HD3 | 2.10 | 0.66 |
| 8:c5:59:PHE:CD2 | 6:M6:12:ILE:HD13 | 2.31 | 0.66 |
| 8:S5:115:MET:CE | 1:X5:75:THR:HG22 | 2.26 | 0.66 |
| 8:W5:130:VAL:HG21 | 8:W5:160:MET:CE | 2.26 | 0.66 |
| 1:Z5:124:ALA:HB1 | 10:k5:699:SER:HB3 | 1.77 | 0.66 |
| 10:j5:1054:SER:N | 1:r7:106:GLU:O | 2.29 | 0.66 |
| 10:k5:178:ILE:HG12 | 10:k5:178:ILE:O | 1.94 | 0.66 |
| 10:k5:804:GLU:OE1 | 9:z7:30:LYS:HE3 | 1.95 | 0.66 |
| 10:k5:1055:SER:CB | 12:k5:1203:CYC:CBB | 2.60 | 0.66 |
| 1:R7:53:LYS:HZ1 | 8:M7:120:GLN:HG3 | 1.59 | 0.66 |
| 8:S7:64:ASP:OD2 | 8:I7:69:GLY:HA3 | 1.96 | 0.66 |
| 8:g7:102:THR:HB | 8:g7:103:PRO:HD2 | 1.76 | 0.66 |
| 8:c7:96:ILE:HG13 | 8:c7:152:TYR:CB | 2.23 | 0.66 |
| 12:c7:201:CYC:HMD1 | 12:c7:201:CYC:NC | 2.02 | 0.66 |
| 8:q7:120:GLN:HG3 | 1:v7:53:LYS:NZ | 2.09 | 0.66 |
| 4:M8:99:VAL:HB | 3:Q8:1:MET:CE | 2.23 | 0.66 |
| 5:Z8:14:LYS:HE2 | 5:Z8:50:LEU:CD2 | 2.26 | 0.66 |
| 5:Z8:20:ILE:HG21 | 5:Z8:60:ILE:CD1 | 2.26 | 0.66 |
| 5:Z8:22:LEU:HD21 | 5:Z8:26:LEU:CD2 | 2.08 | 0.66 |
| 5:Z8:42:SER:HA | 12:Z8:301:CYC:HMA2 | 0.73 | 0.66 |
| 3:F9:36:LYS:HB2 | 3:F9:156:LEU:HD11 | 1.77 | 0.66 |
| 12:G9:201:CYC:HMD1 | 12:G9:201:CYC:NC | 2.09 | 0.66 |
| 11:a9:106:LEU:HD23 | 11:a9:106:LEU:C | 2.21 | 0.66 |
| 11:a9:714:ARG:HG2 | 11:a9:808:LEU:O | 1.96 | 0.66 |
| 11:aA:587:THR:OG1 | 11:aA:588:VAL:N | 2.29 | 0.66 |
| 11:aA:714:ARG:HG2 | 11:aA:808:LEU:O | 1.96 | 0.66 |
| 5:N1:20:ILE:HD13 | 5:N1:60:ILE:HD13 | 1.78 | 0.66 |
| 3:FA:68:ARG:CZ | 3:ZA:68:ARG:CZ | 2.72 | 0.65 |
| 3:FA:158:ASN:OD1 | 3:FA:158:ASN:N | 2.28 | 0.65 |
| 2:A1:60:TYR:CG | 2:A1:67:THR:CG2 | 2.79 | 0.65 |
| 12:D4:201:CYC:HC | 12:D4:201:CYC:CMD | 1.99 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:N3:39:PRO:HB3 | 3:T3:113:LEU:CA | 2.18 | 0.65 |
| 4:M4:100:SER:N | 3:Q4:1:MET:HE2 | 2.06 | 0.65 |
| 3:O4:112:GLY:O | 5:Z4:70:ILE:CB | 2.35 | 0.65 |
| 12:K5:201:CYC:O1D | 1:J5:62:TYR:CZ | 2.49 | 0.65 |
| 5:Z4:20:ILE:HD13 | 5:Z4:60:ILE:HD13 | 1.78 | 0.65 |
| 12:F5:201:CYC:HBB2 | 10:k5:588:VAL:HG21 | 1.78 | 0.65 |
| 1:d5:127:VAL:HB | 10:j5:698:GLY:HA3 | 1.78 | 0.65 |
| 1:f5:19:LEU:HD11 | 10:j5:172:LEU:HD12 | 1.75 | 0.65 |
| 1:P5:114:GLU:HG3 | 10:k5:496:GLU:OE2 | 1.95 | 0.65 |
| 12:T5:201:CYC:O2A | 10:j5:483:PHE:CE1 | 2.48 | 0.65 |
| 1:X5:50:THR:HG21 | 8:a5:49:ARG:HH12 | 1.53 | 0.65 |
| 10:k5:277:ILE:HG23 | 10:k5:284:PRO:N | 2.11 | 0.65 |
| 10:k5:743:VAL:HG12 | 12:D7:201:CYC:CGD | 2.26 | 0.65 |
| 8:k7:68:PRO:HG2 | 11:a9:334:LYS:CG | 2.26 | 0.65 |
| 8:a7:66:VAL:HG12 | 8:a7:66:VAL:O | 1.96 | 0.65 |
| 8:c7:54:ALA:HB2 | 8:c7:133:MET:HA | 1.76 | 0.65 |
| 2:A8:60:TYR:CG | 2:A8:67:THR:CG2 | 2.79 | 0.65 |
| 8:m7:66:VAL:O | 8:m7:66:VAL:HG12 | 1.96 | 0.65 |
| 8:o7:39:ILE:HD11 | 8:o7:145:ASP:CB | 2.26 | 0.65 |
| 8:q7:66:VAL:CG1 | 11:aA:61:TYR:CD1 | 2.79 | 0.65 |
| 8:u7:94:TYR:HH | 1:v7:17:LYS:C | 1.93 | 0.65 |
| 12:T8:201:CYC:HMD1 | 12:T8:201:CYC:NC | 2.09 | 0.65 |
| 2:X8:69:PRO:N | 2:S9:42:ARG:HE | 1.93 | 0.65 |
| 4:M8:17:VAL:O | 4:M8:44:SER:HA | 1.95 | 0.65 |
| 3:L9:14:LEU:CD1 | 11:a9:358:PRO:HB2 | 2.24 | 0.65 |
| 12:L9:202:CYC:O2A | 11:a9:404:TYR:N | 2.29 | 0.65 |
| 4:M9:41:ASN:HD21 | 3:B9:119:ALA:CB | 2.09 | 0.65 |
| 12:I9:201:CYC:HMD1 | 12:I9:201:CYC:NC | 2.09 | 0.65 |
| 12:R9:202:CYC:HC | 12:R9:202:CYC:CMD | 1.99 | 0.65 |
| 11:a9:283:GLN:CG | 11:a9:284:PRO:HD2 | 2.25 | 0.65 |
| 11:a9:365:LYS:NZ | 11:a9:365:LYS:HB2 | 2.10 | 0.65 |
| 11:aA:620:ALA:O | 3:H1:70:GLY:HA2 | 1.97 | 0.65 |
| 2:K1:115:GLU:CD | 2:K1:118:ARG:HH12 | 2.04 | 0.65 |
| 3:HA:113:LEU:HD11 | 12:HA:202:CYC:C2B | 2.25 | 0.65 |
| 2:IA:1:MET:HE1 | 2:IA:108:TYR:HE1 | 1.59 | 0.65 |
| 2:OA:60:TYR:CG | 2:OA:67:THR:CG2 | 2.79 | 0.65 |
| 3:B3:82:CYS:SG | 12:B3:202:CYC:HAC1 | 2.31 | 0.65 |
| 3:D4:150:ARG:HH11 | 2:C1:140:SER:CB | 2.09 | 0.65 |
| 3:F4:110:LEU:HD11 | 3:F4:167:ALA:HA | 1.78 | 0.65 |
| 4:M4:113:ILE:HD11 | 4:M4:143:VAL:CG2 | 2.21 | 0.65 |
| 2:N4:33:ARG:NE | 2:X4:28:ASN:HD21 | 1.91 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:O5:75:GLU:CD | 8:i7:56:ASP:OD2 | 2.40 | 0.65 |
| 5:Z4:41:GLN:CG | 12:Z4:301:CYC:C3B | 2.68 | 0.65 |
| 8:I5:66:VAL:HG12 | 8:I5:66:VAL:O | 1.96 | 0.65 |
| 8:c5:73:TYR:HE2 | 6:M6:9:ARG:HH12 | 1.41 | 0.65 |
| 8:Q5:130:VAL:HG21 | 8:Q5:160:MET:CE | 2.26 | 0.65 |
| 8:S5:14:GLU:HG2 | 10:j5:538:PHE:HZ | 1.58 | 0.65 |
| 8:S5:107:ILE:CD1 | 1:T5:13:ASP:CG | 2.69 | 0.65 |
| 6:M6:250:GLY:HA2 | 3:H6:120:LEU:HA | 1.77 | 0.65 |
| 7:N6:49:LEU:HD11 | 3:B6:88:ILE:HD11 | 1.77 | 0.65 |
| 10:j5:141:GLU:OE2 | 10:j5:141:GLU:N | 2.24 | 0.65 |
| 10:j5:388:ARG:NH2 | 10:j5:392:SER:HA | 2.10 | 0.65 |
| 10:k5:822:ARG:HB2 | 10:k5:822:ARG:NH1 | 2.04 | 0.65 |
| 10:k5:974:LEU:CG | 1:p7:106:GLU:OE2 | 2.43 | 0.65 |
| 10:k5:1077:ILE:HG22 | 12:k5:1203:CYC:CBA | 2.26 | 0.65 |
| 1:J7:75:THR:HB | 8:K7:112:VAL:N | 2.09 | 0.65 |
| 12:d7:201:CYC:C1B | 9:x7:38:PHE:HE1 | 2.08 | 0.65 |
| 3:F8:106:GLU:O | 4:M8:6:THR:O | 2.13 | 0.65 |
| 3:H8:14:LEU:HD13 | 11:a9:85:ALA:HB1 | 1.77 | 0.65 |
| 3:F1:107:ASP:HB3 | 11:aA:646:ASN:ND2 | 2.11 | 0.65 |
| 3:H9:116:THR:HG21 | 11:a9:449:ASN:HD21 | 1.59 | 0.65 |
| 11:a9:524:MET:O | 11:a9:524:MET:HG3 | 1.95 | 0.65 |
| 11:aA:99:ALA:CB | 11:aA:100:PRO:HD3 | 2.02 | 0.65 |
| 11:aA:445:THR:O | 11:aA:542:ALA:O | 2.14 | 0.65 |
| 12:YA:201:CYC:HMD1 | 12:YA:201:CYC:NC | 2.09 | 0.65 |
| 3:J2:84:ARG:CD | 6:M2:185:PHE:CZ | 2.58 | 0.65 |
| 3:D3:68:ARG:NH1 | 3:X3:68:ARG:HH12 | 1.94 | 0.65 |
| 4:M4:5:THR:C | 4:M4:6:THR:HG1 | 1.97 | 0.65 |
| 4:M4:99:VAL:HB | 3:Q4:1:MET:HE1 | 1.78 | 0.65 |
| 4:M4:214:GLY:CA | 5:Z4:28:HIS:CD2 | 2.78 | 0.65 |
| 3:O4:111:ASN:O | 5:Z4:67:ILE:HG22 | 1.96 | 0.65 |
| 8:A5:66:VAL:HG12 | 8:A5:66:VAL:O | 1.96 | 0.65 |
| 8:A5:90:ARG:HD3 | 1:B5:18:TYR:CD1 | 2.31 | 0.65 |
| 8:E5:72:ALA:HB2 | 12:E5:201:CYC:C1C | 2.25 | 0.65 |
| 12:J5:201:CYC:HBB2 | 9:i5:42:GLN:HE21 | 1.60 | 0.65 |
| 8:c5:66:VAL:HG12 | 8:c5:66:VAL:O | 1.96 | 0.65 |
| 8:W5:17:TYR:HB2 | 1:X5:45:SER:HB3 | 1.76 | 0.65 |
| 1:Z5:83:ARG:CZ | 10:k5:379:PHE:HE2 | 2.07 | 0.65 |
| 1:b5:114:GLU:HB3 | 10:k5:491:THR:OG1 | 1.96 | 0.65 |
| 7:N6:48:LEU:HD23 | 12:N6:101:CYC:HAA1 | 1.77 | 0.65 |
| 10:j5:965:GLN:N | 1:t7:69:GLY:HA3 | 2.09 | 0.65 |
| 10:j5:1005:LEU:CD1 | 10:j5:1016:LEU:HD21 | 2.26 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:k5:298:ARG:NH2 | 10:k5:310:LYS:HD3 | 2.09 | 0.65 |
| 10:k5:929:PRO:CB | 1:D7:147:LYS:HG2 | 2.26 | 0.65 |
| 8:S7:161:GLN:NE2 | 1:H7:49:THR:HG22 | 2.11 | 0.65 |
| 8:E7:66:VAL:HG12 | 8:E7:66:VAL:O | 1.96 | 0.65 |
| 8:g7:29:PHE:HE1 | 8:g7:98:ALA:C | 2.02 | 0.65 |
| 8:Y7:66:VAL:HG12 | 8:Y7:66:VAL:O | 1.96 | 0.65 |
| 8:u7:16:ARG:O | 1:v7:94:TYR:CE1 | 2.49 | 0.65 |
| 2:X8:28:ASN:HD21 | 2:N8:33:ARG:HE | 1.44 | 0.65 |
| 3:L8:68:ARG:C | 3:L8:69:PRO:O | 2.40 | 0.65 |
| 3:L8:82:CYS:HA | 12:a9:901:CYC:C1D | 2.25 | 0.65 |
| 3:L8:113:LEU:CD1 | 12:a9:901:CYC:CHB | 2.74 | 0.65 |
| 12:M8:302:CYC:OC | 3:S8:78:ARG:NE | 2.28 | 0.65 |
| 2:I9:37:SER:O | 2:I9:97:LEU:CG | 2.43 | 0.65 |
| 11:aA:287:ALA:H | 11:aA:289:THR:HG23 | 1.62 | 0.65 |
| 12:E2:201:CYC:HMD1 | 12:E2:201:CYC:NC | 2.10 | 0.65 |
| 4:MA:273:ILE:HD13 | 3:VA:75:PRO:HG3 | 1.73 | 0.65 |
| 2:O1:60:TYR:CG | 2:O1:67:THR:CG2 | 2.79 | 0.65 |
| 3:B3:127:VAL:N | 12:B3:202:CYC:HMC1 | 2.11 | 0.65 |
| 4:M3:260:ARG:HG3 | 4:M3:260:ARG:NH1 | 2.09 | 0.65 |
| 12:S3:201:CYC:HMD1 | 12:S3:201:CYC:NC | 2.10 | 0.65 |
| 12:H4:201:CYC:HAA1 | 11:aA:264:ASP:OD1 | 1.96 | 0.65 |
| 12:M4:301:CYC:C3B | 3:Y4:88:ILE:HD12 | 2.27 | 0.65 |
| 1:N5:110:ASN:HD21 | 10:k5:692:LEU:HB2 | 1.51 | 0.65 |
| 12:D5:201:CYC:CBB | 9:z5:42:GLN:NE2 | 2.59 | 0.65 |
| 8:G5:121:THR:HG23 | 12:G5:201:CYC:C1C | 2.25 | 0.65 |
| 1:H5:14:VAL:CG1 | 10:j5:555:ALA:HA | 2.26 | 0.65 |
| 8:I5:102:THR:HB | 8:I5:103:PRO:HD2 | 1.76 | 0.65 |
| 8:c5:120:GLN:HG3 | 1:f5:53:LYS:HZ1 | 1.60 | 0.65 |
| 12:X5:201:CYC:HBB2 | 10:j5:520:ARG:CG | 2.26 | 0.65 |
| 2:K6:28:ASN:HD21 | 2:A6:33:ARG:HE | 1.44 | 0.65 |
| 8:A7:66:VAL:HG12 | 8:A7:66:VAL:O | 1.96 | 0.65 |
| 10:j5:1069:ARG:HG3 | 10:j5:1069:ARG:HH11 | 1.61 | 0.65 |
| 10:j5:1070:ALA:HB1 | 10:j5:1071:PRO:CD | 2.26 | 0.65 |
| 10:k5:985:ALA:O | 10:k5:988:ALA:HB3 | 1.96 | 0.65 |
| 8:O7:66:VAL:HG12 | 8:O7:66:VAL:O | 1.96 | 0.65 |
| 12:j7:201:CYC:HMA2 | 9:y7:38:PHE:HD1 | 1.60 | 0.65 |
| 8:e7:66:VAL:O | 8:e7:66:VAL:HG12 | 1.96 | 0.65 |
| 8:o7:2:SER:CB | 1:p7:5:ILE:HB | 2.26 | 0.65 |
| 8:o7:17:TYR:OH | 1:p7:89:LEU:HG | 1.96 | 0.65 |
| 5:N9:70:ILE:CG2 | 3:T9:116:THR:HA | 2.17 | 0.65 |
| 2:O9:60:TYR:CG | 2:O9:67:THR:CG2 | 2.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:K9:15:GLN:HA | 11:a9:393:ARG:HD2 | 1.79 | 0.65 |
| 11:a9:245:ALA:HB3 | 12:a9:901:CYC:CBB | 2.26 | 0.65 |
| 11:a9:371:VAL:CG1 | 11:a9:507:PHE:CD2 | 2.80 | 0.65 |
| 11:a9:377:VAL:HG11 | 11:a9:390:ALA:C | 2.21 | 0.65 |
| 11:a9:643:LEU:HD13 | 11:a9:766:ASN:CB | 2.26 | 0.65 |
| 11:aA:821:ARG:CZ | 3:L1:120:LEU:O | 2.45 | 0.65 |
| 4:M1:188:LEU:HD22 | 12:Z1:202:CYC:HMA2 | 1.76 | 0.65 |
| 12:EA:201:CYC:HMD1 | 12:EA:201:CYC:NC | 2.10 | 0.65 |
| 4:MA:263:PRO:CB | 3:VA:119:ALA:HB2 | 2.11 | 0.65 |
| 4:MA:267:LEU:HD11 | 3:VA:120:LEU:HA | 1.78 | 0.65 |
| 2:K3:28:ASN:HD21 | 2:A3:33:ARG:HE | 1.44 | 0.65 |
| 6:M2:45:ILE:HD12 | 8:i7:78:THR:HG22 | 1.78 | 0.65 |
| 6:M2:57:GLU:CD | 8:i7:76:LYS:HE3 | 2.22 | 0.65 |
| 5:N3:20:ILE:HG21 | 5:N3:60:ILE:CD1 | 2.26 | 0.65 |
| 12:E4:201:CYC:HMD1 | 12:E4:201:CYC:NC | 2.09 | 0.65 |
| 3:F4:109:CYS:O | 4:M4:6:THR:CG2 | 2.44 | 0.65 |
| 4:M4:100:SER:OG | 2:P4:13:ASP:OD2 | 2.14 | 0.65 |
| 2:N4:112:GLY:HA2 | 5:Z4:33:GLY:C | 2.21 | 0.65 |
| 3:Q4:52:ILE:HD11 | 3:Q4:87:GLU:HA | 1.78 | 0.65 |
| 8:K5:29:PHE:CE1 | 8:K5:99:GLY:HA3 | 2.31 | 0.65 |
| 3:Y4:89:ILE:CA | 3:Y4:92:TYR:CZ | 2.76 | 0.65 |
| 1:B5:11:ASN:HA | 10:k5:552:VAL:HG21 | 1.78 | 0.65 |
| 12:C5:201:CYC:HC | 12:C5:201:CYC:CMD | 2.10 | 0.65 |
| 8:G5:16:ARG:O | 1:H5:94:TYR:OH | 2.08 | 0.65 |
| 1:T5:87:TYR:HE2 | 10:j5:483:PHE:CE2 | 2.13 | 0.65 |
| 1:T5:110:ASN:OD1 | 10:j5:692:LEU:HB3 | 1.96 | 0.65 |
| 12:A7:201:CYC:CMD | 12:A7:201:CYC:HC | 2.10 | 0.65 |
| 9:z5:23:LEU:O | 9:z5:23:LEU:HD12 | 1.96 | 0.65 |
| 9:i5:23:LEU:HD12 | 9:i5:23:LEU:O | 1.96 | 0.65 |
| 10:j5:985:ALA:O | 10:j5:988:ALA:HB3 | 1.96 | 0.65 |
| 10:k5:822:ARG:HG3 | 1:B7:106:GLU:OE2 | 1.96 | 0.65 |
| 10:k5:1064:LYS:HD2 | 10:k5:1065:HIS:CA | 2.27 | 0.65 |
| 12:C7:201:CYC:HC | 12:C7:201:CYC:CMD | 2.10 | 0.65 |
| 1:H7:140:LEU:CD1 | 11:aA:561:ALA:CA | 2.74 | 0.65 |
| 8:I7:102:THR:CB | 8:I7:103:PRO:CD | 2.64 | 0.65 |
| 8:g7:37:LEU:HD21 | 1:h7:27:LEU:HD12 | 1.77 | 0.65 |
| 8:o7:97:VAL:CG2 | 1:p7:19:LEU:HD11 | 2.26 | 0.65 |
| 8:o7:121:THR:HG23 | 12:o7:201:CYC:CMC | 2.14 | 0.65 |
| 2:X8:74:TYR:HE1 | 2:S9:35:THR:HG23 | 1.41 | 0.65 |
| 4:M8:98:ASP:O | 4:M8:99:VAL:HG23 | 1.95 | 0.65 |
| 4:M8:228:SER:HA | 3:Y8:88:ILE:HD12 | 1.77 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:O8:92:TYR:OH | 3:O8:108:ARG:CD | 2.38 | 0.65 |
| 3:Q8:102:ALA:CB | 3:Q8:166:LYS:CD | 2.64 | 0.65 |
| 3:L9:84:ARG:HH21 | 11:a9:406:LEU:HA | 1.62 | 0.65 |
| 4:M9:274:VAL:H | 3:V9:77:ARG:HG2 | 1.59 | 0.65 |
| 5:N9:20:ILE:HD13 | 5:N9:60:ILE:HD13 | 1.78 | 0.65 |
| 11:a9:734:PHE:CE1 | 11:a9:816:LEU:HD11 | 2.31 | 0.65 |
| 11:aA:708:HIS:CB | 3:L1:108:ARG:NH2 | 2.35 | 0.65 |
| 11:aA:742:GLN:CG | 3:L1:88:ILE:HD12 | 1.82 | 0.65 |
| 5:N1:21:ALA:CB | 5:N1:68:LEU:HD11 | 2.23 | 0.65 |
| 3:FA:153:CYS:SG | 12:F9:302:CYC:C4C | 2.84 | 0.65 |
| 12:IA:201:CYC:HMD1 | 12:IA:201:CYC:NC | 2.09 | 0.65 |
| 5:NA:1:MET:C | 5:NA:3:VAL:N | 2.50 | 0.65 |
| 2:QA:29:GLY:HA3 | 2:UA:25:GLN:O | 1.97 | 0.65 |
| 2:QA:149:GLU:OE1 | 2:UA:21:ASN:OD1 | 2.15 | 0.65 |
| 4:M3:118:TYR:CG | 3:X3:84:ARG:NE | 2.63 | 0.65 |
| 5:N3:21:ALA:CB | 5:N3:68:LEU:HD11 | 2.23 | 0.65 |
| 3:B1:111:ASN:OD1 | 4:M1:76:ALA:CB | 2.45 | 0.65 |
| 12:J4:201:CYC:HMA3 | 11:aA:176:ASN:HD21 | 1.59 | 0.65 |
| 3:O4:107:ASP:CA | 5:Z4:66:ARG:CB | 2.74 | 0.65 |
| 8:M5:115:MET:CE | 1:R5:75:THR:HG22 | 2.26 | 0.65 |
| 8:O5:76:LYS:CG | 8:O5:77:MET:HE3 | 2.24 | 0.65 |
| 12:A5:201:CYC:HMD1 | 12:A5:201:CYC:NC | 2.02 | 0.65 |
| 8:C5:66:VAL:O | 8:C5:66:VAL:HG12 | 1.96 | 0.65 |
| 8:Q5:23:LEU:HD22 | 1:R5:38:VAL:HG13 | 1.79 | 0.65 |
| 8:U5:59:PHE:CD2 | 6:M6:37:GLU:CD | 2.73 | 0.65 |
| 10:j5:77:VAL:HG11 | 10:j5:141:GLU:HG2 | 1.79 | 0.65 |
| 10:j5:182:ASN:N | 10:j5:182:ASN:HD22 | 1.94 | 0.65 |
| 10:j5:194:CYS:HB2 | 12:j5:1201:CYC:HAC1 | 1.79 | 0.65 |
| 10:j5:964:GLY:C | 1:t7:69:GLY:CA | 2.68 | 0.65 |
| 10:k5:362:LYS:HD3 | 10:k5:362:LYS:C | 2.21 | 0.65 |
| 10:k5:742:GLY:HA2 | 12:D7:201:CYC:O1D | 1.96 | 0.65 |
| 2:A6:60:TYR:CG | 2:A6:67:THR:CG2 | 2.79 | 0.65 |
| 3:F6:130:ALA:HB3 | 12:F6:201:CYC:HBC3 | 1.77 | 0.65 |
| 12:O7:201:CYC:CMD | 12:O7:201:CYC:HC | 2.10 | 0.65 |
| 8:Q7:66:VAL:HG12 | 8:Q7:66:VAL:O | 1.96 | 0.65 |
| 8:i7:25:ARG:HH12 | 8:s7:6:LYS:CA | 2.09 | 0.65 |
| 8:k7:64:ASP:HB3 | 11:a9:69:ARG:NH2 | 2.06 | 0.65 |
| 8:c7:54:ALA:HB2 | 8:c7:133:MET:CG | 2.26 | 0.65 |
| 8:q7:66:VAL:O | 8:q7:66:VAL:HG12 | 1.96 | 0.65 |
| 8:u7:30:VAL:HG12 | 1:v7:31:PHE:CD1 | 2.31 | 0.65 |
| 4:M8:128:ALA:CB | 4:M8:142:PHE:HE1 | 2.09 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:Q8:84:ARG:NH1 | 5:Z8:36:THR:HG23 | 2.12 | 0.65 |
| 5:Z8:20:ILE:HD13 | 5:Z8:60:ILE:HD13 | 1.78 | 0.65 |
| 12:S9:201:CYC:HMD1 | 12:S9:201:CYC:NC | 2.09 | 0.65 |
| 11:a9:274:LEU:O | 11:a9:278:LEU:HD11 | 1.96 | 0.65 |
| 11:a9:639:GLN:HE21 | 11:a9:639:GLN:C | 2.04 | 0.65 |
| 11:aA:89:ALA:HB1 | 11:aA:92:LYS:HZ2 | 1.60 | 0.65 |
| 5:N1:37:HIS:CD2 | 12:T1:301:CYC:CMA | 2.79 | 0.65 |
| 3:DA:68:ARG:NH2 | 3:XA:68:ARG:CZ | 2.56 | 0.65 |
| 4:MA:160:THR:CG2 | 4:MA:257:GLN:HB2 | 2.07 | 0.65 |
| 2:QA:33:ARG:NE | 12:VA:202:CYC:CBB | 2.53 | 0.65 |
| 3:Z3:119:ALA:CB | 4:M3:263:PRO:CB | 2.61 | 0.65 |
| 3:B4:119:ALA:CB | 4:M4:69:ILE:CG2 | 2.61 | 0.65 |
| 2:C4:114:ARG:HH11 | 11:aA:134:GLU:CD | 2.05 | 0.65 |
| 3:U4:108:ARG:C | 4:M4:246:ALA:CB | 2.70 | 0.65 |
| 12:K4:201:CYC:HMD1 | 12:K4:201:CYC:NC | 2.09 | 0.65 |
| 3:L4:68:ARG:O | 3:L4:69:PRO:C | 2.38 | 0.65 |
| 8:K5:98:ALA:HA | 1:L5:5:ILE:HG21 | 1.79 | 0.65 |
| 8:M5:107:ILE:CD1 | 1:N5:13:ASP:CG | 2.69 | 0.65 |
| 12:O5:201:CYC:HC | 12:O5:201:CYC:CMD | 2.10 | 0.65 |
| 3:Y4:89:ILE:HA | 3:Y4:92:TYR:HE2 | 0.84 | 0.65 |
| 8:A5:115:MET:HE3 | 12:A5:201:CYC:CHB | 2.26 | 0.65 |
| 1:D5:62:TYR:CZ | 12:E5:201:CYC:O1D | 2.49 | 0.65 |
| 1:D5:62:TYR:N | 12:E5:201:CYC:O2A | 2.26 | 0.65 |
| 8:G5:115:MET:HE3 | 12:G5:201:CYC:CHB | 2.26 | 0.65 |
| 12:I5:201:CYC:CMD | 12:I5:201:CYC:HC | 2.10 | 0.65 |
| 1:f5:30:TYR:HH | 10:j5:47:PHE:HZ | 0.70 | 0.65 |
| 8:a5:66:VAL:HG12 | 8:a5:66:VAL:O | 1.96 | 0.65 |
| 10:j5:209:ASN:C | 10:j5:209:ASN:HD22 | 2.05 | 0.65 |
| 10:j5:362:LYS:CD | 10:j5:363:HIS:NE2 | 2.60 | 0.65 |
| 10:j5:1147:TYR:HE1 | 11:aA:35:ARG:HB3 | 1.59 | 0.65 |
| 10:k5:1151:GLN:CA | 1:p7:122:PRO:HB3 | 2.24 | 0.65 |
| 12:g7:201:CYC:CMD | 12:g7:201:CYC:HC | 2.10 | 0.65 |
| 8:a7:63:PRO:CD | 11:a9:336:ILE:HG21 | 1.87 | 0.65 |
| 12:B8:202:CYC:HHA | 4:M8:54:ALA:CB | 2.07 | 0.65 |
| 8:o7:36:ARG:HG2 | 8:o7:36:ARG:NH2 | 2.10 | 0.65 |
| 5:N9:14:LYS:HE2 | 5:N9:50:LEU:CD2 | 2.26 | 0.65 |
| 5:N9:16:PHE:HE2 | 5:N9:50:LEU:HA | 1.62 | 0.65 |
| 5:Z8:29:HIS:HB2 | 5:Z8:31:TRP:HD1 | 1.61 | 0.65 |
| 12:C9:201:CYC:HMD1 | 12:C9:201:CYC:NC | 2.10 | 0.65 |
| 11:a9:245:ALA:H | 12:a9:901:CYC:HBB3 | 1.61 | 0.65 |
| 11:aA:707:PHE:HE2 | 3:L1:108:ARG:HH12 | 1.37 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M1:246:ALA:CA | 12:X1:201:CYC:HBB2 | 2.26 | 0.65 |
| 2:A2:60:TYR:CG | 2:A2:67:THR:CG2 | 2.79 | 0.65 |
| 2:IA:4:VAL:HG23 | 2:IA:100:GLY:O | 1.96 | 0.65 |
| 2:KA:15:GLN:HA | 11:aA:393:ARG:HD2 | 1.79 | 0.65 |
| 2:QA:33:ARG:HB3 | 2:UA:25:GLN:HG2 | 1.77 | 0.65 |
| 2:A4:33:ARG:HE | 2:K4:28:ASN:HD21 | 1.44 | 0.65 |
| 3:B1:86:MET:HG3 | 12:B1:202:CYC:CBC | 2.26 | 0.65 |
| 3:L4:68:ARG:CZ | 11:aA:81:ASP:N | 2.58 | 0.65 |
| 2:N4:60:TYR:CG | 2:N4:67:THR:CG2 | 2.79 | 0.65 |
| 12:Q4:201:CYC:HC | 12:Q4:201:CYC:CMD | 1.99 | 0.65 |
| 12:L5:201:CYC:HMA3 | 10:j5:591:ILE:CG2 | 2.26 | 0.65 |
| 12:M5:201:CYC:CMD | 12:M5:201:CYC:HC | 2.10 | 0.65 |
| 5:Z4:20:ILE:HG21 | 5:Z4:60:ILE:CD1 | 2.26 | 0.65 |
| 1:D5:20:ASP:O | 1:D5:21:GLY:C | 2.33 | 0.65 |
| 8:Q5:66:VAL:HG12 | 8:Q5:66:VAL:O | 1.96 | 0.65 |
| 12:S5:201:CYC:HC | 12:S5:201:CYC:CMD | 2.10 | 0.65 |
| 1:V5:114:GLU:OE1 | 10:j5:496:GLU:CG | 2.44 | 0.65 |
| 1:Z5:28:LYS:HD3 | 1:t7:143:PRO:HG3 | 1.63 | 0.65 |
| 1:Z5:161:SER:OG | 10:k5:695:GLY:O | 2.14 | 0.65 |
| 12:a5:201:CYC:HC | 12:a5:201:CYC:CMD | 2.10 | 0.65 |
| 9:i5:11:ILE:CD1 | 9:i5:28:PHE:CE2 | 2.79 | 0.65 |
| 10:j5:953:LEU:HD11 | 8:u7:48:GLU:OE1 | 1.97 | 0.65 |
| 10:j5:1064:LYS:CG | 10:j5:1065:HIS:H | 2.10 | 0.65 |
| 8:g7:25:ARG:HH22 | 8:u7:25:ARG:NH1 | 1.89 | 0.65 |
| 8:i7:43:LEU:CD1 | 8:i7:141:LEU:HD21 | 2.26 | 0.65 |
| 8:W7:126:VAL:CG2 | 12:W7:201:CYC:HMC1 | 2.27 | 0.65 |
| 8:u7:29:PHE:CE2 | 1:v7:5:ILE:CD1 | 2.80 | 0.65 |
| 8:u7:39:ILE:HD11 | 8:u7:145:ASP:CB | 2.26 | 0.65 |
| 8:u7:66:VAL:O | 8:u7:66:VAL:HG12 | 1.96 | 0.65 |
| 8:u7:97:VAL:CG2 | 1:v7:19:LEU:HD11 | 2.26 | 0.65 |
| 4:M8:86:ALA:HB1 | 3:Y8:77:ARG:HH11 | 1.61 | 0.65 |
| 2:N8:115:GLU:HB3 | 5:Z8:33:GLY:N | 2.11 | 0.65 |
| 5:Z8:22:LEU:HD23 | 5:Z8:26:LEU:CD1 | 1.83 | 0.65 |
| 5:Z8:37:HIS:NE2 | 12:Z8:301:CYC:C1A | 2.59 | 0.65 |
| 5:Z8:38:GLU:HB2 | 12:Z8:301:CYC:HMB1 | 1.62 | 0.65 |
| 2:A9:60:TYR:CG | 2:A9:67:THR:CG2 | 2.79 | 0.65 |
| 11:a9:448:ASN:OD1 | 11:a9:474:PHE:CD1 | 2.49 | 0.65 |
| 11:aA:377:VAL:HG11 | 11:aA:390:ALA:C | 2.21 | 0.65 |
| 11:aA:629:LYS:HA | 11:aA:629:LYS:HZ3 | 1.59 | 0.65 |
| 3:FA:145:PRO:HD2 | 12:F9:302:CYC:CMC | 2.26 | 0.65 |
| 4:MA:159:CYS:C | 3:VA:108:ARG:HG3 | 2.21 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:MA:222:ARG:HG3 | 4:MA:222:ARG:NH1 | 2.01 | 0.65 |
| 12:QA:201:CYC:HMA1 | 3:TA:79:MET:HE3 | 1.79 | 0.65 |
| 12:J3:202:CYC:HBB2 | 11:a9:795:ASP:O | 1.94 | 0.65 |
| 2:C3:140:SER:CB | 3:D8:150:ARG:HG3 | 2.10 | 0.65 |
| 3:D3:68:ARG:NH2 | 3:X3:68:ARG:NH1 | 2.45 | 0.65 |
| 12:B4:202:CYC:CHA | 4:M4:54:ALA:HB2 | 2.24 | 0.65 |
| 5:N3:31:TRP:CD1 | 2:S3:16:GLY:N | 2.64 | 0.65 |
| 5:N3:61:LYS:HZ2 | 12:R3:201:CYC:CBB | 2.09 | 0.65 |
| 3:F4:108:ARG:HE | 4:M4:9:GLN:HG3 | 0.82 | 0.65 |
| 2:N4:112:GLY:HA2 | 5:Z4:33:GLY:CA | 2.26 | 0.65 |
| 3:Q4:7:LYS:CD | 3:Q4:101:ASP:OD1 | 2.44 | 0.65 |
| 1:L5:79:ALA:HB1 | 8:G5:114:GLU:HB2 | 1.79 | 0.65 |
| 8:G5:103:PRO:CA | 10:j5:557:VAL:HG11 | 2.22 | 0.65 |
| 8:G5:107:ILE:HG13 | 10:j5:557:VAL:HG12 | 1.78 | 0.65 |
| 1:J5:20:ASP:O | 1:J5:21:GLY:C | 2.34 | 0.65 |
| 8:e5:66:VAL:HG12 | 8:e5:66:VAL:O | 1.96 | 0.65 |
| 12:Y5:201:CYC:HC | 12:Y5:201:CYC:CMD | 2.10 | 0.65 |
| 1:b5:30:TYR:CE2 | 10:k5:47:PHE:CE1 | 2.84 | 0.65 |
| 10:j5:761:ARG:HD2 | 10:j5:761:ARG:C | 2.21 | 0.65 |
| 10:j5:1064:LYS:HD2 | 10:j5:1065:HIS:CA | 2.27 | 0.65 |
| 10:j5:1119:LEU:HD13 | 1:t7:87:TYR:CZ | 2.32 | 0.65 |
| 10:k5:286:VAL:CG2 | 10:k5:324:LYS:O | 2.45 | 0.65 |
| 10:k5:388:ARG:NH2 | 10:k5:392:SER:HA | 2.10 | 0.65 |
| 12:I6:201:CYC:HMD1 | 12:I6:201:CYC:NC | 2.10 | 0.65 |
| 8:K7:126:VAL:CG2 | 12:K7:201:CYC:HMC1 | 2.27 | 0.65 |
| 8:a7:10:ASN:HD22 | 8:o7:10:ASN:HD21 | 1.44 | 0.65 |
| 8:o7:16:ARG:O | 1:p7:94:TYR:CE1 | 2.50 | 0.65 |
| 4:M8:215:GLU:CD | 4:M8:215:GLU:C | 2.65 | 0.65 |
| 3:F1:119:ALA:HB3 | 4:M1:41:ASN:HD21 | 1.62 | 0.65 |
| 4:M9:96:LYS:HE3 | 3:P9:111:ASN:ND2 | 2.12 | 0.65 |
| 3:F9:36:LYS:CB | 3:F9:156:LEU:CD1 | 2.75 | 0.65 |
| 3:F9:68:ARG:CZ | 3:Z9:68:ARG:HH22 | 2.09 | 0.65 |
| 3:F9:142:VAL:O | 12:F9:303:CYC:HMC3 | 1.97 | 0.65 |
| 11:a9:287:ALA:H | 11:a9:289:THR:HG23 | 1.62 | 0.65 |
| 11:a9:360:ALA:HA | 11:a9:363:GLN:OE1 | 1.96 | 0.65 |
| 11:a9:445:THR:O | 11:a9:542:ALA:O | 2.14 | 0.65 |
| 11:aA:360:ALA:HA | 11:aA:363:GLN:NE2 | 2.11 | 0.65 |
| 4:MA:274:VAL:N | 3:VA:77:ARG:CG | 2.38 | 0.65 |
| 5:NA:20:ILE:HD13 | 5:NA:60:ILE:HD13 | 1.78 | 0.65 |
| 3:S4:82:CYS:HB2 | 12:S4:202:CYC:HAC2 | 1.79 | 0.65 |
| 3:U4:120:LEU:HD21 | 12:U4:201:CYC:CBD | 2.27 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:M4:144:ARG:HG3 | 4:M4:204:ILE:HG21 | 1.76 | 0.65 |
| 8:M5:140:LEU:CD2 | 1:J7:140:LEU:HG | 2.26 | 0.65 |
| 3:Y4:87:GLU:O | 3:Y4:91:ARG:HG3 | 1.96 | 0.65 |
| 8:G5:90:ARG:HD3 | 1:H5:18:TYR:CD1 | 2.31 | 0.65 |
| 8:e5:29:PHE:HE1 | 8:e5:98:ALA:C | 2.01 | 0.65 |
| 8:Q5:9:VAL:HG22 | 1:R5:107:ARG:HH12 | 1.61 | 0.65 |
| 10:j5:924:ASP:CG | 1:J7:26:LYS:NZ | 2.50 | 0.65 |
| 10:k5:209:ASN:HD22 | 10:k5:209:ASN:C | 2.05 | 0.65 |
| 10:k5:252:ASP:OD1 | 10:k5:252:ASP:N | 2.26 | 0.65 |
| 10:k5:1008:PHE:CD1 | 1:p7:87:TYR:OH | 2.46 | 0.65 |
| 10:k5:1064:LYS:CD | 10:k5:1065:HIS:CD2 | 2.77 | 0.65 |
| 10:k5:1064:LYS:CG | 10:k5:1065:HIS:H | 2.10 | 0.65 |
| 8:G7:66:VAL:O | 8:G7:66:VAL:HG12 | 1.96 | 0.65 |
| 8:K7:25:ARG:HB3 | 8:U7:25:ARG:NH2 | 2.10 | 0.65 |
| 8:i7:47:ARG:CG | 1:j7:18:TYR:CE2 | 2.78 | 0.65 |
| 8:o7:23:LEU:HA | 1:p7:38:VAL:CG2 | 2.25 | 0.65 |
| 4:M8:99:VAL:HA | 3:Q8:108:ARG:HH11 | 1.61 | 0.65 |
| 3:L9:111:ASN:O | 11:a9:532:ALA:CA | 2.45 | 0.65 |
| 4:M9:159:CYS:C | 3:V9:108:ARG:HG3 | 2.21 | 0.65 |
| 5:Z8:16:PHE:HE2 | 5:Z8:50:LEU:HA | 1.62 | 0.65 |
| 12:K9:201:CYC:HMD1 | 12:K9:201:CYC:NC | 2.10 | 0.65 |
| 11:a9:245:ALA:HA | 12:a9:901:CYC:OB | 1.97 | 0.65 |
| 11:a9:414:ALA:CB | 11:a9:428:PHE:HE1 | 2.10 | 0.65 |
| 11:aA:325:LEU:HD23 | 11:aA:325:LEU:H | 1.60 | 0.65 |
| 11:aA:371:VAL:CG1 | 11:aA:507:PHE:HD2 | 2.10 | 0.65 |
| 11:aA:807:GLN:O | 3:L1:111:ASN:ND2 | 2.30 | 0.65 |
| 3:HA:72:ASN:OD1 | 12:HA:202:CYC:CMD | 2.45 | 0.64 |
| 12:LA:202:CYC:O2A | 11:aA:404:TYR:N | 2.29 | 0.64 |
| 5:NA:14:LYS:HE2 | 5:NA:50:LEU:CD2 | 2.26 | 0.64 |
| 2:QA:116:VAL:CG1 | 3:TA:79:MET:CG | 2.75 | 0.64 |
| 2:SA:39:GLU:CA | 2:X4:69:PRO:HB3 | 2.27 | 0.64 |
| 12:P1:202:CYC:HC | 12:P1:202:CYC:CMD | 1.99 | 0.64 |
| 4:M4:100:SER:H | 3:Q4:1:MET:HE3 | 1.55 | 0.64 |
| 5:Z4:16:PHE:HE2 | 5:Z4:50:LEU:HA | 1.62 | 0.64 |
| 1:B5:76:ARG:HD2 | 9:z5:14:LEU:C | 2.22 | 0.64 |
| 8:E5:161:GLN:CD | 1:P5:49:THR:CG2 | 2.70 | 0.64 |
| 8:Q5:17:TYR:HB2 | 1:R5:45:SER:HB3 | 1.76 | 0.64 |
| 8:W5:126:VAL:CG2 | 12:W5:201:CYC:HMC1 | 2.27 | 0.64 |
| 10:j5:642:ARG:HG2 | 10:j5:642:ARG:NH1 | 2.02 | 0.64 |
| 10:j5:1037:ARG:HG2 | 10:j5:1037:ARG:O | 1.97 | 0.64 |
| 10:j5:1118:THR:HG21 | 1:t7:83:ARG:CZ | 2.26 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:k5:143:ILE:HD12 | 10:k5:146:ALA:HB3 | 1.80 | 0.64 |
| 10:k5:1070:ALA:HB1 | 10:k5:1071:PRO:CD | 2.26 | 0.64 |
| 12:F6:202:CYC:HC | 12:F6:202:CYC:CMD | 1.98 | 0.64 |
| 8:C7:66:VAL:O | 8:C7:66:VAL:HG12 | 1.96 | 0.64 |
| 8:I7:29:PHE:HE1 | 8:I7:98:ALA:C | 2.01 | 0.64 |
| 8:g7:48:GLU:HA | 11:aA:318:TRP:CZ3 | 2.25 | 0.64 |
| 8:i7:47:ARG:HD3 | 1:j7:18:TYR:CD1 | 2.30 | 0.64 |
| 1:T7:14:VAL:HG12 | 9:w7:64:ASN:HD21 | 1.59 | 0.64 |
| 12:U7:201:CYC:HC | 12:U7:201:CYC:CMD | 2.10 | 0.64 |
| 12:a7:201:CYC:HC | 12:a7:201:CYC:CMD | 2.10 | 0.64 |
| 12:d7:201:CYC:HMA2 | 9:x7:38:PHE:CD1 | 2.28 | 0.64 |
| 3:B8:116:THR:HG22 | 4:M8:53:LEU:HA | 1.75 | 0.64 |
| 12:m7:201:CYC:HC | 12:m7:201:CYC:CMD | 2.10 | 0.64 |
| 8:o7:29:PHE:CE2 | 1:p7:5:ILE:CD1 | 2.80 | 0.64 |
| 9:z7:7:VAL:HG11 | 9:z7:37:TRP:CZ3 | 2.33 | 0.64 |
| 2:X8:16:GLY:C | 4:M8:228:SER:HB3 | 2.22 | 0.64 |
| 4:M8:151:LEU:O | 4:M8:155:ARG:HG3 | 1.98 | 0.64 |
| 2:N8:60:TYR:CG | 2:N8:67:THR:CG2 | 2.79 | 0.64 |
| 3:O8:108:ARG:NE | 5:Z8:61:LYS:HG2 | 1.85 | 0.64 |
| 3:Q8:82:CYS:CA | 12:Z8:301:CYC:HAC2 | 2.21 | 0.64 |
| 3:Q8:89:ILE:CG1 | 3:Q8:92:TYR:HE2 | 2.10 | 0.64 |
| 3:L9:84:ARG:NE | 11:a9:406:LEU:CD2 | 2.60 | 0.64 |
| 2:O9:33:ARG:HE | 2:Y9:28:ASN:HD21 | 1.44 | 0.64 |
| 3:F9:36:LYS:CB | 3:F9:156:LEU:HD11 | 2.26 | 0.64 |
| 11:a9:371:VAL:CG1 | 11:a9:507:PHE:HD2 | 2.10 | 0.64 |
| 11:a9:644:ARG:O | 11:a9:645:PRO:O | 2.13 | 0.64 |
| 11:aA:32:ARG:C | 11:aA:33:MET:HG2 | 2.21 | 0.64 |
| 11:aA:804:ARG:NH2 | 3:J1:121:GLY:CA | 2.60 | 0.64 |
| 4:M1:188:LEU:CD2 | 12:Z1:202:CYC:NB | 2.59 | 0.64 |
| 5:N1:20:ILE:HG21 | 5:N1:60:ILE:CD1 | 2.26 | 0.64 |
| 3:FA:145:PRO:CG | 12:F9:302:CYC:HMC3 | 2.13 | 0.64 |
| 3:HA:116:THR:HG21 | 11:aA:449:ASN:HD21 | 1.58 | 0.64 |
| 4:MA:148:LYS:CD | 4:MA:197:ASP:OD1 | 2.37 | 0.64 |
| 12:OA:201:CYC:HMD1 | 12:OA:201:CYC:NC | 2.09 | 0.64 |
| 3:B3:111:ASN:OD1 | 4:M3:76:ALA:CB | 2.45 | 0.64 |
| 4:M4:215:GLU:CD | 4:M4:215:GLU:C | 2.65 | 0.64 |
| 4:M4:225:LYS:NZ | 3:Y4:81:ALA:HB2 | 2.13 | 0.64 |
| 4:M4:232:VAL:CA | 12:M4:301:CYC:CBB | 2.76 | 0.64 |
| 8:K5:109:ILE:HD12 | 8:K5:109:ILE:O | 1.96 | 0.64 |
| 5:Z4:14:LYS:HE2 | 5:Z4:50:LEU:CD2 | 2.26 | 0.64 |
| 8:A5:107:ILE:HD13 | 1:B5:13:ASP:OD1 | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:G5:12:ASP:CG | 1:H5:91:TYR:CE1 | 2.75 | 0.64 |
| 8:G5:66:VAL:O | 8:G5:66:VAL:HG12 | 1.96 | 0.64 |
| 10:j5:286:VAL:CG2 | 10:j5:324:LYS:O | 2.45 | 0.64 |
| 10:j5:1155:ARG:HB3 | 10:j5:1155:ARG:NH2 | 2.07 | 0.64 |
| 10:k5:761:ARG:HD2 | 10:k5:761:ARG:C | 2.21 | 0.64 |
| 12:S7:201:CYC:CMD | 12:S7:201:CYC:HC | 2.10 | 0.64 |
| 12:M7:201:CYC:HC | 12:M7:201:CYC:CMD | 2.10 | 0.64 |
| 8:g7:66:VAL:HG12 | 8:g7:66:VAL:O | 1.96 | 0.64 |
| 12:j7:201:CYC:NB | 9:y7:38:PHE:HE1 | 1.93 | 0.64 |
| 12:Y7:201:CYC:HC | 12:Y7:201:CYC:CMD | 2.10 | 0.64 |
| 2:C8:114:ARG:NH1 | 11:a9:134:GLU:OE1 | 2.30 | 0.64 |
| 8:u7:17:TYR:OH | 1:v7:89:LEU:HG | 1.96 | 0.64 |
| 4:M8:128:ALA:HB1 | 4:M8:142:PHE:HE1 | 1.56 | 0.64 |
| 12:M8:301:CYC:HMC3 | 3:Y8:122:THR:HG23 | 1.78 | 0.64 |
| 3:Y8:89:ILE:CG1 | 3:Y8:92:TYR:CE2 | 2.81 | 0.64 |
| 3:F9:43:ALA:CB | 3:F9:142:VAL:HG22 | 2.27 | 0.64 |
| 11:aA:371:VAL:HG11 | 11:aA:507:PHE:HD2 | 1.61 | 0.64 |
| 11:aA:711:SER:HB2 | 3:L1:111:ASN:O | 1.95 | 0.64 |
| 4:MA:29:PRO:HD2 | 11:aA:378:GLU:OE1 | 1.96 | 0.64 |
| 5:NA:53:LEU:HB3 | 12:TA:301:CYC:HAA1 | 1.76 | 0.64 |
| 12:WA:201:CYC:HMD1 | 12:WA:201:CYC:NC | 2.10 | 0.64 |
| 3:B4:120:LEU:N | 4:M4:52:LEU:HD13 | 2.12 | 0.64 |
| 3:L3:120:LEU:O | 11:a9:821:ARG:CZ | 2.45 | 0.64 |
| 5:N3:14:LYS:HE2 | 5:N3:50:LEU:CD2 | 2.26 | 0.64 |
| 8:K5:23:LEU:HD13 | 1:L5:42:ALA:HB2 | 1.78 | 0.64 |
| 12:H5:201:CYC:HBB2 | 9:i5:21:ARG:CA | 2.22 | 0.64 |
| 12:e5:201:CYC:HC | 12:e5:201:CYC:CMD | 2.10 | 0.64 |
| 1:P5:123:ILE:HG22 | 10:k5:11:VAL:CG2 | 2.28 | 0.64 |
| 8:Q5:17:TYR:CZ | 1:R5:44:ILE:HG21 | 2.16 | 0.64 |
| 8:W5:9:VAL:HG22 | 1:X5:107:ARG:HH12 | 1.60 | 0.64 |
| 10:j5:362:LYS:HD3 | 10:j5:362:LYS:C | 2.22 | 0.64 |
| 10:j5:931:VAL:CG2 | 1:J7:30:TYR:CA | 2.74 | 0.64 |
| 10:j5:1150:TYR:OH | 11:aA:39:PRO:HD3 | 1.97 | 0.64 |
| 10:k5:66:MET:HE3 | 10:k5:66:MET:CA | 2.23 | 0.64 |
| 10:k5:277:ILE:CG2 | 10:k5:284:PRO:HA | 2.27 | 0.64 |
| 10:k5:1081:VAL:HG11 | 12:k5:1203:CYC:CMA | 2.20 | 0.64 |
| 10:k5:1085:GLY:CA | 1:l7:87:TYR:OH | 2.46 | 0.64 |
| 2:C6:69:PRO:HG2 | 3:J8:125:ARG:NH1 | 2.11 | 0.64 |
| 12:E6:201:CYC:HMD1 | 12:E6:201:CYC:NC | 2.10 | 0.64 |
| 8:Q7:126:VAL:CG2 | 12:Q7:201:CYC:HMC1 | 2.27 | 0.64 |
| 8:E7:126:VAL:HG22 | 12:E7:201:CYC:CMC | 2.27 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:G7:201:CYC:HC | 12:G7:201:CYC:CMD | 2.10 | 0.64 |
| 1:H7:54:GLU:OE2 | 11:aA:563:PHE:HD2 | 1.81 | 0.64 |
| 8:i7:92:VAL:CG2 | 8:i7:156:LEU:CD1 | 2.69 | 0.64 |
| 12:k7:201:CYC:CMD | 12:k7:201:CYC:HC | 2.10 | 0.64 |
| 8:U7:66:VAL:HG12 | 8:U7:66:VAL:O | 1.96 | 0.64 |
| 12:C8:201:CYC:HMD1 | 12:C8:201:CYC:NC | 2.09 | 0.64 |
| 2:X8:69:PRO:HG2 | 2:S9:39:GLU:N | 2.11 | 0.64 |
| 2:X8:108:TYR:CE1 | 4:M8:273:ILE:CD1 | 2.80 | 0.64 |
| 12:H8:201:CYC:HAA1 | 11:a9:264:ASP:OD1 | 1.98 | 0.64 |
| 4:M8:148:LYS:HE3 | 4:M8:197:ASP:CG | 2.22 | 0.64 |
| 5:N9:22:LEU:HD21 | 5:N9:26:LEU:CD2 | 2.08 | 0.64 |
| 5:Z8:34:LEU:O | 5:Z8:34:LEU:CG | 2.44 | 0.64 |
| 11:a9:197:ILE:HD12 | 11:a9:278:LEU:HD22 | 1.78 | 0.64 |
| 11:a9:312:ASP:O | 11:a9:314:SER:C | 2.41 | 0.64 |
| 11:aA:425:VAL:HG21 | 11:aA:502:ASN:O | 1.98 | 0.64 |
| 11:aA:800:THR:HG21 | 12:aA:901:CYC:HAA2 | 1.76 | 0.64 |
| 12:BA:202:CYC:HC | 12:BA:202:CYC:CMD | 1.99 | 0.64 |
| 12:KA:201:CYC:HMD1 | 12:KA:201:CYC:NC | 2.10 | 0.64 |
| 4:MA:210:ILE:HD13 | 5:NA:59:ARG:HH11 | 1.62 | 0.64 |
| 6:M2:127:SER:CA | 12:F2:201:CYC:O2A | 2.40 | 0.64 |
| 2:A4:60:TYR:CG | 2:A4:67:THR:CG2 | 2.79 | 0.64 |
| 5:N3:62:ARG:CZ | 2:Q3:14:SER:HB2 | 2.26 | 0.64 |
| 8:K5:66:VAL:O | 8:K5:66:VAL:HG12 | 1.96 | 0.64 |
| 8:O5:66:VAL:O | 8:O5:66:VAL:HG12 | 1.96 | 0.64 |
| 8:Q5:126:VAL:HG22 | 12:Q5:201:CYC:CMC | 2.27 | 0.64 |
| 8:U5:78:THR:HG22 | 6:M6:35:GLY:CA | 2.24 | 0.64 |
| 8:W5:23:LEU:HD22 | 1:X5:38:VAL:HG13 | 1.79 | 0.64 |
| 1:b5:24:LEU:O | 10:k5:54:ILE:HD13 | 1.98 | 0.64 |
| 1:b5:30:TYR:OH | 10:k5:47:PHE:CE2 | 2.41 | 0.64 |
| 9:z5:11:ILE:CD1 | 9:z5:28:PHE:CE2 | 2.79 | 0.64 |
| 10:j5:889:LEU:HD23 | 12:J7:201:CYC:OB | 1.97 | 0.64 |
| 8:i7:21:GLY:H | 8:s7:101:VAL:HG22 | 0.53 | 0.64 |
| 8:o7:66:VAL:HG12 | 8:o7:66:VAL:O | 1.96 | 0.64 |
| 12:s7:201:CYC:CMD | 12:s7:201:CYC:HC | 2.10 | 0.64 |
| 9:w7:18:ARG:HB3 | 9:w7:22:GLU:OE2 | 1.97 | 0.64 |
| 9:y7:40:GLU:OE2 | 9:y7:43:ARG:HD3 | 1.98 | 0.64 |
| 4:M8:227:GLN:HB2 | 4:M8:230:GLN:OE1 | 1.98 | 0.64 |
| 4:M8:232:VAL:HG21 | 3:Y8:113:LEU:HD21 | 1.79 | 0.64 |
| 3:O8:107:ASP:OD1 | 5:Z8:66:ARG:NH1 | 2.29 | 0.64 |
| 4:M9:151:LEU:O | 4:M9:155:ARG:HG3 | 1.97 | 0.64 |
| 4:M9:210:ILE:HD13 | 5:N9:59:ARG:HH11 | 1.62 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:M9:267:LEU:HD11 | 3:V9:120:LEU:HA | 1.78 | 0.64 |
| 5:Z8:1:MET:C | 5:Z8:3:VAL:N | 2.50 | 0.64 |
| 11:aA:283:GLN:CG | 11:aA:284:PRO:HD2 | 2.25 | 0.64 |
| 11:aA:312:ASP:O | 11:aA:314:SER:C | 2.41 | 0.64 |
| 3:H1:78:ARG:HA | 12:H1:201:CYC:CMD | 2.26 | 0.64 |
| 1:A:18:TYR:CE1 | 8:a5:90:ARG:HB2 | 2.33 | 0.64 |
| 2:AA:149:GLU:OE2 | 2:KA:21:ASN:ND2 | 2.31 | 0.64 |
| 3:FA:68:ARG:CZ | 3:ZA:68:ARG:HH22 | 2.09 | 0.64 |
| 2:IA:4:VAL:HG11 | 2:IA:30:ARG:HB2 | 1.79 | 0.64 |
| 3:JA:119:ALA:CA | 11:aA:365:LYS:CE | 2.69 | 0.64 |
| 3:LA:14:LEU:HG | 11:aA:358:PRO:HB2 | 1.75 | 0.64 |
| 3:LA:84:ARG:NE | 11:aA:406:LEU:CD2 | 2.61 | 0.64 |
| 3:LA:111:ASN:OD1 | 11:aA:366:LEU:CD1 | 2.46 | 0.64 |
| 12:LA:202:CYC:HMA1 | 11:aA:534:SER:HB3 | 1.79 | 0.64 |
| 4:MA:96:LYS:HE3 | 3:PA:111:ASN:ND2 | 2.12 | 0.64 |
| 12:QA:201:CYC:CGD | 3:TA:57:HIS:CD2 | 2.75 | 0.64 |
| 3:L2:75:PRO:CG | 3:L2:78:ARG:CG | 2.75 | 0.64 |
| 2:A3:63:PHE:HB2 | 2:A3:66:LEU:CG | 2.28 | 0.64 |
| 12:F3:201:CYC:OB | 4:M3:28:HIS:NE2 | 2.21 | 0.64 |
| 3:B4:119:ALA:HB2 | 4:M4:69:ILE:HD12 | 1.79 | 0.64 |
| 2:C4:114:ARG:NH1 | 11:aA:134:GLU:OE1 | 2.30 | 0.64 |
| 3:U4:108:ARG:CB | 4:M4:246:ALA:CB | 2.58 | 0.64 |
| 4:M4:197:ASP:CB | 5:Z4:52:ARG:HG3 | 2.27 | 0.64 |
| 8:O5:76:LYS:CD | 8:O5:77:MET:HE3 | 2.07 | 0.64 |
| 5:Z4:42:SER:HA | 12:Z4:301:CYC:C3A | 2.27 | 0.64 |
| 8:E5:29:PHE:CE1 | 8:E5:99:GLY:HA3 | 2.31 | 0.64 |
| 1:J5:76:ARG:NH1 | 9:i5:67:VAL:HG11 | 2.11 | 0.64 |
| 8:c5:90:ARG:HA | 1:d5:18:TYR:CE2 | 2.33 | 0.64 |
| 1:f5:38:VAL:HG11 | 10:j5:40:VAL:HG12 | 1.80 | 0.64 |
| 1:b5:18:TYR:OH | 10:k5:165:ARG:N | 2.30 | 0.64 |
| 9:z5:16:ARG:O | 9:z5:16:ARG:NE | 2.26 | 0.64 |
| 10:j5:1146:THR:OG1 | 1:v7:71:MEN:HE21 | 1.98 | 0.64 |
| 10:k5:1015:TYR:O | 10:k5:1017:ARG:N | 2.30 | 0.64 |
| 10:k5:1054:SER:HG | 1:l7:110:ASN:HB3 | 1.60 | 0.64 |
| 8:Q7:25:ARG:HE | 8:C7:25:ARG:NH2 | 1.95 | 0.64 |
| 12:Q7:201:CYC:HMD1 | 12:Q7:201:CYC:NC | 2.02 | 0.64 |
| 1:D7:76:ARG:N | 8:E7:110:ILE:O | 2.31 | 0.64 |
| 2:C8:114:ARG:HH11 | 11:a9:134:GLU:CD | 2.05 | 0.64 |
| 8:m7:102:THR:HB | 8:m7:103:PRO:HD2 | 1.76 | 0.64 |
| 8:o7:27:LYS:CD | 1:p7:35:ALA:HB2 | 2.27 | 0.64 |
| 4:M8:56:MET:CE | 4:M8:66:VAL:CG2 | 2.57 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 5:N9:21:ALA:CB | 5:N9:68:LEU:HD11 | 2.23 | 0.64 |
| 11:a9:32:ARG:C | 11:a9:33:MET:HG2 | 2.21 | 0.64 |
| 11:a9:425:VAL:HG21 | 11:a9:502:ASN:O | 1.98 | 0.64 |
| 11:a9:594:ARG:HH11 | 11:a9:594:ARG:CG | 2.10 | 0.64 |
| 11:a9:624:GLY:O | 11:a9:628:THR:HG23 | 1.92 | 0.64 |
| 11:aA:33:MET:O | 11:aA:34:ILE:HD12 | 1.97 | 0.64 |
| 11:aA:56:ILE:HG22 | 11:aA:56:ILE:O | 1.96 | 0.64 |
| 11:aA:197:ILE:HD12 | 11:aA:278:LEU:HD22 | 1.78 | 0.64 |
| 11:aA:274:LEU:O | 11:aA:278:LEU:HD11 | 1.96 | 0.64 |
| 11:aA:537:ASP:HB3 | 11:aA:543:GLN:HB2 | 1.79 | 0.64 |
| 12:W1:201:CYC:HMD1 | 12:W1:201:CYC:NC | 2.09 | 0.64 |
| 5:NA:21:ALA:CB | 5:NA:68:LEU:HD11 | 2.23 | 0.64 |
| 5:NA:24:PRO:CG | 5:NA:35:ASP:O | 2.46 | 0.64 |
| 3:TA:24:LEU:HD22 | 2:X4:68:GLN:NE2 | 2.12 | 0.64 |
| 12:K3:201:CYC:HMD1 | 12:K3:201:CYC:NC | 2.10 | 0.64 |
| 2:C3:140:SER:CB | 3:D8:150:ARG:HH11 | 2.09 | 0.64 |
| 3:F3:119:ALA:HB3 | 4:M3:41:ASN:HD21 | 1.62 | 0.64 |
| 3:L3:115:GLU:HB2 | 11:a9:809:ARG:HH22 | 1.63 | 0.64 |
| 12:L4:202:CYC:HAB1 | 11:aA:239:TYR:HE1 | 1.61 | 0.64 |
| 4:M4:148:LYS:HE3 | 4:M4:197:ASP:CG | 2.22 | 0.64 |
| 4:M4:197:ASP:O | 5:Z4:52:ARG:NH2 | 2.31 | 0.64 |
| 8:A5:12:ASP:OD1 | 1:B5:91:TYR:OH | 2.15 | 0.64 |
| 8:C5:26:ILE:O | 8:C5:26:ILE:HG23 | 1.98 | 0.64 |
| 8:C5:102:THR:HB | 8:C5:103:PRO:HD2 | 1.77 | 0.64 |
| 1:J5:118:SER:HB3 | 9:i5:56:LEU:HD11 | 1.78 | 0.64 |
| 12:c5:201:CYC:CMD | 12:c5:201:CYC:HC | 2.10 | 0.64 |
| 10:j5:277:ILE:CG2 | 10:j5:284:PRO:HA | 2.27 | 0.64 |
| 10:j5:1153:VAL:O | 10:j5:1155:ARG:HD2 | 1.97 | 0.64 |
| 10:k5:199:THR:CG2 | 12:k5:1201:CYC:HBC2 | 2.26 | 0.64 |
| 10:k5:547:ARG:HD2 | 10:k5:547:ARG:C | 2.16 | 0.64 |
| 12:I7:201:CYC:HC | 12:I7:201:CYC:CMD | 2.10 | 0.64 |
| 2:A8:63:PHE:HB2 | 2:A8:66:LEU:CG | 2.28 | 0.64 |
| 3:B8:82:CYS:CB | 12:B8:202:CYC:OC | 2.45 | 0.64 |
| 12:o7:201:CYC:CMD | 12:o7:201:CYC:HC | 2.10 | 0.64 |
| 9:w7:15:LYS:HE3 | 9:w7:16:ARG:HD3 | 1.79 | 0.64 |
| 4:M8:139:VAL:HG22 | 4:M8:216:ASN:HA | 1.75 | 0.64 |
| 4:M8:235:PHE:CA | 12:M8:301:CYC:HAA1 | 2.27 | 0.64 |
| 3:Q8:89:ILE:CG1 | 3:Q8:92:TYR:CE2 | 2.81 | 0.64 |
| 5:N9:53:LEU:HB3 | 12:T9:301:CYC:HAA1 | 1.76 | 0.64 |
| 3:H9:72:ASN:OD1 | 12:H9:202:CYC:CMD | 2.45 | 0.64 |
| 11:aA:426:ARG:O | 11:aA:426:ARG:HG3 | 1.91 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:XA:202:CYC:HC | 12:XA:202:CYC:CMD | 1.98 | 0.64 |
| 12:J3:202:CYC:HBA1 | 11:a9:667:THR:CG2 | 2.23 | 0.64 |
| 3:B3:127:VAL:HA | 12:B3:202:CYC:HMC1 | 1.80 | 0.64 |
| 3:L4:68:ARG:C | 3:L4:69:PRO:O | 2.41 | 0.64 |
| 4:M4:104:ALA:CB | 2:P4:13:ASP:C | 2.66 | 0.64 |
| 8:M5:66:VAL:HG12 | 8:M5:66:VAL:O | 1.96 | 0.64 |
| 3:Y4:93:VAL:HA | 3:Y4:105:LEU:HD12 | 1.80 | 0.64 |
| 12:E5:201:CYC:CMD | 12:E5:201:CYC:HC | 2.10 | 0.64 |
| 8:G5:100:ASP:CG | 8:S5:20:PRO:CG | 2.71 | 0.64 |
| 1:f5:18:TYR:CZ | 10:j5:165:ARG:CG | 2.81 | 0.64 |
| 8:W5:126:VAL:HG22 | 12:W5:201:CYC:CMC | 2.27 | 0.64 |
| 8:A7:90:ARG:HA | 1:B7:18:TYR:CE2 | 2.33 | 0.64 |
| 10:j5:990:ARG:HH11 | 10:j5:990:ARG:CG | 2.10 | 0.64 |
| 10:j5:1002:ARG:HG2 | 10:j5:1002:ARG:O | 1.98 | 0.64 |
| 10:j5:1015:TYR:O | 10:j5:1017:ARG:N | 2.30 | 0.64 |
| 10:k5:426:LEU:HD12 | 10:k5:426:LEU:O | 1.98 | 0.64 |
| 10:k5:990:ARG:HH11 | 10:k5:990:ARG:CG | 2.10 | 0.64 |
| 10:k5:1139:SER:O | 11:a9:32:ARG:NH1 | 2.23 | 0.64 |
| 8:G7:48:GLU:HG2 | 11:a9:578:MET:SD | 2.38 | 0.64 |
| 8:I7:66:VAL:HG12 | 8:I7:66:VAL:O | 1.96 | 0.64 |
| 8:M7:66:VAL:HG12 | 8:M7:66:VAL:O | 1.96 | 0.64 |
| 8:W7:126:VAL:HG22 | 12:W7:201:CYC:CMC | 2.27 | 0.64 |
| 3:B8:82:CYS:O | 12:B8:202:CYC:CAC | 2.41 | 0.64 |
| 8:o7:18:LEU:HD22 | 1:p7:97:LEU:CD1 | 2.20 | 0.64 |
| 8:s7:102:THR:HB | 8:s7:103:PRO:HD2 | 1.76 | 0.64 |
| 3:L8:109:CYS:HA | 12:a9:901:CYC:HAB2 | 1.79 | 0.64 |
| 5:Z8:38:GLU:CG | 12:Z8:301:CYC:HMB2 | 2.28 | 0.64 |
| 11:a9:95:ILE:HD13 | 11:a9:237:PHE:CZ | 2.33 | 0.64 |
| 11:a9:732:SER:HB3 | 11:a9:824:VAL:HG21 | 1.80 | 0.64 |
| 1:Z:110:ASN:O | 10:j5:434:TRP:HA | 1.98 | 0.64 |
| 2:AA:33:ARG:HE | 2:KA:28:ASN:HD21 | 1.44 | 0.64 |
| 3:BA:119:ALA:CB | 4:MA:41:ASN:HD21 | 2.09 | 0.64 |
| 4:MA:118:TYR:CD2 | 12:ZA:202:CYC:O2A | 2.51 | 0.64 |
| 12:G3:201:CYC:HMD1 | 12:G3:201:CYC:NC | 2.09 | 0.64 |
| 3:H3:70:GLY:HA2 | 11:a9:620:ALA:O | 1.97 | 0.64 |
| 12:J3:202:CYC:HB | 11:a9:666:ASN:CB | 2.02 | 0.64 |
| 12:A3:201:CYC:HMD1 | 12:A3:201:CYC:NC | 2.10 | 0.64 |
| 3:F3:119:ALA:HB2 | 4:M3:41:ASN:HD21 | 1.63 | 0.64 |
| 3:B4:119:ALA:HB3 | 4:M4:52:LEU:HD11 | 1.75 | 0.64 |
| 4:M4:85:VAL:HG12 | 4:M4:85:VAL:O | 1.97 | 0.64 |
| 2:N4:118:ARG:HH12 | 5:Z4:32:PRO:HG3 | 1.63 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 12:K5:201:CYC:CMD | 12:K5:201:CYC:HC | 2.10 | 0.64 |
| 3:Y4:89:ILE:CG1 | 3:Y4:92:TYR:CE2 | 2.81 | 0.64 |
| 10:j5:1143:LEU:CD1 | 8:q7:103:PRO:HA | 2.27 | 0.64 |
| 10:k5:542:GLN:NE2 | 10:k5:560:VAL:HG12 | 2.13 | 0.64 |
| 10:k5:984:ILE:C | 10:k5:984:ILE:HD12 | 2.23 | 0.64 |
| 10:k5:1046:ARG:NH2 | 8:k7:9:VAL:CG1 | 2.58 | 0.64 |
| 10:k5:1069:ARG:HG3 | 10:k5:1069:ARG:HH11 | 1.60 | 0.64 |
| 10:k5:1076:GLU:O | 10:k5:1078:SER:N | 2.30 | 0.64 |
| 10:k5:1150:TYR:CE1 | 11:a9:38:VAL:HG13 | 2.31 | 0.64 |
| 8:g7:19:SER:CB | 8:g7:20:PRO:CD | 2.76 | 0.64 |
| 8:i7:25:ARG:HH21 | 8:s7:3:VAL:C | 2.06 | 0.64 |
| 8:U7:102:THR:HB | 8:U7:103:PRO:HD2 | 1.76 | 0.64 |
| 8:m7:27:LYS:O | 8:m7:30:VAL:HG23 | 1.98 | 0.64 |
| 8:q7:90:ARG:HA | 1:r7:18:TYR:CE2 | 2.33 | 0.64 |
| 2:X8:64:PRO:C | 3:T9:25:ASN:CB | 2.54 | 0.64 |
| 4:M8:200:ILE:CB | 5:Z8:52:ARG:NH2 | 2.61 | 0.64 |
| 11:a9:371:VAL:HG12 | 11:a9:371:VAL:O | 1.98 | 0.64 |
| 11:aA:61:TYR:O | 11:aA:63:ASP:N | 2.31 | 0.64 |
| 11:aA:734:PHE:CE1 | 11:aA:816:LEU:HD11 | 2.31 | 0.64 |
| 4:M1:120:LEU:CD2 | 3:X1:84:ARG:HH11 | 2.00 | 0.64 |
| 1:A:31:PHE:CE2 | 8:a5:37:LEU:HD11 | 2.31 | 0.64 |
| 1:Z:158:SER:HB2 | 1:X5:11:ASN:HD22 | 1.60 | 0.64 |
| 3:DA:115:GLU:OE2 | 4:MA:78:GLY:HA2 | 1.98 | 0.64 |
| 12:GA:201:CYC:HMD1 | 12:GA:201:CYC:NC | 2.09 | 0.64 |
| 3:JA:78:ARG:CZ | 11:aA:359:ASP:HA | 2.15 | 0.64 |
| 3:LA:51:ILE:HD13 | 3:LA:90:LEU:HD11 | 1.79 | 0.64 |
| 4:MA:77:LEU:CD2 | 3:ZA:115:GLU:OE2 | 2.46 | 0.64 |
| 4:MA:153:LYS:NZ | 2:UA:14:SER:OG | 2.31 | 0.64 |
| 6:M2:34:ARG:HD2 | 8:O5:52:LYS:CB | 2.24 | 0.64 |
| 3:D4:14:LEU:HD11 | 3:Y4:125:ARG:CD | 2.13 | 0.64 |
| 3:D4:150:ARG:CG | 2:C1:140:SER:HB3 | 2.10 | 0.64 |
| 2:O3:33:ARG:HE | 2:Y3:28:ASN:HD21 | 1.45 | 0.64 |
| 12:V3:202:CYC:HC | 12:V3:202:CYC:CMD | 1.99 | 0.64 |
| 3:U4:112:GLY:HA2 | 4:M4:74:LEU:HD22 | 1.73 | 0.64 |
| 4:M4:58:TYR:HA | 4:M4:61:ASN:ND2 | 2.13 | 0.64 |
| 3:Q4:77:ARG:H | 5:Z4:34:LEU:HD13 | 1.63 | 0.64 |
| 8:A5:12:ASP:CG | 1:B5:91:TYR:CE1 | 2.75 | 0.64 |
| 8:I5:26:ILE:HG23 | 8:I5:26:ILE:O | 1.98 | 0.64 |
| 8:U5:59:PHE:HD2 | 6:M6:37:GLU:CD | 2.04 | 0.64 |
| 9:z5:8:THR:HG22 | 9:z5:52:LEU:HD12 | 1.80 | 0.64 |
| 10:j5:1056:PRO:CD | 10:j5:1057:LYS:N | 2.57 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:S7:90:ARG:HA | 1:T7:18:TYR:CE2 | 2.33 | 0.64 |
| 8:E7:126:VAL:CG2 | 12:E7:201:CYC:HMC1 | 2.27 | 0.64 |
| 8:K7:126:VAL:HG22 | 12:K7:201:CYC:CMC | 2.27 | 0.64 |
| 8:g7:107:ILE:HD13 | 1:h7:13:ASP:OD1 | 1.98 | 0.64 |
| 8:i7:25:ARG:HH11 | 8:s7:6:LYS:HG2 | 1.60 | 0.64 |
| 1:d7:107:ARG:O | 9:x7:45:GLN:NE2 | 2.31 | 0.64 |
| 3:B8:68:ARG:HH22 | 3:U8:68:ARG:NH1 | 1.94 | 0.64 |
| 8:o7:48:GLU:O | 8:o7:48:GLU:HG3 | 1.98 | 0.64 |
| 8:u7:23:LEU:HD22 | 1:v7:38:VAL:CG2 | 2.28 | 0.64 |
| 8:u7:97:VAL:CG2 | 1:v7:19:LEU:HD12 | 2.25 | 0.64 |
| 9:z7:18:ARG:HB3 | 9:z7:22:GLU:OE2 | 1.97 | 0.64 |
| 9:x7:40:GLU:OE2 | 9:x7:43:ARG:HD3 | 1.98 | 0.64 |
| 2:X8:69:PRO:CB | 2:S9:39:GLU:CA | 2.73 | 0.64 |
| 4:M8:190:ARG:HH11 | 4:M8:202:SER:HB3 | 1.63 | 0.64 |
| 12:M8:301:CYC:HMC1 | 3:Y8:127:VAL:CG2 | 2.28 | 0.64 |
| 3:Q8:117:TYR:C | 3:Q8:120:LEU:HG | 2.22 | 0.64 |
| 4:M9:78:GLY:HA2 | 3:D9:115:GLU:OE2 | 1.98 | 0.64 |
| 4:M9:153:LYS:NZ | 2:U9:14:SER:OG | 2.31 | 0.64 |
| 2:A9:33:ARG:HE | 2:K9:28:ASN:HD21 | 1.44 | 0.64 |
| 3:D9:68:ARG:HH12 | 3:X9:65:ASP:HB3 | 1.63 | 0.64 |
| 2:I9:4:VAL:HG23 | 2:I9:100:GLY:O | 1.96 | 0.64 |
| 11:a9:823:ILE:HD13 | 11:a9:823:ILE:O | 1.98 | 0.64 |
| 11:aA:290:ASP:O | 11:aA:291:TYR:HD1 | 1.73 | 0.64 |
| 5:N1:16:PHE:HE2 | 5:N1:50:LEU:HA | 1.62 | 0.64 |
| 3:JA:65:ASP:OD2 | 11:aA:354:VAL:HG21 | 1.98 | 0.64 |
| 3:LA:56:ALA:CA | 3:LA:86:MET:HE1 | 2.28 | 0.64 |
| 12:PA:202:CYC:HC | 12:PA:202:CYC:CMD | 1.98 | 0.64 |
| 2:K3:112:GLY:HA3 | 11:a9:670:LEU:HD21 | 1.74 | 0.64 |
| 12:B4:202:CYC:CBD | 4:M4:53:LEU:HB3 | 2.26 | 0.64 |
| 12:B1:201:CYC:HC | 12:B1:201:CYC:CMD | 1.98 | 0.64 |
| 3:L4:69:PRO:HD2 | 11:aA:81:ASP:HA | 1.80 | 0.64 |
| 2:N4:33:ARG:CZ | 2:X4:28:ASN:ND2 | 2.61 | 0.64 |
| 5:Z4:34:LEU:CG | 5:Z4:34:LEU:O | 2.44 | 0.64 |
| 8:A5:114:GLU:HB2 | 1:F5:79:ALA:HB1 | 1.78 | 0.64 |
| 8:E5:98:ALA:HA | 1:F5:5:ILE:HG21 | 1.79 | 0.64 |
| 1:H5:76:ARG:HD2 | 9:i5:14:LEU:HB2 | 1.78 | 0.64 |
| 8:U5:48:GLU:CA | 6:M6:34:ARG:HH12 | 2.09 | 0.64 |
| 9:i5:10:CYS:O | 9:i5:49:GLY:HA2 | 1.98 | 0.64 |
| 10:j5:86:GLU:HA | 10:j5:89:LYS:HE2 | 1.80 | 0.64 |
| 10:j5:187:ARG:HE | 10:j5:237:ASP:CG | 2.04 | 0.64 |
| 10:j5:934:ALA:HB1 | 1:J7:32:THR:HG21 | 0.66 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:k5:19:THR:OG1 | 10:k5:19:THR:O | 2.04 | 0.64 |
| 10:k5:182:ASN:HD22 | 10:k5:182:ASN:N | 1.94 | 0.64 |
| 10:k5:974:LEU:HD22 | 10:k5:974:LEU:O | 1.98 | 0.64 |
| 10:k5:1150:TYR:CD2 | 1:p7:69:GLY:O | 2.50 | 0.64 |
| 1:J7:76:ARG:N | 8:K7:110:ILE:O | 2.31 | 0.64 |
| 8:K7:126:VAL:HG22 | 12:K7:201:CYC:HMC1 | 1.80 | 0.64 |
| 8:M7:90:ARG:HA | 1:N7:18:TYR:CE2 | 2.33 | 0.64 |
| 1:X7:118:SER:O | 9:w7:61:GLN:CG | 2.46 | 0.64 |
| 12:E1:201:CYC:HMD1 | 12:E1:201:CYC:NC | 2.10 | 0.64 |
| 3:B8:82:CYS:CA | 12:B8:202:CYC:OC | 2.44 | 0.64 |
| 8:o7:29:PHE:HE2 | 1:p7:5:ILE:CD1 | 2.10 | 0.64 |
| 8:o7:97:VAL:CG2 | 1:p7:19:LEU:HD12 | 2.25 | 0.64 |
| 8:u7:48:GLU:O | 8:u7:48:GLU:HG3 | 1.98 | 0.64 |
| 4:M8:86:ALA:CB | 3:Y8:77:ARG:NH1 | 2.61 | 0.64 |
| 4:M9:76:ALA:CB | 3:D9:112:GLY:N | 2.52 | 0.64 |
| 3:Y8:89:ILE:CG1 | 3:Y8:92:TYR:HE2 | 2.10 | 0.64 |
| 5:Z8:41:GLN:C | 12:Z8:301:CYC:HMA2 | 2.23 | 0.64 |
| 3:D9:68:ARG:NH2 | 3:X9:68:ARG:CZ | 2.56 | 0.64 |
| 11:a9:32:ARG:HH11 | 11:a9:32:ARG:CG | 2.10 | 0.64 |
| 11:a9:95:ILE:O | 11:a9:99:ALA:N | 2.30 | 0.64 |
| 11:a9:377:VAL:O | 11:a9:391:VAL:CG2 | 2.44 | 0.64 |
| 11:a9:632:ILE:H | 11:a9:632:ILE:HD12 | 1.62 | 0.64 |
| 11:aA:95:ILE:O | 11:aA:99:ALA:N | 2.30 | 0.64 |
| 11:aA:632:ILE:H | 11:aA:632:ILE:HD12 | 1.62 | 0.64 |
| 5:N1:14:LYS:HE2 | 5:N1:50:LEU:CD2 | 2.26 | 0.64 |
| 12:U1:201:CYC:HMD1 | 12:U1:201:CYC:NC | 2.09 | 0.64 |
| 1:A:17:LYS:O | 8:a5:94:TYR:OH | 2.14 | 0.63 |
| 3:LA:84:ARG:HH21 | 11:aA:406:LEU:HA | 1.62 | 0.63 |
| 2:Q1:14:SER:HB2 | 5:N1:62:ARG:CZ | 2.26 | 0.63 |
| 3:H3:62:GLU:OE1 | 8:k7:49:ARG:CZ | 2.45 | 0.63 |
| 4:M3:151:LEU:O | 4:M3:155:ARG:HG3 | 1.98 | 0.63 |
| 2:O3:33:ARG:CZ | 2:Y3:28:ASN:ND2 | 2.62 | 0.63 |
| 3:B1:127:VAL:CA | 12:B1:202:CYC:HMC1 | 2.23 | 0.63 |
| 4:M4:86:ALA:HB1 | 3:Y4:77:ARG:HH11 | 1.61 | 0.63 |
| 4:M4:134:ASN:C | 4:M4:135:GLY:O | 2.21 | 0.63 |
| 8:G5:12:ASP:OD1 | 1:H5:91:TYR:OH | 2.15 | 0.63 |
| 8:S5:59:PHE:CD2 | 8:E7:68:PRO:HB3 | 2.33 | 0.63 |
| 8:U5:27:LYS:O | 8:U5:30:VAL:HG23 | 1.98 | 0.63 |
| 1:b5:9:ILE:HG22 | 10:k5:17:PHE:HZ | 1.63 | 0.63 |
| 10:j5:246:VAL:HG23 | 10:j5:257:THR:HG22 | 1.80 | 0.63 |
| 10:j5:261:ILE:O | 10:j5:261:ILE:HG13 | 1.95 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:990:ARG:HD3 | 1:f7:76:ARG:HD2 | 1.80 | 0.63 |
| 10:k5:931:VAL:HG22 | 1:D7:30:TYR:CA | 2.26 | 0.63 |
| 8:O7:27:LYS:O | 8:O7:30:VAL:HG23 | 1.98 | 0.63 |
| 8:W7:126:VAL:HG22 | 12:W7:201:CYC:HMC1 | 1.80 | 0.63 |
| 8:c7:11:ALA:HB1 | 1:d7:94:TYR:HE1 | 1.57 | 0.63 |
| 12:e7:201:CYC:HC | 12:e7:201:CYC:CMD | 2.10 | 0.63 |
| 12:B8:201:CYC:HC | 12:B8:201:CYC:CMD | 1.99 | 0.63 |
| 9:z7:5:PHE:CE2 | 9:z7:37:TRP:CD1 | 2.86 | 0.63 |
| 3:L8:68:ARG:O | 3:L8:69:PRO:C | 2.38 | 0.63 |
| 3:L9:111:ASN:ND2 | 11:a9:531:ASP:H | 1.96 | 0.63 |
| 3:Y8:89:ILE:CB | 3:Y8:92:TYR:OH | 2.46 | 0.63 |
| 5:Z8:38:GLU:CA | 12:Z8:301:CYC:CMB | 2.70 | 0.63 |
| 3:J9:112:GLY:HA3 | 11:a9:519:ARG:HA | 1.78 | 0.63 |
| 11:a9:312:ASP:OD1 | 11:a9:316:GLY:CA | 2.46 | 0.63 |
| 3:LA:106:GLU:O | 3:LA:111:ASN:HB2 | 1.98 | 0.63 |
| 5:NA:16:PHE:HE2 | 5:NA:50:LEU:HA | 1.62 | 0.63 |
| 3:L2:65:ASP:CG | 1:h7:64:ASP:CG | 2.59 | 0.63 |
| 3:F3:107:ASP:HB3 | 11:a9:646:ASN:ND2 | 2.13 | 0.63 |
| 3:B4:68:ARG:HH22 | 3:U4:68:ARG:NH1 | 1.94 | 0.63 |
| 3:B4:119:ALA:O | 4:M4:15:PHE:CE2 | 2.51 | 0.63 |
| 4:M3:85:VAL:HG12 | 4:M3:85:VAL:O | 1.97 | 0.63 |
| 2:U3:46:SER:OG | 2:Q9:74:TYR:HD1 | 1.65 | 0.63 |
| 2:N4:111:ALA:C | 5:Z4:34:LEU:CA | 2.66 | 0.63 |
| 2:N4:112:GLY:N | 5:Z4:34:LEU:H | 1.96 | 0.63 |
| 8:G5:15:ALA:HB1 | 1:H5:90:ARG:NH2 | 2.14 | 0.63 |
| 8:c5:73:TYR:CE2 | 6:M6:9:ARG:NH1 | 2.55 | 0.63 |
| 1:X5:64:ASP:HB3 | 10:j5:704:THR:CG2 | 2.29 | 0.63 |
| 1:b5:18:TYR:CD1 | 10:k5:165:ARG:CG | 2.80 | 0.63 |
| 1:b5:18:TYR:CZ | 10:k5:165:ARG:CG | 2.81 | 0.63 |
| 1:b5:18:TYR:CE1 | 10:k5:165:ARG:CB | 2.72 | 0.63 |
| 10:j5:345:ARG:O | 10:j5:345:ARG:HG2 | 1.98 | 0.63 |
| 10:k5:77:VAL:HG11 | 10:k5:141:GLU:HG2 | 1.79 | 0.63 |
| 10:k5:362:LYS:CD | 10:k5:363:HIS:NE2 | 2.60 | 0.63 |
| 10:k5:619:GLU:HB3 | 10:k5:620:PRO:CD | 2.28 | 0.63 |
| 10:k5:1037:ARG:HG2 | 10:k5:1037:ARG:O | 1.97 | 0.63 |
| 10:k5:1143:LEU:HA | 1:l7:10:ASN:HD21 | 1.63 | 0.63 |
| 10:k5:1153:VAL:O | 10:k5:1155:ARG:HD2 | 1.97 | 0.63 |
| 8:O7:22:GLU:HG2 | 8:O7:25:ARG:HH12 | 1.58 | 0.63 |
| 8:k7:90:ARG:HA | 1:l7:18:TYR:CE2 | 2.33 | 0.63 |
| 8:s7:27:LYS:O | 8:s7:30:VAL:HG23 | 1.98 | 0.63 |
| 2:X8:107:ASP:CB | 4:M8:273:ILE:CG2 | 2.76 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:L8:70:GLY:O | 3:L8:71:GLY:C | 2.39 | 0.63 |
| 3:L9:14:LEU:CD2 | 11:a9:358:PRO:CA | 2.51 | 0.63 |
| 4:M9:134:ASN:HD21 | 5:N9:1:MET:N | 1.96 | 0.63 |
| 11:a9:33:MET:O | 11:a9:34:ILE:HD12 | 1.97 | 0.63 |
| 11:a9:245:ALA:CA | 12:a9:901:CYC:OB | 2.47 | 0.63 |
| 11:a9:278:LEU:HD12 | 11:a9:278:LEU:N | 2.07 | 0.63 |
| 11:a9:291:TYR:C | 11:a9:293:LEU:H | 2.05 | 0.63 |
| 3:HA:120:LEU:HD13 | 12:HA:202:CYC:C1A | 2.29 | 0.63 |
| 2:IA:37:SER:HB3 | 2:IA:97:LEU:CD1 | 2.28 | 0.63 |
| 3:LA:120:LEU:HA | 11:aA:539:GLY:HA3 | 1.80 | 0.63 |
| 2:QA:76:ASP:N | 2:U1:141:GLN:HA | 2.13 | 0.63 |
| 2:A1:33:ARG:HE | 2:K1:28:ASN:HD21 | 1.44 | 0.63 |
| 6:M2:276:PRO:CB | 1:j7:63:SER:OG | 2.32 | 0.63 |
| 4:M3:116:ASN:ND2 | 12:X3:201:CYC:OB | 2.29 | 0.63 |
| 5:N3:2:SER:O | 5:N3:2:SER:OG | 2.16 | 0.63 |
| 4:M4:95:ALA:CA | 5:Z4:38:GLU:HG3 | 2.27 | 0.63 |
| 4:M4:200:ILE:HB | 5:Z4:52:ARG:NH2 | 2.13 | 0.63 |
| 4:M4:235:PHE:HZ | 3:Y4:113:LEU:HA | 1.63 | 0.63 |
| 2:N4:63:PHE:HB2 | 2:N4:66:LEU:HD12 | 1.70 | 0.63 |
| 8:K5:20:PRO:HG3 | 8:U5:151:PHE:C | 2.24 | 0.63 |
| 8:O5:35:ARG:NH2 | 8:O5:144:ASP:CB | 2.61 | 0.63 |
| 1:F5:12:TYR:CZ | 1:F5:23:ALA:HB2 | 2.34 | 0.63 |
| 12:U5:201:CYC:CMD | 12:U5:201:CYC:HC | 2.10 | 0.63 |
| 9:i5:56:LEU:HD12 | 9:i5:56:LEU:H | 1.61 | 0.63 |
| 10:j5:386:ILE:HG23 | 10:j5:387:VAL:O | 1.98 | 0.63 |
| 10:j5:987:ASP:O | 1:h7:106:GLU:CD | 2.41 | 0.63 |
| 10:k5:386:ILE:HG23 | 10:k5:387:VAL:O | 1.98 | 0.63 |
| 8:I7:27:LYS:O | 8:I7:30:VAL:HG23 | 1.98 | 0.63 |
| 8:g7:16:ARG:HH11 | 8:g7:16:ARG:HG3 | 1.64 | 0.63 |
| 8:i7:39:ILE:HD11 | 8:i7:148:GLU:HB3 | 1.59 | 0.63 |
| 1:j7:87:TYR:CE2 | 9:y7:38:PHE:CE1 | 2.77 | 0.63 |
| 8:U7:29:PHE:HE1 | 8:U7:98:ALA:C | 2.01 | 0.63 |
| 8:a7:102:THR:HB | 8:a7:103:PRO:HD2 | 1.76 | 0.63 |
| 8:m7:29:PHE:HE1 | 8:m7:98:ALA:C | 2.01 | 0.63 |
| 8:u7:23:LEU:HA | 1:v7:38:VAL:HG22 | 1.79 | 0.63 |
| 8:u7:36:ARG:HG2 | 8:u7:36:ARG:NH2 | 2.10 | 0.63 |
| 12:u7:201:CYC:HC | 12:u7:201:CYC:CMD | 2.10 | 0.63 |
| 9:w7:7:VAL:HG11 | 9:w7:37:TRP:CZ3 | 2.33 | 0.63 |
| 2:X8:69:PRO:HB3 | 2:S9:39:GLU:CA | 2.27 | 0.63 |
| 3:L8:65:ASP:O | 11:a9:82:GLN:CD | 2.39 | 0.63 |
| 4:M8:126:THR:CG2 | 12:M8:302:CYC:O2A | 2.45 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:M8:134:ASN:C | 4:M8:135:GLY:O | 2.21 | 0.63 |
| 2:N8:118:ARG:HH12 | 5:Z8:32:PRO:HB3 | 1.62 | 0.63 |
| 3:Q8:85:ASP:HB2 | 12:Z8:301:CYC:HBC2 | 1.73 | 0.63 |
| 3:F1:113:LEU:HD13 | 4:M1:38:PRO:CB | 2.28 | 0.63 |
| 3:L9:56:ALA:CA | 3:L9:86:MET:HE1 | 2.28 | 0.63 |
| 3:L9:111:ASN:OD1 | 11:a9:366:LEU:CD1 | 2.47 | 0.63 |
| 3:Y8:110:LEU:HD11 | 3:Y8:166:LYS:HB3 | 1.81 | 0.63 |
| 5:Z8:24:PRO:CG | 5:Z8:35:ASP:O | 2.46 | 0.63 |
| 2:A9:114:ARG:NH1 | 11:a9:407:GLU:CD | 2.56 | 0.63 |
| 3:H9:59:LEU:CD2 | 12:H9:202:CYC:CBC | 2.75 | 0.63 |
| 2:I9:4:VAL:HG11 | 2:I9:30:ARG:HB2 | 1.79 | 0.63 |
| 11:a9:710:THR:HG21 | 11:a9:807:GLN:CD | 2.21 | 0.63 |
| 5:N1:24:PRO:CG | 5:N1:35:ASP:O | 2.46 | 0.63 |
| 2:KA:24:LEU:HD22 | 3:LA:38:LEU:CD2 | 2.24 | 0.63 |
| 4:MA:85:VAL:HG12 | 4:MA:85:VAL:O | 1.97 | 0.63 |
| 12:S1:201:CYC:HMD1 | 12:S1:201:CYC:NC | 2.10 | 0.63 |
| 3:B3:68:ARG:NH1 | 3:V3:68:ARG:HH12 | 1.92 | 0.63 |
| 12:E3:201:CYC:HMD1 | 12:E3:201:CYC:NC | 2.09 | 0.63 |
| 2:U3:141:GLN:HA | 2:Q9:76:ASP:N | 2.05 | 0.63 |
| 3:H4:84:ARG:HG2 | 11:aA:131:TYR:CZ | 2.26 | 0.63 |
| 4:M4:215:GLU:OE1 | 12:Z4:301:CYC:HAB1 | 1.96 | 0.63 |
| 12:X4:201:CYC:HMD1 | 12:X4:201:CYC:NC | 2.09 | 0.63 |
| 1:F5:10:ASN:HB2 | 9:z5:65:THR:OG1 | 1.96 | 0.63 |
| 1:d5:155:TYR:HE2 | 1:T5:113:LYS:NZ | 1.91 | 0.63 |
| 8:U5:63:PRO:HB3 | 6:M6:39:ARG:NH1 | 2.12 | 0.63 |
| 1:b5:12:TYR:CZ | 1:b5:23:ALA:HB2 | 2.33 | 0.63 |
| 6:M6:277:GLY:CA | 1:d7:62:TYR:HB2 | 2.28 | 0.63 |
| 10:j5:820:HIS:ND1 | 10:j5:859:ILE:HD13 | 1.93 | 0.63 |
| 10:j5:1008:PHE:CE1 | 12:v7:201:CYC:C3B | 2.82 | 0.63 |
| 10:k5:391:SER:O | 10:k5:392:SER:CB | 2.47 | 0.63 |
| 10:k5:1118:THR:HA | 12:k5:1204:CYC:HBA1 | 1.80 | 0.63 |
| 10:k5:1124:TYR:OH | 1:n7:119:LEU:HD21 | 1.99 | 0.63 |
| 3:D1:68:ARG:NH2 | 3:X1:68:ARG:NH1 | 2.45 | 0.63 |
| 8:O7:102:THR:HB | 8:O7:103:PRO:HD2 | 1.76 | 0.63 |
| 8:Q7:126:VAL:HG22 | 12:Q7:201:CYC:CMC | 2.27 | 0.63 |
| 8:Q7:126:VAL:HG22 | 12:Q7:201:CYC:HMC1 | 1.80 | 0.63 |
| 8:M7:60:GLN:NE2 | 3:J9:114:LYS:HD3 | 2.13 | 0.63 |
| 8:i7:47:ARG:CD | 1:j7:18:TYR:OH | 2.44 | 0.63 |
| 1:j7:12:TYR:CZ | 1:j7:23:ALA:HB2 | 2.34 | 0.63 |
| 8:U7:27:LYS:O | 8:U7:30:VAL:HG23 | 1.98 | 0.63 |
| 1:X7:12:TYR:CZ | 1:X7:23:ALA:HB2 | 2.33 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:a7:107:ILE:HD13 | 1:b7:13:ASP:OD1 | 1.98 | 0.63 |
| 2:A8:33:ARG:CZ | 2:K8:28:ASN:ND2 | 2.61 | 0.63 |
| 1:v7:12:TYR:CZ | 1:v7:23:ALA:HB2 | 2.34 | 0.63 |
| 4:M8:58:TYR:HA | 4:M8:61:ASN:ND2 | 2.13 | 0.63 |
| 3:L9:51:ILE:HD13 | 3:L9:90:LEU:HD11 | 1.79 | 0.63 |
| 4:M9:85:VAL:HG12 | 4:M9:85:VAL:O | 1.97 | 0.63 |
| 12:J9:202:CYC:HBB1 | 11:a9:516:GLN:O | 1.98 | 0.63 |
| 2:G1:111:ALA:HB1 | 3:L1:77:ARG:HG2 | 1.81 | 0.63 |
| 11:a9:798:SER:CB | 11:a9:800:THR:HB | 2.18 | 0.63 |
| 11:aA:32:ARG:HH11 | 11:aA:32:ARG:CG | 2.10 | 0.63 |
| 2:AA:33:ARG:CZ | 2:KA:28:ASN:ND2 | 2.61 | 0.63 |
| 3:JA:112:GLY:HA3 | 11:aA:519:ARG:HA | 1.79 | 0.63 |
| 3:LA:111:ASN:O | 11:aA:532:ALA:CA | 2.46 | 0.63 |
| 4:MA:252:LEU:CD1 | 12:ZA:202:CYC:O1D | 2.47 | 0.63 |
| 2:OA:33:ARG:CZ | 2:YA:28:ASN:ND2 | 2.62 | 0.63 |
| 12:QA:201:CYC:O2A | 3:TA:67:ILE:CD1 | 2.46 | 0.63 |
| 2:SA:42:ARG:HD2 | 2:X4:69:PRO:CA | 2.29 | 0.63 |
| 3:TA:32:LYS:NZ | 2:X4:57:GLN:CA | 2.28 | 0.63 |
| 2:K3:28:ASN:ND2 | 2:A3:33:ARG:CZ | 2.61 | 0.63 |
| 2:C3:140:SER:HB3 | 3:D8:150:ARG:CG | 2.10 | 0.63 |
| 12:C4:201:CYC:HMD1 | 12:C4:201:CYC:NC | 2.09 | 0.63 |
| 5:N3:33:GLY:O | 3:T3:84:ARG:CD | 2.40 | 0.63 |
| 3:F4:106:GLU:C | 4:M4:6:THR:O | 2.41 | 0.63 |
| 2:N4:63:PHE:HB2 | 2:N4:66:LEU:CG | 2.27 | 0.63 |
| 8:C5:37:LEU:CD2 | 1:D5:27:LEU:HD12 | 2.29 | 0.63 |
| 8:Y5:90:ARG:HA | 1:Z5:18:TYR:CE2 | 2.33 | 0.63 |
| 1:b5:9:ILE:CG2 | 10:k5:17:PHE:CZ | 2.81 | 0.63 |
| 9:i5:6:LYS:HB3 | 9:i5:55:LYS:HB2 | 0.64 | 0.63 |
| 10:j5:619:GLU:HB2 | 10:j5:620:PRO:HD2 | 1.80 | 0.63 |
| 10:j5:1043:GLU:CD | 8:e7:14:GLU:HG2 | 2.22 | 0.63 |
| 10:k5:386:ILE:HG22 | 10:k5:395:SER:C | 2.18 | 0.63 |
| 10:k5:889:LEU:HD23 | 12:D7:201:CYC:OB | 1.99 | 0.63 |
| 10:k5:971:VAL:HG11 | 1:n7:76:ARG:HH12 | 1.61 | 0.63 |
| 2:A6:63:PHE:HB2 | 2:A6:66:LEU:CG | 2.28 | 0.63 |
| 8:S7:6:LYS:HZ1 | 8:G7:22:GLU:CD | 2.06 | 0.63 |
| 8:c7:25:ARG:NH2 | 8:m7:6:LYS:HZ3 | 1.89 | 0.63 |
| 8:o7:23:LEU:HD22 | 1:p7:38:VAL:CG2 | 2.28 | 0.63 |
| 8:q7:68:PRO:HB2 | 11:aA:334:LYS:NZ | 2.14 | 0.63 |
| 3:U8:114:LYS:NZ | 4:M8:13:LYS:HZ2 | 1.86 | 0.63 |
| 2:X8:28:ASN:ND2 | 2:N8:33:ARG:CZ | 2.61 | 0.63 |
| 2:X8:68:GLN:NE2 | 3:T9:24:LEU:HD22 | 2.12 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M8:29:PRO:HG3 | 11:a9:226:PHE:CA | 2.28 | 0.63 |
| 4:M8:29:PRO:HG2 | 11:a9:230:THR:OG1 | 1.99 | 0.63 |
| 4:M8:235:PHE:HA | 12:M8:301:CYC:HAA1 | 1.79 | 0.63 |
| 12:P8:201:CYC:HMD1 | 12:P8:201:CYC:NC | 2.10 | 0.63 |
| 4:M9:252:LEU:CD1 | 12:Z9:202:CYC:O1D | 2.47 | 0.63 |
| 2:G1:111:ALA:CB | 3:L1:77:ARG:CG | 2.68 | 0.63 |
| 11:a9:643:LEU:HD13 | 11:a9:766:ASN:HB3 | 1.81 | 0.63 |
| 11:aA:312:ASP:OD1 | 11:aA:316:GLY:CA | 2.46 | 0.63 |
| 2:AA:19:LEU:O | 3:BA:45:THR:HG21 | 1.99 | 0.63 |
| 3:HA:59:LEU:CD2 | 12:HA:202:CYC:CBC | 2.76 | 0.63 |
| 2:OA:19:LEU:O | 3:PA:45:THR:HG21 | 1.99 | 0.63 |
| 12:R1:201:CYC:CBB | 5:N1:61:LYS:NZ | 2.62 | 0.63 |
| 2:A1:19:LEU:O | 3:B1:45:THR:HG21 | 1.99 | 0.63 |
| 3:J2:119:ALA:HB3 | 6:M2:260:THR:OG1 | 1.99 | 0.63 |
| 2:A4:33:ARG:CZ | 2:K4:28:ASN:ND2 | 2.61 | 0.63 |
| 2:A4:63:PHE:HB2 | 2:A4:66:LEU:CG | 2.28 | 0.63 |
| 12:B4:202:CYC:CMB | 4:M4:57:THR:CG2 | 2.74 | 0.63 |
| 3:F4:91:ARG:HH21 | 11:aA:140:GLN:NE2 | 1.96 | 0.63 |
| 1:f5:5:ILE:CD1 | 10:j5:46:PHE:CE1 | 2.80 | 0.63 |
| 2:K6:28:ASN:ND2 | 2:A6:33:ARG:CZ | 2.61 | 0.63 |
| 9:z5:10:CYS:O | 9:z5:49:GLY:HA2 | 1.98 | 0.63 |
| 10:j5:138:PRO:CB | 10:j5:201:VAL:CG1 | 2.52 | 0.63 |
| 10:j5:974:LEU:HD22 | 10:j5:974:LEU:O | 1.98 | 0.63 |
| 10:j5:1016:LEU:CB | 10:j5:1044:ASN:ND2 | 2.62 | 0.63 |
| 10:k5:141:GLU:OE2 | 10:k5:141:GLU:N | 2.23 | 0.63 |
| 10:k5:187:ARG:HE | 10:k5:237:ASP:CG | 2.05 | 0.63 |
| 8:O7:20:PRO:O | 8:O7:23:LEU:HB2 | 1.98 | 0.63 |
| 8:I7:37:LEU:HD11 | 1:J7:31:PHE:HE2 | 1.64 | 0.63 |
| 8:a7:16:ARG:HG3 | 8:a7:16:ARG:HH11 | 1.64 | 0.63 |
| 12:B8:202:CYC:CBD | 4:M8:53:LEU:HB3 | 2.27 | 0.63 |
| 8:m7:37:LEU:HD11 | 1:n7:31:PHE:HE2 | 1.64 | 0.63 |
| 2:X8:57:GLN:C | 3:T9:32:LYS:NZ | 2.56 | 0.63 |
| 2:X8:69:PRO:CA | 2:S9:42:ARG:HD2 | 2.29 | 0.63 |
| 4:M8:85:VAL:HG12 | 4:M8:85:VAL:O | 1.97 | 0.63 |
| 4:M8:134:ASN:OD1 | 5:Z8:1:MET:HE1 | 1.97 | 0.63 |
| 2:I9:37:SER:HB3 | 2:I9:97:LEU:CD1 | 2.28 | 0.63 |
| 11:a9:61:TYR:O | 11:a9:63:ASP:N | 2.31 | 0.63 |
| 11:a9:245:ALA:HB2 | 12:a9:901:CYC:OB | 1.96 | 0.63 |
| 11:aA:338:VAL:CG2 | 11:aA:340:PRO:HD3 | 2.25 | 0.63 |
| 11:aA:813:PRO:CA | 3:L1:119:ALA:HB2 | 2.27 | 0.63 |
| 11:aA:823:ILE:O | 11:aA:823:ILE:HD13 | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:MA:151:LEU:O | 4:MA:155:ARG:HG3 | 1.97 | 0.63 |
| 2:QA:81:LYS:NZ | 3:TA:67:ILE:HD13 | 2.13 | 0.63 |
| 2:O1:33:ARG:HE | 2:Y1:28:ASN:HD21 | 1.45 | 0.63 |
| 12:I3:201:CYC:HMD1 | 12:I3:201:CYC:NC | 2.09 | 0.63 |
| 12:I2:201:CYC:HMD1 | 12:I2:201:CYC:NC | 2.10 | 0.63 |
| 2:K2:28:ASN:ND2 | 2:A2:33:ARG:CZ | 2.61 | 0.63 |
| 5:N3:24:PRO:CG | 5:N3:35:ASP:O | 2.46 | 0.63 |
| 4:M4:232:VAL:HG21 | 3:Y4:113:LEU:HB2 | 1.81 | 0.63 |
| 3:O4:116:THR:N | 5:Z4:70:ILE:CG2 | 2.62 | 0.63 |
| 8:K5:23:LEU:HD12 | 8:U5:151:PHE:CD1 | 2.34 | 0.63 |
| 3:Y4:89:ILE:CB | 3:Y4:92:TYR:OH | 2.46 | 0.63 |
| 3:Y4:89:ILE:CG1 | 3:Y4:92:TYR:HE2 | 2.10 | 0.63 |
| 8:G5:107:ILE:HD13 | 1:H5:13:ASP:OD1 | 1.97 | 0.63 |
| 8:I5:37:LEU:CD2 | 1:J5:27:LEU:HD12 | 2.29 | 0.63 |
| 2:C1:115:GLU:OE2 | 4:M1:33:LEU:HD21 | 1.91 | 0.63 |
| 8:Q5:8:ILE:HG21 | 1:R5:94:TYR:HB3 | 1.80 | 0.63 |
| 8:Q5:126:VAL:CG2 | 12:Q5:201:CYC:HMC1 | 2.27 | 0.63 |
| 1:R5:12:TYR:CZ | 1:R5:23:ALA:HB2 | 2.34 | 0.63 |
| 8:a5:102:THR:HB | 8:a5:103:PRO:HD2 | 1.76 | 0.63 |
| 9:i5:8:THR:CG2 | 9:i5:52:LEU:HD12 | 2.29 | 0.63 |
| 10:j5:388:ARG:CD | 10:j5:393:MET:N | 2.61 | 0.63 |
| 10:j5:949:ARG:HB2 | 10:j5:950:PRO:HD2 | 1.80 | 0.63 |
| 10:k5:614:ARG:HH11 | 10:k5:614:ARG:HG2 | 1.64 | 0.63 |
| 10:k5:619:GLU:HB3 | 10:k5:620:PRO:HD3 | 1.81 | 0.63 |
| 10:k5:800:THR:HA | 9:z7:30:LYS:HB2 | 1.81 | 0.63 |
| 10:k5:826:THR:HG21 | 12:B7:201:CYC:HMA2 | 1.79 | 0.63 |
| 10:k5:973:THR:O | 10:k5:977:GLN:NE2 | 2.32 | 0.63 |
| 10:k5:1085:GLY:HA2 | 1:l7:87:TYR:CE1 | 2.34 | 0.63 |
| 3:U8:5:PHE:CD2 | 3:U8:27:LEU:HD22 | 2.34 | 0.63 |
| 3:L8:69:PRO:HD2 | 11:a9:81:ASP:HA | 1.81 | 0.63 |
| 3:Q8:89:ILE:CB | 3:Q8:92:TYR:CZ | 2.81 | 0.63 |
| 3:Q8:92:TYR:CE1 | 3:Q8:105:LEU:HD13 | 2.34 | 0.63 |
| 3:Q8:122:THR:HG21 | 12:Z8:301:CYC:HMC2 | 1.79 | 0.63 |
| 4:M9:36:TYR:O | 12:B9:201:CYC:HMA3 | 1.98 | 0.63 |
| 4:M9:188:LEU:HD21 | 12:V9:201:CYC:NB | 2.12 | 0.63 |
| 2:O9:19:LEU:O | 3:P9:45:THR:HG21 | 1.99 | 0.63 |
| 2:K9:15:GLN:HG2 | 11:a9:393:ARG:NH1 | 2.12 | 0.63 |
| 12:G1:201:CYC:HMD1 | 12:G1:201:CYC:NC | 2.09 | 0.63 |
| 11:a9:640:ALA:CB | 11:a9:767:THR:HG23 | 2.26 | 0.63 |
| 1:A:161:SER:OG | 1:R5:14:VAL:HG21 | 1.78 | 0.63 |
| 4:MA:159:CYS:N | 3:VA:108:ARG:HG3 | 2.13 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:OA:63:PHE:HB2 | 2:OA:66:LEU:CG | 2.28 | 0.63 |
| 3:TA:32:LYS:NZ | 2:X4:57:GLN:C | 2.56 | 0.63 |
| 6:M2:153:PHE:HA | 6:M2:254:GLN:HE22 | 1.64 | 0.63 |
| 12:A4:201:CYC:HMD1 | 12:A4:201:CYC:NC | 2.09 | 0.63 |
| 12:Q3:201:CYC:HMD1 | 12:Q3:201:CYC:NC | 2.10 | 0.63 |
| 2:N4:19:LEU:O | 3:O4:45:THR:HG21 | 1.99 | 0.63 |
| 5:Z4:1:MET:C | 5:Z4:3:VAL:N | 2.50 | 0.63 |
| 5:Z4:21:ALA:CB | 5:Z4:68:LEU:HD11 | 2.23 | 0.63 |
| 8:A5:90:ARG:HD3 | 1:B5:18:TYR:CE1 | 2.34 | 0.63 |
| 1:D5:14:VAL:O | 1:D5:14:VAL:HG23 | 1.98 | 0.63 |
| 8:G5:71:ASN:CG | 12:G5:201:CYC:HMD3 | 2.24 | 0.63 |
| 1:H5:107:ARG:NH2 | 9:i5:21:ARG:HD3 | 2.13 | 0.63 |
| 8:U5:83:ARG:HG3 | 6:M6:31:ASP:CB | 2.28 | 0.63 |
| 9:i5:8:THR:HG22 | 9:i5:52:LEU:HD12 | 1.80 | 0.63 |
| 9:i5:23:LEU:N | 9:i5:25:ASN:H | 1.97 | 0.63 |
| 10:j5:221:LYS:HB3 | 10:j5:221:LYS:NZ | 2.14 | 0.63 |
| 10:j5:823:TYR:O | 1:H7:107:ARG:HD2 | 1.99 | 0.63 |
| 10:j5:931:VAL:CG2 | 1:J7:30:TYR:N | 2.60 | 0.63 |
| 8:g7:27:LYS:O | 8:g7:30:VAL:HG23 | 1.98 | 0.63 |
| 1:b7:75:THR:HB | 8:c7:111:GLY:C | 2.24 | 0.63 |
| 8:o7:29:PHE:CD2 | 1:p7:31:PHE:CE1 | 2.58 | 0.63 |
| 8:q7:76:LYS:HZ2 | 11:aA:605:PRO:CB | 1.97 | 0.63 |
| 9:z7:21:ARG:O | 9:z7:22:GLU:C | 2.40 | 0.63 |
| 9:y7:3:ARG:NH1 | 9:y7:67:VAL:HG11 | 2.14 | 0.63 |
| 2:X8:57:GLN:HE22 | 3:T9:32:LYS:HG2 | 1.63 | 0.63 |
| 3:L8:130:ALA:CB | 12:a9:901:CYC:CBC | 2.77 | 0.63 |
| 4:M8:230:GLN:C | 12:M8:301:CYC:HBB3 | 2.13 | 0.63 |
| 4:M8:267:LEU:C | 4:M8:269:SER:O | 2.42 | 0.63 |
| 3:O8:5:PHE:CD2 | 3:O8:27:LEU:HD22 | 2.34 | 0.63 |
| 3:O8:107:ASP:HB3 | 5:Z8:66:ARG:CA | 2.28 | 0.63 |
| 12:L9:202:CYC:HMA1 | 11:a9:534:SER:HB3 | 1.80 | 0.63 |
| 4:M9:118:TYR:CD2 | 12:Z9:202:CYC:O2A | 2.51 | 0.63 |
| 5:N9:6:GLY:HA3 | 3:R9:108:ARG:C | 2.24 | 0.63 |
| 3:Y8:5:PHE:CD2 | 3:Y8:27:LEU:HD22 | 2.34 | 0.63 |
| 11:aA:95:ILE:HD13 | 11:aA:237:PHE:CZ | 2.33 | 0.63 |
| 11:aA:371:VAL:CG1 | 11:aA:507:PHE:CD2 | 2.80 | 0.63 |
| 11:aA:716:ILE:HD12 | 11:aA:738:LEU:HD21 | 1.81 | 0.63 |
| 5:NA:1:MET:CB | 5:NA:3:VAL:CG2 | 2.76 | 0.63 |
| 12:QA:201:CYC:O2A | 3:TA:67:ILE:HD12 | 1.98 | 0.63 |
| 2:O1:19:LEU:O | 3:P1:45:THR:HG21 | 1.99 | 0.63 |
| 2:G3:111:ALA:HB1 | 3:L3:77:ARG:HG2 | 1.81 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:H3:84:ARG:CD | 11:a9:776:TYR:CZ | 2.82 | 0.63 |
| 2:A3:19:LEU:O | 3:B3:45:THR:HG21 | 1.99 | 0.63 |
| 5:N3:16:PHE:HE2 | 5:N3:50:LEU:HA | 1.62 | 0.63 |
| 5:N3:36:THR:HG1 | 12:T3:301:CYC:HB | 1.35 | 0.63 |
| 3:B1:91:ARG:NH1 | 11:aA:677:GLN:HE22 | 1.97 | 0.63 |
| 3:F4:110:LEU:N | 4:M4:6:THR:HG22 | 2.07 | 0.63 |
| 4:M4:151:LEU:O | 4:M4:155:ARG:HG3 | 1.98 | 0.63 |
| 8:G5:125:ALA:HB3 | 12:G5:201:CYC:HMC2 | 1.81 | 0.63 |
| 8:c5:114:GLU:OE1 | 10:j5:312:TYR:C | 2.41 | 0.63 |
| 1:d5:155:TYR:OH | 1:T5:113:LYS:NZ | 2.24 | 0.63 |
| 1:f5:12:TYR:CZ | 1:f5:23:ALA:HB2 | 2.33 | 0.63 |
| 1:X5:12:TYR:CZ | 1:X5:23:ALA:HB2 | 2.34 | 0.63 |
| 6:M6:153:PHE:HA | 6:M6:254:GLN:HE22 | 1.64 | 0.63 |
| 7:N6:49:LEU:HD12 | 3:B6:84:ARG:NE | 2.14 | 0.63 |
| 10:j5:143:ILE:HD12 | 10:j5:146:ALA:HB3 | 1.79 | 0.63 |
| 10:j5:391:SER:O | 10:j5:392:SER:CB | 2.47 | 0.63 |
| 10:j5:984:ILE:C | 10:j5:984:ILE:HD12 | 2.23 | 0.63 |
| 10:k5:298:ARG:NH1 | 10:k5:298:ARG:HG2 | 2.14 | 0.63 |
| 10:k5:820:HIS:HE1 | 10:k5:859:ILE:CD1 | 1.95 | 0.63 |
| 10:k5:1043:GLU:OE1 | 8:Y7:14:GLU:HG2 | 1.99 | 0.63 |
| 10:k5:1125:ARG:NH2 | 1:n7:114:GLU:HB2 | 2.12 | 0.63 |
| 8:O7:37:LEU:HD11 | 1:P7:31:PHE:HE2 | 1.64 | 0.63 |
| 1:F7:12:TYR:CZ | 1:F7:23:ALA:HB2 | 2.34 | 0.63 |
| 8:G7:90:ARG:HA | 1:H7:18:TYR:CE2 | 2.32 | 0.63 |
| 8:K7:25:ARG:CD | 8:U7:25:ARG:HH22 | 2.11 | 0.63 |
| 8:K7:25:ARG:CB | 8:U7:25:ARG:HH21 | 2.07 | 0.63 |
| 1:L7:12:TYR:CZ | 1:L7:23:ALA:HB2 | 2.34 | 0.63 |
| 8:i7:37:LEU:CD1 | 1:j7:31:PHE:CD2 | 2.78 | 0.63 |
| 3:D8:5:PHE:CD2 | 3:D8:27:LEU:HD22 | 2.34 | 0.63 |
| 3:L8:71:GLY:CA | 11:a9:82:GLN:CD | 2.71 | 0.63 |
| 2:N8:63:PHE:HB2 | 2:N8:66:LEU:CG | 2.27 | 0.63 |
| 3:Q8:5:PHE:CD2 | 3:Q8:27:LEU:HD22 | 2.34 | 0.63 |
| 4:M9:160:THR:H | 3:V9:108:ARG:HG2 | 1.59 | 0.63 |
| 3:P9:5:PHE:CD2 | 3:P9:27:LEU:HD22 | 2.34 | 0.63 |
| 3:H9:66:LEU:HD22 | 12:H9:202:CYC:C1C | 2.19 | 0.63 |
| 3:V9:5:PHE:CD2 | 3:V9:27:LEU:HD22 | 2.34 | 0.63 |
| 11:a9:275:THR:CA | 11:a9:278:LEU:HD13 | 2.03 | 0.63 |
| 11:a9:537:ASP:HB3 | 11:a9:543:GLN:HB2 | 1.79 | 0.63 |
| 3:L1:5:PHE:CD2 | 3:L1:27:LEU:HD22 | 2.34 | 0.63 |
| 4:M1:151:LEU:O | 4:M1:155:ARG:HG3 | 1.98 | 0.63 |
| 4:M1:188:LEU:HD22 | 12:Z1:202:CYC:HB | 1.63 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:X1:5:PHE:CD2 | 3:X1:27:LEU:HD22 | 2.34 | 0.63 |
| 2:A2:19:LEU:O | 3:B2:45:THR:HG21 | 1.99 | 0.63 |
| 3:D2:5:PHE:CD2 | 3:D2:27:LEU:HD22 | 2.34 | 0.63 |
| 1:A:62:TYR:HD1 | 10:k5:155:LYS:HZ1 | 1.46 | 0.62 |
| 2:AA:63:PHE:HB2 | 2:AA:66:LEU:CG | 2.27 | 0.62 |
| 12:BA:201:CYC:HMA3 | 4:MA:36:TYR:O | 1.98 | 0.62 |
| 5:NA:6:GLY:HA3 | 3:RA:108:ARG:C | 2.24 | 0.62 |
| 2:QA:116:VAL:CG1 | 3:TA:79:MET:HG2 | 2.29 | 0.62 |
| 2:A3:63:PHE:CB | 2:A3:66:LEU:HG | 2.29 | 0.62 |
| 12:B3:202:CYC:HBA1 | 11:a9:684:ASN:ND2 | 2.13 | 0.62 |
| 3:D4:5:PHE:CD2 | 3:D4:27:LEU:HD22 | 2.34 | 0.62 |
| 2:U3:140:SER:O | 2:Q9:76:ASP:HB2 | 1.99 | 0.62 |
| 4:M4:197:ASP:CB | 5:Z4:52:ARG:HG2 | 2.18 | 0.62 |
| 1:L5:12:TYR:CZ | 1:L5:23:ALA:HB2 | 2.34 | 0.62 |
| 1:L5:119:LEU:CD2 | 10:j5:546:PHE:CD2 | 2.76 | 0.62 |
| 8:M5:14:GLU:HG2 | 10:k5:538:PHE:CZ | 2.34 | 0.62 |
| 8:C5:2:SER:C | 8:C5:100:ASP:HB3 | 2.24 | 0.62 |
| 8:E5:161:GLN:NE2 | 1:P5:49:THR:CG2 | 2.62 | 0.62 |
| 6:M6:104:ARG:NH1 | 2:G6:16:GLY:HA2 | 2.13 | 0.62 |
| 10:j5:619:GLU:HB3 | 10:j5:620:PRO:HD3 | 1.81 | 0.62 |
| 10:k5:246:VAL:HG23 | 10:k5:257:THR:HG22 | 1.80 | 0.62 |
| 10:k5:362:LYS:CE | 10:k5:363:HIS:HD2 | 2.08 | 0.62 |
| 10:k5:539:LYS:O | 10:k5:539:LYS:HG3 | 1.97 | 0.62 |
| 3:B6:5:PHE:CD2 | 3:B6:27:LEU:HD22 | 2.34 | 0.62 |
| 8:I7:35:ARG:NH2 | 8:I7:144:ASP:CB | 2.61 | 0.62 |
| 8:U7:37:LEU:HD11 | 1:V7:31:PHE:HE2 | 1.64 | 0.62 |
| 8:o7:23:LEU:HA | 1:p7:38:VAL:HG22 | 1.79 | 0.62 |
| 12:q7:201:CYC:HC | 12:q7:201:CYC:CMD | 2.10 | 0.62 |
| 9:w7:5:PHE:CE2 | 9:w7:37:TRP:CD1 | 2.86 | 0.62 |
| 3:J8:5:PHE:CD2 | 3:J8:27:LEU:HD22 | 2.34 | 0.62 |
| 3:L8:5:PHE:CD2 | 3:L8:27:LEU:HD22 | 2.34 | 0.62 |
| 3:S8:5:PHE:CD2 | 3:S8:27:LEU:HD22 | 2.34 | 0.62 |
| 3:F1:119:ALA:HB2 | 4:M1:41:ASN:HD21 | 1.63 | 0.62 |
| 4:M9:77:LEU:CD2 | 3:Z9:115:GLU:OE2 | 2.46 | 0.62 |
| 4:M9:188:LEU:HD11 | 3:V9:88:ILE:HD11 | 1.81 | 0.62 |
| 3:J9:119:ALA:CA | 11:a9:365:LYS:CE | 2.69 | 0.62 |
| 11:a9:371:VAL:CG1 | 11:a9:507:PHE:CB | 2.77 | 0.62 |
| 11:aA:809:ARG:HH22 | 3:L1:115:GLU:HB2 | 1.64 | 0.62 |
| 5:N1:33:GLY:O | 3:T1:84:ARG:CD | 2.40 | 0.62 |
| 3:B2:5:PHE:CD2 | 3:B2:27:LEU:HD22 | 2.34 | 0.62 |
| 1:Z:27:LEU:HD13 | 8:e5:37:LEU:HD21 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AA:114:ARG:NH1 | 11:aA:407:GLU:CD | 2.56 | 0.62 |
| 3:DA:68:ARG:HH12 | 3:XA:65:ASP:HB3 | 1.63 | 0.62 |
| 12:JA:202:CYC:HBB1 | 11:aA:516:GLN:O | 1.99 | 0.62 |
| 4:MA:160:THR:HG22 | 4:MA:257:GLN:HB3 | 1.73 | 0.62 |
| 3:XA:5:PHE:CD2 | 3:XA:27:LEU:HD22 | 2.34 | 0.62 |
| 2:O1:2:LYS:HE2 | 2:Y1:22:THR:HG21 | 1.81 | 0.62 |
| 3:R1:5:PHE:CD2 | 3:R1:27:LEU:HD22 | 2.34 | 0.62 |
| 3:H2:5:PHE:CD2 | 3:H2:27:LEU:HD22 | 2.34 | 0.62 |
| 3:H2:121:GLY:HA3 | 6:M2:251:LYS:HZ1 | 1.63 | 0.62 |
| 3:L2:5:PHE:CD2 | 3:L2:27:LEU:HD22 | 2.34 | 0.62 |
| 2:C3:115:GLU:OE2 | 4:M3:33:LEU:HD21 | 1.91 | 0.62 |
| 2:A4:63:PHE:CB | 2:A4:66:LEU:HG | 2.29 | 0.62 |
| 2:O3:19:LEU:O | 3:P3:45:THR:HG21 | 1.99 | 0.62 |
| 3:H4:14:LEU:HD11 | 11:aA:86:ASP:H | 1.64 | 0.62 |
| 3:Q4:91:ARG:HH11 | 3:Q4:95:TYR:HD2 | 1.45 | 0.62 |
| 12:N5:201:CYC:HBB2 | 10:k5:482:GLN:NE2 | 2.13 | 0.62 |
| 8:A5:125:ALA:HB3 | 12:A5:201:CYC:HMC2 | 1.81 | 0.62 |
| 8:G5:25:ARG:NH2 | 8:S5:25:ARG:HE | 1.96 | 0.62 |
| 1:d5:67:ARG:NH2 | 10:j5:708:GLY:HA3 | 2.13 | 0.62 |
| 8:e5:27:LYS:O | 8:e5:30:VAL:HG23 | 1.98 | 0.62 |
| 8:e5:35:ARG:NH2 | 8:e5:144:ASP:CB | 2.61 | 0.62 |
| 12:J6:202:CYC:O2A | 6:M6:185:PHE:CD2 | 2.41 | 0.62 |
| 10:j5:344:ARG:HH11 | 10:j5:344:ARG:HG2 | 1.64 | 0.62 |
| 10:j5:614:ARG:HH11 | 10:j5:614:ARG:HG2 | 1.64 | 0.62 |
| 10:k5:275:THR:CG2 | 10:k5:286:VAL:HG12 | 2.29 | 0.62 |
| 3:F6:82:CYS:HB2 | 12:F6:201:CYC:C2D | 2.29 | 0.62 |
| 8:C7:102:THR:HB | 8:C7:103:PRO:HD2 | 1.76 | 0.62 |
| 8:g7:90:ARG:CZ | 1:h7:16:GLY:C | 2.73 | 0.62 |
| 8:i7:42:THR:CB | 8:i7:141:LEU:CD2 | 2.76 | 0.62 |
| 8:a7:2:SER:C | 8:a7:100:ASP:HB3 | 2.24 | 0.62 |
| 2:A8:19:LEU:O | 3:B8:45:THR:HG21 | 1.99 | 0.62 |
| 12:B8:202:CYC:HMB3 | 4:M8:57:THR:HG23 | 1.81 | 0.62 |
| 8:o7:94:TYR:HH | 1:p7:17:LYS:C | 1.95 | 0.62 |
| 8:s7:37:LEU:HD11 | 1:t7:31:PHE:HE2 | 1.64 | 0.62 |
| 1:v7:139:GLY:HA3 | 11:aA:342:ARG:HE | 1.64 | 0.62 |
| 3:F1:5:PHE:CD2 | 3:F1:27:LEU:HD22 | 2.34 | 0.62 |
| 2:A9:33:ARG:CZ | 2:K9:28:ASN:ND2 | 2.61 | 0.62 |
| 11:aA:50:LEU:O | 11:aA:53:VAL:N | 2.33 | 0.62 |
| 4:M1:245:ASP:CB | 3:X1:108:ARG:O | 2.41 | 0.62 |
| 3:HA:5:PHE:CD2 | 3:HA:27:LEU:HD22 | 2.34 | 0.62 |
| 2:IA:4:VAL:HB | 2:IA:30:ARG:HG3 | 1.80 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:JA:20:SER:O | 3:JA:22:GLN:CA | 2.46 | 0.62 |
| 12:JA:202:CYC:CGA | 11:aA:511:LYS:HD2 | 2.26 | 0.62 |
| 3:LA:120:LEU:HD23 | 11:aA:539:GLY:H | 1.65 | 0.62 |
| 4:MA:134:ASN:CB | 12:RA:201:CYC:HAA1 | 2.21 | 0.62 |
| 4:MA:188:LEU:HD21 | 12:VA:201:CYC:NB | 2.12 | 0.62 |
| 2:QA:116:VAL:HG22 | 3:TA:79:MET:C | 2.24 | 0.62 |
| 3:RA:5:PHE:CD2 | 3:RA:27:LEU:HD22 | 2.34 | 0.62 |
| 2:O1:33:ARG:CZ | 2:Y1:28:ASN:ND2 | 2.62 | 0.62 |
| 3:J3:84:ARG:NH2 | 2:K3:115:GLU:OE2 | 2.26 | 0.62 |
| 2:A4:19:LEU:O | 3:B4:45:THR:HG21 | 1.99 | 0.62 |
| 3:B4:120:LEU:HD11 | 4:M4:53:LEU:H | 1.61 | 0.62 |
| 3:L3:5:PHE:CD2 | 3:L3:27:LEU:HD22 | 2.34 | 0.62 |
| 5:N3:61:LYS:NZ | 12:R3:201:CYC:CBB | 2.62 | 0.62 |
| 3:P3:5:PHE:CD2 | 3:P3:27:LEU:HD22 | 2.34 | 0.62 |
| 3:V3:5:PHE:CD2 | 3:V3:27:LEU:HD22 | 2.34 | 0.62 |
| 12:G4:201:CYC:HMD1 | 12:G4:201:CYC:NC | 2.09 | 0.62 |
| 3:H4:5:PHE:CD2 | 3:H4:27:LEU:HD22 | 2.34 | 0.62 |
| 3:H4:84:ARG:CD | 11:aA:131:TYR:CZ | 2.82 | 0.62 |
| 4:M4:232:VAL:CG2 | 3:Y4:113:LEU:HB2 | 2.30 | 0.62 |
| 3:O4:120:LEU:HD23 | 5:Z4:14:LYS:HZ2 | 1.64 | 0.62 |
| 3:Q4:5:PHE:CD2 | 3:Q4:27:LEU:HD22 | 2.34 | 0.62 |
| 1:L5:106:GLU:HG3 | 9:i5:58:THR:HG23 | 1.80 | 0.62 |
| 8:O5:2:SER:C | 8:O5:100:ASP:HB3 | 2.25 | 0.62 |
| 8:O5:76:LYS:O | 8:O5:77:MET:C | 2.43 | 0.62 |
| 3:Y4:93:VAL:HG22 | 3:Y4:105:LEU:HD11 | 1.81 | 0.62 |
| 8:E5:128:GLU:OE1 | 8:E5:128:GLU:HA | 1.99 | 0.62 |
| 1:f5:9:ILE:HG21 | 10:j5:17:PHE:CZ | 2.33 | 0.62 |
| 1:P5:114:GLU:CB | 10:k5:496:GLU:CG | 2.62 | 0.62 |
| 2:K6:22:THR:HG21 | 2:A6:2:LYS:HE2 | 1.81 | 0.62 |
| 9:z5:8:THR:CG2 | 9:z5:52:LEU:HD12 | 2.29 | 0.62 |
| 10:j5:309:LEU:HD13 | 10:j5:342:LEU:HD13 | 1.81 | 0.62 |
| 10:j5:539:LYS:O | 10:j5:539:LYS:HG3 | 1.98 | 0.62 |
| 10:j5:1071:PRO:O | 10:j5:1071:PRO:HD2 | 1.99 | 0.62 |
| 10:k5:345:ARG:HG2 | 10:k5:345:ARG:O | 1.98 | 0.62 |
| 10:k5:1002:ARG:HG2 | 10:k5:1002:ARG:O | 1.98 | 0.62 |
| 10:k5:1155:ARG:HB3 | 10:k5:1155:ARG:NH2 | 2.07 | 0.62 |
| 1:R7:12:TYR:CZ | 1:R7:23:ALA:HB2 | 2.34 | 0.62 |
| 8:i7:96:ILE:HA | 8:i7:152:TYR:CE1 | 2.30 | 0.62 |
| 8:a7:19:SER:CB | 8:a7:20:PRO:CD | 2.76 | 0.62 |
| 8:c7:39:ILE:HG23 | 8:c7:149:ALA:HB2 | 1.81 | 0.62 |
| 8:u7:29:PHE:HE2 | 1:v7:5:ILE:CD1 | 2.10 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:W8:5:PHE:CD2 | 3:W8:27:LEU:HD22 | 2.34 | 0.62 |
| 3:H8:1:MET:H2 | 11:a9:96:THR:CG2 | 2.12 | 0.62 |
| 3:H8:5:PHE:CD2 | 3:H8:27:LEU:HD22 | 2.34 | 0.62 |
| 4:M8:144:ARG:HD3 | 4:M8:204:ILE:HG21 | 1.81 | 0.62 |
| 2:N8:63:PHE:CB | 2:N8:66:LEU:HG | 2.29 | 0.62 |
| 3:L9:120:LEU:HA | 11:a9:539:GLY:HA3 | 1.79 | 0.62 |
| 4:M9:73:ASP:HA | 3:D9:111:ASN:HD21 | 1.65 | 0.62 |
| 4:M9:263:PRO:O | 3:V9:119:ALA:HB1 | 1.99 | 0.62 |
| 2:O9:33:ARG:CZ | 2:Y9:28:ASN:ND2 | 2.62 | 0.62 |
| 5:Z8:69:GLU:O | 5:Z8:70:ILE:HG12 | 1.99 | 0.62 |
| 3:J9:5:PHE:CD2 | 3:J9:27:LEU:HD22 | 2.34 | 0.62 |
| 11:a9:327:SER:O | 11:a9:328:GLN:C | 2.40 | 0.62 |
| 11:aA:298:ILE:C | 11:aA:300:GLY:N | 2.48 | 0.62 |
| 4:M1:80:PRO:CA | 3:X1:111:ASN:HD21 | 2.11 | 0.62 |
| 4:M1:85:VAL:HG12 | 4:M1:85:VAL:O | 1.97 | 0.62 |
| 5:N1:69:GLU:O | 5:N1:70:ILE:HG12 | 1.99 | 0.62 |
| 2:A2:63:PHE:CB | 2:A2:66:LEU:HG | 2.30 | 0.62 |
| 3:F2:5:PHE:CD2 | 3:F2:27:LEU:HD22 | 2.34 | 0.62 |
| 4:MA:134:ASN:HD21 | 5:NA:1:MET:N | 1.96 | 0.62 |
| 2:QA:149:GLU:OE2 | 2:UA:21:ASN:OD1 | 2.17 | 0.62 |
| 3:H3:5:PHE:CD2 | 3:H3:27:LEU:HD22 | 2.34 | 0.62 |
| 3:J3:121:GLY:CA | 11:a9:804:ARG:NH2 | 2.62 | 0.62 |
| 7:N2:49:LEU:HD12 | 3:B2:84:ARG:NE | 2.14 | 0.62 |
| 3:B3:91:ARG:NH1 | 11:a9:677:GLN:HE22 | 1.97 | 0.62 |
| 3:F3:5:PHE:CD2 | 3:F3:27:LEU:HD22 | 2.34 | 0.62 |
| 3:B4:108:ARG:HA | 4:M4:61:ASN:O | 1.99 | 0.62 |
| 2:O3:2:LYS:HE2 | 2:Y3:22:THR:HG21 | 1.81 | 0.62 |
| 3:J4:5:PHE:CD2 | 3:J4:27:LEU:HD22 | 2.34 | 0.62 |
| 4:M4:82:ILE:HD12 | 12:M4:301:CYC:O2D | 1.90 | 0.62 |
| 8:A5:16:ARG:O | 1:B5:94:TYR:OH | 2.08 | 0.62 |
| 12:G5:201:CYC:HMD1 | 12:G5:201:CYC:NC | 2.02 | 0.62 |
| 8:c5:14:GLU:OE2 | 10:j5:393:MET:HA | 1.98 | 0.62 |
| 1:d5:28:LYS:CE | 1:n7:143:PRO:HB3 | 2.11 | 0.62 |
| 1:d5:127:VAL:CG1 | 10:j5:698:GLY:N | 2.42 | 0.62 |
| 8:W5:17:TYR:HB2 | 1:X5:45:SER:CB | 2.30 | 0.62 |
| 1:b5:114:GLU:HB3 | 10:k5:491:THR:CB | 2.29 | 0.62 |
| 3:J6:119:ALA:HB3 | 6:M6:260:THR:OG1 | 1.99 | 0.62 |
| 10:j5:77:VAL:HG22 | 10:j5:141:GLU:CB | 2.28 | 0.62 |
| 10:j5:141:GLU:CD | 10:j5:141:GLU:H | 2.07 | 0.62 |
| 10:j5:426:LEU:HD12 | 10:j5:426:LEU:O | 1.98 | 0.62 |
| 10:k5:77:VAL:HG22 | 10:k5:141:GLU:CB | 2.28 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:O7:2:SER:C | 8:O7:100:ASP:HB3 | 2.25 | 0.62 |
| 8:O7:35:ARG:NE | 8:O7:145:ASP:OD1 | 2.33 | 0.62 |
| 8:C7:27:LYS:O | 8:C7:30:VAL:HG23 | 1.99 | 0.62 |
| 8:C7:37:LEU:HD11 | 1:D7:31:PHE:HE2 | 1.64 | 0.62 |
| 8:g7:52:LYS:CD | 11:aA:321:ALA:HB2 | 2.24 | 0.62 |
| 8:U7:21:GLY:HA2 | 8:U7:24:ASP:CG | 2.25 | 0.62 |
| 3:B8:5:PHE:CD2 | 3:B8:27:LEU:HD22 | 2.34 | 0.62 |
| 3:D8:116:THR:OG1 | 4:M8:38:PRO:HB2 | 1.99 | 0.62 |
| 8:u7:27:LYS:HE3 | 1:v7:35:ALA:CA | 2.29 | 0.62 |
| 9:z7:15:LYS:HE3 | 9:z7:16:ARG:HD3 | 1.79 | 0.62 |
| 2:X8:22:THR:HG21 | 2:N8:2:LYS:HE2 | 1.81 | 0.62 |
| 3:F8:1:MET:HB2 | 4:M8:10:ARG:HA | 1.81 | 0.62 |
| 3:Q8:81:ALA:HB2 | 5:Z8:36:THR:HG21 | 1.81 | 0.62 |
| 4:M9:251:ASN:H | 4:M9:251:ASN:ND2 | 1.95 | 0.62 |
| 5:Z8:37:HIS:CG | 12:Z8:301:CYC:C4B | 2.81 | 0.62 |
| 2:A9:63:PHE:CB | 2:A9:66:LEU:HG | 2.29 | 0.62 |
| 3:D9:5:PHE:CD2 | 3:D9:27:LEU:HD22 | 2.34 | 0.62 |
| 4:M1:263:PRO:HB2 | 3:Z1:119:ALA:HB3 | 1.78 | 0.62 |
| 1:Z:31:PHE:HE2 | 8:e5:37:LEU:HD11 | 1.64 | 0.62 |
| 3:BA:5:PHE:CD2 | 3:BA:27:LEU:HD22 | 2.34 | 0.62 |
| 4:MA:37:GLU:CD | 11:aA:381:PRO:HG3 | 2.24 | 0.62 |
| 4:MA:51:ARG:NH2 | 11:aA:430:ARG:NE | 2.48 | 0.62 |
| 3:ZA:5:PHE:CD2 | 3:ZA:27:LEU:HD22 | 2.34 | 0.62 |
| 6:M2:28:ASN:HB3 | 8:O5:80:LEU:HD21 | 0.66 | 0.62 |
| 7:N2:29:LEU:HG | 2:A2:115:GLU:OE2 | 2.00 | 0.62 |
| 3:B3:5:PHE:CD2 | 3:B3:27:LEU:HD22 | 2.34 | 0.62 |
| 3:B4:5:PHE:CD2 | 3:B4:27:LEU:HD22 | 2.34 | 0.62 |
| 5:N3:69:GLU:O | 5:N3:70:ILE:HG12 | 1.99 | 0.62 |
| 2:N4:33:ARG:HE | 2:X4:28:ASN:HD21 | 1.44 | 0.62 |
| 3:O4:112:GLY:C | 5:Z4:70:ILE:HB | 2.24 | 0.62 |
| 8:E5:161:GLN:CD | 1:P5:49:THR:HG22 | 2.24 | 0.62 |
| 3:J6:5:PHE:CD2 | 3:J6:27:LEU:HD22 | 2.35 | 0.62 |
| 10:j5:275:THR:CG2 | 10:j5:286:VAL:HG12 | 2.29 | 0.62 |
| 10:j5:973:THR:O | 10:j5:977:GLN:NE2 | 2.32 | 0.62 |
| 10:k5:86:GLU:HA | 10:k5:89:LYS:HE2 | 1.80 | 0.62 |
| 10:k5:1046:ARG:HD2 | 8:k7:13:ALA:HB2 | 1.79 | 0.62 |
| 3:H6:5:PHE:CD2 | 3:H6:27:LEU:HD22 | 2.34 | 0.62 |
| 8:g7:25:ARG:NE | 8:u7:25:ARG:NE | 2.45 | 0.62 |
| 8:U7:2:SER:C | 8:U7:100:ASP:HB3 | 2.25 | 0.62 |
| 8:c7:12:ASP:OD2 | 1:d7:91:TYR:HE1 | 1.77 | 0.62 |
| 8:c7:42:THR:CB | 8:c7:141:LEU:CD2 | 2.75 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:B8:202:CYC:HMA1 | 4:M8:58:TYR:CB | 2.19 | 0.62 |
| 3:F8:5:PHE:CD2 | 3:F8:27:LEU:HD22 | 2.34 | 0.62 |
| 3:O8:111:ASN:OD1 | 5:Z8:68:LEU:C | 2.43 | 0.62 |
| 3:Q8:89:ILE:CG1 | 3:Q8:92:TYR:OH | 2.48 | 0.62 |
| 3:L9:106:GLU:O | 3:L9:111:ASN:HB2 | 1.98 | 0.62 |
| 4:M9:159:CYS:N | 3:V9:108:ARG:HG3 | 2.13 | 0.62 |
| 4:M9:274:VAL:HG12 | 3:V9:77:ARG:CZ | 2.29 | 0.62 |
| 5:N9:24:PRO:CG | 5:N9:35:ASP:O | 2.46 | 0.62 |
| 3:F9:68:ARG:CZ | 3:Z9:68:ARG:HH12 | 1.95 | 0.62 |
| 11:a9:523:GLN:HE21 | 11:a9:548:LEU:HD13 | 1.60 | 0.62 |
| 11:aA:735:VAL:C | 12:aA:902:CYC:O2A | 2.14 | 0.62 |
| 3:T1:5:PHE:CD2 | 3:T1:27:LEU:HD22 | 2.34 | 0.62 |
| 12:A2:201:CYC:HMD1 | 12:A2:201:CYC:NC | 2.10 | 0.62 |
| 12:JA:201:CYC:HC | 12:JA:201:CYC:CMD | 1.98 | 0.62 |
| 4:MA:134:ASN:CG | 5:NA:1:MET:H1 | 2.08 | 0.62 |
| 2:OA:63:PHE:CB | 2:OA:66:LEU:HG | 2.30 | 0.62 |
| 3:TA:5:PHE:CD2 | 3:TA:27:LEU:HD22 | 2.35 | 0.62 |
| 2:A1:63:PHE:CB | 2:A1:66:LEU:HG | 2.29 | 0.62 |
| 3:H3:111:ASN:O | 11:a9:782:ALA:HB3 | 1.99 | 0.62 |
| 3:B3:85:ASP:OD2 | 12:B3:202:CYC:NA | 2.32 | 0.62 |
| 3:F3:113:LEU:HD13 | 4:M3:38:PRO:CB | 2.29 | 0.62 |
| 3:U4:5:PHE:CD2 | 3:U4:27:LEU:HD22 | 2.34 | 0.62 |
| 3:W4:5:PHE:CD2 | 3:W4:27:LEU:HD22 | 2.34 | 0.62 |
| 3:H4:111:ASN:CG | 11:aA:291:TYR:HH | 1.75 | 0.62 |
| 12:I4:201:CYC:HMD1 | 12:I4:201:CYC:NC | 2.10 | 0.62 |
| 3:L4:5:PHE:CD2 | 3:L4:27:LEU:HD22 | 2.34 | 0.62 |
| 4:M4:29:PRO:HG2 | 11:aA:226:PHE:HA | 1.80 | 0.62 |
| 4:M4:136:SER:CB | 5:Z4:2:SER:HB2 | 2.28 | 0.62 |
| 12:R4:201:CYC:HMD1 | 12:R4:201:CYC:NC | 2.10 | 0.62 |
| 3:Y4:5:PHE:CD2 | 3:Y4:27:LEU:HD22 | 2.34 | 0.62 |
| 8:a5:2:SER:C | 8:a5:100:ASP:HB3 | 2.25 | 0.62 |
| 10:j5:902:ASN:HD22 | 10:j5:902:ASN:C | 2.02 | 0.62 |
| 1:D7:76:ARG:HD3 | 8:E7:110:ILE:CD1 | 2.29 | 0.62 |
| 8:M7:60:GLN:NE2 | 3:J9:114:LYS:CD | 2.62 | 0.62 |
| 8:g7:25:ARG:HH21 | 8:u7:25:ARG:CD | 2.12 | 0.62 |
| 1:V7:53:LYS:HZ1 | 8:W7:120:GLN:CD | 2.08 | 0.62 |
| 8:a7:33:GLY:C | 1:b7:31:PHE:HE2 | 2.08 | 0.62 |
| 8:a7:35:ARG:NH2 | 8:a7:144:ASP:CB | 2.61 | 0.62 |
| 8:a7:90:ARG:CZ | 1:b7:16:GLY:C | 2.73 | 0.62 |
| 1:d7:12:TYR:CZ | 1:d7:23:ALA:HB2 | 2.34 | 0.62 |
| 1:p7:12:TYR:CZ | 1:p7:23:ALA:HB2 | 2.34 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:x7:3:ARG:NH1 | 9:x7:67:VAL:HG11 | 2.14 | 0.62 |
| 2:T8:111:ALA:CB | 4:M8:87:ILE:HG21 | 2.28 | 0.62 |
| 3:L8:86:MET:HG3 | 12:a9:901:CYC:CBC | 2.25 | 0.62 |
| 5:N9:61:LYS:HB3 | 3:T9:108:ARG:HA | 1.81 | 0.62 |
| 5:N9:69:GLU:O | 5:N9:70:ILE:HG12 | 1.99 | 0.62 |
| 3:Y8:89:ILE:CA | 3:Y8:92:TYR:CZ | 2.76 | 0.62 |
| 3:H9:108:ARG:O | 3:H9:108:ARG:HD2 | 2.00 | 0.62 |
| 11:a9:30:MET:HG2 | 11:a9:34:ILE:O | 2.00 | 0.62 |
| 4:M1:190:ARG:HH11 | 4:M1:202:SER:HB3 | 1.63 | 0.62 |
| 5:N1:39:PRO:HB3 | 3:T1:113:LEU:CA | 2.18 | 0.62 |
| 1:A:107:ARG:HH12 | 8:a5:9:VAL:HG22 | 1.63 | 0.62 |
| 3:DA:111:ASN:HD21 | 4:MA:73:ASP:HA | 1.65 | 0.62 |
| 3:JA:114:LYS:HG2 | 8:S7:60:GLN:HE21 | 1.62 | 0.62 |
| 3:LA:5:PHE:CD2 | 3:LA:27:LEU:HD22 | 2.34 | 0.62 |
| 4:MA:132:LEU:HD13 | 4:MA:142:PHE:HB2 | 1.82 | 0.62 |
| 4:MA:188:LEU:HD11 | 3:VA:88:ILE:HD11 | 1.81 | 0.62 |
| 2:QA:81:LYS:HE2 | 3:TA:67:ILE:CD1 | 2.29 | 0.62 |
| 2:QA:149:GLU:OE2 | 2:UA:21:ASN:CG | 2.43 | 0.62 |
| 5:N3:1:MET:HE3 | 5:N3:1:MET:CA | 2.17 | 0.62 |
| 4:M4:94:TRP:CE3 | 3:Q4:88:ILE:HG12 | 2.35 | 0.62 |
| 3:O4:5:PHE:CD2 | 3:O4:27:LEU:HD22 | 2.34 | 0.62 |
| 1:N5:113:LYS:CE | 1:Z5:155:TYR:OH | 2.47 | 0.62 |
| 8:A5:15:ALA:HB1 | 1:B5:90:ARG:NH2 | 2.14 | 0.62 |
| 8:W5:126:VAL:HG22 | 12:W5:201:CYC:HMC1 | 1.80 | 0.62 |
| 8:a5:27:LYS:O | 8:a5:30:VAL:HG23 | 1.98 | 0.62 |
| 7:N6:29:LEU:HG | 2:A6:115:GLU:OE2 | 2.00 | 0.62 |
| 10:j5:1016:LEU:CG | 10:j5:1017:ARG:H | 2.12 | 0.62 |
| 1:P7:53:LYS:NZ | 8:Q7:120:GLN:CD | 2.58 | 0.62 |
| 1:D7:53:LYS:HZ1 | 8:E7:120:GLN:CD | 2.08 | 0.62 |
| 1:H7:68:PRO:CB | 1:J7:14:VAL:C | 2.67 | 0.62 |
| 8:g7:2:SER:C | 8:g7:100:ASP:HB3 | 2.25 | 0.62 |
| 8:a7:27:LYS:O | 8:a7:30:VAL:HG23 | 1.98 | 0.62 |
| 8:o7:23:LEU:CD2 | 1:p7:38:VAL:CG2 | 2.77 | 0.62 |
| 8:u7:90:ARG:HB2 | 1:v7:18:TYR:CE1 | 2.34 | 0.62 |
| 3:U8:115:GLU:CD | 4:M8:74:LEU:HD12 | 2.24 | 0.62 |
| 4:M8:200:ILE:HB | 5:Z8:52:ARG:HH21 | 1.65 | 0.62 |
| 3:Q8:120:LEU:HD12 | 3:Q8:121:GLY:C | 2.24 | 0.62 |
| 3:F1:84:ARG:CZ | 4:M1:35:THR:CB | 2.78 | 0.62 |
| 5:N9:39:PRO:HB3 | 3:P9:116:THR:OG1 | 2.00 | 0.62 |
| 3:H9:5:PHE:CD2 | 3:H9:27:LEU:HD22 | 2.34 | 0.62 |
| 11:a9:716:ILE:HD12 | 11:a9:738:LEU:HD21 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:Z1:5:PHE:CD2 | 3:Z1:27:LEU:HD22 | 2.34 | 0.62 |
| 3:LA:111:ASN:ND2 | 11:aA:531:ASP:H | 1.98 | 0.62 |
| 3:P1:5:PHE:CD2 | 3:P1:27:LEU:HD22 | 2.34 | 0.62 |
| 2:A1:33:ARG:CZ | 2:K1:28:ASN:ND2 | 2.61 | 0.62 |
| 2:K2:28:ASN:HD21 | 2:A2:33:ARG:HE | 1.44 | 0.62 |
| 3:X3:5:PHE:CD2 | 3:X3:27:LEU:HD22 | 2.34 | 0.62 |
| 3:S4:5:PHE:CD2 | 3:S4:27:LEU:HD22 | 2.34 | 0.62 |
| 3:O4:92:TYR:OH | 3:O4:108:ARG:HD2 | 1.99 | 0.62 |
| 12:O4:201:CYC:HBB3 | 5:Z4:57:MET:HB3 | 1.82 | 0.62 |
| 8:O5:27:LYS:O | 8:O5:30:VAL:HG23 | 1.98 | 0.62 |
| 8:A5:119:LEU:HD11 | 12:A5:201:CYC:CAA | 2.30 | 0.62 |
| 8:E5:23:LEU:CD1 | 1:F5:42:ALA:HB2 | 2.29 | 0.62 |
| 8:E5:78:THR:O | 8:E5:81:CYS:HB3 | 2.00 | 0.62 |
| 8:G5:119:LEU:HD11 | 12:G5:201:CYC:CAA | 2.30 | 0.62 |
| 1:H5:10:ASN:ND2 | 10:j5:557:VAL:O | 2.33 | 0.62 |
| 1:H5:87:TYR:CE1 | 9:i5:20:GLY:HA2 | 2.34 | 0.62 |
| 8:e5:2:SER:C | 8:e5:100:ASP:HB3 | 2.25 | 0.62 |
| 8:U5:2:SER:C | 8:U5:100:ASP:HB3 | 2.24 | 0.62 |
| 12:X5:201:CYC:HBB2 | 10:j5:520:ARG:CZ | 2.30 | 0.62 |
| 10:j5:742:GLY:CA | 12:J7:201:CYC:O1D | 2.46 | 0.62 |
| 10:j5:1074:GLN:CD | 1:r7:119:LEU:HD21 | 2.25 | 0.62 |
| 10:k5:1064:LYS:HA | 10:k5:1069:ARG:N | 2.15 | 0.62 |
| 1:D7:53:LYS:NZ | 8:E7:120:GLN:CD | 2.58 | 0.62 |
| 1:J7:53:LYS:NZ | 8:K7:120:GLN:CD | 2.58 | 0.62 |
| 8:a7:107:ILE:HG21 | 1:b7:13:ASP:OD1 | 2.00 | 0.62 |
| 2:A8:2:LYS:HE2 | 2:K8:22:THR:HG21 | 1.81 | 0.62 |
| 8:o7:90:ARG:HB2 | 1:p7:18:TYR:CE1 | 2.34 | 0.62 |
| 8:s7:2:SER:C | 8:s7:100:ASP:HB3 | 2.25 | 0.62 |
| 4:M8:93:LEU:C | 4:M8:216:ASN:HD21 | 2.07 | 0.62 |
| 2:N8:120:PHE:CE2 | 3:Q8:83:LEU:HD11 | 2.34 | 0.62 |
| 3:O8:92:TYR:OH | 3:O8:108:ARG:HD2 | 1.99 | 0.62 |
| 3:O8:107:ASP:HA | 5:Z8:66:ARG:HH11 | 1.63 | 0.62 |
| 3:Q8:78:ARG:NH1 | 12:Z8:301:CYC:CAD | 2.54 | 0.62 |
| 5:Z8:31:TRP:HB3 | 5:Z8:32:PRO:CD | 2.25 | 0.62 |
| 2:I9:4:VAL:HB | 2:I9:30:ARG:HG3 | 1.80 | 0.62 |
| 11:aA:30:MET:HG2 | 11:aA:34:ILE:O | 2.00 | 0.62 |
| 11:aA:338:VAL:HG13 | 11:aA:340:PRO:HD3 | 1.82 | 0.62 |
| 11:aA:414:ALA:CB | 11:aA:428:PHE:HE1 | 2.10 | 0.62 |
| 11:aA:623:ASP:HB3 | 3:H1:78:ARG:HH22 | 1.35 | 0.62 |
| 4:M1:172:HIS:CE1 | 4:M1:249:ASP:OD2 | 2.52 | 0.62 |
| 3:DA:5:PHE:CD2 | 3:DA:27:LEU:HD22 | 2.34 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:IA:97:LEU:HD13 | 2:IA:97:LEU:O | 1.99 | 0.62 |
| 3:LA:14:LEU:HD11 | 11:aA:358:PRO:HB2 | 1.76 | 0.62 |
| 4:MA:190:ARG:HH11 | 4:MA:202:SER:HB3 | 1.63 | 0.62 |
| 3:J2:5:PHE:CD2 | 3:J2:27:LEU:HD22 | 2.34 | 0.62 |
| 6:M2:39:ARG:NH2 | 8:O5:66:VAL:CG1 | 2.60 | 0.62 |
| 6:M2:127:SER:CA | 12:F2:201:CYC:HBA1 | 2.28 | 0.62 |
| 12:Z3:201:CYC:NB | 4:M3:188:LEU:CD2 | 2.59 | 0.62 |
| 3:B4:41:VAL:HG21 | 3:B4:98:LEU:HB2 | 1.82 | 0.62 |
| 2:O3:63:PHE:CB | 2:O3:66:LEU:HG | 2.30 | 0.62 |
| 4:M4:138:SER:CB | 12:Z4:301:CYC:CBB | 2.51 | 0.62 |
| 5:Z4:42:SER:HA | 12:Z4:301:CYC:HMA3 | 1.70 | 0.62 |
| 8:A5:126:VAL:HG23 | 12:A5:201:CYC:CMC | 2.30 | 0.62 |
| 8:C5:35:ARG:NE | 8:C5:145:ASP:OD1 | 2.33 | 0.62 |
| 8:G5:90:ARG:HD3 | 1:H5:18:TYR:CE1 | 2.34 | 0.62 |
| 8:I5:2:SER:C | 8:I5:100:ASP:HB3 | 2.24 | 0.62 |
| 8:I5:35:ARG:NE | 8:I5:145:ASP:OD1 | 2.33 | 0.62 |
| 1:J5:14:VAL:HG23 | 1:J5:14:VAL:O | 1.98 | 0.62 |
| 3:L6:5:PHE:CD2 | 3:L6:27:LEU:HD22 | 2.34 | 0.62 |
| 10:j5:619:GLU:HB3 | 10:j5:620:PRO:CD | 2.28 | 0.62 |
| 10:j5:642:ARG:HH11 | 10:j5:642:ARG:CG | 2.07 | 0.62 |
| 10:j5:1020:GLU:O | 10:j5:1024:LYS:HG3 | 2.00 | 0.62 |
| 10:j5:1067:LEU:HD13 | 10:j5:1101:GLU:HG2 | 1.78 | 0.62 |
| 10:k5:959:PHE:HD2 | 1:n7:67:ARG:HH12 | 1.47 | 0.62 |
| 8:C7:2:SER:C | 8:C7:100:ASP:HB3 | 2.25 | 0.62 |
| 8:E7:126:VAL:HG22 | 12:E7:201:CYC:HMC1 | 1.80 | 0.62 |
| 8:i7:126:VAL:HG22 | 12:i7:201:CYC:HMC1 | 1.82 | 0.62 |
| 8:c7:18:LEU:HD22 | 1:d7:97:LEU:HD11 | 1.82 | 0.62 |
| 8:u7:30:VAL:HB | 1:v7:31:PHE:CA | 2.30 | 0.62 |
| 2:N8:111:ALA:HB1 | 5:Z8:35:ASP:OD2 | 1.99 | 0.62 |
| 2:N8:112:GLY:CA | 5:Z8:34:LEU:CA | 2.65 | 0.62 |
| 3:L9:5:PHE:CD2 | 3:L9:27:LEU:HD22 | 2.34 | 0.62 |
| 4:M9:274:VAL:CG2 | 2:W9:111:ALA:CB | 2.77 | 0.62 |
| 3:F9:5:PHE:CD2 | 3:F9:27:LEU:HD22 | 2.34 | 0.62 |
| 3:H9:84:ARG:NH1 | 11:a9:475:ASN:HA | 2.15 | 0.62 |
| 3:J9:20:SER:O | 3:J9:22:GLN:CA | 2.46 | 0.62 |
| 11:a9:194:GLN:OE1 | 11:a9:278:LEU:HB2 | 2.00 | 0.62 |
| 11:a9:312:ASP:CB | 11:a9:315:LEU:HD13 | 2.19 | 0.62 |
| 11:aA:75:ALA:HB1 | 11:aA:81:ASP:CA | 2.28 | 0.62 |
| 11:aA:371:VAL:O | 11:aA:371:VAL:HG12 | 1.98 | 0.62 |
| 11:aA:388:VAL:HG12 | 11:aA:392:ILE:CD1 | 2.30 | 0.62 |
| 11:aA:668:TYR:HB2 | 3:J1:84:ARG:CD | 2.21 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:V1:5:PHE:CD2 | 3:V1:27:LEU:HD22 | 2.34 | 0.62 |
| 3:JA:5:PHE:CD2 | 3:JA:27:LEU:HD22 | 2.34 | 0.62 |
| 5:NA:22:LEU:HD21 | 5:NA:26:LEU:CD2 | 2.08 | 0.62 |
| 3:J3:5:PHE:CD2 | 3:J3:27:LEU:HD22 | 2.34 | 0.62 |
| 3:J3:77:ARG:HH12 | 2:K3:107:ASP:CG | 2.07 | 0.62 |
| 6:M2:276:PRO:O | 1:j7:62:TYR:O | 2.18 | 0.62 |
| 12:D3:201:CYC:HC | 12:D3:201:CYC:CMD | 1.99 | 0.62 |
| 4:M3:80:PRO:CA | 3:X3:111:ASN:HD21 | 2.10 | 0.62 |
| 3:T3:5:PHE:CD2 | 3:T3:27:LEU:HD22 | 2.34 | 0.62 |
| 12:U4:202:CYC:HC | 12:U4:202:CYC:CMD | 1.99 | 0.62 |
| 3:F4:5:PHE:CD2 | 3:F4:27:LEU:HD22 | 2.34 | 0.62 |
| 4:M4:61:ASN:C | 4:M4:63:GLY:H | 2.08 | 0.62 |
| 4:M4:148:LYS:HD2 | 5:Z4:52:ARG:NE | 2.13 | 0.62 |
| 4:M4:190:ARG:HH11 | 4:M4:202:SER:HB3 | 1.63 | 0.62 |
| 4:M4:232:VAL:HG12 | 3:Y4:109:CYS:C | 2.24 | 0.62 |
| 3:Q4:89:ILE:HA | 3:Q4:92:TYR:CE2 | 2.34 | 0.62 |
| 8:A5:71:ASN:CG | 12:A5:201:CYC:HMD3 | 2.24 | 0.62 |
| 8:E5:23:LEU:HD22 | 1:F5:38:VAL:HG13 | 1.81 | 0.62 |
| 1:H5:11:ASN:HA | 10:j5:552:VAL:HG21 | 1.80 | 0.62 |
| 8:Q5:16:ARG:C | 1:R5:90:ARG:HH11 | 2.06 | 0.62 |
| 1:T5:110:ASN:HD21 | 10:j5:692:LEU:CA | 2.06 | 0.62 |
| 1:X5:50:THR:CG2 | 8:a5:49:ARG:NH2 | 2.58 | 0.62 |
| 1:X5:106:GLU:HG3 | 10:j5:505:VAL:HA | 1.81 | 0.62 |
| 6:M6:65:VAL:HB | 1:b7:59:ALA:O | 2.00 | 0.62 |
| 7:N6:48:LEU:HB3 | 12:N6:101:CYC:HBA2 | 1.81 | 0.62 |
| 10:j5:804:GLU:CD | 9:w7:30:LYS:CE | 2.72 | 0.62 |
| 10:j5:1076:GLU:O | 10:j5:1078:SER:N | 2.30 | 0.62 |
| 10:k5:1020:GLU:O | 10:k5:1024:LYS:HG3 | 1.99 | 0.62 |
| 8:g7:107:ILE:HG21 | 1:h7:13:ASP:OD1 | 2.00 | 0.62 |
| 8:i7:12:ASP:CG | 9:y7:46:LYS:NZ | 2.55 | 0.62 |
| 8:W7:12:ASP:C | 9:w7:46:LYS:HZ3 | 2.05 | 0.62 |
| 8:o7:27:LYS:HE3 | 1:p7:35:ALA:CA | 2.29 | 0.62 |
| 8:u7:23:LEU:CD2 | 1:v7:38:VAL:CG2 | 2.77 | 0.62 |
| 8:u7:47:ARG:HG2 | 8:u7:47:ARG:NH2 | 2.11 | 0.62 |
| 3:U8:114:LYS:HE2 | 4:M8:13:LYS:HE3 | 1.75 | 0.62 |
| 12:I8:201:CYC:HMD1 | 12:I8:201:CYC:NC | 2.10 | 0.62 |
| 3:L8:109:CYS:SG | 12:a9:901:CYC:HAB2 | 2.40 | 0.62 |
| 12:N8:201:CYC:HMD1 | 12:N8:201:CYC:NC | 2.09 | 0.62 |
| 3:Q8:110:LEU:HB3 | 3:Q8:170:SER:CB | 2.30 | 0.62 |
| 4:M9:37:GLU:CD | 11:a9:381:PRO:HG3 | 2.25 | 0.62 |
| 5:N9:54:LEU:HD21 | 3:T9:84:ARG:CD | 2.24 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:Z8:2:SER:OG | 5:Z8:2:SER:O | 2.15 | 0.62 |
| 5:Z8:29:HIS:ND1 | 5:Z8:31:TRP:CG | 2.66 | 0.62 |
| 2:A9:63:PHE:HB2 | 2:A9:66:LEU:CG | 2.27 | 0.62 |
| 3:B9:107:ASP:HA | 11:a9:382:ASN:ND2 | 2.15 | 0.62 |
| 11:aA:430:ARG:HG2 | 11:aA:430:ARG:O | 2.00 | 0.62 |
| 11:aA:670:LEU:HD21 | 3:J1:80:ALA:HB3 | 1.82 | 0.62 |
| 3:H1:5:PHE:CD2 | 3:H1:27:LEU:HD22 | 2.34 | 0.62 |
| 2:AA:63:PHE:CB | 2:AA:66:LEU:HG | 2.29 | 0.61 |
| 3:FA:5:PHE:CD2 | 3:FA:27:LEU:HD22 | 2.34 | 0.61 |
| 3:FA:68:ARG:NH2 | 3:ZA:68:ARG:NH1 | 2.48 | 0.61 |
| 3:FA:150:ARG:CG | 3:F9:150:ARG:CB | 2.54 | 0.61 |
| 3:HA:84:ARG:NH1 | 11:aA:475:ASN:HA | 2.15 | 0.61 |
| 4:MA:22:SER:HB3 | 4:MA:23:PRO:HD2 | 1.82 | 0.61 |
| 4:MA:153:LYS:HD3 | 2:UA:14:SER:HB2 | 1.83 | 0.61 |
| 5:NA:61:LYS:HB3 | 3:TA:108:ARG:HA | 1.81 | 0.61 |
| 2:QA:119:THR:HB | 3:TA:83:LEU:HD11 | 1.75 | 0.61 |
| 3:VA:5:PHE:CD2 | 3:VA:27:LEU:HD22 | 2.34 | 0.61 |
| 3:J3:77:ARG:HG2 | 2:K3:111:ALA:HB1 | 1.80 | 0.61 |
| 3:H2:14:LEU:CD1 | 6:M2:69:ALA:HB2 | 2.30 | 0.61 |
| 3:D3:5:PHE:CD2 | 3:D3:27:LEU:HD22 | 2.34 | 0.61 |
| 2:C4:114:ARG:NH1 | 11:aA:134:GLU:CD | 2.58 | 0.61 |
| 3:U4:120:LEU:CD1 | 4:M4:254:LEU:CG | 2.65 | 0.61 |
| 8:K5:23:LEU:HD22 | 1:L5:38:VAL:HG13 | 1.81 | 0.61 |
| 8:K5:23:LEU:CD1 | 1:L5:42:ALA:HB2 | 2.29 | 0.61 |
| 1:D5:75:THR:HG21 | 8:E5:112:VAL:CB | 2.30 | 0.61 |
| 8:S5:110:ILE:HD12 | 10:j5:533:LEU:HD12 | 1.82 | 0.61 |
| 8:W5:8:ILE:HG21 | 1:X5:94:TYR:HB3 | 1.80 | 0.61 |
| 12:L6:202:CYC:HC | 12:L6:202:CYC:CMD | 1.98 | 0.61 |
| 10:j5:545:GLY:HA2 | 10:j5:596:GLY:HA3 | 1.82 | 0.61 |
| 10:j5:974:LEU:O | 10:j5:974:LEU:HD13 | 2.00 | 0.61 |
| 10:k5:619:GLU:HB2 | 10:k5:620:PRO:HD2 | 1.80 | 0.61 |
| 10:k5:1012:PRO:O | 10:k5:1014:SER:N | 2.33 | 0.61 |
| 8:g7:35:ARG:NE | 8:g7:145:ASP:OD1 | 2.33 | 0.61 |
| 8:o7:23:LEU:CD2 | 1:p7:38:VAL:CB | 2.74 | 0.61 |
| 9:x7:4:TYR:CB | 9:x7:58:THR:OG1 | 2.40 | 0.61 |
| 12:M8:302:CYC:HMD3 | 3:S8:77:ARG:HH22 | 0.62 | 0.61 |
| 3:O8:112:GLY:C | 5:Z8:70:ILE:HB | 2.23 | 0.61 |
| 4:M9:134:ASN:CB | 12:R9:201:CYC:HAA1 | 2.21 | 0.61 |
| 3:J9:65:ASP:CG | 11:a9:354:VAL:HG21 | 2.25 | 0.61 |
| 11:a9:92:LYS:O | 11:a9:94:GLY:N | 2.33 | 0.61 |
| 11:aA:371:VAL:CG1 | 11:aA:507:PHE:CB | 2.77 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:HA:108:ARG:O | 3:HA:108:ARG:HD2 | 2.00 | 0.61 |
| 2:OA:2:LYS:HE2 | 2:YA:22:THR:HG21 | 1.81 | 0.61 |
| 3:PA:5:PHE:CD2 | 3:PA:27:LEU:HD22 | 2.34 | 0.61 |
| 3:TA:32:LYS:HG2 | 2:X4:57:GLN:HE22 | 1.63 | 0.61 |
| 2:S1:13:ASP:O | 5:N1:31:TRP:NE1 | 2.23 | 0.61 |
| 12:H3:201:CYC:HC | 12:H3:201:CYC:CMD | 1.99 | 0.61 |
| 3:Z3:5:PHE:CD2 | 3:Z3:27:LEU:HD22 | 2.34 | 0.61 |
| 2:A4:49:ASP:O | 2:A4:52:VAL:N | 2.33 | 0.61 |
| 4:M3:172:HIS:CE1 | 4:M3:249:ASP:OD2 | 2.52 | 0.61 |
| 12:Y3:201:CYC:HMD1 | 12:Y3:201:CYC:NC | 2.09 | 0.61 |
| 3:B1:5:PHE:CD2 | 3:B1:27:LEU:HD22 | 2.34 | 0.61 |
| 4:M4:205:ASP:HB3 | 5:Z4:59:ARG:CZ | 2.29 | 0.61 |
| 4:M4:215:GLU:N | 5:Z4:28:HIS:O | 2.29 | 0.61 |
| 12:M4:301:CYC:HAB2 | 3:Y4:89:ILE:HG12 | 1.83 | 0.61 |
| 2:N4:13:ASP:HB2 | 3:O4:108:ARG:HH12 | 1.65 | 0.61 |
| 8:K5:23:LEU:CD1 | 8:U5:151:PHE:CD1 | 2.83 | 0.61 |
| 8:K5:78:THR:O | 8:K5:81:CYS:HB3 | 2.00 | 0.61 |
| 5:Z4:34:LEU:O | 5:Z4:35:ASP:C | 2.41 | 0.61 |
| 5:Z4:69:GLU:O | 5:Z4:70:ILE:HG12 | 1.99 | 0.61 |
| 8:I5:35:ARG:NH2 | 8:I5:144:ASP:CB | 2.61 | 0.61 |
| 12:P5:201:CYC:HBA2 | 10:k5:472:TYR:OH | 2.00 | 0.61 |
| 6:M6:69:ALA:HB2 | 3:H6:14:LEU:CD1 | 2.30 | 0.61 |
| 6:M6:278:ARG:NH2 | 1:d7:64:ASP:N | 2.48 | 0.61 |
| 10:k5:1085:GLY:HA3 | 1:l7:87:TYR:OH | 1.99 | 0.61 |
| 10:k5:1119:LEU:HD12 | 10:k5:1119:LEU:O | 2.00 | 0.61 |
| 3:F6:126:SER:C | 12:F6:201:CYC:HMC3 | 2.22 | 0.61 |
| 3:D1:5:PHE:CD2 | 3:D1:27:LEU:HD22 | 2.34 | 0.61 |
| 8:C7:35:ARG:NE | 8:C7:145:ASP:OD1 | 2.33 | 0.61 |
| 8:I7:29:PHE:CZ | 8:I7:98:ALA:C | 2.76 | 0.61 |
| 8:a7:37:LEU:CD1 | 1:b7:24:LEU:HD21 | 2.30 | 0.61 |
| 1:b7:27:LEU:HD23 | 1:b7:27:LEU:N | 2.15 | 0.61 |
| 8:c7:49:ARG:NE | 8:c7:140:LEU:HD21 | 2.14 | 0.61 |
| 3:B8:120:LEU:HD21 | 4:M8:49:LEU:O | 2.00 | 0.61 |
| 3:D8:116:THR:OG1 | 4:M8:38:PRO:HA | 2.00 | 0.61 |
| 9:w7:19:THR:O | 9:w7:19:THR:HG23 | 2.01 | 0.61 |
| 4:M8:104:ALA:O | 2:P8:14:SER:HB2 | 1.99 | 0.61 |
| 4:M8:197:ASP:CB | 5:Z8:52:ARG:CG | 2.42 | 0.61 |
| 4:M8:226:SER:OG | 3:Y8:84:ARG:C | 2.43 | 0.61 |
| 12:N8:201:CYC:HBB2 | 3:Q8:75:PRO:CB | 2.29 | 0.61 |
| 3:L9:120:LEU:HD23 | 11:a9:539:GLY:H | 1.64 | 0.61 |
| 4:M9:132:LEU:HD13 | 4:M9:142:PHE:HB2 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:B9:5:PHE:CD2 | 3:B9:27:LEU:HD22 | 2.34 | 0.61 |
| 3:Z9:5:PHE:CD2 | 3:Z9:27:LEU:HD22 | 2.34 | 0.61 |
| 11:a9:824:VAL:O | 11:a9:824:VAL:HG12 | 2.00 | 0.61 |
| 11:aA:632:ILE:HG23 | 11:aA:634:ALA:HB2 | 1.82 | 0.61 |
| 11:aA:776:TYR:H | 12:H1:201:CYC:CGA | 2.11 | 0.61 |
| 12:I1:201:CYC:HMD1 | 12:I1:201:CYC:NC | 2.09 | 0.61 |
| 4:M1:273:ILE:HA | 3:Z1:77:ARG:NH2 | 2.16 | 0.61 |
| 2:GA:119:THR:HG21 | 3:LA:83:LEU:HD11 | 1.83 | 0.61 |
| 3:JA:114:LYS:HE2 | 8:S7:60:GLN:NE2 | 2.15 | 0.61 |
| 4:MA:185:ALA:HB2 | 12:VA:201:CYC:CGA | 2.29 | 0.61 |
| 5:NA:39:PRO:HB3 | 3:PA:116:THR:OG1 | 2.00 | 0.61 |
| 5:NA:69:GLU:O | 5:NA:70:ILE:HG12 | 1.99 | 0.61 |
| 2:QA:25:GLN:HE22 | 2:UA:100:GLY:C | 2.08 | 0.61 |
| 2:QA:112:GLY:O | 3:TA:80:ALA:HB2 | 2.01 | 0.61 |
| 3:TA:32:LYS:HZ2 | 2:X4:60:TYR:HB2 | 1.63 | 0.61 |
| 2:O1:63:PHE:CB | 2:O1:66:LEU:HG | 2.30 | 0.61 |
| 2:K3:115:GLU:OE2 | 11:a9:670:LEU:HA | 2.01 | 0.61 |
| 2:K2:22:THR:HG21 | 2:A2:2:LYS:HE2 | 1.81 | 0.61 |
| 3:D4:116:THR:HG1 | 4:M4:38:PRO:HB2 | 1.62 | 0.61 |
| 3:R3:5:PHE:CD2 | 3:R3:27:LEU:HD22 | 2.34 | 0.61 |
| 3:F4:107:ASP:OD2 | 4:M4:9:GLN:CA | 2.49 | 0.61 |
| 3:J4:108:ARG:HH22 | 11:aA:171:ARG:CB | 2.08 | 0.61 |
| 3:L4:68:ARG:NH1 | 11:aA:75:ALA:CB | 2.58 | 0.61 |
| 2:N4:2:LYS:HE2 | 2:X4:22:THR:HG21 | 1.81 | 0.61 |
| 3:Q4:7:LYS:HE3 | 3:Q4:101:ASP:CG | 2.24 | 0.61 |
| 3:Q4:102:ALA:HB2 | 3:Q4:166:LYS:NZ | 2.15 | 0.61 |
| 8:M5:105:GLU:OE1 | 10:k5:532:THR:CG2 | 2.49 | 0.61 |
| 3:Y4:110:LEU:HD21 | 3:Y4:167:ALA:HA | 1.80 | 0.61 |
| 8:A5:49:ARG:NH2 | 8:A5:140:LEU:HD22 | 2.15 | 0.61 |
| 8:G5:161:GLN:HG2 | 1:T5:49:THR:HG21 | 1.82 | 0.61 |
| 1:f5:18:TYR:CE1 | 10:j5:165:ARG:HB2 | 2.31 | 0.61 |
| 8:W5:16:ARG:C | 1:X5:90:ARG:HH11 | 2.05 | 0.61 |
| 8:W5:23:LEU:HD13 | 1:X5:42:ALA:HB2 | 1.82 | 0.61 |
| 10:j5:925:ILE:HD12 | 10:j5:925:ILE:O | 2.00 | 0.61 |
| 10:j5:1002:ARG:HA | 10:j5:1007:VAL:HG13 | 1.82 | 0.61 |
| 10:k5:182:ASN:CB | 12:k5:1201:CYC:HAB2 | 2.30 | 0.61 |
| 10:k5:385:PRO:O | 10:k5:386:ILE:CG2 | 2.48 | 0.61 |
| 10:k5:748:ARG:NE | 8:E7:106:GLU:CD | 2.56 | 0.61 |
| 2:A6:63:PHE:CB | 2:A6:66:LEU:HG | 2.29 | 0.61 |
| 3:D6:5:PHE:CD2 | 3:D6:27:LEU:HD22 | 2.34 | 0.61 |
| 3:F6:5:PHE:CD2 | 3:F6:27:LEU:HD22 | 2.34 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:O7:21:GLY:O | 8:O7:22:GLU:C | 2.42 | 0.61 |
| 8:I7:2:SER:C | 8:I7:100:ASP:HB3 | 2.25 | 0.61 |
| 8:I7:25:ARG:NH2 | 8:W7:25:ARG:HE | 1.97 | 0.61 |
| 1:b7:75:THR:HB | 8:c7:112:VAL:HA | 1.82 | 0.61 |
| 2:A8:63:PHE:CB | 2:A8:66:LEU:HG | 2.29 | 0.61 |
| 8:o7:30:VAL:HB | 1:p7:31:PHE:CA | 2.30 | 0.61 |
| 3:U8:108:ARG:NH2 | 4:M8:245:ASP:OD2 | 2.33 | 0.61 |
| 4:M9:172:HIS:CE1 | 4:M9:249:ASP:OD2 | 2.53 | 0.61 |
| 4:M9:274:VAL:CG2 | 3:V9:77:ARG:CB | 2.73 | 0.61 |
| 2:A9:19:LEU:O | 3:B9:45:THR:HG21 | 1.99 | 0.61 |
| 2:G1:111:ALA:HB3 | 3:L1:77:ARG:CD | 2.30 | 0.61 |
| 11:aA:334:LYS:HG3 | 11:aA:334:LYS:O | 2.00 | 0.61 |
| 11:aA:734:PHE:O | 11:aA:738:LEU:HG | 2.00 | 0.61 |
| 3:FA:37:ARG:CA | 3:FA:156:LEU:HD21 | 2.30 | 0.61 |
| 3:JA:20:SER:C | 3:JA:22:GLN:N | 2.46 | 0.61 |
| 4:MA:77:LEU:HD21 | 3:ZA:115:GLU:OE2 | 2.00 | 0.61 |
| 5:NA:70:ILE:CG2 | 3:TA:116:THR:HA | 2.17 | 0.61 |
| 12:J2:202:CYC:O2A | 6:M2:185:PHE:CD2 | 2.41 | 0.61 |
| 6:M2:34:ARG:CD | 8:O5:52:LYS:HD2 | 2.30 | 0.61 |
| 3:F3:84:ARG:CZ | 4:M3:35:THR:CB | 2.78 | 0.61 |
| 3:Z3:77:ARG:NH2 | 4:M3:273:ILE:HA | 2.16 | 0.61 |
| 5:N3:66:ARG:NH1 | 5:N3:66:ARG:HB2 | 2.16 | 0.61 |
| 12:O3:201:CYC:HMD1 | 12:O3:201:CYC:NC | 2.10 | 0.61 |
| 2:N4:13:ASP:OD2 | 3:O4:108:ARG:CZ | 2.46 | 0.61 |
| 8:K5:23:LEU:CD1 | 8:U5:151:PHE:CE1 | 2.83 | 0.61 |
| 1:L5:69:GLY:C | 10:j5:554:ASN:HD22 | 2.08 | 0.61 |
| 8:M5:106:GLU:HG2 | 10:k5:533:LEU:HD21 | 1.82 | 0.61 |
| 8:O5:29:PHE:CZ | 8:O5:98:ALA:C | 2.76 | 0.61 |
| 3:Y4:85:ASP:CA | 3:Y4:88:ILE:HG12 | 2.30 | 0.61 |
| 8:Q5:17:TYR:HB2 | 1:R5:45:SER:CB | 2.30 | 0.61 |
| 8:Q5:126:VAL:HG22 | 12:Q5:201:CYC:HMC1 | 1.81 | 0.61 |
| 1:b5:38:VAL:CG1 | 10:k5:40:VAL:HG13 | 2.01 | 0.61 |
| 10:j5:1055:SER:OG | 12:r7:201:CYC:CBB | 2.27 | 0.61 |
| 10:k5:949:ARG:HB2 | 10:k5:950:PRO:HD2 | 1.80 | 0.61 |
| 10:k5:1016:LEU:CG | 10:k5:1017:ARG:H | 2.12 | 0.61 |
| 10:k5:1071:PRO:O | 10:k5:1071:PRO:HD2 | 1.99 | 0.61 |
| 2:A6:19:LEU:O | 3:B6:45:THR:HG21 | 1.99 | 0.61 |
| 8:g7:33:GLY:C | 1:h7:31:PHE:HE2 | 2.08 | 0.61 |
| 8:i7:39:ILE:HG23 | 8:i7:149:ALA:HB2 | 1.81 | 0.61 |
| 3:B8:116:THR:CG2 | 4:M8:53:LEU:HD12 | 2.27 | 0.61 |
| 8:o7:47:ARG:HG2 | 8:o7:47:ARG:NH2 | 2.11 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:o7:58:LEU:HD12 | 8:o7:58:LEU:C | 2.25 | 0.61 |
| 3:L8:108:ARG:O | 12:a9:901:CYC:CBB | 2.38 | 0.61 |
| 4:M8:27:HIS:CD2 | 4:M8:34:ASP:HB3 | 2.34 | 0.61 |
| 12:M8:301:CYC:CMC | 3:Y8:127:VAL:HG23 | 2.29 | 0.61 |
| 2:N8:13:ASP:CB | 3:O8:108:ARG:HH12 | 2.13 | 0.61 |
| 2:O9:63:PHE:HB2 | 2:O9:66:LEU:CG | 2.28 | 0.61 |
| 5:Z8:29:HIS:ND1 | 5:Z8:31:TRP:CD1 | 2.68 | 0.61 |
| 11:a9:50:LEU:O | 11:a9:53:VAL:N | 2.33 | 0.61 |
| 11:a9:290:ASP:O | 11:a9:291:TYR:HD1 | 1.73 | 0.61 |
| 11:a9:338:VAL:HG13 | 11:a9:340:PRO:HD3 | 1.82 | 0.61 |
| 11:aA:112:GLU:O | 11:aA:113:ALA:C | 2.44 | 0.61 |
| 3:J1:5:PHE:CD2 | 3:J1:27:LEU:HD22 | 2.34 | 0.61 |
| 5:N1:1:MET:C | 5:N1:3:VAL:N | 2.50 | 0.61 |
| 1:A:73:TYR:OH | 10:k5:162:TRP:CE2 | 2.54 | 0.61 |
| 4:MA:192:GLN:CG | 3:VA:84:ARG:HG3 | 2.29 | 0.61 |
| 2:QA:13:ASP:OD1 | 3:RA:91:ARG:NH1 | 2.32 | 0.61 |
| 2:QA:18:PHE:CE1 | 3:RA:48:ALA:HB1 | 2.35 | 0.61 |
| 2:QA:33:ARG:NH2 | 12:VA:202:CYC:HBB2 | 2.15 | 0.61 |
| 2:SA:42:ARG:CD | 2:X4:69:PRO:HD2 | 2.31 | 0.61 |
| 2:O1:63:PHE:HB2 | 2:O1:66:LEU:CG | 2.28 | 0.61 |
| 3:L3:107:ASP:O | 11:a9:710:THR:O | 2.18 | 0.61 |
| 3:H4:80:ALA:C | 3:H4:84:ARG:HH11 | 2.08 | 0.61 |
| 2:N4:63:PHE:CB | 2:N4:66:LEU:HG | 2.29 | 0.61 |
| 8:M5:107:ILE:HD13 | 1:N5:13:ASP:OD1 | 2.00 | 0.61 |
| 3:Y4:89:ILE:CG1 | 3:Y4:92:TYR:OH | 2.48 | 0.61 |
| 8:A5:64:ASP:HA | 8:A5:67:SER:CB | 2.30 | 0.61 |
| 10:j5:793:SER:HB3 | 12:T7:201:CYC:CBA | 2.29 | 0.61 |
| 10:j5:1007:VAL:HG22 | 10:j5:1007:VAL:O | 1.99 | 0.61 |
| 10:k5:844:GLN:O | 10:k5:844:GLN:HG3 | 2.00 | 0.61 |
| 10:k5:1055:SER:HB2 | 12:k5:1203:CYC:HAB2 | 1.80 | 0.61 |
| 10:k5:1119:LEU:HD11 | 12:k5:1204:CYC:C4B | 2.28 | 0.61 |
| 8:i7:94:TYR:CG | 1:j7:9:ILE:CG2 | 2.82 | 0.61 |
| 8:a7:102:THR:CB | 8:a7:103:PRO:CD | 2.64 | 0.61 |
| 2:X8:69:PRO:HD2 | 2:S9:42:ARG:CD | 2.31 | 0.61 |
| 3:H8:84:ARG:CD | 11:a9:131:TYR:CE1 | 2.79 | 0.61 |
| 3:O8:108:ARG:HB3 | 5:Z8:61:LYS:CD | 2.20 | 0.61 |
| 3:O8:111:ASN:HB3 | 5:Z8:67:ILE:CB | 2.10 | 0.61 |
| 3:L9:38:LEU:HD23 | 3:L9:98:LEU:HD11 | 1.83 | 0.61 |
| 5:Z8:37:HIS:CE1 | 12:Z8:301:CYC:HMA3 | 2.35 | 0.61 |
| 11:a9:278:LEU:CD1 | 11:a9:278:LEU:H | 1.95 | 0.61 |
| 11:a9:734:PHE:O | 11:a9:738:LEU:HG | 2.00 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:aA:710:THR:HG21 | 11:aA:807:GLN:CD | 2.21 | 0.61 |
| 11:aA:798:SER:HB2 | 11:aA:800:THR:CG2 | 2.20 | 0.61 |
| 4:M1:61:ASN:C | 4:M1:63:GLY:H | 2.08 | 0.61 |
| 4:M1:132:LEU:HD13 | 4:M1:142:PHE:HB2 | 1.82 | 0.61 |
| 5:N1:22:LEU:HD21 | 5:N1:26:LEU:CG | 2.29 | 0.61 |
| 1:A:127:VAL:HG11 | 1:R5:15:GLN:CB | 2.29 | 0.61 |
| 2:QA:149:GLU:CD | 2:UA:21:ASN:OD1 | 2.43 | 0.61 |
| 2:G2:16:GLY:HA2 | 6:M2:104:ARG:NH1 | 2.13 | 0.61 |
| 12:G2:201:CYC:HB | 12:G2:201:CYC:HMA2 | 1.66 | 0.61 |
| 2:O3:63:PHE:HB2 | 2:O3:66:LEU:CG | 2.27 | 0.61 |
| 12:L4:202:CYC:CBB | 11:aA:245:ALA:HB2 | 2.22 | 0.61 |
| 2:N4:49:ASP:O | 2:N4:52:VAL:N | 2.33 | 0.61 |
| 8:M5:20:PRO:HB2 | 8:A5:100:ASP:OD2 | 1.98 | 0.61 |
| 5:Z4:28:HIS:HB3 | 5:Z4:35:ASP:CA | 2.30 | 0.61 |
| 8:E5:17:TYR:CB | 1:F5:45:SER:CB | 2.79 | 0.61 |
| 8:G5:126:VAL:HG23 | 12:G5:201:CYC:CMC | 2.30 | 0.61 |
| 1:H5:83:ARG:HD2 | 9:i5:18:ARG:O | 1.99 | 0.61 |
| 12:P5:201:CYC:CBB | 10:k5:623:VAL:CG2 | 2.75 | 0.61 |
| 8:a5:35:ARG:NE | 8:a5:145:ASP:OD1 | 2.33 | 0.61 |
| 1:b5:5:ILE:CD1 | 10:k5:46:PHE:HE1 | 2.08 | 0.61 |
| 3:J6:84:ARG:HD2 | 6:M6:185:PHE:CZ | 2.35 | 0.61 |
| 10:j5:385:PRO:O | 10:j5:386:ILE:CG2 | 2.48 | 0.61 |
| 10:k5:1152:TYR:HE2 | 8:G7:68:PRO:CG | 1.84 | 0.61 |
| 8:i7:25:ARG:NH2 | 8:s7:3:VAL:C | 2.57 | 0.61 |
| 1:V7:53:LYS:NZ | 8:W7:120:GLN:CD | 2.58 | 0.61 |
| 3:F8:118:VAL:CG1 | 3:Y8:119:ALA:HA | 2.30 | 0.61 |
| 3:J8:108:ARG:HH22 | 11:a9:171:ARG:CB | 2.06 | 0.61 |
| 3:L8:59:LEU:CD2 | 12:a9:901:CYC:CMC | 2.68 | 0.61 |
| 3:Y8:89:ILE:CG1 | 3:Y8:92:TYR:OH | 2.48 | 0.61 |
| 3:J9:65:ASP:OD2 | 11:a9:354:VAL:HG21 | 1.99 | 0.61 |
| 11:aA:194:GLN:OE1 | 11:aA:278:LEU:HB2 | 2.00 | 0.61 |
| 11:aA:312:ASP:C | 11:aA:314:SER:N | 2.45 | 0.61 |
| 2:A2:49:ASP:O | 2:A2:52:VAL:N | 2.33 | 0.61 |
| 1:Z:76:ARG:HH21 | 10:j5:16:LEU:CD1 | 2.14 | 0.61 |
| 12:DA:202:CYC:HC | 12:DA:202:CYC:CMD | 1.99 | 0.61 |
| 4:MA:61:ASN:C | 4:MA:63:GLY:H | 2.08 | 0.61 |
| 4:MA:172:HIS:CE1 | 4:MA:249:ASP:OD2 | 2.53 | 0.61 |
| 5:NA:6:GLY:N | 3:RA:111:ASN:O | 2.34 | 0.61 |
| 5:NA:66:ARG:NH1 | 3:TA:111:ASN:OD1 | 2.30 | 0.61 |
| 2:G3:107:ASP:CG | 3:L3:77:ARG:HH12 | 2.08 | 0.61 |
| 7:N2:49:LEU:HG | 12:N2:101:CYC:HB | 1.65 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:A3:49:ASP:O | 2:A3:52:VAL:N | 2.33 | 0.61 |
| 12:Z3:201:CYC:HB | 4:M3:188:LEU:HD22 | 1.63 | 0.61 |
| 3:Y4:88:ILE:HA | 3:Y4:91:ARG:NH2 | 2.15 | 0.61 |
| 8:A5:106:GLU:OE1 | 10:k5:557:VAL:CG1 | 2.43 | 0.61 |
| 8:A5:122:PRO:HG2 | 12:A5:201:CYC:CMC | 2.27 | 0.61 |
| 1:P5:114:GLU:OE1 | 10:k5:496:GLU:CG | 2.47 | 0.61 |
| 8:S5:107:ILE:HD13 | 1:T5:13:ASP:OD1 | 2.00 | 0.61 |
| 12:X5:201:CYC:CBB | 10:j5:520:ARG:CZ | 2.79 | 0.61 |
| 10:k5:344:ARG:HH11 | 10:k5:344:ARG:HG2 | 1.64 | 0.61 |
| 3:F6:82:CYS:CB | 12:F6:201:CYC:HMD3 | 2.17 | 0.61 |
| 1:J7:76:ARG:HD3 | 8:K7:110:ILE:CD1 | 2.29 | 0.61 |
| 8:i7:54:ALA:HB2 | 8:i7:133:MET:CG | 2.26 | 0.61 |
| 8:i7:96:ILE:CA | 8:i7:152:TYR:CD2 | 2.84 | 0.61 |
| 8:U7:17:TYR:CZ | 1:V7:90:ARG:HA | 2.36 | 0.61 |
| 8:c7:12:ASP:HA | 1:d7:90:ARG:HH11 | 1.64 | 0.61 |
| 8:o7:30:VAL:CB | 1:p7:31:PHE:O | 2.47 | 0.61 |
| 9:x7:6:LYS:HG2 | 9:x7:6:LYS:O | 2.01 | 0.61 |
| 4:M8:104:ALA:HB3 | 2:P8:14:SER:HA | 1.81 | 0.61 |
| 2:N8:13:ASP:HB2 | 3:O8:108:ARG:HH12 | 1.65 | 0.61 |
| 2:N8:19:LEU:O | 3:O8:45:THR:HG21 | 1.99 | 0.61 |
| 12:F1:201:CYC:OB | 4:M1:28:HIS:NE2 | 2.21 | 0.61 |
| 11:aA:403:THR:CG2 | 11:aA:536:THR:HG23 | 1.95 | 0.61 |
| 4:M1:118:TYR:CD2 | 3:X1:84:ARG:CZ | 2.84 | 0.61 |
| 1:A:16:GLY:CA | 8:a5:90:ARG:CZ | 2.79 | 0.61 |
| 12:BA:201:CYC:HBB2 | 4:MA:38:PRO:HD3 | 1.82 | 0.61 |
| 3:FA:150:ARG:CG | 3:F9:150:ARG:CA | 2.69 | 0.61 |
| 3:JA:65:ASP:CG | 11:aA:354:VAL:HG21 | 2.25 | 0.61 |
| 3:LA:38:LEU:HD23 | 3:LA:98:LEU:HD11 | 1.83 | 0.61 |
| 4:MA:232:VAL:HG11 | 3:XA:111:ASN:O | 1.95 | 0.61 |
| 12:R1:201:CYC:O1D | 5:N1:50:LEU:HD21 | 2.01 | 0.61 |
| 2:A1:49:ASP:O | 2:A1:52:VAL:N | 2.33 | 0.61 |
| 3:U4:115:GLU:CG | 4:M4:71:PRO:HD2 | 2.30 | 0.61 |
| 4:M4:53:LEU:HD12 | 4:M4:53:LEU:O | 2.01 | 0.61 |
| 4:M4:128:ALA:HB1 | 4:M4:142:PHE:HE1 | 1.59 | 0.61 |
| 3:Q4:120:LEU:HD11 | 5:Z4:39:PRO:C | 2.25 | 0.61 |
| 3:Y4:110:LEU:HD22 | 3:Y4:170:SER:HB3 | 1.83 | 0.61 |
| 5:Z4:66:ARG:NH1 | 5:Z4:66:ARG:HB2 | 2.16 | 0.61 |
| 1:f5:5:ILE:HD13 | 10:j5:46:PHE:HZ | 1.65 | 0.61 |
| 12:R5:201:CYC:HBB2 | 10:k5:520:ARG:HG2 | 1.82 | 0.61 |
| 1:Z5:127:VAL:CB | 10:k5:698:GLY:CA | 2.77 | 0.61 |
| 10:j5:774:GLN:HA | 10:j5:774:GLN:HE21 | 1.65 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:k5:849:LYS:HG2 | 10:k5:849:LYS:O | 2.00 | 0.61 |
| 10:k5:925:ILE:O | 10:k5:925:ILE:HD12 | 2.00 | 0.61 |
| 10:k5:974:LEU:O | 10:k5:974:LEU:HD13 | 2.00 | 0.61 |
| 10:k5:1002:ARG:HA | 10:k5:1007:VAL:HG13 | 1.82 | 0.61 |
| 10:k5:1077:ILE:HG22 | 12:k5:1203:CYC:CAA | 2.31 | 0.61 |
| 1:R7:107:ARG:HG2 | 9:z7:45:GLN:HB2 | 1.82 | 0.61 |
| 1:h7:27:LEU:N | 1:h7:27:LEU:HD23 | 2.15 | 0.61 |
| 2:C8:114:ARG:NH1 | 11:a9:134:GLU:CD | 2.59 | 0.61 |
| 8:u7:30:VAL:CB | 1:v7:31:PHE:O | 2.47 | 0.61 |
| 3:T9:5:PHE:CD2 | 3:T9:27:LEU:HD22 | 2.35 | 0.61 |
| 11:a9:388:VAL:HG12 | 11:a9:392:ILE:CD1 | 2.30 | 0.61 |
| 11:a9:763:PHE:CE1 | 11:a9:769:PRO:HA | 2.36 | 0.61 |
| 11:aA:716:ILE:HD11 | 11:aA:738:LEU:HD23 | 1.83 | 0.61 |
| 11:aA:782:ALA:HB3 | 3:H1:111:ASN:O | 2.01 | 0.61 |
| 2:OA:33:ARG:CZ | 2:YA:28:ASN:CG | 2.74 | 0.61 |
| 2:OA:49:ASP:O | 2:OA:52:VAL:N | 2.33 | 0.61 |
| 2:SA:39:GLU:CA | 2:X4:69:PRO:CB | 2.73 | 0.61 |
| 12:G2:201:CYC:OB | 3:L2:74:TYR:O | 2.19 | 0.61 |
| 2:A4:2:LYS:HE2 | 2:K4:22:THR:HG21 | 1.81 | 0.61 |
| 4:M3:22:SER:HB3 | 4:M3:23:PRO:HD2 | 1.82 | 0.61 |
| 5:N3:16:PHE:CZ | 3:R3:120:LEU:HD21 | 2.35 | 0.61 |
| 4:M4:22:SER:HB3 | 4:M4:23:PRO:HD2 | 1.83 | 0.61 |
| 4:M4:82:ILE:HD12 | 12:M4:301:CYC:CGD | 2.24 | 0.61 |
| 2:N4:13:ASP:CB | 3:O4:108:ARG:HH12 | 2.13 | 0.61 |
| 2:N4:111:ALA:N | 5:Z4:34:LEU:HD12 | 2.16 | 0.61 |
| 3:Y4:113:LEU:HD11 | 3:Y4:171:ILE:HG23 | 1.82 | 0.61 |
| 12:H5:201:CYC:CAA | 9:i5:26:THR:HG21 | 2.31 | 0.61 |
| 1:d5:62:TYR:CE1 | 12:e5:201:CYC:O1D | 2.54 | 0.61 |
| 8:Q5:23:LEU:HD13 | 1:R5:42:ALA:HB2 | 1.82 | 0.61 |
| 8:U5:76:LYS:O | 8:U5:77:MET:C | 2.43 | 0.61 |
| 8:a5:2:SER:C | 8:a5:100:ASP:CB | 2.74 | 0.61 |
| 12:K6:201:CYC:HMD1 | 12:K6:201:CYC:NC | 2.09 | 0.61 |
| 7:N6:5:VAL:HG23 | 3:F6:108:ARG:NH1 | 2.16 | 0.61 |
| 9:i5:8:THR:HB | 9:i5:52:LEU:HB2 | 1.83 | 0.61 |
| 10:j5:732:ARG:CZ | 1:J7:69:GLY:HA3 | 2.30 | 0.61 |
| 10:k5:1018:LEU:HD13 | 10:k5:1035:PHE:HE2 | 1.53 | 0.61 |
| 10:k5:1118:THR:C | 12:k5:1204:CYC:HMA2 | 2.24 | 0.61 |
| 3:F6:84:ARG:NH2 | 12:F6:201:CYC:O2A | 2.33 | 0.61 |
| 8:g7:33:GLY:C | 1:h7:31:PHE:CE2 | 2.79 | 0.61 |
| 8:c7:13:ALA:HA | 9:x7:46:LYS:HE3 | 1.81 | 0.61 |
| 2:A8:49:ASP:O | 2:A8:52:VAL:N | 2.33 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 3:H8:84:ARG:CD | 11:a9:131:TYR:CB | 2.74 | 0.61 |
| 12:K8:201:CYC:HMA2 | 12:K8:201:CYC:HB | 1.66 | 0.61 |
| 4:M8:100:SER:HA | 4:M8:103:GLN:HB3 | 1.83 | 0.61 |
| 4:M8:141:GLU:OE1 | 4:M8:144:ARG:NE | 2.33 | 0.61 |
| 4:M8:172:HIS:CE1 | 4:M8:249:ASP:OD2 | 2.52 | 0.61 |
| 4:M9:77:LEU:HD21 | 3:Z9:115:GLU:OE2 | 2.00 | 0.61 |
| 4:M9:185:ALA:HB2 | 12:V9:201:CYC:CGA | 2.29 | 0.61 |
| 2:O9:49:ASP:O | 2:O9:52:VAL:N | 2.33 | 0.61 |
| 2:O9:63:PHE:CB | 2:O9:66:LEU:HG | 2.30 | 0.61 |
| 3:Y8:95:TYR:HB2 | 3:Y8:104:VAL:HG11 | 1.82 | 0.61 |
| 3:F9:68:ARG:NH2 | 3:Z9:68:ARG:NH1 | 2.48 | 0.61 |
| 3:X9:5:PHE:CD2 | 3:X9:27:LEU:HD22 | 2.34 | 0.61 |
| 11:a9:274:LEU:O | 11:a9:278:LEU:CD1 | 2.49 | 0.61 |
| 3:FA:150:ARG:HD2 | 3:F9:150:ARG:CD | 2.31 | 0.61 |
| 3:HA:84:ARG:O | 11:aA:478:HIS:CE1 | 2.54 | 0.61 |
| 2:IA:1:MET:HE1 | 2:IA:108:TYR:CE1 | 2.36 | 0.61 |
| 4:MA:53:LEU:HD12 | 4:MA:53:LEU:O | 2.01 | 0.61 |
| 12:QA:201:CYC:HMA2 | 12:QA:201:CYC:HB | 1.66 | 0.61 |
| 2:O1:2:LYS:HE2 | 2:Y1:22:THR:CB | 2.31 | 0.61 |
| 2:K3:22:THR:CB | 2:A3:2:LYS:HE2 | 2.31 | 0.61 |
| 3:J2:84:ARG:HD2 | 6:M2:185:PHE:CZ | 2.35 | 0.61 |
| 12:K2:201:CYC:HMD1 | 12:K2:201:CYC:NC | 2.09 | 0.61 |
| 4:M3:132:LEU:HD13 | 4:M3:142:PHE:HB2 | 1.82 | 0.61 |
| 2:T4:115:GLU:OE2 | 3:Y4:84:ARG:NH2 | 2.28 | 0.61 |
| 4:M4:172:HIS:CE1 | 4:M4:249:ASP:OD2 | 2.53 | 0.61 |
| 3:Q4:7:LYS:CE | 3:Q4:101:ASP:CG | 2.74 | 0.61 |
| 1:L5:75:THR:CB | 8:G5:112:VAL:HA | 2.28 | 0.61 |
| 12:H5:201:CYC:OB | 9:i5:23:LEU:N | 2.34 | 0.61 |
| 8:c5:14:GLU:OE2 | 10:j5:393:MET:CG | 2.48 | 0.61 |
| 1:f5:18:TYR:CD2 | 10:j5:165:ARG:CG | 2.82 | 0.61 |
| 1:P5:87:TYR:CE2 | 10:k5:649:PHE:CZ | 2.88 | 0.61 |
| 8:Q5:17:TYR:CB | 1:R5:45:SER:CB | 2.78 | 0.61 |
| 8:U5:2:SER:C | 8:U5:100:ASP:CB | 2.74 | 0.61 |
| 9:z5:8:THR:HB | 9:z5:52:LEU:HB2 | 1.83 | 0.61 |
| 10:k5:1007:VAL:HG22 | 10:k5:1007:VAL:O | 1.99 | 0.61 |
| 10:k5:1009:ALA:CA | 1:p7:87:TYR:HE1 | 2.13 | 0.61 |
| 2:A6:49:ASP:O | 2:A6:52:VAL:N | 2.33 | 0.61 |
| 2:C6:69:PRO:HG2 | 3:J8:125:ARG:CZ | 2.30 | 0.61 |
| 8:O7:2:SER:C | 8:O7:100:ASP:CB | 2.74 | 0.61 |
| 8:C7:2:SER:C | 8:C7:100:ASP:CB | 2.74 | 0.61 |
| 8:g7:37:LEU:CD1 | 1:h7:24:LEU:HD21 | 2.30 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:A8:2:LYS:HE2 | 2:K8:22:THR:CB | 2.31 | 0.61 |
| 8:m7:2:SER:C | 8:m7:100:ASP:HB3 | 2.25 | 0.61 |
| 8:m7:16:ARG:HH12 | 8:m7:19:SER:HB3 | 1.64 | 0.61 |
| 8:u7:2:SER:HB3 | 1:v7:5:ILE:HG21 | 1.83 | 0.61 |
| 4:M8:260:ARG:HG3 | 4:M8:260:ARG:HH11 | 1.66 | 0.61 |
| 4:M9:22:SER:HB3 | 4:M9:23:PRO:HD2 | 1.82 | 0.61 |
| 2:O9:2:LYS:HE2 | 2:Y9:22:THR:HG21 | 1.81 | 0.61 |
| 2:A9:149:GLU:OE2 | 2:K9:21:ASN:ND2 | 2.31 | 0.61 |
| 2:I9:97:LEU:HD13 | 2:I9:97:LEU:O | 1.99 | 0.61 |
| 2:G1:107:ASP:CG | 3:L1:77:ARG:HH12 | 2.08 | 0.61 |
| 11:a9:75:ALA:HB1 | 11:a9:81:ASP:CA | 2.28 | 0.61 |
| 1:A:13:ASP:CG | 8:a5:107:ILE:CD1 | 2.74 | 0.60 |
| 4:MA:159:CYS:O | 3:VA:107:ASP:O | 2.19 | 0.60 |
| 3:R1:120:LEU:HD21 | 5:N1:16:PHE:CZ | 2.35 | 0.60 |
| 2:A1:2:LYS:HE2 | 2:K1:22:THR:HG21 | 1.81 | 0.60 |
| 2:A1:33:ARG:CZ | 2:K1:28:ASN:CG | 2.74 | 0.60 |
| 2:A1:63:PHE:HB2 | 2:A1:66:LEU:CG | 2.28 | 0.60 |
| 3:J3:77:ARG:CD | 2:K3:111:ALA:HB3 | 2.30 | 0.60 |
| 3:J3:84:ARG:HB2 | 11:a9:668:TYR:CD2 | 2.34 | 0.60 |
| 6:M2:34:ARG:CD | 8:O5:52:LYS:HB2 | 2.26 | 0.60 |
| 7:N2:5:VAL:HG23 | 3:F2:108:ARG:NH1 | 2.16 | 0.60 |
| 3:B3:127:VAL:HG22 | 12:B3:202:CYC:C3C | 2.29 | 0.60 |
| 3:B4:120:LEU:CD1 | 4:M4:53:LEU:HA | 2.21 | 0.60 |
| 5:N3:31:TRP:HZ2 | 3:T3:92:TYR:HH | 1.42 | 0.60 |
| 2:O3:2:LYS:HE2 | 2:Y3:22:THR:CB | 2.31 | 0.60 |
| 2:O3:49:ASP:O | 2:O3:52:VAL:N | 2.33 | 0.60 |
| 3:O4:92:TYR:OH | 3:O4:108:ARG:CD | 2.39 | 0.60 |
| 8:K5:17:TYR:CB | 1:L5:45:SER:CB | 2.79 | 0.60 |
| 8:K5:128:GLU:HA | 8:K5:128:GLU:OE1 | 1.99 | 0.60 |
| 5:Z4:29:HIS:HE2 | 5:Z4:38:GLU:N | 1.99 | 0.60 |
| 8:A5:114:GLU:HB2 | 1:F5:79:ALA:HB2 | 1.83 | 0.60 |
| 8:C5:2:SER:C | 8:C5:100:ASP:CB | 2.74 | 0.60 |
| 12:F5:201:CYC:OB | 10:k5:588:VAL:CG2 | 2.49 | 0.60 |
| 8:G5:53:GLN:HE21 | 8:G5:57:GLN:HE21 | 1.49 | 0.60 |
| 6:M6:247:THR:OG1 | 12:H6:201:CYC:HBA2 | 2.01 | 0.60 |
| 9:z5:10:CYS:N | 9:z5:50:LYS:O | 2.32 | 0.60 |
| 10:j5:372:ARG:NH2 | 10:j5:376:GLN:HE21 | 1.99 | 0.60 |
| 10:j5:932:GLN:HG2 | 10:j5:932:GLN:O | 2.01 | 0.60 |
| 10:k5:961:GLY:O | 1:p7:15:GLN:HG2 | 2.01 | 0.60 |
| 3:D1:68:ARG:HH12 | 3:X1:68:ARG:NH2 | 1.97 | 0.60 |
| 8:g7:2:SER:C | 8:g7:100:ASP:CB | 2.74 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:E8:1:MET:H3 | 4:M8:10:ARG:NH2 | 1.98 | 0.60 |
| 8:o7:94:TYR:CD1 | 1:p7:19:LEU:HG | 2.36 | 0.60 |
| 8:u7:94:TYR:CD1 | 1:v7:19:LEU:HG | 2.36 | 0.60 |
| 2:X8:22:THR:CB | 2:N8:2:LYS:HE2 | 2.31 | 0.60 |
| 3:Q8:110:LEU:HD13 | 3:Q8:170:SER:HB2 | 1.82 | 0.60 |
| 3:Q8:127:VAL:CG2 | 12:Z8:301:CYC:HMC3 | 2.04 | 0.60 |
| 4:M9:58:TYR:CD2 | 11:a9:496:ARG:CZ | 2.72 | 0.60 |
| 4:M9:232:VAL:HG11 | 3:X9:111:ASN:O | 1.95 | 0.60 |
| 2:O9:33:ARG:CZ | 2:Y9:28:ASN:CG | 2.74 | 0.60 |
| 3:B9:26:GLN:O | 3:B9:30:LEU:HD11 | 1.98 | 0.60 |
| 3:R9:5:PHE:CD2 | 3:R9:27:LEU:HD22 | 2.34 | 0.60 |
| 11:a9:89:ALA:CA | 11:a9:92:LYS:NZ | 2.64 | 0.60 |
| 11:a9:98:ILE:HG22 | 11:a9:99:ALA:O | 2.01 | 0.60 |
| 11:a9:308:LEU:HD23 | 11:a9:308:LEU:C | 2.26 | 0.60 |
| 11:aA:274:LEU:O | 11:aA:278:LEU:CD1 | 2.49 | 0.60 |
| 11:aA:327:SER:O | 11:aA:328:GLN:C | 2.40 | 0.60 |
| 4:M1:22:SER:HB3 | 4:M1:23:PRO:HD2 | 1.82 | 0.60 |
| 2:A2:63:PHE:HB2 | 2:A2:66:LEU:CG | 2.28 | 0.60 |
| 1:Z:62:TYR:HD1 | 10:j5:155:LYS:HZ1 | 1.49 | 0.60 |
| 2:AA:33:ARG:CZ | 2:KA:28:ASN:CG | 2.74 | 0.60 |
| 4:MA:263:PRO:O | 3:VA:119:ALA:HB1 | 1.99 | 0.60 |
| 2:OA:2:LYS:HE2 | 2:YA:22:THR:CB | 2.31 | 0.60 |
| 12:QA:201:CYC:HMA1 | 3:TA:79:MET:CE | 2.31 | 0.60 |
| 2:O1:49:ASP:O | 2:O1:52:VAL:N | 2.33 | 0.60 |
| 12:T4:201:CYC:HMA2 | 12:T4:201:CYC:HB | 1.66 | 0.60 |
| 4:M4:128:ALA:O | 4:M4:142:PHE:HE1 | 1.81 | 0.60 |
| 4:M4:232:VAL:CA | 12:M4:301:CYC:HBB2 | 2.30 | 0.60 |
| 2:N4:33:ARG:CZ | 2:X4:28:ASN:CG | 2.74 | 0.60 |
| 3:Q4:85:ASP:HB3 | 3:Q4:88:ILE:HD12 | 1.83 | 0.60 |
| 8:M5:38:ARG:CD | 1:J7:144:ASP:OD1 | 2.49 | 0.60 |
| 12:N5:201:CYC:CBB | 10:k5:482:GLN:NE2 | 2.64 | 0.60 |
| 3:Y4:108:ARG:O | 3:Y4:109:CYS:HB3 | 2.00 | 0.60 |
| 5:Z4:44:TYR:O | 5:Z4:44:TYR:CD2 | 2.53 | 0.60 |
| 8:C5:35:ARG:NH2 | 8:C5:144:ASP:CB | 2.61 | 0.60 |
| 8:G5:6:LYS:HZ3 | 8:S5:19:SER:CB | 1.90 | 0.60 |
| 8:G5:64:ASP:HA | 8:G5:67:SER:CB | 2.30 | 0.60 |
| 8:I5:2:SER:C | 8:I5:100:ASP:CB | 2.74 | 0.60 |
| 1:P5:61:ILE:HB | 12:Q5:201:CYC:O2A | 2.01 | 0.60 |
| 1:Z5:62:TYR:CE1 | 12:a5:201:CYC:O1D | 2.54 | 0.60 |
| 2:K6:28:ASN:CG | 2:A6:33:ARG:CZ | 2.75 | 0.60 |
| 10:k5:388:ARG:CD | 10:k5:393:MET:N | 2.61 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:k5:390:GLN:HA | 10:k5:390:GLN:OE1 | 2.02 | 0.60 |
| 10:k5:742:GLY:CA | 12:D7:201:CYC:O1D | 2.48 | 0.60 |
| 10:k5:803:LYS:CE | 9:z7:43:ARG:HH11 | 2.14 | 0.60 |
| 10:k5:948:SER:O | 10:k5:948:SER:OG | 2.16 | 0.60 |
| 10:k5:1155:ARG:HH21 | 10:k5:1155:ARG:CB | 2.09 | 0.60 |
| 8:i7:21:GLY:HA3 | 8:s7:100:ASP:CG | 2.17 | 0.60 |
| 8:i7:21:GLY:CA | 8:s7:101:VAL:H | 2.14 | 0.60 |
| 8:a7:2:SER:C | 8:a7:100:ASP:CB | 2.74 | 0.60 |
| 3:L8:84:ARG:NH2 | 12:a9:901:CYC:O2A | 2.35 | 0.60 |
| 4:M8:29:PRO:CG | 11:a9:230:THR:OG1 | 2.49 | 0.60 |
| 4:M8:61:ASN:C | 4:M8:63:GLY:H | 2.08 | 0.60 |
| 4:M8:100:SER:H | 3:Q8:1:MET:CE | 2.13 | 0.60 |
| 4:M9:38:PRO:HD3 | 12:B9:201:CYC:HBB2 | 1.82 | 0.60 |
| 4:M9:61:ASN:C | 4:M9:63:GLY:H | 2.08 | 0.60 |
| 4:M9:92:GLU:O | 4:M9:92:GLU:HG3 | 1.99 | 0.60 |
| 5:N9:6:GLY:N | 3:R9:111:ASN:O | 2.34 | 0.60 |
| 12:O9:201:CYC:HMD1 | 12:O9:201:CYC:NC | 2.09 | 0.60 |
| 11:a9:627:GLN:N | 11:a9:627:GLN:OE1 | 2.35 | 0.60 |
| 11:aA:92:LYS:O | 11:aA:94:GLY:N | 2.33 | 0.60 |
| 11:aA:275:THR:CA | 11:aA:278:LEU:HD13 | 2.03 | 0.60 |
| 11:aA:667:THR:CG2 | 12:aA:901:CYC:HBA1 | 2.22 | 0.60 |
| 4:MA:5:THR:C | 4:MA:6:THR:HG1 | 2.02 | 0.60 |
| 12:O1:201:CYC:HB | 12:O1:201:CYC:HMA2 | 1.67 | 0.60 |
| 12:P1:201:CYC:CBA | 4:M1:130:SER:O | 2.49 | 0.60 |
| 2:G3:111:ALA:HB3 | 3:L3:77:ARG:CD | 2.31 | 0.60 |
| 12:P4:201:CYC:HMA2 | 12:P4:201:CYC:HB | 1.67 | 0.60 |
| 8:K5:107:ILE:HG22 | 8:K5:107:ILE:O | 2.01 | 0.60 |
| 5:Z4:3:VAL:O | 5:Z4:4:LEU:C | 2.44 | 0.60 |
| 8:G5:49:ARG:NH2 | 8:G5:140:LEU:HD22 | 2.15 | 0.60 |
| 1:P5:87:TYR:HE2 | 10:k5:649:PHE:CZ | 2.14 | 0.60 |
| 1:V5:61:ILE:HB | 12:W5:201:CYC:O2A | 2.01 | 0.60 |
| 8:a5:93:THR:O | 8:a5:97:VAL:HG22 | 2.02 | 0.60 |
| 6:M6:287:TYR:HB3 | 8:Y7:73:TYR:OH | 2.01 | 0.60 |
| 10:j5:588:VAL:O | 10:j5:588:VAL:HG13 | 2.00 | 0.60 |
| 10:j5:868:ASP:C | 9:w7:43:ARG:NE | 2.36 | 0.60 |
| 10:j5:1012:PRO:O | 10:j5:1014:SER:N | 2.33 | 0.60 |
| 10:j5:1119:LEU:HD12 | 10:j5:1119:LEU:O | 2.00 | 0.60 |
| 10:k5:309:LEU:HD13 | 10:k5:342:LEU:HD13 | 1.81 | 0.60 |
| 10:k5:545:GLY:HA2 | 10:k5:596:GLY:HA3 | 1.82 | 0.60 |
| 10:k5:774:GLN:HA | 10:k5:774:GLN:HE21 | 1.65 | 0.60 |
| 10:k5:932:GLN:HG2 | 10:k5:932:GLN:O | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:k5:1001:TYR:OH | 10:k5:1018:LEU:HG | 2.01 | 0.60 |
| 10:k5:1150:TYR:HE1 | 11:a9:38:VAL:HG13 | 1.66 | 0.60 |
| 8:i7:49:ARG:NE | 8:i7:140:LEU:HD21 | 2.14 | 0.60 |
| 12:b7:201:CYC:HBB1 | 9:x7:21:ARG:CZ | 2.30 | 0.60 |
| 8:c7:20:PRO:HD2 | 8:m7:155:TYR:CD1 | 2.37 | 0.60 |
| 1:d7:110:ASN:HD21 | 9:x7:51:VAL:H | 1.49 | 0.60 |
| 1:f7:67:ARG:HD3 | 11:aA:311:LEU:CG | 2.29 | 0.60 |
| 3:B8:81:ALA:HB1 | 12:B8:202:CYC:HMD1 | 0.61 | 0.60 |
| 8:s7:35:ARG:NE | 8:s7:145:ASP:OD1 | 2.33 | 0.60 |
| 12:T8:201:CYC:HMA2 | 12:T8:201:CYC:HB | 1.66 | 0.60 |
| 3:U8:120:LEU:HD23 | 3:U8:122:THR:OG1 | 2.01 | 0.60 |
| 3:L8:82:CYS:CB | 12:a9:901:CYC:NC | 2.64 | 0.60 |
| 4:M8:22:SER:HB3 | 4:M8:23:PRO:HD2 | 1.83 | 0.60 |
| 4:M8:86:ALA:HB3 | 3:Y8:77:ARG:HD2 | 1.83 | 0.60 |
| 3:L9:84:ARG:CZ | 11:a9:406:LEU:HD23 | 2.31 | 0.60 |
| 5:N9:22:LEU:HD21 | 5:N9:26:LEU:CD1 | 2.15 | 0.60 |
| 3:Y8:89:ILE:HG12 | 3:Y8:92:TYR:CE2 | 2.37 | 0.60 |
| 3:Y8:93:VAL:HG22 | 3:Y8:105:LEU:HD21 | 1.83 | 0.60 |
| 5:Z8:22:LEU:HD21 | 5:Z8:26:LEU:CG | 2.29 | 0.60 |
| 11:a9:89:ALA:O | 11:a9:92:LYS:N | 2.34 | 0.60 |
| 11:a9:430:ARG:HG2 | 11:a9:430:ARG:O | 2.00 | 0.60 |
| 12:K1:201:CYC:HB | 12:K1:201:CYC:HMA2 | 1.66 | 0.60 |
| 4:M1:148:LYS:CD | 4:M1:197:ASP:OD1 | 2.37 | 0.60 |
| 4:M1:160:THR:HG22 | 4:M1:257:GLN:HB3 | 1.73 | 0.60 |
| 5:N1:2:SER:O | 5:N1:2:SER:OG | 2.16 | 0.60 |
| 3:BA:107:ASP:HA | 11:aA:382:ASN:ND2 | 2.15 | 0.60 |
| 3:HA:117:TYR:CE1 | 12:HA:202:CYC:NA | 2.69 | 0.60 |
| 12:O1:201:CYC:CBB | 3:R1:74:TYR:CE1 | 2.83 | 0.60 |
| 12:A1:201:CYC:HMD1 | 12:A1:201:CYC:NC | 2.10 | 0.60 |
| 3:H3:125:ARG:NH2 | 8:k7:45:GLU:OE1 | 2.34 | 0.60 |
| 2:K3:22:THR:HG21 | 2:A3:2:LYS:HE2 | 1.81 | 0.60 |
| 12:H2:201:CYC:HBA2 | 6:M2:247:THR:OG1 | 2.01 | 0.60 |
| 7:N2:48:LEU:HB3 | 12:N2:101:CYC:HBA2 | 1.81 | 0.60 |
| 3:Z3:84:ARG:HH11 | 4:M3:189:ASP:CG | 2.09 | 0.60 |
| 3:B4:105:LEU:HD11 | 3:B4:110:LEU:HD21 | 1.81 | 0.60 |
| 5:N3:53:LEU:HB3 | 12:R3:201:CYC:HBA2 | 1.83 | 0.60 |
| 12:H4:201:CYC:HBA2 | 11:aA:261:SER:OG | 2.01 | 0.60 |
| 4:M4:86:ALA:CB | 3:Y4:77:ARG:HH11 | 2.14 | 0.60 |
| 4:M4:226:SER:OG | 3:Y4:85:ASP:HA | 2.00 | 0.60 |
| 3:O4:104:VAL:HA | 5:Z4:61:LYS:CE | 2.31 | 0.60 |
| 8:K5:23:LEU:HD12 | 8:U5:151:PHE:HD1 | 1.66 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:K5:36:ARG:HH12 | 8:U5:24:ASP:CG | 1.97 | 0.60 |
| 1:R5:106:GLU:HG2 | 10:k5:505:VAL:HA | 1.82 | 0.60 |
| 1:T5:53:LYS:HZ3 | 8:U5:120:GLN:HG3 | 1.67 | 0.60 |
| 8:U5:35:ARG:NE | 8:U5:145:ASP:OD1 | 2.33 | 0.60 |
| 1:b5:24:LEU:HD22 | 10:k5:54:ILE:HG23 | 1.82 | 0.60 |
| 9:z5:5:PHE:HA | 9:z5:55:LYS:O | 2.01 | 0.60 |
| 10:j5:190:LEU:HD22 | 10:j5:194:CYS:SG | 2.41 | 0.60 |
| 10:j5:283:ARG:HD3 | 10:j5:283:ARG:C | 2.27 | 0.60 |
| 10:j5:344:ARG:NH1 | 10:j5:344:ARG:HG2 | 2.16 | 0.60 |
| 10:j5:1147:TYR:O | 10:j5:1147:TYR:HD1 | 1.85 | 0.60 |
| 10:k5:930:LEU:CD1 | 1:D7:33:THR:HB | 2.27 | 0.60 |
| 10:k5:1150:TYR:CD1 | 11:a9:38:VAL:HG22 | 2.32 | 0.60 |
| 12:C6:201:CYC:HMD1 | 12:C6:201:CYC:NC | 2.10 | 0.60 |
| 8:I7:2:SER:C | 8:I7:100:ASP:CB | 2.74 | 0.60 |
| 8:i7:20:PRO:N | 8:s7:101:VAL:HG21 | 2.17 | 0.60 |
| 8:U7:93:THR:O | 8:U7:97:VAL:HG22 | 2.02 | 0.60 |
| 8:c7:23:LEU:CD1 | 1:d7:42:ALA:HB2 | 2.31 | 0.60 |
| 8:m7:35:ARG:NE | 8:m7:145:ASP:OD1 | 2.33 | 0.60 |
| 1:v7:136:VAL:CG1 | 11:aA:342:ARG:NH1 | 2.61 | 0.60 |
| 2:X8:13:ASP:OD1 | 4:M8:229:GLY:C | 2.42 | 0.60 |
| 12:G8:201:CYC:HMA2 | 12:G8:201:CYC:HB | 1.67 | 0.60 |
| 3:J8:108:ARG:HH21 | 11:a9:171:ARG:HB3 | 1.65 | 0.60 |
| 4:M8:210:ILE:HD13 | 5:Z8:25:THR:O | 2.00 | 0.60 |
| 3:Q8:102:ALA:HB2 | 3:Q8:166:LYS:HZ3 | 1.59 | 0.60 |
| 4:M9:51:ARG:NH2 | 11:a9:430:ARG:NE | 2.49 | 0.60 |
| 3:H9:84:ARG:O | 11:a9:478:HIS:CE1 | 2.54 | 0.60 |
| 3:H9:113:LEU:HD13 | 12:H9:202:CYC:C2B | 2.31 | 0.60 |
| 11:a9:112:GLU:O | 11:a9:113:ALA:C | 2.44 | 0.60 |
| 11:aA:85:ALA:O | 11:aA:86:ASP:HB2 | 2.01 | 0.60 |
| 11:aA:91:THR:HG22 | 11:aA:91:THR:O | 2.01 | 0.60 |
| 11:aA:98:ILE:HG22 | 11:aA:99:ALA:O | 2.01 | 0.60 |
| 11:aA:763:PHE:CE1 | 11:aA:769:PRO:HA | 2.36 | 0.60 |
| 11:aA:803:ASN:C | 3:J1:119:ALA:O | 2.44 | 0.60 |
| 4:M1:53:LEU:HD12 | 4:M1:53:LEU:O | 2.01 | 0.60 |
| 12:Y1:201:CYC:HMD1 | 12:Y1:201:CYC:NC | 2.09 | 0.60 |
| 2:IA:24:LEU:HB3 | 12:JA:201:CYC:HAB2 | 1.82 | 0.60 |
| 5:NA:66:ARG:NH1 | 5:NA:66:ARG:HB2 | 2.16 | 0.60 |
| 4:M3:259:ARG:NH2 | 4:M3:259:ARG:HG3 | 2.17 | 0.60 |
| 4:M3:260:ARG:HG3 | 4:M3:260:ARG:HH11 | 1.66 | 0.60 |
| 5:N3:50:LEU:HD12 | 5:N3:50:LEU:O | 2.02 | 0.60 |
| 4:M4:94:TRP:CG | 3:Q4:88:ILE:HG12 | 2.36 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 12:O4:201:CYC:OB | 5:Z4:54:LEU:HD12 | 2.02 | 0.60 |
| 3:Q4:85:ASP:CG | 3:Q4:88:ILE:HD12 | 2.26 | 0.60 |
| 3:Y4:89:ILE:CB | 3:Y4:92:TYR:HE2 | 2.08 | 0.60 |
| 5:Z4:31:TRP:HB3 | 5:Z4:32:PRO:CD | 2.25 | 0.60 |
| 8:U5:75:GLU:OE1 | 6:M6:43:TRP:CE2 | 2.50 | 0.60 |
| 1:Z5:161:SER:HB2 | 10:k5:695:GLY:C | 2.25 | 0.60 |
| 9:i5:11:ILE:HD12 | 9:i5:28:PHE:CE2 | 2.27 | 0.60 |
| 10:j5:879:ASP:OD1 | 10:j5:879:ASP:N | 2.29 | 0.60 |
| 10:j5:974:LEU:HD23 | 1:v7:1:MET:H2 | 1.65 | 0.60 |
| 10:j5:1118:THR:HG23 | 12:j5:1202:CYC:CBA | 2.31 | 0.60 |
| 8:Q7:13:ALA:CA | 9:z7:46:LYS:HD3 | 2.32 | 0.60 |
| 8:C7:93:THR:O | 8:C7:97:VAL:HG22 | 2.02 | 0.60 |
| 8:G7:51:VAL:HG11 | 11:a9:579:PHE:HE1 | 1.66 | 0.60 |
| 8:U7:2:SER:C | 8:U7:100:ASP:CB | 2.74 | 0.60 |
| 8:U7:35:ARG:NE | 8:U7:145:ASP:OD1 | 2.33 | 0.60 |
| 8:W7:101:VAL:O | 8:W7:102:THR:C | 2.45 | 0.60 |
| 12:A8:201:CYC:HMA2 | 12:A8:201:CYC:HB | 1.67 | 0.60 |
| 8:m7:17:TYR:CZ | 1:n7:90:ARG:HA | 2.37 | 0.60 |
| 8:m7:35:ARG:NH2 | 8:m7:144:ASP:CB | 2.61 | 0.60 |
| 9:w7:5:PHE:CD2 | 9:w7:37:TRP:CD1 | 2.90 | 0.60 |
| 4:M8:205:ASP:CG | 5:Z8:59:ARG:NE | 2.56 | 0.60 |
| 12:R8:201:CYC:HMA2 | 12:R8:201:CYC:HB | 1.67 | 0.60 |
| 12:C9:201:CYC:HMA2 | 12:C9:201:CYC:HB | 1.67 | 0.60 |
| 3:F9:36:LYS:C | 3:F9:156:LEU:HD21 | 2.24 | 0.60 |
| 2:I9:24:LEU:HB3 | 12:J9:201:CYC:HAB2 | 1.82 | 0.60 |
| 11:a9:95:ILE:HG22 | 11:a9:95:ILE:O | 2.01 | 0.60 |
| 11:aA:578:MET:CE | 11:aA:582:MET:HE1 | 2.30 | 0.60 |
| 5:N1:37:HIS:O | 12:T1:301:CYC:CMA | 2.50 | 0.60 |
| 12:C2:201:CYC:HB | 12:C2:201:CYC:HMA2 | 1.67 | 0.60 |
| 1:A:127:VAL:HG13 | 1:R5:15:GLN:OE1 | 2.01 | 0.60 |
| 1:Z:76:ARG:NH1 | 10:j5:262:TYR:CZ | 2.69 | 0.60 |
| 12:AA:201:CYC:HMA2 | 12:AA:201:CYC:HB | 1.67 | 0.60 |
| 3:LA:51:ILE:CG2 | 3:LA:90:LEU:HD12 | 2.24 | 0.60 |
| 5:NA:3:VAL:O | 5:NA:4:LEU:C | 2.44 | 0.60 |
| 3:J3:80:ALA:HB3 | 11:a9:670:LEU:HD21 | 1.82 | 0.60 |
| 12:E3:201:CYC:HMA2 | 12:E3:201:CYC:HB | 1.67 | 0.60 |
| 2:C4:15:GLN:HG2 | 11:aA:102:GLN:HE21 | 1.66 | 0.60 |
| 12:K4:201:CYC:HB | 12:K4:201:CYC:HMA2 | 1.66 | 0.60 |
| 4:M4:260:ARG:HG3 | 4:M4:260:ARG:HH11 | 1.66 | 0.60 |
| 8:M5:54:ALA:HA | 8:M5:132:ALA:HB1 | 1.84 | 0.60 |
| 8:O5:93:THR:O | 8:O5:97:VAL:HG22 | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:Z4:1:MET:CB | 5:Z4:3:VAL:CG2 | 2.76 | 0.60 |
| 5:Z4:22:LEU:CD1 | 12:Z4:301:CYC:C4B | 2.56 | 0.60 |
| 1:D5:87:TYR:HE2 | 9:z5:38:PHE:HE2 | 1.48 | 0.60 |
| 12:H5:201:CYC:CBB | 9:i5:21:ARG:HA | 2.25 | 0.60 |
| 8:c5:101:VAL:O | 8:c5:102:THR:C | 2.45 | 0.60 |
| 10:j5:147:ARG:HA | 10:j5:147:ARG:HE | 1.67 | 0.60 |
| 10:j5:298:ARG:HG2 | 10:j5:298:ARG:NH1 | 2.14 | 0.60 |
| 10:j5:449:ARG:HH21 | 10:j5:449:ARG:CG | 2.10 | 0.60 |
| 10:j5:849:LYS:HG2 | 10:j5:849:LYS:O | 2.00 | 0.60 |
| 10:j5:989:THR:HG21 | 8:g7:106:GLU:OE2 | 1.97 | 0.60 |
| 10:j5:1150:TYR:CE1 | 11:aA:38:VAL:HG13 | 2.37 | 0.60 |
| 10:k5:1106:PHE:O | 10:k5:1110:ILE:CD1 | 2.49 | 0.60 |
| 12:G6:201:CYC:HMA2 | 12:G6:201:CYC:HB | 1.66 | 0.60 |
| 8:O7:35:ARG:NH2 | 8:O7:144:ASP:CB | 2.61 | 0.60 |
| 8:C7:35:ARG:NH2 | 8:C7:144:ASP:CB | 2.61 | 0.60 |
| 8:c7:9:VAL:HG22 | 1:d7:107:ARG:HH12 | 1.66 | 0.60 |
| 8:e7:101:VAL:O | 8:e7:102:THR:C | 2.45 | 0.60 |
| 3:H8:84:ARG:CG | 11:a9:131:TYR:CE1 | 2.83 | 0.60 |
| 3:L8:130:ALA:CB | 12:a9:901:CYC:HBC2 | 2.32 | 0.60 |
| 2:N8:115:GLU:N | 5:Z8:32:PRO:HB2 | 2.16 | 0.60 |
| 3:O8:107:ASP:O | 5:Z8:67:ILE:N | 2.31 | 0.60 |
| 12:P8:201:CYC:HMA2 | 12:P8:201:CYC:HB | 1.67 | 0.60 |
| 3:Q8:89:ILE:HG12 | 3:Q8:92:TYR:CE2 | 2.36 | 0.60 |
| 4:M9:153:LYS:HD3 | 2:U9:14:SER:HB2 | 1.83 | 0.60 |
| 4:M9:274:VAL:N | 3:V9:77:ARG:CG | 2.40 | 0.60 |
| 2:O9:2:LYS:HE2 | 2:Y9:22:THR:CB | 2.31 | 0.60 |
| 12:W9:201:CYC:HMD1 | 12:W9:201:CYC:NC | 2.10 | 0.60 |
| 11:aA:89:ALA:CA | 11:aA:92:LYS:NZ | 2.64 | 0.60 |
| 11:aA:638:ALA:O | 11:aA:639:GLN:NE2 | 2.34 | 0.60 |
| 4:M1:92:GLU:HG3 | 4:M1:92:GLU:O | 1.99 | 0.60 |
| 4:M1:189:ASP:CG | 3:Z1:84:ARG:HH11 | 2.09 | 0.60 |
| 1:A:27:LEU:HD13 | 8:a5:37:LEU:HD21 | 1.83 | 0.60 |
| 2:AA:49:ASP:O | 2:AA:52:VAL:N | 2.33 | 0.60 |
| 3:DA:112:GLY:CA | 4:MA:76:ALA:HB1 | 2.31 | 0.60 |
| 12:SA:201:CYC:HB | 12:SA:201:CYC:HMA2 | 1.67 | 0.60 |
| 2:O1:33:ARG:CZ | 2:Y1:28:ASN:CG | 2.74 | 0.60 |
| 12:A1:201:CYC:HMA2 | 12:A1:201:CYC:HB | 1.67 | 0.60 |
| 3:H3:125:ARG:CZ | 8:k7:45:GLU:OE1 | 2.49 | 0.60 |
| 3:J3:77:ARG:CG | 2:K3:111:ALA:CB | 2.68 | 0.60 |
| 2:K2:22:THR:CB | 2:A2:2:LYS:HE2 | 2.31 | 0.60 |
| 2:A4:33:ARG:CZ | 2:K4:28:ASN:CG | 2.74 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M3:53:LEU:HD12 | 4:M3:53:LEU:O | 2.01 | 0.60 |
| 4:M3:61:ASN:C | 4:M3:63:GLY:H | 2.08 | 0.60 |
| 4:M3:232:VAL:HG21 | 3:V3:113:LEU:CA | 2.32 | 0.60 |
| 3:F4:110:LEU:O | 3:F4:112:GLY:N | 2.35 | 0.60 |
| 3:H4:108:ARG:CZ | 11:aA:97:ALA:HB2 | 2.32 | 0.60 |
| 4:M4:232:VAL:HG22 | 4:M4:235:PHE:CE2 | 2.31 | 0.60 |
| 8:M5:90:ARG:CZ | 1:N5:16:GLY:HA2 | 2.32 | 0.60 |
| 8:A5:126:VAL:HG22 | 12:A5:201:CYC:HBC3 | 1.83 | 0.60 |
| 8:E5:107:ILE:HG22 | 8:E5:107:ILE:O | 2.01 | 0.60 |
| 8:G5:126:VAL:HG22 | 12:G5:201:CYC:HBC3 | 1.82 | 0.60 |
| 8:c5:54:ALA:HA | 8:c5:132:ALA:HB1 | 1.84 | 0.60 |
| 8:e5:93:THR:O | 8:e5:97:VAL:HG22 | 2.02 | 0.60 |
| 1:R5:65:LEU:CD1 | 10:k5:706:PRO:CG | 2.67 | 0.60 |
| 8:U5:93:THR:O | 8:U5:97:VAL:HG22 | 2.02 | 0.60 |
| 12:K6:201:CYC:HMA2 | 12:K6:201:CYC:HB | 1.66 | 0.60 |
| 10:j5:353:ASN:HB3 | 10:j5:382:ILE:HD12 | 1.84 | 0.60 |
| 10:j5:844:GLN:O | 10:j5:844:GLN:HG3 | 2.00 | 0.60 |
| 10:k5:966:SER:OG | 1:p7:14:VAL:CG1 | 2.50 | 0.60 |
| 10:k5:1052:PRO:CB | 11:a9:32:ARG:NH2 | 2.62 | 0.60 |
| 8:O7:6:LYS:HZ2 | 8:E7:21:GLY:HA3 | 1.65 | 0.60 |
| 8:I7:93:THR:O | 8:I7:97:VAL:HG22 | 2.02 | 0.60 |
| 8:g7:25:ARG:NE | 8:u7:25:ARG:CZ | 2.64 | 0.60 |
| 8:Y7:104:ILE:CG2 | 8:Y7:156:LEU:HD21 | 2.32 | 0.60 |
| 8:a7:35:ARG:NE | 8:a7:145:ASP:OD1 | 2.33 | 0.60 |
| 8:u7:5:THR:N | 1:v7:3:ASP:OD2 | 2.35 | 0.60 |
| 9:y7:32:VAL:O | 9:y7:32:VAL:HG13 | 2.01 | 0.60 |
| 3:H8:14:LEU:HD11 | 11:a9:86:ASP:H | 1.65 | 0.60 |
| 4:M8:144:ARG:HD3 | 4:M8:204:ILE:CG2 | 2.31 | 0.60 |
| 4:M8:235:PHE:CD2 | 12:M8:301:CYC:C3A | 2.84 | 0.60 |
| 3:L9:83:LEU:HD11 | 2:G9:119:THR:HG21 | 1.83 | 0.60 |
| 5:N9:66:ARG:NH1 | 5:N9:66:ARG:HB2 | 2.16 | 0.60 |
| 5:N9:66:ARG:NH1 | 3:T9:111:ASN:OD1 | 2.30 | 0.60 |
| 11:a9:85:ALA:O | 11:a9:86:ASP:HB2 | 2.02 | 0.60 |
| 11:aA:54:ARG:HD2 | 11:aA:610:ALA:CB | 2.32 | 0.60 |
| 11:aA:95:ILE:HG22 | 11:aA:95:ILE:O | 2.01 | 0.60 |
| 4:MA:92:GLU:O | 4:MA:92:GLU:HG3 | 1.99 | 0.60 |
| 4:MA:251:ASN:H | 4:MA:251:ASN:ND2 | 1.95 | 0.60 |
| 2:QA:120:PHE:CE2 | 3:TA:83:LEU:HD11 | 2.37 | 0.60 |
| 3:L2:75:PRO:CD | 3:L2:78:ARG:CB | 2.71 | 0.60 |
| 12:C3:201:CYC:HB | 12:C3:201:CYC:HMA2 | 1.67 | 0.60 |
| 3:D3:68:ARG:HH12 | 3:X3:68:ARG:NH2 | 1.97 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:B4:86:MET:N | 12:B4:202:CYC:CAC | 2.64 | 0.60 |
| 5:N3:14:LYS:CE | 5:N3:50:LEU:CD2 | 2.80 | 0.60 |
| 5:N3:50:LEU:HD21 | 12:R3:201:CYC:O1D | 2.01 | 0.60 |
| 4:M4:205:ASP:OD2 | 5:Z4:59:ARG:CG | 2.50 | 0.60 |
| 2:N4:44:LEU:CD1 | 2:N4:142:LEU:HD11 | 2.32 | 0.60 |
| 1:L5:68:PRO:CB | 1:H5:14:VAL:O | 2.50 | 0.60 |
| 8:M5:101:VAL:O | 8:M5:102:THR:C | 2.45 | 0.60 |
| 8:O5:2:SER:C | 8:O5:100:ASP:CB | 2.74 | 0.60 |
| 5:Z4:50:LEU:HD12 | 5:Z4:50:LEU:O | 2.02 | 0.60 |
| 8:G5:101:VAL:O | 8:G5:102:THR:C | 2.45 | 0.60 |
| 12:C1:201:CYC:HB | 12:C1:201:CYC:HMA2 | 1.67 | 0.60 |
| 8:S5:59:PHE:HB3 | 8:E7:68:PRO:HB2 | 1.84 | 0.60 |
| 8:a5:35:ARG:NH2 | 8:a5:144:ASP:CB | 2.61 | 0.60 |
| 1:b5:5:ILE:HD11 | 10:k5:46:PHE:CE1 | 2.36 | 0.60 |
| 10:j5:1119:LEU:CD1 | 1:t7:87:TYR:OH | 2.49 | 0.60 |
| 10:k5:372:ARG:NH2 | 10:k5:376:GLN:HE21 | 1.99 | 0.60 |
| 2:A6:44:LEU:CD1 | 2:A6:142:LEU:HD11 | 2.32 | 0.60 |
| 12:A6:201:CYC:HMA2 | 12:A6:201:CYC:HB | 1.67 | 0.60 |
| 12:I6:201:CYC:HMA2 | 12:I6:201:CYC:HB | 1.67 | 0.60 |
| 8:C7:17:TYR:CZ | 1:D7:90:ARG:HA | 2.36 | 0.60 |
| 8:I7:17:TYR:CZ | 1:J7:90:ARG:HA | 2.36 | 0.60 |
| 8:a7:10:ASN:ND2 | 8:o7:10:ASN:HD22 | 1.98 | 0.60 |
| 8:a7:33:GLY:C | 1:b7:31:PHE:CE2 | 2.79 | 0.60 |
| 8:c7:20:PRO:CD | 8:m7:155:TYR:CD1 | 2.84 | 0.60 |
| 2:E8:15:GLN:HG3 | 11:a9:163:ASP:CG | 2.27 | 0.60 |
| 8:m7:2:SER:C | 8:m7:100:ASP:CB | 2.74 | 0.60 |
| 8:o7:5:THR:N | 1:p7:3:ASP:OD2 | 2.35 | 0.60 |
| 1:p7:68:PRO:O | 11:a9:42:ARG:CZ | 2.50 | 0.60 |
| 8:s7:2:SER:C | 8:s7:100:ASP:CB | 2.74 | 0.60 |
| 8:s7:29:PHE:CZ | 8:s7:98:ALA:C | 2.76 | 0.60 |
| 8:u7:17:TYR:CE2 | 1:v7:93:THR:HG21 | 2.35 | 0.60 |
| 5:Z8:22:LEU:HD21 | 5:Z8:26:LEU:CD1 | 2.15 | 0.60 |
| 5:Z8:50:LEU:HD12 | 5:Z8:50:LEU:O | 2.02 | 0.60 |
| 11:a9:638:ALA:O | 11:a9:639:GLN:NE2 | 2.34 | 0.60 |
| 11:aA:594:ARG:HH11 | 11:aA:594:ARG:CG | 2.10 | 0.60 |
| 3:H1:81:ALA:HB1 | 12:H1:201:CYC:C4D | 2.31 | 0.60 |
| 5:N1:66:ARG:NH1 | 5:N1:66:ARG:HB2 | 2.16 | 0.60 |
| 1:Z:16:GLY:C | 8:e5:90:ARG:CZ | 2.75 | 0.60 |
| 2:AA:44:LEU:CD1 | 2:AA:142:LEU:HD11 | 2.32 | 0.60 |
| 4:MA:274:VAL:CG2 | 3:VA:77:ARG:HB2 | 2.07 | 0.60 |
| 12:Q1:201:CYC:HMA2 | 12:Q1:201:CYC:HB | 1.67 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:M2:32:MET:HA | 8:O5:79:ALA:CB | 2.31 | 0.60 |
| 12:B3:202:CYC:HBA2 | 11:a9:684:ASN:N | 2.17 | 0.60 |
| 3:B4:92:TYR:OH | 12:B4:202:CYC:CAB | 2.49 | 0.60 |
| 5:N3:61:LYS:HD3 | 3:R3:108:ARG:O | 2.02 | 0.60 |
| 5:Z4:14:LYS:CE | 5:Z4:50:LEU:CD2 | 2.80 | 0.60 |
| 5:Z4:38:GLU:O | 5:Z4:39:PRO:C | 2.43 | 0.60 |
| 5:Z4:42:SER:CA | 12:Z4:301:CYC:HMA3 | 2.26 | 0.60 |
| 1:B5:14:VAL:O | 1:F5:68:PRO:CB | 2.50 | 0.60 |
| 1:B5:76:ARG:HD2 | 9:z5:14:LEU:CB | 2.27 | 0.60 |
| 8:e5:2:SER:C | 8:e5:100:ASP:CB | 2.74 | 0.60 |
| 8:A7:104:ILE:CG2 | 8:A7:156:LEU:HD21 | 2.32 | 0.60 |
| 10:j5:275:THR:HG21 | 10:j5:286:VAL:CA | 2.32 | 0.60 |
| 10:j5:878:GLU:HG3 | 9:w7:28:PHE:CD2 | 2.37 | 0.60 |
| 10:k5:275:THR:HG21 | 10:k5:286:VAL:CA | 2.31 | 0.60 |
| 10:k5:804:GLU:OE1 | 9:z7:30:LYS:CE | 2.50 | 0.60 |
| 8:S7:104:ILE:CG2 | 8:S7:156:LEU:HD21 | 2.32 | 0.60 |
| 1:J7:67:ARG:O | 1:J7:68:PRO:O | 2.20 | 0.60 |
| 8:a7:6:LYS:HZ2 | 8:o7:16:ARG:NH2 | 2.00 | 0.60 |
| 3:B8:119:ALA:HB3 | 4:M8:52:LEU:CD1 | 2.32 | 0.60 |
| 9:z7:5:PHE:CD2 | 9:z7:37:TRP:CD1 | 2.90 | 0.60 |
| 9:w7:21:ARG:O | 9:w7:22:GLU:C | 2.40 | 0.60 |
| 9:x7:23:LEU:HD12 | 9:x7:23:LEU:C | 2.25 | 0.60 |
| 9:x7:32:VAL:O | 9:x7:32:VAL:HG13 | 2.01 | 0.60 |
| 2:X8:28:ASN:CG | 2:N8:33:ARG:CZ | 2.74 | 0.60 |
| 12:H8:201:CYC:HBA1 | 11:a9:261:SER:HB2 | 1.84 | 0.60 |
| 4:M8:100:SER:HA | 4:M8:103:GLN:CB | 2.32 | 0.60 |
| 2:N8:44:LEU:CD1 | 2:N8:142:LEU:HD11 | 2.32 | 0.60 |
| 3:Q8:113:LEU:C | 3:Q8:115:GLU:H | 2.10 | 0.60 |
| 4:M9:260:ARG:HG3 | 4:M9:260:ARG:HH11 | 1.66 | 0.60 |
| 3:Y8:117:TYR:HB2 | 3:Y8:124:THR:HG22 | 1.84 | 0.60 |
| 2:K9:17:ARG:HB3 | 2:K9:17:ARG:CZ | 2.32 | 0.60 |
| 12:S9:201:CYC:HMA2 | 12:S9:201:CYC:HB | 1.67 | 0.60 |
| 12:Y9:201:CYC:HB | 12:Y9:201:CYC:HMA2 | 1.66 | 0.60 |
| 11:a9:716:ILE:CD1 | 11:a9:738:LEU:CD2 | 2.80 | 0.60 |
| 11:aA:50:LEU:O | 11:aA:53:VAL:CA | 2.49 | 0.60 |
| 11:aA:312:ASP:CB | 11:aA:315:LEU:HD13 | 2.19 | 0.60 |
| 11:aA:325:LEU:O | 11:aA:329:ASN:OD1 | 2.19 | 0.60 |
| 12:I1:201:CYC:HMA2 | 12:I1:201:CYC:HB | 1.67 | 0.60 |
| 2:A2:44:LEU:CD1 | 2:A2:142:LEU:HD11 | 2.32 | 0.60 |
| 12:DA:201:CYC:CBB | 4:MA:6:THR:CG2 | 2.80 | 0.60 |
| 4:MA:260:ARG:HG3 | 4:MA:260:ARG:HH11 | 1.66 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:P1:201:CYC:HBA2 | 4:M1:134:ASN:N | 2.17 | 0.60 |
| 3:R1:108:ARG:O | 5:N1:61:LYS:HD3 | 2.02 | 0.60 |
| 2:A1:2:LYS:HE2 | 2:K1:22:THR:CB | 2.31 | 0.60 |
| 4:M3:118:TYR:CD2 | 3:X3:84:ARG:CZ | 2.84 | 0.60 |
| 2:O3:44:LEU:CD1 | 2:O3:142:LEU:HD11 | 2.32 | 0.60 |
| 3:L4:71:GLY:HA3 | 11:aA:82:GLN:HG2 | 1.74 | 0.60 |
| 4:M4:86:ALA:HB1 | 3:Y4:77:ARG:NH1 | 2.17 | 0.60 |
| 3:Q4:97:LEU:CA | 3:Q4:163:TYR:CE2 | 2.82 | 0.60 |
| 8:M5:14:GLU:HG2 | 10:k5:538:PHE:CE2 | 2.36 | 0.60 |
| 3:Y4:89:ILE:HG12 | 3:Y4:92:TYR:CE2 | 2.37 | 0.60 |
| 9:z5:6:LYS:HB3 | 9:z5:55:LYS:HB2 | 0.64 | 0.60 |
| 9:z5:23:LEU:N | 9:z5:25:ASN:H | 1.97 | 0.60 |
| 10:j5:1064:LYS:HA | 10:j5:1069:ARG:N | 2.15 | 0.60 |
| 10:k5:190:LEU:HD22 | 10:k5:194:CYS:SG | 2.41 | 0.60 |
| 10:k5:905:THR:HG22 | 10:k5:906:ARG:HG2 | 1.84 | 0.60 |
| 10:k5:1016:LEU:CB | 10:k5:1044:ASN:ND2 | 2.62 | 0.60 |
| 10:k5:1124:TYR:CZ | 1:n7:119:LEU:HD21 | 2.37 | 0.60 |
| 12:B7:201:CYC:HB | 12:B7:201:CYC:CMA | 1.99 | 0.60 |
| 8:G7:104:ILE:CG2 | 8:G7:156:LEU:HD21 | 2.32 | 0.60 |
| 8:Y7:54:ALA:HA | 8:Y7:132:ALA:HB1 | 1.84 | 0.60 |
| 8:Y7:118:SER:HB2 | 1:d7:82:ILE:CD1 | 2.31 | 0.60 |
| 8:a7:63:PRO:CG | 11:a9:334:LYS:HA | 2.32 | 0.60 |
| 2:E1:114:ARG:NH1 | 11:aA:671:GLU:CD | 2.60 | 0.60 |
| 12:E8:201:CYC:HB | 12:E8:201:CYC:HMA2 | 1.67 | 0.60 |
| 8:o7:27:LYS:CE | 1:p7:35:ALA:CA | 2.80 | 0.60 |
| 8:q7:120:GLN:CG | 1:v7:53:LYS:HZ1 | 2.13 | 0.60 |
| 8:u7:27:LYS:CD | 1:v7:35:ALA:HB2 | 2.28 | 0.60 |
| 8:u7:101:VAL:O | 8:u7:102:THR:C | 2.45 | 0.60 |
| 4:M9:232:VAL:CG1 | 3:X9:111:ASN:C | 2.71 | 0.60 |
| 5:N9:50:LEU:HD12 | 5:N9:50:LEU:O | 2.02 | 0.60 |
| 5:Z8:14:LYS:CE | 5:Z8:50:LEU:CD2 | 2.80 | 0.60 |
| 3:B9:27:LEU:HD23 | 3:B9:30:LEU:HD22 | 1.84 | 0.60 |
| 2:I9:1:MET:HE1 | 2:I9:108:TYR:CE1 | 2.36 | 0.60 |
| 12:Y9:201:CYC:HMD1 | 12:Y9:201:CYC:NC | 2.09 | 0.60 |
| 11:a9:353:ALA:O | 11:a9:356:ALA:HB2 | 2.02 | 0.60 |
| 11:a9:371:VAL:HG11 | 11:a9:507:PHE:HD2 | 1.61 | 0.60 |
| 11:aA:707:PHE:CD2 | 3:L1:108:ARG:NH1 | 2.68 | 0.60 |
| 4:M1:260:ARG:HG3 | 4:M1:260:ARG:HH11 | 1.66 | 0.60 |
| 3:LA:84:ARG:CZ | 11:aA:406:LEU:HD23 | 2.31 | 0.59 |
| 4:MA:274:VAL:OXT | 3:VA:77:ARG:CZ | 2.50 | 0.59 |
| 2:QA:116:VAL:HG13 | 3:TA:79:MET:HG2 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:A1:44:LEU:CD1 | 2:A1:142:LEU:HD11 | 2.32 | 0.59 |
| 2:K3:15:GLN:C | 11:a9:745:GLY:HA3 | 2.23 | 0.59 |
| 3:B4:82:CYS:HB2 | 12:B4:202:CYC:C1C | 2.27 | 0.59 |
| 2:E4:15:GLN:HG3 | 11:aA:163:ASP:CG | 2.26 | 0.59 |
| 4:M4:225:LYS:CE | 3:Y4:81:ALA:CB | 2.69 | 0.59 |
| 8:O5:36:ARG:HD3 | 8:O5:96:ILE:O | 2.02 | 0.59 |
| 1:f5:9:ILE:CG2 | 10:j5:17:PHE:CZ | 2.85 | 0.59 |
| 1:R5:83:ARG:HD3 | 10:k5:516:THR:HG22 | 1.84 | 0.59 |
| 8:Y5:101:VAL:O | 8:Y5:102:THR:C | 2.45 | 0.59 |
| 2:K6:22:THR:CB | 2:A6:2:LYS:HE2 | 2.31 | 0.59 |
| 10:j5:750:ARG:NH2 | 10:j5:884:TRP:O | 2.35 | 0.59 |
| 10:j5:888:THR:HG21 | 1:J7:83:ARG:NH1 | 2.17 | 0.59 |
| 10:k5:588:VAL:O | 10:k5:588:VAL:HG13 | 2.00 | 0.59 |
| 3:B6:77:ARG:HH11 | 3:B6:77:ARG:HG2 | 1.67 | 0.59 |
| 3:F6:120:LEU:HD11 | 12:F6:201:CYC:HAA1 | 1.84 | 0.59 |
| 8:O7:93:THR:O | 8:O7:97:VAL:HG22 | 2.02 | 0.59 |
| 8:M7:104:ILE:CG2 | 8:M7:156:LEU:HD21 | 2.32 | 0.59 |
| 8:c7:126:VAL:HG22 | 12:c7:201:CYC:HMC1 | 1.82 | 0.59 |
| 8:o7:37:LEU:HD22 | 1:p7:24:LEU:CD1 | 2.32 | 0.59 |
| 8:o7:101:VAL:O | 8:o7:102:THR:C | 2.45 | 0.59 |
| 3:Q8:80:ALA:CB | 5:Z8:33:GLY:HA3 | 2.32 | 0.59 |
| 3:L9:37:ARG:HD3 | 3:L9:98:LEU:HA | 1.84 | 0.59 |
| 4:M9:53:LEU:HD12 | 4:M9:53:LEU:O | 2.01 | 0.59 |
| 12:Q9:201:CYC:HB | 12:Q9:201:CYC:HMA2 | 1.66 | 0.59 |
| 12:G9:201:CYC:HMA2 | 12:G9:201:CYC:HB | 1.67 | 0.59 |
| 12:H9:202:CYC:OB | 11:a9:448:ASN:HB2 | 2.02 | 0.59 |
| 12:K9:201:CYC:HMA2 | 12:K9:201:CYC:HB | 1.66 | 0.59 |
| 12:G1:201:CYC:HB | 12:G1:201:CYC:HMA2 | 1.67 | 0.59 |
| 11:a9:30:MET:CE | 11:a9:35:ARG:HD3 | 2.32 | 0.59 |
| 11:a9:50:LEU:O | 11:a9:53:VAL:CA | 2.49 | 0.59 |
| 11:a9:716:ILE:HD11 | 11:a9:738:LEU:HD23 | 1.83 | 0.59 |
| 11:aA:425:VAL:HG23 | 11:aA:502:ASN:HA | 1.83 | 0.59 |
| 11:aA:710:THR:O | 3:L1:107:ASP:O | 2.19 | 0.59 |
| 12:CA:201:CYC:HB | 12:CA:201:CYC:HMA2 | 1.67 | 0.59 |
| 3:DA:112:GLY:N | 4:MA:76:ALA:CB | 2.52 | 0.59 |
| 12:KA:201:CYC:HB | 12:KA:201:CYC:HMA2 | 1.66 | 0.59 |
| 2:K2:28:ASN:CG | 2:A2:33:ARG:CZ | 2.74 | 0.59 |
| 12:A3:201:CYC:HMA2 | 12:A3:201:CYC:HB | 1.67 | 0.59 |
| 4:M3:134:ASN:HD21 | 5:N3:1:MET:H1 | 1.50 | 0.59 |
| 5:N3:22:LEU:HD21 | 5:N3:26:LEU:CG | 2.29 | 0.59 |
| 2:O3:33:ARG:CZ | 2:Y3:28:ASN:CG | 2.74 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 12:Y3:201:CYC:HMA2 | 12:Y3:201:CYC:HB | 1.67 | 0.59 |
| 4:M4:268:ARG:CZ | 3:Y4:111:ASN:HB3 | 2.32 | 0.59 |
| 1:L5:79:ALA:HB2 | 8:G5:114:GLU:HB2 | 1.83 | 0.59 |
| 8:O5:76:LYS:CD | 8:O5:77:MET:HE1 | 2.14 | 0.59 |
| 8:C5:93:THR:O | 8:C5:97:VAL:HG22 | 2.02 | 0.59 |
| 8:S5:104:ILE:CG2 | 8:S5:156:LEU:HD21 | 2.32 | 0.59 |
| 8:U5:75:GLU:CG | 6:M6:32:MET:CE | 2.81 | 0.59 |
| 8:W5:101:VAL:O | 8:W5:102:THR:C | 2.45 | 0.59 |
| 10:j5:743:VAL:CA | 12:J7:201:CYC:O2D | 2.48 | 0.59 |
| 10:j5:1118:THR:O | 10:j5:1118:THR:HG22 | 2.02 | 0.59 |
| 10:k5:298:ARG:CG | 10:k5:298:ARG:HH11 | 2.15 | 0.59 |
| 10:k5:722:ILE:HD11 | 8:E7:82:LEU:HD12 | 1.84 | 0.59 |
| 10:k5:1146:THR:HG23 | 10:k5:1146:THR:O | 2.02 | 0.59 |
| 1:D7:67:ARG:O | 1:D7:68:PRO:O | 2.20 | 0.59 |
| 8:g7:93:THR:O | 8:g7:97:VAL:HG22 | 2.02 | 0.59 |
| 8:a7:63:PRO:CG | 11:a9:333:GLN:O | 2.50 | 0.59 |
| 9:x7:21:ARG:HD3 | 9:x7:21:ARG:C | 2.27 | 0.59 |
| 4:M8:251:ASN:HD22 | 4:M8:251:ASN:N | 1.92 | 0.59 |
| 12:M8:302:CYC:CMC | 3:S8:72:ASN:HD21 | 1.69 | 0.59 |
| 12:M8:302:CYC:HBC1 | 3:S8:81:ALA:HB3 | 1.84 | 0.59 |
| 4:M9:65:ARG:CD | 3:F9:111:ASN:HD21 | 2.12 | 0.59 |
| 4:M9:159:CYS:O | 3:V9:107:ASP:O | 2.19 | 0.59 |
| 11:a9:334:LYS:O | 11:a9:334:LYS:HG3 | 2.00 | 0.59 |
| 11:a9:425:VAL:HG23 | 11:a9:502:ASN:HA | 1.83 | 0.59 |
| 11:aA:89:ALA:O | 11:aA:92:LYS:N | 2.34 | 0.59 |
| 11:aA:95:ILE:HD13 | 11:aA:237:PHE:CE1 | 2.34 | 0.59 |
| 3:B2:77:ARG:HH11 | 3:B2:77:ARG:HG2 | 1.67 | 0.59 |
| 12:Z:201:CYC:HBB2 | 10:j5:256:LEU:HD11 | 1.83 | 0.59 |
| 12:CA:201:CYC:HMD1 | 12:CA:201:CYC:NC | 2.10 | 0.59 |
| 3:DA:112:GLY:HA3 | 4:MA:4:LEU:HD12 | 1.85 | 0.59 |
| 2:KA:17:ARG:HB3 | 2:KA:17:ARG:CZ | 2.32 | 0.59 |
| 3:LA:120:LEU:HD22 | 11:aA:538:ARG:CB | 2.27 | 0.59 |
| 4:MA:259:ARG:NH2 | 4:MA:259:ARG:HG3 | 2.17 | 0.59 |
| 2:OA:44:LEU:CD1 | 2:OA:142:LEU:HD11 | 2.32 | 0.59 |
| 12:QA:201:CYC:HBA1 | 3:TA:67:ILE:HG22 | 1.84 | 0.59 |
| 3:R1:111:ASN:ND2 | 5:N1:66:ARG:HH12 | 1.94 | 0.59 |
| 12:R1:201:CYC:HBA2 | 5:N1:53:LEU:HB3 | 1.83 | 0.59 |
| 2:K3:28:ASN:CG | 2:A3:33:ARG:CZ | 2.74 | 0.59 |
| 3:F3:119:ALA:CB | 4:M3:41:ASN:ND2 | 2.62 | 0.59 |
| 2:A4:2:LYS:HE2 | 2:K4:22:THR:CB | 2.31 | 0.59 |
| 3:B4:108:ARG:HA | 4:M4:61:ASN:CB | 2.30 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:M3:164:ARG:NH1 | 4:M3:259:ARG:O | 2.33 | 0.59 |
| 3:B1:88:ILE:HD13 | 12:B1:202:CYC:C1B | 2.31 | 0.59 |
| 12:L4:202:CYC:HBB3 | 11:aA:245:ALA:N | 2.16 | 0.59 |
| 12:M4:301:CYC:C4B | 3:Y4:88:ILE:CD1 | 2.79 | 0.59 |
| 8:C5:2:SER:CB | 1:D5:3:ASP:OD2 | 2.49 | 0.59 |
| 8:I5:36:ARG:HD3 | 8:I5:96:ILE:O | 2.02 | 0.59 |
| 8:e5:36:ARG:HD3 | 8:e5:96:ILE:O | 2.02 | 0.59 |
| 1:f5:5:ILE:HD13 | 10:j5:46:PHE:CZ | 2.36 | 0.59 |
| 8:S5:54:ALA:HA | 8:S5:132:ALA:HB1 | 1.84 | 0.59 |
| 1:X5:143:PRO:HB2 | 8:a5:38:ARG:CZ | 2.32 | 0.59 |
| 9:i5:56:LEU:H | 9:i5:56:LEU:CD1 | 2.15 | 0.59 |
| 10:j5:619:GLU:CB | 10:j5:620:PRO:HD2 | 2.32 | 0.59 |
| 10:k5:1067:LEU:HD12 | 10:k5:1101:GLU:OE1 | 2.02 | 0.59 |
| 10:k5:1078:SER:HA | 12:k5:1203:CYC:CBA | 2.32 | 0.59 |
| 10:k5:1147:TYR:HD1 | 10:k5:1147:TYR:O | 1.85 | 0.59 |
| 8:O7:17:TYR:CZ | 1:P7:90:ARG:HA | 2.36 | 0.59 |
| 8:S7:54:ALA:HA | 8:S7:132:ALA:HB1 | 1.84 | 0.59 |
| 8:C7:36:ARG:HD3 | 8:C7:96:ILE:O | 2.02 | 0.59 |
| 8:I7:101:VAL:CG2 | 8:W7:20:PRO:HG2 | 2.32 | 0.59 |
| 1:J7:75:THR:HB | 8:K7:111:GLY:C | 2.28 | 0.59 |
| 1:b7:75:THR:HB | 8:c7:112:VAL:CA | 2.32 | 0.59 |
| 8:e7:54:ALA:HA | 8:e7:132:ALA:HB1 | 1.84 | 0.59 |
| 12:C8:201:CYC:HMA2 | 12:C8:201:CYC:HB | 1.67 | 0.59 |
| 8:o7:5:THR:HG1 | 1:p7:3:ASP:CG | 2.03 | 0.59 |
| 9:y7:21:ARG:HD3 | 9:y7:21:ARG:C | 2.27 | 0.59 |
| 12:H8:201:CYC:HBA2 | 11:a9:261:SER:OG | 2.01 | 0.59 |
| 4:M8:141:GLU:OE1 | 4:M8:144:ARG:CB | 2.43 | 0.59 |
| 4:M8:162:ASN:O | 4:M8:166:THR:CG2 | 2.51 | 0.59 |
| 4:M9:251:ASN:HD22 | 4:M9:251:ASN:N | 1.92 | 0.59 |
| 5:N9:14:LYS:CE | 5:N9:50:LEU:CD2 | 2.80 | 0.59 |
| 2:A9:49:ASP:O | 2:A9:52:VAL:N | 2.33 | 0.59 |
| 11:aA:558:VAL:HG12 | 11:aA:558:VAL:O | 2.01 | 0.59 |
| 11:aA:640:ALA:CB | 11:aA:767:THR:HG23 | 2.26 | 0.59 |
| 1:A:110:ASN:ND2 | 10:k5:462:TYR:HE2 | 1.90 | 0.59 |
| 3:BA:84:ARG:CZ | 4:MA:35:THR:HB | 2.33 | 0.59 |
| 12:HA:202:CYC:OB | 11:aA:448:ASN:HB2 | 2.02 | 0.59 |
| 5:NA:14:LYS:CE | 5:NA:50:LEU:CD2 | 2.80 | 0.59 |
| 2:O1:44:LEU:CD1 | 2:O1:142:LEU:HD11 | 2.32 | 0.59 |
| 4:M3:196:TYR:HB3 | 2:Y3:14:SER:O | 2.03 | 0.59 |
| 5:N3:1:MET:CB | 5:N3:3:VAL:CG2 | 2.76 | 0.59 |
| 12:U3:201:CYC:HMA2 | 12:U3:201:CYC:HB | 1.67 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M4:104:ALA:HB3 | 2:P4:13:ASP:C | 2.25 | 0.59 |
| 4:M4:214:GLY:HA2 | 5:Z4:28:HIS:NE2 | 2.17 | 0.59 |
| 4:M4:215:GLU:H | 5:Z4:28:HIS:C | 2.10 | 0.59 |
| 4:M4:232:VAL:O | 4:M4:235:PHE:HD2 | 1.69 | 0.59 |
| 2:N4:2:LYS:HE2 | 2:X4:22:THR:CB | 2.31 | 0.59 |
| 8:K5:112:VAL:CB | 1:J5:75:THR:HG21 | 2.30 | 0.59 |
| 7:N6:1:MET:HE2 | 7:N6:1:MET:N | 2.18 | 0.59 |
| 9:i5:5:PHE:HA | 9:i5:55:LYS:O | 2.01 | 0.59 |
| 9:i5:16:ARG:O | 9:i5:16:ARG:NE | 2.26 | 0.59 |
| 10:j5:1001:TYR:OH | 10:j5:1018:LEU:HG | 2.01 | 0.59 |
| 10:j5:1008:PHE:CZ | 12:v7:201:CYC:NB | 2.71 | 0.59 |
| 10:j5:1008:PHE:HD1 | 12:v7:201:CYC:HBB3 | 1.59 | 0.59 |
| 10:k5:284:PRO:CD | 10:k5:326:GLY:C | 2.61 | 0.59 |
| 10:k5:750:ARG:NH2 | 10:k5:884:TRP:O | 2.35 | 0.59 |
| 8:S7:101:VAL:O | 8:S7:102:THR:C | 2.45 | 0.59 |
| 8:I7:36:ARG:HD3 | 8:I7:96:ILE:O | 2.03 | 0.59 |
| 8:U7:36:ARG:HD3 | 8:U7:96:ILE:O | 2.03 | 0.59 |
| 8:c7:131:ARG:HH11 | 8:c7:131:ARG:CB | 2.15 | 0.59 |
| 2:A8:44:LEU:CD1 | 2:A8:142:LEU:HD11 | 2.32 | 0.59 |
| 8:s7:17:TYR:CZ | 1:t7:90:ARG:HA | 2.36 | 0.59 |
| 9:y7:6:LYS:HG2 | 9:y7:6:LYS:O | 2.01 | 0.59 |
| 4:M8:94:TRP:CG | 3:Q8:88:ILE:HG12 | 2.38 | 0.59 |
| 12:F1:201:CYC:HBA1 | 4:M1:36:TYR:H | 1.67 | 0.59 |
| 3:L9:84:ARG:NE | 11:a9:406:LEU:HD23 | 2.17 | 0.59 |
| 4:M9:274:VAL:HG13 | 3:V9:77:ARG:CG | 2.22 | 0.59 |
| 3:Y8:89:ILE:CB | 3:Y8:92:TYR:HE2 | 2.08 | 0.59 |
| 5:Z8:3:VAL:O | 5:Z8:4:LEU:C | 2.44 | 0.59 |
| 12:A9:201:CYC:HB | 12:A9:201:CYC:HMA2 | 1.67 | 0.59 |
| 11:a9:91:THR:HG22 | 11:a9:91:THR:O | 2.01 | 0.59 |
| 11:a9:275:THR:O | 11:a9:278:LEU:HD13 | 2.02 | 0.59 |
| 11:a9:325:LEU:O | 11:a9:329:ASN:OD1 | 2.19 | 0.59 |
| 11:a9:819:SER:O | 11:a9:819:SER:OG | 2.15 | 0.59 |
| 11:aA:426:ARG:HE | 11:aA:496:ARG:HD3 | 1.68 | 0.59 |
| 11:aA:627:GLN:N | 11:aA:627:GLN:OE1 | 2.35 | 0.59 |
| 11:aA:716:ILE:CD1 | 11:aA:738:LEU:CD2 | 2.80 | 0.59 |
| 11:aA:808:LEU:HD23 | 3:L1:111:ASN:HD21 | 1.67 | 0.59 |
| 4:M1:116:ASN:ND2 | 12:X1:201:CYC:OB | 2.29 | 0.59 |
| 4:M1:232:VAL:HG21 | 3:V1:113:LEU:CA | 2.32 | 0.59 |
| 4:M1:259:ARG:HG3 | 4:M1:259:ARG:NH2 | 2.17 | 0.59 |
| 12:WA:201:CYC:HB | 12:WA:201:CYC:HMA2 | 1.67 | 0.59 |
| 6:M2:238:LEU:CD1 | 6:M2:258:VAL:HG11 | 2.33 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 5:N3:62:ARG:CZ | 2:Q3:14:SER:CB | 2.79 | 0.59 |
| 12:G4:201:CYC:HB | 12:G4:201:CYC:HMA2 | 1.67 | 0.59 |
| 12:N4:201:CYC:HB | 12:N4:201:CYC:HMA2 | 1.67 | 0.59 |
| 1:N5:107:ARG:CZ | 10:k5:482:GLN:CD | 2.76 | 0.59 |
| 5:Z4:41:GLN:HB3 | 12:Z4:301:CYC:C4B | 2.32 | 0.59 |
| 8:S5:90:ARG:CZ | 1:T5:16:GLY:HA2 | 2.32 | 0.59 |
| 1:V5:161:SER:HB3 | 10:j5:11:VAL:HG21 | 1.83 | 0.59 |
| 7:N6:49:LEU:HG | 12:N6:101:CYC:HB | 1.65 | 0.59 |
| 10:j5:284:PRO:CD | 10:j5:326:GLY:C | 2.61 | 0.59 |
| 10:j5:357:LEU:CD2 | 10:j5:401:LEU:HD13 | 2.33 | 0.59 |
| 10:j5:924:ASP:CG | 1:J7:26:LYS:HZ3 | 2.08 | 0.59 |
| 10:j5:1069:ARG:HH11 | 10:j5:1069:ARG:CG | 2.15 | 0.59 |
| 1:D7:75:THR:HB | 8:E7:111:GLY:C | 2.28 | 0.59 |
| 8:g7:36:ARG:HD3 | 8:g7:96:ILE:O | 2.03 | 0.59 |
| 1:j7:82:ILE:CD1 | 8:e7:118:SER:HB2 | 2.32 | 0.59 |
| 8:k7:104:ILE:CG2 | 8:k7:156:LEU:HD21 | 2.32 | 0.59 |
| 8:W7:104:ILE:CG2 | 8:W7:156:LEU:HD21 | 2.32 | 0.59 |
| 8:a7:36:ARG:HD3 | 8:a7:96:ILE:O | 2.03 | 0.59 |
| 8:u7:37:LEU:HD22 | 1:v7:24:LEU:CD1 | 2.32 | 0.59 |
| 9:x7:30:LYS:HG3 | 9:x7:30:LYS:O | 2.03 | 0.59 |
| 9:y7:21:ARG:HD3 | 9:y7:21:ARG:O | 2.03 | 0.59 |
| 4:M8:268:ARG:NH1 | 3:Y8:112:GLY:H | 2.01 | 0.59 |
| 2:N8:49:ASP:O | 2:N8:52:VAL:N | 2.33 | 0.59 |
| 3:L9:111:ASN:C | 11:a9:532:ALA:HB3 | 2.28 | 0.59 |
| 4:M9:274:VAL:CG2 | 3:V9:77:ARG:CG | 2.80 | 0.59 |
| 3:H9:78:ARG:HD3 | 12:H9:202:CYC:CBD | 2.31 | 0.59 |
| 3:H9:120:LEU:HD13 | 12:H9:202:CYC:HAA2 | 1.82 | 0.59 |
| 11:a9:426:ARG:CZ | 11:a9:496:ARG:HD3 | 2.33 | 0.59 |
| 4:M1:164:ARG:NH1 | 4:M1:259:ARG:O | 2.33 | 0.59 |
| 12:W1:201:CYC:HB | 12:W1:201:CYC:HMA2 | 1.67 | 0.59 |
| 3:FA:68:ARG:NH2 | 3:ZA:68:ARG:CZ | 2.66 | 0.59 |
| 5:NA:50:LEU:HD12 | 5:NA:50:LEU:O | 2.02 | 0.59 |
| 12:OA:201:CYC:HB | 12:OA:201:CYC:HMA2 | 1.67 | 0.59 |
| 12:UA:201:CYC:HMA2 | 12:UA:201:CYC:HB | 1.67 | 0.59 |
| 3:P1:112:GLY:HA3 | 5:N1:4:LEU:O | 2.02 | 0.59 |
| 2:A4:44:LEU:CD1 | 2:A4:142:LEU:HD11 | 2.32 | 0.59 |
| 12:V4:201:CYC:HB | 12:V4:201:CYC:HMA2 | 1.67 | 0.59 |
| 2:K4:13:ASP:O | 11:aA:242:GLY:HA2 | 2.02 | 0.59 |
| 4:M4:227:GLN:C | 3:Y4:88:ILE:HG22 | 2.21 | 0.59 |
| 4:M4:259:ARG:NH2 | 4:M4:259:ARG:HG3 | 2.17 | 0.59 |
| 1:L5:46:SER:HB3 | 8:U5:154:ASP:HB3 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:A5:53:GLN:HE21 | 8:A5:57:GLN:HE21 | 1.49 | 0.59 |
| 1:H5:76:ARG:HD2 | 9:i5:14:LEU:C | 2.26 | 0.59 |
| 8:Q5:101:VAL:O | 8:Q5:102:THR:C | 2.45 | 0.59 |
| 8:Q5:104:ILE:CG2 | 8:Q5:156:LEU:HD21 | 2.33 | 0.59 |
| 8:S5:101:VAL:O | 8:S5:102:THR:C | 2.45 | 0.59 |
| 8:U5:35:ARG:NH2 | 8:U5:144:ASP:CB | 2.61 | 0.59 |
| 1:Z5:107:ARG:HD2 | 10:k5:351:PHE:O | 2.02 | 0.59 |
| 8:a5:29:PHE:CZ | 8:a5:98:ALA:C | 2.76 | 0.59 |
| 10:j5:905:THR:HG22 | 10:j5:906:ARG:HG2 | 1.84 | 0.59 |
| 10:j5:971:VAL:CG1 | 1:t7:76:ARG:CZ | 2.79 | 0.59 |
| 10:k5:147:ARG:HA | 10:k5:147:ARG:HE | 1.67 | 0.59 |
| 10:k5:221:LYS:HB3 | 10:k5:221:LYS:NZ | 2.14 | 0.59 |
| 10:k5:277:ILE:C | 10:k5:284:PRO:HA | 2.27 | 0.59 |
| 10:k5:911:LEU:O | 10:k5:913:VAL:N | 2.36 | 0.59 |
| 10:k5:929:PRO:HB3 | 1:D7:147:LYS:HG2 | 1.83 | 0.59 |
| 10:k5:1034:GLU:CD | 10:k5:1037:ARG:HH21 | 2.10 | 0.59 |
| 12:E6:201:CYC:HMA2 | 12:E6:201:CYC:HB | 1.67 | 0.59 |
| 8:Y7:101:VAL:O | 8:Y7:102:THR:C | 2.45 | 0.59 |
| 8:a7:51:VAL:HB | 11:a9:318:TRP:CZ3 | 2.38 | 0.59 |
| 12:b7:201:CYC:CBB | 9:x7:21:ARG:CD | 2.64 | 0.59 |
| 8:c7:12:ASP:HA | 1:d7:90:ARG:HH12 | 1.67 | 0.59 |
| 2:A8:33:ARG:CZ | 2:K8:28:ASN:CG | 2.74 | 0.59 |
| 8:s7:36:ARG:HD3 | 8:s7:96:ILE:O | 2.02 | 0.59 |
| 8:u7:58:LEU:HD12 | 8:u7:58:LEU:C | 2.25 | 0.59 |
| 8:u7:104:ILE:CG2 | 8:u7:156:LEU:HD21 | 2.32 | 0.59 |
| 12:V8:201:CYC:HMA2 | 12:V8:201:CYC:HB | 1.67 | 0.59 |
| 2:X8:16:GLY:O | 3:Y8:91:ARG:NH1 | 2.35 | 0.59 |
| 4:M8:53:LEU:HD12 | 4:M8:53:LEU:O | 2.01 | 0.59 |
| 4:M8:225:LYS:CD | 3:Y8:81:ALA:HB2 | 2.33 | 0.59 |
| 12:M8:302:CYC:CMD | 3:S8:77:ARG:CZ | 2.77 | 0.59 |
| 3:Q8:77:ARG:CA | 5:Z8:34:LEU:CB | 2.65 | 0.59 |
| 3:L9:113:LEU:HD12 | 3:L9:113:LEU:O | 2.03 | 0.59 |
| 4:M9:6:THR:CG2 | 12:D9:201:CYC:CBB | 2.80 | 0.59 |
| 4:M9:274:VAL:CG1 | 2:W9:111:ALA:CB | 2.68 | 0.59 |
| 2:A9:44:LEU:CD1 | 2:A9:142:LEU:HD11 | 2.32 | 0.59 |
| 3:H9:117:TYR:CE1 | 12:H9:202:CYC:NA | 2.70 | 0.59 |
| 12:W9:201:CYC:HMA2 | 12:W9:201:CYC:HB | 1.67 | 0.59 |
| 11:a9:54:ARG:HD2 | 11:a9:610:ALA:CB | 2.32 | 0.59 |
| 11:a9:376:ALA:HB2 | 11:a9:504:VAL:O | 2.03 | 0.59 |
| 11:a9:495:TYR:C | 11:a9:495:TYR:CD1 | 2.80 | 0.59 |
| 11:aA:776:TYR:N | 12:H1:201:CYC:HBA2 | 2.13 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:U1:43:ALA:O | 2:U1:47:ASN:CG | 2.46 | 0.59 |
| 12:K2:201:CYC:HB | 12:K2:201:CYC:HMA2 | 1.66 | 0.59 |
| 12:W3:201:CYC:HMA2 | 12:W3:201:CYC:HB | 1.67 | 0.59 |
| 3:F4:112:GLY:HA2 | 4:M4:76:ALA:HB1 | 1.83 | 0.59 |
| 12:R4:201:CYC:HB | 12:R4:201:CYC:HMA2 | 1.67 | 0.59 |
| 8:K5:112:VAL:HG22 | 8:K5:112:VAL:O | 2.03 | 0.59 |
| 8:A5:101:VAL:O | 8:A5:102:THR:C | 2.45 | 0.59 |
| 1:B5:76:ARG:HG3 | 9:z5:14:LEU:O | 2.03 | 0.59 |
| 1:J5:38:VAL:O | 1:J5:39:ARG:C | 2.37 | 0.59 |
| 6:M6:127:SER:O | 12:F6:201:CYC:HBA2 | 2.01 | 0.59 |
| 8:A7:54:ALA:HA | 8:A7:132:ALA:HB1 | 1.84 | 0.59 |
| 10:j5:232:ARG:HB2 | 10:j5:232:ARG:NH1 | 2.18 | 0.59 |
| 10:k5:141:GLU:H | 10:k5:141:GLU:CD | 2.08 | 0.59 |
| 10:k5:412:THR:O | 10:k5:412:THR:OG1 | 2.19 | 0.59 |
| 10:k5:1069:ARG:HH11 | 10:k5:1069:ARG:CG | 2.15 | 0.59 |
| 8:E7:104:ILE:CG2 | 8:E7:156:LEU:HD21 | 2.33 | 0.59 |
| 8:G7:54:ALA:HA | 8:G7:132:ALA:HB1 | 1.84 | 0.59 |
| 8:i7:101:VAL:O | 8:i7:102:THR:C | 2.45 | 0.59 |
| 8:i7:131:ARG:HH11 | 8:i7:131:ARG:CB | 2.15 | 0.59 |
| 1:V7:75:THR:HB | 8:W7:111:GLY:C | 2.27 | 0.59 |
| 8:m7:36:ARG:HD3 | 8:m7:96:ILE:O | 2.02 | 0.59 |
| 8:m7:93:THR:O | 8:m7:97:VAL:HG22 | 2.02 | 0.59 |
| 8:s7:93:THR:O | 8:s7:97:VAL:HG22 | 2.02 | 0.59 |
| 8:u7:157:VAL:O | 8:u7:161:GLN:HG3 | 2.03 | 0.59 |
| 9:y7:4:TYR:CB | 9:y7:58:THR:OG1 | 2.40 | 0.59 |
| 12:X8:201:CYC:HMA2 | 12:X8:201:CYC:HB | 1.66 | 0.59 |
| 4:M8:128:ALA:CA | 4:M8:142:PHE:CE1 | 2.83 | 0.59 |
| 4:M8:232:VAL:HG22 | 4:M8:235:PHE:CE2 | 2.31 | 0.59 |
| 4:M8:259:ARG:HG3 | 4:M8:259:ARG:NH2 | 2.17 | 0.59 |
| 12:L9:202:CYC:CMA | 11:a9:534:SER:CB | 2.81 | 0.59 |
| 4:M9:274:VAL:HG22 | 3:V9:77:ARG:CG | 2.32 | 0.59 |
| 5:N9:57:MET:HE1 | 3:T9:116:THR:OG1 | 2.03 | 0.59 |
| 2:A9:33:ARG:CZ | 2:K9:28:ASN:CG | 2.74 | 0.59 |
| 11:aA:30:MET:CE | 11:aA:35:ARG:HD3 | 2.32 | 0.59 |
| 11:aA:308:LEU:HD23 | 11:aA:308:LEU:C | 2.26 | 0.59 |
| 11:aA:495:TYR:CD1 | 11:aA:495:TYR:C | 2.80 | 0.59 |
| 12:A2:201:CYC:HMA2 | 12:A2:201:CYC:HB | 1.67 | 0.59 |
| 1:A:18:TYR:OH | 8:a5:89:LEU:HB3 | 2.02 | 0.59 |
| 1:Z:31:PHE:CE2 | 8:e5:37:LEU:HD11 | 2.38 | 0.59 |
| 3:FA:111:ASN:HD21 | 4:MA:65:ARG:CD | 2.12 | 0.59 |
| 3:LA:14:LEU:CD1 | 11:aA:358:PRO:HB2 | 2.25 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:MA:120:LEU:O | 4:MA:123:GLU:CB | 2.51 | 0.59 |
| 12:YA:201:CYC:HMA2 | 12:YA:201:CYC:HB | 1.66 | 0.59 |
| 3:H2:10:VAL:CG1 | 6:M2:69:ALA:HB1 | 2.29 | 0.59 |
| 4:M3:130:SER:O | 12:P3:201:CYC:CBA | 2.49 | 0.59 |
| 3:B1:85:ASP:OD2 | 12:B1:202:CYC:NA | 2.36 | 0.59 |
| 2:E4:1:MET:N | 4:M4:10:ARG:CZ | 2.59 | 0.59 |
| 12:E4:201:CYC:HMA2 | 12:E4:201:CYC:HB | 1.67 | 0.59 |
| 12:H4:201:CYC:HBA1 | 11:aA:261:SER:HB2 | 1.84 | 0.59 |
| 4:M4:164:ARG:NH1 | 4:M4:259:ARG:O | 2.33 | 0.59 |
| 2:N4:115:GLU:OE1 | 5:Z4:33:GLY:CA | 2.49 | 0.59 |
| 8:c5:104:ILE:CG2 | 8:c5:156:LEU:HD21 | 2.32 | 0.59 |
| 12:R5:201:CYC:CBB | 10:k5:520:ARG:CZ | 2.80 | 0.59 |
| 1:T5:87:TYR:CZ | 10:j5:483:PHE:HE2 | 2.21 | 0.59 |
| 12:X5:201:CYC:CBB | 10:j5:520:ARG:NE | 2.62 | 0.59 |
| 9:z5:8:THR:O | 9:z5:52:LEU:N | 2.35 | 0.59 |
| 10:j5:77:VAL:CG2 | 10:j5:141:GLU:HB3 | 2.32 | 0.59 |
| 10:j5:362:LYS:CD | 10:j5:363:HIS:HD2 | 1.83 | 0.59 |
| 10:j5:724:GLU:HA | 10:j5:727:THR:HG23 | 1.85 | 0.59 |
| 8:G7:101:VAL:O | 8:G7:102:THR:C | 2.45 | 0.59 |
| 8:c7:17:TYR:CB | 1:d7:45:SER:HB3 | 2.31 | 0.59 |
| 8:c7:50:ILE:CD1 | 8:c7:137:ALA:CB | 2.80 | 0.59 |
| 8:o7:72:ALA:HB2 | 12:o7:201:CYC:OC | 2.03 | 0.59 |
| 8:s7:35:ARG:NH2 | 8:s7:144:ASP:CB | 2.61 | 0.59 |
| 3:U8:115:GLU:CD | 4:M8:74:LEU:CD1 | 2.75 | 0.59 |
| 4:M8:181:GLN:HG3 | 4:M8:181:GLN:O | 2.03 | 0.59 |
| 4:M9:181:GLN:HG3 | 4:M9:181:GLN:O | 2.03 | 0.59 |
| 5:Z8:1:MET:CB | 5:Z8:3:VAL:CG2 | 2.76 | 0.59 |
| 5:Z8:29:HIS:CD2 | 5:Z8:36:THR:HG22 | 2.33 | 0.59 |
| 3:F9:68:ARG:NH2 | 3:Z9:68:ARG:CZ | 2.66 | 0.59 |
| 11:a9:89:ALA:CB | 11:a9:92:LYS:HZ2 | 2.16 | 0.59 |
| 11:a9:283:GLN:CG | 11:a9:284:PRO:CD | 2.80 | 0.59 |
| 11:a9:578:MET:CE | 11:a9:582:MET:HE1 | 2.30 | 0.59 |
| 11:aA:582:MET:O | 11:aA:586:LEU:HD23 | 2.03 | 0.59 |
| 3:H1:77:ARG:NH2 | 12:H1:201:CYC:O2D | 2.36 | 0.59 |
| 4:M1:251:ASN:HD22 | 4:M1:251:ASN:N | 1.92 | 0.59 |
| 5:N1:14:LYS:CE | 5:N1:50:LEU:CD2 | 2.80 | 0.59 |
| 12:GA:201:CYC:HB | 12:GA:201:CYC:HMA2 | 1.67 | 0.59 |
| 12:IA:201:CYC:HMA2 | 12:IA:201:CYC:HB | 1.67 | 0.59 |
| 3:JA:78:ARG:NH2 | 11:aA:359:ASP:N | 2.50 | 0.59 |
| 4:MA:230:GLN:O | 4:MA:230:GLN:HG2 | 2.03 | 0.59 |
| 5:NA:57:MET:HE1 | 3:TA:116:THR:OG1 | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:QA:162:SER:O | 2:WA:118:ARG:HD2 | 2.00 | 0.59 |
| 12:K3:201:CYC:HB | 12:K3:201:CYC:HMA2 | 1.66 | 0.59 |
| 12:I2:201:CYC:HMA2 | 12:I2:201:CYC:HB | 1.67 | 0.59 |
| 12:A4:201:CYC:HMA2 | 12:A4:201:CYC:HB | 1.67 | 0.59 |
| 3:B4:82:CYS:SG | 12:B4:202:CYC:C2C | 2.89 | 0.59 |
| 3:L3:111:ASN:HD21 | 11:a9:808:LEU:HD23 | 1.66 | 0.59 |
| 4:M3:190:ARG:HH11 | 4:M3:202:SER:HB3 | 1.63 | 0.59 |
| 12:O3:201:CYC:HB | 12:O3:201:CYC:HMA2 | 1.67 | 0.59 |
| 3:B1:127:VAL:HG22 | 12:B1:202:CYC:CMC | 2.33 | 0.59 |
| 3:F4:113:LEU:HA | 4:M4:5:THR:OG1 | 2.03 | 0.59 |
| 4:M4:217:VAL:HG13 | 5:Z4:30:PRO:HB3 | 1.83 | 0.59 |
| 4:M4:230:GLN:HG2 | 4:M4:230:GLN:O | 2.03 | 0.59 |
| 8:C5:36:ARG:HD3 | 8:C5:96:ILE:O | 2.02 | 0.59 |
| 8:G5:61:ILE:HD11 | 8:o7:68:PRO:HD2 | 1.82 | 0.59 |
| 1:J5:73:TYR:O | 1:J5:77:ARG:NE | 2.36 | 0.59 |
| 1:P5:114:GLU:HB3 | 10:k5:496:GLU:HG3 | 1.79 | 0.59 |
| 8:W5:126:VAL:HG23 | 12:W5:201:CYC:CMC | 2.33 | 0.59 |
| 6:M6:243:ALA:HA | 12:H6:201:CYC:CBB | 2.33 | 0.59 |
| 9:z5:23:LEU:C | 9:z5:25:ASN:H | 2.09 | 0.59 |
| 9:i5:56:LEU:O | 9:i5:58:THR:N | 2.30 | 0.59 |
| 10:j5:869:GLY:N | 9:w7:43:ARG:CZ | 2.43 | 0.59 |
| 10:j5:1151:GLN:C | 1:v7:122:PRO:CB | 2.75 | 0.59 |
| 10:k5:275:THR:HG22 | 10:k5:286:VAL:O | 2.03 | 0.59 |
| 10:k5:353:ASN:HB3 | 10:k5:382:ILE:HD12 | 1.84 | 0.59 |
| 8:O7:45:GLU:O | 1:r7:113:LYS:NZ | 2.33 | 0.59 |
| 8:Q7:101:VAL:O | 8:Q7:102:THR:C | 2.45 | 0.59 |
| 8:Q7:104:ILE:CG2 | 8:Q7:156:LEU:HD21 | 2.32 | 0.59 |
| 8:K7:101:VAL:O | 8:K7:102:THR:C | 2.45 | 0.59 |
| 8:g7:10:ASN:ND2 | 8:u7:10:ASN:HD22 | 1.99 | 0.59 |
| 8:a7:93:THR:O | 8:a7:97:VAL:HG22 | 2.02 | 0.59 |
| 8:c7:18:LEU:HD22 | 1:d7:97:LEU:HD13 | 1.84 | 0.59 |
| 8:q7:54:ALA:HA | 8:q7:132:ALA:HB1 | 1.84 | 0.59 |
| 4:M8:98:ASP:O | 3:Q8:1:MET:HE1 | 2.03 | 0.59 |
| 2:N8:111:ALA:CB | 5:Z8:35:ASP:OD2 | 2.51 | 0.59 |
| 3:Y8:113:LEU:HD13 | 3:Y8:171:ILE:HG13 | 1.84 | 0.59 |
| 2:I9:37:SER:HA | 2:I9:97:LEU:CD2 | 2.27 | 0.59 |
| 12:I9:201:CYC:HB | 12:I9:201:CYC:HMA2 | 1.67 | 0.59 |
| 2:S9:42:ARG:NH1 | 3:T9:21:GLU:CD | 2.59 | 0.59 |
| 11:a9:388:VAL:HG12 | 11:a9:392:ILE:HD12 | 1.84 | 0.59 |
| 11:a9:818:ARG:HH11 | 11:a9:818:ARG:CG | 2.10 | 0.59 |
| 12:Y1:201:CYC:HMA2 | 12:Y1:201:CYC:HB | 1.67 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 4:MA:144:ARG:NH2 | 5:NA:52:ARG:NH2 | 2.51 | 0.59 |
| 3:H3:78:ARG:NH1 | 11:a9:623:ASP:HB2 | 2.17 | 0.59 |
| 3:J3:119:ALA:O | 11:a9:803:ASN:C | 2.45 | 0.59 |
| 3:B3:127:VAL:CG2 | 12:B3:202:CYC:CMC | 2.81 | 0.59 |
| 4:M3:230:GLN:HG2 | 4:M3:230:GLN:O | 2.03 | 0.59 |
| 3:H4:1:MET:N | 11:aA:96:THR:CG2 | 2.66 | 0.59 |
| 3:H4:80:ALA:C | 3:H4:84:ARG:NH1 | 2.61 | 0.59 |
| 4:M4:93:LEU:HB3 | 4:M4:216:ASN:OD1 | 2.03 | 0.59 |
| 4:M4:129:GLU:HG3 | 4:M4:142:PHE:CE2 | 2.38 | 0.59 |
| 1:L5:106:GLU:CG | 9:i5:58:THR:CG2 | 2.81 | 0.59 |
| 12:X4:201:CYC:HMA2 | 12:X4:201:CYC:HB | 1.66 | 0.59 |
| 8:E5:112:VAL:HG22 | 8:E5:112:VAL:O | 2.03 | 0.59 |
| 8:G5:63:PRO:HG2 | 8:U5:68:PRO:HB2 | 1.84 | 0.59 |
| 1:d5:127:VAL:HG12 | 10:j5:698:GLY:HA3 | 1.82 | 0.59 |
| 9:z5:56:LEU:C | 9:z5:58:THR:H | 2.11 | 0.59 |
| 10:j5:750:ARG:HH11 | 10:j5:750:ARG:HG2 | 1.67 | 0.59 |
| 10:j5:939:GLN:O | 10:j5:943:THR:CG2 | 2.50 | 0.59 |
| 10:j5:1034:GLU:CD | 10:j5:1037:ARG:HH21 | 2.10 | 0.59 |
| 10:j5:1043:GLU:HB2 | 8:e7:14:GLU:OE2 | 2.03 | 0.59 |
| 10:k5:986:PRO:HD3 | 9:x7:24:GLN:NE2 | 2.18 | 0.59 |
| 10:k5:1025:LEU:HD22 | 10:k5:1035:PHE:CB | 2.15 | 0.59 |
| 1:P7:75:THR:HB | 8:Q7:111:GLY:C | 2.27 | 0.59 |
| 8:I7:35:ARG:NE | 8:I7:145:ASP:OD1 | 2.33 | 0.59 |
| 8:c7:96:ILE:CA | 8:c7:152:TYR:CD2 | 2.84 | 0.59 |
| 8:c7:101:VAL:O | 8:c7:102:THR:C | 2.45 | 0.59 |
| 3:B8:82:CYS:CA | 12:B8:202:CYC:C2C | 2.76 | 0.59 |
| 8:q7:101:VAL:O | 8:q7:102:THR:C | 2.45 | 0.59 |
| 8:q7:104:ILE:CG2 | 8:q7:156:LEU:HD21 | 2.33 | 0.59 |
| 9:z7:19:THR:O | 9:z7:19:THR:HG23 | 2.01 | 0.59 |
| 9:y7:30:LYS:O | 9:y7:30:LYS:HG3 | 2.03 | 0.59 |
| 4:M8:26:SER:CB | 11:a9:228:GLU:CD | 2.76 | 0.59 |
| 4:M8:164:ARG:NH1 | 4:M8:259:ARG:O | 2.33 | 0.59 |
| 12:M8:301:CYC:OC | 3:Y8:72:ASN:CB | 2.51 | 0.59 |
| 3:L9:120:LEU:CD2 | 11:a9:538:ARG:CB | 2.81 | 0.59 |
| 4:M9:35:THR:HB | 3:B9:84:ARG:NH1 | 2.18 | 0.59 |
| 5:N9:1:MET:C | 5:N9:3:VAL:N | 2.50 | 0.59 |
| 2:O9:44:LEU:CD1 | 2:O9:142:LEU:HD11 | 2.32 | 0.59 |
| 2:Y9:62:LYS:HG2 | 2:Y9:129:GLU:HG2 | 1.85 | 0.59 |
| 11:a9:112:GLU:O | 11:a9:115:VAL:N | 2.36 | 0.59 |
| 4:M1:120:LEU:O | 4:M1:123:GLU:CB | 2.51 | 0.59 |
| 5:N1:50:LEU:HD12 | 5:N1:50:LEU:O | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:NA:57:MET:SD | 12:TA:301:CYC:HMA3 | 2.43 | 0.58 |
| 5:NA:62:ARG:HE | 2:SA:14:SER:HA | 1.66 | 0.58 |
| 2:Q1:62:LYS:HG2 | 2:Q1:129:GLU:HG2 | 1.85 | 0.58 |
| 12:G3:201:CYC:HB | 12:G3:201:CYC:HMA2 | 1.67 | 0.58 |
| 2:I2:62:LYS:HG2 | 2:I2:129:GLU:HG2 | 1.85 | 0.58 |
| 12:B3:202:CYC:CMA | 11:a9:684:ASN:ND2 | 2.66 | 0.58 |
| 2:E3:62:LYS:HG2 | 2:E3:129:GLU:HG2 | 1.85 | 0.58 |
| 3:B4:120:LEU:HD13 | 4:M4:53:LEU:CB | 2.00 | 0.58 |
| 3:L3:1:MET:HE2 | 3:L3:108:ARG:HH12 | 1.67 | 0.58 |
| 4:M3:251:ASN:HD22 | 4:M3:251:ASN:N | 1.92 | 0.58 |
| 5:N3:37:HIS:O | 12:T3:301:CYC:CMA | 2.50 | 0.58 |
| 2:Q3:62:LYS:HG2 | 2:Q3:129:GLU:HG2 | 1.85 | 0.58 |
| 2:U3:62:LYS:HG2 | 2:U3:129:GLU:HG2 | 1.85 | 0.58 |
| 3:U4:120:LEU:CG | 4:M4:254:LEU:CD2 | 2.71 | 0.58 |
| 4:M4:231:THR:C | 12:M4:301:CYC:HBB3 | 2.27 | 0.58 |
| 8:M5:104:ILE:CG2 | 8:M5:156:LEU:HD21 | 2.32 | 0.58 |
| 8:O5:35:ARG:NE | 8:O5:145:ASP:OD1 | 2.33 | 0.58 |
| 1:B5:2:GLN:NE2 | 10:k5:551:MET:HG2 | 2.17 | 0.58 |
| 1:D5:73:TYR:O | 1:D5:77:ARG:NE | 2.36 | 0.58 |
| 8:G5:104:ILE:CG2 | 8:G5:156:LEU:HD21 | 2.32 | 0.58 |
| 8:I5:93:THR:O | 8:I5:97:VAL:HG22 | 2.02 | 0.58 |
| 1:b5:9:ILE:HG22 | 10:k5:17:PHE:CZ | 2.37 | 0.58 |
| 6:M6:238:LEU:CD1 | 6:M6:258:VAL:HG11 | 2.33 | 0.58 |
| 12:N6:101:CYC:H3C | 3:B6:127:VAL:HG22 | 1.85 | 0.58 |
| 8:A7:101:VAL:O | 8:A7:102:THR:C | 2.45 | 0.58 |
| 9:i5:8:THR:O | 9:i5:52:LEU:N | 2.36 | 0.58 |
| 9:i5:56:LEU:C | 9:i5:58:THR:H | 2.11 | 0.58 |
| 10:j5:362:LYS:HD2 | 10:j5:363:HIS:CD2 | 2.34 | 0.58 |
| 10:j5:1119:LEU:HD11 | 12:j5:1202:CYC:HBB3 | 1.84 | 0.58 |
| 10:j5:1146:THR:O | 10:j5:1146:THR:HG23 | 2.02 | 0.58 |
| 10:k5:159:ASP:OD2 | 12:k5:1201:CYC:NC | 2.36 | 0.58 |
| 10:k5:964:GLY:HA3 | 1:n7:69:GLY:HA3 | 1.85 | 0.58 |
| 10:k5:971:VAL:O | 10:k5:971:VAL:HG13 | 2.02 | 0.58 |
| 8:k7:54:ALA:HA | 8:k7:132:ALA:HB1 | 1.84 | 0.58 |
| 8:o7:104:ILE:CG2 | 8:o7:156:LEU:HD21 | 2.32 | 0.58 |
| 8:o7:157:VAL:O | 8:o7:161:GLN:HG3 | 2.03 | 0.58 |
| 8:u7:17:TYR:CE2 | 1:v7:93:THR:CG2 | 2.86 | 0.58 |
| 2:K8:13:ASP:O | 11:a9:242:GLY:HA2 | 2.03 | 0.58 |
| 4:M9:120:LEU:O | 4:M9:123:GLU:CB | 2.51 | 0.58 |
| 4:M9:134:ASN:CG | 5:N9:1:MET:H1 | 2.10 | 0.58 |
| 4:M9:162:ASN:O | 4:M9:166:THR:CG2 | 2.50 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M9:230:GLN:HG2 | 4:M9:230:GLN:O | 2.03 | 0.58 |
| 4:M9:259:ARG:HG3 | 4:M9:259:ARG:NH2 | 2.17 | 0.58 |
| 5:Z8:29:HIS:CG | 5:Z8:31:TRP:HD1 | 2.21 | 0.58 |
| 2:S9:62:LYS:HG2 | 2:S9:129:GLU:HG2 | 1.85 | 0.58 |
| 11:aA:376:ALA:HB2 | 11:aA:504:VAL:O | 2.03 | 0.58 |
| 11:aA:624:GLY:O | 11:aA:628:THR:HG23 | 1.92 | 0.58 |
| 4:M1:162:ASN:O | 4:M1:166:THR:CG2 | 2.50 | 0.58 |
| 1:A:83:ARG:HD3 | 10:k5:259:PRO:HD3 | 1.85 | 0.58 |
| 1:Z:73:TYR:CZ | 10:j5:162:TRP:HZ2 | 2.14 | 0.58 |
| 3:HA:84:ARG:HA | 11:aA:478:HIS:CE1 | 2.38 | 0.58 |
| 12:LA:202:CYC:CMA | 11:aA:534:SER:CB | 2.81 | 0.58 |
| 5:NA:53:LEU:CA | 12:TA:301:CYC:HBA2 | 2.33 | 0.58 |
| 2:YA:62:LYS:HG2 | 2:YA:129:GLU:HG2 | 1.85 | 0.58 |
| 3:J3:127:VAL:HG22 | 12:J3:202:CYC:H3C | 1.86 | 0.58 |
| 2:A3:44:LEU:CD1 | 2:A3:142:LEU:HD11 | 2.32 | 0.58 |
| 3:B4:85:ASP:N | 12:B4:202:CYC:CAC | 2.57 | 0.58 |
| 12:C4:201:CYC:HB | 12:C4:201:CYC:HMA2 | 1.67 | 0.58 |
| 3:B1:86:MET:SD | 12:B1:202:CYC:HBC1 | 2.43 | 0.58 |
| 2:K4:62:LYS:HG2 | 2:K4:129:GLU:HG2 | 1.86 | 0.58 |
| 8:M5:53:GLN:HB2 | 8:M5:136:VAL:HG21 | 1.86 | 0.58 |
| 1:D5:38:VAL:O | 1:D5:39:ARG:C | 2.37 | 0.58 |
| 6:M6:271:VAL:CG2 | 1:d7:127:VAL:CG1 | 2.81 | 0.58 |
| 10:j5:187:ARG:CZ | 10:j5:196:ILE:HD13 | 2.33 | 0.58 |
| 10:j5:1052:PRO:CB | 11:aA:32:ARG:NH2 | 2.64 | 0.58 |
| 10:k5:1144:SER:HB3 | 1:l7:13:ASP:OD2 | 2.03 | 0.58 |
| 2:G6:62:LYS:HG2 | 2:G6:129:GLU:HG2 | 1.85 | 0.58 |
| 12:G6:201:CYC:HB | 12:G6:201:CYC:CMA | 2.16 | 0.58 |
| 8:K7:126:VAL:HG23 | 12:K7:201:CYC:CMC | 2.33 | 0.58 |
| 1:h7:53:LYS:HG2 | 1:h7:53:LYS:O | 2.03 | 0.58 |
| 8:k7:52:LYS:HB2 | 11:a9:52:MET:HE1 | 1.83 | 0.58 |
| 8:a7:90:ARG:HB2 | 1:b7:18:TYR:CE1 | 2.38 | 0.58 |
| 8:c7:122:PRO:O | 8:c7:125:ALA:N | 2.36 | 0.58 |
| 3:B8:119:ALA:CB | 4:M8:52:LEU:CD1 | 2.72 | 0.58 |
| 8:u7:23:LEU:CD2 | 1:v7:38:VAL:CB | 2.74 | 0.58 |
| 8:u7:23:LEU:HD13 | 1:v7:38:VAL:HG12 | 1.84 | 0.58 |
| 8:u7:72:ALA:HB2 | 12:u7:201:CYC:OC | 2.03 | 0.58 |
| 9:x7:21:ARG:HD3 | 9:x7:21:ARG:O | 2.03 | 0.58 |
| 3:H8:108:ARG:CZ | 11:a9:97:ALA:HB2 | 2.33 | 0.58 |
| 4:M8:1:MET:HG3 | 4:M8:43:TYR:OH | 2.04 | 0.58 |
| 3:Q8:84:ARG:HD2 | 5:Z8:31:TRP:NE1 | 2.16 | 0.58 |
| 12:J9:202:CYC:HBA1 | 11:a9:512:TYR:N | 2.18 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:W9:62:LYS:HG2 | 2:W9:129:GLU:HG2 | 1.85 | 0.58 |
| 2:G1:111:ALA:HB2 | 3:L1:77:ARG:HE | 1.69 | 0.58 |
| 11:aA:56:ILE:CD1 | 11:aA:612:TYR:CZ | 2.87 | 0.58 |
| 11:aA:288:ARG:O | 11:aA:288:ARG:HG2 | 2.02 | 0.58 |
| 11:aA:353:ALA:O | 11:aA:356:ALA:HB2 | 2.02 | 0.58 |
| 11:aA:388:VAL:HG12 | 11:aA:392:ILE:HD12 | 1.84 | 0.58 |
| 12:U1:201:CYC:HMA2 | 12:U1:201:CYC:HB | 1.67 | 0.58 |
| 2:KA:62:LYS:HG2 | 2:KA:129:GLU:HG2 | 1.86 | 0.58 |
| 3:LA:113:LEU:O | 3:LA:113:LEU:HD12 | 2.03 | 0.58 |
| 5:NA:54:LEU:HD21 | 3:TA:84:ARG:NE | 2.14 | 0.58 |
| 12:YA:201:CYC:HB | 12:YA:201:CYC:CMA | 2.16 | 0.58 |
| 3:R1:111:ASN:ND2 | 5:N1:66:ARG:HH11 | 1.96 | 0.58 |
| 2:A1:56:VAL:HG22 | 2:A1:82:CYS:SG | 2.44 | 0.58 |
| 2:G3:62:LYS:HG2 | 2:G3:129:GLU:HG2 | 1.85 | 0.58 |
| 3:H2:127:VAL:HG22 | 12:H2:201:CYC:H3C | 1.86 | 0.58 |
| 12:H2:201:CYC:HBB2 | 6:M2:243:ALA:CA | 2.34 | 0.58 |
| 7:N2:1:MET:HE2 | 7:N2:1:MET:N | 2.18 | 0.58 |
| 4:M3:134:ASN:N | 12:P3:201:CYC:HBA2 | 2.17 | 0.58 |
| 12:S3:201:CYC:HB | 12:S3:201:CYC:HMA2 | 1.67 | 0.58 |
| 2:E4:62:LYS:HG2 | 2:E4:129:GLU:HG2 | 1.85 | 0.58 |
| 3:H4:84:ARG:HD2 | 11:aA:131:TYR:CD1 | 2.34 | 0.58 |
| 3:O4:127:VAL:HG22 | 12:O4:201:CYC:H3C | 1.85 | 0.58 |
| 8:A5:114:GLU:CB | 1:F5:79:ALA:HB1 | 2.34 | 0.58 |
| 8:G5:61:ILE:CG1 | 8:o7:68:PRO:CD | 2.53 | 0.58 |
| 8:G5:121:THR:CG2 | 12:G5:201:CYC:CHD | 2.80 | 0.58 |
| 1:T5:53:LYS:HZ3 | 8:U5:120:GLN:CG | 2.15 | 0.58 |
| 8:W5:104:ILE:CG2 | 8:W5:156:LEU:HD21 | 2.33 | 0.58 |
| 10:j5:820:HIS:C | 10:j5:820:HIS:CD2 | 2.80 | 0.58 |
| 10:j5:1067:LEU:HD12 | 10:j5:1101:GLU:OE1 | 2.02 | 0.58 |
| 10:k5:1069:ARG:HD3 | 10:k5:1115:ARG:HH11 | 1.69 | 0.58 |
| 12:C6:201:CYC:CMA | 12:C6:201:CYC:HB | 2.17 | 0.58 |
| 8:Q7:126:VAL:HG23 | 12:Q7:201:CYC:CMC | 2.33 | 0.58 |
| 8:I7:6:LYS:HZ3 | 8:W7:22:GLU:N | 2.02 | 0.58 |
| 8:M7:54:ALA:HA | 8:M7:132:ALA:HB1 | 1.84 | 0.58 |
| 8:M7:101:VAL:O | 8:M7:102:THR:C | 2.45 | 0.58 |
| 8:g7:29:PHE:CZ | 8:g7:98:ALA:C | 2.76 | 0.58 |
| 8:W7:126:VAL:HG23 | 12:W7:201:CYC:CMC | 2.33 | 0.58 |
| 8:c7:12:ASP:CB | 1:d7:94:TYR:CE2 | 2.85 | 0.58 |
| 3:B8:82:CYS:HA | 12:B8:202:CYC:H2C | 1.84 | 0.58 |
| 3:B8:82:CYS:O | 12:B8:202:CYC:H2C | 2.03 | 0.58 |
| 3:W8:127:VAL:HG22 | 12:W8:201:CYC:H3C | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:I8:201:CYC:HB | 12:I8:201:CYC:HMA2 | 1.67 | 0.58 |
| 4:M8:96:LYS:HE3 | 3:Q8:89:ILE:CG1 | 2.33 | 0.58 |
| 4:M8:251:ASN:H | 4:M8:251:ASN:ND2 | 1.95 | 0.58 |
| 2:N8:56:VAL:HG22 | 2:N8:82:CYS:SG | 2.44 | 0.58 |
| 12:O8:201:CYC:CGA | 5:Z8:50:LEU:CD1 | 2.81 | 0.58 |
| 4:M9:35:THR:HB | 3:B9:84:ARG:CZ | 2.33 | 0.58 |
| 12:Q9:201:CYC:HB | 12:Q9:201:CYC:CMA | 2.16 | 0.58 |
| 3:B9:14:LEU:HD13 | 3:X9:125:ARG:HD2 | 1.85 | 0.58 |
| 3:B9:27:LEU:CA | 3:B9:30:LEU:HD13 | 2.33 | 0.58 |
| 12:E9:201:CYC:HB | 12:E9:201:CYC:HMA2 | 1.67 | 0.58 |
| 12:U9:201:CYC:HB | 12:U9:201:CYC:HMA2 | 1.67 | 0.58 |
| 3:X9:127:VAL:HG22 | 12:X9:201:CYC:H3C | 1.86 | 0.58 |
| 11:a9:93:LEU:HD21 | 11:a9:252:ARG:HH12 | 1.65 | 0.58 |
| 11:a9:245:ALA:CB | 12:a9:901:CYC:OB | 2.50 | 0.58 |
| 11:a9:296:VAL:HG13 | 11:a9:298:ILE:H | 1.68 | 0.58 |
| 11:aA:621:THR:CG2 | 3:J1:14:LEU:HD11 | 2.26 | 0.58 |
| 2:I1:62:LYS:HG2 | 2:I1:129:GLU:HG2 | 1.86 | 0.58 |
| 4:M1:230:GLN:O | 4:M1:230:GLN:HG2 | 2.03 | 0.58 |
| 12:W1:201:CYC:HB | 12:W1:201:CYC:CMA | 2.17 | 0.58 |
| 12:E2:201:CYC:HMA2 | 12:E2:201:CYC:HB | 1.67 | 0.58 |
| 1:Z:76:ARG:N | 10:j5:261:ILE:HD11 | 2.19 | 0.58 |
| 1:Z:131:GLN:HG3 | 1:X5:17:LYS:HZ1 | 0.76 | 0.58 |
| 12:IA:201:CYC:HB | 12:IA:201:CYC:CMA | 2.17 | 0.58 |
| 12:JA:202:CYC:HBA1 | 11:aA:512:TYR:N | 2.19 | 0.58 |
| 4:MA:159:CYS:O | 3:VA:107:ASP:HB3 | 2.04 | 0.58 |
| 2:QA:116:VAL:CG2 | 3:TA:80:ALA:CA | 2.81 | 0.58 |
| 3:TA:24:LEU:HB3 | 2:X4:68:GLN:CG | 2.32 | 0.58 |
| 2:O1:56:VAL:HG22 | 2:O1:82:CYS:SG | 2.44 | 0.58 |
| 12:S1:201:CYC:HB | 12:S1:201:CYC:HMA2 | 1.67 | 0.58 |
| 3:D3:127:VAL:HG22 | 12:D3:202:CYC:H3C | 1.86 | 0.58 |
| 12:F3:201:CYC:HBA1 | 4:M3:36:TYR:H | 1.67 | 0.58 |
| 3:D4:14:LEU:CD1 | 3:Y4:125:ARG:NE | 2.57 | 0.58 |
| 3:L3:104:VAL:CG1 | 3:L3:108:ARG:NH2 | 2.62 | 0.58 |
| 4:M3:210:ILE:CD1 | 5:N3:59:ARG:NH1 | 2.66 | 0.58 |
| 5:N3:4:LEU:O | 3:P3:112:GLY:HA3 | 2.02 | 0.58 |
| 3:V3:127:VAL:HG22 | 12:V3:201:CYC:H3C | 1.86 | 0.58 |
| 12:H4:201:CYC:OB | 11:aA:129:ASN:CB | 2.51 | 0.58 |
| 4:M4:101:ASP:CA | 2:P4:13:ASP:CG | 2.75 | 0.58 |
| 4:M4:226:SER:CB | 3:Y4:85:ASP:HA | 2.33 | 0.58 |
| 8:A5:104:ILE:CG2 | 8:A5:156:LEU:HD21 | 2.32 | 0.58 |
| 8:G5:61:ILE:HG23 | 8:o7:68:PRO:HG2 | 1.83 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:G5:122:PRO:HG2 | 12:G5:201:CYC:CMC | 2.27 | 0.58 |
| 8:I5:29:PHE:CZ | 8:I5:98:ALA:C | 2.76 | 0.58 |
| 8:U5:79:ALA:HB1 | 6:M6:32:MET:N | 2.19 | 0.58 |
| 10:j5:778:LYS:NZ | 12:L7:201:CYC:OB | 2.36 | 0.58 |
| 10:j5:822:ARG:CD | 1:H7:106:GLU:OE2 | 2.51 | 0.58 |
| 10:j5:1064:LYS:HD2 | 10:j5:1065:HIS:CG | 2.39 | 0.58 |
| 10:j5:1153:VAL:HG21 | 1:v7:125:ALA:CA | 2.32 | 0.58 |
| 10:k5:247:ARG:HG2 | 10:k5:247:ARG:O | 2.04 | 0.58 |
| 10:k5:750:ARG:HH11 | 10:k5:750:ARG:HG2 | 1.67 | 0.58 |
| 10:k5:1146:THR:N | 1:p7:77:ARG:HH22 | 2.00 | 0.58 |
| 2:A6:63:PHE:CB | 2:A6:66:LEU:CG | 2.82 | 0.58 |
| 3:H6:127:VAL:HG22 | 12:H6:201:CYC:H3C | 1.86 | 0.58 |
| 3:D1:68:ARG:HH12 | 3:X1:68:ARG:CZ | 2.17 | 0.58 |
| 8:O7:161:GLN:HG2 | 1:F7:49:THR:CG2 | 2.33 | 0.58 |
| 8:Q7:13:ALA:HA | 9:z7:46:LYS:HD3 | 1.85 | 0.58 |
| 1:T7:68:PRO:CB | 1:V7:14:VAL:C | 2.67 | 0.58 |
| 8:U7:44:THR:HG23 | 1:V7:18:TYR:CD2 | 2.39 | 0.58 |
| 8:a7:52:LYS:CD | 11:a9:321:ALA:HB2 | 2.24 | 0.58 |
| 2:C8:15:GLN:HG2 | 11:a9:102:GLN:HE21 | 1.68 | 0.58 |
| 1:r7:17:LYS:HZ1 | 11:aA:41:ASP:CG | 1.96 | 0.58 |
| 2:K8:62:LYS:HG2 | 2:K8:129:GLU:HG2 | 1.86 | 0.58 |
| 3:L8:69:PRO:O | 11:a9:82:GLN:CG | 2.50 | 0.58 |
| 2:N8:13:ASP:OD2 | 3:O8:108:ARG:CZ | 2.46 | 0.58 |
| 2:N8:112:GLY:CA | 5:Z8:33:GLY:CA | 2.77 | 0.58 |
| 4:M9:120:LEU:O | 4:M9:123:GLU:HB2 | 2.04 | 0.58 |
| 12:O9:201:CYC:HMA2 | 12:O9:201:CYC:HB | 1.67 | 0.58 |
| 12:C9:201:CYC:HB | 12:C9:201:CYC:CMA | 2.17 | 0.58 |
| 3:F9:127:VAL:HG22 | 12:F9:301:CYC:H3C | 1.85 | 0.58 |
| 3:H9:78:ARG:CG | 12:H9:202:CYC:HAD1 | 2.32 | 0.58 |
| 3:H9:120:LEU:CD1 | 12:H9:202:CYC:C1A | 2.78 | 0.58 |
| 11:aA:312:ASP:HB2 | 11:aA:315:LEU:HB3 | 0.72 | 0.58 |
| 11:aA:508:ARG:HB2 | 11:aA:513:GLN:HE22 | 1.68 | 0.58 |
| 11:aA:623:ASP:HB2 | 3:H1:78:ARG:NH1 | 2.18 | 0.58 |
| 12:aA:902:CYC:H3C | 3:L1:127:VAL:HG22 | 1.85 | 0.58 |
| 2:C2:62:LYS:HG2 | 2:C2:129:GLU:HG2 | 1.86 | 0.58 |
| 2:E2:62:LYS:HG2 | 2:E2:129:GLU:HG2 | 1.86 | 0.58 |
| 3:BA:27:LEU:HD23 | 3:BA:30:LEU:HD22 | 1.84 | 0.58 |
| 3:DA:127:VAL:HG22 | 12:DA:201:CYC:H3C | 1.86 | 0.58 |
| 12:HA:202:CYC:OB | 11:aA:448:ASN:OD1 | 2.22 | 0.58 |
| 3:LA:111:ASN:OD1 | 11:aA:366:LEU:HD12 | 2.04 | 0.58 |
| 4:MA:196:TYR:H | 2:UA:15:GLN:HA | 1.68 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:OA:56:VAL:HG22 | 2:OA:82:CYS:SG | 2.44 | 0.58 |
| 2:QA:68:GLN:O | 2:QA:74:TYR:HB3 | 2.03 | 0.58 |
| 12:QA:201:CYC:HB | 12:QA:201:CYC:CMA | 2.16 | 0.58 |
| 2:SA:42:ARG:NH1 | 3:TA:21:GLU:CD | 2.59 | 0.58 |
| 12:SA:201:CYC:HB | 12:SA:201:CYC:CMA | 2.17 | 0.58 |
| 3:XA:127:VAL:HG22 | 12:XA:201:CYC:H3C | 1.86 | 0.58 |
| 3:P1:127:VAL:HG22 | 12:P1:201:CYC:H3C | 1.86 | 0.58 |
| 12:Q1:201:CYC:HB | 12:Q1:201:CYC:CMA | 2.17 | 0.58 |
| 2:G2:62:LYS:HG2 | 2:G2:129:GLU:HG2 | 1.85 | 0.58 |
| 12:C4:201:CYC:HB | 12:C4:201:CYC:CMA | 2.17 | 0.58 |
| 3:D4:127:VAL:HG22 | 12:D4:202:CYC:H3C | 1.86 | 0.58 |
| 3:L3:75:PRO:CG | 11:a9:823:ILE:CD1 | 2.81 | 0.58 |
| 4:M3:120:LEU:O | 4:M3:123:GLU:CB | 2.51 | 0.58 |
| 3:U4:127:VAL:HG22 | 12:U4:201:CYC:H3C | 1.86 | 0.58 |
| 12:G4:201:CYC:HB | 12:G4:201:CYC:CMA | 2.17 | 0.58 |
| 12:K4:201:CYC:HB | 12:K4:201:CYC:CMA | 2.16 | 0.58 |
| 3:L4:127:VAL:HG22 | 12:L4:202:CYC:H3C | 1.86 | 0.58 |
| 4:M4:96:LYS:HZ3 | 4:M4:96:LYS:HB3 | 1.69 | 0.58 |
| 2:N4:56:VAL:HG22 | 2:N4:82:CYS:SG | 2.44 | 0.58 |
| 8:C5:98:ALA:HA | 1:D5:5:ILE:CG2 | 2.33 | 0.58 |
| 1:Z5:62:TYR:HE1 | 12:a5:201:CYC:O1D | 1.86 | 0.58 |
| 10:j5:156:SER:OG | 12:j5:1201:CYC:HHD | 2.03 | 0.58 |
| 10:j5:974:LEU:HD21 | 1:v7:1:MET:H3 | 1.62 | 0.58 |
| 10:k5:344:ARG:NH1 | 10:k5:344:ARG:HG2 | 2.17 | 0.58 |
| 12:A6:201:CYC:HB | 12:A6:201:CYC:CMA | 2.17 | 0.58 |
| 8:O7:22:GLU:HA | 8:O7:25:ARG:HG2 | 1.85 | 0.58 |
| 8:O7:25:ARG:NH2 | 8:E7:25:ARG:CD | 2.66 | 0.58 |
| 8:c7:96:ILE:HD11 | 8:c7:152:TYR:HB2 | 1.85 | 0.58 |
| 8:e7:104:ILE:CG2 | 8:e7:156:LEU:HD21 | 2.32 | 0.58 |
| 2:E1:62:LYS:HG2 | 2:E1:129:GLU:HG2 | 1.85 | 0.58 |
| 3:B8:120:LEU:HD13 | 4:M8:53:LEU:HB2 | 1.76 | 0.58 |
| 12:E8:201:CYC:HB | 12:E8:201:CYC:CMA | 2.17 | 0.58 |
| 8:m7:44:THR:HG23 | 1:n7:18:TYR:CD2 | 2.39 | 0.58 |
| 8:o7:17:TYR:CE2 | 1:p7:93:THR:CG2 | 2.86 | 0.58 |
| 12:H8:201:CYC:OB | 11:a9:129:ASN:CB | 2.51 | 0.58 |
| 12:K8:201:CYC:HB | 12:K8:201:CYC:CMA | 2.16 | 0.58 |
| 4:M8:120:LEU:O | 4:M8:123:GLU:CB | 2.51 | 0.58 |
| 12:M8:302:CYC:C2C | 3:S8:78:ARG:HG2 | 2.32 | 0.58 |
| 4:M9:38:PRO:HD3 | 12:B9:201:CYC:CBB | 2.34 | 0.58 |
| 4:M9:76:ALA:HB1 | 3:D9:112:GLY:CA | 2.31 | 0.58 |
| 4:M9:192:GLN:CG | 3:V9:84:ARG:HG3 | 2.29 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 4:M9:274:VAL:CG2 | 3:V9:77:ARG:HG2 | 2.33 | 0.58 |
| 3:Y8:87:GLU:HG2 | 3:Y8:91:ARG:NE | 2.18 | 0.58 |
| 5:Z8:37:HIS:CE1 | 12:Z8:301:CYC:HMA1 | 2.38 | 0.58 |
| 3:F9:153:CYS:CB | 12:F9:303:CYC:C4C | 2.81 | 0.58 |
| 11:a9:245:ALA:CB | 12:a9:901:CYC:HBB2 | 2.32 | 0.58 |
| 4:M1:19:MET:HG2 | 4:M1:59:ILE:HD13 | 1.86 | 0.58 |
| 4:M1:120:LEU:O | 4:M1:123:GLU:HB2 | 2.04 | 0.58 |
| 3:BA:127:VAL:HG22 | 12:BA:201:CYC:H3C | 1.86 | 0.58 |
| 3:LA:37:ARG:HD3 | 3:LA:98:LEU:HA | 1.84 | 0.58 |
| 3:RA:127:VAL:HG22 | 12:RA:201:CYC:H3C | 1.86 | 0.58 |
| 3:H3:127:VAL:HG22 | 12:H3:202:CYC:H3C | 1.85 | 0.58 |
| 12:I2:201:CYC:HB | 12:I2:201:CYC:CMA | 2.17 | 0.58 |
| 3:J2:84:ARG:HG3 | 6:M2:189:HIS:CG | 2.39 | 0.58 |
| 3:L2:127:VAL:HG22 | 12:L2:201:CYC:H3C | 1.86 | 0.58 |
| 3:B4:120:LEU:CD2 | 4:M4:52:LEU:CB | 2.69 | 0.58 |
| 3:L3:1:MET:CE | 11:a9:708:HIS:ND1 | 2.67 | 0.58 |
| 2:T4:62:LYS:HG2 | 2:T4:129:GLU:HG2 | 1.86 | 0.58 |
| 12:V4:201:CYC:HB | 12:V4:201:CYC:CMA | 2.17 | 0.58 |
| 3:H4:127:VAL:HG22 | 12:H4:201:CYC:H3C | 1.86 | 0.58 |
| 12:J4:201:CYC:CMA | 11:aA:176:ASN:ND2 | 2.56 | 0.58 |
| 3:L4:68:ARG:HB2 | 11:aA:82:GLN:CA | 2.32 | 0.58 |
| 4:M4:138:SER:CB | 12:Z4:301:CYC:CAB | 2.82 | 0.58 |
| 2:N4:63:PHE:CB | 2:N4:66:LEU:CG | 2.82 | 0.58 |
| 5:Z4:28:HIS:HB2 | 5:Z4:35:ASP:HA | 1.84 | 0.58 |
| 8:W5:126:VAL:CG2 | 12:W5:201:CYC:HMC3 | 2.34 | 0.58 |
| 8:Y5:104:ILE:CG2 | 8:Y5:156:LEU:HD21 | 2.32 | 0.58 |
| 3:J6:127:VAL:HG22 | 12:J6:202:CYC:H3C | 1.86 | 0.58 |
| 3:L6:127:VAL:HG22 | 12:L6:201:CYC:H3C | 1.86 | 0.58 |
| 10:k5:194:CYS:CB | 12:k5:1201:CYC:HAC1 | 2.32 | 0.58 |
| 10:k5:217:GLU:HA | 10:k5:217:GLU:OE1 | 2.02 | 0.58 |
| 10:k5:283:ARG:HD3 | 10:k5:283:ARG:C | 2.27 | 0.58 |
| 10:k5:724:GLU:HA | 10:k5:727:THR:HG23 | 1.85 | 0.58 |
| 1:B7:136:VAL:CA | 11:a9:563:PHE:CZ | 2.87 | 0.58 |
| 8:i7:96:ILE:CG1 | 8:i7:152:TYR:CE1 | 2.82 | 0.58 |
| 8:k7:66:VAL:HG12 | 11:a9:65:LEU:HD22 | 1.84 | 0.58 |
| 1:T7:110:ASN:HD21 | 9:w7:57:PHE:CA | 2.15 | 0.58 |
| 8:U7:37:LEU:HD11 | 1:V7:31:PHE:CE2 | 2.39 | 0.58 |
| 8:c7:49:ARG:NH2 | 8:c7:140:LEU:CD2 | 2.67 | 0.58 |
| 8:q7:79:ALA:CA | 11:aA:53:VAL:HG21 | 2.34 | 0.58 |
| 8:s7:37:LEU:HD11 | 1:t7:31:PHE:CE2 | 2.38 | 0.58 |
| 2:A9:63:PHE:CB | 2:A9:66:LEU:CG | 2.82 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:E9:33:ARG:CG | 2:I9:25:GLN:HE22 | 2.16 | 0.58 |
| 3:V1:127:VAL:HG22 | 12:V1:201:CYC:H3C | 1.86 | 0.58 |
| 1:Z:131:GLN:CB | 1:X5:17:LYS:HZ3 | 2.08 | 0.58 |
| 12:EA:201:CYC:HMA2 | 12:EA:201:CYC:HB | 1.67 | 0.58 |
| 12:O1:201:CYC:HBB3 | 3:R1:74:TYR:HE1 | 1.65 | 0.58 |
| 12:I3:201:CYC:HB | 12:I3:201:CYC:CMA | 2.17 | 0.58 |
| 12:I3:201:CYC:HB | 12:I3:201:CYC:HMA2 | 1.67 | 0.58 |
| 3:J2:127:VAL:HG22 | 12:J2:202:CYC:H3C | 1.86 | 0.58 |
| 2:K2:62:LYS:HG2 | 2:K2:129:GLU:HG2 | 1.86 | 0.58 |
| 2:E3:114:ARG:NH1 | 11:a9:671:GLU:CD | 2.62 | 0.58 |
| 3:L3:112:GLY:O | 11:a9:809:ARG:NH2 | 2.37 | 0.58 |
| 4:M3:120:LEU:O | 4:M3:123:GLU:HB2 | 2.04 | 0.58 |
| 2:O3:63:PHE:CB | 2:O3:66:LEU:CG | 2.82 | 0.58 |
| 3:X3:127:VAL:HG22 | 12:X3:201:CYC:H3C | 1.85 | 0.58 |
| 3:S4:72:ASN:HD22 | 3:S4:123:PRO:HD3 | 0.66 | 0.58 |
| 3:F4:107:ASP:OD2 | 4:M4:9:GLN:HA | 2.04 | 0.58 |
| 3:F4:112:GLY:HA3 | 4:M4:4:LEU:HD12 | 1.86 | 0.58 |
| 12:I4:201:CYC:HMA2 | 12:I4:201:CYC:HB | 1.67 | 0.58 |
| 4:M4:201:ASP:CG | 5:Z4:59:ARG:HD2 | 2.28 | 0.58 |
| 12:R4:201:CYC:HB | 12:R4:201:CYC:CMA | 2.17 | 0.58 |
| 8:K5:80:LEU:HD12 | 12:K5:201:CYC:HAD1 | 1.82 | 0.58 |
| 8:M5:90:ARG:CA | 1:N5:18:TYR:CZ | 2.87 | 0.58 |
| 8:A5:112:VAL:HA | 1:F5:75:THR:CB | 2.28 | 0.58 |
| 1:d5:127:VAL:CB | 10:j5:698:GLY:CA | 2.81 | 0.58 |
| 8:Q5:17:TYR:HD2 | 1:R5:93:THR:CG2 | 2.12 | 0.58 |
| 8:Q5:126:VAL:HG23 | 12:Q5:201:CYC:CMC | 2.33 | 0.58 |
| 7:N6:22:GLN:OE1 | 7:N6:39:TYR:CE2 | 2.57 | 0.58 |
| 9:z5:56:LEU:H | 9:z5:56:LEU:CD1 | 2.15 | 0.58 |
| 10:j5:252:ASP:OD1 | 10:j5:252:ASP:N | 2.26 | 0.58 |
| 10:j5:390:GLN:HA | 10:j5:390:GLN:OE1 | 2.02 | 0.58 |
| 10:j5:911:LEU:O | 10:j5:913:VAL:N | 2.33 | 0.58 |
| 10:j5:986:PRO:HD3 | 9:y7:24:GLN:NE2 | 2.19 | 0.58 |
| 10:k5:138:PRO:CB | 10:k5:201:VAL:CG1 | 2.52 | 0.58 |
| 10:k5:778:LYS:CE | 12:F7:201:CYC:CBB | 2.82 | 0.58 |
| 10:k5:978:LEU:HD11 | 1:p7:107:ARG:CZ | 2.33 | 0.58 |
| 1:P7:53:LYS:HZ1 | 8:Q7:120:GLN:CD | 2.11 | 0.58 |
| 8:E7:101:VAL:O | 8:E7:102:THR:C | 2.45 | 0.58 |
| 8:I7:101:VAL:HG21 | 8:W7:20:PRO:HG2 | 1.85 | 0.58 |
| 8:K7:104:ILE:CG2 | 8:K7:156:LEU:HD21 | 2.32 | 0.58 |
| 8:i7:96:ILE:HD11 | 8:i7:152:TYR:HB2 | 1.86 | 0.58 |
| 8:i7:122:PRO:O | 8:i7:125:ALA:N | 2.36 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:W7:13:ALA:C | 9:w7:46:LYS:HZ2 | 2.10 | 0.58 |
| 12:E1:201:CYC:HMA2 | 12:E1:201:CYC:HB | 1.67 | 0.58 |
| 12:B8:202:CYC:C4D | 4:M8:53:LEU:HG | 2.34 | 0.58 |
| 12:C8:201:CYC:HB | 12:C8:201:CYC:CMA | 2.17 | 0.58 |
| 4:M8:235:PHE:CD2 | 12:M8:301:CYC:C4A | 2.87 | 0.58 |
| 3:Q8:92:TYR:HE1 | 3:Q8:105:LEU:HD13 | 1.67 | 0.58 |
| 3:Q8:117:TYR:HA | 3:Q8:120:LEU:HG | 1.86 | 0.58 |
| 4:M9:134:ASN:OD1 | 3:R9:116:THR:HG23 | 2.03 | 0.58 |
| 5:N9:62:ARG:HE | 2:S9:14:SER:HA | 1.66 | 0.58 |
| 2:Q9:62:LYS:HG2 | 2:Q9:129:GLU:HG2 | 1.85 | 0.58 |
| 12:A9:201:CYC:HB | 12:A9:201:CYC:CMA | 2.17 | 0.58 |
| 2:I9:62:LYS:HG2 | 2:I9:129:GLU:HG2 | 1.85 | 0.58 |
| 3:T9:127:VAL:HG22 | 12:T9:301:CYC:H3C | 1.85 | 0.58 |
| 3:Z9:127:VAL:HG22 | 12:Z9:202:CYC:H3C | 1.86 | 0.58 |
| 11:a9:95:ILE:HD12 | 11:a9:237:PHE:CD1 | 2.38 | 0.58 |
| 11:aA:72:ASP:HB3 | 11:aA:73:TYR:HA | 1.86 | 0.58 |
| 11:aA:426:ARG:CZ | 11:aA:496:ARG:HD3 | 2.33 | 0.58 |
| 3:T1:127:VAL:HG22 | 12:T1:301:CYC:H3C | 1.85 | 0.58 |
| 2:U1:62:LYS:HG2 | 2:U1:129:GLU:HG2 | 1.85 | 0.58 |
| 2:W1:62:LYS:HG2 | 2:W1:129:GLU:HG2 | 1.86 | 0.58 |
| 2:Y1:62:LYS:HG2 | 2:Y1:129:GLU:HG2 | 1.86 | 0.58 |
| 2:A2:56:VAL:HG22 | 2:A2:82:CYS:SG | 2.44 | 0.58 |
| 3:BA:84:ARG:NH1 | 4:MA:35:THR:HB | 2.18 | 0.58 |
| 3:FA:36:LYS:C | 3:FA:156:LEU:CD2 | 2.76 | 0.58 |
| 12:KA:201:CYC:HB | 12:KA:201:CYC:CMA | 2.17 | 0.58 |
| 4:MA:1:MET:HG3 | 4:MA:43:TYR:OH | 2.04 | 0.58 |
| 4:MA:159:CYS:C | 3:VA:108:ARG:CG | 2.77 | 0.58 |
| 4:MA:232:VAL:CG1 | 3:XA:111:ASN:C | 2.71 | 0.58 |
| 12:UA:201:CYC:HB | 12:UA:201:CYC:CMA | 2.17 | 0.58 |
| 2:A1:63:PHE:CB | 2:A1:66:LEU:CG | 2.82 | 0.58 |
| 2:I3:62:LYS:HG2 | 2:I3:129:GLU:HG2 | 1.86 | 0.58 |
| 12:K3:201:CYC:HB | 12:K3:201:CYC:CMA | 2.17 | 0.58 |
| 12:G2:201:CYC:HB | 12:G2:201:CYC:CMA | 2.16 | 0.58 |
| 3:R3:127:VAL:HG22 | 12:R3:201:CYC:H3C | 1.85 | 0.58 |
| 12:U3:201:CYC:HB | 12:U3:201:CYC:CMA | 2.17 | 0.58 |
| 2:Y3:62:LYS:HG2 | 2:Y3:129:GLU:HG2 | 1.86 | 0.58 |
| 12:E4:201:CYC:HB | 12:E4:201:CYC:CMA | 2.17 | 0.58 |
| 4:M4:120:LEU:O | 4:M4:123:GLU:CB | 2.51 | 0.58 |
| 4:M4:144:ARG:HH12 | 5:Z4:59:ARG:NH1 | 2.01 | 0.58 |
| 8:M5:68:PRO:CB | 8:e5:59:PHE:CB | 2.80 | 0.58 |
| 12:X4:201:CYC:HB | 12:X4:201:CYC:CMA | 2.17 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:E5:29:PHE:HE1 | 8:E5:99:GLY:HA3 | 1.68 | 0.58 |
| 8:G5:71:ASN:OD1 | 12:G5:201:CYC:HMD1 | 2.00 | 0.58 |
| 1:f5:118:SER:OG | 10:j5:491:THR:O | 2.22 | 0.58 |
| 8:S5:14:GLU:OE2 | 10:j5:538:PHE:CE2 | 2.56 | 0.58 |
| 8:U5:36:ARG:HD3 | 8:U5:96:ILE:O | 2.03 | 0.58 |
| 8:U5:80:LEU:HA | 8:U5:83:ARG:CZ | 2.34 | 0.58 |
| 2:K6:62:LYS:HG2 | 2:K6:129:GLU:HG2 | 1.86 | 0.58 |
| 6:M6:243:ALA:CA | 12:H6:201:CYC:HBB2 | 2.33 | 0.58 |
| 10:j5:217:GLU:OE1 | 10:j5:217:GLU:HA | 2.02 | 0.58 |
| 10:j5:1105:ILE:CD1 | 10:j5:1115:ARG:HH21 | 2.12 | 0.58 |
| 10:k5:187:ARG:CZ | 10:k5:196:ILE:HD13 | 2.33 | 0.58 |
| 10:k5:328:ILE:HG12 | 10:k5:328:ILE:O | 2.04 | 0.58 |
| 10:k5:619:GLU:CB | 10:k5:620:PRO:HD2 | 2.32 | 0.58 |
| 10:k5:741:GLN:CG | 1:D7:77:ARG:NH2 | 2.56 | 0.58 |
| 8:K7:25:ARG:CD | 8:U7:25:ARG:NH2 | 2.67 | 0.58 |
| 8:M7:60:GLN:HE22 | 3:J9:114:LYS:CD | 2.15 | 0.58 |
| 8:i7:89:LEU:HD13 | 8:i7:153:PHE:HZ | 1.67 | 0.58 |
| 8:W7:126:VAL:CG2 | 12:W7:201:CYC:HMC3 | 2.34 | 0.58 |
| 8:o7:17:TYR:CE2 | 1:p7:93:THR:HG21 | 2.35 | 0.58 |
| 3:L8:82:CYS:HB2 | 12:a9:901:CYC:NC | 2.18 | 0.58 |
| 4:M8:15:PHE:CD1 | 4:M8:71:PRO:HA | 2.38 | 0.58 |
| 12:P8:201:CYC:HB | 12:P8:201:CYC:CMA | 2.17 | 0.58 |
| 4:M9:6:THR:HG21 | 3:D9:108:ARG:O | 1.96 | 0.58 |
| 4:M9:19:MET:HG2 | 4:M9:59:ILE:HD13 | 1.86 | 0.58 |
| 4:M9:159:CYS:O | 3:V9:107:ASP:HB3 | 2.04 | 0.58 |
| 2:O9:63:PHE:CB | 2:O9:66:LEU:CG | 2.82 | 0.58 |
| 3:J9:2:GLN:HG2 | 3:J9:6:THR:HG22 | 1.86 | 0.58 |
| 12:Y9:201:CYC:HB | 12:Y9:201:CYC:CMA | 2.16 | 0.58 |
| 11:a9:288:ARG:HG2 | 11:a9:288:ARG:O | 2.02 | 0.58 |
| 11:aA:112:GLU:O | 11:aA:115:VAL:N | 2.36 | 0.58 |
| 3:H1:77:ARG:NH1 | 12:H1:201:CYC:O1D | 2.37 | 0.58 |
| 4:M1:103:GLN:HA | 4:M1:103:GLN:OE1 | 2.04 | 0.58 |
| 4:MA:274:VAL:CG2 | 2:WA:111:ALA:CB | 2.77 | 0.58 |
| 2:QA:18:PHE:CE1 | 3:RA:48:ALA:CB | 2.87 | 0.58 |
| 2:QA:62:LYS:HG2 | 2:QA:129:GLU:HG2 | 1.85 | 0.58 |
| 2:QA:68:GLN:C | 2:U1:46:SER:HB3 | 2.29 | 0.58 |
| 12:WA:201:CYC:HB | 12:WA:201:CYC:CMA | 2.17 | 0.58 |
| 3:H2:14:LEU:HD11 | 6:M2:69:ALA:HB2 | 1.86 | 0.58 |
| 3:L2:75:PRO:HG2 | 3:L2:78:ARG:CA | 2.34 | 0.58 |
| 12:C3:201:CYC:HB | 12:C3:201:CYC:CMA | 2.17 | 0.58 |
| 4:M3:19:MET:HG2 | 4:M3:59:ILE:HD13 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M3:181:GLN:O | 4:M3:181:GLN:HG3 | 2.03 | 0.58 |
| 3:P3:2:GLN:HG2 | 3:P3:6:THR:HG22 | 1.86 | 0.58 |
| 3:X3:2:GLN:HG2 | 3:X3:6:THR:HG22 | 1.86 | 0.58 |
| 3:F4:127:VAL:HG22 | 12:F4:202:CYC:H3C | 1.86 | 0.58 |
| 2:I4:62:LYS:HG2 | 2:I4:129:GLU:HG2 | 1.86 | 0.58 |
| 3:L4:71:GLY:HA2 | 11:aA:82:GLN:CG | 2.29 | 0.58 |
| 12:L4:202:CYC:C4B | 11:aA:239:TYR:CE1 | 2.87 | 0.58 |
| 4:M4:19:MET:HG2 | 4:M4:59:ILE:HD13 | 1.86 | 0.58 |
| 3:O4:2:GLN:HG2 | 3:O4:6:THR:HG22 | 1.86 | 0.58 |
| 8:K5:20:PRO:CB | 8:U5:151:PHE:HB3 | 2.29 | 0.58 |
| 5:Z4:26:LEU:HD21 | 5:Z4:63:ASN:HB2 | 1.77 | 0.58 |
| 12:C1:201:CYC:HB | 12:C1:201:CYC:CMA | 2.17 | 0.58 |
| 1:d5:83:ARG:CZ | 10:j5:379:PHE:HE2 | 2.14 | 0.58 |
| 1:f5:38:VAL:CG1 | 10:j5:40:VAL:HG13 | 2.09 | 0.58 |
| 8:Y5:54:ALA:HA | 8:Y5:132:ALA:HB1 | 1.84 | 0.58 |
| 12:L6:201:CYC:HBB2 | 6:M6:229:ALA:HB2 | 1.86 | 0.58 |
| 6:M6:50:LEU:HD23 | 8:c7:79:ALA:O | 1.93 | 0.58 |
| 6:M6:69:ALA:HB2 | 3:H6:14:LEU:HD11 | 1.86 | 0.58 |
| 9:i5:6:LYS:CG | 9:i5:55:LYS:CB | 2.64 | 0.58 |
| 10:k5:241:ALA:N | 10:k5:242:PRO:HD3 | 2.19 | 0.58 |
| 10:k5:878:GLU:HG3 | 9:z7:28:PHE:CE2 | 2.39 | 0.58 |
| 10:k5:1052:PRO:CA | 1:l7:106:GLU:HG2 | 2.34 | 0.58 |
| 10:k5:1064:LYS:HD2 | 10:k5:1065:HIS:CG | 2.39 | 0.58 |
| 12:E6:201:CYC:HB | 12:E6:201:CYC:CMA | 2.17 | 0.58 |
| 3:F6:2:GLN:HG2 | 3:F6:6:THR:HG22 | 1.86 | 0.58 |
| 3:D1:127:VAL:HG22 | 12:D1:202:CYC:H3C | 1.85 | 0.58 |
| 8:O7:36:ARG:HD3 | 8:O7:96:ILE:O | 2.02 | 0.58 |
| 8:O7:37:LEU:HD11 | 1:P7:31:PHE:CE2 | 2.39 | 0.58 |
| 8:C7:37:LEU:HD11 | 1:D7:31:PHE:CE2 | 2.39 | 0.58 |
| 8:C7:44:THR:HG23 | 1:D7:18:TYR:CD2 | 2.39 | 0.58 |
| 12:h7:201:CYC:HB | 12:h7:201:CYC:HMA2 | 1.69 | 0.58 |
| 8:i7:126:VAL:CG2 | 12:i7:201:CYC:HMC1 | 2.33 | 0.58 |
| 2:A8:56:VAL:HG22 | 2:A8:82:CYS:SG | 2.44 | 0.58 |
| 8:o7:23:LEU:HD13 | 1:p7:38:VAL:HG12 | 1.85 | 0.58 |
| 8:o7:29:PHE:HZ | 1:p7:31:PHE:HZ | 1.52 | 0.58 |
| 8:o7:37:LEU:HD22 | 1:p7:24:LEU:CB | 2.33 | 0.58 |
| 4:M8:140:ARG:O | 4:M8:144:ARG:N | 2.34 | 0.58 |
| 3:Q8:72:ASN:O | 12:Z8:301:CYC:HMD2 | 2.04 | 0.58 |
| 12:R8:201:CYC:HB | 12:R8:201:CYC:CMA | 2.17 | 0.58 |
| 12:O9:201:CYC:HB | 12:O9:201:CYC:CMA | 2.17 | 0.58 |
| 12:K9:201:CYC:HB | 12:K9:201:CYC:CMA | 2.17 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:S9:201:CYC:HB | 12:S9:201:CYC:CMA | 2.17 | 0.58 |
| 11:a9:365:LYS:HZ2 | 11:a9:365:LYS:CB | 2.16 | 0.58 |
| 11:aA:798:SER:C | 11:aA:800:THR:HG23 | 2.28 | 0.58 |
| 11:aA:823:ILE:HD13 | 3:L1:77:ARG:HD2 | 1.86 | 0.58 |
| 4:M1:15:PHE:CD1 | 4:M1:71:PRO:HA | 2.38 | 0.58 |
| 2:A2:63:PHE:CB | 2:A2:66:LEU:CG | 2.82 | 0.58 |
| 2:AA:56:VAL:HG22 | 2:AA:82:CYS:SG | 2.44 | 0.58 |
| 12:AA:201:CYC:HB | 12:AA:201:CYC:CMA | 2.17 | 0.58 |
| 3:LA:84:ARG:NE | 11:aA:406:LEU:HD23 | 2.18 | 0.58 |
| 4:MA:120:LEU:HD22 | 2:UA:115:GLU:OE2 | 2.04 | 0.58 |
| 4:MA:162:ASN:O | 4:MA:166:THR:CG2 | 2.50 | 0.58 |
| 3:PA:127:VAL:HG22 | 12:PA:201:CYC:H3C | 1.85 | 0.58 |
| 3:TA:127:VAL:HG22 | 12:TA:301:CYC:H3C | 1.86 | 0.58 |
| 3:ZA:127:VAL:HG22 | 12:ZA:202:CYC:H3C | 1.86 | 0.58 |
| 12:G2:201:CYC:HBB3 | 3:L2:74:TYR:CE1 | 2.39 | 0.58 |
| 7:N2:22:GLN:OE1 | 7:N2:39:TYR:CE2 | 2.57 | 0.58 |
| 12:N2:101:CYC:H3C | 3:B2:127:VAL:HG22 | 1.85 | 0.58 |
| 2:C3:62:LYS:HG2 | 2:C3:129:GLU:HG2 | 1.86 | 0.58 |
| 2:A4:56:VAL:HG22 | 2:A4:82:CYS:SG | 2.44 | 0.58 |
| 3:D4:116:THR:OG1 | 4:M4:38:PRO:CA | 2.52 | 0.58 |
| 3:L3:1:MET:CG | 3:L3:104:VAL:HG12 | 2.32 | 0.58 |
| 4:M3:251:ASN:H | 4:M3:251:ASN:ND2 | 1.95 | 0.58 |
| 12:O3:201:CYC:HB | 12:O3:201:CYC:CMA | 2.17 | 0.58 |
| 12:Q3:201:CYC:HB | 12:Q3:201:CYC:CMA | 2.17 | 0.58 |
| 12:Q3:201:CYC:HB | 12:Q3:201:CYC:HMA2 | 1.67 | 0.58 |
| 3:W4:2:GLN:HG2 | 3:W4:6:THR:HG22 | 1.86 | 0.58 |
| 3:J4:127:VAL:HG22 | 12:J4:201:CYC:H3C | 1.85 | 0.58 |
| 3:L4:68:ARG:HB3 | 3:L4:69:PRO:HD2 | 1.86 | 0.58 |
| 4:M4:214:GLY:CA | 5:Z4:28:HIS:CE1 | 2.87 | 0.58 |
| 3:Q4:120:LEU:HD11 | 5:Z4:39:PRO:HA | 1.86 | 0.58 |
| 3:Q4:120:LEU:CD1 | 5:Z4:39:PRO:CA | 2.81 | 0.58 |
| 8:C5:90:ARG:HD2 | 1:D5:17:LYS:O | 2.04 | 0.58 |
| 1:T5:107:ARG:NH1 | 10:j5:482:GLN:OE1 | 2.37 | 0.58 |
| 8:Y5:53:GLN:HB2 | 8:Y5:136:VAL:HG21 | 1.86 | 0.58 |
| 1:b5:30:TYR:CZ | 10:k5:47:PHE:CE2 | 2.92 | 0.58 |
| 9:z5:6:LYS:HZ3 | 9:z5:29:THR:CG2 | 2.17 | 0.58 |
| 10:j5:19:THR:HB | 10:j5:173:ALA:CB | 2.34 | 0.58 |
| 10:j5:1064:LYS:CE | 10:j5:1065:HIS:CD2 | 2.87 | 0.58 |
| 10:j5:1153:VAL:CG2 | 1:v7:125:ALA:HA | 2.34 | 0.58 |
| 10:k5:77:VAL:CG1 | 10:k5:141:GLU:HG2 | 2.34 | 0.58 |
| 10:k5:190:LEU:O | 10:k5:194:CYS:SG | 2.62 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:k5:937:GLU:HG3 | 10:k5:937:GLU:O | 2.00 | 0.58 |
| 10:k5:1064:LYS:CE | 10:k5:1065:HIS:CD2 | 2.87 | 0.58 |
| 12:C6:201:CYC:HB | 12:C6:201:CYC:HMA2 | 1.67 | 0.58 |
| 3:H6:2:GLN:HG2 | 3:H6:6:THR:HG22 | 1.86 | 0.58 |
| 8:O7:44:THR:HG23 | 1:P7:18:TYR:CD2 | 2.39 | 0.58 |
| 8:Q7:21:GLY:HA3 | 8:C7:6:LYS:NZ | 2.19 | 0.58 |
| 8:Q7:126:VAL:CG2 | 12:Q7:201:CYC:HMC3 | 2.34 | 0.58 |
| 8:k7:101:VAL:O | 8:k7:102:THR:C | 2.45 | 0.58 |
| 8:a7:161:GLN:OE1 | 1:p7:49:THR:HG22 | 2.04 | 0.58 |
| 8:e7:106:GLU:OE2 | 9:y7:68:GLY:C | 2.47 | 0.58 |
| 12:A8:201:CYC:HB | 12:A8:201:CYC:CMA | 2.17 | 0.58 |
| 3:H8:127:VAL:HG22 | 12:H8:201:CYC:H3C | 1.86 | 0.58 |
| 2:I8:112:GLY:H | 11:a9:133:LEU:CD2 | 2.16 | 0.58 |
| 4:M8:100:SER:N | 3:Q8:1:MET:HE2 | 2.17 | 0.58 |
| 3:Q8:89:ILE:CA | 3:Q8:92:TYR:CZ | 2.78 | 0.58 |
| 4:M9:120:LEU:HD22 | 2:U9:115:GLU:OE2 | 2.04 | 0.58 |
| 5:N9:57:MET:SD | 12:T9:301:CYC:HMA3 | 2.43 | 0.58 |
| 2:O9:56:VAL:HG22 | 2:O9:82:CYS:SG | 2.44 | 0.58 |
| 2:A9:56:VAL:HG22 | 2:A9:82:CYS:SG | 2.44 | 0.58 |
| 11:a9:56:ILE:CD1 | 11:a9:612:TYR:CZ | 2.87 | 0.58 |
| 5:N1:3:VAL:O | 5:N1:4:LEU:C | 2.44 | 0.58 |
| 5:N1:37:HIS:CD2 | 12:T1:301:CYC:HMA3 | 2.39 | 0.58 |
| 3:BA:30:LEU:HD12 | 3:BA:30:LEU:N | 2.19 | 0.57 |
| 12:CA:201:CYC:HB | 12:CA:201:CYC:CMA | 2.17 | 0.57 |
| 3:FA:36:LYS:CB | 3:FA:156:LEU:HD11 | 2.28 | 0.57 |
| 5:NA:13:SER:HB3 | 5:NA:14:LYS:HD3 | 1.86 | 0.57 |
| 3:TA:2:GLN:HG2 | 3:TA:6:THR:HG22 | 1.86 | 0.57 |
| 3:VA:2:GLN:HG2 | 3:VA:6:THR:HG22 | 1.87 | 0.57 |
| 3:J3:2:GLN:HG2 | 3:J3:6:THR:HG22 | 1.86 | 0.57 |
| 12:G2:201:CYC:HBB3 | 3:L2:74:TYR:CZ | 2.39 | 0.57 |
| 12:H2:201:CYC:CBB | 6:M2:243:ALA:HA | 2.33 | 0.57 |
| 7:N2:49:LEU:HD11 | 3:B2:88:ILE:CD1 | 2.34 | 0.57 |
| 3:Z3:127:VAL:HG22 | 12:Z3:201:CYC:H3C | 1.86 | 0.57 |
| 2:W3:62:LYS:HG2 | 2:W3:129:GLU:HG2 | 1.86 | 0.57 |
| 3:B1:84:ARG:HH22 | 12:B1:202:CYC:CGA | 2.16 | 0.57 |
| 12:B1:202:CYC:HAA1 | 11:aA:684:ASN:OD1 | 1.96 | 0.57 |
| 3:F4:2:GLN:HG2 | 3:F4:6:THR:HG22 | 1.86 | 0.57 |
| 4:M4:144:ARG:NH1 | 5:Z4:59:ARG:CZ | 2.67 | 0.57 |
| 2:N4:118:ARG:HH12 | 5:Z4:32:PRO:CG | 2.17 | 0.57 |
| 3:Y4:105:LEU:CD1 | 3:Y4:163:TYR:HB3 | 2.32 | 0.57 |
| 3:Y4:127:VAL:CG1 | 3:Y4:171:ILE:HG21 | 2.33 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 5:Z4:13:SER:HB3 | 5:Z4:14:LYS:HD3 | 1.86 | 0.57 |
| 8:C5:29:PHE:HE2 | 1:D5:5:ILE:HD11 | 1.69 | 0.57 |
| 8:e5:35:ARG:NE | 8:e5:145:ASP:OD1 | 2.33 | 0.57 |
| 6:M6:69:ALA:HB1 | 3:H6:10:VAL:CG1 | 2.29 | 0.57 |
| 7:N6:49:LEU:HD11 | 3:B6:88:ILE:CD1 | 2.34 | 0.57 |
| 9:i5:10:CYS:N | 9:i5:50:LYS:O | 2.32 | 0.57 |
| 10:j5:77:VAL:CG1 | 10:j5:141:GLU:HG2 | 2.34 | 0.57 |
| 10:j5:190:LEU:C | 10:j5:194:CYS:SG | 2.87 | 0.57 |
| 10:j5:277:ILE:C | 10:j5:284:PRO:HA | 2.27 | 0.57 |
| 10:j5:971:VAL:HG11 | 1:t7:76:ARG:NH1 | 1.89 | 0.57 |
| 10:j5:1025:LEU:HD21 | 10:j5:1035:PHE:HB2 | 0.58 | 0.57 |
| 10:j5:1150:TYR:CD1 | 11:aA:38:VAL:HG22 | 2.37 | 0.57 |
| 10:k5:357:LEU:CD2 | 10:k5:401:LEU:HD13 | 2.33 | 0.57 |
| 10:k5:1067:LEU:HD13 | 10:k5:1101:GLU:HG2 | 1.78 | 0.57 |
| 1:B7:136:VAL:CA | 11:a9:563:PHE:HZ | 2.17 | 0.57 |
| 8:g7:63:PRO:CG | 11:aA:336:ILE:HG23 | 2.33 | 0.57 |
| 8:g7:90:ARG:HB2 | 1:h7:18:TYR:CE1 | 2.38 | 0.57 |
| 2:A8:63:PHE:CB | 2:A8:66:LEU:CG | 2.82 | 0.57 |
| 3:F8:2:GLN:HG2 | 3:F8:6:THR:HG22 | 1.86 | 0.57 |
| 4:M8:148:LYS:HD2 | 4:M8:197:ASP:OD1 | 2.04 | 0.57 |
| 12:M8:302:CYC:CBC | 3:S8:81:ALA:HB3 | 2.34 | 0.57 |
| 3:Q8:78:ARG:NH1 | 12:Z8:301:CYC:HAD1 | 2.17 | 0.57 |
| 3:Q8:89:ILE:CB | 3:Q8:92:TYR:OH | 2.49 | 0.57 |
| 4:M9:20:THR:CG2 | 4:M9:67:LEU:HD11 | 2.34 | 0.57 |
| 4:M9:185:ALA:HB2 | 12:V9:201:CYC:O1A | 2.04 | 0.57 |
| 3:B9:2:GLN:HG2 | 3:B9:6:THR:HG22 | 1.86 | 0.57 |
| 11:a9:426:ARG:HE | 11:a9:496:ARG:HD3 | 1.68 | 0.57 |
| 11:a9:816:LEU:O | 11:a9:816:LEU:HD23 | 2.04 | 0.57 |
| 12:A2:201:CYC:HB | 12:A2:201:CYC:CMA | 2.17 | 0.57 |
| 2:GA:62:LYS:HG2 | 2:GA:129:GLU:HG2 | 1.85 | 0.57 |
| 12:GA:201:CYC:HB | 12:GA:201:CYC:CMA | 2.17 | 0.57 |
| 3:HA:84:ARG:CA | 11:aA:478:HIS:CE1 | 2.87 | 0.57 |
| 3:HA:120:LEU:CD1 | 12:HA:202:CYC:C1A | 2.82 | 0.57 |
| 3:JA:127:VAL:HG22 | 12:JA:202:CYC:H3C | 1.85 | 0.57 |
| 12:LA:202:CYC:CGD | 11:aA:538:ARG:HB3 | 2.34 | 0.57 |
| 4:MA:120:LEU:O | 4:MA:123:GLU:HB2 | 2.04 | 0.57 |
| 4:MA:260:ARG:HH11 | 4:MA:260:ARG:CG | 2.18 | 0.57 |
| 3:TA:24:LEU:CD2 | 2:X4:68:GLN:NE2 | 2.67 | 0.57 |
| 2:G3:111:ALA:HB2 | 3:L3:77:ARG:HE | 1.69 | 0.57 |
| 2:A3:56:VAL:HG22 | 2:A3:82:CYS:SG | 2.44 | 0.57 |
| 2:A3:63:PHE:CB | 2:A3:66:LEU:CG | 2.82 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 12:A3:201:CYC:HB | 12:A3:201:CYC:CMA | 2.17 | 0.57 |
| 3:F3:127:VAL:HG22 | 12:F3:201:CYC:H3C | 1.86 | 0.57 |
| 3:B4:2:GLN:HG2 | 3:B4:6:THR:HG22 | 1.86 | 0.57 |
| 12:B4:202:CYC:C4D | 4:M4:53:LEU:HG | 2.34 | 0.57 |
| 4:M3:15:PHE:CD1 | 4:M3:71:PRO:HA | 2.38 | 0.57 |
| 4:M3:20:THR:CG2 | 4:M3:67:LEU:HD11 | 2.34 | 0.57 |
| 5:N3:3:VAL:O | 5:N3:4:LEU:C | 2.44 | 0.57 |
| 3:B1:88:ILE:HG22 | 12:B1:202:CYC:CMB | 2.18 | 0.57 |
| 12:T4:201:CYC:HB | 12:T4:201:CYC:CMA | 2.17 | 0.57 |
| 4:M4:144:ARG:NH2 | 4:M4:204:ILE:HG22 | 2.17 | 0.57 |
| 12:P4:201:CYC:HB | 12:P4:201:CYC:CMA | 2.17 | 0.57 |
| 5:Z4:29:HIS:NE2 | 5:Z4:37:HIS:C | 2.61 | 0.57 |
| 8:A5:94:TYR:OH | 1:B5:17:LYS:O | 2.20 | 0.57 |
| 1:B5:14:VAL:HG13 | 10:k5:556:GLY:H | 1.69 | 0.57 |
| 1:J5:76:ARG:HH12 | 9:i5:67:VAL:CB | 2.18 | 0.57 |
| 2:C1:62:LYS:HG2 | 2:C1:129:GLU:HG2 | 1.86 | 0.57 |
| 1:P5:110:ASN:OD1 | 10:k5:490:SER:OG | 2.21 | 0.57 |
| 8:S5:53:GLN:HB2 | 8:S5:136:VAL:HG21 | 1.86 | 0.57 |
| 8:a5:36:ARG:HD3 | 8:a5:96:ILE:O | 2.02 | 0.57 |
| 3:J6:84:ARG:HG3 | 6:M6:189:HIS:CG | 2.39 | 0.57 |
| 8:A7:53:GLN:HB2 | 8:A7:136:VAL:HG21 | 1.86 | 0.57 |
| 9:z5:6:LYS:NZ | 9:z5:29:THR:CG2 | 2.67 | 0.57 |
| 10:j5:971:VAL:HG13 | 10:j5:971:VAL:O | 2.02 | 0.57 |
| 10:j5:992:GLU:OE2 | 10:j5:992:GLU:N | 2.37 | 0.57 |
| 10:j5:1109:ASP:OD1 | 10:j5:1109:ASP:N | 2.35 | 0.57 |
| 10:k5:53:ARG:C | 10:k5:56:ILE:HG22 | 2.28 | 0.57 |
| 10:k5:190:LEU:C | 10:k5:194:CYS:SG | 2.87 | 0.57 |
| 10:k5:1005:LEU:CD1 | 10:k5:1016:LEU:CD2 | 2.82 | 0.57 |
| 10:k5:1008:PHE:CE2 | 1:p7:83:ARG:NH1 | 2.72 | 0.57 |
| 10:k5:1026:LYS:C | 10:k5:1028:ASN:H | 2.12 | 0.57 |
| 10:k5:1148:THR:O | 10:k5:1148:THR:HG23 | 2.03 | 0.57 |
| 3:F6:130:ALA:HB1 | 12:F6:201:CYC:HBC1 | 1.84 | 0.57 |
| 2:I6:62:LYS:HG2 | 2:I6:129:GLU:HG2 | 1.86 | 0.57 |
| 8:I7:44:THR:HG23 | 1:J7:18:TYR:CD2 | 2.39 | 0.57 |
| 8:o7:80:LEU:HD12 | 12:o7:201:CYC:HAD1 | 1.86 | 0.57 |
| 8:s7:44:THR:HG23 | 1:t7:18:TYR:CD2 | 2.39 | 0.57 |
| 12:X8:201:CYC:HB | 12:X8:201:CYC:CMA | 2.17 | 0.57 |
| 4:M8:92:GLU:OE2 | 4:M8:217:VAL:HG22 | 1.95 | 0.57 |
| 12:M8:302:CYC:C3C | 3:S8:78:ARG:HG2 | 2.33 | 0.57 |
| 12:M8:302:CYC:HBB3 | 5:Z8:9:GLN:OE1 | 2.04 | 0.57 |
| 3:O8:111:ASN:O | 5:Z8:67:ILE:CB | 2.52 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:O8:111:ASN:ND2 | 5:Z8:68:LEU:CG | 2.66 | 0.57 |
| 3:L9:77:ARG:NH1 | 11:a9:538:ARG:HH21 | 2.01 | 0.57 |
| 4:M9:1:MET:HG3 | 4:M9:43:TYR:OH | 2.04 | 0.57 |
| 4:M9:53:LEU:HA | 12:F9:301:CYC:HMA2 | 1.86 | 0.57 |
| 5:N9:13:SER:HB3 | 5:N9:14:LYS:HD3 | 1.86 | 0.57 |
| 5:Z8:13:SER:HB3 | 5:Z8:14:LYS:HD3 | 1.86 | 0.57 |
| 3:J9:78:ARG:NH2 | 11:a9:359:ASP:N | 2.50 | 0.57 |
| 12:W9:201:CYC:HB | 12:W9:201:CYC:CMA | 2.17 | 0.57 |
| 11:aA:338:VAL:CG2 | 11:aA:340:PRO:CD | 2.78 | 0.57 |
| 4:M1:210:ILE:CD1 | 5:N1:59:ARG:NH1 | 2.66 | 0.57 |
| 12:U1:201:CYC:HB | 12:U1:201:CYC:CMA | 2.17 | 0.57 |
| 3:X1:2:GLN:HG2 | 3:X1:6:THR:HG22 | 1.86 | 0.57 |
| 12:C2:201:CYC:HB | 12:C2:201:CYC:CMA | 2.17 | 0.57 |
| 2:AA:63:PHE:CB | 2:AA:66:LEU:CG | 2.82 | 0.57 |
| 2:IA:62:LYS:HG2 | 2:IA:129:GLU:HG2 | 1.85 | 0.57 |
| 2:QA:32:GLN:HG2 | 2:UA:28:ASN:ND2 | 2.14 | 0.57 |
| 2:UA:62:LYS:HG2 | 2:UA:129:GLU:HG2 | 1.85 | 0.57 |
| 3:VA:127:VAL:HG22 | 12:VA:201:CYC:H3C | 1.86 | 0.57 |
| 3:R1:2:GLN:HG2 | 3:R1:6:THR:HG22 | 1.86 | 0.57 |
| 2:K3:62:LYS:HG2 | 2:K3:129:GLU:HG2 | 1.85 | 0.57 |
| 2:I2:80:ALA:HB2 | 11:aA:297:ASP:CG | 2.29 | 0.57 |
| 12:E3:201:CYC:HB | 12:E3:201:CYC:CMA | 2.17 | 0.57 |
| 3:B4:107:ASP:O | 4:M4:61:ASN:HA | 2.04 | 0.57 |
| 3:L3:104:VAL:HG11 | 3:L3:108:ARG:HH22 | 1.67 | 0.57 |
| 4:M3:1:MET:HG3 | 4:M3:43:TYR:OH | 2.04 | 0.57 |
| 4:M3:160:THR:HG21 | 4:M3:257:GLN:CB | 2.29 | 0.57 |
| 2:S3:62:LYS:HG2 | 2:S3:129:GLU:HG2 | 1.85 | 0.57 |
| 12:W3:201:CYC:HB | 12:W3:201:CYC:CMA | 2.17 | 0.57 |
| 3:J4:2:GLN:HG2 | 3:J4:6:THR:HG22 | 1.86 | 0.57 |
| 4:M4:20:THR:CG2 | 4:M4:67:LEU:HD11 | 2.35 | 0.57 |
| 4:M4:120:LEU:O | 4:M4:123:GLU:HB2 | 2.04 | 0.57 |
| 4:M4:200:ILE:HB | 5:Z4:52:ARG:HH22 | 1.69 | 0.57 |
| 1:D5:1:MET:O | 1:D5:1:MET:HG3 | 2.03 | 0.57 |
| 1:D5:70:GLY:O | 1:D5:77:ARG:NH1 | 2.38 | 0.57 |
| 8:I5:98:ALA:HA | 1:J5:5:ILE:CG2 | 2.33 | 0.57 |
| 8:c5:53:GLN:HB2 | 8:c5:136:VAL:HG21 | 1.86 | 0.57 |
| 1:Z5:127:VAL:HB | 10:k5:698:GLY:HA3 | 1.85 | 0.57 |
| 10:j5:247:ARG:HG2 | 10:j5:247:ARG:O | 2.03 | 0.57 |
| 10:j5:853:LEU:HD12 | 10:j5:853:LEU:O | 2.04 | 0.57 |
| 10:k5:647:ARG:HG2 | 10:k5:647:ARG:O | 2.04 | 0.57 |
| 8:E7:126:VAL:HG23 | 12:E7:201:CYC:CMC | 2.33 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:i7:21:GLY:N | 8:s7:101:VAL:H | 2.02 | 0.57 |
| 8:i7:49:ARG:NH2 | 8:i7:140:LEU:CD2 | 2.67 | 0.57 |
| 8:i7:50:ILE:CD1 | 8:i7:137:ALA:CB | 2.80 | 0.57 |
| 8:Y7:53:GLN:HB2 | 8:Y7:136:VAL:HG21 | 1.86 | 0.57 |
| 8:c7:96:ILE:HA | 8:c7:152:TYR:CE1 | 2.30 | 0.57 |
| 12:D8:201:CYC:HB | 12:D8:201:CYC:CMA | 2.18 | 0.57 |
| 8:m7:37:LEU:HD11 | 1:n7:31:PHE:CE2 | 2.39 | 0.57 |
| 12:W8:202:CYC:CMA | 12:W8:202:CYC:HB | 2.18 | 0.57 |
| 3:H8:1:MET:N | 11:a9:96:THR:CG2 | 2.68 | 0.57 |
| 3:H8:2:GLN:HG2 | 3:H8:6:THR:HG22 | 1.86 | 0.57 |
| 3:J8:127:VAL:HG22 | 12:J8:201:CYC:H3C | 1.85 | 0.57 |
| 4:M8:232:VAL:HG21 | 3:Y8:113:LEU:HD11 | 1.86 | 0.57 |
| 2:N8:63:PHE:CB | 2:N8:66:LEU:CG | 2.82 | 0.57 |
| 3:Y8:88:ILE:O | 3:Y8:92:TYR:HD2 | 1.87 | 0.57 |
| 12:E9:201:CYC:HB | 12:E9:201:CYC:CMA | 2.17 | 0.57 |
| 3:R9:2:GLN:HG2 | 3:R9:6:THR:HG22 | 1.86 | 0.57 |
| 11:a9:582:MET:O | 11:a9:586:LEU:HD23 | 2.03 | 0.57 |
| 11:aA:89:ALA:CB | 11:aA:92:LYS:HZ2 | 2.18 | 0.57 |
| 11:aA:95:ILE:HD12 | 11:aA:237:PHE:CD1 | 2.38 | 0.57 |
| 11:aA:280:ASP:OD1 | 11:aA:281:PRO:CD | 2.34 | 0.57 |
| 12:aA:901:CYC:H3C | 3:J1:127:VAL:HG22 | 1.86 | 0.57 |
| 12:E2:201:CYC:HB | 12:E2:201:CYC:CMA | 2.17 | 0.57 |
| 3:DA:68:ARG:NH2 | 3:XA:68:ARG:NH2 | 2.52 | 0.57 |
| 12:LA:202:CYC:C1B | 11:aA:404:TYR:OH | 2.53 | 0.57 |
| 4:MA:263:PRO:HG2 | 3:VA:115:GLU:C | 2.30 | 0.57 |
| 12:O1:201:CYC:HB | 12:O1:201:CYC:CMA | 2.17 | 0.57 |
| 3:P1:2:GLN:HG2 | 3:P1:6:THR:HG22 | 1.86 | 0.57 |
| 3:B3:2:GLN:HG2 | 3:B3:6:THR:HG22 | 1.86 | 0.57 |
| 5:N3:37:HIS:CD2 | 12:T3:301:CYC:HMA3 | 2.39 | 0.57 |
| 2:O3:56:VAL:HG22 | 2:O3:82:CYS:SG | 2.44 | 0.57 |
| 3:R3:2:GLN:HG2 | 3:R3:6:THR:HG22 | 1.86 | 0.57 |
| 3:T3:127:VAL:HG22 | 12:T3:301:CYC:H3C | 1.85 | 0.57 |
| 3:U4:2:GLN:HG2 | 3:U4:6:THR:HG22 | 1.86 | 0.57 |
| 3:W4:127:VAL:HG22 | 12:W4:201:CYC:H3C | 1.86 | 0.57 |
| 3:H4:2:GLN:HG2 | 3:H4:6:THR:HG22 | 1.86 | 0.57 |
| 12:N4:201:CYC:HB | 12:N4:201:CYC:CMA | 2.17 | 0.57 |
| 8:I5:2:SER:CB | 1:J5:3:ASP:OD2 | 2.49 | 0.57 |
| 8:Q5:126:VAL:CG2 | 12:Q5:201:CYC:HMC3 | 2.34 | 0.57 |
| 1:X5:106:GLU:CG | 10:j5:505:VAL:HA | 2.35 | 0.57 |
| 12:Z5:201:CYC:HB | 12:Z5:201:CYC:HMA2 | 1.69 | 0.57 |
| 3:L6:2:GLN:HG2 | 3:L6:6:THR:HG22 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 6:M6:117:MET:HE2 | 3:H6:77:ARG:HH12 | 1.55 | 0.57 |
| 8:A7:19:SER:OG | 8:M7:100:ASP:OD1 | 2.14 | 0.57 |
| 10:j5:241:ALA:N | 10:j5:242:PRO:HD3 | 2.19 | 0.57 |
| 10:k5:232:ARG:HB2 | 10:k5:232:ARG:NH1 | 2.18 | 0.57 |
| 12:k5:1202:CYC:HMA2 | 12:k5:1202:CYC:HB | 1.69 | 0.57 |
| 2:E6:62:LYS:HG2 | 2:E6:129:GLU:HG2 | 1.85 | 0.57 |
| 12:H6:202:CYC:CMA | 12:H6:202:CYC:HB | 2.18 | 0.57 |
| 8:O7:15:ALA:C | 1:P7:90:ARG:CZ | 2.78 | 0.57 |
| 8:M7:53:GLN:HB2 | 8:M7:136:VAL:HG21 | 1.86 | 0.57 |
| 8:i7:20:PRO:CD | 8:s7:155:TYR:CE2 | 2.87 | 0.57 |
| 9:x7:32:VAL:HG11 | 9:x7:37:TRP:HE3 | 1.70 | 0.57 |
| 9:y7:28:PHE:CD1 | 9:y7:28:PHE:N | 2.72 | 0.57 |
| 12:T8:201:CYC:HB | 12:T8:201:CYC:CMA | 2.17 | 0.57 |
| 12:V8:201:CYC:HB | 12:V8:201:CYC:CMA | 2.17 | 0.57 |
| 3:F8:91:ARG:HH21 | 11:a9:140:GLN:NE2 | 1.95 | 0.57 |
| 12:G8:201:CYC:HB | 12:G8:201:CYC:CMA | 2.17 | 0.57 |
| 2:I8:62:LYS:HG2 | 2:I8:129:GLU:HG2 | 1.86 | 0.57 |
| 3:L8:82:CYS:SG | 12:a9:901:CYC:H2C | 2.44 | 0.57 |
| 4:M8:160:THR:HG21 | 4:M8:257:GLN:CB | 2.30 | 0.57 |
| 12:L9:202:CYC:C1B | 11:a9:404:TYR:OH | 2.52 | 0.57 |
| 4:M9:4:LEU:HD12 | 3:D9:112:GLY:HA3 | 1.85 | 0.57 |
| 4:M9:159:CYS:C | 3:V9:108:ARG:CG | 2.77 | 0.57 |
| 5:N9:3:VAL:O | 5:N9:4:LEU:C | 2.44 | 0.57 |
| 5:Z8:66:ARG:HB2 | 5:Z8:66:ARG:NH1 | 2.16 | 0.57 |
| 3:F9:68:ARG:HH22 | 3:Z9:68:ARG:NH1 | 2.02 | 0.57 |
| 3:H9:84:ARG:HA | 11:a9:478:HIS:CE1 | 2.37 | 0.57 |
| 3:T9:2:GLN:HG2 | 3:T9:6:THR:HG22 | 1.86 | 0.57 |
| 3:Z9:2:GLN:HG2 | 3:Z9:6:THR:HG22 | 1.86 | 0.57 |
| 12:Z9:201:CYC:CMA | 12:Z9:201:CYC:HB | 2.18 | 0.57 |
| 11:aA:595:ARG:CG | 11:aA:596:THR:N | 2.68 | 0.57 |
| 11:aA:668:TYR:HH | 2:K1:115:GLU:CG | 2.05 | 0.57 |
| 11:aA:745:GLY:HA2 | 2:K1:15:GLN:C | 2.29 | 0.57 |
| 11:aA:798:SER:HB3 | 11:aA:800:THR:HG23 | 0.58 | 0.57 |
| 3:Z1:2:GLN:HG2 | 3:Z1:6:THR:HG22 | 1.87 | 0.57 |
| 1:A:17:LYS:C | 8:a5:90:ARG:HD2 | 2.29 | 0.57 |
| 1:Z:131:GLN:HB3 | 1:X5:17:LYS:HZ3 | 1.70 | 0.57 |
| 12:JA:201:CYC:CMA | 12:JA:201:CYC:HB | 2.18 | 0.57 |
| 4:MA:134:ASN:OD1 | 3:RA:116:THR:HG23 | 2.03 | 0.57 |
| 2:QA:95:TYR:CD2 | 3:RA:9:ILE:HG23 | 2.40 | 0.57 |
| 12:QA:201:CYC:O2A | 3:TA:67:ILE:HG21 | 2.02 | 0.57 |
| 12:QA:201:CYC:CMA | 3:TA:79:MET:HG2 | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:TA:32:LYS:CE | 2:X4:57:GLN:HA | 2.34 | 0.57 |
| 7:N2:48:LEU:HB3 | 12:N2:101:CYC:CBA | 2.34 | 0.57 |
| 2:A4:63:PHE:CB | 2:A4:66:LEU:CG | 2.82 | 0.57 |
| 3:B4:92:TYR:OH | 12:B4:202:CYC:HAB1 | 2.05 | 0.57 |
| 3:L3:77:ARG:HB3 | 11:a9:824:VAL:OXT | 2.04 | 0.57 |
| 3:L3:119:ALA:HB2 | 11:a9:813:PRO:CA | 2.25 | 0.57 |
| 3:S4:2:GLN:HG2 | 3:S4:6:THR:HG22 | 1.86 | 0.57 |
| 12:U4:202:CYC:CMA | 12:U4:202:CYC:HB | 2.18 | 0.57 |
| 12:L4:201:CYC:CMA | 12:L4:201:CYC:HB | 2.18 | 0.57 |
| 3:Q4:105:LEU:HD22 | 3:Q4:166:LYS:HD3 | 1.86 | 0.57 |
| 3:Q4:120:LEU:CD1 | 5:Z4:39:PRO:HA | 2.35 | 0.57 |
| 2:R4:62:LYS:HG2 | 2:R4:129:GLU:HG2 | 1.85 | 0.57 |
| 8:A5:122:PRO:O | 12:A5:201:CYC:HMC2 | 2.01 | 0.57 |
| 1:H5:14:VAL:HG11 | 10:j5:555:ALA:CA | 2.33 | 0.57 |
| 1:H5:106:GLU:OE2 | 10:j5:560:VAL:HG12 | 2.05 | 0.57 |
| 8:I5:29:PHE:HE2 | 1:J5:5:ILE:HD11 | 1.69 | 0.57 |
| 1:d5:110:ASN:HD22 | 10:j5:451:LYS:HB3 | 1.64 | 0.57 |
| 8:Q5:18:LEU:HD22 | 1:R5:97:LEU:HD13 | 1.87 | 0.57 |
| 8:S5:90:ARG:CA | 1:T5:18:TYR:CZ | 2.87 | 0.57 |
| 12:K6:201:CYC:HB | 12:K6:201:CYC:CMA | 2.16 | 0.57 |
| 7:N6:29:LEU:HD21 | 3:D6:80:ALA:HB3 | 1.86 | 0.57 |
| 9:i5:6:LYS:NZ | 9:i5:29:THR:CG2 | 2.67 | 0.57 |
| 10:j5:211:ALA:O | 10:j5:212:ARG:C | 2.46 | 0.57 |
| 10:j5:275:THR:HG22 | 10:j5:286:VAL:O | 2.03 | 0.57 |
| 10:j5:286:VAL:HB | 10:j5:293:LYS:CE | 2.35 | 0.57 |
| 10:j5:965:GLN:CB | 1:t7:69:GLY:HA2 | 2.33 | 0.57 |
| 10:j5:1119:LEU:CD2 | 1:t7:87:TYR:CE1 | 2.85 | 0.57 |
| 10:k5:803:LYS:NZ | 9:z7:43:ARG:NH1 | 2.40 | 0.57 |
| 8:E7:126:VAL:CG2 | 12:E7:201:CYC:HMC3 | 2.34 | 0.57 |
| 8:i7:25:ARG:CZ | 8:s7:3:VAL:O | 2.52 | 0.57 |
| 8:U7:15:ALA:C | 1:V7:90:ARG:CZ | 2.78 | 0.57 |
| 3:B8:86:MET:HG3 | 12:B8:202:CYC:HBC2 | 1.85 | 0.57 |
| 12:B8:201:CYC:CMA | 12:B8:201:CYC:HB | 2.18 | 0.57 |
| 8:m7:29:PHE:CZ | 8:m7:98:ALA:C | 2.76 | 0.57 |
| 8:s7:15:ALA:HB1 | 1:t7:90:ARG:HH22 | 1.70 | 0.57 |
| 4:M8:20:THR:CG2 | 4:M8:67:LEU:HD11 | 2.35 | 0.57 |
| 4:M8:127:SER:HA | 12:M8:302:CYC:HMA1 | 0.62 | 0.57 |
| 12:S8:201:CYC:HB | 12:S8:201:CYC:CMA | 2.18 | 0.57 |
| 3:L9:120:LEU:HD22 | 11:a9:538:ARG:CB | 2.26 | 0.57 |
| 4:M9:144:ARG:NH2 | 5:N9:52:ARG:NH2 | 2.51 | 0.57 |
| 2:E9:152:ALA:CB | 2:I9:21:ASN:HD21 | 2.16 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:G9:201:CYC:HB | 12:G9:201:CYC:CMA | 2.17 | 0.57 |
| 12:I9:201:CYC:HB | 12:I9:201:CYC:CMA | 2.17 | 0.57 |
| 12:T9:302:CYC:CMA | 12:T9:302:CYC:HB | 2.18 | 0.57 |
| 12:U9:201:CYC:HB | 12:U9:201:CYC:CMA | 2.17 | 0.57 |
| 11:a9:508:ARG:HB2 | 11:a9:513:GLN:HE22 | 1.68 | 0.57 |
| 4:M1:196:TYR:HB3 | 2:Y1:14:SER:O | 2.03 | 0.57 |
| 3:T1:2:GLN:HG2 | 3:T1:6:THR:HG22 | 1.86 | 0.57 |
| 12:X1:202:CYC:HB | 12:X1:202:CYC:CMA | 2.17 | 0.57 |
| 1:A:13:ASP:OD2 | 8:a5:107:ILE:HG12 | 2.04 | 0.57 |
| 12:A:201:CYC:HB | 12:A:201:CYC:HMA2 | 1.69 | 0.57 |
| 3:BA:14:LEU:HD13 | 3:XA:125:ARG:HD2 | 1.85 | 0.57 |
| 12:BA:201:CYC:CBB | 4:MA:38:PRO:HD3 | 2.34 | 0.57 |
| 12:EA:201:CYC:HB | 12:EA:201:CYC:CMA | 2.17 | 0.57 |
| 3:LA:127:VAL:HG22 | 12:LA:202:CYC:H3C | 1.85 | 0.57 |
| 4:MA:133:ARG:HB3 | 12:RA:201:CYC:CGA | 2.34 | 0.57 |
| 4:MA:185:ALA:CA | 12:VA:201:CYC:CBA | 2.82 | 0.57 |
| 12:QA:201:CYC:HBA1 | 3:TA:79:MET:CE | 2.34 | 0.57 |
| 3:XA:2:GLN:HG2 | 3:XA:6:THR:HG22 | 1.86 | 0.57 |
| 3:J3:80:ALA:CB | 11:a9:670:LEU:CD2 | 2.83 | 0.57 |
| 7:N2:29:LEU:HD21 | 3:D2:80:ALA:HB3 | 1.86 | 0.57 |
| 3:D3:68:ARG:HH12 | 3:X3:68:ARG:CZ | 2.16 | 0.57 |
| 12:F3:201:CYC:HAA1 | 4:M3:36:TYR:CE2 | 2.39 | 0.57 |
| 3:B4:82:CYS:CA | 12:B4:202:CYC:H2C | 2.34 | 0.57 |
| 3:B4:120:LEU:HG | 4:M4:52:LEU:HB3 | 1.87 | 0.57 |
| 2:C4:62:LYS:HG2 | 2:C4:129:GLU:HG2 | 1.86 | 0.57 |
| 3:D4:2:GLN:HG2 | 3:D4:6:THR:HG22 | 1.86 | 0.57 |
| 3:P3:127:VAL:HG22 | 12:P3:201:CYC:H3C | 1.86 | 0.57 |
| 12:X3:202:CYC:CMA | 12:X3:202:CYC:HB | 2.17 | 0.57 |
| 2:G4:62:LYS:HG2 | 2:G4:129:GLU:HG2 | 1.85 | 0.57 |
| 3:L4:2:GLN:HG2 | 3:L4:6:THR:HG22 | 1.86 | 0.57 |
| 4:M4:1:MET:HG3 | 4:M4:43:TYR:OH | 2.04 | 0.57 |
| 4:M4:260:ARG:HH11 | 4:M4:260:ARG:CG | 2.18 | 0.57 |
| 2:X4:62:LYS:HG2 | 2:X4:129:GLU:HG2 | 1.86 | 0.57 |
| 8:E5:17:TYR:HB3 | 1:F5:45:SER:CB | 2.32 | 0.57 |
| 8:I5:90:ARG:HD2 | 1:J5:17:LYS:O | 2.04 | 0.57 |
| 8:S5:90:ARG:CA | 1:T5:18:TYR:CE2 | 2.87 | 0.57 |
| 12:a5:201:CYC:HC | 12:a5:201:CYC:HMD3 | 1.70 | 0.57 |
| 6:M6:127:SER:CA | 12:F6:201:CYC:O2A | 2.52 | 0.57 |
| 10:j5:11:VAL:O | 10:j5:11:VAL:HG12 | 2.03 | 0.57 |
| 10:j5:298:ARG:CG | 10:j5:298:ARG:HH11 | 2.15 | 0.57 |
| 10:j5:357:LEU:HD21 | 10:j5:382:ILE:HG12 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:k5:11:VAL:HG12 | 10:k5:11:VAL:O | 2.03 | 0.57 |
| 10:k5:19:THR:HB | 10:k5:173:ALA:CB | 2.34 | 0.57 |
| 10:k5:187:ARG:CB | 10:k5:237:ASP:OD1 | 2.53 | 0.57 |
| 10:k5:934:ALA:HB1 | 1:D7:32:THR:HG21 | 0.59 | 0.57 |
| 10:k5:1118:THR:O | 10:k5:1118:THR:HG22 | 2.03 | 0.57 |
| 3:D6:2:GLN:HG2 | 3:D6:6:THR:HG22 | 1.86 | 0.57 |
| 8:W7:13:ALA:C | 9:w7:46:LYS:NZ | 2.61 | 0.57 |
| 12:X7:201:CYC:HB | 12:X7:201:CYC:HMA2 | 1.69 | 0.57 |
| 8:c7:126:VAL:CG2 | 12:c7:201:CYC:HMC1 | 2.34 | 0.57 |
| 1:f7:110:ASN:ND2 | 9:y7:57:PHE:O | 2.38 | 0.57 |
| 2:E8:62:LYS:HG2 | 2:E8:129:GLU:HG2 | 1.85 | 0.57 |
| 8:m7:15:ALA:HB1 | 1:n7:90:ARG:HH22 | 1.70 | 0.57 |
| 9:y7:34:TYR:C | 9:y7:34:TYR:CD1 | 2.83 | 0.57 |
| 3:U8:127:VAL:HG22 | 12:U8:201:CYC:H3C | 1.86 | 0.57 |
| 2:V8:62:LYS:HG2 | 2:V8:129:GLU:HG2 | 1.85 | 0.57 |
| 2:X8:62:LYS:HG2 | 2:X8:129:GLU:HG2 | 1.86 | 0.57 |
| 3:J8:108:ARG:NH2 | 11:a9:171:ARG:CA | 2.68 | 0.57 |
| 4:M8:98:ASP:HB2 | 4:M8:101:ASP:HB2 | 1.86 | 0.57 |
| 4:M8:235:PHE:N | 12:M8:301:CYC:HMA1 | 2.18 | 0.57 |
| 4:M8:260:ARG:HH11 | 4:M8:260:ARG:CG | 2.18 | 0.57 |
| 12:M8:302:CYC:CBC | 3:S8:78:ARG:O | 2.49 | 0.57 |
| 3:S8:116:THR:CG2 | 3:S8:117:TYR:N | 2.67 | 0.57 |
| 4:M9:190:ARG:HH11 | 4:M9:202:SER:HB3 | 1.63 | 0.57 |
| 2:C9:62:LYS:HG2 | 2:C9:129:GLU:HG2 | 1.86 | 0.57 |
| 3:D9:2:GLN:HG2 | 3:D9:6:THR:HG22 | 1.86 | 0.57 |
| 12:J9:201:CYC:HC | 12:J9:201:CYC:HMD2 | 1.70 | 0.57 |
| 12:G1:201:CYC:HB | 12:G1:201:CYC:CMA | 2.17 | 0.57 |
| 11:a9:331:TYR:HA | 11:a9:333:GLN:HE21 | 1.66 | 0.57 |
| 11:a9:587:THR:OG1 | 11:a9:588:VAL:N | 2.29 | 0.57 |
| 11:aA:75:ALA:CB | 11:aA:81:ASP:OD1 | 2.25 | 0.57 |
| 11:aA:816:LEU:HD23 | 11:aA:816:LEU:O | 2.04 | 0.57 |
| 3:X1:127:VAL:HG22 | 12:X1:201:CYC:H3C | 1.85 | 0.57 |
| 12:F2:202:CYC:CMA | 12:F2:202:CYC:HB | 2.18 | 0.57 |
| 12:JA:202:CYC:HBB3 | 11:aA:516:GLN:HG2 | 1.86 | 0.57 |
| 12:LA:201:CYC:CMA | 12:LA:201:CYC:HB | 2.18 | 0.57 |
| 4:MA:19:MET:HG2 | 4:MA:59:ILE:HD13 | 1.86 | 0.57 |
| 4:MA:103:GLN:HA | 4:MA:103:GLN:OE1 | 2.04 | 0.57 |
| 2:SA:62:LYS:HG2 | 2:SA:129:GLU:HG2 | 1.85 | 0.57 |
| 2:O1:63:PHE:CB | 2:O1:66:LEU:CG | 2.82 | 0.57 |
| 2:Q1:14:SER:CB | 5:N1:62:ARG:CZ | 2.79 | 0.57 |
| 12:R1:202:CYC:CMA | 12:R1:202:CYC:HB | 2.18 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:F3:201:CYC:CMD | 12:F3:201:CYC:HC | 2.18 | 0.57 |
| 3:Z3:2:GLN:HG2 | 3:Z3:6:THR:HG22 | 1.87 | 0.57 |
| 12:H4:201:CYC:CBB | 11:aA:259:ALA:HB2 | 2.24 | 0.57 |
| 2:K4:13:ASP:O | 11:aA:242:GLY:CA | 2.52 | 0.57 |
| 4:M4:27:HIS:NE2 | 4:M4:34:ASP:OD1 | 2.36 | 0.57 |
| 3:Q4:4:ALA:N | 3:Q4:99:ALA:O | 2.37 | 0.57 |
| 12:Q4:201:CYC:CMA | 12:Q4:201:CYC:HB | 2.18 | 0.57 |
| 12:M5:201:CYC:HC | 12:M5:201:CYC:HMD3 | 1.70 | 0.57 |
| 12:f5:201:CYC:HB | 12:f5:201:CYC:HMA2 | 1.69 | 0.57 |
| 12:L6:202:CYC:CMA | 12:L6:202:CYC:HB | 2.18 | 0.57 |
| 6:M6:251:LYS:NZ | 3:H6:121:GLY:HA3 | 2.20 | 0.57 |
| 10:j5:965:GLN:HG3 | 1:t7:69:GLY:C | 2.22 | 0.57 |
| 10:k5:286:VAL:HB | 10:k5:293:LYS:CE | 2.35 | 0.57 |
| 2:C6:62:LYS:HG2 | 2:C6:129:GLU:HG2 | 1.86 | 0.57 |
| 12:I6:201:CYC:HB | 12:I6:201:CYC:CMA | 2.17 | 0.57 |
| 12:j7:201:CYC:HB | 12:j7:201:CYC:HMA2 | 1.69 | 0.57 |
| 8:c7:4:LEU:O | 8:c7:8:ILE:HG13 | 2.05 | 0.57 |
| 12:B8:202:CYC:CMD | 12:B8:202:CYC:HC | 2.18 | 0.57 |
| 8:s7:15:ALA:C | 1:t7:90:ARG:CZ | 2.78 | 0.57 |
| 4:M8:140:ARG:HH22 | 4:M8:210:ILE:CG1 | 2.13 | 0.57 |
| 3:Q8:117:TYR:HA | 3:Q8:120:LEU:CG | 2.33 | 0.57 |
| 3:Q8:120:LEU:HD12 | 3:Q8:121:GLY:N | 2.19 | 0.57 |
| 12:F1:201:CYC:HAA1 | 4:M1:36:TYR:CE2 | 2.39 | 0.57 |
| 3:D9:68:ARG:NH2 | 3:X9:68:ARG:NH2 | 2.52 | 0.57 |
| 3:V9:127:VAL:HG22 | 12:V9:201:CYC:H3C | 1.86 | 0.57 |
| 11:a9:239:TYR:CD1 | 12:a9:901:CYC:HBA1 | 2.38 | 0.57 |
| 11:aA:577:GLU:HA | 11:aA:577:GLU:OE2 | 2.05 | 0.57 |
| 11:aA:670:LEU:CD2 | 3:J1:80:ALA:CB | 2.83 | 0.57 |
| 12:I1:201:CYC:HB | 12:I1:201:CYC:CMA | 2.17 | 0.57 |
| 12:K1:201:CYC:HB | 12:K1:201:CYC:CMA | 2.17 | 0.57 |
| 4:M1:163:ASN:ND2 | 12:Z1:202:CYC:HMA1 | 2.20 | 0.57 |
| 4:M1:250:THR:HG21 | 3:X1:120:LEU:HD21 | 1.87 | 0.57 |
| 3:D2:127:VAL:HG22 | 12:D2:201:CYC:H3C | 1.86 | 0.57 |
| 3:F2:2:GLN:HG2 | 3:F2:6:THR:HG22 | 1.86 | 0.57 |
| 2:CA:62:LYS:HG2 | 2:CA:129:GLU:HG2 | 1.86 | 0.57 |
| 3:DA:108:ARG:NH1 | 4:MA:9:GLN:OE1 | 2.38 | 0.57 |
| 12:FA:301:CYC:HC | 12:FA:301:CYC:CMD | 2.18 | 0.57 |
| 3:HA:113:LEU:HD13 | 12:HA:202:CYC:C2B | 2.34 | 0.57 |
| 3:PA:2:GLN:HG2 | 3:PA:6:THR:HG22 | 1.86 | 0.57 |
| 2:QA:21:ASN:HB3 | 2:UA:153:TYR:OH | 2.05 | 0.57 |
| 3:TA:24:LEU:C | 2:X4:68:GLN:CD | 2.73 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:R1:201:CYC:CMD | 12:R1:201:CYC:HC | 2.18 | 0.57 |
| 12:S1:201:CYC:HB | 12:S1:201:CYC:CMA | 2.17 | 0.57 |
| 12:L2:201:CYC:HC | 12:L2:201:CYC:CMD | 2.18 | 0.57 |
| 6:M2:258:VAL:O | 6:M2:258:VAL:HG23 | 2.05 | 0.57 |
| 3:B4:116:THR:CG2 | 3:B4:117:TYR:N | 2.67 | 0.57 |
| 12:B4:202:CYC:HC | 12:B4:202:CYC:CMD | 2.18 | 0.57 |
| 12:P3:202:CYC:CMA | 12:P3:202:CYC:HB | 2.18 | 0.57 |
| 12:B1:201:CYC:HB | 12:B1:201:CYC:CMA | 2.18 | 0.57 |
| 3:S4:120:LEU:HD13 | 12:S4:202:CYC:C4D | 2.35 | 0.57 |
| 3:U4:108:ARG:HG2 | 4:M4:246:ALA:HB2 | 1.87 | 0.57 |
| 12:F4:201:CYC:HC | 12:F4:201:CYC:HMD2 | 1.70 | 0.57 |
| 12:F4:201:CYC:CMA | 12:F4:201:CYC:HB | 2.18 | 0.57 |
| 3:H4:84:ARG:CG | 11:aA:131:TYR:CE1 | 2.84 | 0.57 |
| 12:I4:201:CYC:HB | 12:I4:201:CYC:CMA | 2.17 | 0.57 |
| 12:O4:202:CYC:HC | 12:O4:202:CYC:HMD2 | 1.70 | 0.57 |
| 2:P4:62:LYS:HG2 | 2:P4:129:GLU:HG2 | 1.85 | 0.57 |
| 3:Q4:116:THR:HB | 5:Z4:40:SER:HB3 | 1.87 | 0.57 |
| 1:L5:79:ALA:HB1 | 8:G5:114:GLU:CB | 2.34 | 0.57 |
| 8:U5:76:LYS:CD | 8:U5:77:MET:HE3 | 2.07 | 0.57 |
| 8:U5:78:THR:CG2 | 6:M6:35:GLY:HA2 | 2.28 | 0.57 |
| 8:U5:79:ALA:CA | 6:M6:31:ASP:O | 2.50 | 0.57 |
| 3:J6:119:ALA:CB | 6:M6:261:LYS:N | 2.67 | 0.57 |
| 10:j5:187:ARG:NE | 10:j5:237:ASP:OD2 | 2.37 | 0.57 |
| 10:j5:732:ARG:NH2 | 1:J7:68:PRO:O | 2.31 | 0.57 |
| 10:j5:869:GLY:O | 9:w7:43:ARG:CZ | 2.53 | 0.57 |
| 10:k5:601:LYS:O | 10:k5:601:LYS:HG3 | 2.05 | 0.57 |
| 12:D1:201:CYC:CMA | 12:D1:201:CYC:HB | 2.18 | 0.57 |
| 1:H7:54:GLU:CD | 11:aA:563:PHE:CD2 | 2.83 | 0.57 |
| 8:g7:35:ARG:NH2 | 8:g7:144:ASP:CB | 2.61 | 0.57 |
| 8:c7:50:ILE:HA | 8:c7:136:VAL:CG1 | 2.34 | 0.57 |
| 8:c7:92:VAL:CG2 | 8:c7:156:LEU:HD12 | 2.34 | 0.57 |
| 12:e7:201:CYC:HC | 12:e7:201:CYC:HMD3 | 1.70 | 0.57 |
| 12:p7:201:CYC:HB | 12:p7:201:CYC:HMA2 | 1.69 | 0.57 |
| 2:T8:62:LYS:HG2 | 2:T8:129:GLU:HG2 | 1.86 | 0.57 |
| 2:X8:57:GLN:C | 3:T9:32:LYS:HZ1 | 2.12 | 0.57 |
| 2:X8:68:GLN:CD | 3:T9:24:LEU:C | 2.73 | 0.57 |
| 12:H8:202:CYC:CMA | 12:H8:202:CYC:HB | 2.18 | 0.57 |
| 2:R8:62:LYS:HG2 | 2:R8:129:GLU:HG2 | 1.85 | 0.57 |
| 3:L9:127:VAL:HG22 | 12:L9:202:CYC:H3C | 1.85 | 0.57 |
| 12:L9:202:CYC:CGD | 11:a9:538:ARG:HB3 | 2.34 | 0.57 |
| 4:M9:103:GLN:OE1 | 4:M9:103:GLN:HA | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:M9:164:ARG:NH1 | 4:M9:259:ARG:O | 2.33 | 0.57 |
| 4:M9:196:TYR:H | 2:U9:15:GLN:HA | 1.68 | 0.57 |
| 5:N9:1:MET:HG2 | 3:R9:119:ALA:CB | 1.98 | 0.57 |
| 5:N9:1:MET:CB | 5:N9:3:VAL:CG2 | 2.76 | 0.57 |
| 3:Y8:2:GLN:HG2 | 3:Y8:6:THR:HG22 | 1.86 | 0.57 |
| 5:Z8:37:HIS:HD2 | 12:Z8:301:CYC:C4A | 2.07 | 0.57 |
| 5:Z8:41:GLN:CB | 12:Z8:301:CYC:CMB | 2.64 | 0.57 |
| 12:D9:202:CYC:CMA | 12:D9:202:CYC:HB | 2.18 | 0.57 |
| 12:H9:202:CYC:CMD | 12:H9:202:CYC:HC | 2.18 | 0.57 |
| 11:aA:798:SER:C | 11:aA:800:THR:N | 2.62 | 0.57 |
| 4:M1:1:MET:HG3 | 4:M1:43:TYR:OH | 2.04 | 0.57 |
| 2:U1:47:ASN:O | 2:U1:51:LEU:CG | 2.53 | 0.57 |
| 1:A:118:SER:OG | 10:k5:9:SER:HB2 | 2.04 | 0.57 |
| 2:EA:62:LYS:HG2 | 2:EA:129:GLU:HG2 | 1.85 | 0.57 |
| 3:FA:127:VAL:HG22 | 12:FA:301:CYC:H3C | 1.85 | 0.57 |
| 3:HA:2:GLN:HG2 | 3:HA:6:THR:HG22 | 1.86 | 0.57 |
| 12:JA:202:CYC:HC | 12:JA:202:CYC:CMD | 2.18 | 0.57 |
| 2:OA:63:PHE:CB | 2:OA:66:LEU:CG | 2.82 | 0.57 |
| 12:PA:202:CYC:CMA | 12:PA:202:CYC:HB | 2.18 | 0.57 |
| 12:RA:202:CYC:CMA | 12:RA:202:CYC:HB | 2.18 | 0.57 |
| 12:ZA:202:CYC:HC | 12:ZA:202:CYC:CMD | 2.18 | 0.57 |
| 12:H2:202:CYC:HB | 12:H2:202:CYC:CMA | 2.18 | 0.57 |
| 12:L2:202:CYC:HB | 12:L2:202:CYC:CMA | 2.18 | 0.57 |
| 12:N2:101:CYC:HC | 12:N2:101:CYC:CMD | 2.18 | 0.57 |
| 12:F3:202:CYC:CMA | 12:F3:202:CYC:HB | 2.18 | 0.57 |
| 3:B4:116:THR:CA | 4:M4:56:MET:CG | 2.69 | 0.57 |
| 12:V3:202:CYC:CMA | 12:V3:202:CYC:HB | 2.18 | 0.57 |
| 12:X3:201:CYC:CMD | 12:X3:201:CYC:HC | 2.18 | 0.57 |
| 2:I4:14:SER:CB | 11:aA:170:PHE:CE2 | 2.88 | 0.57 |
| 4:M4:87:ILE:CD1 | 3:Y4:77:ARG:HG2 | 2.27 | 0.57 |
| 4:M4:148:LYS:HD2 | 4:M4:197:ASP:OD1 | 2.04 | 0.57 |
| 1:B5:143:PRO:CG | 8:W7:41:GLN:HE22 | 2.06 | 0.57 |
| 8:C5:29:PHE:CZ | 8:C5:98:ALA:C | 2.76 | 0.57 |
| 8:E5:4:LEU:O | 8:E5:8:ILE:HG13 | 2.05 | 0.57 |
| 1:H5:10:ASN:OD1 | 10:j5:557:VAL:CB | 2.52 | 0.57 |
| 1:H5:87:TYR:CZ | 9:i5:19:THR:O | 2.56 | 0.57 |
| 12:H5:201:CYC:HB | 12:H5:201:CYC:HMA2 | 1.70 | 0.57 |
| 1:d5:62:TYR:HE1 | 12:e5:201:CYC:O1D | 1.87 | 0.57 |
| 12:d5:201:CYC:NB | 10:j5:379:PHE:HZ | 2.01 | 0.57 |
| 1:R5:106:GLU:CG | 10:k5:505:VAL:CA | 2.76 | 0.57 |
| 8:W5:8:ILE:CG2 | 1:X5:94:TYR:HB3 | 2.35 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:W5:16:ARG:CA | 1:X5:90:ARG:CD | 2.45 | 0.57 |
| 1:b5:18:TYR:CE2 | 10:k5:165:ARG:HG3 | 2.38 | 0.57 |
| 12:b5:201:CYC:HB | 12:b5:201:CYC:HMA2 | 1.69 | 0.57 |
| 12:J6:201:CYC:CMA | 12:J6:201:CYC:HB | 2.18 | 0.57 |
| 12:A7:201:CYC:HC | 12:A7:201:CYC:HMD3 | 1.70 | 0.57 |
| 9:i5:23:LEU:C | 9:i5:25:ASN:H | 2.09 | 0.57 |
| 10:j5:586:LEU:HD12 | 10:j5:607:LEU:HD23 | 1.77 | 0.57 |
| 10:j5:733:SER:CB | 1:D7:154:ASP:OD2 | 2.51 | 0.57 |
| 10:j5:1148:THR:O | 10:j5:1148:THR:HG23 | 2.04 | 0.57 |
| 10:k5:990:ARG:HD3 | 1:Z7:76:ARG:HD2 | 1.86 | 0.57 |
| 10:k5:1025:LEU:HD21 | 10:k5:1035:PHE:HB2 | 0.58 | 0.57 |
| 2:A6:56:VAL:HG22 | 2:A6:82:CYS:SG | 2.44 | 0.57 |
| 12:B6:201:CYC:CMA | 12:B6:201:CYC:HB | 2.18 | 0.57 |
| 8:Q7:4:LEU:O | 8:Q7:8:ILE:HG13 | 2.05 | 0.57 |
| 8:K7:4:LEU:O | 8:K7:8:ILE:HG13 | 2.05 | 0.57 |
| 8:a7:90:ARG:HD3 | 1:b7:18:TYR:CD1 | 2.40 | 0.57 |
| 12:b7:201:CYC:HB | 12:b7:201:CYC:HMA2 | 1.69 | 0.57 |
| 12:d7:201:CYC:C4B | 9:x7:38:PHE:HE1 | 2.03 | 0.57 |
| 3:D8:2:GLN:HG2 | 3:D8:6:THR:HG22 | 1.86 | 0.57 |
| 8:m7:15:ALA:C | 1:n7:90:ARG:CZ | 2.78 | 0.57 |
| 8:o7:4:LEU:O | 8:o7:8:ILE:HG13 | 2.05 | 0.57 |
| 8:o7:80:LEU:CD1 | 12:o7:201:CYC:CAD | 2.82 | 0.57 |
| 8:s7:15:ALA:CB | 1:t7:90:ARG:NH2 | 2.68 | 0.57 |
| 12:v7:201:CYC:HB | 12:v7:201:CYC:HMA2 | 1.69 | 0.57 |
| 9:w7:15:LYS:HD2 | 9:w7:16:ARG:HB3 | 1.86 | 0.57 |
| 3:O8:111:ASN:CB | 5:Z8:67:ILE:HB | 2.24 | 0.57 |
| 3:F1:119:ALA:CB | 4:M1:41:ASN:ND2 | 2.62 | 0.57 |
| 3:L9:2:GLN:HG2 | 3:L9:6:THR:HG22 | 1.86 | 0.57 |
| 3:B9:127:VAL:HG22 | 12:B9:201:CYC:H3C | 1.86 | 0.57 |
| 3:H9:84:ARG:CA | 11:a9:478:HIS:CE1 | 2.87 | 0.57 |
| 11:a9:72:ASP:HB3 | 11:a9:73:TYR:HA | 1.86 | 0.57 |
| 11:a9:419:ARG:HH11 | 11:a9:419:ARG:HG3 | 1.69 | 0.57 |
| 11:a9:454:LEU:HD22 | 11:a9:535:ASP:OD2 | 2.00 | 0.57 |
| 11:aA:29:ARG:O | 11:aA:29:ARG:HG2 | 2.04 | 0.57 |
| 11:aA:654:ALA:CB | 2:I1:15:GLN:HG2 | 2.35 | 0.57 |
| 11:aA:694:ARG:HH22 | 4:M1:51:ARG:HH22 | 1.48 | 0.57 |
| 11:aA:731:GLN:HG3 | 3:L1:120:LEU:HD21 | 1.87 | 0.57 |
| 4:M1:269:SER:HA | 3:V1:111:ASN:ND2 | 2.20 | 0.57 |
| 5:N1:13:SER:HB3 | 5:N1:14:LYS:HD3 | 1.86 | 0.57 |
| 1:A:18:TYR:CZ | 8:a5:90:ARG:HA | 2.40 | 0.57 |
| 3:HA:78:ARG:HD3 | 12:HA:202:CYC:CBD | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:HA:113:LEU:HD21 | 12:HA:202:CYC:HMB3 | 1.86 | 0.57 |
| 12:HA:201:CYC:CMA | 12:HA:201:CYC:HB | 2.18 | 0.57 |
| 3:LA:111:ASN:C | 11:aA:532:ALA:HB3 | 2.29 | 0.57 |
| 12:TA:302:CYC:CMA | 12:TA:302:CYC:HB | 2.18 | 0.57 |
| 2:S1:62:LYS:HG2 | 2:S1:129:GLU:HG2 | 1.85 | 0.57 |
| 12:G3:201:CYC:HB | 12:G3:201:CYC:CMA | 2.17 | 0.57 |
| 2:K3:15:GLN:C | 11:a9:745:GLY:HA2 | 2.29 | 0.57 |
| 12:K2:201:CYC:HB | 12:K2:201:CYC:CMA | 2.16 | 0.57 |
| 12:D3:201:CYC:CMA | 12:D3:201:CYC:HB | 2.18 | 0.57 |
| 3:F3:2:GLN:HG2 | 3:F3:6:THR:HG22 | 1.86 | 0.57 |
| 12:A4:201:CYC:HB | 12:A4:201:CYC:CMA | 2.17 | 0.57 |
| 3:B4:116:THR:CG2 | 4:M4:56:MET:HG2 | 2.33 | 0.57 |
| 3:B4:120:LEU:N | 4:M4:52:LEU:CD1 | 2.68 | 0.57 |
| 3:L3:75:PRO:HG2 | 11:a9:823:ILE:CD1 | 2.35 | 0.57 |
| 3:T3:2:GLN:HG2 | 3:T3:6:THR:HG22 | 1.86 | 0.57 |
| 12:Y3:201:CYC:HB | 12:Y3:201:CYC:CMA | 2.17 | 0.57 |
| 12:W4:202:CYC:HB | 12:W4:202:CYC:CMA | 2.18 | 0.57 |
| 8:K5:24:ASP:OD2 | 8:U5:36:ARG:NH1 | 2.34 | 0.57 |
| 8:M5:14:GLU:OE2 | 10:k5:538:PHE:HE2 | 1.88 | 0.57 |
| 5:Z4:42:SER:CA | 12:Z4:301:CYC:HMA1 | 2.18 | 0.57 |
| 12:F5:201:CYC:HMA2 | 12:F5:201:CYC:HB | 1.69 | 0.57 |
| 8:G5:94:TYR:OH | 1:H5:17:LYS:O | 2.20 | 0.57 |
| 1:f5:38:VAL:CG1 | 10:j5:40:VAL:HG11 | 2.34 | 0.57 |
| 12:X5:201:CYC:HB | 12:X5:201:CYC:HMA2 | 1.69 | 0.57 |
| 12:J6:202:CYC:CMD | 12:J6:202:CYC:HC | 2.18 | 0.57 |
| 12:L6:201:CYC:CMD | 12:L6:201:CYC:HC | 2.18 | 0.57 |
| 10:k5:182:ASN:HB2 | 12:k5:1201:CYC:HAB2 | 1.87 | 0.57 |
| 10:k5:820:HIS:HE1 | 10:k5:859:ILE:HD13 | 1.59 | 0.57 |
| 10:k5:1118:THR:CA | 12:k5:1204:CYC:HBA1 | 2.34 | 0.57 |
| 3:D6:127:VAL:HG22 | 12:D6:201:CYC:H3C | 1.86 | 0.57 |
| 8:O7:15:ALA:CB | 1:P7:90:ARG:NH2 | 2.67 | 0.57 |
| 8:i7:47:ARG:CZ | 1:j7:18:TYR:CD2 | 2.88 | 0.57 |
| 3:B8:2:GLN:HG2 | 3:B8:6:THR:HG22 | 1.86 | 0.57 |
| 8:s7:107:ILE:HD13 | 1:t7:13:ASP:CG | 2.30 | 0.57 |
| 8:u7:29:PHE:HZ | 1:v7:31:PHE:HZ | 1.52 | 0.57 |
| 12:W8:201:CYC:CMD | 12:W8:201:CYC:HC | 2.18 | 0.57 |
| 12:H8:201:CYC:CMD | 12:H8:201:CYC:HC | 2.18 | 0.57 |
| 3:O8:104:VAL:CA | 5:Z8:61:LYS:HE3 | 2.29 | 0.57 |
| 2:P8:18:PHE:HA | 3:Q8:91:ARG:NH2 | 1.92 | 0.57 |
| 3:Q8:2:GLN:HG2 | 3:Q8:6:THR:HG22 | 1.86 | 0.57 |
| 12:Q8:201:CYC:CMA | 12:Q8:201:CYC:HB | 2.18 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 12:L9:201:CYC:CMA | 12:L9:201:CYC:HB | 2.18 | 0.57 |
| 3:P9:2:GLN:HG2 | 3:P9:6:THR:HG22 | 1.86 | 0.57 |
| 3:J9:127:VAL:HG22 | 12:J9:202:CYC:H3C | 1.85 | 0.57 |
| 2:K9:62:LYS:HG2 | 2:K9:129:GLU:HG2 | 1.85 | 0.57 |
| 12:R9:202:CYC:HB | 12:R9:202:CYC:CMA | 2.18 | 0.57 |
| 3:V9:2:GLN:HG2 | 3:V9:6:THR:HG22 | 1.87 | 0.57 |
| 2:G1:62:LYS:HG2 | 2:G1:129:GLU:HG2 | 1.85 | 0.57 |
| 12:T1:302:CYC:CMA | 12:T1:302:CYC:HB | 2.18 | 0.57 |
| 12:Z1:201:CYC:CMA | 12:Z1:201:CYC:HB | 2.18 | 0.57 |
| 12:Z1:202:CYC:HC | 12:Z1:202:CYC:CMD | 2.18 | 0.57 |
| 12:B2:201:CYC:HB | 12:B2:201:CYC:CMA | 2.18 | 0.57 |
| 12:D2:201:CYC:HC | 12:D2:201:CYC:CMD | 2.18 | 0.57 |
| 3:FA:68:ARG:HH22 | 3:ZA:68:ARG:NH1 | 2.02 | 0.56 |
| 3:JA:65:ASP:HB2 | 11:aA:354:VAL:HG21 | 1.76 | 0.56 |
| 4:MA:20:THR:CG2 | 4:MA:67:LEU:HD11 | 2.34 | 0.56 |
| 12:OA:201:CYC:HB | 12:OA:201:CYC:CMA | 2.17 | 0.56 |
| 12:RA:201:CYC:HC | 12:RA:201:CYC:CMD | 2.18 | 0.56 |
| 12:P1:202:CYC:HB | 12:P1:202:CYC:CMA | 2.18 | 0.56 |
| 3:H2:121:GLY:HA3 | 6:M2:251:LYS:NZ | 2.20 | 0.56 |
| 12:H2:202:CYC:HC | 12:H2:202:CYC:HMD2 | 1.70 | 0.56 |
| 12:B3:201:CYC:CMA | 12:B3:201:CYC:HB | 2.18 | 0.56 |
| 3:L3:119:ALA:HB2 | 11:a9:813:PRO:C | 2.26 | 0.56 |
| 12:L3:202:CYC:O2A | 11:a9:735:VAL:C | 2.13 | 0.56 |
| 4:M3:250:THR:HG21 | 3:X3:120:LEU:HD21 | 1.87 | 0.56 |
| 4:M3:252:LEU:HD13 | 3:X3:77:ARG:HH12 | 1.69 | 0.56 |
| 12:V3:201:CYC:HC | 12:V3:201:CYC:CMD | 2.18 | 0.56 |
| 4:M4:101:ASP:N | 2:P4:13:ASP:OD2 | 2.38 | 0.56 |
| 4:M4:144:ARG:HH21 | 4:M4:204:ILE:HG22 | 1.70 | 0.56 |
| 3:Y4:88:ILE:O | 3:Y4:92:TYR:HD2 | 1.87 | 0.56 |
| 8:A5:138:THR:HG21 | 8:u7:75:GLU:HG2 | 1.87 | 0.56 |
| 12:B5:201:CYC:HBB2 | 9:z5:21:ARG:CB | 2.35 | 0.56 |
| 1:J5:70:GLY:O | 1:J5:77:ARG:NH1 | 2.38 | 0.56 |
| 12:P5:201:CYC:O2D | 10:k5:642:ARG:NH2 | 2.38 | 0.56 |
| 6:M6:115:TYR:HD2 | 12:H6:201:CYC:O2A | 1.88 | 0.56 |
| 10:j5:159:ASP:OD2 | 12:j5:1201:CYC:NC | 2.37 | 0.56 |
| 10:j5:187:ARG:CB | 10:j5:237:ASP:OD1 | 2.53 | 0.56 |
| 10:j5:1153:VAL:CG1 | 1:v7:59:ALA:O | 2.52 | 0.56 |
| 10:k5:199:THR:HG22 | 12:k5:1201:CYC:HBC1 | 1.87 | 0.56 |
| 10:k5:853:LEU:O | 10:k5:853:LEU:HD12 | 2.04 | 0.56 |
| 10:k5:939:GLN:O | 10:k5:943:THR:CG2 | 2.50 | 0.56 |
| 10:k5:992:GLU:OE2 | 10:k5:992:GLU:N | 2.37 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:k5:1052:PRO:HB3 | 11:a9:32:ARG:CZ | 2.34 | 0.56 |
| 3:D1:2:GLN:HG2 | 3:D1:6:THR:HG22 | 1.86 | 0.56 |
| 8:I7:6:LYS:HZ1 | 8:W7:19:SER:HB3 | 1.68 | 0.56 |
| 8:i7:6:LYS:HE2 | 8:s7:10:ASN:HB3 | 1.87 | 0.56 |
| 8:i7:20:PRO:HD2 | 8:s7:101:VAL:CG2 | 2.25 | 0.56 |
| 8:c7:25:ARG:NH2 | 8:m7:6:LYS:CE | 2.67 | 0.56 |
| 8:e7:53:GLN:HB2 | 8:e7:136:VAL:HG21 | 1.86 | 0.56 |
| 2:C8:62:LYS:HG2 | 2:C8:129:GLU:HG2 | 1.86 | 0.56 |
| 12:D8:202:CYC:HC | 12:D8:202:CYC:CMD | 2.18 | 0.56 |
| 12:q7:201:CYC:HC | 12:q7:201:CYC:HMD3 | 1.70 | 0.56 |
| 3:F8:115:GLU:CG | 4:M8:3:VAL:HG21 | 2.30 | 0.56 |
| 12:F8:201:CYC:CMA | 12:F8:201:CYC:HB | 2.18 | 0.56 |
| 4:M8:134:ASN:OD1 | 5:Z8:1:MET:CE | 2.52 | 0.56 |
| 12:M8:301:CYC:CMD | 12:M8:301:CYC:HC | 2.18 | 0.56 |
| 3:Q8:89:ILE:CB | 3:Q8:92:TYR:HE2 | 2.11 | 0.56 |
| 12:D9:201:CYC:CMD | 12:D9:201:CYC:HC | 2.18 | 0.56 |
| 2:E9:62:LYS:HG2 | 2:E9:129:GLU:HG2 | 1.85 | 0.56 |
| 12:F9:303:CYC:HB | 12:F9:303:CYC:CMA | 2.18 | 0.56 |
| 2:G9:62:LYS:HG2 | 2:G9:129:GLU:HG2 | 1.85 | 0.56 |
| 2:U9:62:LYS:HG2 | 2:U9:129:GLU:HG2 | 1.85 | 0.56 |
| 12:X9:201:CYC:HC | 12:X9:201:CYC:CMD | 2.18 | 0.56 |
| 11:aA:278:LEU:CD1 | 11:aA:278:LEU:H | 1.95 | 0.56 |
| 11:aA:622:ALA:N | 3:J1:14:LEU:HD21 | 2.04 | 0.56 |
| 11:aA:809:ARG:NH2 | 3:L1:112:GLY:O | 2.38 | 0.56 |
| 12:L1:201:CYC:CMA | 12:L1:201:CYC:HB | 2.18 | 0.56 |
| 4:M1:251:ASN:H | 4:M1:251:ASN:ND2 | 1.95 | 0.56 |
| 3:Z1:127:VAL:HG22 | 12:Z1:202:CYC:H3C | 1.86 | 0.56 |
| 1:Z:127:VAL:CG1 | 1:X5:15:GLN:CD | 2.76 | 0.56 |
| 12:FA:301:CYC:HMA2 | 4:MA:53:LEU:HA | 1.86 | 0.56 |
| 3:RA:2:GLN:HG2 | 3:RA:6:THR:HG22 | 1.86 | 0.56 |
| 2:WA:62:LYS:HG2 | 2:WA:129:GLU:HG2 | 1.85 | 0.56 |
| 3:D3:2:GLN:HG2 | 3:D3:6:THR:HG22 | 1.86 | 0.56 |
| 3:B4:82:CYS:CA | 12:B4:202:CYC:NC | 2.63 | 0.56 |
| 12:B4:201:CYC:CMA | 12:B4:201:CYC:HB | 2.18 | 0.56 |
| 3:L3:127:VAL:HG22 | 12:L3:202:CYC:H3C | 1.85 | 0.56 |
| 4:M3:103:GLN:HA | 4:M3:103:GLN:OE1 | 2.04 | 0.56 |
| 12:T3:301:CYC:HC | 12:T3:301:CYC:CMD | 2.18 | 0.56 |
| 3:B1:68:ARG:NH1 | 3:V1:68:ARG:HH12 | 1.92 | 0.56 |
| 3:S4:116:THR:CG2 | 3:S4:117:TYR:N | 2.67 | 0.56 |
| 12:U4:201:CYC:CMD | 12:U4:201:CYC:HC | 2.18 | 0.56 |
| 12:L4:202:CYC:CMD | 12:L4:202:CYC:HC | 2.18 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:O4:201:CYC:HC | 12:O4:201:CYC:CMD | 2.18 | 0.56 |
| 12:O4:202:CYC:HB | 12:O4:202:CYC:CMA | 2.18 | 0.56 |
| 8:M5:90:ARG:CA | 1:N5:18:TYR:CE2 | 2.87 | 0.56 |
| 12:C5:201:CYC:HC | 12:C5:201:CYC:HMD3 | 1.70 | 0.56 |
| 8:Q5:8:ILE:CG2 | 1:R5:94:TYR:HB3 | 2.35 | 0.56 |
| 8:S5:68:PRO:HB2 | 8:a5:59:PHE:HB2 | 1.81 | 0.56 |
| 6:M6:127:SER:HB2 | 12:F6:201:CYC:O2A | 2.05 | 0.56 |
| 10:j5:778:LYS:CE | 12:L7:201:CYC:HBB2 | 2.34 | 0.56 |
| 10:j5:1008:PHE:HZ | 1:v7:87:TYR:CE2 | 1.76 | 0.56 |
| 12:H6:201:CYC:CMD | 12:H6:201:CYC:HC | 2.18 | 0.56 |
| 8:E7:4:LEU:O | 8:E7:8:ILE:HG13 | 2.05 | 0.56 |
| 8:I7:15:ALA:CB | 1:J7:90:ARG:NH2 | 2.68 | 0.56 |
| 12:I7:201:CYC:HC | 12:I7:201:CYC:HMD3 | 1.70 | 0.56 |
| 8:M7:62:ARG:O | 8:M7:65:VAL:HG22 | 2.05 | 0.56 |
| 8:M7:94:TYR:OH | 1:N7:17:LYS:O | 2.24 | 0.56 |
| 8:i7:94:TYR:CE1 | 1:j7:9:ILE:CG2 | 2.77 | 0.56 |
| 8:i7:94:TYR:CD1 | 1:j7:9:ILE:CG2 | 2.88 | 0.56 |
| 12:T7:201:CYC:HB | 12:T7:201:CYC:HMA2 | 1.69 | 0.56 |
| 1:X7:118:SER:O | 9:w7:61:GLN:HG2 | 2.05 | 0.56 |
| 8:a7:89:LEU:HB3 | 1:b7:18:TYR:OH | 2.05 | 0.56 |
| 8:q7:62:ARG:O | 8:q7:65:VAL:HG22 | 2.05 | 0.56 |
| 8:u7:90:ARG:HB2 | 1:v7:18:TYR:OH | 2.05 | 0.56 |
| 9:y7:33:PRO:HG2 | 9:y7:33:PRO:O | 2.04 | 0.56 |
| 2:X8:68:GLN:CG | 3:T9:24:LEU:HB3 | 2.32 | 0.56 |
| 3:H8:84:ARG:HD2 | 11:a9:131:TYR:CZ | 2.39 | 0.56 |
| 12:J8:201:CYC:CMA | 11:a9:176:ASN:ND2 | 2.55 | 0.56 |
| 2:K8:13:ASP:O | 11:a9:242:GLY:CA | 2.53 | 0.56 |
| 3:L8:2:GLN:HG2 | 3:L8:6:THR:HG22 | 1.86 | 0.56 |
| 4:M8:120:LEU:O | 4:M8:123:GLU:HB2 | 2.04 | 0.56 |
| 3:O8:127:VAL:HG22 | 12:O8:201:CYC:H3C | 1.85 | 0.56 |
| 4:M9:205:ASP:OD2 | 5:N9:52:ARG:NH2 | 2.37 | 0.56 |
| 3:P9:127:VAL:HG22 | 12:P9:201:CYC:H3C | 1.85 | 0.56 |
| 12:J9:202:CYC:C1B | 11:a9:512:TYR:HB2 | 2.31 | 0.56 |
| 3:X9:2:GLN:HG2 | 3:X9:6:THR:HG22 | 1.86 | 0.56 |
| 12:X9:202:CYC:CMA | 12:X9:202:CYC:HB | 2.18 | 0.56 |
| 11:a9:29:ARG:HG2 | 11:a9:29:ARG:O | 2.04 | 0.56 |
| 11:a9:338:VAL:HG13 | 11:a9:340:PRO:CD | 2.35 | 0.56 |
| 11:a9:601:ALA:HB1 | 11:a9:602:PRO:CD | 2.35 | 0.56 |
| 11:aA:587:THR:OG1 | 11:aA:588:VAL:HG23 | 2.05 | 0.56 |
| 11:aA:823:ILE:CD1 | 3:L1:75:PRO:CG | 2.83 | 0.56 |
| 2:K1:62:LYS:HG2 | 2:K1:129:GLU:HG2 | 1.85 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:D2:202:CYC:HB | 12:D2:202:CYC:CMA | 2.18 | 0.56 |
| 1:Z:73:TYR:OH | 10:j5:162:TRP:NE1 | 2.38 | 0.56 |
| 12:DA:201:CYC:HC | 12:DA:201:CYC:CMD | 2.18 | 0.56 |
| 12:DA:202:CYC:HB | 12:DA:202:CYC:CMA | 2.18 | 0.56 |
| 2:EA:152:ALA:CB | 2:IA:21:ASN:HD21 | 2.16 | 0.56 |
| 3:JA:2:GLN:HG2 | 3:JA:6:THR:HG22 | 1.86 | 0.56 |
| 3:JA:114:LYS:CE | 8:S7:60:GLN:NE2 | 2.67 | 0.56 |
| 2:KA:17:ARG:CZ | 2:KA:17:ARG:CB | 2.83 | 0.56 |
| 2:KA:18:PHE:HE2 | 3:LA:48:ALA:HB1 | 1.67 | 0.56 |
| 4:MA:7:SER:C | 4:MA:14:LEU:HD13 | 2.08 | 0.56 |
| 4:MA:274:VAL:CG2 | 3:VA:77:ARG:CG | 2.83 | 0.56 |
| 5:NA:61:LYS:CD | 12:TA:301:CYC:CBB | 2.83 | 0.56 |
| 12:PA:201:CYC:HC | 12:PA:201:CYC:CMD | 2.18 | 0.56 |
| 3:ZA:2:GLN:HG2 | 3:ZA:6:THR:HG22 | 1.86 | 0.56 |
| 12:ZA:201:CYC:CMA | 12:ZA:201:CYC:HB | 2.18 | 0.56 |
| 12:P1:201:CYC:HC | 12:P1:201:CYC:CMD | 2.18 | 0.56 |
| 12:R1:202:CYC:HC | 12:R1:202:CYC:HMD2 | 1.70 | 0.56 |
| 3:H3:2:GLN:HG2 | 3:H3:6:THR:HG22 | 1.86 | 0.56 |
| 2:K3:14:SER:HA | 11:a9:746:TYR:CB | 2.31 | 0.56 |
| 12:H2:201:CYC:HC | 12:H2:201:CYC:CMD | 2.18 | 0.56 |
| 12:L2:201:CYC:HBB2 | 6:M2:229:ALA:HB2 | 1.86 | 0.56 |
| 7:N2:22:GLN:O | 7:N2:37:SER:OG | 2.24 | 0.56 |
| 3:B4:108:ARG:C | 4:M4:61:ASN:CB | 2.78 | 0.56 |
| 3:L3:2:GLN:HG2 | 3:L3:6:THR:HG22 | 1.86 | 0.56 |
| 12:L3:201:CYC:CMA | 12:L3:201:CYC:HB | 2.18 | 0.56 |
| 4:M3:51:ARG:HH22 | 11:a9:694:ARG:HH22 | 1.49 | 0.56 |
| 4:M3:92:GLU:O | 4:M3:92:GLU:HG3 | 1.99 | 0.56 |
| 12:S3:201:CYC:HB | 12:S3:201:CYC:CMA | 2.17 | 0.56 |
| 3:B1:2:GLN:HG2 | 3:B1:6:THR:HG22 | 1.86 | 0.56 |
| 12:S4:201:CYC:CMA | 12:S4:201:CYC:HB | 2.18 | 0.56 |
| 2:V4:62:LYS:HG2 | 2:V4:129:GLU:HG2 | 1.85 | 0.56 |
| 12:F4:202:CYC:HC | 12:F4:202:CYC:CMD | 2.18 | 0.56 |
| 12:H4:201:CYC:HC | 12:H4:201:CYC:CMD | 2.18 | 0.56 |
| 12:J4:201:CYC:HC | 12:J4:201:CYC:CMD | 2.18 | 0.56 |
| 4:M4:214:GLY:C | 5:Z4:27:ALA:CA | 2.78 | 0.56 |
| 4:M4:273:ILE:HG22 | 2:X4:107:ASP:OD2 | 2.06 | 0.56 |
| 12:M4:301:CYC:HC | 12:M4:301:CYC:CMD | 2.18 | 0.56 |
| 2:N4:63:PHE:HB3 | 2:N4:66:LEU:HG | 1.88 | 0.56 |
| 3:O4:111:ASN:O | 5:Z4:67:ILE:CB | 2.53 | 0.56 |
| 3:O4:111:ASN:HD22 | 5:Z4:66:ARG:HB2 | 1.71 | 0.56 |
| 3:Q4:120:LEU:CD1 | 5:Z4:39:PRO:C | 2.78 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:Y4:110:LEU:CD1 | 3:Y4:166:LYS:HB3 | 2.36 | 0.56 |
| 12:Y4:201:CYC:CMA | 12:Y4:201:CYC:HB | 2.18 | 0.56 |
| 1:J5:1:MET:O | 1:J5:1:MET:HG3 | 2.03 | 0.56 |
| 1:f5:114:GLU:CD | 10:j5:491:THR:OG1 | 2.47 | 0.56 |
| 12:U5:201:CYC:HC | 12:U5:201:CYC:HMD3 | 1.71 | 0.56 |
| 3:J6:2:GLN:HG2 | 3:J6:6:THR:HG22 | 1.86 | 0.56 |
| 12:N6:101:CYC:CMD | 12:N6:101:CYC:HC | 2.18 | 0.56 |
| 10:j5:53:ARG:C | 10:j5:56:ILE:HG22 | 2.28 | 0.56 |
| 10:j5:540:LEU:O | 10:j5:540:LEU:HG | 2.05 | 0.56 |
| 10:j5:601:LYS:HG3 | 10:j5:601:LYS:O | 2.05 | 0.56 |
| 10:k5:929:PRO:HG2 | 1:D7:147:LYS:CE | 2.33 | 0.56 |
| 10:k5:955:LEU:HD13 | 8:o7:80:LEU:CD2 | 2.35 | 0.56 |
| 10:k5:966:SER:OG | 1:p7:14:VAL:HG11 | 2.03 | 0.56 |
| 10:k5:971:VAL:O | 10:k5:971:VAL:HG22 | 2.06 | 0.56 |
| 2:A6:63:PHE:HB3 | 2:A6:66:LEU:HG | 1.88 | 0.56 |
| 12:D6:202:CYC:CMA | 12:D6:202:CYC:HB | 2.18 | 0.56 |
| 12:F6:201:CYC:CMD | 12:F6:201:CYC:HC | 2.18 | 0.56 |
| 12:F6:202:CYC:CMA | 12:F6:202:CYC:HB | 2.18 | 0.56 |
| 8:O7:15:ALA:HB1 | 1:P7:90:ARG:HH22 | 1.70 | 0.56 |
| 8:O7:107:ILE:HD13 | 1:P7:13:ASP:CG | 2.30 | 0.56 |
| 12:O7:201:CYC:HC | 12:O7:201:CYC:HMD3 | 1.70 | 0.56 |
| 12:P7:201:CYC:HB | 12:P7:201:CYC:HMA2 | 1.69 | 0.56 |
| 1:R7:118:SER:C | 9:z7:61:GLN:NE2 | 2.59 | 0.56 |
| 12:R7:201:CYC:HB | 12:R7:201:CYC:HMA2 | 1.69 | 0.56 |
| 12:S7:201:CYC:HC | 12:S7:201:CYC:HMD3 | 1.70 | 0.56 |
| 1:B7:54:GLU:OE2 | 11:a9:563:PHE:CG | 2.57 | 0.56 |
| 8:C7:107:ILE:HD13 | 1:D7:13:ASP:CG | 2.30 | 0.56 |
| 8:G7:62:ARG:O | 8:G7:65:VAL:HG22 | 2.06 | 0.56 |
| 8:I7:15:ALA:C | 1:J7:90:ARG:CZ | 2.78 | 0.56 |
| 8:K7:126:VAL:CG2 | 12:K7:201:CYC:HMC3 | 2.34 | 0.56 |
| 12:g7:201:CYC:HC | 12:g7:201:CYC:HMD3 | 1.70 | 0.56 |
| 1:h7:62:TYR:HE1 | 12:i7:201:CYC:O1D | 1.88 | 0.56 |
| 8:i7:88:TYR:HB3 | 8:i7:156:LEU:HD13 | 1.87 | 0.56 |
| 8:k7:53:GLN:HB2 | 8:k7:136:VAL:HG21 | 1.86 | 0.56 |
| 8:W7:4:LEU:O | 8:W7:8:ILE:HG13 | 2.05 | 0.56 |
| 8:a7:6:LYS:NZ | 8:o7:16:ARG:NH2 | 2.53 | 0.56 |
| 1:b7:53:LYS:HG2 | 1:b7:53:LYS:O | 2.03 | 0.56 |
| 8:c7:15:ALA:HA | 1:d7:90:ARG:NH1 | 2.08 | 0.56 |
| 8:c7:25:ARG:HH22 | 8:m7:6:LYS:HZ2 | 1.44 | 0.56 |
| 12:E1:201:CYC:HB | 12:E1:201:CYC:CMA | 2.17 | 0.56 |
| 3:B8:81:ALA:HB2 | 12:B8:202:CYC:HMD1 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:D8:202:CYC:CMA | 4:M8:35:THR:OG1 | 2.53 | 0.56 |
| 12:r7:201:CYC:HMA2 | 12:r7:201:CYC:HB | 1.70 | 0.56 |
| 12:s7:201:CYC:HC | 12:s7:201:CYC:HMD3 | 1.70 | 0.56 |
| 8:u7:34:GLU:HG3 | 1:v7:28:LYS:HD3 | 1.87 | 0.56 |
| 9:x7:34:TYR:C | 9:x7:34:TYR:CD1 | 2.83 | 0.56 |
| 9:y7:29:THR:HG22 | 9:y7:29:THR:O | 2.06 | 0.56 |
| 9:y7:32:VAL:HG11 | 9:y7:37:TRP:HE3 | 1.70 | 0.56 |
| 12:U8:202:CYC:CMA | 12:U8:202:CYC:HB | 2.18 | 0.56 |
| 2:X8:68:GLN:NE2 | 3:T9:24:LEU:CD2 | 2.67 | 0.56 |
| 12:F8:202:CYC:CMD | 12:F8:202:CYC:HC | 2.18 | 0.56 |
| 2:G8:62:LYS:HG2 | 2:G8:129:GLU:HG2 | 1.85 | 0.56 |
| 12:I8:201:CYC:HB | 12:I8:201:CYC:CMA | 2.17 | 0.56 |
| 3:J8:2:GLN:HG2 | 3:J8:6:THR:HG22 | 1.86 | 0.56 |
| 12:J8:201:CYC:HC | 12:J8:201:CYC:CMD | 2.18 | 0.56 |
| 12:L8:201:CYC:HB | 12:L8:201:CYC:CMA | 2.18 | 0.56 |
| 4:M8:19:MET:HG2 | 4:M8:59:ILE:HD13 | 1.86 | 0.56 |
| 4:M8:200:ILE:CG2 | 5:Z8:52:ARG:NH2 | 2.69 | 0.56 |
| 4:M8:225:LYS:C | 12:M8:301:CYC:O1A | 2.44 | 0.56 |
| 4:M8:268:ARG:HH12 | 3:Y8:112:GLY:H | 1.53 | 0.56 |
| 2:N8:99:ALA:HB2 | 3:O8:9:ILE:CD1 | 2.36 | 0.56 |
| 3:O8:107:ASP:CG | 5:Z8:66:ARG:CG | 2.78 | 0.56 |
| 3:O8:111:ASN:CG | 5:Z8:68:LEU:HD23 | 2.29 | 0.56 |
| 3:O8:116:THR:N | 5:Z8:70:ILE:HG22 | 2.15 | 0.56 |
| 3:Q8:88:ILE:O | 3:Q8:92:TYR:HD2 | 1.88 | 0.56 |
| 12:F1:201:CYC:HBB2 | 4:M1:38:PRO:HD3 | 1.86 | 0.56 |
| 4:M9:9:GLN:OE1 | 3:D9:108:ARG:NH1 | 2.38 | 0.56 |
| 4:M9:133:ARG:HB3 | 12:R9:201:CYC:CGA | 2.34 | 0.56 |
| 4:M9:263:PRO:HG2 | 3:V9:115:GLU:C | 2.30 | 0.56 |
| 2:O9:60:TYR:CB | 2:O9:67:THR:CG2 | 2.83 | 0.56 |
| 12:P9:201:CYC:CMD | 12:P9:201:CYC:HC | 2.18 | 0.56 |
| 3:Y8:92:TYR:HD1 | 3:Y8:105:LEU:HD22 | 1.70 | 0.56 |
| 3:Y8:113:LEU:O | 3:Y8:114:LYS:C | 2.48 | 0.56 |
| 12:D9:202:CYC:HC | 12:D9:202:CYC:HMD2 | 1.70 | 0.56 |
| 2:K9:17:ARG:CZ | 2:K9:17:ARG:CB | 2.83 | 0.56 |
| 3:R9:127:VAL:HG22 | 12:R9:201:CYC:H3C | 1.86 | 0.56 |
| 12:T9:301:CYC:HC | 12:T9:301:CYC:CMD | 2.18 | 0.56 |
| 11:a9:22:ALA:O | 11:a9:26:PRO:HD3 | 2.06 | 0.56 |
| 11:a9:632:ILE:HG23 | 11:a9:634:ALA:HB2 | 1.82 | 0.56 |
| 11:aA:22:ALA:O | 11:aA:26:PRO:HD3 | 2.05 | 0.56 |
| 11:aA:405:ILE:HG22 | 11:aA:405:ILE:O | 2.05 | 0.56 |
| 11:aA:419:ARG:HH11 | 11:aA:419:ARG:HG3 | 1.69 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:aA:450:ARG:NE | 11:aA:543:GLN:OE1 | 2.38 | 0.56 |
| 11:aA:746:TYR:HB2 | 2:K1:14:SER:CB | 2.34 | 0.56 |
| 11:aA:820:GLY:O | 11:aA:821:ARG:O | 2.24 | 0.56 |
| 12:aA:902:CYC:HC | 12:aA:902:CYC:CMD | 2.18 | 0.56 |
| 12:J1:201:CYC:HB | 12:J1:201:CYC:CMA | 2.18 | 0.56 |
| 4:M1:252:LEU:HD13 | 3:X1:77:ARG:HH12 | 1.69 | 0.56 |
| 5:N1:1:MET:CB | 5:N1:3:VAL:CG2 | 2.76 | 0.56 |
| 3:V1:2:GLN:HG2 | 3:V1:6:THR:HG22 | 1.86 | 0.56 |
| 12:Y1:201:CYC:HB | 12:Y1:201:CYC:CMA | 2.17 | 0.56 |
| 12:D2:202:CYC:HC | 12:D2:202:CYC:HMD2 | 1.70 | 0.56 |
| 12:F2:201:CYC:CMD | 12:F2:201:CYC:HC | 2.18 | 0.56 |
| 12:BA:202:CYC:CMA | 12:BA:202:CYC:HB | 2.18 | 0.56 |
| 3:FA:2:GLN:HG2 | 3:FA:6:THR:HG22 | 1.86 | 0.56 |
| 3:LA:120:LEU:CD2 | 11:aA:538:ARG:CB | 2.83 | 0.56 |
| 4:MA:251:ASN:HD22 | 4:MA:251:ASN:N | 1.92 | 0.56 |
| 5:NA:1:MET:CG | 3:RA:119:ALA:HB2 | 1.92 | 0.56 |
| 2:QA:19:LEU:O | 3:RA:45:THR:HG21 | 2.06 | 0.56 |
| 12:RA:202:CYC:HC | 12:RA:202:CYC:HMD2 | 1.70 | 0.56 |
| 12:XA:202:CYC:CMA | 12:XA:202:CYC:HB | 2.18 | 0.56 |
| 3:H3:70:GLY:CA | 11:a9:620:ALA:O | 2.53 | 0.56 |
| 3:J3:77:ARG:NH1 | 2:K3:107:ASP:CG | 2.63 | 0.56 |
| 12:J3:202:CYC:O1D | 11:a9:802:ARG:CD | 2.52 | 0.56 |
| 12:J2:202:CYC:HC | 12:J2:202:CYC:CMD | 2.18 | 0.56 |
| 12:Z3:202:CYC:HC | 12:Z3:202:CYC:HMD2 | 1.70 | 0.56 |
| 5:N3:34:LEU:CB | 3:T3:84:ARG:HH11 | 2.17 | 0.56 |
| 3:V3:2:GLN:HG2 | 3:V3:6:THR:HG22 | 1.86 | 0.56 |
| 12:L4:202:CYC:CBB | 11:aA:245:ALA:N | 2.69 | 0.56 |
| 4:M4:273:ILE:HD12 | 2:X4:108:TYR:CE1 | 2.36 | 0.56 |
| 3:Q4:2:GLN:HG2 | 3:Q4:6:THR:HG22 | 1.86 | 0.56 |
| 8:K5:29:PHE:HE1 | 8:K5:99:GLY:HA3 | 1.68 | 0.56 |
| 12:N5:201:CYC:HBB1 | 10:k5:482:GLN:HE22 | 1.70 | 0.56 |
| 8:A5:122:PRO:HG2 | 12:A5:201:CYC:OC | 2.06 | 0.56 |
| 12:D5:201:CYC:HB | 12:D5:201:CYC:HMA2 | 1.69 | 0.56 |
| 1:f5:5:ILE:HD12 | 10:j5:46:PHE:HZ | 1.59 | 0.56 |
| 8:U5:59:PHE:HE2 | 6:M6:37:GLU:OE2 | 1.76 | 0.56 |
| 7:N6:48:LEU:HB3 | 12:N6:101:CYC:CBA | 2.34 | 0.56 |
| 10:j5:328:ILE:HG12 | 10:j5:328:ILE:O | 2.04 | 0.56 |
| 10:j5:1146:THR:OG1 | 1:v7:71:MEN:CE2 | 2.52 | 0.56 |
| 10:k5:211:ALA:O | 10:k5:212:ARG:C | 2.46 | 0.56 |
| 10:k5:388:ARG:HD2 | 10:k5:393:MET:N | 2.13 | 0.56 |
| 10:k5:544:VAL:HG13 | 10:k5:564:VAL:HG21 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:C7:15:ALA:C | 1:D7:90:ARG:CZ | 2.78 | 0.56 |
| 8:g7:90:ARG:HD3 | 1:h7:18:TYR:CD1 | 2.40 | 0.56 |
| 8:Y7:62:ARG:O | 8:Y7:65:VAL:HG22 | 2.05 | 0.56 |
| 8:u7:37:LEU:HD22 | 1:v7:24:LEU:CB | 2.33 | 0.56 |
| 3:U8:2:GLN:HG2 | 3:U8:6:THR:HG22 | 1.86 | 0.56 |
| 12:W8:202:CYC:HC | 12:W8:202:CYC:HMD2 | 1.70 | 0.56 |
| 3:F8:127:VAL:HG22 | 12:F8:202:CYC:H3C | 1.86 | 0.56 |
| 4:M8:102:VAL:HG13 | 4:M8:132:LEU:HD23 | 1.88 | 0.56 |
| 12:M8:301:CYC:CMB | 3:Y8:89:ILE:HG12 | 2.34 | 0.56 |
| 12:F1:201:CYC:CMD | 12:F1:201:CYC:HC | 2.18 | 0.56 |
| 4:M9:28:HIS:NE2 | 12:B9:201:CYC:OB | 2.29 | 0.56 |
| 5:N9:53:LEU:CA | 12:T9:301:CYC:HBA2 | 2.33 | 0.56 |
| 3:B9:30:LEU:HD12 | 3:B9:30:LEU:N | 2.19 | 0.56 |
| 3:B9:107:ASP:CG | 11:a9:382:ASN:ND2 | 2.58 | 0.56 |
| 12:H9:201:CYC:CMA | 12:H9:201:CYC:HB | 2.18 | 0.56 |
| 12:V9:202:CYC:CMA | 12:V9:202:CYC:HB | 2.18 | 0.56 |
| 12:Z9:202:CYC:CMD | 12:Z9:202:CYC:HC | 2.18 | 0.56 |
| 11:aA:819:SER:O | 11:aA:819:SER:OG | 2.15 | 0.56 |
| 11:aA:823:ILE:O | 11:aA:823:ILE:HG23 | 2.04 | 0.56 |
| 12:aA:901:CYC:CMD | 12:aA:901:CYC:HC | 2.18 | 0.56 |
| 3:J1:2:GLN:HG2 | 3:J1:6:THR:HG22 | 1.86 | 0.56 |
| 4:M1:20:THR:CG2 | 4:M1:67:LEU:HD11 | 2.34 | 0.56 |
| 12:T1:301:CYC:HC | 12:T1:301:CYC:CMD | 2.18 | 0.56 |
| 2:EA:33:ARG:CG | 2:IA:25:GLN:HE22 | 2.16 | 0.56 |
| 2:EA:99:ALA:HB2 | 3:FA:9:ILE:CD1 | 2.36 | 0.56 |
| 3:FA:151:GLY:O | 3:F9:150:ARG:CZ | 2.54 | 0.56 |
| 4:MA:205:ASP:OD2 | 5:NA:52:ARG:NH2 | 2.37 | 0.56 |
| 4:MA:274:VAL:HG22 | 3:VA:77:ARG:CG | 2.35 | 0.56 |
| 12:TA:301:CYC:HC | 12:TA:301:CYC:CMD | 2.18 | 0.56 |
| 12:XA:201:CYC:CMD | 12:XA:201:CYC:HC | 2.18 | 0.56 |
| 2:O1:99:ALA:HB2 | 3:P1:9:ILE:CD1 | 2.36 | 0.56 |
| 3:R1:127:VAL:HG22 | 12:R1:201:CYC:H3C | 1.85 | 0.56 |
| 2:G3:107:ASP:CB | 3:L3:77:ARG:NH1 | 2.69 | 0.56 |
| 12:H3:201:CYC:CMA | 12:H3:201:CYC:HB | 2.18 | 0.56 |
| 3:L2:77:ARG:NH1 | 6:M2:70:GLU:HG2 | 2.13 | 0.56 |
| 12:D3:202:CYC:CMD | 12:D3:202:CYC:HC | 2.18 | 0.56 |
| 12:D4:201:CYC:CMA | 12:D4:201:CYC:HB | 2.18 | 0.56 |
| 12:P3:201:CYC:HC | 12:P3:201:CYC:CMD | 2.18 | 0.56 |
| 12:R3:202:CYC:CMA | 12:R3:202:CYC:HB | 2.18 | 0.56 |
| 12:T3:302:CYC:CMA | 12:T3:302:CYC:HB | 2.18 | 0.56 |
| 3:B1:85:ASP:CG | 12:B1:202:CYC:HD | 2.10 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M4:95:ALA:H | 3:Q4:88:ILE:CD1 | 2.18 | 0.56 |
| 4:M4:103:GLN:HA | 4:M4:103:GLN:OE1 | 2.04 | 0.56 |
| 3:O4:104:VAL:HG22 | 5:Z4:61:LYS:NZ | 2.20 | 0.56 |
| 3:Q4:72:ASN:O | 12:Z4:301:CYC:HMD1 | 2.03 | 0.56 |
| 8:M5:90:ARG:CZ | 1:N5:16:GLY:C | 2.78 | 0.56 |
| 5:Z4:41:GLN:HG3 | 12:Z4:301:CYC:CAB | 2.35 | 0.56 |
| 8:A5:65:VAL:HG23 | 8:A5:66:VAL:N | 2.21 | 0.56 |
| 8:G5:122:PRO:O | 12:G5:201:CYC:HMC2 | 2.01 | 0.56 |
| 8:c5:62:ARG:O | 8:c5:65:VAL:HG22 | 2.05 | 0.56 |
| 1:X5:143:PRO:HG2 | 8:a5:38:ARG:NE | 2.20 | 0.56 |
| 8:Y5:114:GLU:OE1 | 10:k5:312:TYR:C | 2.47 | 0.56 |
| 10:j5:66:MET:HE3 | 10:j5:66:MET:CA | 2.23 | 0.56 |
| 10:j5:221:LYS:HZ1 | 10:j5:221:LYS:C | 2.12 | 0.56 |
| 10:j5:286:VAL:HB | 10:j5:293:LYS:HE2 | 1.88 | 0.56 |
| 10:j5:431:GLN:HA | 10:j5:431:GLN:NE2 | 2.20 | 0.56 |
| 10:j5:971:VAL:HG13 | 1:t7:76:ARG:CZ | 2.35 | 0.56 |
| 10:j5:974:LEU:CG | 1:v7:1:MET:H2 | 2.12 | 0.56 |
| 10:j5:1026:LYS:C | 10:j5:1028:ASN:H | 2.12 | 0.56 |
| 10:k5:431:GLN:HA | 10:k5:431:GLN:NE2 | 2.20 | 0.56 |
| 10:k5:540:LEU:O | 10:k5:540:LEU:HG | 2.06 | 0.56 |
| 10:k5:723:GLN:HE21 | 10:k5:723:GLN:CA | 2.18 | 0.56 |
| 10:k5:1043:GLU:CD | 8:Y7:14:GLU:HG2 | 2.31 | 0.56 |
| 2:C6:99:ALA:HB2 | 3:D6:9:ILE:CD1 | 2.36 | 0.56 |
| 8:G7:53:GLN:HB2 | 8:G7:136:VAL:HG21 | 1.86 | 0.56 |
| 8:I7:37:LEU:HD11 | 1:J7:31:PHE:CE2 | 2.39 | 0.56 |
| 8:i7:4:LEU:O | 8:i7:8:ILE:HG13 | 2.05 | 0.56 |
| 12:U7:201:CYC:HC | 12:U7:201:CYC:HMD3 | 1.70 | 0.56 |
| 12:a7:201:CYC:HC | 12:a7:201:CYC:HMD3 | 1.71 | 0.56 |
| 1:f7:67:ARG:CG | 11:aA:311:LEU:CD2 | 2.76 | 0.56 |
| 3:D8:127:VAL:HG22 | 12:D8:202:CYC:H3C | 1.86 | 0.56 |
| 3:W8:2:GLN:HG2 | 3:W8:6:THR:HG22 | 1.86 | 0.56 |
| 3:O8:2:GLN:HG2 | 3:O8:6:THR:HG22 | 1.86 | 0.56 |
| 3:S8:116:THR:HG23 | 3:S8:117:TYR:H | 1.70 | 0.56 |
| 12:J9:202:CYC:CMD | 12:J9:202:CYC:HC | 2.18 | 0.56 |
| 2:G1:107:ASP:CB | 3:L1:77:ARG:NH1 | 2.69 | 0.56 |
| 12:a9:901:CYC:CMD | 12:a9:901:CYC:HC | 2.18 | 0.56 |
| 11:aA:338:VAL:HG13 | 11:aA:340:PRO:CD | 2.35 | 0.56 |
| 3:L1:2:GLN:HG2 | 3:L1:6:THR:HG22 | 1.86 | 0.56 |
| 1:A:76:ARG:HH21 | 10:k5:16:LEU:HD12 | 1.69 | 0.56 |
| 2:GA:99:ALA:HB2 | 3:HA:9:ILE:CD1 | 2.36 | 0.56 |
| 2:IA:99:ALA:HB2 | 3:JA:9:ILE:CD1 | 2.36 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:QA:84:ARG:NH1 | 3:TA:67:ILE:HD12 | 2.18 | 0.56 |
| 3:J3:77:ARG:HE | 2:K3:111:ALA:HB2 | 1.68 | 0.56 |
| 2:K3:115:GLU:OE2 | 11:a9:670:LEU:HD23 | 2.06 | 0.56 |
| 3:H2:2:GLN:HG2 | 3:H2:6:THR:HG22 | 1.86 | 0.56 |
| 6:M2:26:PHE:CA | 8:O5:83:ARG:HD2 | 2.35 | 0.56 |
| 2:A3:63:PHE:HB3 | 2:A3:66:LEU:HG | 1.88 | 0.56 |
| 3:B4:85:ASP:C | 12:B4:202:CYC:HBC3 | 2.29 | 0.56 |
| 3:D4:150:ARG:HH11 | 2:C1:140:SER:HB2 | 1.68 | 0.56 |
| 2:S3:99:ALA:HB2 | 3:T3:9:ILE:CD1 | 2.36 | 0.56 |
| 3:B1:127:VAL:CG2 | 12:B1:202:CYC:HMC3 | 2.36 | 0.56 |
| 2:I4:112:GLY:H | 11:aA:133:LEU:CD2 | 2.18 | 0.56 |
| 4:M4:95:ALA:N | 3:Q4:88:ILE:HD13 | 2.19 | 0.56 |
| 4:M4:144:ARG:NH2 | 5:Z4:59:ARG:HH11 | 1.87 | 0.56 |
| 3:Q4:82:CYS:CA | 12:Z4:301:CYC:HAC2 | 2.33 | 0.56 |
| 3:Q4:84:ARG:NH1 | 5:Z4:31:TRP:HB2 | 2.21 | 0.56 |
| 3:Q4:103:SER:O | 3:Q4:105:LEU:N | 2.38 | 0.56 |
| 8:M5:62:ARG:O | 8:M5:65:VAL:HG22 | 2.06 | 0.56 |
| 3:Y4:2:GLN:HG2 | 3:Y4:6:THR:HG22 | 1.86 | 0.56 |
| 12:J5:201:CYC:HB | 12:J5:201:CYC:HMA2 | 1.69 | 0.56 |
| 12:T5:201:CYC:HB | 12:T5:201:CYC:HMA2 | 1.69 | 0.56 |
| 8:Y5:65:VAL:HG23 | 8:Y5:66:VAL:N | 2.21 | 0.56 |
| 6:M6:68:THR:N | 3:H6:14:LEU:HD21 | 2.21 | 0.56 |
| 9:i5:8:THR:CB | 9:i5:52:LEU:HB2 | 2.36 | 0.56 |
| 10:j5:227:ILE:HG22 | 10:j5:227:ILE:O | 2.06 | 0.56 |
| 10:j5:929:PRO:CB | 1:J7:147:LYS:HG2 | 2.35 | 0.56 |
| 10:j5:1025:LEU:CA | 10:j5:1030:ILE:CG2 | 2.79 | 0.56 |
| 10:j5:1146:THR:OG1 | 1:v7:71:MEN:ND2 | 2.38 | 0.56 |
| 10:k5:286:VAL:CB | 10:k5:293:LYS:HE2 | 2.36 | 0.56 |
| 10:k5:965:GLN:CA | 1:n7:69:GLY:HA2 | 2.29 | 0.56 |
| 1:D7:67:ARG:O | 1:D7:68:PRO:C | 2.49 | 0.56 |
| 1:J7:67:ARG:O | 1:J7:68:PRO:C | 2.49 | 0.56 |
| 8:i7:46:ALA:HB3 | 8:i7:140:LEU:HD12 | 1.85 | 0.56 |
| 8:U7:35:ARG:NH2 | 8:U7:144:ASP:CB | 2.61 | 0.56 |
| 12:Y7:201:CYC:HC | 12:Y7:201:CYC:HMD3 | 1.70 | 0.56 |
| 1:b7:75:THR:HG22 | 8:c7:115:MET:CE | 2.34 | 0.56 |
| 8:c7:43:LEU:HD21 | 8:c7:149:ALA:CB | 2.32 | 0.56 |
| 2:E8:99:ALA:HB2 | 3:F8:9:ILE:CD1 | 2.36 | 0.56 |
| 8:m7:107:ILE:HD13 | 1:n7:13:ASP:CG | 2.30 | 0.56 |
| 8:o7:34:GLU:HG3 | 1:p7:28:LYS:HD3 | 1.87 | 0.56 |
| 1:t7:75:THR:HG22 | 8:u7:115:MET:SD | 2.45 | 0.56 |
| 9:z7:15:LYS:HD2 | 9:z7:16:ARG:HB3 | 1.86 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:W8:75:PRO:HB2 | 2:X8:108:TYR:O | 2.06 | 0.56 |
| 2:X8:57:GLN:HA | 3:T9:32:LYS:CE | 2.34 | 0.56 |
| 3:F8:91:ARG:NH2 | 11:a9:140:GLN:HE21 | 2.00 | 0.56 |
| 2:I8:112:GLY:N | 11:a9:133:LEU:HD21 | 2.20 | 0.56 |
| 12:J8:202:CYC:HB | 12:J8:202:CYC:CMA | 2.18 | 0.56 |
| 3:S8:2:GLN:HG2 | 3:S8:6:THR:HG22 | 1.86 | 0.56 |
| 3:F1:127:VAL:HG22 | 12:F1:201:CYC:H3C | 1.86 | 0.56 |
| 2:Q9:99:ALA:HB2 | 3:R9:9:ILE:CD1 | 2.36 | 0.56 |
| 12:Y8:201:CYC:CMA | 12:Y8:201:CYC:HB | 2.18 | 0.56 |
| 12:B9:202:CYC:HB | 12:B9:202:CYC:CMA | 2.18 | 0.56 |
| 12:F9:302:CYC:HC | 12:F9:302:CYC:HMD2 | 1.70 | 0.56 |
| 12:F9:302:CYC:CMA | 12:F9:302:CYC:HB | 2.18 | 0.56 |
| 2:I9:99:ALA:HB2 | 3:J9:9:ILE:CD1 | 2.36 | 0.56 |
| 12:J9:201:CYC:CMA | 12:J9:201:CYC:HB | 2.18 | 0.56 |
| 12:R9:201:CYC:HC | 12:R9:201:CYC:CMD | 2.18 | 0.56 |
| 12:V9:201:CYC:HC | 12:V9:201:CYC:CMD | 2.18 | 0.56 |
| 2:W9:99:ALA:HB2 | 3:X9:9:ILE:CD1 | 2.36 | 0.56 |
| 11:a9:75:ALA:CB | 11:a9:81:ASP:HB3 | 1.92 | 0.56 |
| 11:a9:577:GLU:OE2 | 11:a9:577:GLU:HA | 2.05 | 0.56 |
| 11:a9:581:ARG:HG3 | 11:a9:581:ARG:NH1 | 2.17 | 0.56 |
| 3:H1:2:GLN:HG2 | 3:H1:6:THR:HG22 | 1.86 | 0.56 |
| 12:V1:201:CYC:CMD | 12:V1:201:CYC:HC | 2.18 | 0.56 |
| 1:Z:18:TYR:CZ | 8:e5:90:ARG:CA | 2.88 | 0.56 |
| 1:Z:83:ARG:HD3 | 10:j5:259:PRO:HD3 | 1.88 | 0.56 |
| 3:HA:78:ARG:CG | 12:HA:202:CYC:HAD1 | 2.35 | 0.56 |
| 3:HA:107:ASP:HB3 | 11:aA:445:THR:HG23 | 1.88 | 0.56 |
| 4:MA:192:GLN:O | 4:MA:192:GLN:HG3 | 2.05 | 0.56 |
| 2:SA:39:GLU:N | 2:X4:69:PRO:HG2 | 2.11 | 0.56 |
| 3:J2:2:GLN:HG2 | 3:J2:6:THR:HG22 | 1.86 | 0.56 |
| 12:J2:201:CYC:CMA | 12:J2:201:CYC:HB | 2.18 | 0.56 |
| 6:M2:45:ILE:HD12 | 8:i7:78:THR:CG2 | 2.35 | 0.56 |
| 6:M2:53:LEU:CD2 | 8:i7:80:LEU:CG | 2.53 | 0.56 |
| 12:F3:201:CYC:HBB2 | 4:M3:38:PRO:HD3 | 1.86 | 0.56 |
| 2:A4:108:TYR:O | 3:D4:75:PRO:HB2 | 2.06 | 0.56 |
| 4:M3:91:VAL:HG12 | 4:M3:91:VAL:O | 2.06 | 0.56 |
| 5:N3:66:ARG:HH12 | 3:R3:111:ASN:ND2 | 1.94 | 0.56 |
| 12:S4:202:CYC:CMD | 12:S4:202:CYC:HC | 2.18 | 0.56 |
| 3:U4:75:PRO:HB2 | 2:V4:108:TYR:O | 2.06 | 0.56 |
| 12:W4:202:CYC:HC | 12:W4:202:CYC:HMD2 | 1.70 | 0.56 |
| 3:L4:68:ARG:HH12 | 11:aA:75:ALA:HB3 | 1.65 | 0.56 |
| 12:M4:301:CYC:NA | 3:Y4:85:ASP:OD2 | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:K5:4:LEU:O | 8:K5:8:ILE:HG13 | 2.05 | 0.56 |
| 3:Y4:124:THR:C | 3:Y4:172:ALA:HA | 2.31 | 0.56 |
| 8:G5:106:GLU:OE1 | 10:j5:557:VAL:CB | 2.48 | 0.56 |
| 8:S5:90:ARG:CZ | 1:T5:16:GLY:C | 2.78 | 0.56 |
| 9:i5:6:LYS:HZ1 | 9:i5:29:THR:HG21 | 1.71 | 0.56 |
| 10:j5:1069:ARG:HD3 | 10:j5:1115:ARG:HH11 | 1.69 | 0.56 |
| 10:k5:77:VAL:CG2 | 10:k5:141:GLU:HB3 | 2.32 | 0.56 |
| 10:k5:138:PRO:CG | 10:k5:201:VAL:HG11 | 2.34 | 0.56 |
| 10:k5:1078:SER:OG | 12:k5:1203:CYC:O1A | 2.21 | 0.56 |
| 3:B6:2:GLN:HG2 | 3:B6:6:THR:HG22 | 1.86 | 0.56 |
| 12:D6:201:CYC:CMD | 12:D6:201:CYC:HC | 2.18 | 0.56 |
| 8:S7:53:GLN:HB2 | 8:S7:136:VAL:HG21 | 1.86 | 0.56 |
| 1:B7:136:VAL:CG1 | 11:a9:563:PHE:HZ | 2.08 | 0.56 |
| 12:F7:201:CYC:HMA2 | 12:F7:201:CYC:HB | 1.69 | 0.56 |
| 8:G7:94:TYR:OH | 1:H7:17:LYS:O | 2.24 | 0.56 |
| 8:g7:63:PRO:CG | 11:aA:334:LYS:HA | 2.36 | 0.56 |
| 8:g7:89:LEU:HB3 | 1:h7:18:TYR:OH | 2.05 | 0.56 |
| 8:i7:20:PRO:CD | 8:s7:101:VAL:CG2 | 2.81 | 0.56 |
| 12:k7:201:CYC:HC | 12:k7:201:CYC:HMD3 | 1.71 | 0.56 |
| 8:o7:17:TYR:CD2 | 1:p7:93:THR:CB | 2.89 | 0.56 |
| 8:q7:53:GLN:HB2 | 8:q7:136:VAL:HG21 | 1.86 | 0.56 |
| 8:u7:4:LEU:O | 8:u7:8:ILE:HG13 | 2.05 | 0.56 |
| 8:u7:90:ARG:CB | 1:v7:18:TYR:CE2 | 2.88 | 0.56 |
| 8:u7:90:ARG:HG3 | 1:v7:18:TYR:CD2 | 2.41 | 0.56 |
| 9:x7:33:PRO:HG2 | 9:x7:33:PRO:O | 2.04 | 0.56 |
| 12:U8:202:CYC:HC | 12:U8:202:CYC:HMD2 | 1.70 | 0.56 |
| 4:M8:82:ILE:HD11 | 12:M8:301:CYC:O2D | 2.06 | 0.56 |
| 4:M8:239:PHE:CZ | 3:Y8:120:LEU:HD21 | 2.41 | 0.56 |
| 12:O8:202:CYC:CMA | 12:O8:202:CYC:HB | 2.18 | 0.56 |
| 2:P8:62:LYS:HG2 | 2:P8:129:GLU:HG2 | 1.85 | 0.56 |
| 4:M9:160:THR:HG22 | 4:M9:257:GLN:HB3 | 1.73 | 0.56 |
| 12:Y8:201:CYC:HC | 12:Y8:201:CYC:HMD2 | 1.70 | 0.56 |
| 2:C9:99:ALA:HB2 | 3:D9:9:ILE:CD1 | 2.36 | 0.56 |
| 2:U9:108:TYR:O | 3:Z9:75:PRO:HB2 | 2.06 | 0.56 |
| 2:G1:107:ASP:CG | 3:L1:77:ARG:NH1 | 2.64 | 0.56 |
| 5:N1:34:LEU:CB | 3:T1:84:ARG:HH11 | 2.17 | 0.56 |
| 3:B2:77:ARG:HH11 | 3:B2:77:ARG:CG | 2.18 | 0.56 |
| 3:F2:82:CYS:SG | 12:F2:201:CYC:HAC1 | 2.35 | 0.56 |
| 2:OA:99:ALA:HB2 | 3:PA:9:ILE:CD1 | 2.36 | 0.56 |
| 12:VA:202:CYC:CMA | 12:VA:202:CYC:HB | 2.18 | 0.56 |
| 2:A1:99:ALA:HB2 | 3:B1:9:ILE:CD1 | 2.36 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:J3:77:ARG:NH1 | 2:K3:107:ASP:CB | 2.68 | 0.56 |
| 2:K3:99:ALA:HB2 | 3:L3:9:ILE:CD1 | 2.36 | 0.56 |
| 12:F3:201:CYC:CBB | 4:M3:38:PRO:HD3 | 2.35 | 0.56 |
| 3:B4:85:ASP:C | 12:B4:202:CYC:HAC1 | 2.27 | 0.56 |
| 4:M3:205:ASP:OD2 | 5:N3:52:ARG:NH2 | 2.39 | 0.56 |
| 3:S4:9:ILE:CD1 | 2:R4:99:ALA:HB2 | 2.36 | 0.56 |
| 2:T4:99:ALA:HB2 | 3:U4:9:ILE:CD1 | 2.36 | 0.56 |
| 3:F4:107:ASP:O | 4:M4:6:THR:O | 2.23 | 0.56 |
| 3:J4:75:PRO:HB2 | 2:K4:108:TYR:O | 2.06 | 0.56 |
| 4:M4:137:ILE:HA | 5:Z4:44:TYR:HE1 | 1.71 | 0.56 |
| 3:Q4:102:ALA:HB1 | 3:Q4:166:LYS:CE | 2.16 | 0.56 |
| 8:O5:69:GLY:O | 8:A5:64:ASP:OD2 | 2.24 | 0.56 |
| 3:Y4:85:ASP:O | 3:Y4:88:ILE:HG12 | 2.06 | 0.56 |
| 5:Z4:2:SER:O | 5:Z4:2:SER:OG | 2.16 | 0.56 |
| 8:A5:103:PRO:HB3 | 10:k5:557:VAL:HG21 | 1.87 | 0.56 |
| 1:F5:106:GLU:HG3 | 9:z5:58:THR:CG2 | 2.36 | 0.56 |
| 1:H5:87:TYR:HE1 | 9:i5:20:GLY:HA2 | 1.71 | 0.56 |
| 2:C1:99:ALA:HB2 | 3:D1:9:ILE:CD1 | 2.36 | 0.56 |
| 2:C1:108:TYR:O | 3:F1:75:PRO:HB2 | 2.06 | 0.56 |
| 12:d5:201:CYC:HB | 12:d5:201:CYC:HMA2 | 1.69 | 0.56 |
| 12:e5:201:CYC:HC | 12:e5:201:CYC:HMD3 | 1.70 | 0.56 |
| 8:Q5:4:LEU:O | 8:Q5:8:ILE:HG13 | 2.05 | 0.56 |
| 12:Y5:201:CYC:HC | 12:Y5:201:CYC:HMD3 | 1.70 | 0.56 |
| 6:M6:45:ILE:HD11 | 8:c7:78:THR:CG2 | 2.36 | 0.56 |
| 6:M6:258:VAL:O | 6:M6:258:VAL:HG23 | 2.05 | 0.56 |
| 6:M6:271:VAL:HG13 | 1:d7:124:ALA:HB1 | 1.87 | 0.56 |
| 8:A7:62:ARG:O | 8:A7:65:VAL:HG22 | 2.06 | 0.56 |
| 10:j5:207:ARG:HG3 | 10:j5:224:SER:HA | 1.88 | 0.56 |
| 10:j5:1153:VAL:O | 10:j5:1153:VAL:HG12 | 2.05 | 0.56 |
| 12:j5:1202:CYC:HB | 12:j5:1202:CYC:CMA | 1.99 | 0.56 |
| 10:k5:357:LEU:HD21 | 10:k5:382:ILE:HG12 | 1.86 | 0.56 |
| 10:k5:489:ASN:C | 10:k5:490:SER:OG | 2.38 | 0.56 |
| 2:G6:99:ALA:HB2 | 3:H6:9:ILE:CD1 | 2.36 | 0.56 |
| 8:C7:29:PHE:CZ | 8:C7:98:ALA:C | 2.76 | 0.56 |
| 8:G7:120:GLN:CG | 1:L7:53:LYS:HZ1 | 2.19 | 0.56 |
| 8:K7:25:ARG:CB | 8:U7:25:ARG:NH2 | 2.67 | 0.56 |
| 12:N7:201:CYC:HB | 12:N7:201:CYC:HMA2 | 1.69 | 0.56 |
| 8:i7:50:ILE:HA | 8:i7:136:VAL:CG1 | 2.34 | 0.56 |
| 8:U7:107:ILE:HD13 | 1:V7:13:ASP:CG | 2.30 | 0.56 |
| 12:V7:201:CYC:HBB2 | 9:w7:21:ARG:HA | 1.88 | 0.56 |
| 8:c7:24:ASP:OD2 | 8:m7:36:ARG:NH1 | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:e7:65:VAL:HG23 | 8:e7:66:VAL:N | 2.21 | 0.56 |
| 8:u7:2:SER:CB | 1:v7:5:ILE:CG2 | 2.80 | 0.56 |
| 12:u7:201:CYC:HC | 12:u7:201:CYC:HMD3 | 1.70 | 0.56 |
| 12:U8:201:CYC:HC | 12:U8:201:CYC:CMD | 2.18 | 0.56 |
| 3:F8:84:ARG:NH2 | 11:a9:143:SER:CB | 2.66 | 0.56 |
| 12:M8:302:CYC:CMD | 12:M8:302:CYC:HC | 2.18 | 0.56 |
| 5:N9:61:LYS:CD | 12:T9:301:CYC:CBB | 2.83 | 0.56 |
| 5:Z8:37:HIS:NE2 | 12:Z8:301:CYC:NA | 2.52 | 0.56 |
| 3:D9:127:VAL:HG22 | 12:D9:201:CYC:H3C | 1.86 | 0.56 |
| 3:F9:142:VAL:O | 12:F9:303:CYC:CMC | 2.54 | 0.56 |
| 12:F9:301:CYC:CMD | 12:F9:301:CYC:HC | 2.18 | 0.56 |
| 3:H9:2:GLN:HG2 | 3:H9:6:THR:HG22 | 1.86 | 0.56 |
| 2:G1:99:ALA:HB2 | 3:H1:9:ILE:CD1 | 2.36 | 0.56 |
| 11:a9:245:ALA:HB2 | 12:a9:901:CYC:CAB | 2.35 | 0.56 |
| 11:aA:93:LEU:HD21 | 11:aA:252:ARG:HH12 | 1.65 | 0.56 |
| 11:aA:521:PHE:C | 11:aA:521:PHE:CD1 | 2.84 | 0.56 |
| 2:K1:99:ALA:HB2 | 3:L1:9:ILE:CD1 | 2.36 | 0.56 |
| 5:N1:36:THR:HB | 3:T1:84:ARG:CZ | 2.36 | 0.56 |
| 2:U1:108:TYR:O | 3:Z1:75:PRO:HB2 | 2.06 | 0.56 |
| 12:X1:201:CYC:HC | 12:X1:201:CYC:CMD | 2.18 | 0.56 |
| 2:AA:108:TYR:O | 3:DA:75:PRO:HB2 | 2.06 | 0.56 |
| 3:BA:2:GLN:HG2 | 3:BA:6:THR:HG22 | 1.86 | 0.56 |
| 2:IA:23:GLU:HA | 2:IA:23:GLU:OE2 | 2.06 | 0.56 |
| 3:JA:106:GLU:HB3 | 11:aA:556:LEU:HD21 | 1.88 | 0.56 |
| 2:KA:99:ALA:HB2 | 3:LA:9:ILE:CD1 | 2.36 | 0.56 |
| 2:OA:63:PHE:HB3 | 2:OA:66:LEU:HG | 1.88 | 0.56 |
| 2:UA:99:ALA:HB2 | 3:VA:9:ILE:CD1 | 2.36 | 0.56 |
| 12:VA:201:CYC:HC | 12:VA:201:CYC:CMD | 2.18 | 0.56 |
| 2:Q1:99:ALA:HB2 | 3:R1:9:ILE:CD1 | 2.36 | 0.56 |
| 12:A1:201:CYC:HB | 12:A1:201:CYC:CMA | 2.17 | 0.56 |
| 3:H3:78:ARG:CZ | 11:a9:623:ASP:CB | 2.63 | 0.56 |
| 12:B3:202:CYC:HMA1 | 11:a9:684:ASN:ND2 | 2.21 | 0.56 |
| 12:Z3:201:CYC:HC | 12:Z3:201:CYC:CMD | 2.18 | 0.56 |
| 3:B4:117:TYR:CD1 | 4:M4:53:LEU:HD13 | 2.41 | 0.56 |
| 12:L3:202:CYC:CMD | 12:L3:202:CYC:HC | 2.18 | 0.56 |
| 4:M3:260:ARG:HH11 | 4:M3:260:ARG:CG | 2.18 | 0.56 |
| 3:W4:75:PRO:HB2 | 2:X4:108:TYR:O | 2.06 | 0.56 |
| 2:E4:99:ALA:HB2 | 3:F4:9:ILE:CD1 | 2.36 | 0.56 |
| 12:H4:202:CYC:CMA | 12:H4:202:CYC:HB | 2.18 | 0.56 |
| 3:L4:68:ARG:HH11 | 11:aA:75:ALA:CB | 2.17 | 0.56 |
| 4:M4:192:GLN:O | 4:M4:192:GLN:HG3 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:M4:233:GLU:OE2 | 4:M4:268:ARG:NH1 | 2.39 | 0.56 |
| 2:N4:108:TYR:O | 3:Q4:75:PRO:HB2 | 2.06 | 0.56 |
| 8:M5:65:VAL:HG23 | 8:M5:66:VAL:N | 2.21 | 0.56 |
| 8:O5:76:LYS:C | 8:O5:78:THR:N | 2.64 | 0.56 |
| 1:X5:64:ASP:HB3 | 10:j5:704:THR:HG21 | 1.88 | 0.56 |
| 8:Y5:120:GLN:CG | 1:b5:53:LYS:HZ1 | 2.18 | 0.56 |
| 1:b5:114:GLU:CA | 10:k5:491:THR:HG23 | 2.35 | 0.56 |
| 10:j5:284:PRO:CG | 10:j5:326:GLY:HA2 | 2.19 | 0.56 |
| 10:j5:286:VAL:CB | 10:j5:293:LYS:HE2 | 2.36 | 0.56 |
| 10:j5:755:GLN:HB3 | 10:j5:879:ASP:CB | 2.36 | 0.56 |
| 10:j5:862:LEU:O | 10:j5:862:LEU:HD12 | 2.06 | 0.56 |
| 10:k5:1105:ILE:CD1 | 10:k5:1115:ARG:HH21 | 2.12 | 0.56 |
| 1:B7:136:VAL:CB | 11:a9:563:PHE:CZ | 2.89 | 0.56 |
| 8:M7:41:GLN:NE2 | 3:H9:125:ARG:HE | 2.04 | 0.56 |
| 12:M7:201:CYC:HC | 12:M7:201:CYC:HMD3 | 1.70 | 0.56 |
| 8:c7:8:ILE:CG2 | 1:d7:94:TYR:HB3 | 2.36 | 0.56 |
| 2:E1:99:ALA:HB2 | 3:F1:9:ILE:CD1 | 2.36 | 0.56 |
| 2:A8:63:PHE:HB3 | 2:A8:66:LEU:HG | 1.88 | 0.56 |
| 8:o7:2:SER:HB3 | 1:p7:5:ILE:HG21 | 1.83 | 0.56 |
| 8:u7:17:TYR:CD2 | 1:v7:93:THR:CB | 2.89 | 0.56 |
| 2:X8:16:GLY:HA2 | 4:M8:228:SER:HB3 | 1.82 | 0.56 |
| 2:O9:108:TYR:O | 3:R9:75:PRO:HB2 | 2.06 | 0.56 |
| 2:A9:99:ALA:HB2 | 3:B9:9:ILE:CD1 | 2.36 | 0.56 |
| 12:B9:201:CYC:HC | 12:B9:201:CYC:CMD | 2.18 | 0.56 |
| 3:F9:2:GLN:HG2 | 3:F9:6:THR:HG22 | 1.86 | 0.56 |
| 2:G1:108:TYR:O | 3:L1:75:PRO:HB2 | 2.06 | 0.56 |
| 11:a9:25:GLU:C | 11:a9:27:PHE:H | 2.14 | 0.56 |
| 11:aA:38:VAL:CG1 | 11:aA:39:PRO:HD2 | 2.36 | 0.56 |
| 11:aA:620:ALA:O | 3:H1:70:GLY:CA | 2.53 | 0.56 |
| 4:M1:192:GLN:O | 4:M1:192:GLN:HG3 | 2.05 | 0.56 |
| 3:V1:75:PRO:HB2 | 2:W1:108:TYR:O | 2.06 | 0.56 |
| 3:B2:2:GLN:HG2 | 3:B2:6:THR:HG22 | 1.86 | 0.56 |
| 2:E2:99:ALA:HB2 | 3:F2:9:ILE:CD1 | 2.36 | 0.56 |
| 1:Z:18:TYR:CZ | 8:e5:90:ARG:HA | 2.41 | 0.56 |
| 2:AA:99:ALA:HB2 | 3:BA:9:ILE:CD1 | 2.36 | 0.56 |
| 2:CA:99:ALA:HB2 | 3:DA:9:ILE:CD1 | 2.36 | 0.56 |
| 3:HA:75:PRO:HB2 | 2:IA:108:TYR:O | 2.06 | 0.56 |
| 3:HA:120:LEU:HD13 | 12:HA:202:CYC:HAA2 | 1.83 | 0.56 |
| 3:LA:109:CYS:O | 11:aA:532:ALA:CB | 2.50 | 0.56 |
| 2:OA:108:TYR:O | 3:RA:75:PRO:HB2 | 2.06 | 0.56 |
| 2:SA:99:ALA:HB2 | 3:TA:9:ILE:CD1 | 2.36 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:P1:75:PRO:HB2 | 2:S1:108:TYR:O | 2.06 | 0.56 |
| 12:H2:201:CYC:O2A | 6:M2:115:TYR:HD2 | 1.88 | 0.56 |
| 2:A4:99:ALA:HB2 | 3:B4:9:ILE:CD1 | 2.36 | 0.56 |
| 5:N3:36:THR:HB | 3:T3:84:ARG:CZ | 2.36 | 0.56 |
| 12:R3:201:CYC:HC | 12:R3:201:CYC:CMD | 2.18 | 0.56 |
| 12:R3:202:CYC:HC | 12:R3:202:CYC:HMD2 | 1.70 | 0.56 |
| 3:H4:75:PRO:HB2 | 2:I4:108:TYR:O | 2.06 | 0.56 |
| 4:M4:100:SER:CA | 3:Q4:1:MET:HE2 | 2.36 | 0.56 |
| 1:L5:49:THR:HG22 | 8:U5:161:GLN:NE2 | 2.21 | 0.56 |
| 5:Z4:41:GLN:CD | 12:Z4:301:CYC:HBB2 | 2.29 | 0.56 |
| 12:Z4:301:CYC:CMD | 12:Z4:301:CYC:HC | 2.19 | 0.56 |
| 12:c5:201:CYC:HC | 12:c5:201:CYC:HMD3 | 1.70 | 0.56 |
| 8:Q5:17:TYR:CD2 | 1:R5:44:ILE:HG22 | 2.40 | 0.56 |
| 1:b5:9:ILE:HG21 | 10:k5:17:PHE:CZ | 2.41 | 0.56 |
| 6:M6:127:SER:CB | 12:F6:201:CYC:O2A | 2.54 | 0.56 |
| 10:j5:246:VAL:CG2 | 10:j5:257:THR:CG2 | 2.83 | 0.56 |
| 10:j5:298:ARG:HG2 | 10:j5:298:ARG:HH11 | 1.71 | 0.56 |
| 10:j5:1008:PHE:CD1 | 12:v7:201:CYC:OB | 2.59 | 0.56 |
| 10:k5:755:GLN:HB3 | 10:k5:879:ASP:CB | 2.36 | 0.56 |
| 10:k5:1146:THR:HB | 1:p7:77:ARG:CZ | 2.23 | 0.56 |
| 10:k5:1153:VAL:O | 10:k5:1153:VAL:HG12 | 2.05 | 0.56 |
| 3:H6:75:PRO:HB2 | 2:I6:108:TYR:O | 2.06 | 0.56 |
| 12:D1:202:CYC:CMD | 12:D1:202:CYC:HC | 2.18 | 0.56 |
| 8:C7:15:ALA:HB1 | 1:D7:90:ARG:HH22 | 1.70 | 0.56 |
| 8:U7:52:LYS:NZ | 11:a9:29:ARG:NH1 | 2.53 | 0.56 |
| 8:a7:37:LEU:HA | 8:a7:97:VAL:HG12 | 1.88 | 0.56 |
| 8:a7:63:PRO:CB | 11:a9:333:GLN:O | 2.54 | 0.56 |
| 12:d7:201:CYC:HMA2 | 12:d7:201:CYC:HB | 1.69 | 0.56 |
| 12:B8:202:CYC:O2D | 4:M8:50:ASP:HA | 2.05 | 0.56 |
| 2:C8:99:ALA:HB2 | 3:D8:9:ILE:CD1 | 2.36 | 0.56 |
| 1:n7:75:THR:HG22 | 8:o7:115:MET:SD | 2.46 | 0.56 |
| 8:o7:90:ARG:CB | 1:p7:18:TYR:CE2 | 2.88 | 0.56 |
| 8:u7:80:LEU:HD12 | 12:u7:201:CYC:HAD1 | 1.86 | 0.56 |
| 2:I8:14:SER:CB | 11:a9:170:PHE:CE2 | 2.89 | 0.56 |
| 4:M8:139:VAL:HG23 | 4:M8:216:ASN:CA | 2.22 | 0.56 |
| 4:M8:228:SER:HA | 3:Y8:88:ILE:CD1 | 2.33 | 0.56 |
| 3:L9:9:ILE:CD1 | 2:K9:99:ALA:HB2 | 2.36 | 0.56 |
| 3:L9:75:PRO:HB2 | 2:G9:108:TYR:O | 2.06 | 0.56 |
| 12:L9:202:CYC:HC | 12:L9:202:CYC:CMD | 2.18 | 0.56 |
| 12:P9:202:CYC:CMA | 12:P9:202:CYC:HB | 2.18 | 0.56 |
| 3:H9:126:SER:HB3 | 12:H9:202:CYC:HMC1 | 1.59 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:S9:99:ALA:HB2 | 3:T9:9:ILE:CD1 | 2.36 | 0.56 |
| 11:a9:56:ILE:O | 11:a9:56:ILE:CG2 | 2.54 | 0.56 |
| 11:a9:346:TYR:C | 11:a9:346:TYR:CD1 | 2.84 | 0.56 |
| 11:a9:587:THR:OG1 | 11:a9:588:VAL:HG23 | 2.05 | 0.56 |
| 11:aA:588:VAL:CA | 11:aA:590:PRO:CD | 2.84 | 0.56 |
| 11:aA:798:SER:C | 11:aA:800:THR:H | 2.14 | 0.56 |
| 12:H1:201:CYC:CMD | 12:H1:201:CYC:HC | 2.18 | 0.56 |
| 12:H1:202:CYC:HB | 12:H1:202:CYC:CMA | 2.18 | 0.56 |
| 12:BA:201:CYC:CMD | 12:BA:201:CYC:HC | 2.18 | 0.55 |
| 3:DA:2:GLN:HG2 | 3:DA:6:THR:HG22 | 1.86 | 0.55 |
| 3:JA:75:PRO:HB2 | 2:KA:108:TYR:O | 2.06 | 0.55 |
| 3:LA:89:ILE:HB | 3:LA:134:MET:HE1 | 1.88 | 0.55 |
| 4:MA:181:GLN:O | 4:MA:181:GLN:HG3 | 2.03 | 0.55 |
| 3:XA:75:PRO:HB2 | 2:YA:108:TYR:O | 2.06 | 0.55 |
| 2:G3:107:ASP:CG | 3:L3:77:ARG:NH1 | 2.64 | 0.55 |
| 2:G3:107:ASP:CB | 3:L3:77:ARG:CZ | 2.84 | 0.55 |
| 12:J3:202:CYC:HC | 12:J3:202:CYC:CMD | 2.18 | 0.55 |
| 2:I2:99:ALA:HB2 | 3:J2:9:ILE:CD1 | 2.36 | 0.55 |
| 2:K2:99:ALA:HB2 | 3:L2:9:ILE:CD1 | 2.36 | 0.55 |
| 3:L2:2:GLN:HG2 | 3:L2:6:THR:HG22 | 1.86 | 0.55 |
| 3:B4:75:PRO:HB2 | 2:E4:108:TYR:O | 2.06 | 0.55 |
| 12:X3:202:CYC:HC | 12:X3:202:CYC:HMD2 | 1.70 | 0.55 |
| 3:L4:65:ASP:HB2 | 11:aA:82:GLN:NE2 | 2.21 | 0.55 |
| 4:M4:48:PRO:O | 4:M4:48:PRO:HG2 | 2.06 | 0.55 |
| 3:Q4:117:TYR:CE1 | 5:Z4:39:PRO:HB2 | 2.41 | 0.55 |
| 8:G5:161:GLN:CG | 1:T5:49:THR:HG21 | 2.36 | 0.55 |
| 8:W5:4:LEU:O | 8:W5:8:ILE:HG13 | 2.05 | 0.55 |
| 8:W5:17:TYR:CD2 | 1:X5:93:THR:CB | 2.89 | 0.55 |
| 8:Y5:62:ARG:O | 8:Y5:65:VAL:HG22 | 2.05 | 0.55 |
| 8:A7:120:GLN:CG | 1:F7:53:LYS:HZ1 | 2.15 | 0.55 |
| 9:i5:34:TYR:C | 9:i5:34:TYR:CD1 | 2.83 | 0.55 |
| 10:j5:722:ILE:HD13 | 8:K7:82:LEU:HB2 | 1.89 | 0.55 |
| 8:I7:107:ILE:HD13 | 1:J7:13:ASP:CG | 2.30 | 0.55 |
| 8:c7:46:ALA:HB3 | 8:c7:140:LEU:HD12 | 1.85 | 0.55 |
| 8:c7:53:GLN:HB2 | 8:c7:136:VAL:HG21 | 1.88 | 0.55 |
| 2:C8:108:TYR:O | 3:F8:75:PRO:HB2 | 2.06 | 0.55 |
| 2:T8:99:ALA:HB2 | 3:U8:9:ILE:CD1 | 2.36 | 0.55 |
| 2:T8:115:GLU:OE2 | 3:Y8:84:ARG:NH2 | 2.28 | 0.55 |
| 2:G8:99:ALA:HB2 | 3:H8:9:ILE:CD1 | 2.36 | 0.55 |
| 3:J8:75:PRO:HB2 | 2:K8:108:TYR:O | 2.06 | 0.55 |
| 3:O8:75:PRO:HB2 | 2:R8:108:TYR:O | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:O8:201:CYC:CMD | 12:O8:201:CYC:HC | 2.18 | 0.55 |
| 4:M9:224:PHE:O | 4:M9:235:PHE:HE2 | 1.89 | 0.55 |
| 3:B9:75:PRO:HB2 | 2:E9:108:TYR:O | 2.06 | 0.55 |
| 3:V9:75:PRO:HB2 | 2:W9:108:TYR:O | 2.06 | 0.55 |
| 11:aA:426:ARG:HH21 | 11:aA:496:ARG:NE | 2.04 | 0.55 |
| 11:aA:482:TYR:CD1 | 11:aA:482:TYR:C | 2.84 | 0.55 |
| 4:M1:260:ARG:HH11 | 4:M1:260:ARG:CG | 2.18 | 0.55 |
| 2:Y1:99:ALA:HB2 | 3:Z1:9:ILE:CD1 | 2.36 | 0.55 |
| 12:DA:201:CYC:CBB | 4:MA:6:THR:HG21 | 2.36 | 0.55 |
| 2:IA:1:MET:CE | 2:IA:108:TYR:CE1 | 2.83 | 0.55 |
| 2:IA:21:ASN:O | 2:IA:22:THR:C | 2.49 | 0.55 |
| 3:LA:2:GLN:HG2 | 3:LA:6:THR:HG22 | 1.86 | 0.55 |
| 4:MA:160:THR:HG21 | 4:MA:257:GLN:CB | 2.30 | 0.55 |
| 2:QA:115:GLU:HB2 | 3:TA:80:ALA:HB1 | 1.88 | 0.55 |
| 3:TA:25:ASN:HA | 2:X4:68:GLN:HG2 | 1.88 | 0.55 |
| 12:H3:202:CYC:CMD | 12:H3:202:CYC:HC | 2.18 | 0.55 |
| 3:J3:75:PRO:HB2 | 2:K3:108:TYR:O | 2.06 | 0.55 |
| 3:J2:75:PRO:HB2 | 2:K2:108:TYR:O | 2.06 | 0.55 |
| 6:M2:31:ASP:HB3 | 8:O5:82:LEU:HB2 | 1.87 | 0.55 |
| 3:Z3:119:ALA:HB3 | 4:M3:263:PRO:HB2 | 1.78 | 0.55 |
| 12:Z3:201:CYC:HMA1 | 4:M3:163:ASN:ND2 | 2.20 | 0.55 |
| 12:Z3:201:CYC:CMA | 4:M3:163:ASN:HD21 | 2.19 | 0.55 |
| 12:B4:202:CYC:O2D | 4:M4:50:ASP:HA | 2.06 | 0.55 |
| 4:M3:224:PHE:O | 4:M3:235:PHE:HE2 | 1.89 | 0.55 |
| 5:N3:29:HIS:NE2 | 12:T3:301:CYC:OB | 2.40 | 0.55 |
| 2:O3:99:ALA:HB2 | 3:P3:9:ILE:CD1 | 2.36 | 0.55 |
| 2:O3:108:TYR:O | 3:R3:75:PRO:HB2 | 2.06 | 0.55 |
| 3:U4:108:ARG:O | 4:M4:246:ALA:CB | 2.52 | 0.55 |
| 3:F4:108:ARG:HE | 4:M4:9:GLN:CB | 2.14 | 0.55 |
| 2:G4:99:ALA:HB2 | 3:H4:9:ILE:CD1 | 2.36 | 0.55 |
| 4:M4:15:PHE:CD1 | 4:M4:71:PRO:HA | 2.38 | 0.55 |
| 4:M4:214:GLY:HA3 | 5:Z4:28:HIS:O | 2.06 | 0.55 |
| 3:Y4:87:GLU:HB3 | 3:Y4:91:ARG:HH12 | 1.70 | 0.55 |
| 1:B5:1:MET:O | 10:k5:559:THR:HB | 2.05 | 0.55 |
| 8:E5:123:ILE:O | 8:E5:126:VAL:HB | 2.07 | 0.55 |
| 8:G5:65:VAL:HG23 | 8:G5:66:VAL:N | 2.21 | 0.55 |
| 1:J5:12:TYR:CE2 | 1:J5:23:ALA:HB2 | 2.40 | 0.55 |
| 8:e5:49:ARG:NH2 | 1:R5:50:THR:CG2 | 2.66 | 0.55 |
| 8:Q5:127:ALA:HB2 | 8:Q5:161:GLN:HE22 | 1.72 | 0.55 |
| 8:S5:65:VAL:HG23 | 8:S5:66:VAL:N | 2.21 | 0.55 |
| 8:W5:18:LEU:HD22 | 1:X5:97:LEU:HD13 | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:W5:123:ILE:O | 8:W5:126:VAL:HB | 2.06 | 0.55 |
| 2:K6:99:ALA:HB2 | 3:L6:9:ILE:CD1 | 2.36 | 0.55 |
| 9:z5:10:CYS:O | 9:z5:49:GLY:CA | 2.55 | 0.55 |
| 10:j5:1150:TYR:HE1 | 11:aA:38:VAL:HG13 | 1.70 | 0.55 |
| 10:k5:298:ARG:HG2 | 10:k5:298:ARG:HH11 | 1.71 | 0.55 |
| 10:k5:946:ASP:OD1 | 10:k5:946:ASP:N | 2.38 | 0.55 |
| 3:F6:127:VAL:CA | 12:F6:201:CYC:HMC2 | 2.36 | 0.55 |
| 12:D1:202:CYC:HMA2 | 4:M1:53:LEU:HA | 1.88 | 0.55 |
| 12:C7:201:CYC:HC | 12:C7:201:CYC:HMD3 | 1.70 | 0.55 |
| 8:M7:41:GLN:HE21 | 3:H9:125:ARG:NE | 2.02 | 0.55 |
| 1:Z7:10:ASN:HD21 | 9:x7:65:THR:C | 2.15 | 0.55 |
| 1:Z7:67:ARG:HD3 | 11:a9:311:LEU:CG | 2.35 | 0.55 |
| 8:c7:88:TYR:HB3 | 8:c7:156:LEU:HD13 | 1.87 | 0.55 |
| 9:x7:29:THR:HG22 | 9:x7:29:THR:O | 2.06 | 0.55 |
| 2:X8:68:GLN:HG2 | 3:T9:25:ASN:HA | 1.88 | 0.55 |
| 4:M8:96:LYS:HZ3 | 3:Q8:113:LEU:HD22 | 1.71 | 0.55 |
| 4:M8:200:ILE:HG22 | 5:Z8:52:ARG:NH2 | 2.20 | 0.55 |
| 2:N8:63:PHE:HB3 | 2:N8:66:LEU:HG | 1.88 | 0.55 |
| 3:F1:2:GLN:HG2 | 3:F1:6:THR:HG22 | 1.86 | 0.55 |
| 12:F1:201:CYC:CBB | 4:M1:38:PRO:HD3 | 2.35 | 0.55 |
| 4:M9:6:THR:HG21 | 12:D9:201:CYC:CBB | 2.36 | 0.55 |
| 5:N9:62:ARG:NE | 2:S9:14:SER:CA | 2.56 | 0.55 |
| 2:O9:63:PHE:HB3 | 2:O9:66:LEU:HG | 1.88 | 0.55 |
| 2:G9:99:ALA:HB2 | 3:H9:9:ILE:CD1 | 2.36 | 0.55 |
| 11:a9:25:GLU:O | 11:a9:27:PHE:N | 2.40 | 0.55 |
| 11:a9:67:GLN:C | 11:a9:68:THR:CG2 | 2.79 | 0.55 |
| 11:a9:823:ILE:O | 11:a9:823:ILE:HG23 | 2.04 | 0.55 |
| 11:aA:629:LYS:CE | 11:aA:629:LYS:CA | 2.84 | 0.55 |
| 11:aA:707:PHE:CE2 | 3:L1:108:ARG:CZ | 2.87 | 0.55 |
| 11:aA:802:ARG:HB2 | 3:J1:120:LEU:HD23 | 1.87 | 0.55 |
| 3:B2:75:PRO:HB2 | 2:E2:108:TYR:O | 2.06 | 0.55 |
| 3:D2:2:GLN:HG2 | 3:D2:6:THR:HG22 | 1.86 | 0.55 |
| 1:A:76:ARG:HA | 10:k5:261:ILE:HD11 | 1.88 | 0.55 |
| 1:A:76:ARG:N | 10:k5:261:ILE:HD11 | 2.22 | 0.55 |
| 2:QA:68:GLN:HG3 | 2:QA:69:PRO:CD | 2.36 | 0.55 |
| 2:QA:81:LYS:CE | 3:TA:67:ILE:CD1 | 2.83 | 0.55 |
| 3:H2:75:PRO:HB2 | 2:I2:108:TYR:O | 2.06 | 0.55 |
| 3:H2:120:LEU:C | 6:M2:251:LYS:HZ3 | 2.14 | 0.55 |
| 12:B3:202:CYC:HMA2 | 11:a9:684:ASN:HD22 | 1.71 | 0.55 |
| 12:Z3:202:CYC:CMA | 12:Z3:202:CYC:HB | 2.18 | 0.55 |
| 12:W4:201:CYC:HC | 12:W4:201:CYC:CMD | 2.18 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:F4:110:LEU:HD21 | 3:F4:167:ALA:HA | 1.88 | 0.55 |
| 3:H4:119:ALA:CA | 11:aA:266:ASN:HD22 | 2.13 | 0.55 |
| 12:J4:202:CYC:CMA | 12:J4:202:CYC:HB | 2.18 | 0.55 |
| 4:M4:27:HIS:HD1 | 4:M4:35:THR:H | 1.25 | 0.55 |
| 2:N4:99:ALA:HB2 | 3:O4:9:ILE:CD1 | 2.36 | 0.55 |
| 3:Q4:72:ASN:CG | 12:Z4:301:CYC:CMD | 2.57 | 0.55 |
| 3:Q4:124:THR:HB | 3:Q4:172:ALA:HA | 1.89 | 0.55 |
| 12:H5:201:CYC:C4B | 9:i5:23:LEU:HB2 | 2.36 | 0.55 |
| 1:f5:27:LEU:CD1 | 10:j5:172:LEU:HD22 | 2.36 | 0.55 |
| 8:U5:83:ARG:NE | 6:M6:27:ALA:C | 2.61 | 0.55 |
| 12:V5:201:CYC:NB | 10:j5:649:PHE:CZ | 2.74 | 0.55 |
| 10:j5:1005:LEU:CD1 | 10:j5:1016:LEU:CD2 | 2.82 | 0.55 |
| 10:j5:1035:PHE:C | 10:j5:1035:PHE:CD1 | 2.84 | 0.55 |
| 10:j5:1119:LEU:HD13 | 1:t7:87:TYR:CE2 | 2.41 | 0.55 |
| 10:j5:1153:VAL:HG22 | 1:v7:125:ALA:HB1 | 1.77 | 0.55 |
| 10:k5:913:VAL:HG12 | 10:k5:913:VAL:O | 2.06 | 0.55 |
| 2:A6:99:ALA:HB2 | 3:B6:9:ILE:CD1 | 2.36 | 0.55 |
| 8:g7:25:ARG:HE | 8:u7:25:ARG:CZ | 2.18 | 0.55 |
| 8:k7:62:ARG:O | 8:k7:65:VAL:HG22 | 2.05 | 0.55 |
| 8:k7:65:VAL:HG23 | 8:k7:66:VAL:N | 2.21 | 0.55 |
| 8:U7:29:PHE:CZ | 8:U7:98:ALA:C | 2.76 | 0.55 |
| 12:V7:201:CYC:HB | 12:V7:201:CYC:HMA2 | 1.69 | 0.55 |
| 8:o7:90:ARG:HG3 | 1:p7:18:TYR:CD2 | 2.41 | 0.55 |
| 8:q7:65:VAL:HG23 | 8:q7:66:VAL:N | 2.21 | 0.55 |
| 9:y7:23:LEU:HD12 | 9:y7:23:LEU:C | 2.25 | 0.55 |
| 3:L8:78:ARG:NH2 | 11:a9:88:ALA:H | 2.03 | 0.55 |
| 3:L8:109:CYS:HA | 12:a9:901:CYC:HBB2 | 1.74 | 0.55 |
| 3:Q8:92:TYR:CE2 | 3:Q8:109:CYS:SG | 2.98 | 0.55 |
| 2:U9:99:ALA:HB2 | 3:V9:9:ILE:CD1 | 2.36 | 0.55 |
| 11:a9:38:VAL:CG1 | 11:a9:39:PRO:HD2 | 2.36 | 0.55 |
| 11:a9:166:LYS:HE3 | 11:a9:209:TYR:CE1 | 2.42 | 0.55 |
| 11:a9:588:VAL:CA | 11:a9:590:PRO:CD | 2.84 | 0.55 |
| 11:a9:731:GLN:HG2 | 11:a9:817:LEU:HD21 | 1.88 | 0.55 |
| 11:aA:56:ILE:O | 11:aA:56:ILE:CG2 | 2.54 | 0.55 |
| 11:aA:166:LYS:HE3 | 11:aA:209:TYR:CE1 | 2.42 | 0.55 |
| 11:aA:454:LEU:HD22 | 11:aA:535:ASP:OD2 | 2.00 | 0.55 |
| 3:J1:75:PRO:HB2 | 2:K1:108:TYR:O | 2.06 | 0.55 |
| 4:M1:81:ASP:N | 3:X1:111:ASN:HD21 | 2.02 | 0.55 |
| 2:U1:99:ALA:HB2 | 3:V1:9:ILE:CD1 | 2.36 | 0.55 |
| 2:EA:152:ALA:CB | 2:IA:21:ASN:OD1 | 2.54 | 0.55 |
| 12:FA:301:CYC:HBA1 | 4:MA:53:LEU:HB2 | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 4:MA:48:PRO:HG2 | 4:MA:48:PRO:O | 2.07 | 0.55 |
| 4:MA:164:ARG:NH1 | 4:MA:259:ARG:O | 2.33 | 0.55 |
| 2:QA:33:ARG:CG | 2:UA:25:GLN:CG | 2.85 | 0.55 |
| 3:TA:24:LEU:CD2 | 2:X4:68:GLN:HE21 | 2.16 | 0.55 |
| 3:J3:84:ARG:CZ | 11:a9:668:TYR:HB3 | 2.36 | 0.55 |
| 12:J3:201:CYC:CMA | 12:J3:201:CYC:HB | 2.18 | 0.55 |
| 2:K3:19:LEU:HD13 | 3:L3:98:LEU:HD22 | 1.89 | 0.55 |
| 3:B3:75:PRO:HB2 | 2:E3:108:TYR:O | 2.06 | 0.55 |
| 2:C3:99:ALA:HB2 | 3:D3:9:ILE:CD1 | 2.36 | 0.55 |
| 2:C3:108:TYR:O | 3:F3:75:PRO:HB2 | 2.06 | 0.55 |
| 5:N3:13:SER:HB3 | 5:N3:14:LYS:HD3 | 1.86 | 0.55 |
| 5:N3:66:ARG:HH11 | 3:R3:111:ASN:ND2 | 1.96 | 0.55 |
| 3:V3:75:PRO:HB2 | 2:W3:108:TYR:O | 2.06 | 0.55 |
| 2:G4:108:TYR:O | 3:L4:75:PRO:HB2 | 2.06 | 0.55 |
| 2:K4:19:LEU:HD13 | 3:L4:98:LEU:HD22 | 1.89 | 0.55 |
| 3:L4:78:ARG:NH2 | 11:aA:88:ALA:H | 2.03 | 0.55 |
| 2:N4:115:GLU:OE1 | 3:Q4:84:ARG:NH2 | 2.39 | 0.55 |
| 12:L5:201:CYC:HMA3 | 10:j5:591:ILE:HG23 | 1.88 | 0.55 |
| 1:D5:71:MEN:O | 1:D5:77:ARG:NH1 | 2.39 | 0.55 |
| 1:H5:76:ARG:CD | 9:i5:14:LEU:O | 2.55 | 0.55 |
| 8:c5:65:VAL:HG23 | 8:c5:66:VAL:N | 2.20 | 0.55 |
| 12:P5:201:CYC:HB | 12:P5:201:CYC:HMA2 | 1.69 | 0.55 |
| 8:S5:65:VAL:HG23 | 8:S5:66:VAL:HG23 | 1.89 | 0.55 |
| 8:U5:29:PHE:CZ | 8:U5:98:ALA:C | 2.76 | 0.55 |
| 8:A7:104:ILE:HG23 | 8:A7:156:LEU:HD21 | 1.89 | 0.55 |
| 10:j5:182:ASN:CB | 12:j5:1201:CYC:HAB2 | 2.36 | 0.55 |
| 10:j5:647:ARG:HG2 | 10:j5:647:ARG:O | 2.05 | 0.55 |
| 10:j5:1077:ILE:O | 12:r7:201:CYC:HBA1 | 2.06 | 0.55 |
| 10:k5:307:ARG:HH12 | 10:k5:346:GLU:CD | 2.10 | 0.55 |
| 10:k5:320:GLU:HG2 | 10:k5:320:GLU:O | 2.06 | 0.55 |
| 10:k5:743:VAL:CB | 12:D7:201:CYC:O2D | 2.50 | 0.55 |
| 10:k5:820:HIS:CD2 | 10:k5:820:HIS:C | 2.80 | 0.55 |
| 10:k5:1105:ILE:HD13 | 10:k5:1115:ARG:NH2 | 2.15 | 0.55 |
| 10:k5:1109:ASP:OD1 | 10:k5:1109:ASP:N | 2.36 | 0.55 |
| 12:L7:201:CYC:HMA2 | 12:L7:201:CYC:HB | 1.69 | 0.55 |
| 8:M7:65:VAL:HG23 | 8:M7:66:VAL:N | 2.21 | 0.55 |
| 8:W7:123:ILE:O | 8:W7:126:VAL:HB | 2.06 | 0.55 |
| 1:b7:75:THR:O | 8:c7:111:GLY:HA3 | 2.05 | 0.55 |
| 8:c7:20:PRO:CD | 8:m7:155:TYR:CG | 2.90 | 0.55 |
| 1:f7:10:ASN:CB | 9:y7:65:THR:HG1 | 2.14 | 0.55 |
| 8:m7:15:ALA:CB | 1:n7:90:ARG:NH2 | 2.68 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:q7:49:ARG:NH2 | 3:H1:62:GLU:CD | 2.64 | 0.55 |
| 8:u7:80:LEU:CD1 | 12:u7:201:CYC:CAD | 2.82 | 0.55 |
| 12:M8:302:CYC:C1D | 3:S8:77:ARG:HH12 | 2.19 | 0.55 |
| 12:M8:302:CYC:HAC1 | 3:S8:81:ALA:HB3 | 1.89 | 0.55 |
| 2:Q9:108:TYR:O | 3:T9:75:PRO:HB2 | 2.06 | 0.55 |
| 2:E9:99:ALA:HB2 | 3:F9:9:ILE:CD1 | 2.36 | 0.55 |
| 12:J9:202:CYC:HBB3 | 11:a9:516:GLN:HG2 | 1.85 | 0.55 |
| 2:Y9:19:LEU:HD13 | 3:Z9:98:LEU:HD22 | 1.89 | 0.55 |
| 2:Y9:99:ALA:HB2 | 3:Z9:9:ILE:CD1 | 2.36 | 0.55 |
| 11:a9:426:ARG:HH21 | 11:a9:496:ARG:NE | 2.04 | 0.55 |
| 11:a9:820:GLY:O | 11:a9:821:ARG:O | 2.24 | 0.55 |
| 11:aA:601:ALA:HB1 | 11:aA:602:PRO:CD | 2.35 | 0.55 |
| 11:aA:640:ALA:HB2 | 11:aA:770:TYR:CE2 | 2.41 | 0.55 |
| 11:aA:813:PRO:C | 3:L1:119:ALA:HB2 | 2.27 | 0.55 |
| 2:A2:63:PHE:HB3 | 2:A2:66:LEU:HG | 1.88 | 0.55 |
| 2:A2:99:ALA:HB2 | 3:B2:9:ILE:CD1 | 2.36 | 0.55 |
| 1:Z:16:GLY:O | 8:e5:90:ARG:NE | 2.39 | 0.55 |
| 2:QA:69:PRO:HB3 | 2:U1:47:ASN:CA | 2.21 | 0.55 |
| 2:QA:69:PRO:HD3 | 2:U1:46:SER:CA | 2.35 | 0.55 |
| 2:SA:42:ARG:NE | 2:X4:69:PRO:N | 2.54 | 0.55 |
| 2:S1:99:ALA:HB2 | 3:T1:9:ILE:CD1 | 2.36 | 0.55 |
| 2:G3:99:ALA:HB2 | 3:H3:9:ILE:CD1 | 2.36 | 0.55 |
| 3:H3:5:PHE:CZ | 3:H3:30:LEU:HD22 | 2.42 | 0.55 |
| 3:H3:75:PRO:HB2 | 2:I3:108:TYR:O | 2.06 | 0.55 |
| 2:I3:19:LEU:HD13 | 3:J3:98:LEU:HD22 | 1.89 | 0.55 |
| 2:G2:99:ALA:HB2 | 3:H2:9:ILE:CD1 | 2.36 | 0.55 |
| 3:B3:127:VAL:HG22 | 12:B3:202:CYC:CMC | 2.37 | 0.55 |
| 2:C3:19:LEU:HD13 | 3:D3:98:LEU:HD22 | 1.89 | 0.55 |
| 3:B1:68:ARG:NH1 | 3:V1:68:ARG:HH22 | 2.04 | 0.55 |
| 12:H4:201:CYC:CBB | 11:aA:259:ALA:CB | 2.79 | 0.55 |
| 4:M4:113:ILE:CD1 | 4:M4:143:VAL:HA | 2.36 | 0.55 |
| 8:G5:116:TYR:HE1 | 12:G5:201:CYC:HD | 1.54 | 0.55 |
| 1:J5:71:MEN:O | 1:J5:77:ARG:NH1 | 2.39 | 0.55 |
| 1:T5:87:TYR:CZ | 10:j5:483:PHE:CE2 | 2.95 | 0.55 |
| 8:W5:127:ALA:HB2 | 8:W5:161:GLN:HE22 | 1.72 | 0.55 |
| 6:M6:117:MET:HE3 | 3:H6:77:ARG:CD | 2.37 | 0.55 |
| 9:z5:8:THR:CB | 9:z5:52:LEU:HB2 | 2.36 | 0.55 |
| 9:z5:16:ARG:HE | 9:z5:16:ARG:CA | 2.20 | 0.55 |
| 9:z5:24:GLN:O | 9:z5:25:ASN:C | 2.31 | 0.55 |
| 9:z5:56:LEU:O | 9:z5:58:THR:N | 2.30 | 0.55 |
| 10:j5:411:TYR:CD1 | 10:j5:411:TYR:C | 2.84 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:544:VAL:HG13 | 10:j5:564:VAL:HG21 | 1.87 | 0.55 |
| 10:j5:723:GLN:HE21 | 10:j5:723:GLN:CA | 2.18 | 0.55 |
| 10:j5:769:THR:O | 10:j5:769:THR:OG1 | 2.19 | 0.55 |
| 10:k5:207:ARG:HG3 | 10:k5:224:SER:HA | 1.88 | 0.55 |
| 10:k5:230:VAL:O | 10:k5:234:LEU:CD1 | 2.55 | 0.55 |
| 2:E6:99:ALA:HB2 | 3:F6:9:ILE:CD1 | 2.36 | 0.55 |
| 3:F6:5:PHE:CZ | 3:F6:30:LEU:HD22 | 2.42 | 0.55 |
| 12:G7:201:CYC:HC | 12:G7:201:CYC:HMD3 | 1.70 | 0.55 |
| 8:I7:15:ALA:HB1 | 1:J7:90:ARG:HH22 | 1.70 | 0.55 |
| 8:M7:65:VAL:HG23 | 8:M7:66:VAL:HG23 | 1.89 | 0.55 |
| 1:d7:76:ARG:NH1 | 9:x7:3:ARG:HH22 | 2.05 | 0.55 |
| 8:o7:90:ARG:HG3 | 1:p7:18:TYR:CG | 2.42 | 0.55 |
| 8:q7:79:ALA:CB | 11:aA:53:VAL:CG2 | 2.70 | 0.55 |
| 2:K8:99:ALA:HB2 | 3:L8:9:ILE:CD1 | 2.36 | 0.55 |
| 4:M8:91:VAL:O | 4:M8:91:VAL:HG12 | 2.06 | 0.55 |
| 4:M8:197:ASP:OD1 | 5:Z8:52:ARG:NE | 2.39 | 0.55 |
| 2:O9:99:ALA:HB2 | 3:P9:9:ILE:CD1 | 2.36 | 0.55 |
| 2:E9:152:ALA:CB | 2:I9:21:ASN:OD1 | 2.54 | 0.55 |
| 2:G1:107:ASP:CB | 3:L1:77:ARG:CZ | 2.85 | 0.55 |
| 11:aA:283:GLN:CG | 11:aA:284:PRO:CD | 2.80 | 0.55 |
| 2:I1:99:ALA:HB2 | 3:J1:9:ILE:CD1 | 2.36 | 0.55 |
| 4:M1:17:VAL:HG12 | 4:M1:18:THR:N | 2.22 | 0.55 |
| 4:M1:224:PHE:O | 4:M1:235:PHE:HE2 | 1.89 | 0.55 |
| 2:W1:99:ALA:HB2 | 3:X1:9:ILE:CD1 | 2.36 | 0.55 |
| 2:A2:108:TYR:O | 3:D2:75:PRO:HB2 | 2.06 | 0.55 |
| 2:AA:65:TYR:O | 2:AA:71:GLN:CG | 2.54 | 0.55 |
| 2:CA:108:TYR:O | 3:FA:75:PRO:HB2 | 2.06 | 0.55 |
| 2:WA:19:LEU:HD13 | 3:XA:98:LEU:HD22 | 1.89 | 0.55 |
| 3:R1:5:PHE:CZ | 3:R1:30:LEU:HD22 | 2.42 | 0.55 |
| 3:H3:68:ARG:HD2 | 11:a9:615:ARG:O | 2.01 | 0.55 |
| 6:M2:50:LEU:HD21 | 8:i7:79:ALA:O | 2.00 | 0.55 |
| 3:Z3:9:ILE:CD1 | 2:Y3:99:ALA:HB2 | 2.36 | 0.55 |
| 3:Z3:75:PRO:HB2 | 2:U3:108:TYR:O | 2.06 | 0.55 |
| 3:D4:107:ASP:OD2 | 11:aA:109:ASN:OD1 | 2.16 | 0.55 |
| 3:L3:77:ARG:HD2 | 11:a9:823:ILE:HD13 | 1.87 | 0.55 |
| 3:L3:116:THR:OG1 | 11:a9:713:ASN:ND2 | 2.40 | 0.55 |
| 4:M3:17:VAL:HG12 | 4:M3:18:THR:N | 2.22 | 0.55 |
| 3:P3:5:PHE:CZ | 3:P3:30:LEU:HD22 | 2.42 | 0.55 |
| 2:Q3:108:TYR:O | 3:T3:75:PRO:HB2 | 2.06 | 0.55 |
| 3:U4:5:PHE:CZ | 3:U4:30:LEU:HD22 | 2.42 | 0.55 |
| 4:M4:27:HIS:ND1 | 4:M4:34:ASP:C | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:M4:162:ASN:O | 4:M4:166:THR:CG2 | 2.51 | 0.55 |
| 1:D5:12:TYR:CE2 | 1:D5:23:ALA:HB2 | 2.40 | 0.55 |
| 8:G5:104:ILE:HG23 | 8:G5:156:LEU:HD21 | 1.89 | 0.55 |
| 12:I5:201:CYC:HC | 12:I5:201:CYC:HMD3 | 1.70 | 0.55 |
| 3:J6:9:ILE:CD1 | 2:I6:99:ALA:HB2 | 2.36 | 0.55 |
| 3:J6:108:ARG:HH22 | 6:M6:155:ASN:CG | 2.15 | 0.55 |
| 8:A7:37:LEU:HD22 | 1:B7:24:LEU:HD22 | 1.89 | 0.55 |
| 9:z5:56:LEU:C | 9:z5:58:THR:N | 2.61 | 0.55 |
| 10:j5:283:ARG:HD3 | 10:j5:283:ARG:O | 2.06 | 0.55 |
| 10:j5:799:GLU:O | 9:w7:30:LYS:HA | 2.06 | 0.55 |
| 10:k5:930:LEU:CA | 1:D7:33:THR:HG21 | 2.32 | 0.55 |
| 8:S7:104:ILE:HG23 | 8:S7:156:LEU:HD21 | 1.89 | 0.55 |
| 12:H7:201:CYC:HB | 12:H7:201:CYC:CMA | 1.99 | 0.55 |
| 8:U7:15:ALA:CB | 9:w7:20:GLY:HA2 | 2.37 | 0.55 |
| 1:l7:17:LYS:HG2 | 11:a9:43:GLU:HG3 | 1.89 | 0.55 |
| 8:o7:2:SER:HB3 | 1:p7:5:ILE:HG22 | 1.87 | 0.55 |
| 2:T8:108:TYR:O | 3:Y8:75:PRO:HB2 | 2.06 | 0.55 |
| 4:M8:104:ALA:HB1 | 2:P8:14:SER:N | 1.93 | 0.55 |
| 2:N8:115:GLU:OE1 | 5:Z8:32:PRO:CD | 2.49 | 0.55 |
| 4:M9:185:ALA:CA | 12:V9:201:CYC:HBA2 | 2.37 | 0.55 |
| 4:M9:185:ALA:CA | 12:V9:201:CYC:CBA | 2.82 | 0.55 |
| 4:M9:233:GLU:OE2 | 4:M9:268:ARG:NH1 | 2.39 | 0.55 |
| 3:P9:75:PRO:HB2 | 2:S9:108:TYR:O | 2.06 | 0.55 |
| 2:A9:108:TYR:O | 3:D9:75:PRO:HB2 | 2.06 | 0.55 |
| 3:V9:5:PHE:CZ | 3:V9:30:LEU:HD22 | 2.42 | 0.55 |
| 11:a9:456:PHE:CD1 | 11:a9:462:ARG:NH1 | 2.75 | 0.55 |
| 11:aA:456:PHE:CD1 | 11:aA:462:ARG:NH1 | 2.75 | 0.55 |
| 3:H1:5:PHE:CZ | 3:H1:30:LEU:HD22 | 2.42 | 0.55 |
| 3:H1:75:PRO:HB2 | 2:I1:108:TYR:O | 2.06 | 0.55 |
| 2:K1:19:LEU:HD13 | 3:L1:98:LEU:HD22 | 1.89 | 0.55 |
| 12:V1:202:CYC:CMA | 12:V1:202:CYC:HB | 2.18 | 0.55 |
| 2:C2:99:ALA:HB2 | 3:D2:9:ILE:CD1 | 2.36 | 0.55 |
| 1:A:127:VAL:HG11 | 1:R5:15:GLN:HB3 | 1.87 | 0.55 |
| 3:DA:68:ARG:NH1 | 3:XA:68:ARG:HH12 | 2.04 | 0.55 |
| 2:GA:119:THR:CG2 | 3:LA:83:LEU:HD13 | 2.34 | 0.55 |
| 12:HA:202:CYC:CMD | 12:HA:202:CYC:HC | 2.18 | 0.55 |
| 2:IA:148:THR:HG21 | 12:F9:302:CYC:HMB3 | 1.89 | 0.55 |
| 12:LA:202:CYC:CMD | 12:LA:202:CYC:HC | 2.18 | 0.55 |
| 4:MA:209:TYR:C | 4:MA:209:TYR:CD1 | 2.85 | 0.55 |
| 4:MA:224:PHE:O | 4:MA:235:PHE:HE2 | 1.89 | 0.55 |
| 4:MA:233:GLU:OE2 | 4:MA:268:ARG:NH1 | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:MA:274:VAL:CG1 | 2:WA:111:ALA:CB | 2.68 | 0.55 |
| 2:QA:22:THR:O | 2:UA:4:VAL:HG22 | 2.07 | 0.55 |
| 2:UA:108:TYR:O | 3:ZA:75:PRO:HB2 | 2.06 | 0.55 |
| 3:ZA:5:PHE:CZ | 3:ZA:30:LEU:HD22 | 2.42 | 0.55 |
| 2:G3:19:LEU:HD13 | 3:H3:98:LEU:HD22 | 1.89 | 0.55 |
| 2:G3:108:TYR:O | 3:L3:75:PRO:HB2 | 2.06 | 0.55 |
| 12:H3:202:CYC:HMA2 | 11:a9:776:TYR:HB3 | 1.89 | 0.55 |
| 3:H2:84:ARG:O | 3:H2:87:GLU:N | 2.40 | 0.55 |
| 6:M2:57:GLU:OE1 | 8:i7:76:LYS:NZ | 2.33 | 0.55 |
| 2:A3:99:ALA:HB2 | 3:B3:9:ILE:CD1 | 2.36 | 0.55 |
| 3:L3:104:VAL:HG12 | 3:L3:108:ARG:NH1 | 2.21 | 0.55 |
| 5:N3:37:HIS:O | 5:N3:38:GLU:C | 2.49 | 0.55 |
| 2:E4:19:LEU:HD13 | 3:F4:98:LEU:HD22 | 1.89 | 0.55 |
| 3:H4:1:MET:H2 | 11:aA:96:THR:CG2 | 2.19 | 0.55 |
| 3:J4:108:ARG:NH2 | 11:aA:171:ARG:CA | 2.69 | 0.55 |
| 4:M4:128:ALA:O | 4:M4:142:PHE:CZ | 2.46 | 0.55 |
| 8:O5:20:PRO:HB3 | 8:E5:152:TYR:CZ | 2.41 | 0.55 |
| 12:E5:201:CYC:HC | 12:E5:201:CYC:HMD3 | 1.70 | 0.55 |
| 8:G5:119:LEU:HD21 | 12:G5:201:CYC:HAA2 | 1.89 | 0.55 |
| 8:e5:29:PHE:CZ | 8:e5:98:ALA:C | 2.76 | 0.55 |
| 1:f5:9:ILE:CG2 | 10:j5:17:PHE:HZ | 2.19 | 0.55 |
| 1:f5:114:GLU:CA | 10:j5:491:THR:CG2 | 2.84 | 0.55 |
| 8:U5:76:LYS:CG | 8:U5:77:MET:H | 2.19 | 0.55 |
| 3:J6:75:PRO:HB2 | 2:K6:108:TYR:O | 2.06 | 0.55 |
| 7:N6:22:GLN:O | 7:N6:37:SER:OG | 2.24 | 0.55 |
| 10:j5:723:GLN:HE21 | 10:j5:723:GLN:HA | 1.72 | 0.55 |
| 10:k5:879:ASP:OD1 | 10:k5:879:ASP:N | 2.29 | 0.55 |
| 10:k5:1035:PHE:CD1 | 10:k5:1035:PHE:C | 2.84 | 0.55 |
| 10:k5:1055:SER:HG | 12:k5:1203:CYC:CBB | 1.97 | 0.55 |
| 1:D7:75:THR:C | 8:E7:111:GLY:HA3 | 2.32 | 0.55 |
| 1:h7:24:LEU:O | 1:h7:24:LEU:HD23 | 2.06 | 0.55 |
| 8:i7:25:ARG:HH12 | 8:s7:6:LYS:CG | 2.09 | 0.55 |
| 8:i7:46:ALA:HB2 | 8:i7:140:LEU:HD12 | 1.87 | 0.55 |
| 8:Y7:65:VAL:HG23 | 8:Y7:66:VAL:HG23 | 1.89 | 0.55 |
| 2:A8:65:TYR:O | 2:A8:71:GLN:CG | 2.54 | 0.55 |
| 3:U8:115:GLU:OE1 | 4:M8:74:LEU:HD12 | 1.99 | 0.55 |
| 2:V8:19:LEU:HD13 | 3:W8:98:LEU:HD22 | 1.89 | 0.55 |
| 2:X8:68:GLN:HE21 | 3:T9:24:LEU:CD2 | 2.16 | 0.55 |
| 3:F8:107:ASP:C | 4:M8:8:SER:O | 2.49 | 0.55 |
| 2:I8:99:ALA:HB2 | 3:J8:9:ILE:CD1 | 2.36 | 0.55 |
| 3:J8:5:PHE:CZ | 3:J8:30:LEU:HD22 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:M8:5:THR:C | 4:M8:6:THR:HG1 | 2.05 | 0.55 |
| 3:Q8:81:ALA:HB2 | 5:Z8:36:THR:CB | 2.36 | 0.55 |
| 3:L9:111:ASN:OD1 | 11:a9:366:LEU:HD12 | 2.05 | 0.55 |
| 4:M9:263:PRO:HG2 | 3:V9:115:GLU:O | 2.07 | 0.55 |
| 4:M9:274:VAL:OXT | 3:V9:77:ARG:NH2 | 2.40 | 0.55 |
| 2:A9:63:PHE:HB3 | 2:A9:66:LEU:HG | 1.88 | 0.55 |
| 3:J9:110:LEU:C | 11:a9:518:ALA:CB | 2.80 | 0.55 |
| 3:T9:5:PHE:CZ | 3:T9:30:LEU:HD22 | 2.42 | 0.55 |
| 11:a9:287:ALA:O | 11:a9:288:ARG:CD | 2.55 | 0.55 |
| 11:a9:450:ARG:NE | 11:a9:543:GLN:OE1 | 2.38 | 0.55 |
| 11:a9:521:PHE:CD1 | 11:a9:521:PHE:C | 2.84 | 0.55 |
| 3:B2:5:PHE:CZ | 3:B2:30:LEU:HD22 | 2.42 | 0.55 |
| 1:Z:75:THR:HG1 | 10:j5:182:ASN:HA | 1.71 | 0.55 |
| 4:MA:158:PHE:CE2 | 2:UA:10:ALA:HB1 | 2.41 | 0.55 |
| 4:MA:185:ALA:CA | 12:VA:201:CYC:HBA2 | 2.37 | 0.55 |
| 4:MA:185:ALA:HB2 | 12:VA:201:CYC:O1A | 2.04 | 0.55 |
| 2:YA:99:ALA:HB2 | 3:ZA:9:ILE:CD1 | 2.36 | 0.55 |
| 2:A1:63:PHE:HB3 | 2:A1:66:LEU:HG | 1.88 | 0.55 |
| 2:I3:99:ALA:HB2 | 3:J3:9:ILE:CD1 | 2.36 | 0.55 |
| 2:G2:113:LEU:HA | 3:L2:76:ASN:HD22 | 1.62 | 0.55 |
| 3:H2:14:LEU:HD21 | 6:M2:69:ALA:N | 2.22 | 0.55 |
| 3:B4:5:PHE:CZ | 3:B4:30:LEU:HD22 | 2.42 | 0.55 |
| 2:C4:19:LEU:HD13 | 3:D4:98:LEU:HD22 | 1.89 | 0.55 |
| 2:C4:99:ALA:HB2 | 3:D4:9:ILE:CD1 | 2.36 | 0.55 |
| 12:D4:202:CYC:CMD | 12:D4:202:CYC:HC | 2.18 | 0.55 |
| 3:L3:5:PHE:CZ | 3:L3:30:LEU:HD22 | 2.42 | 0.55 |
| 4:M3:222:ARG:HH11 | 4:M3:222:ARG:CG | 2.13 | 0.55 |
| 2:Q3:99:ALA:HB2 | 3:R3:9:ILE:CD1 | 2.36 | 0.55 |
| 3:V3:5:PHE:CZ | 3:V3:30:LEU:HD22 | 2.42 | 0.55 |
| 2:V4:19:LEU:HD13 | 3:W4:98:LEU:HD22 | 1.89 | 0.55 |
| 3:F4:5:PHE:CZ | 3:F4:30:LEU:HD22 | 2.42 | 0.55 |
| 3:F4:84:ARG:NH2 | 11:aA:143:SER:HB3 | 2.22 | 0.55 |
| 2:I4:99:ALA:HB2 | 3:J4:9:ILE:CD1 | 2.36 | 0.55 |
| 2:K4:99:ALA:HB2 | 3:L4:9:ILE:CD1 | 2.36 | 0.55 |
| 3:L4:5:PHE:CZ | 3:L4:30:LEU:HD22 | 2.42 | 0.55 |
| 1:N5:110:ASN:ND2 | 10:k5:692:LEU:CB | 2.12 | 0.55 |
| 2:X4:99:ALA:HB2 | 3:Y4:9:ILE:CD1 | 2.36 | 0.55 |
| 3:Y4:104:VAL:HA | 3:Y4:108:ARG:HB3 | 1.88 | 0.55 |
| 2:C1:19:LEU:HD13 | 3:D1:98:LEU:HD22 | 1.89 | 0.55 |
| 8:c5:37:LEU:HD22 | 1:d5:24:LEU:HD22 | 1.89 | 0.55 |
| 8:Q5:17:TYR:CD2 | 1:R5:93:THR:CB | 2.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:a5:37:LEU:HA | 8:a5:97:VAL:HG12 | 1.89 | 0.55 |
| 10:j5:192:LYS:HA | 10:j5:192:LYS:HZ1 | 1.69 | 0.55 |
| 10:j5:971:VAL:O | 10:j5:971:VAL:HG22 | 2.05 | 0.55 |
| 10:j5:1008:PHE:CZ | 1:v7:83:ARG:NH1 | 2.74 | 0.55 |
| 10:k5:33:ARG:NH2 | 10:k5:39:GLU:OE2 | 2.40 | 0.55 |
| 10:k5:782:SER:OG | 1:F7:83:ARG:HD2 | 2.07 | 0.55 |
| 10:k5:862:LEU:O | 10:k5:862:LEU:HD12 | 2.06 | 0.55 |
| 2:E6:19:LEU:HD13 | 3:F6:98:LEU:HD22 | 1.89 | 0.55 |
| 3:H6:5:PHE:CZ | 3:H6:30:LEU:HD22 | 2.42 | 0.55 |
| 3:D1:5:PHE:CZ | 3:D1:30:LEU:HD22 | 2.42 | 0.55 |
| 8:Q7:22:GLU:N | 8:C7:6:LYS:HZ3 | 2.05 | 0.55 |
| 8:S7:62:ARG:O | 8:S7:65:VAL:HG22 | 2.06 | 0.55 |
| 8:C7:37:LEU:HA | 8:C7:97:VAL:HG12 | 1.89 | 0.55 |
| 8:K7:104:ILE:HG23 | 8:K7:156:LEU:HD21 | 1.89 | 0.55 |
| 8:i7:53:GLN:HB2 | 8:i7:136:VAL:HG21 | 1.88 | 0.55 |
| 8:k7:37:LEU:HD22 | 1:l7:24:LEU:HD22 | 1.89 | 0.55 |
| 1:b7:24:LEU:HD23 | 1:b7:24:LEU:O | 2.07 | 0.55 |
| 8:c7:89:LEU:HD13 | 8:c7:153:PHE:HZ | 1.67 | 0.55 |
| 8:e7:62:ARG:O | 8:e7:65:VAL:HG22 | 2.06 | 0.55 |
| 2:A8:108:TYR:O | 3:D8:75:PRO:HB2 | 2.06 | 0.55 |
| 8:m7:90:ARG:CZ | 1:n7:16:GLY:HA2 | 2.37 | 0.55 |
| 12:m7:201:CYC:HC | 12:m7:201:CYC:HMD3 | 1.70 | 0.55 |
| 8:o7:123:ILE:O | 8:o7:126:VAL:HB | 2.07 | 0.55 |
| 8:q7:104:ILE:HG23 | 8:q7:156:LEU:HD21 | 1.89 | 0.55 |
| 1:r7:17:LYS:CE | 11:aA:41:ASP:OD2 | 2.54 | 0.55 |
| 9:x7:28:PHE:N | 9:x7:28:PHE:CD1 | 2.72 | 0.55 |
| 2:X8:99:ALA:HB2 | 3:Y8:9:ILE:CD1 | 2.36 | 0.55 |
| 2:N8:115:GLU:CD | 5:Z8:31:TRP:HB3 | 2.31 | 0.55 |
| 3:L9:5:PHE:CZ | 3:L9:30:LEU:HD22 | 2.42 | 0.55 |
| 4:M9:158:PHE:CE2 | 2:U9:10:ALA:HB1 | 2.41 | 0.55 |
| 3:Y8:88:ILE:O | 3:Y8:92:TYR:CD2 | 2.60 | 0.55 |
| 2:C9:108:TYR:O | 3:F9:75:PRO:HB2 | 2.06 | 0.55 |
| 3:H9:5:PHE:CZ | 3:H9:30:LEU:HD22 | 2.42 | 0.55 |
| 3:J9:19:LEU:HD12 | 3:J9:24:LEU:HD21 | 1.89 | 0.55 |
| 3:X9:5:PHE:CZ | 3:X9:30:LEU:HD22 | 2.42 | 0.55 |
| 2:G1:19:LEU:HD13 | 3:H1:98:LEU:HD22 | 1.89 | 0.55 |
| 11:a9:578:MET:HE3 | 11:a9:582:MET:CE | 2.34 | 0.55 |
| 11:aA:91:THR:HG22 | 11:aA:96:THR:CA | 2.21 | 0.55 |
| 11:aA:776:TYR:CD1 | 12:H1:201:CYC:NB | 2.73 | 0.55 |
| 3:J1:5:PHE:CZ | 3:J1:30:LEU:HD22 | 2.42 | 0.55 |
| 4:M1:95:ALA:HB2 | 5:N1:38:GLU:OE1 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 4:M1:181:GLN:O | 4:M1:181:GLN:HG3 | 2.03 | 0.55 |
| 4:M1:233:GLU:OE2 | 4:M1:268:ARG:NH1 | 2.39 | 0.55 |
| 2:C2:108:TYR:O | 3:F2:75:PRO:HB2 | 2.06 | 0.55 |
| 3:JA:65:ASP:HB2 | 11:aA:354:VAL:HG22 | 1.79 | 0.55 |
| 4:MA:17:VAL:HG12 | 4:MA:18:THR:N | 2.22 | 0.55 |
| 4:MA:37:GLU:CD | 4:MA:40:GLN:NE2 | 2.62 | 0.55 |
| 5:NA:54:LEU:HB3 | 12:TA:301:CYC:O2A | 2.07 | 0.55 |
| 3:RA:5:PHE:CZ | 3:RA:30:LEU:HD22 | 2.42 | 0.55 |
| 3:TA:25:ASN:CB | 2:X4:64:PRO:C | 2.54 | 0.55 |
| 2:WA:99:ALA:HB2 | 3:XA:9:ILE:CD1 | 2.36 | 0.55 |
| 2:YA:19:LEU:HD13 | 3:ZA:98:LEU:HD22 | 1.89 | 0.55 |
| 3:J3:77:ARG:CZ | 2:K3:107:ASP:CB | 2.85 | 0.55 |
| 3:B3:68:ARG:NH1 | 3:V3:68:ARG:HH22 | 2.04 | 0.55 |
| 2:W3:99:ALA:HB2 | 3:X3:9:ILE:CD1 | 2.36 | 0.55 |
| 3:S4:75:PRO:HB2 | 2:P4:108:TYR:O | 2.06 | 0.55 |
| 2:T4:108:TYR:O | 3:Y4:75:PRO:HB2 | 2.06 | 0.55 |
| 2:V4:99:ALA:HB2 | 3:W4:9:ILE:CD1 | 2.36 | 0.55 |
| 3:O4:75:PRO:HB2 | 2:R4:108:TYR:O | 2.06 | 0.55 |
| 3:Q4:89:ILE:HG21 | 3:Q4:131:VAL:HG22 | 1.89 | 0.55 |
| 1:L5:82:ILE:HD12 | 8:G5:118:SER:HB2 | 1.86 | 0.55 |
| 8:M5:66:VAL:HG12 | 8:K7:68:PRO:HG3 | 1.80 | 0.55 |
| 1:D5:75:THR:HB | 8:E5:112:VAL:CA | 2.37 | 0.55 |
| 8:c5:104:ILE:HG23 | 8:c5:156:LEU:HD21 | 1.89 | 0.55 |
| 1:d5:107:ARG:HD2 | 10:j5:351:PHE:O | 2.07 | 0.55 |
| 1:f5:30:TYR:CE2 | 10:j5:47:PHE:CZ | 2.95 | 0.55 |
| 2:K6:19:LEU:HD13 | 3:L6:98:LEU:HD22 | 1.89 | 0.55 |
| 8:A7:65:VAL:HG23 | 8:A7:66:VAL:HG23 | 1.89 | 0.55 |
| 9:z5:6:LYS:CG | 9:z5:55:LYS:CB | 2.64 | 0.55 |
| 10:j5:20:VAL:O | 10:j5:24:THR:CG2 | 2.51 | 0.55 |
| 10:j5:1118:THR:OG1 | 12:j5:1202:CYC:CGA | 2.54 | 0.55 |
| 10:k5:66:MET:CE | 10:k5:66:MET:CA | 2.84 | 0.55 |
| 10:k5:822:ARG:CD | 1:B7:106:GLU:OE2 | 2.55 | 0.55 |
| 12:k5:1202:CYC:HB | 12:k5:1202:CYC:HMA3 | 1.72 | 0.55 |
| 12:k5:1204:CYC:HMA2 | 12:k5:1204:CYC:HB | 1.70 | 0.55 |
| 2:C6:108:TYR:O | 3:F6:75:PRO:HB2 | 2.06 | 0.55 |
| 1:B7:75:THR:HB | 8:C7:111:GLY:C | 2.32 | 0.55 |
| 12:J7:201:CYC:HB | 12:J7:201:CYC:HMA2 | 1.69 | 0.55 |
| 8:U7:15:ALA:CB | 1:V7:90:ARG:NH2 | 2.68 | 0.55 |
| 8:U7:37:LEU:HA | 8:U7:97:VAL:HG12 | 1.88 | 0.55 |
| 8:U7:90:ARG:CZ | 1:V7:16:GLY:HA2 | 2.37 | 0.55 |
| 8:W7:13:ALA:CA | 9:w7:46:LYS:HD3 | 2.36 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:W7:104:ILE:HG23 | 8:W7:156:LEU:HD21 | 1.89 | 0.55 |
| 8:c7:95:GLY:O | 8:c7:152:TYR:CE2 | 2.54 | 0.55 |
| 12:f7:201:CYC:HMA2 | 12:f7:201:CYC:HB | 1.69 | 0.55 |
| 1:l7:75:THR:HB | 8:m7:111:GLY:C | 2.32 | 0.55 |
| 8:s7:37:LEU:HA | 8:s7:97:VAL:HG12 | 1.89 | 0.55 |
| 8:u7:123:ILE:O | 8:u7:126:VAL:HB | 2.07 | 0.55 |
| 9:y7:9:ALA:HB3 | 9:y7:44:ILE:HD11 | 1.89 | 0.55 |
| 2:V8:99:ALA:HB2 | 3:W8:9:ILE:CD1 | 2.36 | 0.55 |
| 3:F8:104:VAL:HA | 3:F8:107:ASP:OD1 | 2.07 | 0.55 |
| 4:M8:61:ASN:OD1 | 4:M8:62:LYS:HG2 | 2.07 | 0.55 |
| 4:M8:192:GLN:O | 4:M8:192:GLN:HG3 | 2.05 | 0.55 |
| 12:F1:202:CYC:CMA | 12:F1:202:CYC:HB | 2.18 | 0.55 |
| 4:M9:91:VAL:O | 4:M9:91:VAL:HG12 | 2.06 | 0.55 |
| 3:D9:68:ARG:NH1 | 3:X9:68:ARG:HH12 | 2.04 | 0.55 |
| 2:E9:19:LEU:HD13 | 3:F9:98:LEU:HD22 | 1.89 | 0.55 |
| 2:I9:23:GLU:OE2 | 2:I9:23:GLU:HA | 2.06 | 0.55 |
| 3:J9:5:PHE:CZ | 3:J9:30:LEU:HD22 | 2.42 | 0.55 |
| 3:R9:5:PHE:CZ | 3:R9:30:LEU:HD22 | 2.42 | 0.55 |
| 2:S9:19:LEU:HD13 | 3:T9:98:LEU:HD22 | 1.89 | 0.55 |
| 11:a9:351:THR:CB | 11:a9:352:PRO:CD | 2.33 | 0.55 |
| 11:aA:426:ARG:NE | 11:aA:496:ARG:HD3 | 2.22 | 0.55 |
| 11:aA:668:TYR:HE2 | 3:J1:80:ALA:HB1 | 1.62 | 0.55 |
| 11:aA:776:TYR:CD2 | 11:aA:776:TYR:C | 2.83 | 0.55 |
| 3:F2:5:PHE:CZ | 3:F2:30:LEU:HD22 | 2.42 | 0.55 |
| 1:Z:107:ARG:HH12 | 8:e5:9:VAL:HG22 | 1.72 | 0.55 |
| 3:DA:5:PHE:CZ | 3:DA:30:LEU:HD22 | 2.42 | 0.55 |
| 12:VA:202:CYC:HC | 12:VA:202:CYC:HMD2 | 1.71 | 0.55 |
| 2:Q1:108:TYR:O | 3:T1:75:PRO:HB2 | 2.06 | 0.55 |
| 2:I2:19:LEU:HD13 | 3:J2:98:LEU:HD22 | 1.89 | 0.55 |
| 3:L2:5:PHE:CZ | 3:L2:30:LEU:HD22 | 2.42 | 0.55 |
| 3:D3:5:PHE:CZ | 3:D3:30:LEU:HD22 | 2.42 | 0.55 |
| 12:D3:202:CYC:HMA2 | 4:M3:53:LEU:HA | 1.88 | 0.55 |
| 3:B4:107:ASP:O | 4:M4:61:ASN:C | 2.49 | 0.55 |
| 3:B4:116:THR:CA | 4:M4:56:MET:CB | 2.80 | 0.55 |
| 3:D4:5:PHE:CZ | 3:D4:30:LEU:HD22 | 2.42 | 0.55 |
| 4:M3:233:GLU:OE2 | 4:M3:268:ARG:NH1 | 2.39 | 0.55 |
| 2:I4:19:LEU:HD13 | 3:J4:98:LEU:HD22 | 1.89 | 0.55 |
| 3:L4:71:GLY:CA | 11:aA:82:GLN:CD | 2.80 | 0.55 |
| 4:M4:217:VAL:HG11 | 5:Z4:30:PRO:HB3 | 1.88 | 0.55 |
| 8:K5:123:ILE:O | 8:K5:126:VAL:HB | 2.07 | 0.55 |
| 8:M5:104:ILE:HG23 | 8:M5:156:LEU:HD21 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:O5:37:LEU:HA | 8:O5:97:VAL:HG12 | 1.89 | 0.55 |
| 1:B5:2:GLN:OE1 | 10:k5:551:MET:SD | 2.64 | 0.55 |
| 8:S5:62:ARG:O | 8:S5:65:VAL:HG22 | 2.06 | 0.55 |
| 12:S5:201:CYC:HC | 12:S5:201:CYC:HMD3 | 1.70 | 0.55 |
| 8:W5:17:TYR:HD2 | 1:X5:93:THR:CG2 | 2.12 | 0.55 |
| 12:Z5:201:CYC:HMA2 | 10:k5:379:PHE:CE1 | 2.42 | 0.55 |
| 9:z5:9:ALA:HA | 9:z5:51:VAL:HA | 1.89 | 0.55 |
| 10:k5:49:ASP:OD1 | 10:k5:49:ASP:N | 2.39 | 0.55 |
| 2:A6:108:TYR:O | 3:D6:75:PRO:HB2 | 2.06 | 0.55 |
| 3:F6:82:CYS:SG | 12:F6:201:CYC:NC | 2.79 | 0.55 |
| 1:N7:106:GLU:HG3 | 9:z7:58:THR:CG2 | 2.31 | 0.55 |
| 8:g7:16:ARG:HG3 | 8:g7:16:ARG:NH1 | 2.20 | 0.55 |
| 8:i7:43:LEU:HD21 | 8:i7:149:ALA:CB | 2.32 | 0.55 |
| 8:c7:24:ASP:CG | 8:m7:36:ARG:NH1 | 2.65 | 0.55 |
| 3:B8:75:PRO:HB2 | 2:E8:108:TYR:O | 2.06 | 0.55 |
| 1:r7:75:THR:HB | 8:s7:111:GLY:C | 2.32 | 0.55 |
| 9:x7:32:VAL:HG23 | 9:x7:33:PRO:HD2 | 1.89 | 0.55 |
| 9:y7:32:VAL:HG23 | 9:y7:33:PRO:HD2 | 1.89 | 0.55 |
| 3:U8:5:PHE:CZ | 3:U8:30:LEU:HD22 | 2.42 | 0.55 |
| 2:N8:14:SER:CA | 5:Z8:62:ARG:HD2 | 2.37 | 0.55 |
| 2:R8:99:ALA:HB2 | 3:S8:9:ILE:CD1 | 2.36 | 0.55 |
| 4:M9:17:VAL:HG12 | 4:M9:18:THR:N | 2.22 | 0.55 |
| 12:P9:202:CYC:HC | 12:P9:202:CYC:HMD2 | 1.70 | 0.55 |
| 3:F9:5:PHE:CZ | 3:F9:30:LEU:HD22 | 2.42 | 0.55 |
| 11:a9:798:SER:C | 11:a9:800:THR:N | 2.62 | 0.55 |
| 3:V1:5:PHE:CZ | 3:V1:30:LEU:HD22 | 2.42 | 0.55 |
| 3:X1:75:PRO:HB2 | 2:Y1:108:TYR:O | 2.06 | 0.55 |
| 3:BA:75:PRO:HB2 | 2:EA:108:TYR:O | 2.06 | 0.54 |
| 2:CA:19:LEU:HD13 | 3:DA:98:LEU:HD22 | 1.89 | 0.54 |
| 2:GA:108:TYR:O | 3:LA:75:PRO:HB2 | 2.06 | 0.54 |
| 3:JA:5:PHE:CZ | 3:JA:30:LEU:HD22 | 2.42 | 0.54 |
| 3:LA:37:ARG:NH1 | 3:LA:97:LEU:HD12 | 2.22 | 0.54 |
| 3:LA:77:ARG:NH1 | 11:aA:538:ARG:HH21 | 2.02 | 0.54 |
| 4:MA:15:PHE:CD1 | 4:MA:71:PRO:HA | 2.38 | 0.54 |
| 4:MA:130:SER:O | 12:RA:201:CYC:HBA1 | 2.07 | 0.54 |
| 2:QA:76:ASP:HB2 | 2:U1:140:SER:C | 2.32 | 0.54 |
| 3:VA:75:PRO:HB2 | 2:WA:108:TYR:O | 2.06 | 0.54 |
| 2:O1:63:PHE:HB3 | 2:O1:66:LEU:HG | 1.88 | 0.54 |
| 2:G3:111:ALA:CB | 3:L3:77:ARG:CG | 2.68 | 0.54 |
| 3:B3:5:PHE:CZ | 3:B3:30:LEU:HD22 | 2.42 | 0.54 |
| 3:Z3:5:PHE:CZ | 3:Z3:30:LEU:HD22 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M3:1:MET:O | 4:M3:2:ASN:O | 2.26 | 0.54 |
| 4:M3:162:ASN:O | 4:M3:166:THR:CG2 | 2.50 | 0.54 |
| 3:S4:5:PHE:CZ | 3:S4:30:LEU:HD22 | 2.42 | 0.54 |
| 3:J4:5:PHE:CZ | 3:J4:30:LEU:HD22 | 2.42 | 0.54 |
| 3:O4:95:TYR:HE2 | 3:O4:108:ARG:NH2 | 2.01 | 0.54 |
| 12:O4:201:CYC:C4B | 5:Z4:54:LEU:HD12 | 2.37 | 0.54 |
| 12:K5:201:CYC:CGD | 1:J5:62:TYR:HH | 2.17 | 0.54 |
| 12:L5:201:CYC:HB | 12:L5:201:CYC:CMA | 1.99 | 0.54 |
| 12:O5:201:CYC:HC | 12:O5:201:CYC:HMD3 | 1.70 | 0.54 |
| 3:Y4:88:ILE:O | 3:Y4:92:TYR:CD2 | 2.60 | 0.54 |
| 12:D5:201:CYC:HB | 12:D5:201:CYC:HMA3 | 1.73 | 0.54 |
| 8:c5:82:LEU:CD1 | 6:M6:15:ILE:HG13 | 2.33 | 0.54 |
| 8:Q5:123:ILE:O | 8:Q5:126:VAL:HB | 2.06 | 0.54 |
| 8:Y5:37:LEU:HD22 | 1:Z5:24:LEU:HD22 | 1.89 | 0.54 |
| 3:L6:75:PRO:HB2 | 2:G6:108:TYR:O | 2.07 | 0.54 |
| 9:i5:10:CYS:O | 9:i5:49:GLY:CA | 2.55 | 0.54 |
| 10:j5:306:GLU:OE2 | 10:j5:362:LYS:CE | 2.55 | 0.54 |
| 10:j5:456:ILE:O | 10:j5:456:ILE:HG13 | 2.06 | 0.54 |
| 10:j5:1052:PRO:HB3 | 11:aA:32:ARG:CZ | 2.37 | 0.54 |
| 10:k5:156:SER:OG | 12:k5:1201:CYC:HHD | 2.07 | 0.54 |
| 10:k5:723:GLN:HE21 | 10:k5:723:GLN:HA | 1.72 | 0.54 |
| 10:k5:969:VAL:O | 10:k5:969:VAL:HG22 | 2.07 | 0.54 |
| 8:i7:101:VAL:HB | 8:i7:155:TYR:OH | 2.08 | 0.54 |
| 8:c7:36:ARG:HH12 | 8:m7:24:ASP:CG | 2.11 | 0.54 |
| 8:q7:37:LEU:HD22 | 1:r7:24:LEU:HD22 | 1.89 | 0.54 |
| 9:x7:4:TYR:N | 9:x7:58:THR:OG1 | 2.40 | 0.54 |
| 3:F8:84:ARG:NH2 | 11:a9:143:SER:HB3 | 2.22 | 0.54 |
| 3:L8:5:PHE:CZ | 3:L8:30:LEU:HD22 | 2.42 | 0.54 |
| 12:M8:302:CYC:HAC2 | 3:S8:78:ARG:CB | 2.36 | 0.54 |
| 2:P8:108:TYR:O | 3:S8:75:PRO:HB2 | 2.06 | 0.54 |
| 3:Q8:89:ILE:HG12 | 3:Q8:92:TYR:CZ | 2.42 | 0.54 |
| 4:M9:260:ARG:HH11 | 4:M9:260:ARG:CG | 2.18 | 0.54 |
| 5:Z8:23:SER:C | 5:Z8:25:THR:H | 2.15 | 0.54 |
| 5:Z8:31:TRP:CB | 5:Z8:32:PRO:HD2 | 2.32 | 0.54 |
| 12:F9:303:CYC:HC | 12:F9:303:CYC:HMD2 | 1.70 | 0.54 |
| 3:J9:119:ALA:C | 11:a9:365:LYS:HE3 | 2.12 | 0.54 |
| 11:a9:245:ALA:N | 12:a9:901:CYC:HBB3 | 2.21 | 0.54 |
| 11:aA:558:VAL:HG12 | 11:aA:560:SER:OG | 2.06 | 0.54 |
| 11:aA:643:LEU:CD1 | 11:aA:766:ASN:CA | 2.85 | 0.54 |
| 11:aA:716:ILE:HD12 | 11:aA:738:LEU:CD2 | 2.37 | 0.54 |
| 4:M1:91:VAL:HG12 | 4:M1:91:VAL:O | 2.06 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:Y1:19:LEU:HD13 | 3:Z1:98:LEU:HD22 | 1.89 | 0.54 |
| 3:Z1:5:PHE:CZ | 3:Z1:30:LEU:HD22 | 2.42 | 0.54 |
| 3:FA:43:ALA:HB3 | 3:FA:142:VAL:HG22 | 1.89 | 0.54 |
| 3:HA:5:PHE:CZ | 3:HA:30:LEU:HD22 | 2.42 | 0.54 |
| 2:IA:16:GLY:HA3 | 11:aA:514:VAL:CG1 | 2.36 | 0.54 |
| 4:MA:263:PRO:HG2 | 3:VA:115:GLU:O | 2.07 | 0.54 |
| 3:PA:5:PHE:CZ | 3:PA:30:LEU:HD22 | 2.42 | 0.54 |
| 3:PA:75:PRO:HB2 | 2:SA:108:TYR:O | 2.06 | 0.54 |
| 12:QA:201:CYC:HBA2 | 3:TA:79:MET:HE1 | 1.90 | 0.54 |
| 3:H2:14:LEU:HD21 | 6:M2:68:THR:N | 2.21 | 0.54 |
| 3:H2:88:ILE:CD1 | 6:M2:115:TYR:OH | 2.56 | 0.54 |
| 2:A3:108:TYR:O | 3:D3:75:PRO:HB2 | 2.06 | 0.54 |
| 2:E3:99:ALA:HB2 | 3:F3:9:ILE:CD1 | 2.36 | 0.54 |
| 12:Z3:201:CYC:HBA1 | 4:M3:188:LEU:HD23 | 1.89 | 0.54 |
| 2:A4:63:PHE:HB3 | 2:A4:66:LEU:HG | 1.88 | 0.54 |
| 4:M3:95:ALA:HB2 | 5:N3:38:GLU:OE1 | 2.07 | 0.54 |
| 4:M3:209:TYR:CD1 | 4:M3:209:TYR:C | 2.85 | 0.54 |
| 2:O3:63:PHE:HB3 | 2:O3:66:LEU:HG | 1.88 | 0.54 |
| 2:U3:99:ALA:HB2 | 3:V3:9:ILE:CD1 | 2.36 | 0.54 |
| 2:T4:19:LEU:HD13 | 3:U4:98:LEU:HD22 | 1.89 | 0.54 |
| 3:F4:104:VAL:HA | 3:F4:107:ASP:OD1 | 2.07 | 0.54 |
| 3:F4:107:ASP:OD2 | 4:M4:9:GLN:C | 2.50 | 0.54 |
| 2:G4:19:LEU:HD13 | 3:H4:98:LEU:HD22 | 1.89 | 0.54 |
| 4:M4:90:LYS:HE3 | 4:M4:220:TYR:CZ | 2.43 | 0.54 |
| 4:M4:220:TYR:C | 4:M4:220:TYR:CD1 | 2.85 | 0.54 |
| 3:O4:120:LEU:HD23 | 5:Z4:14:LYS:NZ | 2.22 | 0.54 |
| 8:K5:17:TYR:HB3 | 1:L5:45:SER:CB | 2.32 | 0.54 |
| 8:A5:65:VAL:HG23 | 8:A5:66:VAL:HG23 | 1.89 | 0.54 |
| 8:A5:119:LEU:HD21 | 12:A5:201:CYC:HAA2 | 1.89 | 0.54 |
| 8:G5:88:TYR:OH | 12:G5:201:CYC:HMB2 | 2.07 | 0.54 |
| 8:G5:115:MET:SD | 12:G5:201:CYC:C1B | 2.96 | 0.54 |
| 8:G5:122:PRO:HG2 | 12:G5:201:CYC:OC | 2.06 | 0.54 |
| 1:d5:110:ASN:O | 10:j5:352:ILE:HD11 | 2.05 | 0.54 |
| 12:R5:201:CYC:HB | 12:R5:201:CYC:HMA2 | 1.70 | 0.54 |
| 8:W5:126:VAL:HG23 | 12:W5:201:CYC:HMC3 | 1.89 | 0.54 |
| 1:X5:107:ARG:HB3 | 10:j5:520:ARG:HH22 | 1.72 | 0.54 |
| 1:X5:120:GLY:O | 10:j5:703:LEU:HD11 | 2.07 | 0.54 |
| 10:j5:1054:SER:HG | 1:r7:110:ASN:HB3 | 1.71 | 0.54 |
| 10:k5:286:VAL:HB | 10:k5:293:LYS:HE2 | 1.88 | 0.54 |
| 3:B6:75:PRO:HB2 | 2:E6:108:TYR:O | 2.06 | 0.54 |
| 8:O7:37:LEU:HA | 8:O7:97:VAL:HG12 | 1.88 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:Q7:123:ILE:O | 8:Q7:126:VAL:HB | 2.07 | 0.54 |
| 8:g7:37:LEU:CD2 | 1:h7:24:LEU:HD21 | 2.38 | 0.54 |
| 8:g7:161:GLN:HG2 | 1:v7:49:THR:HG21 | 1.90 | 0.54 |
| 8:i7:92:VAL:CG2 | 8:i7:156:LEU:HD12 | 2.34 | 0.54 |
| 8:k7:66:VAL:HG11 | 11:a9:61:TYR:HE1 | 1.70 | 0.54 |
| 8:k7:104:ILE:HG23 | 8:k7:156:LEU:HD21 | 1.89 | 0.54 |
| 1:Z7:67:ARG:CG | 11:a9:311:LEU:CD2 | 2.80 | 0.54 |
| 8:c7:9:VAL:HG22 | 1:d7:107:ARG:HH22 | 1.71 | 0.54 |
| 8:c7:58:LEU:HD13 | 8:c7:128:GLU:HB3 | 1.89 | 0.54 |
| 8:e7:65:VAL:HG23 | 8:e7:66:VAL:HG23 | 1.89 | 0.54 |
| 3:B8:5:PHE:CZ | 3:B8:30:LEU:HD22 | 2.42 | 0.54 |
| 3:B8:109:CYS:HA | 4:M8:60:LYS:HZ1 | 1.72 | 0.54 |
| 8:o7:17:TYR:OH | 1:p7:90:ARG:HA | 2.06 | 0.54 |
| 8:o7:56:ASP:OD1 | 8:o7:56:ASP:N | 2.37 | 0.54 |
| 3:W8:5:PHE:CZ | 3:W8:30:LEU:HD22 | 2.43 | 0.54 |
| 2:X8:16:GLY:CA | 4:M8:228:SER:HB3 | 2.30 | 0.54 |
| 3:F8:5:PHE:CZ | 3:F8:30:LEU:HD22 | 2.42 | 0.54 |
| 3:H8:5:PHE:CZ | 3:H8:30:LEU:HD22 | 2.42 | 0.54 |
| 3:O8:5:PHE:CZ | 3:O8:30:LEU:HD22 | 2.42 | 0.54 |
| 3:L9:37:ARG:NH1 | 3:L9:97:LEU:HD12 | 2.22 | 0.54 |
| 4:M9:15:PHE:CD1 | 4:M9:71:PRO:HA | 2.38 | 0.54 |
| 4:M9:53:LEU:HB2 | 12:F9:301:CYC:HBA1 | 1.87 | 0.54 |
| 4:M9:209:TYR:C | 4:M9:209:TYR:CD1 | 2.85 | 0.54 |
| 5:N9:54:LEU:HD13 | 3:T9:84:ARG:CZ | 2.36 | 0.54 |
| 5:Z8:27:ALA:HB2 | 12:Z8:301:CYC:HAB1 | 1.86 | 0.54 |
| 3:D9:5:PHE:CZ | 3:D9:30:LEU:HD22 | 2.42 | 0.54 |
| 3:H9:107:ASP:HB3 | 11:a9:445:THR:HG23 | 1.88 | 0.54 |
| 3:X9:75:PRO:HB2 | 2:Y9:108:TYR:O | 2.06 | 0.54 |
| 11:a9:462:ARG:HH11 | 11:a9:462:ARG:HG2 | 1.71 | 0.54 |
| 3:L1:5:PHE:CZ | 3:L1:30:LEU:HD22 | 2.42 | 0.54 |
| 4:M1:134:ASN:HD21 | 5:N1:1:MET:H1 | 1.55 | 0.54 |
| 3:D2:5:PHE:CZ | 3:D2:30:LEU:HD22 | 2.42 | 0.54 |
| 1:A:127:VAL:HG11 | 1:R5:15:GLN:CD | 2.32 | 0.54 |
| 1:Z:161:SER:HG | 1:X5:14:VAL:HG21 | 1.70 | 0.54 |
| 2:AA:63:PHE:HB3 | 2:AA:66:LEU:HG | 1.88 | 0.54 |
| 3:BA:27:LEU:CA | 3:BA:30:LEU:HD13 | 2.33 | 0.54 |
| 2:QA:23:GLU:OE2 | 2:UA:2:LYS:NZ | 2.40 | 0.54 |
| 3:TA:5:PHE:CZ | 3:TA:30:LEU:HD22 | 2.42 | 0.54 |
| 12:TA:302:CYC:HC | 12:TA:302:CYC:HMD2 | 1.70 | 0.54 |
| 3:P1:5:PHE:CZ | 3:P1:30:LEU:HD22 | 2.42 | 0.54 |
| 12:H3:202:CYC:HB | 11:a9:776:TYR:HB3 | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 3:J3:5:PHE:CZ | 3:J3:30:LEU:HD22 | 2.42 | 0.54 |
| 3:J3:120:LEU:CG | 11:a9:800:THR:HG21 | 2.34 | 0.54 |
| 7:N2:43:VAL:HG21 | 7:N2:51:GLU:HG2 | 1.88 | 0.54 |
| 3:F3:5:PHE:CZ | 3:F3:30:LEU:HD22 | 2.42 | 0.54 |
| 2:C4:108:TYR:O | 3:F4:75:PRO:HB2 | 2.06 | 0.54 |
| 5:N3:31:TRP:CZ2 | 3:T3:92:TYR:OH | 2.56 | 0.54 |
| 2:O3:65:TYR:O | 2:O3:71:GLN:CG | 2.54 | 0.54 |
| 3:H4:5:PHE:CZ | 3:H4:30:LEU:HD22 | 2.42 | 0.54 |
| 4:M4:61:ASN:C | 4:M4:63:GLY:N | 2.64 | 0.54 |
| 4:M4:181:GLN:O | 4:M4:181:GLN:HG3 | 2.03 | 0.54 |
| 2:P4:99:ALA:HB2 | 3:Q4:9:ILE:CD1 | 2.36 | 0.54 |
| 12:K5:201:CYC:HC | 12:K5:201:CYC:HMD3 | 1.70 | 0.54 |
| 8:M5:65:VAL:HG23 | 8:M5:66:VAL:HG23 | 1.89 | 0.54 |
| 8:A5:118:SER:HB2 | 1:F5:82:ILE:HD12 | 1.86 | 0.54 |
| 8:c5:14:GLU:OE2 | 10:j5:393:MET:HG3 | 2.07 | 0.54 |
| 1:Z5:64:ASP:HB2 | 10:k5:705:THR:HG21 | 1.82 | 0.54 |
| 8:a5:29:PHE:CD1 | 8:a5:99:GLY:HA3 | 2.43 | 0.54 |
| 6:M6:277:GLY:HA2 | 1:d7:62:TYR:HB2 | 1.90 | 0.54 |
| 10:j5:320:GLU:HG2 | 10:j5:320:GLU:O | 2.06 | 0.54 |
| 10:j5:820:HIS:HE1 | 10:j5:859:ILE:HD13 | 1.59 | 0.54 |
| 10:k5:361:PHE:HZ | 10:k5:378:TYR:CE2 | 2.25 | 0.54 |
| 10:k5:1052:PRO:CA | 1:l7:106:GLU:CG | 2.85 | 0.54 |
| 12:k5:1204:CYC:HB | 12:k5:1204:CYC:HMA3 | 1.73 | 0.54 |
| 8:Q7:21:GLY:CA | 8:C7:6:LYS:HZ3 | 2.19 | 0.54 |
| 8:Q7:104:ILE:HG23 | 8:Q7:156:LEU:HD21 | 1.89 | 0.54 |
| 8:K7:123:ILE:O | 8:K7:126:VAL:HB | 2.07 | 0.54 |
| 8:K7:126:VAL:HG23 | 12:K7:201:CYC:HMC3 | 1.89 | 0.54 |
| 8:i7:95:GLY:O | 8:i7:152:TYR:CE2 | 2.54 | 0.54 |
| 1:Z7:10:ASN:ND2 | 9:x7:65:THR:C | 2.65 | 0.54 |
| 2:A8:99:ALA:HB2 | 3:B8:9:ILE:CD1 | 2.36 | 0.54 |
| 2:C8:19:LEU:HD13 | 3:D8:98:LEU:HD22 | 1.89 | 0.54 |
| 12:p7:201:CYC:HB | 12:p7:201:CYC:HMA3 | 1.73 | 0.54 |
| 8:q7:65:VAL:HG23 | 8:q7:66:VAL:HG23 | 1.89 | 0.54 |
| 2:G8:19:LEU:HD13 | 3:H8:98:LEU:HD22 | 1.89 | 0.54 |
| 4:M8:233:GLU:OE2 | 4:M8:268:ARG:NH1 | 2.39 | 0.54 |
| 2:N8:115:GLU:HA | 5:Z8:32:PRO:HB2 | 1.86 | 0.54 |
| 3:Q8:78:ARG:CD | 12:Z8:301:CYC:CMD | 2.85 | 0.54 |
| 3:F1:5:PHE:CZ | 3:F1:30:LEU:HD22 | 2.42 | 0.54 |
| 4:M9:1:MET:O | 4:M9:2:ASN:O | 2.26 | 0.54 |
| 4:M9:90:LYS:HE3 | 4:M9:220:TYR:CZ | 2.43 | 0.54 |
| 3:Y8:106:GLU:HB2 | 3:Y8:166:LYS:HD3 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:A9:65:TYR:O | 2:A9:71:GLN:CG | 2.54 | 0.54 |
| 2:C9:19:LEU:HD13 | 3:D9:98:LEU:HD22 | 1.89 | 0.54 |
| 3:H9:75:PRO:HB2 | 2:I9:108:TYR:O | 2.06 | 0.54 |
| 2:I9:19:LEU:HD12 | 3:J9:41:VAL:HG13 | 1.89 | 0.54 |
| 11:a9:388:VAL:HG11 | 11:a9:419:ARG:HH11 | 1.73 | 0.54 |
| 11:a9:482:TYR:C | 11:a9:482:TYR:CD1 | 2.84 | 0.54 |
| 11:aA:643:LEU:HD11 | 11:aA:766:ASN:HA | 1.89 | 0.54 |
| 2:I1:19:LEU:HD13 | 3:J1:98:LEU:HD22 | 1.89 | 0.54 |
| 4:M1:205:ASP:OD2 | 5:N1:52:ARG:NH2 | 2.39 | 0.54 |
| 5:N1:29:HIS:NE2 | 12:T1:301:CYC:OB | 2.40 | 0.54 |
| 3:J2:119:ALA:CB | 6:M2:261:LYS:N | 2.67 | 0.54 |
| 3:B3:126:SER:CB | 12:B3:202:CYC:HMC2 | 2.37 | 0.54 |
| 3:Z3:98:LEU:HD22 | 2:Y3:19:LEU:HD13 | 1.89 | 0.54 |
| 4:M3:220:TYR:C | 4:M3:220:TYR:CD1 | 2.85 | 0.54 |
| 3:X3:75:PRO:HB2 | 2:Y3:108:TYR:O | 2.06 | 0.54 |
| 3:B1:84:ARG:HD3 | 11:aA:680:SER:OG | 2.07 | 0.54 |
| 4:M4:1:MET:O | 4:M4:2:ASN:O | 2.26 | 0.54 |
| 4:M4:17:VAL:HG12 | 4:M4:18:THR:N | 2.22 | 0.54 |
| 4:M4:129:GLU:HG3 | 4:M4:142:PHE:HE2 | 1.71 | 0.54 |
| 4:M4:273:ILE:CG2 | 2:X4:107:ASP:CB | 2.85 | 0.54 |
| 1:L5:1:MET:O | 1:L5:1:MET:HG3 | 2.04 | 0.54 |
| 2:X4:19:LEU:HD13 | 3:Y4:98:LEU:HD22 | 1.89 | 0.54 |
| 8:G5:161:GLN:HG2 | 1:T5:49:THR:CG2 | 2.36 | 0.54 |
| 12:V5:201:CYC:HB | 12:V5:201:CYC:HMA2 | 1.69 | 0.54 |
| 8:W5:18:LEU:HD22 | 1:X5:97:LEU:HD11 | 1.90 | 0.54 |
| 8:W5:104:ILE:HG23 | 8:W5:156:LEU:HD21 | 1.89 | 0.54 |
| 7:N6:43:VAL:HG21 | 7:N6:51:GLU:HG2 | 1.88 | 0.54 |
| 10:j5:70:ARG:HG2 | 10:j5:209:ASN:OD1 | 2.08 | 0.54 |
| 10:j5:138:PRO:CG | 10:j5:201:VAL:HG11 | 2.34 | 0.54 |
| 10:j5:230:VAL:O | 10:j5:234:LEU:CD1 | 2.54 | 0.54 |
| 10:j5:878:GLU:CG | 9:w7:28:PHE:CE2 | 2.89 | 0.54 |
| 10:k5:825:ASN:CB | 12:B7:201:CYC:HBB2 | 2.36 | 0.54 |
| 10:k5:1064:LYS:HE2 | 10:k5:1065:HIS:CD2 | 2.42 | 0.54 |
| 2:G6:19:LEU:HD13 | 3:H6:98:LEU:HD22 | 1.89 | 0.54 |
| 8:G7:104:ILE:HG23 | 8:G7:156:LEU:HD21 | 1.89 | 0.54 |
| 8:M7:37:LEU:HD22 | 1:N7:24:LEU:HD22 | 1.89 | 0.54 |
| 1:T7:75:THR:HB | 8:U7:111:GLY:C | 2.32 | 0.54 |
| 8:e7:104:ILE:HG23 | 8:e7:156:LEU:HD21 | 1.89 | 0.54 |
| 8:q7:45:GLU:OE2 | 3:H1:125:ARG:NH2 | 2.40 | 0.54 |
| 12:r7:201:CYC:HB | 12:r7:201:CYC:HMA3 | 1.73 | 0.54 |
| 8:s7:90:ARG:CZ | 1:t7:16:GLY:HA2 | 2.37 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:u7:30:VAL:CA | 1:v7:31:PHE:HD1 | 2.20 | 0.54 |
| 9:w7:7:VAL:HG11 | 9:w7:37:TRP:CE3 | 2.43 | 0.54 |
| 3:F8:113:LEU:N | 4:M8:5:THR:HG23 | 2.21 | 0.54 |
| 12:H8:201:CYC:CBB | 11:a9:259:ALA:CB | 2.80 | 0.54 |
| 4:M8:1:MET:O | 4:M8:2:ASN:O | 2.26 | 0.54 |
| 4:M8:17:VAL:HG12 | 4:M8:18:THR:N | 2.22 | 0.54 |
| 3:S8:5:PHE:CZ | 3:S8:30:LEU:HD22 | 2.42 | 0.54 |
| 4:M9:48:PRO:HG2 | 4:M9:48:PRO:O | 2.07 | 0.54 |
| 5:N9:39:PRO:CA | 3:P9:116:THR:OG1 | 2.56 | 0.54 |
| 3:Y8:89:ILE:C | 3:Y8:92:TYR:CE2 | 2.82 | 0.54 |
| 3:J9:75:PRO:HB2 | 2:K9:108:TYR:O | 2.06 | 0.54 |
| 12:J9:202:CYC:CBA | 11:a9:510:PHE:O | 2.49 | 0.54 |
| 3:Z9:5:PHE:CZ | 3:Z9:30:LEU:HD22 | 2.42 | 0.54 |
| 11:aA:346:TYR:CD1 | 11:aA:346:TYR:C | 2.84 | 0.54 |
| 4:M1:163:ASN:HD21 | 12:Z1:202:CYC:CMA | 2.19 | 0.54 |
| 4:M1:209:TYR:C | 4:M1:209:TYR:CD1 | 2.85 | 0.54 |
| 4:M1:220:TYR:C | 4:M1:220:TYR:CD1 | 2.85 | 0.54 |
| 3:X1:5:PHE:CZ | 3:X1:30:LEU:HD22 | 2.42 | 0.54 |
| 1:A:18:TYR:CZ | 8:a5:90:ARG:CA | 2.91 | 0.54 |
| 1:Z:18:TYR:OH | 8:e5:89:LEU:CB | 2.56 | 0.54 |
| 2:AA:38:MET:CE | 3:BA:28:THR:OG1 | 2.56 | 0.54 |
| 2:IA:19:LEU:HD12 | 3:JA:41:VAL:HG13 | 1.89 | 0.54 |
| 4:MA:91:VAL:HG12 | 4:MA:91:VAL:O | 2.06 | 0.54 |
| 4:MA:95:ALA:CB | 5:NA:38:GLU:OE2 | 2.56 | 0.54 |
| 12:QA:201:CYC:HBB3 | 3:TA:74:TYR:CE2 | 2.43 | 0.54 |
| 3:H2:5:PHE:CZ | 3:H2:30:LEU:HD22 | 2.42 | 0.54 |
| 3:J2:88:ILE:HD11 | 6:M2:185:PHE:CZ | 2.43 | 0.54 |
| 7:N2:22:GLN:OE1 | 7:N2:39:TYR:HE2 | 1.91 | 0.54 |
| 3:B4:82:CYS:CB | 12:B4:202:CYC:OC | 2.48 | 0.54 |
| 4:M3:48:PRO:HG2 | 4:M3:48:PRO:O | 2.06 | 0.54 |
| 4:M3:81:ASP:N | 3:X3:111:ASN:HD21 | 2.02 | 0.54 |
| 3:P3:75:PRO:HB2 | 2:S3:108:TYR:O | 2.06 | 0.54 |
| 3:B1:75:PRO:HB2 | 2:E1:108:TYR:O | 2.06 | 0.54 |
| 3:B1:84:ARG:NH1 | 11:aA:680:SER:CB | 2.71 | 0.54 |
| 3:F4:115:GLU:CB | 4:M4:3:VAL:HG11 | 2.24 | 0.54 |
| 3:Q4:5:PHE:CZ | 3:Q4:30:LEU:HD22 | 2.42 | 0.54 |
| 8:K5:106:GLU:OE1 | 9:i5:66:GLY:N | 2.38 | 0.54 |
| 12:N5:201:CYC:HB | 12:N5:201:CYC:HMA2 | 1.69 | 0.54 |
| 1:B5:107:ARG:NH2 | 9:z5:21:ARG:HD3 | 2.22 | 0.54 |
| 8:C5:29:PHE:CD1 | 8:C5:99:GLY:HA3 | 2.43 | 0.54 |
| 12:F5:201:CYC:HB | 12:F5:201:CYC:HMA3 | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:G5:107:ILE:CD1 | 1:H5:13:ASP:OD2 | 2.55 | 0.54 |
| 8:U5:37:LEU:HA | 8:U5:97:VAL:HG12 | 1.89 | 0.54 |
| 8:W5:17:TYR:CD2 | 1:X5:44:ILE:HG22 | 2.40 | 0.54 |
| 8:Y5:65:VAL:HG23 | 8:Y5:66:VAL:HG23 | 1.89 | 0.54 |
| 7:N6:22:GLN:OE1 | 7:N6:39:TYR:HE2 | 1.91 | 0.54 |
| 10:j5:221:LYS:CA | 10:j5:221:LYS:CE | 2.85 | 0.54 |
| 10:j5:386:ILE:CG2 | 10:j5:387:VAL:N | 2.36 | 0.54 |
| 10:j5:1018:LEU:HB3 | 10:j5:1021:ALA:HB3 | 0.68 | 0.54 |
| 10:j5:1118:THR:HG23 | 12:j5:1202:CYC:HBA1 | 1.90 | 0.54 |
| 10:j5:1155:ARG:HH21 | 10:j5:1155:ARG:CB | 2.09 | 0.54 |
| 10:k5:283:ARG:HD3 | 10:k5:283:ARG:O | 2.06 | 0.54 |
| 12:k5:1203:CYC:HB | 12:k5:1203:CYC:HMA3 | 1.73 | 0.54 |
| 1:B7:54:GLU:OE1 | 11:a9:563:PHE:CD2 | 2.61 | 0.54 |
| 8:G7:65:VAL:HG23 | 8:G7:66:VAL:HG23 | 1.89 | 0.54 |
| 1:H7:75:THR:HB | 8:I7:111:GLY:C | 2.32 | 0.54 |
| 8:M7:104:ILE:HG23 | 8:M7:156:LEU:HD21 | 1.89 | 0.54 |
| 8:Y7:104:ILE:HG23 | 8:Y7:156:LEU:HD21 | 1.89 | 0.54 |
| 8:u7:17:TYR:OH | 1:v7:90:ARG:HA | 2.06 | 0.54 |
| 9:z7:39:THR:O | 9:z7:39:THR:OG1 | 2.22 | 0.54 |
| 3:U8:115:GLU:CD | 4:M8:70:SER:HB2 | 2.32 | 0.54 |
| 2:X8:69:PRO:N | 2:S9:42:ARG:NE | 2.54 | 0.54 |
| 3:F8:108:ARG:HE | 4:M8:9:GLN:CA | 2.20 | 0.54 |
| 2:G8:108:TYR:O | 3:L8:75:PRO:HB2 | 2.06 | 0.54 |
| 12:N8:201:CYC:HB | 12:N8:201:CYC:CMA | 2.17 | 0.54 |
| 3:Q8:102:ALA:CB | 3:Q8:166:LYS:NZ | 2.32 | 0.54 |
| 4:M9:37:GLU:CD | 4:M9:40:GLN:NE2 | 2.62 | 0.54 |
| 4:M9:95:ALA:CB | 5:N9:38:GLU:OE2 | 2.56 | 0.54 |
| 4:M9:192:GLN:O | 4:M9:192:GLN:HG3 | 2.05 | 0.54 |
| 5:N9:11:ARG:HD2 | 3:R9:108:ARG:NH2 | 2.23 | 0.54 |
| 5:Z8:41:GLN:H | 12:Z8:301:CYC:CHB | 2.21 | 0.54 |
| 11:a9:512:TYR:CD1 | 11:a9:512:TYR:C | 2.86 | 0.54 |
| 11:aA:55:ASP:CB | 11:aA:612:TYR:CG | 2.91 | 0.54 |
| 11:aA:379:LEU:HD13 | 11:aA:391:VAL:CG2 | 2.30 | 0.54 |
| 4:M1:1:MET:O | 4:M1:2:ASN:O | 2.26 | 0.54 |
| 4:M1:61:ASN:O | 4:M1:63:GLY:N | 2.40 | 0.54 |
| 4:M1:90:LYS:HE3 | 4:M1:220:TYR:CZ | 2.43 | 0.54 |
| 4:MA:274:VAL:CG2 | 3:VA:77:ARG:CB | 2.73 | 0.54 |
| 3:XA:5:PHE:CZ | 3:XA:30:LEU:HD22 | 2.42 | 0.54 |
| 2:A1:108:TYR:O | 3:D1:75:PRO:HB2 | 2.06 | 0.54 |
| 3:T3:5:PHE:CZ | 3:T3:30:LEU:HD22 | 2.42 | 0.54 |
| 3:B1:5:PHE:CZ | 3:B1:30:LEU:HD22 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:F4:110:LEU:O | 3:F4:111:ASN:C | 2.51 | 0.54 |
| 4:M4:131:LEU:HD21 | 5:Z4:2:SER:HA | 1.87 | 0.54 |
| 4:M4:209:TYR:CD1 | 4:M4:209:TYR:C | 2.85 | 0.54 |
| 3:O4:5:PHE:CZ | 3:O4:30:LEU:HD22 | 2.42 | 0.54 |
| 3:O4:119:ALA:CB | 5:Z4:72:GLU:H | 2.20 | 0.54 |
| 3:Q4:37:ARG:HD3 | 3:Q4:98:LEU:HD12 | 1.90 | 0.54 |
| 8:M5:38:ARG:CD | 1:J7:144:ASP:CG | 2.81 | 0.54 |
| 8:e5:37:LEU:HA | 8:e5:97:VAL:HG12 | 1.88 | 0.54 |
| 8:S5:90:ARG:CZ | 1:T5:16:GLY:CA | 2.86 | 0.54 |
| 8:W5:8:ILE:CG2 | 1:X5:94:TYR:CG | 2.90 | 0.54 |
| 1:Z5:28:LYS:HD3 | 1:t7:143:PRO:CG | 2.05 | 0.54 |
| 1:b5:90:ARG:HA | 10:k5:34:TYR:CE1 | 2.41 | 0.54 |
| 6:M6:69:ALA:N | 3:H6:14:LEU:HD21 | 2.22 | 0.54 |
| 6:M6:115:TYR:OH | 3:H6:88:ILE:CD1 | 2.56 | 0.54 |
| 10:k5:306:GLU:OE2 | 10:k5:362:LYS:CE | 2.56 | 0.54 |
| 10:k5:411:TYR:C | 10:k5:411:TYR:CD1 | 2.84 | 0.54 |
| 10:k5:929:PRO:HG3 | 1:D7:147:LYS:NZ | 2.21 | 0.54 |
| 10:k5:989:THR:HG21 | 8:a7:106:GLU:OE2 | 2.02 | 0.54 |
| 10:k5:1018:LEU:HB3 | 10:k5:1021:ALA:HB3 | 0.68 | 0.54 |
| 10:k5:1150:TYR:CE1 | 11:a9:38:VAL:CG2 | 2.62 | 0.54 |
| 12:k5:1203:CYC:HMA2 | 12:k5:1203:CYC:HB | 1.70 | 0.54 |
| 3:F6:86:MET:CG | 12:F6:201:CYC:HBC1 | 2.37 | 0.54 |
| 8:C7:90:ARG:CZ | 1:D7:16:GLY:HA2 | 2.37 | 0.54 |
| 12:D7:201:CYC:HB | 12:D7:201:CYC:HMA2 | 1.70 | 0.54 |
| 8:E7:123:ILE:O | 8:E7:126:VAL:HB | 2.07 | 0.54 |
| 8:E7:126:VAL:HG23 | 12:E7:201:CYC:HMC3 | 1.89 | 0.54 |
| 8:G7:65:VAL:HG23 | 8:G7:66:VAL:N | 2.21 | 0.54 |
| 8:I7:29:PHE:CD1 | 8:I7:99:GLY:HA3 | 2.43 | 0.54 |
| 8:I7:44:THR:OG1 | 1:J7:18:TYR:HD2 | 1.91 | 0.54 |
| 1:h7:30:TYR:CD2 | 1:h7:30:TYR:C | 2.86 | 0.54 |
| 1:T7:1:MET:O | 9:w7:66:GLY:HA3 | 2.07 | 0.54 |
| 8:a7:63:PRO:CG | 11:a9:336:ILE:CG2 | 2.80 | 0.54 |
| 8:o7:23:LEU:CA | 1:p7:38:VAL:CG2 | 2.85 | 0.54 |
| 12:o7:201:CYC:HC | 12:o7:201:CYC:HMD3 | 1.70 | 0.54 |
| 8:u7:37:LEU:HD21 | 1:v7:24:LEU:CD2 | 2.21 | 0.54 |
| 8:u7:90:ARG:HG3 | 1:v7:18:TYR:CG | 2.42 | 0.54 |
| 3:H8:75:PRO:HB2 | 2:I8:108:TYR:O | 2.06 | 0.54 |
| 3:H8:84:ARG:CD | 11:a9:131:TYR:CZ | 2.89 | 0.54 |
| 2:I8:19:LEU:HD13 | 3:J8:98:LEU:HD22 | 1.89 | 0.54 |
| 4:M8:91:VAL:HG22 | 2:P8:15:GLN:CA | 2.38 | 0.54 |
| 4:M8:140:ARG:NH1 | 4:M8:210:ILE:HG13 | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M8:160:THR:HG22 | 4:M8:257:GLN:HB3 | 1.73 | 0.54 |
| 4:M8:209:TYR:CD1 | 4:M8:209:TYR:C | 2.85 | 0.54 |
| 4:M8:232:VAL:HA | 12:M8:301:CYC:C1B | 2.38 | 0.54 |
| 12:O8:201:CYC:HBB3 | 5:Z8:57:MET:HB3 | 1.89 | 0.54 |
| 4:M9:130:SER:O | 12:R9:201:CYC:HBA1 | 2.07 | 0.54 |
| 5:N9:53:LEU:C | 12:T9:301:CYC:HBA1 | 2.29 | 0.54 |
| 3:P9:5:PHE:CZ | 3:P9:30:LEU:HD22 | 2.42 | 0.54 |
| 2:Q9:19:LEU:HD13 | 3:R9:98:LEU:HD22 | 1.89 | 0.54 |
| 3:Y8:5:PHE:CZ | 3:Y8:30:LEU:HD22 | 2.42 | 0.54 |
| 3:F9:37:ARG:N | 3:F9:156:LEU:HD21 | 2.22 | 0.54 |
| 2:I9:13:ASP:OD1 | 3:J9:92:TYR:OH | 2.20 | 0.54 |
| 11:a9:640:ALA:HB2 | 11:a9:770:TYR:CE2 | 2.41 | 0.54 |
| 11:a9:643:LEU:CD1 | 11:a9:766:ASN:CA | 2.85 | 0.54 |
| 11:a9:798:SER:C | 11:a9:800:THR:H | 2.14 | 0.54 |
| 11:aA:462:ARG:HH11 | 11:aA:462:ARG:HG2 | 1.71 | 0.54 |
| 11:aA:812:ASP:O | 11:aA:816:LEU:N | 2.39 | 0.54 |
| 3:LA:84:ARG:HE | 11:aA:406:LEU:CD2 | 2.21 | 0.54 |
| 4:MA:220:TYR:C | 4:MA:220:TYR:CD1 | 2.85 | 0.54 |
| 2:OA:2:LYS:NZ | 2:YA:23:GLU:OE2 | 2.41 | 0.54 |
| 2:O1:2:LYS:HE2 | 2:Y1:22:THR:CG2 | 2.38 | 0.54 |
| 2:O1:2:LYS:NZ | 2:Y1:23:GLU:OE2 | 2.41 | 0.54 |
| 2:A1:2:LYS:NZ | 2:K1:23:GLU:OE2 | 2.41 | 0.54 |
| 3:H2:77:ARG:HH12 | 6:M2:117:MET:HE2 | 1.55 | 0.54 |
| 3:S4:98:LEU:HD22 | 2:R4:19:LEU:HD13 | 1.89 | 0.54 |
| 4:M4:17:VAL:CG1 | 4:M4:18:THR:N | 2.71 | 0.54 |
| 4:M4:96:LYS:NZ | 3:Q4:92:TYR:OH | 2.40 | 0.54 |
| 4:M4:141:GLU:CG | 4:M4:145:LEU:HD12 | 2.38 | 0.54 |
| 4:M4:205:ASP:HB3 | 5:Z4:59:ARG:HH11 | 1.72 | 0.54 |
| 4:M4:205:ASP:HB3 | 5:Z4:59:ARG:NH1 | 2.22 | 0.54 |
| 3:O4:111:ASN:O | 5:Z4:67:ILE:HB | 2.08 | 0.54 |
| 8:O5:76:LYS:CG | 8:O5:77:MET:H | 2.18 | 0.54 |
| 3:Y4:5:PHE:CZ | 3:Y4:30:LEU:HD22 | 2.42 | 0.54 |
| 5:Z4:41:GLN:CB | 12:Z4:301:CYC:C4B | 2.85 | 0.54 |
| 8:A5:116:TYR:HE1 | 12:A5:201:CYC:HD | 1.54 | 0.54 |
| 8:c5:9:VAL:CG1 | 10:j5:344:ARG:NH1 | 2.60 | 0.54 |
| 8:Q5:160:MET:HB2 | 8:Q5:161:GLN:HE21 | 1.73 | 0.54 |
| 8:U5:76:LYS:C | 8:U5:78:THR:N | 2.64 | 0.54 |
| 3:J6:5:PHE:CZ | 3:J6:30:LEU:HD22 | 2.42 | 0.54 |
| 3:J6:98:LEU:HD22 | 2:I6:19:LEU:HD13 | 1.89 | 0.54 |
| 7:N6:5:VAL:HB | 2:E6:13:ASP:OD2 | 2.08 | 0.54 |
| 8:A7:65:VAL:HG23 | 8:A7:66:VAL:N | 2.21 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:990:ARG:HE | 10:j5:1026:LYS:HZ1 | 1.34 | 0.54 |
| 3:F6:86:MET:HG2 | 12:F6:201:CYC:HBC1 | 1.88 | 0.54 |
| 3:H6:84:ARG:O | 3:H6:87:GLU:N | 2.40 | 0.54 |
| 8:Q7:126:VAL:HG23 | 12:Q7:201:CYC:HMC3 | 1.89 | 0.54 |
| 8:g7:37:LEU:HA | 8:g7:97:VAL:HG12 | 1.88 | 0.54 |
| 8:g7:51:VAL:HB | 11:aA:318:TRP:CZ3 | 2.42 | 0.54 |
| 12:j7:201:CYC:HB | 12:j7:201:CYC:HMA3 | 1.72 | 0.54 |
| 8:k7:68:PRO:HB2 | 11:a9:334:LYS:NZ | 2.23 | 0.54 |
| 8:Y7:49:ARG:HG3 | 8:Y7:52:LYS:HZ2 | 1.71 | 0.54 |
| 3:B8:92:TYR:OH | 12:B8:202:CYC:HAB1 | 2.08 | 0.54 |
| 2:E8:19:LEU:HD13 | 3:F8:98:LEU:HD22 | 1.89 | 0.54 |
| 8:m7:37:LEU:HA | 8:m7:97:VAL:HG12 | 1.88 | 0.54 |
| 8:o7:18:LEU:CD1 | 1:p7:97:LEU:HD13 | 2.37 | 0.54 |
| 3:F8:113:LEU:HD13 | 4:M8:5:THR:HG21 | 1.89 | 0.54 |
| 12:J8:202:CYC:HC | 12:J8:202:CYC:HMD2 | 1.70 | 0.54 |
| 3:L8:86:MET:HG3 | 12:a9:901:CYC:CAC | 2.37 | 0.54 |
| 4:M8:139:VAL:HG23 | 4:M8:215:GLU:O | 2.06 | 0.54 |
| 4:M9:158:PHE:CE1 | 2:U9:10:ALA:CA | 2.91 | 0.54 |
| 5:N9:34:LEU:CB | 3:P9:84:ARG:HH11 | 2.21 | 0.54 |
| 11:a9:405:ILE:HG22 | 11:a9:405:ILE:O | 2.05 | 0.54 |
| 11:aA:512:TYR:CD1 | 11:aA:512:TYR:C | 2.86 | 0.54 |
| 11:aA:615:ARG:O | 3:H1:68:ARG:HD2 | 2.03 | 0.54 |
| 11:aA:731:GLN:HG2 | 11:aA:817:LEU:HD21 | 1.88 | 0.54 |
| 4:M1:17:VAL:CG1 | 4:M1:18:THR:N | 2.71 | 0.54 |
| 3:F2:127:VAL:CG2 | 12:F2:201:CYC:HMC2 | 2.38 | 0.54 |
| 1:A:161:SER:OXT | 1:R5:14:VAL:HG21 | 2.08 | 0.54 |
| 12:A:201:CYC:HB | 12:A:201:CYC:HMA3 | 1.73 | 0.54 |
| 3:HA:66:LEU:HD22 | 12:HA:202:CYC:C1C | 2.23 | 0.54 |
| 3:JA:110:LEU:C | 11:aA:518:ALA:CB | 2.80 | 0.54 |
| 4:MA:17:VAL:CG1 | 4:MA:18:THR:N | 2.71 | 0.54 |
| 5:NA:34:LEU:CB | 3:PA:84:ARG:HH11 | 2.21 | 0.54 |
| 5:NA:67:ILE:N | 5:NA:67:ILE:HD13 | 2.23 | 0.54 |
| 3:J2:5:PHE:CZ | 3:J2:30:LEU:HD22 | 2.42 | 0.54 |
| 2:K2:22:THR:CG2 | 2:A2:2:LYS:HE2 | 2.38 | 0.54 |
| 6:M2:45:ILE:HD11 | 8:i7:78:THR:HB | 1.89 | 0.54 |
| 2:A4:2:LYS:HE2 | 2:K4:22:THR:CG2 | 2.38 | 0.54 |
| 5:N3:31:TRP:HZ2 | 3:T3:92:TYR:OH | 1.89 | 0.54 |
| 4:M4:225:LYS:CD | 3:Y4:81:ALA:HB2 | 2.36 | 0.54 |
| 8:M5:105:GLU:OE1 | 10:k5:532:THR:HG22 | 2.07 | 0.54 |
| 8:A5:126:VAL:HG23 | 12:A5:201:CYC:HMC1 | 1.89 | 0.54 |
| 8:E5:80:LEU:HD12 | 12:E5:201:CYC:HAD1 | 1.82 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:G5:65:VAL:HG23 | 8:G5:66:VAL:HG23 | 1.89 | 0.54 |
| 8:G5:126:VAL:HG23 | 12:G5:201:CYC:HMC1 | 1.89 | 0.54 |
| 8:Q5:15:ALA:HB2 | 10:k5:521:GLY:HA2 | 1.89 | 0.54 |
| 8:W5:160:MET:HB2 | 8:W5:161:GLN:HE21 | 1.73 | 0.54 |
| 8:Y5:14:GLU:OE2 | 10:k5:393:MET:CG | 2.56 | 0.54 |
| 9:i5:16:ARG:HE | 9:i5:16:ARG:CA | 2.20 | 0.54 |
| 10:j5:190:LEU:CA | 10:j5:194:CYS:HG | 2.21 | 0.54 |
| 10:j5:306:GLU:OE2 | 10:j5:362:LYS:HE2 | 2.08 | 0.54 |
| 10:j5:872:TYR:HB3 | 9:w7:43:ARG:HH12 | 1.73 | 0.54 |
| 10:j5:969:VAL:HG22 | 10:j5:969:VAL:O | 2.08 | 0.54 |
| 10:j5:1064:LYS:HE2 | 10:j5:1065:HIS:CD2 | 2.42 | 0.54 |
| 10:k5:18:ARG:HH12 | 10:k5:268:SER:HB3 | 1.73 | 0.54 |
| 10:k5:549:LYS:HD3 | 10:k5:549:LYS:C | 2.33 | 0.54 |
| 8:Q7:21:GLY:HA3 | 8:C7:6:LYS:HD3 | 1.90 | 0.54 |
| 8:S7:65:VAL:HG23 | 8:S7:66:VAL:HG23 | 1.89 | 0.54 |
| 8:G7:37:LEU:HD22 | 1:H7:24:LEU:HD22 | 1.89 | 0.54 |
| 8:I7:37:LEU:HA | 8:I7:97:VAL:HG12 | 1.89 | 0.54 |
| 8:k7:65:VAL:HG23 | 8:k7:66:VAL:HG23 | 1.89 | 0.54 |
| 8:Y7:65:VAL:HG23 | 8:Y7:66:VAL:N | 2.21 | 0.54 |
| 8:a7:63:PRO:CG | 11:a9:336:ILE:HG23 | 2.37 | 0.54 |
| 8:o7:2:SER:CB | 1:p7:5:ILE:HG21 | 2.38 | 0.54 |
| 12:v7:201:CYC:HB | 12:v7:201:CYC:HMA3 | 1.73 | 0.54 |
| 9:x7:9:ALA:HB3 | 9:x7:44:ILE:HD11 | 1.89 | 0.54 |
| 3:U8:75:PRO:HB2 | 2:V8:108:TYR:O | 2.06 | 0.54 |
| 3:Q8:5:PHE:CZ | 3:Q8:30:LEU:HD22 | 2.42 | 0.54 |
| 3:Q8:84:ARG:HD3 | 5:Z8:29:HIS:CG | 2.42 | 0.54 |
| 3:Q8:88:ILE:O | 3:Q8:92:TYR:CD2 | 2.61 | 0.54 |
| 3:L9:89:ILE:HB | 3:L9:134:MET:HE1 | 1.88 | 0.54 |
| 2:O9:38:MET:CE | 3:P9:28:THR:OG1 | 2.56 | 0.54 |
| 3:Y8:110:LEU:HD13 | 3:Y8:170:SER:HB2 | 1.89 | 0.54 |
| 12:X9:202:CYC:HC | 12:X9:202:CYC:HMD2 | 1.70 | 0.54 |
| 11:a9:629:LYS:CE | 11:a9:629:LYS:CA | 2.84 | 0.54 |
| 11:aA:581:ARG:HG3 | 11:aA:581:ARG:NH1 | 2.17 | 0.54 |
| 11:aA:703:LYS:C | 11:aA:708:HIS:HD2 | 2.13 | 0.54 |
| 4:M1:95:ALA:CB | 5:N1:38:GLU:OE1 | 2.56 | 0.54 |
| 3:T1:5:PHE:CZ | 3:T1:30:LEU:HD22 | 2.42 | 0.54 |
| 2:W1:19:LEU:HD13 | 3:X1:98:LEU:HD22 | 1.89 | 0.54 |
| 12:Z:201:CYC:HB | 12:Z:201:CYC:HMA2 | 1.69 | 0.54 |
| 3:BA:26:GLN:C | 3:BA:30:LEU:HD13 | 2.31 | 0.54 |
| 3:FA:5:PHE:CZ | 3:FA:30:LEU:HD22 | 2.42 | 0.54 |
| 3:FA:125:ARG:HD2 | 3:VA:14:LEU:HD11 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:LA:5:PHE:CZ | 3:LA:30:LEU:HD22 | 2.42 | 0.54 |
| 5:NA:39:PRO:CA | 3:PA:116:THR:OG1 | 2.56 | 0.54 |
| 2:QA:21:ASN:HB3 | 2:UA:153:TYR:CZ | 2.43 | 0.54 |
| 2:QA:120:PHE:CZ | 3:TA:79:MET:SD | 3.01 | 0.54 |
| 2:A1:2:LYS:HE2 | 2:K1:22:THR:CG2 | 2.38 | 0.54 |
| 2:A1:38:MET:CE | 3:B1:28:THR:OG1 | 2.56 | 0.54 |
| 3:J3:14:LEU:HD11 | 11:a9:621:THR:CG2 | 2.27 | 0.54 |
| 2:K3:16:GLY:N | 11:a9:745:GLY:HA2 | 2.23 | 0.54 |
| 3:H2:77:ARG:CD | 6:M2:117:MET:HE3 | 2.36 | 0.54 |
| 2:C3:140:SER:HB2 | 3:D8:150:ARG:HH11 | 1.68 | 0.54 |
| 2:A4:38:MET:CE | 3:B4:28:THR:OG1 | 2.56 | 0.54 |
| 4:M3:95:ALA:CB | 5:N3:38:GLU:OE1 | 2.56 | 0.54 |
| 2:O3:38:MET:CE | 3:P3:28:THR:OG1 | 2.56 | 0.54 |
| 3:R3:5:PHE:CZ | 3:R3:30:LEU:HD22 | 2.42 | 0.54 |
| 3:S4:85:ASP:OD2 | 12:S4:202:CYC:HHD | 2.08 | 0.54 |
| 3:U4:108:ARG:HB3 | 4:M4:246:ALA:CB | 2.34 | 0.54 |
| 4:M4:215:GLU:HB3 | 5:Z4:28:HIS:H | 1.72 | 0.54 |
| 12:M4:301:CYC:CMB | 3:Y4:89:ILE:CD1 | 2.73 | 0.54 |
| 2:N4:38:MET:CE | 3:O4:28:THR:OG1 | 2.56 | 0.54 |
| 8:M5:38:ARG:HD3 | 1:J7:144:ASP:CG | 2.33 | 0.54 |
| 8:O5:29:PHE:CD1 | 8:O5:99:GLY:HA3 | 2.43 | 0.54 |
| 8:A5:88:TYR:OH | 12:A5:201:CYC:HMB2 | 2.07 | 0.54 |
| 8:A5:107:ILE:CD1 | 1:B5:13:ASP:OD2 | 2.55 | 0.54 |
| 8:A5:115:MET:SD | 12:A5:201:CYC:C1B | 2.95 | 0.54 |
| 8:C5:37:LEU:HA | 8:C5:97:VAL:HG12 | 1.89 | 0.54 |
| 8:C5:88:TYR:CE2 | 12:C5:201:CYC:CMB | 2.91 | 0.54 |
| 8:U5:75:GLU:HG2 | 6:M6:32:MET:CE | 2.37 | 0.54 |
| 3:L6:77:ARG:NE | 6:M6:70:GLU:OE2 | 2.41 | 0.54 |
| 9:z5:34:TYR:C | 9:z5:34:TYR:CD1 | 2.83 | 0.54 |
| 10:j5:16:LEU:N | 10:j5:16:LEU:HD13 | 2.22 | 0.54 |
| 10:k5:227:ILE:HG22 | 10:k5:227:ILE:O | 2.06 | 0.54 |
| 10:k5:456:ILE:O | 10:k5:456:ILE:HG13 | 2.07 | 0.54 |
| 10:k5:1125:ARG:NH1 | 1:n7:114:GLU:HB3 | 2.22 | 0.54 |
| 3:B6:5:PHE:CZ | 3:B6:30:LEU:HD22 | 2.42 | 0.54 |
| 3:D6:5:PHE:CZ | 3:D6:30:LEU:HD22 | 2.42 | 0.54 |
| 1:R7:49:THR:HG22 | 8:C7:161:GLN:CG | 2.31 | 0.54 |
| 12:f7:201:CYC:HB | 12:f7:201:CYC:HMA3 | 1.72 | 0.54 |
| 3:D8:107:ASP:OD2 | 11:a9:109:ASN:OD1 | 2.18 | 0.54 |
| 8:o7:30:VAL:CG1 | 1:p7:31:PHE:HD1 | 2.21 | 0.54 |
| 8:o7:80:LEU:CD1 | 12:o7:201:CYC:HAD2 | 2.38 | 0.54 |
| 8:o7:104:ILE:HG23 | 8:o7:156:LEU:HD21 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:u7:23:LEU:CA | 1:v7:38:VAL:CG2 | 2.85 | 0.54 |
| 9:w7:7:VAL:O | 9:w7:7:VAL:HG23 | 2.08 | 0.54 |
| 3:F8:91:ARG:HH21 | 11:a9:140:GLN:HE21 | 1.56 | 0.54 |
| 2:K8:19:LEU:HD13 | 3:L8:98:LEU:HD22 | 1.89 | 0.54 |
| 3:L8:68:ARG:HB3 | 3:L8:69:PRO:HD2 | 1.89 | 0.54 |
| 2:N8:65:TYR:O | 2:N8:71:GLN:CG | 2.54 | 0.54 |
| 5:N9:67:ILE:N | 5:N9:67:ILE:HD13 | 2.23 | 0.54 |
| 5:Z8:37:HIS:HB2 | 12:Z8:301:CYC:C3B | 2.38 | 0.54 |
| 5:Z8:37:HIS:O | 5:Z8:38:GLU:C | 2.49 | 0.54 |
| 2:I9:21:ASN:O | 2:I9:22:THR:C | 2.49 | 0.54 |
| 11:a9:716:ILE:HD12 | 11:a9:738:LEU:CD2 | 2.37 | 0.54 |
| 11:aA:585:GLU:HA | 11:aA:588:VAL:O | 2.06 | 0.54 |
| 4:M1:188:LEU:HD23 | 12:Z1:202:CYC:HBA1 | 1.89 | 0.54 |
| 12:BA:201:CYC:OB | 4:MA:28:HIS:NE2 | 2.29 | 0.54 |
| 3:HA:125:ARG:NE | 8:S7:41:GLN:HE21 | 1.99 | 0.54 |
| 12:JA:202:CYC:CBB | 11:aA:516:GLN:HG3 | 2.35 | 0.54 |
| 4:MA:58:TYR:CD2 | 11:aA:496:ARG:NH1 | 2.75 | 0.54 |
| 5:NA:54:LEU:HD13 | 3:TA:84:ARG:CZ | 2.36 | 0.54 |
| 2:QA:81:LYS:HZ1 | 3:TA:67:ILE:CD1 | 2.19 | 0.54 |
| 3:VA:5:PHE:CZ | 3:VA:30:LEU:HD22 | 2.42 | 0.54 |
| 3:B3:127:VAL:HG23 | 12:B3:202:CYC:HMC3 | 1.89 | 0.54 |
| 12:L3:202:CYC:HMA1 | 11:a9:713:ASN:OD1 | 2.08 | 0.54 |
| 2:O3:2:LYS:HE2 | 2:Y3:22:THR:CG2 | 2.38 | 0.54 |
| 2:O3:2:LYS:NZ | 2:Y3:23:GLU:OE2 | 2.41 | 0.54 |
| 3:X3:5:PHE:CZ | 3:X3:30:LEU:HD22 | 2.42 | 0.54 |
| 3:F4:84:ARG:NH2 | 11:aA:143:SER:CB | 2.66 | 0.54 |
| 4:M4:61:ASN:O | 4:M4:63:GLY:N | 2.40 | 0.54 |
| 3:Q4:7:LYS:HD2 | 3:Q4:101:ASP:OD1 | 2.07 | 0.54 |
| 12:L5:201:CYC:CMA | 10:j5:591:ILE:CG2 | 2.85 | 0.54 |
| 12:N5:201:CYC:HB | 12:N5:201:CYC:HMA3 | 1.73 | 0.54 |
| 3:Y4:104:VAL:HA | 3:Y4:108:ARG:CB | 2.37 | 0.54 |
| 8:E5:17:TYR:CG | 1:F5:45:SER:HB3 | 2.43 | 0.54 |
| 8:G5:6:LYS:HE2 | 8:S5:21:GLY:HA3 | 1.89 | 0.54 |
| 8:Q5:104:ILE:HG23 | 8:Q5:156:LEU:HD21 | 1.89 | 0.54 |
| 8:Q5:126:VAL:HG23 | 12:Q5:201:CYC:HMC3 | 1.89 | 0.54 |
| 8:W5:127:ALA:HB2 | 8:W5:161:GLN:NE2 | 2.22 | 0.54 |
| 12:J6:201:CYC:HC | 12:J6:201:CYC:HMD2 | 1.70 | 0.54 |
| 6:M6:104:ARG:NE | 2:G6:16:GLY:HA3 | 2.23 | 0.54 |
| 9:i5:9:ALA:HA | 9:i5:51:VAL:HA | 1.89 | 0.54 |
| 10:j5:33:ARG:NH2 | 10:j5:39:GLU:OE2 | 2.40 | 0.54 |
| 10:j5:913:VAL:HG12 | 10:j5:913:VAL:O | 2.06 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:j5:929:PRO:HB3 | 1:J7:147:LYS:HG2 | 1.89 | 0.54 |
| 10:j5:1025:LEU:HD22 | 10:j5:1035:PHE:CB | 2.15 | 0.54 |
| 10:j5:1052:PRO:HB3 | 1:r7:106:GLU:OE2 | 2.08 | 0.54 |
| 10:j5:1151:GLN:C | 1:v7:122:PRO:HB3 | 2.33 | 0.54 |
| 10:k5:221:LYS:CA | 10:k5:221:LYS:CE | 2.85 | 0.54 |
| 10:k5:756:SER:HB2 | 9:z7:24:GLN:HG2 | 1.90 | 0.54 |
| 3:F6:82:CYS:HA | 12:F6:201:CYC:C1D | 2.38 | 0.54 |
| 8:S7:37:LEU:HD22 | 1:T7:24:LEU:HD22 | 1.89 | 0.54 |
| 8:S7:65:VAL:HG23 | 8:S7:66:VAL:N | 2.21 | 0.54 |
| 12:F7:201:CYC:HB | 12:F7:201:CYC:HMA3 | 1.72 | 0.54 |
| 8:I7:90:ARG:CZ | 1:J7:16:GLY:HA2 | 2.37 | 0.54 |
| 8:M7:60:GLN:NE2 | 3:J9:114:LYS:HG2 | 2.22 | 0.54 |
| 8:a7:16:ARG:HG3 | 8:a7:16:ARG:NH1 | 2.20 | 0.54 |
| 1:b7:30:TYR:CD2 | 1:b7:30:TYR:C | 2.85 | 0.54 |
| 1:d7:77:ARG:NH2 | 9:x7:63:ALA:HB2 | 2.17 | 0.54 |
| 2:E1:19:LEU:HD13 | 3:F1:98:LEU:HD22 | 1.89 | 0.54 |
| 8:s7:44:THR:OG1 | 1:t7:18:TYR:HD2 | 1.90 | 0.54 |
| 8:u7:80:LEU:CD1 | 12:u7:201:CYC:HAD2 | 2.38 | 0.54 |
| 9:z7:27:PHE:CD1 | 9:z7:27:PHE:C | 2.86 | 0.54 |
| 9:y7:4:TYR:N | 9:y7:58:THR:OG1 | 2.40 | 0.54 |
| 2:X8:22:THR:CG2 | 2:N8:2:LYS:HE2 | 2.38 | 0.54 |
| 3:L8:82:CYS:CB | 12:a9:901:CYC:C4C | 2.85 | 0.54 |
| 4:M8:200:ILE:CG2 | 5:Z8:52:ARG:HH21 | 2.21 | 0.54 |
| 4:M8:226:SER:OG | 3:Y8:88:ILE:HG13 | 2.08 | 0.54 |
| 12:O8:202:CYC:HC | 12:O8:202:CYC:HMD2 | 1.70 | 0.54 |
| 2:R8:19:LEU:HD13 | 3:S8:98:LEU:HD22 | 1.89 | 0.54 |
| 3:L9:84:ARG:HE | 11:a9:406:LEU:CD2 | 2.20 | 0.54 |
| 4:M9:58:TYR:CD2 | 11:a9:496:ARG:NH1 | 2.76 | 0.54 |
| 3:Y8:89:ILE:HG12 | 3:Y8:92:TYR:CZ | 2.43 | 0.54 |
| 5:Z8:22:LEU:O | 5:Z8:37:HIS:HE1 | 1.91 | 0.54 |
| 3:B9:26:GLN:C | 3:B9:30:LEU:HD13 | 2.31 | 0.54 |
| 2:W9:19:LEU:HD13 | 3:X9:98:LEU:HD22 | 1.89 | 0.54 |
| 11:a9:90:GLN:O | 11:a9:93:LEU:HD13 | 2.08 | 0.54 |
| 11:a9:419:ARG:HH11 | 11:a9:419:ARG:CG | 2.20 | 0.54 |
| 11:a9:585:GLU:HA | 11:a9:588:VAL:O | 2.06 | 0.54 |
| 11:a9:615:ARG:HH11 | 11:a9:615:ARG:CB | 2.20 | 0.54 |
| 11:aA:25:GLU:C | 11:aA:27:PHE:H | 2.16 | 0.54 |
| 11:aA:75:ALA:HB1 | 11:aA:81:ASP:N | 2.23 | 0.54 |
| 11:aA:800:THR:CG2 | 12:aA:901:CYC:HAA2 | 2.29 | 0.54 |
| 4:M1:28:HIS:HE1 | 4:M1:37:GLU:OE1 | 1.91 | 0.54 |
| 2:U1:19:LEU:HD13 | 3:V1:98:LEU:HD22 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:A2:38:MET:CE | 3:B2:28:THR:OG1 | 2.56 | 0.54 |
| 2:E2:19:LEU:HD13 | 3:F2:98:LEU:HD22 | 1.89 | 0.54 |
| 12:JA:202:CYC:C1B | 11:aA:512:TYR:HB2 | 2.32 | 0.53 |
| 4:MA:90:LYS:HE3 | 4:MA:220:TYR:CZ | 2.43 | 0.53 |
| 5:NA:23:SER:C | 5:NA:25:THR:H | 2.15 | 0.53 |
| 2:SA:19:LEU:HD13 | 3:TA:98:LEU:HD22 | 1.89 | 0.53 |
| 2:O1:60:TYR:CB | 2:O1:67:THR:CG2 | 2.83 | 0.53 |
| 2:Q1:19:LEU:HD13 | 3:R1:98:LEU:HD22 | 1.89 | 0.53 |
| 6:M2:127:SER:C | 12:F2:201:CYC:HMA2 | 2.33 | 0.53 |
| 4:M3:61:ASN:O | 4:M3:63:GLY:N | 2.40 | 0.53 |
| 4:M3:90:LYS:HE3 | 4:M3:220:TYR:CZ | 2.43 | 0.53 |
| 2:Q3:19:LEU:HD13 | 3:R3:98:LEU:HD22 | 1.89 | 0.53 |
| 2:W3:19:LEU:HD13 | 3:X3:98:LEU:HD22 | 1.89 | 0.53 |
| 3:S4:116:THR:HG23 | 3:S4:117:TYR:H | 1.70 | 0.53 |
| 2:N4:65:TYR:O | 2:N4:71:GLN:CG | 2.54 | 0.53 |
| 3:O4:112:GLY:HA3 | 5:Z4:69:GLU:C | 2.33 | 0.53 |
| 12:L5:201:CYC:OB | 10:j5:588:VAL:CG2 | 2.56 | 0.53 |
| 8:O5:151:PHE:CB | 8:E5:20:PRO:HB3 | 2.26 | 0.53 |
| 5:Z4:38:GLU:O | 5:Z4:38:GLU:HG2 | 2.08 | 0.53 |
| 5:Z4:67:ILE:HD13 | 5:Z4:67:ILE:N | 2.23 | 0.53 |
| 8:A5:15:ALA:HA | 1:B5:90:ARG:NH1 | 2.23 | 0.53 |
| 8:A5:71:ASN:OD1 | 12:A5:201:CYC:HMD1 | 2.00 | 0.53 |
| 1:D5:5:ILE:HG22 | 1:D5:5:ILE:O | 2.08 | 0.53 |
| 12:D5:201:CYC:C4B | 9:z5:38:PHE:CE2 | 2.91 | 0.53 |
| 8:E5:77:MET:O | 12:E5:201:CYC:HMD3 | 2.08 | 0.53 |
| 12:H5:201:CYC:HBB2 | 9:i5:21:ARG:CG | 2.38 | 0.53 |
| 12:J5:201:CYC:HBB1 | 9:i5:42:GLN:NE2 | 2.21 | 0.53 |
| 12:Z5:201:CYC:HB | 12:Z5:201:CYC:HMA3 | 1.73 | 0.53 |
| 2:K6:23:GLU:OE2 | 2:A6:2:LYS:NZ | 2.41 | 0.53 |
| 3:L6:65:ASP:OD2 | 1:b7:64:ASP:CB | 2.56 | 0.53 |
| 9:z5:11:ILE:HD12 | 9:z5:28:PHE:CE2 | 2.27 | 0.53 |
| 10:j5:1139:SER:HB2 | 12:v7:201:CYC:O2D | 2.07 | 0.53 |
| 10:k5:199:THR:CG2 | 12:k5:1201:CYC:CBC | 2.80 | 0.53 |
| 10:k5:965:GLN:C | 1:p7:14:VAL:HG12 | 2.33 | 0.53 |
| 10:k5:1102:TYR:C | 10:k5:1102:TYR:CD1 | 2.85 | 0.53 |
| 2:A6:38:MET:CE | 3:B6:28:THR:OG1 | 2.56 | 0.53 |
| 3:F6:72:ASN:OD1 | 12:F6:201:CYC:HBD2 | 2.08 | 0.53 |
| 8:O7:29:PHE:CD1 | 8:O7:99:GLY:HA3 | 2.43 | 0.53 |
| 8:O7:95:GLY:H | 8:O7:104:ILE:HD11 | 1.73 | 0.53 |
| 1:P7:75:THR:C | 8:Q7:111:GLY:HA3 | 2.33 | 0.53 |
| 1:H7:136:VAL:CA | 11:aA:563:PHE:CZ | 2.88 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:J7:75:THR:C | 8:K7:111:GLY:HA3 | 2.32 | 0.53 |
| 8:U7:44:THR:OG1 | 1:V7:18:TYR:HD2 | 1.91 | 0.53 |
| 8:U7:52:LYS:HB2 | 11:a9:27:PHE:CE2 | 2.43 | 0.53 |
| 8:a7:29:PHE:CZ | 8:a7:98:ALA:C | 2.76 | 0.53 |
| 2:A8:2:LYS:NZ | 2:K8:23:GLU:OE2 | 2.41 | 0.53 |
| 3:D8:5:PHE:CZ | 3:D8:30:LEU:HD22 | 2.42 | 0.53 |
| 8:o7:4:LEU:HD23 | 8:o7:26:ILE:CD1 | 2.38 | 0.53 |
| 9:y7:9:ALA:CB | 9:y7:44:ILE:HD11 | 2.39 | 0.53 |
| 2:T8:19:LEU:HD13 | 3:U8:98:LEU:HD22 | 1.89 | 0.53 |
| 3:Q8:85:ASP:CB | 12:Z8:301:CYC:HBC3 | 2.04 | 0.53 |
| 5:N9:54:LEU:HB3 | 12:T9:301:CYC:O2A | 2.07 | 0.53 |
| 3:Y8:87:GLU:HG2 | 3:Y8:91:ARG:HE | 1.73 | 0.53 |
| 3:Y8:114:LYS:HA | 3:Y8:124:THR:HG21 | 1.89 | 0.53 |
| 2:A9:60:TYR:CB | 2:A9:67:THR:CG2 | 2.82 | 0.53 |
| 3:F9:125:ARG:HD2 | 3:V9:14:LEU:HD11 | 1.89 | 0.53 |
| 11:a9:643:LEU:HD11 | 11:a9:766:ASN:HA | 1.90 | 0.53 |
| 11:aA:287:ALA:O | 11:aA:288:ARG:CD | 2.55 | 0.53 |
| 11:aA:616:PRO:HA | 3:H1:69:PRO:O | 2.08 | 0.53 |
| 11:aA:640:ALA:CB | 11:aA:767:THR:HG21 | 2.38 | 0.53 |
| 5:N1:41:GLN:HG2 | 5:N1:44:TYR:CE1 | 2.44 | 0.53 |
| 2:AA:60:TYR:CB | 2:AA:67:THR:CG2 | 2.83 | 0.53 |
| 3:L3:120:LEU:HD21 | 11:a9:731:GLN:HG3 | 1.86 | 0.53 |
| 4:M3:152:TYR:CD1 | 4:M3:152:TYR:C | 2.87 | 0.53 |
| 2:U3:19:LEU:HD13 | 3:V3:98:LEU:HD22 | 1.89 | 0.53 |
| 3:W4:5:PHE:CZ | 3:W4:30:LEU:HD22 | 2.43 | 0.53 |
| 8:K5:17:TYR:CG | 1:L5:45:SER:HB3 | 2.43 | 0.53 |
| 1:L5:76:ARG:CA | 8:G5:111:GLY:HA3 | 2.36 | 0.53 |
| 8:M5:90:ARG:CZ | 1:N5:16:GLY:CA | 2.86 | 0.53 |
| 8:C5:35:ARG:NH2 | 8:C5:145:ASP:OD1 | 2.42 | 0.53 |
| 1:X5:3:ASP:H | 1:X5:6:THR:HG1 | 1.56 | 0.53 |
| 12:a5:201:CYC:HB | 12:a5:201:CYC:CMA | 2.21 | 0.53 |
| 1:b5:24:LEU:HD21 | 10:k5:57:VAL:CG1 | 2.37 | 0.53 |
| 10:j5:361:PHE:HZ | 10:j5:378:TYR:CE2 | 2.25 | 0.53 |
| 10:j5:489:ASN:HD22 | 10:j5:492:ILE:HG12 | 1.73 | 0.53 |
| 10:j5:1102:TYR:C | 10:j5:1102:TYR:CD1 | 2.85 | 0.53 |
| 10:k5:70:ARG:HG2 | 10:k5:209:ASN:OD1 | 2.08 | 0.53 |
| 10:k5:283:ARG:N | 10:k5:283:ARG:CD | 2.72 | 0.53 |
| 10:k5:1118:THR:HG23 | 12:k5:1204:CYC:C3A | 2.38 | 0.53 |
| 10:k5:1119:LEU:CD2 | 1:n7:87:TYR:OH | 2.53 | 0.53 |
| 1:H7:140:LEU:HG | 11:aA:561:ALA:CB | 2.20 | 0.53 |
| 12:N7:201:CYC:HB | 12:N7:201:CYC:HMA3 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:h7:62:TYR:CE1 | 12:i7:201:CYC:O1D | 2.61 | 0.53 |
| 8:U7:52:LYS:HD2 | 11:a9:27:PHE:CG | 2.43 | 0.53 |
| 1:V7:75:THR:C | 8:W7:111:GLY:HA3 | 2.32 | 0.53 |
| 8:W7:4:LEU:HD23 | 8:W7:26:ILE:CD1 | 2.38 | 0.53 |
| 3:B8:119:ALA:CB | 4:M8:69:ILE:CG2 | 2.67 | 0.53 |
| 8:m7:27:LYS:O | 8:m7:30:VAL:HG22 | 2.09 | 0.53 |
| 8:o7:44:THR:HG22 | 8:o7:44:THR:O | 2.08 | 0.53 |
| 1:v7:139:GLY:HA3 | 11:aA:342:ARG:NE | 2.23 | 0.53 |
| 3:L8:109:CYS:SG | 12:a9:901:CYC:HMB1 | 2.47 | 0.53 |
| 4:M8:224:PHE:C | 12:M8:301:CYC:CGA | 2.65 | 0.53 |
| 4:M9:81:ASP:N | 3:Z9:111:ASN:HD21 | 2.06 | 0.53 |
| 5:N9:41:GLN:HG2 | 5:N9:44:TYR:CE1 | 2.43 | 0.53 |
| 2:O9:2:LYS:NZ | 2:Y9:23:GLU:OE2 | 2.41 | 0.53 |
| 2:G9:19:LEU:HD13 | 3:H9:98:LEU:HD22 | 1.89 | 0.53 |
| 11:aA:388:VAL:HG11 | 11:aA:419:ARG:HH11 | 1.73 | 0.53 |
| 11:aA:419:ARG:HH11 | 11:aA:419:ARG:CG | 2.20 | 0.53 |
| 4:M1:48:PRO:HG2 | 4:M1:48:PRO:O | 2.06 | 0.53 |
| 5:N1:37:HIS:O | 5:N1:37:HIS:HD2 | 1.92 | 0.53 |
| 2:EA:19:LEU:HD13 | 3:FA:98:LEU:HD22 | 1.89 | 0.53 |
| 2:GA:19:LEU:HD13 | 3:HA:98:LEU:HD22 | 1.89 | 0.53 |
| 5:NA:11:ARG:HD2 | 3:RA:108:ARG:NH2 | 2.23 | 0.53 |
| 2:QA:32:GLN:CG | 2:UA:28:ASN:HD21 | 2.14 | 0.53 |
| 2:S1:19:LEU:HD13 | 3:T1:98:LEU:HD22 | 1.89 | 0.53 |
| 2:I3:15:GLN:HG2 | 11:a9:654:ALA:CB | 2.36 | 0.53 |
| 3:L2:75:PRO:HD3 | 3:L2:78:ARG:HE | 1.73 | 0.53 |
| 2:A3:38:MET:CE | 3:B3:28:THR:OG1 | 2.56 | 0.53 |
| 3:L3:88:ILE:CD1 | 3:L3:91:ARG:HH21 | 2.21 | 0.53 |
| 4:M3:17:VAL:CG1 | 4:M3:18:THR:N | 2.71 | 0.53 |
| 4:M3:28:HIS:HE1 | 4:M3:37:GLU:OE1 | 1.91 | 0.53 |
| 3:U4:120:LEU:CD1 | 4:M4:254:LEU:HD21 | 2.38 | 0.53 |
| 4:M4:110:TYR:CE2 | 4:M4:124:ARG:NH1 | 2.77 | 0.53 |
| 3:Q4:84:ARG:NH2 | 5:Z4:33:GLY:O | 2.41 | 0.53 |
| 1:N5:113:LYS:HE2 | 1:Z5:155:TYR:OH | 2.07 | 0.53 |
| 8:O5:35:ARG:NH2 | 8:O5:145:ASP:OD1 | 2.42 | 0.53 |
| 5:Z4:39:PRO:CG | 12:Z4:301:CYC:HHD | 2.38 | 0.53 |
| 12:C5:201:CYC:HB | 12:C5:201:CYC:CMA | 2.21 | 0.53 |
| 8:G5:15:ALA:HA | 1:H5:90:ARG:NH1 | 2.23 | 0.53 |
| 8:c5:65:VAL:HG23 | 8:c5:66:VAL:HG23 | 1.89 | 0.53 |
| 12:T5:201:CYC:HB | 12:T5:201:CYC:HMA3 | 1.73 | 0.53 |
| 8:Y5:104:ILE:HG23 | 8:Y5:156:LEU:HD21 | 1.89 | 0.53 |
| 6:M6:141:ARG:NH2 | 6:M6:202:ASP:OD1 | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:1052:PRO:HB3 | 11:aA:32:ARG:HH21 | 1.72 | 0.53 |
| 10:k5:306:GLU:OE2 | 10:k5:362:LYS:HE2 | 2.08 | 0.53 |
| 2:C6:19:LEU:HD13 | 3:D6:98:LEU:HD22 | 1.89 | 0.53 |
| 8:O7:90:ARG:CZ | 1:P7:16:GLY:HA2 | 2.37 | 0.53 |
| 8:O7:111:GLY:C | 1:N7:75:THR:HB | 2.32 | 0.53 |
| 8:S7:49:ARG:HH11 | 11:aA:550:PHE:HE1 | 1.56 | 0.53 |
| 8:c7:94:TYR:CD2 | 1:d7:9:ILE:CG2 | 2.91 | 0.53 |
| 8:o7:90:ARG:HB2 | 1:p7:18:TYR:OH | 2.05 | 0.53 |
| 2:X8:19:LEU:HD13 | 3:Y8:98:LEU:HD22 | 1.89 | 0.53 |
| 2:X8:23:GLU:OE2 | 2:N8:2:LYS:NZ | 2.41 | 0.53 |
| 4:M8:28:HIS:HE1 | 4:M8:37:GLU:OE1 | 1.91 | 0.53 |
| 4:M8:110:TYR:CE2 | 4:M8:124:ARG:NH1 | 2.77 | 0.53 |
| 4:M8:152:TYR:C | 4:M8:152:TYR:CD1 | 2.87 | 0.53 |
| 4:M8:225:LYS:HE3 | 3:Y8:81:ALA:CB | 2.25 | 0.53 |
| 3:O8:88:ILE:HD11 | 5:Z8:54:LEU:CD1 | 2.37 | 0.53 |
| 4:M9:185:ALA:HB1 | 12:V9:201:CYC:O1A | 2.08 | 0.53 |
| 11:a9:615:ARG:HB3 | 11:a9:615:ARG:NH1 | 2.20 | 0.53 |
| 11:a9:640:ALA:CB | 11:a9:767:THR:HG21 | 2.38 | 0.53 |
| 11:aA:90:GLN:O | 11:aA:93:LEU:HD13 | 2.08 | 0.53 |
| 11:aA:325:LEU:HD23 | 11:aA:325:LEU:N | 2.23 | 0.53 |
| 11:aA:818:ARG:HH11 | 11:aA:818:ARG:CG | 2.10 | 0.53 |
| 3:L1:88:ILE:CD1 | 3:L1:91:ARG:HH21 | 2.21 | 0.53 |
| 3:JA:19:LEU:HD12 | 3:JA:24:LEU:HD21 | 1.89 | 0.53 |
| 4:MA:81:ASP:N | 3:ZA:111:ASN:HD21 | 2.06 | 0.53 |
| 4:MA:185:ALA:CA | 12:VA:201:CYC:O2A | 2.51 | 0.53 |
| 2:UA:19:LEU:HD13 | 3:VA:98:LEU:HD22 | 1.89 | 0.53 |
| 2:K3:23:GLU:OE2 | 2:A3:2:LYS:NZ | 2.41 | 0.53 |
| 2:K2:19:LEU:HD13 | 3:L2:98:LEU:HD22 | 1.89 | 0.53 |
| 3:B3:85:ASP:OD2 | 12:B3:202:CYC:ND | 2.30 | 0.53 |
| 3:L3:1:MET:HE2 | 11:a9:708:HIS:ND1 | 2.24 | 0.53 |
| 4:M3:192:GLN:O | 4:M3:192:GLN:HG3 | 2.05 | 0.53 |
| 5:N3:23:SER:C | 5:N3:25:THR:H | 2.15 | 0.53 |
| 2:S3:19:LEU:HD13 | 3:T3:98:LEU:HD22 | 1.89 | 0.53 |
| 3:B1:127:VAL:HG22 | 12:B1:202:CYC:HMC3 | 1.90 | 0.53 |
| 3:F4:113:LEU:CB | 4:M4:5:THR:HG21 | 2.26 | 0.53 |
| 4:M4:233:GLU:HG3 | 3:Y4:112:GLY:CA | 2.39 | 0.53 |
| 3:O4:107:ASP:O | 5:Z4:67:ILE:N | 2.41 | 0.53 |
| 3:Q4:116:THR:O | 3:Q4:119:ALA:N | 2.40 | 0.53 |
| 8:K5:125:ALA:O | 8:K5:128:GLU:HB3 | 2.09 | 0.53 |
| 1:L5:75:THR:CG2 | 8:G5:115:MET:CE | 2.75 | 0.53 |
| 12:L5:201:CYC:CBB | 10:j5:588:VAL:HG21 | 2.38 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 12:E5:201:CYC:HB | 12:E5:201:CYC:CMA | 2.21 | 0.53 |
| 8:G5:109:ILE:HD13 | 8:G5:159:ALA:HB1 | 1.91 | 0.53 |
| 8:Q5:4:LEU:HD23 | 8:Q5:26:ILE:CD1 | 2.38 | 0.53 |
| 8:Q5:8:ILE:CG2 | 1:R5:94:TYR:CG | 2.90 | 0.53 |
| 8:S5:14:GLU:CD | 10:j5:538:PHE:HE2 | 2.17 | 0.53 |
| 8:S5:104:ILE:HG23 | 8:S5:156:LEU:HD21 | 1.89 | 0.53 |
| 8:U5:79:ALA:HB1 | 6:M6:31:ASP:C | 2.33 | 0.53 |
| 1:X5:106:GLU:HG3 | 10:j5:505:VAL:CA | 2.38 | 0.53 |
| 12:X5:201:CYC:HB | 12:X5:201:CYC:HMA3 | 1.72 | 0.53 |
| 3:J6:88:ILE:HD11 | 6:M6:185:PHE:CZ | 2.43 | 0.53 |
| 2:K6:22:THR:CG2 | 2:A6:2:LYS:HE2 | 2.38 | 0.53 |
| 9:z5:16:ARG:NE | 9:z5:16:ARG:HA | 2.23 | 0.53 |
| 9:i5:56:LEU:C | 9:i5:58:THR:N | 2.61 | 0.53 |
| 10:j5:218:ALA:O | 10:j5:221:LYS:HB2 | 2.09 | 0.53 |
| 10:j5:489:ASN:ND2 | 10:j5:492:ILE:HG12 | 2.24 | 0.53 |
| 10:j5:1105:ILE:HD13 | 10:j5:1115:ARG:NH2 | 2.15 | 0.53 |
| 10:k5:820:HIS:ND1 | 10:k5:859:ILE:HD13 | 1.93 | 0.53 |
| 12:D7:201:CYC:HB | 12:D7:201:CYC:HMA3 | 1.73 | 0.53 |
| 8:g7:35:ARG:NH2 | 8:g7:145:ASP:OD1 | 2.42 | 0.53 |
| 1:j7:83:ARG:NH1 | 9:y7:38:PHE:CE1 | 2.76 | 0.53 |
| 8:W7:126:VAL:HG23 | 12:W7:201:CYC:HMC3 | 1.89 | 0.53 |
| 8:a7:27:LYS:O | 8:a7:30:VAL:HG22 | 2.09 | 0.53 |
| 8:m7:44:THR:OG1 | 1:n7:18:TYR:HD2 | 1.90 | 0.53 |
| 8:s7:27:LYS:O | 8:s7:30:VAL:HG22 | 2.09 | 0.53 |
| 8:s7:35:ARG:NH2 | 8:s7:145:ASP:OD1 | 2.41 | 0.53 |
| 9:z7:7:VAL:HG11 | 9:z7:37:TRP:CE3 | 2.43 | 0.53 |
| 4:M8:48:PRO:HG2 | 4:M8:48:PRO:O | 2.06 | 0.53 |
| 4:M8:215:GLU:O | 4:M8:215:GLU:CG | 2.57 | 0.53 |
| 4:M9:17:VAL:CG1 | 4:M9:18:THR:N | 2.71 | 0.53 |
| 4:M9:176:ARG:HH11 | 4:M9:176:ARG:HG2 | 1.74 | 0.53 |
| 2:A9:38:MET:CE | 3:B9:28:THR:OG1 | 2.56 | 0.53 |
| 3:F9:150:ARG:HH11 | 12:F9:302:CYC:C2C | 2.19 | 0.53 |
| 2:U9:19:LEU:HD13 | 3:V9:98:LEU:HD22 | 1.89 | 0.53 |
| 11:a9:312:ASP:HB2 | 11:a9:315:LEU:HB3 | 0.72 | 0.53 |
| 11:aA:643:LEU:HD13 | 11:aA:766:ASN:HB3 | 1.80 | 0.53 |
| 4:M1:185:ALA:HA | 12:Z1:202:CYC:HBA2 | 1.90 | 0.53 |
| 3:BA:107:ASP:CG | 11:aA:382:ASN:ND2 | 2.59 | 0.53 |
| 12:BA:201:CYC:O2A | 4:MA:35:THR:CA | 2.54 | 0.53 |
| 2:IA:113:LEU:CD2 | 2:IA:161:LEU:HD23 | 2.18 | 0.53 |
| 3:JA:88:ILE:CD1 | 11:aA:512:TYR:CG | 2.92 | 0.53 |
| 12:JA:202:CYC:CBA | 11:aA:510:PHE:O | 2.50 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:MA:158:PHE:CZ | 2:UA:10:ALA:CB | 2.92 | 0.53 |
| 2:K3:22:THR:CG2 | 2:A3:2:LYS:HE2 | 2.38 | 0.53 |
| 3:B3:88:ILE:CG2 | 12:B3:202:CYC:HMB1 | 2.37 | 0.53 |
| 2:E3:19:LEU:HD13 | 3:F3:98:LEU:HD22 | 1.89 | 0.53 |
| 12:F3:201:CYC:HBA2 | 4:M3:36:TYR:CD2 | 2.43 | 0.53 |
| 3:B4:107:ASP:O | 4:M4:61:ASN:CA | 2.57 | 0.53 |
| 5:N3:22:LEU:O | 5:N3:37:HIS:HE1 | 1.92 | 0.53 |
| 2:I4:112:GLY:N | 11:aA:133:LEU:HD21 | 2.23 | 0.53 |
| 3:L4:65:ASP:C | 11:aA:82:GLN:OE1 | 2.48 | 0.53 |
| 2:N4:2:LYS:HE2 | 2:X4:22:THR:CG2 | 2.38 | 0.53 |
| 8:K5:22:GLU:OE2 | 8:U5:6:LYS:NZ | 2.41 | 0.53 |
| 5:Z4:24:PRO:HD2 | 12:Z4:301:CYC:O2A | 2.07 | 0.53 |
| 1:f5:114:GLU:HG2 | 10:j5:491:THR:CB | 2.34 | 0.53 |
| 8:W5:17:TYR:CZ | 1:X5:44:ILE:HG21 | 2.16 | 0.53 |
| 1:X5:65:LEU:CG | 10:j5:706:PRO:HG3 | 2.37 | 0.53 |
| 1:b5:24:LEU:HB3 | 10:k5:54:ILE:HG23 | 1.91 | 0.53 |
| 3:L6:5:PHE:CZ | 3:L6:30:LEU:HD22 | 2.42 | 0.53 |
| 10:j5:221:LYS:HA | 10:j5:221:LYS:CE | 2.37 | 0.53 |
| 10:j5:549:LYS:HD3 | 10:j5:549:LYS:C | 2.33 | 0.53 |
| 10:j5:756:SER:O | 9:w7:21:ARG:HD3 | 2.08 | 0.53 |
| 10:j5:965:GLN:H | 1:t7:69:GLY:HA3 | 1.54 | 0.53 |
| 10:j5:1009:ALA:CA | 1:v7:87:TYR:HE1 | 2.20 | 0.53 |
| 10:k5:16:LEU:N | 10:k5:16:LEU:HD13 | 2.22 | 0.53 |
| 10:k5:20:VAL:O | 10:k5:24:THR:CG2 | 2.51 | 0.53 |
| 10:k5:489:ASN:HD22 | 10:k5:492:ILE:HG12 | 1.73 | 0.53 |
| 10:k5:1067:LEU:CD1 | 10:k5:1101:GLU:OE1 | 2.56 | 0.53 |
| 3:B6:77:ARG:HH11 | 3:B6:77:ARG:CG | 2.18 | 0.53 |
| 12:R7:201:CYC:CGA | 9:z7:34:TYR:OH | 2.53 | 0.53 |
| 1:J7:53:LYS:HZ1 | 8:K7:120:GLN:CD | 2.17 | 0.53 |
| 12:J7:201:CYC:HB | 12:J7:201:CYC:HMA3 | 1.73 | 0.53 |
| 12:h7:201:CYC:HBB1 | 9:y7:21:ARG:NE | 2.22 | 0.53 |
| 8:i7:21:GLY:N | 8:s7:101:VAL:CG2 | 2.21 | 0.53 |
| 12:f7:201:CYC:HMD1 | 12:f7:201:CYC:NC | 2.09 | 0.53 |
| 3:L8:65:ASP:C | 11:a9:82:GLN:HE22 | 2.16 | 0.53 |
| 4:M8:205:ASP:CB | 5:Z8:59:ARG:NH1 | 2.69 | 0.53 |
| 3:O8:115:GLU:HB3 | 5:Z8:70:ILE:O | 2.08 | 0.53 |
| 12:F1:201:CYC:CBA | 4:M1:36:TYR:CE2 | 2.92 | 0.53 |
| 4:M9:134:ASN:N | 12:R9:201:CYC:HBA2 | 2.24 | 0.53 |
| 4:M9:139:VAL:HG12 | 4:M9:139:VAL:O | 2.09 | 0.53 |
| 2:O9:2:LYS:HE2 | 2:Y9:22:THR:CG2 | 2.38 | 0.53 |
| 5:Z8:67:ILE:N | 5:Z8:67:ILE:HD13 | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:I9:113:LEU:CD2 | 2:I9:161:LEU:HD23 | 2.18 | 0.53 |
| 11:a9:537:ASP:HB3 | 11:a9:543:GLN:CB | 2.38 | 0.53 |
| 3:H1:81:ALA:HB1 | 12:H1:201:CYC:C2D | 2.30 | 0.53 |
| 2:C2:19:LEU:HD13 | 3:D2:98:LEU:HD22 | 1.89 | 0.53 |
| 5:NA:22:LEU:O | 5:NA:37:HIS:HE1 | 1.92 | 0.53 |
| 2:QA:76:ASP:CB | 2:U1:140:SER:C | 2.80 | 0.53 |
| 2:G2:19:LEU:HD13 | 3:H2:98:LEU:HD22 | 1.89 | 0.53 |
| 3:J2:108:ARG:CZ | 6:M2:155:ASN:O | 2.55 | 0.53 |
| 6:M2:141:ARG:NH2 | 6:M2:202:ASP:OD1 | 2.42 | 0.53 |
| 3:B4:105:LEU:HG | 3:B4:110:LEU:HD11 | 1.90 | 0.53 |
| 4:M3:110:TYR:CE2 | 4:M3:124:ARG:NH1 | 2.77 | 0.53 |
| 5:N3:41:GLN:HG2 | 5:N3:44:TYR:CE1 | 2.44 | 0.53 |
| 4:M4:61:ASN:OD1 | 4:M4:62:LYS:HG2 | 2.07 | 0.53 |
| 2:N4:112:GLY:CA | 5:Z4:34:LEU:CA | 2.83 | 0.53 |
| 8:K5:127:ALA:O | 8:K5:157:VAL:HG22 | 2.08 | 0.53 |
| 8:A5:5:THR:HG21 | 10:k5:559:THR:HG21 | 1.91 | 0.53 |
| 8:A5:88:TYR:CE2 | 12:A5:201:CYC:HMB3 | 2.44 | 0.53 |
| 8:A5:104:ILE:HG23 | 8:A5:156:LEU:HD21 | 1.89 | 0.53 |
| 8:A5:109:ILE:HD13 | 8:A5:159:ALA:HB1 | 1.91 | 0.53 |
| 8:A5:115:MET:HE2 | 1:F5:75:THR:CG2 | 2.34 | 0.53 |
| 12:H5:201:CYC:HB | 12:H5:201:CYC:HMA3 | 1.73 | 0.53 |
| 8:I5:88:TYR:CE2 | 12:I5:201:CYC:CMB | 2.91 | 0.53 |
| 8:Q5:127:ALA:HB2 | 8:Q5:161:GLN:NE2 | 2.22 | 0.53 |
| 6:M6:205:GLU:OE1 | 6:M6:219:ARG:NH2 | 2.42 | 0.53 |
| 10:j5:542:GLN:HE21 | 10:j5:560:VAL:CG1 | 2.13 | 0.53 |
| 10:j5:741:GLN:HG3 | 1:J7:77:ARG:CZ | 2.30 | 0.53 |
| 10:k5:218:ALA:O | 10:k5:221:LYS:HB2 | 2.09 | 0.53 |
| 10:k5:221:LYS:HE2 | 10:k5:221:LYS:CA | 2.37 | 0.53 |
| 10:k5:1118:THR:HG21 | 1:n7:83:ARG:NH1 | 2.23 | 0.53 |
| 8:S7:25:ARG:CZ | 8:G7:25:ARG:NE | 2.71 | 0.53 |
| 8:C7:27:LYS:O | 8:C7:30:VAL:HG22 | 2.09 | 0.53 |
| 8:C7:95:GLY:H | 8:C7:104:ILE:HD11 | 1.74 | 0.53 |
| 8:E7:104:ILE:HG23 | 8:E7:156:LEU:HD21 | 1.89 | 0.53 |
| 8:G7:109:ILE:HD13 | 8:G7:159:ALA:HB1 | 1.91 | 0.53 |
| 8:I7:35:ARG:NH2 | 8:I7:145:ASP:OD1 | 2.42 | 0.53 |
| 8:i7:122:PRO:HB2 | 8:i7:125:ALA:H | 1.74 | 0.53 |
| 12:X7:201:CYC:O1A | 9:w7:34:TYR:OH | 2.27 | 0.53 |
| 8:a7:11:ALA:O | 8:a7:12:ASP:C | 2.50 | 0.53 |
| 8:a7:29:PHE:CD1 | 8:a7:99:GLY:HA3 | 2.43 | 0.53 |
| 8:a7:95:GLY:H | 8:a7:104:ILE:HD11 | 1.74 | 0.53 |
| 1:b7:75:THR:HG21 | 8:c7:112:VAL:HG23 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:c7:101:VAL:HB | 8:c7:155:TYR:OH | 2.08 | 0.53 |
| 8:e7:109:ILE:HD13 | 8:e7:159:ALA:HB1 | 1.91 | 0.53 |
| 2:A8:60:TYR:CB | 2:A8:67:THR:CG2 | 2.83 | 0.53 |
| 4:M8:230:GLN:O | 4:M8:231:THR:HG23 | 2.09 | 0.53 |
| 12:F1:201:CYC:HBA2 | 4:M1:36:TYR:CD2 | 2.43 | 0.53 |
| 5:N9:23:SER:C | 5:N9:25:THR:H | 2.15 | 0.53 |
| 3:F9:68:ARG:HH22 | 3:Z9:68:ARG:CZ | 2.22 | 0.53 |
| 11:aA:615:ARG:NH1 | 11:aA:615:ARG:CB | 2.72 | 0.53 |
| 11:aA:801:ASN:HD22 | 11:aA:801:ASN:C | 2.10 | 0.53 |
| 4:M1:152:TYR:CD1 | 4:M1:152:TYR:C | 2.87 | 0.53 |
| 5:N1:31:TRP:HZ2 | 3:T1:92:TYR:OH | 1.89 | 0.53 |
| 1:A:75:THR:HG1 | 10:k5:182:ASN:HA | 1.72 | 0.53 |
| 2:IA:13:ASP:OD1 | 11:aA:515:GLY:HA2 | 2.09 | 0.53 |
| 2:IA:16:GLY:CA | 11:aA:514:VAL:HG11 | 2.36 | 0.53 |
| 4:MA:134:ASN:N | 12:RA:201:CYC:HBA2 | 2.24 | 0.53 |
| 5:NA:2:SER:O | 5:NA:2:SER:OG | 2.16 | 0.53 |
| 2:OA:2:LYS:HE2 | 2:YA:22:THR:CG2 | 2.38 | 0.53 |
| 2:OA:38:MET:CE | 3:PA:28:THR:OG1 | 2.56 | 0.53 |
| 2:A4:2:LYS:NZ | 2:K4:23:GLU:OE2 | 2.41 | 0.53 |
| 3:B4:85:ASP:HB3 | 12:B4:202:CYC:H3C | 1.85 | 0.53 |
| 3:B1:82:CYS:SG | 12:B1:202:CYC:C4C | 2.97 | 0.53 |
| 3:S4:127:VAL:CG2 | 12:S4:202:CYC:HMC2 | 2.39 | 0.53 |
| 4:M4:100:SER:CA | 3:Q4:1:MET:HE3 | 2.28 | 0.53 |
| 4:M4:215:GLU:O | 4:M4:215:GLU:CG | 2.57 | 0.53 |
| 8:K5:112:VAL:CA | 1:J5:75:THR:HB | 2.37 | 0.53 |
| 8:O5:95:GLY:H | 8:O5:104:ILE:HD11 | 1.74 | 0.53 |
| 8:E5:26:ILE:O | 8:E5:30:VAL:HG13 | 2.09 | 0.53 |
| 8:I5:29:PHE:CD1 | 8:I5:99:GLY:HA3 | 2.43 | 0.53 |
| 8:U5:79:ALA:O | 8:U5:83:ARG:HG3 | 2.09 | 0.53 |
| 8:U5:109:ILE:HD13 | 8:U5:159:ALA:HB1 | 1.91 | 0.53 |
| 6:M6:67:GLY:CA | 3:H6:14:LEU:HD22 | 2.38 | 0.53 |
| 10:j5:49:ASP:OD1 | 10:j5:49:ASP:N | 2.39 | 0.53 |
| 10:j5:221:LYS:NZ | 10:j5:221:LYS:CB | 2.72 | 0.53 |
| 10:j5:682:GLU:HG2 | 10:j5:682:GLU:O | 2.08 | 0.53 |
| 10:k5:275:THR:HG21 | 10:k5:286:VAL:HG12 | 1.87 | 0.53 |
| 3:F6:59:LEU:HD21 | 12:F6:201:CYC:C2C | 2.39 | 0.53 |
| 8:G7:51:VAL:HG11 | 11:a9:579:PHE:CE1 | 2.43 | 0.53 |
| 8:i7:88:TYR:O | 8:i7:156:LEU:HD11 | 2.09 | 0.53 |
| 8:U7:109:ILE:HD13 | 8:U7:159:ALA:HB1 | 1.91 | 0.53 |
| 12:X7:201:CYC:HB | 12:X7:201:CYC:HMA3 | 1.73 | 0.53 |
| 8:a7:35:ARG:NH2 | 8:a7:145:ASP:OD1 | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:c7:11:ALA:HB1 | 1:d7:94:TYR:OH | 2.08 | 0.53 |
| 8:c7:88:TYR:O | 8:c7:156:LEU:HD11 | 2.09 | 0.53 |
| 8:m7:29:PHE:CD1 | 8:m7:99:GLY:HA3 | 2.43 | 0.53 |
| 9:x7:3:ARG:CD | 9:x7:67:VAL:HG13 | 2.38 | 0.53 |
| 3:H8:119:ALA:CA | 11:a9:266:ASN:HD22 | 2.11 | 0.53 |
| 4:M8:96:LYS:HB3 | 3:Q8:109:CYS:SG | 2.49 | 0.53 |
| 4:M8:140:ARG:HH12 | 4:M8:210:ILE:HG13 | 1.73 | 0.53 |
| 2:N8:14:SER:CB | 5:Z8:62:ARG:HD2 | 2.36 | 0.53 |
| 4:M9:110:TYR:CE2 | 4:M9:124:ARG:NH1 | 2.77 | 0.53 |
| 5:N9:22:LEU:O | 5:N9:37:HIS:HE1 | 1.92 | 0.53 |
| 11:a9:581:ARG:HH11 | 11:a9:581:ARG:CG | 2.14 | 0.53 |
| 11:a9:598:SER:HB3 | 11:a9:599:PRO:HB3 | 1.90 | 0.53 |
| 11:aA:275:THR:O | 11:aA:278:LEU:HD13 | 2.02 | 0.53 |
| 11:aA:632:ILE:CG2 | 11:aA:634:ALA:CA | 2.86 | 0.53 |
| 11:aA:713:ASN:ND2 | 3:L1:116:THR:OG1 | 2.41 | 0.53 |
| 4:M1:245:ASP:CB | 3:X1:108:ARG:HA | 2.38 | 0.53 |
| 2:IA:19:LEU:HD12 | 3:JA:41:VAL:CG1 | 2.39 | 0.53 |
| 4:MA:61:ASN:O | 4:MA:63:GLY:N | 2.40 | 0.53 |
| 4:MA:158:PHE:CZ | 2:UA:10:ALA:O | 2.62 | 0.53 |
| 7:N2:5:VAL:HB | 2:E2:13:ASP:OD2 | 2.08 | 0.53 |
| 7:N2:34:LEU:HB2 | 12:D2:201:CYC:OB | 2.09 | 0.53 |
| 3:B4:116:THR:HG23 | 3:B4:117:TYR:H | 1.70 | 0.53 |
| 4:M3:245:ASP:CB | 3:X3:108:ARG:HA | 2.38 | 0.53 |
| 5:N3:24:PRO:HD3 | 12:T3:301:CYC:HBA2 | 1.90 | 0.53 |
| 5:N3:67:ILE:N | 5:N3:67:ILE:HD13 | 2.23 | 0.53 |
| 3:B1:84:ARG:NH1 | 11:aA:680:SER:HB3 | 2.24 | 0.53 |
| 3:F4:116:THR:N | 4:M4:3:VAL:HG12 | 2.23 | 0.53 |
| 4:M4:140:ARG:HH11 | 4:M4:144:ARG:NE | 2.02 | 0.53 |
| 4:M4:215:GLU:OE2 | 12:Z4:301:CYC:HAB1 | 1.98 | 0.53 |
| 3:Q4:117:TYR:HE1 | 5:Z4:39:PRO:CG | 2.22 | 0.53 |
| 8:O5:27:LYS:O | 8:O5:30:VAL:HG22 | 2.09 | 0.53 |
| 1:B5:106:GLU:O | 10:k5:543:ASN:ND2 | 2.40 | 0.53 |
| 1:D5:4:ALA:HB2 | 1:D5:98:ALA:O | 2.09 | 0.53 |
| 8:I5:37:LEU:HA | 8:I5:97:VAL:HG12 | 1.89 | 0.53 |
| 1:J5:4:ALA:HB2 | 1:J5:98:ALA:O | 2.09 | 0.53 |
| 1:d5:28:LYS:CE | 1:n7:143:PRO:HG2 | 2.24 | 0.53 |
| 8:Q5:109:ILE:HD13 | 8:Q5:159:ALA:HB1 | 1.91 | 0.53 |
| 8:S5:41:GLN:NE2 | 1:D7:143:PRO:HG3 | 2.17 | 0.53 |
| 8:U5:27:LYS:O | 8:U5:30:VAL:HG22 | 2.09 | 0.53 |
| 8:a5:27:LYS:O | 8:a5:30:VAL:HG22 | 2.09 | 0.53 |
| 3:L6:132:GLN:NE2 | 1:d7:15:GLN:OE1 | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:156:SER:OG | 12:j5:1201:CYC:CAC | 2.56 | 0.53 |
| 10:j5:190:LEU:CD2 | 12:j5:1201:CYC:ND | 2.67 | 0.53 |
| 10:j5:542:GLN:NE2 | 10:j5:560:VAL:HG13 | 2.12 | 0.53 |
| 10:j5:824:PRO:HD3 | 1:h7:106:GLU:O | 2.09 | 0.53 |
| 10:k5:187:ARG:HB3 | 10:k5:237:ASP:OD1 | 2.08 | 0.53 |
| 10:k5:367:ARG:NH1 | 10:k5:410:GLU:OE2 | 2.42 | 0.53 |
| 10:k5:1085:GLY:HA2 | 1:l7:87:TYR:HE1 | 1.73 | 0.53 |
| 3:F6:59:LEU:HD21 | 12:F6:201:CYC:CMC | 2.38 | 0.53 |
| 8:I7:6:LYS:HZ1 | 8:W7:22:GLU:HG3 | 1.73 | 0.53 |
| 12:L7:201:CYC:HB | 12:L7:201:CYC:HMA3 | 1.72 | 0.53 |
| 8:Y7:109:ILE:HD13 | 8:Y7:159:ALA:HB1 | 1.91 | 0.53 |
| 8:a7:107:ILE:CD1 | 1:b7:13:ASP:OD2 | 2.57 | 0.53 |
| 8:o7:45:GLU:OE2 | 8:o7:45:GLU:HA | 2.09 | 0.53 |
| 8:s7:109:ILE:HD13 | 8:s7:159:ALA:HB1 | 1.91 | 0.53 |
| 8:u7:2:SER:CB | 1:v7:5:ILE:HG21 | 2.38 | 0.53 |
| 8:u7:18:LEU:CD1 | 1:v7:97:LEU:HD13 | 2.37 | 0.53 |
| 8:u7:26:ILE:O | 8:u7:30:VAL:HG13 | 2.09 | 0.53 |
| 4:M8:90:LYS:HE3 | 4:M8:220:TYR:CZ | 2.43 | 0.53 |
| 4:M8:230:GLN:CD | 12:M8:301:CYC:HMA2 | 2.34 | 0.53 |
| 3:Q8:85:ASP:OD2 | 12:Z8:301:CYC:CAC | 2.57 | 0.53 |
| 4:M9:61:ASN:O | 4:M9:63:GLY:N | 2.40 | 0.53 |
| 4:M9:158:PHE:CZ | 2:U9:10:ALA:O | 2.62 | 0.53 |
| 4:M9:220:TYR:CD1 | 4:M9:220:TYR:C | 2.85 | 0.53 |
| 11:a9:59:ARG:HA | 11:a9:62:MET:HG2 | 1.90 | 0.53 |
| 11:a9:632:ILE:CG2 | 11:a9:634:ALA:CA | 2.86 | 0.53 |
| 11:aA:425:VAL:CG2 | 11:aA:502:ASN:HA | 2.38 | 0.53 |
| 11:aA:523:GLN:HE22 | 11:aA:548:LEU:HD13 | 1.73 | 0.53 |
| 2:A2:65:TYR:O | 2:A2:71:GLN:CG | 2.54 | 0.53 |
| 12:F3:202:CYC:HC | 12:F3:202:CYC:HMD2 | 1.70 | 0.53 |
| 4:M3:269:SER:HA | 3:V3:111:ASN:ND2 | 2.20 | 0.53 |
| 4:M4:148:LYS:O | 4:M4:148:LYS:HG2 | 2.09 | 0.53 |
| 2:N4:2:LYS:NZ | 2:X4:23:GLU:OE2 | 2.41 | 0.53 |
| 8:A5:26:ILE:O | 8:A5:30:VAL:HG13 | 2.09 | 0.53 |
| 1:B5:14:VAL:HG13 | 10:k5:556:GLY:N | 2.24 | 0.53 |
| 8:C5:95:GLY:H | 8:C5:104:ILE:HD11 | 1.74 | 0.53 |
| 12:d5:201:CYC:HMA2 | 10:j5:379:PHE:CE1 | 2.44 | 0.53 |
| 12:P5:201:CYC:HBB2 | 10:k5:623:VAL:CB | 2.39 | 0.53 |
| 8:Q5:26:ILE:O | 8:Q5:30:VAL:HG13 | 2.09 | 0.53 |
| 8:S5:109:ILE:HD13 | 8:S5:159:ALA:HB1 | 1.91 | 0.53 |
| 8:U5:83:ARG:CG | 6:M6:31:ASP:CB | 2.87 | 0.53 |
| 8:W5:116:TYR:HB3 | 8:W5:123:ILE:HG12 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:Y5:109:ILE:HD13 | 8:Y5:159:ALA:HB1 | 1.91 | 0.53 |
| 12:Z5:201:CYC:NB | 10:k5:379:PHE:HZ | 2.05 | 0.53 |
| 1:b5:24:LEU:HD21 | 10:k5:57:VAL:HG12 | 1.91 | 0.53 |
| 10:j5:1026:LYS:C | 10:j5:1028:ASN:N | 2.66 | 0.53 |
| 10:j5:1067:LEU:CD1 | 10:j5:1101:GLU:OE1 | 2.56 | 0.53 |
| 10:k5:372:ARG:O | 10:k5:372:ARG:HG3 | 2.09 | 0.53 |
| 10:k5:682:GLU:O | 10:k5:682:GLU:HG2 | 2.08 | 0.53 |
| 10:k5:1023:SER:CA | 12:k5:1202:CYC:HBA1 | 2.39 | 0.53 |
| 8:C7:109:ILE:HD13 | 8:C7:159:ALA:HB1 | 1.91 | 0.53 |
| 8:I7:6:LYS:NZ | 8:W7:22:GLU:HG3 | 2.24 | 0.53 |
| 8:I7:25:ARG:HH22 | 8:W7:25:ARG:NE | 2.00 | 0.53 |
| 8:I7:109:ILE:HD13 | 8:I7:159:ALA:HB1 | 1.91 | 0.53 |
| 1:L7:49:THR:HG21 | 8:U7:161:GLN:HG2 | 1.91 | 0.53 |
| 8:M7:109:ILE:HD13 | 8:M7:159:ALA:HB1 | 1.91 | 0.53 |
| 8:i7:58:LEU:HD13 | 8:i7:128:GLU:HB3 | 1.90 | 0.53 |
| 1:j7:110:ASN:ND2 | 9:y7:51:VAL:H | 2.07 | 0.53 |
| 1:T7:110:ASN:ND2 | 9:w7:57:PHE:C | 2.67 | 0.53 |
| 8:c7:20:PRO:HD3 | 8:m7:155:TYR:HB2 | 1.80 | 0.53 |
| 8:c7:122:PRO:HB2 | 8:c7:125:ALA:H | 1.74 | 0.53 |
| 8:e7:26:ILE:O | 8:e7:30:VAL:HG13 | 2.09 | 0.53 |
| 8:o7:26:ILE:O | 8:o7:30:VAL:HG13 | 2.09 | 0.53 |
| 8:o7:30:VAL:CA | 1:p7:31:PHE:HD1 | 2.20 | 0.53 |
| 8:q7:75:GLU:CA | 11:aA:53:VAL:HG11 | 2.39 | 0.53 |
| 8:u7:94:TYR:HE1 | 1:v7:18:TYR:HA | 1.74 | 0.53 |
| 8:u7:104:ILE:HG23 | 8:u7:156:LEU:HD21 | 1.89 | 0.53 |
| 8:u7:109:ILE:HD13 | 8:u7:159:ALA:HB1 | 1.91 | 0.53 |
| 9:y7:14:LEU:HD13 | 9:y7:14:LEU:O | 2.09 | 0.53 |
| 3:L8:130:ALA:HB1 | 12:a9:901:CYC:CBC | 2.39 | 0.53 |
| 3:O8:112:GLY:CA | 5:Z8:69:GLU:C | 2.82 | 0.53 |
| 12:L9:202:CYC:O1D | 11:a9:538:ARG:NE | 2.37 | 0.53 |
| 4:M9:152:TYR:C | 4:M9:152:TYR:CD1 | 2.87 | 0.53 |
| 4:M9:273:ILE:CG2 | 2:W9:107:ASP:O | 2.57 | 0.53 |
| 5:Z8:38:GLU:N | 12:Z8:301:CYC:CMB | 2.70 | 0.53 |
| 3:J9:88:ILE:CD1 | 11:a9:512:TYR:CG | 2.91 | 0.53 |
| 12:J9:202:CYC:CBB | 11:a9:516:GLN:HG3 | 2.35 | 0.53 |
| 11:a9:93:LEU:N | 11:a9:93:LEU:CD1 | 2.72 | 0.53 |
| 11:a9:425:VAL:CG2 | 11:a9:502:ASN:HA | 2.38 | 0.53 |
| 11:aA:50:LEU:HD22 | 11:aA:600:THR:HG21 | 1.91 | 0.53 |
| 11:aA:59:ARG:HA | 11:aA:62:MET:HG2 | 1.90 | 0.53 |
| 11:aA:537:ASP:HB3 | 11:aA:543:GLN:CB | 2.38 | 0.53 |
| 11:aA:581:ARG:CZ | 11:aA:581:ARG:HB3 | 2.38 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 11:aA:741:TYR:OH | 2:K1:13:ASP:CG | 2.50 | 0.53 |
| 11:aA:823:ILE:CD1 | 3:L1:75:PRO:HG2 | 2.36 | 0.53 |
| 4:MA:110:TYR:CE2 | 4:MA:124:ARG:NH1 | 2.77 | 0.53 |
| 5:NA:41:GLN:HG2 | 5:NA:44:TYR:CE1 | 2.43 | 0.53 |
| 5:NA:74:GLU:HA | 3:RA:111:ASN:HD21 | 1.74 | 0.53 |
| 2:QA:120:PHE:HZ | 3:TA:60:PHE:HE2 | 1.56 | 0.53 |
| 3:J3:77:ARG:CD | 2:K3:107:ASP:O | 2.57 | 0.53 |
| 12:J2:201:CYC:HC | 12:J2:201:CYC:HMD2 | 1.70 | 0.53 |
| 2:K2:23:GLU:OE2 | 2:A2:2:LYS:NZ | 2.41 | 0.53 |
| 3:B4:112:GLY:H | 4:M4:60:LYS:HB2 | 1.74 | 0.53 |
| 12:B4:202:CYC:C2D | 4:M4:53:LEU:HD23 | 2.39 | 0.53 |
| 4:M4:176:ARG:HH11 | 4:M4:176:ARG:HG2 | 1.74 | 0.53 |
| 8:E5:125:ALA:O | 8:E5:128:GLU:HB3 | 2.09 | 0.53 |
| 8:E5:127:ALA:O | 8:E5:157:VAL:HG22 | 2.08 | 0.53 |
| 8:G5:26:ILE:O | 8:G5:30:VAL:HG13 | 2.09 | 0.53 |
| 8:e5:29:PHE:CD1 | 8:e5:99:GLY:HA3 | 2.43 | 0.53 |
| 8:e5:95:GLY:H | 8:e5:104:ILE:HD11 | 1.74 | 0.53 |
| 12:b5:201:CYC:HB | 12:b5:201:CYC:HMA3 | 1.73 | 0.53 |
| 9:i5:6:LYS:HB2 | 9:i5:55:LYS:HB3 | 1.84 | 0.53 |
| 10:j5:43:LEU:CD2 | 10:j5:43:LEU:N | 2.72 | 0.53 |
| 10:j5:187:ARG:HB3 | 10:j5:237:ASP:OD1 | 2.08 | 0.53 |
| 10:j5:540:LEU:HD11 | 10:j5:544:VAL:CG2 | 2.39 | 0.53 |
| 10:j5:676:GLU:O | 10:j5:676:GLU:HG3 | 2.02 | 0.53 |
| 10:k5:284:PRO:HG3 | 10:k5:326:GLY:HA2 | 1.68 | 0.53 |
| 10:k5:431:GLN:NE2 | 10:k5:431:GLN:CA | 2.72 | 0.53 |
| 10:k5:1024:LYS:HD2 | 10:k5:1038:ARG:HH12 | 1.73 | 0.53 |
| 10:k5:1043:GLU:HB2 | 8:Y7:14:GLU:OE2 | 2.09 | 0.53 |
| 8:Q7:25:ARG:HD3 | 8:C7:25:ARG:NH2 | 2.08 | 0.53 |
| 1:H7:53:LYS:HD3 | 8:I7:118:SER:O | 2.09 | 0.53 |
| 1:j7:3:ASP:H | 1:j7:6:THR:HG1 | 1.57 | 0.53 |
| 8:u7:90:ARG:HA | 1:v7:18:TYR:HE2 | 1.63 | 0.53 |
| 8:u7:121:THR:HG22 | 12:u7:201:CYC:HMC3 | 1.81 | 0.53 |
| 4:M8:91:VAL:HA | 2:P8:15:GLN:CA | 2.35 | 0.53 |
| 4:M8:220:TYR:CD1 | 4:M8:220:TYR:C | 2.85 | 0.53 |
| 4:M9:259:ARG:HH12 | 3:V9:116:THR:N | 2.07 | 0.53 |
| 11:a9:55:ASP:CB | 11:a9:612:TYR:CG | 2.91 | 0.53 |
| 11:a9:426:ARG:NE | 11:a9:496:ARG:HD3 | 2.22 | 0.53 |
| 11:a9:595:ARG:CG | 11:a9:596:THR:O | 2.55 | 0.53 |
| 12:J1:201:CYC:HC | 12:J1:201:CYC:HMD2 | 1.70 | 0.53 |
| 4:M1:110:TYR:CE2 | 4:M1:124:ARG:NH1 | 2.77 | 0.53 |
| 4:M1:250:THR:OG1 | 12:X1:201:CYC:HAA1 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:MA:185:ALA:HB1 | 12:VA:201:CYC:O1A | 2.08 | 0.52 |
| 5:NA:37:HIS:O | 5:NA:37:HIS:HD2 | 1.92 | 0.52 |
| 2:O1:38:MET:CE | 3:P1:28:THR:OG1 | 2.56 | 0.52 |
| 2:G3:107:ASP:O | 3:L3:77:ARG:CD | 2.57 | 0.52 |
| 6:M2:278:ARG:HH21 | 1:j7:67:ARG:NH1 | 2.00 | 0.52 |
| 12:Z3:201:CYC:HBA2 | 4:M3:185:ALA:HA | 1.90 | 0.52 |
| 3:B4:86:MET:CB | 12:B4:202:CYC:HBC1 | 2.38 | 0.52 |
| 4:M4:100:SER:O | 2:P4:13:ASP:HB2 | 2.09 | 0.52 |
| 4:M4:232:VAL:CB | 12:M4:301:CYC:CBB | 2.73 | 0.52 |
| 8:K5:77:MET:O | 12:K5:201:CYC:HMD3 | 2.08 | 0.52 |
| 5:Z4:44:TYR:CZ | 5:Z4:46:THR:OG1 | 2.56 | 0.52 |
| 8:A5:110:ILE:CG1 | 1:F5:76:ARG:HD3 | 2.38 | 0.52 |
| 1:B5:2:GLN:HE22 | 10:k5:551:MET:HG2 | 1.74 | 0.52 |
| 1:F5:14:VAL:HG12 | 9:z5:64:ASN:ND2 | 2.24 | 0.52 |
| 8:G5:88:TYR:CE2 | 12:G5:201:CYC:CMB | 2.92 | 0.52 |
| 8:e5:35:ARG:NH2 | 8:e5:145:ASP:OD1 | 2.42 | 0.52 |
| 8:U5:87:TYR:CZ | 6:M6:26:PHE:CD2 | 2.79 | 0.52 |
| 1:X5:86:ASP:CG | 1:X5:90:ARG:NE | 2.67 | 0.52 |
| 3:J6:108:ARG:CZ | 6:M6:155:ASN:O | 2.55 | 0.52 |
| 7:N6:1:MET:N | 7:N6:1:MET:CE | 2.72 | 0.52 |
| 8:A7:109:ILE:HD13 | 8:A7:159:ALA:HB1 | 1.91 | 0.52 |
| 9:i5:5:PHE:CA | 9:i5:55:LYS:O | 2.57 | 0.52 |
| 9:i5:24:GLN:O | 9:i5:25:ASN:C | 2.31 | 0.52 |
| 10:j5:431:GLN:NE2 | 10:j5:431:GLN:CA | 2.72 | 0.52 |
| 10:j5:748:ARG:HE | 8:K7:106:GLU:CD | 2.08 | 0.52 |
| 10:j5:946:ASP:OD1 | 10:j5:946:ASP:N | 2.38 | 0.52 |
| 10:j5:995:VAL:CG2 | 8:u7:14:GLU:OE2 | 2.56 | 0.52 |
| 10:j5:1125:ARG:NH1 | 1:t7:114:GLU:HB3 | 2.22 | 0.52 |
| 10:k5:53:ARG:O | 10:k5:56:ILE:CG2 | 2.43 | 0.52 |
| 10:k5:221:LYS:HA | 10:k5:221:LYS:CE | 2.37 | 0.52 |
| 10:k5:489:ASN:ND2 | 10:k5:492:ILE:HG12 | 2.24 | 0.52 |
| 10:k5:938:GLN:HE22 | 1:D7:28:LYS:HB3 | 1.74 | 0.52 |
| 8:O7:118:SER:O | 1:N7:53:LYS:HD3 | 2.09 | 0.52 |
| 8:E7:4:LEU:HD23 | 8:E7:26:ILE:CD1 | 2.38 | 0.52 |
| 8:E7:109:ILE:HD13 | 8:E7:159:ALA:HB1 | 1.91 | 0.52 |
| 1:Z7:110:ASN:ND2 | 9:x7:57:PHE:O | 2.42 | 0.52 |
| 8:a7:52:LYS:HE3 | 11:a9:321:ALA:HA | 1.91 | 0.52 |
| 8:a7:63:PRO:HB2 | 11:a9:333:GLN:O | 2.09 | 0.52 |
| 8:c7:126:VAL:HG22 | 12:c7:201:CYC:CMC | 2.39 | 0.52 |
| 8:m7:95:GLY:H | 8:m7:104:ILE:HD11 | 1.74 | 0.52 |
| 8:s7:95:GLY:H | 8:s7:104:ILE:HD11 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:M8:51:ARG:HB3 | 4:M8:51:ARG:NH1 | 2.23 | 0.52 |
| 4:M8:198:ALA:HB2 | 5:Z8:55:PRO:CG | 2.37 | 0.52 |
| 3:O8:107:ASP:OD1 | 5:Z8:66:ARG:CB | 2.52 | 0.52 |
| 5:Z8:29:HIS:HE1 | 5:Z8:31:TRP:CB | 2.09 | 0.52 |
| 2:G1:107:ASP:O | 3:L1:77:ARG:CD | 2.57 | 0.52 |
| 11:a9:95:ILE:HD13 | 11:a9:237:PHE:CE1 | 2.34 | 0.52 |
| 11:aA:75:ALA:CB | 11:aA:81:ASP:N | 2.72 | 0.52 |
| 11:aA:800:THR:CB | 3:J1:120:LEU:HD21 | 2.38 | 0.52 |
| 3:FA:68:ARG:HH22 | 3:ZA:68:ARG:CZ | 2.22 | 0.52 |
| 4:MA:1:MET:O | 4:MA:2:ASN:O | 2.26 | 0.52 |
| 4:MA:245:ASP:HB3 | 3:ZA:108:ARG:O | 2.09 | 0.52 |
| 2:S1:16:GLY:HA3 | 5:N1:31:TRP:CG | 2.44 | 0.52 |
| 3:H3:69:PRO:O | 11:a9:616:PRO:HA | 2.08 | 0.52 |
| 2:K2:33:ARG:CG | 2:A2:25:GLN:HG2 | 2.39 | 0.52 |
| 4:M3:245:ASP:HB2 | 3:X3:108:ARG:HA | 1.91 | 0.52 |
| 5:N3:22:LEU:HD21 | 5:N3:26:LEU:CD1 | 2.14 | 0.52 |
| 4:M4:28:HIS:HE1 | 4:M4:37:GLU:OE1 | 1.91 | 0.52 |
| 3:Q4:4:ALA:CA | 3:Q4:99:ALA:O | 2.57 | 0.52 |
| 8:K5:26:ILE:O | 8:K5:30:VAL:HG13 | 2.09 | 0.52 |
| 12:M5:201:CYC:HB | 12:M5:201:CYC:CMA | 2.21 | 0.52 |
| 12:N5:201:CYC:O2A | 10:k5:483:PHE:CE1 | 2.57 | 0.52 |
| 3:Y4:89:ILE:HG12 | 3:Y4:92:TYR:CZ | 2.43 | 0.52 |
| 8:G5:161:GLN:CG | 1:T5:49:THR:CG2 | 2.87 | 0.52 |
| 12:R5:201:CYC:CBB | 10:k5:520:ARG:CG | 2.88 | 0.52 |
| 8:W5:17:TYR:CD2 | 1:X5:93:THR:OG1 | 2.46 | 0.52 |
| 8:Y5:26:ILE:O | 8:Y5:30:VAL:HG13 | 2.09 | 0.52 |
| 10:j5:612:ILE:HD12 | 10:j5:612:ILE:N | 2.06 | 0.52 |
| 10:j5:1139:SER:O | 11:aA:32:ARG:NH1 | 2.28 | 0.52 |
| 10:k5:187:ARG:NE | 10:k5:237:ASP:OD2 | 2.37 | 0.52 |
| 10:k5:221:LYS:NZ | 10:k5:221:LYS:CB | 2.72 | 0.52 |
| 10:k5:902:ASN:HD22 | 10:k5:902:ASN:C | 2.03 | 0.52 |
| 10:k5:1026:LYS:C | 10:k5:1028:ASN:N | 2.66 | 0.52 |
| 2:A6:65:TYR:O | 2:A6:71:GLN:CG | 2.54 | 0.52 |
| 12:P7:201:CYC:OB | 9:z7:21:ARG:O | 2.27 | 0.52 |
| 8:Q7:26:ILE:O | 8:Q7:30:VAL:HG13 | 2.09 | 0.52 |
| 8:Q7:116:TYR:HB3 | 8:Q7:123:ILE:HG12 | 1.92 | 0.52 |
| 8:S7:9:VAL:HG21 | 9:w7:69:ALA:HB1 | 1.90 | 0.52 |
| 8:C7:29:PHE:CD1 | 8:C7:99:GLY:HA3 | 2.43 | 0.52 |
| 8:I7:95:GLY:H | 8:I7:104:ILE:HD11 | 1.74 | 0.52 |
| 8:K7:116:TYR:HB3 | 8:K7:123:ILE:HG12 | 1.91 | 0.52 |
| 8:i7:26:ILE:O | 8:i7:30:VAL:HG13 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:d7:201:CYC:HB | 12:d7:201:CYC:HMA3 | 1.73 | 0.52 |
| 8:o7:37:LEU:CD1 | 1:p7:24:LEU:HB3 | 2.38 | 0.52 |
| 8:o7:94:TYR:HE1 | 1:p7:18:TYR:HA | 1.74 | 0.52 |
| 8:q7:26:ILE:O | 8:q7:30:VAL:HG13 | 2.09 | 0.52 |
| 8:q7:90:ARG:HB2 | 1:r7:18:TYR:CZ | 2.44 | 0.52 |
| 8:u7:44:THR:HG22 | 8:u7:44:THR:O | 2.08 | 0.52 |
| 9:z7:3:ARG:NE | 9:z7:67:VAL:HG13 | 2.24 | 0.52 |
| 9:y7:3:ARG:CD | 9:y7:67:VAL:HG13 | 2.38 | 0.52 |
| 5:Z8:37:HIS:HD2 | 5:Z8:37:HIS:O | 1.92 | 0.52 |
| 11:a9:615:ARG:CB | 11:a9:615:ARG:NH1 | 2.72 | 0.52 |
| 11:a9:776:TYR:HA | 11:a9:780:GLN:HE22 | 1.75 | 0.52 |
| 11:aA:25:GLU:O | 11:aA:27:PHE:N | 2.42 | 0.52 |
| 11:aA:331:TYR:HA | 11:aA:333:GLN:HE21 | 1.66 | 0.52 |
| 11:aA:598:SER:HB3 | 11:aA:599:PRO:HB3 | 1.90 | 0.52 |
| 1:Z:16:GLY:CA | 8:e5:90:ARG:NH1 | 2.68 | 0.52 |
| 3:DA:108:ARG:O | 4:MA:6:THR:HG21 | 1.96 | 0.52 |
| 2:IA:37:SER:HA | 2:IA:97:LEU:CD2 | 2.27 | 0.52 |
| 3:LA:44:ILE:HG22 | 3:LA:90:LEU:HD21 | 1.88 | 0.52 |
| 4:MA:144:ARG:NH2 | 4:MA:205:ASP:OD1 | 2.43 | 0.52 |
| 4:MA:152:TYR:CD1 | 4:MA:152:TYR:C | 2.87 | 0.52 |
| 2:OA:60:TYR:CB | 2:OA:67:THR:CG2 | 2.83 | 0.52 |
| 2:QA:116:VAL:HG23 | 3:TA:80:ALA:CA | 2.39 | 0.52 |
| 2:A1:60:TYR:CB | 2:A1:67:THR:CG2 | 2.83 | 0.52 |
| 6:M2:50:LEU:HD21 | 8:i7:79:ALA:HA | 1.91 | 0.52 |
| 4:M3:112:GLN:HG2 | 4:M3:219:PRO:O | 2.10 | 0.52 |
| 4:M3:144:ARG:NH2 | 4:M3:205:ASP:OD1 | 2.43 | 0.52 |
| 4:M3:232:VAL:HG21 | 3:V3:113:LEU:HA | 1.91 | 0.52 |
| 4:M4:29:PRO:CG | 11:aA:226:PHE:O | 2.55 | 0.52 |
| 4:M4:82:ILE:HD12 | 12:M4:301:CYC:O1D | 2.03 | 0.52 |
| 4:M4:112:GLN:HG2 | 4:M4:219:PRO:O | 2.09 | 0.52 |
| 4:M4:227:GLN:C | 3:Y4:91:ARG:HH21 | 2.14 | 0.52 |
| 3:O4:88:ILE:HD11 | 5:Z4:54:LEU:CD1 | 2.38 | 0.52 |
| 3:Q4:85:ASP:CB | 12:Z4:301:CYC:CBC | 2.84 | 0.52 |
| 8:A5:88:TYR:CE2 | 12:A5:201:CYC:CMB | 2.92 | 0.52 |
| 8:I5:95:GLY:H | 8:I5:104:ILE:HD11 | 1.74 | 0.52 |
| 12:I5:201:CYC:HB | 12:I5:201:CYC:CMA | 2.21 | 0.52 |
| 12:e5:201:CYC:HB | 12:e5:201:CYC:CMA | 2.21 | 0.52 |
| 1:f5:113:LYS:HE2 | 1:V5:105:ASP:OD2 | 2.09 | 0.52 |
| 1:R5:64:ASP:HB3 | 10:k5:704:THR:CG2 | 2.39 | 0.52 |
| 1:b5:118:SER:OG | 10:k5:491:THR:O | 2.26 | 0.52 |
| 9:z5:42:GLN:HA | 9:z5:45:GLN:HG2 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:i5:16:ARG:NE | 9:i5:16:ARG:HA | 2.23 | 0.52 |
| 10:j5:362:LYS:CE | 10:j5:363:HIS:HD2 | 2.08 | 0.52 |
| 10:k5:43:LEU:N | 10:k5:43:LEU:CD2 | 2.72 | 0.52 |
| 10:k5:802:VAL:O | 10:k5:802:VAL:HG12 | 2.10 | 0.52 |
| 12:P7:201:CYC:HB | 12:P7:201:CYC:HMA3 | 1.73 | 0.52 |
| 12:P7:201:CYC:HBB2 | 9:z7:21:ARG:CG | 2.39 | 0.52 |
| 8:Q7:109:ILE:HD13 | 8:Q7:159:ALA:HB1 | 1.91 | 0.52 |
| 8:S7:26:ILE:O | 8:S7:30:VAL:HG13 | 2.09 | 0.52 |
| 8:C7:15:ALA:CB | 1:D7:90:ARG:NH2 | 2.68 | 0.52 |
| 8:E7:126:VAL:HG22 | 12:E7:201:CYC:H3C | 1.91 | 0.52 |
| 8:i7:3:VAL:CG2 | 8:s7:25:ARG:NH2 | 2.73 | 0.52 |
| 8:i7:4:LEU:HD23 | 8:i7:26:ILE:CD1 | 2.38 | 0.52 |
| 8:i7:49:ARG:NH2 | 8:i7:140:LEU:HD21 | 2.24 | 0.52 |
| 8:i7:126:VAL:HG22 | 12:i7:201:CYC:CMC | 2.39 | 0.52 |
| 2:A8:2:LYS:HE2 | 2:K8:22:THR:CG2 | 2.38 | 0.52 |
| 8:m7:109:ILE:HD13 | 8:m7:159:ALA:HB1 | 1.91 | 0.52 |
| 9:z7:7:VAL:O | 9:z7:7:VAL:HG23 | 2.08 | 0.52 |
| 9:z7:34:TYR:C | 9:z7:34:TYR:CD1 | 2.87 | 0.52 |
| 9:w7:27:PHE:C | 9:w7:27:PHE:CD1 | 2.86 | 0.52 |
| 3:F8:109:CYS:HA | 4:M8:6:THR:CG2 | 2.36 | 0.52 |
| 4:M8:58:TYR:OH | 11:a9:223:ARG:NH1 | 2.42 | 0.52 |
| 4:M8:91:VAL:HG21 | 2:P8:14:SER:O | 1.93 | 0.52 |
| 4:M9:14:LEU:HD12 | 4:M9:14:LEU:N | 2.24 | 0.52 |
| 5:N9:16:PHE:HE1 | 3:T9:120:LEU:HD23 | 1.64 | 0.52 |
| 2:I9:16:GLY:HA3 | 11:a9:514:VAL:CG1 | 2.36 | 0.52 |
| 11:a9:75:ALA:HB1 | 11:a9:81:ASP:N | 2.23 | 0.52 |
| 11:a9:801:ASN:HD22 | 11:a9:801:ASN:C | 2.10 | 0.52 |
| 11:aA:328:GLN:NE2 | 11:aA:328:GLN:N | 2.58 | 0.52 |
| 11:aA:419:ARG:CG | 11:aA:419:ARG:NH1 | 2.71 | 0.52 |
| 11:aA:745:GLY:HA2 | 2:K1:16:GLY:N | 2.24 | 0.52 |
| 11:aA:776:TYR:CA | 12:H1:201:CYC:HBA1 | 2.35 | 0.52 |
| 1:A:158:SER:OG | 1:R5:11:ASN:ND2 | 2.38 | 0.52 |
| 2:IA:13:ASP:OD1 | 3:JA:92:TYR:OH | 2.20 | 0.52 |
| 4:MA:153:LYS:NZ | 2:UA:14:SER:CB | 2.72 | 0.52 |
| 2:G2:16:GLY:HA3 | 6:M2:104:ARG:NE | 2.23 | 0.52 |
| 4:M3:176:ARG:HH11 | 4:M3:176:ARG:HG2 | 1.74 | 0.52 |
| 5:N3:53:LEU:HB3 | 12:R3:201:CYC:CBA | 2.39 | 0.52 |
| 3:B1:125:ARG:HD2 | 3:X1:14:LEU:CD1 | 2.39 | 0.52 |
| 3:S4:72:ASN:HB3 | 12:S4:202:CYC:OC | 2.09 | 0.52 |
| 12:H4:201:CYC:HBB2 | 11:aA:259:ALA:CA | 2.38 | 0.52 |
| 8:K5:161:GLN:CD | 1:V5:49:THR:HG22 | 2.34 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:O5:109:ILE:HD13 | 8:O5:159:ALA:HB1 | 1.91 | 0.52 |
| 3:Y4:127:VAL:HG11 | 3:Y4:171:ILE:HG21 | 1.91 | 0.52 |
| 12:R5:201:CYC:CBB | 10:k5:520:ARG:CD | 2.87 | 0.52 |
| 10:j5:935:LEU:CD1 | 1:J7:25:ASP:O | 2.57 | 0.52 |
| 10:j5:1124:TYR:CE2 | 1:t7:119:LEU:CD2 | 2.87 | 0.52 |
| 12:j5:1202:CYC:HMD1 | 12:j5:1202:CYC:NC | 2.09 | 0.52 |
| 1:T7:53:LYS:HD3 | 8:U7:118:SER:O | 2.09 | 0.52 |
| 8:U7:95:GLY:H | 8:U7:104:ILE:HD11 | 1.73 | 0.52 |
| 8:c7:4:LEU:HD23 | 8:c7:26:ILE:CD1 | 2.38 | 0.52 |
| 8:c7:46:ALA:HB1 | 8:c7:140:LEU:HD11 | 1.90 | 0.52 |
| 12:D8:202:CYC:CAA | 4:M8:35:THR:OG1 | 2.52 | 0.52 |
| 12:D8:202:CYC:HMA2 | 4:M8:35:THR:OG1 | 2.10 | 0.52 |
| 8:o7:80:LEU:HD12 | 12:o7:201:CYC:HAD2 | 1.90 | 0.52 |
| 1:r7:53:LYS:HD3 | 8:s7:118:SER:O | 2.09 | 0.52 |
| 8:u7:37:LEU:CD1 | 1:v7:24:LEU:HB3 | 2.38 | 0.52 |
| 2:G8:15:GLN:HB3 | 11:a9:120:ARG:HH11 | 1.75 | 0.52 |
| 4:M8:17:VAL:CG1 | 4:M8:18:THR:N | 2.71 | 0.52 |
| 4:M8:112:GLN:HG2 | 4:M8:219:PRO:O | 2.10 | 0.52 |
| 4:M8:225:LYS:H | 12:M8:301:CYC:CGA | 2.15 | 0.52 |
| 3:L9:98:LEU:O | 3:L9:99:ALA:C | 2.48 | 0.52 |
| 4:M9:188:LEU:HD12 | 4:M9:188:LEU:C | 2.35 | 0.52 |
| 5:N9:37:HIS:O | 5:N9:38:GLU:C | 2.49 | 0.52 |
| 5:Z8:22:LEU:O | 12:Z8:301:CYC:HMA3 | 2.09 | 0.52 |
| 3:H9:126:SER:HB2 | 12:H9:202:CYC:HMC3 | 1.78 | 0.52 |
| 3:J9:70:GLY:C | 11:a9:357:THR:H | 2.17 | 0.52 |
| 11:a9:581:ARG:C | 11:a9:581:ARG:HD2 | 2.35 | 0.52 |
| 11:a9:802:ARG:HH11 | 11:a9:802:ARG:CG | 2.22 | 0.52 |
| 11:aA:365:LYS:HZ2 | 11:aA:365:LYS:CB | 2.17 | 0.52 |
| 11:aA:426:ARG:NH2 | 11:aA:496:ARG:CD | 2.58 | 0.52 |
| 4:M1:61:ASN:C | 4:M1:63:GLY:N | 2.64 | 0.52 |
| 3:F2:78:ARG:HG2 | 12:F2:201:CYC:HAD1 | 1.91 | 0.52 |
| 12:Z:201:CYC:HB | 12:Z:201:CYC:HMA3 | 1.73 | 0.52 |
| 3:HA:125:ARG:NE | 8:S7:41:GLN:NE2 | 2.53 | 0.52 |
| 2:QA:69:PRO:HD3 | 2:U1:46:SER:HA | 1.90 | 0.52 |
| 3:L2:65:ASP:OD1 | 1:h7:64:ASP:CG | 2.51 | 0.52 |
| 6:M2:34:ARG:HD2 | 8:O5:52:LYS:HD2 | 1.89 | 0.52 |
| 4:M3:14:LEU:HD12 | 4:M3:14:LEU:N | 2.25 | 0.52 |
| 3:H4:14:LEU:HD21 | 11:aA:86:ASP:N | 2.25 | 0.52 |
| 4:M4:128:ALA:CA | 4:M4:142:PHE:CZ | 2.93 | 0.52 |
| 2:N4:115:GLU:HB2 | 5:Z4:32:PRO:HG2 | 1.91 | 0.52 |
| 12:K5:201:CYC:HB | 12:K5:201:CYC:CMA | 2.21 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:C5:84:ASP:OD2 | 12:C5:201:CYC:NA | 2.43 | 0.52 |
| 8:G5:88:TYR:CE2 | 12:G5:201:CYC:HMB3 | 2.44 | 0.52 |
| 1:J5:5:ILE:HG22 | 1:J5:5:ILE:O | 2.08 | 0.52 |
| 8:c5:26:ILE:O | 8:c5:30:VAL:HG13 | 2.09 | 0.52 |
| 8:e5:27:LYS:O | 8:e5:30:VAL:HG22 | 2.09 | 0.52 |
| 1:f5:38:VAL:CG1 | 10:j5:40:VAL:HG12 | 2.27 | 0.52 |
| 6:M6:43:TRP:CZ2 | 8:c7:56:ASP:OD2 | 2.63 | 0.52 |
| 9:i5:18:ARG:HB3 | 9:i5:22:GLU:CD | 2.30 | 0.52 |
| 10:j5:238:ARG:CG | 10:j5:238:ARG:NH1 | 2.72 | 0.52 |
| 10:j5:826:THR:HG21 | 12:H7:201:CYC:CMA | 2.38 | 0.52 |
| 10:j5:965:GLN:CD | 1:t7:69:GLY:O | 2.51 | 0.52 |
| 10:k5:246:VAL:CG2 | 10:k5:257:THR:CG2 | 2.83 | 0.52 |
| 10:k5:886:PHE:N | 10:k5:886:PHE:CD1 | 2.77 | 0.52 |
| 10:k5:974:LEU:CD1 | 1:p7:106:GLU:CD | 2.80 | 0.52 |
| 10:k5:1008:PHE:CZ | 12:p7:201:CYC:C4B | 2.92 | 0.52 |
| 10:k5:1119:LEU:CD1 | 12:k5:1204:CYC:CBB | 2.87 | 0.52 |
| 8:Q7:126:VAL:HG22 | 12:Q7:201:CYC:H3C | 1.91 | 0.52 |
| 12:R7:201:CYC:HB | 12:R7:201:CYC:HMA3 | 1.73 | 0.52 |
| 8:S7:90:ARG:HB2 | 1:T7:18:TYR:CZ | 2.45 | 0.52 |
| 8:S7:109:ILE:HD13 | 8:S7:159:ALA:HB1 | 1.91 | 0.52 |
| 1:B7:53:LYS:HD3 | 8:C7:118:SER:O | 2.09 | 0.52 |
| 8:C7:35:ARG:NH2 | 8:C7:145:ASP:OD1 | 2.41 | 0.52 |
| 8:g7:95:GLY:H | 8:g7:104:ILE:HD11 | 1.74 | 0.52 |
| 8:i7:131:ARG:CB | 8:i7:131:ARG:NH1 | 2.73 | 0.52 |
| 8:W7:116:TYR:HB3 | 8:W7:123:ILE:HG12 | 1.91 | 0.52 |
| 1:n7:75:THR:OG1 | 8:o7:110:ILE:O | 2.27 | 0.52 |
| 8:o7:37:LEU:HD21 | 1:p7:24:LEU:CD2 | 2.21 | 0.52 |
| 8:q7:109:ILE:HD13 | 8:q7:159:ALA:HB1 | 1.91 | 0.52 |
| 8:u7:2:SER:HB3 | 1:v7:5:ILE:HG22 | 1.87 | 0.52 |
| 8:u7:90:ARG:CA | 1:v7:18:TYR:CZ | 2.93 | 0.52 |
| 4:M8:61:ASN:C | 4:M8:63:GLY:N | 2.64 | 0.52 |
| 4:M8:176:ARG:HH11 | 4:M8:176:ARG:HG2 | 1.74 | 0.52 |
| 2:N8:115:GLU:CA | 5:Z8:32:PRO:CB | 2.76 | 0.52 |
| 3:L9:14:LEU:HD21 | 11:a9:358:PRO:CD | 2.40 | 0.52 |
| 4:M9:36:TYR:CZ | 12:B9:201:CYC:HAA1 | 2.45 | 0.52 |
| 5:Z8:37:HIS:HD2 | 12:Z8:301:CYC:CHB | 2.15 | 0.52 |
| 2:A9:31:PHE:CG | 3:B9:34:SER:HB2 | 2.45 | 0.52 |
| 12:H9:202:CYC:OB | 11:a9:448:ASN:OD1 | 2.27 | 0.52 |
| 11:aA:578:MET:HE3 | 11:aA:582:MET:CE | 2.34 | 0.52 |
| 11:aA:615:ARG:HB3 | 11:aA:615:ARG:NH1 | 2.20 | 0.52 |
| 5:N1:67:ILE:N | 5:N1:67:ILE:HD13 | 2.23 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Z:18:TYR:OH | 8:e5:90:ARG:N | 2.43 | 0.52 |
| 2:AA:114:ARG:NH1 | 11:aA:407:GLU:OE2 | 2.43 | 0.52 |
| 3:J3:81:ALA:O | 11:a9:668:TYR:CE2 | 2.63 | 0.52 |
| 2:E4:14:SER:C | 11:aA:163:ASP:OD2 | 2.53 | 0.52 |
| 8:M5:109:ILE:HD13 | 8:M5:159:ALA:HB1 | 1.91 | 0.52 |
| 1:D5:76:ARG:HG3 | 1:D5:77:ARG:N | 2.25 | 0.52 |
| 1:H5:76:ARG:CD | 9:i5:14:LEU:HB2 | 2.40 | 0.52 |
| 8:S5:90:ARG:HD2 | 1:T5:18:TYR:N | 2.24 | 0.52 |
| 8:W5:126:VAL:HG22 | 12:W5:201:CYC:H3C | 1.91 | 0.52 |
| 8:Y5:90:ARG:HB2 | 1:Z5:18:TYR:CZ | 2.45 | 0.52 |
| 10:j5:357:LEU:CD1 | 10:j5:379:PHE:CA | 2.84 | 0.52 |
| 10:j5:886:PHE:CD1 | 10:j5:886:PHE:N | 2.77 | 0.52 |
| 10:k5:931:VAL:CA | 1:D7:29:ALA:O | 2.51 | 0.52 |
| 10:k5:1151:GLN:O | 1:p7:122:PRO:HB3 | 2.07 | 0.52 |
| 8:Q7:4:LEU:HD23 | 8:Q7:26:ILE:CD1 | 2.38 | 0.52 |
| 8:G7:90:ARG:HB2 | 1:H7:18:TYR:CZ | 2.45 | 0.52 |
| 8:i7:3:VAL:HG13 | 8:s7:25:ARG:HH21 | 1.22 | 0.52 |
| 8:i7:46:ALA:HB2 | 8:i7:140:LEU:CD1 | 2.39 | 0.52 |
| 8:k7:109:ILE:HD13 | 8:k7:159:ALA:HB1 | 1.91 | 0.52 |
| 8:U7:27:LYS:O | 8:U7:30:VAL:HG22 | 2.09 | 0.52 |
| 8:u7:36:ARG:NH2 | 8:u7:36:ARG:CG | 2.71 | 0.52 |
| 2:N8:14:SER:OG | 5:Z8:62:ARG:CZ | 2.57 | 0.52 |
| 2:N8:60:TYR:CB | 2:N8:67:THR:CG2 | 2.83 | 0.52 |
| 3:L9:107:ASP:O | 11:a9:531:ASP:CG | 2.52 | 0.52 |
| 2:O9:25:GLN:HG2 | 2:Y9:33:ARG:CG | 2.38 | 0.52 |
| 2:O9:34:ALA:HB1 | 3:P9:31:VAL:HG21 | 1.92 | 0.52 |
| 11:a9:581:ARG:HB3 | 11:a9:581:ARG:CZ | 2.38 | 0.52 |
| 11:a9:629:LYS:HD3 | 11:a9:629:LYS:C | 2.35 | 0.52 |
| 3:F2:72:ASN:O | 12:F2:201:CYC:CMD | 2.57 | 0.52 |
| 1:Z:18:TYR:CD1 | 8:e5:90:ARG:HD3 | 2.45 | 0.52 |
| 2:AA:114:ARG:NH1 | 11:aA:407:GLU:OE1 | 2.25 | 0.52 |
| 2:IA:19:LEU:CD1 | 3:JA:41:VAL:HG11 | 2.40 | 0.52 |
| 12:LA:202:CYC:O1D | 11:aA:538:ARG:NE | 2.38 | 0.52 |
| 4:MA:188:LEU:HD12 | 4:MA:188:LEU:C | 2.35 | 0.52 |
| 4:MA:273:ILE:CG2 | 2:WA:107:ASP:O | 2.57 | 0.52 |
| 5:NA:37:HIS:O | 5:NA:38:GLU:C | 2.49 | 0.52 |
| 2:OA:34:ALA:HB1 | 3:PA:31:VAL:HG21 | 1.92 | 0.52 |
| 2:A1:31:PHE:CG | 3:B1:34:SER:HB2 | 2.45 | 0.52 |
| 2:A1:65:TYR:O | 2:A1:71:GLN:CG | 2.54 | 0.52 |
| 3:H3:62:GLU:CD | 8:k7:49:ARG:NH2 | 2.68 | 0.52 |
| 2:A4:31:PHE:CG | 3:B4:34:SER:HB2 | 2.45 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:B4:86:MET:HG3 | 12:B4:202:CYC:HBC1 | 1.90 | 0.52 |
| 3:B4:120:LEU:HD12 | 4:M4:53:LEU:CB | 2.13 | 0.52 |
| 4:M3:188:LEU:HD12 | 4:M3:188:LEU:C | 2.35 | 0.52 |
| 2:O3:34:ALA:HB1 | 3:P3:31:VAL:HG21 | 1.92 | 0.52 |
| 4:M4:139:VAL:O | 4:M4:139:VAL:HG12 | 2.09 | 0.52 |
| 3:Q4:72:ASN:HD21 | 12:Z4:301:CYC:CBD | 2.03 | 0.52 |
| 8:M5:26:ILE:O | 8:M5:30:VAL:HG13 | 2.09 | 0.52 |
| 1:J5:76:ARG:HH12 | 9:i5:67:VAL:HB | 1.74 | 0.52 |
| 8:c5:109:ILE:HD13 | 8:c5:159:ALA:HB1 | 1.91 | 0.52 |
| 8:U5:29:PHE:HE1 | 8:U5:99:GLY:N | 2.08 | 0.52 |
| 8:a5:109:ILE:HD13 | 8:a5:159:ALA:HB1 | 1.91 | 0.52 |
| 1:b5:9:ILE:CG2 | 10:k5:17:PHE:HZ | 2.21 | 0.52 |
| 8:A7:26:ILE:O | 8:A7:30:VAL:HG13 | 2.10 | 0.52 |
| 8:A7:51:VAL:HG11 | 11:aA:579:PHE:CE1 | 2.41 | 0.52 |
| 10:k5:362:LYS:HD2 | 10:k5:363:HIS:CD2 | 2.34 | 0.52 |
| 10:k5:964:GLY:C | 1:n7:69:GLY:CA | 2.81 | 0.52 |
| 10:k5:1046:ARG:CZ | 8:k7:9:VAL:CG1 | 2.88 | 0.52 |
| 10:k5:1119:LEU:CD2 | 1:n7:87:TYR:CZ | 2.93 | 0.52 |
| 2:A6:34:ALA:HB1 | 3:B6:31:VAL:HG21 | 1.92 | 0.52 |
| 3:F6:78:ARG:HG2 | 12:F6:201:CYC:O1D | 2.09 | 0.52 |
| 12:i7:201:CYC:HB | 12:i7:201:CYC:CMA | 2.21 | 0.52 |
| 8:U7:15:ALA:HB1 | 1:V7:90:ARG:HH22 | 1.70 | 0.52 |
| 8:c7:131:ARG:CB | 8:c7:131:ARG:NH1 | 2.73 | 0.52 |
| 8:u7:30:VAL:CG1 | 1:v7:31:PHE:HD1 | 2.21 | 0.52 |
| 3:F8:104:VAL:O | 3:F8:107:ASP:OD1 | 2.28 | 0.52 |
| 4:M8:14:LEU:N | 4:M8:14:LEU:HD12 | 2.25 | 0.52 |
| 4:M8:112:GLN:NE2 | 4:M8:172:HIS:O | 2.43 | 0.52 |
| 12:M8:302:CYC:CAC | 3:S8:81:ALA:HB3 | 2.40 | 0.52 |
| 4:M9:153:LYS:NZ | 2:U9:14:SER:CB | 2.72 | 0.52 |
| 4:M9:274:VAL:H | 3:V9:77:ARG:CG | 2.19 | 0.52 |
| 2:A9:114:ARG:NH1 | 11:a9:407:GLU:OE2 | 2.43 | 0.52 |
| 11:a9:418:LEU:HD22 | 11:a9:428:PHE:CD2 | 2.45 | 0.52 |
| 11:a9:632:ILE:H | 11:a9:632:ILE:CD1 | 2.22 | 0.52 |
| 11:a9:812:ASP:O | 11:a9:816:LEU:N | 2.39 | 0.52 |
| 4:M1:112:GLN:HG2 | 4:M1:219:PRO:O | 2.10 | 0.52 |
| 5:N1:22:LEU:O | 5:N1:37:HIS:HE1 | 1.92 | 0.52 |
| 2:AA:31:PHE:CG | 3:BA:34:SER:HB2 | 2.45 | 0.52 |
| 2:A3:31:PHE:CG | 3:B3:34:SER:HB2 | 2.45 | 0.52 |
| 5:N3:3:VAL:CG1 | 3:P3:115:GLU:HB2 | 2.36 | 0.52 |
| 2:O3:31:PHE:CG | 3:P3:34:SER:HB2 | 2.45 | 0.52 |
| 3:L4:88:ILE:HD13 | 11:aA:239:TYR:CZ | 2.45 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M4:235:PHE:CZ | 3:Y4:113:LEU:HA | 2.43 | 0.52 |
| 3:Q4:84:ARG:O | 3:Q4:88:ILE:HG13 | 2.10 | 0.52 |
| 1:L5:68:PRO:CA | 1:H5:14:VAL:O | 2.58 | 0.52 |
| 1:L5:76:ARG:HD3 | 8:G5:110:ILE:CG1 | 2.37 | 0.52 |
| 1:B5:10:ASN:ND2 | 10:k5:557:VAL:CB | 2.68 | 0.52 |
| 1:B5:14:VAL:CG1 | 10:k5:555:ALA:CA | 2.85 | 0.52 |
| 1:B5:14:VAL:O | 1:F5:68:PRO:CA | 2.58 | 0.52 |
| 1:J5:76:ARG:HG3 | 1:J5:77:ARG:N | 2.25 | 0.52 |
| 8:c5:9:VAL:CG1 | 10:j5:344:ARG:NE | 2.73 | 0.52 |
| 8:Q5:116:TYR:HB3 | 8:Q5:123:ILE:HG12 | 1.91 | 0.52 |
| 1:R5:3:ASP:H | 1:R5:6:THR:HG1 | 1.56 | 0.52 |
| 8:U5:95:GLY:H | 8:U5:104:ILE:HD11 | 1.74 | 0.52 |
| 8:a5:35:ARG:NH2 | 8:a5:145:ASP:OD1 | 2.42 | 0.52 |
| 1:b5:18:TYR:CD1 | 10:k5:165:ARG:HG3 | 2.43 | 0.52 |
| 10:j5:1153:VAL:CG2 | 1:v7:65:LEU:HD11 | 2.27 | 0.52 |
| 10:k5:357:LEU:CD1 | 10:k5:379:PHE:CA | 2.84 | 0.52 |
| 10:k5:965:GLN:H | 1:n7:69:GLY:C | 2.14 | 0.52 |
| 10:k5:978:LEU:HD22 | 1:p7:107:ARG:NH2 | 1.92 | 0.52 |
| 8:O7:27:LYS:O | 8:O7:30:VAL:HG22 | 2.09 | 0.52 |
| 8:O7:109:ILE:HD13 | 8:O7:159:ALA:HB1 | 1.91 | 0.52 |
| 8:I7:29:PHE:HE1 | 8:I7:99:GLY:N | 2.08 | 0.52 |
| 8:g7:27:LYS:O | 8:g7:30:VAL:HG22 | 2.09 | 0.52 |
| 8:g7:52:LYS:HE3 | 11:aA:321:ALA:HA | 1.92 | 0.52 |
| 1:h7:75:THR:HB | 8:i7:112:VAL:CA | 2.40 | 0.52 |
| 8:a7:56:ASP:OD1 | 11:a9:325:LEU:CB | 2.58 | 0.52 |
| 8:c7:95:GLY:C | 8:c7:152:TYR:CD2 | 2.87 | 0.52 |
| 3:B8:107:ASP:C | 4:M8:61:ASN:HA | 2.31 | 0.52 |
| 9:w7:3:ARG:NE | 9:w7:67:VAL:HG13 | 2.24 | 0.52 |
| 3:F8:107:ASP:CG | 4:M8:8:SER:C | 2.65 | 0.52 |
| 2:N8:34:ALA:HB1 | 3:O8:31:VAL:HG21 | 1.92 | 0.52 |
| 5:N9:53:LEU:CB | 12:T9:301:CYC:CBA | 2.53 | 0.52 |
| 5:N9:57:MET:HE2 | 5:N9:67:ILE:HG13 | 1.92 | 0.52 |
| 11:aA:776:TYR:HB3 | 12:H1:201:CYC:O2A | 2.10 | 0.52 |
| 5:N1:24:PRO:HD3 | 12:T1:301:CYC:HBA2 | 1.90 | 0.52 |
| 2:AA:34:ALA:HB1 | 3:BA:31:VAL:HG21 | 1.92 | 0.52 |
| 3:FA:150:ARG:HD2 | 3:F9:150:ARG:CG | 2.39 | 0.52 |
| 4:MA:112:GLN:HG2 | 4:MA:219:PRO:O | 2.10 | 0.52 |
| 2:O1:25:GLN:HG2 | 2:Y1:33:ARG:CG | 2.38 | 0.52 |
| 3:P1:84:ARG:CZ | 4:M1:130:SER:HB3 | 2.40 | 0.52 |
| 2:G3:107:ASP:CG | 3:L3:77:ARG:NH2 | 2.67 | 0.52 |
| 6:M2:259:THR:O | 6:M2:262:ASP:N | 2.22 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:C3:140:SER:HB3 | 3:D8:150:ARG:HH11 | 1.75 | 0.52 |
| 12:F3:201:CYC:CBA | 4:M3:36:TYR:CE2 | 2.92 | 0.52 |
| 3:B4:108:ARG:O | 4:M4:61:ASN:CA | 2.58 | 0.52 |
| 3:B4:117:TYR:HE1 | 4:M4:53:LEU:HD21 | 1.75 | 0.52 |
| 3:B4:119:ALA:HB3 | 4:M4:52:LEU:CD1 | 2.37 | 0.52 |
| 4:M3:250:THR:OG1 | 12:X3:201:CYC:HAA1 | 2.09 | 0.52 |
| 5:N3:37:HIS:O | 5:N3:37:HIS:HD2 | 1.92 | 0.52 |
| 5:N3:57:MET:HE2 | 5:N3:67:ILE:HG13 | 1.92 | 0.52 |
| 4:M4:14:LEU:HD12 | 4:M4:14:LEU:N | 2.25 | 0.52 |
| 4:M4:27:HIS:CE1 | 4:M4:35:THR:HG22 | 2.45 | 0.52 |
| 4:M4:29:PRO:CD | 11:aA:230:THR:OG1 | 2.58 | 0.52 |
| 4:M4:273:ILE:HG21 | 2:X4:108:TYR:CE1 | 2.44 | 0.52 |
| 8:Q5:126:VAL:HG22 | 12:Q5:201:CYC:H3C | 1.91 | 0.52 |
| 9:z5:5:PHE:CA | 9:z5:55:LYS:O | 2.57 | 0.52 |
| 10:j5:388:ARG:HD2 | 10:j5:393:MET:N | 2.13 | 0.52 |
| 10:k5:501:ILE:H | 10:k5:501:ILE:CD1 | 2.17 | 0.52 |
| 8:K7:26:ILE:O | 8:K7:30:VAL:HG13 | 2.09 | 0.52 |
| 8:K7:109:ILE:HD13 | 8:K7:159:ALA:HB1 | 1.91 | 0.52 |
| 1:N7:106:GLU:CG | 9:z7:58:THR:CG2 | 2.87 | 0.52 |
| 8:g7:11:ALA:O | 8:g7:12:ASP:C | 2.50 | 0.52 |
| 8:U7:35:ARG:NH2 | 8:U7:145:ASP:OD1 | 2.42 | 0.52 |
| 8:Y7:106:GLU:OE2 | 9:x7:68:GLY:C | 2.53 | 0.52 |
| 1:b7:76:ARG:CA | 8:c7:110:ILE:O | 2.58 | 0.52 |
| 8:c7:46:ALA:HB2 | 8:c7:140:LEU:CD1 | 2.39 | 0.52 |
| 1:d7:77:ARG:CZ | 9:x7:63:ALA:CB | 2.73 | 0.52 |
| 1:l7:53:LYS:HD3 | 8:m7:118:SER:O | 2.09 | 0.52 |
| 8:m7:35:ARG:NH2 | 8:m7:145:ASP:OD1 | 2.41 | 0.52 |
| 4:M8:96:LYS:NZ | 3:Q8:113:LEU:HD22 | 2.24 | 0.52 |
| 3:O8:95:TYR:HE2 | 3:O8:108:ARG:NH2 | 2.01 | 0.52 |
| 3:Q8:113:LEU:C | 3:Q8:115:GLU:N | 2.68 | 0.52 |
| 4:M9:245:ASP:HB3 | 3:Z9:108:ARG:O | 2.09 | 0.52 |
| 5:N9:37:HIS:O | 5:N9:37:HIS:HD2 | 1.92 | 0.52 |
| 5:N9:54:LEU:HD21 | 3:T9:84:ARG:NE | 2.14 | 0.52 |
| 2:I9:19:LEU:HD12 | 3:J9:41:VAL:CG1 | 2.39 | 0.52 |
| 2:I9:19:LEU:CD1 | 3:J9:41:VAL:HG11 | 2.40 | 0.52 |
| 11:a9:75:ALA:CB | 11:a9:81:ASP:N | 2.73 | 0.52 |
| 11:aA:95:ILE:HD13 | 11:aA:237:PHE:CE2 | 2.45 | 0.52 |
| 11:aA:629:LYS:HD3 | 11:aA:629:LYS:C | 2.35 | 0.52 |
| 11:aA:632:ILE:H | 11:aA:632:ILE:CD1 | 2.22 | 0.52 |
| 11:aA:776:TYR:HA | 11:aA:780:GLN:HE22 | 1.75 | 0.52 |
| 11:aA:803:ASN:CB | 3:J1:119:ALA:C | 2.80 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:M1:14:LEU:HD12 | 4:M1:14:LEU:N | 2.25 | 0.52 |
| 4:M1:245:ASP:HB2 | 3:X1:108:ARG:HA | 1.91 | 0.52 |
| 2:A2:31:PHE:CG | 3:B2:34:SER:HB2 | 2.45 | 0.52 |
| 2:G2:15:GLN:C | 6:M2:104:ARG:CD | 2.83 | 0.52 |
| 3:J2:108:ARG:HH22 | 6:M2:155:ASN:CG | 2.15 | 0.52 |
| 12:B4:202:CYC:HHA | 4:M4:54:ALA:CB | 2.07 | 0.52 |
| 4:M3:259:ARG:HG3 | 4:M3:259:ARG:HH21 | 1.75 | 0.52 |
| 4:M4:228:SER:HB3 | 2:X4:16:GLY:C | 2.34 | 0.52 |
| 2:N4:34:ALA:HB1 | 3:O4:31:VAL:HG21 | 1.92 | 0.52 |
| 3:Q4:90:LEU:HB2 | 3:Q4:134:MET:SD | 2.50 | 0.52 |
| 5:Z4:1:MET:O | 5:Z4:3:VAL:N | 2.43 | 0.52 |
| 8:C5:29:PHE:CE2 | 1:D5:5:ILE:CD1 | 2.93 | 0.52 |
| 8:E5:4:LEU:HD23 | 8:E5:26:ILE:CD1 | 2.38 | 0.52 |
| 8:G5:81:CYS:SG | 12:G5:201:CYC:HAC2 | 2.50 | 0.52 |
| 6:M6:43:TRP:NE1 | 8:c7:56:ASP:OD2 | 2.42 | 0.52 |
| 7:N6:34:LEU:HB2 | 12:D6:201:CYC:OB | 2.09 | 0.52 |
| 9:i5:42:GLN:HA | 9:i5:45:GLN:HG2 | 1.91 | 0.52 |
| 10:j5:303:GLN:HG2 | 10:j5:421:PRO:HB2 | 1.91 | 0.52 |
| 10:j5:1097:VAL:HG12 | 10:j5:1097:VAL:O | 2.10 | 0.52 |
| 10:k5:386:ILE:HG21 | 10:k5:395:SER:C | 2.14 | 0.52 |
| 10:k5:822:ARG:CG | 1:B7:106:GLU:OE2 | 2.58 | 0.52 |
| 8:G7:26:ILE:O | 8:G7:30:VAL:HG13 | 2.10 | 0.52 |
| 8:g7:107:ILE:CD1 | 1:h7:13:ASP:OD2 | 2.57 | 0.52 |
| 8:a7:37:LEU:CD2 | 1:b7:24:LEU:HD21 | 2.38 | 0.52 |
| 2:A8:38:MET:CE | 3:B8:28:THR:OG1 | 2.56 | 0.52 |
| 3:F8:111:ASN:ND2 | 4:M8:73:ASP:HA | 2.25 | 0.52 |
| 4:M8:87:ILE:HD13 | 3:Y8:77:ARG:CB | 2.30 | 0.52 |
| 4:M8:235:PHE:CG | 12:M8:301:CYC:C3A | 2.93 | 0.52 |
| 4:M9:35:THR:CA | 12:B9:201:CYC:O2A | 2.54 | 0.52 |
| 4:M9:259:ARG:HG3 | 4:M9:259:ARG:HH21 | 1.75 | 0.52 |
| 11:a9:50:LEU:HD22 | 11:a9:600:THR:HG21 | 1.91 | 0.52 |
| 11:a9:776:TYR:HA | 11:a9:780:GLN:NE2 | 2.25 | 0.52 |
| 11:aA:713:ASN:OD1 | 12:aA:902:CYC:HMA1 | 2.10 | 0.52 |
| 4:M1:144:ARG:NH2 | 4:M1:205:ASP:OD1 | 2.43 | 0.52 |
| 3:LA:14:LEU:CD2 | 11:aA:358:PRO:CA | 2.53 | 0.51 |
| 4:MA:74:LEU:O | 4:MA:77:LEU:CD1 | 2.59 | 0.51 |
| 2:OA:65:TYR:O | 2:OA:71:GLN:CG | 2.54 | 0.51 |
| 2:QA:75:GLY:HA2 | 2:U1:141:GLN:HG2 | 1.91 | 0.51 |
| 3:J3:77:ARG:NH2 | 2:K3:107:ASP:CG | 2.68 | 0.51 |
| 12:N2:101:CYC:HB | 12:N2:101:CYC:HMA2 | 1.76 | 0.51 |
| 3:B3:88:ILE:CG2 | 12:B3:202:CYC:HMB2 | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 3:B3:127:VAL:CG2 | 12:B3:202:CYC:HMC1 | 2.40 | 0.51 |
| 2:A4:34:ALA:HB1 | 3:B4:31:VAL:HG21 | 1.92 | 0.51 |
| 3:B4:82:CYS:CA | 12:B4:202:CYC:HAC2 | 2.40 | 0.51 |
| 4:M3:20:THR:HG23 | 4:M3:67:LEU:HD11 | 1.92 | 0.51 |
| 4:M3:139:VAL:O | 4:M3:139:VAL:HG12 | 2.09 | 0.51 |
| 2:G4:15:GLN:HB3 | 11:aA:120:ARG:HH11 | 1.75 | 0.51 |
| 4:M4:188:LEU:HD12 | 4:M4:188:LEU:C | 2.35 | 0.51 |
| 8:O5:29:PHE:HE1 | 8:O5:99:GLY:N | 2.08 | 0.51 |
| 8:O5:161:GLN:NE2 | 1:F5:49:THR:HG22 | 2.26 | 0.51 |
| 5:Z4:1:MET:HB2 | 5:Z4:3:VAL:HG23 | 1.91 | 0.51 |
| 8:A5:121:THR:CG2 | 12:A5:201:CYC:CHD | 2.80 | 0.51 |
| 1:B5:14:VAL:CG1 | 10:k5:556:GLY:N | 2.74 | 0.51 |
| 8:C5:29:PHE:HE1 | 8:C5:99:GLY:N | 2.08 | 0.51 |
| 8:I5:84:ASP:OD2 | 12:I5:201:CYC:NA | 2.43 | 0.51 |
| 8:S5:68:PRO:HG3 | 8:a5:59:PHE:HB3 | 1.91 | 0.51 |
| 8:U5:82:LEU:HB2 | 6:M6:31:ASP:HB3 | 1.92 | 0.51 |
| 8:W5:26:ILE:O | 8:W5:30:VAL:HG13 | 2.09 | 0.51 |
| 8:a5:29:PHE:HE1 | 8:a5:99:GLY:N | 2.08 | 0.51 |
| 1:b5:6:THR:HG21 | 10:k5:22:THR:HG23 | 1.90 | 0.51 |
| 6:M6:104:ARG:CD | 2:G6:15:GLN:C | 2.83 | 0.51 |
| 10:j5:182:ASN:HB2 | 12:j5:1201:CYC:HAB2 | 1.92 | 0.51 |
| 10:j5:450:ARG:HG3 | 10:j5:494:PRO:O | 2.10 | 0.51 |
| 10:j5:614:ARG:HG2 | 10:j5:614:ARG:NH1 | 2.21 | 0.51 |
| 10:j5:1054:SER:CB | 10:j5:1056:PRO:HD3 | 2.40 | 0.51 |
| 10:k5:192:LYS:HA | 10:k5:192:LYS:HZ1 | 1.69 | 0.51 |
| 10:k5:284:PRO:HD2 | 10:k5:326:GLY:C | 2.35 | 0.51 |
| 10:k5:793:SER:HB3 | 12:N7:201:CYC:HBA1 | 1.92 | 0.51 |
| 10:k5:951:MET:HE3 | 10:k5:951:MET:C | 2.34 | 0.51 |
| 10:k5:1052:PRO:C | 1:l7:106:GLU:HG2 | 2.34 | 0.51 |
| 10:k5:1118:THR:HG23 | 12:k5:1204:CYC:O2A | 2.08 | 0.51 |
| 2:A6:60:TYR:CB | 2:A6:67:THR:CG2 | 2.83 | 0.51 |
| 1:D7:76:ARG:CA | 8:E7:110:ILE:O | 2.58 | 0.51 |
| 8:M7:90:ARG:HB2 | 1:N7:18:TYR:CZ | 2.45 | 0.51 |
| 8:k7:120:GLN:CG | 1:p7:53:LYS:HZ1 | 2.23 | 0.51 |
| 8:Y7:26:ILE:O | 8:Y7:30:VAL:HG13 | 2.09 | 0.51 |
| 8:a7:29:PHE:HE1 | 8:a7:99:GLY:N | 2.08 | 0.51 |
| 8:o7:37:LEU:HD22 | 1:p7:24:LEU:HD13 | 1.92 | 0.51 |
| 8:u7:37:LEU:HD22 | 1:v7:24:LEU:HD13 | 1.92 | 0.51 |
| 4:M8:20:THR:HG23 | 4:M8:67:LEU:HD11 | 1.92 | 0.51 |
| 4:M9:153:LYS:HZ2 | 2:U9:14:SER:CB | 2.24 | 0.51 |
| 5:N9:1:MET:O | 5:N9:3:VAL:N | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:I9:13:ASP:OD1 | 11:a9:515:GLY:HA2 | 2.09 | 0.51 |
| 11:a9:90:GLN:C | 11:a9:92:LYS:H | 2.17 | 0.51 |
| 11:aA:581:ARG:HD2 | 11:aA:581:ARG:C | 2.35 | 0.51 |
| 11:aA:775:LYS:HA | 12:H1:201:CYC:CBA | 2.25 | 0.51 |
| 4:M1:112:GLN:NE2 | 4:M1:172:HIS:O | 2.43 | 0.51 |
| 4:MA:139:VAL:O | 4:MA:139:VAL:HG12 | 2.09 | 0.51 |
| 2:QA:81:LYS:HZ3 | 12:QA:201:CYC:CGA | 2.24 | 0.51 |
| 12:R1:201:CYC:CBA | 5:N1:53:LEU:HB3 | 2.39 | 0.51 |
| 12:J2:202:CYC:HB | 12:J2:202:CYC:HMA2 | 1.76 | 0.51 |
| 6:M2:26:PHE:HD1 | 8:O5:83:ARG:HG2 | 1.74 | 0.51 |
| 3:B3:84:ARG:NH1 | 11:a9:680:SER:CB | 2.73 | 0.51 |
| 3:B3:125:ARG:HD2 | 3:X3:14:LEU:CD1 | 2.39 | 0.51 |
| 3:B3:127:VAL:N | 12:B3:202:CYC:CMC | 2.73 | 0.51 |
| 3:L3:84:ARG:CD | 11:a9:739:ASP:HA | 2.39 | 0.51 |
| 4:M3:74:LEU:O | 4:M3:77:LEU:CD1 | 2.59 | 0.51 |
| 4:M3:93:LEU:HD21 | 4:M3:102:VAL:HG22 | 1.92 | 0.51 |
| 3:B1:112:GLY:H | 4:M1:76:ALA:HB1 | 1.73 | 0.51 |
| 3:Y4:106:GLU:HA | 3:Y4:110:LEU:HD12 | 1.91 | 0.51 |
| 8:A5:81:CYS:SG | 12:A5:201:CYC:HAC2 | 2.50 | 0.51 |
| 12:F5:201:CYC:HMD1 | 12:F5:201:CYC:NC | 2.09 | 0.51 |
| 12:H5:201:CYC:HBA1 | 9:i5:26:THR:CG2 | 2.35 | 0.51 |
| 8:I5:61:ILE:HG22 | 8:I5:62:ARG:HG2 | 1.93 | 0.51 |
| 8:Q5:18:LEU:HD22 | 1:R5:97:LEU:HD11 | 1.90 | 0.51 |
| 10:j5:18:ARG:HH12 | 10:j5:268:SER:HB3 | 1.73 | 0.51 |
| 10:j5:925:ILE:HD12 | 10:j5:925:ILE:C | 2.36 | 0.51 |
| 10:j5:1008:PHE:CG | 12:v7:201:CYC:OB | 2.63 | 0.51 |
| 10:k5:449:ARG:HH21 | 10:k5:449:ARG:CG | 2.10 | 0.51 |
| 10:k5:540:LEU:HD11 | 10:k5:544:VAL:CG2 | 2.39 | 0.51 |
| 10:k5:776:PHE:HB3 | 10:k5:780:ILE:CG1 | 2.40 | 0.51 |
| 2:A6:31:PHE:CG | 3:B6:34:SER:HB2 | 2.45 | 0.51 |
| 1:R7:107:ARG:HA | 9:z7:45:GLN:NE2 | 2.26 | 0.51 |
| 1:J7:76:ARG:CA | 8:K7:110:ILE:O | 2.58 | 0.51 |
| 8:i7:8:ILE:HG23 | 1:j7:94:TYR:CE1 | 2.45 | 0.51 |
| 8:W7:126:VAL:HG22 | 12:W7:201:CYC:H3C | 1.91 | 0.51 |
| 1:d7:3:ASP:H | 1:d7:6:THR:HG1 | 1.57 | 0.51 |
| 8:o7:30:VAL:CG1 | 1:p7:31:PHE:HA | 2.40 | 0.51 |
| 8:o7:90:ARG:CA | 1:p7:18:TYR:CZ | 2.93 | 0.51 |
| 8:o7:121:THR:HG22 | 12:o7:201:CYC:HMC3 | 1.81 | 0.51 |
| 8:u7:30:VAL:CG1 | 1:v7:31:PHE:HA | 2.40 | 0.51 |
| 3:U8:115:GLU:CG | 4:M8:74:LEU:CD1 | 2.71 | 0.51 |
| 2:N8:31:PHE:CG | 3:O8:34:SER:HB2 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:N8:38:MET:CE | 3:O8:28:THR:OG1 | 2.56 | 0.51 |
| 3:S8:116:THR:CG2 | 3:S8:117:TYR:H | 2.24 | 0.51 |
| 11:a9:419:ARG:CG | 11:a9:419:ARG:NH1 | 2.71 | 0.51 |
| 11:aA:418:LEU:HD22 | 11:aA:428:PHE:CD2 | 2.45 | 0.51 |
| 3:LA:41:VAL:HG21 | 3:LA:98:LEU:HD13 | 1.93 | 0.51 |
| 3:LA:107:ASP:O | 11:aA:531:ASP:CG | 2.53 | 0.51 |
| 5:NA:50:LEU:C | 5:NA:50:LEU:CD1 | 2.84 | 0.51 |
| 3:H2:14:LEU:HD22 | 6:M2:67:GLY:CA | 2.38 | 0.51 |
| 12:J4:201:CYC:HB | 12:J4:201:CYC:HMA2 | 1.76 | 0.51 |
| 4:M4:27:HIS:NE2 | 4:M4:34:ASP:N | 2.57 | 0.51 |
| 2:N4:25:GLN:HG2 | 2:X4:33:ARG:CG | 2.38 | 0.51 |
| 3:Q4:124:THR:HB | 3:Q4:172:ALA:CA | 2.40 | 0.51 |
| 8:K5:12:ASP:HA | 1:L5:94:TYR:OH | 2.10 | 0.51 |
| 1:N5:107:ARG:NH2 | 10:k5:482:GLN:CD | 2.69 | 0.51 |
| 8:O5:151:PHE:O | 8:E5:20:PRO:HG3 | 2.10 | 0.51 |
| 5:Z4:29:HIS:CB | 5:Z4:31:TRP:HD1 | 2.23 | 0.51 |
| 1:D5:62:TYR:HH | 12:E5:201:CYC:CGD | 2.15 | 0.51 |
| 8:G5:12:ASP:CG | 1:H5:91:TYR:HE1 | 2.18 | 0.51 |
| 8:c5:90:ARG:HB2 | 1:d5:18:TYR:CZ | 2.45 | 0.51 |
| 8:W5:109:ILE:HD13 | 8:W5:159:ALA:HB1 | 1.91 | 0.51 |
| 12:J6:202:CYC:HMA2 | 12:J6:202:CYC:HB | 1.76 | 0.51 |
| 12:L6:201:CYC:HMA2 | 12:L6:201:CYC:HB | 1.76 | 0.51 |
| 6:M6:271:VAL:HG21 | 1:d7:127:VAL:CG2 | 2.40 | 0.51 |
| 9:z5:6:LYS:HB2 | 9:z5:55:LYS:HB3 | 1.84 | 0.51 |
| 10:j5:254:PRO:HG2 | 10:j5:434:TRP:CH2 | 2.45 | 0.51 |
| 10:j5:929:PRO:HG3 | 1:J7:147:LYS:NZ | 2.24 | 0.51 |
| 10:j5:978:LEU:HD21 | 1:v7:107:ARG:NE | 2.20 | 0.51 |
| 10:k5:303:GLN:HG2 | 10:k5:421:PRO:HB2 | 1.91 | 0.51 |
| 10:k5:990:ARG:CG | 10:k5:990:ARG:NH1 | 2.72 | 0.51 |
| 10:k5:1006:ASP:OD1 | 10:k5:1065:HIS:CD2 | 2.64 | 0.51 |
| 10:k5:1144:SER:CB | 1:l7:13:ASP:OD2 | 2.58 | 0.51 |
| 12:F6:201:CYC:HB | 12:F6:201:CYC:HMA2 | 1.75 | 0.51 |
| 8:Q7:17:TYR:CE2 | 1:R7:90:ARG:HA | 2.46 | 0.51 |
| 8:E7:26:ILE:O | 8:E7:30:VAL:HG13 | 2.09 | 0.51 |
| 8:K7:17:TYR:CE2 | 1:L7:90:ARG:HA | 2.46 | 0.51 |
| 8:k7:26:ILE:O | 8:k7:30:VAL:HG13 | 2.09 | 0.51 |
| 8:W7:109:ILE:HD13 | 8:W7:159:ALA:HB1 | 1.91 | 0.51 |
| 12:B8:202:CYC:C2D | 4:M8:53:LEU:HD23 | 2.39 | 0.51 |
| 8:m7:90:ARG:NH1 | 1:n7:16:GLY:HA2 | 2.25 | 0.51 |
| 12:p7:201:CYC:HMD1 | 12:p7:201:CYC:NC | 2.09 | 0.51 |
| 9:x7:9:ALA:CB | 9:x7:44:ILE:HD11 | 2.39 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:x7:14:LEU:HD13 | 9:x7:14:LEU:O | 2.09 | 0.51 |
| 3:F8:1:MET:CB | 4:M8:10:ARG:HA | 2.35 | 0.51 |
| 4:M8:259:ARG:HG3 | 4:M8:259:ARG:HH21 | 1.75 | 0.51 |
| 3:Q8:72:ASN:OD1 | 12:Z8:301:CYC:NC | 2.42 | 0.51 |
| 3:Q8:116:THR:C | 5:Z8:40:SER:HA | 2.35 | 0.51 |
| 3:L9:109:CYS:O | 11:a9:532:ALA:CB | 2.49 | 0.51 |
| 4:M9:93:LEU:HD21 | 4:M9:102:VAL:HG22 | 1.92 | 0.51 |
| 4:M9:112:GLN:HG2 | 4:M9:219:PRO:O | 2.10 | 0.51 |
| 5:N9:22:LEU:HD21 | 5:N9:26:LEU:CG | 2.29 | 0.51 |
| 11:a9:91:THR:HG22 | 11:a9:96:THR:CA | 2.21 | 0.51 |
| 11:a9:291:TYR:C | 11:a9:293:LEU:N | 2.68 | 0.51 |
| 11:aA:613:TYR:N | 11:aA:613:TYR:CD1 | 2.76 | 0.51 |
| 4:M1:74:LEU:O | 4:M1:77:LEU:CD1 | 2.59 | 0.51 |
| 4:M1:268:ARG:O | 3:V1:111:ASN:ND2 | 2.44 | 0.51 |
| 5:N1:23:SER:C | 5:N1:25:THR:H | 2.15 | 0.51 |
| 5:N1:57:MET:HE2 | 5:N1:67:ILE:HG13 | 1.92 | 0.51 |
| 2:A2:34:ALA:HB1 | 3:B2:31:VAL:HG21 | 1.92 | 0.51 |
| 1:Z:59:ALA:O | 1:Z:60:LEU:HD23 | 2.11 | 0.51 |
| 4:MA:20:THR:HG23 | 4:MA:67:LEU:HD11 | 1.92 | 0.51 |
| 4:MA:181:GLN:CD | 3:VA:120:LEU:CD2 | 2.78 | 0.51 |
| 2:A1:34:ALA:HB1 | 3:B1:31:VAL:HG21 | 1.92 | 0.51 |
| 12:L2:201:CYC:HMA2 | 12:L2:201:CYC:HB | 1.76 | 0.51 |
| 2:A3:60:TYR:CB | 2:A3:67:THR:CG2 | 2.83 | 0.51 |
| 12:P3:201:CYC:HMA2 | 12:P3:201:CYC:HB | 1.76 | 0.51 |
| 12:U4:201:CYC:HMA2 | 12:U4:201:CYC:HB | 1.76 | 0.51 |
| 3:F4:84:ARG:HH22 | 11:aA:143:SER:HB3 | 1.75 | 0.51 |
| 4:M4:29:PRO:HG2 | 11:aA:230:THR:OG1 | 2.10 | 0.51 |
| 1:L5:76:ARG:CA | 8:G5:110:ILE:O | 2.59 | 0.51 |
| 8:A5:53:GLN:O | 8:A5:53:GLN:HG3 | 2.10 | 0.51 |
| 8:A5:110:ILE:O | 1:F5:76:ARG:CA | 2.59 | 0.51 |
| 1:d5:127:VAL:CG1 | 10:j5:697:PHE:C | 2.82 | 0.51 |
| 8:e5:109:ILE:HD13 | 8:e5:159:ALA:HB1 | 1.91 | 0.51 |
| 8:S5:26:ILE:O | 8:S5:30:VAL:HG13 | 2.09 | 0.51 |
| 1:T5:53:LYS:CE | 8:U5:120:GLN:NE2 | 2.69 | 0.51 |
| 8:U5:76:LYS:CD | 8:U5:77:MET:HE1 | 2.14 | 0.51 |
| 1:Z5:63:SER:OG | 10:k5:703:LEU:O | 2.28 | 0.51 |
| 12:Z5:201:CYC:O2D | 10:k5:372:ARG:NH1 | 2.29 | 0.51 |
| 6:M6:65:VAL:HG12 | 1:b7:59:ALA:CA | 2.40 | 0.51 |
| 6:M6:271:VAL:CG2 | 1:d7:127:VAL:CB | 2.84 | 0.51 |
| 6:M6:278:ARG:HH21 | 1:d7:64:ASP:N | 2.08 | 0.51 |
| 10:j5:1020:GLU:HG3 | 1:f7:87:TYR:OH | 2.09 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:k5:213:LEU:HD12 | 10:k5:213:LEU:N | 2.26 | 0.51 |
| 10:k5:1034:GLU:OE2 | 10:k5:1034:GLU:HA | 2.09 | 0.51 |
| 8:O7:90:ARG:NH1 | 1:P7:16:GLY:HA2 | 2.25 | 0.51 |
| 8:C7:61:ILE:HG22 | 8:C7:62:ARG:HG2 | 1.93 | 0.51 |
| 1:H7:136:VAL:CA | 11:aA:563:PHE:HZ | 2.21 | 0.51 |
| 8:g7:29:PHE:HE1 | 8:g7:99:GLY:N | 2.08 | 0.51 |
| 8:g7:29:PHE:CD1 | 8:g7:99:GLY:HA3 | 2.43 | 0.51 |
| 8:U7:29:PHE:HE1 | 8:U7:99:GLY:N | 2.08 | 0.51 |
| 8:U7:90:ARG:NH1 | 1:V7:16:GLY:HA2 | 2.25 | 0.51 |
| 8:a7:61:ILE:HG22 | 8:a7:62:ARG:HG2 | 1.92 | 0.51 |
| 2:A8:31:PHE:CG | 3:B8:34:SER:HB2 | 2.45 | 0.51 |
| 8:o7:58:LEU:HG | 8:o7:59:PHE:CD1 | 2.46 | 0.51 |
| 8:q7:94:TYR:OH | 1:r7:17:LYS:O | 2.24 | 0.51 |
| 12:U8:201:CYC:HB | 12:U8:201:CYC:HMA2 | 1.76 | 0.51 |
| 3:L8:71:GLY:HA2 | 11:a9:82:GLN:CG | 2.38 | 0.51 |
| 4:M8:96:LYS:HE3 | 3:Q8:89:ILE:HG12 | 1.93 | 0.51 |
| 4:M8:148:LYS:HG2 | 4:M8:148:LYS:O | 2.09 | 0.51 |
| 4:M8:235:PHE:CB | 12:M8:301:CYC:CMA | 2.83 | 0.51 |
| 12:O8:201:CYC:OB | 5:Z8:54:LEU:HD12 | 2.11 | 0.51 |
| 5:N9:74:GLU:HA | 3:R9:111:ASN:HD21 | 1.74 | 0.51 |
| 5:Z8:37:HIS:CE1 | 12:Z8:301:CYC:HBA1 | 2.45 | 0.51 |
| 5:Z8:41:GLN:O | 5:Z8:41:GLN:HG3 | 2.10 | 0.51 |
| 2:A9:34:ALA:HB1 | 3:B9:31:VAL:HG21 | 1.92 | 0.51 |
| 3:B9:14:LEU:CD1 | 3:X9:125:ARG:HD2 | 2.40 | 0.51 |
| 4:M1:51:ARG:HB3 | 4:M1:51:ARG:NH1 | 2.23 | 0.51 |
| 4:M1:139:VAL:O | 4:M1:139:VAL:HG12 | 2.09 | 0.51 |
| 1:A:75:THR:OG1 | 10:k5:182:ASN:CA | 2.50 | 0.51 |
| 1:A:161:SER:C | 1:R5:14:VAL:HG21 | 2.35 | 0.51 |
| 3:JA:78:ARG:HH12 | 11:aA:359:ASP:CA | 2.04 | 0.51 |
| 3:JA:88:ILE:HD13 | 11:aA:512:TYR:CG | 2.46 | 0.51 |
| 2:OA:31:PHE:CG | 3:PA:34:SER:HB2 | 2.45 | 0.51 |
| 2:QA:68:GLN:CG | 2:QA:69:PRO:CD | 2.88 | 0.51 |
| 2:O1:31:PHE:CG | 3:P1:34:SER:HB2 | 2.45 | 0.51 |
| 2:S1:16:GLY:HA2 | 5:N1:31:TRP:NE1 | 2.25 | 0.51 |
| 2:A3:16:GLY:CA | 11:a9:677:GLN:CD | 2.80 | 0.51 |
| 2:A4:65:TYR:O | 2:A4:71:GLN:CG | 2.54 | 0.51 |
| 4:M3:22:SER:HB3 | 4:M3:23:PRO:CD | 2.41 | 0.51 |
| 4:M3:130:SER:HB3 | 3:P3:84:ARG:CZ | 2.40 | 0.51 |
| 3:S4:116:THR:CG2 | 3:S4:117:TYR:H | 2.24 | 0.51 |
| 4:M4:74:LEU:O | 4:M4:77:LEU:CD1 | 2.59 | 0.51 |
| 2:N4:112:GLY:N | 5:Z4:34:LEU:HA | 2.21 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 3:Q4:84:ARG:HH11 | 5:Z4:29:HIS:HB2 | 1.75 | 0.51 |
| 3:Q4:105:LEU:HD22 | 3:Q4:166:LYS:CD | 2.41 | 0.51 |
| 8:K5:116:TYR:HB3 | 8:K5:123:ILE:HG12 | 1.93 | 0.51 |
| 1:B5:76:ARG:CD | 9:z5:14:LEU:O | 2.58 | 0.51 |
| 1:D5:62:TYR:HE1 | 12:E5:201:CYC:O1D | 1.94 | 0.51 |
| 8:I5:109:ILE:HD13 | 8:I5:159:ALA:HB1 | 1.91 | 0.51 |
| 8:U5:35:ARG:NH2 | 8:U5:145:ASP:OD1 | 2.42 | 0.51 |
| 1:X5:64:ASP:CB | 10:j5:704:THR:CG2 | 2.88 | 0.51 |
| 8:a5:95:GLY:H | 8:a5:104:ILE:HD11 | 1.74 | 0.51 |
| 9:i5:6:LYS:HZ3 | 9:i5:29:THR:CG2 | 2.22 | 0.51 |
| 10:j5:776:PHE:HB3 | 10:j5:780:ILE:CG1 | 2.40 | 0.51 |
| 10:k5:1009:ALA:CA | 1:p7:87:TYR:CE1 | 2.91 | 0.51 |
| 10:k5:1105:ILE:HD11 | 10:k5:1115:ARG:HH22 | 1.71 | 0.51 |
| 8:O7:29:PHE:HE1 | 8:O7:99:GLY:N | 2.08 | 0.51 |
| 8:C7:90:ARG:NH1 | 1:D7:16:GLY:HA2 | 2.25 | 0.51 |
| 1:F7:3:ASP:H | 1:F7:6:THR:HG1 | 1.58 | 0.51 |
| 8:I7:27:LYS:O | 8:I7:30:VAL:HG22 | 2.09 | 0.51 |
| 8:I7:90:ARG:NH1 | 1:J7:16:GLY:HA2 | 2.25 | 0.51 |
| 8:M7:49:ARG:HD2 | 11:a9:550:PHE:CZ | 2.33 | 0.51 |
| 8:g7:61:ILE:HG22 | 8:g7:62:ARG:HG2 | 1.93 | 0.51 |
| 8:i7:54:ALA:HB3 | 8:i7:133:MET:HG3 | 1.85 | 0.51 |
| 8:c7:130:VAL:O | 8:c7:130:VAL:HG12 | 2.10 | 0.51 |
| 2:A8:34:ALA:HB1 | 3:B8:31:VAL:HG21 | 1.92 | 0.51 |
| 3:B8:85:ASP:CG | 3:B8:117:TYR:OH | 2.53 | 0.51 |
| 9:w7:34:TYR:CD1 | 9:w7:34:TYR:C | 2.87 | 0.51 |
| 4:M8:74:LEU:O | 4:M8:77:LEU:CD1 | 2.58 | 0.51 |
| 3:Q8:72:ASN:CG | 12:Z8:301:CYC:HMD1 | 2.30 | 0.51 |
| 3:L9:14:LEU:HD11 | 11:a9:358:PRO:HB2 | 1.76 | 0.51 |
| 12:L9:201:CYC:HAB2 | 2:K9:24:LEU:CB | 2.34 | 0.51 |
| 4:M9:61:ASN:C | 4:M9:63:GLY:N | 2.64 | 0.51 |
| 4:M9:144:ARG:NH2 | 4:M9:205:ASP:OD1 | 2.43 | 0.51 |
| 4:M9:158:PHE:CZ | 2:U9:10:ALA:CB | 2.92 | 0.51 |
| 2:O9:31:PHE:CG | 3:P9:34:SER:HB2 | 2.45 | 0.51 |
| 12:H9:202:CYC:HB | 12:H9:202:CYC:HMA2 | 1.76 | 0.51 |
| 3:J9:88:ILE:HD13 | 11:a9:512:TYR:CG | 2.46 | 0.51 |
| 11:a9:358:PRO:HG2 | 11:a9:358:PRO:O | 2.11 | 0.51 |
| 11:aA:34:ILE:O | 11:aA:34:ILE:HG22 | 2.09 | 0.51 |
| 11:aA:67:GLN:C | 11:aA:68:THR:CG2 | 2.79 | 0.51 |
| 11:aA:445:THR:HB | 11:aA:542:ALA:O | 2.11 | 0.51 |
| 11:aA:668:TYR:HD1 | 3:J1:84:ARG:CD | 2.19 | 0.51 |
| 4:M1:188:LEU:HD12 | 4:M1:188:LEU:C | 2.35 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:Z1:202:CYC:HB | 12:Z1:202:CYC:HMA2 | 1.76 | 0.51 |
| 1:A:59:ALA:O | 1:A:60:LEU:HD23 | 2.11 | 0.51 |
| 2:AA:138:VAL:HG12 | 2:AA:138:VAL:O | 2.11 | 0.51 |
| 2:EA:152:ALA:HB1 | 2:IA:21:ASN:CG | 2.36 | 0.51 |
| 3:HA:123:PRO:HG2 | 12:HA:202:CYC:HMC1 | 1.92 | 0.51 |
| 2:KA:18:PHE:CB | 3:LA:45:THR:HG23 | 2.40 | 0.51 |
| 3:LA:51:ILE:HG21 | 3:LA:90:LEU:HD11 | 1.86 | 0.51 |
| 3:J3:81:ALA:HA | 11:a9:668:TYR:CD2 | 2.46 | 0.51 |
| 2:K3:33:ARG:CG | 2:A3:25:GLN:HG2 | 2.38 | 0.51 |
| 6:M2:55:PRO:HA | 1:h7:62:TYR:CG | 2.46 | 0.51 |
| 7:N2:1:MET:N | 7:N2:1:MET:CE | 2.72 | 0.51 |
| 3:B3:84:ARG:NH1 | 11:a9:680:SER:HB3 | 2.26 | 0.51 |
| 3:B3:112:GLY:H | 4:M3:76:ALA:HB1 | 1.73 | 0.51 |
| 3:B4:116:THR:CG2 | 3:B4:117:TYR:H | 2.23 | 0.51 |
| 4:M3:112:GLN:NE2 | 4:M3:172:HIS:O | 2.43 | 0.51 |
| 12:F4:202:CYC:CMA | 11:aA:144:LEU:HD23 | 2.40 | 0.51 |
| 4:M4:259:ARG:HG3 | 4:M4:259:ARG:HH21 | 1.75 | 0.51 |
| 1:N5:59:ALA:O | 1:N5:60:LEU:HD23 | 2.11 | 0.51 |
| 8:E5:12:ASP:HA | 1:F5:94:TYR:OH | 2.10 | 0.51 |
| 1:F5:1:MET:O | 1:F5:1:MET:HG3 | 2.03 | 0.51 |
| 1:F5:14:VAL:HG12 | 9:z5:64:ASN:HD21 | 1.76 | 0.51 |
| 1:d5:124:ALA:HB1 | 10:j5:699:SER:CB | 2.37 | 0.51 |
| 12:d5:201:CYC:HB | 12:d5:201:CYC:HMA3 | 1.73 | 0.51 |
| 12:d5:201:CYC:HMA2 | 10:j5:379:PHE:CZ | 2.46 | 0.51 |
| 8:W5:17:TYR:CE2 | 1:X5:93:THR:CB | 2.91 | 0.51 |
| 10:j5:307:ARG:HH12 | 10:j5:346:GLU:CD | 2.10 | 0.51 |
| 10:j5:1023:SER:CA | 12:f7:201:CYC:HBA1 | 2.40 | 0.51 |
| 10:k5:77:VAL:CG2 | 10:k5:141:GLU:CB | 2.89 | 0.51 |
| 10:k5:254:PRO:HG2 | 10:k5:434:TRP:CH2 | 2.45 | 0.51 |
| 10:k5:605:ARG:O | 10:k5:605:ARG:HG2 | 2.11 | 0.51 |
| 10:k5:1025:LEU:CA | 10:k5:1030:ILE:CG2 | 2.79 | 0.51 |
| 8:S7:61:ILE:HG22 | 8:S7:62:ARG:HG2 | 1.93 | 0.51 |
| 8:E7:116:TYR:HB3 | 8:E7:123:ILE:HG12 | 1.91 | 0.51 |
| 8:M7:26:ILE:O | 8:M7:30:VAL:HG13 | 2.09 | 0.51 |
| 12:h7:201:CYC:HB | 12:h7:201:CYC:HMA3 | 1.73 | 0.51 |
| 8:k7:66:VAL:CG1 | 11:a9:65:LEU:HD22 | 2.40 | 0.51 |
| 8:k7:90:ARG:HB2 | 1:l7:18:TYR:CZ | 2.45 | 0.51 |
| 8:W7:26:ILE:O | 8:W7:30:VAL:HG13 | 2.09 | 0.51 |
| 8:Y7:110:ILE:O | 1:d7:76:ARG:N | 2.43 | 0.51 |
| 4:M8:103:GLN:O | 4:M8:104:ALA:C | 2.53 | 0.51 |
| 2:N8:115:GLU:HB3 | 5:Z8:33:GLY:CA | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:M9:264:LYS:N | 3:V9:119:ALA:CB | 2.74 | 0.51 |
| 5:N9:37:HIS:O | 12:P9:201:CYC:CMA | 2.59 | 0.51 |
| 3:Y8:113:LEU:HB3 | 3:Y8:171:ILE:HA | 1.92 | 0.51 |
| 2:C9:138:VAL:HG12 | 2:C9:138:VAL:O | 2.11 | 0.51 |
| 2:I9:1:MET:CE | 2:I9:108:TYR:CE1 | 2.83 | 0.51 |
| 2:U9:138:VAL:O | 2:U9:138:VAL:HG12 | 2.11 | 0.51 |
| 12:X9:201:CYC:HB | 12:X9:201:CYC:HMA2 | 1.76 | 0.51 |
| 11:a9:93:LEU:CD1 | 11:a9:93:LEU:H | 2.23 | 0.51 |
| 11:a9:325:LEU:HD23 | 11:a9:325:LEU:N | 2.23 | 0.51 |
| 11:a9:455:ASN:OD1 | 11:a9:455:ASN:N | 2.40 | 0.51 |
| 11:a9:613:TYR:CD1 | 11:a9:613:TYR:N | 2.76 | 0.51 |
| 11:aA:93:LEU:N | 11:aA:93:LEU:CD1 | 2.72 | 0.51 |
| 11:aA:776:TYR:HA | 11:aA:780:GLN:NE2 | 2.25 | 0.51 |
| 11:aA:802:ARG:O | 11:aA:804:ARG:N | 2.43 | 0.51 |
| 5:N1:29:HIS:HD2 | 5:N1:36:THR:HG23 | 1.76 | 0.51 |
| 3:B2:77:ARG:CG | 3:B2:77:ARG:NH1 | 2.72 | 0.51 |
| 1:Z:127:VAL:HG13 | 1:X5:15:GLN:OE1 | 2.08 | 0.51 |
| 3:BA:14:LEU:CD1 | 3:XA:125:ARG:HD2 | 2.40 | 0.51 |
| 2:IA:16:GLY:CA | 3:JA:91:ARG:HH11 | 2.20 | 0.51 |
| 3:LA:14:LEU:HD21 | 11:aA:358:PRO:CD | 2.40 | 0.51 |
| 4:MA:14:LEU:HD12 | 4:MA:14:LEU:N | 2.24 | 0.51 |
| 5:NA:6:GLY:HA3 | 3:RA:108:ARG:O | 2.11 | 0.51 |
| 12:P1:201:CYC:HMA2 | 12:P1:201:CYC:HB | 1.76 | 0.51 |
| 3:J3:77:ARG:HD2 | 2:K3:107:ASP:O | 2.11 | 0.51 |
| 3:L2:77:ARG:HH22 | 6:M2:70:GLU:CG | 2.16 | 0.51 |
| 2:A4:25:GLN:HG2 | 2:K4:33:ARG:CG | 2.38 | 0.51 |
| 4:M4:152:TYR:CD1 | 4:M4:152:TYR:C | 2.87 | 0.51 |
| 4:M4:227:GLN:C | 3:Y4:91:ARG:NH2 | 2.68 | 0.51 |
| 3:O4:119:ALA:HB2 | 5:Z4:72:GLU:N | 2.19 | 0.51 |
| 8:A5:111:GLY:HA3 | 1:F5:76:ARG:CA | 2.36 | 0.51 |
| 8:A5:126:VAL:N | 12:A5:201:CYC:HMC1 | 2.26 | 0.51 |
| 8:C5:109:ILE:HD13 | 8:C5:159:ALA:HB1 | 1.91 | 0.51 |
| 12:D5:201:CYC:NB | 9:z5:38:PHE:CE2 | 2.78 | 0.51 |
| 8:e5:29:PHE:HE1 | 8:e5:99:GLY:N | 2.08 | 0.51 |
| 1:Z5:127:VAL:HB | 10:k5:698:GLY:CA | 2.40 | 0.51 |
| 1:b5:3:ASP:H | 1:b5:6:THR:HG1 | 1.57 | 0.51 |
| 6:M6:127:SER:C | 12:F6:201:CYC:HBA1 | 2.30 | 0.51 |
| 10:j5:540:LEU:HD11 | 10:j5:544:VAL:HG22 | 1.93 | 0.51 |
| 10:k5:357:LEU:HD23 | 10:k5:401:LEU:HD13 | 1.93 | 0.51 |
| 10:k5:955:LEU:HD13 | 8:o7:80:LEU:HD21 | 1.92 | 0.51 |
| 10:k5:1097:VAL:O | 10:k5:1097:VAL:HG12 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:k5:1136:ILE:O | 10:k5:1136:ILE:HG22 | 2.09 | 0.51 |
| 12:D6:201:CYC:HMA2 | 12:D6:201:CYC:HB | 1.76 | 0.51 |
| 3:F6:82:CYC:SG | 12:F6:201:CYC:C3C | 2.98 | 0.51 |
| 8:O7:47:ARG:HD3 | 1:P7:18:TYR:CE1 | 2.46 | 0.51 |
| 8:S7:120:GLN:CG | 1:X7:53:LYS:HZ1 | 2.21 | 0.51 |
| 8:I7:47:ARG:HD3 | 1:J7:18:TYR:CE1 | 2.46 | 0.51 |
| 8:M7:61:ILE:HG22 | 8:M7:62:ARG:HG2 | 1.93 | 0.51 |
| 1:Z7:67:ARG:NH1 | 11:a9:307:ARG:CG | 2.72 | 0.51 |
| 8:a7:109:ILE:HD13 | 8:a7:159:ALA:HB1 | 1.91 | 0.51 |
| 1:b7:119:LEU:HD21 | 9:x7:12:PRO:HB3 | 1.93 | 0.51 |
| 8:c7:17:TYR:HE2 | 1:d7:93:THR:OG1 | 1.86 | 0.51 |
| 2:C8:138:VAL:HG12 | 2:C8:138:VAL:O | 2.11 | 0.51 |
| 8:m7:61:ILE:HG22 | 8:m7:62:ARG:HG2 | 1.93 | 0.51 |
| 8:o7:109:ILE:HD13 | 8:o7:159:ALA:HB1 | 1.91 | 0.51 |
| 8:u7:45:GLU:HA | 8:u7:45:GLU:OE2 | 2.09 | 0.51 |
| 12:W8:201:CYC:HMA2 | 12:W8:201:CYC:HB | 1.76 | 0.51 |
| 12:H8:201:CYC:HMA2 | 12:H8:201:CYC:HB | 1.76 | 0.51 |
| 4:M8:176:ARG:CG | 4:M8:176:ARG:NH1 | 2.70 | 0.51 |
| 12:N8:201:CYC:C2B | 3:Q8:76:ASN:ND2 | 2.73 | 0.51 |
| 3:F9:43:ALA:HB3 | 3:F9:142:VAL:HG22 | 1.91 | 0.51 |
| 12:J9:202:CYC:HBA2 | 11:a9:510:PHE:C | 2.33 | 0.51 |
| 12:V9:201:CYC:HB | 12:V9:201:CYC:HMA2 | 1.76 | 0.51 |
| 11:a9:75:ALA:CB | 11:a9:81:ASP:OD1 | 2.25 | 0.51 |
| 11:aA:90:GLN:C | 11:aA:92:LYS:H | 2.17 | 0.51 |
| 11:aA:320:ASP:O | 11:aA:321:ALA:C | 2.50 | 0.51 |
| 11:aA:412:VAL:CA | 11:aA:415:GLU:OE2 | 2.59 | 0.51 |
| 5:N1:37:HIS:O | 5:N1:38:GLU:C | 2.49 | 0.51 |
| 2:E2:138:VAL:HG12 | 2:E2:138:VAL:O | 2.11 | 0.51 |
| 3:F2:78:ARG:NH1 | 12:F2:201:CYC:O2D | 2.40 | 0.51 |
| 12:BA:201:CYC:HAA1 | 4:MA:36:TYR:CZ | 2.45 | 0.51 |
| 3:JA:70:GLY:C | 11:aA:357:THR:H | 2.17 | 0.51 |
| 3:LA:98:LEU:O | 3:LA:99:ALA:C | 2.48 | 0.51 |
| 4:MA:112:GLN:NE2 | 4:MA:172:HIS:O | 2.43 | 0.51 |
| 5:NA:37:HIS:O | 12:PA:201:CYC:CMA | 2.59 | 0.51 |
| 2:K3:22:THR:HB | 2:A3:2:LYS:HE2 | 1.93 | 0.51 |
| 3:J2:88:ILE:HD11 | 6:M2:185:PHE:HE1 | 1.74 | 0.51 |
| 7:N2:49:LEU:CD1 | 3:B2:84:ARG:NE | 2.74 | 0.51 |
| 3:F4:112:GLY:HA2 | 4:M4:76:ALA:CB | 2.40 | 0.51 |
| 4:M4:112:GLN:NE2 | 4:M4:172:HIS:O | 2.43 | 0.51 |
| 1:L5:59:ALA:O | 1:L5:60:LEU:HD23 | 2.11 | 0.51 |
| 5:Z4:36:THR:OG1 | 5:Z4:37:HIS:N | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:Z4:57:MET:HE2 | 5:Z4:67:ILE:HG13 | 1.92 | 0.51 |
| 1:B5:59:ALA:O | 1:B5:60:LEU:HD23 | 2.11 | 0.51 |
| 1:H5:59:ALA:O | 1:H5:60:LEU:HD23 | 2.11 | 0.51 |
| 1:Z5:161:SER:OG | 10:k5:696:ARG:CA | 2.55 | 0.51 |
| 6:M6:245:SER:OG | 12:H6:201:CYC:HMA1 | 2.11 | 0.51 |
| 8:A7:90:ARG:HB2 | 1:B7:18:TYR:CZ | 2.45 | 0.51 |
| 8:A7:94:TYR:OH | 1:B7:17:LYS:O | 2.24 | 0.51 |
| 10:j5:298:ARG:HH11 | 10:j5:298:ARG:HA | 1.76 | 0.51 |
| 10:j5:511:ARG:NH1 | 10:j5:683:ARG:O | 2.44 | 0.51 |
| 10:j5:722:ILE:O | 10:j5:722:ILE:HG22 | 2.11 | 0.51 |
| 10:j5:1043:GLU:CD | 8:e7:14:GLU:CG | 2.84 | 0.51 |
| 10:k5:192:LYS:CE | 10:k5:192:LYS:CA | 2.85 | 0.51 |
| 10:k5:612:ILE:HD12 | 10:k5:612:ILE:N | 2.06 | 0.51 |
| 10:k5:1081:VAL:HG21 | 12:k5:1203:CYC:HMA2 | 1.90 | 0.51 |
| 12:P7:201:CYC:HBB2 | 9:z7:21:ARG:HA | 1.93 | 0.51 |
| 1:h7:75:THR:HG22 | 8:i7:115:MET:HE1 | 1.88 | 0.51 |
| 8:a7:161:GLN:CG | 1:p7:49:THR:CG2 | 2.89 | 0.51 |
| 8:c7:126:VAL:O | 8:c7:126:VAL:HG12 | 2.11 | 0.51 |
| 1:r7:59:ALA:O | 1:r7:60:LEU:HD23 | 2.11 | 0.51 |
| 8:s7:90:ARG:NH1 | 1:t7:16:GLY:HA2 | 2.25 | 0.51 |
| 12:F8:202:CYC:CMA | 11:a9:144:LEU:HD23 | 2.41 | 0.51 |
| 12:J8:201:CYC:HMA2 | 12:J8:201:CYC:HB | 1.76 | 0.51 |
| 4:M8:205:ASP:CB | 5:Z8:59:ARG:HH11 | 2.24 | 0.51 |
| 12:M8:301:CYC:CAC | 3:Y8:82:CYS:SG | 2.95 | 0.51 |
| 2:N8:115:GLU:OE2 | 5:Z8:32:PRO:HD2 | 2.06 | 0.51 |
| 3:Q8:84:ARG:HH12 | 5:Z8:36:THR:HG23 | 1.76 | 0.51 |
| 5:N9:6:GLY:HA3 | 3:R9:108:ARG:O | 2.11 | 0.51 |
| 5:N9:36:THR:OG1 | 12:P9:201:CYC:CMA | 2.59 | 0.51 |
| 2:O9:2:LYS:HE2 | 2:Y9:22:THR:HB | 1.93 | 0.51 |
| 2:O9:138:VAL:O | 2:O9:138:VAL:HG12 | 2.11 | 0.51 |
| 5:Z8:1:MET:O | 5:Z8:3:VAL:N | 2.44 | 0.51 |
| 5:Z8:57:MET:HE2 | 5:Z8:67:ILE:HG13 | 1.92 | 0.51 |
| 3:F9:148:VAL:O | 3:F9:149:THR:O | 2.29 | 0.51 |
| 3:H9:108:ARG:NH2 | 11:a9:477:TYR:CZ | 2.79 | 0.51 |
| 3:H9:120:LEU:HD13 | 12:H9:202:CYC:CHA | 2.40 | 0.51 |
| 2:I9:16:GLY:CA | 3:J9:91:ARG:HH11 | 2.19 | 0.51 |
| 2:G1:107:ASP:O | 3:L1:77:ARG:HD2 | 2.11 | 0.51 |
| 11:a9:61:TYR:HA | 11:a9:65:LEU:CB | 2.41 | 0.51 |
| 11:a9:412:VAL:CA | 11:a9:415:GLU:OE2 | 2.59 | 0.51 |
| 2:EA:21:ASN:ND2 | 12:F9:302:CYC:HBB1 | 2.26 | 0.51 |
| 4:MA:205:ASP:OD2 | 5:NA:52:ARG:CZ | 2.59 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:MA:259:ARG:HH12 | 3:VA:116:THR:N | 2.07 | 0.51 |
| 5:NA:36:THR:OG1 | 12:PA:201:CYC:CMA | 2.59 | 0.51 |
| 2:I3:138:VAL:HG12 | 2:I3:138:VAL:O | 2.11 | 0.51 |
| 12:Z3:201:CYC:HB | 12:Z3:201:CYC:HMA2 | 1.76 | 0.51 |
| 3:D4:107:ASP:CB | 11:aA:109:ASN:HB3 | 2.41 | 0.51 |
| 3:L3:77:ARG:HD3 | 11:a9:824:VAL:O | 2.09 | 0.51 |
| 5:N3:21:ALA:HA | 5:N3:42:SER:O | 2.11 | 0.51 |
| 12:X3:201:CYC:HMA2 | 12:X3:201:CYC:HB | 1.76 | 0.51 |
| 4:M4:93:LEU:HD21 | 4:M4:102:VAL:HG22 | 1.92 | 0.51 |
| 2:N4:60:TYR:CB | 2:N4:67:THR:CG2 | 2.83 | 0.51 |
| 2:N4:138:VAL:O | 2:N4:138:VAL:HG12 | 2.11 | 0.51 |
| 3:O4:116:THR:OG1 | 5:Z4:70:ILE:HD12 | 2.11 | 0.51 |
| 3:O4:119:ALA:HB1 | 5:Z4:72:GLU:CD | 2.22 | 0.51 |
| 8:M5:90:ARG:HD2 | 1:N5:18:TYR:N | 2.24 | 0.51 |
| 12:Z4:301:CYC:HMA2 | 12:Z4:301:CYC:HB | 1.76 | 0.51 |
| 8:C5:61:ILE:HG22 | 8:C5:62:ARG:HG2 | 1.93 | 0.51 |
| 8:E5:151:PHE:HE1 | 1:P5:42:ALA:HB2 | 1.76 | 0.51 |
| 8:c5:61:ILE:HG22 | 8:c5:62:ARG:HG2 | 1.93 | 0.51 |
| 1:d5:127:VAL:HB | 10:j5:698:GLY:CA | 2.40 | 0.51 |
| 1:V5:59:ALA:O | 1:V5:60:LEU:HD23 | 2.11 | 0.51 |
| 8:W5:8:ILE:HG23 | 1:X5:94:TYR:CG | 2.46 | 0.51 |
| 12:X5:201:CYC:OB | 10:j5:520:ARG:HG2 | 2.10 | 0.51 |
| 2:K6:22:THR:HB | 2:A6:2:LYS:HE2 | 1.93 | 0.51 |
| 6:M6:50:LEU:HB3 | 8:c7:83:ARG:HG3 | 1.92 | 0.51 |
| 9:z5:16:ARG:NE | 9:z5:16:ARG:CA | 2.73 | 0.51 |
| 9:i5:16:ARG:NE | 9:i5:16:ARG:CA | 2.73 | 0.51 |
| 10:j5:489:ASN:C | 10:j5:490:SER:OG | 2.38 | 0.51 |
| 10:j5:948:SER:O | 10:j5:948:SER:OG | 2.16 | 0.51 |
| 10:j5:1020:GLU:HG2 | 1:f7:87:TYR:CZ | 2.45 | 0.51 |
| 10:j5:1052:PRO:CB | 1:r7:106:GLU:OE2 | 2.59 | 0.51 |
| 10:k5:249:SER:HB2 | 10:k5:254:PRO:O | 2.10 | 0.51 |
| 10:k5:309:LEU:CD1 | 10:k5:342:LEU:HD13 | 2.41 | 0.51 |
| 10:k5:477:ASP:OD1 | 10:k5:477:ASP:N | 2.41 | 0.51 |
| 10:k5:511:ARG:NH1 | 10:k5:683:ARG:O | 2.44 | 0.51 |
| 10:k5:546:PHE:CD1 | 10:k5:561:GLU:OE1 | 2.64 | 0.51 |
| 10:k5:676:GLU:O | 10:k5:676:GLU:HG3 | 2.02 | 0.51 |
| 10:k5:1008:PHE:CE1 | 12:p7:201:CYC:C3B | 2.94 | 0.51 |
| 10:k5:1051:GLU:HB3 | 10:k5:1052:PRO:HD3 | 1.93 | 0.51 |
| 10:k5:1054:SER:CB | 10:k5:1056:PRO:HD3 | 2.40 | 0.51 |
| 1:B7:59:ALA:O | 1:B7:60:LEU:HD23 | 2.11 | 0.51 |
| 1:B7:136:VAL:HG22 | 11:a9:563:PHE:CE1 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:C7:29:PHE:HE1 | 8:C7:99:GLY:N | 2.08 | 0.51 |
| 1:L7:59:ALA:O | 1:L7:60:LEU:HD23 | 2.11 | 0.51 |
| 8:U7:47:ARG:HD3 | 1:V7:18:TYR:CE1 | 2.46 | 0.51 |
| 1:b7:59:ALA:O | 1:b7:60:LEU:HD23 | 2.11 | 0.51 |
| 1:f7:59:ALA:O | 1:f7:60:LEU:HD23 | 2.11 | 0.51 |
| 2:E8:138:VAL:O | 2:E8:138:VAL:HG12 | 2.11 | 0.51 |
| 1:n7:59:ALA:O | 1:n7:60:LEU:HD23 | 2.11 | 0.51 |
| 1:n7:75:THR:HB | 8:o7:111:GLY:O | 2.11 | 0.51 |
| 8:s7:29:PHE:HE1 | 8:s7:99:GLY:N | 2.08 | 0.51 |
| 8:u7:58:LEU:HG | 8:u7:59:PHE:CD1 | 2.46 | 0.51 |
| 3:H8:84:ARG:NE | 11:a9:131:TYR:CD1 | 2.78 | 0.51 |
| 4:M9:20:THR:HG23 | 4:M9:67:LEU:HD11 | 1.92 | 0.51 |
| 4:M9:112:GLN:NE2 | 4:M9:172:HIS:O | 2.43 | 0.51 |
| 4:M9:185:ALA:CA | 12:V9:201:CYC:O2A | 2.51 | 0.51 |
| 4:M9:259:ARG:HH12 | 3:V9:116:THR:H | 1.59 | 0.51 |
| 2:I9:16:GLY:CA | 11:a9:514:VAL:HG11 | 2.36 | 0.51 |
| 11:a9:319:LEU:O | 11:a9:322:ALA:HB3 | 2.11 | 0.51 |
| 11:a9:328:GLN:NE2 | 11:a9:328:GLN:N | 2.58 | 0.51 |
| 5:N1:1:MET:O | 5:N1:3:VAL:N | 2.43 | 0.51 |
| 4:MA:158:PHE:CE1 | 2:UA:10:ALA:CA | 2.91 | 0.51 |
| 4:MA:259:ARG:HG3 | 4:MA:259:ARG:HH21 | 1.75 | 0.51 |
| 2:QA:18:PHE:CZ | 3:RA:48:ALA:HB2 | 2.43 | 0.51 |
| 2:O1:2:LYS:HE2 | 2:Y1:22:THR:HB | 1.93 | 0.51 |
| 12:R1:201:CYC:HB | 12:R1:201:CYC:HMA2 | 1.76 | 0.51 |
| 12:H3:202:CYC:HMA2 | 12:H3:202:CYC:HB | 1.76 | 0.51 |
| 5:N3:29:HIS:HD2 | 5:N3:36:THR:HG23 | 1.76 | 0.51 |
| 2:O3:2:LYS:HE2 | 2:Y3:22:THR:HB | 1.93 | 0.51 |
| 3:B1:120:LEU:HD13 | 12:B1:202:CYC:HBD1 | 1.93 | 0.51 |
| 3:L4:71:GLY:HA2 | 11:aA:82:GLN:CD | 2.36 | 0.51 |
| 4:M4:29:PRO:CB | 11:aA:225:VAL:C | 2.48 | 0.51 |
| 4:M4:140:ARG:HH12 | 4:M4:144:ARG:HH11 | 1.48 | 0.51 |
| 8:C5:37:LEU:CD2 | 1:D5:27:LEU:HD13 | 2.25 | 0.51 |
| 8:E5:102:THR:N | 8:E5:103:PRO:CD | 2.74 | 0.51 |
| 8:G5:126:VAL:N | 12:G5:201:CYC:HMC1 | 2.26 | 0.51 |
| 8:I5:29:PHE:CE2 | 1:J5:5:ILE:CD1 | 2.93 | 0.51 |
| 8:I5:35:ARG:NH2 | 8:I5:145:ASP:OD1 | 2.42 | 0.51 |
| 1:d5:59:ALA:O | 1:d5:60:LEU:HD23 | 2.11 | 0.51 |
| 12:R5:201:CYC:HB | 12:R5:201:CYC:HMA3 | 1.73 | 0.51 |
| 1:b5:59:ALA:O | 1:b5:60:LEU:HD23 | 2.11 | 0.51 |
| 6:M6:69:ALA:HB2 | 3:H6:14:LEU:HG | 1.93 | 0.51 |
| 10:j5:367:ARG:NH1 | 10:j5:410:GLU:OE2 | 2.42 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:j5:1136:ILE:O | 10:j5:1136:ILE:HG22 | 2.09 | 0.51 |
| 10:k5:43:LEU:N | 10:k5:43:LEU:HD22 | 2.26 | 0.51 |
| 10:k5:1119:LEU:HD22 | 1:n7:87:TYR:CZ | 2.46 | 0.51 |
| 12:D1:202:CYC:HMA2 | 12:D1:202:CYC:HB | 1.76 | 0.51 |
| 8:g7:90:ARG:NH2 | 1:h7:16:GLY:HA2 | 2.26 | 0.51 |
| 1:h7:75:THR:CG2 | 8:i7:115:MET:CE | 2.81 | 0.51 |
| 12:b7:201:CYC:HB | 12:b7:201:CYC:HMA3 | 1.73 | 0.51 |
| 8:m7:47:ARG:HD3 | 1:n7:18:TYR:CE1 | 2.46 | 0.51 |
| 8:m7:57:GLN:O | 8:m7:61:ILE:HD13 | 2.11 | 0.51 |
| 1:t7:59:ALA:O | 1:t7:60:LEU:HD23 | 2.11 | 0.51 |
| 8:u7:116:TYR:HB3 | 8:u7:123:ILE:HG12 | 1.91 | 0.51 |
| 1:v7:59:ALA:O | 1:v7:60:LEU:HD23 | 2.12 | 0.51 |
| 3:L9:45:THR:HG23 | 2:K9:18:PHE:CB | 2.40 | 0.51 |
| 4:M9:185:ALA:HA | 12:V9:201:CYC:HBA2 | 1.93 | 0.51 |
| 2:Q9:138:VAL:O | 2:Q9:138:VAL:HG12 | 2.11 | 0.51 |
| 3:D9:68:ARG:NH2 | 3:X9:68:ARG:HH22 | 2.09 | 0.51 |
| 11:a9:25:GLU:HB3 | 11:a9:26:PRO:HD3 | 1.93 | 0.51 |
| 11:a9:95:ILE:HD13 | 11:a9:237:PHE:CE2 | 2.45 | 0.51 |
| 11:a9:338:VAL:CG2 | 11:a9:340:PRO:CD | 2.78 | 0.51 |
| 11:a9:445:THR:HB | 11:a9:542:ALA:O | 2.11 | 0.51 |
| 11:a9:802:ARG:O | 11:a9:804:ARG:N | 2.43 | 0.51 |
| 11:aA:93:LEU:CD1 | 11:aA:93:LEU:H | 2.24 | 0.51 |
| 4:M1:16:LYS:HB2 | 4:M1:46:VAL:HG22 | 1.93 | 0.51 |
| 12:F2:201:CYC:HMA2 | 12:F2:201:CYC:HB | 1.75 | 0.51 |
| 4:MA:93:LEU:HD21 | 4:MA:102:VAL:HG22 | 1.92 | 0.50 |
| 4:MA:170:PHE:HD1 | 4:MA:174:LEU:HD12 | 1.77 | 0.50 |
| 5:NA:29:HIS:HD2 | 5:NA:36:THR:HG23 | 1.76 | 0.50 |
| 2:G2:138:VAL:O | 2:G2:138:VAL:HG12 | 2.11 | 0.50 |
| 6:M2:283:VAL:HG12 | 6:M2:284:SER:N | 2.25 | 0.50 |
| 3:D4:150:ARG:HH11 | 2:C1:140:SER:HB3 | 1.75 | 0.50 |
| 2:N4:31:PHE:CG | 3:O4:34:SER:HB2 | 2.45 | 0.50 |
| 8:K5:79:ALA:C | 8:K5:81:CYS:N | 2.68 | 0.50 |
| 8:K5:154:ASP:HB3 | 1:V5:46:SER:HB3 | 1.93 | 0.50 |
| 3:Y4:88:ILE:HG13 | 3:Y4:89:ILE:N | 2.26 | 0.50 |
| 5:Z4:39:PRO:HG3 | 12:Z4:301:CYC:H3C | 1.92 | 0.50 |
| 12:J5:201:CYC:HB | 12:J5:201:CYC:HMA3 | 1.73 | 0.50 |
| 1:R5:86:ASP:CG | 1:R5:90:ARG:NE | 2.67 | 0.50 |
| 1:X5:59:ALA:O | 1:X5:60:LEU:HD23 | 2.11 | 0.50 |
| 1:Z5:59:ALA:O | 1:Z5:60:LEU:HD23 | 2.11 | 0.50 |
| 10:j5:56:ILE:CG2 | 10:j5:57:VAL:H | 2.22 | 0.50 |
| 10:j5:175:ASP:OD1 | 10:j5:175:ASP:N | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:j5:275:THR:HG23 | 10:j5:286:VAL:CG1 | 2.32 | 0.50 |
| 10:j5:1124:TYR:CG | 12:j5:1202:CYC:HAA1 | 2.46 | 0.50 |
| 10:k5:614:ARG:HG2 | 10:k5:614:ARG:NH1 | 2.21 | 0.50 |
| 8:O7:29:PHE:CZ | 8:O7:98:ALA:C | 2.76 | 0.50 |
| 8:O7:61:ILE:HG22 | 8:O7:62:ARG:HG2 | 1.93 | 0.50 |
| 1:B7:136:VAL:HA | 11:a9:563:PHE:CE1 | 2.46 | 0.50 |
| 8:G7:61:ILE:HG22 | 8:G7:62:ARG:HG2 | 1.93 | 0.50 |
| 8:g7:61:ILE:O | 11:aA:336:ILE:CB | 2.59 | 0.50 |
| 8:i7:126:VAL:O | 8:i7:126:VAL:HG12 | 2.11 | 0.50 |
| 1:j7:76:ARG:N | 8:e7:110:ILE:O | 2.43 | 0.50 |
| 1:T7:110:ASN:ND2 | 9:w7:57:PHE:CD2 | 2.79 | 0.50 |
| 1:V7:59:ALA:O | 1:V7:60:LEU:HD23 | 2.11 | 0.50 |
| 1:Z7:59:ALA:O | 1:Z7:60:LEU:HD23 | 2.11 | 0.50 |
| 8:c7:49:ARG:NH2 | 8:c7:140:LEU:HD21 | 2.24 | 0.50 |
| 8:m7:29:PHE:HE1 | 8:m7:99:GLY:N | 2.08 | 0.50 |
| 8:o7:116:TYR:HB3 | 8:o7:123:ILE:HG12 | 1.91 | 0.50 |
| 8:q7:75:GLU:CA | 11:aA:53:VAL:CG1 | 2.88 | 0.50 |
| 2:X8:15:GLN:HG2 | 4:M8:211:GLN:HE22 | 1.76 | 0.50 |
| 3:F8:84:ARG:CG | 11:a9:139:ILE:HG21 | 2.41 | 0.50 |
| 3:H8:81:ALA:HA | 3:H8:84:ARG:HH21 | 1.74 | 0.50 |
| 4:M9:16:LYS:HB2 | 4:M9:46:VAL:HG22 | 1.93 | 0.50 |
| 5:N9:21:ALA:HA | 5:N9:42:SER:O | 2.11 | 0.50 |
| 5:N9:29:HIS:HD2 | 5:N9:36:THR:HG23 | 1.76 | 0.50 |
| 2:E9:138:VAL:O | 2:E9:138:VAL:HG12 | 2.11 | 0.50 |
| 11:a9:95:ILE:HD13 | 11:a9:237:PHE:CD1 | 2.46 | 0.50 |
| 11:a9:403:THR:HB | 11:a9:441:ARG:HH21 | 1.76 | 0.50 |
| 11:a9:586:LEU:N | 11:a9:586:LEU:CD2 | 2.73 | 0.50 |
| 11:aA:25:GLU:HB3 | 11:aA:26:PRO:HD3 | 1.93 | 0.50 |
| 11:aA:358:PRO:HG2 | 11:aA:358:PRO:O | 2.11 | 0.50 |
| 11:aA:365:LYS:NZ | 11:aA:365:LYS:CB | 2.72 | 0.50 |
| 11:aA:667:THR:CG2 | 11:aA:800:THR:HG22 | 2.40 | 0.50 |
| 4:M1:232:VAL:HG21 | 3:V1:113:LEU:HA | 1.91 | 0.50 |
| 2:U1:138:VAL:HG12 | 2:U1:138:VAL:O | 2.11 | 0.50 |
| 1:Z:114:GLU:OE1 | 10:j5:6:THR:HB | 2.12 | 0.50 |
| 2:EA:138:VAL:HG12 | 2:EA:138:VAL:O | 2.11 | 0.50 |
| 12:FA:301:CYC:HB | 12:FA:301:CYC:HMA2 | 1.76 | 0.50 |
| 3:JA:88:ILE:HD13 | 11:aA:512:TYR:CE1 | 2.25 | 0.50 |
| 4:MA:22:SER:HB3 | 4:MA:23:PRO:CD | 2.41 | 0.50 |
| 5:NA:39:PRO:CB | 3:PA:116:THR:OG1 | 2.60 | 0.50 |
| 5:NA:57:MET:HE2 | 5:NA:67:ILE:HG13 | 1.92 | 0.50 |
| 12:TA:301:CYC:HB | 12:TA:301:CYC:HMA2 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 3:J2:87:GLU:OE1 | 6:M2:189:HIS:NE2 | 2.31 | 0.50 |
| 6:M2:205:GLU:OE1 | 6:M2:219:ARG:NH2 | 2.42 | 0.50 |
| 2:A3:65:TYR:O | 2:A3:71:GLN:CG | 2.54 | 0.50 |
| 2:A4:60:TYR:CB | 2:A4:67:THR:CG2 | 2.83 | 0.50 |
| 3:B4:113:LEU:HD13 | 4:M4:60:LYS:CE | 2.37 | 0.50 |
| 4:M3:16:LYS:HB2 | 4:M3:46:VAL:HG22 | 1.93 | 0.50 |
| 3:B1:85:ASP:OD1 | 12:B1:202:CYC:NA | 2.44 | 0.50 |
| 2:V4:138:VAL:O | 2:V4:138:VAL:HG12 | 2.11 | 0.50 |
| 3:F4:104:VAL:O | 3:F4:107:ASP:OD1 | 2.28 | 0.50 |
| 3:H4:108:ARG:NH2 | 11:aA:97:ALA:HB2 | 2.26 | 0.50 |
| 4:M4:20:THR:HG23 | 4:M4:67:LEU:HD11 | 1.92 | 0.50 |
| 4:M4:27:HIS:CG | 4:M4:34:ASP:HA | 2.43 | 0.50 |
| 4:M4:215:GLU:HB3 | 5:Z4:28:HIS:N | 2.26 | 0.50 |
| 8:M5:90:ARG:HA | 1:N5:18:TYR:CZ | 2.47 | 0.50 |
| 1:D5:59:ALA:O | 1:D5:60:LEU:HD23 | 2.11 | 0.50 |
| 8:G5:61:ILE:HG13 | 8:o7:68:PRO:CG | 2.39 | 0.50 |
| 8:I5:29:PHE:HE1 | 8:I5:99:GLY:N | 2.08 | 0.50 |
| 8:e5:4:LEU:HD23 | 8:e5:26:ILE:HD13 | 1.91 | 0.50 |
| 1:P5:114:GLU:HB3 | 10:k5:496:GLU:CG | 2.39 | 0.50 |
| 1:b5:18:TYR:CE2 | 10:k5:165:ARG:CG | 2.94 | 0.50 |
| 6:M6:75:LYS:HZ3 | 3:H6:2:GLN:NE2 | 2.08 | 0.50 |
| 10:j5:59:LYS:NZ | 10:j5:213:LEU:O | 2.45 | 0.50 |
| 10:j5:77:VAL:CG2 | 10:j5:141:GLU:CB | 2.89 | 0.50 |
| 10:j5:190:LEU:O | 10:j5:194:CYS:SG | 2.62 | 0.50 |
| 10:j5:194:CYS:CB | 12:j5:1201:CYC:HAC1 | 2.40 | 0.50 |
| 10:j5:867:VAL:O | 9:w7:43:ARG:NH2 | 2.23 | 0.50 |
| 10:j5:1125:ARG:HH22 | 1:t7:114:GLU:HB3 | 1.74 | 0.50 |
| 10:k5:549:LYS:C | 10:k5:549:LYS:CD | 2.84 | 0.50 |
| 10:k5:773:VAL:O | 10:k5:773:VAL:HG12 | 2.12 | 0.50 |
| 10:k5:929:PRO:CG | 1:D7:147:LYS:HG2 | 2.39 | 0.50 |
| 10:k5:1008:PHE:CG | 12:p7:201:CYC:OB | 2.64 | 0.50 |
| 12:H6:201:CYC:HMA2 | 12:H6:201:CYC:HB | 1.76 | 0.50 |
| 1:D7:59:ALA:O | 1:D7:60:LEU:HD23 | 2.11 | 0.50 |
| 8:E7:17:TYR:CE2 | 1:F7:90:ARG:HA | 2.46 | 0.50 |
| 1:N7:59:ALA:O | 1:N7:60:LEU:HD23 | 2.11 | 0.50 |
| 1:V7:76:ARG:HD3 | 8:W7:110:ILE:HD11 | 1.93 | 0.50 |
| 8:W7:17:TYR:CE2 | 1:X7:90:ARG:HA | 2.46 | 0.50 |
| 12:b7:201:CYC:OB | 9:x7:23:LEU:HB2 | 2.11 | 0.50 |
| 8:c7:26:ILE:O | 8:c7:30:VAL:HG13 | 2.10 | 0.50 |
| 8:c7:43:LEU:HD13 | 8:c7:141:LEU:HD21 | 1.94 | 0.50 |
| 2:E1:138:VAL:HG12 | 2:E1:138:VAL:O | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:B8:81:ALA:O | 12:B8:202:CYC:HMD3 | 2.10 | 0.50 |
| 3:B8:113:LEU:HB2 | 4:M8:60:LYS:CE | 2.35 | 0.50 |
| 8:s7:57:GLN:O | 8:s7:61:ILE:HD13 | 2.12 | 0.50 |
| 8:u7:56:ASP:N | 8:u7:56:ASP:OD1 | 2.37 | 0.50 |
| 8:u7:80:LEU:HD12 | 12:u7:201:CYC:HAD2 | 1.90 | 0.50 |
| 9:w7:15:LYS:O | 9:w7:15:LYS:HG3 | 2.11 | 0.50 |
| 4:M8:96:LYS:CE | 3:Q8:113:LEU:HD22 | 2.41 | 0.50 |
| 3:L9:51:ILE:HG21 | 3:L9:90:LEU:HD11 | 1.86 | 0.50 |
| 4:M9:74:LEU:O | 4:M9:77:LEU:CD1 | 2.59 | 0.50 |
| 5:N9:37:HIS:C | 5:N9:37:HIS:CD2 | 2.90 | 0.50 |
| 5:N9:54:LEU:CD1 | 12:T9:301:CYC:C1B | 2.89 | 0.50 |
| 5:Z8:29:HIS:CG | 5:Z8:31:TRP:CD1 | 2.99 | 0.50 |
| 5:Z8:29:HIS:NE2 | 5:Z8:33:GLY:O | 2.44 | 0.50 |
| 5:Z8:37:HIS:HB2 | 12:Z8:301:CYC:C4B | 2.41 | 0.50 |
| 11:a9:34:ILE:O | 11:a9:34:ILE:HG22 | 2.09 | 0.50 |
| 11:a9:252:ARG:NH2 | 11:a9:291:TYR:HB3 | 2.26 | 0.50 |
| 11:a9:588:VAL:CA | 11:a9:590:PRO:HD2 | 2.42 | 0.50 |
| 11:a9:802:ARG:CG | 11:a9:802:ARG:NH1 | 2.72 | 0.50 |
| 11:aA:586:LEU:N | 11:aA:586:LEU:CD2 | 2.73 | 0.50 |
| 11:aA:798:SER:CB | 12:aA:901:CYC:HMA1 | 2.30 | 0.50 |
| 4:M1:20:THR:HG23 | 4:M1:67:LEU:HD11 | 1.92 | 0.50 |
| 4:M1:269:SER:CA | 3:V1:111:ASN:HD22 | 2.24 | 0.50 |
| 2:YA:138:VAL:HG12 | 2:YA:138:VAL:O | 2.11 | 0.50 |
| 3:P1:115:GLU:HB2 | 5:N1:3:VAL:CG1 | 2.36 | 0.50 |
| 2:A1:138:VAL:HG12 | 2:A1:138:VAL:O | 2.11 | 0.50 |
| 2:G3:107:ASP:O | 3:L3:77:ARG:HD2 | 2.11 | 0.50 |
| 2:A3:138:VAL:HG12 | 2:A3:138:VAL:O | 2.11 | 0.50 |
| 3:B3:115:GLU:OE2 | 4:M3:78:GLY:CA | 2.59 | 0.50 |
| 3:B4:85:ASP:H | 12:B4:202:CYC:CAC | 2.22 | 0.50 |
| 5:N3:37:HIS:CD2 | 5:N3:37:HIS:C | 2.90 | 0.50 |
| 3:F4:108:ARG:NH2 | 4:M4:9:GLN:HE21 | 2.07 | 0.50 |
| 4:M4:22:SER:HB3 | 4:M4:23:PRO:CD | 2.41 | 0.50 |
| 4:M4:226:SER:CB | 3:Y4:85:ASP:N | 2.75 | 0.50 |
| 3:Q4:105:LEU:HD12 | 3:Q4:105:LEU:N | 2.27 | 0.50 |
| 8:O5:61:ILE:HG22 | 8:O5:62:ARG:HG2 | 1.93 | 0.50 |
| 3:Y4:113:LEU:O | 3:Y4:114:LYS:C | 2.54 | 0.50 |
| 8:C5:94:TYR:HB3 | 1:D5:9:ILE:HD13 | 1.94 | 0.50 |
| 8:I5:94:TYR:HB3 | 1:J5:9:ILE:HD13 | 1.93 | 0.50 |
| 12:V5:201:CYC:HB | 12:V5:201:CYC:HMA3 | 1.73 | 0.50 |
| 12:Z5:201:CYC:HBB2 | 10:k5:353:ASN:HB2 | 1.93 | 0.50 |
| 10:j5:19:THR:HB | 10:j5:173:ALA:HB1 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:j5:182:ASN:N | 10:j5:182:ASN:ND2 | 2.60 | 0.50 |
| 10:j5:216:ASP:HA | 10:j5:220:SER:HB2 | 1.94 | 0.50 |
| 10:j5:1150:TYR:CE1 | 11:aA:38:VAL:CG2 | 2.66 | 0.50 |
| 10:k5:1024:LYS:CD | 10:k5:1038:ARG:NH1 | 2.68 | 0.50 |
| 2:A6:138:VAL:HG12 | 2:A6:138:VAL:O | 2.11 | 0.50 |
| 2:I6:138:VAL:HG12 | 2:I6:138:VAL:O | 2.11 | 0.50 |
| 1:H7:59:ALA:O | 1:H7:60:LEU:HD23 | 2.11 | 0.50 |
| 8:K7:4:LEU:HD23 | 8:K7:26:ILE:CD1 | 2.38 | 0.50 |
| 8:K7:126:VAL:HG22 | 12:K7:201:CYC:H3C | 1.91 | 0.50 |
| 12:N7:201:CYC:HMD1 | 12:N7:201:CYC:NC | 2.09 | 0.50 |
| 12:T7:201:CYC:HB | 12:T7:201:CYC:HMA3 | 1.73 | 0.50 |
| 1:t7:75:THR:OG1 | 8:u7:110:ILE:O | 2.28 | 0.50 |
| 8:u7:23:LEU:C | 1:v7:38:VAL:HG21 | 2.36 | 0.50 |
| 3:F8:84:ARG:HH22 | 11:a9:143:SER:HB3 | 1.75 | 0.50 |
| 3:F8:112:GLY:HA3 | 4:M8:4:LEU:O | 2.11 | 0.50 |
| 3:L8:68:ARG:HB2 | 11:a9:82:GLN:CA | 2.39 | 0.50 |
| 4:M8:140:ARG:NH1 | 4:M8:204:ILE:O | 2.42 | 0.50 |
| 2:E9:152:ALA:HB1 | 2:I9:21:ASN:CG | 2.36 | 0.50 |
| 3:J9:119:ALA:C | 11:a9:365:LYS:NZ | 2.61 | 0.50 |
| 11:aA:490:ILE:N | 11:aA:490:ILE:HD13 | 2.26 | 0.50 |
| 11:aA:776:TYR:CB | 12:H1:201:CYC:HBA1 | 2.41 | 0.50 |
| 12:aA:902:CYC:CAB | 3:L1:88:ILE:HG21 | 2.41 | 0.50 |
| 4:M1:259:ARG:HG3 | 4:M1:259:ARG:HH21 | 1.75 | 0.50 |
| 1:A:16:GLY:C | 8:a5:90:ARG:CZ | 2.85 | 0.50 |
| 1:A:78:TYR:CE2 | 12:k5:1201:CYC:HAA1 | 2.46 | 0.50 |
| 2:AA:25:GLN:HG2 | 2:KA:33:ARG:CG | 2.38 | 0.50 |
| 3:JA:68:ARG:HB3 | 11:aA:353:ALA:HB2 | 1.93 | 0.50 |
| 4:MA:264:LYS:N | 3:VA:119:ALA:CB | 2.74 | 0.50 |
| 5:NA:1:MET:O | 5:NA:3:VAL:N | 2.43 | 0.50 |
| 2:S1:138:VAL:O | 2:S1:138:VAL:HG12 | 2.11 | 0.50 |
| 12:J3:202:CYC:HMA2 | 12:J3:202:CYC:HB | 1.76 | 0.50 |
| 12:H2:201:CYC:HBB3 | 6:M2:243:ALA:HA | 1.94 | 0.50 |
| 12:D3:202:CYC:HMA2 | 12:D3:202:CYC:HB | 1.76 | 0.50 |
| 2:Q3:138:VAL:HG12 | 2:Q3:138:VAL:O | 2.11 | 0.50 |
| 12:V3:201:CYC:HB | 12:V3:201:CYC:HMA2 | 1.76 | 0.50 |
| 12:H4:201:CYC:HMA2 | 12:H4:201:CYC:HB | 1.76 | 0.50 |
| 3:Y4:101:ASP:C | 3:Y4:103:SER:H | 2.19 | 0.50 |
| 12:B5:201:CYC:CBB | 9:z5:21:ARG:CA | 2.81 | 0.50 |
| 8:S5:61:ILE:HG22 | 8:S5:62:ARG:HG2 | 1.93 | 0.50 |
| 8:S5:90:ARG:N | 1:T5:18:TYR:OH | 2.44 | 0.50 |
| 8:U5:82:LEU:HD12 | 6:M6:34:ARG:HB2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:Z5:110:ASN:O | 10:k5:352:ILE:HD11 | 2.11 | 0.50 |
| 9:z5:6:LYS:HZ1 | 9:z5:29:THR:HG21 | 1.75 | 0.50 |
| 10:j5:190:LEU:HD21 | 12:j5:1201:CYC:C4D | 2.41 | 0.50 |
| 10:j5:213:LEU:HD12 | 10:j5:213:LEU:N | 2.26 | 0.50 |
| 10:j5:249:SER:HB2 | 10:j5:254:PRO:O | 2.10 | 0.50 |
| 10:j5:284:PRO:HD2 | 10:j5:326:GLY:C | 2.36 | 0.50 |
| 10:j5:802:VAL:O | 10:j5:802:VAL:HG12 | 2.10 | 0.50 |
| 10:j5:1006:ASP:OD1 | 10:j5:1065:HIS:CD2 | 2.64 | 0.50 |
| 10:j5:1018:LEU:HD11 | 10:j5:1035:PHE:HZ | 1.39 | 0.50 |
| 10:j5:1024:LYS:CD | 10:j5:1038:ARG:NH1 | 2.68 | 0.50 |
| 10:k5:803:LYS:HZ2 | 9:z7:43:ARG:NH1 | 2.06 | 0.50 |
| 10:k5:1141:SER:HB2 | 8:k7:106:GLU:CD | 2.36 | 0.50 |
| 8:O7:21:GLY:O | 8:O7:23:LEU:N | 2.44 | 0.50 |
| 8:g7:10:ASN:HD21 | 8:u7:10:ASN:HD22 | 1.58 | 0.50 |
| 8:g7:63:PRO:CG | 11:aA:333:GLN:O | 2.59 | 0.50 |
| 8:g7:109:ILE:HD13 | 8:g7:159:ALA:HB1 | 1.91 | 0.50 |
| 1:h7:52:ILE:HG22 | 1:h7:52:ILE:O | 2.11 | 0.50 |
| 1:j7:59:ALA:O | 1:j7:60:LEU:HD23 | 2.11 | 0.50 |
| 8:c7:96:ILE:CG1 | 8:c7:152:TYR:CE1 | 2.81 | 0.50 |
| 1:p7:59:ALA:O | 1:p7:60:LEU:HD23 | 2.11 | 0.50 |
| 8:s7:47:ARG:HD3 | 1:t7:18:TYR:CE1 | 2.46 | 0.50 |
| 9:w7:39:THR:O | 9:w7:39:THR:OG1 | 2.22 | 0.50 |
| 9:y7:11:ILE:CD1 | 9:y7:28:PHE:HE1 | 2.25 | 0.50 |
| 2:G8:138:VAL:HG12 | 2:G8:138:VAL:O | 2.11 | 0.50 |
| 3:H8:119:ALA:C | 11:a9:266:ASN:ND2 | 2.69 | 0.50 |
| 3:L8:68:ARG:HD2 | 11:a9:82:GLN:N | 1.90 | 0.50 |
| 12:M8:301:CYC:OC | 3:Y8:72:ASN:CG | 2.55 | 0.50 |
| 2:N8:10:ALA:O | 5:Z8:62:ARG:CZ | 2.59 | 0.50 |
| 2:Y9:138:VAL:O | 2:Y9:138:VAL:HG12 | 2.11 | 0.50 |
| 2:G1:107:ASP:CG | 3:L1:77:ARG:NH2 | 2.68 | 0.50 |
| 11:a9:632:ILE:N | 11:a9:632:ILE:HD12 | 2.27 | 0.50 |
| 4:M1:93:LEU:HD21 | 4:M1:102:VAL:HG22 | 1.92 | 0.50 |
| 1:A:18:TYR:OH | 8:a5:90:ARG:N | 2.44 | 0.50 |
| 12:Z:201:CYC:HMD1 | 12:Z:201:CYC:NC | 2.10 | 0.50 |
| 2:IA:19:LEU:HD13 | 3:JA:41:VAL:HG11 | 1.92 | 0.50 |
| 2:KA:24:LEU:CB | 12:LA:201:CYC:HAB2 | 2.34 | 0.50 |
| 12:LA:202:CYC:HMA2 | 12:LA:202:CYC:HB | 1.76 | 0.50 |
| 4:MA:188:LEU:HG | 3:VA:84:ARG:NE | 2.26 | 0.50 |
| 12:XA:201:CYC:HMA2 | 12:XA:201:CYC:HB | 1.76 | 0.50 |
| 2:G3:138:VAL:O | 2:G3:138:VAL:HG12 | 2.11 | 0.50 |
| 12:J3:202:CYC:CGD | 11:a9:802:ARG:NE | 2.69 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:H2:14:LEU:HG | 6:M2:69:ALA:HB2 | 1.93 | 0.50 |
| 12:H2:201:CYC:HMA1 | 6:M2:245:SER:OG | 2.11 | 0.50 |
| 12:B3:202:CYC:HMA2 | 12:B3:202:CYC:HB | 1.76 | 0.50 |
| 3:B4:86:MET:H | 12:B4:202:CYC:CAC | 2.23 | 0.50 |
| 4:M3:170:PHE:HD1 | 4:M3:174:LEU:HD12 | 1.77 | 0.50 |
| 4:M3:268:ARG:O | 3:V3:111:ASN:ND2 | 2.44 | 0.50 |
| 5:N3:1:MET:O | 5:N3:3:VAL:N | 2.44 | 0.50 |
| 3:B1:115:GLU:OE2 | 4:M1:78:GLY:CA | 2.59 | 0.50 |
| 2:E4:138:VAL:HG12 | 2:E4:138:VAL:O | 2.11 | 0.50 |
| 2:N4:115:GLU:OE1 | 5:Z4:33:GLY:N | 2.45 | 0.50 |
| 8:K5:101:VAL:C | 8:K5:103:PRO:HD2 | 2.37 | 0.50 |
| 1:L5:75:THR:HG22 | 8:G5:115:MET:SD | 2.51 | 0.50 |
| 1:B5:13:ASP:OD2 | 10:k5:556:GLY:HA3 | 2.12 | 0.50 |
| 8:E5:116:TYR:HB3 | 8:E5:123:ILE:HG12 | 1.93 | 0.50 |
| 8:G5:6:LYS:CE | 8:S5:21:GLY:HA3 | 2.42 | 0.50 |
| 8:G5:69:GLY:HA3 | 8:U5:64:ASP:OD1 | 2.12 | 0.50 |
| 1:R5:59:ALA:O | 1:R5:60:LEU:HD23 | 2.11 | 0.50 |
| 8:U5:29:PHE:CD1 | 8:U5:99:GLY:HA3 | 2.43 | 0.50 |
| 8:U5:57:GLN:O | 8:U5:61:ILE:HD13 | 2.12 | 0.50 |
| 6:M6:57:GLU:HA | 8:c7:76:LYS:NZ | 2.26 | 0.50 |
| 9:i5:56:LEU:N | 9:i5:56:LEU:CD1 | 2.73 | 0.50 |
| 10:j5:773:VAL:HG12 | 10:j5:773:VAL:O | 2.12 | 0.50 |
| 10:j5:937:GLU:O | 10:j5:937:GLU:HG3 | 2.00 | 0.50 |
| 10:j5:1008:PHE:CD1 | 12:v7:201:CYC:C4B | 2.94 | 0.50 |
| 10:j5:1023:SER:O | 10:j5:1027:ASN:HB2 | 2.12 | 0.50 |
| 10:k5:298:ARG:HH11 | 10:k5:298:ARG:HA | 1.76 | 0.50 |
| 10:k5:328:ILE:HG21 | 10:k5:336:ARG:CZ | 2.42 | 0.50 |
| 10:k5:450:ARG:HG3 | 10:k5:494:PRO:O | 2.10 | 0.50 |
| 10:k5:586:LEU:HD12 | 10:k5:607:LEU:HD23 | 1.77 | 0.50 |
| 10:k5:930:LEU:C | 1:D7:33:THR:CG2 | 2.53 | 0.50 |
| 10:k5:964:GLY:HA2 | 1:n7:69:GLY:CA | 2.35 | 0.50 |
| 10:k5:1118:THR:CG2 | 12:k5:1204:CYC:CMA | 2.88 | 0.50 |
| 8:M7:106:GLU:OE2 | 9:z7:68:GLY:HA3 | 2.10 | 0.50 |
| 1:T7:59:ALA:O | 1:T7:60:LEU:HD23 | 2.11 | 0.50 |
| 8:Y7:61:ILE:HG22 | 8:Y7:62:ARG:HG2 | 1.93 | 0.50 |
| 1:t7:75:THR:HB | 8:u7:111:GLY:O | 2.11 | 0.50 |
| 9:x7:11:ILE:CD1 | 9:x7:28:PHE:HE1 | 2.25 | 0.50 |
| 12:J8:201:CYC:HMA1 | 11:a9:176:ASN:ND2 | 2.20 | 0.50 |
| 4:M8:26:SER:CB | 11:a9:228:GLU:HG3 | 2.42 | 0.50 |
| 3:L9:41:VAL:HG21 | 3:L9:98:LEU:HD13 | 1.93 | 0.50 |
| 3:L9:83:LEU:CD1 | 2:G9:119:THR:CG2 | 2.86 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 12:L9:202:CYC:HB | 12:L9:202:CYC:HMA2 | 1.76 | 0.50 |
| 2:G9:138:VAL:HG12 | 2:G9:138:VAL:O | 2.11 | 0.50 |
| 11:a9:90:GLN:C | 11:a9:92:LYS:N | 2.70 | 0.50 |
| 4:M1:232:VAL:HG21 | 3:V1:113:LEU:HB2 | 1.94 | 0.50 |
| 2:OA:2:LYS:HE2 | 2:YA:22:THR:HB | 1.93 | 0.50 |
| 2:UA:138:VAL:HG12 | 2:UA:138:VAL:O | 2.11 | 0.50 |
| 2:Q1:138:VAL:HG12 | 2:Q1:138:VAL:O | 2.11 | 0.50 |
| 3:B4:109:CYS:HA | 12:B4:202:CYC:HMB2 | 1.93 | 0.50 |
| 2:Y3:138:VAL:HG12 | 2:Y3:138:VAL:O | 2.11 | 0.50 |
| 3:F4:113:LEU:H | 4:M4:5:THR:CB | 2.23 | 0.50 |
| 2:I4:14:SER:HA | 11:aA:170:PHE:CE2 | 2.45 | 0.50 |
| 3:L4:68:ARG:CG | 11:aA:82:GLN:N | 2.72 | 0.50 |
| 4:M4:170:PHE:HD1 | 4:M4:174:LEU:HD12 | 1.77 | 0.50 |
| 12:M4:301:CYC:CMD | 3:Y4:78:ARG:HG2 | 2.41 | 0.50 |
| 1:N5:87:TYR:CE2 | 10:k5:483:PHE:HE2 | 2.29 | 0.50 |
| 8:E5:131:ARG:CZ | 8:E5:157:VAL:HG11 | 2.42 | 0.50 |
| 1:f5:59:ALA:O | 1:f5:60:LEU:HD23 | 2.11 | 0.50 |
| 8:S5:90:ARG:N | 1:T5:18:TYR:CZ | 2.80 | 0.50 |
| 1:V5:114:GLU:CD | 10:j5:496:GLU:CB | 2.84 | 0.50 |
| 1:X5:86:ASP:O | 1:X5:90:ARG:HG3 | 2.12 | 0.50 |
| 8:Y5:65:VAL:CG2 | 8:Y5:66:VAL:N | 2.75 | 0.50 |
| 8:a5:61:ILE:HG22 | 8:a5:62:ARG:HG2 | 1.93 | 0.50 |
| 10:j5:43:LEU:N | 10:j5:43:LEU:HD22 | 2.26 | 0.50 |
| 10:j5:357:LEU:HD23 | 10:j5:401:LEU:HD13 | 1.93 | 0.50 |
| 10:j5:549:LYS:HG2 | 10:j5:551:MET:CG | 2.42 | 0.50 |
| 10:j5:965:GLN:C | 1:t7:69:GLY:HA2 | 2.37 | 0.50 |
| 10:j5:1051:GLU:HB3 | 10:j5:1052:PRO:HD3 | 1.93 | 0.50 |
| 10:j5:1118:THR:HG21 | 12:j5:1202:CYC:O2A | 2.07 | 0.50 |
| 10:k5:59:LYS:NZ | 10:k5:213:LEU:O | 2.45 | 0.50 |
| 10:k5:182:ASN:HB3 | 12:k5:1201:CYC:HAB2 | 1.93 | 0.50 |
| 10:k5:277:ILE:CG2 | 10:k5:284:PRO:CA | 2.87 | 0.50 |
| 10:k5:283:ARG:O | 10:k5:284:PRO:C | 2.53 | 0.50 |
| 10:k5:825:ASN:CB | 12:B7:201:CYC:OB | 2.51 | 0.50 |
| 10:k5:1017:ARG:O | 10:k5:1018:LEU:HG | 2.12 | 0.50 |
| 12:k5:1203:CYC:HMD1 | 12:k5:1203:CYC:NC | 2.09 | 0.50 |
| 12:H6:201:CYC:HB | 12:H6:201:CYC:CMA | 2.25 | 0.50 |
| 8:E7:4:LEU:HD21 | 8:E7:26:ILE:HD13 | 1.93 | 0.50 |
| 8:G7:23:LEU:HD22 | 1:H7:38:VAL:HG13 | 1.94 | 0.50 |
| 8:I7:57:GLN:O | 8:I7:61:ILE:HD13 | 2.12 | 0.50 |
| 8:I7:61:ILE:HG22 | 8:I7:62:ARG:HG2 | 1.93 | 0.50 |
| 8:M7:23:LEU:HD22 | 1:N7:38:VAL:HG13 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:c7:12:ASP:CA | 1:d7:94:TYR:CE2 | 2.94 | 0.50 |
| 8:o7:23:LEU:C | 1:p7:38:VAL:HG21 | 2.36 | 0.50 |
| 8:q7:57:GLN:O | 8:q7:61:ILE:HD13 | 2.12 | 0.50 |
| 4:M8:96:LYS:CD | 3:Q8:113:LEU:HD22 | 2.41 | 0.50 |
| 4:M8:170:PHE:HD1 | 4:M8:174:LEU:HD12 | 1.77 | 0.50 |
| 4:M8:188:LEU:HD12 | 4:M8:188:LEU:C | 2.35 | 0.50 |
| 4:M8:231:THR:H | 12:M8:301:CYC:HBB3 | 0.68 | 0.50 |
| 4:M8:232:VAL:CG2 | 3:Y8:113:LEU:HD21 | 2.41 | 0.50 |
| 12:N8:201:CYC:C2B | 3:Q8:76:ASN:HD21 | 2.24 | 0.50 |
| 3:Q8:122:THR:HG23 | 12:Z8:301:CYC:C1C | 2.41 | 0.50 |
| 4:M9:22:SER:HB3 | 4:M9:23:PRO:CD | 2.41 | 0.50 |
| 4:M9:51:ARG:HB3 | 4:M9:51:ARG:NH1 | 2.23 | 0.50 |
| 5:N9:1:MET:HB2 | 5:N9:3:VAL:HG23 | 1.90 | 0.50 |
| 2:O9:65:TYR:O | 2:O9:71:GLN:CG | 2.54 | 0.50 |
| 5:Z8:21:ALA:HA | 5:Z8:42:SER:O | 2.11 | 0.50 |
| 11:a9:89:ALA:CA | 11:a9:92:LYS:HZ2 | 2.25 | 0.50 |
| 11:aA:745:GLY:HA3 | 2:K1:15:GLN:C | 2.24 | 0.50 |
| 3:H1:78:ARG:CA | 12:H1:201:CYC:CMD | 2.90 | 0.50 |
| 12:H1:201:CYC:HMA2 | 12:H1:201:CYC:HB | 1.76 | 0.50 |
| 4:M1:5:THR:C | 4:M1:6:THR:HG1 | 2.06 | 0.50 |
| 4:M1:252:LEU:HD12 | 12:X1:201:CYC:O1D | 2.06 | 0.50 |
| 1:A:127:VAL:HG11 | 1:R5:15:GLN:OE1 | 2.12 | 0.50 |
| 1:Z:110:ASN:OD1 | 10:j5:462:TYR:CD1 | 2.53 | 0.50 |
| 3:FA:150:ARG:HD2 | 3:F9:150:ARG:HD3 | 1.93 | 0.50 |
| 3:HA:119:ALA:CA | 8:S7:49:ARG:NH1 | 2.50 | 0.50 |
| 3:JA:19:LEU:HD13 | 3:JA:24:LEU:CD2 | 2.41 | 0.50 |
| 2:KA:17:ARG:NH1 | 2:KA:17:ARG:CB | 2.73 | 0.50 |
| 2:KA:25:GLN:O | 2:KA:26:ALA:O | 2.28 | 0.50 |
| 5:NA:53:LEU:C | 12:TA:301:CYC:HBA1 | 2.29 | 0.50 |
| 2:QA:116:VAL:HG21 | 3:TA:76:ASN:O | 2.12 | 0.50 |
| 2:SA:42:ARG:HD2 | 2:X4:69:PRO:CB | 2.42 | 0.50 |
| 3:J3:84:ARG:CZ | 11:a9:669:ILE:C | 2.57 | 0.50 |
| 3:J3:120:LEU:CD2 | 11:a9:802:ARG:HB2 | 2.42 | 0.50 |
| 12:H2:201:CYC:HMA2 | 12:H2:201:CYC:HB | 1.76 | 0.50 |
| 12:J2:202:CYC:HB | 12:J2:202:CYC:CMA | 2.25 | 0.50 |
| 2:C3:138:VAL:O | 2:C3:138:VAL:HG12 | 2.11 | 0.50 |
| 3:B4:88:ILE:HG21 | 12:B4:202:CYC:HMB1 | 1.93 | 0.50 |
| 12:U4:201:CYC:HB | 12:U4:201:CYC:CMA | 2.25 | 0.50 |
| 3:J4:125:ARG:NH1 | 2:C2:69:PRO:CG | 2.69 | 0.50 |
| 12:L4:202:CYC:HMA2 | 12:L4:202:CYC:HB | 1.76 | 0.50 |
| 12:O4:201:CYC:CGA | 5:Z4:50:LEU:HD13 | 2.41 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:Q4:80:ALA:HB1 | 5:Z4:33:GLY:HA3 | 1.94 | 0.50 |
| 3:Q4:103:SER:C | 3:Q4:105:LEU:N | 2.67 | 0.50 |
| 8:M5:90:ARG:N | 1:N5:18:TYR:CZ | 2.80 | 0.50 |
| 8:C5:90:ARG:HD3 | 1:D5:18:TYR:CD1 | 2.47 | 0.50 |
| 1:H5:10:ASN:OD1 | 10:j5:557:VAL:HG22 | 2.11 | 0.50 |
| 8:c5:120:GLN:CD | 1:f5:53:LYS:HZ2 | 2.20 | 0.50 |
| 8:S5:41:GLN:CD | 1:D7:143:PRO:CD | 2.85 | 0.50 |
| 8:S5:57:GLN:O | 8:S5:61:ILE:HD13 | 2.12 | 0.50 |
| 8:U5:95:GLY:N | 8:U5:104:ILE:HD11 | 2.27 | 0.50 |
| 8:W5:57:GLN:O | 8:W5:61:ILE:HD13 | 2.12 | 0.50 |
| 9:z5:6:LYS:HG2 | 9:z5:55:LYS:CB | 2.39 | 0.50 |
| 10:j5:238:ARG:O | 10:j5:238:ARG:HD2 | 2.11 | 0.50 |
| 10:j5:1034:GLU:OE2 | 10:j5:1034:GLU:HA | 2.09 | 0.50 |
| 10:k5:190:LEU:CA | 10:k5:194:CYS:SG | 3.00 | 0.50 |
| 10:k5:540:LEU:HD11 | 10:k5:544:VAL:HG22 | 1.93 | 0.50 |
| 10:k5:966:SER:CA | 1:p7:14:VAL:HG13 | 2.14 | 0.50 |
| 10:k5:990:ARG:CZ | 10:k5:1026:LYS:NZ | 2.67 | 0.50 |
| 10:k5:1025:LEU:HD21 | 10:k5:1035:PHE:CA | 2.33 | 0.50 |
| 10:k5:1146:THR:CA | 1:p7:77:ARG:NH2 | 2.64 | 0.50 |
| 10:k5:1150:TYR:HE1 | 11:a9:38:VAL:CG1 | 2.24 | 0.50 |
| 3:F6:127:VAL:HA | 12:F6:201:CYC:HMC2 | 1.93 | 0.50 |
| 8:S7:64:ASP:OD2 | 8:I7:69:GLY:O | 2.30 | 0.50 |
| 8:C7:15:ALA:HA | 1:D7:90:ARG:NH1 | 2.27 | 0.50 |
| 8:I7:15:ALA:HA | 1:J7:90:ARG:NH1 | 2.27 | 0.50 |
| 8:i7:50:ILE:HG12 | 8:i7:137:ALA:CB | 2.41 | 0.50 |
| 8:e7:61:ILE:HG22 | 8:e7:62:ARG:HG2 | 1.93 | 0.50 |
| 12:D8:202:CYC:HMA2 | 12:D8:202:CYC:HB | 1.76 | 0.50 |
| 8:s7:15:ALA:HA | 1:t7:90:ARG:NH1 | 2.27 | 0.50 |
| 8:s7:61:ILE:HG22 | 8:s7:62:ARG:HG2 | 1.93 | 0.50 |
| 3:F8:112:GLY:C | 4:M8:5:THR:HA | 2.36 | 0.50 |
| 3:O8:111:ASN:O | 5:Z8:67:ILE:HB | 2.12 | 0.50 |
| 12:O8:201:CYC:HMA2 | 12:O8:201:CYC:HB | 1.76 | 0.50 |
| 4:M9:170:PHE:HD1 | 4:M9:174:LEU:HD12 | 1.76 | 0.50 |
| 4:M9:205:ASP:OD2 | 5:N9:52:ARG:CZ | 2.59 | 0.50 |
| 3:H9:117:TYR:CE1 | 12:H9:202:CYC:C4A | 2.94 | 0.50 |
| 2:G1:107:ASP:N | 3:L1:77:ARG:NH2 | 2.60 | 0.50 |
| 2:G1:138:VAL:O | 2:G1:138:VAL:HG12 | 2.11 | 0.50 |
| 11:a9:581:ARG:C | 11:a9:581:ARG:CD | 2.85 | 0.50 |
| 11:aA:595:ARG:CG | 11:aA:596:THR:O | 2.55 | 0.50 |
| 11:aA:731:GLN:NE2 | 12:aA:902:CYC:HAA1 | 2.27 | 0.50 |
| 11:aA:742:GLN:HB3 | 3:L1:88:ILE:HD11 | 1.85 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 4:M1:245:ASP:OD2 | 3:X1:108:ARG:HB3 | 2.11 | 0.50 |
| 4:M1:252:LEU:CD1 | 3:X1:77:ARG:NH1 | 2.75 | 0.50 |
| 5:NA:21:ALA:HA | 5:NA:42:SER:O | 2.11 | 0.50 |
| 2:QA:145:GLN:HG3 | 12:VA:202:CYC:HMA3 | 1.93 | 0.50 |
| 2:O1:34:ALA:HB1 | 3:P1:31:VAL:HG21 | 1.92 | 0.50 |
| 2:K3:13:ASP:CG | 11:a9:741:TYR:OH | 2.51 | 0.50 |
| 6:M2:127:SER:HA | 12:F2:201:CYC:CGA | 2.38 | 0.50 |
| 3:L3:88:ILE:HG21 | 12:L3:202:CYC:CAB | 2.41 | 0.50 |
| 4:M3:245:ASP:OD2 | 3:X3:108:ARG:HB3 | 2.11 | 0.50 |
| 2:O3:138:VAL:O | 2:O3:138:VAL:HG12 | 2.11 | 0.50 |
| 4:M4:16:LYS:HB2 | 4:M4:46:VAL:HG22 | 1.93 | 0.50 |
| 4:M4:51:ARG:HB3 | 4:M4:51:ARG:NH1 | 2.23 | 0.50 |
| 4:M4:232:VAL:CA | 12:M4:301:CYC:HBB3 | 2.39 | 0.50 |
| 2:P4:138:VAL:HG12 | 2:P4:138:VAL:O | 2.11 | 0.50 |
| 3:Q4:52:ILE:CD1 | 3:Q4:87:GLU:HA | 2.41 | 0.50 |
| 8:M5:90:ARG:N | 1:N5:18:TYR:OH | 2.44 | 0.50 |
| 12:B5:201:CYC:HAA1 | 9:z5:26:THR:HG21 | 1.89 | 0.50 |
| 1:F5:59:ALA:O | 1:F5:60:LEU:HD23 | 2.11 | 0.50 |
| 8:G5:65:VAL:CG2 | 8:G5:66:VAL:N | 2.75 | 0.50 |
| 8:c5:65:VAL:CG2 | 8:c5:66:VAL:N | 2.75 | 0.50 |
| 1:P5:59:ALA:O | 1:P5:60:LEU:HD23 | 2.11 | 0.50 |
| 8:S5:90:ARG:HA | 1:T5:18:TYR:CZ | 2.47 | 0.50 |
| 1:T5:59:ALA:O | 1:T5:60:LEU:HD23 | 2.11 | 0.50 |
| 1:V5:114:GLU:CD | 10:j5:496:GLU:HB2 | 2.36 | 0.50 |
| 8:W5:17:TYR:CB | 1:X5:45:SER:CB | 2.78 | 0.50 |
| 12:L6:201:CYC:HB | 12:L6:201:CYC:CMA | 2.25 | 0.50 |
| 6:M6:243:ALA:HA | 12:H6:201:CYC:HBB3 | 1.94 | 0.50 |
| 10:j5:1017:ARG:O | 10:j5:1018:LEU:HG | 2.12 | 0.50 |
| 10:j5:1024:LYS:HD2 | 10:j5:1038:ARG:HH12 | 1.73 | 0.50 |
| 10:j5:1153:VAL:HG23 | 1:v7:125:ALA:HA | 1.91 | 0.50 |
| 10:k5:19:THR:HB | 10:k5:173:ALA:HB1 | 1.93 | 0.50 |
| 10:k5:56:ILE:CG2 | 10:k5:57:VAL:H | 2.23 | 0.50 |
| 10:k5:289:SER:O | 10:k5:289:SER:OG | 2.19 | 0.50 |
| 10:k5:325:ASN:ND2 | 10:k5:325:ASN:C | 2.69 | 0.50 |
| 10:k5:722:ILE:O | 10:k5:722:ILE:HG22 | 2.11 | 0.50 |
| 10:k5:863:ILE:O | 10:k5:863:ILE:HG22 | 2.11 | 0.50 |
| 10:k5:925:ILE:HD12 | 10:k5:925:ILE:C | 2.36 | 0.50 |
| 10:k5:1009:ALA:CB | 1:p7:87:TYR:OH | 2.54 | 0.50 |
| 10:k5:1117:PRO:O | 10:k5:1117:PRO:HG2 | 2.12 | 0.50 |
| 2:C6:138:VAL:HG12 | 2:C6:138:VAL:O | 2.11 | 0.50 |
| 8:O7:35:ARG:NH2 | 8:O7:145:ASP:OD1 | 2.42 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:O7:95:GLY:N | 8:O7:104:ILE:HD11 | 2.27 | 0.50 |
| 8:C7:47:ARG:HD3 | 1:D7:18:TYR:CE1 | 2.46 | 0.50 |
| 12:F7:201:CYC:HMD1 | 12:F7:201:CYC:NC | 2.09 | 0.50 |
| 8:i7:50:ILE:HG12 | 8:i7:137:ALA:CA | 2.42 | 0.50 |
| 8:k7:66:VAL:CG1 | 11:a9:61:TYR:CE1 | 2.94 | 0.50 |
| 8:U7:57:GLN:O | 8:U7:61:ILE:HD13 | 2.12 | 0.50 |
| 8:U7:61:ILE:HG22 | 8:U7:62:ARG:HG2 | 1.93 | 0.50 |
| 8:a7:61:ILE:O | 11:a9:336:ILE:CB | 2.55 | 0.50 |
| 8:a7:95:GLY:N | 8:a7:104:ILE:HD11 | 2.27 | 0.50 |
| 2:A8:2:LYS:HE2 | 2:K8:22:THR:HB | 1.93 | 0.50 |
| 1:l7:68:PRO:CB | 1:n7:14:VAL:C | 2.67 | 0.50 |
| 8:o7:2:SER:CB | 1:p7:5:ILE:CG2 | 2.80 | 0.50 |
| 8:u7:97:VAL:HG22 | 1:v7:19:LEU:HD12 | 1.91 | 0.50 |
| 12:H8:201:CYC:CBB | 11:a9:259:ALA:HB2 | 2.25 | 0.50 |
| 2:N8:138:VAL:HG12 | 2:N8:138:VAL:O | 2.11 | 0.50 |
| 4:M9:160:THR:C | 3:V9:108:ARG:HG2 | 2.37 | 0.50 |
| 5:N9:39:PRO:CB | 3:P9:116:THR:OG1 | 2.60 | 0.50 |
| 3:D9:68:ARG:CZ | 3:X9:68:ARG:HH22 | 2.25 | 0.50 |
| 12:F9:301:CYC:HB | 12:F9:301:CYC:HMA2 | 1.76 | 0.50 |
| 3:H9:113:LEU:HD21 | 12:H9:202:CYC:HMB3 | 1.89 | 0.50 |
| 11:aA:548:LEU:C | 11:aA:551:PRO:HD2 | 2.37 | 0.50 |
| 4:M1:160:THR:HG21 | 4:M1:257:GLN:CB | 2.29 | 0.50 |
| 12:D2:201:CYC:HMA2 | 12:D2:201:CYC:HB | 1.76 | 0.50 |
| 3:FA:151:GLY:C | 3:F9:150:ARG:HH22 | 2.09 | 0.50 |
| 3:JA:107:ASP:O | 11:aA:517:ALA:HB1 | 2.11 | 0.50 |
| 5:NA:26:LEU:CD2 | 5:NA:26:LEU:C | 2.85 | 0.50 |
| 2:QA:120:PHE:HZ | 3:TA:60:PHE:CE2 | 2.29 | 0.50 |
| 12:VA:201:CYC:CMA | 12:VA:201:CYC:HB | 2.25 | 0.50 |
| 2:A4:138:VAL:HG12 | 2:A4:138:VAL:O | 2.11 | 0.50 |
| 2:T4:111:ALA:CB | 4:M4:87:ILE:HG21 | 2.40 | 0.50 |
| 12:W4:201:CYC:HMA2 | 12:W4:201:CYC:HB | 1.76 | 0.50 |
| 2:G4:138:VAL:O | 2:G4:138:VAL:HG12 | 2.11 | 0.50 |
| 3:H4:84:ARG:NE | 11:aA:131:TYR:CB | 2.75 | 0.50 |
| 3:L4:70:GLY:O | 3:L4:71:GLY:O | 2.30 | 0.50 |
| 4:M4:226:SER:OG | 3:Y4:84:ARG:C | 2.54 | 0.50 |
| 3:O4:119:ALA:CB | 5:Z4:72:GLU:N | 2.74 | 0.50 |
| 8:K5:161:GLN:NE2 | 1:V5:49:THR:CG2 | 2.70 | 0.50 |
| 8:A5:12:ASP:CG | 1:B5:91:TYR:HE1 | 2.18 | 0.50 |
| 8:A5:64:ASP:OD1 | 8:A5:65:VAL:N | 2.45 | 0.50 |
| 8:E5:151:PHE:HE1 | 1:P5:42:ALA:CB | 2.24 | 0.50 |
| 8:I5:95:GLY:N | 8:I5:104:ILE:HD11 | 2.27 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:C1:138:VAL:O | 2:C1:138:VAL:HG12 | 2.11 | 0.50 |
| 8:c5:23:LEU:HD22 | 1:d5:38:VAL:HG13 | 1.94 | 0.50 |
| 8:e5:19:SER:HB3 | 8:e5:22:GLU:HB2 | 1.93 | 0.50 |
| 8:e5:95:GLY:N | 8:e5:104:ILE:HD11 | 2.27 | 0.50 |
| 12:P5:201:CYC:HB | 12:P5:201:CYC:HMA3 | 1.73 | 0.50 |
| 1:Z5:67:ARG:NH2 | 10:k5:708:GLY:HA3 | 2.26 | 0.50 |
| 12:Z5:201:CYC:HMD1 | 12:Z5:201:CYC:NC | 2.09 | 0.50 |
| 8:a5:25:ARG:C | 8:a5:27:LYS:H | 2.19 | 0.50 |
| 8:a5:57:GLN:O | 8:a5:61:ILE:HD13 | 2.12 | 0.50 |
| 1:b5:31:PHE:CG | 10:k5:50:GLY:HA3 | 2.47 | 0.50 |
| 8:A7:57:GLN:O | 8:A7:61:ILE:HD13 | 2.12 | 0.50 |
| 10:j5:325:ASN:ND2 | 10:j5:325:ASN:C | 2.69 | 0.50 |
| 10:j5:501:ILE:CD1 | 10:j5:501:ILE:C | 2.85 | 0.50 |
| 10:j5:605:ARG:O | 10:j5:605:ARG:HG2 | 2.11 | 0.50 |
| 10:k5:238:ARG:CD | 10:k5:238:ARG:C | 2.85 | 0.50 |
| 10:k5:346:GLU:O | 10:k5:346:GLU:HG3 | 2.07 | 0.50 |
| 10:k5:549:LYS:HG2 | 10:k5:551:MET:CG | 2.42 | 0.50 |
| 1:R7:59:ALA:O | 1:R7:60:LEU:HD23 | 2.11 | 0.50 |
| 1:h7:59:ALA:O | 1:h7:60:LEU:HD23 | 2.11 | 0.50 |
| 8:i7:4:LEU:HD21 | 8:i7:26:ILE:HD13 | 1.93 | 0.50 |
| 8:W7:57:GLN:O | 8:W7:61:ILE:HD13 | 2.12 | 0.50 |
| 8:Y7:106:GLU:OE2 | 9:x7:68:GLY:O | 2.30 | 0.50 |
| 1:b7:52:ILE:HG22 | 1:b7:52:ILE:O | 2.11 | 0.50 |
| 2:E8:14:SER:C | 11:a9:163:ASP:OD2 | 2.55 | 0.50 |
| 8:q7:61:ILE:HG22 | 8:q7:62:ARG:HG2 | 1.93 | 0.50 |
| 8:s7:29:PHE:CD1 | 8:s7:99:GLY:HA3 | 2.43 | 0.50 |
| 8:s7:95:GLY:N | 8:s7:104:ILE:HD11 | 2.27 | 0.50 |
| 4:M8:96:LYS:HD3 | 3:Q8:113:LEU:CD2 | 2.42 | 0.50 |
| 4:M8:190:ARG:HH12 | 4:M8:202:SER:HB2 | 1.68 | 0.50 |
| 12:M8:301:CYC:HMA2 | 12:M8:301:CYC:HB | 1.76 | 0.50 |
| 2:N8:14:SER:CA | 5:Z8:62:ARG:CD | 2.90 | 0.50 |
| 3:O8:107:ASP:OD2 | 5:Z8:66:ARG:HD2 | 2.05 | 0.50 |
| 12:O8:201:CYC:CMA | 12:O8:201:CYC:HB | 2.25 | 0.50 |
| 3:L9:44:ILE:CG2 | 3:L9:90:LEU:CD2 | 2.84 | 0.50 |
| 4:M9:262:ASP:OD1 | 4:M9:263:PRO:HD2 | 2.12 | 0.50 |
| 11:a9:290:ASP:O | 11:a9:291:TYR:CE1 | 2.56 | 0.50 |
| 11:a9:327:SER:O | 11:a9:329:ASN:N | 2.45 | 0.50 |
| 11:a9:595:ARG:HG3 | 11:a9:596:THR:C | 2.36 | 0.50 |
| 11:aA:56:ILE:HD11 | 11:aA:612:TYR:CZ | 2.38 | 0.50 |
| 11:aA:327:SER:C | 11:aA:329:ASN:N | 2.67 | 0.50 |
| 11:aA:823:ILE:HG13 | 3:L1:75:PRO:CD | 2.37 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:N1:50:LEU:C | 5:N1:50:LEU:CD1 | 2.84 | 0.50 |
| 2:C2:138:VAL:O | 2:C2:138:VAL:HG12 | 2.11 | 0.50 |
| 4:MA:211:GLN:O | 5:NA:28:HIS:CE1 | 2.64 | 0.49 |
| 2:OA:60:TYR:CE1 | 2:OA:73:GLY:HA3 | 2.47 | 0.49 |
| 2:O1:138:VAL:O | 2:O1:138:VAL:HG12 | 2.11 | 0.49 |
| 2:A1:2:LYS:HE2 | 2:K1:22:THR:HB | 1.93 | 0.49 |
| 2:I2:138:VAL:HG12 | 2:I2:138:VAL:O | 2.11 | 0.49 |
| 2:K2:138:VAL:O | 2:K2:138:VAL:HG12 | 2.11 | 0.49 |
| 6:M2:45:ILE:HD11 | 8:i7:78:THR:CG2 | 2.41 | 0.49 |
| 12:N2:101:CYC:HB | 12:N2:101:CYC:CMA | 2.25 | 0.49 |
| 12:S4:202:CYC:HMA2 | 12:S4:202:CYC:HB | 1.76 | 0.49 |
| 4:M4:230:GLN:CG | 4:M4:231:THR:O | 2.60 | 0.49 |
| 3:Y4:85:ASP:HA | 3:Y4:88:ILE:CG1 | 2.38 | 0.49 |
| 3:Y4:113:LEU:HD13 | 3:Y4:117:TYR:HB2 | 1.94 | 0.49 |
| 12:B5:201:CYC:HB | 12:B5:201:CYC:CMA | 1.99 | 0.49 |
| 8:C5:27:LYS:C | 8:C5:30:VAL:HG22 | 2.36 | 0.49 |
| 1:D5:74:THR:OG1 | 1:D5:77:ARG:CD | 2.59 | 0.49 |
| 8:G5:53:GLN:O | 8:G5:53:GLN:HG3 | 2.11 | 0.49 |
| 8:I5:102:THR:CB | 8:I5:103:PRO:HD3 | 2.33 | 0.49 |
| 8:c5:57:GLN:O | 8:c5:61:ILE:HD13 | 2.12 | 0.49 |
| 6:M6:271:VAL:HG21 | 1:d7:127:VAL:CG1 | 2.41 | 0.49 |
| 10:j5:549:LYS:C | 10:j5:549:LYS:CD | 2.84 | 0.49 |
| 10:j5:879:ASP:OD1 | 9:w7:25:ASN:CG | 2.55 | 0.49 |
| 10:k5:216:ASP:HA | 10:k5:220:SER:CB | 2.42 | 0.49 |
| 10:k5:238:ARG:O | 10:k5:238:ARG:HD2 | 2.11 | 0.49 |
| 10:k5:289:SER:HB2 | 10:k5:292:GLU:OE2 | 2.10 | 0.49 |
| 10:k5:985:ALA:O | 10:k5:988:ALA:CB | 2.60 | 0.49 |
| 8:O7:15:ALA:HA | 1:P7:90:ARG:NH1 | 2.27 | 0.49 |
| 8:O7:21:GLY:C | 8:O7:23:LEU:N | 2.68 | 0.49 |
| 8:O7:52:LYS:HE3 | 11:aA:29:ARG:CZ | 2.33 | 0.49 |
| 1:P7:59:ALA:O | 1:P7:60:LEU:HD23 | 2.11 | 0.49 |
| 8:E7:128:GLU:HA | 8:E7:128:GLU:OE1 | 2.12 | 0.49 |
| 8:K7:128:GLU:HA | 8:K7:128:GLU:OE1 | 2.12 | 0.49 |
| 8:i7:54:ALA:HB2 | 8:i7:133:MET:CA | 2.42 | 0.49 |
| 1:j7:77:ARG:HH22 | 9:y7:63:ALA:CB | 2.05 | 0.49 |
| 8:k7:23:LEU:HD22 | 1:l7:38:VAL:HG13 | 1.94 | 0.49 |
| 8:U7:15:ALA:HB2 | 9:w7:20:GLY:HA2 | 1.94 | 0.49 |
| 8:U7:29:PHE:CD1 | 8:U7:99:GLY:HA3 | 2.43 | 0.49 |
| 8:W7:4:LEU:HD21 | 8:W7:26:ILE:HD13 | 1.93 | 0.49 |
| 1:X7:59:ALA:O | 1:X7:60:LEU:HD23 | 2.11 | 0.49 |
| 8:a7:90:ARG:NE | 1:b7:16:GLY:O | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:a7:90:ARG:NH2 | 1:b7:16:GLY:HA2 | 2.26 | 0.49 |
| 8:e7:57:GLN:O | 8:e7:61:ILE:HD13 | 2.12 | 0.49 |
| 8:u7:4:LEU:HD23 | 8:u7:26:ILE:CD1 | 2.38 | 0.49 |
| 8:u7:94:TYR:CE1 | 1:v7:18:TYR:HA | 2.47 | 0.49 |
| 9:z7:15:LYS:O | 9:z7:15:LYS:HG3 | 2.11 | 0.49 |
| 3:F8:106:GLU:O | 4:M8:6:THR:C | 2.54 | 0.49 |
| 4:M8:22:SER:HB3 | 4:M8:23:PRO:CD | 2.41 | 0.49 |
| 4:M8:61:ASN:O | 4:M8:63:GLY:N | 2.40 | 0.49 |
| 4:M8:226:SER:OG | 3:Y8:85:ASP:HA | 2.11 | 0.49 |
| 12:M8:301:CYC:CMA | 12:M8:301:CYC:HB | 2.25 | 0.49 |
| 4:M9:21:LEU:HD12 | 4:M9:21:LEU:C | 2.37 | 0.49 |
| 4:M9:41:ASN:HD21 | 3:B9:119:ALA:HB2 | 1.76 | 0.49 |
| 5:N9:38:GLU:HB3 | 5:N9:41:GLN:HE21 | 1.77 | 0.49 |
| 5:N9:50:LEU:C | 5:N9:50:LEU:CD1 | 2.84 | 0.49 |
| 12:Z8:301:CYC:HMD1 | 12:Z8:301:CYC:NC | 2.12 | 0.49 |
| 3:J9:19:LEU:HD13 | 3:J9:24:LEU:CD2 | 2.41 | 0.49 |
| 2:W9:138:VAL:HG12 | 2:W9:138:VAL:O | 2.11 | 0.49 |
| 11:a9:379:LEU:HD13 | 11:a9:391:VAL:CG2 | 2.30 | 0.49 |
| 11:a9:816:LEU:C | 11:a9:816:LEU:CD2 | 2.85 | 0.49 |
| 11:aA:327:SER:O | 11:aA:329:ASN:N | 2.45 | 0.49 |
| 11:aA:633:THR:O | 11:aA:633:THR:OG1 | 2.29 | 0.49 |
| 2:A2:138:VAL:HG12 | 2:A2:138:VAL:O | 2.11 | 0.49 |
| 1:A:76:ARG:CA | 10:k5:261:ILE:HD11 | 2.42 | 0.49 |
| 1:A:110:ASN:O | 10:k5:434:TRP:HA | 2.12 | 0.49 |
| 1:Z:131:GLN:CD | 1:X5:17:LYS:NZ | 2.65 | 0.49 |
| 12:HA:202:CYC:HMA2 | 12:HA:202:CYC:HB | 1.76 | 0.49 |
| 3:JA:19:LEU:HD13 | 3:JA:24:LEU:HG | 1.94 | 0.49 |
| 2:KA:138:VAL:O | 2:KA:138:VAL:HG12 | 2.11 | 0.49 |
| 4:MA:133:ARG:HD2 | 12:RA:201:CYC:O2A | 2.11 | 0.49 |
| 5:NA:54:LEU:HB2 | 12:TA:301:CYC:CGA | 2.42 | 0.49 |
| 2:QA:23:GLU:OE2 | 2:UA:2:LYS:CE | 2.60 | 0.49 |
| 12:VA:201:CYC:HB | 12:VA:201:CYC:HMA2 | 1.76 | 0.49 |
| 12:D4:202:CYC:CMA | 12:D4:202:CYC:HB | 2.26 | 0.49 |
| 12:D4:202:CYC:HB | 12:D4:202:CYC:HMA2 | 1.76 | 0.49 |
| 12:L3:202:CYC:HAA1 | 11:a9:731:GLN:NE2 | 2.27 | 0.49 |
| 4:M3:232:VAL:HG21 | 3:V3:113:LEU:HB2 | 1.94 | 0.49 |
| 4:M3:274:VAL:CG1 | 2:U3:111:ALA:HB1 | 2.42 | 0.49 |
| 5:N3:31:TRP:NE1 | 2:S3:16:GLY:HA2 | 2.25 | 0.49 |
| 12:R3:201:CYC:HB | 12:R3:201:CYC:HMA2 | 1.76 | 0.49 |
| 2:W3:138:VAL:HG12 | 2:W3:138:VAL:O | 2.11 | 0.49 |
| 12:S4:202:CYC:HB | 12:S4:202:CYC:CMA | 2.25 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:T4:138:VAL:HG12 | 2:T4:138:VAL:O | 2.11 | 0.49 |
| 3:F4:113:LEU:N | 4:M4:5:THR:CB | 2.76 | 0.49 |
| 3:F4:120:LEU:HD11 | 11:aA:147:ASN:ND2 | 2.27 | 0.49 |
| 12:F4:202:CYC:HMA2 | 12:F4:202:CYC:HB | 1.76 | 0.49 |
| 4:M4:222:ARG:HH11 | 4:M4:222:ARG:CG | 2.13 | 0.49 |
| 4:M4:262:ASP:OD1 | 4:M4:263:PRO:HD2 | 2.12 | 0.49 |
| 2:N4:60:TYR:CE1 | 2:N4:73:GLY:HA3 | 2.47 | 0.49 |
| 2:R4:138:VAL:O | 2:R4:138:VAL:HG12 | 2.11 | 0.49 |
| 8:K5:102:THR:N | 8:K5:103:PRO:CD | 2.74 | 0.49 |
| 8:M5:61:ILE:HG22 | 8:M5:62:ARG:HG2 | 1.93 | 0.49 |
| 8:O5:24:ASP:O | 8:O5:26:ILE:N | 2.46 | 0.49 |
| 8:G5:108:GLY:HA2 | 12:G5:201:CYC:HAB1 | 1.94 | 0.49 |
| 1:J5:38:VAL:O | 1:J5:39:ARG:O | 2.31 | 0.49 |
| 8:c5:114:GLU:CD | 10:j5:312:TYR:C | 2.80 | 0.49 |
| 8:e5:61:ILE:HG22 | 8:e5:62:ARG:HG2 | 1.93 | 0.49 |
| 8:Q5:8:ILE:HG23 | 1:R5:94:TYR:CG | 2.46 | 0.49 |
| 8:Q5:17:TYR:CD2 | 1:R5:93:THR:CG2 | 2.92 | 0.49 |
| 8:S5:90:ARG:HB2 | 1:T5:18:TYR:CZ | 2.48 | 0.49 |
| 1:X5:65:LEU:HD12 | 10:j5:706:PRO:HG2 | 1.89 | 0.49 |
| 1:Z5:28:LYS:CE | 1:t7:143:PRO:HB3 | 2.22 | 0.49 |
| 3:L6:70:GLY:HA3 | 6:M6:67:GLY:HA2 | 1.91 | 0.49 |
| 6:M6:259:THR:O | 6:M6:262:ASP:N | 2.22 | 0.49 |
| 9:i5:8:THR:HG22 | 9:i5:52:LEU:HB2 | 1.93 | 0.49 |
| 10:j5:277:ILE:CG2 | 10:j5:284:PRO:CA | 2.87 | 0.49 |
| 10:j5:309:LEU:CD1 | 10:j5:342:LEU:HD13 | 2.41 | 0.49 |
| 10:j5:328:ILE:HG21 | 10:j5:336:ARG:CZ | 2.42 | 0.49 |
| 10:j5:346:GLU:O | 10:j5:346:GLU:HG3 | 2.07 | 0.49 |
| 10:j5:492:ILE:HG22 | 10:j5:492:ILE:O | 2.11 | 0.49 |
| 10:j5:951:MET:HE1 | 10:j5:955:LEU:CD2 | 2.42 | 0.49 |
| 10:j5:1105:ILE:HD13 | 10:j5:1115:ARG:HH21 | 1.75 | 0.49 |
| 10:k5:501:ILE:CD1 | 10:k5:501:ILE:C | 2.85 | 0.49 |
| 10:k5:1151:GLN:C | 1:p7:122:PRO:HB3 | 2.36 | 0.49 |
| 12:F6:201:CYC:HB | 12:F6:201:CYC:CMA | 2.25 | 0.49 |
| 1:P7:76:ARG:CA | 8:Q7:110:ILE:O | 2.60 | 0.49 |
| 8:M7:57:GLN:O | 8:M7:61:ILE:HD13 | 2.12 | 0.49 |
| 8:g7:95:GLY:N | 8:g7:104:ILE:HD11 | 2.27 | 0.49 |
| 12:h7:201:CYC:OB | 9:y7:23:LEU:HB2 | 2.11 | 0.49 |
| 1:V7:76:ARG:CA | 8:W7:110:ILE:O | 2.60 | 0.49 |
| 3:B8:111:ASN:H | 4:M8:60:LYS:HD2 | 1.77 | 0.49 |
| 8:s7:21:GLY:C | 8:s7:23:LEU:H | 2.21 | 0.49 |
| 3:U8:114:LYS:HZ1 | 4:M8:13:LYS:HD3 | 1.32 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:X8:69:PRO:CB | 2:S9:42:ARG:HD2 | 2.42 | 0.49 |
| 12:F8:202:CYC:CMA | 12:F8:202:CYC:HB | 2.25 | 0.49 |
| 4:M8:262:ASP:OD1 | 4:M8:263:PRO:HD2 | 2.12 | 0.49 |
| 2:N8:60:TYR:CE1 | 2:N8:73:GLY:HA3 | 2.47 | 0.49 |
| 4:M9:133:ARG:HD2 | 12:R9:201:CYC:O2A | 2.11 | 0.49 |
| 4:M9:160:THR:HG21 | 4:M9:257:GLN:CB | 2.30 | 0.49 |
| 4:M9:230:GLN:CG | 4:M9:231:THR:O | 2.60 | 0.49 |
| 5:N9:54:LEU:HB2 | 12:T9:301:CYC:CGA | 2.42 | 0.49 |
| 5:Z8:29:HIS:CB | 5:Z8:31:TRP:HD1 | 2.23 | 0.49 |
| 5:Z8:37:HIS:CD2 | 5:Z8:37:HIS:C | 2.90 | 0.49 |
| 2:K9:138:VAL:HG12 | 2:K9:138:VAL:O | 2.11 | 0.49 |
| 12:T9:301:CYC:HB | 12:T9:301:CYC:HMA2 | 1.76 | 0.49 |
| 11:aA:632:ILE:N | 11:aA:632:ILE:HD12 | 2.27 | 0.49 |
| 5:N1:26:LEU:CD2 | 5:N1:26:LEU:C | 2.85 | 0.49 |
| 5:N1:37:HIS:CD2 | 5:N1:37:HIS:C | 2.90 | 0.49 |
| 2:W1:138:VAL:O | 2:W1:138:VAL:HG12 | 2.11 | 0.49 |
| 2:A2:60:TYR:CE1 | 2:A2:73:GLY:HA3 | 2.47 | 0.49 |
| 1:Z:127:VAL:HG11 | 1:X5:15:GLN:CB | 2.38 | 0.49 |
| 3:DA:68:ARG:CZ | 3:XA:68:ARG:HH22 | 2.25 | 0.49 |
| 4:MA:21:LEU:HD12 | 4:MA:21:LEU:C | 2.37 | 0.49 |
| 4:MA:160:THR:C | 3:VA:108:ARG:HG2 | 2.37 | 0.49 |
| 5:NA:1:MET:HG2 | 3:RA:119:ALA:CB | 1.98 | 0.49 |
| 2:QA:81:LYS:HE2 | 3:TA:67:ILE:HD11 | 1.93 | 0.49 |
| 12:QA:201:CYC:CBB | 3:TA:75:PRO:HA | 2.36 | 0.49 |
| 2:K3:138:VAL:O | 2:K3:138:VAL:HG12 | 2.11 | 0.49 |
| 2:G2:15:GLN:C | 6:M2:104:ARG:NE | 2.70 | 0.49 |
| 3:H2:2:GLN:NE2 | 6:M2:75:LYS:NZ | 2.60 | 0.49 |
| 3:L2:70:GLY:HA3 | 6:M2:67:GLY:HA2 | 1.91 | 0.49 |
| 2:A3:34:ALA:HB1 | 3:B3:31:VAL:HG21 | 1.92 | 0.49 |
| 3:D3:68:ARG:NH1 | 3:X3:68:ARG:NH1 | 2.56 | 0.49 |
| 12:D3:202:CYC:HB | 12:D3:202:CYC:CMA | 2.25 | 0.49 |
| 3:B4:92:TYR:OH | 12:B4:202:CYC:HAB2 | 2.12 | 0.49 |
| 2:C4:138:VAL:O | 2:C4:138:VAL:HG12 | 2.11 | 0.49 |
| 4:M3:190:ARG:NH1 | 4:M3:202:SER:HG | 2.08 | 0.49 |
| 4:M3:230:GLN:CG | 4:M3:231:THR:O | 2.61 | 0.49 |
| 2:E4:1:MET:H2 | 4:M4:10:ARG:NE | 2.09 | 0.49 |
| 3:F4:116:THR:O | 3:F4:120:LEU:HG | 2.12 | 0.49 |
| 4:M4:58:TYR:O | 4:M4:61:ASN:OD1 | 2.31 | 0.49 |
| 4:M4:131:LEU:CD2 | 5:Z4:2:SER:HA | 2.42 | 0.49 |
| 4:M4:226:SER:OG | 3:Y4:84:ARG:O | 2.30 | 0.49 |
| 3:Q4:124:THR:CB | 3:Q4:172:ALA:HA | 2.41 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:K5:151:PHE:HE1 | 1:V5:42:ALA:HB2 | 1.77 | 0.49 |
| 8:M5:105:GLU:OE1 | 10:k5:532:THR:HG21 | 2.10 | 0.49 |
| 8:O5:57:GLN:O | 8:O5:61:ILE:HD13 | 2.12 | 0.49 |
| 8:A5:108:GLY:HA2 | 12:A5:201:CYC:HAB1 | 1.94 | 0.49 |
| 8:A5:115:MET:SD | 1:F5:75:THR:HG22 | 2.51 | 0.49 |
| 8:C5:110:ILE:CD1 | 9:z5:15:LYS:HB3 | 2.34 | 0.49 |
| 8:G5:6:LYS:CE | 8:S5:19:SER:OG | 2.60 | 0.49 |
| 1:J5:74:THR:OG1 | 1:J5:77:ARG:CD | 2.59 | 0.49 |
| 8:Q5:57:GLN:O | 8:Q5:61:ILE:HD13 | 2.12 | 0.49 |
| 8:Y5:57:GLN:O | 8:Y5:61:ILE:HD13 | 2.12 | 0.49 |
| 8:Y5:61:ILE:HG22 | 8:Y5:62:ARG:HG2 | 1.93 | 0.49 |
| 2:K6:138:VAL:HG12 | 2:K6:138:VAL:O | 2.11 | 0.49 |
| 3:L6:77:ARG:HE | 6:M6:70:GLU:CG | 2.25 | 0.49 |
| 6:M6:75:LYS:NZ | 3:H6:2:GLN:NE2 | 2.60 | 0.49 |
| 9:z5:8:THR:HG22 | 9:z5:52:LEU:HB2 | 1.93 | 0.49 |
| 9:z5:56:LEU:N | 9:z5:56:LEU:CD1 | 2.73 | 0.49 |
| 9:i5:6:LYS:HG2 | 9:i5:55:LYS:CB | 2.39 | 0.49 |
| 10:k5:600:VAL:O | 10:k5:600:VAL:HG12 | 2.12 | 0.49 |
| 10:k5:741:GLN:HG3 | 1:D7:77:ARG:CZ | 2.37 | 0.49 |
| 10:k5:969:VAL:HG12 | 1:n7:77:ARG:HH22 | 1.76 | 0.49 |
| 8:g7:90:ARG:NE | 1:h7:16:GLY:O | 2.45 | 0.49 |
| 8:U7:15:ALA:HA | 1:V7:90:ARG:NH1 | 2.27 | 0.49 |
| 8:U7:95:GLY:N | 8:U7:104:ILE:HD11 | 2.27 | 0.49 |
| 8:m7:95:GLY:N | 8:m7:104:ILE:HD11 | 2.27 | 0.49 |
| 12:U8:201:CYC:HB | 12:U8:201:CYC:CMA | 2.25 | 0.49 |
| 12:F8:202:CYC:HB | 12:F8:202:CYC:HMA2 | 1.76 | 0.49 |
| 4:M8:33:LEU:HD13 | 4:M8:33:LEU:O | 2.13 | 0.49 |
| 12:M8:302:CYC:HMA2 | 12:M8:302:CYC:HB | 1.76 | 0.49 |
| 5:N9:26:LEU:CD2 | 5:N9:26:LEU:C | 2.85 | 0.49 |
| 2:A9:60:TYR:CE1 | 2:A9:73:GLY:HA3 | 2.48 | 0.49 |
| 3:J9:107:ASP:O | 11:a9:517:ALA:HB1 | 2.11 | 0.49 |
| 11:aA:289:THR:O | 11:aA:293:LEU:HA | 2.13 | 0.49 |
| 11:aA:403:THR:HB | 11:aA:441:ARG:HH21 | 1.76 | 0.49 |
| 4:M1:22:SER:HB3 | 4:M1:23:PRO:CD | 2.41 | 0.49 |
| 4:M1:262:ASP:OD1 | 4:M1:263:PRO:HD2 | 2.12 | 0.49 |
| 3:DA:108:ARG:HA | 4:MA:6:THR:HB | 1.95 | 0.49 |
| 3:FA:153:CYS:SG | 12:F9:302:CYC:C3C | 3.00 | 0.49 |
| 4:MA:274:VAL:CG2 | 3:VA:77:ARG:HG2 | 2.41 | 0.49 |
| 2:OA:138:VAL:O | 2:OA:138:VAL:HG12 | 2.11 | 0.49 |
| 2:QA:9:ILE:HG23 | 3:RA:95:TYR:CG | 2.47 | 0.49 |
| 12:QA:201:CYC:HBA2 | 3:TA:79:MET:CE | 2.41 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:O1:65:TYR:O | 2:O1:71:GLN:CG | 2.54 | 0.49 |
| 2:A1:60:TYR:CE1 | 2:A1:73:GLY:HA3 | 2.48 | 0.49 |
| 3:J3:120:LEU:HD21 | 11:a9:800:THR:HG23 | 1.76 | 0.49 |
| 2:G2:113:LEU:CA | 3:L2:76:ASN:HD22 | 2.22 | 0.49 |
| 12:J2:202:CYC:HMA3 | 6:M2:160:ASN:HD21 | 1.76 | 0.49 |
| 2:K2:22:THR:HB | 2:A2:2:LYS:HE2 | 1.93 | 0.49 |
| 6:M2:34:ARG:HD2 | 8:O5:52:LYS:CD | 2.42 | 0.49 |
| 2:A3:60:TYR:CE1 | 2:A3:73:GLY:HA3 | 2.48 | 0.49 |
| 4:M3:252:LEU:CD1 | 3:X3:77:ARG:NH1 | 2.75 | 0.49 |
| 2:S3:138:VAL:HG12 | 2:S3:138:VAL:O | 2.11 | 0.49 |
| 3:B1:91:ARG:HH22 | 11:aA:677:GLN:CD | 2.20 | 0.49 |
| 3:F4:113:LEU:HA | 4:M4:5:THR:CG2 | 2.29 | 0.49 |
| 12:J4:201:CYC:CMA | 12:J4:201:CYC:HB | 2.25 | 0.49 |
| 12:L4:202:CYC:HB | 12:L4:202:CYC:CMA | 2.25 | 0.49 |
| 4:M4:180:ASN:HD21 | 3:Y4:108:ARG:HE | 1.59 | 0.49 |
| 12:K5:201:CYC:O2A | 1:J5:66:THR:OG1 | 2.29 | 0.49 |
| 5:Z4:50:LEU:C | 5:Z4:50:LEU:CD1 | 2.84 | 0.49 |
| 8:E5:101:VAL:C | 8:E5:103:PRO:HD2 | 2.37 | 0.49 |
| 8:G5:64:ASP:OD1 | 8:G5:65:VAL:N | 2.45 | 0.49 |
| 1:J5:59:ALA:O | 1:J5:60:LEU:HD23 | 2.11 | 0.49 |
| 3:J6:88:ILE:HD11 | 6:M6:185:PHE:HE1 | 1.74 | 0.49 |
| 3:L6:65:ASP:OD2 | 1:b7:64:ASP:HB2 | 2.11 | 0.49 |
| 7:N6:49:LEU:CD1 | 3:B6:84:ARG:NE | 2.74 | 0.49 |
| 12:N6:101:CYC:HB | 12:N6:101:CYC:HMA2 | 1.76 | 0.49 |
| 10:j5:547:ARG:C | 10:j5:547:ARG:CD | 2.85 | 0.49 |
| 10:j5:1023:SER:HG | 12:f7:201:CYC:CGA | 2.05 | 0.49 |
| 10:j5:1146:THR:HA | 1:v7:77:ARG:NH2 | 2.22 | 0.49 |
| 10:k5:888:THR:OG1 | 12:D7:201:CYC:O2A | 2.29 | 0.49 |
| 10:k5:1023:SER:O | 10:k5:1027:ASN:HB2 | 2.11 | 0.49 |
| 10:k5:1064:LYS:CD | 10:k5:1064:LYS:C | 2.85 | 0.49 |
| 2:E6:138:VAL:HG12 | 2:E6:138:VAL:O | 2.11 | 0.49 |
| 3:D1:118:VAL:HG22 | 4:M1:254:LEU:HD13 | 1.95 | 0.49 |
| 8:S7:23:LEU:HD22 | 1:T7:38:VAL:HG13 | 1.94 | 0.49 |
| 8:C7:95:GLY:N | 8:C7:104:ILE:HD11 | 2.27 | 0.49 |
| 1:J7:59:ALA:O | 1:J7:60:LEU:HD23 | 2.11 | 0.49 |
| 8:K7:57:GLN:O | 8:K7:61:ILE:HD13 | 2.12 | 0.49 |
| 1:L7:3:ASP:H | 1:L7:6:THR:HG1 | 1.60 | 0.49 |
| 8:U7:60:GLN:CD | 1:p7:117:ASN:CG | 2.63 | 0.49 |
| 8:c7:57:GLN:O | 8:c7:61:ILE:HD13 | 2.12 | 0.49 |
| 1:d7:59:ALA:O | 1:d7:60:LEU:HD23 | 2.11 | 0.49 |
| 2:X8:22:THR:HB | 2:N8:2:LYS:HE2 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:J8:201:CYC:CMA | 12:J8:201:CYC:HB | 2.25 | 0.49 |
| 4:M8:7:SER:C | 4:M8:14:LEU:HD13 | 2.08 | 0.49 |
| 4:M8:235:PHE:CA | 12:M8:301:CYC:HMA1 | 2.43 | 0.49 |
| 12:M8:302:CYC:CMA | 12:M8:302:CYC:HB | 2.26 | 0.49 |
| 2:P8:138:VAL:HG12 | 2:P8:138:VAL:O | 2.11 | 0.49 |
| 3:F1:84:ARG:CZ | 4:M1:35:THR:OG1 | 2.61 | 0.49 |
| 3:L9:52:ILE:CG1 | 3:L9:87:GLU:HA | 2.42 | 0.49 |
| 4:M9:158:PHE:HE1 | 2:U9:13:ASP:HB3 | 1.77 | 0.49 |
| 12:a9:901:CYC:CMA | 12:a9:901:CYC:HB | 2.25 | 0.49 |
| 11:aA:615:ARG:HH11 | 11:aA:615:ARG:CB | 2.20 | 0.49 |
| 12:V1:201:CYC:CMA | 12:V1:201:CYC:HB | 2.26 | 0.49 |
| 12:V1:201:CYC:HB | 12:V1:201:CYC:HMA2 | 1.76 | 0.49 |
| 12:JA:202:CYC:O2A | 11:aA:511:LYS:CD | 2.60 | 0.49 |
| 4:MA:16:LYS:HB2 | 4:MA:46:VAL:HG22 | 1.93 | 0.49 |
| 4:MA:230:GLN:CG | 4:MA:231:THR:O | 2.60 | 0.49 |
| 2:SA:138:VAL:O | 2:SA:138:VAL:HG12 | 2.11 | 0.49 |
| 12:Z3:201:CYC:CBA | 4:M3:185:ALA:HA | 2.42 | 0.49 |
| 12:B4:202:CYC:C4B | 4:M4:61:ASN:HD22 | 2.26 | 0.49 |
| 4:M3:269:SER:CA | 3:V3:111:ASN:HD22 | 2.24 | 0.49 |
| 5:N3:26:LEU:CD2 | 5:N3:26:LEU:C | 2.85 | 0.49 |
| 2:U3:138:VAL:HG12 | 2:U3:138:VAL:O | 2.11 | 0.49 |
| 3:B1:84:ARG:NH2 | 12:B1:202:CYC:C1A | 2.75 | 0.49 |
| 3:F4:84:ARG:CG | 11:aA:139:ILE:HG21 | 2.41 | 0.49 |
| 3:H4:111:ASN:OD1 | 11:aA:291:TYR:HE1 | 1.95 | 0.49 |
| 4:M4:33:LEU:HD13 | 4:M4:33:LEU:O | 2.13 | 0.49 |
| 4:M4:94:TRP:CH2 | 3:Q4:87:GLU:HG2 | 2.48 | 0.49 |
| 3:O4:111:ASN:CB | 5:Z4:67:ILE:HB | 2.37 | 0.49 |
| 8:K5:112:VAL:HG23 | 1:J5:75:THR:HG22 | 1.86 | 0.49 |
| 1:L5:68:PRO:HB3 | 1:H5:14:VAL:O | 2.12 | 0.49 |
| 1:L5:76:ARG:CB | 8:G5:110:ILE:O | 2.60 | 0.49 |
| 3:Y4:85:ASP:C | 3:Y4:88:ILE:HG12 | 2.37 | 0.49 |
| 1:B5:14:VAL:O | 1:F5:68:PRO:HB3 | 2.12 | 0.49 |
| 8:C5:4:LEU:CD2 | 8:C5:4:LEU:C | 2.84 | 0.49 |
| 8:C5:57:GLN:O | 8:C5:61:ILE:HD13 | 2.12 | 0.49 |
| 8:E5:71:ASN:OD1 | 8:E5:121:THR:HA | 2.12 | 0.49 |
| 8:G5:69:GLY:O | 8:U5:64:ASP:CG | 2.55 | 0.49 |
| 8:G5:88:TYR:CZ | 12:G5:201:CYC:HMB3 | 2.48 | 0.49 |
| 8:I5:2:SER:CA | 8:I5:100:ASP:HB3 | 2.43 | 0.49 |
| 8:I5:27:LYS:C | 8:I5:30:VAL:HG22 | 2.36 | 0.49 |
| 8:I5:90:ARG:HD3 | 1:J5:18:TYR:CD1 | 2.47 | 0.49 |
| 12:f5:201:CYC:HB | 12:f5:201:CYC:HMA3 | 1.72 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 12:R5:201:CYC:CMA | 12:R5:201:CYC:NB | 2.74 | 0.49 |
| 8:Y5:23:LEU:HD22 | 1:Z5:38:VAL:HG13 | 1.94 | 0.49 |
| 1:Z5:127:VAL:CG1 | 10:k5:697:PHE:C | 2.83 | 0.49 |
| 12:J6:202:CYC:HB | 12:J6:202:CYC:CMA | 2.25 | 0.49 |
| 6:M6:104:ARG:NE | 2:G6:15:GLN:C | 2.70 | 0.49 |
| 6:M6:251:LYS:HZ3 | 3:H6:120:LEU:C | 2.20 | 0.49 |
| 8:A7:61:ILE:HG22 | 8:A7:62:ARG:HG2 | 1.93 | 0.49 |
| 10:j5:949:ARG:NH2 | 10:j5:954:GLU:OE2 | 2.45 | 0.49 |
| 10:j5:951:MET:HE3 | 10:j5:951:MET:C | 2.34 | 0.49 |
| 10:j5:1060:GLU:C | 10:j5:1063:THR:HG1 | 2.20 | 0.49 |
| 10:j5:1064:LYS:CD | 10:j5:1064:LYS:C | 2.86 | 0.49 |
| 10:j5:1101:GLU:O | 10:j5:1101:GLU:HG3 | 2.13 | 0.49 |
| 10:j5:1151:GLN:HG3 | 1:v7:122:PRO:HA | 1.95 | 0.49 |
| 10:k5:77:VAL:HG23 | 10:k5:77:VAL:O | 2.13 | 0.49 |
| 10:k5:216:ASP:HA | 10:k5:220:SER:HB2 | 1.94 | 0.49 |
| 10:k5:375:VAL:HG11 | 10:k5:456:ILE:HD13 | 1.94 | 0.49 |
| 10:k5:492:ILE:O | 10:k5:492:ILE:HG22 | 2.11 | 0.49 |
| 10:k5:1015:TYR:OH | 8:k7:110:ILE:HG21 | 2.04 | 0.49 |
| 10:k5:1101:GLU:O | 10:k5:1101:GLU:HG3 | 2.13 | 0.49 |
| 12:k5:1202:CYC:HMD1 | 12:k5:1202:CYC:NC | 2.09 | 0.49 |
| 3:D6:52:ILE:HD11 | 3:D6:87:GLU:HA | 1.95 | 0.49 |
| 3:D1:68:ARG:NH1 | 3:X1:68:ARG:NH1 | 2.56 | 0.49 |
| 8:Q7:57:GLN:O | 8:Q7:61:ILE:HD13 | 2.12 | 0.49 |
| 1:F7:59:ALA:O | 1:F7:60:LEU:HD23 | 2.11 | 0.49 |
| 8:I7:95:GLY:N | 8:I7:104:ILE:HD11 | 2.27 | 0.49 |
| 8:I7:161:GLN:NE2 | 1:X7:49:THR:HG22 | 2.26 | 0.49 |
| 8:k7:65:VAL:CG2 | 8:k7:66:VAL:N | 2.75 | 0.49 |
| 12:V7:201:CYC:HB | 12:V7:201:CYC:HMA3 | 1.73 | 0.49 |
| 8:a7:57:GLN:O | 8:a7:61:ILE:HD13 | 2.12 | 0.49 |
| 8:c7:50:ILE:HG12 | 8:c7:137:ALA:CA | 2.42 | 0.49 |
| 8:m7:15:ALA:HA | 1:n7:90:ARG:NH1 | 2.27 | 0.49 |
| 2:V8:138:VAL:HG12 | 2:V8:138:VAL:O | 2.11 | 0.49 |
| 3:Q8:78:ARG:HD2 | 12:Z8:301:CYC:CMD | 2.42 | 0.49 |
| 4:M9:33:LEU:HD13 | 4:M9:33:LEU:O | 2.13 | 0.49 |
| 2:I9:19:LEU:HD13 | 3:J9:41:VAL:HG11 | 1.92 | 0.49 |
| 3:J9:88:ILE:CG1 | 11:a9:512:TYR:CZ | 2.96 | 0.49 |
| 11:a9:338:VAL:CB | 11:a9:340:PRO:HD3 | 2.42 | 0.49 |
| 11:a9:595:ARG:CG | 11:a9:596:THR:N | 2.68 | 0.49 |
| 11:aA:252:ARG:NH2 | 11:aA:291:TYR:HB3 | 2.26 | 0.49 |
| 11:aA:581:ARG:C | 11:aA:581:ARG:CD | 2.85 | 0.49 |
| 2:K1:138:VAL:O | 2:K1:138:VAL:HG12 | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M1:170:PHE:HD1 | 4:M1:174:LEU:HD12 | 1.77 | 0.49 |
| 4:M1:185:ALA:HA | 12:Z1:202:CYC:CBA | 2.42 | 0.49 |
| 3:V1:52:ILE:HD11 | 3:V1:87:GLU:HA | 1.95 | 0.49 |
| 12:X1:201:CYC:HMA2 | 12:X1:201:CYC:HB | 1.76 | 0.49 |
| 3:F2:82:CYS:HB2 | 12:F2:201:CYC:CMD | 2.36 | 0.49 |
| 12:F2:201:CYC:HB | 12:F2:201:CYC:CMA | 2.25 | 0.49 |
| 2:GA:138:VAL:O | 2:GA:138:VAL:HG12 | 2.11 | 0.49 |
| 3:HA:117:TYR:CE1 | 12:HA:202:CYC:C4A | 2.96 | 0.49 |
| 12:HA:202:CYC:CMA | 12:HA:202:CYC:HB | 2.25 | 0.49 |
| 4:MA:33:LEU:HD13 | 4:MA:33:LEU:O | 2.13 | 0.49 |
| 4:MA:158:PHE:HE1 | 2:UA:13:ASP:HB3 | 1.77 | 0.49 |
| 4:MA:262:ASP:OD1 | 4:MA:263:PRO:HD2 | 2.12 | 0.49 |
| 5:NA:38:GLU:HB3 | 5:NA:41:GLN:HE21 | 1.77 | 0.49 |
| 12:QA:201:CYC:HAA1 | 3:TA:79:MET:CE | 2.38 | 0.49 |
| 3:J3:88:ILE:HD12 | 11:a9:668:TYR:OH | 2.12 | 0.49 |
| 12:H2:202:CYC:HC | 12:H2:202:CYC:HMD3 | 1.78 | 0.49 |
| 6:M2:39:ARG:HH21 | 8:O5:66:VAL:HG11 | 1.74 | 0.49 |
| 4:M3:262:ASP:OD1 | 4:M3:263:PRO:HD2 | 2.12 | 0.49 |
| 3:P3:52:ILE:HD11 | 3:P3:87:GLU:HA | 1.95 | 0.49 |
| 12:R3:201:CYC:HB | 12:R3:201:CYC:CMA | 2.25 | 0.49 |
| 3:F4:52:ILE:HD11 | 3:F4:87:GLU:HA | 1.95 | 0.49 |
| 12:F4:202:CYC:CMA | 12:F4:202:CYC:HB | 2.25 | 0.49 |
| 12:H4:201:CYC:HB | 12:H4:201:CYC:CMA | 2.26 | 0.49 |
| 2:K4:138:VAL:HG12 | 2:K4:138:VAL:O | 2.11 | 0.49 |
| 4:M4:268:ARG:HH12 | 3:Y4:112:GLY:HA2 | 1.78 | 0.49 |
| 3:O4:88:ILE:CD1 | 5:Z4:54:LEU:HD11 | 2.41 | 0.49 |
| 3:Q4:93:VAL:HG13 | 3:Q4:163:TYR:CB | 2.42 | 0.49 |
| 8:C5:27:LYS:O | 8:C5:29:PHE:C | 2.56 | 0.49 |
| 1:D5:38:VAL:O | 1:D5:39:ARG:O | 2.30 | 0.49 |
| 8:E5:39:ILE:HG12 | 8:E5:145:ASP:HB3 | 1.95 | 0.49 |
| 12:H5:201:CYC:HBB2 | 9:i5:21:ARG:CB | 2.43 | 0.49 |
| 8:I5:68:PRO:HB3 | 8:Q7:59:PHE:CD2 | 2.47 | 0.49 |
| 1:V5:114:GLU:OE1 | 10:j5:496:GLU:HB2 | 2.10 | 0.49 |
| 8:Y5:14:GLU:OE2 | 10:k5:393:MET:HA | 2.12 | 0.49 |
| 10:j5:216:ASP:HA | 10:j5:220:SER:CB | 2.42 | 0.49 |
| 10:j5:372:ARG:O | 10:j5:372:ARG:HG3 | 2.09 | 0.49 |
| 10:j5:500:PRO:HG2 | 10:j5:500:PRO:O | 2.12 | 0.49 |
| 10:j5:964:GLY:C | 1:t7:69:GLY:HA2 | 2.14 | 0.49 |
| 10:j5:971:VAL:HG12 | 1:t7:76:ARG:NH1 | 2.06 | 0.49 |
| 10:j5:985:ALA:O | 10:j5:988:ALA:CB | 2.60 | 0.49 |
| 10:j5:1018:LEU:CB | 10:j5:1021:ALA:CB | 2.49 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:j5:1052:PRO:O | 10:j5:1053:TYR:CG | 2.65 | 0.49 |
| 10:j5:1117:PRO:HG2 | 10:j5:1117:PRO:O | 2.12 | 0.49 |
| 10:k5:275:THR:HG21 | 10:k5:286:VAL:HA | 1.94 | 0.49 |
| 10:k5:691:SER:O | 10:k5:691:SER:OG | 2.25 | 0.49 |
| 10:k5:803:LYS:CE | 9:z7:43:ARG:NH1 | 2.76 | 0.49 |
| 10:k5:1018:LEU:CB | 10:k5:1021:ALA:CB | 2.49 | 0.49 |
| 12:D1:202:CYC:HB | 12:D1:202:CYC:CMA | 2.25 | 0.49 |
| 1:P7:76:ARG:HD3 | 8:Q7:110:ILE:HD11 | 1.93 | 0.49 |
| 8:C7:44:THR:OG1 | 1:D7:18:TYR:HD2 | 1.91 | 0.49 |
| 8:a7:161:GLN:HG2 | 1:p7:49:THR:CG2 | 2.35 | 0.49 |
| 8:c7:12:ASP:CB | 1:d7:94:TYR:HE2 | 2.24 | 0.49 |
| 12:B8:202:CYC:C4B | 4:M8:61:ASN:HD22 | 2.26 | 0.49 |
| 3:D8:107:ASP:CB | 11:a9:109:ASN:HB3 | 2.42 | 0.49 |
| 8:q7:75:GLU:CB | 11:aA:53:VAL:CG1 | 2.89 | 0.49 |
| 9:w7:29:THR:O | 9:w7:30:LYS:HB3 | 2.13 | 0.49 |
| 3:F8:1:MET:H3 | 4:M8:10:ARG:HB3 | 1.78 | 0.49 |
| 4:M8:92:GLU:OE2 | 4:M8:217:VAL:HG21 | 2.02 | 0.49 |
| 4:M8:99:VAL:HG22 | 3:Q8:108:ARG:CZ | 2.43 | 0.49 |
| 4:M8:205:ASP:OD2 | 5:Z8:59:ARG:NE | 2.46 | 0.49 |
| 4:M9:6:THR:HB | 3:D9:108:ARG:HA | 1.95 | 0.49 |
| 5:Z8:15:LEU:O | 5:Z8:73:GLY:CA | 2.61 | 0.49 |
| 2:A9:138:VAL:O | 2:A9:138:VAL:HG12 | 2.11 | 0.49 |
| 3:F9:37:ARG:HA | 3:F9:156:LEU:HD21 | 1.95 | 0.49 |
| 12:J9:202:CYC:CBB | 11:a9:516:GLN:O | 2.60 | 0.49 |
| 11:a9:308:LEU:CD2 | 11:a9:308:LEU:C | 2.85 | 0.49 |
| 11:a9:327:SER:C | 11:a9:329:ASN:N | 2.67 | 0.49 |
| 11:aA:338:VAL:CB | 11:aA:340:PRO:HD3 | 2.42 | 0.49 |
| 11:aA:668:TYR:HE2 | 3:J1:80:ALA:CB | 2.21 | 0.49 |
| 11:aA:707:PHE:CD2 | 3:L1:108:ARG:CZ | 2.96 | 0.49 |
| 11:aA:709:CYS:O | 11:aA:807:GLN:CB | 2.53 | 0.49 |
| 12:aA:901:CYC:HMA2 | 12:aA:901:CYC:HB | 1.76 | 0.49 |
| 4:M1:162:ASN:HB3 | 12:Z1:202:CYC:OB | 2.09 | 0.49 |
| 4:M1:232:VAL:HG11 | 3:V1:109:CYS:O | 2.12 | 0.49 |
| 2:AA:52:VAL:CG1 | 2:AA:83:ALA:HA | 2.43 | 0.49 |
| 3:BA:26:GLN:O | 3:BA:30:LEU:HD11 | 1.98 | 0.49 |
| 12:FA:301:CYC:HB | 12:FA:301:CYC:CMA | 2.26 | 0.49 |
| 2:IA:138:VAL:HG12 | 2:IA:138:VAL:O | 2.11 | 0.49 |
| 4:MA:176:ARG:HH11 | 4:MA:176:ARG:HG2 | 1.74 | 0.49 |
| 4:MA:259:ARG:HH12 | 3:VA:116:THR:H | 1.59 | 0.49 |
| 5:NA:37:HIS:CD2 | 5:NA:37:HIS:C | 2.90 | 0.49 |
| 2:QA:138:VAL:O | 2:QA:138:VAL:HG12 | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:TA:52:ILE:HD11 | 3:TA:87:GLU:HA | 1.95 | 0.49 |
| 3:ZA:52:ILE:HD11 | 3:ZA:87:GLU:HA | 1.95 | 0.49 |
| 12:R1:201:CYC:HB | 12:R1:201:CYC:CMA | 2.26 | 0.49 |
| 3:J3:77:ARG:NH2 | 2:K3:107:ASP:N | 2.60 | 0.49 |
| 3:J3:119:ALA:C | 11:a9:803:ASN:CB | 2.82 | 0.49 |
| 12:H2:201:CYC:HB | 12:H2:201:CYC:CMA | 2.25 | 0.49 |
| 4:M3:33:LEU:HD13 | 4:M3:33:LEU:O | 2.13 | 0.49 |
| 5:N3:38:GLU:HB3 | 5:N3:41:GLN:HE21 | 1.77 | 0.49 |
| 2:U3:141:GLN:O | 2:Q9:76:ASP:HA | 2.07 | 0.49 |
| 3:H4:119:ALA:C | 11:aA:266:ASN:ND2 | 2.71 | 0.49 |
| 2:I4:138:VAL:HG12 | 2:I4:138:VAL:O | 2.11 | 0.49 |
| 12:L4:202:CYC:CAB | 11:aA:239:TYR:CE1 | 2.93 | 0.49 |
| 4:M4:214:GLY:HA3 | 5:Z4:28:HIS:ND1 | 2.27 | 0.49 |
| 4:M4:227:GLN:N | 3:Y4:88:ILE:HG21 | 2.27 | 0.49 |
| 2:N4:2:LYS:HE2 | 2:X4:22:THR:HB | 1.93 | 0.49 |
| 8:K5:24:ASP:CG | 8:U5:148:GLU:OE2 | 2.53 | 0.49 |
| 8:K5:113:LYS:O | 8:K5:117:ASN:ND2 | 2.45 | 0.49 |
| 12:N5:201:CYC:CBB | 10:k5:482:GLN:HE22 | 2.25 | 0.49 |
| 8:O5:95:GLY:N | 8:O5:104:ILE:HD11 | 2.27 | 0.49 |
| 2:X4:138:VAL:HG12 | 2:X4:138:VAL:O | 2.12 | 0.49 |
| 5:Z4:21:ALA:HA | 5:Z4:42:SER:O | 2.11 | 0.49 |
| 5:Z4:38:GLU:N | 12:Z4:301:CYC:HMB2 | 2.24 | 0.49 |
| 5:Z4:42:SER:N | 12:Z4:301:CYC:HMA3 | 2.23 | 0.49 |
| 12:Z4:301:CYC:CMA | 12:Z4:301:CYC:HB | 2.25 | 0.49 |
| 8:A5:114:GLU:CB | 1:F5:79:ALA:CB | 2.91 | 0.49 |
| 1:B5:107:ARG:CD | 9:z5:21:ARG:HD3 | 2.42 | 0.49 |
| 12:B5:201:CYC:HMD1 | 12:B5:201:CYC:NC | 2.09 | 0.49 |
| 8:C5:2:SER:CA | 8:C5:100:ASP:HB3 | 2.43 | 0.49 |
| 8:G5:61:ILE:HD11 | 8:o7:67:SER:HB2 | 1.80 | 0.49 |
| 8:G5:107:ILE:HG21 | 1:H5:13:ASP:OD1 | 2.13 | 0.49 |
| 1:J5:71:MEN:O | 1:J5:77:ARG:CZ | 2.60 | 0.49 |
| 8:Q5:128:GLU:HA | 8:Q5:128:GLU:OE1 | 2.13 | 0.49 |
| 8:S5:41:GLN:NE2 | 1:D7:143:PRO:CD | 2.76 | 0.49 |
| 8:a5:2:SER:CA | 8:a5:100:ASP:HB3 | 2.43 | 0.49 |
| 8:A7:65:VAL:CG2 | 8:A7:66:VAL:N | 2.75 | 0.49 |
| 10:j5:85:SER:HB2 | 10:j5:157:ILE:HG21 | 1.95 | 0.49 |
| 10:j5:275:THR:HG21 | 10:j5:286:VAL:HA | 1.94 | 0.49 |
| 10:j5:292:GLU:N | 10:j5:292:GLU:OE1 | 2.46 | 0.49 |
| 10:j5:1053:TYR:O | 1:r7:107:ARG:HD2 | 2.12 | 0.49 |
| 10:k5:951:MET:HE1 | 10:k5:955:LEU:CD2 | 2.42 | 0.49 |
| 10:k5:1046:ARG:HD2 | 8:k7:13:ALA:CB | 2.43 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:k5:1052:PRO:O | 10:k5:1053:TYR:CG | 2.65 | 0.49 |
| 10:k5:1081:VAL:HG21 | 12:k5:1203:CYC:CMA | 2.43 | 0.49 |
| 12:D6:201:CYC:HB | 12:D6:201:CYC:CMA | 2.26 | 0.49 |
| 8:C7:57:GLN:O | 8:C7:61:ILE:HD13 | 2.12 | 0.49 |
| 8:E7:57:GLN:O | 8:E7:61:ILE:HD13 | 2.12 | 0.49 |
| 8:k7:57:GLN:O | 8:k7:61:ILE:HD13 | 2.12 | 0.49 |
| 8:U7:2:SER:CA | 8:U7:100:ASP:HB3 | 2.43 | 0.49 |
| 8:W7:12:ASP:O | 9:w7:46:LYS:CE | 2.61 | 0.49 |
| 1:b7:75:THR:C | 8:c7:111:GLY:HA3 | 2.37 | 0.49 |
| 2:E1:114:ARG:HH12 | 11:aA:671:GLU:CD | 2.20 | 0.49 |
| 1:l7:59:ALA:O | 1:l7:60:LEU:HD23 | 2.11 | 0.49 |
| 9:z7:15:LYS:HD2 | 9:z7:15:LYS:C | 2.38 | 0.49 |
| 3:F8:52:ILE:HD11 | 3:F8:87:GLU:HA | 1.95 | 0.49 |
| 2:K8:138:VAL:HG12 | 2:K8:138:VAL:O | 2.11 | 0.49 |
| 3:L8:52:ILE:HD11 | 3:L8:87:GLU:HA | 1.95 | 0.49 |
| 3:L8:68:ARG:CB | 11:a9:82:GLN:HB2 | 2.33 | 0.49 |
| 4:M8:148:LYS:CD | 4:M8:197:ASP:OD1 | 2.61 | 0.49 |
| 3:Q8:52:ILE:HD11 | 3:Q8:87:GLU:HA | 1.95 | 0.49 |
| 4:M9:181:GLN:HA | 4:M9:266:LEU:HD23 | 1.95 | 0.49 |
| 3:H9:52:ILE:HD11 | 3:H9:87:GLU:HA | 1.95 | 0.49 |
| 3:H9:72:ASN:CG | 12:H9:202:CYC:CMD | 2.85 | 0.49 |
| 11:a9:320:ASP:O | 11:a9:321:ALA:C | 2.50 | 0.49 |
| 11:a9:398:GLN:HE21 | 11:a9:505:PRO:HB2 | 1.77 | 0.49 |
| 11:aA:588:VAL:CA | 11:aA:590:PRO:HD2 | 2.42 | 0.49 |
| 11:aA:708:HIS:CA | 3:L1:108:ARG:NH2 | 2.74 | 0.49 |
| 12:aA:901:CYC:CMA | 12:aA:901:CYC:HB | 2.26 | 0.49 |
| 4:M1:230:GLN:HG2 | 4:M1:231:THR:O | 2.13 | 0.49 |
| 4:M1:233:GLU:HG2 | 4:M1:233:GLU:O | 2.13 | 0.49 |
| 4:M1:274:VAL:CG1 | 2:U1:111:ALA:HB1 | 2.42 | 0.49 |
| 2:Y1:138:VAL:HG12 | 2:Y1:138:VAL:O | 2.11 | 0.49 |
| 3:LA:120:LEU:O | 11:aA:539:GLY:HA2 | 2.13 | 0.49 |
| 2:OA:52:VAL:CG1 | 2:OA:83:ALA:HA | 2.43 | 0.49 |
| 3:P1:111:ASN:ND2 | 5:N1:74:GLU:HA | 2.16 | 0.49 |
| 6:M2:130:ARG:NH1 | 12:F2:201:CYC:O2A | 2.46 | 0.49 |
| 2:E3:138:VAL:HG12 | 2:E3:138:VAL:O | 2.11 | 0.49 |
| 3:F3:84:ARG:CZ | 4:M3:35:THR:OG1 | 2.61 | 0.49 |
| 4:M3:21:LEU:HD12 | 4:M3:21:LEU:C | 2.37 | 0.49 |
| 3:V3:52:ILE:HD11 | 3:V3:87:GLU:HA | 1.95 | 0.49 |
| 3:W4:52:ILE:HD11 | 3:W4:87:GLU:HA | 1.95 | 0.49 |
| 12:W4:201:CYC:HB | 12:W4:201:CYC:CMA | 2.26 | 0.49 |
| 3:F4:115:GLU:CA | 4:M4:3:VAL:HG11 | 2.41 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:M4:141:GLU:CG | 4:M4:145:LEU:CD1 | 2.90 | 0.49 |
| 4:M4:235:PHE:CD2 | 12:M4:301:CYC:C3A | 2.59 | 0.49 |
| 3:Q4:93:VAL:HG11 | 3:Q4:164:PHE:CD2 | 2.48 | 0.49 |
| 8:K5:71:ASN:OD1 | 8:K5:121:THR:HA | 2.13 | 0.49 |
| 12:L5:201:CYC:HMD1 | 12:L5:201:CYC:NC | 2.09 | 0.49 |
| 5:Z4:15:LEU:O | 5:Z4:73:GLY:CA | 2.61 | 0.49 |
| 1:B5:2:GLN:CD | 10:k5:551:MET:HG2 | 2.38 | 0.49 |
| 8:C5:29:PHE:HE2 | 1:D5:5:ILE:CD1 | 2.26 | 0.49 |
| 1:D5:71:MEN:O | 1:D5:77:ARG:CZ | 2.61 | 0.49 |
| 12:F5:201:CYC:HMA2 | 10:k5:591:ILE:HG22 | 1.88 | 0.49 |
| 8:I5:57:GLN:O | 8:I5:61:ILE:HD13 | 2.12 | 0.49 |
| 8:S5:41:GLN:CD | 1:D7:143:PRO:HD3 | 2.38 | 0.49 |
| 8:W5:4:LEU:HD23 | 8:W5:26:ILE:CD1 | 2.38 | 0.49 |
| 8:W5:16:ARG:N | 1:X5:90:ARG:CD | 2.39 | 0.49 |
| 3:L6:52:ILE:HD11 | 3:L6:87:GLU:HA | 1.95 | 0.49 |
| 8:A7:86:ASP:CB | 11:aA:579:PHE:HZ | 2.21 | 0.49 |
| 10:j5:301:TYR:HE1 | 10:j5:337:LEU:HD21 | 1.78 | 0.49 |
| 10:j5:974:LEU:CB | 1:v7:1:MET:N | 2.72 | 0.49 |
| 10:j5:1057:LYS:O | 10:j5:1061:LEU:HG | 2.12 | 0.49 |
| 10:k5:803:LYS:HE3 | 9:z7:43:ARG:NH1 | 2.28 | 0.49 |
| 10:k5:1118:THR:HG23 | 12:k5:1204:CYC:CGA | 2.43 | 0.49 |
| 2:G6:138:VAL:HG12 | 2:G6:138:VAL:O | 2.11 | 0.49 |
| 2:I6:53:LYS:HE2 | 11:a9:294:THR:HG22 | 1.93 | 0.49 |
| 8:O7:57:GLN:O | 8:O7:61:ILE:HD13 | 2.12 | 0.49 |
| 8:Q7:4:LEU:HD21 | 8:Q7:26:ILE:HD13 | 1.94 | 0.49 |
| 8:Q7:128:GLU:HA | 8:Q7:128:GLU:OE1 | 2.12 | 0.49 |
| 1:R7:3:ASP:H | 1:R7:6:THR:HG1 | 1.57 | 0.49 |
| 12:F7:201:CYC:CMA | 12:F7:201:CYC:NB | 2.74 | 0.49 |
| 8:k7:61:ILE:HG22 | 8:k7:62:ARG:HG2 | 1.93 | 0.49 |
| 8:W7:39:ILE:HG12 | 8:W7:145:ASP:HB3 | 1.95 | 0.49 |
| 8:Y7:57:GLN:O | 8:Y7:61:ILE:HD13 | 2.12 | 0.49 |
| 8:c7:89:LEU:HD13 | 8:c7:153:PHE:CE1 | 2.48 | 0.49 |
| 8:q7:23:LEU:HD22 | 1:r7:38:VAL:HG13 | 1.94 | 0.49 |
| 3:W8:52:ILE:HD11 | 3:W8:87:GLU:HA | 1.95 | 0.49 |
| 3:H8:14:LEU:HD21 | 11:a9:86:ASP:N | 2.27 | 0.49 |
| 3:L8:120:LEU:CD1 | 12:a9:901:CYC:HAA2 | 2.42 | 0.49 |
| 4:M8:16:LYS:HB2 | 4:M8:46:VAL:HG22 | 1.93 | 0.49 |
| 4:M8:142:PHE:O | 4:M8:146:LEU:HG | 2.13 | 0.49 |
| 3:L9:44:ILE:HG22 | 3:L9:90:LEU:HD21 | 1.88 | 0.49 |
| 3:L9:45:THR:OG1 | 2:K9:19:LEU:O | 2.27 | 0.49 |
| 3:L9:120:LEU:O | 11:a9:539:GLY:HA2 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:M9:158:PHE:CE1 | 2:U9:10:ALA:O | 2.65 | 0.49 |
| 5:N9:3:VAL:CG1 | 3:R9:115:GLU:HB2 | 2.33 | 0.49 |
| 3:Y8:52:ILE:HD11 | 3:Y8:87:GLU:HA | 1.95 | 0.49 |
| 5:Z8:26:LEU:CD2 | 5:Z8:26:LEU:C | 2.85 | 0.49 |
| 12:H9:202:CYC:CMA | 12:H9:202:CYC:HB | 2.25 | 0.49 |
| 3:R9:52:ILE:HD11 | 3:R9:87:GLU:HA | 1.95 | 0.49 |
| 2:G1:111:ALA:HB3 | 3:L1:77:ARG:HG3 | 1.90 | 0.49 |
| 11:a9:817:LEU:O | 11:a9:818:ARG:C | 2.52 | 0.49 |
| 11:aA:582:MET:O | 11:aA:582:MET:HG2 | 2.12 | 0.49 |
| 12:H1:201:CYC:HB | 12:H1:201:CYC:CMA | 2.25 | 0.49 |
| 3:D2:52:ILE:HD11 | 3:D2:87:GLU:HA | 1.95 | 0.49 |
| 3:DA:68:ARG:NH2 | 3:XA:68:ARG:HH22 | 2.09 | 0.49 |
| 3:HA:116:THR:CG2 | 11:aA:449:ASN:ND2 | 2.65 | 0.49 |
| 3:JA:108:ARG:HA | 11:aA:517:ALA:CA | 2.40 | 0.49 |
| 2:KA:30:ARG:HD3 | 2:KA:30:ARG:C | 2.38 | 0.49 |
| 12:LA:202:CYC:CMA | 12:LA:202:CYC:HB | 2.25 | 0.49 |
| 4:MA:158:PHE:CE1 | 2:UA:10:ALA:O | 2.65 | 0.49 |
| 4:MA:210:ILE:HD13 | 5:NA:59:ARG:NH1 | 2.27 | 0.49 |
| 5:NA:54:LEU:HD12 | 12:TA:301:CYC:C1B | 2.33 | 0.49 |
| 2:QA:25:GLN:HE22 | 2:UA:100:GLY:CA | 2.26 | 0.49 |
| 2:QA:159:ASN:OD1 | 3:VA:49:ALA:HB2 | 2.12 | 0.49 |
| 2:O1:60:TYR:CE1 | 2:O1:73:GLY:HA3 | 2.48 | 0.49 |
| 6:M2:50:LEU:CD2 | 8:i7:79:ALA:CA | 2.90 | 0.49 |
| 3:L3:120:LEU:HD23 | 11:a9:731:GLN:HG2 | 1.94 | 0.49 |
| 4:M3:51:ARG:HB3 | 4:M3:51:ARG:NH1 | 2.23 | 0.49 |
| 4:M3:61:ASN:C | 4:M3:63:GLY:N | 2.64 | 0.49 |
| 4:M3:230:GLN:HG2 | 4:M3:231:THR:O | 2.13 | 0.49 |
| 2:O3:60:TYR:CE1 | 2:O3:73:GLY:HA3 | 2.48 | 0.49 |
| 2:U3:46:SER:C | 2:Q9:74:TYR:CE1 | 2.81 | 0.49 |
| 12:X3:201:CYC:HB | 12:X3:201:CYC:CMA | 2.26 | 0.49 |
| 3:F4:108:ARG:NH2 | 4:M4:9:GLN:NE2 | 2.61 | 0.49 |
| 4:M4:176:ARG:HG2 | 4:M4:176:ARG:O | 2.13 | 0.49 |
| 3:O4:107:ASP:CB | 5:Z4:66:ARG:HB2 | 2.34 | 0.49 |
| 12:O4:201:CYC:CGA | 5:Z4:50:LEU:CD1 | 2.91 | 0.49 |
| 3:Q4:72:ASN:OD1 | 12:Z4:301:CYC:NC | 2.43 | 0.49 |
| 8:K5:131:ARG:CZ | 8:K5:157:VAL:HG11 | 2.42 | 0.49 |
| 8:K5:151:PHE:CE1 | 1:V5:42:ALA:HB2 | 2.48 | 0.49 |
| 1:N5:87:TYR:CZ | 10:k5:483:PHE:HE2 | 2.31 | 0.49 |
| 8:O5:76:LYS:HG2 | 8:O5:77:MET:HE3 | 1.93 | 0.49 |
| 8:A5:15:ALA:HB2 | 9:z5:20:GLY:HA3 | 1.95 | 0.49 |
| 1:f5:114:GLU:OE1 | 10:j5:491:THR:OG1 | 2.31 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:S5:65:VAL:CG2 | 8:S5:66:VAL:N | 2.75 | 0.49 |
| 8:U5:61:ILE:HG22 | 8:U5:62:ARG:HG2 | 1.93 | 0.49 |
| 1:b5:17:LYS:C | 10:k5:169:TYR:OH | 2.51 | 0.49 |
| 3:J6:52:ILE:HD11 | 3:J6:87:GLU:HA | 1.95 | 0.49 |
| 8:A7:23:LEU:HD13 | 8:M7:151:PHE:CE1 | 2.48 | 0.49 |
| 10:j5:283:ARG:N | 10:j5:283:ARG:CD | 2.71 | 0.49 |
| 10:k5:878:GLU:HG3 | 9:z7:28:PHE:CD2 | 2.47 | 0.49 |
| 10:k5:990:ARG:HH21 | 10:k5:1026:LYS:HZ1 | 1.30 | 0.49 |
| 2:A6:34:ALA:CB | 3:B6:31:VAL:HG11 | 2.38 | 0.49 |
| 2:A6:52:VAL:CG1 | 2:A6:83:ALA:HA | 2.43 | 0.49 |
| 8:M7:49:ARG:NH1 | 3:H9:119:ALA:CA | 2.54 | 0.49 |
| 1:h7:68:PRO:HD3 | 8:i7:87:TYR:OH | 2.12 | 0.49 |
| 8:i7:90:ARG:CZ | 1:j7:13:ASP:OD1 | 2.58 | 0.49 |
| 8:c7:50:ILE:HG12 | 8:c7:137:ALA:CB | 2.41 | 0.49 |
| 2:A8:52:VAL:CG1 | 2:A8:83:ALA:HA | 2.43 | 0.49 |
| 8:q7:130:VAL:HG12 | 8:q7:157:VAL:HG23 | 1.95 | 0.49 |
| 2:X8:67:THR:OG1 | 3:T9:28:THR:CB | 2.60 | 0.49 |
| 3:J8:52:ILE:HD11 | 3:J8:87:GLU:HA | 1.95 | 0.49 |
| 12:J8:202:CYC:HC | 12:J8:202:CYC:HMD3 | 1.78 | 0.49 |
| 4:M8:130:SER:HB3 | 12:M8:302:CYC:CAA | 2.40 | 0.49 |
| 3:O8:52:ILE:HD11 | 3:O8:87:GLU:HA | 1.95 | 0.49 |
| 4:M9:94:TRP:CH2 | 5:N9:29:HIS:CE1 | 3.01 | 0.49 |
| 4:M9:188:LEU:HG | 3:V9:84:ARG:NE | 2.26 | 0.49 |
| 5:Z8:50:LEU:C | 5:Z8:50:LEU:CD1 | 2.84 | 0.49 |
| 3:J9:19:LEU:HD13 | 3:J9:24:LEU:HG | 1.94 | 0.49 |
| 12:T9:301:CYC:HB | 12:T9:301:CYC:CMA | 2.25 | 0.49 |
| 11:a9:548:LEU:C | 11:a9:551:PRO:HD2 | 2.37 | 0.49 |
| 11:a9:582:MET:O | 11:a9:582:MET:HG2 | 2.12 | 0.49 |
| 11:a9:801:ASN:ND2 | 11:a9:801:ASN:C | 2.71 | 0.49 |
| 11:aA:398:GLN:HE21 | 11:aA:505:PRO:HB2 | 1.77 | 0.49 |
| 11:aA:558:VAL:O | 11:aA:560:SER:N | 2.45 | 0.49 |
| 11:aA:595:ARG:HG3 | 11:aA:596:THR:C | 2.36 | 0.49 |
| 11:aA:710:THR:HA | 11:aA:807:GLN:CB | 2.43 | 0.49 |
| 2:I1:138:VAL:HG12 | 2:I1:138:VAL:O | 2.11 | 0.49 |
| 5:N1:21:ALA:HA | 5:N1:42:SER:O | 2.11 | 0.49 |
| 1:A:73:TYR:OH | 10:k5:162:TRP:CZ2 | 2.66 | 0.49 |
| 2:AA:60:TYR:CE1 | 2:AA:73:GLY:HA3 | 2.48 | 0.49 |
| 3:LA:52:ILE:CG1 | 3:LA:87:GLU:HA | 2.42 | 0.49 |
| 4:MA:185:ALA:N | 12:VA:201:CYC:HBA2 | 2.28 | 0.49 |
| 2:OA:64:PRO:C | 2:OA:66:LEU:N | 2.71 | 0.49 |
| 3:R1:88:ILE:HG21 | 12:R1:201:CYC:HAB2 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:H3:52:ILE:HD11 | 3:H3:87:GLU:HA | 1.95 | 0.49 |
| 12:H3:202:CYC:HB | 12:H3:202:CYC:CMA | 2.25 | 0.49 |
| 12:H3:202:CYC:OB | 11:a9:776:TYR:HB2 | 2.12 | 0.49 |
| 3:J3:84:ARG:NE | 11:a9:668:TYR:HB3 | 2.28 | 0.49 |
| 6:M2:35:GLY:HA2 | 8:O5:78:THR:HG22 | 1.95 | 0.49 |
| 3:B4:85:ASP:CB | 12:B4:202:CYC:HBC3 | 2.43 | 0.49 |
| 3:L3:104:VAL:HB | 3:L3:108:ARG:CZ | 2.34 | 0.49 |
| 12:P3:201:CYC:HB | 12:P3:201:CYC:CMA | 2.25 | 0.49 |
| 3:L4:52:ILE:HD11 | 3:L4:87:GLU:HA | 1.95 | 0.49 |
| 3:O4:52:ILE:HD11 | 3:O4:87:GLU:HA | 1.95 | 0.49 |
| 8:M5:65:VAL:CG2 | 8:M5:66:VAL:N | 2.75 | 0.49 |
| 8:M5:90:ARG:HB2 | 1:N5:18:TYR:CZ | 2.48 | 0.49 |
| 8:O5:130:VAL:HG12 | 8:O5:157:VAL:HG23 | 1.95 | 0.49 |
| 5:Z4:37:HIS:CE1 | 12:Z4:301:CYC:CHA | 2.95 | 0.49 |
| 1:D5:75:THR:HG22 | 8:E5:112:VAL:HG23 | 1.86 | 0.49 |
| 12:D5:201:CYC:CMA | 12:D5:201:CYC:NB | 2.74 | 0.49 |
| 1:R5:64:ASP:HB3 | 10:k5:704:THR:HG21 | 1.94 | 0.49 |
| 6:M6:249:ARG:CB | 12:H6:201:CYC:O1D | 2.61 | 0.49 |
| 8:A7:130:VAL:HG12 | 8:A7:157:VAL:HG23 | 1.95 | 0.49 |
| 9:z5:6:LYS:HB3 | 9:z5:55:LYS:N | 2.28 | 0.49 |
| 10:j5:26:ASN:ND2 | 10:j5:267:ASP:OD1 | 2.46 | 0.49 |
| 10:j5:238:ARG:CD | 10:j5:238:ARG:C | 2.86 | 0.49 |
| 10:j5:804:GLU:CD | 9:w7:30:LYS:HE2 | 2.37 | 0.49 |
| 10:k5:190:LEU:HD21 | 12:k5:1201:CYC:C4D | 2.42 | 0.49 |
| 10:k5:284:PRO:CD | 10:k5:326:GLY:HA3 | 2.23 | 0.49 |
| 10:k5:301:TYR:HE1 | 10:k5:337:LEU:HD21 | 1.78 | 0.49 |
| 10:k5:871:GLU:O | 10:k5:871:GLU:HG2 | 2.12 | 0.49 |
| 10:k5:909:ASP:OD1 | 10:k5:909:ASP:N | 2.46 | 0.49 |
| 8:S7:65:VAL:CG2 | 8:S7:66:VAL:N | 2.75 | 0.49 |
| 8:E7:39:ILE:HG12 | 8:E7:145:ASP:HB3 | 1.95 | 0.49 |
| 8:G7:57:GLN:O | 8:G7:61:ILE:HD13 | 2.12 | 0.49 |
| 8:I7:2:SER:CA | 8:I7:100:ASP:HB3 | 2.43 | 0.49 |
| 8:M7:39:ILE:HG12 | 8:M7:145:ASP:HB3 | 1.95 | 0.49 |
| 8:i7:95:GLY:C | 8:i7:152:TYR:CD2 | 2.87 | 0.49 |
| 8:i7:130:VAL:O | 8:i7:130:VAL:HG12 | 2.10 | 0.49 |
| 8:c7:15:ALA:C | 1:d7:90:ARG:NH2 | 2.55 | 0.49 |
| 2:A8:138:VAL:O | 2:A8:138:VAL:HG12 | 2.11 | 0.49 |
| 8:o7:42:THR:HG21 | 8:o7:141:LEU:HD23 | 1.95 | 0.49 |
| 8:o7:94:TYR:CE1 | 1:p7:18:TYR:HA | 2.47 | 0.49 |
| 8:o7:128:GLU:OE1 | 8:o7:128:GLU:HA | 2.13 | 0.49 |
| 8:q7:65:VAL:CG2 | 8:q7:66:VAL:N | 2.75 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:u7:42:THR:HG21 | 8:u7:141:LEU:HD23 | 1.95 | 0.49 |
| 4:M8:98:ASP:C | 3:Q8:108:ARG:HG3 | 2.38 | 0.49 |
| 3:L9:112:GLY:C | 11:a9:532:ALA:CB | 2.79 | 0.49 |
| 4:M9:133:ARG:CB | 12:R9:201:CYC:HBA2 | 2.35 | 0.49 |
| 2:A9:114:ARG:NH1 | 11:a9:407:GLU:OE1 | 2.26 | 0.49 |
| 12:F9:301:CYC:HB | 12:F9:301:CYC:CMA | 2.26 | 0.49 |
| 3:T9:52:ILE:HD11 | 3:T9:87:GLU:HA | 1.95 | 0.49 |
| 12:V9:201:CYC:CMA | 12:V9:201:CYC:HB | 2.25 | 0.49 |
| 3:X9:88:ILE:HG21 | 12:X9:201:CYC:HAB2 | 1.95 | 0.49 |
| 11:aA:90:GLN:C | 11:aA:92:LYS:N | 2.70 | 0.49 |
| 11:aA:742:GLN:OE1 | 3:L1:88:ILE:HD11 | 2.01 | 0.49 |
| 3:H1:84:ARG:HH22 | 12:H1:201:CYC:C1A | 2.26 | 0.49 |
| 12:Z1:202:CYC:HB | 12:Z1:202:CYC:CMA | 2.25 | 0.49 |
| 3:BA:119:ALA:HB2 | 4:MA:41:ASN:HD21 | 1.76 | 0.48 |
| 12:JA:202:CYC:CBB | 11:aA:516:GLN:O | 2.61 | 0.48 |
| 4:MA:181:GLN:HA | 4:MA:266:LEU:HD23 | 1.95 | 0.48 |
| 5:NA:54:LEU:CD1 | 12:TA:301:CYC:C1B | 2.89 | 0.48 |
| 2:QA:30:ARG:HD3 | 2:QA:30:ARG:C | 2.39 | 0.48 |
| 2:QA:119:THR:CG2 | 3:TA:83:LEU:CD2 | 2.61 | 0.48 |
| 2:WA:138:VAL:HG12 | 2:WA:138:VAL:O | 2.11 | 0.48 |
| 12:O1:201:CYC:OB | 3:R1:74:TYR:CD1 | 2.66 | 0.48 |
| 3:P1:52:ILE:HD11 | 3:P1:87:GLU:HA | 1.95 | 0.48 |
| 3:J3:88:ILE:HG21 | 12:J3:202:CYC:HAB2 | 1.95 | 0.48 |
| 2:K3:14:SER:CB | 11:a9:746:TYR:HB2 | 2.35 | 0.48 |
| 12:B3:202:CYC:CMA | 12:B3:202:CYC:HB | 2.26 | 0.48 |
| 12:Z3:201:CYC:HB | 12:Z3:201:CYC:CMA | 2.25 | 0.48 |
| 4:M3:232:VAL:HG11 | 3:V3:109:CYS:O | 2.12 | 0.48 |
| 2:O3:30:ARG:HD3 | 2:O3:30:ARG:C | 2.38 | 0.48 |
| 3:B1:85:ASP:CG | 12:B1:202:CYC:NA | 2.71 | 0.48 |
| 3:J4:88:ILE:HG21 | 12:J4:201:CYC:HAB2 | 1.95 | 0.48 |
| 4:M4:100:SER:O | 2:P4:13:ASP:CB | 2.61 | 0.48 |
| 4:M4:224:PHE:O | 12:M4:301:CYC:HAD2 | 2.13 | 0.48 |
| 3:Q4:82:CYS:HA | 12:Z4:301:CYC:CAC | 2.38 | 0.48 |
| 3:Q4:120:LEU:HD12 | 5:Z4:40:SER:N | 2.20 | 0.48 |
| 8:M5:39:ILE:HG12 | 8:M5:145:ASP:HB3 | 1.95 | 0.48 |
| 8:M5:130:VAL:HG12 | 8:M5:157:VAL:HG23 | 1.95 | 0.48 |
| 8:A5:65:VAL:CG2 | 8:A5:66:VAL:N | 2.75 | 0.48 |
| 1:B5:87:TYR:CZ | 9:z5:19:THR:O | 2.63 | 0.48 |
| 8:C5:26:ILE:O | 8:C5:26:ILE:HG12 | 2.13 | 0.48 |
| 8:C5:37:LEU:HD22 | 1:D5:27:LEU:HD12 | 1.95 | 0.48 |
| 8:C5:95:GLY:N | 8:C5:104:ILE:HD11 | 2.27 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:G5:106:GLU:OE1 | 10:j5:557:VAL:HG23 | 2.13 | 0.48 |
| 12:d5:201:CYC:HBB2 | 10:j5:353:ASN:HB2 | 1.94 | 0.48 |
| 8:e5:57:GLN:O | 8:e5:61:ILE:HD13 | 2.12 | 0.48 |
| 8:W5:4:LEU:HD21 | 8:W5:26:ILE:HD13 | 1.93 | 0.48 |
| 8:W5:39:ILE:HG12 | 8:W5:145:ASP:HB3 | 1.95 | 0.48 |
| 8:Y5:114:GLU:CD | 10:k5:312:TYR:C | 2.81 | 0.48 |
| 10:j5:277:ILE:CA | 10:j5:284:PRO:HA | 2.43 | 0.48 |
| 10:j5:284:PRO:CD | 10:j5:326:GLY:HA3 | 2.23 | 0.48 |
| 10:j5:619:GLU:HB2 | 10:j5:620:PRO:CD | 2.39 | 0.48 |
| 10:j5:755:GLN:HB3 | 10:j5:879:ASP:HB2 | 1.95 | 0.48 |
| 10:k5:919:ILE:HG22 | 10:k5:919:ILE:O | 2.13 | 0.48 |
| 2:A6:64:PRO:C | 2:A6:66:LEU:N | 2.71 | 0.48 |
| 3:B6:52:ILE:HD11 | 3:B6:87:GLU:HA | 1.95 | 0.48 |
| 3:D1:88:ILE:HG21 | 12:D1:202:CYC:HAB2 | 1.95 | 0.48 |
| 8:I7:40:ALA:HB2 | 8:I7:97:VAL:HG13 | 1.95 | 0.48 |
| 8:c7:112:VAL:HG12 | 8:c7:113:LYS:H | 1.78 | 0.48 |
| 8:m7:40:ALA:HB2 | 8:m7:97:VAL:HG13 | 1.95 | 0.48 |
| 8:o7:23:LEU:CA | 1:p7:38:VAL:HG21 | 2.43 | 0.48 |
| 8:s7:2:SER:CA | 8:s7:100:ASP:HB3 | 2.43 | 0.48 |
| 8:u7:80:LEU:HD12 | 12:u7:201:CYC:C3D | 2.43 | 0.48 |
| 8:u7:128:GLU:HA | 8:u7:128:GLU:OE1 | 2.13 | 0.48 |
| 3:J8:108:ARG:CZ | 11:a9:171:ARG:HA | 2.43 | 0.48 |
| 2:N8:30:ARG:HD3 | 2:N8:30:ARG:C | 2.38 | 0.48 |
| 3:Q8:117:TYR:CA | 3:Q8:120:LEU:HG | 2.42 | 0.48 |
| 3:L9:108:ARG:HA | 11:a9:531:ASP:CB | 2.43 | 0.48 |
| 2:Q9:30:ARG:HD3 | 2:Q9:30:ARG:C | 2.39 | 0.48 |
| 2:A9:64:PRO:C | 2:A9:66:LEU:N | 2.71 | 0.48 |
| 3:J9:68:ARG:HB3 | 11:a9:353:ALA:HB2 | 1.94 | 0.48 |
| 11:a9:490:ILE:N | 11:a9:490:ILE:HD13 | 2.26 | 0.48 |
| 11:aA:70:ALA:N | 11:aA:71:ILE:HD11 | 2.28 | 0.48 |
| 11:aA:308:LEU:CD2 | 11:aA:308:LEU:C | 2.85 | 0.48 |
| 11:aA:319:LEU:O | 11:aA:322:ALA:HB3 | 2.11 | 0.48 |
| 11:aA:371:VAL:HG11 | 11:aA:507:PHE:CG | 2.47 | 0.48 |
| 11:aA:668:TYR:CG | 3:J1:84:ARG:HD3 | 2.47 | 0.48 |
| 4:M1:230:GLN:CG | 4:M1:231:THR:O | 2.61 | 0.48 |
| 4:M1:252:LEU:HD13 | 3:X1:77:ARG:NH1 | 2.28 | 0.48 |
| 2:CA:138:VAL:O | 2:CA:138:VAL:HG12 | 2.11 | 0.48 |
| 2:GA:119:THR:CG2 | 3:LA:83:LEU:CD1 | 2.86 | 0.48 |
| 3:HA:120:LEU:HD13 | 12:HA:202:CYC:CHA | 2.43 | 0.48 |
| 4:MA:230:GLN:HG2 | 4:MA:231:THR:O | 2.13 | 0.48 |
| 3:XA:88:ILE:HG21 | 12:XA:201:CYC:HAB2 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:G3:107:ASP:N | 3:L3:77:ARG:NH2 | 2.60 | 0.48 |
| 3:H3:88:ILE:HG21 | 12:H3:202:CYC:HAB2 | 1.96 | 0.48 |
| 2:A4:60:TYR:CE1 | 2:A4:73:GLY:HA3 | 2.47 | 0.48 |
| 3:P3:88:ILE:HG21 | 12:P3:201:CYC:HAB2 | 1.95 | 0.48 |
| 2:Y3:30:ARG:HD3 | 2:Y3:30:ARG:C | 2.39 | 0.48 |
| 3:S4:52:ILE:HD11 | 3:S4:87:GLU:HA | 1.95 | 0.48 |
| 2:V4:30:ARG:HD3 | 2:V4:30:ARG:C | 2.39 | 0.48 |
| 3:H4:108:ARG:NE | 11:aA:97:ALA:HB2 | 2.28 | 0.48 |
| 3:Q4:103:SER:C | 3:Q4:105:LEU:H | 2.20 | 0.48 |
| 1:L5:106:GLU:HG3 | 9:i5:58:THR:HG22 | 1.93 | 0.48 |
| 8:O5:19:SER:O | 8:O5:23:LEU:HB2 | 2.13 | 0.48 |
| 8:A5:107:ILE:HG21 | 1:B5:13:ASP:OD1 | 2.13 | 0.48 |
| 8:A5:130:VAL:HG12 | 8:A5:157:VAL:HG23 | 1.96 | 0.48 |
| 1:B5:76:ARG:CG | 9:z5:14:LEU:O | 2.61 | 0.48 |
| 8:C5:18:LEU:H | 8:C5:18:LEU:HD12 | 1.78 | 0.48 |
| 8:I5:27:LYS:O | 8:I5:29:PHE:C | 2.56 | 0.48 |
| 8:I5:37:LEU:HD22 | 1:J5:27:LEU:HD12 | 1.95 | 0.48 |
| 8:e5:2:SER:CA | 8:e5:100:ASP:HB3 | 2.43 | 0.48 |
| 8:e5:40:ALA:HB2 | 8:e5:97:VAL:HG13 | 1.95 | 0.48 |
| 8:Y5:130:VAL:HG12 | 8:Y5:157:VAL:HG23 | 1.95 | 0.48 |
| 2:K6:33:ARG:CG | 2:A6:25:GLN:HG2 | 2.39 | 0.48 |
| 6:M6:65:VAL:HG11 | 1:b7:60:LEU:CA | 2.43 | 0.48 |
| 10:j5:71:ALA:HB1 | 10:j5:202:ALA:HB1 | 1.95 | 0.48 |
| 10:j5:755:GLN:H | 10:j5:879:ASP:HB2 | 1.78 | 0.48 |
| 10:j5:863:ILE:O | 10:j5:863:ILE:HG22 | 2.11 | 0.48 |
| 10:j5:990:ARG:HG2 | 8:g7:110:ILE:HD12 | 1.94 | 0.48 |
| 10:k5:547:ARG:C | 10:k5:547:ARG:CD | 2.85 | 0.48 |
| 10:k5:750:ARG:NH1 | 10:k5:750:ARG:CG | 2.74 | 0.48 |
| 10:k5:935:LEU:CD1 | 1:D7:25:ASP:O | 2.55 | 0.48 |
| 2:A6:59:VAL:HG12 | 2:A6:66:LEU:HD13 | 1.95 | 0.48 |
| 2:A6:60:TYR:CE1 | 2:A6:73:GLY:HA3 | 2.47 | 0.48 |
| 8:Q7:22:GLU:H | 8:C7:6:LYS:HZ3 | 1.60 | 0.48 |
| 8:K7:4:LEU:HD21 | 8:K7:26:ILE:HD13 | 1.93 | 0.48 |
| 8:i7:89:LEU:HD13 | 8:i7:153:PHE:CE1 | 2.48 | 0.48 |
| 8:i7:141:LEU:CD1 | 8:i7:146:ALA:HA | 2.43 | 0.48 |
| 12:T7:201:CYC:CMA | 12:T7:201:CYC:NB | 2.74 | 0.48 |
| 8:U7:21:GLY:HA2 | 8:U7:24:ASP:OD2 | 2.12 | 0.48 |
| 8:W7:128:GLU:HA | 8:W7:128:GLU:OE1 | 2.13 | 0.48 |
| 8:Y7:65:VAL:CG2 | 8:Y7:66:VAL:N | 2.76 | 0.48 |
| 8:c7:141:LEU:CD1 | 8:c7:146:ALA:HA | 2.43 | 0.48 |
| 8:e7:151:PHE:HB3 | 8:q7:20:PRO:HB3 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:A8:60:TYR:CE1 | 2:A8:73:GLY:HA3 | 2.47 | 0.48 |
| 8:m7:19:SER:O | 8:m7:20:PRO:C | 2.56 | 0.48 |
| 2:X8:67:THR:O | 3:T9:28:THR:HG23 | 2.13 | 0.48 |
| 4:M8:128:ALA:HB3 | 4:M8:142:PHE:CZ | 2.49 | 0.48 |
| 4:M8:176:ARG:HG2 | 4:M8:176:ARG:O | 2.13 | 0.48 |
| 2:N8:34:ALA:HB3 | 3:O8:31:VAL:CG1 | 2.39 | 0.48 |
| 2:N8:59:VAL:HG12 | 2:N8:66:LEU:HD13 | 1.95 | 0.48 |
| 2:N8:64:PRO:C | 2:N8:66:LEU:N | 2.71 | 0.48 |
| 3:Q8:81:ALA:CB | 5:Z8:36:THR:HG21 | 2.43 | 0.48 |
| 3:L9:41:VAL:HG21 | 3:L9:98:LEU:HB2 | 1.95 | 0.48 |
| 12:L9:202:CYC:CMA | 12:L9:202:CYC:HB | 2.25 | 0.48 |
| 5:N9:54:LEU:HD12 | 12:T9:301:CYC:C1B | 2.33 | 0.48 |
| 2:O9:60:TYR:CE1 | 2:O9:73:GLY:HA3 | 2.47 | 0.48 |
| 2:K9:11:SER:O | 2:K9:15:GLN:HB2 | 2.13 | 0.48 |
| 11:a9:70:ALA:N | 11:a9:71:ILE:CD1 | 2.76 | 0.48 |
| 11:a9:710:THR:HA | 11:a9:807:GLN:CB | 2.43 | 0.48 |
| 11:aA:598:SER:CB | 11:aA:599:PRO:CD | 2.91 | 0.48 |
| 4:M1:176:ARG:HH11 | 4:M1:176:ARG:HG2 | 1.74 | 0.48 |
| 12:X1:201:CYC:HB | 12:X1:201:CYC:CMA | 2.26 | 0.48 |
| 1:A:16:GLY:O | 8:a5:90:ARG:NE | 2.46 | 0.48 |
| 12:A:201:CYC:HBB2 | 10:k5:256:LEU:HD11 | 1.94 | 0.48 |
| 3:DA:52:ILE:HD11 | 3:DA:87:GLU:HA | 1.95 | 0.48 |
| 12:DA:201:CYC:HBB2 | 4:MA:6:THR:CG2 | 2.43 | 0.48 |
| 3:RA:52:ILE:HD11 | 3:RA:87:GLU:HA | 1.95 | 0.48 |
| 12:TA:301:CYC:HB | 12:TA:301:CYC:CMA | 2.25 | 0.48 |
| 2:O1:30:ARG:HD3 | 2:O1:30:ARG:C | 2.38 | 0.48 |
| 2:O1:59:VAL:HG12 | 2:O1:66:LEU:HD13 | 1.96 | 0.48 |
| 12:H2:201:CYC:O1D | 6:M2:249:ARG:CB | 2.61 | 0.48 |
| 12:L2:201:CYC:HB | 12:L2:201:CYC:CMA | 2.25 | 0.48 |
| 6:M2:65:VAL:CG1 | 1:h7:59:ALA:O | 2.57 | 0.48 |
| 2:C3:30:ARG:HD3 | 2:C3:30:ARG:C | 2.39 | 0.48 |
| 2:U3:30:ARG:HD3 | 2:U3:30:ARG:C | 2.38 | 0.48 |
| 4:M4:144:ARG:HH12 | 5:Z4:59:ARG:NH2 | 2.03 | 0.48 |
| 4:M4:230:GLN:HG2 | 4:M4:231:THR:O | 2.13 | 0.48 |
| 2:N4:31:PHE:CD2 | 3:O4:34:SER:HB2 | 2.49 | 0.48 |
| 3:O4:106:GLU:O | 3:O4:111:ASN:CG | 2.56 | 0.48 |
| 12:O4:202:CYC:HC | 12:O4:202:CYC:HMD3 | 1.78 | 0.48 |
| 3:Q4:120:LEU:HD11 | 5:Z4:39:PRO:CA | 2.43 | 0.48 |
| 12:K5:201:CYC:O1D | 1:J5:62:TYR:HE1 | 1.94 | 0.48 |
| 8:A5:88:TYR:CZ | 12:A5:201:CYC:HMB3 | 2.48 | 0.48 |
| 12:B5:201:CYC:HBA1 | 9:z5:26:THR:HG23 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:E5:113:LYS:O | 8:E5:117:ASN:ND2 | 2.46 | 0.48 |
| 8:E5:131:ARG:HG3 | 8:E5:157:VAL:HG21 | 1.95 | 0.48 |
| 8:G5:100:ASP:OD1 | 8:S5:20:PRO:HB3 | 2.05 | 0.48 |
| 8:I5:4:LEU:CD2 | 8:I5:4:LEU:C | 2.84 | 0.48 |
| 2:C1:30:ARG:C | 2:C1:30:ARG:HD3 | 2.39 | 0.48 |
| 8:c5:14:GLU:OE2 | 10:j5:393:MET:CA | 2.61 | 0.48 |
| 1:R5:86:ASP:O | 1:R5:90:ARG:HG3 | 2.12 | 0.48 |
| 8:U5:2:SER:CA | 8:U5:100:ASP:HB3 | 2.43 | 0.48 |
| 8:Y5:14:GLU:OE2 | 10:k5:393:MET:HG3 | 2.12 | 0.48 |
| 8:a5:19:SER:HB3 | 8:a5:22:GLU:HB2 | 1.94 | 0.48 |
| 8:a5:40:ALA:HB2 | 8:a5:97:VAL:HG13 | 1.96 | 0.48 |
| 8:a5:95:GLY:N | 8:a5:104:ILE:HD11 | 2.27 | 0.48 |
| 12:L6:202:CYC:C4B | 2:A6:33:ARG:NH1 | 2.44 | 0.48 |
| 6:M6:47:TYR:CE2 | 8:c7:48:GLU:HG2 | 2.48 | 0.48 |
| 10:j5:241:ALA:O | 10:j5:243:ALA:N | 2.44 | 0.48 |
| 10:j5:725:LEU:CD2 | 8:K7:83:ARG:HD3 | 2.43 | 0.48 |
| 10:k5:238:ARG:C | 10:k5:238:ARG:NE | 2.72 | 0.48 |
| 10:k5:277:ILE:CA | 10:k5:284:PRO:HA | 2.43 | 0.48 |
| 10:k5:851:HIS:ND1 | 10:k5:851:HIS:C | 2.71 | 0.48 |
| 10:k5:1057:LYS:O | 10:k5:1061:LEU:HG | 2.12 | 0.48 |
| 10:k5:1067:LEU:HD22 | 10:k5:1067:LEU:HA | 1.70 | 0.48 |
| 10:k5:1119:LEU:CD1 | 12:k5:1204:CYC:HBB2 | 2.43 | 0.48 |
| 8:O7:44:THR:OG1 | 1:P7:18:TYR:HD2 | 1.91 | 0.48 |
| 8:K7:39:ILE:HG12 | 8:K7:145:ASP:HB3 | 1.95 | 0.48 |
| 8:g7:57:GLN:O | 8:g7:61:ILE:HD13 | 2.12 | 0.48 |
| 8:g7:130:VAL:HG12 | 8:g7:157:VAL:HG23 | 1.95 | 0.48 |
| 1:h7:76:ARG:HA | 8:i7:110:ILE:O | 2.13 | 0.48 |
| 8:U7:40:ALA:HB2 | 8:U7:97:VAL:HG13 | 1.96 | 0.48 |
| 8:Y7:118:SER:HB2 | 1:d7:82:ILE:HD12 | 1.95 | 0.48 |
| 8:c7:54:ALA:HB2 | 8:c7:133:MET:CA | 2.42 | 0.48 |
| 8:e7:17:TYR:CD2 | 1:f7:45:SER:HB3 | 2.48 | 0.48 |
| 8:e7:130:VAL:HG12 | 8:e7:157:VAL:HG23 | 1.96 | 0.48 |
| 2:A8:30:ARG:HD3 | 2:A8:30:ARG:C | 2.39 | 0.48 |
| 8:o7:8:ILE:CD1 | 1:p7:98:ALA:HB2 | 2.44 | 0.48 |
| 8:o7:97:VAL:HG22 | 1:p7:19:LEU:HD12 | 1.91 | 0.48 |
| 8:s7:19:SER:O | 8:s7:20:PRO:C | 2.56 | 0.48 |
| 3:H8:120:LEU:N | 11:a9:266:ASN:CG | 2.72 | 0.48 |
| 3:H8:120:LEU:N | 11:a9:266:ASN:ND2 | 2.61 | 0.48 |
| 2:I8:138:VAL:O | 2:I8:138:VAL:HG12 | 2.12 | 0.48 |
| 2:N8:115:GLU:OE1 | 5:Z8:33:GLY:CA | 2.56 | 0.48 |
| 3:Q8:84:ARG:HG3 | 5:Z8:31:TRP:CD2 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:Q8:110:LEU:CD2 | 3:Q8:170:SER:HB3 | 2.28 | 0.48 |
| 3:F1:52:ILE:HD11 | 3:F1:87:GLU:HA | 1.95 | 0.48 |
| 3:F1:88:ILE:HG21 | 12:F1:201:CYC:HAB2 | 1.95 | 0.48 |
| 4:M9:38:PRO:HB2 | 3:B9:113:LEU:HA | 1.95 | 0.48 |
| 2:O9:52:VAL:CG1 | 2:O9:83:ALA:HA | 2.43 | 0.48 |
| 3:Y8:103:SER:O | 3:Y8:107:ASP:HB2 | 2.13 | 0.48 |
| 2:I9:5:ILE:HG21 | 3:J9:99:ALA:HA | 1.94 | 0.48 |
| 11:a9:643:LEU:CD1 | 11:a9:689:VAL:HG23 | 2.42 | 0.48 |
| 11:aA:68:THR:O | 11:aA:69:ARG:HG3 | 2.14 | 0.48 |
| 11:aA:816:LEU:CD2 | 11:aA:816:LEU:C | 2.85 | 0.48 |
| 12:aA:901:CYC:HAB2 | 3:J1:88:ILE:HG21 | 1.95 | 0.48 |
| 3:H1:88:ILE:HG21 | 12:H1:201:CYC:CAB | 2.42 | 0.48 |
| 4:M1:176:ARG:HG2 | 4:M1:176:ARG:O | 2.13 | 0.48 |
| 2:A2:59:VAL:HG12 | 2:A2:66:LEU:HD13 | 1.95 | 0.48 |
| 12:D2:201:CYC:HB | 12:D2:201:CYC:CMA | 2.26 | 0.48 |
| 3:BA:113:LEU:HA | 4:MA:38:PRO:HB2 | 1.95 | 0.48 |
| 3:HA:52:ILE:HD11 | 3:HA:87:GLU:HA | 1.95 | 0.48 |
| 3:JA:52:ILE:HD11 | 3:JA:87:GLU:HA | 1.95 | 0.48 |
| 2:KA:11:SER:O | 2:KA:15:GLN:HB2 | 2.13 | 0.48 |
| 4:MA:51:ARG:HB3 | 4:MA:51:ARG:NH1 | 2.23 | 0.48 |
| 4:MA:94:TRP:CH2 | 5:NA:29:HIS:CE1 | 3.01 | 0.48 |
| 2:QA:32:GLN:OE1 | 2:UA:32:GLN:OE1 | 2.32 | 0.48 |
| 3:TA:88:ILE:HG21 | 12:TA:301:CYC:HAB2 | 1.95 | 0.48 |
| 12:XA:201:CYC:HB | 12:XA:201:CYC:CMA | 2.25 | 0.48 |
| 2:A1:52:VAL:CG1 | 2:A1:83:ALA:HA | 2.44 | 0.48 |
| 3:J3:77:ARG:HH21 | 2:K3:106:ASP:C | 2.22 | 0.48 |
| 12:J3:202:CYC:CMA | 12:J3:202:CYC:HB | 2.26 | 0.48 |
| 12:J3:202:CYC:HAA1 | 11:a9:800:THR:HB | 1.95 | 0.48 |
| 2:I2:118:ARG:HH22 | 6:M2:118:GLU:CD | 2.19 | 0.48 |
| 4:M3:14:LEU:N | 4:M3:14:LEU:CD1 | 2.77 | 0.48 |
| 4:M3:176:ARG:HH11 | 4:M3:176:ARG:HG3 | 1.78 | 0.48 |
| 3:R3:52:ILE:HD11 | 3:R3:87:GLU:HA | 1.95 | 0.48 |
| 3:T3:52:ILE:HD11 | 3:T3:87:GLU:HA | 1.95 | 0.48 |
| 3:V3:21:GLU:HG2 | 2:Q9:64:PRO:HB3 | 1.95 | 0.48 |
| 4:M4:148:LYS:CD | 4:M4:197:ASP:OD1 | 2.61 | 0.48 |
| 4:M4:228:SER:OG | 2:X4:16:GLY:O | 2.31 | 0.48 |
| 2:N4:5:ILE:HG21 | 3:O4:99:ALA:HA | 1.96 | 0.48 |
| 2:N4:52:VAL:CG1 | 2:N4:83:ALA:HA | 2.43 | 0.48 |
| 8:K5:4:LEU:HD23 | 8:K5:26:ILE:CD1 | 2.38 | 0.48 |
| 3:Y4:89:ILE:C | 3:Y4:92:TYR:CE2 | 2.82 | 0.48 |
| 5:Z4:23:SER:OG | 5:Z4:25:THR:CB | 2.60 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:B5:10:ASN:OD1 | 10:k5:557:VAL:CA | 2.53 | 0.48 |
| 1:D5:62:TYR:OH | 12:E5:201:CYC:CGD | 2.61 | 0.48 |
| 8:I5:4:LEU:O | 8:I5:4:LEU:HD23 | 2.14 | 0.48 |
| 1:V5:118:SER:OG | 10:j5:498:ALA:CB | 2.61 | 0.48 |
| 12:J6:201:CYC:HC | 12:J6:201:CYC:HMD3 | 1.78 | 0.48 |
| 12:J6:202:CYC:HMA3 | 6:M6:160:ASN:HD21 | 1.77 | 0.48 |
| 10:j5:743:VAL:N | 12:J7:201:CYC:CGD | 2.67 | 0.48 |
| 10:j5:829:VAL:O | 10:j5:829:VAL:HG12 | 2.12 | 0.48 |
| 10:k5:85:SER:HB2 | 10:k5:157:ILE:HG21 | 1.95 | 0.48 |
| 10:k5:213:LEU:HD12 | 10:k5:213:LEU:H | 1.79 | 0.48 |
| 10:k5:776:PHE:O | 10:k5:777:ASP:CB | 2.59 | 0.48 |
| 10:k5:949:ARG:NH2 | 10:k5:954:GLU:OE2 | 2.45 | 0.48 |
| 1:R7:53:LYS:HZ2 | 8:M7:120:GLN:CD | 2.20 | 0.48 |
| 8:S7:57:GLN:O | 8:S7:61:ILE:HD13 | 2.12 | 0.48 |
| 8:G7:39:ILE:HG12 | 8:G7:145:ASP:HB3 | 1.95 | 0.48 |
| 8:G7:65:VAL:CG2 | 8:G7:66:VAL:N | 2.76 | 0.48 |
| 8:G7:130:VAL:HG12 | 8:G7:157:VAL:HG23 | 1.95 | 0.48 |
| 1:J7:53:LYS:HZ2 | 8:K7:120:GLN:CD | 2.22 | 0.48 |
| 8:k7:66:VAL:O | 11:a9:65:LEU:CD2 | 2.60 | 0.48 |
| 8:U7:130:VAL:HG12 | 8:U7:157:VAL:HG23 | 1.96 | 0.48 |
| 8:c7:54:ALA:HB3 | 8:c7:133:MET:HG3 | 1.85 | 0.48 |
| 8:e7:65:VAL:CG2 | 8:e7:66:VAL:N | 2.76 | 0.48 |
| 3:B8:68:ARG:HH12 | 3:U8:68:ARG:CZ | 2.26 | 0.48 |
| 8:o7:4:LEU:CD1 | 1:p7:30:TYR:CZ | 2.93 | 0.48 |
| 8:o7:39:ILE:HD11 | 8:o7:145:ASP:HA | 1.95 | 0.48 |
| 12:r7:201:CYC:HMD1 | 12:r7:201:CYC:NC | 2.09 | 0.48 |
| 9:y7:9:ALA:HB2 | 9:y7:44:ILE:CD1 | 2.42 | 0.48 |
| 2:X8:138:VAL:HG12 | 2:X8:138:VAL:O | 2.12 | 0.48 |
| 4:M8:14:LEU:N | 4:M8:14:LEU:CD1 | 2.77 | 0.48 |
| 4:M8:102:VAL:HG12 | 4:M8:106:ILE:HD11 | 1.95 | 0.48 |
| 2:N8:31:PHE:CD2 | 3:O8:34:SER:HB2 | 2.49 | 0.48 |
| 3:F1:119:ALA:HB3 | 4:M1:41:ASN:ND2 | 2.27 | 0.48 |
| 4:M9:185:ALA:N | 12:V9:201:CYC:HBA2 | 2.28 | 0.48 |
| 4:M9:211:GLN:O | 5:N9:28:HIS:CE1 | 2.64 | 0.48 |
| 4:M9:230:GLN:HG2 | 4:M9:231:THR:O | 2.13 | 0.48 |
| 2:O9:34:ALA:CB | 3:P9:31:VAL:HG21 | 2.44 | 0.48 |
| 2:O9:64:PRO:C | 2:O9:66:LEU:N | 2.71 | 0.48 |
| 3:F9:150:ARG:NH1 | 12:F9:302:CYC:C2C | 2.71 | 0.48 |
| 2:I9:138:VAL:O | 2:I9:138:VAL:HG12 | 2.11 | 0.48 |
| 3:J9:65:ASP:HB2 | 11:a9:354:VAL:HG21 | 1.76 | 0.48 |
| 3:J9:88:ILE:HG21 | 12:J9:202:CYC:HAB2 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:a9:598:SER:CB | 11:a9:599:PRO:CD | 2.91 | 0.48 |
| 4:M1:33:LEU:O | 4:M1:33:LEU:HD13 | 2.13 | 0.48 |
| 5:N1:15:LEU:O | 5:N1:73:GLY:CA | 2.61 | 0.48 |
| 3:T1:52:ILE:HD11 | 3:T1:87:GLU:HA | 1.95 | 0.48 |
| 3:Z1:88:ILE:HG21 | 12:Z1:202:CYC:HAB2 | 1.95 | 0.48 |
| 2:A2:64:PRO:C | 2:A2:66:LEU:N | 2.71 | 0.48 |
| 3:DA:88:ILE:HG21 | 12:DA:201:CYC:HAB2 | 1.95 | 0.48 |
| 3:HA:123:PRO:HG2 | 12:HA:202:CYC:CMC | 2.44 | 0.48 |
| 3:LA:41:VAL:HG21 | 3:LA:98:LEU:HB2 | 1.95 | 0.48 |
| 2:QA:145:GLN:OE1 | 12:VA:202:CYC:CHB | 2.62 | 0.48 |
| 12:QA:201:CYC:CBA | 3:TA:79:MET:HE1 | 2.44 | 0.48 |
| 12:P1:201:CYC:HB | 12:P1:201:CYC:CMA | 2.25 | 0.48 |
| 3:J2:88:ILE:HG21 | 12:J2:202:CYC:HAB2 | 1.95 | 0.48 |
| 2:A3:30:ARG:HD3 | 2:A3:30:ARG:C | 2.39 | 0.48 |
| 3:F3:88:ILE:HG21 | 12:F3:201:CYC:HAB2 | 1.95 | 0.48 |
| 3:B4:68:ARG:HH12 | 3:U4:68:ARG:CZ | 2.26 | 0.48 |
| 3:B4:92:TYR:CZ | 12:B4:202:CYC:HAB2 | 2.49 | 0.48 |
| 3:D4:88:ILE:HG21 | 12:D4:202:CYC:HAB2 | 1.95 | 0.48 |
| 4:M3:184:ILE:HA | 4:M3:184:ILE:HD13 | 1.65 | 0.48 |
| 3:S4:108:ARG:O | 12:S4:202:CYC:CBB | 2.54 | 0.48 |
| 3:U4:115:GLU:HB2 | 4:M4:74:LEU:CG | 2.39 | 0.48 |
| 4:M4:251:ASN:H | 4:M4:251:ASN:ND2 | 1.95 | 0.48 |
| 1:N5:107:ARG:CZ | 10:k5:482:GLN:OE1 | 2.61 | 0.48 |
| 8:A5:103:PRO:CA | 10:k5:557:VAL:CG2 | 2.88 | 0.48 |
| 8:I5:26:ILE:O | 8:I5:26:ILE:HG12 | 2.13 | 0.48 |
| 8:c5:94:TYR:OH | 1:d5:17:LYS:O | 2.24 | 0.48 |
| 8:e5:130:VAL:HG12 | 8:e5:157:VAL:HG23 | 1.96 | 0.48 |
| 12:T5:201:CYC:CBB | 10:j5:482:GLN:HE22 | 1.99 | 0.48 |
| 8:U5:82:LEU:CD1 | 6:M6:34:ARG:HB3 | 2.44 | 0.48 |
| 8:a5:130:VAL:HG12 | 8:a5:157:VAL:HG23 | 1.96 | 0.48 |
| 6:M6:42:VAL:HG11 | 8:c7:56:ASP:OD1 | 2.13 | 0.48 |
| 12:N6:101:CYC:HB | 12:N6:101:CYC:CMA | 2.25 | 0.48 |
| 9:z5:6:LYS:HG2 | 9:z5:55:LYS:HB2 | 1.85 | 0.48 |
| 10:j5:558:VAL:O | 10:j5:559:THR:C | 2.57 | 0.48 |
| 10:j5:929:PRO:CG | 1:J7:147:LYS:CG | 2.87 | 0.48 |
| 10:j5:951:MET:HE2 | 10:j5:955:LEU:HD11 | 1.96 | 0.48 |
| 10:k5:26:ASN:ND2 | 10:k5:267:ASP:OD1 | 2.46 | 0.48 |
| 10:k5:71:ALA:HB1 | 10:k5:202:ALA:HB1 | 1.95 | 0.48 |
| 10:k5:275:THR:HG23 | 10:k5:286:VAL:CG1 | 2.32 | 0.48 |
| 10:k5:829:VAL:O | 10:k5:829:VAL:HG12 | 2.13 | 0.48 |
| 10:k5:844:GLN:C | 10:k5:846:GLU:H | 2.21 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:k5:1017:ARG:C | 10:k5:1018:LEU:HG | 2.39 | 0.48 |
| 12:k5:1202:CYC:HMA3 | 12:k5:1202:CYC:NB | 2.29 | 0.48 |
| 12:D1:202:CYC:HAA1 | 4:M1:52:LEU:HD13 | 1.96 | 0.48 |
| 1:P7:14:VAL:O | 1:N7:68:PRO:C | 2.57 | 0.48 |
| 1:R7:53:LYS:HZ1 | 8:M7:120:GLN:CG | 2.26 | 0.48 |
| 1:B7:68:PRO:C | 1:D7:14:VAL:O | 2.57 | 0.48 |
| 8:I7:20:PRO:HB3 | 8:W7:151:PHE:CZ | 2.48 | 0.48 |
| 8:i7:43:LEU:HD13 | 8:i7:141:LEU:HD21 | 1.94 | 0.48 |
| 8:i7:57:GLN:O | 8:i7:61:ILE:HD13 | 2.12 | 0.48 |
| 8:c7:126:VAL:CG2 | 12:c7:201:CYC:CMC | 2.91 | 0.48 |
| 2:E1:30:ARG:HD3 | 2:E1:30:ARG:C | 2.39 | 0.48 |
| 2:A8:59:VAL:HG12 | 2:A8:66:LEU:HD13 | 1.96 | 0.48 |
| 2:A8:64:PRO:C | 2:A8:66:LEU:N | 2.71 | 0.48 |
| 12:D8:202:CYC:CMA | 12:D8:202:CYC:HB | 2.26 | 0.48 |
| 8:o7:80:LEU:HD12 | 12:o7:201:CYC:C3D | 2.43 | 0.48 |
| 9:w7:15:LYS:HD2 | 9:w7:15:LYS:C | 2.38 | 0.48 |
| 3:F8:109:CYS:O | 4:M8:6:THR:CG2 | 2.61 | 0.48 |
| 3:F8:110:LEU:HA | 3:F8:113:LEU:HB2 | 1.94 | 0.48 |
| 3:L8:78:ARG:O | 12:a9:901:CYC:HMD1 | 2.13 | 0.48 |
| 4:M8:141:GLU:OE1 | 4:M8:141:GLU:HA | 2.13 | 0.48 |
| 4:M9:233:GLU:HG2 | 4:M9:233:GLU:O | 2.13 | 0.48 |
| 5:N9:3:VAL:HG11 | 3:R9:115:GLU:HB3 | 1.93 | 0.48 |
| 2:O9:31:PHE:CD2 | 3:P9:34:SER:HB2 | 2.49 | 0.48 |
| 5:Z8:41:GLN:HB2 | 12:Z8:301:CYC:HMB1 | 1.90 | 0.48 |
| 5:Z8:66:ARG:CB | 5:Z8:66:ARG:HH11 | 2.22 | 0.48 |
| 3:T9:88:ILE:HG21 | 12:T9:301:CYC:HAB2 | 1.95 | 0.48 |
| 12:X9:201:CYC:HB | 12:X9:201:CYC:CMA | 2.25 | 0.48 |
| 11:a9:245:ALA:HB3 | 12:a9:901:CYC:HBB3 | 1.80 | 0.48 |
| 11:a9:523:GLN:HE22 | 11:a9:548:LEU:HD13 | 1.73 | 0.48 |
| 11:aA:106:LEU:C | 11:aA:106:LEU:CD2 | 2.85 | 0.48 |
| 11:aA:821:ARG:NH1 | 3:L1:120:LEU:O | 2.47 | 0.48 |
| 3:H1:78:ARG:HG2 | 12:H1:201:CYC:CMD | 2.43 | 0.48 |
| 2:Y1:30:ARG:HD3 | 2:Y1:30:ARG:C | 2.39 | 0.48 |
| 2:AA:59:VAL:HG12 | 2:AA:66:LEU:HD13 | 1.96 | 0.48 |
| 3:DA:115:GLU:CG | 4:MA:78:GLY:HA2 | 2.44 | 0.48 |
| 12:HA:202:CYC:OB | 11:aA:448:ASN:CB | 2.61 | 0.48 |
| 3:LA:111:ASN:CG | 11:aA:366:LEU:CD1 | 2.86 | 0.48 |
| 4:MA:233:GLU:HG2 | 4:MA:233:GLU:O | 2.13 | 0.48 |
| 5:NA:15:LEU:O | 5:NA:73:GLY:CA | 2.61 | 0.48 |
| 2:OA:34:ALA:CB | 3:PA:31:VAL:HG21 | 2.44 | 0.48 |
| 2:WA:30:ARG:HD3 | 2:WA:30:ARG:C | 2.39 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:L2:75:PRO:HG2 | 3:L2:78:ARG:CG | 2.40 | 0.48 |
| 3:L2:125:ARG:NE | 1:h7:69:GLY:O | 2.47 | 0.48 |
| 2:A3:5:ILE:HG21 | 3:B3:99:ALA:HA | 1.96 | 0.48 |
| 2:A4:34:ALA:CB | 3:B4:31:VAL:HG11 | 2.39 | 0.48 |
| 3:L3:52:ILE:HD11 | 3:L3:87:GLU:HA | 1.96 | 0.48 |
| 2:O3:34:ALA:CB | 3:P3:31:VAL:HG21 | 2.44 | 0.48 |
| 3:R3:88:ILE:HG21 | 12:R3:201:CYC:HAB2 | 1.95 | 0.48 |
| 12:V3:201:CYC:HB | 12:V3:201:CYC:CMA | 2.26 | 0.48 |
| 3:U4:52:ILE:HD11 | 3:U4:87:GLU:HA | 1.95 | 0.48 |
| 3:U4:115:GLU:OE1 | 4:M4:74:LEU:HD12 | 2.11 | 0.48 |
| 4:M4:26:SER:CB | 11:aA:228:GLU:HG3 | 2.43 | 0.48 |
| 4:M4:30:TRP:HE1 | 11:aA:105:GLU:CD | 2.22 | 0.48 |
| 4:M4:141:GLU:HG3 | 4:M4:145:LEU:CD1 | 2.43 | 0.48 |
| 4:M4:176:ARG:HH11 | 4:M4:176:ARG:HG3 | 1.78 | 0.48 |
| 4:M4:226:SER:CB | 3:Y4:85:ASP:CA | 2.91 | 0.48 |
| 8:K5:39:ILE:HG12 | 8:K5:145:ASP:HB3 | 1.95 | 0.48 |
| 8:M5:57:GLN:O | 8:M5:61:ILE:HD13 | 2.12 | 0.48 |
| 8:E5:79:ALA:C | 8:E5:81:CYS:H | 2.21 | 0.48 |
| 8:I5:18:LEU:H | 8:I5:18:LEU:HD12 | 1.78 | 0.48 |
| 10:j5:77:VAL:O | 10:j5:77:VAL:HG23 | 2.13 | 0.48 |
| 10:j5:844:GLN:C | 10:j5:846:GLU:H | 2.21 | 0.48 |
| 10:j5:1106:PHE:CE1 | 10:j5:1112:PRO:HA | 2.49 | 0.48 |
| 10:k5:292:GLU:N | 10:k5:292:GLU:OE1 | 2.46 | 0.48 |
| 10:k5:546:PHE:HE1 | 10:k5:561:GLU:OE1 | 1.85 | 0.48 |
| 10:k5:951:MET:HE3 | 10:k5:951:MET:CA | 2.43 | 0.48 |
| 10:k5:1143:LEU:HD23 | 1:l7:10:ASN:HD21 | 1.78 | 0.48 |
| 3:B6:75:PRO:CB | 12:E6:201:CYC:HBB2 | 2.44 | 0.48 |
| 8:O7:2:SER:CA | 8:O7:100:ASP:HB3 | 2.43 | 0.48 |
| 8:O7:40:ALA:HB2 | 8:O7:97:VAL:HG13 | 1.96 | 0.48 |
| 1:D7:76:ARG:HB2 | 8:E7:110:ILE:HG13 | 1.95 | 0.48 |
| 8:i7:94:TYR:CE2 | 1:j7:9:ILE:HG22 | 2.46 | 0.48 |
| 8:a7:2:SER:CA | 8:a7:100:ASP:HB3 | 2.43 | 0.48 |
| 2:A8:25:GLN:HG2 | 2:K8:33:ARG:CG | 2.39 | 0.48 |
| 2:A8:34:ALA:CB | 3:B8:31:VAL:HG21 | 2.44 | 0.48 |
| 3:B8:109:CYS:HA | 4:M8:60:LYS:HZ3 | 1.77 | 0.48 |
| 12:p7:201:CYC:CMA | 12:p7:201:CYC:NB | 2.74 | 0.48 |
| 1:r7:68:PRO:CB | 1:t7:14:VAL:C | 2.67 | 0.48 |
| 9:w7:63:ALA:HB1 | 9:w7:67:VAL:HG21 | 1.95 | 0.48 |
| 2:T8:30:ARG:HD3 | 2:T8:30:ARG:C | 2.39 | 0.48 |
| 2:T8:138:VAL:O | 2:T8:138:VAL:HG12 | 2.11 | 0.48 |
| 12:H8:201:CYC:HB | 12:H8:201:CYC:CMA | 2.26 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M8:29:PRO:CG | 11:a9:226:PHE:HA | 2.41 | 0.48 |
| 4:M8:226:SER:CB | 3:Y8:85:ASP:N | 2.77 | 0.48 |
| 4:M8:235:PHE:CB | 12:M8:301:CYC:HMA1 | 2.41 | 0.48 |
| 12:M8:301:CYC:CMB | 3:Y8:89:ILE:CG1 | 2.80 | 0.48 |
| 2:N8:112:GLY:CA | 5:Z8:33:GLY:C | 2.66 | 0.48 |
| 3:Q8:84:ARG:CG | 5:Z8:31:TRP:HE1 | 2.18 | 0.48 |
| 2:R8:138:VAL:O | 2:R8:138:VAL:HG12 | 2.11 | 0.48 |
| 4:M9:78:GLY:HA2 | 3:D9:115:GLU:CG | 2.44 | 0.48 |
| 3:J9:52:ILE:HD11 | 3:J9:87:GLU:HA | 1.95 | 0.48 |
| 3:Z9:52:ILE:HD11 | 3:Z9:87:GLU:HA | 1.95 | 0.48 |
| 11:aA:95:ILE:HD13 | 11:aA:237:PHE:CD1 | 2.46 | 0.48 |
| 11:aA:197:ILE:CD1 | 11:aA:278:LEU:HD22 | 2.44 | 0.48 |
| 11:aA:595:ARG:HG3 | 11:aA:596:THR:H | 1.79 | 0.48 |
| 11:aA:802:ARG:HB2 | 3:J1:120:LEU:HD22 | 1.94 | 0.48 |
| 2:I1:30:ARG:HD3 | 2:I1:30:ARG:C | 2.39 | 0.48 |
| 4:M1:140:ARG:O | 4:M1:140:ARG:HG2 | 2.13 | 0.48 |
| 2:A2:31:PHE:CD2 | 3:B2:34:SER:HB2 | 2.49 | 0.48 |
| 2:A2:52:VAL:CG1 | 2:A2:83:ALA:HA | 2.43 | 0.48 |
| 2:E2:30:ARG:HD3 | 2:E2:30:ARG:C | 2.39 | 0.48 |
| 2:AA:31:PHE:CD2 | 3:BA:34:SER:HB2 | 2.49 | 0.48 |
| 3:FA:37:ARG:NH2 | 3:FA:159:GLU:CD | 2.58 | 0.48 |
| 3:FA:84:ARG:CZ | 4:MA:53:LEU:CD2 | 2.92 | 0.48 |
| 12:JA:202:CYC:HB | 11:aA:512:TYR:CA | 2.26 | 0.48 |
| 4:MA:153:LYS:HZ3 | 2:UA:14:SER:CB | 2.26 | 0.48 |
| 2:OA:30:ARG:HD3 | 2:OA:30:ARG:C | 2.39 | 0.48 |
| 2:QA:81:LYS:HZ3 | 3:TA:67:ILE:HD13 | 1.79 | 0.48 |
| 3:VA:52:ILE:HD11 | 3:VA:87:GLU:HA | 1.95 | 0.48 |
| 3:H2:52:ILE:HD11 | 3:H2:87:GLU:HA | 1.95 | 0.48 |
| 12:N2:101:CYC:HAB2 | 3:B2:88:ILE:HG21 | 1.96 | 0.48 |
| 3:Z3:52:ILE:HD11 | 3:Z3:87:GLU:HA | 1.95 | 0.48 |
| 3:D4:107:ASP:HB3 | 11:aA:109:ASN:CB | 2.42 | 0.48 |
| 5:N3:31:TRP:CG | 2:S3:16:GLY:HA3 | 2.44 | 0.48 |
| 2:O3:34:ALA:CB | 3:P3:31:VAL:HG11 | 2.38 | 0.48 |
| 2:O3:52:VAL:CG1 | 2:O3:83:ALA:HA | 2.43 | 0.48 |
| 3:H4:88:ILE:HG21 | 12:H4:201:CYC:HAB2 | 1.95 | 0.48 |
| 3:J4:108:ARG:HH21 | 11:aA:171:ARG:HB3 | 1.67 | 0.48 |
| 3:L4:65:ASP:HB2 | 11:aA:82:GLN:HE22 | 1.77 | 0.48 |
| 2:N4:30:ARG:C | 2:N4:30:ARG:HD3 | 2.38 | 0.48 |
| 2:N4:59:VAL:HG12 | 2:N4:66:LEU:HD13 | 1.95 | 0.48 |
| 8:K5:131:ARG:HG3 | 8:K5:157:VAL:HG21 | 1.95 | 0.48 |
| 8:A5:119:LEU:CD2 | 12:A5:201:CYC:HAA2 | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:E5:4:LEU:HD21 | 8:E5:26:ILE:HD13 | 1.93 | 0.48 |
| 1:R5:64:ASP:CB | 10:k5:704:THR:CG2 | 2.91 | 0.48 |
| 8:A7:23:LEU:HD22 | 1:B7:38:VAL:HG13 | 1.94 | 0.48 |
| 10:j5:72:ALA:HB1 | 10:j5:81:PRO:HB2 | 1.96 | 0.48 |
| 10:j5:892:ALA:C | 10:j5:895:PRO:HD2 | 2.39 | 0.48 |
| 10:j5:930:LEU:HB3 | 1:J7:33:THR:HB | 1.95 | 0.48 |
| 10:k5:612:ILE:H | 10:k5:612:ILE:CD1 | 2.03 | 0.48 |
| 10:k5:1143:LEU:HD22 | 1:l7:10:ASN:OD1 | 2.14 | 0.48 |
| 8:O7:130:VAL:HG12 | 8:O7:157:VAL:HG23 | 1.96 | 0.48 |
| 8:C7:130:VAL:HG12 | 8:C7:157:VAL:HG23 | 1.96 | 0.48 |
| 12:L7:201:CYC:HMD1 | 12:L7:201:CYC:NC | 2.09 | 0.48 |
| 8:i7:57:GLN:HB2 | 8:i7:132:ALA:HB1 | 1.96 | 0.48 |
| 8:Y7:17:TYR:CD2 | 1:Z7:45:SER:HB3 | 2.48 | 0.48 |
| 8:Y7:130:VAL:HG12 | 8:Y7:157:VAL:HG23 | 1.96 | 0.48 |
| 8:a7:130:VAL:HG12 | 8:a7:157:VAL:HG23 | 1.95 | 0.48 |
| 12:b7:201:CYC:CMA | 12:b7:201:CYC:NB | 2.74 | 0.48 |
| 8:e7:54:ALA:HB2 | 8:e7:133:MET:HG2 | 1.96 | 0.48 |
| 8:m7:2:SER:CA | 8:m7:100:ASP:HB3 | 2.43 | 0.48 |
| 8:q7:39:ILE:HG12 | 8:q7:145:ASP:HB3 | 1.95 | 0.48 |
| 8:u7:8:ILE:CD1 | 1:v7:98:ALA:HB2 | 2.43 | 0.48 |
| 12:W8:201:CYC:HB | 12:W8:201:CYC:CMA | 2.26 | 0.48 |
| 3:H8:108:ARG:NH2 | 11:a9:97:ALA:HB2 | 2.28 | 0.48 |
| 2:K8:30:ARG:HD3 | 2:K8:30:ARG:C | 2.39 | 0.48 |
| 3:L8:71:GLY:H | 11:a9:82:GLN:CB | 2.27 | 0.48 |
| 4:M8:45:VAL:O | 4:M8:45:VAL:HG12 | 2.14 | 0.48 |
| 4:M8:204:ILE:O | 4:M8:204:ILE:HG22 | 2.14 | 0.48 |
| 4:M8:268:ARG:CZ | 3:Y8:111:ASN:HB3 | 2.44 | 0.48 |
| 12:M8:301:CYC:HBC3 | 3:Y8:127:VAL:HG22 | 1.94 | 0.48 |
| 4:M9:147:ALA:HB2 | 4:M9:173:PHE:CZ | 2.49 | 0.48 |
| 2:A9:52:VAL:CG1 | 2:A9:83:ALA:HA | 2.43 | 0.48 |
| 2:E9:30:ARG:C | 2:E9:30:ARG:HD3 | 2.39 | 0.48 |
| 3:F9:142:VAL:HG13 | 12:F9:303:CYC:HBC2 | 1.95 | 0.48 |
| 2:S9:138:VAL:HG12 | 2:S9:138:VAL:O | 2.11 | 0.48 |
| 11:a9:93:LEU:N | 11:a9:93:LEU:HD12 | 2.29 | 0.48 |
| 11:aA:93:LEU:N | 11:aA:93:LEU:HD12 | 2.29 | 0.48 |
| 11:aA:290:ASP:N | 11:aA:290:ASP:OD1 | 2.47 | 0.48 |
| 3:H1:52:ILE:HD11 | 3:H1:87:GLU:HA | 1.95 | 0.48 |
| 5:N1:38:GLU:HB3 | 5:N1:41:GLN:HE21 | 1.77 | 0.48 |
| 2:A2:60:TYR:CB | 2:A2:67:THR:CG2 | 2.83 | 0.48 |
| 1:Z:16:GLY:HA2 | 8:e5:90:ARG:HH12 | 1.74 | 0.48 |
| 1:Z:89:LEU:HD22 | 1:Z:133:MET:CE | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:Z:201:CYC:HMA3 | 12:Z:201:CYC:NB | 2.29 | 0.48 |
| 2:IA:145:GLN:OE1 | 12:F9:302:CYC:CHB | 2.61 | 0.48 |
| 12:JA:202:CYC:HBA2 | 11:aA:510:PHE:C | 2.34 | 0.48 |
| 3:LA:37:ARG:HH11 | 3:LA:97:LEU:HD12 | 1.79 | 0.48 |
| 12:LA:202:CYC:CMA | 11:aA:534:SER:HB2 | 2.44 | 0.48 |
| 4:MA:147:ALA:HB2 | 4:MA:173:PHE:CZ | 2.49 | 0.48 |
| 2:OA:25:GLN:HG2 | 2:YA:33:ARG:CG | 2.38 | 0.48 |
| 2:OA:34:ALA:CB | 3:PA:31:VAL:HG11 | 2.38 | 0.48 |
| 2:OA:59:VAL:HG12 | 2:OA:66:LEU:HD13 | 1.96 | 0.48 |
| 2:QA:33:ARG:CB | 2:UA:25:GLN:CG | 2.89 | 0.48 |
| 2:O1:5:ILE:HG21 | 3:P1:99:ALA:HA | 1.96 | 0.48 |
| 3:R1:52:ILE:HD11 | 3:R1:87:GLU:HA | 1.95 | 0.48 |
| 2:A1:34:ALA:CB | 3:B1:31:VAL:HG21 | 2.44 | 0.48 |
| 3:J2:52:ILE:HD11 | 3:J2:87:GLU:HA | 1.95 | 0.48 |
| 6:M2:127:SER:O | 12:F2:201:CYC:CMA | 2.61 | 0.48 |
| 2:A3:31:PHE:CD2 | 3:B3:34:SER:HB2 | 2.49 | 0.48 |
| 3:B3:91:ARG:HH22 | 11:a9:677:GLN:CD | 2.21 | 0.48 |
| 12:Z3:201:CYC:OB | 4:M3:162:ASN:HB3 | 2.09 | 0.48 |
| 4:M3:147:ALA:HB2 | 4:M3:173:PHE:CZ | 2.49 | 0.48 |
| 4:M3:233:GLU:HG2 | 4:M3:233:GLU:O | 2.13 | 0.48 |
| 4:M3:252:LEU:HD13 | 3:X3:77:ARG:NH1 | 2.28 | 0.48 |
| 3:U4:120:LEU:HD23 | 3:U4:120:LEU:C | 2.38 | 0.48 |
| 3:F4:115:GLU:CA | 4:M4:3:VAL:CG1 | 2.92 | 0.48 |
| 2:G4:30:ARG:HD3 | 2:G4:30:ARG:C | 2.39 | 0.48 |
| 2:I4:30:ARG:HD3 | 2:I4:30:ARG:C | 2.39 | 0.48 |
| 2:N4:34:ALA:CB | 3:O4:31:VAL:HG11 | 2.38 | 0.48 |
| 8:M5:49:ARG:HH12 | 1:J7:140:LEU:HD21 | 1.79 | 0.48 |
| 8:O5:2:SER:CA | 8:O5:100:ASP:HB3 | 2.43 | 0.48 |
| 3:Y4:124:THR:CG2 | 3:Y4:171:ILE:O | 2.61 | 0.48 |
| 8:G5:130:VAL:HG12 | 8:G5:157:VAL:HG23 | 1.96 | 0.48 |
| 1:f5:9:ILE:HG22 | 10:j5:17:PHE:HZ | 1.78 | 0.48 |
| 1:f5:18:TYR:CE1 | 10:j5:165:ARG:CG | 2.97 | 0.48 |
| 8:U5:130:VAL:HG12 | 8:U5:157:VAL:HG23 | 1.95 | 0.48 |
| 8:Y5:94:TYR:OH | 1:Z5:17:LYS:O | 2.24 | 0.48 |
| 6:M6:259:THR:O | 6:M6:261:LYS:N | 2.47 | 0.48 |
| 10:j5:296:VAL:O | 10:j5:296:VAL:HG12 | 2.14 | 0.48 |
| 10:j5:851:HIS:ND1 | 10:j5:851:HIS:C | 2.71 | 0.48 |
| 10:j5:1017:ARG:C | 10:j5:1018:LEU:HG | 2.39 | 0.48 |
| 10:k5:72:ALA:HB1 | 10:k5:81:PRO:HB2 | 1.96 | 0.48 |
| 10:k5:503:LYS:HB3 | 10:k5:503:LYS:HE3 | 1.59 | 0.48 |
| 10:k5:564:VAL:O | 10:k5:564:VAL:HG12 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:k5:575:ILE:HD12 | 10:k5:607:LEU:HD12 | 1.95 | 0.48 |
| 10:k5:651:ILE:HG21 | 10:k5:651:ILE:HD13 | 1.61 | 0.48 |
| 12:k5:1202:CYC:CMA | 12:k5:1202:CYC:NB | 2.74 | 0.48 |
| 12:k5:1204:CYC:HMA3 | 12:k5:1204:CYC:NB | 2.29 | 0.48 |
| 2:A6:30:ARG:HD3 | 2:A6:30:ARG:C | 2.39 | 0.48 |
| 2:G6:30:ARG:HD3 | 2:G6:30:ARG:C | 2.39 | 0.48 |
| 8:S7:130:VAL:HG12 | 8:S7:157:VAL:HG23 | 1.96 | 0.48 |
| 1:H7:136:VAL:HA | 11:aA:563:PHE:CE1 | 2.47 | 0.48 |
| 8:I7:130:VAL:HG12 | 8:I7:157:VAL:HG23 | 1.96 | 0.48 |
| 1:J7:76:ARG:HB2 | 8:K7:110:ILE:HG13 | 1.95 | 0.48 |
| 8:g7:2:SER:CA | 8:g7:100:ASP:HB3 | 2.43 | 0.48 |
| 8:k7:39:ILE:HG12 | 8:k7:145:ASP:HB3 | 1.96 | 0.48 |
| 8:e7:52:LYS:HB2 | 8:e7:52:LYS:HE3 | 1.53 | 0.48 |
| 3:D8:88:ILE:HG21 | 12:D8:202:CYC:HAB2 | 1.95 | 0.48 |
| 1:l7:68:PRO:C | 1:n7:14:VAL:O | 2.57 | 0.48 |
| 8:o7:23:LEU:HD22 | 1:p7:38:VAL:HG13 | 1.72 | 0.48 |
| 8:q7:79:ALA:CB | 11:aA:50:LEU:HA | 2.43 | 0.48 |
| 8:u7:39:ILE:HD11 | 8:u7:145:ASP:HA | 1.95 | 0.48 |
| 3:H8:52:ILE:HD11 | 3:H8:87:GLU:HA | 1.95 | 0.48 |
| 3:H8:108:ARG:NE | 11:a9:97:ALA:HB2 | 2.28 | 0.48 |
| 3:L8:82:CYS:HB2 | 12:a9:901:CYC:HC | 1.79 | 0.48 |
| 4:M8:29:PRO:CD | 11:a9:230:THR:OG1 | 2.61 | 0.48 |
| 4:M8:200:ILE:CB | 5:Z8:52:ARG:HH21 | 2.22 | 0.48 |
| 4:M8:231:THR:HA | 12:M8:301:CYC:CBB | 2.41 | 0.48 |
| 3:O8:88:ILE:HD11 | 5:Z8:54:LEU:HD11 | 1.94 | 0.48 |
| 2:R8:30:ARG:HD3 | 2:R8:30:ARG:C | 2.39 | 0.48 |
| 4:M9:14:LEU:N | 4:M9:14:LEU:CD1 | 2.76 | 0.48 |
| 4:M9:132:LEU:HD13 | 4:M9:142:PHE:CB | 2.44 | 0.48 |
| 5:N9:15:LEU:O | 5:N9:73:GLY:CA | 2.61 | 0.48 |
| 2:A9:5:ILE:HG21 | 3:B9:99:ALA:HA | 1.96 | 0.48 |
| 3:V9:52:ILE:HD11 | 3:V9:87:GLU:HA | 1.95 | 0.48 |
| 11:a9:68:THR:O | 11:a9:69:ARG:HG3 | 2.14 | 0.48 |
| 11:a9:643:LEU:H | 11:a9:643:LEU:CD1 | 2.03 | 0.48 |
| 11:a9:820:GLY:O | 11:a9:821:ARG:C | 2.56 | 0.48 |
| 11:aA:61:TYR:HA | 11:aA:65:LEU:CB | 2.41 | 0.48 |
| 11:aA:820:GLY:O | 11:aA:821:ARG:C | 2.56 | 0.48 |
| 3:H1:77:ARG:CZ | 12:H1:201:CYC:O2D | 2.61 | 0.48 |
| 4:M1:147:ALA:HB2 | 4:M1:173:PHE:CZ | 2.49 | 0.48 |
| 3:X1:52:ILE:HD11 | 3:X1:87:GLU:HA | 1.95 | 0.48 |
| 3:B2:52:ILE:HD11 | 3:B2:87:GLU:HA | 1.95 | 0.48 |
| 3:BA:52:ILE:HD11 | 3:BA:87:GLU:HA | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:IA:5:ILE:HG21 | 3:JA:99:ALA:HA | 1.94 | 0.48 |
| 3:VA:88:ILE:HG21 | 12:VA:201:CYC:HAB2 | 1.96 | 0.48 |
| 2:O1:34:ALA:CB | 3:P1:31:VAL:HG21 | 2.44 | 0.48 |
| 2:A1:5:ILE:HG21 | 3:B1:99:ALA:HA | 1.96 | 0.48 |
| 3:L2:68:ARG:HB2 | 6:M2:64:ALA:HB2 | 1.96 | 0.48 |
| 3:B3:84:ARG:HD3 | 11:a9:680:SER:OG | 2.09 | 0.48 |
| 3:D3:88:ILE:HG21 | 12:D3:202:CYC:HAB2 | 1.95 | 0.48 |
| 12:D3:202:CYC:HAA1 | 4:M3:52:LEU:HD13 | 1.96 | 0.48 |
| 2:E3:114:ARG:HH12 | 11:a9:671:GLU:CD | 2.21 | 0.48 |
| 2:A4:2:LYS:HE2 | 2:K4:22:THR:HB | 1.93 | 0.48 |
| 3:P3:75:PRO:CB | 12:S3:201:CYC:HBB2 | 2.44 | 0.48 |
| 3:W4:88:ILE:HG21 | 12:W4:201:CYC:HAB2 | 1.95 | 0.48 |
| 3:H4:120:LEU:N | 11:aA:266:ASN:ND2 | 2.62 | 0.48 |
| 3:J4:125:ARG:NH2 | 2:C2:68:GLN:NE2 | 2.62 | 0.48 |
| 4:M4:214:GLY:N | 5:Z4:28:HIS:CE1 | 2.81 | 0.48 |
| 2:N4:44:LEU:HD11 | 2:N4:142:LEU:HD11 | 1.96 | 0.48 |
| 8:G5:140:LEU:HA | 8:o7:52:LYS:NZ | 2.29 | 0.48 |
| 8:c5:39:ILE:HG12 | 8:c5:145:ASP:HB3 | 1.95 | 0.48 |
| 8:S5:54:ALA:HB2 | 8:S5:133:MET:HG2 | 1.96 | 0.48 |
| 8:W5:128:GLU:HA | 8:W5:128:GLU:OE1 | 2.13 | 0.48 |
| 1:Z5:28:LYS:CE | 1:t7:143:PRO:HB2 | 2.24 | 0.48 |
| 3:L6:88:ILE:HG21 | 12:L6:201:CYC:HAB2 | 1.95 | 0.48 |
| 10:j5:851:HIS:O | 10:j5:851:HIS:CG | 2.66 | 0.48 |
| 10:j5:919:ILE:HG22 | 10:j5:919:ILE:O | 2.13 | 0.48 |
| 10:j5:1054:SER:HA | 1:r7:107:ARG:CA | 2.41 | 0.48 |
| 10:k5:500:PRO:HG2 | 10:k5:500:PRO:O | 2.12 | 0.48 |
| 10:k5:851:HIS:O | 10:k5:851:HIS:CG | 2.66 | 0.48 |
| 10:k5:1069:ARG:NH2 | 10:k5:1072:ILE:HD11 | 2.29 | 0.48 |
| 8:O7:22:GLU:HA | 8:O7:25:ARG:HH11 | 1.79 | 0.48 |
| 1:P7:89:LEU:HD22 | 1:P7:133:MET:CE | 2.44 | 0.48 |
| 8:Q7:39:ILE:HG12 | 8:Q7:145:ASP:HB3 | 1.95 | 0.48 |
| 1:B7:89:LEU:HD22 | 1:B7:133:MET:CE | 2.44 | 0.48 |
| 8:C7:2:SER:CA | 8:C7:100:ASP:HB3 | 2.43 | 0.48 |
| 8:C7:40:ALA:HB2 | 8:C7:97:VAL:HG13 | 1.95 | 0.48 |
| 8:M7:65:VAL:CG2 | 8:M7:66:VAL:N | 2.75 | 0.48 |
| 8:g7:63:PRO:CB | 11:aA:333:GLN:O | 2.62 | 0.48 |
| 12:j7:201:CYC:NB | 12:j7:201:CYC:HMA3 | 2.29 | 0.48 |
| 8:k7:130:VAL:HG12 | 8:k7:157:VAL:HG23 | 1.95 | 0.48 |
| 1:T7:89:LEU:HD22 | 1:T7:133:MET:CE | 2.44 | 0.48 |
| 3:B8:92:TYR:CZ | 12:B8:202:CYC:HAB2 | 2.49 | 0.48 |
| 8:m7:130:VAL:HG12 | 8:m7:157:VAL:HG23 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:x7:37:TRP:O | 9:x7:37:TRP:CG | 2.67 | 0.48 |
| 9:y7:37:TRP:O | 9:y7:37:TRP:CG | 2.67 | 0.48 |
| 2:X8:30:ARG:HD3 | 2:X8:30:ARG:C | 2.39 | 0.48 |
| 3:H8:1:MET:H2 | 11:a9:96:THR:HG21 | 1.78 | 0.48 |
| 3:H8:75:PRO:CB | 12:I8:201:CYC:HBB2 | 2.44 | 0.48 |
| 4:M8:21:LEU:HD12 | 4:M8:21:LEU:C | 2.37 | 0.48 |
| 4:M8:269:SER:HA | 3:Y8:108:ARG:O | 2.14 | 0.48 |
| 3:O8:75:PRO:CB | 12:R8:201:CYC:HBB2 | 2.44 | 0.48 |
| 4:M9:53:LEU:CD2 | 3:F9:84:ARG:CZ | 2.92 | 0.48 |
| 4:M9:210:ILE:HD13 | 5:N9:59:ARG:NH1 | 2.27 | 0.48 |
| 3:P9:52:ILE:HD11 | 3:P9:87:GLU:HA | 1.95 | 0.48 |
| 3:P9:88:ILE:HG21 | 12:P9:201:CYC:HAB2 | 1.95 | 0.48 |
| 5:Z8:31:TRP:CB | 5:Z8:32:PRO:CD | 2.90 | 0.48 |
| 2:A9:34:ALA:CB | 3:B9:31:VAL:HG21 | 2.44 | 0.48 |
| 3:F9:52:ILE:HD11 | 3:F9:87:GLU:HA | 1.95 | 0.48 |
| 11:a9:595:ARG:HG3 | 11:a9:596:THR:H | 1.79 | 0.48 |
| 11:a9:643:LEU:CD2 | 11:a9:689:VAL:CG2 | 2.80 | 0.48 |
| 11:a9:709:CYS:O | 11:a9:807:GLN:CB | 2.53 | 0.48 |
| 3:X1:88:ILE:HG21 | 12:X1:201:CYC:HAB2 | 1.96 | 0.48 |
| 2:A2:30:ARG:HD3 | 2:A2:30:ARG:C | 2.38 | 0.48 |
| 3:FA:37:ARG:NH2 | 3:FA:159:GLU:OE2 | 2.43 | 0.48 |
| 3:JA:70:GLY:C | 11:aA:357:THR:O | 2.56 | 0.48 |
| 4:MA:140:ARG:O | 4:MA:140:ARG:HG2 | 2.13 | 0.48 |
| 2:OA:31:PHE:CD2 | 3:PA:34:SER:HB2 | 2.49 | 0.48 |
| 2:OA:44:LEU:HD11 | 2:OA:142:LEU:HD11 | 1.96 | 0.48 |
| 3:PA:75:PRO:CB | 12:SA:201:CYC:HBB2 | 2.44 | 0.48 |
| 2:QA:33:ARG:NH2 | 12:VA:202:CYC:CBB | 2.76 | 0.48 |
| 3:ZA:88:ILE:HG21 | 12:ZA:202:CYC:HAB2 | 1.96 | 0.48 |
| 3:R1:120:LEU:CD2 | 5:N1:16:PHE:CZ | 2.97 | 0.48 |
| 2:I3:30:ARG:HD3 | 2:I3:30:ARG:C | 2.39 | 0.48 |
| 6:M2:39:ARG:HH21 | 8:O5:66:VAL:CG1 | 2.27 | 0.48 |
| 6:M2:54:GLY:C | 1:h7:62:TYR:HB3 | 2.39 | 0.48 |
| 2:A3:52:VAL:CG1 | 2:A3:83:ALA:HA | 2.44 | 0.48 |
| 12:A3:201:CYC:HBB2 | 3:D3:75:PRO:CB | 2.44 | 0.48 |
| 3:Z3:88:ILE:HG21 | 12:Z3:201:CYC:HAB2 | 1.95 | 0.48 |
| 2:A4:31:PHE:CD2 | 3:B4:34:SER:HB2 | 2.49 | 0.48 |
| 2:A4:52:VAL:CG1 | 2:A4:83:ALA:HA | 2.43 | 0.48 |
| 4:M3:140:ARG:O | 4:M3:140:ARG:HG2 | 2.13 | 0.48 |
| 4:M3:181:GLN:HA | 4:M3:266:LEU:HD23 | 1.95 | 0.48 |
| 4:M3:232:VAL:CG2 | 3:V3:113:LEU:HA | 2.44 | 0.48 |
| 2:O3:25:GLN:HG2 | 2:Y3:33:ARG:CG | 2.38 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:O3:59:VAL:HG12 | 2:O3:66:LEU:HD13 | 1.96 | 0.48 |
| 3:X3:88:ILE:HG21 | 12:X3:201:CYC:HAB2 | 1.96 | 0.48 |
| 2:E4:30:ARG:HD3 | 2:E4:30:ARG:C | 2.39 | 0.48 |
| 3:F4:91:ARG:HH21 | 11:aA:140:GLN:HE21 | 1.58 | 0.48 |
| 12:G4:201:CYC:HBB2 | 3:L4:75:PRO:CB | 2.44 | 0.48 |
| 2:K4:30:ARG:HD3 | 2:K4:30:ARG:C | 2.39 | 0.48 |
| 12:L4:202:CYC:CBB | 11:aA:245:ALA:H | 2.26 | 0.48 |
| 4:M4:147:ALA:HB2 | 4:M4:173:PHE:CZ | 2.49 | 0.48 |
| 3:O4:107:ASP:CG | 5:Z4:66:ARG:CG | 2.87 | 0.48 |
| 3:Q4:89:ILE:HB | 3:Q4:134:MET:HE1 | 1.96 | 0.48 |
| 8:K5:17:TYR:OH | 1:L5:89:LEU:CG | 2.62 | 0.48 |
| 8:K5:20:PRO:CG | 8:U5:152:TYR:HA | 2.43 | 0.48 |
| 8:A5:39:ILE:HG12 | 8:A5:145:ASP:HB3 | 1.96 | 0.48 |
| 8:A5:110:ILE:O | 1:F5:76:ARG:CB | 2.60 | 0.48 |
| 8:C5:130:VAL:HG12 | 8:C5:157:VAL:HG23 | 1.96 | 0.48 |
| 8:G5:106:GLU:CD | 10:j5:558:VAL:H | 2.21 | 0.48 |
| 1:H5:89:LEU:HD22 | 1:H5:133:MET:CE | 2.44 | 0.48 |
| 12:C1:201:CYC:HBB2 | 3:F1:75:PRO:CB | 2.44 | 0.48 |
| 12:f5:201:CYC:HMA3 | 12:f5:201:CYC:NB | 2.29 | 0.48 |
| 8:S5:130:VAL:HG12 | 8:S5:157:VAL:HG23 | 1.95 | 0.48 |
| 8:U5:40:ALA:HB2 | 8:U5:97:VAL:HG13 | 1.96 | 0.48 |
| 8:U5:76:LYS:HG2 | 8:U5:77:MET:HE3 | 1.93 | 0.48 |
| 12:X5:201:CYC:HMA3 | 12:X5:201:CYC:NB | 2.29 | 0.48 |
| 1:Z5:89:LEU:HD22 | 1:Z5:133:MET:CE | 2.44 | 0.48 |
| 3:L6:75:PRO:CB | 12:G6:201:CYC:HBB2 | 2.44 | 0.48 |
| 10:j5:190:LEU:CA | 10:j5:194:CYS:SG | 3.00 | 0.48 |
| 10:j5:822:ARG:HD2 | 1:H7:106:GLU:OE2 | 2.14 | 0.48 |
| 10:j5:1069:ARG:NH2 | 10:j5:1072:ILE:HD11 | 2.29 | 0.48 |
| 10:k5:755:GLN:H | 10:k5:879:ASP:HB2 | 1.78 | 0.48 |
| 10:k5:965:GLN:C | 1:p7:14:VAL:CG1 | 2.86 | 0.48 |
| 10:k5:1045:TYR:CD1 | 10:k5:1045:TYR:C | 2.92 | 0.48 |
| 10:k5:1106:PHE:CE1 | 10:k5:1112:PRO:HA | 2.49 | 0.48 |
| 12:k5:1203:CYC:HMA3 | 12:k5:1203:CYC:NB | 2.29 | 0.48 |
| 2:A6:44:LEU:HD11 | 2:A6:142:LEU:HD11 | 1.96 | 0.48 |
| 8:S7:39:ILE:HG12 | 8:S7:145:ASP:HB3 | 1.95 | 0.48 |
| 8:S7:106:GLU:OE2 | 9:w7:68:GLY:CA | 2.58 | 0.48 |
| 1:D7:89:LEU:HD22 | 1:D7:133:MET:CE | 2.44 | 0.48 |
| 12:h7:201:CYC:HBB1 | 9:y7:21:ARG:CZ | 2.44 | 0.48 |
| 8:i7:46:ALA:HB1 | 8:i7:140:LEU:HD11 | 1.90 | 0.48 |
| 12:T7:201:CYC:HMA3 | 12:T7:201:CYC:NB | 2.29 | 0.48 |
| 8:Y7:52:LYS:HE3 | 8:Y7:52:LYS:HB3 | 1.60 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:f7:67:ARG:NH1 | 11:aA:307:ARG:CG | 2.76 | 0.48 |
| 8:q7:49:ARG:NH1 | 3:H1:62:GLU:HB3 | 2.29 | 0.48 |
| 8:q7:79:ALA:CA | 11:aA:53:VAL:CG2 | 2.91 | 0.48 |
| 9:z7:63:ALA:HB1 | 9:z7:67:VAL:HG21 | 1.95 | 0.48 |
| 12:T8:201:CYC:HBB2 | 3:Y8:75:PRO:CB | 2.44 | 0.48 |
| 4:M8:132:LEU:CD1 | 4:M8:142:PHE:HB2 | 2.44 | 0.48 |
| 3:S8:52:ILE:HD11 | 3:S8:87:GLU:HA | 1.95 | 0.48 |
| 4:M9:267:LEU:HD23 | 4:M9:267:LEU:HA | 1.65 | 0.48 |
| 3:Y8:113:LEU:HD13 | 3:Y8:171:ILE:CG1 | 2.44 | 0.48 |
| 2:A9:31:PHE:CD2 | 3:B9:34:SER:HB2 | 2.49 | 0.48 |
| 3:R9:88:ILE:HG21 | 12:R9:201:CYC:HAB2 | 1.95 | 0.48 |
| 2:S9:30:ARG:HD3 | 2:S9:30:ARG:C | 2.39 | 0.48 |
| 3:X9:52:ILE:HD11 | 3:X9:87:GLU:HA | 1.95 | 0.48 |
| 3:Z9:88:ILE:HG21 | 12:Z9:202:CYC:HAB2 | 1.96 | 0.48 |
| 11:a9:70:ALA:N | 11:a9:71:ILE:HD11 | 2.28 | 0.48 |
| 11:a9:81:ASP:OD1 | 11:a9:81:ASP:C | 2.50 | 0.48 |
| 11:a9:629:LYS:C | 11:a9:629:LYS:CD | 2.86 | 0.48 |
| 11:aA:70:ALA:N | 11:aA:71:ILE:CD1 | 2.76 | 0.48 |
| 11:aA:629:LYS:C | 11:aA:629:LYS:CD | 2.85 | 0.48 |
| 2:K1:30:ARG:C | 2:K1:30:ARG:HD3 | 2.39 | 0.48 |
| 4:M1:176:ARG:HH11 | 4:M1:176:ARG:HG3 | 1.78 | 0.48 |
| 2:A2:34:ALA:CB | 3:B2:31:VAL:HG21 | 2.44 | 0.48 |
| 3:BA:14:LEU:CD1 | 3:XA:125:ARG:CD | 2.92 | 0.47 |
| 3:HA:108:ARG:NH2 | 11:aA:477:TYR:CZ | 2.79 | 0.47 |
| 4:MA:16:LYS:HA | 4:MA:46:VAL:HA | 1.96 | 0.47 |
| 4:MA:29:PRO:HB2 | 11:aA:375:GLN:HG3 | 1.96 | 0.47 |
| 5:NA:53:LEU:C | 12:TA:301:CYC:CBA | 2.85 | 0.47 |
| 3:TA:32:LYS:HZ1 | 2:X4:57:GLN:C | 2.08 | 0.47 |
| 2:S1:30:ARG:HD3 | 2:S1:30:ARG:C | 2.39 | 0.47 |
| 2:K2:30:ARG:HD3 | 2:K2:30:ARG:C | 2.39 | 0.47 |
| 3:L2:88:ILE:HG21 | 12:L2:201:CYC:HAB2 | 1.96 | 0.47 |
| 2:A4:34:ALA:HB3 | 3:B4:31:VAL:CG1 | 2.39 | 0.47 |
| 12:C4:201:CYC:HBB2 | 3:F4:75:PRO:CB | 2.44 | 0.47 |
| 4:M3:274:VAL:HG11 | 2:U3:111:ALA:HB1 | 1.96 | 0.47 |
| 3:X3:75:PRO:CB | 12:Y3:201:CYC:HBB2 | 2.45 | 0.47 |
| 3:B1:75:PRO:CB | 12:E1:201:CYC:HBB2 | 2.44 | 0.47 |
| 2:E4:1:MET:C | 4:M4:10:ARG:HH22 | 2.20 | 0.47 |
| 12:M4:301:CYC:HAC1 | 3:Y4:82:CYS:HB2 | 1.86 | 0.47 |
| 12:M4:301:CYC:HB | 12:M4:301:CYC:CMA | 2.25 | 0.47 |
| 8:K5:20:PRO:CG | 8:U5:155:TYR:HB2 | 2.43 | 0.47 |
| 12:N5:201:CYC:HMA3 | 12:N5:201:CYC:NB | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:Z4:29:HIS:HE1 | 5:Z4:38:GLU:OE1 | 1.97 | 0.47 |
| 1:H5:14:VAL:CG1 | 10:j5:555:ALA:CA | 2.92 | 0.47 |
| 8:c5:130:VAL:HG12 | 8:c5:157:VAL:HG23 | 1.95 | 0.47 |
| 1:d5:63:SER:OG | 10:j5:703:LEU:O | 2.32 | 0.47 |
| 8:U5:16:ARG:HH12 | 8:U5:19:SER:HB3 | 1.79 | 0.47 |
| 1:V5:89:LEU:HD22 | 1:V5:133:MET:CE | 2.44 | 0.47 |
| 8:Y5:54:ALA:HB2 | 8:Y5:133:MET:HG2 | 1.96 | 0.47 |
| 8:a5:4:LEU:HD21 | 8:a5:26:ILE:HG23 | 1.96 | 0.47 |
| 3:J6:88:ILE:HG21 | 12:J6:202:CYC:HAB2 | 1.95 | 0.47 |
| 10:j5:283:ARG:O | 10:j5:284:PRO:C | 2.53 | 0.47 |
| 10:j5:472:TYR:N | 10:j5:472:TYR:CD1 | 2.73 | 0.47 |
| 10:j5:743:VAL:CG1 | 12:J7:201:CYC:CGD | 2.88 | 0.47 |
| 10:j5:930:LEU:CD1 | 1:J7:33:THR:HB | 2.25 | 0.47 |
| 10:j5:951:MET:HE3 | 10:j5:951:MET:CA | 2.43 | 0.47 |
| 10:j5:1052:PRO:HG3 | 10:j5:1140:TRP:HA | 1.96 | 0.47 |
| 10:k5:186:LEU:HD21 | 12:k5:1201:CYC:HMB3 | 1.96 | 0.47 |
| 10:k5:641:ASP:HB3 | 10:k5:643:VAL:H | 1.79 | 0.47 |
| 10:k5:892:ALA:C | 10:k5:895:PRO:HD2 | 2.39 | 0.47 |
| 10:k5:1089:LEU:HD22 | 10:k5:1089:LEU:C | 2.39 | 0.47 |
| 10:k5:1143:LEU:HD11 | 8:k7:102:THR:HG22 | 1.96 | 0.47 |
| 3:H6:75:PRO:CB | 12:I6:201:CYC:HBB2 | 2.44 | 0.47 |
| 1:B7:68:PRO:CB | 1:D7:14:VAL:C | 2.67 | 0.47 |
| 12:D7:201:CYC:HMA3 | 12:D7:201:CYC:NB | 2.29 | 0.47 |
| 8:M7:130:VAL:HG12 | 8:M7:157:VAL:HG23 | 1.95 | 0.47 |
| 8:g7:25:ARG:NH2 | 8:u7:25:ARG:NE | 2.49 | 0.47 |
| 12:h7:201:CYC:HMA3 | 12:h7:201:CYC:NB | 2.29 | 0.47 |
| 8:i7:126:VAL:CG2 | 12:i7:201:CYC:CMC | 2.91 | 0.47 |
| 8:c7:57:GLN:HB2 | 8:c7:132:ALA:HB1 | 1.96 | 0.47 |
| 2:A8:31:PHE:CD2 | 3:B8:34:SER:HB2 | 2.49 | 0.47 |
| 8:m7:2:SER:O | 8:m7:100:ASP:CB | 2.62 | 0.47 |
| 8:u7:4:LEU:HD21 | 8:u7:26:ILE:HD13 | 1.93 | 0.47 |
| 3:F8:110:LEU:O | 3:F8:113:LEU:N | 2.47 | 0.47 |
| 3:H8:88:ILE:HG21 | 12:H8:201:CYC:HAB2 | 1.95 | 0.47 |
| 3:L8:70:GLY:O | 3:L8:71:GLY:O | 2.32 | 0.47 |
| 4:M8:58:TYR:O | 4:M8:61:ASN:OD1 | 2.31 | 0.47 |
| 4:M8:233:GLU:HG2 | 4:M8:233:GLU:O | 2.13 | 0.47 |
| 3:O8:88:ILE:HG21 | 12:O8:201:CYC:HAB2 | 1.95 | 0.47 |
| 3:O8:107:ASP:OD1 | 5:Z8:66:ARG:NE | 2.43 | 0.47 |
| 4:M9:140:ARG:HG2 | 4:M9:140:ARG:O | 2.13 | 0.47 |
| 4:M9:176:ARG:HG2 | 4:M9:176:ARG:O | 2.13 | 0.47 |
| 5:N9:2:SER:O | 5:N9:2:SER:OG | 2.16 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:A9:34:ALA:HB3 | 3:B9:31:VAL:CG1 | 2.39 | 0.47 |
| 3:B9:52:ILE:HD11 | 3:B9:87:GLU:HA | 1.95 | 0.47 |
| 3:J9:70:GLY:C | 11:a9:357:THR:O | 2.55 | 0.47 |
| 12:J9:201:CYC:CMD | 12:J9:201:CYC:NC | 2.75 | 0.47 |
| 11:a9:290:ASP:OD1 | 11:a9:290:ASP:N | 2.47 | 0.47 |
| 11:a9:295:ARG:HA | 11:a9:295:ARG:HE | 1.78 | 0.47 |
| 11:aA:617:ALA:O | 11:aA:620:ALA:HA | 2.15 | 0.47 |
| 3:H1:82:CYS:HA | 12:H1:201:CYC:HAC1 | 1.45 | 0.47 |
| 4:M1:181:GLN:HA | 4:M1:266:LEU:HD23 | 1.95 | 0.47 |
| 4:M1:232:VAL:CG2 | 3:V1:113:LEU:HA | 2.44 | 0.47 |
| 4:M1:263:PRO:HB2 | 3:Z1:119:ALA:HB1 | 1.83 | 0.47 |
| 5:N1:37:HIS:CD2 | 12:T1:301:CYC:HMA2 | 2.48 | 0.47 |
| 1:A:89:LEU:HD22 | 1:A:133:MET:CE | 2.44 | 0.47 |
| 1:Z:118:SER:HG | 10:j5:9:SER:HB2 | 1.78 | 0.47 |
| 2:AA:30:ARG:HD3 | 2:AA:30:ARG:C | 2.39 | 0.47 |
| 3:FA:52:ILE:HD11 | 3:FA:87:GLU:HA | 1.95 | 0.47 |
| 2:OA:64:PRO:C | 2:OA:66:LEU:H | 2.23 | 0.47 |
| 2:QA:119:THR:HG21 | 3:TA:83:LEU:CG | 2.41 | 0.47 |
| 2:G3:30:ARG:HD3 | 2:G3:30:ARG:C | 2.39 | 0.47 |
| 2:G3:106:ASP:C | 3:L3:77:ARG:HH21 | 2.22 | 0.47 |
| 3:H2:88:ILE:HG21 | 12:H2:201:CYC:HAB2 | 1.95 | 0.47 |
| 3:J2:75:PRO:CB | 12:K2:201:CYC:HBB2 | 2.45 | 0.47 |
| 3:B3:52:ILE:HD11 | 3:B3:87:GLU:HA | 1.95 | 0.47 |
| 12:B3:202:CYC:HMD1 | 12:B3:202:CYC:NC | 2.12 | 0.47 |
| 2:E3:30:ARG:HD3 | 2:E3:30:ARG:C | 2.39 | 0.47 |
| 4:M3:130:SER:CA | 12:P3:201:CYC:O2A | 2.59 | 0.47 |
| 4:M3:252:LEU:CD1 | 3:X3:77:ARG:HH12 | 2.28 | 0.47 |
| 2:Q3:30:ARG:HD3 | 2:Q3:30:ARG:C | 2.39 | 0.47 |
| 3:T3:88:ILE:HG21 | 12:T3:301:CYC:HAB2 | 1.96 | 0.47 |
| 3:V3:88:ILE:HG21 | 12:V3:201:CYC:HAB2 | 1.96 | 0.47 |
| 3:B1:52:ILE:HD11 | 3:B1:87:GLU:HA | 1.95 | 0.47 |
| 3:B1:82:CYS:SG | 12:B1:202:CYC:C2C | 3.02 | 0.47 |
| 3:S4:75:PRO:CB | 12:P4:201:CYC:HBB2 | 2.45 | 0.47 |
| 3:F4:91:ARG:NH2 | 11:aA:140:GLN:HE21 | 2.03 | 0.47 |
| 3:J4:75:PRO:CB | 12:K4:201:CYC:HBB2 | 2.44 | 0.47 |
| 4:M4:14:LEU:N | 4:M4:14:LEU:CD1 | 2.77 | 0.47 |
| 4:M4:181:GLN:HA | 4:M4:266:LEU:HD23 | 1.95 | 0.47 |
| 12:K5:201:CYC:CGD | 1:J5:62:TYR:OH | 2.61 | 0.47 |
| 1:L5:75:THR:CG2 | 8:G5:115:MET:HE2 | 2.34 | 0.47 |
| 2:X4:30:ARG:HD3 | 2:X4:30:ARG:C | 2.39 | 0.47 |
| 3:Y4:87:GLU:CB | 3:Y4:91:ARG:NH1 | 2.76 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:B5:76:ARG:HD2 | 9:z5:14:LEU:CA | 2.44 | 0.47 |
| 12:F5:201:CYC:CBB | 10:k5:588:VAL:HG21 | 2.44 | 0.47 |
| 8:G5:115:MET:SD | 12:G5:201:CYC:NB | 2.87 | 0.47 |
| 8:G5:126:VAL:HG22 | 12:G5:201:CYC:CB | 2.45 | 0.47 |
| 8:I5:2:SER:O | 8:I5:100:ASP:CB | 2.62 | 0.47 |
| 8:I5:68:PRO:HB3 | 8:Q7:59:PHE:HD2 | 1.79 | 0.47 |
| 1:T5:89:LEU:HD22 | 1:T5:133:MET:CE | 2.45 | 0.47 |
| 12:T5:201:CYC:HMA3 | 12:T5:201:CYC:NB | 2.29 | 0.47 |
| 1:V5:114:GLU:OE1 | 10:j5:496:GLU:CA | 2.63 | 0.47 |
| 1:X5:89:LEU:HD22 | 1:X5:133:MET:CE | 2.45 | 0.47 |
| 10:j5:375:VAL:HG11 | 10:j5:456:ILE:HD13 | 1.94 | 0.47 |
| 10:j5:575:ILE:HD12 | 10:j5:607:LEU:HD12 | 1.95 | 0.47 |
| 10:j5:600:VAL:O | 10:j5:600:VAL:HG12 | 2.12 | 0.47 |
| 10:j5:938:GLN:CD | 1:J7:28:LYS:CD | 2.53 | 0.47 |
| 10:k5:194:CYS:CB | 12:k5:1201:CYC:CAC | 2.87 | 0.47 |
| 10:k5:238:ARG:CG | 10:k5:238:ARG:NH1 | 2.72 | 0.47 |
| 10:k5:779:ASP:CG | 12:F7:201:CYC:HMA2 | 2.27 | 0.47 |
| 10:k5:827:LYS:HE2 | 10:k5:909:ASP:O | 2.13 | 0.47 |
| 10:k5:1009:ALA:HA | 1:p7:87:TYR:HE1 | 1.78 | 0.47 |
| 12:C6:201:CYC:HBB2 | 3:F6:75:PRO:CB | 2.44 | 0.47 |
| 12:P7:201:CYC:HMD1 | 12:P7:201:CYC:NC | 2.10 | 0.47 |
| 8:S7:64:ASP:OD2 | 8:I7:69:GLY:CA | 2.60 | 0.47 |
| 8:i7:99:GLY:O | 8:s7:21:GLY:HA3 | 2.14 | 0.47 |
| 1:j7:89:LEU:HD22 | 1:j7:133:MET:CE | 2.44 | 0.47 |
| 8:a7:25:ARG:HE | 8:o7:25:ARG:HE | 1.50 | 0.47 |
| 8:c7:8:ILE:CG2 | 1:d7:94:TYR:CD1 | 2.82 | 0.47 |
| 1:d7:89:LEU:HD22 | 1:d7:133:MET:CE | 2.44 | 0.47 |
| 12:d7:201:CYC:NB | 12:d7:201:CYC:CMA | 2.74 | 0.47 |
| 12:d7:201:CYC:NB | 12:d7:201:CYC:HMA3 | 2.29 | 0.47 |
| 12:f7:201:CYC:HMA3 | 12:f7:201:CYC:NB | 2.29 | 0.47 |
| 1:l7:89:LEU:HD22 | 1:l7:133:MET:CE | 2.44 | 0.47 |
| 8:o7:97:VAL:HG11 | 1:p7:24:LEU:HD21 | 1.97 | 0.47 |
| 9:z7:29:THR:O | 9:z7:30:LYS:HB3 | 2.13 | 0.47 |
| 9:z7:35:GLU:N | 9:z7:35:GLU:CD | 2.73 | 0.47 |
| 2:X8:68:GLN:NE2 | 3:T9:24:LEU:HB3 | 2.29 | 0.47 |
| 3:F8:110:LEU:O | 3:F8:111:ASN:C | 2.57 | 0.47 |
| 12:G8:201:CYC:HBB2 | 3:L8:75:PRO:CB | 2.44 | 0.47 |
| 3:J8:75:PRO:CB | 12:K8:201:CYC:HBB2 | 2.44 | 0.47 |
| 3:L8:69:PRO:O | 11:a9:82:GLN:HG2 | 2.12 | 0.47 |
| 4:M8:138:SER:HB3 | 12:Z8:301:CYC:HBB1 | 1.96 | 0.47 |
| 4:M8:217:VAL:HG23 | 5:Z8:30:PRO:HD3 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:N8:34:ALA:CB | 3:O8:31:VAL:HG21 | 2.44 | 0.47 |
| 2:N8:44:LEU:HD11 | 2:N8:142:LEU:HD11 | 1.96 | 0.47 |
| 3:Q8:81:ALA:HB2 | 5:Z8:36:THR:CG2 | 2.44 | 0.47 |
| 3:P9:75:PRO:CB | 12:S9:201:CYC:HBB2 | 2.44 | 0.47 |
| 12:Q9:201:CYC:HBB2 | 3:T9:75:PRO:CB | 2.44 | 0.47 |
| 5:Z8:41:GLN:CB | 12:Z8:301:CYC:NB | 2.58 | 0.47 |
| 2:A9:30:ARG:C | 2:A9:30:ARG:HD3 | 2.39 | 0.47 |
| 3:B9:88:ILE:HG21 | 12:B9:201:CYC:HAB2 | 1.95 | 0.47 |
| 2:I9:30:ARG:HD3 | 2:I9:30:ARG:C | 2.39 | 0.47 |
| 3:J9:78:ARG:HH12 | 11:a9:359:ASP:CA | 2.05 | 0.47 |
| 2:K9:30:ARG:HD3 | 2:K9:30:ARG:C | 2.38 | 0.47 |
| 3:V9:75:PRO:CB | 12:W9:201:CYC:HBB2 | 2.44 | 0.47 |
| 3:V9:88:ILE:HG21 | 12:V9:201:CYC:HAB2 | 1.96 | 0.47 |
| 2:W9:30:ARG:HD3 | 2:W9:30:ARG:C | 2.39 | 0.47 |
| 11:a9:338:VAL:CG1 | 11:a9:340:PRO:HD3 | 2.44 | 0.47 |
| 11:aA:550:PHE:N | 11:aA:551:PRO:CD | 2.77 | 0.47 |
| 5:N1:40:SER:O | 5:N1:40:SER:OG | 2.30 | 0.47 |
| 12:A:201:CYC:HMA3 | 12:A:201:CYC:NB | 2.29 | 0.47 |
| 3:BA:88:ILE:HG21 | 12:BA:201:CYC:HAB2 | 1.95 | 0.47 |
| 3:FA:148:VAL:HG11 | 12:F9:302:CYC:C4C | 2.43 | 0.47 |
| 2:IA:30:ARG:HD3 | 2:IA:30:ARG:C | 2.39 | 0.47 |
| 2:IA:97:LEU:CD1 | 2:IA:97:LEU:C | 2.85 | 0.47 |
| 3:JA:68:ARG:CB | 11:aA:353:ALA:CB | 2.92 | 0.47 |
| 3:JA:88:ILE:HG21 | 12:JA:202:CYC:HAB2 | 1.95 | 0.47 |
| 3:JA:119:ALA:C | 11:aA:365:LYS:HE3 | 2.12 | 0.47 |
| 4:MA:185:ALA:HA | 12:VA:201:CYC:HBA2 | 1.93 | 0.47 |
| 2:QA:65:TYR:CD1 | 2:WA:65:TYR:CE1 | 3.02 | 0.47 |
| 3:TA:24:LEU:HB3 | 2:X4:68:GLN:NE2 | 2.29 | 0.47 |
| 3:VA:75:PRO:CB | 12:WA:201:CYC:HBB2 | 2.44 | 0.47 |
| 2:O1:31:PHE:CD2 | 3:P1:34:SER:HB2 | 2.49 | 0.47 |
| 2:O1:52:VAL:CG1 | 2:O1:83:ALA:HA | 2.43 | 0.47 |
| 2:Q1:30:ARG:HD3 | 2:Q1:30:ARG:C | 2.39 | 0.47 |
| 12:Q1:201:CYC:HBB2 | 3:T1:75:PRO:CB | 2.44 | 0.47 |
| 3:D3:118:VAL:HG22 | 4:M3:254:LEU:HD13 | 1.95 | 0.47 |
| 2:A4:30:ARG:HD3 | 2:A4:30:ARG:C | 2.39 | 0.47 |
| 2:A4:34:ALA:CB | 3:B4:31:VAL:HG21 | 2.44 | 0.47 |
| 2:C4:30:ARG:HD3 | 2:C4:30:ARG:C | 2.39 | 0.47 |
| 4:M3:144:ARG:HH21 | 5:N3:52:ARG:NH2 | 2.09 | 0.47 |
| 12:O3:201:CYC:HBB2 | 3:R3:75:PRO:CB | 2.45 | 0.47 |
| 3:S4:82:CYS:SG | 12:S4:202:CYC:HBC1 | 2.53 | 0.47 |
| 3:H4:120:LEU:N | 11:aA:266:ASN:CG | 2.72 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M4:176:ARG:CG | 4:M4:176:ARG:NH1 | 2.70 | 0.47 |
| 12:N4:201:CYC:HBB2 | 3:Q4:75:PRO:CB | 2.45 | 0.47 |
| 8:K5:79:ALA:C | 8:K5:81:CYS:H | 2.21 | 0.47 |
| 8:M5:54:ALA:HB2 | 8:M5:133:MET:HG2 | 1.96 | 0.47 |
| 8:E5:79:ALA:C | 8:E5:81:CYS:N | 2.68 | 0.47 |
| 8:E5:132:ALA:C | 8:E5:134:LYS:N | 2.69 | 0.47 |
| 12:F5:201:CYC:HMA3 | 12:F5:201:CYC:NB | 2.29 | 0.47 |
| 8:G5:39:ILE:HG12 | 8:G5:145:ASP:HB3 | 1.96 | 0.47 |
| 1:J5:3:ASP:HB2 | 1:J5:4:ALA:H | 1.48 | 0.47 |
| 8:e5:2:SER:O | 8:e5:100:ASP:CB | 2.63 | 0.47 |
| 1:f5:89:LEU:HD22 | 1:f5:133:MET:CE | 2.44 | 0.47 |
| 8:U5:48:GLU:HA | 6:M6:34:ARG:NH1 | 2.14 | 0.47 |
| 12:Z5:201:CYC:NB | 12:Z5:201:CYC:HMA3 | 2.29 | 0.47 |
| 1:b5:3:ASP:CG | 10:k5:21:MET:CB | 2.80 | 0.47 |
| 10:j5:415:PHE:O | 10:j5:416:GLY:C | 2.53 | 0.47 |
| 10:k5:362:LYS:CD | 10:k5:362:LYS:C | 2.85 | 0.47 |
| 3:F6:52:ILE:HD11 | 3:F6:87:GLU:HA | 1.95 | 0.47 |
| 8:O7:25:ARG:NH2 | 8:E7:25:ARG:HE | 2.11 | 0.47 |
| 12:N7:201:CYC:HMA3 | 12:N7:201:CYC:NB | 2.29 | 0.47 |
| 8:g7:90:ARG:NH1 | 1:h7:16:GLY:CA | 2.74 | 0.47 |
| 1:h7:89:LEU:HD22 | 1:h7:133:MET:CE | 2.44 | 0.47 |
| 8:i7:47:ARG:HB3 | 1:j7:18:TYR:CE2 | 2.48 | 0.47 |
| 8:U7:2:SER:O | 8:U7:100:ASP:CB | 2.62 | 0.47 |
| 1:f7:89:LEU:HD22 | 1:f7:133:MET:CE | 2.44 | 0.47 |
| 1:n7:89:LEU:HD22 | 1:n7:133:MET:CE | 2.44 | 0.47 |
| 8:u7:23:LEU:CA | 1:v7:38:VAL:HG21 | 2.43 | 0.47 |
| 1:v7:89:LEU:HD22 | 1:v7:133:MET:CE | 2.44 | 0.47 |
| 2:V8:30:ARG:HD3 | 2:V8:30:ARG:C | 2.39 | 0.47 |
| 2:X8:67:THR:HG1 | 3:T9:28:THR:HG22 | 1.68 | 0.47 |
| 3:F8:88:ILE:HG21 | 12:F8:202:CYC:HAB2 | 1.96 | 0.47 |
| 3:J8:88:ILE:HG21 | 12:J8:201:CYC:HAB2 | 1.95 | 0.47 |
| 4:M8:96:LYS:NZ | 3:Q8:109:CYS:SG | 2.86 | 0.47 |
| 12:M8:301:CYC:C1C | 3:Y8:72:ASN:OD1 | 2.62 | 0.47 |
| 12:L9:202:CYC:NB | 11:a9:404:TYR:CE1 | 2.82 | 0.47 |
| 4:M9:6:THR:CG2 | 12:D9:201:CYC:HBB2 | 2.43 | 0.47 |
| 5:N9:53:LEU:C | 12:T9:301:CYC:CBA | 2.85 | 0.47 |
| 5:Z8:29:HIS:NE2 | 5:Z8:36:THR:HG22 | 2.28 | 0.47 |
| 2:C9:38:MET:HE2 | 2:C9:38:MET:HB3 | 1.81 | 0.47 |
| 3:H9:108:ARG:NH2 | 11:a9:477:TYR:OH | 2.47 | 0.47 |
| 2:G1:30:ARG:C | 2:G1:30:ARG:HD3 | 2.39 | 0.47 |
| 12:G1:201:CYC:HBB2 | 3:L1:75:PRO:CB | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 11:a9:389:GLN:NE2 | 11:a9:389:GLN:CA | 2.72 | 0.47 |
| 11:a9:588:VAL:C | 11:a9:590:PRO:HD2 | 2.30 | 0.47 |
| 11:aA:38:VAL:HA | 11:aA:39:PRO:HD3 | 1.85 | 0.47 |
| 11:aA:456:PHE:CD1 | 11:aA:460:LEU:HD12 | 2.49 | 0.47 |
| 4:M1:14:LEU:N | 4:M1:14:LEU:CD1 | 2.77 | 0.47 |
| 4:M1:200:ILE:HD13 | 4:M1:200:ILE:HA | 1.54 | 0.47 |
| 2:W1:30:ARG:HD3 | 2:W1:30:ARG:C | 2.39 | 0.47 |
| 2:A2:5:ILE:HG21 | 3:B2:99:ALA:HA | 1.96 | 0.47 |
| 12:Z:201:CYC:CMA | 12:Z:201:CYC:NB | 2.74 | 0.47 |
| 2:CA:30:ARG:HD3 | 2:CA:30:ARG:C | 2.39 | 0.47 |
| 3:FA:88:ILE:HG21 | 12:FA:301:CYC:HAB2 | 1.96 | 0.47 |
| 12:JA:202:CYC:O2A | 11:aA:511:LYS:HD2 | 2.14 | 0.47 |
| 4:MA:14:LEU:N | 4:MA:14:LEU:CD1 | 2.77 | 0.47 |
| 4:MA:61:ASN:C | 4:MA:63:GLY:N | 2.64 | 0.47 |
| 4:MA:176:ARG:HH11 | 4:MA:176:ARG:HG3 | 1.78 | 0.47 |
| 2:A1:31:PHE:CD2 | 3:B1:34:SER:HB2 | 2.49 | 0.47 |
| 3:J3:52:ILE:HD11 | 3:J3:87:GLU:HA | 1.95 | 0.47 |
| 3:J3:75:PRO:CB | 12:K3:201:CYC:HBB2 | 2.44 | 0.47 |
| 3:B3:75:PRO:CB | 12:E3:201:CYC:HBB2 | 2.44 | 0.47 |
| 3:D3:52:ILE:HD11 | 3:D3:87:GLU:HA | 1.95 | 0.47 |
| 3:B4:75:PRO:CB | 12:E4:201:CYC:HBB2 | 2.44 | 0.47 |
| 12:B4:202:CYC:NA | 4:M4:57:THR:OG1 | 2.40 | 0.47 |
| 3:D4:150:ARG:NH1 | 2:C1:140:SER:O | 2.48 | 0.47 |
| 5:N3:57:MET:CE | 5:N3:67:ILE:HG13 | 2.44 | 0.47 |
| 3:H4:84:ARG:NE | 11:aA:131:TYR:HB3 | 2.30 | 0.47 |
| 4:M4:233:GLU:HG2 | 4:M4:233:GLU:O | 2.13 | 0.47 |
| 3:Y4:52:ILE:HD11 | 3:Y4:87:GLU:HA | 1.95 | 0.47 |
| 5:Z4:57:MET:CE | 5:Z4:67:ILE:HG13 | 2.44 | 0.47 |
| 8:C5:4:LEU:O | 8:C5:4:LEU:HD23 | 2.13 | 0.47 |
| 1:J5:89:LEU:HD22 | 1:J5:133:MET:CE | 2.44 | 0.47 |
| 12:R5:201:CYC:HMA3 | 12:R5:201:CYC:NB | 2.29 | 0.47 |
| 1:X5:87:TYR:OH | 10:j5:521:GLY:HA3 | 2.13 | 0.47 |
| 1:Z5:161:SER:HG | 10:k5:696:ARG:HA | 1.76 | 0.47 |
| 6:M6:277:GLY:HA2 | 1:d7:62:TYR:CB | 2.45 | 0.47 |
| 8:A7:39:ILE:HG12 | 8:A7:145:ASP:HB3 | 1.95 | 0.47 |
| 10:j5:288:LEU:HD23 | 10:j5:288:LEU:HA | 1.77 | 0.47 |
| 10:j5:767:LEU:C | 10:j5:767:LEU:CD2 | 2.84 | 0.47 |
| 10:k5:221:LYS:NZ | 10:k5:221:LYS:C | 2.73 | 0.47 |
| 10:k5:951:MET:HE2 | 10:k5:955:LEU:HD11 | 1.96 | 0.47 |
| 10:k5:1105:ILE:HD13 | 10:k5:1115:ARG:HH21 | 1.75 | 0.47 |
| 12:A6:201:CYC:HBB2 | 3:D6:75:PRO:CB | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:E6:30:ARG:HD3 | 2:E6:30:ARG:C | 2.39 | 0.47 |
| 3:H6:88:ILE:HG21 | 12:H6:201:CYC:HAB2 | 1.96 | 0.47 |
| 8:O7:2:SER:O | 8:O7:100:ASP:CB | 2.63 | 0.47 |
| 8:Q7:21:GLY:HA3 | 8:C7:6:LYS:HZ3 | 1.78 | 0.47 |
| 8:C7:2:SER:O | 8:C7:100:ASP:CB | 2.62 | 0.47 |
| 1:F7:89:LEU:HD22 | 1:F7:133:MET:CE | 2.44 | 0.47 |
| 1:H7:68:PRO:C | 1:J7:14:VAL:O | 2.57 | 0.47 |
| 8:K7:25:ARG:HD3 | 8:U7:25:ARG:HH22 | 1.78 | 0.47 |
| 12:L7:201:CYC:HMA3 | 12:L7:201:CYC:NB | 2.29 | 0.47 |
| 1:j7:82:ILE:HD12 | 8:e7:118:SER:HB2 | 1.95 | 0.47 |
| 1:T7:106:GLU:HG3 | 9:w7:58:THR:HG22 | 1.90 | 0.47 |
| 1:V7:75:THR:HG21 | 8:W7:112:VAL:HB | 1.97 | 0.47 |
| 3:B8:109:CYS:CA | 4:M8:60:LYS:HZ3 | 2.27 | 0.47 |
| 1:r7:68:PRO:C | 1:t7:14:VAL:O | 2.57 | 0.47 |
| 8:u7:97:VAL:HG11 | 1:v7:24:LEU:HD21 | 1.97 | 0.47 |
| 12:v7:201:CYC:NB | 12:v7:201:CYC:HMA3 | 2.29 | 0.47 |
| 3:F8:107:ASP:O | 4:M8:6:THR:C | 2.55 | 0.47 |
| 2:I8:30:ARG:C | 2:I8:30:ARG:HD3 | 2.39 | 0.47 |
| 4:M8:16:LYS:HA | 4:M8:46:VAL:HA | 1.96 | 0.47 |
| 4:M8:100:SER:HB2 | 2:P8:10:ALA:HA | 1.95 | 0.47 |
| 3:L9:75:PRO:CB | 12:G9:201:CYC:HBB2 | 2.44 | 0.47 |
| 3:L9:83:LEU:HD13 | 2:G9:119:THR:CG2 | 2.34 | 0.47 |
| 3:L9:111:ASN:CG | 11:a9:366:LEU:CD1 | 2.87 | 0.47 |
| 12:L9:201:CYC:C4B | 2:A9:33:ARG:NH1 | 2.44 | 0.47 |
| 4:M9:45:VAL:O | 4:M9:45:VAL:HG12 | 2.14 | 0.47 |
| 12:O9:201:CYC:HBB2 | 3:R9:75:PRO:CB | 2.45 | 0.47 |
| 5:Z8:37:HIS:HE1 | 12:Z8:301:CYC:HBA1 | 1.78 | 0.47 |
| 3:B9:14:LEU:CD1 | 3:X9:125:ARG:CD | 2.92 | 0.47 |
| 12:J9:202:CYC:O2A | 11:a9:511:LYS:HD2 | 2.14 | 0.47 |
| 11:a9:64:ARG:O | 11:a9:65:LEU:C | 2.57 | 0.47 |
| 11:a9:289:THR:HG22 | 11:a9:292:ALA:HB3 | 1.96 | 0.47 |
| 11:a9:801:ASN:HB3 | 11:a9:807:GLN:HE21 | 1.79 | 0.47 |
| 11:aA:338:VAL:CG1 | 11:aA:340:PRO:HD3 | 2.44 | 0.47 |
| 11:aA:632:ILE:CD1 | 3:J1:107:ASP:OD1 | 2.62 | 0.47 |
| 3:V1:75:PRO:CB | 12:W1:201:CYC:HBB2 | 2.45 | 0.47 |
| 3:V1:88:ILE:HG21 | 12:V1:201:CYC:HAB2 | 1.96 | 0.47 |
| 12:A2:201:CYC:HBB2 | 3:D2:75:PRO:CB | 2.44 | 0.47 |
| 2:AA:34:ALA:CB | 3:BA:31:VAL:HG21 | 2.44 | 0.47 |
| 12:CA:201:CYC:HBB2 | 3:FA:75:PRO:CB | 2.45 | 0.47 |
| 3:HA:72:ASN:CG | 12:HA:202:CYC:CMD | 2.88 | 0.47 |
| 3:P1:75:PRO:CB | 12:S1:201:CYC:HBB2 | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:A1:30:ARG:HD3 | 2:A1:30:ARG:C | 2.39 | 0.47 |
| 12:A1:201:CYC:HBB2 | 3:D1:75:PRO:CB | 2.44 | 0.47 |
| 3:L2:75:PRO:HG3 | 3:L2:78:ARG:CG | 2.42 | 0.47 |
| 2:A3:59:VAL:HG12 | 2:A3:66:LEU:HD13 | 1.96 | 0.47 |
| 12:Z3:202:CYC:C4B | 2:O3:33:ARG:NH1 | 2.44 | 0.47 |
| 3:B4:108:ARG:CA | 4:M4:61:ASN:CB | 2.92 | 0.47 |
| 3:L3:75:PRO:HG3 | 11:a9:823:ILE:HD12 | 1.95 | 0.47 |
| 4:M3:132:LEU:HD13 | 4:M3:142:PHE:CB | 2.44 | 0.47 |
| 3:J4:52:ILE:HD11 | 3:J4:87:GLU:HA | 1.95 | 0.47 |
| 2:P4:30:ARG:HD3 | 2:P4:30:ARG:C | 2.39 | 0.47 |
| 8:O5:40:ALA:HB2 | 8:O5:97:VAL:HG13 | 1.96 | 0.47 |
| 1:D5:89:LEU:HD22 | 1:D5:133:MET:CE | 2.44 | 0.47 |
| 12:D5:201:CYC:HMA3 | 12:D5:201:CYC:NB | 2.29 | 0.47 |
| 1:d5:89:LEU:HD22 | 1:d5:133:MET:CE | 2.44 | 0.47 |
| 1:f5:18:TYR:CG | 10:j5:165:ARG:CD | 2.91 | 0.47 |
| 1:b5:89:LEU:HD22 | 1:b5:133:MET:CE | 2.44 | 0.47 |
| 2:K6:30:ARG:HD3 | 2:K6:30:ARG:C | 2.39 | 0.47 |
| 10:j5:361:PHE:CZ | 10:j5:378:TYR:CE2 | 3.02 | 0.47 |
| 10:j5:477:ASP:OD1 | 10:j5:477:ASP:N | 2.42 | 0.47 |
| 10:j5:964:GLY:CA | 1:t7:69:GLY:CA | 2.75 | 0.47 |
| 10:k5:930:LEU:HG | 1:D7:148:GLU:HB2 | 1.97 | 0.47 |
| 8:M7:54:ALA:HB2 | 8:M7:133:MET:HG2 | 1.96 | 0.47 |
| 8:i7:36:ARG:NH2 | 8:i7:152:TYR:HH | 2.08 | 0.47 |
| 1:T7:68:PRO:C | 1:V7:14:VAL:O | 2.57 | 0.47 |
| 1:V7:89:LEU:HD22 | 1:V7:133:MET:CE | 2.44 | 0.47 |
| 12:b7:201:CYC:HMD1 | 12:b7:201:CYC:NC | 2.09 | 0.47 |
| 8:c7:11:ALA:HB1 | 1:d7:94:TYR:CZ | 2.44 | 0.47 |
| 12:p7:201:CYC:NB | 12:p7:201:CYC:HMA3 | 2.29 | 0.47 |
| 9:x7:35:GLU:N | 9:x7:35:GLU:CD | 2.72 | 0.47 |
| 3:U8:88:ILE:HG21 | 12:U8:201:CYC:HAB2 | 1.96 | 0.47 |
| 3:W8:88:ILE:HG21 | 12:W8:201:CYC:HAB2 | 1.95 | 0.47 |
| 3:F8:107:ASP:OD2 | 4:M8:8:SER:O | 2.25 | 0.47 |
| 2:I8:14:SER:HA | 11:a9:170:PHE:CE2 | 2.44 | 0.47 |
| 4:M8:217:VAL:HG23 | 5:Z8:30:PRO:CD | 2.43 | 0.47 |
| 2:N8:5:ILE:HG21 | 3:O8:99:ALA:HA | 1.96 | 0.47 |
| 2:N8:52:VAL:CG1 | 2:N8:83:ALA:HA | 2.44 | 0.47 |
| 12:O8:202:CYC:CMD | 12:O8:202:CYC:NC | 2.75 | 0.47 |
| 4:M9:188:LEU:CG | 3:V9:84:ARG:CZ | 2.84 | 0.47 |
| 4:M9:204:ILE:HG22 | 4:M9:204:ILE:O | 2.14 | 0.47 |
| 5:N9:36:THR:HA | 12:P9:201:CYC:HBA1 | 1.95 | 0.47 |
| 2:O9:44:LEU:HD11 | 2:O9:142:LEU:HD11 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:Z8:14:LYS:HE3 | 5:Z8:50:LEU:CD2 | 2.45 | 0.47 |
| 3:D9:88:ILE:HG21 | 12:D9:201:CYC:HAB2 | 1.95 | 0.47 |
| 12:U9:201:CYC:HBB2 | 3:Z9:75:PRO:CB | 2.45 | 0.47 |
| 3:X9:75:PRO:CB | 12:Y9:201:CYC:HBB2 | 2.45 | 0.47 |
| 2:Y9:30:ARG:HD3 | 2:Y9:30:ARG:C | 2.39 | 0.47 |
| 11:a9:371:VAL:HG11 | 11:a9:507:PHE:CG | 2.47 | 0.47 |
| 11:aA:95:ILE:HG23 | 11:aA:98:ILE:HB | 1.96 | 0.47 |
| 3:J1:52:ILE:HD11 | 3:J1:87:GLU:HA | 1.95 | 0.47 |
| 2:A2:44:LEU:HD11 | 2:A2:142:LEU:HD11 | 1.96 | 0.47 |
| 3:D2:88:ILE:HG21 | 12:D2:201:CYC:HAB2 | 1.96 | 0.47 |
| 1:A:107:ARG:NH1 | 8:a5:9:VAL:HG22 | 2.28 | 0.47 |
| 1:Z:76:ARG:NH1 | 10:j5:262:TYR:HE2 | 1.98 | 0.47 |
| 3:DA:68:ARG:HH12 | 3:XA:68:ARG:HH12 | 1.63 | 0.47 |
| 3:JA:19:LEU:CD1 | 3:JA:24:LEU:CD2 | 2.93 | 0.47 |
| 12:OA:201:CYC:HBB2 | 3:RA:75:PRO:CB | 2.44 | 0.47 |
| 2:QA:76:ASP:HB2 | 2:U1:141:GLN:C | 2.39 | 0.47 |
| 3:XA:52:ILE:HD11 | 3:XA:87:GLU:HA | 1.95 | 0.47 |
| 12:J3:202:CYC:HMA1 | 11:a9:798:SER:CB | 2.32 | 0.47 |
| 2:G2:15:GLN:CA | 6:M2:104:ARG:HD3 | 2.42 | 0.47 |
| 3:L2:52:ILE:HD11 | 3:L2:87:GLU:HA | 1.95 | 0.47 |
| 2:E3:38:MET:HE2 | 2:E3:38:MET:HB3 | 1.81 | 0.47 |
| 3:L3:120:LEU:O | 11:a9:821:ARG:NH1 | 2.47 | 0.47 |
| 4:M3:5:THR:C | 4:M3:6:THR:OG1 | 2.56 | 0.47 |
| 4:M3:45:VAL:O | 4:M3:45:VAL:HG12 | 2.14 | 0.47 |
| 4:M3:176:ARG:HG2 | 4:M3:176:ARG:O | 2.13 | 0.47 |
| 5:N3:16:PHE:CZ | 3:R3:120:LEU:CD2 | 2.97 | 0.47 |
| 2:O3:31:PHE:CD2 | 3:P3:34:SER:HB2 | 2.49 | 0.47 |
| 12:Q3:201:CYC:HBB2 | 3:T3:75:PRO:CB | 2.44 | 0.47 |
| 3:F4:88:ILE:HG21 | 12:F4:202:CYC:HAB2 | 1.95 | 0.47 |
| 3:L4:71:GLY:H | 11:aA:82:GLN:CB | 2.27 | 0.47 |
| 1:N5:12:TYR:CZ | 1:N5:23:ALA:HB2 | 2.50 | 0.47 |
| 3:Y4:93:VAL:HA | 3:Y4:105:LEU:CD1 | 2.44 | 0.47 |
| 8:A5:115:MET:SD | 12:A5:201:CYC:NB | 2.87 | 0.47 |
| 8:G5:107:ILE:O | 12:G5:201:CYC:HAB2 | 2.14 | 0.47 |
| 1:H5:12:TYR:CZ | 1:H5:23:ALA:HB2 | 2.50 | 0.47 |
| 1:H5:13:ASP:OD2 | 10:j5:556:GLY:HA3 | 2.15 | 0.47 |
| 8:I5:2:SER:C | 8:I5:100:ASP:HB2 | 2.40 | 0.47 |
| 8:I5:29:PHE:HE2 | 1:J5:5:ILE:CD1 | 2.26 | 0.47 |
| 8:Q5:17:TYR:N | 1:R5:90:ARG:HH11 | 2.13 | 0.47 |
| 8:Q5:39:ILE:HG12 | 8:Q5:145:ASP:HB3 | 1.95 | 0.47 |
| 12:Z5:201:CYC:HMA2 | 10:k5:379:PHE:CZ | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:j5:379:PHE:O | 10:j5:379:PHE:CG | 2.67 | 0.47 |
| 10:k5:415:PHE:O | 10:k5:416:GLY:C | 2.53 | 0.47 |
| 2:A6:5:ILE:HG21 | 3:B6:99:ALA:HA | 1.96 | 0.47 |
| 2:A6:31:PHE:CD2 | 3:B6:34:SER:HB2 | 2.49 | 0.47 |
| 3:F6:127:VAL:HG22 | 12:F6:201:CYC:H3C | 1.95 | 0.47 |
| 8:O7:2:SER:C | 8:O7:100:ASP:HB2 | 2.40 | 0.47 |
| 1:J7:75:THR:HG21 | 8:K7:112:VAL:HB | 1.97 | 0.47 |
| 8:g7:2:SER:O | 8:g7:100:ASP:CB | 2.63 | 0.47 |
| 8:g7:40:ALA:HB2 | 8:g7:97:VAL:HG13 | 1.96 | 0.47 |
| 1:j7:75:THR:HB | 8:e7:112:VAL:N | 2.29 | 0.47 |
| 8:k7:66:VAL:HG11 | 11:a9:61:TYR:CD1 | 2.50 | 0.47 |
| 8:W7:12:ASP:C | 9:w7:46:LYS:NZ | 2.70 | 0.47 |
| 1:Z7:89:LEU:HD22 | 1:Z7:133:MET:CE | 2.44 | 0.47 |
| 2:E8:30:ARG:C | 2:E8:30:ARG:HD3 | 2.39 | 0.47 |
| 1:p7:89:LEU:HD22 | 1:p7:133:MET:CE | 2.44 | 0.47 |
| 8:q7:66:VAL:HG13 | 11:aA:61:TYR:CE1 | 2.41 | 0.47 |
| 8:s7:40:ALA:HB2 | 8:s7:97:VAL:HG13 | 1.96 | 0.47 |
| 4:M8:181:GLN:HA | 4:M8:266:LEU:HD23 | 1.95 | 0.47 |
| 2:N8:112:GLY:C | 5:Z8:33:GLY:HA2 | 2.40 | 0.47 |
| 12:O8:202:CYC:HC | 12:O8:202:CYC:HMD3 | 1.78 | 0.47 |
| 3:Q8:104:VAL:HG22 | 3:Q8:105:LEU:N | 2.29 | 0.47 |
| 4:M9:77:LEU:C | 3:D9:115:GLU:OE2 | 2.54 | 0.47 |
| 12:Y8:201:CYC:HC | 12:Y8:201:CYC:HMD3 | 1.78 | 0.47 |
| 5:Z8:57:MET:CE | 5:Z8:67:ILE:HG13 | 2.44 | 0.47 |
| 2:C9:30:ARG:HD3 | 2:C9:30:ARG:C | 2.39 | 0.47 |
| 2:G9:30:ARG:HD3 | 2:G9:30:ARG:C | 2.39 | 0.47 |
| 2:U9:30:ARG:HD3 | 2:U9:30:ARG:C | 2.39 | 0.47 |
| 11:a9:197:ILE:CD1 | 11:a9:278:LEU:HD22 | 2.44 | 0.47 |
| 11:a9:551:PRO:O | 11:a9:554:ARG:HG2 | 2.15 | 0.47 |
| 11:aA:455:ASN:OD1 | 11:aA:455:ASN:N | 2.40 | 0.47 |
| 4:M1:16:LYS:HA | 4:M1:46:VAL:HA | 1.96 | 0.47 |
| 4:M1:274:VAL:HG11 | 2:U1:111:ALA:HB1 | 1.96 | 0.47 |
| 5:N1:1:MET:HB2 | 5:N1:3:VAL:HG23 | 1.91 | 0.47 |
| 5:N1:66:ARG:HH11 | 5:N1:66:ARG:CB | 2.22 | 0.47 |
| 2:AA:34:ALA:CB | 3:BA:31:VAL:HG11 | 2.38 | 0.47 |
| 2:AA:64:PRO:C | 2:AA:66:LEU:N | 2.71 | 0.47 |
| 2:CA:38:MET:HE2 | 2:CA:38:MET:HB3 | 1.81 | 0.47 |
| 2:EA:30:ARG:HD3 | 2:EA:30:ARG:C | 2.39 | 0.47 |
| 2:IA:45:THR:HG23 | 3:JA:18:PHE:CD2 | 2.50 | 0.47 |
| 3:JA:88:ILE:CG1 | 11:aA:512:TYR:CZ | 2.97 | 0.47 |
| 5:NA:16:PHE:HE1 | 3:TA:120:LEU:HD23 | 1.64 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:NA:36:THR:HA | 12:PA:201:CYC:HBA1 | 1.95 | 0.47 |
| 3:PA:52:ILE:HD11 | 3:PA:87:GLU:HA | 1.95 | 0.47 |
| 2:SA:30:ARG:HD3 | 2:SA:30:ARG:C | 2.39 | 0.47 |
| 2:UA:30:ARG:HD3 | 2:UA:30:ARG:C | 2.39 | 0.47 |
| 12:UA:201:CYC:HBB2 | 3:ZA:75:PRO:CB | 2.45 | 0.47 |
| 2:YA:30:ARG:HD3 | 2:YA:30:ARG:C | 2.39 | 0.47 |
| 2:A1:64:PRO:C | 2:A1:66:LEU:N | 2.71 | 0.47 |
| 3:H3:75:PRO:CB | 12:I3:201:CYC:HBB2 | 2.45 | 0.47 |
| 3:J3:119:ALA:HB1 | 11:a9:803:ASN:HB3 | 1.97 | 0.47 |
| 2:K3:30:ARG:HD3 | 2:K3:30:ARG:C | 2.39 | 0.47 |
| 2:G2:30:ARG:HD3 | 2:G2:30:ARG:C | 2.39 | 0.47 |
| 3:H2:75:PRO:CB | 12:I2:201:CYC:HBB2 | 2.44 | 0.47 |
| 3:B3:91:ARG:NH2 | 11:a9:677:GLN:HE21 | 2.04 | 0.47 |
| 3:F3:52:ILE:HD11 | 3:F3:87:GLU:HA | 1.95 | 0.47 |
| 12:Z3:201:CYC:HMA2 | 4:M3:188:LEU:HD23 | 1.97 | 0.47 |
| 2:A4:59:VAL:HG12 | 2:A4:66:LEU:HD13 | 1.96 | 0.47 |
| 3:B4:68:ARG:NH2 | 3:U4:68:ARG:CZ | 2.50 | 0.47 |
| 3:B4:112:GLY:O | 3:B4:114:LYS:N | 2.46 | 0.47 |
| 3:B4:113:LEU:CD1 | 4:M4:60:LYS:HE2 | 2.39 | 0.47 |
| 4:M3:204:ILE:HG22 | 4:M3:204:ILE:O | 2.14 | 0.47 |
| 5:N3:50:LEU:C | 5:N3:50:LEU:CD1 | 2.84 | 0.47 |
| 2:U3:45:THR:HG22 | 2:Q9:69:PRO:HD3 | 1.96 | 0.47 |
| 3:V3:75:PRO:CB | 12:W3:201:CYC:HBB2 | 2.45 | 0.47 |
| 3:X3:52:ILE:HD11 | 3:X3:87:GLU:HA | 1.95 | 0.47 |
| 3:B1:91:ARG:NH2 | 11:aA:677:GLN:HE21 | 2.04 | 0.47 |
| 3:B1:127:VAL:HA | 12:B1:202:CYC:CMC | 2.30 | 0.47 |
| 2:T4:30:ARG:HD3 | 2:T4:30:ARG:C | 2.39 | 0.47 |
| 3:F4:112:GLY:C | 3:F4:114:LYS:H | 2.17 | 0.47 |
| 3:F4:113:LEU:HD13 | 4:M4:5:THR:HG21 | 1.97 | 0.47 |
| 3:H4:52:ILE:HD11 | 3:H4:87:GLU:HA | 1.95 | 0.47 |
| 3:H4:75:PRO:CB | 12:I4:201:CYC:HBB2 | 2.44 | 0.47 |
| 3:L4:88:ILE:HG21 | 12:L4:202:CYC:HAB2 | 1.96 | 0.47 |
| 4:M4:26:SER:CB | 11:aA:228:GLU:OE1 | 2.63 | 0.47 |
| 4:M4:93:LEU:O | 4:M4:216:ASN:CG | 2.57 | 0.47 |
| 4:M4:99:VAL:C | 3:Q4:1:MET:HE1 | 2.36 | 0.47 |
| 4:M4:137:ILE:HG22 | 5:Z4:44:TYR:OH | 2.14 | 0.47 |
| 4:M4:204:ILE:HG22 | 4:M4:204:ILE:O | 2.14 | 0.47 |
| 4:M4:216:ASN:HB3 | 5:Z4:29:HIS:HA | 1.97 | 0.47 |
| 2:N4:64:PRO:C | 2:N4:66:LEU:H | 2.23 | 0.47 |
| 3:O4:75:PRO:CB | 12:R4:201:CYC:HBB2 | 2.44 | 0.47 |
| 3:Q4:74:TYR:O | 3:Q4:78:ARG:NE | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:L5:89:LEU:HD22 | 1:L5:133:MET:CE | 2.44 | 0.47 |
| 8:A5:115:MET:CE | 1:F5:75:THR:CG2 | 2.75 | 0.47 |
| 1:B5:89:LEU:HD22 | 1:B5:133:MET:CE | 2.44 | 0.47 |
| 8:C5:40:ALA:HB2 | 8:C5:97:VAL:HG13 | 1.96 | 0.47 |
| 1:D5:83:ARG:NH1 | 9:z5:38:PHE:CE2 | 2.82 | 0.47 |
| 8:G5:119:LEU:CD2 | 12:G5:201:CYC:HAA2 | 2.44 | 0.47 |
| 8:I5:40:ALA:HB2 | 8:I5:97:VAL:HG13 | 1.96 | 0.47 |
| 8:c5:54:ALA:HB2 | 8:c5:133:MET:HG2 | 1.96 | 0.47 |
| 12:P5:201:CYC:HMA3 | 12:P5:201:CYC:NB | 2.29 | 0.47 |
| 1:R5:89:LEU:HD22 | 1:R5:133:MET:CE | 2.44 | 0.47 |
| 8:S5:39:ILE:HG12 | 8:S5:145:ASP:HB3 | 1.95 | 0.47 |
| 12:V5:201:CYC:NB | 12:V5:201:CYC:HMA3 | 2.29 | 0.47 |
| 1:X5:47:ASN:OD1 | 8:a5:140:LEU:HD23 | 2.14 | 0.47 |
| 1:Z5:12:TYR:CZ | 1:Z5:23:ALA:HB2 | 2.50 | 0.47 |
| 3:L6:68:ARG:HB2 | 6:M6:64:ALA:HB2 | 1.96 | 0.47 |
| 9:z5:27:PHE:CD1 | 9:z5:27:PHE:C | 2.93 | 0.47 |
| 10:j5:199:THR:CG2 | 12:j5:1201:CYC:HBC2 | 2.41 | 0.47 |
| 10:j5:221:LYS:NZ | 10:j5:221:LYS:C | 2.73 | 0.47 |
| 10:j5:238:ARG:C | 10:j5:238:ARG:NE | 2.72 | 0.47 |
| 10:j5:348:TYR:CD1 | 10:j5:398:LEU:HD13 | 2.50 | 0.47 |
| 10:j5:930:LEU:HD12 | 1:J7:148:GLU:HG2 | 1.97 | 0.47 |
| 10:j5:947:MET:HB2 | 10:j5:947:MET:HE3 | 1.42 | 0.47 |
| 10:j5:1013:PRO:O | 10:j5:1014:SER:C | 2.58 | 0.47 |
| 10:j5:1035:PHE:CD1 | 10:j5:1035:PHE:O | 2.68 | 0.47 |
| 10:j5:1045:TYR:C | 10:j5:1045:TYR:CD1 | 2.92 | 0.47 |
| 10:j5:1105:ILE:HD11 | 10:j5:1115:ARG:HH22 | 1.71 | 0.47 |
| 10:k5:190:LEU:CD2 | 12:k5:1201:CYC:ND | 2.67 | 0.47 |
| 10:k5:241:ALA:O | 10:k5:243:ALA:N | 2.44 | 0.47 |
| 10:k5:472:TYR:CD1 | 10:k5:472:TYR:N | 2.73 | 0.47 |
| 10:k5:931:VAL:HG21 | 1:D7:30:TYR:HA | 1.90 | 0.47 |
| 10:k5:955:LEU:HA | 10:k5:955:LEU:HD23 | 1.55 | 0.47 |
| 10:k5:1035:PHE:CD1 | 10:k5:1035:PHE:O | 2.68 | 0.47 |
| 10:k5:1052:PRO:HG3 | 10:k5:1140:TRP:HA | 1.96 | 0.47 |
| 10:k5:1054:SER:C | 10:k5:1056:PRO:CD | 2.87 | 0.47 |
| 10:k5:1106:PHE:O | 10:k5:1110:ILE:CG1 | 2.63 | 0.47 |
| 10:k5:1119:LEU:HD11 | 12:k5:1204:CYC:C3B | 2.43 | 0.47 |
| 2:A6:34:ALA:CB | 3:B6:31:VAL:HG21 | 2.44 | 0.47 |
| 3:H6:84:ARG:O | 3:H6:86:MET:N | 2.45 | 0.47 |
| 2:I6:30:ARG:HD3 | 2:I6:30:ARG:C | 2.39 | 0.47 |
| 12:P7:201:CYC:HMA3 | 12:P7:201:CYC:NB | 2.29 | 0.47 |
| 8:C7:2:SER:C | 8:C7:100:ASP:HB2 | 2.40 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:D7:12:TYR:CZ | 1:D7:23:ALA:HB2 | 2.50 | 0.47 |
| 1:H7:89:LEU:HD22 | 1:H7:133:MET:CE | 2.44 | 0.47 |
| 12:J7:201:CYC:HMA3 | 12:J7:201:CYC:NB | 2.29 | 0.47 |
| 1:L7:89:LEU:HD22 | 1:L7:133:MET:CE | 2.44 | 0.47 |
| 1:N7:12:TYR:CZ | 1:N7:23:ALA:HB2 | 2.50 | 0.47 |
| 8:g7:161:GLN:CD | 1:v7:49:THR:HG22 | 2.39 | 0.47 |
| 8:k7:120:GLN:CD | 1:p7:53:LYS:HZ2 | 2.23 | 0.47 |
| 12:V7:201:CYC:HMA3 | 12:V7:201:CYC:NB | 2.29 | 0.47 |
| 12:X7:201:CYC:HMA3 | 12:X7:201:CYC:NB | 2.29 | 0.47 |
| 8:Y7:75:GLU:HG2 | 8:Y7:76:LYS:N | 2.30 | 0.47 |
| 8:Y7:110:ILE:HG13 | 1:d7:76:ARG:HB2 | 1.96 | 0.47 |
| 8:a7:40:ALA:HB2 | 8:a7:97:VAL:HG13 | 1.96 | 0.47 |
| 1:b7:51:ILE:HD11 | 1:b7:140:LEU:HD23 | 1.97 | 0.47 |
| 8:c7:20:PRO:HG2 | 8:m7:155:TYR:CG | 2.44 | 0.47 |
| 3:B8:52:ILE:HD11 | 3:B8:87:GLU:HA | 1.96 | 0.47 |
| 3:D8:77:ARG:CG | 4:M8:33:LEU:HD11 | 2.45 | 0.47 |
| 8:m7:22:GLU:H | 8:m7:22:GLU:HG2 | 1.37 | 0.47 |
| 1:p7:3:ASP:H | 1:p7:6:THR:HG1 | 1.61 | 0.47 |
| 1:r7:15:GLN:HA | 11:aA:42:ARG:HG2 | 1.96 | 0.47 |
| 8:s7:2:SER:C | 8:s7:100:ASP:HB2 | 2.40 | 0.47 |
| 1:t7:89:LEU:HD22 | 1:t7:133:MET:CE | 2.44 | 0.47 |
| 9:w7:35:GLU:N | 9:w7:35:GLU:CD | 2.73 | 0.47 |
| 9:y7:35:GLU:N | 9:y7:35:GLU:CD | 2.72 | 0.47 |
| 3:U8:52:ILE:HD11 | 3:U8:87:GLU:HA | 1.95 | 0.47 |
| 3:U8:112:GLY:C | 4:M8:74:LEU:HD21 | 2.35 | 0.47 |
| 3:W8:75:PRO:CB | 12:X8:201:CYC:HBB2 | 2.45 | 0.47 |
| 4:M8:91:VAL:CG2 | 2:P8:15:GLN:HA | 2.43 | 0.47 |
| 4:M8:226:SER:OG | 3:Y8:84:ARG:O | 2.33 | 0.47 |
| 4:M8:231:THR:C | 12:M8:301:CYC:HBB2 | 2.40 | 0.47 |
| 12:M8:301:CYC:C1C | 3:Y8:122:THR:HG23 | 2.44 | 0.47 |
| 2:N8:14:SER:CB | 5:Z8:62:ARG:HD3 | 2.40 | 0.47 |
| 2:N8:119:THR:HG21 | 3:Q8:83:LEU:HD13 | 1.96 | 0.47 |
| 3:O8:104:VAL:HG22 | 5:Z8:61:LYS:HE3 | 1.87 | 0.47 |
| 12:P8:201:CYC:HBB2 | 3:S8:75:PRO:CB | 2.45 | 0.47 |
| 4:M9:51:ARG:HH11 | 4:M9:51:ARG:CG | 2.27 | 0.47 |
| 2:O9:5:ILE:HG21 | 3:P9:99:ALA:HA | 1.96 | 0.47 |
| 2:O9:59:VAL:HG12 | 2:O9:66:LEU:HD13 | 1.96 | 0.47 |
| 12:Z8:301:CYC:CMA | 12:Z8:301:CYC:HB | 2.25 | 0.47 |
| 2:A9:25:GLN:HG2 | 2:K9:33:ARG:CG | 2.38 | 0.47 |
| 2:A9:44:LEU:HD11 | 2:A9:142:LEU:HD11 | 1.96 | 0.47 |
| 12:A9:201:CYC:HBB2 | 3:D9:75:PRO:CB | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:D9:52:ILE:HD11 | 3:D9:87:GLU:HA | 1.95 | 0.47 |
| 12:D9:202:CYC:CMD | 12:D9:202:CYC:NC | 2.75 | 0.47 |
| 3:F9:88:ILE:HG21 | 12:F9:301:CYC:HAB2 | 1.96 | 0.47 |
| 12:F9:303:CYC:HC | 12:F9:303:CYC:HMD3 | 1.78 | 0.47 |
| 3:J9:19:LEU:CD1 | 3:J9:24:LEU:CD2 | 2.93 | 0.47 |
| 11:a9:95:ILE:HG23 | 11:a9:98:ILE:HB | 1.96 | 0.47 |
| 11:a9:412:VAL:HA | 11:a9:415:GLU:OE2 | 2.15 | 0.47 |
| 11:a9:456:PHE:CD1 | 11:a9:460:LEU:HD12 | 2.49 | 0.47 |
| 11:a9:550:PHE:N | 11:a9:551:PRO:CD | 2.77 | 0.47 |
| 11:a9:553:SER:O | 11:a9:554:ARG:C | 2.56 | 0.47 |
| 11:a9:600:THR:O | 11:a9:600:THR:HG22 | 2.14 | 0.47 |
| 11:a9:716:ILE:CD1 | 11:a9:738:LEU:HD23 | 2.44 | 0.47 |
| 11:aA:623:ASP:CB | 3:H1:78:ARG:CZ | 2.65 | 0.47 |
| 11:aA:818:ARG:HA | 11:aA:818:ARG:HD2 | 1.57 | 0.47 |
| 3:H1:75:PRO:CB | 12:I1:201:CYC:HBB2 | 2.45 | 0.47 |
| 4:M1:5:THR:C | 4:M1:6:THR:OG1 | 2.56 | 0.47 |
| 4:M1:74:LEU:HA | 4:M1:74:LEU:HD23 | 1.68 | 0.47 |
| 12:T1:301:CYC:HB | 12:T1:301:CYC:CMA | 2.25 | 0.47 |
| 2:U1:30:ARG:HD3 | 2:U1:30:ARG:C | 2.38 | 0.47 |
| 3:F2:52:ILE:HD11 | 3:F2:87:GLU:HA | 1.95 | 0.47 |
| 3:F2:130:ALA:CB | 12:F2:201:CYC:CBC | 2.92 | 0.47 |
| 1:A:18:TYR:CD1 | 8:a5:90:ARG:HD3 | 2.49 | 0.47 |
| 1:Z:18:TYR:CZ | 8:e5:90:ARG:N | 2.82 | 0.47 |
| 4:MA:45:VAL:HG12 | 4:MA:45:VAL:O | 2.14 | 0.47 |
| 2:QA:111:ALA:O | 3:TA:77:ARG:HA | 2.15 | 0.47 |
| 2:O1:64:PRO:C | 2:O1:66:LEU:H | 2.22 | 0.47 |
| 2:A1:59:VAL:HG12 | 2:A1:66:LEU:HD13 | 1.96 | 0.47 |
| 6:M2:53:LEU:HD21 | 8:i7:76:LYS:O | 2.14 | 0.47 |
| 6:M2:259:THR:O | 6:M2:261:LYS:N | 2.47 | 0.47 |
| 2:A3:59:VAL:O | 2:A3:66:LEU:CD1 | 2.62 | 0.47 |
| 3:B4:108:ARG:HB3 | 12:B4:202:CYC:HBB1 | 1.95 | 0.47 |
| 3:B4:116:THR:N | 4:M4:56:MET:CE | 2.77 | 0.47 |
| 4:M3:16:LYS:HA | 4:M3:46:VAL:HA | 1.96 | 0.47 |
| 5:N3:37:HIS:CD2 | 12:T3:301:CYC:HMA2 | 2.48 | 0.47 |
| 2:O3:64:PRO:C | 2:O3:66:LEU:H | 2.22 | 0.47 |
| 12:B1:202:CYC:HMD1 | 12:B1:202:CYC:NC | 2.12 | 0.47 |
| 3:U4:112:GLY:N | 4:M4:74:LEU:CD2 | 2.72 | 0.47 |
| 3:L4:68:ARG:CG | 11:aA:81:ASP:C | 2.88 | 0.47 |
| 2:P4:12:ALA:HB1 | 3:Q4:95:TYR:HH | 1.79 | 0.47 |
| 3:Q4:84:ARG:NH1 | 5:Z4:29:HIS:HB2 | 2.30 | 0.47 |
| 8:O5:2:SER:O | 8:O5:100:ASP:CB | 2.63 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:Y4:103:SER:O | 3:Y4:108:ARG:HB2 | 2.15 | 0.47 |
| 1:B5:12:TYR:CZ | 1:B5:23:ALA:HB2 | 2.50 | 0.47 |
| 8:G5:52:LYS:HE3 | 8:G5:52:LYS:HB3 | 1.44 | 0.47 |
| 12:d5:201:CYC:NB | 12:d5:201:CYC:HMA3 | 2.29 | 0.47 |
| 8:Q5:4:LEU:HD21 | 8:Q5:26:ILE:HD13 | 1.93 | 0.47 |
| 3:L6:78:ARG:HH22 | 6:M6:70:GLU:N | 2.13 | 0.47 |
| 6:M6:69:ALA:HB2 | 3:H6:14:LEU:CG | 2.45 | 0.47 |
| 6:M6:249:ARG:HB3 | 12:H6:201:CYC:O1D | 2.15 | 0.47 |
| 10:j5:53:ARG:O | 10:j5:56:ILE:CG2 | 2.43 | 0.47 |
| 10:j5:213:LEU:HD12 | 10:j5:213:LEU:H | 1.79 | 0.47 |
| 10:j5:743:VAL:HG13 | 12:J7:201:CYC:CGD | 2.44 | 0.47 |
| 10:j5:802:VAL:O | 10:j5:806:VAL:HG23 | 2.15 | 0.47 |
| 10:j5:1125:ARG:HH22 | 1:t7:114:GLU:CB | 2.21 | 0.47 |
| 10:k5:140:PHE:O | 10:k5:140:PHE:CG | 2.68 | 0.47 |
| 10:k5:152:ARG:CZ | 10:k5:193:SER:HB2 | 2.44 | 0.47 |
| 10:k5:190:LEU:HD13 | 12:k5:1201:CYC:NC | 2.30 | 0.47 |
| 10:k5:382:ILE:HD13 | 10:k5:382:ILE:HG21 | 1.58 | 0.47 |
| 10:k5:755:GLN:HB3 | 10:k5:879:ASP:HB2 | 1.95 | 0.47 |
| 10:k5:1143:LEU:HD23 | 1:l7:10:ASN:CG | 2.39 | 0.47 |
| 8:O7:25:ARG:NH2 | 8:E7:25:ARG:NE | 2.63 | 0.47 |
| 8:i7:44:THR:HG23 | 1:j7:18:TYR:HD2 | 1.79 | 0.47 |
| 8:Y7:39:ILE:HG12 | 8:Y7:145:ASP:HB3 | 1.95 | 0.47 |
| 8:e7:39:ILE:HG12 | 8:e7:145:ASP:HB3 | 1.95 | 0.47 |
| 12:A8:201:CYC:HBB2 | 3:D8:75:PRO:CB | 2.44 | 0.47 |
| 3:D8:52:ILE:HD11 | 3:D8:87:GLU:HA | 1.95 | 0.47 |
| 1:n7:12:TYR:CZ | 1:n7:23:ALA:HB2 | 2.50 | 0.47 |
| 8:s7:2:SER:O | 8:s7:100:ASP:CB | 2.62 | 0.47 |
| 8:u7:4:LEU:CD1 | 1:v7:30:TYR:CZ | 2.93 | 0.47 |
| 3:U8:75:PRO:CB | 12:V8:201:CYC:HBB2 | 2.44 | 0.47 |
| 3:F8:109:CYS:O | 4:M8:6:THR:HG23 | 2.15 | 0.47 |
| 12:M8:301:CYC:HMC2 | 3:Y8:126:SER:HB2 | 1.96 | 0.47 |
| 2:P8:30:ARG:HD3 | 2:P8:30:ARG:C | 2.39 | 0.47 |
| 2:O9:30:ARG:HD3 | 2:O9:30:ARG:C | 2.39 | 0.47 |
| 2:E9:152:ALA:HB3 | 2:I9:21:ASN:OD1 | 2.14 | 0.47 |
| 3:H9:75:PRO:CB | 12:I9:201:CYC:HBB2 | 2.44 | 0.47 |
| 3:J9:68:ARG:HB2 | 11:a9:353:ALA:CB | 2.45 | 0.47 |
| 3:J9:116:THR:CG2 | 11:a9:521:PHE:CG | 2.87 | 0.47 |
| 12:J9:201:CYC:HC | 12:J9:201:CYC:HMD3 | 1.78 | 0.47 |
| 2:G1:106:ASP:C | 3:L1:77:ARG:HH21 | 2.22 | 0.47 |
| 11:a9:632:ILE:HG23 | 11:a9:634:ALA:N | 2.24 | 0.47 |
| 3:H1:109:CYS:HA | 12:H1:201:CYC:HBB2 | 1.94 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:M1:1:MET:HE3 | 4:M1:45:VAL:HA | 1.29 | 0.47 |
| 3:Z1:52:ILE:HD11 | 3:Z1:87:GLU:HA | 1.95 | 0.47 |
| 12:A:201:CYC:HMD1 | 12:A:201:CYC:NC | 2.10 | 0.47 |
| 2:GA:30:ARG:HD3 | 2:GA:30:ARG:C | 2.39 | 0.47 |
| 2:IA:9:ILE:HG23 | 3:JA:95:TYR:HB3 | 1.97 | 0.47 |
| 3:JA:68:ARG:HB2 | 11:aA:353:ALA:CB | 2.44 | 0.47 |
| 3:LA:44:ILE:CG2 | 3:LA:90:LEU:CD2 | 2.84 | 0.47 |
| 3:RA:88:ILE:HG21 | 12:RA:201:CYC:HAB2 | 1.96 | 0.47 |
| 3:TA:28:THR:HG23 | 2:X4:67:THR:O | 2.13 | 0.47 |
| 2:O1:44:LEU:HD11 | 2:O1:142:LEU:HD11 | 1.96 | 0.47 |
| 12:B3:202:CYC:HMA2 | 11:a9:684:ASN:ND2 | 2.29 | 0.47 |
| 3:B4:82:CYS:HG | 12:B4:202:CYC:H2C | 1.76 | 0.47 |
| 3:B4:116:THR:CG2 | 4:M4:56:MET:CG | 2.89 | 0.47 |
| 4:M3:176:ARG:CG | 4:M3:176:ARG:NH1 | 2.70 | 0.47 |
| 2:W3:30:ARG:HD3 | 2:W3:30:ARG:C | 2.39 | 0.47 |
| 2:G4:38:MET:HE2 | 2:G4:38:MET:HB3 | 1.81 | 0.47 |
| 4:M4:74:LEU:O | 4:M4:77:LEU:HD11 | 2.15 | 0.47 |
| 2:N4:34:ALA:CB | 3:O4:31:VAL:HG21 | 2.44 | 0.47 |
| 2:N4:119:THR:HG21 | 3:Q4:83:LEU:HD22 | 1.97 | 0.47 |
| 8:K5:116:TYR:O | 8:K5:120:GLN:N | 2.48 | 0.47 |
| 1:N5:87:TYR:OH | 10:k5:483:PHE:HE2 | 1.95 | 0.47 |
| 8:A5:126:VAL:HG22 | 12:A5:201:CYC:CBC | 2.45 | 0.47 |
| 8:C5:2:SER:O | 8:C5:100:ASP:CB | 2.62 | 0.47 |
| 8:E5:116:TYR:O | 8:E5:120:GLN:N | 2.48 | 0.47 |
| 1:P5:89:LEU:HD22 | 1:P5:133:MET:CE | 2.44 | 0.47 |
| 1:T5:12:TYR:CZ | 1:T5:23:ALA:HB2 | 2.50 | 0.47 |
| 6:M6:69:ALA:CB | 3:H6:14:LEU:HD11 | 2.45 | 0.47 |
| 12:N6:101:CYC:HAB2 | 3:B6:88:ILE:HG21 | 1.96 | 0.47 |
| 9:i5:15:LYS:C | 9:i5:15:LYS:CD | 2.88 | 0.47 |
| 10:j5:19:THR:HB | 10:j5:173:ALA:HB2 | 1.97 | 0.47 |
| 10:j5:28:ILE:HD13 | 10:j5:28:ILE:HG21 | 1.59 | 0.47 |
| 10:j5:275:THR:HG21 | 10:j5:286:VAL:C | 2.40 | 0.47 |
| 10:j5:275:THR:HG21 | 10:j5:286:VAL:HG12 | 1.86 | 0.47 |
| 10:j5:822:ARG:HA | 1:H7:106:GLU:HG2 | 1.96 | 0.47 |
| 10:j5:1089:LEU:HD22 | 10:j5:1089:LEU:C | 2.39 | 0.47 |
| 10:k5:214:PHE:N | 10:k5:214:PHE:CD1 | 2.83 | 0.47 |
| 10:k5:1013:PRO:O | 10:k5:1014:SER:C | 2.58 | 0.47 |
| 12:F7:201:CYC:HMA3 | 12:F7:201:CYC:NB | 2.29 | 0.47 |
| 1:J7:89:LEU:HD22 | 1:J7:133:MET:CE | 2.44 | 0.47 |
| 8:i7:37:LEU:CD2 | 1:j7:31:PHE:CE2 | 2.97 | 0.47 |
| 12:j7:201:CYC:HBB2 | 9:y7:42:GLN:CD | 2.37 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:X7:89:LEU:HD22 | 1:X7:133:MET:CE | 2.44 | 0.47 |
| 8:a7:2:SER:O | 8:a7:100:ASP:CB | 2.63 | 0.47 |
| 2:A8:5:ILE:HG21 | 3:B8:99:ALA:HA | 1.96 | 0.47 |
| 2:A8:34:ALA:CB | 3:B8:31:VAL:HG11 | 2.39 | 0.47 |
| 3:B8:75:PRO:CB | 12:E8:201:CYC:HBB2 | 2.44 | 0.47 |
| 8:q7:54:ALA:HB2 | 8:q7:133:MET:HG2 | 1.96 | 0.47 |
| 8:q7:82:LEU:CD1 | 11:aA:52:MET:SD | 3.03 | 0.47 |
| 12:r7:201:CYC:HMA3 | 12:r7:201:CYC:NB | 2.29 | 0.47 |
| 8:s7:21:GLY:C | 8:s7:23:LEU:N | 2.72 | 0.47 |
| 8:u7:30:VAL:CA | 1:v7:31:PHE:CD1 | 2.86 | 0.47 |
| 3:U8:108:ARG:CG | 4:M8:246:ALA:HB2 | 2.40 | 0.47 |
| 3:F8:107:ASP:OD1 | 3:F8:108:ARG:N | 2.48 | 0.47 |
| 4:M8:226:SER:HG | 3:Y8:88:ILE:HG12 | 1.77 | 0.47 |
| 3:Q8:117:TYR:O | 3:Q8:120:LEU:CG | 2.53 | 0.47 |
| 3:F1:84:ARG:NH2 | 4:M1:35:THR:OG1 | 2.48 | 0.47 |
| 3:F1:113:LEU:HD13 | 4:M1:38:PRO:HB2 | 1.97 | 0.47 |
| 3:L9:48:ALA:HB1 | 2:K9:18:PHE:HE2 | 1.67 | 0.47 |
| 4:M9:16:LYS:HA | 4:M9:46:VAL:HA | 1.96 | 0.47 |
| 4:M9:160:THR:CG2 | 4:M9:257:GLN:CG | 2.93 | 0.47 |
| 2:A9:59:VAL:HG12 | 2:A9:66:LEU:HD13 | 1.96 | 0.47 |
| 11:a9:617:ALA:O | 11:a9:620:ALA:HA | 2.14 | 0.47 |
| 11:a9:818:ARG:HD2 | 11:a9:818:ARG:HA | 1.57 | 0.47 |
| 11:aA:504:VAL:HG12 | 11:aA:505:PRO:HD2 | 1.97 | 0.47 |
| 11:aA:817:LEU:HD12 | 3:L1:119:ALA:C | 2.28 | 0.47 |
| 11:aA:817:LEU:O | 11:aA:818:ARG:C | 2.52 | 0.47 |
| 3:H1:84:ARG:NH2 | 12:H1:201:CYC:C1A | 2.78 | 0.47 |
| 5:N1:57:MET:CE | 5:N1:67:ILE:HG13 | 2.44 | 0.47 |
| 2:C2:30:ARG:C | 2:C2:30:ARG:HD3 | 2.39 | 0.47 |
| 1:A:12:TYR:CZ | 1:A:23:ALA:HB2 | 2.50 | 0.47 |
| 3:FA:151:GLY:N | 3:F9:150:ARG:CZ | 2.51 | 0.47 |
| 2:GA:128:ILE:HG22 | 2:GA:132:LYS:HE3 | 1.97 | 0.47 |
| 12:GA:201:CYC:HBB2 | 3:LA:75:PRO:CB | 2.44 | 0.47 |
| 3:HA:75:PRO:CB | 12:IA:201:CYC:HBB2 | 2.44 | 0.47 |
| 4:MA:204:ILE:HG22 | 4:MA:204:ILE:O | 2.14 | 0.47 |
| 2:QA:21:ASN:CB | 2:UA:153:TYR:CZ | 2.98 | 0.47 |
| 2:QA:25:GLN:HE22 | 2:UA:100:GLY:HA2 | 1.80 | 0.47 |
| 2:A1:16:GLY:CA | 11:aA:677:GLN:CD | 2.80 | 0.47 |
| 3:H2:84:ARG:O | 3:H2:86:MET:N | 2.45 | 0.47 |
| 2:I2:30:ARG:HD3 | 2:I2:30:ARG:C | 2.39 | 0.47 |
| 6:M2:28:ASN:O | 8:O5:79:ALA:HB1 | 2.15 | 0.47 |
| 2:A3:34:ALA:CB | 3:B3:31:VAL:HG21 | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:A4:44:LEU:HD11 | 2:A4:142:LEU:HD11 | 1.97 | 0.47 |
| 4:M3:160:THR:CG2 | 4:M3:257:GLN:CG | 2.93 | 0.47 |
| 2:U3:46:SER:C | 2:Q9:74:TYR:CE2 | 2.93 | 0.47 |
| 3:U4:75:PRO:CB | 12:V4:201:CYC:HBB2 | 2.44 | 0.47 |
| 3:U4:88:ILE:HG21 | 12:U4:201:CYC:HAB2 | 1.96 | 0.47 |
| 3:W4:75:PRO:CB | 12:X4:201:CYC:HBB2 | 2.45 | 0.47 |
| 2:N4:64:PRO:C | 2:N4:66:LEU:N | 2.71 | 0.47 |
| 3:O4:111:ASN:ND2 | 5:Z4:66:ARG:HB2 | 2.30 | 0.47 |
| 2:R4:30:ARG:HD3 | 2:R4:30:ARG:C | 2.39 | 0.47 |
| 8:K5:25:ARG:HH22 | 8:U5:6:LYS:HD3 | 1.80 | 0.47 |
| 8:A5:125:ALA:HB3 | 12:A5:201:CYC:CMC | 2.45 | 0.47 |
| 8:E5:72:ALA:HB2 | 12:E5:201:CYC:OC | 2.15 | 0.47 |
| 8:E5:113:LYS:O | 8:E5:117:ASN:CG | 2.58 | 0.47 |
| 1:F5:89:LEU:HD22 | 1:F5:133:MET:CE | 2.44 | 0.47 |
| 12:F5:201:CYC:HMA2 | 10:k5:591:ILE:HG23 | 1.88 | 0.47 |
| 12:F5:201:CYC:CMA | 12:F5:201:CYC:NB | 2.74 | 0.47 |
| 8:G5:68:PRO:HB2 | 8:U5:63:PRO:HG2 | 1.97 | 0.47 |
| 12:J5:201:CYC:HMA3 | 12:J5:201:CYC:NB | 2.29 | 0.47 |
| 12:T5:201:CYC:CMA | 12:T5:201:CYC:NB | 2.74 | 0.47 |
| 6:M6:43:TRP:CZ3 | 8:c7:52:LYS:CB | 2.98 | 0.47 |
| 6:M6:283:VAL:HG22 | 6:M6:284:SER:N | 2.30 | 0.47 |
| 10:j5:45:GLN:O | 10:j5:49:ASP:OD1 | 2.33 | 0.47 |
| 10:j5:59:LYS:O | 10:j5:63:ASN:OD1 | 2.33 | 0.47 |
| 10:j5:641:ASP:HB3 | 10:j5:643:VAL:H | 1.79 | 0.47 |
| 10:j5:750:ARG:HH11 | 10:j5:750:ARG:CG | 2.25 | 0.47 |
| 10:j5:1129:ARG:HA | 10:j5:1133:GLU:HB3 | 1.96 | 0.47 |
| 10:k5:59:LYS:O | 10:k5:63:ASN:OD1 | 2.33 | 0.47 |
| 10:k5:767:LEU:CD2 | 10:k5:767:LEU:C | 2.84 | 0.47 |
| 10:k5:822:ARG:HD2 | 1:B7:106:GLU:OE2 | 2.15 | 0.47 |
| 2:C6:30:ARG:HD3 | 2:C6:30:ARG:C | 2.39 | 0.47 |
| 3:D6:88:ILE:HG21 | 12:D6:201:CYC:HAB2 | 1.96 | 0.47 |
| 1:R7:89:LEU:HD22 | 1:R7:133:MET:CE | 2.44 | 0.47 |
| 12:R7:201:CYC:HMA3 | 12:R7:201:CYC:NB | 2.29 | 0.47 |
| 12:B7:201:CYC:HMD1 | 12:B7:201:CYC:NC | 2.09 | 0.47 |
| 1:D7:75:THR:HG21 | 8:E7:112:VAL:HB | 1.97 | 0.47 |
| 8:G7:54:ALA:HB2 | 8:G7:133:MET:HG2 | 1.96 | 0.47 |
| 8:G7:86:ASP:CB | 11:a9:579:PHE:HZ | 2.17 | 0.47 |
| 1:J7:12:TYR:CZ | 1:J7:23:ALA:HB2 | 2.50 | 0.47 |
| 8:a7:2:SER:C | 8:a7:100:ASP:HB2 | 2.40 | 0.47 |
| 1:b7:89:LEU:HD22 | 1:b7:133:MET:CE | 2.44 | 0.47 |
| 2:A8:44:LEU:HD11 | 2:A8:142:LEU:HD11 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:C8:30:ARG:HD3 | 2:C8:30:ARG:C | 2.39 | 0.47 |
| 3:D8:107:ASP:HB3 | 11:a9:109:ASN:CB | 2.43 | 0.47 |
| 1:r7:89:LEU:HD22 | 1:r7:133:MET:CE | 2.44 | 0.47 |
| 12:L9:202:CYC:CMA | 11:a9:534:SER:HB2 | 2.44 | 0.47 |
| 12:C9:201:CYC:HBB2 | 3:F9:75:PRO:CB | 2.45 | 0.47 |
| 11:a9:376:ALA:HB3 | 11:a9:504:VAL:H | 1.79 | 0.47 |
| 11:a9:616:PRO:O | 11:a9:616:PRO:HG2 | 2.14 | 0.47 |
| 11:a9:643:LEU:CD1 | 11:a9:766:ASN:HA | 2.45 | 0.47 |
| 11:aA:412:VAL:HA | 11:aA:415:GLU:OE2 | 2.15 | 0.47 |
| 11:aA:588:VAL:C | 11:aA:590:PRO:HD2 | 2.30 | 0.47 |
| 11:aA:643:LEU:CD1 | 11:aA:689:VAL:HG23 | 2.43 | 0.47 |
| 11:aA:714:ARG:NH2 | 11:aA:810:GLN:OE1 | 2.45 | 0.47 |
| 12:J1:201:CYC:HC | 12:J1:201:CYC:HMD3 | 1.78 | 0.47 |
| 2:K1:115:GLU:CD | 2:K1:118:ARG:NH1 | 2.71 | 0.47 |
| 5:N1:22:LEU:HD21 | 5:N1:26:LEU:CD1 | 2.14 | 0.47 |
| 3:X1:75:PRO:CB | 12:Y1:201:CYC:HBB2 | 2.45 | 0.47 |
| 12:C2:201:CYC:HBB2 | 3:F2:75:PRO:CB | 2.44 | 0.47 |
| 2:AA:44:LEU:HD11 | 2:AA:142:LEU:HD11 | 1.96 | 0.46 |
| 2:EA:128:ILE:HG22 | 2:EA:132:LYS:HE3 | 1.98 | 0.46 |
| 3:JA:116:THR:CG2 | 11:aA:521:PHE:CD2 | 2.88 | 0.46 |
| 3:LA:107:ASP:O | 3:LA:111:ASN:CB | 2.64 | 0.46 |
| 2:OA:5:ILE:HG21 | 3:PA:99:ALA:HA | 1.96 | 0.46 |
| 2:YA:38:MET:HE2 | 2:YA:38:MET:HB3 | 1.81 | 0.46 |
| 3:P1:88:ILE:HG21 | 12:P1:201:CYC:HAB2 | 1.95 | 0.46 |
| 3:B4:52:ILE:HD11 | 3:B4:87:GLU:HA | 1.96 | 0.46 |
| 3:D4:52:ILE:HD11 | 3:D4:87:GLU:HA | 1.95 | 0.46 |
| 3:L3:75:PRO:CG | 11:a9:823:ILE:HD12 | 2.45 | 0.46 |
| 4:M3:74:LEU:O | 4:M3:77:LEU:HD11 | 2.15 | 0.46 |
| 8:M5:107:ILE:CG1 | 1:N5:13:ASP:OD2 | 2.59 | 0.46 |
| 1:J5:76:ARG:HG3 | 1:J5:77:ARG:HG3 | 1.97 | 0.46 |
| 1:d5:12:TYR:CZ | 1:d5:23:ALA:HB2 | 2.50 | 0.46 |
| 1:f5:114:GLU:HA | 10:j5:491:THR:CG2 | 2.45 | 0.46 |
| 12:b5:201:CYC:HMA3 | 12:b5:201:CYC:NB | 2.29 | 0.46 |
| 6:M6:53:LEU:HB3 | 8:c7:80:LEU:HD21 | 1.98 | 0.46 |
| 10:j5:794:ARG:HH21 | 12:T7:201:CYC:C4B | 2.27 | 0.46 |
| 10:j5:871:GLU:O | 10:j5:871:GLU:HG2 | 2.12 | 0.46 |
| 10:j5:1015:TYR:OH | 8:q7:110:ILE:HG22 | 2.14 | 0.46 |
| 10:k5:352:ILE:HG22 | 10:k5:353:ASN:N | 2.30 | 0.46 |
| 10:k5:471:PRO:O | 10:k5:501:ILE:CG1 | 2.57 | 0.46 |
| 10:k5:1052:PRO:HB3 | 11:a9:32:ARG:HH21 | 1.70 | 0.46 |
| 1:R7:53:LYS:NZ | 8:M7:120:GLN:CG | 2.78 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:j7:76:ARG:HB2 | 8:e7:110:ILE:HG13 | 1.96 | 0.46 |
| 8:Y7:112:VAL:N | 1:d7:75:THR:HB | 2.29 | 0.46 |
| 8:a7:48:GLU:O | 11:a9:318:TRP:HZ3 | 1.98 | 0.46 |
| 8:c7:11:ALA:HB1 | 1:d7:94:TYR:HH | 1.79 | 0.46 |
| 2:A8:38:MET:HE2 | 2:A8:38:MET:HB3 | 1.81 | 0.46 |
| 8:o7:130:VAL:HG21 | 8:o7:160:MET:HE3 | 1.97 | 0.46 |
| 8:q7:76:LYS:NZ | 11:aA:604:ALA:HB1 | 2.30 | 0.46 |
| 1:v7:3:ASP:H | 1:v7:6:THR:HG1 | 1.61 | 0.46 |
| 3:J8:108:ARG:NE | 11:a9:171:ARG:O | 2.48 | 0.46 |
| 3:L8:68:ARG:CD | 11:a9:82:GLN:N | 2.62 | 0.46 |
| 2:N8:110:VAL:O | 2:N8:111:ALA:C | 2.56 | 0.46 |
| 3:L9:107:ASP:O | 11:a9:531:ASP:HB2 | 2.15 | 0.46 |
| 4:M9:95:ALA:HB2 | 5:N9:38:GLU:OE1 | 2.16 | 0.46 |
| 5:N9:57:MET:CE | 5:N9:67:ILE:HG13 | 2.44 | 0.46 |
| 5:Z8:23:SER:C | 5:Z8:25:THR:N | 2.73 | 0.46 |
| 2:E9:128:ILE:HG22 | 2:E9:132:LYS:HE3 | 1.98 | 0.46 |
| 3:J9:75:PRO:CB | 12:K9:201:CYC:HBB2 | 2.45 | 0.46 |
| 2:S9:128:ILE:HG22 | 2:S9:132:LYS:HE3 | 1.97 | 0.46 |
| 11:aA:616:PRO:HG2 | 11:aA:616:PRO:O | 2.14 | 0.46 |
| 11:aA:643:LEU:CD1 | 11:aA:766:ASN:HA | 2.44 | 0.46 |
| 11:aA:801:ASN:HB3 | 11:aA:807:GLN:HE21 | 1.79 | 0.46 |
| 3:J1:75:PRO:CB | 12:K1:201:CYC:HBB2 | 2.44 | 0.46 |
| 3:L1:52:ILE:HD11 | 3:L1:87:GLU:HA | 1.96 | 0.46 |
| 4:M1:45:VAL:O | 4:M1:45:VAL:HG12 | 2.14 | 0.46 |
| 3:JA:114:LYS:HG2 | 8:S7:60:GLN:HE22 | 1.60 | 0.46 |
| 12:LA:202:CYC:NB | 11:aA:404:TYR:CE1 | 2.83 | 0.46 |
| 4:MA:200:ILE:HD13 | 4:MA:200:ILE:HA | 1.54 | 0.46 |
| 4:MA:274:VAL:H | 3:VA:77:ARG:CG | 2.15 | 0.46 |
| 2:QA:116:VAL:CG1 | 3:TA:79:MET:HG3 | 2.37 | 0.46 |
| 12:P1:201:CYC:O2A | 4:M1:130:SER:CA | 2.59 | 0.46 |
| 2:A1:64:PRO:C | 2:A1:66:LEU:H | 2.22 | 0.46 |
| 12:G3:201:CYC:HBB2 | 3:L3:75:PRO:CB | 2.44 | 0.46 |
| 12:C3:201:CYC:HBB2 | 3:F3:75:PRO:CB | 2.44 | 0.46 |
| 2:A4:59:VAL:O | 2:A4:66:LEU:CD1 | 2.62 | 0.46 |
| 3:B4:97:LEU:HA | 3:B4:163:TYR:CE2 | 2.50 | 0.46 |
| 3:B4:112:GLY:C | 3:B4:114:LYS:N | 2.67 | 0.46 |
| 4:M3:51:ARG:HH11 | 4:M3:51:ARG:CG | 2.27 | 0.46 |
| 4:M3:232:VAL:HG21 | 3:V3:113:LEU:CB | 2.45 | 0.46 |
| 4:M3:252:LEU:HD12 | 12:X3:201:CYC:O1D | 2.06 | 0.46 |
| 2:O3:44:LEU:HD11 | 2:O3:142:LEU:HD11 | 1.96 | 0.46 |
| 2:S3:30:ARG:HD3 | 2:S3:30:ARG:C | 2.39 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M4:45:VAL:O | 4:M4:45:VAL:HG12 | 2.14 | 0.46 |
| 4:M4:152:TYR:CD1 | 4:M4:152:TYR:O | 2.69 | 0.46 |
| 2:N4:13:ASP:OD2 | 3:O4:108:ARG:CD | 2.64 | 0.46 |
| 2:N4:128:ILE:HG22 | 2:N4:132:LYS:HE3 | 1.98 | 0.46 |
| 5:Z4:39:PRO:HG3 | 12:Z4:301:CYC:HHD | 1.95 | 0.46 |
| 1:D5:75:THR:HB | 8:E5:111:GLY:C | 2.41 | 0.46 |
| 12:H5:201:CYC:HMA3 | 12:H5:201:CYC:NB | 2.30 | 0.46 |
| 8:I5:130:VAL:HG12 | 8:I5:157:VAL:HG23 | 1.96 | 0.46 |
| 1:f5:3:ASP:H | 1:f5:6:THR:HG1 | 1.60 | 0.46 |
| 1:R5:87:TYR:HE1 | 10:k5:521:GLY:CA | 2.28 | 0.46 |
| 8:U5:76:LYS:HG3 | 8:U5:77:MET:CA | 2.43 | 0.46 |
| 8:Y5:39:ILE:HG12 | 8:Y5:145:ASP:HB3 | 1.95 | 0.46 |
| 8:a5:2:SER:C | 8:a5:100:ASP:HB2 | 2.40 | 0.46 |
| 9:z5:18:ARG:HB3 | 9:z5:22:GLU:CD | 2.30 | 0.46 |
| 10:j5:66:MET:O | 10:j5:70:ARG:HD3 | 2.15 | 0.46 |
| 10:j5:140:PHE:O | 10:j5:140:PHE:CG | 2.68 | 0.46 |
| 10:k5:66:MET:O | 10:k5:70:ARG:HD3 | 2.15 | 0.46 |
| 10:k5:361:PHE:CZ | 10:k5:378:TYR:CE2 | 3.03 | 0.46 |
| 10:k5:966:SER:HB2 | 1:p7:14:VAL:HG11 | 1.83 | 0.46 |
| 2:A6:34:ALA:HB3 | 3:B6:31:VAL:CG1 | 2.39 | 0.46 |
| 3:D1:52:ILE:HD11 | 3:D1:87:GLU:HA | 1.95 | 0.46 |
| 1:P7:12:TYR:CZ | 1:P7:23:ALA:HB2 | 2.50 | 0.46 |
| 1:P7:75:THR:HG21 | 8:Q7:112:VAL:HB | 1.96 | 0.46 |
| 8:S7:54:ALA:HB2 | 8:S7:133:MET:HG2 | 1.96 | 0.46 |
| 8:g7:2:SER:C | 8:g7:100:ASP:HB2 | 2.40 | 0.46 |
| 1:V7:12:TYR:CZ | 1:V7:23:ALA:HB2 | 2.50 | 0.46 |
| 8:c7:122:PRO:C | 8:c7:125:ALA:H | 2.23 | 0.46 |
| 1:r7:12:TYR:CZ | 1:r7:23:ALA:HB2 | 2.50 | 0.46 |
| 8:s7:130:VAL:HG12 | 8:s7:157:VAL:HG23 | 1.96 | 0.46 |
| 8:u7:5:THR:OG1 | 1:v7:6:THR:HG23 | 2.12 | 0.46 |
| 9:w7:29:THR:HG22 | 9:w7:30:LYS:N | 2.31 | 0.46 |
| 4:M8:160:THR:CG2 | 4:M8:257:GLN:CG | 2.93 | 0.46 |
| 2:N8:34:ALA:CB | 3:O8:31:VAL:HG11 | 2.38 | 0.46 |
| 2:P8:128:ILE:HG22 | 2:P8:132:LYS:HE3 | 1.97 | 0.46 |
| 4:M9:29:PRO:HB2 | 11:a9:375:GLN:HG3 | 1.97 | 0.46 |
| 3:B9:75:PRO:CB | 12:E9:201:CYC:HBB2 | 2.45 | 0.46 |
| 12:J9:202:CYC:HB | 11:a9:512:TYR:CA | 2.25 | 0.46 |
| 2:K9:128:ILE:HG22 | 2:K9:132:LYS:HE3 | 1.98 | 0.46 |
| 11:a9:642:GLU:HG3 | 11:a9:643:LEU:N | 2.29 | 0.46 |
| 11:a9:817:LEU:HD23 | 11:a9:817:LEU:HA | 1.50 | 0.46 |
| 4:M1:164:ARG:O | 4:M1:164:ARG:HG3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 5:N1:37:HIS:CD2 | 5:N1:38:GLU:O | 2.69 | 0.46 |
| 1:Z:161:SER:CB | 1:X5:14:VAL:CB | 2.37 | 0.46 |
| 2:AA:5:ILE:HG21 | 3:BA:99:ALA:HA | 1.96 | 0.46 |
| 2:KA:18:PHE:HZ | 3:LA:90:LEU:HD22 | 1.80 | 0.46 |
| 4:MA:176:ARG:HG2 | 4:MA:176:ARG:O | 2.13 | 0.46 |
| 3:PA:88:ILE:HG21 | 12:PA:201:CYC:HAB2 | 1.95 | 0.46 |
| 2:QA:33:ARG:HB2 | 2:UA:25:GLN:HG2 | 1.96 | 0.46 |
| 12:RA:202:CYC:HC | 12:RA:202:CYC:HMD3 | 1.78 | 0.46 |
| 12:R1:202:CYC:HC | 12:R1:202:CYC:HMD3 | 1.78 | 0.46 |
| 3:B3:88:ILE:HG22 | 12:B3:202:CYC:HMB1 | 1.96 | 0.46 |
| 3:D4:108:ARG:CD | 11:aA:107:ARG:CZ | 2.36 | 0.46 |
| 4:M3:152:TYR:CD1 | 4:M3:152:TYR:O | 2.69 | 0.46 |
| 2:O3:5:ILE:HG21 | 3:P3:99:ALA:HA | 1.96 | 0.46 |
| 12:W4:202:CYC:HC | 12:W4:202:CYC:HMD3 | 1.77 | 0.46 |
| 4:M4:95:ALA:HB2 | 5:Z4:38:GLU:CB | 2.37 | 0.46 |
| 4:M4:164:ARG:O | 4:M4:164:ARG:HG3 | 2.15 | 0.46 |
| 4:M4:214:GLY:CA | 5:Z4:28:HIS:ND1 | 2.79 | 0.46 |
| 3:O4:88:ILE:HG21 | 12:O4:201:CYC:HAB2 | 1.95 | 0.46 |
| 3:O4:108:ARG:HG2 | 3:O4:108:ARG:O | 2.15 | 0.46 |
| 12:O4:202:CYC:CMD | 12:O4:202:CYC:NC | 2.75 | 0.46 |
| 2:R4:128:ILE:HG22 | 2:R4:132:LYS:HE3 | 1.98 | 0.46 |
| 8:K5:113:LYS:O | 8:K5:117:ASN:CG | 2.58 | 0.46 |
| 1:N5:89:LEU:HD22 | 1:N5:133:MET:CE | 2.45 | 0.46 |
| 8:O5:151:PHE:HB3 | 8:E5:20:PRO:CB | 2.28 | 0.46 |
| 8:A5:107:ILE:O | 12:A5:201:CYC:HAB2 | 2.14 | 0.46 |
| 8:C5:6:LYS:O | 8:C5:6:LYS:HG3 | 2.15 | 0.46 |
| 12:X5:201:CYC:CMA | 12:X5:201:CYC:NB | 2.74 | 0.46 |
| 12:b5:201:CYC:HMD1 | 12:b5:201:CYC:NC | 2.09 | 0.46 |
| 3:J6:75:PRO:CB | 12:K6:201:CYC:HBB2 | 2.45 | 0.46 |
| 6:M6:268:LYS:O | 1:d7:158:SER:HB3 | 2.15 | 0.46 |
| 10:j5:564:VAL:O | 10:j5:564:VAL:HG12 | 2.14 | 0.46 |
| 10:j5:935:LEU:HD13 | 1:J7:29:ALA:HB2 | 0.74 | 0.46 |
| 10:j5:990:ARG:CG | 10:j5:990:ARG:NH1 | 2.72 | 0.46 |
| 10:j5:1067:LEU:HD13 | 10:j5:1101:GLU:CG | 2.41 | 0.46 |
| 10:k5:284:PRO:CG | 10:k5:326:GLY:HA2 | 2.19 | 0.46 |
| 10:k5:305:PHE:CE2 | 10:k5:337:LEU:HD23 | 2.51 | 0.46 |
| 10:k5:348:TYR:CD1 | 10:k5:398:LEU:HD13 | 2.50 | 0.46 |
| 10:k5:1009:ALA:HA | 1:p7:87:TYR:CE1 | 2.50 | 0.46 |
| 10:k5:1019:SER:C | 10:k5:1021:ALA:H | 2.23 | 0.46 |
| 10:k5:1124:TYR:CE2 | 1:n7:119:LEU:HD21 | 2.49 | 0.46 |
| 10:k5:1140:TRP:O | 11:a9:32:ARG:NH2 | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 12:k5:1204:CYC:HMD1 | 12:k5:1204:CYC:NC | 2.09 | 0.46 |
| 3:H6:52:ILE:HD11 | 3:H6:87:GLU:HA | 1.95 | 0.46 |
| 3:D1:108:ARG:O | 4:M1:60:LYS:HD3 | 2.16 | 0.46 |
| 3:D1:111:ASN:HD21 | 4:M1:65:ARG:HD2 | 1.80 | 0.46 |
| 8:O7:25:ARG:HH22 | 8:E7:25:ARG:NE | 2.14 | 0.46 |
| 8:Q7:13:ALA:N | 9:z7:46:LYS:CE | 2.77 | 0.46 |
| 8:S7:49:ARG:NH2 | 11:aA:553:SER:HB2 | 2.30 | 0.46 |
| 8:I7:2:SER:O | 8:I7:100:ASP:CB | 2.62 | 0.46 |
| 8:i7:3:VAL:HG22 | 8:s7:25:ARG:NH2 | 2.29 | 0.46 |
| 8:Y7:54:ALA:HB2 | 8:Y7:133:MET:HG2 | 1.96 | 0.46 |
| 12:b7:201:CYC:HMA3 | 12:b7:201:CYC:NB | 2.29 | 0.46 |
| 8:e7:75:GLU:HG2 | 8:e7:76:LYS:N | 2.30 | 0.46 |
| 8:o7:97:VAL:HG22 | 1:p7:19:LEU:HD11 | 1.93 | 0.46 |
| 9:x7:34:TYR:CD1 | 9:x7:34:TYR:O | 2.68 | 0.46 |
| 9:y7:3:ARG:NH1 | 9:y7:67:VAL:CG1 | 2.71 | 0.46 |
| 2:G8:30:ARG:HD3 | 2:G8:30:ARG:C | 2.39 | 0.46 |
| 4:M8:233:GLU:HG3 | 3:Y8:112:GLY:CA | 2.27 | 0.46 |
| 3:Q8:116:THR:O | 5:Z8:40:SER:HA | 2.15 | 0.46 |
| 4:M9:152:TYR:CD1 | 4:M9:152:TYR:O | 2.69 | 0.46 |
| 2:O9:34:ALA:HB3 | 3:P9:31:VAL:CG1 | 2.39 | 0.46 |
| 2:A9:64:PRO:C | 2:A9:66:LEU:H | 2.23 | 0.46 |
| 3:B9:30:LEU:CD1 | 3:B9:30:LEU:H | 2.28 | 0.46 |
| 11:a9:823:ILE:O | 11:a9:824:VAL:OXT | 2.32 | 0.46 |
| 11:aA:668:TYR:CD1 | 3:J1:84:ARG:HB2 | 2.51 | 0.46 |
| 11:aA:694:ARG:HH12 | 4:M1:51:ARG:HH22 | 1.56 | 0.46 |
| 11:aA:803:ASN:HB3 | 3:J1:119:ALA:HB1 | 1.97 | 0.46 |
| 3:BA:30:LEU:CD1 | 3:BA:30:LEU:H | 2.28 | 0.46 |
| 3:BA:75:PRO:CB | 12:EA:201:CYC:HBB2 | 2.45 | 0.46 |
| 3:FA:150:ARG:HD2 | 3:F9:150:ARG:HG2 | 1.83 | 0.46 |
| 5:NA:57:MET:CE | 5:NA:67:ILE:HG13 | 2.45 | 0.46 |
| 2:QA:81:LYS:HE2 | 3:TA:67:ILE:HD12 | 1.96 | 0.46 |
| 2:UA:128:ILE:HG22 | 2:UA:132:LYS:HE3 | 1.98 | 0.46 |
| 2:A1:25:GLN:HG2 | 2:K1:33:ARG:CG | 2.38 | 0.46 |
| 3:H2:14:LEU:CG | 6:M2:69:ALA:HB2 | 2.45 | 0.46 |
| 3:L2:78:ARG:HH22 | 6:M2:70:GLU:N | 2.13 | 0.46 |
| 6:M2:50:LEU:HD21 | 8:i7:79:ALA:CA | 2.46 | 0.46 |
| 6:M2:62:ARG:CZ | 1:h7:58:LYS:HA | 2.34 | 0.46 |
| 2:A3:44:LEU:HD11 | 2:A3:142:LEU:HD11 | 1.96 | 0.46 |
| 3:B3:92:TYR:CE2 | 12:B3:202:CYC:HBB1 | 2.50 | 0.46 |
| 3:F3:84:ARG:NH2 | 4:M3:35:THR:OG1 | 2.48 | 0.46 |
| 3:Z3:75:PRO:CB | 12:U3:201:CYC:HBB2 | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:A4:19:LEU:O | 3:B4:45:THR:CG2 | 2.64 | 0.46 |
| 2:A4:128:ILE:HG22 | 2:A4:132:LYS:HE3 | 1.98 | 0.46 |
| 5:N3:14:LYS:HE3 | 5:N3:50:LEU:CD2 | 2.45 | 0.46 |
| 12:F4:201:CYC:CMD | 12:F4:201:CYC:NC | 2.75 | 0.46 |
| 4:M4:131:LEU:HB3 | 4:M4:137:ILE:HG12 | 1.98 | 0.46 |
| 4:M4:205:ASP:CG | 5:Z4:59:ARG:HE | 2.23 | 0.46 |
| 4:M4:215:GLU:OE1 | 12:Z4:301:CYC:CAB | 2.60 | 0.46 |
| 4:M4:215:GLU:CB | 5:Z4:28:HIS:N | 2.73 | 0.46 |
| 3:O4:104:VAL:CA | 5:Z4:61:LYS:CE | 2.94 | 0.46 |
| 2:X4:18:PHE:CZ | 3:Y4:91:ARG:HG2 | 2.51 | 0.46 |
| 8:E5:17:TYR:CG | 1:F5:45:SER:CB | 2.99 | 0.46 |
| 8:E5:72:ALA:HB2 | 12:E5:201:CYC:NC | 2.30 | 0.46 |
| 1:H5:2:GLN:NE2 | 10:j5:551:MET:HG2 | 2.30 | 0.46 |
| 8:I5:6:LYS:O | 8:I5:6:LYS:HG3 | 2.15 | 0.46 |
| 12:d5:201:CYC:HMD1 | 12:d5:201:CYC:NC | 2.09 | 0.46 |
| 8:Q5:11:ALA:HB1 | 1:R5:94:TYR:CZ | 2.30 | 0.46 |
| 3:L6:132:GLN:CD | 1:d7:15:GLN:OE1 | 2.58 | 0.46 |
| 10:j5:283:ARG:CB | 10:j5:284:PRO:CD | 2.76 | 0.46 |
| 10:j5:1004:VAL:O | 10:j5:1004:VAL:HG12 | 2.14 | 0.46 |
| 10:j5:1019:SER:C | 10:j5:1021:ALA:H | 2.23 | 0.46 |
| 10:j5:1119:LEU:HD11 | 12:j5:1202:CYC:CBB | 2.45 | 0.46 |
| 10:k5:764:PHE:CD1 | 10:k5:764:PHE:C | 2.94 | 0.46 |
| 10:k5:779:ASP:OD2 | 12:F7:201:CYC:CMA | 2.40 | 0.46 |
| 10:k5:822:ARG:HA | 1:B7:106:GLU:HG2 | 1.96 | 0.46 |
| 10:k5:971:VAL:HG13 | 1:n7:76:ARG:NH1 | 2.29 | 0.46 |
| 8:I7:2:SER:C | 8:I7:100:ASP:HB2 | 2.40 | 0.46 |
| 12:h7:201:CYC:CMA | 12:h7:201:CYC:NB | 2.74 | 0.46 |
| 12:j7:201:CYC:CMA | 12:j7:201:CYC:NB | 2.74 | 0.46 |
| 8:a7:62:ARG:HA | 11:a9:336:ILE:CG2 | 2.45 | 0.46 |
| 8:a7:90:ARG:NH1 | 1:b7:16:GLY:CA | 2.74 | 0.46 |
| 8:a7:97:VAL:HG21 | 1:b7:19:LEU:HD11 | 1.96 | 0.46 |
| 2:E1:128:ILE:HG22 | 2:E1:132:LYS:HE3 | 1.98 | 0.46 |
| 2:A8:33:ARG:NH1 | 12:L8:201:CYC:C4B | 2.44 | 0.46 |
| 8:q7:52:LYS:HB3 | 8:q7:52:LYS:HE2 | 1.41 | 0.46 |
| 9:x7:9:ALA:HB2 | 9:x7:44:ILE:CD1 | 2.42 | 0.46 |
| 9:y7:34:TYR:CD1 | 9:y7:34:TYR:O | 2.68 | 0.46 |
| 2:X8:128:ILE:HG22 | 2:X8:132:LYS:HE3 | 1.98 | 0.46 |
| 3:F8:116:THR:N | 4:M8:3:VAL:HG12 | 2.29 | 0.46 |
| 12:J8:202:CYC:CMD | 12:J8:202:CYC:NC | 2.75 | 0.46 |
| 4:M8:211:GLN:O | 5:Z8:28:HIS:CE1 | 2.68 | 0.46 |
| 4:M8:231:THR:H | 12:M8:301:CYC:C3B | 2.29 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:R8:128:ILE:HG22 | 2:R8:132:LYS:HE3 | 1.97 | 0.46 |
| 4:M9:103:GLN:O | 4:M9:103:GLN:HG3 | 2.16 | 0.46 |
| 5:N9:14:LYS:HE3 | 5:N9:50:LEU:CD2 | 2.45 | 0.46 |
| 5:N9:37:HIS:CD2 | 5:N9:38:GLU:O | 2.69 | 0.46 |
| 2:G9:128:ILE:HG22 | 2:G9:132:LYS:HE3 | 1.97 | 0.46 |
| 11:a9:504:VAL:HG12 | 11:a9:505:PRO:HD2 | 1.97 | 0.46 |
| 11:aA:581:ARG:NH1 | 11:aA:581:ARG:CG | 2.72 | 0.46 |
| 2:I1:128:ILE:HG22 | 2:I1:132:LYS:HE3 | 1.98 | 0.46 |
| 4:M1:131:LEU:HB3 | 4:M1:137:ILE:HG12 | 1.98 | 0.46 |
| 3:B2:75:PRO:CB | 12:E2:201:CYC:HBB2 | 2.44 | 0.46 |
| 2:C2:128:ILE:HG22 | 2:C2:132:LYS:HE3 | 1.98 | 0.46 |
| 1:Z:107:ARG:NH1 | 8:e5:9:VAL:HG22 | 2.30 | 0.46 |
| 2:EA:152:ALA:HB3 | 2:IA:21:ASN:OD1 | 2.14 | 0.46 |
| 4:MA:164:ARG:O | 4:MA:164:ARG:HG3 | 2.15 | 0.46 |
| 5:NA:37:HIS:CD2 | 5:NA:38:GLU:O | 2.69 | 0.46 |
| 2:OA:19:LEU:O | 3:PA:45:THR:CG2 | 2.64 | 0.46 |
| 3:TA:28:THR:CB | 2:X4:67:THR:OG1 | 2.60 | 0.46 |
| 12:H2:201:CYC:O1D | 6:M2:249:ARG:HB3 | 2.15 | 0.46 |
| 3:D3:108:ARG:O | 4:M3:60:LYS:HD3 | 2.16 | 0.46 |
| 2:A4:64:PRO:C | 2:A4:66:LEU:N | 2.71 | 0.46 |
| 3:L3:75:PRO:CD | 11:a9:823:ILE:HG13 | 2.35 | 0.46 |
| 2:Y3:128:ILE:HG22 | 2:Y3:132:LYS:HE3 | 1.98 | 0.46 |
| 2:T4:128:ILE:HG22 | 2:T4:132:LYS:HE3 | 1.98 | 0.46 |
| 3:L4:68:ARG:CG | 11:aA:81:ASP:HA | 2.30 | 0.46 |
| 3:L4:88:ILE:HG12 | 11:aA:239:TYR:OH | 2.16 | 0.46 |
| 4:M4:225:LYS:CD | 3:Y4:81:ALA:CB | 2.93 | 0.46 |
| 5:Z4:14:LYS:HE3 | 5:Z4:50:LEU:CD2 | 2.45 | 0.46 |
| 8:E5:96:ILE:HD13 | 8:E5:96:ILE:HG21 | 1.60 | 0.46 |
| 8:G5:125:ALA:HB3 | 12:G5:201:CYC:CMC | 2.45 | 0.46 |
| 8:c5:59:PHE:HD2 | 6:M6:12:ILE:HD13 | 1.79 | 0.46 |
| 1:d5:61:ILE:O | 10:j5:712:ARG:NH2 | 2.49 | 0.46 |
| 1:P5:107:ARG:NE | 10:k5:619:GLU:O | 2.48 | 0.46 |
| 1:V5:83:ARG:HH12 | 10:j5:649:PHE:HE2 | 0.84 | 0.46 |
| 1:V5:114:GLU:OE1 | 10:j5:496:GLU:HA | 2.14 | 0.46 |
| 8:W5:17:TYR:N | 1:X5:90:ARG:HH11 | 2.13 | 0.46 |
| 1:X5:50:THR:OG1 | 8:a5:49:ARG:NH2 | 2.49 | 0.46 |
| 6:M6:45:ILE:HD12 | 8:c7:78:THR:CG2 | 2.37 | 0.46 |
| 6:M6:259:THR:C | 6:M6:261:LYS:N | 2.74 | 0.46 |
| 9:i5:27:PHE:C | 9:i5:27:PHE:CD1 | 2.93 | 0.46 |
| 10:j5:761:ARG:C | 10:j5:761:ARG:CD | 2.87 | 0.46 |
| 10:j5:990:ARG:CZ | 10:j5:1026:LYS:NZ | 2.67 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:j5:1050:PHE:CD2 | 10:j5:1058:VAL:HG11 | 2.45 | 0.46 |
| 10:k5:612:ILE:N | 10:k5:612:ILE:CD1 | 2.73 | 0.46 |
| 10:k5:1004:VAL:O | 10:k5:1004:VAL:HG12 | 2.14 | 0.46 |
| 10:k5:1067:LEU:HD11 | 10:k5:1101:GLU:CG | 2.14 | 0.46 |
| 10:k5:1145:PRO:O | 1:l7:14:VAL:CG1 | 2.64 | 0.46 |
| 2:C6:38:MET:HE2 | 2:C6:38:MET:HB3 | 1.81 | 0.46 |
| 2:C6:128:ILE:HG22 | 2:C6:132:LYS:HE3 | 1.98 | 0.46 |
| 8:C7:21:GLY:C | 8:C7:23:LEU:N | 2.72 | 0.46 |
| 1:N7:89:LEU:HD22 | 1:N7:133:MET:CE | 2.44 | 0.46 |
| 1:T7:12:TYR:CZ | 1:T7:23:ALA:HB2 | 2.50 | 0.46 |
| 8:Y7:134:LYS:O | 8:Y7:138:THR:HB | 2.16 | 0.46 |
| 8:a7:90:ARG:HH12 | 1:b7:16:GLY:HA2 | 1.79 | 0.46 |
| 8:c7:24:ASP:CG | 8:m7:36:ARG:HH12 | 2.24 | 0.46 |
| 8:c7:58:LEU:HD13 | 8:c7:128:GLU:CB | 2.46 | 0.46 |
| 8:m7:17:TYR:OH | 1:n7:89:LEU:HG | 2.16 | 0.46 |
| 8:o7:30:VAL:HB | 1:p7:31:PHE:HB3 | 1.97 | 0.46 |
| 8:u7:39:ILE:O | 8:u7:39:ILE:HG22 | 2.15 | 0.46 |
| 2:T8:128:ILE:HG22 | 2:T8:132:LYS:HE3 | 1.98 | 0.46 |
| 4:M8:147:ALA:HB2 | 4:M8:173:PHE:CZ | 2.49 | 0.46 |
| 3:L9:83:LEU:HD23 | 3:L9:83:LEU:HA | 1.53 | 0.46 |
| 4:M9:34:ASP:O | 12:B9:201:CYC:O2A | 2.33 | 0.46 |
| 4:M9:38:PRO:CB | 3:B9:113:LEU:HD13 | 2.45 | 0.46 |
| 4:M9:160:THR:C | 3:V9:108:ARG:HA | 2.41 | 0.46 |
| 2:O9:128:ILE:HG22 | 2:O9:132:LYS:HE3 | 1.98 | 0.46 |
| 5:Z8:42:SER:C | 12:Z8:301:CYC:HMA2 | 2.30 | 0.46 |
| 3:F9:36:LYS:HE2 | 3:F9:156:LEU:CD1 | 2.44 | 0.46 |
| 12:F9:302:CYC:HC | 12:F9:302:CYC:HMD3 | 1.78 | 0.46 |
| 2:K9:25:GLN:O | 2:K9:26:ALA:O | 2.28 | 0.46 |
| 11:a9:426:ARG:NH2 | 11:a9:496:ARG:CZ | 2.78 | 0.46 |
| 11:aA:98:ILE:N | 11:aA:98:ILE:HD13 | 2.30 | 0.46 |
| 11:aA:426:ARG:HH21 | 11:aA:496:ARG:CZ | 2.29 | 0.46 |
| 11:aA:426:ARG:NH2 | 11:aA:496:ARG:CZ | 2.78 | 0.46 |
| 11:aA:579:PHE:O | 11:aA:580:THR:C | 2.57 | 0.46 |
| 4:M1:19:MET:O | 4:M1:42:SER:HA | 2.16 | 0.46 |
| 4:M1:162:ASN:H | 12:Z1:202:CYC:HBB3 | 1.81 | 0.46 |
| 4:M1:205:ASP:CG | 5:N1:52:ARG:HH22 | 2.23 | 0.46 |
| 3:T1:88:ILE:HG21 | 12:T1:301:CYC:HAB2 | 1.96 | 0.46 |
| 2:A2:128:ILE:HG22 | 2:A2:132:LYS:HE3 | 1.98 | 0.46 |
| 12:AA:201:CYC:HBB2 | 3:DA:75:PRO:CB | 2.45 | 0.46 |
| 12:DA:201:CYC:HB | 12:DA:201:CYC:CMA | 2.26 | 0.46 |
| 3:HA:108:ARG:NH2 | 11:aA:477:TYR:OH | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:JA:75:PRO:CB | 12:KA:201:CYC:HBB2 | 2.45 | 0.46 |
| 3:JA:88:ILE:HG21 | 12:JA:202:CYC:CAB | 2.46 | 0.46 |
| 12:LA:202:CYC:CGD | 11:aA:538:ARG:CB | 2.93 | 0.46 |
| 4:MA:110:TYR:HE2 | 4:MA:124:ARG:NH1 | 2.13 | 0.46 |
| 6:M2:28:ASN:O | 8:O5:79:ALA:CB | 2.64 | 0.46 |
| 6:M2:50:LEU:HD23 | 8:i7:79:ALA:CB | 2.42 | 0.46 |
| 6:M2:259:THR:C | 6:M2:261:LYS:N | 2.74 | 0.46 |
| 2:E3:128:ILE:HG22 | 2:E3:132:LYS:HE3 | 1.98 | 0.46 |
| 3:B4:85:ASP:OD2 | 4:M4:53:LEU:HD21 | 2.15 | 0.46 |
| 3:B4:119:ALA:C | 4:M4:52:LEU:HD11 | 2.36 | 0.46 |
| 3:B4:120:LEU:HD23 | 4:M4:52:LEU:HB3 | 1.87 | 0.46 |
| 4:M3:110:TYR:HE2 | 4:M3:124:ARG:NH1 | 2.13 | 0.46 |
| 5:N3:16:PHE:CE1 | 3:R3:120:LEU:HD23 | 2.51 | 0.46 |
| 12:R3:202:CYC:HC | 12:R3:202:CYC:HMD3 | 1.78 | 0.46 |
| 12:T4:201:CYC:HBB2 | 3:Y4:75:PRO:CB | 2.44 | 0.46 |
| 2:P4:128:ILE:HG22 | 2:P4:132:LYS:HE3 | 1.97 | 0.46 |
| 8:K5:72:ALA:HB2 | 12:K5:201:CYC:NC | 2.30 | 0.46 |
| 1:L5:42:ALA:HB2 | 8:U5:151:PHE:HE1 | 1.79 | 0.46 |
| 3:Y4:2:GLN:HB2 | 3:Y4:103:SER:HB2 | 1.94 | 0.46 |
| 12:D5:201:CYC:HMD1 | 12:D5:201:CYC:NC | 2.10 | 0.46 |
| 8:E5:17:TYR:OH | 1:F5:89:LEU:CG | 2.62 | 0.46 |
| 1:P5:12:TYR:CZ | 1:P5:23:ALA:HB2 | 2.50 | 0.46 |
| 8:U5:2:SER:C | 8:U5:100:ASP:HB2 | 2.40 | 0.46 |
| 8:U5:2:SER:O | 8:U5:100:ASP:CB | 2.63 | 0.46 |
| 8:U5:22:GLU:HA | 8:U5:25:ARG:HH11 | 1.81 | 0.46 |
| 12:V5:201:CYC:CBB | 10:j5:623:VAL:CG2 | 2.89 | 0.46 |
| 8:a5:2:SER:O | 8:a5:100:ASP:CB | 2.62 | 0.46 |
| 3:J6:88:ILE:HG21 | 12:J6:202:CYC:CAB | 2.46 | 0.46 |
| 6:M6:50:LEU:HD23 | 8:c7:79:ALA:C | 2.37 | 0.46 |
| 9:z5:15:LYS:C | 9:z5:15:LYS:CD | 2.88 | 0.46 |
| 10:j5:357:LEU:HD11 | 10:j5:379:PHE:N | 2.30 | 0.46 |
| 10:j5:930:LEU:CA | 1:J7:33:THR:HG21 | 2.43 | 0.46 |
| 10:j5:1024:LYS:HD2 | 10:j5:1038:ARG:NH1 | 2.30 | 0.46 |
| 10:k5:275:THR:HG21 | 10:k5:286:VAL:C | 2.40 | 0.46 |
| 10:k5:669:GLU:O | 10:k5:669:GLU:HG2 | 2.15 | 0.46 |
| 10:k5:870:GLU:OE2 | 10:k5:870:GLU:HA | 2.15 | 0.46 |
| 10:k5:878:GLU:CG | 9:z7:28:PHE:CE2 | 2.99 | 0.46 |
| 10:k5:1129:ARG:HA | 10:k5:1133:GLU:HB3 | 1.96 | 0.46 |
| 2:G6:128:ILE:HG22 | 2:G6:132:LYS:HE3 | 1.98 | 0.46 |
| 3:H6:84:ARG:C | 3:H6:86:MET:N | 2.74 | 0.46 |
| 8:S7:120:GLN:CD | 1:X7:53:LYS:HZ2 | 2.24 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:C7:94:TYR:O | 8:C7:97:VAL:HG23 | 2.16 | 0.46 |
| 8:g7:21:GLY:C | 8:g7:23:LEU:H | 2.23 | 0.46 |
| 8:g7:134:LYS:O | 8:g7:138:THR:HB | 2.16 | 0.46 |
| 8:i7:47:ARG:CB | 1:j7:18:TYR:HE2 | 2.26 | 0.46 |
| 8:a7:94:TYR:O | 8:a7:97:VAL:HG23 | 2.16 | 0.46 |
| 8:c7:13:ALA:CA | 9:x7:46:LYS:HE3 | 2.45 | 0.46 |
| 1:f7:12:TYR:CZ | 1:f7:23:ALA:HB2 | 2.50 | 0.46 |
| 2:A8:19:LEU:O | 3:B8:45:THR:CG2 | 2.64 | 0.46 |
| 3:B8:81:ALA:O | 12:B8:202:CYC:C4C | 2.63 | 0.46 |
| 12:C8:201:CYC:HBB2 | 3:F8:75:PRO:CB | 2.44 | 0.46 |
| 2:E8:1:MET:CA | 4:M8:10:ARG:HH21 | 2.20 | 0.46 |
| 8:o7:39:ILE:O | 8:o7:39:ILE:HG22 | 2.15 | 0.46 |
| 2:G8:128:ILE:HG22 | 2:G8:132:LYS:HE3 | 1.98 | 0.46 |
| 3:O8:108:ARG:CB | 5:Z8:61:LYS:CE | 2.85 | 0.46 |
| 3:F1:113:LEU:HA | 4:M1:38:PRO:HB2 | 1.98 | 0.46 |
| 4:M9:19:MET:O | 4:M9:42:SER:HA | 2.16 | 0.46 |
| 4:M9:176:ARG:HH11 | 4:M9:176:ARG:HG3 | 1.78 | 0.46 |
| 12:D9:202:CYC:HC | 12:D9:202:CYC:HMD3 | 1.78 | 0.46 |
| 12:H9:202:CYC:OB | 11:a9:448:ASN:CB | 2.63 | 0.46 |
| 2:K9:15:GLN:HA | 11:a9:393:ARG:NH1 | 2.00 | 0.46 |
| 11:a9:245:ALA:HB3 | 12:a9:901:CYC:HBB2 | 1.96 | 0.46 |
| 11:a9:802:ARG:HH11 | 11:a9:802:ARG:HG3 | 1.80 | 0.46 |
| 11:aA:376:ALA:HB3 | 11:aA:504:VAL:H | 1.79 | 0.46 |
| 4:M1:152:TYR:CD1 | 4:M1:152:TYR:O | 2.69 | 0.46 |
| 1:A:66:THR:HB | 12:k5:1201:CYC:HBA1 | 1.98 | 0.46 |
| 2:AA:64:PRO:C | 2:AA:66:LEU:H | 2.23 | 0.46 |
| 2:CA:128:ILE:HG22 | 2:CA:132:LYS:HE3 | 1.98 | 0.46 |
| 2:EA:152:ALA:HB1 | 2:IA:21:ASN:OD1 | 2.16 | 0.46 |
| 3:LA:51:ILE:CG2 | 3:LA:90:LEU:HD13 | 2.45 | 0.46 |
| 4:MA:74:LEU:HD23 | 4:MA:74:LEU:HA | 1.68 | 0.46 |
| 3:XA:75:PRO:CB | 12:YA:201:CYC:HBB2 | 2.45 | 0.46 |
| 3:ZA:88:ILE:HG21 | 12:ZA:202:CYC:CAB | 2.46 | 0.46 |
| 2:A1:34:ALA:CB | 3:B1:31:VAL:HG11 | 2.38 | 0.46 |
| 3:J3:88:ILE:HG21 | 12:J3:202:CYC:CAB | 2.46 | 0.46 |
| 7:N2:9:THR:HG23 | 7:N2:12:GLY:H | 1.80 | 0.46 |
| 2:A3:64:PRO:C | 2:A3:66:LEU:H | 2.22 | 0.46 |
| 3:F3:119:ALA:HB3 | 4:M3:41:ASN:ND2 | 2.27 | 0.46 |
| 3:Z3:111:ASN:HD21 | 4:M3:258:LYS:HG2 | 1.81 | 0.46 |
| 12:A4:201:CYC:HBB2 | 3:D4:75:PRO:CB | 2.44 | 0.46 |
| 4:M3:19:MET:O | 4:M3:42:SER:HA | 2.16 | 0.46 |
| 5:N3:15:LEU:O | 5:N3:73:GLY:CA | 2.61 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:F4:107:ASP:OD1 | 3:F4:108:ARG:N | 2.48 | 0.46 |
| 12:H4:201:CYC:HMA1 | 11:aA:261:SER:HB2 | 1.98 | 0.46 |
| 4:M4:233:GLU:HG3 | 3:Y4:112:GLY:H | 1.81 | 0.46 |
| 3:Y4:96:ALA:HB2 | 3:Y4:105:LEU:HB2 | 1.98 | 0.46 |
| 1:D5:76:ARG:HG3 | 1:D5:77:ARG:HG3 | 1.97 | 0.46 |
| 8:c5:64:ASP:O | 8:c5:67:SER:HB2 | 2.16 | 0.46 |
| 8:e5:16:ARG:HG3 | 8:e5:16:ARG:NH1 | 2.31 | 0.46 |
| 8:a5:16:ARG:HG3 | 8:a5:16:ARG:NH1 | 2.31 | 0.46 |
| 2:K6:128:ILE:HG22 | 2:K6:132:LYS:HE3 | 1.98 | 0.46 |
| 10:j5:501:ILE:H | 10:j5:501:ILE:CD1 | 2.17 | 0.46 |
| 10:j5:651:ILE:HD13 | 10:j5:651:ILE:HG21 | 1.61 | 0.46 |
| 10:j5:885:GLN:HE21 | 10:j5:885:GLN:HB3 | 1.52 | 0.46 |
| 10:j5:1054:SER:C | 10:j5:1056:PRO:CD | 2.87 | 0.46 |
| 10:k5:357:LEU:HD11 | 10:k5:379:PHE:N | 2.30 | 0.46 |
| 10:k5:802:VAL:O | 10:k5:806:VAL:HG23 | 2.15 | 0.46 |
| 10:k5:826:THR:HG21 | 12:B7:201:CYC:CMA | 2.43 | 0.46 |
| 8:O7:17:TYR:OH | 1:P7:89:LEU:HG | 2.16 | 0.46 |
| 8:O7:52:LYS:HB2 | 11:aA:27:PHE:CE2 | 2.50 | 0.46 |
| 8:Q7:134:LYS:O | 8:Q7:138:THR:HB | 2.16 | 0.46 |
| 1:B7:12:TYR:CZ | 1:B7:23:ALA:HB2 | 2.50 | 0.46 |
| 8:I7:161:GLN:HG2 | 1:X7:49:THR:CB | 2.44 | 0.46 |
| 8:K7:134:LYS:O | 8:K7:138:THR:HB | 2.16 | 0.46 |
| 8:g7:56:ASP:OD1 | 11:aA:325:LEU:CB | 2.63 | 0.46 |
| 1:h7:51:ILE:HD11 | 1:h7:140:LEU:HD23 | 1.97 | 0.46 |
| 8:U7:17:TYR:OH | 1:V7:89:LEU:HG | 2.16 | 0.46 |
| 12:V7:201:CYC:CMA | 12:V7:201:CYC:NB | 2.74 | 0.46 |
| 8:c7:23:LEU:HD21 | 1:d7:41:ALA:HB3 | 1.97 | 0.46 |
| 2:A8:64:PRO:C | 2:A8:66:LEU:H | 2.23 | 0.46 |
| 3:B8:116:THR:HG23 | 4:M8:53:LEU:HA | 1.89 | 0.46 |
| 8:m7:2:SER:C | 8:m7:100:ASP:HB2 | 2.40 | 0.46 |
| 1:t7:12:TYR:CZ | 1:t7:23:ALA:HB2 | 2.50 | 0.46 |
| 2:X8:33:ARG:CG | 2:N8:25:GLN:HG2 | 2.38 | 0.46 |
| 4:M8:230:GLN:NE2 | 12:M8:301:CYC:CMA | 2.76 | 0.46 |
| 2:N8:19:LEU:O | 3:O8:45:THR:CG2 | 2.64 | 0.46 |
| 2:R8:64:PRO:CB | 3:T9:21:GLU:HB3 | 2.43 | 0.46 |
| 3:L9:107:ASP:O | 3:L9:111:ASN:CB | 2.64 | 0.46 |
| 4:M9:74:LEU:O | 4:M9:77:LEU:HD11 | 2.15 | 0.46 |
| 2:O9:19:LEU:O | 3:P9:45:THR:CG2 | 2.64 | 0.46 |
| 3:J9:68:ARG:CB | 11:a9:353:ALA:CB | 2.93 | 0.46 |
| 12:J9:202:CYC:O2A | 11:a9:511:LYS:CD | 2.60 | 0.46 |
| 11:a9:98:ILE:N | 11:a9:98:ILE:HD13 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:a9:312:ASP:C | 11:a9:315:LEU:HB3 | 2.33 | 0.46 |
| 11:a9:320:ASP:HA | 11:a9:323:ARG:HG2 | 1.98 | 0.46 |
| 11:a9:729:TYR:CD1 | 11:a9:784:VAL:HG21 | 2.51 | 0.46 |
| 11:aA:823:ILE:HD12 | 3:L1:75:PRO:HG3 | 1.97 | 0.46 |
| 12:aA:901:CYC:CAB | 3:J1:88:ILE:HG21 | 2.46 | 0.46 |
| 2:K1:128:ILE:HG22 | 2:K1:132:LYS:HE3 | 1.97 | 0.46 |
| 4:M1:7:SER:C | 4:M1:14:LEU:HD13 | 2.08 | 0.46 |
| 5:N1:14:LYS:HE3 | 5:N1:50:LEU:CD2 | 2.45 | 0.46 |
| 12:D2:202:CYC:HC | 12:D2:202:CYC:HMD3 | 1.78 | 0.46 |
| 3:DA:111:ASN:HD21 | 4:MA:73:ASP:CA | 2.28 | 0.46 |
| 4:MA:131:LEU:HB3 | 4:MA:137:ILE:HG12 | 1.98 | 0.46 |
| 5:NA:14:LYS:HE3 | 5:NA:50:LEU:CD2 | 2.45 | 0.46 |
| 2:QA:2:LYS:NZ | 2:UA:17:ARG:NH2 | 2.64 | 0.46 |
| 3:P1:88:ILE:HG21 | 12:P1:201:CYC:CAB | 2.46 | 0.46 |
| 2:A1:44:LEU:HD11 | 2:A1:142:LEU:HD11 | 1.96 | 0.46 |
| 2:G3:128:ILE:HG22 | 2:G3:132:LYS:HE3 | 1.98 | 0.46 |
| 3:H3:88:ILE:HG21 | 12:H3:202:CYC:CAB | 2.46 | 0.46 |
| 2:I3:128:ILE:HG22 | 2:I3:132:LYS:HE3 | 1.98 | 0.46 |
| 3:D3:88:ILE:HG21 | 12:D3:202:CYC:CAB | 2.46 | 0.46 |
| 3:B4:68:ARG:HH12 | 3:U4:68:ARG:NH1 | 2.14 | 0.46 |
| 4:M3:164:ARG:O | 4:M3:164:ARG:HG3 | 2.15 | 0.46 |
| 2:O3:64:PRO:C | 2:O3:66:LEU:N | 2.70 | 0.46 |
| 2:O3:128:ILE:HG22 | 2:O3:132:LYS:HE3 | 1.98 | 0.46 |
| 3:X3:88:ILE:HG21 | 12:X3:201:CYC:CAB | 2.46 | 0.46 |
| 2:G4:128:ILE:HG22 | 2:G4:132:LYS:HE3 | 1.98 | 0.46 |
| 4:M4:235:PHE:CA | 12:M4:301:CYC:HAA1 | 2.44 | 0.46 |
| 8:K5:161:GLN:HG2 | 1:V5:49:THR:HB | 1.97 | 0.46 |
| 8:A5:134:LYS:O | 8:A5:138:THR:HB | 2.16 | 0.46 |
| 8:E5:134:LYS:O | 8:E5:138:THR:HB | 2.16 | 0.46 |
| 8:G5:138:THR:HG21 | 8:o7:75:GLU:HG2 | 1.97 | 0.46 |
| 12:H5:201:CYC:CMA | 12:H5:201:CYC:NB | 2.74 | 0.46 |
| 8:I5:94:TYR:O | 8:I5:97:VAL:HG23 | 2.16 | 0.46 |
| 8:U5:134:LYS:O | 8:U5:138:THR:HB | 2.16 | 0.46 |
| 1:V5:12:TYR:CZ | 1:V5:23:ALA:HB2 | 2.50 | 0.46 |
| 12:V5:201:CYC:C4B | 10:j5:649:PHE:CE1 | 2.99 | 0.46 |
| 8:a5:94:TYR:O | 8:a5:97:VAL:HG23 | 2.16 | 0.46 |
| 7:N6:20:VAL:CG2 | 7:N6:39:TYR:CZ | 2.99 | 0.46 |
| 8:A7:54:ALA:HB2 | 8:A7:133:MET:HG2 | 1.96 | 0.46 |
| 9:i5:17:VAL:O | 9:i5:17:VAL:HG23 | 2.16 | 0.46 |
| 10:j5:214:PHE:N | 10:j5:214:PHE:CD1 | 2.83 | 0.46 |
| 10:j5:409:GLU:HA | 10:j5:409:GLU:OE2 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 10:j5:549:LYS:CE | 10:j5:551:MET:HB2 | 2.45 | 0.46 |
| 10:j5:630:ILE:O | 10:j5:630:ILE:HG22 | 2.14 | 0.46 |
| 10:j5:748:ARG:NE | 8:K7:106:GLU:CD | 2.71 | 0.46 |
| 10:k5:292:GLU:CD | 10:k5:292:GLU:N | 2.74 | 0.46 |
| 10:k5:391:SER:O | 10:k5:392:SER:HB3 | 2.16 | 0.46 |
| 10:k5:1153:VAL:HG13 | 1:p7:65:LEU:HD12 | 1.98 | 0.46 |
| 2:A6:128:ILE:HG22 | 2:A6:132:LYS:HE3 | 1.97 | 0.46 |
| 8:S7:134:LYS:O | 8:S7:138:THR:HB | 2.16 | 0.46 |
| 8:g7:94:TYR:O | 8:g7:97:VAL:HG23 | 2.16 | 0.46 |
| 8:i7:58:LEU:HD13 | 8:i7:128:GLU:CB | 2.46 | 0.46 |
| 8:k7:54:ALA:HB2 | 8:k7:133:MET:HG2 | 1.96 | 0.46 |
| 8:U7:2:SER:C | 8:U7:100:ASP:HB2 | 2.40 | 0.46 |
| 8:W7:134:LYS:O | 8:W7:138:THR:HB | 2.16 | 0.46 |
| 12:X7:201:CYC:CMA | 12:X7:201:CYC:NB | 2.74 | 0.46 |
| 8:a7:134:LYS:O | 8:a7:138:THR:HB | 2.16 | 0.46 |
| 2:A8:128:ILE:HG22 | 2:A8:132:LYS:HE3 | 1.98 | 0.46 |
| 3:B8:107:ASP:O | 4:M8:61:ASN:O | 2.33 | 0.46 |
| 8:m7:21:GLY:C | 8:m7:23:LEU:H | 2.24 | 0.46 |
| 8:m7:94:TYR:O | 8:m7:97:VAL:HG23 | 2.16 | 0.46 |
| 8:o7:90:ARG:HB2 | 1:p7:18:TYR:HH | 1.78 | 0.46 |
| 8:q7:134:LYS:O | 8:q7:138:THR:HB | 2.16 | 0.46 |
| 2:X8:69:PRO:CD | 2:S9:42:ARG:CD | 2.92 | 0.46 |
| 12:M8:301:CYC:CBC | 3:Y8:127:VAL:HG22 | 2.46 | 0.46 |
| 2:N8:112:GLY:O | 5:Z8:33:GLY:HA2 | 2.16 | 0.46 |
| 2:R8:68:GLN:HG3 | 3:T9:22:GLN:HG3 | 1.98 | 0.46 |
| 4:M9:110:TYR:HE2 | 4:M9:124:ARG:NH1 | 2.13 | 0.46 |
| 3:F9:88:ILE:HG21 | 12:F9:301:CYC:CAB | 2.46 | 0.46 |
| 3:J9:119:ALA:HB1 | 11:a9:365:LYS:CE | 2.35 | 0.46 |
| 2:Y9:128:ILE:HG22 | 2:Y9:132:LYS:HE3 | 1.98 | 0.46 |
| 11:a9:684:ASN:OD1 | 11:a9:686:SER:CB | 2.64 | 0.46 |
| 11:a9:714:ARG:NH2 | 11:a9:810:GLN:OE1 | 2.45 | 0.46 |
| 11:a9:732:SER:HB2 | 11:a9:824:VAL:HG21 | 1.98 | 0.46 |
| 11:aA:383:PHE:CD1 | 11:aA:383:PHE:O | 2.69 | 0.46 |
| 3:L1:88:ILE:HD12 | 3:L1:91:ARG:HH21 | 1.81 | 0.46 |
| 4:M1:56:MET:HE2 | 4:M1:56:MET:HB3 | 1.75 | 0.46 |
| 4:M1:258:LYS:HG2 | 3:Z1:111:ASN:HD21 | 1.81 | 0.46 |
| 5:N1:23:SER:C | 5:N1:25:THR:N | 2.74 | 0.46 |
| 12:U1:201:CYC:HBB2 | 3:Z1:75:PRO:CB | 2.45 | 0.46 |
| 2:AA:19:LEU:O | 3:BA:45:THR:CG2 | 2.64 | 0.46 |
| 3:BA:107:ASP:HB3 | 11:aA:382:ASN:CB | 2.46 | 0.46 |
| 3:BA:113:LEU:HD13 | 4:MA:38:PRO:CB | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:MA:19:MET:O | 4:MA:42:SER:HA | 2.16 | 0.46 |
| 3:PA:88:ILE:HG21 | 12:PA:201:CYC:CAB | 2.46 | 0.46 |
| 2:QA:116:VAL:HG11 | 3:TA:79:MET:HG2 | 1.98 | 0.46 |
| 3:TA:88:ILE:HG21 | 12:TA:301:CYC:CAB | 2.46 | 0.46 |
| 3:VA:88:ILE:HG21 | 12:VA:201:CYC:CAB | 2.46 | 0.46 |
| 3:XA:88:ILE:HG21 | 12:XA:201:CYC:CAB | 2.46 | 0.46 |
| 3:H2:2:GLN:NE2 | 6:M2:75:LYS:HZ3 | 2.14 | 0.46 |
| 6:M2:238:LEU:CD1 | 6:M2:258:VAL:CG1 | 2.94 | 0.46 |
| 4:M3:131:LEU:HB3 | 4:M3:137:ILE:HG12 | 1.98 | 0.46 |
| 2:W3:128:ILE:HG22 | 2:W3:132:LYS:HE3 | 1.98 | 0.46 |
| 12:B1:202:CYC:HB | 12:B1:202:CYC:CMA | 2.26 | 0.46 |
| 3:F4:107:ASP:CG | 4:M4:9:GLN:HA | 2.41 | 0.46 |
| 3:H4:1:MET:N | 11:aA:96:THR:HG21 | 2.31 | 0.46 |
| 3:Q4:7:LYS:CD | 3:Q4:101:ASP:CG | 2.86 | 0.46 |
| 8:M5:38:ARG:HD2 | 1:J7:144:ASP:CG | 2.41 | 0.46 |
| 1:N5:53:LYS:HZ1 | 8:O5:120:GLN:HE21 | 0.47 | 0.46 |
| 8:O5:2:SER:C | 8:O5:100:ASP:HB2 | 2.40 | 0.46 |
| 8:O5:94:TYR:O | 8:O5:97:VAL:HG23 | 2.16 | 0.46 |
| 8:e5:2:SER:C | 8:e5:100:ASP:HB2 | 2.40 | 0.46 |
| 8:e5:134:LYS:O | 8:e5:138:THR:HB | 2.16 | 0.46 |
| 8:S5:64:ASP:O | 8:S5:67:SER:HB2 | 2.16 | 0.46 |
| 1:T5:110:ASN:ND2 | 10:j5:692:LEU:HB2 | 2.03 | 0.46 |
| 8:U5:94:TYR:O | 8:U5:97:VAL:HG23 | 2.16 | 0.46 |
| 8:W5:134:LYS:O | 8:W5:138:THR:HB | 2.16 | 0.46 |
| 8:Y5:134:LYS:O | 8:Y5:138:THR:HB | 2.16 | 0.46 |
| 1:b5:1:MET:HE1 | 10:k5:25:ILE:HD13 | 1.97 | 0.46 |
| 10:j5:187:ARG:HD3 | 10:j5:234:LEU:HB3 | 1.97 | 0.46 |
| 10:j5:826:THR:CG2 | 12:H7:201:CYC:CMA | 2.94 | 0.46 |
| 10:j5:930:LEU:HG | 1:J7:148:GLU:HB2 | 1.97 | 0.46 |
| 10:j5:1016:LEU:CG | 10:j5:1017:ARG:N | 2.73 | 0.46 |
| 10:k5:45:GLN:O | 10:k5:49:ASP:OD1 | 2.33 | 0.46 |
| 10:k5:76:PHE:HB2 | 10:k5:81:PRO:HG3 | 1.97 | 0.46 |
| 10:k5:184:LEU:HA | 10:k5:184:LEU:HD23 | 1.50 | 0.46 |
| 10:k5:965:GLN:O | 1:p7:14:VAL:HG12 | 2.16 | 0.46 |
| 8:O7:6:LYS:NZ | 8:E7:21:GLY:CA | 2.76 | 0.46 |
| 8:g7:97:VAL:HG21 | 1:h7:19:LEU:HD11 | 1.96 | 0.46 |
| 1:j7:107:ARG:O | 9:y7:45:GLN:NE2 | 2.49 | 0.46 |
| 8:c7:11:ALA:CA | 1:d7:94:TYR:OH | 2.58 | 0.46 |
| 8:m7:134:LYS:O | 8:m7:138:THR:HB | 2.16 | 0.46 |
| 8:s7:94:TYR:O | 8:s7:97:VAL:HG23 | 2.16 | 0.46 |
| 8:u7:47:ARG:CD | 8:u7:47:ARG:C | 2.89 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:u7:134:LYS:O | 8:u7:138:THR:HB | 2.16 | 0.46 |
| 9:x7:21:ARG:NE | 9:x7:21:ARG:HA | 2.30 | 0.46 |
| 3:U8:108:ARG:CB | 4:M8:246:ALA:CB | 2.64 | 0.46 |
| 4:M8:19:MET:O | 4:M8:42:SER:HA | 2.16 | 0.46 |
| 4:M8:131:LEU:HB3 | 4:M8:137:ILE:HG12 | 1.98 | 0.46 |
| 2:N8:13:ASP:OD2 | 3:O8:108:ARG:CD | 2.64 | 0.46 |
| 2:N8:128:ILE:HG22 | 2:N8:132:LYS:HE3 | 1.98 | 0.46 |
| 3:L9:90:LEU:HD22 | 2:K9:18:PHE:HZ | 1.80 | 0.46 |
| 12:L9:202:CYC:CGD | 11:a9:538:ARG:CB | 2.93 | 0.46 |
| 2:O9:64:PRO:C | 2:O9:66:LEU:H | 2.23 | 0.46 |
| 3:Y8:110:LEU:CD2 | 3:Y8:167:ALA:HA | 2.46 | 0.46 |
| 3:B9:30:LEU:HD12 | 3:B9:30:LEU:H | 1.80 | 0.46 |
| 2:I9:9:ILE:HG23 | 3:J9:95:TYR:HB3 | 1.97 | 0.46 |
| 2:I9:45:THR:HG23 | 3:J9:18:PHE:CD2 | 2.50 | 0.46 |
| 2:I9:97:LEU:CD1 | 2:I9:97:LEU:C | 2.85 | 0.46 |
| 11:aA:522:ASP:OD1 | 11:aA:522:ASP:N | 2.31 | 0.46 |
| 11:aA:572:THR:HG22 | 11:aA:573:SER:N | 2.31 | 0.46 |
| 4:M1:192:GLN:CG | 3:Z1:84:ARG:HG3 | 2.40 | 0.46 |
| 4:M1:204:ILE:O | 4:M1:204:ILE:HG22 | 2.14 | 0.46 |
| 4:M1:232:VAL:HG21 | 3:V1:113:LEU:CB | 2.45 | 0.46 |
| 5:N1:38:GLU:HG2 | 5:N1:40:SER:H | 1.81 | 0.46 |
| 3:T1:88:ILE:HG21 | 12:T1:301:CYC:CAB | 2.46 | 0.46 |
| 2:U1:38:MET:HE2 | 2:U1:38:MET:HB3 | 1.81 | 0.46 |
| 1:Z:12:TYR:CZ | 1:Z:23:ALA:HB2 | 2.50 | 0.46 |
| 3:BA:88:ILE:HG21 | 12:BA:201:CYC:CAB | 2.46 | 0.46 |
| 4:MA:95:ALA:HB2 | 5:NA:38:GLU:OE1 | 2.16 | 0.46 |
| 4:MA:132:LEU:HD13 | 4:MA:142:PHE:CB | 2.44 | 0.46 |
| 2:O1:128:ILE:HG22 | 2:O1:132:LYS:HE3 | 1.98 | 0.46 |
| 12:R1:202:CYC:CMD | 12:R1:202:CYC:NC | 2.75 | 0.46 |
| 3:H2:14:LEU:HD11 | 6:M2:69:ALA:CB | 2.45 | 0.46 |
| 2:C4:128:ILE:HG22 | 2:C4:132:LYS:HE3 | 1.98 | 0.46 |
| 2:U3:128:ILE:HG22 | 2:U3:132:LYS:HE3 | 1.98 | 0.46 |
| 2:G4:15:GLN:HB3 | 11:aA:120:ARG:NH1 | 2.30 | 0.46 |
| 2:I4:128:ILE:HG22 | 2:I4:132:LYS:HE3 | 1.98 | 0.46 |
| 3:J4:108:ARG:CZ | 11:aA:171:ARG:HA | 2.45 | 0.46 |
| 3:L4:88:ILE:HG21 | 12:L4:202:CYC:CAB | 2.46 | 0.46 |
| 4:M4:19:MET:O | 4:M4:42:SER:HA | 2.16 | 0.46 |
| 4:M4:190:ARG:NH1 | 4:M4:202:SER:HG | 2.13 | 0.46 |
| 4:M4:226:SER:HB3 | 3:Y4:85:ASP:N | 2.30 | 0.46 |
| 8:K5:4:LEU:HD21 | 8:K5:26:ILE:HD13 | 1.93 | 0.46 |
| 8:K5:17:TYR:CG | 1:L5:45:SER:CB | 2.99 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:K5:161:GLN:CD | 1:V5:49:THR:CG2 | 2.89 | 0.46 |
| 8:O5:134:LYS:O | 8:O5:138:THR:HB | 2.16 | 0.46 |
| 5:Z4:24:PRO:HG3 | 5:Z4:37:HIS:NE2 | 2.30 | 0.46 |
| 8:E5:107:ILE:HG21 | 8:E5:107:ILE:HD13 | 1.61 | 0.46 |
| 8:E5:132:ALA:C | 8:E5:134:LYS:H | 2.24 | 0.46 |
| 3:L6:88:ILE:HG21 | 12:L6:201:CYC:CAB | 2.46 | 0.46 |
| 10:k5:187:ARG:HD3 | 10:k5:234:LEU:HB3 | 1.96 | 0.46 |
| 8:S7:49:ARG:HD2 | 11:aA:550:PHE:CZ | 2.30 | 0.46 |
| 8:I7:17:TYR:OH | 1:J7:89:LEU:HG | 2.16 | 0.46 |
| 8:g7:37:LEU:CG | 1:h7:24:LEU:HD21 | 2.46 | 0.46 |
| 8:g7:90:ARG:HD2 | 1:h7:18:TYR:N | 2.31 | 0.46 |
| 8:i7:25:ARG:HH21 | 8:s7:3:VAL:CA | 2.27 | 0.46 |
| 8:a7:21:GLY:C | 8:a7:23:LEU:H | 2.23 | 0.46 |
| 8:c7:4:LEU:HD21 | 8:c7:26:ILE:HD13 | 1.93 | 0.46 |
| 8:o7:37:LEU:HD22 | 1:p7:24:LEU:HB3 | 1.98 | 0.46 |
| 12:W8:202:CYC:HC | 12:W8:202:CYC:HMD3 | 1.77 | 0.46 |
| 3:F8:88:ILE:HG21 | 12:F8:202:CYC:CAB | 2.46 | 0.46 |
| 2:I8:128:ILE:HG22 | 2:I8:132:LYS:HE3 | 1.98 | 0.46 |
| 3:J8:88:ILE:HG21 | 12:J8:201:CYC:CAB | 2.46 | 0.46 |
| 3:F1:88:ILE:HG21 | 12:F1:201:CYC:CAB | 2.46 | 0.46 |
| 4:M9:131:LEU:HB3 | 4:M9:137:ILE:HG12 | 1.98 | 0.46 |
| 2:A9:128:ILE:HG22 | 2:A9:132:LYS:HE3 | 1.98 | 0.46 |
| 12:F9:303:CYC:NC | 12:F9:303:CYC:CMD | 2.75 | 0.46 |
| 11:a9:95:ILE:O | 11:a9:96:THR:C | 2.57 | 0.46 |
| 11:a9:426:ARG:HH21 | 11:a9:496:ARG:CZ | 2.29 | 0.46 |
| 11:aA:337:GLU:CD | 11:aA:337:GLU:C | 2.84 | 0.46 |
| 11:aA:729:TYR:CD1 | 11:aA:784:VAL:HG21 | 2.51 | 0.46 |
| 4:M1:21:LEU:HD12 | 4:M1:21:LEU:C | 2.37 | 0.46 |
| 4:M1:184:ILE:HD13 | 4:M1:184:ILE:HA | 1.65 | 0.46 |
| 2:A2:38:MET:HE2 | 2:A2:38:MET:HB3 | 1.81 | 0.46 |
| 2:A2:64:PRO:C | 2:A2:66:LEU:H | 2.23 | 0.46 |
| 1:A:131:GLN:HG3 | 1:R5:17:LYS:HZ3 | 0.63 | 0.45 |
| 2:EA:128:ILE:CG2 | 2:EA:132:LYS:HE3 | 2.47 | 0.45 |
| 3:LA:107:ASP:O | 11:aA:531:ASP:HB2 | 2.16 | 0.45 |
| 4:MA:103:GLN:O | 4:MA:103:GLN:HG3 | 2.16 | 0.45 |
| 4:MA:152:TYR:CD1 | 4:MA:152:TYR:O | 2.69 | 0.45 |
| 4:MA:267:LEU:HD23 | 4:MA:267:LEU:HA | 1.65 | 0.45 |
| 5:NA:57:MET:SD | 12:TA:301:CYC:CMA | 3.05 | 0.45 |
| 2:OA:128:ILE:HG22 | 2:OA:132:LYS:HE3 | 1.98 | 0.45 |
| 2:QA:116:VAL:HG22 | 3:TA:80:ALA:CA | 2.44 | 0.45 |
| 2:WA:128:ILE:HG22 | 2:WA:132:LYS:HE3 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:R1:88:ILE:HG21 | 12:R1:201:CYC:CAB | 2.46 | 0.45 |
| 3:R1:120:LEU:HD23 | 5:N1:16:PHE:CE1 | 2.51 | 0.45 |
| 12:J2:201:CYC:HC | 12:J2:201:CYC:HMD3 | 1.78 | 0.45 |
| 2:A3:31:PHE:CG | 3:B3:34:SER:CB | 2.99 | 0.45 |
| 3:Z3:84:ARG:HG3 | 4:M3:192:GLN:CG | 2.40 | 0.45 |
| 3:Z3:88:ILE:HG21 | 12:Z3:201:CYC:CAB | 2.46 | 0.45 |
| 5:N3:37:HIS:CD2 | 5:N3:38:GLU:O | 2.69 | 0.45 |
| 3:R3:88:ILE:HG21 | 12:R3:201:CYC:CAB | 2.46 | 0.45 |
| 3:T3:88:ILE:HG21 | 12:T3:301:CYC:CAB | 2.46 | 0.45 |
| 3:F4:88:ILE:HG21 | 12:F4:202:CYC:CAB | 2.46 | 0.45 |
| 3:F4:110:LEU:HB3 | 3:F4:111:ASN:H | 1.51 | 0.45 |
| 4:M4:92:GLU:OE1 | 4:M4:217:VAL:CA | 1.97 | 0.45 |
| 4:M4:225:LYS:HE3 | 3:Y4:81:ALA:CA | 2.46 | 0.45 |
| 8:K5:132:ALA:C | 8:K5:134:LYS:N | 2.71 | 0.45 |
| 8:C5:94:TYR:O | 8:C5:97:VAL:HG23 | 2.16 | 0.45 |
| 8:E5:110:ILE:HD13 | 8:E5:110:ILE:HG21 | 1.59 | 0.45 |
| 8:Q5:160:MET:HB2 | 8:Q5:161:GLN:H | 1.62 | 0.45 |
| 8:U5:48:GLU:CB | 6:M6:34:ARG:NH2 | 2.12 | 0.45 |
| 12:N6:101:CYC:CAB | 3:B6:88:ILE:HG21 | 2.46 | 0.45 |
| 9:z5:18:ARG:N | 9:z5:18:ARG:CD | 2.78 | 0.45 |
| 9:i5:18:ARG:N | 9:i5:18:ARG:CD | 2.78 | 0.45 |
| 10:j5:156:SER:OG | 12:j5:1201:CYC:CHD | 2.64 | 0.45 |
| 10:j5:423:LEU:HD23 | 10:j5:423:LEU:HA | 1.76 | 0.45 |
| 10:j5:1002:ARG:NH1 | 8:u7:13:ALA:O | 2.49 | 0.45 |
| 10:j5:1006:ASP:CG | 10:j5:1065:HIS:HE2 | 2.24 | 0.45 |
| 10:k5:277:ILE:O | 10:k5:277:ILE:HG23 | 2.16 | 0.45 |
| 10:k5:549:LYS:CE | 10:k5:551:MET:HB2 | 2.45 | 0.45 |
| 10:k5:1004:VAL:HG13 | 10:k5:1066:PHE:CZ | 2.52 | 0.45 |
| 3:D6:88:ILE:HG21 | 12:D6:201:CYC:CAB | 2.46 | 0.45 |
| 8:S7:120:GLN:CG | 1:X7:53:LYS:NZ | 2.78 | 0.45 |
| 8:E7:134:LYS:O | 8:E7:138:THR:HB | 2.16 | 0.45 |
| 8:M7:52:LYS:HE2 | 8:M7:52:LYS:HB3 | 1.53 | 0.45 |
| 8:g7:102:THR:CB | 8:g7:103:PRO:HD3 | 2.34 | 0.45 |
| 8:i7:47:ARG:HD3 | 1:j7:18:TYR:CG | 2.51 | 0.45 |
| 8:i7:137:ALA:O | 8:i7:138:THR:C | 2.56 | 0.45 |
| 1:j7:75:THR:HB | 8:e7:111:GLY:C | 2.41 | 0.45 |
| 8:Y7:64:ASP:O | 8:Y7:67:SER:HB2 | 2.17 | 0.45 |
| 8:Y7:111:GLY:C | 1:d7:75:THR:HB | 2.41 | 0.45 |
| 1:Z7:12:TYR:CZ | 1:Z7:23:ALA:HB2 | 2.50 | 0.45 |
| 8:c7:8:ILE:CG2 | 1:d7:94:TYR:CB | 2.95 | 0.45 |
| 2:A8:31:PHE:CG | 3:B8:34:SER:CB | 3.00 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:D8:88:ILE:HG21 | 12:D8:202:CYC:CAB | 2.46 | 0.45 |
| 1:l7:12:TYR:CZ | 1:l7:23:ALA:HB2 | 2.50 | 0.45 |
| 8:o7:90:ARG:HA | 1:p7:18:TYR:HE2 | 1.63 | 0.45 |
| 8:s7:17:TYR:OH | 1:t7:89:LEU:HG | 2.16 | 0.45 |
| 8:s7:134:LYS:O | 8:s7:138:THR:HB | 2.16 | 0.45 |
| 8:u7:51:VAL:O | 8:u7:51:VAL:HG12 | 2.16 | 0.45 |
| 8:u7:130:VAL:HG21 | 8:u7:160:MET:HE3 | 1.97 | 0.45 |
| 3:U8:88:ILE:HG21 | 12:U8:201:CYC:CAB | 2.46 | 0.45 |
| 2:I8:14:SER:CA | 11:a9:170:PHE:CZ | 2.82 | 0.45 |
| 4:M8:51:ARG:HH11 | 4:M8:51:ARG:CG | 2.27 | 0.45 |
| 4:M8:74:LEU:O | 4:M8:77:LEU:HD11 | 2.15 | 0.45 |
| 4:M8:110:TYR:HE2 | 4:M8:124:ARG:NH1 | 2.14 | 0.45 |
| 4:M8:164:ARG:O | 4:M8:164:ARG:HG3 | 2.15 | 0.45 |
| 4:M8:205:ASP:CB | 5:Z8:59:ARG:CZ | 2.66 | 0.45 |
| 3:Q8:92:TYR:CE1 | 3:Q8:109:CYS:SG | 3.05 | 0.45 |
| 3:L9:37:ARG:HH11 | 3:L9:97:LEU:HD12 | 1.79 | 0.45 |
| 4:M9:52:LEU:HD13 | 12:F9:301:CYC:HAA1 | 1.98 | 0.45 |
| 4:M9:185:ALA:HB1 | 12:V9:201:CYC:CGA | 2.42 | 0.45 |
| 5:N9:36:THR:HB | 12:P9:201:CYC:O2A | 2.17 | 0.45 |
| 3:Y8:106:GLU:HA | 3:Y8:110:LEU:CD1 | 2.46 | 0.45 |
| 3:B9:107:ASP:HB3 | 11:a9:382:ASN:CB | 2.45 | 0.45 |
| 2:U9:128:ILE:HG22 | 2:U9:132:LYS:HE3 | 1.98 | 0.45 |
| 11:a9:581:ARG:NH1 | 11:a9:581:ARG:CG | 2.72 | 0.45 |
| 11:a9:609:LEU:HD12 | 11:a9:609:LEU:HA | 1.72 | 0.45 |
| 11:aA:38:VAL:CG1 | 11:aA:39:PRO:CD | 2.95 | 0.45 |
| 11:aA:81:ASP:O | 11:aA:82:GLN:C | 2.59 | 0.45 |
| 4:M1:132:LEU:HD13 | 4:M1:142:PHE:CB | 2.44 | 0.45 |
| 5:N1:36:THR:HB | 3:T1:84:ARG:NH2 | 2.31 | 0.45 |
| 3:DA:115:GLU:OE2 | 4:MA:77:LEU:C | 2.54 | 0.45 |
| 3:DA:115:GLU:OE1 | 4:MA:76:ALA:O | 2.34 | 0.45 |
| 12:FA:301:CYC:HAA1 | 4:MA:52:LEU:HD13 | 1.98 | 0.45 |
| 3:HA:66:LEU:HD21 | 12:HA:202:CYC:HMC1 | 1.98 | 0.45 |
| 2:KA:128:ILE:HG22 | 2:KA:132:LYS:HE3 | 1.98 | 0.45 |
| 3:LA:109:CYS:C | 3:LA:111:ASN:N | 2.71 | 0.45 |
| 4:MA:160:THR:C | 3:VA:108:ARG:HA | 2.41 | 0.45 |
| 2:QA:128:ILE:HG22 | 2:QA:132:LYS:HE3 | 1.98 | 0.45 |
| 12:VA:202:CYC:HC | 12:VA:202:CYC:HMD3 | 1.78 | 0.45 |
| 2:O1:64:PRO:C | 2:O1:66:LEU:N | 2.70 | 0.45 |
| 2:A1:31:PHE:CG | 3:B1:34:SER:CB | 2.99 | 0.45 |
| 2:G2:65:TYR:CD1 | 2:A2:65:TYR:CD1 | 3.05 | 0.45 |
| 4:M3:5:THR:C | 4:M3:6:THR:HG1 | 2.08 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M3:51:ARG:NH1 | 4:M3:51:ARG:CG | 2.77 | 0.45 |
| 5:N3:23:SER:C | 5:N3:25:THR:N | 2.74 | 0.45 |
| 12:X3:202:CYC:HC | 12:X3:202:CYC:HMD3 | 1.77 | 0.45 |
| 2:Y3:128:ILE:CG2 | 2:Y3:132:LYS:HE3 | 2.47 | 0.45 |
| 2:V4:38:MET:HE2 | 2:V4:38:MET:HB3 | 1.81 | 0.45 |
| 4:M4:98:ASP:HB3 | 3:Q4:92:TYR:CB | 2.39 | 0.45 |
| 4:M4:251:ASN:HD22 | 4:M4:251:ASN:N | 1.92 | 0.45 |
| 2:P4:38:MET:HE2 | 2:P4:38:MET:HB3 | 1.81 | 0.45 |
| 8:K5:107:ILE:HG21 | 8:K5:107:ILE:HD13 | 1.61 | 0.45 |
| 8:M5:134:LYS:O | 8:M5:138:THR:HB | 2.16 | 0.45 |
| 8:W5:8:ILE:CG2 | 1:X5:94:TYR:CD1 | 2.93 | 0.45 |
| 8:a5:134:LYS:O | 8:a5:138:THR:HB | 2.16 | 0.45 |
| 6:M6:43:TRP:CH2 | 8:c7:52:LYS:HB2 | 2.51 | 0.45 |
| 6:M6:238:LEU:CD1 | 6:M6:258:VAL:CG1 | 2.94 | 0.45 |
| 8:A7:134:LYS:O | 8:A7:138:THR:HB | 2.16 | 0.45 |
| 9:i5:6:LYS:HB3 | 9:i5:55:LYS:N | 2.28 | 0.45 |
| 10:j5:277:ILE:O | 10:j5:277:ILE:HG23 | 2.16 | 0.45 |
| 10:j5:352:ILE:HG22 | 10:j5:353:ASN:N | 2.30 | 0.45 |
| 10:j5:391:SER:O | 10:j5:392:SER:HB3 | 2.16 | 0.45 |
| 10:j5:750:ARG:HG2 | 10:j5:750:ARG:NH1 | 2.31 | 0.45 |
| 10:j5:1146:THR:CB | 1:v7:71:MEN:HE21 | 2.47 | 0.45 |
| 10:k5:19:THR:HB | 10:k5:173:ALA:HB2 | 1.97 | 0.45 |
| 3:B6:77:ARG:CG | 3:B6:77:ARG:NH1 | 2.72 | 0.45 |
| 2:I6:53:LYS:HE3 | 11:a9:295:ARG:HB2 | 1.99 | 0.45 |
| 8:O7:6:LYS:NZ | 8:E7:19:SER:HB3 | 2.30 | 0.45 |
| 8:O7:94:TYR:O | 8:O7:97:VAL:HG23 | 2.16 | 0.45 |
| 8:G7:82:LEU:CB | 11:a9:579:PHE:CD1 | 3.00 | 0.45 |
| 1:J7:72:MET:HE2 | 1:J7:72:MET:HB3 | 1.87 | 0.45 |
| 8:M7:60:GLN:NE2 | 3:J9:114:LYS:CG | 2.80 | 0.45 |
| 8:M7:134:LYS:O | 8:M7:138:THR:HB | 2.16 | 0.45 |
| 8:g7:63:PRO:HB2 | 11:aA:333:GLN:O | 2.17 | 0.45 |
| 8:i7:25:ARG:HH12 | 8:s7:6:LYS:HG2 | 1.66 | 0.45 |
| 8:U7:94:TYR:O | 8:U7:97:VAL:HG23 | 2.16 | 0.45 |
| 8:a7:37:LEU:CG | 1:b7:24:LEU:HD21 | 2.46 | 0.45 |
| 8:c7:20:PRO:HB3 | 8:m7:151:PHE:C | 2.41 | 0.45 |
| 8:c7:23:LEU:HB3 | 1:d7:38:VAL:HG13 | 1.98 | 0.45 |
| 12:B8:202:CYC:NA | 4:M8:57:THR:OG1 | 2.40 | 0.45 |
| 8:o7:94:TYR:HD1 | 1:p7:19:LEU:HG | 1.78 | 0.45 |
| 8:u7:37:LEU:HD22 | 1:v7:24:LEU:HB3 | 1.98 | 0.45 |
| 8:u7:90:ARG:HB2 | 1:v7:18:TYR:HH | 1.81 | 0.45 |
| 8:u7:94:TYR:OH | 1:v7:17:LYS:C | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:F8:110:LEU:O | 3:F8:112:GLY:N | 2.50 | 0.45 |
| 2:K8:128:ILE:HG22 | 2:K8:132:LYS:HE3 | 1.97 | 0.45 |
| 4:M8:152:TYR:CD1 | 4:M8:152:TYR:O | 2.69 | 0.45 |
| 12:M8:302:CYC:HMD1 | 3:S8:77:ARG:NH2 | 2.19 | 0.45 |
| 3:Q8:117:TYR:CE1 | 12:Z8:301:CYC:H3C | 2.52 | 0.45 |
| 5:N9:34:LEU:HB3 | 3:P9:84:ARG:NH1 | 2.31 | 0.45 |
| 3:D9:88:ILE:HG21 | 12:D9:201:CYC:CAB | 2.46 | 0.45 |
| 3:J9:88:ILE:HD13 | 11:a9:512:TYR:CE1 | 2.25 | 0.45 |
| 2:S9:42:ARG:NH2 | 3:T9:25:ASN:OD1 | 2.46 | 0.45 |
| 2:Y9:128:ILE:CG2 | 2:Y9:132:LYS:HE3 | 2.47 | 0.45 |
| 11:a9:81:ASP:O | 11:a9:82:GLN:C | 2.59 | 0.45 |
| 11:a9:383:PHE:CD1 | 11:a9:383:PHE:O | 2.69 | 0.45 |
| 11:a9:781:ALA:O | 11:a9:782:ALA:C | 2.60 | 0.45 |
| 11:aA:290:ASP:O | 11:aA:291:TYR:CE1 | 2.56 | 0.45 |
| 11:aA:609:LEU:HD12 | 11:aA:609:LEU:HA | 1.72 | 0.45 |
| 2:K1:128:ILE:CG2 | 2:K1:132:LYS:HE3 | 2.47 | 0.45 |
| 4:M1:222:ARG:HH11 | 4:M1:222:ARG:CG | 2.13 | 0.45 |
| 4:M1:252:LEU:CD1 | 3:X1:77:ARG:HH12 | 2.28 | 0.45 |
| 2:U1:128:ILE:HG22 | 2:U1:132:LYS:HE3 | 1.98 | 0.45 |
| 12:BA:201:CYC:O2A | 4:MA:34:ASP:O | 2.33 | 0.45 |
| 3:DA:88:ILE:HG21 | 12:DA:201:CYC:CAB | 2.46 | 0.45 |
| 3:HA:127:VAL:HA | 12:HA:202:CYC:HBC3 | 1.97 | 0.45 |
| 4:MA:74:LEU:O | 4:MA:77:LEU:HD11 | 2.15 | 0.45 |
| 2:OA:34:ALA:HB3 | 3:PA:31:VAL:CG1 | 2.39 | 0.45 |
| 3:TA:21:GLU:HB3 | 2:R4:64:PRO:CB | 2.43 | 0.45 |
| 3:TA:22:GLN:HG3 | 2:R4:68:GLN:HG3 | 1.98 | 0.45 |
| 2:O1:31:PHE:CG | 3:P1:34:SER:CB | 3.00 | 0.45 |
| 2:Q1:128:ILE:HG22 | 2:Q1:132:LYS:HE3 | 1.98 | 0.45 |
| 2:A1:65:TYR:CD1 | 2:G1:65:TYR:CD1 | 3.05 | 0.45 |
| 2:G3:111:ALA:HB3 | 3:L3:77:ARG:HG3 | 1.90 | 0.45 |
| 2:K3:128:ILE:HG22 | 2:K3:132:LYS:HE3 | 1.97 | 0.45 |
| 7:N2:18:ILE:HD11 | 7:N2:48:LEU:HD11 | 1.98 | 0.45 |
| 2:A3:64:PRO:C | 2:A3:66:LEU:N | 2.71 | 0.45 |
| 2:C3:140:SER:O | 3:D8:150:ARG:NH1 | 2.48 | 0.45 |
| 2:A4:64:PRO:C | 2:A4:66:LEU:H | 2.23 | 0.45 |
| 3:S4:113:LEU:HD13 | 12:S4:202:CYC:HMB2 | 1.98 | 0.45 |
| 2:K4:128:ILE:HG22 | 2:K4:132:LYS:HE3 | 1.97 | 0.45 |
| 3:L4:69:PRO:O | 11:aA:82:GLN:CG | 2.63 | 0.45 |
| 4:M4:16:LYS:HA | 4:M4:46:VAL:HA | 1.96 | 0.45 |
| 4:M4:29:PRO:CG | 11:aA:230:THR:OG1 | 2.65 | 0.45 |
| 2:N4:31:PHE:CG | 3:O4:34:SER:CB | 3.00 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:M5:64:ASP:O | 8:M5:67:SER:HB2 | 2.16 | 0.45 |
| 3:Y4:106:GLU:HB2 | 3:Y4:166:LYS:CD | 2.40 | 0.45 |
| 8:C5:2:SER:C | 8:C5:100:ASP:HB2 | 2.40 | 0.45 |
| 1:H5:2:GLN:OE1 | 10:j5:551:MET:HG2 | 2.16 | 0.45 |
| 1:H5:110:ASN:CG | 10:j5:547:ARG:HD3 | 2.41 | 0.45 |
| 2:C1:128:ILE:HG22 | 2:C1:132:LYS:HE3 | 1.98 | 0.45 |
| 8:c5:134:LYS:O | 8:c5:138:THR:HB | 2.16 | 0.45 |
| 1:P5:123:ILE:HG22 | 10:k5:11:VAL:HG23 | 1.97 | 0.45 |
| 8:S5:90:ARG:NE | 1:T5:16:GLY:O | 2.50 | 0.45 |
| 7:N6:9:THR:HG23 | 7:N6:12:GLY:H | 1.80 | 0.45 |
| 9:i5:14:LEU:HD13 | 9:i5:15:LYS:HB3 | 1.98 | 0.45 |
| 10:j5:245:ILE:H | 10:j5:245:ILE:HG12 | 1.45 | 0.45 |
| 10:j5:384:SER:HA | 10:j5:385:PRO:HD2 | 1.58 | 0.45 |
| 10:j5:886:PHE:N | 10:j5:886:PHE:HD1 | 2.15 | 0.45 |
| 10:k5:182:ASN:N | 10:k5:182:ASN:ND2 | 2.59 | 0.45 |
| 10:k5:388:ARG:NH2 | 10:k5:392:SER:CA | 2.74 | 0.45 |
| 10:k5:409:GLU:OE2 | 10:k5:409:GLU:HA | 2.16 | 0.45 |
| 10:k5:729:ILE:HB | 1:D7:64:ASP:OD1 | 2.16 | 0.45 |
| 10:k5:1143:LEU:HD23 | 1:l7:10:ASN:ND2 | 2.31 | 0.45 |
| 2:A6:59:VAL:O | 2:A6:66:LEU:CD1 | 2.62 | 0.45 |
| 2:A6:65:TYR:CD1 | 2:G6:65:TYR:CD1 | 3.05 | 0.45 |
| 8:O7:22:GLU:O | 8:O7:26:ILE:HG13 | 2.16 | 0.45 |
| 8:S7:64:ASP:O | 8:S7:67:SER:HB2 | 2.16 | 0.45 |
| 2:V8:128:ILE:HG22 | 2:V8:132:LYS:HE3 | 1.98 | 0.45 |
| 2:X8:128:ILE:CG2 | 2:X8:132:LYS:HE3 | 2.47 | 0.45 |
| 4:M8:130:SER:CB | 12:M8:302:CYC:HAA1 | 2.41 | 0.45 |
| 2:N8:64:PRO:C | 2:N8:66:LEU:H | 2.23 | 0.45 |
| 3:O8:107:ASP:HA | 5:Z8:66:ARG:NH1 | 2.27 | 0.45 |
| 4:M9:5:THR:C | 4:M9:6:THR:OG1 | 2.56 | 0.45 |
| 3:B9:65:ASP:OD1 | 3:B9:65:ASP:N | 2.49 | 0.45 |
| 3:B9:88:ILE:HG21 | 12:B9:201:CYC:CAB | 2.46 | 0.45 |
| 3:D9:68:ARG:HH12 | 3:X9:68:ARG:HH12 | 1.63 | 0.45 |
| 2:K9:128:ILE:CG2 | 2:K9:132:LYS:HE3 | 2.47 | 0.45 |
| 3:T9:88:ILE:HG21 | 12:T9:301:CYC:CAB | 2.46 | 0.45 |
| 11:a9:38:VAL:CG1 | 11:a9:39:PRO:CD | 2.95 | 0.45 |
| 11:a9:337:GLU:CD | 11:a9:337:GLU:C | 2.84 | 0.45 |
| 11:aA:95:ILE:O | 11:aA:96:THR:C | 2.57 | 0.45 |
| 11:aA:600:THR:O | 11:aA:600:THR:HG22 | 2.14 | 0.45 |
| 2:AA:65:TYR:CD1 | 2:GA:65:TYR:CD1 | 3.05 | 0.45 |
| 3:BA:65:ASP:OD1 | 3:BA:65:ASP:N | 2.49 | 0.45 |
| 4:MA:133:ARG:CB | 12:RA:201:CYC:HBA2 | 2.35 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:NA:34:LEU:HD22 | 5:NA:34:LEU:HA | 1.71 | 0.45 |
| 5:NA:38:GLU:HG2 | 5:NA:40:SER:H | 1.81 | 0.45 |
| 2:SA:128:ILE:CG2 | 2:SA:132:LYS:HE3 | 2.47 | 0.45 |
| 3:H3:78:ARG:NH2 | 11:a9:623:ASP:CA | 2.61 | 0.45 |
| 3:J3:14:LEU:HD21 | 11:a9:622:ALA:N | 2.04 | 0.45 |
| 3:J2:108:ARG:CZ | 6:M2:155:ASN:HA | 2.46 | 0.45 |
| 6:M2:39:ARG:CZ | 8:O5:66:VAL:HG21 | 2.46 | 0.45 |
| 7:N2:20:VAL:HG21 | 7:N2:39:TYR:CE1 | 2.51 | 0.45 |
| 2:C3:128:ILE:CG2 | 2:C3:132:LYS:HE3 | 2.47 | 0.45 |
| 3:F3:113:LEU:HA | 4:M3:38:PRO:HB2 | 1.98 | 0.45 |
| 12:Z3:201:CYC:HBB3 | 4:M3:162:ASN:H | 1.81 | 0.45 |
| 3:D4:88:ILE:HG21 | 12:D4:202:CYC:CAB | 2.46 | 0.45 |
| 4:M3:93:LEU:HA | 4:M3:93:LEU:HD12 | 1.66 | 0.45 |
| 4:M3:205:ASP:CG | 5:N3:52:ARG:HH22 | 2.23 | 0.45 |
| 2:O3:19:LEU:O | 3:P3:45:THR:CG2 | 2.64 | 0.45 |
| 3:U4:108:ARG:NH2 | 4:M4:245:ASP:OD2 | 2.50 | 0.45 |
| 2:V4:128:ILE:CG2 | 2:V4:132:LYS:HE3 | 2.47 | 0.45 |
| 12:F4:201:CYC:HC | 12:F4:201:CYC:HMD3 | 1.78 | 0.45 |
| 3:H4:88:ILE:HG21 | 12:H4:201:CYC:CAB | 2.46 | 0.45 |
| 8:K5:72:ALA:HB2 | 12:K5:201:CYC:OC | 2.15 | 0.45 |
| 8:M5:90:ARG:NE | 1:N5:16:GLY:O | 2.50 | 0.45 |
| 8:Y5:64:ASP:O | 8:Y5:67:SER:HB2 | 2.16 | 0.45 |
| 8:a5:4:LEU:HD23 | 8:a5:26:ILE:HD13 | 1.97 | 0.45 |
| 1:b5:10:ASN:OD1 | 10:k5:17:PHE:CZ | 2.69 | 0.45 |
| 3:J6:108:ARG:CZ | 6:M6:155:ASN:HA | 2.46 | 0.45 |
| 2:K6:38:MET:HE2 | 2:K6:38:MET:HB3 | 1.81 | 0.45 |
| 7:N6:5:VAL:HG23 | 3:F6:108:ARG:HH12 | 1.81 | 0.45 |
| 10:j5:357:LEU:CD1 | 10:j5:379:PHE:N | 2.80 | 0.45 |
| 10:j5:669:GLU:O | 10:j5:669:GLU:HG2 | 2.15 | 0.45 |
| 10:j5:984:ILE:C | 10:j5:984:ILE:CD1 | 2.85 | 0.45 |
| 10:j5:1020:GLU:CG | 1:f7:87:TYR:CE1 | 2.83 | 0.45 |
| 10:k5:732:ARG:NE | 1:D7:69:GLY:HA3 | 2.31 | 0.45 |
| 10:k5:761:ARG:C | 10:k5:761:ARG:CD | 2.87 | 0.45 |
| 10:k5:1020:GLU:HG3 | 1:Z7:87:TYR:OH | 2.13 | 0.45 |
| 2:A6:128:ILE:CG2 | 2:A6:132:LYS:HE3 | 2.47 | 0.45 |
| 8:Q7:21:GLY:CA | 8:C7:6:LYS:NZ | 2.79 | 0.45 |
| 1:H7:12:TYR:CZ | 1:H7:23:ALA:HB2 | 2.50 | 0.45 |
| 1:h7:51:ILE:HD11 | 1:h7:140:LEU:CD2 | 2.46 | 0.45 |
| 8:i7:122:PRO:C | 8:i7:125:ALA:H | 2.23 | 0.45 |
| 12:j7:201:CYC:HMA2 | 9:y7:38:PHE:CD1 | 2.45 | 0.45 |
| 8:k7:120:GLN:CG | 1:p7:53:LYS:NZ | 2.78 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:T7:201:CYC:HMD1 | 12:T7:201:CYC:NC | 2.09 | 0.45 |
| 1:b7:51:ILE:HD11 | 1:b7:140:LEU:CD2 | 2.46 | 0.45 |
| 8:e7:134:LYS:O | 8:e7:138:THR:HB | 2.16 | 0.45 |
| 9:x7:28:PHE:O | 9:x7:28:PHE:CG | 2.69 | 0.45 |
| 2:V8:128:ILE:CG2 | 2:V8:132:LYS:HE3 | 2.47 | 0.45 |
| 3:F8:111:ASN:HB3 | 4:M8:6:THR:CA | 2.38 | 0.45 |
| 2:G8:15:GLN:HB3 | 11:a9:120:ARG:NH1 | 2.30 | 0.45 |
| 3:H8:88:ILE:HG21 | 12:H8:201:CYC:CAB | 2.46 | 0.45 |
| 4:M8:92:GLU:HG2 | 4:M8:217:VAL:CG2 | 2.29 | 0.45 |
| 2:N8:31:PHE:CG | 3:O8:34:SER:CB | 3.00 | 0.45 |
| 2:N8:59:VAL:O | 2:N8:66:LEU:CD1 | 2.62 | 0.45 |
| 3:Q8:127:VAL:CG2 | 12:Z8:301:CYC:HMC2 | 2.17 | 0.45 |
| 4:M9:53:LEU:HD22 | 3:F9:84:ARG:CZ | 2.47 | 0.45 |
| 2:C9:128:ILE:CG2 | 2:C9:132:LYS:HE3 | 2.47 | 0.45 |
| 2:S9:128:ILE:CG2 | 2:S9:132:LYS:HE3 | 2.47 | 0.45 |
| 2:W9:128:ILE:HG22 | 2:W9:132:LYS:HE3 | 1.98 | 0.45 |
| 11:aA:373:PRO:HG2 | 11:aA:373:PRO:O | 2.17 | 0.45 |
| 11:aA:419:ARG:O | 11:aA:420:ASN:C | 2.58 | 0.45 |
| 11:aA:632:ILE:HG23 | 11:aA:634:ALA:N | 2.24 | 0.45 |
| 4:M1:74:LEU:O | 4:M1:77:LEU:HD11 | 2.15 | 0.45 |
| 2:W1:128:ILE:CG2 | 2:W1:132:LYS:HE3 | 2.47 | 0.45 |
| 2:AA:2:LYS:NZ | 2:KA:17:ARG:NH2 | 2.65 | 0.45 |
| 2:IA:33:ARG:HH12 | 12:F9:302:CYC:HMA3 | 1.82 | 0.45 |
| 3:LA:108:ARG:HA | 11:aA:531:ASP:CB | 2.44 | 0.45 |
| 5:NA:22:LEU:HD21 | 5:NA:26:LEU:CG | 2.29 | 0.45 |
| 5:NA:54:LEU:CG | 3:TA:84:ARG:CZ | 2.93 | 0.45 |
| 2:OA:31:PHE:CG | 3:PA:34:SER:CB | 3.00 | 0.45 |
| 2:QA:4:VAL:HG22 | 2:UA:22:THR:O | 2.15 | 0.45 |
| 2:QA:68:GLN:C | 2:U1:46:SER:CB | 2.88 | 0.45 |
| 2:QA:101:GLY:CA | 2:UA:22:THR:OG1 | 2.62 | 0.45 |
| 2:SA:42:ARG:NH1 | 3:TA:24:LEU:HD13 | 2.32 | 0.45 |
| 2:G3:128:ILE:CG2 | 2:G3:132:LYS:HE3 | 2.47 | 0.45 |
| 3:J3:107:ASP:OD1 | 11:a9:632:ILE:CD1 | 2.64 | 0.45 |
| 2:K3:128:ILE:CG2 | 2:K3:132:LYS:HE3 | 2.47 | 0.45 |
| 3:H2:84:ARG:C | 3:H2:86:MET:N | 2.74 | 0.45 |
| 2:K2:128:ILE:HG22 | 2:K2:132:LYS:HE3 | 1.98 | 0.45 |
| 12:N2:101:CYC:CAB | 3:B2:88:ILE:HG21 | 2.47 | 0.45 |
| 2:A3:38:MET:HE2 | 2:A3:38:MET:HB3 | 1.81 | 0.45 |
| 2:C4:128:ILE:CG2 | 2:C4:132:LYS:HE3 | 2.47 | 0.45 |
| 4:M3:103:GLN:O | 4:M3:103:GLN:HG3 | 2.16 | 0.45 |
| 5:N3:36:THR:HB | 3:T3:84:ARG:NH2 | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:U3:128:ILE:CG2 | 2:U3:132:LYS:HE3 | 2.47 | 0.45 |
| 3:F4:112:GLY:C | 4:M4:5:THR:HA | 2.28 | 0.45 |
| 3:L4:66:LEU:HD23 | 3:L4:66:LEU:HA | 1.98 | 0.45 |
| 4:M4:103:GLN:O | 4:M4:103:GLN:HG3 | 2.16 | 0.45 |
| 4:M4:113:ILE:HD11 | 4:M4:143:VAL:HA | 1.98 | 0.45 |
| 12:M4:301:CYC:C3B | 3:Y4:88:ILE:CD1 | 2.93 | 0.45 |
| 2:R4:128:ILE:CG2 | 2:R4:132:LYS:HE3 | 2.47 | 0.45 |
| 8:K5:80:LEU:HD13 | 12:K5:201:CYC:CHA | 2.47 | 0.45 |
| 8:M5:41:GLN:CD | 1:J7:143:PRO:CD | 2.90 | 0.45 |
| 2:X4:128:ILE:HG22 | 2:X4:132:LYS:HE3 | 1.98 | 0.45 |
| 8:G5:134:LYS:O | 8:G5:138:THR:HB | 2.16 | 0.45 |
| 1:d5:72:MET:HE2 | 1:d5:72:MET:HB3 | 1.87 | 0.45 |
| 8:Q5:8:ILE:CG2 | 1:R5:94:TYR:CD1 | 2.93 | 0.45 |
| 1:X5:72:MET:HE2 | 1:X5:72:MET:HB3 | 1.87 | 0.45 |
| 12:X5:201:CYC:CBB | 10:j5:520:ARG:CD | 2.90 | 0.45 |
| 9:z5:14:LEU:HD13 | 9:z5:15:LYS:HB3 | 1.98 | 0.45 |
| 10:j5:76:PHE:HB2 | 10:j5:81:PRO:HG3 | 1.97 | 0.45 |
| 10:j5:305:PHE:CE2 | 10:j5:337:LEU:HD23 | 2.51 | 0.45 |
| 10:j5:540:LEU:HB2 | 10:j5:567:LEU:HG | 1.99 | 0.45 |
| 10:j5:576:PHE:CD1 | 10:j5:576:PHE:N | 2.84 | 0.45 |
| 10:j5:729:ILE:HB | 1:J7:64:ASP:OD1 | 2.17 | 0.45 |
| 10:j5:965:GLN:HB2 | 1:t7:69:GLY:C | 2.42 | 0.45 |
| 10:k5:889:LEU:HD23 | 12:D7:201:CYC:C4B | 2.46 | 0.45 |
| 2:A6:64:PRO:C | 2:A6:66:LEU:H | 2.23 | 0.45 |
| 2:E6:128:ILE:CG2 | 2:E6:132:LYS:HE3 | 2.47 | 0.45 |
| 3:F6:84:ARG:CZ | 12:F6:201:CYC:O2A | 2.64 | 0.45 |
| 3:D1:88:ILE:HG21 | 12:D1:202:CYC:CAB | 2.46 | 0.45 |
| 12:R7:201:CYC:CMA | 12:R7:201:CYC:NB | 2.74 | 0.45 |
| 8:G7:134:LYS:O | 8:G7:138:THR:HB | 2.16 | 0.45 |
| 8:I7:94:TYR:O | 8:I7:97:VAL:HG23 | 2.16 | 0.45 |
| 8:M7:64:ASP:O | 8:M7:67:SER:HB2 | 2.17 | 0.45 |
| 1:h7:79:ALA:HB2 | 8:i7:111:GLY:O | 2.16 | 0.45 |
| 8:i7:20:PRO:HD3 | 8:s7:155:TYR:CG | 2.31 | 0.45 |
| 8:c7:137:ALA:O | 8:c7:138:THR:C | 2.55 | 0.45 |
| 3:B8:113:LEU:N | 4:M8:60:LYS:HD3 | 2.32 | 0.45 |
| 2:C8:128:ILE:CG2 | 2:C8:132:LYS:HE3 | 2.47 | 0.45 |
| 2:E8:128:ILE:CG2 | 2:E8:132:LYS:HE3 | 2.47 | 0.45 |
| 8:o7:94:TYR:OH | 1:p7:17:LYS:C | 2.50 | 0.45 |
| 8:q7:64:ASP:O | 8:q7:67:SER:HB2 | 2.17 | 0.45 |
| 12:U8:202:CYC:HC | 12:U8:202:CYC:HMD3 | 1.78 | 0.45 |
| 3:W8:88:ILE:HG21 | 12:W8:201:CYC:CAB | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M9:7:SER:C | 4:M9:14:LEU:HD13 | 2.08 | 0.45 |
| 4:M9:73:ASP:CA | 3:D9:111:ASN:HD21 | 2.28 | 0.45 |
| 5:N9:40:SER:O | 5:N9:40:SER:OG | 2.30 | 0.45 |
| 3:P9:88:ILE:HG21 | 12:P9:201:CYC:CAB | 2.46 | 0.45 |
| 2:I9:1:MET:HE2 | 2:I9:108:TYR:CE1 | 2.45 | 0.45 |
| 2:S9:42:ARG:NH1 | 3:T9:24:LEU:HD13 | 2.32 | 0.45 |
| 11:a9:572:THR:HG22 | 11:a9:573:SER:N | 2.31 | 0.45 |
| 11:a9:710:THR:HB | 11:a9:807:GLN:HB3 | 1.96 | 0.45 |
| 11:aA:823:ILE:HD12 | 3:L1:75:PRO:CG | 2.46 | 0.45 |
| 3:L1:84:ARG:O | 3:L1:88:ILE:HG12 | 2.16 | 0.45 |
| 4:M1:153:LYS:O | 4:M1:157:PHE:HB3 | 2.17 | 0.45 |
| 2:Y1:128:ILE:CG2 | 2:Y1:132:LYS:HE3 | 2.47 | 0.45 |
| 3:Z1:88:ILE:HG21 | 12:Z1:202:CYC:CAB | 2.46 | 0.45 |
| 1:Z:76:ARG:HG2 | 10:j5:262:TYR:CD2 | 2.52 | 0.45 |
| 3:BA:30:LEU:HD12 | 3:BA:30:LEU:H | 1.81 | 0.45 |
| 2:EA:2:LYS:NZ | 2:IA:17:ARG:CZ | 2.69 | 0.45 |
| 3:HA:126:SER:CB | 12:HA:202:CYC:HMC1 | 2.31 | 0.45 |
| 4:MA:91:VAL:O | 4:MA:218:VAL:HG23 | 2.17 | 0.45 |
| 4:MA:160:THR:CG2 | 4:MA:257:GLN:CG | 2.93 | 0.45 |
| 5:NA:3:VAL:HG11 | 3:RA:115:GLU:HB3 | 1.93 | 0.45 |
| 5:NA:36:THR:HB | 12:PA:201:CYC:O2A | 2.17 | 0.45 |
| 2:OA:65:TYR:CD1 | 2:UA:65:TYR:CD1 | 3.05 | 0.45 |
| 2:QA:119:THR:O | 3:TA:53:SER:HB2 | 2.16 | 0.45 |
| 3:RA:88:ILE:HG21 | 12:RA:201:CYC:CAB | 2.46 | 0.45 |
| 2:WA:38:MET:HE2 | 2:WA:38:MET:HB3 | 1.81 | 0.45 |
| 2:O1:19:LEU:O | 3:P1:45:THR:CG2 | 2.64 | 0.45 |
| 3:J2:88:ILE:HG21 | 12:J2:202:CYC:CAB | 2.46 | 0.45 |
| 7:N2:20:VAL:CG2 | 7:N2:39:TYR:CZ | 2.99 | 0.45 |
| 2:A3:19:LEU:O | 3:B3:45:THR:CG2 | 2.64 | 0.45 |
| 2:A3:128:ILE:CG2 | 2:A3:132:LYS:HE3 | 2.47 | 0.45 |
| 2:E3:128:ILE:CG2 | 2:E3:132:LYS:HE3 | 2.47 | 0.45 |
| 3:B4:111:ASN:HD21 | 4:M4:65:ARG:HG2 | 1.80 | 0.45 |
| 3:B4:117:TYR:HE1 | 4:M4:53:LEU:CD2 | 2.30 | 0.45 |
| 5:N3:37:HIS:O | 5:N3:37:HIS:CD2 | 2.70 | 0.45 |
| 3:X3:67:ILE:HD12 | 12:Y3:201:CYC:O2A | 2.17 | 0.45 |
| 3:B1:125:ARG:HD2 | 3:X1:14:LEU:HD13 | 1.97 | 0.45 |
| 2:T4:128:ILE:CG2 | 2:T4:132:LYS:HE3 | 2.47 | 0.45 |
| 3:U4:120:LEU:CD1 | 4:M4:254:LEU:CD2 | 2.94 | 0.45 |
| 3:F4:115:GLU:OE2 | 4:M4:3:VAL:HG21 | 2.06 | 0.45 |
| 2:G4:128:ILE:CG2 | 2:G4:132:LYS:HE3 | 2.47 | 0.45 |
| 4:M4:57:THR:O | 4:M4:60:LYS:HG2 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 4:M4:226:SER:HG | 3:Y4:84:ARG:C | 2.25 | 0.45 |
| 2:N4:128:ILE:CG2 | 2:N4:132:LYS:HE3 | 2.47 | 0.45 |
| 8:O5:76:LYS:HG3 | 8:O5:77:MET:CA | 2.43 | 0.45 |
| 12:B5:201:CYC:OB | 9:z5:22:GLU:N | 2.50 | 0.45 |
| 8:C5:16:ARG:HH11 | 8:C5:16:ARG:CG | 2.29 | 0.45 |
| 8:E5:71:ASN:CG | 8:E5:121:THR:HA | 2.41 | 0.45 |
| 8:G5:50:ILE:HA | 8:G5:136:VAL:HG11 | 1.99 | 0.45 |
| 1:J5:15:GLN:HE21 | 1:J5:15:GLN:HB2 | 1.56 | 0.45 |
| 2:C1:128:ILE:CG2 | 2:C1:132:LYS:HE3 | 2.47 | 0.45 |
| 12:d5:201:CYC:CMA | 12:d5:201:CYC:NB | 2.74 | 0.45 |
| 8:e5:94:TYR:O | 8:e5:97:VAL:HG23 | 2.16 | 0.45 |
| 8:Q5:134:LYS:O | 8:Q5:138:THR:HB | 2.16 | 0.45 |
| 1:Z5:62:TYR:OH | 12:a5:201:CYC:O1D | 2.30 | 0.45 |
| 2:K6:128:ILE:CG2 | 2:K6:132:LYS:HE3 | 2.47 | 0.45 |
| 6:M6:38:SER:O | 6:M6:38:SER:OG | 2.31 | 0.45 |
| 10:j5:182:ASN:HB3 | 12:j5:1201:CYC:HAB2 | 1.98 | 0.45 |
| 10:j5:750:ARG:CG | 10:j5:750:ARG:NH1 | 2.74 | 0.45 |
| 10:j5:820:HIS:CD2 | 10:j5:820:HIS:O | 2.69 | 0.45 |
| 10:j5:1064:LYS:CD | 10:j5:1065:HIS:H | 2.25 | 0.45 |
| 10:k5:190:LEU:CD1 | 12:k5:1201:CYC:NC | 2.79 | 0.45 |
| 10:k5:394:PRO:HB2 | 10:k5:395:SER:H | 1.56 | 0.45 |
| 10:k5:756:SER:CB | 9:z7:24:GLN:HG2 | 2.47 | 0.45 |
| 10:k5:888:THR:O | 12:D7:201:CYC:HMA2 | 2.17 | 0.45 |
| 10:k5:1023:SER:HA | 12:k5:1202:CYC:HBA1 | 1.99 | 0.45 |
| 10:k5:1150:TYR:OH | 11:a9:38:VAL:HG13 | 2.17 | 0.45 |
| 2:I6:128:ILE:HG22 | 2:I6:132:LYS:HE3 | 1.98 | 0.45 |
| 8:S7:49:ARG:CD | 11:aA:550:PHE:CD1 | 2.84 | 0.45 |
| 8:g7:10:ASN:HD21 | 8:u7:10:ASN:ND2 | 2.09 | 0.45 |
| 8:i7:21:GLY:HA2 | 8:s7:100:ASP:CA | 2.36 | 0.45 |
| 8:i7:90:ARG:NH2 | 1:j7:13:ASP:OD1 | 2.50 | 0.45 |
| 1:d7:72:MET:HE2 | 1:d7:72:MET:HB3 | 1.87 | 0.45 |
| 2:A8:65:TYR:CD1 | 2:G8:65:TYR:CD1 | 3.05 | 0.45 |
| 3:B8:68:ARG:HH12 | 3:U8:68:ARG:NH1 | 2.14 | 0.45 |
| 2:E8:128:ILE:HG22 | 2:E8:132:LYS:HE3 | 1.98 | 0.45 |
| 9:z7:6:LYS:O | 9:z7:6:LYS:HG3 | 2.15 | 0.45 |
| 9:w7:6:LYS:O | 9:w7:6:LYS:HG3 | 2.15 | 0.45 |
| 9:y7:15:LYS:HB2 | 9:y7:15:LYS:HE3 | 1.33 | 0.45 |
| 9:y7:28:PHE:O | 9:y7:28:PHE:CG | 2.69 | 0.45 |
| 12:H8:201:CYC:CBA | 11:a9:261:SER:CB | 2.95 | 0.45 |
| 2:I8:112:GLY:N | 11:a9:133:LEU:CD2 | 2.80 | 0.45 |
| 2:K8:128:ILE:CG2 | 2:K8:132:LYS:HE3 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M8:57:THR:O | 4:M8:60:LYS:HG2 | 2.16 | 0.45 |
| 2:P8:128:ILE:CG2 | 2:P8:132:LYS:HE3 | 2.47 | 0.45 |
| 2:O9:128:ILE:CG2 | 2:O9:132:LYS:HE3 | 2.47 | 0.45 |
| 5:Z8:37:HIS:CD2 | 5:Z8:37:HIS:O | 2.70 | 0.45 |
| 5:Z8:41:GLN:CG | 12:Z8:301:CYC:CAB | 2.56 | 0.45 |
| 2:E9:152:ALA:HB1 | 2:I9:21:ASN:OD1 | 2.16 | 0.45 |
| 3:J9:88:ILE:HG21 | 12:J9:202:CYC:CAB | 2.46 | 0.45 |
| 3:J9:88:ILE:HG12 | 11:a9:512:TYR:CZ | 2.51 | 0.45 |
| 12:J9:202:CYC:HB | 12:J9:202:CYC:CMA | 2.26 | 0.45 |
| 2:W9:128:ILE:CG2 | 2:W9:132:LYS:HE3 | 2.47 | 0.45 |
| 11:a9:548:LEU:O | 11:a9:552:LEU:HB2 | 2.17 | 0.45 |
| 11:aA:64:ARG:O | 11:aA:65:LEU:C | 2.56 | 0.45 |
| 11:aA:320:ASP:HA | 11:aA:323:ARG:HG2 | 1.98 | 0.45 |
| 11:aA:328:GLN:HE21 | 11:aA:328:GLN:CA | 2.30 | 0.45 |
| 11:aA:710:THR:HA | 11:aA:807:GLN:HB2 | 1.99 | 0.45 |
| 11:aA:716:ILE:HD11 | 11:aA:738:LEU:CD2 | 2.47 | 0.45 |
| 3:H1:84:ARG:HH22 | 12:H1:201:CYC:CHA | 2.30 | 0.45 |
| 2:I1:128:ILE:CG2 | 2:I1:132:LYS:HE3 | 2.47 | 0.45 |
| 4:M1:103:GLN:O | 4:M1:103:GLN:HG3 | 2.16 | 0.45 |
| 4:M1:160:THR:CG2 | 4:M1:257:GLN:CG | 2.93 | 0.45 |
| 2:E2:128:ILE:HG22 | 2:E2:132:LYS:HE3 | 1.98 | 0.45 |
| 3:F2:88:ILE:HG21 | 12:F2:201:CYC:HAB2 | 1.99 | 0.45 |
| 3:F2:127:VAL:HG22 | 12:F2:201:CYC:HMC2 | 1.97 | 0.45 |
| 1:A:18:TYR:OH | 8:a5:89:LEU:CB | 2.64 | 0.45 |
| 2:AA:31:PHE:CG | 3:BA:34:SER:CB | 3.00 | 0.45 |
| 2:IA:37:SER:CA | 2:IA:97:LEU:CD2 | 2.92 | 0.45 |
| 4:MA:222:ARG:HH11 | 4:MA:222:ARG:CG | 2.13 | 0.45 |
| 4:MA:232:VAL:HG13 | 3:XA:111:ASN:C | 2.18 | 0.45 |
| 2:QA:68:GLN:CA | 2:U1:46:SER:CB | 2.53 | 0.45 |
| 2:SA:42:ARG:NH2 | 3:TA:25:ASN:OD1 | 2.46 | 0.45 |
| 2:UA:128:ILE:CG2 | 2:UA:132:LYS:HE3 | 2.47 | 0.45 |
| 2:YA:128:ILE:CG2 | 2:YA:132:LYS:HE3 | 2.47 | 0.45 |
| 12:P1:201:CYC:HBA2 | 4:M1:133:ARG:HB3 | 1.99 | 0.45 |
| 12:Q1:201:CYC:O2A | 3:T1:67:ILE:HD12 | 2.17 | 0.45 |
| 2:S1:128:ILE:HG22 | 2:S1:132:LYS:HE3 | 1.98 | 0.45 |
| 2:G3:65:TYR:CD1 | 2:A3:65:TYR:CD1 | 3.05 | 0.45 |
| 3:J3:77:ARG:HG3 | 2:K3:111:ALA:HB3 | 1.90 | 0.45 |
| 3:H2:88:ILE:HG21 | 12:H2:201:CYC:CAB | 2.46 | 0.45 |
| 2:I2:128:ILE:HG22 | 2:I2:132:LYS:HE3 | 1.98 | 0.45 |
| 2:C3:128:ILE:HG22 | 2:C3:132:LYS:HE3 | 1.98 | 0.45 |
| 3:D3:111:ASN:HD21 | 4:M3:65:ARG:HD2 | 1.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:A4:65:TYR:CD1 | 2:G4:65:TYR:CD1 | 3.05 | 0.45 |
| 2:A4:128:ILE:CG2 | 2:A4:132:LYS:HE3 | 2.47 | 0.45 |
| 3:B4:67:ILE:HD12 | 12:E4:201:CYC:O2A | 2.17 | 0.45 |
| 4:M3:19:MET:HE2 | 4:M3:59:ILE:CD1 | 2.46 | 0.45 |
| 5:N3:66:ARG:HH11 | 5:N3:66:ARG:CB | 2.22 | 0.45 |
| 2:O3:128:ILE:CG2 | 2:O3:132:LYS:HE3 | 2.47 | 0.45 |
| 3:P3:67:ILE:HD12 | 12:S3:201:CYC:O2A | 2.17 | 0.45 |
| 3:U4:88:ILE:HG21 | 12:U4:201:CYC:CAB | 2.46 | 0.45 |
| 3:F4:112:GLY:C | 3:F4:114:LYS:N | 2.74 | 0.45 |
| 2:K4:128:ILE:CG2 | 2:K4:132:LYS:HE3 | 2.47 | 0.45 |
| 8:O5:29:PHE:CE2 | 1:P5:31:PHE:HE1 | 2.34 | 0.45 |
| 3:Y4:88:ILE:CA | 3:Y4:91:ARG:NH2 | 2.80 | 0.45 |
| 8:c5:120:GLN:CG | 1:f5:53:LYS:HZ1 | 2.26 | 0.45 |
| 12:P5:201:CYC:CMA | 12:P5:201:CYC:NB | 2.74 | 0.45 |
| 12:X5:201:CYC:HMD1 | 12:X5:201:CYC:NC | 2.09 | 0.45 |
| 7:N6:20:VAL:HG21 | 7:N6:39:TYR:CE1 | 2.51 | 0.45 |
| 10:j5:44:ASP:O | 10:j5:48:GLY:N | 2.48 | 0.45 |
| 10:j5:186:LEU:HD21 | 12:j5:1201:CYC:HMB3 | 1.98 | 0.45 |
| 10:j5:1008:PHE:CE1 | 12:v7:201:CYC:CBB | 2.93 | 0.45 |
| 10:j5:1009:ALA:HB2 | 1:v7:87:TYR:OH | 2.15 | 0.45 |
| 10:j5:1017:ARG:O | 10:j5:1018:LEU:HD23 | 2.17 | 0.45 |
| 10:k5:355:ARG:NH1 | 10:k5:358:GLU:OE1 | 2.48 | 0.45 |
| 10:k5:1147:TYR:CD1 | 10:k5:1147:TYR:O | 2.69 | 0.45 |
| 8:C7:17:TYR:OH | 1:D7:89:LEU:HG | 2.16 | 0.45 |
| 8:G7:82:LEU:HB3 | 11:a9:579:PHE:CD1 | 2.52 | 0.45 |
| 8:G7:120:GLN:CG | 1:L7:53:LYS:NZ | 2.78 | 0.45 |
| 1:h7:52:ILE:HG12 | 1:h7:133:MET:HE3 | 1.98 | 0.45 |
| 8:k7:94:TYR:OH | 1:l7:17:LYS:O | 2.24 | 0.45 |
| 1:b7:30:TYR:CD2 | 1:b7:30:TYR:O | 2.70 | 0.45 |
| 12:A8:201:CYC:O2A | 3:D8:67:ILE:HD12 | 2.17 | 0.45 |
| 8:o7:36:ARG:NH2 | 8:o7:36:ARG:CG | 2.71 | 0.45 |
| 8:u7:42:THR:HG21 | 8:u7:141:LEU:CD2 | 2.47 | 0.45 |
| 3:O8:67:ILE:HD12 | 12:R8:201:CYC:O2A | 2.17 | 0.45 |
| 3:L9:41:VAL:HG21 | 3:L9:98:LEU:CD1 | 2.47 | 0.45 |
| 4:M9:73:ASP:HA | 3:D9:111:ASN:ND2 | 2.31 | 0.45 |
| 2:O9:34:ALA:CB | 3:P9:31:VAL:HG11 | 2.38 | 0.45 |
| 12:P9:202:CYC:CMD | 12:P9:202:CYC:NC | 2.75 | 0.45 |
| 3:Y8:84:ARG:O | 3:Y8:88:ILE:HG12 | 2.16 | 0.45 |
| 2:C9:128:ILE:HG22 | 2:C9:132:LYS:HE3 | 1.98 | 0.45 |
| 2:E9:128:ILE:CG2 | 2:E9:132:LYS:HE3 | 2.47 | 0.45 |
| 2:G9:128:ILE:CG2 | 2:G9:132:LYS:HE3 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:I9:128:ILE:HG22 | 2:I9:132:LYS:HE3 | 1.98 | 0.45 |
| 3:R9:88:ILE:HG21 | 12:R9:201:CYC:CAB | 2.46 | 0.45 |
| 12:T9:301:CYC:HC | 12:T9:301:CYC:HMD3 | 1.82 | 0.45 |
| 3:V9:88:ILE:HG21 | 12:V9:201:CYC:CAB | 2.46 | 0.45 |
| 2:G1:128:ILE:HG22 | 2:G1:132:LYS:HE3 | 1.98 | 0.45 |
| 11:a9:388:VAL:HG12 | 11:a9:392:ILE:HD11 | 1.99 | 0.45 |
| 11:a9:446:ALA:C | 11:a9:447:SER:O | 2.59 | 0.45 |
| 11:a9:522:ASP:OD1 | 11:a9:522:ASP:N | 2.31 | 0.45 |
| 11:aA:93:LEU:HD13 | 11:aA:93:LEU:H | 1.81 | 0.45 |
| 11:aA:438:TYR:O | 11:aA:438:TYR:CD1 | 2.70 | 0.45 |
| 11:aA:731:GLN:HG2 | 3:L1:120:LEU:HD23 | 1.96 | 0.45 |
| 4:M1:110:TYR:HE2 | 4:M1:124:ARG:NH1 | 2.13 | 0.45 |
| 3:X1:67:ILE:HD12 | 12:Y1:201:CYC:O2A | 2.17 | 0.45 |
| 2:A2:31:PHE:CG | 3:B2:34:SER:CB | 3.00 | 0.45 |
| 3:JA:116:THR:CG2 | 11:aA:521:PHE:CG | 2.88 | 0.45 |
| 4:MA:163:ASN:CG | 12:VA:201:CYC:HMA3 | 2.41 | 0.45 |
| 5:NA:34:LEU:HB3 | 3:PA:84:ARG:NH1 | 2.31 | 0.45 |
| 12:RA:201:CYC:HB | 12:RA:201:CYC:CMA | 2.26 | 0.45 |
| 2:SA:128:ILE:HG22 | 2:SA:132:LYS:HE3 | 1.97 | 0.45 |
| 2:YA:128:ILE:HG22 | 2:YA:132:LYS:HE3 | 1.98 | 0.45 |
| 2:A1:128:ILE:HG22 | 2:A1:132:LYS:HE3 | 1.98 | 0.45 |
| 3:L2:88:ILE:HG21 | 12:L2:201:CYC:CAB | 2.46 | 0.45 |
| 3:F3:88:ILE:HG21 | 12:F3:201:CYC:CAB | 2.46 | 0.45 |
| 12:F3:202:CYC:HC | 12:F3:202:CYC:HMD3 | 1.78 | 0.45 |
| 3:L3:84:ARG:O | 3:L3:88:ILE:HG12 | 2.16 | 0.45 |
| 12:L3:202:CYC:CMA | 11:a9:713:ASN:OD1 | 2.64 | 0.45 |
| 4:M3:137:ILE:HB | 4:M3:141:GLU:HB3 | 1.99 | 0.45 |
| 5:N3:22:LEU:O | 5:N3:37:HIS:CE1 | 2.70 | 0.45 |
| 2:E4:128:ILE:CG2 | 2:E4:132:LYS:HE3 | 2.47 | 0.45 |
| 3:J4:67:ILE:HD12 | 12:K4:201:CYC:O2A | 2.17 | 0.45 |
| 3:L4:71:GLY:HA3 | 11:aA:82:GLN:CG | 2.41 | 0.45 |
| 4:M4:96:LYS:HE3 | 3:Q4:171:ILE:CG1 | 2.46 | 0.45 |
| 3:O4:67:ILE:HD12 | 12:R4:201:CYC:O2A | 2.17 | 0.45 |
| 2:P4:19:LEU:HD21 | 3:Q4:95:TYR:HE1 | 1.44 | 0.45 |
| 8:K5:134:LYS:O | 8:K5:138:THR:HB | 2.16 | 0.45 |
| 8:M5:37:LEU:HD22 | 1:N5:24:LEU:HD22 | 1.99 | 0.45 |
| 2:X4:128:ILE:CG2 | 2:X4:132:LYS:HE3 | 2.47 | 0.45 |
| 1:H5:2:GLN:CD | 10:j5:551:MET:HG2 | 2.41 | 0.45 |
| 1:H5:10:ASN:OD1 | 10:j5:557:VAL:CG2 | 2.65 | 0.45 |
| 8:I5:95:GLY:CA | 8:I5:104:ILE:HD11 | 2.47 | 0.45 |
| 8:e5:94:TYR:O | 8:e5:97:VAL:CG2 | 2.65 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:P5:161:SER:HB3 | 10:k5:11:VAL:HG21 | 1.99 | 0.45 |
| 1:R5:87:TYR:CE1 | 10:k5:521:GLY:HA3 | 2.51 | 0.45 |
| 10:j5:965:GLN:HB3 | 10:j5:969:VAL:CG1 | 2.44 | 0.45 |
| 10:j5:1004:VAL:HG13 | 10:j5:1066:PHE:CZ | 2.52 | 0.45 |
| 10:k5:357:LEU:CD1 | 10:k5:379:PHE:N | 2.80 | 0.45 |
| 10:k5:1008:PHE:CZ | 1:p7:87:TYR:OH | 2.60 | 0.45 |
| 3:H6:67:ILE:HD12 | 12:I6:201:CYC:O2A | 2.17 | 0.45 |
| 8:O7:94:TYR:O | 8:O7:97:VAL:CG2 | 2.65 | 0.45 |
| 8:O7:161:GLN:CD | 1:F7:49:THR:HG22 | 2.41 | 0.45 |
| 8:S7:94:TYR:OH | 1:T7:17:LYS:O | 2.23 | 0.45 |
| 8:I7:134:LYS:O | 8:I7:138:THR:HB | 2.16 | 0.45 |
| 1:N7:106:GLU:HG2 | 9:z7:58:THR:HG23 | 1.96 | 0.45 |
| 8:g7:25:ARG:NH2 | 8:u7:25:ARG:CD | 2.80 | 0.45 |
| 1:h7:76:ARG:CA | 8:i7:110:ILE:O | 2.65 | 0.45 |
| 8:i7:25:ARG:NH1 | 8:s7:6:LYS:CA | 2.69 | 0.45 |
| 1:Z7:67:ARG:HH22 | 11:a9:307:ARG:HB3 | 0.50 | 0.45 |
| 8:a7:59:PHE:HB3 | 11:a9:331:TYR:CE1 | 2.52 | 0.45 |
| 8:c7:20:PRO:HD3 | 8:m7:155:TYR:CD1 | 2.52 | 0.45 |
| 8:c7:53:GLN:HB2 | 8:c7:136:VAL:CG2 | 2.47 | 0.45 |
| 2:C8:128:ILE:HG22 | 2:C8:132:LYS:HE3 | 1.98 | 0.45 |
| 8:o7:34:GLU:HG3 | 1:p7:28:LYS:CD | 2.46 | 0.45 |
| 8:o7:37:LEU:HD23 | 8:o7:37:LEU:HA | 1.59 | 0.45 |
| 8:o7:134:LYS:O | 8:o7:138:THR:HB | 2.16 | 0.45 |
| 8:u7:81:CYS:HA | 12:u7:201:CYC:HAC1 | 1.23 | 0.45 |
| 2:X8:15:GLN:CG | 4:M8:211:GLN:HE22 | 2.30 | 0.45 |
| 3:F8:116:THR:N | 4:M8:3:VAL:CG1 | 2.79 | 0.45 |
| 12:H8:201:CYC:HMA1 | 11:a9:261:SER:HB2 | 1.97 | 0.45 |
| 12:H8:201:CYC:CBA | 11:a9:261:SER:HB2 | 2.47 | 0.45 |
| 3:L8:117:TYR:CE1 | 12:a9:901:CYC:NA | 2.85 | 0.45 |
| 3:L9:84:ARG:HE | 11:a9:406:LEU:HD22 | 1.82 | 0.45 |
| 3:L9:90:LEU:CD2 | 2:K9:18:PHE:CZ | 3.00 | 0.45 |
| 2:A9:152:ALA:HB1 | 2:K9:21:ASN:HB2 | 1.99 | 0.45 |
| 3:H9:67:ILE:HD12 | 12:I9:201:CYC:O2A | 2.17 | 0.45 |
| 3:J9:19:LEU:CD1 | 3:J9:24:LEU:HD21 | 2.47 | 0.45 |
| 2:K9:38:MET:HE2 | 2:K9:38:MET:HB3 | 1.81 | 0.45 |
| 3:Z9:88:ILE:HG21 | 12:Z9:202:CYC:CAB | 2.46 | 0.45 |
| 11:a9:438:TYR:CD1 | 11:a9:438:TYR:O | 2.70 | 0.45 |
| 11:a9:643:LEU:CD1 | 11:a9:766:ASN:O | 2.65 | 0.45 |
| 11:aA:371:VAL:HG11 | 11:aA:507:PHE:CB | 2.47 | 0.45 |
| 11:aA:485:GLU:OE2 | 11:aA:485:GLU:HA | 2.17 | 0.45 |
| 11:aA:643:LEU:CD2 | 11:aA:689:VAL:CG2 | 2.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:aA:775:LYS:O | 11:aA:777:GLN:HG2 | 2.17 | 0.45 |
| 4:M1:273:ILE:HA | 3:Z1:77:ARG:CZ | 2.47 | 0.45 |
| 5:N1:37:HIS:O | 5:N1:37:HIS:CD2 | 2.70 | 0.45 |
| 2:Y1:128:ILE:HG22 | 2:Y1:132:LYS:HE3 | 1.98 | 0.45 |
| 2:C2:128:ILE:CG2 | 2:C2:132:LYS:HE3 | 2.47 | 0.45 |
| 3:F2:85:ASP:OD2 | 12:F2:201:CYC:NA | 2.49 | 0.45 |
| 1:A:127:VAL:CG1 | 1:R5:15:GLN:HG2 | 2.38 | 0.45 |
| 2:AA:59:VAL:O | 2:AA:66:LEU:CD1 | 2.62 | 0.45 |
| 2:AA:128:ILE:CG2 | 2:AA:132:LYS:HE3 | 2.47 | 0.45 |
| 3:JA:119:ALA:HB1 | 11:aA:365:LYS:CE | 2.34 | 0.45 |
| 3:LA:41:VAL:HG21 | 3:LA:98:LEU:CD1 | 2.47 | 0.45 |
| 2:O1:65:TYR:CD1 | 2:U1:65:TYR:CD1 | 3.04 | 0.45 |
| 2:Q1:128:ILE:CG2 | 2:Q1:132:LYS:HE3 | 2.47 | 0.45 |
| 2:A1:59:VAL:O | 2:A1:66:LEU:CD1 | 2.62 | 0.45 |
| 2:G2:128:ILE:HG22 | 2:G2:132:LYS:HE3 | 1.98 | 0.45 |
| 3:L2:78:ARG:HH22 | 6:M2:70:GLU:HA | 1.82 | 0.45 |
| 3:B3:125:ARG:HD2 | 3:X3:14:LEU:HD13 | 1.97 | 0.45 |
| 12:Z3:202:CYC:CMD | 12:Z3:202:CYC:NC | 2.75 | 0.45 |
| 2:O3:60:TYR:CB | 2:O3:67:THR:CG2 | 2.83 | 0.45 |
| 3:P3:88:ILE:HG21 | 12:P3:201:CYC:CAB | 2.46 | 0.45 |
| 12:X3:201:CYC:HC | 12:X3:201:CYC:HMD3 | 1.82 | 0.45 |
| 3:J4:88:ILE:HG21 | 12:J4:201:CYC:CAB | 2.46 | 0.45 |
| 4:M4:26:SER:CB | 11:aA:228:GLU:CG | 2.94 | 0.45 |
| 4:M4:160:THR:CG2 | 4:M4:257:GLN:CG | 2.93 | 0.45 |
| 3:O4:120:LEU:CD2 | 5:Z4:14:LYS:HZ1 | 2.30 | 0.45 |
| 1:D5:39:ARG:C | 1:D5:41:ALA:N | 2.70 | 0.45 |
| 8:I5:16:ARG:HH11 | 8:I5:16:ARG:HG2 | 1.82 | 0.45 |
| 8:S5:37:LEU:HD22 | 1:T5:24:LEU:HD22 | 1.99 | 0.45 |
| 12:b5:201:CYC:CMA | 12:b5:201:CYC:NB | 2.74 | 0.45 |
| 6:M6:104:ARG:HD3 | 2:G6:15:GLN:CA | 2.42 | 0.45 |
| 9:z5:27:PHE:HE2 | 9:z5:52:LEU:HD11 | 1.82 | 0.45 |
| 10:j5:825:ASN:CB | 12:H7:201:CYC:OB | 2.52 | 0.45 |
| 10:j5:959:PHE:HD2 | 1:t7:67:ARG:HH12 | 1.65 | 0.45 |
| 10:j5:984:ILE:HD12 | 10:j5:984:ILE:O | 2.17 | 0.45 |
| 10:j5:1008:PHE:HZ | 1:v7:83:ARG:NH1 | 2.15 | 0.45 |
| 10:j5:1150:TYR:HE1 | 11:aA:38:VAL:CG1 | 2.29 | 0.45 |
| 10:k5:166:TYR:HB3 | 10:k5:179:LEU:CD2 | 2.47 | 0.45 |
| 10:k5:724:GLU:O | 10:k5:724:GLU:CG | 2.65 | 0.45 |
| 10:k5:984:ILE:HD12 | 10:k5:984:ILE:O | 2.17 | 0.45 |
| 12:C6:201:CYC:O2A | 3:F6:67:ILE:HD12 | 2.17 | 0.45 |
| 3:H6:88:ILE:HG21 | 12:H6:201:CYC:CAB | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:O7:95:GLY:CA | 8:O7:104:ILE:HD11 | 2.47 | 0.45 |
| 8:C7:15:ALA:HA | 1:D7:90:ARG:CZ | 2.47 | 0.45 |
| 8:i7:92:VAL:CG2 | 8:i7:156:LEU:HG | 2.47 | 0.45 |
| 3:B8:82:CYS:CA | 12:B8:202:CYC:H2C | 2.45 | 0.45 |
| 3:B8:85:ASP:OD2 | 3:B8:117:TYR:OH | 2.33 | 0.45 |
| 8:o7:39:ILE:HD11 | 8:o7:145:ASP:CA | 2.47 | 0.45 |
| 2:G8:38:MET:HE2 | 2:G8:38:MET:HB3 | 1.81 | 0.45 |
| 4:M8:5:THR:C | 4:M8:6:THR:OG1 | 2.56 | 0.45 |
| 4:M8:51:ARG:NH1 | 4:M8:51:ARG:CG | 2.77 | 0.45 |
| 4:M8:231:THR:H | 12:M8:301:CYC:C4B | 2.29 | 0.45 |
| 2:Q9:128:ILE:CG2 | 2:Q9:132:LYS:HE3 | 2.47 | 0.45 |
| 12:Q9:201:CYC:O2A | 3:T9:67:ILE:HD12 | 2.17 | 0.45 |
| 2:A9:34:ALA:CB | 3:B9:31:VAL:HG11 | 2.39 | 0.45 |
| 12:C9:201:CYC:O2A | 3:F9:67:ILE:HD12 | 2.17 | 0.45 |
| 2:E9:2:LYS:NZ | 2:I9:17:ARG:CZ | 2.69 | 0.45 |
| 2:E9:38:MET:HE2 | 2:E9:38:MET:HB3 | 1.81 | 0.45 |
| 3:X9:67:ILE:HD12 | 12:Y9:201:CYC:O2A | 2.17 | 0.45 |
| 12:G1:201:CYC:O2A | 3:L1:67:ILE:HD12 | 2.17 | 0.45 |
| 11:a9:337:GLU:CG | 11:a9:339:GLU:HG2 | 2.47 | 0.45 |
| 11:a9:710:THR:HA | 11:a9:807:GLN:HB2 | 1.99 | 0.45 |
| 11:a9:775:LYS:O | 11:a9:777:GLN:HG2 | 2.17 | 0.45 |
| 11:a9:809:ARG:HG3 | 11:a9:810:GLN:H | 1.82 | 0.45 |
| 11:aA:30:MET:HE3 | 11:aA:35:ARG:CA | 2.46 | 0.45 |
| 11:aA:527:LEU:HD23 | 11:aA:527:LEU:HA | 1.62 | 0.45 |
| 11:aA:615:ARG:H | 11:aA:615:ARG:HG2 | 1.55 | 0.45 |
| 11:aA:643:LEU:HD13 | 11:aA:766:ASN:CG | 2.41 | 0.45 |
| 12:A:201:CYC:CMA | 12:A:201:CYC:NB | 2.74 | 0.45 |
| 1:Z:13:ASP:OD2 | 8:e5:107:ILE:CD1 | 2.65 | 0.45 |
| 2:IA:128:ILE:CG2 | 2:IA:132:LYS:HE3 | 2.47 | 0.45 |
| 5:NA:62:ARG:NE | 2:SA:14:SER:CA | 2.56 | 0.45 |
| 3:PA:67:ILE:HD12 | 12:SA:201:CYC:O2A | 2.17 | 0.45 |
| 2:QA:2:LYS:NZ | 2:UA:17:ARG:CZ | 2.80 | 0.45 |
| 2:QA:128:ILE:CG2 | 2:QA:132:LYS:HE3 | 2.47 | 0.45 |
| 3:TA:29:ASN:ND2 | 2:X4:61:ASN:HA | 2.31 | 0.45 |
| 12:UA:201:CYC:O2A | 3:ZA:67:ILE:HD12 | 2.17 | 0.45 |
| 12:G3:201:CYC:O2A | 3:L3:67:ILE:HD12 | 2.17 | 0.45 |
| 3:J3:84:ARG:NH1 | 11:a9:668:TYR:CB | 2.61 | 0.45 |
| 3:J2:67:ILE:HD12 | 12:K2:201:CYC:O2A | 2.17 | 0.45 |
| 2:K2:128:ILE:CG2 | 2:K2:132:LYS:HE3 | 2.47 | 0.45 |
| 2:C3:38:MET:HE2 | 2:C3:38:MET:HB3 | 1.81 | 0.45 |
| 3:Z3:77:ARG:CZ | 4:M3:273:ILE:HA | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:B4:117:TYR:CE1 | 4:M4:53:LEU:CD1 | 3.00 | 0.45 |
| 2:O3:65:TYR:CD1 | 2:U3:65:TYR:CD1 | 3.04 | 0.45 |
| 3:W4:88:ILE:HG21 | 12:W4:201:CYC:CAB | 2.46 | 0.45 |
| 2:G4:15:GLN:HE21 | 11:aA:120:ARG:HH11 | 1.64 | 0.45 |
| 12:H4:201:CYC:HC | 12:H4:201:CYC:HMD3 | 1.82 | 0.45 |
| 3:J4:108:ARG:NE | 11:aA:171:ARG:O | 2.50 | 0.45 |
| 3:L4:65:ASP:CA | 11:aA:82:GLN:OE1 | 2.65 | 0.45 |
| 4:M4:153:LYS:O | 4:M4:157:PHE:HB3 | 2.17 | 0.45 |
| 4:M4:261:VAL:HG11 | 4:M4:266:LEU:HD13 | 1.99 | 0.45 |
| 3:O4:88:ILE:HG21 | 12:O4:201:CYC:CAB | 2.46 | 0.45 |
| 3:Q4:116:THR:O | 3:Q4:117:TYR:C | 2.60 | 0.45 |
| 8:O5:19:SER:OG | 8:O5:20:PRO:HD2 | 2.17 | 0.45 |
| 2:X4:38:MET:HE2 | 2:X4:38:MET:HB3 | 1.81 | 0.45 |
| 8:A5:52:LYS:HB3 | 8:A5:52:LYS:HE3 | 1.43 | 0.45 |
| 8:C5:16:ARG:CG | 8:C5:16:ARG:NH1 | 2.77 | 0.45 |
| 8:E5:101:VAL:O | 8:E5:102:THR:C | 2.57 | 0.45 |
| 8:I5:94:TYR:O | 8:I5:97:VAL:CG2 | 2.65 | 0.45 |
| 8:I5:134:LYS:O | 8:I5:138:THR:HB | 2.16 | 0.45 |
| 12:J5:201:CYC:CMA | 12:J5:201:CYC:NB | 2.74 | 0.45 |
| 7:N6:17:LYS:HB3 | 7:N6:66:GLU:HB2 | 1.99 | 0.45 |
| 9:z5:17:VAL:O | 9:z5:17:VAL:HG23 | 2.16 | 0.45 |
| 9:z5:45:GLN:HG2 | 9:z5:45:GLN:H | 1.66 | 0.45 |
| 10:j5:558:VAL:HG13 | 10:j5:561:GLU:HB2 | 1.99 | 0.45 |
| 10:j5:1023:SER:HA | 12:f7:201:CYC:HBA1 | 1.99 | 0.45 |
| 10:j5:1067:LEU:CD1 | 10:j5:1101:GLU:CD | 2.90 | 0.45 |
| 10:k5:82:MET:HE3 | 10:k5:82:MET:HB3 | 1.73 | 0.45 |
| 10:k5:283:ARG:CD | 10:k5:283:ARG:H | 2.30 | 0.45 |
| 10:k5:576:PHE:N | 10:k5:576:PHE:CD1 | 2.84 | 0.45 |
| 10:k5:729:ILE:HD13 | 10:k5:729:ILE:HG21 | 1.72 | 0.45 |
| 10:k5:764:PHE:CD1 | 10:k5:764:PHE:O | 2.70 | 0.45 |
| 10:k5:970:GLY:HA3 | 1:n7:77:ARG:NH2 | 2.12 | 0.45 |
| 10:k5:1106:PHE:C | 10:k5:1110:ILE:HD12 | 2.38 | 0.45 |
| 10:k5:1145:PRO:O | 1:l7:14:VAL:HG11 | 2.17 | 0.45 |
| 2:A6:19:LEU:O | 3:B6:45:THR:CG2 | 2.64 | 0.45 |
| 2:E6:128:ILE:HG22 | 2:E6:132:LYS:HE3 | 1.98 | 0.45 |
| 8:G7:64:ASP:O | 8:G7:67:SER:HB2 | 2.16 | 0.45 |
| 1:H7:71:MEN:O | 1:H7:77:ARG:HD3 | 2.18 | 0.45 |
| 8:I7:27:LYS:HA | 8:I7:30:VAL:HG22 | 1.99 | 0.45 |
| 8:g7:90:ARG:NH2 | 1:h7:16:GLY:CA | 2.80 | 0.45 |
| 8:U7:134:LYS:O | 8:U7:138:THR:HB | 2.16 | 0.45 |
| 8:a7:95:GLY:CA | 8:a7:104:ILE:HD11 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:b7:76:ARG:HD3 | 8:c7:110:ILE:CD1 | 2.46 | 0.45 |
| 1:d7:76:ARG:NH2 | 9:x7:67:VAL:HG11 | 2.32 | 0.45 |
| 8:e7:64:ASP:O | 8:e7:67:SER:HB2 | 2.17 | 0.45 |
| 2:A8:128:ILE:CG2 | 2:A8:132:LYS:HE3 | 2.47 | 0.45 |
| 8:o7:23:LEU:HD13 | 1:p7:38:VAL:O | 2.17 | 0.45 |
| 8:s7:95:GLY:CA | 8:s7:104:ILE:HD11 | 2.47 | 0.45 |
| 8:u7:23:LEU:HD13 | 1:v7:38:VAL:O | 2.17 | 0.45 |
| 8:u7:37:LEU:HD23 | 8:u7:37:LEU:HA | 1.59 | 0.45 |
| 2:X8:61:ASN:HA | 3:T9:29:ASN:ND2 | 2.31 | 0.45 |
| 12:H8:201:CYC:OB | 11:a9:129:ASN:CG | 2.58 | 0.45 |
| 2:I8:128:ILE:CG2 | 2:I8:132:LYS:HE3 | 2.47 | 0.45 |
| 4:M8:96:LYS:H | 4:M8:96:LYS:HG2 | 1.58 | 0.45 |
| 4:M8:129:GLU:HA | 4:M8:142:PHE:CZ | 2.52 | 0.45 |
| 4:M8:268:ARG:HH12 | 3:Y8:112:GLY:N | 2.14 | 0.45 |
| 3:O8:107:ASP:OD1 | 5:Z8:66:ARG:CZ | 2.65 | 0.45 |
| 2:P8:38:MET:HE2 | 2:P8:38:MET:HB3 | 1.81 | 0.45 |
| 3:Q8:37:ARG:NH1 | 3:Q8:97:LEU:O | 2.42 | 0.45 |
| 5:N9:37:HIS:O | 5:N9:37:HIS:CD2 | 2.70 | 0.45 |
| 2:Q9:128:ILE:HG22 | 2:Q9:132:LYS:HE3 | 1.98 | 0.45 |
| 5:Z8:41:GLN:O | 12:Z8:301:CYC:HMA2 | 1.90 | 0.45 |
| 2:A9:19:LEU:O | 3:B9:45:THR:CG2 | 2.64 | 0.45 |
| 12:A9:201:CYC:O2A | 3:D9:67:ILE:HD12 | 2.17 | 0.45 |
| 3:X9:88:ILE:HG21 | 12:X9:201:CYC:CAB | 2.46 | 0.45 |
| 11:a9:328:GLN:CA | 11:a9:328:GLN:HE21 | 2.30 | 0.45 |
| 11:a9:615:ARG:HA | 11:a9:616:PRO:HD2 | 1.32 | 0.45 |
| 11:a9:643:LEU:HD13 | 11:a9:766:ASN:CG | 2.42 | 0.45 |
| 3:H1:67:ILE:HD12 | 12:I1:201:CYC:O2A | 2.17 | 0.45 |
| 4:M1:52:LEU:HD22 | 4:M1:52:LEU:O | 2.17 | 0.45 |
| 2:A2:34:ALA:CB | 3:B2:31:VAL:HG11 | 2.39 | 0.45 |
| 3:D2:88:ILE:HG21 | 12:D2:201:CYC:CAB | 2.46 | 0.45 |
| 2:CA:128:ILE:CG2 | 2:CA:132:LYS:HE3 | 2.47 | 0.44 |
| 3:FA:84:ARG:CZ | 4:MA:53:LEU:HD22 | 2.47 | 0.44 |
| 2:GA:128:ILE:CG2 | 2:GA:132:LYS:HE3 | 2.47 | 0.44 |
| 4:MA:29:PRO:HG3 | 11:aA:378:GLU:HG3 | 1.99 | 0.44 |
| 4:MA:185:ALA:HB1 | 12:VA:201:CYC:CGA | 2.42 | 0.44 |
| 4:MA:235:PHE:CD1 | 4:MA:235:PHE:O | 2.70 | 0.44 |
| 2:QA:33:ARG:CD | 12:VA:202:CYC:HBB3 | 2.43 | 0.44 |
| 12:QA:201:CYC:CGA | 3:TA:67:ILE:HD13 | 2.47 | 0.44 |
| 12:TA:301:CYC:HC | 12:TA:301:CYC:HMD3 | 1.82 | 0.44 |
| 2:O1:38:MET:HE2 | 2:O1:38:MET:HB3 | 1.81 | 0.44 |
| 12:P1:201:CYC:HC | 12:P1:201:CYC:HMD3 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:A1:19:LEU:O | 3:B1:45:THR:CG2 | 2.64 | 0.44 |
| 12:J2:201:CYC:CMD | 12:J2:201:CYC:NC | 2.75 | 0.44 |
| 12:A3:201:CYC:O2A | 3:D3:67:ILE:HD12 | 2.17 | 0.44 |
| 3:B3:88:ILE:HB | 12:B3:202:CYC:HMB2 | 1.99 | 0.44 |
| 3:B3:126:SER:HB2 | 12:B3:202:CYC:HMC2 | 1.98 | 0.44 |
| 12:C3:201:CYC:O2A | 3:F3:67:ILE:HD12 | 2.17 | 0.44 |
| 3:F3:113:LEU:HD13 | 4:M3:38:PRO:HB2 | 1.98 | 0.44 |
| 12:F3:201:CYC:HBB2 | 4:M3:38:PRO:CD | 2.47 | 0.44 |
| 3:B4:120:LEU:HD23 | 4:M4:49:LEU:O | 2.16 | 0.44 |
| 12:C4:201:CYC:O2A | 3:F4:67:ILE:HD12 | 2.17 | 0.44 |
| 3:L3:119:ALA:HB1 | 11:a9:813:PRO:CA | 2.39 | 0.44 |
| 4:M3:74:LEU:HD23 | 4:M3:74:LEU:HA | 1.68 | 0.44 |
| 4:M3:91:VAL:O | 4:M3:218:VAL:HG23 | 2.17 | 0.44 |
| 12:H4:201:CYC:CBA | 11:aA:261:SER:OG | 2.66 | 0.44 |
| 2:I4:128:ILE:CG2 | 2:I4:132:LYS:HE3 | 2.47 | 0.44 |
| 2:N4:34:ALA:HB3 | 3:O4:31:VAL:CG1 | 2.39 | 0.44 |
| 8:K5:17:TYR:CB | 1:L5:45:SER:HB2 | 2.48 | 0.44 |
| 8:K5:71:ASN:CG | 8:K5:121:THR:HA | 2.42 | 0.44 |
| 8:K5:111:GLY:C | 1:J5:75:THR:HB | 2.41 | 0.44 |
| 12:N5:201:CYC:HMD1 | 12:N5:201:CYC:NC | 2.09 | 0.44 |
| 8:C5:134:LYS:O | 8:C5:138:THR:HB | 2.16 | 0.44 |
| 1:D5:74:THR:OG1 | 1:D5:76:ARG:HG2 | 2.17 | 0.44 |
| 8:c5:120:GLN:CG | 1:f5:53:LYS:NZ | 2.78 | 0.44 |
| 1:f5:18:TYR:CG | 10:j5:165:ARG:CG | 2.98 | 0.44 |
| 12:V5:201:CYC:O2D | 10:j5:642:ARG:NH2 | 2.47 | 0.44 |
| 8:W5:116:TYR:CB | 8:W5:123:ILE:HG12 | 2.48 | 0.44 |
| 3:L6:78:ARG:HH22 | 6:M6:70:GLU:HA | 1.82 | 0.44 |
| 6:M6:10:LYS:HB3 | 6:M6:11:VAL:H | 1.58 | 0.44 |
| 8:A7:64:ASP:O | 8:A7:67:SER:HB2 | 2.16 | 0.44 |
| 10:j5:287:ASN:HD22 | 10:j5:287:ASN:HA | 1.55 | 0.44 |
| 10:j5:764:PHE:CD1 | 10:j5:764:PHE:C | 2.94 | 0.44 |
| 10:k5:296:VAL:O | 10:k5:296:VAL:HG12 | 2.14 | 0.44 |
| 10:k5:966:SER:OG | 1:p7:14:VAL:HG13 | 2.16 | 0.44 |
| 8:C7:95:GLY:CA | 8:C7:104:ILE:HD11 | 2.47 | 0.44 |
| 8:k7:134:LYS:O | 8:k7:138:THR:HB | 2.16 | 0.44 |
| 8:a7:90:ARG:NH2 | 1:b7:16:GLY:CA | 2.80 | 0.44 |
| 3:B8:68:ARG:NH2 | 3:U8:68:ARG:NH1 | 2.64 | 0.44 |
| 1:n7:72:MET:HE2 | 1:n7:72:MET:HB3 | 1.87 | 0.44 |
| 8:s7:94:TYR:O | 8:s7:97:VAL:CG2 | 2.65 | 0.44 |
| 8:u7:23:LEU:HA | 1:v7:38:VAL:HG21 | 1.97 | 0.44 |
| 8:u7:30:VAL:HB | 1:v7:31:PHE:HB3 | 1.97 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:u7:80:LEU:HA | 8:u7:80:LEU:HD23 | 1.63 | 0.44 |
| 8:u7:94:TYR:HD1 | 1:v7:19:LEU:HG | 1.79 | 0.44 |
| 3:F8:111:ASN:C | 4:M8:76:ALA:HB1 | 2.42 | 0.44 |
| 12:F8:202:CYC:HC | 12:F8:202:CYC:HMD3 | 1.82 | 0.44 |
| 2:G8:128:ILE:CG2 | 2:G8:132:LYS:HE3 | 2.47 | 0.44 |
| 3:L8:120:LEU:CD1 | 12:a9:901:CYC:CAA | 2.91 | 0.44 |
| 4:M8:153:LYS:O | 4:M8:157:PHE:HB3 | 2.17 | 0.44 |
| 4:M8:231:THR:N | 12:M8:301:CYC:OB | 2.50 | 0.44 |
| 4:M8:261:VAL:HG11 | 4:M8:266:LEU:HD13 | 1.99 | 0.44 |
| 2:N8:128:ILE:CG2 | 2:N8:132:LYS:HE3 | 2.47 | 0.44 |
| 3:Q8:120:LEU:CD1 | 3:Q8:120:LEU:C | 2.89 | 0.44 |
| 2:R8:128:ILE:CG2 | 2:R8:132:LYS:HE3 | 2.47 | 0.44 |
| 3:L9:109:CYS:C | 3:L9:111:ASN:N | 2.71 | 0.44 |
| 4:M9:153:LYS:O | 4:M9:157:PHE:HB3 | 2.17 | 0.44 |
| 4:M9:191:TYR:OH | 2:U9:16:GLY:HA2 | 2.17 | 0.44 |
| 4:M9:258:LYS:HG3 | 3:V9:111:ASN:HD21 | 1.76 | 0.44 |
| 12:O9:201:CYC:O2A | 3:R9:67:ILE:HD12 | 2.17 | 0.44 |
| 3:Y8:101:ASP:C | 3:Y8:103:SER:H | 2.24 | 0.44 |
| 5:Z8:29:HIS:NE2 | 5:Z8:36:THR:CG2 | 2.79 | 0.44 |
| 2:A9:65:TYR:CD1 | 2:G9:65:TYR:CD1 | 3.05 | 0.44 |
| 11:a9:25:GLU:C | 11:a9:27:PHE:N | 2.75 | 0.44 |
| 11:aA:388:VAL:HG12 | 11:aA:392:ILE:HD11 | 1.99 | 0.44 |
| 11:aA:615:ARG:HA | 11:aA:616:PRO:HD2 | 1.32 | 0.44 |
| 4:M1:91:VAL:O | 4:M1:218:VAL:HG23 | 2.17 | 0.44 |
| 3:V1:67:ILE:HD12 | 12:W1:201:CYC:O2A | 2.17 | 0.44 |
| 3:V1:88:ILE:HG21 | 12:V1:201:CYC:CAB | 2.46 | 0.44 |
| 3:X1:88:ILE:HG21 | 12:X1:201:CYC:CAB | 2.46 | 0.44 |
| 1:A:83:ARG:CD | 10:k5:259:PRO:HD3 | 2.47 | 0.44 |
| 3:FA:88:ILE:HG21 | 12:FA:301:CYC:CAB | 2.46 | 0.44 |
| 12:HA:202:CYC:HC | 12:HA:202:CYC:HMD3 | 1.82 | 0.44 |
| 3:JA:19:LEU:CD1 | 3:JA:24:LEU:HD21 | 2.47 | 0.44 |
| 12:JA:202:CYC:HB | 12:JA:202:CYC:CMA | 2.26 | 0.44 |
| 2:KA:18:PHE:CZ | 3:LA:90:LEU:CD2 | 3.00 | 0.44 |
| 2:OA:59:VAL:O | 2:OA:66:LEU:CD1 | 2.62 | 0.44 |
| 3:H3:124:THR:HB | 3:H3:171:ILE:O | 2.18 | 0.44 |
| 12:Z3:201:CYC:HC | 12:Z3:201:CYC:HMD3 | 1.82 | 0.44 |
| 2:O3:31:PHE:CG | 3:P3:34:SER:CB | 3.00 | 0.44 |
| 2:O3:34:ALA:HB3 | 3:P3:31:VAL:CG1 | 2.39 | 0.44 |
| 2:S3:128:ILE:CG2 | 2:S3:132:LYS:HE3 | 2.47 | 0.44 |
| 12:T3:301:CYC:HC | 12:T3:301:CYC:HMD3 | 1.82 | 0.44 |
| 3:S4:67:ILE:HD12 | 12:P4:201:CYC:O2A | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:T4:65:TYR:CD1 | 2:N4:65:TYR:CD1 | 3.05 | 0.44 |
| 12:T4:201:CYC:O2A | 3:Y4:67:ILE:HD12 | 2.17 | 0.44 |
| 12:W4:202:CYC:CMD | 12:W4:202:CYC:NC | 2.75 | 0.44 |
| 12:G4:201:CYC:O2A | 3:L4:67:ILE:HD12 | 2.17 | 0.44 |
| 4:M4:56:MET:SD | 4:M4:66:VAL:HG22 | 2.55 | 0.44 |
| 4:M4:197:ASP:OD1 | 5:Z4:52:ARG:CD | 2.60 | 0.44 |
| 4:M4:232:VAL:HA | 12:M4:301:CYC:C3B | 2.47 | 0.44 |
| 2:N4:19:LEU:O | 3:O4:45:THR:CG2 | 2.64 | 0.44 |
| 2:N4:38:MET:HE2 | 2:N4:38:MET:HB3 | 1.81 | 0.44 |
| 2:P4:128:ILE:CG2 | 2:P4:132:LYS:HE3 | 2.47 | 0.44 |
| 8:C5:26:ILE:HD13 | 8:C5:26:ILE:HG21 | 1.60 | 0.44 |
| 8:E5:80:LEU:HD13 | 12:E5:201:CYC:CHA | 2.47 | 0.44 |
| 1:J5:74:THR:OG1 | 1:J5:76:ARG:HG2 | 2.17 | 0.44 |
| 8:e5:27:LYS:HA | 8:e5:30:VAL:HG22 | 1.99 | 0.44 |
| 8:S5:41:GLN:NE2 | 1:D7:143:PRO:CG | 2.78 | 0.44 |
| 8:W5:17:TYR:CD2 | 1:X5:93:THR:CG2 | 2.92 | 0.44 |
| 3:J6:67:ILE:HD12 | 12:K6:201:CYC:O2A | 2.17 | 0.44 |
| 9:i5:11:ILE:HD11 | 9:i5:28:PHE:CE2 | 2.52 | 0.44 |
| 10:j5:309:LEU:HD13 | 10:j5:342:LEU:CD1 | 2.46 | 0.44 |
| 10:j5:1025:LEU:N | 10:j5:1030:ILE:HG22 | 2.33 | 0.44 |
| 10:k5:379:PHE:O | 10:k5:379:PHE:CG | 2.68 | 0.44 |
| 10:k5:820:HIS:CD2 | 10:k5:820:HIS:O | 2.69 | 0.44 |
| 2:A6:31:PHE:CG | 3:B6:34:SER:CB | 3.00 | 0.44 |
| 2:E6:38:MET:HE2 | 2:E6:38:MET:HB3 | 1.81 | 0.44 |
| 12:D7:201:CYC:CMA | 12:D7:201:CYC:NB | 2.74 | 0.44 |
| 12:N7:201:CYC:CMA | 12:N7:201:CYC:NB | 2.74 | 0.44 |
| 1:b7:52:ILE:HG12 | 1:b7:133:MET:HE3 | 1.98 | 0.44 |
| 3:B8:107:ASP:O | 4:M8:61:ASN:C | 2.61 | 0.44 |
| 3:D8:77:ARG:HD2 | 4:M8:33:LEU:HD11 | 1.98 | 0.44 |
| 8:q7:90:ARG:HB2 | 1:r7:18:TYR:CE1 | 2.52 | 0.44 |
| 9:z7:29:THR:HG22 | 9:z7:30:LYS:N | 2.31 | 0.44 |
| 3:W8:67:ILE:HD12 | 12:X8:201:CYC:O2A | 2.17 | 0.44 |
| 12:M8:301:CYC:C4B | 3:Y8:88:ILE:CG2 | 2.80 | 0.44 |
| 3:O8:88:ILE:HG21 | 12:O8:201:CYC:CAB | 2.46 | 0.44 |
| 3:S8:124:THR:HB | 3:S8:171:ILE:O | 2.18 | 0.44 |
| 4:M9:51:ARG:NH1 | 4:M9:51:ARG:CG | 2.78 | 0.44 |
| 5:N9:38:GLU:HG2 | 5:N9:40:SER:H | 1.81 | 0.44 |
| 5:N9:57:MET:SD | 12:T9:301:CYC:CMA | 3.05 | 0.44 |
| 2:O9:65:TYR:CD1 | 2:U9:65:TYR:CD1 | 3.05 | 0.44 |
| 12:P9:202:CYC:HC | 12:P9:202:CYC:HMD3 | 1.78 | 0.44 |
| 2:A9:128:ILE:CG2 | 2:A9:132:LYS:HE3 | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:R9:201:CYC:HB | 12:R9:201:CYC:CMA | 2.26 | 0.44 |
| 2:G1:128:ILE:CG2 | 2:G1:132:LYS:HE3 | 2.47 | 0.44 |
| 11:a9:67:GLN:C | 11:a9:68:THR:HG23 | 2.42 | 0.44 |
| 11:aA:479:LYS:HB3 | 11:aA:479:LYS:HE2 | 1.68 | 0.44 |
| 11:aA:712:ASN:CG | 3:L1:108:ARG:O | 2.52 | 0.44 |
| 11:aA:809:ARG:HG3 | 11:aA:810:GLN:H | 1.82 | 0.44 |
| 3:Z1:124:THR:HB | 3:Z1:171:ILE:O | 2.18 | 0.44 |
| 12:C2:201:CYC:O2A | 3:F2:67:ILE:HD12 | 2.17 | 0.44 |
| 12:D2:202:CYC:CMD | 12:D2:202:CYC:NC | 2.75 | 0.44 |
| 1:A:16:GLY:CA | 8:a5:90:ARG:NH1 | 2.72 | 0.44 |
| 1:Z:13:ASP:OD2 | 8:e5:107:ILE:CG1 | 2.62 | 0.44 |
| 1:Z:73:TYR:OH | 10:j5:162:TRP:CE2 | 2.71 | 0.44 |
| 3:BA:14:LEU:HD11 | 3:XA:125:ARG:HD3 | 1.99 | 0.44 |
| 3:FA:144:SER:O | 3:FA:144:SER:OG | 2.30 | 0.44 |
| 3:JA:88:ILE:HG12 | 11:aA:512:TYR:CZ | 2.52 | 0.44 |
| 4:MA:153:LYS:O | 4:MA:157:PHE:HB3 | 2.17 | 0.44 |
| 4:MA:252:LEU:CD1 | 3:ZA:77:ARG:NH1 | 2.80 | 0.44 |
| 2:OA:24:LEU:HB3 | 12:PA:202:CYC:HAB2 | 2.00 | 0.44 |
| 2:SA:38:MET:HE2 | 2:SA:38:MET:HB3 | 1.81 | 0.44 |
| 12:TA:302:CYC:CMD | 12:TA:302:CYC:NC | 2.75 | 0.44 |
| 2:WA:128:ILE:CG2 | 2:WA:132:LYS:HE3 | 2.47 | 0.44 |
| 2:O1:128:ILE:CG2 | 2:O1:132:LYS:HE3 | 2.47 | 0.44 |
| 2:S1:128:ILE:CG2 | 2:S1:132:LYS:HE3 | 2.47 | 0.44 |
| 2:I3:128:ILE:CG2 | 2:I3:132:LYS:HE3 | 2.47 | 0.44 |
| 3:H2:67:ILE:HD12 | 12:I2:201:CYC:O2A | 2.17 | 0.44 |
| 2:I2:76:ASP:OD2 | 11:aA:298:ILE:HG12 | 2.17 | 0.44 |
| 2:I2:128:ILE:CG2 | 2:I2:132:LYS:HE3 | 2.47 | 0.44 |
| 6:M2:26:PHE:C | 8:O5:83:ARG:HD2 | 2.42 | 0.44 |
| 6:M2:127:SER:HB3 | 3:F2:84:ARG:NE | 2.19 | 0.44 |
| 7:N2:17:LYS:HB3 | 7:N2:66:GLU:HB2 | 1.99 | 0.44 |
| 2:Q3:128:ILE:CG2 | 2:Q3:132:LYS:HE3 | 2.47 | 0.44 |
| 2:S3:128:ILE:HG22 | 2:S3:132:LYS:HE3 | 1.98 | 0.44 |
| 3:V3:124:THR:HB | 3:V3:171:ILE:O | 2.18 | 0.44 |
| 2:W3:128:ILE:CG2 | 2:W3:132:LYS:HE3 | 2.47 | 0.44 |
| 12:W4:201:CYC:HC | 12:W4:201:CYC:HMD3 | 1.82 | 0.44 |
| 4:M4:93:LEU:HA | 4:M4:93:LEU:HD12 | 1.65 | 0.44 |
| 4:M4:214:GLY:CA | 5:Z4:27:ALA:C | 2.73 | 0.44 |
| 4:M4:267:LEU:HD23 | 4:M4:267:LEU:HA | 1.65 | 0.44 |
| 3:Q4:77:ARG:HG2 | 5:Z4:36:THR:HB | 1.99 | 0.44 |
| 3:Q4:127:VAL:HG22 | 12:Z4:301:CYC:CMC | 2.47 | 0.44 |
| 8:M5:21:GLY:H | 8:A5:6:LYS:NZ | 2.12 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:O5:94:TYR:O | 8:O5:97:VAL:CG2 | 2.65 | 0.44 |
| 3:Y4:87:GLU:CD | 3:Y4:91:ARG:NH1 | 2.76 | 0.44 |
| 8:C5:37:LEU:HD11 | 1:D5:31:PHE:HE2 | 1.82 | 0.44 |
| 8:C5:95:GLY:CA | 8:C5:104:ILE:HD11 | 2.47 | 0.44 |
| 8:C5:102:THR:CB | 8:C5:103:PRO:HD3 | 2.33 | 0.44 |
| 1:H5:2:GLN:OE1 | 10:j5:551:MET:CE | 2.62 | 0.44 |
| 12:J5:201:CYC:HMD1 | 12:J5:201:CYC:NC | 2.09 | 0.44 |
| 1:P5:110:ASN:OD1 | 10:k5:489:ASN:O | 2.35 | 0.44 |
| 8:S5:134:LYS:O | 8:S5:138:THR:HB | 2.16 | 0.44 |
| 8:Y5:90:ARG:HB2 | 1:Z5:18:TYR:CE1 | 2.53 | 0.44 |
| 6:M6:243:ALA:HA | 12:H6:201:CYC:HBB2 | 1.94 | 0.44 |
| 9:z5:9:ALA:CA | 9:z5:50:LYS:O | 2.63 | 0.44 |
| 9:z5:16:ARG:HE | 9:z5:16:ARG:HA | 1.82 | 0.44 |
| 10:j5:388:ARG:HA | 10:j5:394:PRO:CG | 2.46 | 0.44 |
| 10:k5:322:LYS:NZ | 10:k5:336:ARG:NH1 | 2.66 | 0.44 |
| 10:k5:544:VAL:HG13 | 10:k5:564:VAL:CG2 | 2.48 | 0.44 |
| 10:k5:630:ILE:O | 10:k5:630:ILE:HG22 | 2.14 | 0.44 |
| 10:k5:1067:LEU:CD1 | 10:k5:1101:GLU:CD | 2.90 | 0.44 |
| 8:O7:134:LYS:O | 8:O7:138:THR:HB | 2.16 | 0.44 |
| 8:S7:25:ARG:NH2 | 8:G7:25:ARG:CZ | 2.80 | 0.44 |
| 1:B7:71:MEN:O | 1:B7:77:ARG:HD3 | 2.18 | 0.44 |
| 8:C7:134:LYS:O | 8:C7:138:THR:HB | 2.16 | 0.44 |
| 8:E7:116:TYR:CB | 8:E7:123:ILE:HG12 | 2.47 | 0.44 |
| 8:I7:6:LYS:HZ3 | 8:W7:22:GLU:H | 1.64 | 0.44 |
| 8:I7:94:TYR:O | 8:I7:97:VAL:CG2 | 2.65 | 0.44 |
| 1:L7:72:MET:HE2 | 1:L7:72:MET:HB3 | 1.87 | 0.44 |
| 8:g7:95:GLY:CA | 8:g7:104:ILE:HD11 | 2.47 | 0.44 |
| 8:k7:67:SER:HB3 | 8:k7:68:PRO:HD2 | 1.99 | 0.44 |
| 8:U7:15:ALA:HA | 1:V7:90:ARG:CZ | 2.47 | 0.44 |
| 8:W7:116:TYR:CB | 8:W7:123:ILE:HG12 | 2.47 | 0.44 |
| 8:a7:94:TYR:O | 8:a7:97:VAL:CG2 | 2.65 | 0.44 |
| 8:c7:12:ASP:CA | 1:d7:94:TYR:OH | 2.65 | 0.44 |
| 8:c7:92:VAL:CG2 | 8:c7:156:LEU:HG | 2.47 | 0.44 |
| 8:e7:106:GLU:OE2 | 9:y7:68:GLY:O | 2.35 | 0.44 |
| 12:f7:201:CYC:CMA | 12:f7:201:CYC:NB | 2.74 | 0.44 |
| 12:B8:202:CYC:HMA2 | 4:M8:58:TYR:CA | 2.39 | 0.44 |
| 12:B8:202:CYC:HMD3 | 12:B8:202:CYC:HC | 1.82 | 0.44 |
| 8:o7:8:ILE:O | 8:o7:11:ALA:N | 2.51 | 0.44 |
| 12:v7:201:CYC:CMA | 12:v7:201:CYC:NB | 2.74 | 0.44 |
| 2:T8:65:TYR:CD1 | 2:N8:65:TYR:CD1 | 3.05 | 0.44 |
| 3:H8:81:ALA:HA | 3:H8:84:ARG:NH2 | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:O8:107:ASP:HB3 | 5:Z8:66:ARG:HA | 2.00 | 0.44 |
| 3:O8:112:GLY:HA2 | 5:Z8:69:GLU:CA | 2.44 | 0.44 |
| 3:Q8:1:MET:SD | 3:Q8:104:VAL:HB | 2.58 | 0.44 |
| 4:M9:160:THR:HA | 3:V9:107:ASP:O | 2.18 | 0.44 |
| 4:M9:192:GLN:HE22 | 3:V9:87:GLU:HB3 | 1.82 | 0.44 |
| 3:P9:124:THR:HB | 3:P9:171:ILE:O | 2.18 | 0.44 |
| 3:Y8:92:TYR:CD1 | 3:Y8:105:LEU:HD22 | 2.52 | 0.44 |
| 2:A9:2:LYS:NZ | 2:K9:17:ARG:NH2 | 2.65 | 0.44 |
| 3:B9:14:LEU:HD11 | 3:X9:125:ARG:HD3 | 1.99 | 0.44 |
| 2:E9:99:ALA:HB2 | 3:F9:9:ILE:HD13 | 2.00 | 0.44 |
| 3:J9:116:THR:CG2 | 11:a9:521:PHE:CD2 | 2.87 | 0.44 |
| 11:a9:93:LEU:HD13 | 11:a9:93:LEU:H | 1.81 | 0.44 |
| 11:a9:245:ALA:CA | 12:a9:901:CYC:HBB3 | 2.43 | 0.44 |
| 11:a9:332:SER:H | 11:a9:333:GLN:HE21 | 1.64 | 0.44 |
| 11:a9:368:ILE:HG21 | 11:a9:368:ILE:HD13 | 1.68 | 0.44 |
| 11:a9:611:GLY:HA3 | 11:a9:614:SER:HB3 | 2.00 | 0.44 |
| 11:aA:337:GLU:CG | 11:aA:339:GLU:HG2 | 2.47 | 0.44 |
| 11:aA:346:TYR:CD1 | 11:aA:346:TYR:O | 2.70 | 0.44 |
| 11:aA:495:TYR:CD1 | 11:aA:495:TYR:O | 2.70 | 0.44 |
| 11:aA:548:LEU:O | 11:aA:552:LEU:HB2 | 2.17 | 0.44 |
| 11:aA:642:GLU:HG3 | 11:aA:643:LEU:N | 2.29 | 0.44 |
| 11:aA:643:LEU:CD1 | 11:aA:766:ASN:O | 2.65 | 0.44 |
| 11:aA:787:ARG:NH2 | 11:aA:819:SER:HB3 | 2.27 | 0.44 |
| 3:H1:81:ALA:HB3 | 12:H1:201:CYC:HMD1 | 1.98 | 0.44 |
| 5:N1:13:SER:HB3 | 5:N1:14:LYS:H | 1.55 | 0.44 |
| 12:FA:301:CYC:HC | 12:FA:301:CYC:HMD3 | 1.83 | 0.44 |
| 3:HA:84:ARG:NH1 | 11:aA:475:ASN:OD1 | 2.50 | 0.44 |
| 3:JA:67:ILE:HD12 | 12:KA:201:CYC:O2A | 2.17 | 0.44 |
| 4:MA:56:MET:HE2 | 4:MA:56:MET:HB3 | 1.75 | 0.44 |
| 3:VA:124:THR:HB | 3:VA:171:ILE:O | 2.18 | 0.44 |
| 3:XA:67:ILE:HD12 | 12:YA:201:CYC:O2A | 2.17 | 0.44 |
| 2:G3:38:MET:HE2 | 2:G3:38:MET:HB3 | 1.81 | 0.44 |
| 3:J3:77:ARG:NH2 | 2:K3:106:ASP:C | 2.76 | 0.44 |
| 3:J3:81:ALA:HA | 11:a9:668:TYR:CG | 2.53 | 0.44 |
| 6:M2:127:SER:O | 12:F2:201:CYC:CAA | 2.61 | 0.44 |
| 7:N2:45:LEU:HD21 | 12:N2:101:CYC:O1D | 2.18 | 0.44 |
| 2:A3:128:ILE:HG22 | 2:A3:132:LYS:HE3 | 1.98 | 0.44 |
| 3:B3:67:ILE:HD12 | 12:E3:201:CYC:O2A | 2.17 | 0.44 |
| 5:N3:39:PRO:HD2 | 12:T3:301:CYC:HBB2 | 1.99 | 0.44 |
| 3:P3:65:ASP:OD1 | 3:P3:65:ASP:N | 2.47 | 0.44 |
| 2:Q3:128:ILE:HG22 | 2:Q3:132:LYS:HE3 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:V3:88:ILE:HG21 | 12:V3:201:CYC:CAB | 2.46 | 0.44 |
| 2:E4:128:ILE:HG22 | 2:E4:132:LYS:HE3 | 1.98 | 0.44 |
| 3:F4:2:GLN:HA | 3:F4:6:THR:HG21 | 2.00 | 0.44 |
| 5:Z4:1:MET:CE | 5:Z4:1:MET:CA | 2.85 | 0.44 |
| 5:Z4:26:LEU:HD11 | 5:Z4:63:ASN:HB2 | 1.99 | 0.44 |
| 1:D5:73:TYR:CE1 | 12:E5:201:CYC:HBB2 | 2.53 | 0.44 |
| 8:e5:95:GLY:CA | 8:e5:104:ILE:HD11 | 2.47 | 0.44 |
| 1:P5:114:GLU:CG | 10:k5:496:GLU:CB | 2.72 | 0.44 |
| 8:U5:95:GLY:CA | 8:U5:104:ILE:HD11 | 2.47 | 0.44 |
| 6:M6:283:VAL:HG22 | 6:M6:284:SER:H | 1.81 | 0.44 |
| 7:N6:1:MET:CE | 7:N6:1:MET:H3 | 2.30 | 0.44 |
| 10:j5:56:ILE:HD11 | 10:j5:219:ASP:HB3 | 1.88 | 0.44 |
| 10:j5:152:ARG:CZ | 10:j5:193:SER:HB2 | 2.44 | 0.44 |
| 10:j5:851:HIS:ND1 | 10:j5:851:HIS:O | 2.51 | 0.44 |
| 10:k5:21:MET:HE3 | 10:k5:25:ILE:HD11 | 2.00 | 0.44 |
| 10:k5:222:LEU:HA | 10:k5:222:LEU:HD23 | 1.51 | 0.44 |
| 10:k5:305:PHE:HE2 | 10:k5:337:LEU:HD23 | 1.83 | 0.44 |
| 12:k5:1203:CYC:CMA | 12:k5:1203:CYC:NB | 2.74 | 0.44 |
| 2:C6:128:ILE:CG2 | 2:C6:132:LYS:HE3 | 2.47 | 0.44 |
| 12:D6:201:CYC:HC | 12:D6:201:CYC:HMD3 | 1.83 | 0.44 |
| 8:Q7:13:ALA:HB2 | 9:z7:46:LYS:HD3 | 2.00 | 0.44 |
| 8:Q7:67:SER:HB3 | 8:Q7:68:PRO:HD2 | 2.00 | 0.44 |
| 8:G7:120:GLN:CD | 1:L7:53:LYS:HZ2 | 2.26 | 0.44 |
| 8:g7:115:MET:CE | 1:f7:75:THR:HG22 | 2.48 | 0.44 |
| 12:X7:201:CYC:HMD1 | 12:X7:201:CYC:NC | 2.09 | 0.44 |
| 1:Z7:67:ARG:NH2 | 11:a9:307:ARG:CB | 2.28 | 0.44 |
| 1:b7:75:THR:HG21 | 8:c7:112:VAL:CB | 2.48 | 0.44 |
| 8:c7:43:LEU:CD1 | 8:c7:141:LEU:HD11 | 2.31 | 0.44 |
| 2:E1:128:ILE:CG2 | 2:E1:132:LYS:HE3 | 2.47 | 0.44 |
| 8:m7:94:TYR:O | 8:m7:97:VAL:CG2 | 2.65 | 0.44 |
| 8:o7:30:VAL:HB | 1:p7:31:PHE:CB | 2.48 | 0.44 |
| 8:o7:42:THR:HG21 | 8:o7:141:LEU:CD2 | 2.47 | 0.44 |
| 9:x7:63:ALA:HB1 | 9:x7:64:ASN:H | 1.42 | 0.44 |
| 12:G8:201:CYC:O2A | 3:L8:67:ILE:HD12 | 2.17 | 0.44 |
| 4:M9:29:PRO:HG3 | 11:a9:378:GLU:HG3 | 1.99 | 0.44 |
| 3:Y8:87:GLU:CD | 3:Y8:91:ARG:CZ | 2.90 | 0.44 |
| 11:a9:107:ARG:CB | 11:a9:108:PRO:HD2 | 2.35 | 0.44 |
| 11:a9:346:TYR:CD1 | 11:a9:346:TYR:O | 2.70 | 0.44 |
| 11:a9:462:ARG:CG | 11:a9:462:ARG:NH1 | 2.71 | 0.44 |
| 11:aA:30:MET:HE3 | 11:aA:35:ARG:CD | 2.44 | 0.44 |
| 11:aA:91:THR:C | 11:aA:92:LYS:HE3 | 2.40 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:aA:426:ARG:HD2 | 11:aA:490:ILE:HG23 | 1.99 | 0.44 |
| 12:A2:201:CYC:O2A | 3:D2:67:ILE:HD12 | 2.17 | 0.44 |
| 2:AA:99:ALA:HB2 | 3:BA:9:ILE:HD13 | 2.00 | 0.44 |
| 2:AA:128:ILE:HG22 | 2:AA:132:LYS:HE3 | 1.98 | 0.44 |
| 2:AA:152:ALA:HB1 | 2:KA:21:ASN:HB2 | 1.99 | 0.44 |
| 12:AA:201:CYC:O2A | 3:DA:67:ILE:HD12 | 2.17 | 0.44 |
| 2:KA:128:ILE:CG2 | 2:KA:132:LYS:HE3 | 2.47 | 0.44 |
| 3:LA:83:LEU:HD23 | 3:LA:83:LEU:HA | 1.53 | 0.44 |
| 4:MA:51:ARG:HH11 | 4:MA:51:ARG:CG | 2.27 | 0.44 |
| 4:MA:52:LEU:HD22 | 4:MA:52:LEU:O | 2.17 | 0.44 |
| 2:QA:38:MET:HE2 | 2:QA:38:MET:HB3 | 1.81 | 0.44 |
| 2:QA:81:LYS:HZ1 | 3:TA:67:ILE:HD13 | 1.82 | 0.44 |
| 3:J3:124:THR:HB | 3:J3:171:ILE:O | 2.18 | 0.44 |
| 12:J3:202:CYC:HBA1 | 11:a9:667:THR:N | 2.33 | 0.44 |
| 12:G2:201:CYC:O2A | 3:L2:67:ILE:HD12 | 2.17 | 0.44 |
| 7:N2:4:ASN:OD1 | 3:F2:108:ARG:HB3 | 2.17 | 0.44 |
| 3:D3:68:ARG:CZ | 3:X3:68:ARG:HH12 | 2.31 | 0.44 |
| 2:A4:31:PHE:CG | 3:B4:34:SER:CB | 3.00 | 0.44 |
| 2:C4:99:ALA:HB2 | 3:D4:9:ILE:HD13 | 2.00 | 0.44 |
| 12:D4:202:CYC:HC | 12:D4:202:CYC:HMD3 | 1.83 | 0.44 |
| 4:M3:132:LEU:CD1 | 4:M3:142:PHE:CB | 2.95 | 0.44 |
| 5:N3:6:GLY:N | 3:P3:111:ASN:O | 2.50 | 0.44 |
| 12:S4:202:CYC:HC | 12:S4:202:CYC:HMD3 | 1.82 | 0.44 |
| 3:W4:67:ILE:HD12 | 12:X4:201:CYC:O2A | 2.17 | 0.44 |
| 3:L4:63:GLN:C | 3:L4:65:ASP:O | 2.60 | 0.44 |
| 3:O4:112:GLY:HA2 | 5:Z4:69:GLU:HA | 1.98 | 0.44 |
| 2:P4:19:LEU:CD2 | 3:Q4:95:TYR:CZ | 2.98 | 0.44 |
| 8:O5:23:LEU:HD22 | 1:P5:38:VAL:HG13 | 2.00 | 0.44 |
| 3:Y4:85:ASP:O | 3:Y4:88:ILE:CG1 | 2.65 | 0.44 |
| 3:Y4:131:VAL:HA | 3:Y4:134:MET:HE2 | 1.98 | 0.44 |
| 8:A5:17:TYR:CD2 | 1:B5:45:SER:HB3 | 2.52 | 0.44 |
| 1:B5:71:MEN:O | 1:B5:77:ARG:HD3 | 2.18 | 0.44 |
| 8:C5:16:ARG:HH11 | 8:C5:16:ARG:HG2 | 1.82 | 0.44 |
| 8:G5:67:SER:HB3 | 8:G5:68:PRO:HD2 | 2.00 | 0.44 |
| 8:I5:67:SER:HB3 | 8:I5:68:PRO:HD2 | 2.00 | 0.44 |
| 8:Q5:158:GLY:O | 8:Q5:161:GLN:C | 2.61 | 0.44 |
| 1:R5:71:MEN:O | 1:R5:77:ARG:HD3 | 2.18 | 0.44 |
| 1:R5:106:GLU:HG3 | 10:k5:505:VAL:CG2 | 2.47 | 0.44 |
| 8:S5:105:GLU:OE1 | 10:j5:532:THR:HG22 | 2.17 | 0.44 |
| 8:U5:94:TYR:O | 8:U5:97:VAL:CG2 | 2.65 | 0.44 |
| 8:a5:5:THR:C | 8:a5:7:ALA:H | 2.25 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:j5:292:GLU:CD | 10:j5:292:GLU:N | 2.74 | 0.44 |
| 10:j5:292:GLU:OE1 | 10:j5:292:GLU:CA | 2.66 | 0.44 |
| 10:j5:393:MET:HA | 10:j5:394:PRO:HD3 | 1.68 | 0.44 |
| 10:j5:764:PHE:CD1 | 10:j5:764:PHE:O | 2.70 | 0.44 |
| 10:j5:1050:PHE:CD1 | 10:j5:1050:PHE:O | 2.70 | 0.44 |
| 10:k5:540:LEU:HD21 | 10:k5:544:VAL:HG21 | 2.00 | 0.44 |
| 10:k5:1006:ASP:CG | 10:k5:1065:HIS:HE2 | 2.24 | 0.44 |
| 10:k5:1017:ARG:O | 10:k5:1018:LEU:HD23 | 2.17 | 0.44 |
| 10:k5:1081:VAL:HG11 | 12:k5:1203:CYC:HB | 1.82 | 0.44 |
| 12:A6:201:CYC:O2A | 3:D6:67:ILE:HD12 | 2.17 | 0.44 |
| 1:P7:72:MET:HE2 | 1:P7:72:MET:HB3 | 1.86 | 0.44 |
| 8:I7:15:ALA:HA | 1:J7:90:ARG:CZ | 2.47 | 0.44 |
| 8:M7:90:ARG:HB2 | 1:N7:18:TYR:CE1 | 2.53 | 0.44 |
| 1:h7:71:MEN:O | 1:h7:77:ARG:HD3 | 2.18 | 0.44 |
| 8:k7:64:ASP:O | 8:k7:67:SER:HB2 | 2.17 | 0.44 |
| 8:k7:90:ARG:HB2 | 1:l7:18:TYR:CE1 | 2.52 | 0.44 |
| 8:U7:94:TYR:O | 8:U7:97:VAL:CG2 | 2.65 | 0.44 |
| 1:b7:46:SER:HB2 | 8:o7:157:VAL:HG12 | 1.99 | 0.44 |
| 8:m7:37:LEU:HD23 | 8:m7:97:VAL:HG12 | 2.00 | 0.44 |
| 8:o7:23:LEU:HD13 | 1:p7:38:VAL:HG13 | 1.73 | 0.44 |
| 8:o7:47:ARG:CD | 8:o7:47:ARG:C | 2.89 | 0.44 |
| 8:o7:116:TYR:CB | 8:o7:123:ILE:HG12 | 2.48 | 0.44 |
| 8:s7:15:ALA:HA | 1:t7:90:ARG:CZ | 2.47 | 0.44 |
| 8:u7:67:SER:HB3 | 8:u7:68:PRO:HD2 | 2.00 | 0.44 |
| 3:U8:67:ILE:HD12 | 12:V8:201:CYC:O2A | 2.17 | 0.44 |
| 3:H8:124:THR:HB | 3:H8:171:ILE:O | 2.18 | 0.44 |
| 3:J8:124:THR:HB | 3:J8:171:ILE:O | 2.18 | 0.44 |
| 12:M8:302:CYC:C2D | 3:S8:77:ARG:HH12 | 2.30 | 0.44 |
| 2:N8:24:LEU:HB3 | 12:O8:202:CYC:HAB2 | 2.00 | 0.44 |
| 12:F1:201:CYC:HBB2 | 4:M1:38:PRO:CD | 2.46 | 0.44 |
| 4:M9:200:ILE:HD13 | 4:M9:200:ILE:HA | 1.54 | 0.44 |
| 4:M9:252:LEU:CD1 | 3:Z9:77:ARG:NH1 | 2.81 | 0.44 |
| 2:O9:31:PHE:CG | 3:P9:34:SER:CB | 3.00 | 0.44 |
| 5:Z8:22:LEU:O | 5:Z8:37:HIS:CE1 | 2.70 | 0.44 |
| 5:Z8:41:GLN:CG | 12:Z8:301:CYC:NB | 2.71 | 0.44 |
| 2:A9:31:PHE:CG | 3:B9:34:SER:CB | 3.00 | 0.44 |
| 3:F9:2:GLN:HA | 3:F9:6:THR:HG21 | 2.00 | 0.44 |
| 2:I9:24:LEU:HB3 | 12:J9:201:CYC:CAB | 2.47 | 0.44 |
| 2:U9:128:ILE:CG2 | 2:U9:132:LYS:HE3 | 2.47 | 0.44 |
| 12:V9:201:CYC:HC | 12:V9:201:CYC:HMD3 | 1.83 | 0.44 |
| 11:a9:562:TYR:CD1 | 11:a9:562:TYR:O | 2.71 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:a9:681:LEU:HD23 | 11:a9:684:ASN:HD21 | 1.83 | 0.44 |
| 11:aA:643:LEU:HD21 | 11:aA:689:VAL:HG22 | 1.91 | 0.44 |
| 3:J1:67:ILE:HD12 | 12:K1:201:CYC:O2A | 2.17 | 0.44 |
| 2:K1:38:MET:HE2 | 2:K1:38:MET:HB3 | 1.81 | 0.44 |
| 12:U1:201:CYC:O2A | 3:Z1:67:ILE:HD12 | 2.17 | 0.44 |
| 3:BA:14:LEU:HD13 | 3:XA:125:ARG:CD | 2.47 | 0.44 |
| 3:BA:124:THR:HB | 3:BA:171:ILE:O | 2.18 | 0.44 |
| 3:DA:2:GLN:HA | 3:DA:6:THR:HG21 | 2.00 | 0.44 |
| 3:FA:124:THR:HB | 3:FA:171:ILE:O | 2.18 | 0.44 |
| 3:FA:125:ARG:CD | 3:VA:14:LEU:HD11 | 2.47 | 0.44 |
| 4:MA:93:LEU:HD12 | 4:MA:93:LEU:HA | 1.66 | 0.44 |
| 4:MA:160:THR:HA | 3:VA:107:ASP:O | 2.18 | 0.44 |
| 4:MA:191:TYR:OH | 2:UA:16:GLY:HA2 | 2.17 | 0.44 |
| 5:NA:1:MET:HB2 | 5:NA:3:VAL:HG23 | 1.91 | 0.44 |
| 2:OA:99:ALA:HB2 | 3:PA:9:ILE:HD13 | 2.00 | 0.44 |
| 3:PA:124:THR:HB | 3:PA:171:ILE:O | 2.18 | 0.44 |
| 2:QA:18:PHE:CE2 | 3:RA:48:ALA:HB2 | 2.52 | 0.44 |
| 2:G3:106:ASP:C | 3:L3:77:ARG:NH2 | 2.76 | 0.44 |
| 3:H3:67:ILE:HD12 | 12:I3:201:CYC:O2A | 2.17 | 0.44 |
| 2:G2:128:ILE:CG2 | 2:G2:132:LYS:HE3 | 2.47 | 0.44 |
| 3:B3:84:ARG:CZ | 12:B3:202:CYC:O2A | 2.66 | 0.44 |
| 3:F3:2:GLN:HA | 3:F3:6:THR:HG21 | 2.00 | 0.44 |
| 12:F3:201:CYC:HC | 12:F3:201:CYC:HMD3 | 1.82 | 0.44 |
| 3:Z3:67:ILE:HD12 | 12:U3:201:CYC:O2A | 2.17 | 0.44 |
| 3:L3:1:MET:HE1 | 11:a9:708:HIS:CE1 | 2.50 | 0.44 |
| 4:M3:133:ARG:HB3 | 12:P3:201:CYC:HBA2 | 1.99 | 0.44 |
| 4:M3:153:LYS:O | 4:M3:157:PHE:HB3 | 2.17 | 0.44 |
| 4:M3:200:ILE:HA | 4:M3:200:ILE:HD13 | 1.54 | 0.44 |
| 3:T3:124:THR:HB | 3:T3:171:ILE:O | 2.18 | 0.44 |
| 12:V3:201:CYC:HC | 12:V3:201:CYC:HMD3 | 1.82 | 0.44 |
| 3:B1:67:ILE:HD12 | 12:E1:201:CYC:O2A | 2.17 | 0.44 |
| 2:V4:128:ILE:HG22 | 2:V4:132:LYS:HE3 | 1.98 | 0.44 |
| 3:H4:67:ILE:HD12 | 12:I4:201:CYC:O2A | 2.17 | 0.44 |
| 12:H4:201:CYC:CBA | 11:aA:261:SER:CB | 2.95 | 0.44 |
| 12:L4:202:CYC:HC | 12:L4:202:CYC:HMD3 | 1.83 | 0.44 |
| 4:M4:110:TYR:HE2 | 4:M4:124:ARG:NH1 | 2.13 | 0.44 |
| 8:M5:25:ARG:HE | 8:A5:25:ARG:HH22 | 1.58 | 0.44 |
| 8:O5:67:SER:HB3 | 8:O5:68:PRO:HD2 | 2.00 | 0.44 |
| 8:A5:50:ILE:HA | 8:A5:136:VAL:HG11 | 1.99 | 0.44 |
| 1:B5:107:ARG:NH1 | 9:z5:21:ARG:CB | 2.81 | 0.44 |
| 1:H5:14:VAL:HG13 | 10:j5:556:GLY:H | 1.81 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:Q5:16:ARG:CA | 1:R5:90:ARG:CD | 2.45 | 0.44 |
| 1:R5:86:ASP:OD1 | 1:R5:90:ARG:NE | 2.51 | 0.44 |
| 1:T5:72:MET:HE2 | 1:T5:72:MET:HB3 | 1.87 | 0.44 |
| 12:T5:201:CYC:HMD1 | 12:T5:201:CYC:NC | 2.10 | 0.44 |
| 1:X5:143:PRO:HB2 | 8:a5:38:ARG:HH11 | 1.76 | 0.44 |
| 1:b5:24:LEU:HB3 | 10:k5:54:ILE:CG2 | 2.47 | 0.44 |
| 1:b5:31:PHE:CZ | 10:k5:50:GLY:HA2 | 2.53 | 0.44 |
| 3:L6:77:ARG:NH2 | 6:M6:70:GLU:HG2 | 2.23 | 0.44 |
| 12:N6:101:CYC:HC | 12:N6:101:CYC:HMD3 | 1.82 | 0.44 |
| 8:A7:67:SER:HB3 | 8:A7:68:PRO:HD2 | 2.00 | 0.44 |
| 9:z5:8:THR:O | 9:z5:51:VAL:HG13 | 2.18 | 0.44 |
| 10:j5:226:TYR:HD1 | 10:j5:226:TYR:HA | 1.55 | 0.44 |
| 10:j5:277:ILE:HG12 | 10:j5:284:PRO:HB3 | 0.62 | 0.44 |
| 10:j5:367:ARG:NH1 | 10:j5:410:GLU:OE1 | 2.51 | 0.44 |
| 10:j5:924:ASP:CG | 1:J7:26:LYS:HZ1 | 2.16 | 0.44 |
| 10:j5:1018:LEU:CA | 10:j5:1021:ALA:HB3 | 2.40 | 0.44 |
| 10:k5:540:LEU:HB2 | 10:k5:567:LEU:HG | 1.99 | 0.44 |
| 10:k5:549:LYS:HB2 | 10:k5:550:GLY:H | 1.47 | 0.44 |
| 10:k5:1024:LYS:HD2 | 10:k5:1038:ARG:NH1 | 2.30 | 0.44 |
| 2:A6:24:LEU:HB3 | 12:B6:201:CYC:HAB2 | 2.00 | 0.44 |
| 3:F6:82:CYS:SG | 12:F6:201:CYC:CHD | 3.06 | 0.44 |
| 2:G6:128:ILE:CG2 | 2:G6:132:LYS:HE3 | 2.47 | 0.44 |
| 8:O7:15:ALA:HA | 1:P7:90:ARG:CZ | 2.47 | 0.44 |
| 8:O7:27:LYS:HA | 8:O7:30:VAL:HG22 | 2.00 | 0.44 |
| 8:g7:37:LEU:HD23 | 8:g7:97:VAL:HG12 | 1.99 | 0.44 |
| 8:g7:94:TYR:O | 8:g7:97:VAL:CG2 | 2.65 | 0.44 |
| 1:V7:71:MEN:O | 1:V7:77:ARG:HD3 | 2.18 | 0.44 |
| 8:Y7:67:SER:HB3 | 8:Y7:68:PRO:HD2 | 1.99 | 0.44 |
| 1:b7:71:MEN:O | 1:b7:77:ARG:HD3 | 2.18 | 0.44 |
| 8:c7:112:VAL:O | 8:c7:115:MET:HB3 | 2.17 | 0.44 |
| 3:D8:124:THR:HB | 3:D8:171:ILE:O | 2.18 | 0.44 |
| 1:l7:71:MEN:O | 1:l7:77:ARG:HD3 | 2.18 | 0.44 |
| 8:m7:27:LYS:HA | 8:m7:30:VAL:HG22 | 1.99 | 0.44 |
| 1:r7:71:MEN:O | 1:r7:77:ARG:HD3 | 2.18 | 0.44 |
| 8:u7:39:ILE:HD11 | 8:u7:145:ASP:CA | 2.47 | 0.44 |
| 3:F8:124:THR:HB | 3:F8:171:ILE:O | 2.18 | 0.44 |
| 3:H8:67:ILE:HD12 | 12:I8:201:CYC:O2A | 2.17 | 0.44 |
| 12:M8:301:CYC:CBC | 3:Y8:127:VAL:HA | 2.42 | 0.44 |
| 3:O8:104:VAL:HG22 | 5:Z8:61:LYS:CE | 2.46 | 0.44 |
| 3:P9:67:ILE:HD12 | 12:S9:201:CYC:O2A | 2.17 | 0.44 |
| 3:Y8:109:CYS:SG | 3:Y8:110:LEU:N | 2.87 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:A9:99:ALA:HB2 | 3:B9:9:ILE:HD13 | 2.00 | 0.44 |
| 3:F9:125:ARG:CD | 3:V9:14:LEU:HD11 | 2.47 | 0.44 |
| 2:I9:128:ILE:CG2 | 2:I9:132:LYS:HE3 | 2.47 | 0.44 |
| 3:J9:19:LEU:HB3 | 3:J9:24:LEU:HG | 1.99 | 0.44 |
| 11:a9:562:TYR:CD1 | 11:a9:562:TYR:C | 2.94 | 0.44 |
| 11:a9:615:ARG:H | 11:a9:615:ARG:HG2 | 1.55 | 0.44 |
| 11:aA:708:HIS:CE1 | 11:aA:709:CYS:SG | 3.10 | 0.44 |
| 11:aA:812:ASP:HA | 11:aA:813:PRO:HD3 | 1.69 | 0.44 |
| 2:K1:115:GLU:OE1 | 2:K1:118:ARG:NH1 | 2.50 | 0.44 |
| 4:M1:137:ILE:HB | 4:M1:141:GLU:HB3 | 1.99 | 0.44 |
| 3:T1:2:GLN:HA | 3:T1:6:THR:HG21 | 2.00 | 0.44 |
| 2:U1:128:ILE:CG2 | 2:U1:132:LYS:HE3 | 2.47 | 0.44 |
| 2:W1:128:ILE:HG22 | 2:W1:132:LYS:HE3 | 1.98 | 0.44 |
| 2:A2:128:ILE:CG2 | 2:A2:132:LYS:HE3 | 2.47 | 0.44 |
| 12:GA:201:CYC:O2A | 3:LA:67:ILE:HD12 | 2.18 | 0.44 |
| 3:HA:67:ILE:HD12 | 12:IA:201:CYC:O2A | 2.17 | 0.44 |
| 2:IA:128:ILE:HG22 | 2:IA:132:LYS:HE3 | 1.98 | 0.44 |
| 3:JA:19:LEU:HB3 | 3:JA:24:LEU:HG | 1.99 | 0.44 |
| 3:LA:124:THR:HB | 3:LA:171:ILE:O | 2.18 | 0.44 |
| 4:MA:95:ALA:HB2 | 5:NA:38:GLU:CD | 2.43 | 0.44 |
| 5:NA:22:LEU:O | 5:NA:37:HIS:CE1 | 2.70 | 0.44 |
| 2:QA:162:SER:HA | 2:WA:118:ARG:HG2 | 1.99 | 0.44 |
| 3:P1:2:GLN:HA | 3:P1:6:THR:HG21 | 2.00 | 0.44 |
| 3:P1:111:ASN:O | 5:N1:6:GLY:N | 2.50 | 0.44 |
| 2:A1:24:LEU:HB3 | 12:B1:201:CYC:HAB2 | 2.00 | 0.44 |
| 2:A1:128:ILE:CG2 | 2:A1:132:LYS:HE3 | 2.47 | 0.44 |
| 12:A1:201:CYC:O2A | 3:D1:67:ILE:HD12 | 2.17 | 0.44 |
| 3:L2:74:TYR:O | 3:L2:74:TYR:CD1 | 2.70 | 0.44 |
| 2:A3:99:ALA:HB2 | 3:B3:9:ILE:HD13 | 2.00 | 0.44 |
| 2:C3:99:ALA:HB2 | 3:D3:9:ILE:HD13 | 2.00 | 0.44 |
| 12:D3:202:CYC:HC | 12:D3:202:CYC:HMD3 | 1.83 | 0.44 |
| 3:B4:124:THR:HB | 3:B4:171:ILE:O | 2.18 | 0.44 |
| 5:N3:38:GLU:HG2 | 5:N3:40:SER:H | 1.81 | 0.44 |
| 2:O3:24:LEU:HB3 | 12:P3:202:CYC:HAB2 | 1.99 | 0.44 |
| 3:L4:2:GLN:HA | 3:L4:6:THR:HG21 | 2.00 | 0.44 |
| 4:M4:205:ASP:OD1 | 4:M4:205:ASP:C | 2.58 | 0.44 |
| 12:M4:301:CYC:HC | 12:M4:301:CYC:HMD3 | 1.82 | 0.44 |
| 1:N5:87:TYR:HH | 10:k5:483:PHE:HE2 | 1.46 | 0.44 |
| 3:Y4:124:THR:O | 3:Y4:172:ALA:HA | 2.17 | 0.44 |
| 8:A5:67:SER:HB3 | 8:A5:68:PRO:HD2 | 2.00 | 0.44 |
| 1:D5:74:THR:HG1 | 1:D5:77:ARG:CD | 2.28 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 8:I5:37:LEU:HD23 | 8:I5:97:VAL:HG12 | 2.00 | 0.44 |
| 1:d5:71:MEN:O | 1:d5:77:ARG:HD3 | 2.18 | 0.44 |
| 12:T5:201:CYC:NB | 10:j5:483:PHE:CE2 | 2.85 | 0.44 |
| 1:V5:123:ILE:HG22 | 10:j5:11:VAL:CG2 | 2.48 | 0.44 |
| 8:W5:158:GLY:O | 8:W5:161:GLN:C | 2.61 | 0.44 |
| 6:M6:278:ARG:HG2 | 1:d7:62:TYR:O | 2.18 | 0.44 |
| 10:j5:199:THR:HG22 | 12:j5:1201:CYC:HBC1 | 1.98 | 0.44 |
| 10:j5:289:SER:HB2 | 10:j5:292:GLU:OE2 | 2.10 | 0.44 |
| 10:j5:364:PHE:CD1 | 10:j5:406:ILE:HD11 | 2.53 | 0.44 |
| 10:j5:756:SER:OG | 9:w7:22:GLU:HA | 2.18 | 0.44 |
| 10:j5:971:VAL:HG12 | 1:t7:76:ARG:HH22 | 1.83 | 0.44 |
| 10:j5:1041:ARG:O | 10:j5:1041:ARG:HG3 | 2.18 | 0.44 |
| 10:j5:1143:LEU:HD23 | 10:j5:1143:LEU:HA | 1.62 | 0.44 |
| 10:k5:886:PHE:N | 10:k5:886:PHE:HD1 | 2.15 | 0.44 |
| 10:k5:947:MET:CE | 10:k5:948:SER:HB3 | 2.47 | 0.44 |
| 10:k5:1025:LEU:N | 10:k5:1030:ILE:HG22 | 2.33 | 0.44 |
| 10:k5:1085:GLY:HA2 | 1:l7:87:TYR:OH | 2.16 | 0.44 |
| 3:B6:67:ILE:HD12 | 12:E6:201:CYC:O2A | 2.17 | 0.44 |
| 2:E6:99:ALA:HB2 | 3:F6:9:ILE:HD13 | 2.00 | 0.44 |
| 12:G6:201:CYC:CMA | 12:G6:201:CYC:NB | 2.81 | 0.44 |
| 2:I6:38:MET:HE2 | 2:I6:38:MET:HB3 | 1.81 | 0.44 |
| 2:I6:128:ILE:CG2 | 2:I6:132:LYS:HE3 | 2.47 | 0.44 |
| 1:D7:71:MEN:O | 1:D7:77:ARG:HD3 | 2.18 | 0.44 |
| 8:I7:95:GLY:CA | 8:I7:104:ILE:HD11 | 2.47 | 0.44 |
| 12:J7:201:CYC:HMD1 | 12:J7:201:CYC:NC | 2.10 | 0.44 |
| 8:K7:116:TYR:CB | 8:K7:123:ILE:HG12 | 2.47 | 0.44 |
| 12:K7:201:CYC:HB | 12:K7:201:CYC:CMA | 2.21 | 0.44 |
| 1:h7:30:TYR:CD2 | 1:h7:30:TYR:O | 2.70 | 0.44 |
| 8:i7:48:GLU:O | 8:i7:52:LYS:HG3 | 2.18 | 0.44 |
| 8:i7:53:GLN:HB2 | 8:i7:136:VAL:CG2 | 2.47 | 0.44 |
| 1:T7:71:MEN:O | 1:T7:77:ARG:HD3 | 2.18 | 0.44 |
| 8:U7:95:GLY:CA | 8:U7:104:ILE:HD11 | 2.47 | 0.44 |
| 1:Z7:75:THR:HG22 | 8:a7:115:MET:CE | 2.48 | 0.44 |
| 8:c7:112:VAL:O | 8:c7:116:TYR:N | 2.41 | 0.44 |
| 1:d7:71:MEN:O | 1:d7:77:ARG:HD3 | 2.18 | 0.44 |
| 2:A8:99:ALA:HB2 | 3:B8:9:ILE:HD13 | 2.00 | 0.44 |
| 3:B8:2:GLN:HA | 3:B8:6:THR:HG21 | 2.00 | 0.44 |
| 8:m7:95:GLY:CA | 8:m7:104:ILE:HD11 | 2.47 | 0.44 |
| 8:o7:16:ARG:N | 1:p7:94:TYR:OH | 2.50 | 0.44 |
| 1:v7:71:MEN:O | 1:v7:77:ARG:HD3 | 2.18 | 0.44 |
| 9:z7:38:PHE:O | 9:z7:38:PHE:CG | 2.68 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:y7:21:ARG:NE | 9:y7:21:ARG:HA | 2.30 | 0.44 |
| 2:T8:128:ILE:CG2 | 2:T8:132:LYS:HE3 | 2.47 | 0.44 |
| 3:U8:124:THR:HB | 3:U8:171:ILE:O | 2.18 | 0.44 |
| 2:X8:68:GLN:CB | 3:T9:25:ASN:OD1 | 2.64 | 0.44 |
| 3:H8:84:ARG:HD3 | 11:a9:131:TYR:CG | 2.13 | 0.44 |
| 3:L8:68:ARG:CG | 11:a9:82:GLN:N | 2.74 | 0.44 |
| 4:M8:52:LEU:HD22 | 4:M8:52:LEU:O | 2.17 | 0.44 |
| 4:M8:87:ILE:HD12 | 3:Y8:77:ARG:HG2 | 1.87 | 0.44 |
| 4:M8:96:LYS:HB2 | 3:Q8:88:ILE:CG2 | 2.48 | 0.44 |
| 4:M8:140:ARG:O | 4:M8:143:VAL:N | 2.50 | 0.44 |
| 4:M8:205:ASP:OD1 | 4:M8:205:ASP:C | 2.59 | 0.44 |
| 4:M8:231:THR:C | 12:M8:301:CYC:CBB | 2.90 | 0.44 |
| 2:N8:99:ALA:HB2 | 3:O8:9:ILE:HD13 | 2.00 | 0.44 |
| 3:O8:124:THR:HB | 3:O8:171:ILE:O | 2.18 | 0.44 |
| 3:Q8:110:LEU:HD13 | 3:Q8:170:SER:CB | 2.46 | 0.44 |
| 3:L9:95:TYR:CD2 | 2:K9:9:ILE:HG23 | 2.53 | 0.44 |
| 4:M9:52:LEU:HD22 | 4:M9:52:LEU:O | 2.17 | 0.44 |
| 4:M9:91:VAL:O | 4:M9:218:VAL:HG23 | 2.17 | 0.44 |
| 4:M9:261:VAL:HG11 | 4:M9:266:LEU:HD13 | 1.99 | 0.44 |
| 12:B9:201:CYC:CMA | 12:B9:201:CYC:HB | 2.25 | 0.44 |
| 3:H9:84:ARG:NH1 | 11:a9:475:ASN:OD1 | 2.50 | 0.44 |
| 3:R9:124:THR:HB | 3:R9:171:ILE:O | 2.18 | 0.44 |
| 3:Z9:124:THR:HB | 3:Z9:171:ILE:O | 2.18 | 0.44 |
| 2:G1:106:ASP:C | 3:L1:77:ARG:NH2 | 2.76 | 0.44 |
| 11:a9:92:LYS:HD3 | 11:a9:92:LYS:HA | 1.54 | 0.44 |
| 11:a9:643:LEU:HD12 | 11:a9:766:ASN:O | 2.18 | 0.44 |
| 11:aA:67:GLN:C | 11:aA:68:THR:HG23 | 2.42 | 0.44 |
| 11:aA:562:TYR:CD1 | 11:aA:562:TYR:O | 2.71 | 0.44 |
| 12:aA:901:CYC:HC | 12:aA:901:CYC:HMD3 | 1.83 | 0.44 |
| 3:H1:2:GLN:HA | 3:H1:6:THR:HG21 | 2.00 | 0.44 |
| 4:M1:19:MET:HE2 | 4:M1:59:ILE:CD1 | 2.46 | 0.44 |
| 3:X1:124:THR:HB | 3:X1:171:ILE:O | 2.18 | 0.44 |
| 12:X1:201:CYC:HC | 12:X1:201:CYC:HMD3 | 1.82 | 0.44 |
| 3:F2:78:ARG:HG2 | 12:F2:201:CYC:CBD | 2.47 | 0.44 |
| 3:F2:126:SER:C | 12:F2:201:CYC:HMC3 | 2.43 | 0.44 |
| 3:F2:130:ALA:CB | 12:F2:201:CYC:HBC2 | 2.47 | 0.44 |
| 12:EA:201:CYC:CMA | 12:EA:201:CYC:NB | 2.81 | 0.44 |
| 3:FA:149:THR:C | 3:F9:150:ARG:HG3 | 2.41 | 0.44 |
| 3:LA:112:GLY:C | 11:aA:532:ALA:CB | 2.79 | 0.44 |
| 4:MA:132:LEU:CD1 | 4:MA:142:PHE:CB | 2.95 | 0.44 |
| 4:MA:192:GLN:HE22 | 3:VA:87:GLU:HB3 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:MA:261:VAL:HG11 | 4:MA:266:LEU:HD13 | 1.99 | 0.44 |
| 5:NA:11:ARG:HD2 | 3:RA:108:ARG:CZ | 2.47 | 0.44 |
| 2:SA:42:ARG:CD | 2:X4:69:PRO:CD | 2.92 | 0.44 |
| 12:ZA:202:CYC:HC | 12:ZA:202:CYC:HMD3 | 1.82 | 0.44 |
| 12:R1:201:CYC:HC | 12:R1:201:CYC:HMD3 | 1.83 | 0.44 |
| 3:B3:2:GLN:HA | 3:B3:6:THR:HG21 | 2.00 | 0.44 |
| 3:B3:127:VAL:HG22 | 12:B3:202:CYC:HMC1 | 1.99 | 0.44 |
| 3:D4:124:THR:HB | 3:D4:171:ILE:O | 2.18 | 0.44 |
| 12:D4:201:CYC:HB | 12:D4:201:CYC:HMA3 | 1.83 | 0.44 |
| 4:M3:70:SER:O | 4:M3:70:SER:OG | 2.35 | 0.44 |
| 5:N3:40:SER:O | 5:N3:40:SER:OG | 2.30 | 0.44 |
| 12:R3:202:CYC:CMD | 12:R3:202:CYC:NC | 2.75 | 0.44 |
| 2:S3:99:ALA:HB2 | 3:T3:9:ILE:HD13 | 2.00 | 0.44 |
| 3:V3:65:ASP:OD1 | 3:V3:65:ASP:N | 2.47 | 0.44 |
| 3:V3:67:ILE:HD12 | 12:W3:201:CYC:O2A | 2.17 | 0.44 |
| 3:B1:124:THR:HB | 3:B1:171:ILE:O | 2.18 | 0.44 |
| 3:S4:124:THR:HB | 3:S4:171:ILE:O | 2.18 | 0.44 |
| 3:U4:67:ILE:HD12 | 12:V4:201:CYC:O2A | 2.17 | 0.44 |
| 3:H4:124:THR:HB | 3:H4:171:ILE:O | 2.18 | 0.44 |
| 4:M4:37:GLU:CD | 11:aA:229:ASN:ND2 | 2.76 | 0.44 |
| 2:N4:24:LEU:HB3 | 12:O4:202:CYC:HAB2 | 2.00 | 0.44 |
| 3:Q4:2:GLN:HA | 3:Q4:6:THR:HG21 | 2.00 | 0.44 |
| 3:Q4:84:ARG:O | 3:Q4:87:GLU:HB3 | 2.18 | 0.44 |
| 8:M5:89:LEU:CB | 1:N5:18:TYR:OH | 2.65 | 0.44 |
| 8:O5:27:LYS:HA | 8:O5:30:VAL:HG22 | 2.00 | 0.44 |
| 3:Y4:112:GLY:O | 3:Y4:113:LEU:C | 2.60 | 0.44 |
| 8:A5:53:GLN:OE1 | 8:A5:53:GLN:HA | 2.17 | 0.44 |
| 1:B5:10:ASN:CG | 10:k5:557:VAL:H | 2.26 | 0.44 |
| 8:C5:37:LEU:HD23 | 8:C5:97:VAL:HG12 | 2.00 | 0.44 |
| 8:C5:94:TYR:O | 8:C5:97:VAL:CG2 | 2.65 | 0.44 |
| 1:P5:71:MEN:O | 1:P5:77:ARG:HD3 | 2.18 | 0.44 |
| 8:U5:29:PHE:CE2 | 1:V5:31:PHE:HE1 | 2.34 | 0.44 |
| 8:a5:95:GLY:CA | 8:a5:104:ILE:HD11 | 2.47 | 0.44 |
| 3:J6:2:GLN:HA | 3:J6:6:THR:HG21 | 2.00 | 0.44 |
| 12:J6:202:CYC:HC | 12:J6:202:CYC:HMD3 | 1.83 | 0.44 |
| 7:N6:4:ASN:OD1 | 3:F6:108:ARG:HB3 | 2.17 | 0.44 |
| 7:N6:45:LEU:HD21 | 12:N6:101:CYC:O1D | 2.18 | 0.44 |
| 10:j5:355:ARG:NH1 | 10:j5:358:GLU:OE1 | 2.48 | 0.44 |
| 10:j5:386:ILE:HG21 | 10:j5:395:SER:O | 2.02 | 0.44 |
| 10:j5:643:VAL:O | 10:j5:643:VAL:HG12 | 2.16 | 0.44 |
| 10:j5:1146:THR:HG21 | 1:v7:71:MEN:HE21 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:k5:328:ILE:HG21 | 10:k5:336:ARG:NH2 | 2.33 | 0.44 |
| 10:k5:364:PHE:CD1 | 10:k5:406:ILE:HD11 | 2.53 | 0.44 |
| 10:k5:739:VAL:O | 10:k5:739:VAL:HG12 | 2.18 | 0.44 |
| 10:k5:823:TYR:O | 1:B7:107:ARG:HD2 | 2.17 | 0.44 |
| 10:k5:955:LEU:HD13 | 8:o7:80:LEU:HD23 | 2.00 | 0.44 |
| 10:k5:1050:PHE:CD1 | 10:k5:1050:PHE:O | 2.70 | 0.44 |
| 10:k5:1058:VAL:O | 10:k5:1062:LEU:HG | 2.18 | 0.44 |
| 3:D6:124:THR:HB | 3:D6:171:ILE:O | 2.18 | 0.44 |
| 3:F6:88:ILE:HG21 | 12:F6:201:CYC:CAB | 2.47 | 0.44 |
| 3:F6:127:VAL:N | 12:F6:201:CYC:CMC | 2.71 | 0.44 |
| 3:H6:77:ARG:NH2 | 12:H6:201:CYC:O1A | 2.51 | 0.44 |
| 3:H6:124:THR:HB | 3:H6:171:ILE:O | 2.18 | 0.44 |
| 12:H6:201:CYC:HC | 12:H6:201:CYC:HMD3 | 1.83 | 0.44 |
| 8:C7:94:TYR:O | 8:C7:97:VAL:CG2 | 2.65 | 0.44 |
| 8:G7:86:ASP:CB | 11:a9:579:PHE:CZ | 2.92 | 0.44 |
| 8:I7:21:GLY:C | 8:I7:23:LEU:N | 2.72 | 0.44 |
| 8:i7:67:SER:HB3 | 8:i7:68:PRO:HD2 | 2.00 | 0.44 |
| 1:j7:76:ARG:NH1 | 9:y7:3:ARG:HH22 | 2.16 | 0.44 |
| 8:U7:37:LEU:HD23 | 8:U7:97:VAL:HG12 | 2.00 | 0.44 |
| 8:m7:15:ALA:HA | 1:n7:90:ARG:CZ | 2.47 | 0.44 |
| 1:p7:68:PRO:O | 11:a9:42:ARG:NE | 2.50 | 0.44 |
| 8:q7:130:VAL:CG1 | 8:q7:157:VAL:HG23 | 2.48 | 0.44 |
| 12:W8:201:CYC:HC | 12:W8:201:CYC:HMD3 | 1.82 | 0.44 |
| 4:M8:201:ASP:HB3 | 5:Z8:59:ARG:HD2 | 1.99 | 0.44 |
| 4:M8:267:LEU:HA | 4:M8:267:LEU:HD23 | 1.65 | 0.44 |
| 3:O8:119:ALA:CB | 5:Z8:72:GLU:N | 2.75 | 0.44 |
| 3:Q8:78:ARG:CD | 12:Z8:301:CYC:HMD2 | 2.46 | 0.44 |
| 3:L9:67:ILE:HD12 | 12:G9:201:CYC:O2A | 2.18 | 0.44 |
| 4:M9:76:ALA:O | 3:D9:115:GLU:OE1 | 2.34 | 0.44 |
| 4:M9:181:GLN:CD | 3:V9:120:LEU:CD2 | 2.78 | 0.44 |
| 5:N9:11:ARG:HD2 | 3:R9:108:ARG:CZ | 2.47 | 0.44 |
| 2:O9:24:LEU:HB3 | 12:P9:202:CYC:HAB2 | 2.00 | 0.44 |
| 5:Z8:26:LEU:HD23 | 12:Z8:301:CYC:OB | 2.17 | 0.44 |
| 3:D9:2:GLN:HA | 3:D9:6:THR:HG21 | 2.00 | 0.44 |
| 2:I9:20:ASN:O | 2:I9:24:LEU:HG | 2.18 | 0.44 |
| 11:a9:371:VAL:HG11 | 11:a9:507:PHE:CB | 2.47 | 0.44 |
| 11:aA:89:ALA:CB | 11:aA:92:LYS:NZ | 2.81 | 0.44 |
| 11:aA:112:GLU:O | 11:aA:114:ASP:N | 2.51 | 0.44 |
| 11:aA:304:ALA:C | 11:aA:306:GLY:H | 2.26 | 0.44 |
| 11:aA:643:LEU:HD12 | 11:aA:766:ASN:O | 2.18 | 0.44 |
| 11:aA:816:LEU:HD23 | 11:aA:816:LEU:C | 2.41 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:aA:902:CYC:HC | 12:aA:902:CYC:HMD3 | 1.83 | 0.44 |
| 3:V1:2:GLN:HA | 3:V1:6:THR:HG21 | 2.00 | 0.44 |
| 3:B2:124:THR:HB | 3:B2:171:ILE:O | 2.18 | 0.44 |
| 3:JA:124:THR:HB | 3:JA:171:ILE:O | 2.18 | 0.44 |
| 3:ZA:124:THR:HB | 3:ZA:171:ILE:O | 2.18 | 0.44 |
| 12:O1:201:CYC:O2A | 3:R1:67:ILE:HD12 | 2.17 | 0.44 |
| 7:N2:25:ASP:OD1 | 7:N2:25:ASP:N | 2.50 | 0.44 |
| 12:F3:201:CYC:CMA | 12:F3:201:CYC:HB | 2.25 | 0.44 |
| 3:Z3:2:GLN:HA | 3:Z3:6:THR:HG21 | 2.00 | 0.44 |
| 2:A4:99:ALA:HB2 | 3:B4:9:ILE:HD13 | 2.00 | 0.44 |
| 3:B4:2:GLN:HA | 3:B4:6:THR:HG21 | 2.00 | 0.44 |
| 4:M3:52:LEU:HD22 | 4:M3:52:LEU:O | 2.17 | 0.44 |
| 3:P3:124:THR:HB | 3:P3:171:ILE:O | 2.18 | 0.44 |
| 3:U4:2:GLN:HA | 3:U4:6:THR:HG21 | 2.00 | 0.44 |
| 3:J4:124:THR:HB | 3:J4:171:ILE:O | 2.18 | 0.44 |
| 4:M4:27:HIS:O | 11:aA:227:GLY:HA2 | 2.14 | 0.44 |
| 3:Q4:79:MET:O | 3:Q4:83:LEU:HG | 2.17 | 0.44 |
| 3:Q4:112:GLY:O | 3:Q4:116:THR:HG23 | 2.18 | 0.44 |
| 8:K5:67:SER:HB3 | 8:K5:68:PRO:HD2 | 2.00 | 0.44 |
| 8:O5:95:GLY:CA | 8:O5:104:ILE:HD11 | 2.47 | 0.44 |
| 1:B5:10:ASN:HD21 | 10:k5:557:VAL:HB | 1.80 | 0.44 |
| 8:e5:16:ARG:HG3 | 8:e5:16:ARG:HH11 | 1.83 | 0.44 |
| 8:Q5:67:SER:HB3 | 8:Q5:68:PRO:HD2 | 2.00 | 0.44 |
| 8:S5:59:PHE:CB | 8:E7:68:PRO:HB2 | 2.46 | 0.44 |
| 1:T5:71:MEN:O | 1:T5:77:ARG:HD3 | 2.18 | 0.44 |
| 8:U5:37:LEU:HD23 | 8:U5:97:VAL:HG12 | 2.00 | 0.44 |
| 8:a5:94:TYR:O | 8:a5:97:VAL:CG2 | 2.65 | 0.44 |
| 3:L6:67:ILE:HD12 | 12:G6:201:CYC:O2A | 2.17 | 0.44 |
| 12:L6:201:CYC:HC | 12:L6:201:CYC:HMD3 | 1.83 | 0.44 |
| 7:N6:25:ASP:OD1 | 7:N6:25:ASP:N | 2.50 | 0.44 |
| 8:A7:90:ARG:HB2 | 1:B7:18:TYR:CE1 | 2.52 | 0.44 |
| 9:z5:7:VAL:HG22 | 9:z5:30:LYS:O | 2.18 | 0.44 |
| 9:z5:11:ILE:HD11 | 9:z5:28:PHE:CE2 | 2.52 | 0.44 |
| 9:i5:27:PHE:HE2 | 9:i5:52:LEU:HD11 | 1.81 | 0.44 |
| 9:i5:44:ILE:HD13 | 9:i5:44:ILE:HG21 | 1.77 | 0.44 |
| 10:j5:21:MET:HE3 | 10:j5:25:ILE:HD11 | 2.00 | 0.44 |
| 10:j5:283:ARG:CD | 10:j5:283:ARG:H | 2.30 | 0.44 |
| 10:j5:764:PHE:O | 10:j5:764:PHE:CG | 2.70 | 0.44 |
| 10:j5:765:ASP:O | 10:j5:769:THR:HG22 | 2.18 | 0.44 |
| 10:j5:820:HIS:NE2 | 10:j5:859:ILE:HD11 | 2.12 | 0.44 |
| 10:j5:844:GLN:O | 10:j5:844:GLN:CG | 2.65 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:j5:947:MET:CE | 10:j5:948:SER:HB3 | 2.48 | 0.44 |
| 10:k5:278:TYR:CE2 | 10:k5:287:ASN:OD1 | 2.71 | 0.44 |
| 10:k5:1143:LEU:HA | 10:k5:1143:LEU:HD23 | 1.62 | 0.44 |
| 12:H6:202:CYC:HB | 12:H6:202:CYC:HMA3 | 1.83 | 0.44 |
| 8:S7:90:ARG:HB2 | 1:T7:18:TYR:CE1 | 2.53 | 0.44 |
| 8:G7:90:ARG:HB2 | 1:H7:18:TYR:CE1 | 2.53 | 0.44 |
| 8:G7:130:VAL:CG1 | 8:G7:157:VAL:HG23 | 2.48 | 0.44 |
| 8:M7:130:VAL:CG1 | 8:M7:157:VAL:HG23 | 2.48 | 0.44 |
| 8:g7:27:LYS:HA | 8:g7:30:VAL:HG22 | 2.00 | 0.44 |
| 8:a7:27:LYS:HA | 8:a7:30:VAL:HG22 | 2.00 | 0.44 |
| 1:b7:72:MET:HE2 | 1:b7:72:MET:HB3 | 1.87 | 0.44 |
| 8:c7:101:VAL:HG12 | 8:c7:155:TYR:CE2 | 2.52 | 0.44 |
| 8:e7:23:LEU:HD22 | 1:f7:38:VAL:HG13 | 2.00 | 0.44 |
| 2:C8:99:ALA:HB2 | 3:D8:9:ILE:HD13 | 2.00 | 0.44 |
| 12:D8:201:CYC:HB | 12:D8:201:CYC:HMA3 | 1.83 | 0.44 |
| 8:m7:18:LEU:HD23 | 8:m7:22:GLU:HB2 | 2.00 | 0.44 |
| 8:o7:3:VAL:O | 8:o7:7:ALA:N | 2.51 | 0.44 |
| 8:o7:4:LEU:HD21 | 8:o7:26:ILE:HD13 | 1.93 | 0.44 |
| 8:o7:67:SER:HB3 | 8:o7:68:PRO:HD2 | 2.00 | 0.44 |
| 1:p7:72:MET:HE2 | 1:p7:72:MET:HB3 | 1.87 | 0.44 |
| 8:s7:67:SER:HB3 | 8:s7:68:PRO:HD2 | 2.00 | 0.44 |
| 9:x7:40:GLU:OE2 | 9:x7:43:ARG:CD | 2.65 | 0.44 |
| 12:W8:202:CYC:CMD | 12:W8:202:CYC:NC | 2.75 | 0.44 |
| 4:M9:222:ARG:NH1 | 4:M9:222:ARG:CG | 2.72 | 0.44 |
| 12:D9:201:CYC:HB | 12:D9:201:CYC:CMA | 2.26 | 0.44 |
| 3:J9:67:ILE:HD12 | 12:K9:201:CYC:O2A | 2.17 | 0.44 |
| 3:V9:67:ILE:HD12 | 12:W9:201:CYC:O2A | 2.17 | 0.44 |
| 12:Y9:201:CYC:CMA | 12:Y9:201:CYC:NB | 2.81 | 0.44 |
| 11:a9:373:PRO:HG2 | 11:a9:373:PRO:O | 2.17 | 0.44 |
| 11:a9:426:ARG:NH1 | 11:a9:430:ARG:HH21 | 2.16 | 0.44 |
| 11:a9:485:GLU:HA | 11:a9:485:GLU:OE2 | 2.17 | 0.44 |
| 11:a9:490:ILE:N | 11:a9:490:ILE:CD1 | 2.80 | 0.44 |
| 11:a9:495:TYR:CD1 | 11:a9:495:TYR:O | 2.70 | 0.44 |
| 11:a9:576:LEU:HD23 | 11:a9:576:LEU:HA | 1.65 | 0.44 |
| 11:aA:371:VAL:CG2 | 11:aA:507:PHE:HD2 | 2.31 | 0.44 |
| 11:aA:426:ARG:NH2 | 11:aA:496:ARG:NE | 2.66 | 0.44 |
| 11:aA:670:LEU:HD12 | 2:K1:111:ALA:HB1 | 1.74 | 0.44 |
| 12:K1:201:CYC:CMA | 12:K1:201:CYC:NB | 2.81 | 0.44 |
| 3:L1:124:THR:HB | 3:L1:171:ILE:O | 2.18 | 0.44 |
| 4:M1:51:ARG:NH1 | 4:M1:51:ARG:CG | 2.77 | 0.44 |
| 12:X1:202:CYC:HB | 12:X1:202:CYC:HMA3 | 1.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:A2:19:LEU:O | 3:B2:45:THR:CG2 | 2.64 | 0.44 |
| 2:E2:128:ILE:CG2 | 2:E2:132:LYS:HE3 | 2.47 | 0.44 |
| 3:F2:124:THR:HB | 3:F2:171:ILE:O | 2.18 | 0.44 |
| 12:BA:201:CYC:CMA | 12:BA:201:CYC:HB | 2.25 | 0.43 |
| 12:JA:202:CYC:HC | 12:JA:202:CYC:HMD3 | 1.82 | 0.43 |
| 5:NA:13:SER:HB3 | 5:NA:14:LYS:H | 1.55 | 0.43 |
| 2:QA:119:THR:CG2 | 3:TA:83:LEU:CD1 | 2.90 | 0.43 |
| 12:XA:202:CYC:HB | 12:XA:202:CYC:HMA3 | 1.83 | 0.43 |
| 2:G2:99:ALA:HB2 | 3:H2:9:ILE:HD13 | 2.00 | 0.43 |
| 3:H2:77:ARG:NH2 | 12:H2:201:CYC:O1A | 2.51 | 0.43 |
| 12:H2:202:CYC:CMD | 12:H2:202:CYC:NC | 2.75 | 0.43 |
| 3:L2:2:GLN:HA | 3:L2:6:THR:HG21 | 2.00 | 0.43 |
| 2:A3:24:LEU:HB3 | 12:B3:201:CYC:HAB2 | 2.00 | 0.43 |
| 12:A4:201:CYC:O2A | 3:D4:67:ILE:HD12 | 2.17 | 0.43 |
| 3:B4:107:ASP:O | 4:M4:60:LYS:O | 2.36 | 0.43 |
| 12:B4:202:CYC:C1D | 4:M4:53:LEU:CD2 | 2.96 | 0.43 |
| 12:O3:201:CYC:O2A | 3:R3:67:ILE:HD12 | 2.17 | 0.43 |
| 12:Y3:201:CYC:CMA | 12:Y3:201:CYC:NB | 2.81 | 0.43 |
| 2:G4:99:ALA:HB2 | 3:H4:9:ILE:HD13 | 2.00 | 0.43 |
| 2:I4:14:SER:CA | 11:aA:170:PHE:CZ | 2.82 | 0.43 |
| 4:M4:160:THR:HG21 | 4:M4:257:GLN:CB | 2.30 | 0.43 |
| 4:M4:223:GLY:O | 12:M4:301:CYC:CGA | 2.66 | 0.43 |
| 4:M4:241:LEU:HA | 4:M4:241:LEU:HD23 | 1.63 | 0.43 |
| 3:O4:124:THR:HB | 3:O4:171:ILE:O | 2.18 | 0.43 |
| 8:O5:130:VAL:CG1 | 8:O5:157:VAL:HG23 | 2.48 | 0.43 |
| 3:Y4:124:THR:HB | 3:Y4:171:ILE:O | 2.18 | 0.43 |
| 8:A5:112:VAL:CG2 | 1:F5:75:THR:HG21 | 2.38 | 0.43 |
| 8:G5:17:TYR:CD2 | 1:H5:45:SER:HB3 | 2.52 | 0.43 |
| 8:G5:53:GLN:OE1 | 8:G5:53:GLN:HA | 2.17 | 0.43 |
| 1:H5:71:MEN:O | 1:H5:77:ARG:HD3 | 2.18 | 0.43 |
| 8:c5:64:ASP:HA | 8:c5:67:SER:CB | 2.49 | 0.43 |
| 8:c5:67:SER:HB3 | 8:c5:68:PRO:HD2 | 2.00 | 0.43 |
| 8:c5:90:ARG:HB2 | 1:d5:18:TYR:CE1 | 2.53 | 0.43 |
| 8:c5:130:VAL:CG1 | 8:c5:157:VAL:HG23 | 2.48 | 0.43 |
| 8:U5:113:LYS:HD2 | 10:j5:582:GLN:HB2 | 1.99 | 0.43 |
| 8:a5:27:LYS:HA | 8:a5:30:VAL:HG22 | 1.99 | 0.43 |
| 3:J6:124:THR:HB | 3:J6:171:ILE:O | 2.18 | 0.43 |
| 6:M6:259:THR:C | 6:M6:261:LYS:H | 2.25 | 0.43 |
| 10:j5:166:TYR:HB3 | 10:j5:179:LEU:CD2 | 2.47 | 0.43 |
| 10:j5:631:HIS:HA | 10:j5:664:MET:CE | 2.48 | 0.43 |
| 10:j5:776:PHE:O | 10:j5:777:ASP:CB | 2.59 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:j5:1147:TYR:CD1 | 10:j5:1147:TYR:O | 2.69 | 0.43 |
| 10:k5:175:ASP:OD1 | 10:k5:175:ASP:N | 2.44 | 0.43 |
| 10:k5:764:PHE:O | 10:k5:764:PHE:CG | 2.70 | 0.43 |
| 10:k5:888:THR:CG2 | 1:D7:83:ARG:NH1 | 2.74 | 0.43 |
| 10:k5:986:PRO:HD3 | 9:x7:24:GLN:HE22 | 1.83 | 0.43 |
| 10:k5:1118:THR:CG2 | 12:k5:1204:CYC:HBA1 | 2.41 | 0.43 |
| 3:B6:2:GLN:HA | 3:B6:6:THR:HG21 | 2.00 | 0.43 |
| 1:P7:71:MEN:O | 1:P7:77:ARG:HD3 | 2.18 | 0.43 |
| 1:R7:71:MEN:O | 1:R7:77:ARG:HD3 | 2.18 | 0.43 |
| 8:C7:21:GLY:C | 8:C7:23:LEU:H | 2.25 | 0.43 |
| 8:C7:37:LEU:HD23 | 8:C7:97:VAL:HG12 | 2.00 | 0.43 |
| 8:C7:67:SER:HB3 | 8:C7:68:PRO:HD2 | 2.00 | 0.43 |
| 1:L7:71:MEN:O | 1:L7:77:ARG:HD3 | 2.18 | 0.43 |
| 8:i7:25:ARG:HG2 | 8:s7:3:VAL:HG13 | 1.99 | 0.43 |
| 8:i7:152:TYR:CZ | 8:s7:20:PRO:HB3 | 2.53 | 0.43 |
| 1:j7:71:MEN:O | 1:j7:77:ARG:HD3 | 2.18 | 0.43 |
| 8:k7:79:ALA:CA | 11:a9:53:VAL:HG21 | 2.47 | 0.43 |
| 8:k7:130:VAL:CG1 | 8:k7:157:VAL:HG23 | 2.48 | 0.43 |
| 1:T7:110:ASN:ND2 | 9:w7:57:PHE:CA | 2.81 | 0.43 |
| 8:U7:27:LYS:HA | 8:U7:30:VAL:HG22 | 2.00 | 0.43 |
| 8:W7:67:SER:HB3 | 8:W7:68:PRO:HD2 | 2.00 | 0.43 |
| 3:B8:67:ILE:HD12 | 12:E8:201:CYC:O2A | 2.17 | 0.43 |
| 3:B8:116:THR:HG23 | 4:M8:52:LEU:O | 2.17 | 0.43 |
| 8:o7:103:PRO:CG | 1:p7:9:ILE:CD1 | 2.66 | 0.43 |
| 8:s7:11:ALA:CB | 8:s7:18:LEU:CD1 | 2.96 | 0.43 |
| 8:u7:16:ARG:N | 1:v7:94:TYR:OH | 2.51 | 0.43 |
| 8:u7:34:GLU:HG3 | 1:v7:28:LYS:CD | 2.46 | 0.43 |
| 2:T8:99:ALA:HB2 | 3:U8:9:ILE:HD13 | 2.00 | 0.43 |
| 2:V8:99:ALA:HB2 | 3:W8:9:ILE:HD13 | 2.00 | 0.43 |
| 2:X8:107:ASP:OD2 | 4:M8:273:ILE:CG2 | 2.57 | 0.43 |
| 3:J8:67:ILE:HD12 | 12:K8:201:CYC:O2A | 2.17 | 0.43 |
| 3:L8:2:GLN:HA | 3:L8:6:THR:HG21 | 2.00 | 0.43 |
| 12:M8:301:CYC:HC | 12:M8:301:CYC:HMD3 | 1.82 | 0.43 |
| 3:O8:105:LEU:O | 3:O8:108:ARG:O | 2.36 | 0.43 |
| 3:Q8:2:GLN:HA | 3:Q8:6:THR:HG21 | 2.00 | 0.43 |
| 4:M9:95:ALA:HB2 | 5:N9:38:GLU:CD | 2.43 | 0.43 |
| 4:M9:158:PHE:CZ | 2:U9:10:ALA:CA | 3.01 | 0.43 |
| 4:M9:164:ARG:O | 4:M9:164:ARG:HG3 | 2.15 | 0.43 |
| 4:M9:235:PHE:CD1 | 4:M9:235:PHE:O | 2.70 | 0.43 |
| 12:P9:201:CYC:HC | 12:P9:201:CYC:HMD3 | 1.82 | 0.43 |
| 5:Z8:27:ALA:HB3 | 12:Z8:301:CYC:HAB1 | 1.97 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:B9:107:ASP:HB3 | 11:a9:382:ASN:CG | 2.40 | 0.43 |
| 2:G9:99:ALA:HB2 | 3:H9:9:ILE:HD13 | 2.00 | 0.43 |
| 3:H9:2:GLN:HA | 3:H9:6:THR:HG21 | 2.00 | 0.43 |
| 12:S9:201:CYC:CMA | 12:S9:201:CYC:NB | 2.81 | 0.43 |
| 3:T9:124:THR:HB | 3:T9:171:ILE:O | 2.18 | 0.43 |
| 2:U9:99:ALA:HB2 | 3:V9:9:ILE:HD13 | 2.00 | 0.43 |
| 3:X9:124:THR:HB | 3:X9:171:ILE:O | 2.18 | 0.43 |
| 2:Y9:99:ALA:HB2 | 3:Z9:9:ILE:HD13 | 2.00 | 0.43 |
| 11:a9:30:MET:HE3 | 11:a9:35:ARG:CD | 2.44 | 0.43 |
| 11:a9:363:GLN:HE21 | 11:a9:363:GLN:H | 1.66 | 0.43 |
| 11:a9:371:VAL:CG2 | 11:a9:507:PHE:HD2 | 2.31 | 0.43 |
| 11:aA:801:ASN:ND2 | 11:aA:801:ASN:C | 2.71 | 0.43 |
| 11:aA:817:LEU:HA | 11:aA:817:LEU:HD23 | 1.50 | 0.43 |
| 2:K1:99:ALA:HB2 | 3:L1:9:ILE:HD13 | 2.00 | 0.43 |
| 4:M1:93:LEU:HD12 | 4:M1:93:LEU:HA | 1.66 | 0.43 |
| 4:M1:176:ARG:CG | 4:M1:176:ARG:NH1 | 2.70 | 0.43 |
| 3:T1:124:THR:HB | 3:T1:171:ILE:O | 2.18 | 0.43 |
| 12:F2:201:CYC:HMD3 | 12:F2:201:CYC:HC | 1.83 | 0.43 |
| 12:F2:202:CYC:HB | 12:F2:202:CYC:HMA3 | 1.83 | 0.43 |
| 1:Z:71:MEN:O | 1:Z:77:ARG:HD3 | 2.18 | 0.43 |
| 12:BA:201:CYC:HC | 12:BA:201:CYC:HMD3 | 1.83 | 0.43 |
| 12:CA:201:CYC:CMA | 12:CA:201:CYC:NB | 2.81 | 0.43 |
| 12:CA:201:CYC:O2A | 3:FA:67:ILE:HD12 | 2.17 | 0.43 |
| 2:EA:99:ALA:HB2 | 3:FA:9:ILE:HD13 | 2.00 | 0.43 |
| 2:IA:99:ALA:HB2 | 3:JA:9:ILE:HD13 | 2.00 | 0.43 |
| 12:KA:201:CYC:CMA | 12:KA:201:CYC:NB | 2.81 | 0.43 |
| 12:LA:202:CYC:HC | 12:LA:202:CYC:HMD3 | 1.83 | 0.43 |
| 5:NA:3:VAL:CG1 | 3:RA:115:GLU:HB2 | 2.33 | 0.43 |
| 5:NA:37:HIS:O | 5:NA:37:HIS:CD2 | 2.70 | 0.43 |
| 2:QA:68:GLN:HA | 2:U1:46:SER:HB3 | 0.69 | 0.43 |
| 12:ZA:201:CYC:HB | 12:ZA:201:CYC:HMA3 | 1.83 | 0.43 |
| 2:O1:24:LEU:HB3 | 12:P1:202:CYC:HAB2 | 2.00 | 0.43 |
| 3:P1:67:ILE:HD12 | 12:S1:201:CYC:O2A | 2.17 | 0.43 |
| 2:I2:38:MET:HE2 | 2:I2:38:MET:HB3 | 1.81 | 0.43 |
| 12:K2:201:CYC:CMA | 12:K2:201:CYC:NB | 2.81 | 0.43 |
| 7:N2:11:TRP:HE1 | 2:E2:107:ASP:CA | 2.31 | 0.43 |
| 2:C3:140:SER:C | 3:D8:150:ARG:NH1 | 2.77 | 0.43 |
| 12:C3:201:CYC:CMA | 12:C3:201:CYC:NB | 2.82 | 0.43 |
| 3:D3:2:GLN:HA | 3:D3:6:THR:HG21 | 2.00 | 0.43 |
| 3:B4:86:MET:CG | 12:B4:202:CYC:HBC1 | 2.48 | 0.43 |
| 12:L3:202:CYC:NB | 11:a9:738:LEU:HD22 | 2.30 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 4:M3:120:LEU:HD11 | 3:X3:84:ARG:HH12 | 1.83 | 0.43 |
| 4:M3:235:PHE:CD1 | 4:M3:235:PHE:O | 2.70 | 0.43 |
| 5:N3:74:GLU:HA | 3:P3:111:ASN:ND2 | 2.16 | 0.43 |
| 12:Q3:201:CYC:O2A | 3:T3:67:ILE:HD12 | 2.17 | 0.43 |
| 12:W3:201:CYC:CMA | 12:W3:201:CYC:NB | 2.81 | 0.43 |
| 4:M4:27:HIS:HD1 | 4:M4:35:THR:C | 2.25 | 0.43 |
| 4:M4:74:LEU:HA | 4:M4:74:LEU:HD23 | 1.68 | 0.43 |
| 8:K5:107:ILE:HG23 | 1:J5:74:THR:HG22 | 2.00 | 0.43 |
| 8:M5:130:VAL:CG1 | 8:M5:157:VAL:HG23 | 2.48 | 0.43 |
| 5:Z4:29:HIS:HB3 | 5:Z4:31:TRP:CD1 | 2.45 | 0.43 |
| 5:Z4:38:GLU:HG2 | 12:Z4:301:CYC:HMB2 | 1.97 | 0.43 |
| 8:G5:119:LEU:HD11 | 12:G5:201:CYC:HAA2 | 2.00 | 0.43 |
| 8:I5:16:ARG:HH11 | 8:I5:16:ARG:CG | 2.29 | 0.43 |
| 8:I5:26:ILE:HG21 | 8:I5:26:ILE:HD13 | 1.61 | 0.43 |
| 8:e5:5:THR:C | 8:e5:7:ALA:H | 2.25 | 0.43 |
| 8:e5:37:LEU:HD23 | 8:e5:97:VAL:HG12 | 2.00 | 0.43 |
| 8:e5:67:SER:HB3 | 8:e5:68:PRO:HD2 | 2.00 | 0.43 |
| 8:Q5:8:ILE:O | 8:Q5:11:ALA:N | 2.51 | 0.43 |
| 8:S5:130:VAL:CG1 | 8:S5:157:VAL:HG23 | 2.48 | 0.43 |
| 1:V5:71:MEN:O | 1:V5:77:ARG:HD3 | 2.18 | 0.43 |
| 1:V5:114:GLU:HG3 | 10:j5:496:GLU:OE2 | 2.16 | 0.43 |
| 8:Y5:130:VAL:CG1 | 8:Y5:157:VAL:HG23 | 2.48 | 0.43 |
| 3:J6:9:ILE:HD13 | 2:I6:99:ALA:HB2 | 2.00 | 0.43 |
| 3:L6:124:THR:HB | 3:L6:171:ILE:O | 2.18 | 0.43 |
| 6:M6:127:SER:HB3 | 3:F6:84:ARG:NE | 2.19 | 0.43 |
| 6:M6:276:PRO:C | 1:d7:62:TYR:O | 2.61 | 0.43 |
| 7:N6:18:ILE:HD11 | 7:N6:48:LEU:HD11 | 1.98 | 0.43 |
| 10:j5:386:ILE:HG21 | 10:j5:395:SER:C | 2.14 | 0.43 |
| 10:j5:1118:THR:HG21 | 1:t7:83:ARG:HH12 | 1.82 | 0.43 |
| 10:k5:528:GLU:O | 10:k5:528:GLU:CG | 2.66 | 0.43 |
| 10:k5:557:VAL:O | 10:k5:559:THR:N | 2.51 | 0.43 |
| 10:k5:750:ARG:HH11 | 10:k5:750:ARG:CG | 2.25 | 0.43 |
| 10:k5:784:ILE:HG21 | 10:k5:784:ILE:HD13 | 1.72 | 0.43 |
| 10:k5:947:MET:HE3 | 10:k5:947:MET:HB2 | 1.42 | 0.43 |
| 10:k5:965:GLN:HB3 | 10:k5:969:VAL:CG1 | 2.43 | 0.43 |
| 3:B6:124:THR:HB | 3:B6:171:ILE:O | 2.18 | 0.43 |
| 3:F6:2:GLN:HA | 3:F6:6:THR:HG21 | 2.00 | 0.43 |
| 8:O7:130:VAL:CG1 | 8:O7:157:VAL:HG23 | 2.49 | 0.43 |
| 8:Q7:116:TYR:CB | 8:Q7:123:ILE:HG12 | 2.48 | 0.43 |
| 8:S7:64:ASP:HA | 8:S7:67:SER:CB | 2.49 | 0.43 |
| 8:C7:27:LYS:HA | 8:C7:30:VAL:HG22 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:G7:67:SER:HB3 | 8:G7:68:PRO:HD2 | 2.00 | 0.43 |
| 8:I7:11:ALA:CB | 8:I7:18:LEU:CD1 | 2.96 | 0.43 |
| 1:N7:71:MEN:O | 1:N7:77:ARG:HD3 | 2.18 | 0.43 |
| 8:g7:48:GLU:O | 11:aA:318:TRP:HZ3 | 2.00 | 0.43 |
| 8:i7:101:VAL:HG12 | 8:i7:155:TYR:CE2 | 2.53 | 0.43 |
| 8:i7:138:THR:O | 8:i7:138:THR:HG23 | 2.18 | 0.43 |
| 1:T7:110:ASN:ND2 | 9:w7:57:PHE:O | 2.51 | 0.43 |
| 8:U7:67:SER:HB3 | 8:U7:68:PRO:HD2 | 2.00 | 0.43 |
| 8:a7:11:ALA:C | 8:a7:13:ALA:N | 2.75 | 0.43 |
| 8:a7:90:ARG:HD2 | 1:b7:18:TYR:N | 2.31 | 0.43 |
| 1:f7:71:MEN:O | 1:f7:77:ARG:HD3 | 2.18 | 0.43 |
| 8:s7:37:LEU:HD23 | 8:s7:97:VAL:HG12 | 2.00 | 0.43 |
| 8:u7:27:LYS:HE3 | 1:v7:35:ALA:C | 2.43 | 0.43 |
| 8:u7:30:VAL:HG12 | 1:v7:31:PHE:HA | 1.99 | 0.43 |
| 9:z7:3:ARG:CZ | 9:z7:67:VAL:HG13 | 2.48 | 0.43 |
| 12:T8:201:CYC:O2A | 3:Y8:67:ILE:HD12 | 2.17 | 0.43 |
| 3:J8:108:ARG:HH22 | 11:a9:171:ARG:CG | 2.30 | 0.43 |
| 4:M8:137:ILE:HD11 | 4:M8:142:PHE:CD1 | 2.53 | 0.43 |
| 4:M8:201:ASP:H | 5:Z8:52:ARG:HH22 | 1.60 | 0.43 |
| 4:M8:201:ASP:CG | 5:Z8:56:GLU:CD | 2.86 | 0.43 |
| 12:M8:302:CYC:H2C | 3:S8:72:ASN:O | 2.18 | 0.43 |
| 3:F1:2:GLN:HA | 3:F1:6:THR:HG21 | 2.00 | 0.43 |
| 3:L9:2:GLN:HA | 3:L9:6:THR:HG21 | 2.00 | 0.43 |
| 4:M9:118:TYR:CD1 | 3:Z9:84:ARG:CZ | 3.01 | 0.43 |
| 4:M9:137:ILE:HB | 4:M9:141:GLU:HB3 | 1.99 | 0.43 |
| 2:O9:99:ALA:HB2 | 3:P9:9:ILE:HD13 | 2.00 | 0.43 |
| 3:B9:2:GLN:HA | 3:B9:6:THR:HG21 | 2.00 | 0.43 |
| 3:F9:37:ARG:CA | 3:F9:156:LEU:HD21 | 2.48 | 0.43 |
| 3:J9:65:ASP:HB2 | 11:a9:354:VAL:HG22 | 1.80 | 0.43 |
| 12:X9:202:CYC:CMD | 12:X9:202:CYC:NC | 2.75 | 0.43 |
| 11:a9:239:TYR:CE1 | 12:a9:901:CYC:CBA | 2.74 | 0.43 |
| 11:a9:376:ALA:HB3 | 11:a9:503:THR:HG22 | 2.01 | 0.43 |
| 11:a9:710:THR:CG2 | 11:a9:807:GLN:OE1 | 2.64 | 0.43 |
| 11:aA:781:ALA:O | 11:aA:782:ALA:C | 2.60 | 0.43 |
| 4:M1:235:PHE:O | 4:M1:235:PHE:CD1 | 2.70 | 0.43 |
| 5:N1:22:LEU:O | 5:N1:37:HIS:CE1 | 2.70 | 0.43 |
| 2:U1:42:ARG:O | 2:U1:46:SER:OG | 2.36 | 0.43 |
| 12:AA:201:CYC:CMA | 12:AA:201:CYC:NB | 2.82 | 0.43 |
| 3:HA:2:GLN:HA | 3:HA:6:THR:HG21 | 2.00 | 0.43 |
| 2:KA:9:ILE:HG23 | 3:LA:95:TYR:CD2 | 2.53 | 0.43 |
| 2:KA:24:LEU:CD2 | 3:LA:38:LEU:HD22 | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:LA:86:MET:O | 3:LA:134:MET:SD | 2.77 | 0.43 |
| 3:LA:111:ASN:C | 11:aA:532:ALA:CB | 2.86 | 0.43 |
| 4:MA:137:ILE:HB | 4:MA:141:GLU:HB3 | 1.99 | 0.43 |
| 12:OA:201:CYC:O2A | 3:RA:67:ILE:HD12 | 2.17 | 0.43 |
| 3:TA:2:GLN:HA | 3:TA:6:THR:HG21 | 2.00 | 0.43 |
| 12:XA:201:CYC:HC | 12:XA:201:CYC:HMD3 | 1.83 | 0.43 |
| 3:H2:2:GLN:HA | 3:H2:6:THR:HG21 | 2.01 | 0.43 |
| 3:H2:124:THR:HB | 3:H2:171:ILE:O | 2.18 | 0.43 |
| 12:J2:201:CYC:HB | 12:J2:201:CYC:HMA3 | 1.84 | 0.43 |
| 6:M2:66:GLY:HA2 | 1:h7:124:ALA:C | 2.43 | 0.43 |
| 3:B3:127:VAL:CG2 | 12:B3:202:CYC:HMC3 | 2.48 | 0.43 |
| 3:B4:82:CYS:CB | 12:B4:202:CYC:C2C | 2.95 | 0.43 |
| 12:L3:202:CYC:HC | 12:L3:202:CYC:HMD3 | 1.83 | 0.43 |
| 4:M3:261:VAL:HG11 | 4:M3:266:LEU:HD13 | 1.99 | 0.43 |
| 3:P3:2:GLN:HA | 3:P3:6:THR:HG21 | 2.00 | 0.43 |
| 3:R3:124:THR:HB | 3:R3:171:ILE:O | 2.18 | 0.43 |
| 2:U3:38:MET:HE2 | 2:U3:38:MET:HB3 | 1.81 | 0.43 |
| 12:S4:201:CYC:HB | 12:S4:201:CYC:HMA3 | 1.83 | 0.43 |
| 2:V4:99:ALA:HB2 | 3:W4:9:ILE:HD13 | 2.00 | 0.43 |
| 3:W4:124:THR:HB | 3:W4:171:ILE:O | 2.18 | 0.43 |
| 12:J4:201:CYC:HC | 12:J4:201:CYC:HMD3 | 1.83 | 0.43 |
| 4:M4:52:LEU:HD22 | 4:M4:52:LEU:O | 2.17 | 0.43 |
| 4:M4:99:VAL:CB | 3:Q4:1:MET:HE1 | 2.47 | 0.43 |
| 4:M4:137:ILE:HG22 | 5:Z4:44:TYR:CE1 | 2.54 | 0.43 |
| 2:N4:99:ALA:HB2 | 3:O4:9:ILE:HD13 | 2.00 | 0.43 |
| 3:Q4:113:LEU:HD22 | 3:Q4:113:LEU:HA | 1.85 | 0.43 |
| 5:Z4:39:PRO:HD3 | 12:Z4:301:CYC:HD | 1.83 | 0.43 |
| 1:D5:74:THR:HG22 | 8:E5:107:ILE:HG23 | 2.00 | 0.43 |
| 1:D5:118:SER:O | 9:z5:56:LEU:HD21 | 2.19 | 0.43 |
| 8:G5:53:GLN:HB3 | 8:G5:136:VAL:HG21 | 2.00 | 0.43 |
| 8:G5:130:VAL:CG1 | 8:G5:157:VAL:HG23 | 2.48 | 0.43 |
| 8:I5:27:LYS:C | 8:I5:29:PHE:H | 2.19 | 0.43 |
| 8:e5:130:VAL:CG1 | 8:e5:157:VAL:HG23 | 2.48 | 0.43 |
| 1:P5:114:GLU:CB | 10:k5:496:GLU:CD | 2.85 | 0.43 |
| 1:X5:71:MEN:O | 1:X5:77:ARG:HD3 | 2.18 | 0.43 |
| 8:Y5:9:VAL:CG1 | 10:k5:344:ARG:NH1 | 2.65 | 0.43 |
| 8:a5:37:LEU:HD23 | 8:a5:97:VAL:HG12 | 2.00 | 0.43 |
| 12:L6:202:CYC:HB | 12:L6:202:CYC:HMA3 | 1.84 | 0.43 |
| 7:N6:2:TYR:CD1 | 7:N6:2:TYR:N | 2.73 | 0.43 |
| 10:j5:187:ARG:NH1 | 10:j5:237:ASP:OD2 | 2.52 | 0.43 |
| 10:j5:278:TYR:CE2 | 10:j5:287:ASN:OD1 | 2.71 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:544:VAL:HG13 | 10:j5:564:VAL:CG2 | 2.48 | 0.43 |
| 10:j5:724:GLU:O | 10:j5:724:GLU:CG | 2.65 | 0.43 |
| 10:j5:729:ILE:HD13 | 10:j5:729:ILE:HG21 | 1.72 | 0.43 |
| 10:j5:1058:VAL:O | 10:j5:1062:LEU:HG | 2.18 | 0.43 |
| 10:k5:141:GLU:O | 10:k5:142:PRO:C | 2.59 | 0.43 |
| 10:k5:297:VAL:O | 10:k5:297:VAL:HG13 | 2.18 | 0.43 |
| 10:k5:352:ILE:HG22 | 10:k5:354:SER:H | 1.83 | 0.43 |
| 10:k5:1152:TYR:CD1 | 10:k5:1152:TYR:N | 2.72 | 0.43 |
| 3:D1:124:THR:HB | 3:D1:171:ILE:O | 2.18 | 0.43 |
| 8:Q7:8:ILE:O | 8:Q7:11:ALA:N | 2.51 | 0.43 |
| 8:K7:67:SER:HB3 | 8:K7:68:PRO:HD2 | 2.00 | 0.43 |
| 8:M7:67:SER:HB3 | 8:M7:68:PRO:HD2 | 2.00 | 0.43 |
| 8:g7:90:ARG:HH12 | 1:h7:16:GLY:HA2 | 1.79 | 0.43 |
| 8:i7:112:VAL:O | 8:i7:115:MET:HB3 | 2.17 | 0.43 |
| 1:T7:1:MET:O | 9:w7:66:GLY:CA | 2.66 | 0.43 |
| 8:a7:25:ARG:CZ | 8:o7:25:ARG:NH2 | 2.66 | 0.43 |
| 12:E1:201:CYC:CMA | 12:E1:201:CYC:NB | 2.81 | 0.43 |
| 12:C8:201:CYC:O2A | 3:F8:67:ILE:HD12 | 2.17 | 0.43 |
| 2:E8:99:ALA:HB2 | 3:F8:9:ILE:HD13 | 2.00 | 0.43 |
| 1:n7:71:MEN:O | 1:n7:77:ARG:HD3 | 2.18 | 0.43 |
| 1:p7:71:MEN:O | 1:p7:77:ARG:HD3 | 2.18 | 0.43 |
| 8:u7:116:TYR:CB | 8:u7:123:ILE:HG12 | 2.47 | 0.43 |
| 9:y7:19:THR:O | 9:y7:19:THR:OG1 | 2.16 | 0.43 |
| 2:X8:99:ALA:HB2 | 3:Y8:9:ILE:HD13 | 2.00 | 0.43 |
| 3:L8:78:ARG:CD | 12:a9:901:CYC:O2D | 2.54 | 0.43 |
| 3:L8:124:THR:HB | 3:L8:171:ILE:O | 2.18 | 0.43 |
| 4:M8:91:VAL:O | 4:M8:218:VAL:HG23 | 2.17 | 0.43 |
| 4:M8:96:LYS:HD3 | 3:Q8:113:LEU:HD22 | 1.98 | 0.43 |
| 4:M8:176:ARG:HH11 | 4:M8:176:ARG:HG3 | 1.78 | 0.43 |
| 3:F1:124:THR:HB | 3:F1:171:ILE:O | 2.18 | 0.43 |
| 12:F1:201:CYC:HC | 12:F1:201:CYC:HMD3 | 1.82 | 0.43 |
| 4:M9:241:LEU:HA | 4:M9:241:LEU:HD23 | 1.63 | 0.43 |
| 5:N9:22:LEU:O | 5:N9:37:HIS:CE1 | 2.70 | 0.43 |
| 2:C9:99:ALA:HB2 | 3:D9:9:ILE:HD13 | 2.00 | 0.43 |
| 12:F9:301:CYC:HC | 12:F9:301:CYC:HMD3 | 1.83 | 0.43 |
| 3:J9:20:SER:O | 3:J9:21:GLU:C | 2.45 | 0.43 |
| 12:U9:201:CYC:O2A | 3:Z9:67:ILE:HD12 | 2.17 | 0.43 |
| 11:a9:312:ASP:CB | 11:a9:315:LEU:CG | 2.63 | 0.43 |
| 11:a9:446:ALA:HB1 | 11:a9:450:ARG:CG | 2.49 | 0.43 |
| 11:aA:112:GLU:CG | 11:aA:113:ALA:N | 2.82 | 0.43 |
| 11:aA:710:THR:CG2 | 11:aA:807:GLN:OE1 | 2.64 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:J1:124:THR:HB | 3:J1:171:ILE:O | 2.18 | 0.43 |
| 4:M1:190:ARG:HH12 | 4:M1:202:SER:HB2 | 1.68 | 0.43 |
| 2:U1:99:ALA:HB2 | 3:V1:9:ILE:HD13 | 2.00 | 0.43 |
| 2:W1:99:ALA:HB2 | 3:X1:9:ILE:HD13 | 2.00 | 0.43 |
| 12:Y1:201:CYC:CMA | 12:Y1:201:CYC:NB | 2.81 | 0.43 |
| 3:BA:2:GLN:HA | 3:BA:6:THR:HG21 | 2.00 | 0.43 |
| 3:JA:68:ARG:HB2 | 11:aA:353:ALA:HB1 | 2.00 | 0.43 |
| 5:NA:23:SER:C | 5:NA:25:THR:N | 2.74 | 0.43 |
| 12:QA:201:CYC:HBB1 | 3:TA:75:PRO:CB | 2.24 | 0.43 |
| 3:RA:124:THR:HB | 3:RA:171:ILE:O | 2.18 | 0.43 |
| 12:TA:302:CYC:HB | 12:TA:302:CYC:HMA3 | 1.83 | 0.43 |
| 2:UA:99:ALA:HB2 | 3:VA:9:ILE:HD13 | 2.00 | 0.43 |
| 3:XA:2:GLN:HA | 3:XA:6:THR:HG21 | 2.01 | 0.43 |
| 2:S1:38:MET:HE2 | 2:S1:38:MET:HB3 | 1.81 | 0.43 |
| 12:S1:201:CYC:CMA | 12:S1:201:CYC:NB | 2.81 | 0.43 |
| 2:K3:99:ALA:HB2 | 3:L3:9:ILE:HD13 | 2.00 | 0.43 |
| 6:M2:65:VAL:HG12 | 1:h7:59:ALA:C | 2.41 | 0.43 |
| 3:D4:2:GLN:HA | 3:D4:6:THR:HG21 | 2.00 | 0.43 |
| 4:M3:134:ASN:ND2 | 5:N3:1:MET:H1 | 2.16 | 0.43 |
| 4:M3:268:ARG:CB | 3:V3:111:ASN:HD21 | 2.32 | 0.43 |
| 12:P3:201:CYC:HC | 12:P3:201:CYC:HMD3 | 1.82 | 0.43 |
| 12:P3:202:CYC:HB | 12:P3:202:CYC:HMA3 | 1.84 | 0.43 |
| 3:S4:120:LEU:CG | 12:S4:202:CYC:HBD1 | 2.45 | 0.43 |
| 3:S4:127:VAL:HG22 | 12:S4:202:CYC:HMC2 | 2.00 | 0.43 |
| 12:F4:202:CYC:HC | 12:F4:202:CYC:HMD3 | 1.82 | 0.43 |
| 4:M4:51:ARG:NH1 | 4:M4:51:ARG:CG | 2.78 | 0.43 |
| 4:M4:91:VAL:O | 4:M4:218:VAL:CG2 | 2.51 | 0.43 |
| 12:M4:301:CYC:C1B | 3:Y4:88:ILE:HD11 | 2.49 | 0.43 |
| 8:K5:80:LEU:HD12 | 12:K5:201:CYC:C3D | 2.48 | 0.43 |
| 1:L5:14:VAL:HG12 | 9:i5:64:ASN:ND2 | 2.34 | 0.43 |
| 1:N5:14:VAL:C | 1:R5:68:PRO:HB3 | 2.41 | 0.43 |
| 8:O5:25:ARG:HH21 | 8:E5:25:ARG:CD | 2.32 | 0.43 |
| 3:Y4:119:ALA:C | 3:Y4:121:GLY:N | 2.76 | 0.43 |
| 1:F5:71:MEN:O | 1:F5:77:ARG:HD3 | 2.18 | 0.43 |
| 8:G5:115:MET:SD | 12:G5:201:CYC:CHB | 3.06 | 0.43 |
| 8:U5:11:ALA:CB | 8:U5:18:LEU:CD1 | 2.96 | 0.43 |
| 1:X5:86:ASP:OD1 | 1:X5:90:ARG:NE | 2.51 | 0.43 |
| 12:X5:201:CYC:O1A | 10:j5:515:PRO:HB3 | 2.18 | 0.43 |
| 1:Z5:71:MEN:O | 1:Z5:77:ARG:HD3 | 2.18 | 0.43 |
| 9:z5:15:LYS:HD2 | 9:z5:16:ARG:N | 2.34 | 0.43 |
| 10:j5:1025:LEU:HD21 | 10:j5:1035:PHE:CA | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:k5:18:ARG:HH12 | 10:k5:268:SER:CB | 2.31 | 0.43 |
| 10:k5:190:LEU:CD2 | 12:k5:1201:CYC:C1D | 2.96 | 0.43 |
| 10:k5:221:LYS:NZ | 10:k5:221:LYS:O | 2.40 | 0.43 |
| 10:k5:292:GLU:OE1 | 10:k5:292:GLU:CA | 2.66 | 0.43 |
| 10:k5:851:HIS:ND1 | 10:k5:851:HIS:O | 2.51 | 0.43 |
| 10:k5:1047:LYS:O | 10:k5:1051:GLU:HB2 | 2.12 | 0.43 |
| 3:F6:124:THR:HB | 3:F6:171:ILE:O | 2.18 | 0.43 |
| 8:O7:37:LEU:HD23 | 8:O7:97:VAL:HG12 | 2.00 | 0.43 |
| 1:F7:71:MEN:O | 1:F7:77:ARG:HD3 | 2.18 | 0.43 |
| 8:K7:8:ILE:O | 8:K7:11:ALA:N | 2.51 | 0.43 |
| 8:g7:130:VAL:CG1 | 8:g7:157:VAL:HG23 | 2.48 | 0.43 |
| 1:X7:71:MEN:O | 1:X7:77:ARG:HD3 | 2.18 | 0.43 |
| 8:a7:67:SER:HB3 | 8:a7:68:PRO:HD2 | 2.00 | 0.43 |
| 8:c7:96:ILE:CG1 | 8:c7:152:TYR:CB | 2.92 | 0.43 |
| 8:e7:37:LEU:HD22 | 1:f7:24:LEU:HD22 | 2.00 | 0.43 |
| 2:E1:138:VAL:O | 2:E1:138:VAL:CG1 | 2.67 | 0.43 |
| 8:o7:27:LYS:HE3 | 1:p7:35:ALA:C | 2.43 | 0.43 |
| 8:o7:30:VAL:HG12 | 1:p7:31:PHE:HA | 1.99 | 0.43 |
| 9:x7:15:LYS:O | 9:x7:16:ARG:HG3 | 2.19 | 0.43 |
| 12:H8:201:CYC:HC | 12:H8:201:CYC:HMD3 | 1.82 | 0.43 |
| 4:M8:74:LEU:HA | 4:M8:74:LEU:HD23 | 1.68 | 0.43 |
| 4:M8:96:LYS:HD3 | 3:Q8:113:LEU:CD1 | 2.48 | 0.43 |
| 4:M8:132:LEU:HD13 | 4:M8:142:PHE:HB2 | 2.00 | 0.43 |
| 4:M8:140:ARG:HH12 | 4:M8:210:ILE:CG1 | 2.31 | 0.43 |
| 2:N8:115:GLU:CA | 5:Z8:32:PRO:CG | 2.90 | 0.43 |
| 12:P8:201:CYC:O2A | 3:S8:67:ILE:HD12 | 2.17 | 0.43 |
| 3:Q8:78:ARG:HD2 | 12:Z8:301:CYC:HMD3 | 2.00 | 0.43 |
| 3:Q8:110:LEU:HD11 | 3:Q8:166:LYS:C | 2.43 | 0.43 |
| 2:R8:99:ALA:HB2 | 3:S8:9:ILE:HD13 | 2.00 | 0.43 |
| 12:L9:202:CYC:C1B | 11:a9:404:TYR:CZ | 3.01 | 0.43 |
| 12:L9:202:CYC:HC | 12:L9:202:CYC:HMD3 | 1.83 | 0.43 |
| 4:M9:62:LYS:HA | 4:M9:62:LYS:HD2 | 1.67 | 0.43 |
| 3:H9:116:THR:CG2 | 11:a9:449:ASN:ND2 | 2.65 | 0.43 |
| 12:R9:201:CYC:HC | 12:R9:201:CYC:HMD3 | 1.83 | 0.43 |
| 2:S9:99:ALA:HB2 | 3:T9:9:ILE:HD13 | 2.00 | 0.43 |
| 12:X9:201:CYC:HC | 12:X9:201:CYC:HMD3 | 1.83 | 0.43 |
| 11:a9:31:SER:HB2 | 11:a9:32:ARG:H | 1.71 | 0.43 |
| 11:a9:112:GLU:O | 11:a9:114:ASP:N | 2.51 | 0.43 |
| 11:a9:787:ARG:NH2 | 11:a9:819:SER:HB3 | 2.27 | 0.43 |
| 11:aA:284:PRO:HG3 | 11:aA:295:ARG:NH2 | 2.33 | 0.43 |
| 11:aA:332:SER:H | 11:aA:333:GLN:HE21 | 1.64 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:aA:558:VAL:HG12 | 11:aA:560:SER:CB | 2.48 | 0.43 |
| 11:aA:745:GLY:CA | 2:K1:14:SER:C | 2.89 | 0.43 |
| 3:H1:124:THR:HB | 3:H1:171:ILE:O | 2.18 | 0.43 |
| 2:I1:138:VAL:O | 2:I1:138:VAL:CG1 | 2.67 | 0.43 |
| 3:L1:2:GLN:HA | 3:L1:6:THR:HG21 | 2.00 | 0.43 |
| 12:B2:201:CYC:HB | 12:B2:201:CYC:HMA3 | 1.83 | 0.43 |
| 1:A:75:THR:HG23 | 10:k5:182:ASN:O | 2.15 | 0.43 |
| 3:LA:84:ARG:NH2 | 11:aA:406:LEU:HD23 | 2.34 | 0.43 |
| 4:MA:176:ARG:CG | 4:MA:176:ARG:NH1 | 2.70 | 0.43 |
| 2:OA:128:ILE:CG2 | 2:OA:132:LYS:HE3 | 2.47 | 0.43 |
| 12:PA:201:CYC:HC | 12:PA:201:CYC:HMD3 | 1.82 | 0.43 |
| 2:QA:67:THR:O | 2:U1:46:SER:HB3 | 2.04 | 0.43 |
| 2:QA:138:VAL:O | 2:QA:138:VAL:CG1 | 2.67 | 0.43 |
| 12:TA:302:CYC:HC | 12:TA:302:CYC:HMD3 | 1.78 | 0.43 |
| 3:P1:124:THR:HB | 3:P1:171:ILE:O | 2.18 | 0.43 |
| 3:R1:124:THR:HB | 3:R1:171:ILE:O | 2.18 | 0.43 |
| 12:I3:201:CYC:CMA | 12:I3:201:CYC:NB | 2.82 | 0.43 |
| 12:H2:201:CYC:HBB2 | 6:M2:243:ALA:HA | 1.95 | 0.43 |
| 12:F3:202:CYC:CMD | 12:F3:202:CYC:NC | 2.75 | 0.43 |
| 2:C4:138:VAL:O | 2:C4:138:VAL:CG1 | 2.67 | 0.43 |
| 3:L3:88:ILE:HD12 | 3:L3:91:ARG:HH21 | 1.81 | 0.43 |
| 2:O3:99:ALA:HB2 | 3:P3:9:ILE:HD13 | 2.00 | 0.43 |
| 2:O3:138:VAL:O | 2:O3:138:VAL:CG1 | 2.67 | 0.43 |
| 12:R3:201:CYC:HC | 12:R3:201:CYC:HMD3 | 1.83 | 0.43 |
| 3:V3:2:GLN:HA | 3:V3:6:THR:HG21 | 2.00 | 0.43 |
| 3:B1:2:GLN:HA | 3:B1:6:THR:HG21 | 2.00 | 0.43 |
| 3:B1:127:VAL:CA | 12:B1:202:CYC:CMC | 2.93 | 0.43 |
| 3:S4:2:GLN:HA | 3:S4:6:THR:HG21 | 2.00 | 0.43 |
| 3:U4:115:GLU:CD | 4:M4:74:LEU:HD12 | 2.43 | 0.43 |
| 12:V4:201:CYC:CMA | 12:V4:201:CYC:NB | 2.82 | 0.43 |
| 12:F4:201:CYC:HB | 12:F4:201:CYC:HMA3 | 1.84 | 0.43 |
| 3:H4:2:GLN:HA | 3:H4:6:THR:HG21 | 2.00 | 0.43 |
| 3:H4:65:ASP:OD1 | 3:H4:65:ASP:N | 2.47 | 0.43 |
| 12:H4:201:CYC:OB | 11:aA:129:ASN:CG | 2.60 | 0.43 |
| 4:M4:142:PHE:O | 4:M4:146:LEU:CG | 2.47 | 0.43 |
| 12:N4:201:CYC:O2A | 3:Q4:67:ILE:HD12 | 2.17 | 0.43 |
| 3:Q4:77:ARG:NH1 | 5:Z4:37:HIS:CE1 | 2.84 | 0.43 |
| 8:O5:37:LEU:HD23 | 8:O5:97:VAL:HG12 | 2.00 | 0.43 |
| 5:Z4:13:SER:HB3 | 5:Z4:14:LYS:H | 1.55 | 0.43 |
| 12:Z4:301:CYC:HMD3 | 12:Z4:301:CYC:HC | 1.83 | 0.43 |
| 2:C1:99:ALA:HB2 | 3:D1:9:ILE:HD13 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:C1:201:CYC:O2A | 3:F1:67:ILE:HD12 | 2.17 | 0.43 |
| 1:f5:114:GLU:HA | 10:j5:491:THR:HG21 | 2.00 | 0.43 |
| 1:P5:118:SER:CB | 10:k5:498:ALA:HB1 | 2.47 | 0.43 |
| 12:Q5:201:CYC:HB | 12:Q5:201:CYC:CMA | 2.21 | 0.43 |
| 1:T5:107:ARG:CZ | 10:j5:482:GLN:CD | 2.91 | 0.43 |
| 8:W5:67:SER:HB3 | 8:W5:68:PRO:HD2 | 2.00 | 0.43 |
| 8:a5:16:ARG:HG3 | 8:a5:16:ARG:HH11 | 1.83 | 0.43 |
| 10:j5:274:MET:HE2 | 10:j5:323:VAL:HG22 | 2.01 | 0.43 |
| 10:j5:382:ILE:HG21 | 10:j5:382:ILE:HD13 | 1.58 | 0.43 |
| 10:j5:637:ARG:HH11 | 10:j5:637:ARG:HD2 | 1.61 | 0.43 |
| 10:k5:190:LEU:HD23 | 10:k5:190:LEU:HA | 1.57 | 0.43 |
| 10:k5:232:ARG:CZ | 10:k5:232:ARG:CB | 2.85 | 0.43 |
| 10:k5:978:LEU:HD21 | 1:p7:107:ARG:HE | 1.78 | 0.43 |
| 10:k5:1052:PRO:CB | 11:a9:32:ARG:CZ | 2.95 | 0.43 |
| 3:D6:2:GLN:HA | 3:D6:6:THR:HG21 | 2.00 | 0.43 |
| 2:G6:138:VAL:O | 2:G6:138:VAL:CG1 | 2.67 | 0.43 |
| 2:I6:138:VAL:O | 2:I6:138:VAL:CG1 | 2.67 | 0.43 |
| 8:E7:8:ILE:O | 8:E7:11:ALA:N | 2.51 | 0.43 |
| 1:F7:72:MET:HE2 | 1:F7:72:MET:HB3 | 1.87 | 0.43 |
| 8:G7:64:ASP:HA | 8:G7:67:SER:CB | 2.49 | 0.43 |
| 8:U7:11:ALA:CB | 8:U7:18:LEU:CD1 | 2.96 | 0.43 |
| 8:U7:21:GLY:O | 8:U7:24:ASP:HB2 | 2.19 | 0.43 |
| 8:W7:8:ILE:O | 8:W7:11:ALA:N | 2.51 | 0.43 |
| 1:X7:3:ASP:H | 1:X7:6:THR:HG1 | 1.63 | 0.43 |
| 1:X7:77:ARG:NH2 | 9:w7:62:GLY:O | 2.52 | 0.43 |
| 8:Y7:64:ASP:HA | 8:Y7:67:SER:CB | 2.48 | 0.43 |
| 1:Z7:71:MEN:O | 1:Z7:77:ARG:HD3 | 2.18 | 0.43 |
| 8:a7:37:LEU:HD23 | 8:a7:97:VAL:HG12 | 1.99 | 0.43 |
| 1:b7:52:ILE:O | 1:b7:52:ILE:CG2 | 2.67 | 0.43 |
| 1:b7:75:THR:HG21 | 8:c7:112:VAL:CG2 | 2.48 | 0.43 |
| 8:c7:36:ARG:NH2 | 8:c7:152:TYR:HH | 2.11 | 0.43 |
| 12:B8:202:CYC:C1D | 4:M8:53:LEU:CD2 | 2.96 | 0.43 |
| 8:o7:2:SER:CB | 1:p7:5:ILE:CB | 2.90 | 0.43 |
| 8:q7:49:ARG:NH1 | 3:H1:63:GLN:HE21 | 2.15 | 0.43 |
| 8:s7:130:VAL:CG1 | 8:s7:157:VAL:HG23 | 2.48 | 0.43 |
| 8:u7:18:LEU:CG | 1:v7:97:LEU:HD13 | 2.49 | 0.43 |
| 12:U8:202:CYC:CMD | 12:U8:202:CYC:NC | 2.75 | 0.43 |
| 4:M8:179:TYR:CZ | 4:M8:230:GLN:HG3 | 2.54 | 0.43 |
| 4:M8:230:GLN:HE22 | 12:M8:301:CYC:HBA1 | 1.84 | 0.43 |
| 4:M8:268:ARG:NH1 | 3:Y8:112:GLY:N | 2.65 | 0.43 |
| 12:M8:302:CYC:HMD3 | 12:M8:302:CYC:HC | 1.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:M8:302:CYC:HAC1 | 3:S8:81:ALA:CB | 2.49 | 0.43 |
| 12:N8:201:CYC:C1B | 3:Q8:76:ASN:OD1 | 2.66 | 0.43 |
| 3:S8:65:ASP:OD1 | 3:S8:65:ASP:N | 2.47 | 0.43 |
| 4:M9:38:PRO:CD | 12:B9:201:CYC:HBB2 | 2.48 | 0.43 |
| 2:Q9:138:VAL:O | 2:Q9:138:VAL:CG1 | 2.67 | 0.43 |
| 5:Z8:14:LYS:HE3 | 5:Z8:14:LYS:HB2 | 1.92 | 0.43 |
| 2:E9:138:VAL:O | 2:E9:138:VAL:CG1 | 2.67 | 0.43 |
| 3:F9:124:THR:HB | 3:F9:171:ILE:O | 2.18 | 0.43 |
| 2:I9:37:SER:HB3 | 2:I9:97:LEU:O | 2.19 | 0.43 |
| 3:J9:68:ARG:HB2 | 11:a9:353:ALA:HB1 | 2.00 | 0.43 |
| 3:J9:124:THR:HB | 3:J9:171:ILE:O | 2.18 | 0.43 |
| 2:K9:138:VAL:O | 2:K9:138:VAL:CG1 | 2.67 | 0.43 |
| 3:X9:2:GLN:HA | 3:X9:6:THR:HG21 | 2.01 | 0.43 |
| 11:a9:50:LEU:HA | 11:a9:50:LEU:HD12 | 1.60 | 0.43 |
| 11:a9:308:LEU:CD2 | 11:a9:312:ASP:HB3 | 2.49 | 0.43 |
| 11:aA:572:THR:CG2 | 11:aA:573:SER:N | 2.82 | 0.43 |
| 11:aA:611:GLY:HA3 | 11:aA:614:SER:HB3 | 2.00 | 0.43 |
| 12:V1:201:CYC:HC | 12:V1:201:CYC:HMD3 | 1.82 | 0.43 |
| 3:B2:67:ILE:HD12 | 12:E2:201:CYC:O2A | 2.17 | 0.43 |
| 2:AA:49:ASP:O | 2:AA:50:SER:C | 2.62 | 0.43 |
| 3:FA:2:GLN:HA | 3:FA:6:THR:HG21 | 2.00 | 0.43 |
| 4:MA:62:LYS:HD2 | 4:MA:62:LYS:HA | 1.67 | 0.43 |
| 4:MA:158:PHE:CZ | 2:UA:10:ALA:CA | 3.01 | 0.43 |
| 4:MA:159:CYS:O | 3:VA:107:ASP:C | 2.62 | 0.43 |
| 2:OA:49:ASP:O | 2:OA:50:SER:C | 2.62 | 0.43 |
| 3:PA:2:GLN:HA | 3:PA:6:THR:HG21 | 2.00 | 0.43 |
| 12:RA:201:CYC:HC | 12:RA:201:CYC:HMD3 | 1.83 | 0.43 |
| 12:RA:202:CYC:HB | 12:RA:202:CYC:HMA3 | 1.84 | 0.43 |
| 2:UA:38:MET:HE2 | 2:UA:38:MET:HB3 | 1.81 | 0.43 |
| 3:VA:67:ILE:HD12 | 12:WA:201:CYC:O2A | 2.17 | 0.43 |
| 12:A1:201:CYC:CMA | 12:A1:201:CYC:NB | 2.82 | 0.43 |
| 3:H3:62:GLU:O | 8:k7:49:ARG:HD2 | 2.19 | 0.43 |
| 12:H3:201:CYC:HB | 12:H3:201:CYC:HMA3 | 1.84 | 0.43 |
| 3:J3:67:ILE:HD12 | 12:K3:201:CYC:O2A | 2.17 | 0.43 |
| 12:G2:201:CYC:CMA | 12:G2:201:CYC:NB | 2.81 | 0.43 |
| 3:J2:124:THR:HB | 3:J2:171:ILE:O | 2.18 | 0.43 |
| 3:L2:70:GLY:HA2 | 6:M2:67:GLY:CA | 2.45 | 0.43 |
| 6:M2:42:VAL:HG11 | 8:i7:56:ASP:OD1 | 2.19 | 0.43 |
| 6:M2:239:TRP:CD1 | 6:M2:241:GLY:H | 2.37 | 0.43 |
| 12:N2:101:CYC:HC | 12:N2:101:CYC:HMD3 | 1.83 | 0.43 |
| 2:E3:138:VAL:O | 2:E3:138:VAL:CG1 | 2.67 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:A4:24:LEU:HB3 | 12:B4:201:CYC:HAB2 | 2.00 | 0.43 |
| 12:B4:201:CYC:HB | 12:B4:201:CYC:HMA3 | 1.84 | 0.43 |
| 3:D4:150:ARG:NH1 | 2:C1:140:SER:C | 2.77 | 0.43 |
| 3:L3:2:GLN:HA | 3:L3:6:THR:HG21 | 2.00 | 0.43 |
| 2:O3:49:ASP:O | 2:O3:50:SER:C | 2.62 | 0.43 |
| 2:Q3:99:ALA:HB2 | 3:R3:9:ILE:HD13 | 2.00 | 0.43 |
| 3:X3:124:THR:HB | 3:X3:171:ILE:O | 2.18 | 0.43 |
| 2:T4:99:ALA:HB2 | 3:U4:9:ILE:HD13 | 2.00 | 0.43 |
| 2:E4:138:VAL:O | 2:E4:138:VAL:CG1 | 2.67 | 0.43 |
| 12:E4:201:CYC:CMA | 12:E4:201:CYC:NB | 2.81 | 0.43 |
| 12:H4:202:CYC:HB | 12:H4:202:CYC:HMA3 | 1.83 | 0.43 |
| 3:L4:68:ARG:HG3 | 11:aA:81:ASP:C | 2.43 | 0.43 |
| 3:L4:69:PRO:C | 3:L4:71:GLY:N | 2.76 | 0.43 |
| 4:M4:27:HIS:ND1 | 4:M4:35:THR:O | 2.49 | 0.43 |
| 4:M4:56:MET:CE | 4:M4:69:ILE:HD11 | 2.48 | 0.43 |
| 4:M4:144:ARG:CZ | 5:Z4:59:ARG:CZ | 2.94 | 0.43 |
| 3:O4:2:GLN:HA | 3:O4:6:THR:HG21 | 2.01 | 0.43 |
| 3:O4:108:ARG:N | 5:Z4:61:LYS:CE | 2.81 | 0.43 |
| 2:P4:138:VAL:O | 2:P4:138:VAL:CG1 | 2.67 | 0.43 |
| 3:Q4:82:CYS:O | 3:Q4:86:MET:HG3 | 2.18 | 0.43 |
| 3:Q4:85:ASP:HA | 3:Q4:88:ILE:CD1 | 2.47 | 0.43 |
| 8:K5:96:ILE:HD13 | 8:K5:96:ILE:HG21 | 1.60 | 0.43 |
| 12:O5:201:CYC:HB | 12:O5:201:CYC:CMA | 2.21 | 0.43 |
| 8:A5:115:MET:SD | 12:A5:201:CYC:CHB | 3.06 | 0.43 |
| 8:A5:119:LEU:HD11 | 12:A5:201:CYC:HAA2 | 2.00 | 0.43 |
| 8:G5:119:LEU:HD13 | 12:G5:201:CYC:HHA | 1.90 | 0.43 |
| 1:J5:76:ARG:HH22 | 9:i5:67:VAL:HG21 | 1.84 | 0.43 |
| 12:P5:201:CYC:HMD1 | 12:P5:201:CYC:NC | 2.09 | 0.43 |
| 1:R5:72:MET:HE2 | 1:R5:72:MET:HB3 | 1.87 | 0.43 |
| 8:Y5:64:ASP:HA | 8:Y5:67:SER:CB | 2.48 | 0.43 |
| 3:J6:88:ILE:CD1 | 6:M6:185:PHE:CZ | 3.01 | 0.43 |
| 6:M6:147:ASP:CG | 2:E6:15:GLN:HG2 | 2.43 | 0.43 |
| 6:M6:239:TRP:CD1 | 6:M6:241:GLY:H | 2.37 | 0.43 |
| 8:A7:64:ASP:HA | 8:A7:67:SER:CB | 2.49 | 0.43 |
| 9:i5:8:THR:O | 9:i5:51:VAL:HG13 | 2.18 | 0.43 |
| 10:j5:144:ASN:OD1 | 10:j5:144:ASN:N | 2.50 | 0.43 |
| 10:j5:156:SER:OG | 12:j5:1201:CYC:C4C | 2.65 | 0.43 |
| 10:j5:184:LEU:HA | 10:j5:184:LEU:HD23 | 1.50 | 0.43 |
| 10:j5:395:SER:HA | 10:j5:400:ALA:HB2 | 2.00 | 0.43 |
| 10:j5:725:LEU:HD23 | 8:K7:83:ARG:HD3 | 2.01 | 0.43 |
| 10:j5:870:GLU:OE2 | 10:j5:870:GLU:HA | 2.15 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:1064:LYS:HD2 | 10:j5:1065:HIS:HA | 2.01 | 0.43 |
| 10:k5:481:ILE:HG21 | 10:k5:481:ILE:HD13 | 1.69 | 0.43 |
| 10:k5:542:GLN:HG3 | 10:k5:560:VAL:HG12 | 1.99 | 0.43 |
| 10:k5:643:VAL:O | 10:k5:643:VAL:HG12 | 2.16 | 0.43 |
| 10:k5:778:LYS:NZ | 12:F7:201:CYC:CBB | 2.60 | 0.43 |
| 2:A6:138:VAL:O | 2:A6:138:VAL:CG1 | 2.67 | 0.43 |
| 8:O7:67:SER:HB3 | 8:O7:68:PRO:HD2 | 2.00 | 0.43 |
| 1:P7:14:VAL:C | 1:N7:68:PRO:CB | 2.67 | 0.43 |
| 1:R7:87:TYR:CE2 | 9:z7:38:PHE:CE1 | 3.03 | 0.43 |
| 8:S7:130:VAL:CG1 | 8:S7:157:VAL:HG23 | 2.48 | 0.43 |
| 8:C7:2:SER:O | 8:C7:100:ASP:OD2 | 2.37 | 0.43 |
| 8:I7:37:LEU:HD23 | 8:I7:97:VAL:HG12 | 2.00 | 0.43 |
| 12:L7:201:CYC:CMA | 12:L7:201:CYC:NB | 2.74 | 0.43 |
| 1:Z7:14:VAL:CG1 | 9:x7:64:ASN:HD21 | 2.32 | 0.43 |
| 2:E1:99:ALA:HB2 | 3:F1:9:ILE:HD13 | 2.00 | 0.43 |
| 2:A8:34:ALA:HB3 | 3:B8:31:VAL:CG1 | 2.39 | 0.43 |
| 12:A8:201:CYC:CMA | 12:A8:201:CYC:NB | 2.82 | 0.43 |
| 12:D8:202:CYC:HC | 12:D8:202:CYC:HMD3 | 1.83 | 0.43 |
| 8:o7:18:LEU:HB2 | 1:p7:97:LEU:HD11 | 2.01 | 0.43 |
| 9:y7:63:ALA:HB1 | 9:y7:64:ASN:H | 1.42 | 0.43 |
| 3:W8:2:GLN:HA | 3:W8:6:THR:HG21 | 2.00 | 0.43 |
| 2:G8:99:ALA:HB2 | 3:H8:9:ILE:HD13 | 2.00 | 0.43 |
| 2:I8:111:ALA:HA | 11:a9:133:LEU:HD13 | 2.01 | 0.43 |
| 3:L8:86:MET:HG2 | 12:a9:901:CYC:CBC | 2.29 | 0.43 |
| 4:M8:19:MET:HE2 | 4:M8:59:ILE:CD1 | 2.46 | 0.43 |
| 4:M8:104:ALA:HA | 2:P8:14:SER:HB3 | 1.80 | 0.43 |
| 2:N8:49:ASP:O | 2:N8:50:SER:C | 2.62 | 0.43 |
| 3:Q8:105:LEU:HD21 | 3:Q8:166:LYS:HB2 | 1.99 | 0.43 |
| 2:Q9:99:ALA:HB2 | 3:R9:9:ILE:HD13 | 2.00 | 0.43 |
| 5:Z8:13:SER:HB3 | 5:Z8:14:LYS:H | 1.55 | 0.43 |
| 2:A9:24:LEU:HB3 | 12:B9:202:CYC:HAB2 | 2.00 | 0.43 |
| 3:H9:124:THR:HB | 3:H9:171:ILE:O | 2.18 | 0.43 |
| 2:I9:8:VAL:CG1 | 2:I9:23:GLU:OE2 | 2.64 | 0.43 |
| 2:S9:38:MET:HE2 | 2:S9:38:MET:HB3 | 1.81 | 0.43 |
| 3:V9:2:GLN:HA | 3:V9:6:THR:HG21 | 2.00 | 0.43 |
| 3:V9:124:THR:HB | 3:V9:171:ILE:O | 2.18 | 0.43 |
| 11:aA:308:LEU:CD2 | 11:aA:312:ASP:HB3 | 2.49 | 0.43 |
| 11:aA:363:GLN:H | 11:aA:363:GLN:HE21 | 1.66 | 0.43 |
| 12:I1:201:CYC:CMA | 12:I1:201:CYC:NB | 2.82 | 0.43 |
| 4:M1:120:LEU:HD11 | 3:X1:84:ARG:HH12 | 1.83 | 0.43 |
| 3:F2:126:SER:CB | 12:F2:201:CYC:HMC1 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:BA:30:LEU:CD1 | 3:BA:30:LEU:N | 2.80 | 0.43 |
| 2:IA:37:SER:HB3 | 2:IA:97:LEU:O | 2.19 | 0.43 |
| 2:KA:138:VAL:O | 2:KA:138:VAL:CG1 | 2.67 | 0.43 |
| 4:MA:5:THR:C | 4:MA:6:THR:OG1 | 2.56 | 0.43 |
| 4:MA:9:GLN:CD | 4:MA:9:GLN:C | 2.87 | 0.43 |
| 5:NA:54:LEU:CD2 | 3:TA:84:ARG:NH1 | 2.67 | 0.43 |
| 12:OA:201:CYC:CMA | 12:OA:201:CYC:NB | 2.82 | 0.43 |
| 2:QA:81:LYS:HZ3 | 3:TA:67:ILE:CD1 | 2.31 | 0.43 |
| 12:QA:201:CYC:CMA | 12:QA:201:CYC:NB | 2.81 | 0.43 |
| 3:XA:124:THR:HB | 3:XA:171:ILE:O | 2.18 | 0.43 |
| 3:R1:69:PRO:HA | 3:R1:74:TYR:CD2 | 2.53 | 0.43 |
| 7:N2:5:VAL:HG23 | 3:F2:108:ARG:HH12 | 1.80 | 0.43 |
| 3:Z3:124:THR:HB | 3:Z3:171:ILE:O | 2.18 | 0.43 |
| 12:Z3:202:CYC:HC | 12:Z3:202:CYC:HMD3 | 1.78 | 0.43 |
| 2:A4:49:ASP:O | 2:A4:50:SER:C | 2.62 | 0.43 |
| 12:D4:202:CYC:O2A | 4:M4:35:THR:CB | 2.57 | 0.43 |
| 3:L3:124:THR:HB | 3:L3:171:ILE:O | 2.18 | 0.43 |
| 4:M3:241:LEU:HD23 | 4:M3:241:LEU:HA | 1.63 | 0.43 |
| 5:N3:53:LEU:HD13 | 12:R3:201:CYC:HAA1 | 2.01 | 0.43 |
| 12:T3:302:CYC:HB | 12:T3:302:CYC:HMA3 | 1.84 | 0.43 |
| 3:S4:3:ASP:H | 3:S4:6:THR:HB | 1.84 | 0.43 |
| 3:L4:124:THR:HB | 3:L4:171:ILE:O | 2.18 | 0.43 |
| 4:M4:37:GLU:HG3 | 4:M4:38:PRO:HD2 | 2.00 | 0.43 |
| 4:M4:205:ASP:OD2 | 5:Z4:59:ARG:HB2 | 2.12 | 0.43 |
| 1:L5:82:ILE:HD13 | 8:G5:118:SER:CB | 2.48 | 0.43 |
| 12:X4:201:CYC:CMA | 12:X4:201:CYC:NB | 2.81 | 0.43 |
| 3:Y4:110:LEU:HB3 | 3:Y4:170:SER:CB | 2.49 | 0.43 |
| 1:B5:14:VAL:HG11 | 10:k5:555:ALA:N | 2.32 | 0.43 |
| 8:G5:6:LYS:CE | 8:S5:21:GLY:H | 2.31 | 0.43 |
| 8:G5:121:THR:HG22 | 12:G5:201:CYC:HMC3 | 2.01 | 0.43 |
| 8:G5:161:GLN:NE2 | 1:T5:49:THR:HG22 | 2.34 | 0.43 |
| 1:J5:39:ARG:C | 1:J5:41:ALA:N | 2.70 | 0.43 |
| 1:f5:71:MEN:O | 1:f5:77:ARG:HD3 | 2.18 | 0.43 |
| 1:P5:101:PRO:HB2 | 1:b5:113:LYS:NZ | 2.33 | 0.43 |
| 1:P5:123:ILE:CG2 | 10:k5:11:VAL:HG23 | 2.49 | 0.43 |
| 8:U5:27:LYS:HA | 8:U5:30:VAL:HG22 | 1.99 | 0.43 |
| 1:b5:71:MEN:O | 1:b5:77:ARG:HD3 | 2.18 | 0.43 |
| 10:j5:277:ILE:CB | 10:j5:284:PRO:HA | 2.49 | 0.43 |
| 10:j5:540:LEU:HD21 | 10:j5:544:VAL:HG21 | 2.00 | 0.43 |
| 10:j5:649:PHE:O | 10:j5:649:PHE:CG | 2.69 | 0.43 |
| 10:j5:971:VAL:CG1 | 1:t7:76:ARG:HH22 | 2.32 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:k5:1033:ARG:NH2 | 10:k5:1098:GLU:HG2 | 2.34 | 0.43 |
| 2:G6:99:ALA:HB2 | 3:H6:9:ILE:HD13 | 2.00 | 0.43 |
| 3:H6:2:GLN:HA | 3:H6:6:THR:HG21 | 2.00 | 0.43 |
| 3:D1:68:ARG:CZ | 3:X1:68:ARG:HH12 | 2.31 | 0.43 |
| 8:O7:6:LYS:HZ1 | 8:E7:19:SER:HB3 | 1.83 | 0.43 |
| 8:E7:67:SER:HB3 | 8:E7:68:PRO:HD2 | 2.00 | 0.43 |
| 8:W7:12:ASP:C | 9:w7:46:LYS:HE2 | 2.44 | 0.43 |
| 8:a7:130:VAL:CG1 | 8:a7:157:VAL:HG23 | 2.48 | 0.43 |
| 8:c7:67:SER:HB3 | 8:c7:68:PRO:HD2 | 2.00 | 0.43 |
| 8:c7:141:LEU:HD12 | 8:c7:146:ALA:HA | 2.01 | 0.43 |
| 8:e7:67:SER:HB3 | 8:e7:68:PRO:HD2 | 2.00 | 0.43 |
| 8:e7:130:VAL:CG1 | 8:e7:157:VAL:HG23 | 2.48 | 0.43 |
| 2:A8:138:VAL:O | 2:A8:138:VAL:CG1 | 2.67 | 0.43 |
| 8:o7:5:THR:OG1 | 1:p7:6:THR:HG23 | 2.12 | 0.43 |
| 8:q7:120:GLN:CG | 1:v7:53:LYS:NZ | 2.78 | 0.43 |
| 8:s7:2:SER:O | 8:s7:100:ASP:OD2 | 2.37 | 0.43 |
| 9:y7:15:LYS:O | 9:y7:16:ARG:HG3 | 2.19 | 0.43 |
| 2:G8:15:GLN:HE21 | 11:a9:120:ARG:HH11 | 1.67 | 0.43 |
| 4:M8:99:VAL:HG13 | 3:Q8:108:ARG:HH12 | 1.83 | 0.43 |
| 4:M8:126:THR:CB | 12:M8:302:CYC:CGA | 2.70 | 0.43 |
| 4:M8:268:ARG:O | 4:M8:269:SER:C | 2.52 | 0.43 |
| 2:N8:138:VAL:O | 2:N8:138:VAL:CG1 | 2.67 | 0.43 |
| 3:Q8:124:THR:HB | 3:Q8:171:ILE:O | 2.18 | 0.43 |
| 3:S8:2:GLN:HA | 3:S8:6:THR:HG21 | 2.00 | 0.43 |
| 3:L9:9:ILE:HD13 | 2:K9:99:ALA:HB2 | 2.00 | 0.43 |
| 3:L9:124:THR:HB | 3:L9:171:ILE:O | 2.18 | 0.43 |
| 4:M9:176:ARG:CG | 4:M9:176:ARG:NH1 | 2.70 | 0.43 |
| 2:O9:138:VAL:O | 2:O9:138:VAL:CG1 | 2.67 | 0.43 |
| 3:P9:2:GLN:HA | 3:P9:6:THR:HG21 | 2.00 | 0.43 |
| 5:Z8:37:HIS:CB | 12:Z8:301:CYC:C4B | 2.97 | 0.43 |
| 3:B9:30:LEU:CD1 | 3:B9:30:LEU:N | 2.80 | 0.43 |
| 3:H9:66:LEU:HD13 | 12:H9:202:CYC:H2C | 2.01 | 0.43 |
| 12:Z9:202:CYC:HC | 12:Z9:202:CYC:HMD3 | 1.82 | 0.43 |
| 11:a9:30:MET:HE3 | 11:a9:35:ARG:CA | 2.46 | 0.43 |
| 11:a9:112:GLU:CG | 11:a9:113:ALA:N | 2.82 | 0.43 |
| 11:a9:419:ARG:O | 11:a9:421:GLY:N | 2.52 | 0.43 |
| 11:a9:581:ARG:HD2 | 11:a9:581:ARG:O | 2.18 | 0.43 |
| 11:aA:538:ARG:HB3 | 11:aA:538:ARG:HE | 1.58 | 0.43 |
| 11:aA:581:ARG:HD2 | 11:aA:581:ARG:O | 2.18 | 0.43 |
| 11:aA:657:ARG:NH1 | 2:I1:15:GLN:O | 2.32 | 0.43 |
| 4:M1:188:LEU:HD23 | 12:Z1:202:CYC:HMA2 | 1.97 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:N1:39:PRO:HD2 | 12:T1:301:CYC:HBB2 | 1.99 | 0.43 |
| 2:Y1:38:MET:HE2 | 2:Y1:38:MET:HB3 | 1.81 | 0.43 |
| 12:Z1:202:CYC:HC | 12:Z1:202:CYC:HMD3 | 1.82 | 0.43 |
| 2:A2:34:ALA:HB3 | 3:B2:31:VAL:CG1 | 2.39 | 0.43 |
| 2:C2:138:VAL:O | 2:C2:138:VAL:CG1 | 2.67 | 0.43 |
| 12:D2:201:CYC:HC | 12:D2:201:CYC:HMD3 | 1.83 | 0.43 |
| 2:AA:24:LEU:HB3 | 12:BA:202:CYC:HAB2 | 2.00 | 0.43 |
| 3:FA:36:LYS:O | 3:FA:156:LEU:CD2 | 2.66 | 0.43 |
| 3:HA:124:THR:HB | 3:HA:171:ILE:O | 2.18 | 0.43 |
| 2:IA:155:ASP:O | 2:IA:159:ASN:OD1 | 2.37 | 0.43 |
| 4:MA:118:TYR:CD1 | 3:ZA:84:ARG:CZ | 3.01 | 0.43 |
| 3:VA:108:ARG:CG | 3:VA:108:ARG:HH21 | 2.32 | 0.43 |
| 3:ZA:2:GLN:HA | 3:ZA:6:THR:HG21 | 2.00 | 0.43 |
| 2:I2:99:ALA:HB2 | 3:J2:9:ILE:HD13 | 2.00 | 0.43 |
| 2:I2:138:VAL:O | 2:I2:138:VAL:CG1 | 2.67 | 0.43 |
| 12:L3:201:CYC:HB | 12:L3:201:CYC:HMA3 | 1.84 | 0.43 |
| 3:T3:2:GLN:HA | 3:T3:6:THR:HG21 | 2.00 | 0.43 |
| 12:V3:202:CYC:HB | 12:V3:202:CYC:HMA3 | 1.84 | 0.43 |
| 3:X3:2:GLN:HA | 3:X3:6:THR:HG21 | 2.00 | 0.43 |
| 12:U4:201:CYC:HC | 12:U4:201:CYC:HMD3 | 1.82 | 0.43 |
| 3:F4:108:ARG:HE | 4:M4:9:GLN:CA | 2.32 | 0.43 |
| 3:J4:2:GLN:HA | 3:J4:6:THR:HG21 | 2.00 | 0.43 |
| 2:K4:138:VAL:O | 2:K4:138:VAL:CG1 | 2.67 | 0.43 |
| 4:M4:21:LEU:HD12 | 4:M4:21:LEU:C | 2.37 | 0.43 |
| 4:M4:94:TRP:CZ2 | 5:Z4:31:TRP:HZ2 | 2.37 | 0.43 |
| 4:M4:232:VAL:HG11 | 3:Y4:110:LEU:HA | 2.01 | 0.43 |
| 2:N4:118:ARG:HH12 | 5:Z4:32:PRO:CB | 2.31 | 0.43 |
| 12:R4:201:CYC:CMA | 12:R4:201:CYC:NB | 2.81 | 0.43 |
| 12:K5:201:CYC:HBB2 | 1:J5:73:TYR:CE1 | 2.53 | 0.43 |
| 8:O5:2:SER:O | 8:O5:100:ASP:OD2 | 2.37 | 0.43 |
| 2:X4:138:VAL:O | 2:X4:138:VAL:CG1 | 2.67 | 0.43 |
| 3:Y4:2:GLN:HA | 3:Y4:6:THR:HG21 | 2.00 | 0.43 |
| 8:A5:130:VAL:CG1 | 8:A5:157:VAL:HG23 | 2.48 | 0.43 |
| 8:C5:67:SER:HB3 | 8:C5:68:PRO:HD2 | 2.00 | 0.43 |
| 1:D5:76:ARG:HH12 | 9:z5:67:VAL:HB | 1.82 | 0.43 |
| 8:E5:80:LEU:HD12 | 12:E5:201:CYC:C3D | 2.48 | 0.43 |
| 8:I5:2:SER:O | 8:I5:100:ASP:OD2 | 2.37 | 0.43 |
| 2:C1:138:VAL:O | 2:C1:138:VAL:CG1 | 2.67 | 0.43 |
| 1:d5:62:TYR:OH | 12:e5:201:CYC:O1D | 2.30 | 0.43 |
| 8:Y5:114:GLU:OE2 | 10:k5:312:TYR:C | 2.61 | 0.43 |
| 8:a5:130:VAL:CG1 | 8:a5:157:VAL:HG23 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 12:J6:201:CYC:CMD | 12:J6:201:CYC:NC | 2.75 | 0.43 |
| 6:M6:43:TRP:CH2 | 8:c7:52:LYS:CB | 3.02 | 0.43 |
| 10:j5:190:LEU:HD23 | 10:j5:190:LEU:HA | 1.57 | 0.43 |
| 10:j5:262:TYR:CD1 | 10:j5:262:TYR:C | 2.97 | 0.43 |
| 10:j5:322:LYS:NZ | 10:j5:336:ARG:NH1 | 2.66 | 0.43 |
| 10:j5:328:ILE:HG21 | 10:j5:336:ARG:NH2 | 2.33 | 0.43 |
| 10:j5:352:ILE:HG22 | 10:j5:354:SER:H | 1.84 | 0.43 |
| 10:j5:362:LYS:HG2 | 10:j5:362:LYS:O | 2.18 | 0.43 |
| 10:j5:630:ILE:HD13 | 10:j5:630:ILE:HG21 | 1.68 | 0.43 |
| 10:j5:793:SER:O | 12:T7:201:CYC:HBA1 | 2.19 | 0.43 |
| 10:j5:978:LEU:HD12 | 10:j5:978:LEU:HA | 1.88 | 0.43 |
| 10:k5:153:MET:HE3 | 10:k5:153:MET:HB3 | 1.94 | 0.43 |
| 10:k5:362:LYS:O | 10:k5:362:LYS:HG2 | 2.18 | 0.43 |
| 10:k5:386:ILE:CG2 | 10:k5:387:VAL:N | 2.36 | 0.43 |
| 10:k5:568:ILE:O | 10:k5:568:ILE:CG2 | 2.66 | 0.43 |
| 10:k5:990:ARG:HG2 | 8:a7:110:ILE:HD12 | 2.01 | 0.43 |
| 10:k5:1001:TYR:CE1 | 10:k5:1016:LEU:HD11 | 2.54 | 0.43 |
| 12:D1:202:CYC:HC | 12:D1:202:CYC:HMD3 | 1.83 | 0.43 |
| 8:I7:2:SER:HA | 8:I7:100:ASP:HB3 | 2.01 | 0.43 |
| 12:h7:201:CYC:HC | 12:h7:201:CYC:CMD | 2.14 | 0.43 |
| 8:i7:109:ILE:HG21 | 8:i7:159:ALA:HB1 | 2.01 | 0.43 |
| 8:i7:112:VAL:HG12 | 8:i7:113:LYS:H | 1.78 | 0.43 |
| 8:U7:33:GLY:HA2 | 8:U7:36:ARG:HB2 | 2.01 | 0.43 |
| 12:W7:201:CYC:HB | 12:W7:201:CYC:CMA | 2.21 | 0.43 |
| 8:a7:2:SER:O | 8:a7:100:ASP:OD2 | 2.37 | 0.43 |
| 8:a7:66:VAL:O | 8:a7:66:VAL:CG1 | 2.66 | 0.43 |
| 8:c7:46:ALA:HB2 | 8:c7:140:LEU:HD12 | 1.87 | 0.43 |
| 8:c7:109:ILE:HG21 | 8:c7:159:ALA:HB1 | 2.01 | 0.43 |
| 8:c7:138:THR:O | 8:c7:138:THR:HG23 | 2.18 | 0.43 |
| 8:m7:33:GLY:HA2 | 8:m7:36:ARG:HB2 | 2.01 | 0.43 |
| 12:U8:201:CYC:HC | 12:U8:201:CYC:HMD3 | 1.82 | 0.43 |
| 3:W8:124:THR:HB | 3:W8:171:ILE:O | 2.18 | 0.43 |
| 3:F8:113:LEU:HB3 | 3:F8:171:ILE:HG12 | 2.01 | 0.43 |
| 3:F8:118:VAL:HG12 | 3:Y8:119:ALA:HA | 2.01 | 0.43 |
| 12:G8:201:CYC:CMA | 12:G8:201:CYC:NB | 2.82 | 0.43 |
| 12:J8:201:CYC:HC | 12:J8:201:CYC:HMD3 | 1.83 | 0.43 |
| 2:N8:112:GLY:HA2 | 5:Z8:34:LEU:N | 1.83 | 0.43 |
| 4:M9:132:LEU:CD1 | 4:M9:142:PHE:CB | 2.95 | 0.43 |
| 3:B9:124:THR:HB | 3:B9:171:ILE:O | 2.18 | 0.43 |
| 12:D9:201:CYC:HC | 12:D9:201:CYC:HMD3 | 1.83 | 0.43 |
| 2:G9:138:VAL:O | 2:G9:138:VAL:CG1 | 2.67 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:R9:2:GLN:HA | 3:R9:6:THR:HG21 | 2.00 | 0.43 |
| 12:V9:202:CYC:HB | 12:V9:202:CYC:HMA3 | 1.84 | 0.43 |
| 2:W9:138:VAL:O | 2:W9:138:VAL:CG1 | 2.67 | 0.43 |
| 11:a9:38:VAL:HG12 | 11:a9:39:PRO:CD | 2.48 | 0.43 |
| 11:a9:486:ILE:HD13 | 11:a9:486:ILE:HA | 1.79 | 0.43 |
| 11:a9:643:LEU:HD21 | 11:a9:689:VAL:HG22 | 1.91 | 0.43 |
| 11:aA:38:VAL:HG12 | 11:aA:39:PRO:CD | 2.48 | 0.43 |
| 11:aA:327:SER:C | 11:aA:329:ASN:H | 2.27 | 0.43 |
| 11:aA:419:ARG:O | 11:aA:421:GLY:N | 2.52 | 0.43 |
| 11:aA:426:ARG:NH1 | 11:aA:430:ARG:HH21 | 2.16 | 0.43 |
| 11:aA:710:THR:HB | 11:aA:807:GLN:HB3 | 1.96 | 0.43 |
| 11:aA:713:ASN:OD1 | 12:aA:902:CYC:CMA | 2.66 | 0.43 |
| 2:K1:138:VAL:O | 2:K1:138:VAL:CG1 | 2.67 | 0.43 |
| 4:M1:134:ASN:CG | 5:N1:1:MET:H2 | 2.27 | 0.43 |
| 2:A2:59:VAL:O | 2:A2:66:LEU:CD1 | 2.62 | 0.43 |
| 2:E2:138:VAL:O | 2:E2:138:VAL:CG1 | 2.67 | 0.43 |
| 3:F2:2:GLN:HA | 3:F2:6:THR:HG21 | 2.00 | 0.43 |
| 12:DA:201:CYC:HC | 12:DA:201:CYC:HMD3 | 1.83 | 0.43 |
| 2:EA:17:ARG:CZ | 2:IA:2:LYS:NZ | 2.82 | 0.43 |
| 12:GA:201:CYC:CMA | 12:GA:201:CYC:NB | 2.82 | 0.43 |
| 2:IA:20:ASN:O | 2:IA:24:LEU:HG | 2.18 | 0.43 |
| 4:MA:51:ARG:NH1 | 4:MA:51:ARG:CG | 2.77 | 0.43 |
| 3:TA:124:THR:HB | 3:TA:171:ILE:O | 2.18 | 0.43 |
| 12:UA:201:CYC:CMA | 12:UA:201:CYC:NB | 2.82 | 0.43 |
| 12:YA:201:CYC:CMA | 12:YA:201:CYC:NB | 2.81 | 0.43 |
| 12:ZA:202:CYC:HB | 12:ZA:202:CYC:CMA | 2.25 | 0.43 |
| 12:P1:202:CYC:HB | 12:P1:202:CYC:HMA3 | 1.84 | 0.43 |
| 3:J2:88:ILE:CD1 | 6:M2:185:PHE:CZ | 3.01 | 0.43 |
| 3:L2:70:GLY:HA2 | 6:M2:68:THR:H | 1.84 | 0.43 |
| 12:L2:201:CYC:HC | 12:L2:201:CYC:HMD3 | 1.83 | 0.43 |
| 12:L2:202:CYC:C4B | 2:A2:33:ARG:NH1 | 2.44 | 0.43 |
| 6:M2:278:ARG:NH2 | 1:j7:67:ARG:HH12 | 2.17 | 0.43 |
| 12:L3:202:CYC:HAA1 | 11:a9:731:GLN:HE21 | 1.84 | 0.43 |
| 4:M3:211:GLN:O | 5:N3:28:HIS:NE2 | 2.45 | 0.43 |
| 5:N3:50:LEU:CD2 | 12:R3:201:CYC:O1D | 2.66 | 0.43 |
| 2:U3:138:VAL:O | 2:U3:138:VAL:CG1 | 2.67 | 0.43 |
| 12:X3:202:CYC:HMD3 | 12:X3:202:CYC:NC | 2.34 | 0.43 |
| 3:B1:3:ASP:H | 3:B1:6:THR:HB | 1.84 | 0.43 |
| 2:E4:99:ALA:HB2 | 3:F4:9:ILE:HD13 | 2.00 | 0.43 |
| 3:F4:124:THR:HB | 3:F4:171:ILE:O | 2.18 | 0.43 |
| 4:M4:29:PRO:CB | 11:aA:226:PHE:HA | 2.45 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M4:94:TRP:HZ3 | 3:Q4:91:ARG:HB3 | 1.83 | 0.43 |
| 4:M4:226:SER:HB2 | 3:Y4:85:ASP:HA | 2.00 | 0.43 |
| 12:P4:201:CYC:CMA | 12:P4:201:CYC:NB | 2.82 | 0.43 |
| 1:L5:71:MEN:O | 1:L5:77:ARG:HD3 | 2.18 | 0.43 |
| 8:A5:53:GLN:HB3 | 8:A5:136:VAL:HG21 | 2.00 | 0.43 |
| 8:A5:71:ASN:CG | 12:A5:201:CYC:CMD | 2.85 | 0.43 |
| 1:D5:76:ARG:NH1 | 9:z5:67:VAL:HG11 | 2.34 | 0.43 |
| 8:I5:37:LEU:HD11 | 1:J5:31:PHE:HE2 | 1.83 | 0.43 |
| 8:e5:2:SER:O | 8:e5:100:ASP:OD2 | 2.37 | 0.43 |
| 8:U5:2:SER:HA | 8:U5:100:ASP:HB3 | 2.01 | 0.43 |
| 8:Y5:120:GLN:CD | 1:b5:53:LYS:HZ2 | 2.27 | 0.43 |
| 3:L6:2:GLN:HA | 3:L6:6:THR:HG21 | 2.00 | 0.43 |
| 7:N6:15:VAL:HA | 7:N6:44:PRO:HA | 2.01 | 0.43 |
| 8:A7:130:VAL:CG1 | 8:A7:157:VAL:HG23 | 2.48 | 0.43 |
| 9:i5:7:VAL:HG22 | 9:i5:30:LYS:O | 2.18 | 0.43 |
| 10:j5:305:PHE:HE2 | 10:j5:337:LEU:HD23 | 1.83 | 0.43 |
| 10:j5:834:LYS:O | 10:j5:834:LYS:CG | 2.66 | 0.43 |
| 10:k5:182:ASN:HD22 | 10:k5:182:ASN:H | 1.67 | 0.43 |
| 10:k5:277:ILE:CB | 10:k5:284:PRO:HA | 2.49 | 0.43 |
| 10:k5:283:ARG:C | 10:k5:283:ARG:CD | 2.84 | 0.43 |
| 10:k5:339:LYS:HB2 | 10:k5:399:TYR:CE1 | 2.54 | 0.43 |
| 10:k5:367:ARG:NH1 | 10:k5:410:GLU:OE1 | 2.51 | 0.43 |
| 10:k5:387:VAL:O | 10:k5:394:PRO:HG3 | 2.05 | 0.43 |
| 10:k5:826:THR:CG2 | 12:B7:201:CYC:CMA | 2.97 | 0.43 |
| 12:F6:201:CYC:HMD3 | 12:F6:201:CYC:HC | 1.82 | 0.43 |
| 8:O7:2:SER:HA | 8:O7:100:ASP:HB3 | 2.01 | 0.43 |
| 8:O7:11:ALA:CB | 8:O7:18:LEU:CD1 | 2.96 | 0.43 |
| 8:S7:67:SER:HB3 | 8:S7:68:PRO:HD2 | 2.00 | 0.43 |
| 8:I7:6:LYS:HD3 | 8:W7:21:GLY:HA3 | 2.01 | 0.43 |
| 8:I7:130:VAL:CG1 | 8:I7:157:VAL:HG23 | 2.49 | 0.43 |
| 8:i7:19:SER:OG | 8:s7:101:VAL:HG21 | 2.18 | 0.43 |
| 8:i7:156:LEU:O | 8:i7:160:MET:HG3 | 2.19 | 0.43 |
| 1:b7:46:SER:HA | 8:o7:158:GLY:HA2 | 2.01 | 0.43 |
| 8:c7:139:SER:O | 8:c7:139:SER:OG | 2.36 | 0.43 |
| 8:c7:141:LEU:HB2 | 8:c7:146:ALA:HB2 | 2.01 | 0.43 |
| 3:B8:124:THR:HB | 3:B8:171:ILE:O | 2.18 | 0.43 |
| 8:m7:67:SER:HB3 | 8:m7:68:PRO:HD2 | 2.00 | 0.43 |
| 8:s7:27:LYS:HA | 8:s7:30:VAL:HG22 | 2.00 | 0.43 |
| 8:u7:3:VAL:O | 8:u7:7:ALA:N | 2.51 | 0.43 |
| 8:u7:8:ILE:O | 8:u7:11:ALA:N | 2.51 | 0.43 |
| 8:u7:18:LEU:HB2 | 1:v7:97:LEU:HD11 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:u7:30:VAL:CG2 | 1:v7:31:PHE:O | 2.66 | 0.43 |
| 8:u7:90:ARG:CG | 1:v7:18:TYR:CE1 | 3.02 | 0.43 |
| 12:v7:201:CYC:HC | 12:v7:201:CYC:CMD | 2.13 | 0.43 |
| 3:U8:120:LEU:O | 3:U8:120:LEU:HG | 2.19 | 0.43 |
| 3:F8:2:GLN:HA | 3:F8:6:THR:HG21 | 2.00 | 0.43 |
| 4:M8:37:GLU:HG3 | 4:M8:38:PRO:HD2 | 2.00 | 0.43 |
| 12:M8:302:CYC:C1C | 3:S8:78:ARG:NH1 | 2.70 | 0.43 |
| 4:M9:1:MET:HE3 | 4:M9:45:VAL:HA | 1.29 | 0.43 |
| 4:M9:159:CYS:O | 3:V9:107:ASP:C | 2.62 | 0.43 |
| 3:Y8:2:GLN:HA | 3:Y8:6:THR:HG21 | 2.00 | 0.43 |
| 12:I9:201:CYC:CMA | 12:I9:201:CYC:NB | 2.81 | 0.43 |
| 12:K9:201:CYC:CMA | 12:K9:201:CYC:NB | 2.81 | 0.43 |
| 2:S9:138:VAL:O | 2:S9:138:VAL:CG1 | 2.67 | 0.43 |
| 2:Y9:138:VAL:O | 2:Y9:138:VAL:CG1 | 2.67 | 0.43 |
| 11:a9:527:LEU:HD23 | 11:a9:527:LEU:HA | 1.62 | 0.43 |
| 11:aA:446:ALA:HB1 | 11:aA:450:ARG:CG | 2.49 | 0.43 |
| 11:aA:465:TYR:CE2 | 11:aA:516:GLN:HA | 2.54 | 0.43 |
| 11:aA:670:LEU:HD22 | 2:K1:112:GLY:HA2 | 0.47 | 0.43 |
| 4:M1:120:LEU:HD23 | 4:M1:120:LEU:HA | 1.89 | 0.43 |
| 4:M1:261:VAL:HG11 | 4:M1:266:LEU:HD13 | 1.99 | 0.43 |
| 2:Y1:138:VAL:O | 2:Y1:138:VAL:CG1 | 2.67 | 0.43 |
| 3:D2:2:GLN:HA | 3:D2:6:THR:HG21 | 2.00 | 0.43 |
| 1:Z:91:TYR:OH | 10:j5:254:PRO:HB3 | 2.19 | 0.43 |
| 2:AA:138:VAL:O | 2:AA:138:VAL:CG1 | 2.67 | 0.43 |
| 3:DA:124:THR:HB | 3:DA:171:ILE:O | 2.18 | 0.43 |
| 2:EA:17:ARG:CZ | 2:IA:2:LYS:HZ1 | 2.31 | 0.43 |
| 2:OA:33:ARG:NH1 | 12:ZA:201:CYC:C4B | 2.44 | 0.43 |
| 12:R1:201:CYC:HAA1 | 5:N1:53:LEU:HD13 | 2.01 | 0.43 |
| 3:H3:2:GLN:HA | 3:H3:6:THR:HG21 | 2.00 | 0.43 |
| 2:I3:99:ALA:HB2 | 3:J3:9:ILE:HD13 | 2.00 | 0.43 |
| 12:J3:201:CYC:HB | 12:J3:201:CYC:HMA3 | 1.83 | 0.43 |
| 2:K3:14:SER:C | 11:a9:745:GLY:CA | 2.91 | 0.43 |
| 12:I2:201:CYC:CMA | 12:I2:201:CYC:NB | 2.82 | 0.43 |
| 12:J2:201:CYC:HMD3 | 12:J2:201:CYC:NC | 2.34 | 0.43 |
| 3:L2:124:THR:HB | 3:L2:171:ILE:O | 2.18 | 0.43 |
| 6:M2:147:ASP:CG | 2:E2:15:GLN:HG2 | 2.43 | 0.43 |
| 6:M2:179:GLY:HA2 | 6:M2:182:GLN:HG2 | 2.01 | 0.43 |
| 7:N2:15:VAL:HA | 7:N2:44:PRO:HA | 2.01 | 0.43 |
| 3:B4:3:ASP:H | 3:B4:6:THR:HB | 1.84 | 0.43 |
| 3:L3:77:ARG:CB | 11:a9:824:VAL:OXT | 2.66 | 0.43 |
| 3:L3:92:TYR:HE1 | 3:L3:108:ARG:HE | 1.67 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:O3:59:VAL:O | 2:O3:66:LEU:CD1 | 2.62 | 0.43 |
| 12:R3:202:CYC:HB | 12:R3:202:CYC:HMA3 | 1.84 | 0.43 |
| 12:X3:202:CYC:HB | 12:X3:202:CYC:HMA3 | 1.83 | 0.43 |
| 3:U4:124:THR:HB | 3:U4:171:ILE:O | 2.18 | 0.43 |
| 2:G4:138:VAL:O | 2:G4:138:VAL:CG1 | 2.67 | 0.43 |
| 12:K4:201:CYC:CMA | 12:K4:201:CYC:NB | 2.81 | 0.43 |
| 4:M4:232:VAL:CG1 | 3:Y4:109:CYS:C | 2.90 | 0.43 |
| 3:Q4:89:ILE:HG21 | 3:Q4:131:VAL:HG13 | 2.00 | 0.43 |
| 8:M5:64:ASP:HA | 8:M5:67:SER:CB | 2.48 | 0.43 |
| 1:N5:71:MEN:O | 1:N5:77:ARG:HD3 | 2.18 | 0.43 |
| 3:Y4:87:GLU:CB | 3:Y4:91:ARG:HH12 | 2.31 | 0.43 |
| 3:Y4:105:LEU:O | 3:Y4:109:CYS:SG | 2.77 | 0.43 |
| 5:Z4:68:LEU:HA | 5:Z4:68:LEU:HD23 | 1.80 | 0.43 |
| 1:B5:72:MET:HE2 | 1:B5:72:MET:HB3 | 1.87 | 0.43 |
| 8:E5:8:ILE:O | 8:E5:11:ALA:N | 2.51 | 0.43 |
| 8:S5:64:ASP:HA | 8:S5:67:SER:CB | 2.48 | 0.43 |
| 8:S5:90:ARG:HA | 1:T5:18:TYR:CD2 | 2.53 | 0.43 |
| 1:T5:14:VAL:C | 1:X5:68:PRO:HB3 | 2.41 | 0.43 |
| 8:U5:67:SER:HB3 | 8:U5:68:PRO:HD2 | 2.00 | 0.43 |
| 8:a5:2:SER:O | 8:a5:100:ASP:OD2 | 2.37 | 0.43 |
| 3:J6:87:GLU:OE1 | 6:M6:189:HIS:NE2 | 2.31 | 0.43 |
| 2:K6:99:ALA:HB2 | 3:L6:9:ILE:HD13 | 2.00 | 0.43 |
| 10:j5:600:VAL:O | 10:j5:600:VAL:CG1 | 2.66 | 0.43 |
| 10:j5:612:ILE:H | 10:j5:612:ILE:CD1 | 2.03 | 0.43 |
| 10:j5:790:ALA:HB2 | 1:T7:87:TYR:OH | 2.18 | 0.43 |
| 10:j5:793:SER:O | 12:T7:201:CYC:CBA | 2.67 | 0.43 |
| 10:j5:909:ASP:OD1 | 10:j5:909:ASP:N | 2.51 | 0.43 |
| 10:j5:1118:THR:HA | 12:j5:1202:CYC:HMA3 | 2.00 | 0.43 |
| 10:j5:1124:TYR:OH | 1:t7:119:LEU:CD2 | 2.58 | 0.43 |
| 10:k5:160:LEU:HD23 | 10:k5:160:LEU:HA | 1.69 | 0.43 |
| 10:k5:440:TYR:N | 10:k5:440:TYR:CD1 | 2.84 | 0.43 |
| 10:k5:813:ALA:CB | 8:M7:14:GLU:OE2 | 2.67 | 0.43 |
| 10:k5:1041:ARG:O | 10:k5:1041:ARG:HG3 | 2.18 | 0.43 |
| 2:C6:38:MET:HE3 | 3:D6:24:LEU:CD2 | 2.49 | 0.43 |
| 12:F6:202:CYC:HB | 12:F6:202:CYC:HMA3 | 1.84 | 0.43 |
| 12:P7:201:CYC:CMA | 12:P7:201:CYC:NB | 2.74 | 0.43 |
| 8:K7:122:PRO:HD2 | 12:K7:201:CYC:OC | 2.19 | 0.43 |
| 8:i7:8:ILE:O | 8:i7:11:ALA:N | 2.51 | 0.43 |
| 8:i7:47:ARG:CD | 1:j7:18:TYR:CG | 3.01 | 0.43 |
| 8:i7:141:LEU:HB2 | 8:i7:146:ALA:HB2 | 2.01 | 0.43 |
| 1:j7:119:LEU:HD21 | 9:y7:5:PHE:HZ | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:a7:16:ARG:NH1 | 8:a7:16:ARG:CG | 2.80 | 0.43 |
| 8:e7:64:ASP:HA | 8:e7:67:SER:CB | 2.48 | 0.43 |
| 2:A8:24:LEU:HB3 | 12:B8:201:CYC:HAB2 | 2.00 | 0.43 |
| 8:m7:2:SER:O | 8:m7:100:ASP:OD2 | 2.37 | 0.43 |
| 12:m7:201:CYC:HB | 12:m7:201:CYC:CMA | 2.21 | 0.43 |
| 8:u7:30:VAL:HB | 1:v7:31:PHE:CB | 2.48 | 0.43 |
| 2:X8:138:VAL:O | 2:X8:138:VAL:CG1 | 2.67 | 0.43 |
| 3:H8:2:GLN:HA | 3:H8:6:THR:HG21 | 2.00 | 0.43 |
| 2:K8:99:ALA:HB2 | 3:L8:9:ILE:HD13 | 2.00 | 0.43 |
| 3:Q8:89:ILE:C | 3:Q8:92:TYR:CE2 | 2.86 | 0.43 |
| 3:S8:3:ASP:H | 3:S8:6:THR:HB | 1.84 | 0.43 |
| 4:M9:9:GLN:CD | 4:M9:9:GLN:C | 2.87 | 0.43 |
| 4:M9:132:LEU:HD12 | 4:M9:137:ILE:HD12 | 2.01 | 0.43 |
| 4:M9:264:LYS:N | 3:V9:119:ALA:HB2 | 2.34 | 0.43 |
| 3:J9:108:ARG:HA | 11:a9:517:ALA:CA | 2.40 | 0.43 |
| 12:X9:202:CYC:HC | 12:X9:202:CYC:HMD3 | 1.78 | 0.43 |
| 11:a9:426:ARG:NH2 | 11:a9:496:ARG:NE | 2.66 | 0.43 |
| 11:aA:667:THR:N | 12:aA:901:CYC:HBA1 | 2.34 | 0.43 |
| 3:H1:65:ASP:OD1 | 3:H1:65:ASP:N | 2.47 | 0.43 |
| 4:M1:80:PRO:C | 3:X1:111:ASN:HD21 | 2.27 | 0.43 |
| 3:Z1:2:GLN:HA | 3:Z1:6:THR:HG21 | 2.00 | 0.43 |
| 1:Z:19:LEU:HD11 | 8:e5:97:VAL:HG21 | 2.01 | 0.42 |
| 2:GA:38:MET:HE2 | 2:GA:38:MET:HB3 | 1.81 | 0.42 |
| 12:JA:201:CYC:HB | 12:JA:201:CYC:HMA3 | 1.83 | 0.42 |
| 2:KA:99:ALA:HB2 | 3:LA:9:ILE:HD13 | 2.00 | 0.42 |
| 3:LA:2:GLN:HA | 3:LA:6:THR:HG21 | 2.00 | 0.42 |
| 3:LA:116:THR:HG22 | 3:LA:117:TYR:N | 2.34 | 0.42 |
| 4:MA:160:THR:O | 3:VA:108:ARG:CG | 2.59 | 0.42 |
| 4:MA:264:LYS:N | 3:VA:119:ALA:HB2 | 2.34 | 0.42 |
| 2:QA:119:THR:HG23 | 3:TA:52:ILE:HG22 | 2.01 | 0.42 |
| 2:WA:138:VAL:O | 2:WA:138:VAL:CG1 | 2.67 | 0.42 |
| 2:O1:59:VAL:O | 2:O1:66:LEU:CD1 | 2.62 | 0.42 |
| 2:Q1:138:VAL:O | 2:Q1:138:VAL:CG1 | 2.67 | 0.42 |
| 3:R1:3:ASP:H | 3:R1:6:THR:HB | 1.84 | 0.42 |
| 12:R1:201:CYC:OB | 5:N1:54:LEU:HD11 | 2.14 | 0.42 |
| 2:S1:99:ALA:HB2 | 3:T1:9:ILE:HD13 | 2.00 | 0.42 |
| 2:A1:49:ASP:O | 2:A1:50:SER:C | 2.62 | 0.42 |
| 2:A1:99:ALA:HB2 | 3:B1:9:ILE:HD13 | 2.00 | 0.42 |
| 3:J2:2:GLN:HA | 3:J2:6:THR:HG21 | 2.00 | 0.42 |
| 12:L2:202:CYC:HB | 12:L2:202:CYC:HMA3 | 1.84 | 0.42 |
| 6:M2:259:THR:C | 6:M2:261:LYS:H | 2.25 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:N2:49:LEU:O | 7:N2:53:GLN:HB2 | 2.19 | 0.42 |
| 2:A3:34:ALA:CB | 3:B3:31:VAL:HG11 | 2.38 | 0.42 |
| 12:B3:202:CYC:CBA | 11:a9:684:ASN:CG | 2.87 | 0.42 |
| 4:M3:233:GLU:HB2 | 3:V3:111:ASN:O | 2.19 | 0.42 |
| 5:N3:59:ARG:HE | 5:N3:59:ARG:HB2 | 1.69 | 0.42 |
| 2:Q3:138:VAL:O | 2:Q3:138:VAL:CG1 | 2.67 | 0.42 |
| 3:R3:3:ASP:H | 3:R3:6:THR:HB | 1.84 | 0.42 |
| 12:U3:201:CYC:CMA | 12:U3:201:CYC:NB | 2.82 | 0.42 |
| 3:S4:9:ILE:HD13 | 2:R4:99:ALA:HB2 | 2.00 | 0.42 |
| 12:T4:201:CYC:CMA | 12:T4:201:CYC:NB | 2.81 | 0.42 |
| 3:W4:2:GLN:HA | 3:W4:6:THR:HG21 | 2.01 | 0.42 |
| 12:H4:201:CYC:CBA | 11:aA:261:SER:HB2 | 2.48 | 0.42 |
| 12:L4:201:CYC:HB | 12:L4:201:CYC:HMA3 | 1.84 | 0.42 |
| 4:M4:128:ALA:CA | 4:M4:142:PHE:CE1 | 3.01 | 0.42 |
| 2:N4:59:VAL:O | 2:N4:66:LEU:CD1 | 2.62 | 0.42 |
| 2:P4:38:MET:HE3 | 3:Q4:24:LEU:CD2 | 2.49 | 0.42 |
| 3:Q4:88:ILE:O | 3:Q4:89:ILE:C | 2.62 | 0.42 |
| 8:M5:67:SER:HB3 | 8:M5:68:PRO:HD2 | 2.00 | 0.42 |
| 8:O5:95:GLY:HA3 | 8:O5:104:ILE:HD11 | 2.01 | 0.42 |
| 8:C5:95:GLY:HA3 | 8:C5:104:ILE:HD11 | 2.01 | 0.42 |
| 1:D5:5:ILE:CG2 | 1:D5:5:ILE:O | 2.67 | 0.42 |
| 8:E5:102:THR:N | 8:E5:103:PRO:HD2 | 2.34 | 0.42 |
| 1:F5:106:GLU:HG3 | 9:z5:58:THR:HG22 | 2.01 | 0.42 |
| 12:C1:201:CYC:CMA | 12:C1:201:CYC:NB | 2.81 | 0.42 |
| 1:R5:107:ARG:C | 10:k5:520:ARG:HH12 | 2.22 | 0.42 |
| 1:V5:72:MET:HE2 | 1:V5:72:MET:HB3 | 1.87 | 0.42 |
| 8:W5:66:VAL:O | 8:W5:66:VAL:CG1 | 2.66 | 0.42 |
| 9:i5:15:LYS:HD2 | 9:i5:16:ARG:N | 2.34 | 0.42 |
| 9:i5:58:THR:HG22 | 9:i5:58:THR:O | 2.19 | 0.42 |
| 10:j5:339:LYS:HB2 | 10:j5:399:TYR:CE1 | 2.54 | 0.42 |
| 10:j5:934:ALA:CB | 1:J7:32:THR:HG22 | 2.31 | 0.42 |
| 10:j5:951:MET:CE | 10:j5:955:LEU:CD1 | 2.97 | 0.42 |
| 10:j5:968:GLU:H | 10:j5:968:GLU:HG2 | 1.61 | 0.42 |
| 10:j5:1140:TRP:O | 11:aA:32:ARG:NH2 | 2.52 | 0.42 |
| 10:k5:190:LEU:HD11 | 12:k5:1201:CYC:HC | 1.83 | 0.42 |
| 10:k5:247:ARG:HA | 10:k5:248:PRO:HD3 | 1.67 | 0.42 |
| 10:k5:309:LEU:HD13 | 10:k5:342:LEU:CD1 | 2.46 | 0.42 |
| 10:k5:765:ASP:O | 10:k5:769:THR:HG22 | 2.18 | 0.42 |
| 2:E6:38:MET:HE3 | 3:F6:24:LEU:CD2 | 2.49 | 0.42 |
| 3:F6:82:CYS:HA | 12:F6:201:CYC:CHD | 2.49 | 0.42 |
| 8:O7:95:GLY:HA3 | 8:O7:104:ILE:HD11 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:S7:201:CYC:HB | 12:S7:201:CYC:CMA | 2.21 | 0.42 |
| 8:C7:130:VAL:CG1 | 8:C7:157:VAL:HG23 | 2.49 | 0.42 |
| 1:h7:37:ARG:NH1 | 1:h7:37:ARG:HG2 | 2.34 | 0.42 |
| 8:U7:130:VAL:CG1 | 8:U7:157:VAL:HG23 | 2.49 | 0.42 |
| 8:Y7:23:LEU:HD22 | 1:Z7:38:VAL:HG13 | 2.00 | 0.42 |
| 1:b7:37:ARG:NH1 | 1:b7:37:ARG:HG2 | 2.34 | 0.42 |
| 8:c7:48:GLU:O | 8:c7:52:LYS:HG3 | 2.18 | 0.42 |
| 2:A8:59:VAL:O | 2:A8:66:LEU:CD1 | 2.62 | 0.42 |
| 3:B8:108:ARG:O | 4:M8:60:LYS:NZ | 2.52 | 0.42 |
| 8:o7:30:VAL:CG2 | 1:p7:31:PHE:O | 2.66 | 0.42 |
| 8:q7:67:SER:HB3 | 8:q7:68:PRO:HD2 | 2.00 | 0.42 |
| 1:t7:71:MEN:O | 1:t7:77:ARG:HD3 | 2.18 | 0.42 |
| 8:u7:160:MET:HE2 | 8:u7:160:MET:HB2 | 1.87 | 0.42 |
| 9:w7:3:ARG:CZ | 9:w7:67:VAL:HG13 | 2.48 | 0.42 |
| 9:x7:56:LEU:HA | 9:x7:56:LEU:HD23 | 1.58 | 0.42 |
| 4:M8:99:VAL:HG22 | 3:Q8:108:ARG:HH12 | 1.81 | 0.42 |
| 3:O8:3:ASP:H | 3:O8:6:THR:HB | 1.84 | 0.42 |
| 3:D9:124:THR:HB | 3:D9:171:ILE:O | 2.18 | 0.42 |
| 3:F9:3:ASP:H | 3:F9:6:THR:HB | 1.84 | 0.42 |
| 12:R9:202:CYC:HB | 12:R9:202:CYC:HMA3 | 1.84 | 0.42 |
| 3:T9:3:ASP:H | 3:T9:6:THR:HB | 1.84 | 0.42 |
| 12:U9:201:CYC:CMA | 12:U9:201:CYC:NB | 2.82 | 0.42 |
| 3:V9:3:ASP:H | 3:V9:6:THR:HB | 1.84 | 0.42 |
| 11:aA:50:LEU:HA | 11:aA:50:LEU:HD12 | 1.60 | 0.42 |
| 11:aA:376:ALA:HB3 | 11:aA:503:THR:HG22 | 2.01 | 0.42 |
| 12:aA:902:CYC:HAB2 | 3:L1:88:ILE:HG21 | 2.01 | 0.42 |
| 3:J1:2:GLN:HA | 3:J1:6:THR:HG21 | 2.00 | 0.42 |
| 4:M1:62:LYS:HD2 | 4:M1:62:LYS:HA | 1.67 | 0.42 |
| 4:M1:140:ARG:NH1 | 4:M1:204:ILE:O | 2.52 | 0.42 |
| 5:N1:37:HIS:H | 12:T1:301:CYC:HMA3 | 1.84 | 0.42 |
| 12:T1:302:CYC:HB | 12:T1:302:CYC:HMA3 | 1.84 | 0.42 |
| 2:A2:99:ALA:HB2 | 3:B2:9:ILE:HD13 | 2.00 | 0.42 |
| 2:E2:99:ALA:HB2 | 3:F2:9:ILE:HD13 | 2.00 | 0.42 |
| 1:Z:76:ARG:CG | 10:j5:262:TYR:CD2 | 3.01 | 0.42 |
| 2:IA:37:SER:CA | 2:IA:97:LEU:CD1 | 2.90 | 0.42 |
| 4:MA:263:PRO:CA | 3:VA:119:ALA:CB | 2.95 | 0.42 |
| 4:MA:273:ILE:HG22 | 2:WA:107:ASP:O | 2.20 | 0.42 |
| 5:NA:61:LYS:HD2 | 12:TA:301:CYC:HBB3 | 1.98 | 0.42 |
| 2:OA:138:VAL:O | 2:OA:138:VAL:CG1 | 2.67 | 0.42 |
| 2:O1:34:ALA:CB | 3:P1:31:VAL:HG11 | 2.38 | 0.42 |
| 2:A3:138:VAL:O | 2:A3:138:VAL:CG1 | 2.67 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:C3:138:VAL:O | 2:C3:138:VAL:CG1 | 2.67 | 0.42 |
| 4:M3:51:ARG:HH22 | 11:a9:694:ARG:HH12 | 1.53 | 0.42 |
| 5:N3:28:HIS:CD2 | 5:N3:28:HIS:H | 2.38 | 0.42 |
| 12:X3:202:CYC:CMD | 12:X3:202:CYC:NC | 2.75 | 0.42 |
| 3:B1:86:MET:CG | 12:B1:202:CYC:CBC | 2.79 | 0.42 |
| 2:T4:38:MET:HE3 | 3:U4:24:LEU:CD2 | 2.49 | 0.42 |
| 2:V4:38:MET:HE3 | 3:W4:24:LEU:CD2 | 2.49 | 0.42 |
| 12:W4:202:CYC:HMD3 | 12:W4:202:CYC:NC | 2.34 | 0.42 |
| 4:M4:19:MET:HE2 | 4:M4:59:ILE:CD1 | 2.46 | 0.42 |
| 4:M4:200:ILE:HD13 | 4:M4:200:ILE:HA | 1.54 | 0.42 |
| 8:O5:11:ALA:CB | 8:O5:18:LEU:CD1 | 2.96 | 0.42 |
| 5:Z4:37:HIS:N | 5:Z4:37:HIS:ND1 | 2.66 | 0.42 |
| 1:B5:2:GLN:OE1 | 10:k5:551:MET:HG2 | 2.19 | 0.42 |
| 8:C5:130:VAL:CG1 | 8:C5:157:VAL:HG23 | 2.49 | 0.42 |
| 8:E5:17:TYR:CB | 1:F5:45:SER:HB2 | 2.47 | 0.42 |
| 8:E5:116:TYR:HB3 | 8:E5:123:ILE:CG1 | 2.49 | 0.42 |
| 8:I5:130:VAL:CG1 | 8:I5:157:VAL:HG23 | 2.49 | 0.42 |
| 12:T5:201:CYC:C4B | 10:j5:483:PHE:CE2 | 3.03 | 0.42 |
| 12:J6:201:CYC:HB | 12:J6:201:CYC:HMA3 | 1.83 | 0.42 |
| 6:M6:68:THR:N | 3:H6:14:LEU:CD2 | 2.82 | 0.42 |
| 7:N6:4:ASN:O | 7:N6:5:VAL:C | 2.61 | 0.42 |
| 10:j5:839:ARG:H | 10:j5:839:ARG:HG2 | 1.60 | 0.42 |
| 10:k5:262:TYR:CD1 | 10:k5:262:TYR:C | 2.97 | 0.42 |
| 10:k5:431:GLN:CA | 10:k5:431:GLN:HE21 | 2.33 | 0.42 |
| 10:k5:1024:LYS:HD3 | 10:k5:1038:ARG:NH1 | 2.23 | 0.42 |
| 2:E6:138:VAL:O | 2:E6:138:VAL:CG1 | 2.67 | 0.42 |
| 8:C7:11:ALA:CB | 8:C7:18:LEU:CD1 | 2.96 | 0.42 |
| 8:C7:33:GLY:HA2 | 8:C7:36:ARG:HB2 | 2.01 | 0.42 |
| 8:I7:67:SER:HB3 | 8:I7:68:PRO:HD2 | 2.00 | 0.42 |
| 8:M7:64:ASP:HA | 8:M7:67:SER:CB | 2.48 | 0.42 |
| 8:g7:2:SER:O | 8:g7:100:ASP:OD2 | 2.37 | 0.42 |
| 8:U7:2:SER:HA | 8:U7:100:ASP:HB3 | 2.01 | 0.42 |
| 8:Y7:130:VAL:CG1 | 8:Y7:157:VAL:HG23 | 2.48 | 0.42 |
| 2:A8:49:ASP:O | 2:A8:50:SER:C | 2.62 | 0.42 |
| 8:m7:2:SER:HA | 8:m7:100:ASP:HB3 | 2.01 | 0.42 |
| 8:o7:76:LYS:O | 8:o7:80:LEU:HG | 2.19 | 0.42 |
| 8:q7:49:ARG:CZ | 3:H1:62:GLU:HB3 | 2.49 | 0.42 |
| 8:s7:95:GLY:HA3 | 8:s7:104:ILE:HD11 | 2.01 | 0.42 |
| 8:s7:102:THR:CB | 8:s7:103:PRO:HD3 | 2.33 | 0.42 |
| 12:W8:202:CYC:HMD3 | 12:W8:202:CYC:NC | 2.34 | 0.42 |
| 3:F8:106:GLU:HA | 3:F8:110:LEU:HB2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:H8:202:CYC:HB | 12:H8:202:CYC:HMA3 | 1.83 | 0.42 |
| 2:I8:38:MET:HE3 | 3:J8:24:LEU:CD2 | 2.50 | 0.42 |
| 2:I8:99:ALA:HB2 | 3:J8:9:ILE:HD13 | 2.00 | 0.42 |
| 3:J8:2:GLN:HA | 3:J8:6:THR:HG21 | 2.00 | 0.42 |
| 4:M8:56:MET:HE1 | 4:M8:66:VAL:CG1 | 2.48 | 0.42 |
| 4:M8:226:SER:HB3 | 3:Y8:84:ARG:HB2 | 2.01 | 0.42 |
| 4:M8:235:PHE:HB3 | 12:M8:301:CYC:HAA1 | 1.75 | 0.42 |
| 3:Q8:3:ASP:H | 3:Q8:6:THR:HB | 1.84 | 0.42 |
| 3:Q8:99:ALA:O | 3:Q8:100:GLY:C | 2.61 | 0.42 |
| 2:R8:38:MET:HE3 | 3:S8:24:LEU:CD2 | 2.50 | 0.42 |
| 12:R8:201:CYC:CMA | 12:R8:201:CYC:NB | 2.81 | 0.42 |
| 3:L9:86:MET:O | 3:L9:134:MET:SD | 2.77 | 0.42 |
| 4:M9:28:HIS:CD2 | 4:M9:35:THR:HG23 | 2.55 | 0.42 |
| 2:A9:59:VAL:O | 2:A9:66:LEU:CD1 | 2.62 | 0.42 |
| 12:B9:201:CYC:HC | 12:B9:201:CYC:HMD3 | 1.83 | 0.42 |
| 12:F9:302:CYC:HB | 12:F9:302:CYC:HMA3 | 1.84 | 0.42 |
| 2:I9:37:SER:CA | 2:I9:97:LEU:CD2 | 2.92 | 0.42 |
| 2:I9:38:MET:HE3 | 3:J9:24:LEU:CD2 | 2.50 | 0.42 |
| 12:J9:201:CYC:HB | 12:J9:201:CYC:HMA3 | 1.83 | 0.42 |
| 12:J9:202:CYC:HC | 12:J9:202:CYC:HMD3 | 1.82 | 0.42 |
| 2:S9:38:MET:HE3 | 3:T9:24:LEU:CD2 | 2.49 | 0.42 |
| 2:U9:138:VAL:O | 2:U9:138:VAL:CG1 | 2.67 | 0.42 |
| 2:G1:99:ALA:HB2 | 3:H1:9:ILE:HD13 | 2.00 | 0.42 |
| 11:a9:327:SER:C | 11:a9:329:ASN:H | 2.27 | 0.42 |
| 11:aA:25:GLU:C | 11:aA:27:PHE:N | 2.77 | 0.42 |
| 11:aA:75:ALA:CB | 11:aA:81:ASP:HB3 | 1.92 | 0.42 |
| 11:aA:776:TYR:HB2 | 12:H1:201:CYC:CMA | 2.42 | 0.42 |
| 2:I1:99:ALA:HB2 | 3:J1:9:ILE:HD13 | 2.00 | 0.42 |
| 4:M1:233:GLU:HB2 | 3:V1:111:ASN:O | 2.19 | 0.42 |
| 2:W1:38:MET:HE3 | 3:X1:24:LEU:CD2 | 2.49 | 0.42 |
| 2:A2:24:LEU:HB3 | 12:B2:201:CYC:HAB2 | 2.00 | 0.42 |
| 2:A2:49:ASP:O | 2:A2:50:SER:C | 2.62 | 0.42 |
| 1:Z:75:THR:C | 10:j5:261:ILE:HD11 | 2.43 | 0.42 |
| 2:CA:38:MET:HE3 | 3:DA:24:LEU:CD2 | 2.49 | 0.42 |
| 2:CA:138:VAL:O | 2:CA:138:VAL:CG1 | 2.67 | 0.42 |
| 2:GA:99:ALA:HB2 | 3:HA:9:ILE:HD13 | 2.00 | 0.42 |
| 3:JA:116:THR:OG1 | 11:aA:521:PHE:CB | 2.55 | 0.42 |
| 3:LA:84:ARG:HE | 11:aA:406:LEU:HD22 | 1.83 | 0.42 |
| 4:MA:23:PRO:HB2 | 4:MA:34:ASP:HB3 | 2.02 | 0.42 |
| 4:MA:28:HIS:HD2 | 4:MA:35:THR:CG2 | 2.33 | 0.42 |
| 4:MA:264:LYS:N | 3:VA:119:ALA:HB1 | 2.30 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:WA:38:MET:HE3 | 3:XA:24:LEU:CD2 | 2.49 | 0.42 |
| 2:YA:138:VAL:O | 2:YA:138:VAL:CG1 | 2.67 | 0.42 |
| 2:S1:138:VAL:O | 2:S1:138:VAL:CG1 | 2.67 | 0.42 |
| 2:A1:138:VAL:O | 2:A1:138:VAL:CG1 | 2.67 | 0.42 |
| 12:H3:202:CYC:HC | 12:H3:202:CYC:HMD3 | 1.82 | 0.42 |
| 3:H2:14:LEU:CD2 | 6:M2:68:THR:N | 2.82 | 0.42 |
| 3:B3:126:SER:HB3 | 12:B3:202:CYC:HMC2 | 2.01 | 0.42 |
| 2:E3:99:ALA:HB2 | 3:F3:9:ILE:HD13 | 2.00 | 0.42 |
| 3:F3:124:THR:HB | 3:F3:171:ILE:O | 2.18 | 0.42 |
| 3:B4:127:VAL:HG22 | 12:B4:202:CYC:CMC | 2.49 | 0.42 |
| 12:B4:202:CYC:OB | 4:M4:58:TYR:HD1 | 2.02 | 0.42 |
| 2:C4:38:MET:HE3 | 3:D4:24:LEU:CD2 | 2.49 | 0.42 |
| 3:L3:88:ILE:HG21 | 12:L3:202:CYC:HAB2 | 2.01 | 0.42 |
| 4:M3:9:GLN:CD | 4:M3:9:GLN:C | 2.87 | 0.42 |
| 4:M3:37:GLU:HG3 | 4:M3:38:PRO:HD2 | 2.00 | 0.42 |
| 4:M3:80:PRO:C | 3:X3:111:ASN:HD21 | 2.27 | 0.42 |
| 4:M3:246:ALA:HA | 12:X3:201:CYC:HBB3 | 1.99 | 0.42 |
| 2:W3:99:ALA:HB2 | 3:X3:9:ILE:HD13 | 2.00 | 0.42 |
| 2:Y3:138:VAL:O | 2:Y3:138:VAL:CG1 | 2.67 | 0.42 |
| 12:B1:201:CYC:HB | 12:B1:201:CYC:HMA3 | 1.84 | 0.42 |
| 3:S4:120:LEU:CD1 | 12:S4:202:CYC:C4D | 2.96 | 0.42 |
| 2:G4:38:MET:HE3 | 3:H4:24:LEU:CD2 | 2.49 | 0.42 |
| 3:H4:111:ASN:ND2 | 11:aA:291:TYR:CE1 | 2.82 | 0.42 |
| 2:I4:38:MET:HE3 | 3:J4:24:LEU:CD2 | 2.50 | 0.42 |
| 2:I4:99:ALA:HB2 | 3:J4:9:ILE:HD13 | 2.00 | 0.42 |
| 4:M4:42:SER:O | 4:M4:42:SER:OG | 2.29 | 0.42 |
| 4:M4:273:ILE:CD1 | 2:X4:108:TYR:CE1 | 2.99 | 0.42 |
| 1:L5:119:LEU:HD21 | 10:j5:546:PHE:CE2 | 2.50 | 0.42 |
| 8:A5:12:ASP:OD2 | 1:B5:91:TYR:HE1 | 2.02 | 0.42 |
| 12:B5:201:CYC:HC | 12:B5:201:CYC:CMD | 2.13 | 0.42 |
| 8:C5:2:SER:O | 8:C5:100:ASP:OD2 | 2.37 | 0.42 |
| 8:E5:67:SER:HB3 | 8:E5:68:PRO:HD2 | 2.00 | 0.42 |
| 8:G5:64:ASP:O | 8:G5:65:VAL:C | 2.61 | 0.42 |
| 1:H5:107:ARG:CD | 9:i5:21:ARG:HD3 | 2.48 | 0.42 |
| 1:J5:1:MET:HB2 | 1:J5:1:MET:HE3 | 1.34 | 0.42 |
| 8:Q5:116:TYR:CB | 8:Q5:123:ILE:HG12 | 2.47 | 0.42 |
| 8:U5:48:GLU:O | 6:M6:34:ARG:NH1 | 2.52 | 0.42 |
| 8:U5:82:LEU:CD1 | 6:M6:34:ARG:CB | 2.98 | 0.42 |
| 8:a5:2:SER:HA | 8:a5:100:ASP:HB3 | 2.01 | 0.42 |
| 2:K6:138:VAL:O | 2:K6:138:VAL:CG1 | 2.67 | 0.42 |
| 6:M6:43:TRP:CZ3 | 8:c7:52:LYS:HB3 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 6:M6:277:GLY:HA3 | 1:d7:62:TYR:HB2 | 2.00 | 0.42 |
| 10:j5:722:ILE:CD1 | 8:K7:82:LEU:HD12 | 2.47 | 0.42 |
| 10:j5:1024:LYS:HD3 | 10:j5:1038:ARG:NH1 | 2.23 | 0.42 |
| 10:j5:1069:ARG:HB2 | 10:j5:1070:ALA:H | 1.67 | 0.42 |
| 10:j5:1102:TYR:O | 10:j5:1102:TYR:CD1 | 2.72 | 0.42 |
| 10:j5:1136:ILE:HG23 | 10:j5:1136:ILE:HD12 | 1.69 | 0.42 |
| 10:k5:89:LYS:HE2 | 10:k5:89:LYS:HB2 | 1.92 | 0.42 |
| 10:k5:395:SER:HA | 10:k5:400:ALA:HB2 | 2.00 | 0.42 |
| 10:k5:750:ARG:HG2 | 10:k5:750:ARG:NH1 | 2.31 | 0.42 |
| 10:k5:848:ILE:HD13 | 10:k5:848:ILE:HG21 | 1.63 | 0.42 |
| 10:k5:931:VAL:CG1 | 1:D7:29:ALA:CB | 2.67 | 0.42 |
| 10:k5:1008:PHE:CD1 | 12:p7:201:CYC:CBB | 3.03 | 0.42 |
| 10:k5:1118:THR:CB | 12:k5:1204:CYC:HBA1 | 2.49 | 0.42 |
| 8:O7:2:SER:O | 8:O7:100:ASP:OD2 | 2.37 | 0.42 |
| 8:I7:33:GLY:HA2 | 8:I7:36:ARG:HB2 | 2.01 | 0.42 |
| 1:J7:71:MEN:O | 1:J7:77:ARG:HD3 | 2.18 | 0.42 |
| 1:L7:49:THR:HG22 | 8:U7:161:GLN:CD | 2.44 | 0.42 |
| 8:M7:49:ARG:HD2 | 11:a9:550:PHE:CD1 | 2.37 | 0.42 |
| 8:k7:76:LYS:NZ | 11:a9:604:ALA:CB | 2.72 | 0.42 |
| 8:U7:2:SER:O | 8:U7:100:ASP:OD2 | 2.37 | 0.42 |
| 2:A8:25:GLN:HG3 | 2:K8:33:ARG:HG2 | 1.99 | 0.42 |
| 3:B8:3:ASP:H | 3:B8:6:THR:HB | 1.84 | 0.42 |
| 2:E8:138:VAL:O | 2:E8:138:VAL:CG1 | 2.67 | 0.42 |
| 8:m7:11:ALA:CB | 8:m7:18:LEU:CD1 | 2.96 | 0.42 |
| 8:o7:6:LYS:HD3 | 8:o7:6:LYS:HA | 1.68 | 0.42 |
| 8:o7:90:ARG:CG | 1:p7:18:TYR:CE1 | 3.02 | 0.42 |
| 8:s7:2:SER:HA | 8:s7:100:ASP:HB3 | 2.01 | 0.42 |
| 3:U8:114:LYS:HE3 | 4:M8:13:LYS:NZ | 2.21 | 0.42 |
| 12:V8:201:CYC:CMA | 12:V8:201:CYC:NB | 2.82 | 0.42 |
| 3:F8:107:ASP:OD1 | 3:F8:108:ARG:HG3 | 2.20 | 0.42 |
| 12:F8:201:CYC:HB | 12:F8:201:CYC:HMA3 | 1.84 | 0.42 |
| 2:I8:14:SER:CA | 11:a9:170:PHE:CE2 | 3.02 | 0.42 |
| 12:I8:201:CYC:CMA | 12:I8:201:CYC:NB | 2.82 | 0.42 |
| 3:L8:109:CYS:C | 12:a9:901:CYC:HBB2 | 2.44 | 0.42 |
| 4:M8:28:HIS:CD2 | 4:M8:35:THR:HG23 | 2.54 | 0.42 |
| 4:M8:95:ALA:CB | 5:Z8:38:GLU:HG3 | 2.36 | 0.42 |
| 4:M8:226:SER:HG | 3:Y8:84:ARG:C | 2.28 | 0.42 |
| 3:O8:2:GLN:HA | 3:O8:6:THR:HG21 | 2.01 | 0.42 |
| 2:P8:138:VAL:O | 2:P8:138:VAL:CG1 | 2.67 | 0.42 |
| 3:L9:84:ARG:NH2 | 11:a9:406:LEU:HD23 | 2.34 | 0.42 |
| 4:M9:28:HIS:HD2 | 4:M9:35:THR:CG2 | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M9:250:THR:O | 4:M9:250:THR:HG22 | 2.19 | 0.42 |
| 2:Q9:38:MET:HE3 | 3:R9:24:LEU:CD2 | 2.50 | 0.42 |
| 3:J9:2:GLN:HA | 3:J9:6:THR:HG21 | 2.00 | 0.42 |
| 3:J9:116:THR:OG1 | 11:a9:521:PHE:CB | 2.54 | 0.42 |
| 2:U9:38:MET:HE3 | 3:V9:24:LEU:CD2 | 2.49 | 0.42 |
| 3:V9:108:ARG:CG | 3:V9:108:ARG:HH21 | 2.32 | 0.42 |
| 3:X9:65:ASP:OD1 | 3:X9:65:ASP:N | 2.47 | 0.42 |
| 12:X9:202:CYC:NC | 12:X9:202:CYC:HMD3 | 2.35 | 0.42 |
| 11:a9:377:VAL:CG1 | 11:a9:390:ALA:HB3 | 2.48 | 0.42 |
| 11:a9:470:ILE:O | 11:a9:470:ILE:HG22 | 2.19 | 0.42 |
| 11:a9:586:LEU:HD13 | 11:a9:586:LEU:HA | 1.43 | 0.42 |
| 11:aA:56:ILE:HD12 | 11:aA:612:TYR:CZ | 2.54 | 0.42 |
| 11:aA:102:GLN:OE1 | 11:aA:102:GLN:HA | 2.19 | 0.42 |
| 11:aA:708:HIS:ND1 | 11:aA:709:CYS:SG | 2.92 | 0.42 |
| 4:M1:245:ASP:O | 12:X1:201:CYC:HBB3 | 2.19 | 0.42 |
| 3:X1:2:GLN:HA | 3:X1:6:THR:HG21 | 2.00 | 0.42 |
| 2:C2:38:MET:HE3 | 3:D2:24:LEU:CD2 | 2.49 | 0.42 |
| 3:HA:3:ASP:H | 3:HA:6:THR:HB | 1.85 | 0.42 |
| 2:KA:38:MET:HE3 | 3:LA:24:LEU:CD2 | 2.50 | 0.42 |
| 2:SA:99:ALA:HB2 | 3:TA:9:ILE:HD13 | 2.00 | 0.42 |
| 3:VA:2:GLN:HA | 3:VA:6:THR:HG21 | 2.00 | 0.42 |
| 3:VA:108:ARG:HG2 | 3:VA:108:ARG:HH21 | 1.84 | 0.42 |
| 2:Q1:38:MET:HE3 | 3:R1:24:LEU:CD2 | 2.50 | 0.42 |
| 12:Q1:201:CYC:CMA | 12:Q1:201:CYC:NB | 2.82 | 0.42 |
| 2:I3:38:MET:HE3 | 3:J3:24:LEU:CD2 | 2.50 | 0.42 |
| 2:I3:138:VAL:O | 2:I3:138:VAL:CG1 | 2.67 | 0.42 |
| 3:J3:2:GLN:HA | 3:J3:6:THR:HG21 | 2.00 | 0.42 |
| 12:J3:202:CYC:HC | 12:J3:202:CYC:HMD3 | 1.83 | 0.42 |
| 2:K3:38:MET:HE3 | 3:L3:24:LEU:CD2 | 2.50 | 0.42 |
| 12:H2:201:CYC:HC | 12:H2:201:CYC:HMD3 | 1.83 | 0.42 |
| 3:J2:108:ARG:NE | 6:M2:155:ASN:C | 2.67 | 0.42 |
| 2:K2:99:ALA:HB2 | 3:L2:9:ILE:HD13 | 2.00 | 0.42 |
| 3:L2:3:ASP:H | 3:L2:6:THR:HB | 1.85 | 0.42 |
| 12:B3:201:CYC:HB | 12:B3:201:CYC:HMA3 | 1.84 | 0.42 |
| 3:D3:124:THR:HB | 3:D3:171:ILE:O | 2.18 | 0.42 |
| 12:E3:201:CYC:CMA | 12:E3:201:CYC:NB | 2.81 | 0.42 |
| 5:N3:1:MET:HB2 | 5:N3:3:VAL:HG23 | 1.91 | 0.42 |
| 5:N3:37:HIS:H | 12:T3:301:CYC:HMA3 | 1.84 | 0.42 |
| 5:N3:53:LEU:C | 5:N3:53:LEU:CD2 | 2.92 | 0.42 |
| 12:O3:201:CYC:CMA | 12:O3:201:CYC:NB | 2.81 | 0.42 |
| 2:S3:38:MET:HE3 | 3:T3:24:LEU:CD2 | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:S3:81:LYS:NZ | 12:S3:201:CYC:O1A | 2.51 | 0.42 |
| 2:T4:138:VAL:O | 2:T4:138:VAL:CG1 | 2.67 | 0.42 |
| 2:V4:138:VAL:O | 2:V4:138:VAL:CG1 | 2.67 | 0.42 |
| 3:F4:3:ASP:H | 3:F4:6:THR:HB | 1.85 | 0.42 |
| 4:M4:28:HIS:HD2 | 4:M4:35:THR:CG2 | 2.33 | 0.42 |
| 3:O4:104:VAL:CG2 | 5:Z4:61:LYS:CE | 2.96 | 0.42 |
| 12:O4:201:CYC:CMA | 12:O4:201:CYC:HB | 2.25 | 0.42 |
| 1:L5:79:ALA:CB | 8:G5:114:GLU:CB | 2.91 | 0.42 |
| 1:N5:53:LYS:CE | 8:O5:120:GLN:NE2 | 2.69 | 0.42 |
| 8:O5:76:LYS:HG2 | 8:O5:77:MET:CE | 2.37 | 0.42 |
| 2:X4:38:MET:HE3 | 3:Y4:24:LEU:CD2 | 2.50 | 0.42 |
| 2:C1:38:MET:HE3 | 3:D1:24:LEU:CD2 | 2.50 | 0.42 |
| 8:Q5:122:PRO:HD2 | 12:Q5:201:CYC:OC | 2.19 | 0.42 |
| 8:S5:107:ILE:HG21 | 1:T5:13:ASP:OD1 | 2.19 | 0.42 |
| 8:U5:78:THR:HG21 | 6:M6:35:GLY:O | 2.19 | 0.42 |
| 8:W5:122:PRO:HD2 | 12:W5:201:CYC:OC | 2.19 | 0.42 |
| 8:a5:67:SER:HB3 | 8:a5:68:PRO:HD2 | 2.00 | 0.42 |
| 3:L6:70:GLY:HA2 | 6:M6:68:THR:H | 1.84 | 0.42 |
| 6:M6:127:SER:CA | 3:F6:84:ARG:NH1 | 2.80 | 0.42 |
| 10:j5:18:ARG:HH12 | 10:j5:268:SER:CB | 2.31 | 0.42 |
| 10:j5:190:LEU:CD2 | 10:j5:194:CYS:SG | 3.08 | 0.42 |
| 10:j5:277:ILE:CA | 10:j5:284:PRO:HB3 | 2.49 | 0.42 |
| 10:j5:414:ILE:HG21 | 10:j5:414:ILE:HD13 | 1.72 | 0.42 |
| 10:j5:431:GLN:HA | 10:j5:431:GLN:HE21 | 1.84 | 0.42 |
| 10:j5:471:PRO:O | 10:j5:501:ILE:CG1 | 2.57 | 0.42 |
| 10:j5:528:GLU:O | 10:j5:528:GLU:CG | 2.66 | 0.42 |
| 10:j5:1118:THR:CG2 | 1:t7:83:ARG:NH1 | 2.77 | 0.42 |
| 10:j5:1146:THR:HA | 1:v7:77:ARG:NH1 | 2.34 | 0.42 |
| 10:j5:1151:GLN:CA | 1:v7:122:PRO:CB | 2.74 | 0.42 |
| 10:k5:262:TYR:CD1 | 10:k5:262:TYR:O | 2.73 | 0.42 |
| 10:k5:284:PRO:HB2 | 10:k5:286:VAL:N | 2.34 | 0.42 |
| 10:k5:631:HIS:HB2 | 10:k5:664:MET:HE1 | 2.01 | 0.42 |
| 10:k5:1067:LEU:HD13 | 10:k5:1101:GLU:CG | 2.41 | 0.42 |
| 10:k5:1097:VAL:O | 10:k5:1097:VAL:CG1 | 2.68 | 0.42 |
| 12:k5:1204:CYC:CMA | 12:k5:1204:CYC:NB | 2.74 | 0.42 |
| 3:B6:3:ASP:H | 3:B6:6:THR:HB | 1.85 | 0.42 |
| 8:Q7:151:PHE:CZ | 8:C7:20:PRO:HB3 | 2.55 | 0.42 |
| 8:I7:95:GLY:HA3 | 8:I7:104:ILE:HD11 | 2.01 | 0.42 |
| 8:i7:27:LYS:NZ | 8:s7:148:GLU:OE1 | 2.45 | 0.42 |
| 8:k7:67:SER:O | 8:k7:68:PRO:C | 2.63 | 0.42 |
| 12:V7:201:CYC:OB | 9:w7:21:ARG:O | 2.37 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:W7:122:PRO:HD2 | 12:W7:201:CYC:OC | 2.19 | 0.42 |
| 8:Y7:37:LEU:HD22 | 1:Z7:24:LEU:HD22 | 2.00 | 0.42 |
| 1:Z7:67:ARG:HH12 | 11:a9:307:ARG:CB | 2.33 | 0.42 |
| 8:c7:50:ILE:HD13 | 8:c7:137:ALA:CB | 2.46 | 0.42 |
| 8:c7:67:SER:O | 8:c7:68:PRO:C | 2.62 | 0.42 |
| 8:o7:51:VAL:O | 8:o7:51:VAL:HG12 | 2.16 | 0.42 |
| 8:o7:80:LEU:CD1 | 12:o7:201:CYC:C3D | 2.97 | 0.42 |
| 2:T8:138:VAL:O | 2:T8:138:VAL:CG1 | 2.67 | 0.42 |
| 12:U8:202:CYC:HB | 12:U8:202:CYC:HMA3 | 1.84 | 0.42 |
| 2:X8:38:MET:HE2 | 2:X8:38:MET:HB3 | 1.81 | 0.42 |
| 3:F8:111:ASN:CG | 3:F8:112:GLY:N | 2.77 | 0.42 |
| 12:J8:202:CYC:HMD3 | 12:J8:202:CYC:NC | 2.34 | 0.42 |
| 2:K8:38:MET:HE3 | 3:L8:24:LEU:CD2 | 2.50 | 0.42 |
| 12:L8:201:CYC:HB | 12:L8:201:CYC:HMA3 | 1.84 | 0.42 |
| 4:M8:28:HIS:HD2 | 4:M8:35:THR:CG2 | 2.33 | 0.42 |
| 4:M8:29:PRO:HG3 | 11:a9:226:PHE:O | 2.19 | 0.42 |
| 4:M8:140:ARG:CD | 4:M8:214:GLY:O | 2.54 | 0.42 |
| 3:Q8:84:ARG:HD2 | 5:Z8:31:TRP:HE1 | 1.82 | 0.42 |
| 12:S8:201:CYC:HB | 12:S8:201:CYC:HMA3 | 1.83 | 0.42 |
| 12:L9:201:CYC:HAB1 | 2:K9:24:LEU:HB3 | 1.96 | 0.42 |
| 4:M9:232:VAL:HG11 | 3:X9:111:ASN:C | 2.40 | 0.42 |
| 12:P9:202:CYC:NC | 12:P9:202:CYC:HMD3 | 2.34 | 0.42 |
| 3:Y8:102:ALA:CB | 3:Y8:105:LEU:HB3 | 2.47 | 0.42 |
| 3:Y8:114:LYS:O | 3:Y8:118:VAL:HB | 2.19 | 0.42 |
| 2:A9:138:VAL:O | 2:A9:138:VAL:CG1 | 2.67 | 0.42 |
| 2:E9:17:ARG:CZ | 2:I9:2:LYS:NZ | 2.82 | 0.42 |
| 2:W9:38:MET:HE3 | 3:X9:24:LEU:CD2 | 2.49 | 0.42 |
| 2:G1:138:VAL:O | 2:G1:138:VAL:CG1 | 2.67 | 0.42 |
| 12:G1:201:CYC:CMA | 12:G1:201:CYC:NB | 2.82 | 0.42 |
| 11:a9:56:ILE:HD12 | 11:a9:612:TYR:CZ | 2.54 | 0.42 |
| 11:a9:816:LEU:HD23 | 11:a9:816:LEU:C | 2.41 | 0.42 |
| 11:aA:365:LYS:HA | 11:aA:365:LYS:HD3 | 1.35 | 0.42 |
| 11:aA:377:VAL:CG1 | 11:aA:390:ALA:HB3 | 2.48 | 0.42 |
| 11:aA:446:ALA:C | 11:aA:447:SER:O | 2.59 | 0.42 |
| 11:aA:470:ILE:O | 11:aA:470:ILE:HG22 | 2.19 | 0.42 |
| 3:J1:3:ASP:H | 3:J1:6:THR:HB | 1.85 | 0.42 |
| 5:N1:53:LEU:C | 5:N1:53:LEU:CD2 | 2.92 | 0.42 |
| 12:U1:201:CYC:CMA | 12:U1:201:CYC:NB | 2.82 | 0.42 |
| 3:X1:3:ASP:H | 3:X1:6:THR:HB | 1.85 | 0.42 |
| 12:Z1:201:CYC:HB | 12:Z1:201:CYC:HMA3 | 1.84 | 0.42 |
| 3:B2:2:GLN:HA | 3:B2:6:THR:HG21 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:F2:3:ASP:H | 3:F2:6:THR:HB | 1.85 | 0.42 |
| 3:F2:78:ARG:HG2 | 12:F2:201:CYC:CAD | 2.48 | 0.42 |
| 2:AA:34:ALA:HB3 | 3:BA:31:VAL:CG1 | 2.39 | 0.42 |
| 2:CA:99:ALA:HB2 | 3:DA:9:ILE:HD13 | 2.00 | 0.42 |
| 2:IA:138:VAL:O | 2:IA:138:VAL:CG1 | 2.67 | 0.42 |
| 3:JA:2:GLN:HA | 3:JA:6:THR:HG21 | 2.00 | 0.42 |
| 12:LA:202:CYC:C1B | 11:aA:404:TYR:CZ | 3.02 | 0.42 |
| 4:MA:132:LEU:HD12 | 4:MA:137:ILE:HD12 | 2.01 | 0.42 |
| 2:SA:138:VAL:O | 2:SA:138:VAL:CG1 | 2.67 | 0.42 |
| 12:SA:201:CYC:CMA | 12:SA:201:CYC:NB | 2.81 | 0.42 |
| 12:TA:302:CYC:NC | 12:TA:302:CYC:HMD3 | 2.34 | 0.42 |
| 2:O1:138:VAL:O | 2:O1:138:VAL:CG1 | 2.67 | 0.42 |
| 2:Q1:99:ALA:HB2 | 3:R1:9:ILE:HD13 | 2.00 | 0.42 |
| 3:R1:120:LEU:CD2 | 5:N1:16:PHE:CE1 | 3.02 | 0.42 |
| 3:L2:77:ARG:NH2 | 6:M2:70:GLU:CG | 2.77 | 0.42 |
| 2:A4:138:VAL:O | 2:A4:138:VAL:CG1 | 2.67 | 0.42 |
| 12:C4:201:CYC:CMA | 12:C4:201:CYC:NB | 2.82 | 0.42 |
| 2:Q3:38:MET:HE3 | 3:R3:24:LEU:CD2 | 2.50 | 0.42 |
| 3:R3:2:GLN:HA | 3:R3:6:THR:HG21 | 2.01 | 0.42 |
| 2:S3:138:VAL:O | 2:S3:138:VAL:CG1 | 2.67 | 0.42 |
| 12:B1:202:CYC:HBA1 | 11:aA:680:SER:O | 2.19 | 0.42 |
| 2:N4:138:VAL:O | 2:N4:138:VAL:CG1 | 2.67 | 0.42 |
| 12:B5:201:CYC:CBB | 9:z5:21:ARG:CB | 2.97 | 0.42 |
| 8:C5:2:SER:HA | 8:C5:100:ASP:HB3 | 2.01 | 0.42 |
| 1:D5:3:ASP:HB2 | 1:D5:4:ALA:H | 1.48 | 0.42 |
| 1:J5:76:ARG:HH12 | 9:i5:67:VAL:HG11 | 1.84 | 0.42 |
| 8:Q5:17:TYR:CD2 | 1:R5:93:THR:OG1 | 2.46 | 0.42 |
| 8:S5:67:SER:HB3 | 8:S5:68:PRO:HD2 | 2.00 | 0.42 |
| 8:U5:82:LEU:HD12 | 6:M6:34:ARG:CB | 2.49 | 0.42 |
| 8:Y5:67:SER:HB3 | 8:Y5:68:PRO:HD2 | 2.00 | 0.42 |
| 3:L6:132:GLN:OE1 | 1:d7:15:GLN:OE1 | 2.36 | 0.42 |
| 6:M6:179:GLY:HA2 | 6:M6:182:GLN:HG2 | 2.01 | 0.42 |
| 6:M6:278:ARG:NH2 | 1:d7:64:ASP:CG | 2.64 | 0.42 |
| 9:i5:9:ALA:CA | 9:i5:50:LYS:O | 2.63 | 0.42 |
| 10:j5:191:GLU:HB3 | 10:j5:196:ILE:CD1 | 2.49 | 0.42 |
| 10:j5:262:TYR:CD1 | 10:j5:262:TYR:O | 2.73 | 0.42 |
| 10:j5:277:ILE:CB | 10:j5:284:PRO:CA | 2.98 | 0.42 |
| 10:k5:1064:LYS:HD2 | 10:k5:1065:HIS:HA | 2.01 | 0.42 |
| 2:C6:99:ALA:HB2 | 3:D6:9:ILE:HD13 | 2.00 | 0.42 |
| 12:E6:201:CYC:CMA | 12:E6:201:CYC:NB | 2.82 | 0.42 |
| 2:G6:38:MET:HE3 | 3:H6:24:LEU:CD2 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:D1:2:GLN:HA | 3:D1:6:THR:HG21 | 2.00 | 0.42 |
| 8:Q7:20:PRO:HG2 | 8:C7:101:VAL:HG21 | 2.02 | 0.42 |
| 1:R7:72:MET:HE2 | 1:R7:72:MET:HB3 | 1.87 | 0.42 |
| 8:g7:33:GLY:HA2 | 8:g7:36:ARG:HB2 | 2.01 | 0.42 |
| 8:i7:49:ARG:CZ | 8:i7:140:LEU:HD22 | 2.49 | 0.42 |
| 8:U7:22:GLU:O | 8:U7:24:ASP:N | 2.52 | 0.42 |
| 8:Y7:4:LEU:CD2 | 8:Y7:26:ILE:HD13 | 2.47 | 0.42 |
| 8:a7:95:GLY:HA3 | 8:a7:104:ILE:HD11 | 2.01 | 0.42 |
| 12:B8:202:CYC:CMA | 12:B8:202:CYC:HB | 2.25 | 0.42 |
| 12:B8:202:CYC:OB | 4:M8:58:TYR:HD1 | 2.02 | 0.42 |
| 8:m7:95:GLY:HA3 | 8:m7:104:ILE:HD11 | 2.01 | 0.42 |
| 8:m7:130:VAL:CG1 | 8:m7:157:VAL:HG23 | 2.48 | 0.42 |
| 1:p7:68:PRO:HB2 | 11:a9:42:ARG:HD3 | 2.01 | 0.42 |
| 2:V8:138:VAL:O | 2:V8:138:VAL:CG1 | 2.67 | 0.42 |
| 3:W8:3:ASP:H | 3:W8:6:THR:HB | 1.85 | 0.42 |
| 2:N8:14:SER:HA | 5:Z8:62:ARG:HD2 | 2.02 | 0.42 |
| 12:O8:201:CYC:HC | 12:O8:201:CYC:HMD3 | 1.82 | 0.42 |
| 5:N9:1:MET:CE | 5:N9:1:MET:CA | 2.85 | 0.42 |
| 3:Y8:105:LEU:HB3 | 3:Y8:106:GLU:H | 1.67 | 0.42 |
| 5:Z8:53:LEU:C | 5:Z8:53:LEU:CD2 | 2.92 | 0.42 |
| 5:Z8:56:GLU:OE2 | 5:Z8:59:ARG:NH2 | 2.51 | 0.42 |
| 3:B9:107:ASP:HB3 | 11:a9:382:ASN:HB3 | 2.02 | 0.42 |
| 3:Z9:2:GLN:HA | 3:Z9:6:THR:HG21 | 2.00 | 0.42 |
| 11:a9:55:ASP:HB3 | 11:a9:612:TYR:CG | 2.47 | 0.42 |
| 11:a9:392:ILE:O | 11:a9:392:ILE:HG22 | 2.19 | 0.42 |
| 11:a9:412:VAL:H | 11:a9:412:VAL:HG22 | 1.57 | 0.42 |
| 11:aA:320:ASP:OD1 | 11:aA:320:ASP:N | 2.50 | 0.42 |
| 11:aA:582:MET:O | 11:aA:582:MET:CG | 2.68 | 0.42 |
| 3:H1:108:ARG:O | 12:H1:201:CYC:CBB | 2.60 | 0.42 |
| 12:H1:201:CYC:HMD3 | 12:H1:201:CYC:HC | 1.82 | 0.42 |
| 12:J1:201:CYC:HB | 12:J1:201:CYC:HMA3 | 1.83 | 0.42 |
| 4:M1:9:GLN:CD | 4:M1:9:GLN:C | 2.87 | 0.42 |
| 4:M1:190:ARG:HE | 4:M1:190:ARG:HB2 | 1.71 | 0.42 |
| 12:V1:202:CYC:HB | 12:V1:202:CYC:HMA3 | 1.84 | 0.42 |
| 2:Y1:99:ALA:HB2 | 3:Z1:9:ILE:HD13 | 2.00 | 0.42 |
| 3:D2:124:THR:HB | 3:D2:171:ILE:O | 2.18 | 0.42 |
| 2:E2:38:MET:HE2 | 2:E2:38:MET:HB3 | 1.81 | 0.42 |
| 1:Z:72:MET:HE2 | 1:Z:72:MET:HB3 | 1.87 | 0.42 |
| 3:HA:125:ARG:NH2 | 8:S7:41:GLN:HG2 | 2.34 | 0.42 |
| 2:KA:19:LEU:O | 3:LA:45:THR:OG1 | 2.27 | 0.42 |
| 2:KA:22:THR:O | 2:KA:22:THR:HG22 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 5:NA:22:LEU:HD21 | 5:NA:26:LEU:CD1 | 2.15 | 0.42 |
| 5:NA:28:HIS:CD2 | 5:NA:28:HIS:H | 2.38 | 0.42 |
| 2:UA:38:MET:HE3 | 3:VA:24:LEU:CD2 | 2.49 | 0.42 |
| 2:YA:99:ALA:HB2 | 3:ZA:9:ILE:HD13 | 2.00 | 0.42 |
| 2:O1:99:ALA:HB2 | 3:P1:9:ILE:HD13 | 2.00 | 0.42 |
| 2:K3:38:MET:HE2 | 2:K3:38:MET:HB3 | 1.81 | 0.42 |
| 12:K3:201:CYC:CMA | 12:K3:201:CYC:NB | 2.81 | 0.42 |
| 2:I2:38:MET:HE3 | 3:J2:24:LEU:CD2 | 2.50 | 0.42 |
| 2:K2:138:VAL:O | 2:K2:138:VAL:CG1 | 2.67 | 0.42 |
| 6:M2:147:ASP:OD2 | 2:E2:15:GLN:NE2 | 2.53 | 0.42 |
| 2:E3:38:MET:HE3 | 3:F3:24:LEU:CD2 | 2.50 | 0.42 |
| 3:F3:3:ASP:H | 3:F3:6:THR:HB | 1.85 | 0.42 |
| 3:Z3:9:ILE:HD13 | 2:Y3:99:ALA:HB2 | 2.00 | 0.42 |
| 4:M3:7:SER:C | 4:M3:14:LEU:HD13 | 2.08 | 0.42 |
| 4:M3:28:HIS:HD2 | 4:M3:35:THR:CG2 | 2.33 | 0.42 |
| 2:O3:30:ARG:NH1 | 3:P3:5:PHE:CE1 | 2.88 | 0.42 |
| 12:R3:202:CYC:HMD3 | 12:R3:202:CYC:NC | 2.35 | 0.42 |
| 2:E4:1:MET:H2 | 4:M4:10:ARG:HE | 1.67 | 0.42 |
| 2:E4:38:MET:HE3 | 3:F4:24:LEU:CD2 | 2.50 | 0.42 |
| 4:M4:225:LYS:HD2 | 4:M4:225:LYS:HA | 1.84 | 0.42 |
| 4:M4:262:ASP:OD1 | 4:M4:263:PRO:CD | 2.68 | 0.42 |
| 12:O4:201:CYC:HC | 12:O4:201:CYC:HMD3 | 1.82 | 0.42 |
| 3:Q4:84:ARG:HE | 5:Z4:29:HIS:HD2 | 1.66 | 0.42 |
| 2:X4:99:ALA:HB2 | 3:Y4:9:ILE:HD13 | 2.00 | 0.42 |
| 5:Z4:39:PRO:HG3 | 12:Z4:301:CYC:CHD | 2.49 | 0.42 |
| 8:E5:151:PHE:CE1 | 1:P5:42:ALA:CB | 3.02 | 0.42 |
| 1:F5:106:GLU:CG | 9:z5:58:THR:CG2 | 2.98 | 0.42 |
| 12:G5:201:CYC:HB | 12:G5:201:CYC:CMA | 2.21 | 0.42 |
| 12:H5:201:CYC:HMD1 | 12:H5:201:CYC:NC | 2.09 | 0.42 |
| 8:c5:120:GLN:CD | 1:f5:53:LYS:NZ | 2.78 | 0.42 |
| 1:f5:30:TYR:HE2 | 10:j5:47:PHE:CE1 | 2.37 | 0.42 |
| 8:Q5:121:THR:HG23 | 12:Q5:201:CYC:NC | 2.35 | 0.42 |
| 8:a5:33:GLY:HA2 | 8:a5:36:ARG:HB2 | 2.01 | 0.42 |
| 7:N6:11:TRP:HE1 | 2:E6:107:ASP:CA | 2.31 | 0.42 |
| 10:j5:1001:TYR:CE1 | 10:j5:1016:LEU:HD11 | 2.54 | 0.42 |
| 10:j5:1097:VAL:O | 10:j5:1097:VAL:CG1 | 2.68 | 0.42 |
| 10:k5:44:ASP:O | 10:k5:48:GLY:N | 2.48 | 0.42 |
| 10:k5:651:ILE:O | 10:k5:651:ILE:CG2 | 2.65 | 0.42 |
| 10:k5:1053:TYR:CA | 1:l7:106:GLU:O | 2.67 | 0.42 |
| 10:k5:1102:TYR:CD1 | 10:k5:1102:TYR:O | 2.72 | 0.42 |
| 12:C6:201:CYC:CMA | 12:C6:201:CYC:NB | 2.82 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:P7:75:THR:HB | 8:Q7:112:VAL:CA | 2.50 | 0.42 |
| 8:Q7:121:THR:HG23 | 12:Q7:201:CYC:NC | 2.35 | 0.42 |
| 8:G7:120:GLN:CD | 1:L7:53:LYS:NZ | 2.78 | 0.42 |
| 1:h7:24:LEU:HD23 | 1:h7:24:LEU:HA | 1.70 | 0.42 |
| 8:i7:17:TYR:OH | 1:j7:86:ASP:OD1 | 2.22 | 0.42 |
| 8:i7:20:PRO:HD2 | 8:s7:155:TYR:CZ | 2.52 | 0.42 |
| 8:U7:95:GLY:HA3 | 8:U7:104:ILE:HD11 | 2.01 | 0.42 |
| 8:c7:92:VAL:HG13 | 8:c7:152:TYR:HB2 | 1.99 | 0.42 |
| 8:c7:156:LEU:O | 8:c7:160:MET:HG3 | 2.19 | 0.42 |
| 8:e7:67:SER:O | 8:e7:68:PRO:C | 2.63 | 0.42 |
| 8:q7:79:ALA:O | 11:aA:49:TRP:HB3 | 2.20 | 0.42 |
| 3:U8:2:GLN:HA | 3:U8:6:THR:HG21 | 2.00 | 0.42 |
| 3:H8:111:ASN:OD1 | 11:a9:291:TYR:HE1 | 1.96 | 0.42 |
| 2:I8:138:VAL:O | 2:I8:138:VAL:CG1 | 2.67 | 0.42 |
| 4:M8:70:SER:O | 4:M8:70:SER:OG | 2.36 | 0.42 |
| 4:M8:126:THR:HB | 12:M8:302:CYC:CBA | 2.46 | 0.42 |
| 4:M8:268:ARG:O | 4:M8:269:SER:O | 2.27 | 0.42 |
| 12:M8:301:CYC:CAC | 3:Y8:127:VAL:HG22 | 2.48 | 0.42 |
| 2:R8:138:VAL:O | 2:R8:138:VAL:CG1 | 2.67 | 0.42 |
| 3:L9:51:ILE:CG2 | 3:L9:90:LEU:HD13 | 2.45 | 0.42 |
| 4:M9:271:ARG:NH2 | 3:V9:78:ARG:NH1 | 2.68 | 0.42 |
| 5:N9:53:LEU:C | 5:N9:53:LEU:CD2 | 2.92 | 0.42 |
| 2:Q9:38:MET:HE2 | 2:Q9:38:MET:HB3 | 1.81 | 0.42 |
| 5:Z8:37:HIS:ND1 | 12:Z8:301:CYC:C4B | 2.79 | 0.42 |
| 12:C9:201:CYC:CMA | 12:C9:201:CYC:NB | 2.81 | 0.42 |
| 2:I9:19:LEU:CD1 | 3:J9:41:VAL:CG1 | 2.98 | 0.42 |
| 3:T9:2:GLN:HA | 3:T9:6:THR:HG21 | 2.00 | 0.42 |
| 3:X9:3:ASP:H | 3:X9:6:THR:HB | 1.85 | 0.42 |
| 3:Z9:3:ASP:H | 3:Z9:6:THR:HB | 1.85 | 0.42 |
| 12:Z9:202:CYC:HB | 12:Z9:202:CYC:CMA | 2.25 | 0.42 |
| 11:a9:102:GLN:OE1 | 11:a9:102:GLN:HA | 2.19 | 0.42 |
| 11:a9:426:ARG:HD2 | 11:a9:490:ILE:HG22 | 1.98 | 0.42 |
| 11:a9:538:ARG:HB3 | 11:a9:538:ARG:HE | 1.58 | 0.42 |
| 11:a9:582:MET:O | 11:a9:582:MET:CG | 2.68 | 0.42 |
| 11:aA:731:GLN:HE21 | 12:aA:902:CYC:HAA1 | 1.83 | 0.42 |
| 3:H1:78:ARG:HG2 | 12:H1:201:CYC:HMD2 | 2.01 | 0.42 |
| 2:I1:38:MET:HE3 | 3:J1:24:LEU:CD2 | 2.50 | 0.42 |
| 4:M1:268:ARG:CB | 3:V1:111:ASN:HD21 | 2.32 | 0.42 |
| 3:V1:124:THR:HB | 3:V1:171:ILE:O | 2.18 | 0.42 |
| 1:A:62:TYR:HA | 10:k5:155:LYS:NZ | 2.35 | 0.42 |
| 1:A:71:MEN:O | 1:A:77:ARG:HD3 | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:FA:3:ASP:H | 3:FA:6:THR:HB | 1.84 | 0.42 |
| 2:IA:24:LEU:HB3 | 12:JA:201:CYC:CAB | 2.47 | 0.42 |
| 5:NA:53:LEU:C | 5:NA:53:LEU:CD2 | 2.92 | 0.42 |
| 2:OA:25:GLN:HG3 | 2:YA:33:ARG:HG2 | 1.99 | 0.42 |
| 2:SA:38:MET:HE3 | 3:TA:24:LEU:CD2 | 2.49 | 0.42 |
| 3:TA:28:THR:HG22 | 2:X4:67:THR:HG1 | 1.70 | 0.42 |
| 12:VA:202:CYC:HMD3 | 12:VA:202:CYC:NC | 2.35 | 0.42 |
| 12:WA:201:CYC:CMA | 12:WA:201:CYC:NB | 2.81 | 0.42 |
| 2:YA:38:MET:HE3 | 3:ZA:24:LEU:CD2 | 2.50 | 0.42 |
| 3:J3:121:GLY:CA | 11:a9:804:ARG:HH21 | 2.23 | 0.42 |
| 2:G2:138:VAL:O | 2:G2:138:VAL:CG1 | 2.67 | 0.42 |
| 12:J2:202:CYC:HC | 12:J2:202:CYC:HMD3 | 1.83 | 0.42 |
| 6:M2:32:MET:HE1 | 8:O5:75:GLU:OE1 | 2.19 | 0.42 |
| 2:A3:30:ARG:NH1 | 3:B3:5:PHE:CE1 | 2.88 | 0.42 |
| 3:B3:3:ASP:H | 3:B3:6:THR:HB | 1.84 | 0.42 |
| 3:B3:127:VAL:HG23 | 12:B3:202:CYC:CMC | 2.47 | 0.42 |
| 5:N3:34:LEU:HD22 | 5:N3:34:LEU:HA | 1.71 | 0.42 |
| 12:Q3:201:CYC:CMA | 12:Q3:201:CYC:NB | 2.82 | 0.42 |
| 2:U3:38:MET:HE3 | 3:V3:24:LEU:CD2 | 2.49 | 0.42 |
| 12:F4:201:CYC:NC | 12:F4:201:CYC:HMD3 | 2.35 | 0.42 |
| 2:I4:138:VAL:O | 2:I4:138:VAL:CG1 | 2.67 | 0.42 |
| 3:J4:3:ASP:H | 3:J4:6:THR:HB | 1.85 | 0.42 |
| 12:J4:202:CYC:HB | 12:J4:202:CYC:HMA3 | 1.84 | 0.42 |
| 2:K4:99:ALA:HB2 | 3:L4:9:ILE:HD13 | 2.00 | 0.42 |
| 3:L4:3:ASP:H | 3:L4:6:THR:HB | 1.85 | 0.42 |
| 4:M4:51:ARG:HH11 | 4:M4:51:ARG:CG | 2.27 | 0.42 |
| 8:K5:101:VAL:O | 8:K5:102:THR:C | 2.57 | 0.42 |
| 8:I5:16:ARG:CG | 8:I5:16:ARG:NH1 | 2.77 | 0.42 |
| 12:P5:201:CYC:HC | 12:P5:201:CYC:CMD | 2.13 | 0.42 |
| 8:Q5:16:ARG:HA | 1:R5:90:ARG:CG | 2.44 | 0.42 |
| 8:Q5:67:SER:O | 8:Q5:68:PRO:C | 2.63 | 0.42 |
| 1:R5:1:MET:N | 10:k5:504:ASP:OD2 | 2.53 | 0.42 |
| 1:R5:106:GLU:HG3 | 10:k5:505:VAL:HG22 | 2.02 | 0.42 |
| 8:W5:16:ARG:HA | 1:X5:90:ARG:CG | 2.44 | 0.42 |
| 8:Y5:120:GLN:CD | 1:b5:53:LYS:NZ | 2.78 | 0.42 |
| 1:b5:6:THR:HG21 | 10:k5:22:THR:CG2 | 2.50 | 0.42 |
| 3:L6:3:ASP:H | 3:L6:6:THR:HB | 1.85 | 0.42 |
| 6:M6:65:VAL:CG1 | 1:b7:60:LEU:N | 2.82 | 0.42 |
| 9:z5:58:THR:HG22 | 9:z5:58:THR:O | 2.19 | 0.42 |
| 10:j5:17:PHE:CD1 | 10:j5:19:THR:CG2 | 3.02 | 0.42 |
| 10:j5:297:VAL:O | 10:j5:297:VAL:HG13 | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:j5:481:ILE:HD13 | 10:j5:481:ILE:HG21 | 1.69 | 0.42 |
| 10:j5:1146:THR:CA | 1:v7:77:ARG:CZ | 2.94 | 0.42 |
| 10:k5:187:ARG:NH1 | 10:k5:237:ASP:OD2 | 2.52 | 0.42 |
| 10:k5:191:GLU:HB3 | 10:k5:196:ILE:CD1 | 2.49 | 0.42 |
| 10:k5:277:ILE:HA | 10:k5:284:PRO:HB3 | 2.02 | 0.42 |
| 10:k5:631:HIS:HA | 10:k5:664:MET:CE | 2.48 | 0.42 |
| 10:k5:1050:PHE:CD2 | 10:k5:1058:VAL:HG11 | 2.45 | 0.42 |
| 10:k5:1118:THR:CB | 12:k5:1204:CYC:O2A | 2.68 | 0.42 |
| 2:A6:49:ASP:O | 2:A6:50:SER:C | 2.62 | 0.42 |
| 3:F6:3:ASP:H | 3:F6:6:THR:HB | 1.85 | 0.42 |
| 8:I7:102:THR:CB | 8:I7:103:PRO:HD3 | 2.33 | 0.42 |
| 8:K7:67:SER:O | 8:K7:68:PRO:C | 2.63 | 0.42 |
| 1:h7:52:ILE:O | 1:h7:52:ILE:CG2 | 2.67 | 0.42 |
| 8:i7:43:LEU:CD1 | 8:i7:141:LEU:HD11 | 2.32 | 0.42 |
| 8:k7:64:ASP:HA | 8:k7:67:SER:CB | 2.49 | 0.42 |
| 8:a7:48:GLU:HA | 11:a9:318:TRP:HH2 | 0.78 | 0.42 |
| 12:d7:201:CYC:HMD1 | 12:d7:201:CYC:NC | 2.09 | 0.42 |
| 12:C8:201:CYC:CMA | 12:C8:201:CYC:NB | 2.82 | 0.42 |
| 8:o7:18:LEU:CG | 1:p7:97:LEU:HD13 | 2.49 | 0.42 |
| 8:o7:81:CYS:HA | 12:o7:201:CYC:HAC1 | 1.23 | 0.42 |
| 8:q7:64:ASP:HA | 8:q7:67:SER:CB | 2.49 | 0.42 |
| 1:v7:139:GLY:CA | 11:aA:342:ARG:HD2 | 2.49 | 0.42 |
| 9:x7:11:ILE:HD11 | 9:x7:28:PHE:CE1 | 2.55 | 0.42 |
| 9:y7:11:ILE:HD11 | 9:y7:28:PHE:CE1 | 2.55 | 0.42 |
| 3:L8:66:LEU:HA | 11:a9:82:GLN:NE2 | 2.34 | 0.42 |
| 4:M8:1:MET:HE3 | 4:M8:45:VAL:HA | 1.29 | 0.42 |
| 4:M8:91:VAL:CA | 2:P8:15:GLN:HA | 2.40 | 0.42 |
| 2:N8:30:ARG:NH1 | 3:O8:5:PHE:CE1 | 2.88 | 0.42 |
| 3:Q8:103:SER:O | 3:Q8:104:VAL:C | 2.62 | 0.42 |
| 3:Q8:122:THR:CG2 | 12:Z8:301:CYC:HMC2 | 2.48 | 0.42 |
| 12:F1:202:CYC:HB | 12:F1:202:CYC:HMA3 | 1.84 | 0.42 |
| 5:N9:54:LEU:HB3 | 5:N9:55:PRO:HD3 | 2.02 | 0.42 |
| 5:N9:54:LEU:CG | 3:T9:84:ARG:CZ | 2.93 | 0.42 |
| 5:N9:68:LEU:HD23 | 5:N9:68:LEU:HA | 1.80 | 0.42 |
| 12:Q9:201:CYC:CMA | 12:Q9:201:CYC:NB | 2.81 | 0.42 |
| 5:Z8:28:HIS:CD2 | 5:Z8:28:HIS:H | 2.38 | 0.42 |
| 12:A9:201:CYC:CMA | 12:A9:201:CYC:NB | 2.81 | 0.42 |
| 12:E9:201:CYC:CMA | 12:E9:201:CYC:NB | 2.81 | 0.42 |
| 12:F9:303:CYC:NC | 12:F9:303:CYC:HMD3 | 2.35 | 0.42 |
| 2:I9:37:SER:CB | 2:I9:97:LEU:CD1 | 2.97 | 0.42 |
| 3:J9:3:ASP:H | 3:J9:6:THR:HB | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:W9:99:ALA:HB2 | 3:X9:9:ILE:HD13 | 2.00 | 0.42 |
| 11:a9:572:THR:CG2 | 11:a9:573:SER:N | 2.82 | 0.42 |
| 12:a9:901:CYC:HMD3 | 12:a9:901:CYC:HC | 1.83 | 0.42 |
| 11:aA:490:ILE:N | 11:aA:490:ILE:CD1 | 2.80 | 0.42 |
| 11:aA:552:LEU:HA | 11:aA:552:LEU:HD23 | 1.64 | 0.42 |
| 4:M1:37:GLU:HG3 | 4:M1:38:PRO:HD2 | 2.00 | 0.42 |
| 4:M1:246:ALA:HA | 12:X1:201:CYC:HBB3 | 1.99 | 0.42 |
| 4:M1:262:ASP:OD1 | 4:M1:263:PRO:CD | 2.68 | 0.42 |
| 5:N1:14:LYS:HE3 | 5:N1:14:LYS:HB2 | 1.92 | 0.42 |
| 2:U1:38:MET:HE3 | 3:V1:24:LEU:CD2 | 2.49 | 0.42 |
| 12:D2:202:CYC:HB | 12:D2:202:CYC:HMA3 | 1.84 | 0.42 |
| 2:GA:38:MET:HE3 | 3:HA:24:LEU:CD2 | 2.50 | 0.42 |
| 2:KA:19:LEU:HA | 2:KA:19:LEU:HD23 | 1.75 | 0.42 |
| 4:MA:59:ILE:HD13 | 4:MA:59:ILE:HG21 | 1.67 | 0.42 |
| 4:MA:252:LEU:HD12 | 12:ZA:202:CYC:O1D | 2.20 | 0.42 |
| 5:NA:54:LEU:HB3 | 5:NA:55:PRO:HD3 | 2.02 | 0.42 |
| 2:UA:138:VAL:O | 2:UA:138:VAL:CG1 | 2.67 | 0.42 |
| 12:R1:202:CYC:HMD3 | 12:R1:202:CYC:NC | 2.35 | 0.42 |
| 12:H3:202:CYC:HBA1 | 11:a9:776:TYR:H | 1.85 | 0.42 |
| 6:M2:38:SER:O | 6:M2:38:SER:OG | 2.31 | 0.42 |
| 3:F3:111:ASN:O | 4:M3:39:SER:CB | 2.61 | 0.42 |
| 3:Z3:24:LEU:CD2 | 2:Y3:38:MET:HE3 | 2.50 | 0.42 |
| 12:Z3:202:CYC:NC | 12:Z3:202:CYC:HMD3 | 2.35 | 0.42 |
| 3:B4:117:TYR:CE1 | 4:M4:53:LEU:HD13 | 2.54 | 0.42 |
| 2:C4:38:MET:HE2 | 2:C4:38:MET:HB3 | 1.81 | 0.42 |
| 4:M3:140:ARG:NH1 | 4:M3:204:ILE:O | 2.52 | 0.42 |
| 3:V3:3:ASP:H | 3:V3:6:THR:HB | 1.84 | 0.42 |
| 3:S4:24:LEU:CD2 | 2:R4:38:MET:HE3 | 2.50 | 0.42 |
| 3:F4:116:THR:N | 4:M4:3:VAL:CG1 | 2.78 | 0.42 |
| 3:L4:91:ARG:NH2 | 11:aA:239:TYR:OH | 2.53 | 0.42 |
| 4:M4:62:LYS:HD2 | 4:M4:62:LYS:HA | 1.67 | 0.42 |
| 2:P4:99:ALA:HB2 | 3:Q4:9:ILE:HD13 | 2.00 | 0.42 |
| 3:Q4:75:PRO:HD3 | 3:Q4:78:ARG:HH21 | 1.85 | 0.42 |
| 1:L5:42:ALA:HB2 | 8:U5:151:PHE:CE1 | 2.55 | 0.42 |
| 8:M5:90:ARG:CD | 1:N5:18:TYR:N | 2.83 | 0.42 |
| 8:M5:90:ARG:HH12 | 1:N5:16:GLY:HA2 | 1.84 | 0.42 |
| 8:O5:105:GLU:HG2 | 8:O5:110:ILE:HG23 | 2.02 | 0.42 |
| 3:Y4:117:TYR:O | 3:Y4:122:THR:N | 2.53 | 0.42 |
| 3:Y4:128:ALA:HB2 | 3:Y4:172:ALA:HB2 | 2.02 | 0.42 |
| 5:Z4:29:HIS:NE2 | 5:Z4:38:GLU:N | 2.67 | 0.42 |
| 5:Z4:37:HIS:NE2 | 12:Z4:301:CYC:C1A | 2.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:C5:27:LYS:C | 8:C5:29:PHE:H | 2.19 | 0.42 |
| 1:D5:5:ILE:HG21 | 1:D5:5:ILE:HD13 | 1.68 | 0.42 |
| 1:D5:71:MEN:C | 1:D5:77:ARG:CZ | 2.96 | 0.42 |
| 1:J5:5:ILE:CG2 | 1:J5:5:ILE:O | 2.67 | 0.42 |
| 2:C1:38:MET:HE2 | 2:C1:38:MET:HB3 | 1.81 | 0.42 |
| 8:e5:25:ARG:H | 8:e5:25:ARG:HG3 | 1.65 | 0.42 |
| 8:Q5:22:GLU:O | 8:Q5:26:ILE:HG13 | 2.20 | 0.42 |
| 8:U5:33:GLY:HA2 | 8:U5:36:ARG:HB2 | 2.01 | 0.42 |
| 8:W5:67:SER:O | 8:W5:68:PRO:C | 2.63 | 0.42 |
| 8:a5:25:ARG:C | 8:a5:27:LYS:N | 2.78 | 0.42 |
| 8:a5:95:GLY:HA3 | 8:a5:104:ILE:HD11 | 2.01 | 0.42 |
| 1:b5:18:TYR:CZ | 10:k5:165:ARG:N | 2.88 | 0.42 |
| 10:j5:631:HIS:CA | 10:j5:664:MET:HE1 | 2.50 | 0.42 |
| 10:j5:806:VAL:O | 10:j5:806:VAL:HG12 | 2.20 | 0.42 |
| 10:j5:813:ALA:CB | 8:S7:14:GLU:OE2 | 2.67 | 0.42 |
| 10:j5:1069:ARG:HD3 | 10:j5:1115:ARG:NH1 | 2.34 | 0.42 |
| 10:j5:1071:PRO:CD | 10:j5:1071:PRO:O | 2.65 | 0.42 |
| 10:j5:1146:THR:HA | 1:v7:77:ARG:CZ | 2.49 | 0.42 |
| 10:k5:19:THR:O | 10:k5:21:MET:N | 2.53 | 0.42 |
| 10:k5:747:LYS:O | 10:k5:750:ARG:NH1 | 2.53 | 0.42 |
| 10:k5:793:SER:CB | 12:N7:201:CYC:O2A | 2.64 | 0.42 |
| 10:k5:951:MET:CE | 10:k5:955:LEU:CD1 | 2.97 | 0.42 |
| 10:k5:1041:ARG:H | 10:k5:1041:ARG:HG2 | 1.53 | 0.42 |
| 10:k5:1145:PRO:HG2 | 1:l7:14:VAL:HG11 | 2.01 | 0.42 |
| 2:A6:30:ARG:NH1 | 3:B6:5:PHE:CE1 | 2.88 | 0.42 |
| 2:A6:99:ALA:HB2 | 3:B6:9:ILE:HD13 | 2.00 | 0.42 |
| 2:C6:138:VAL:O | 2:C6:138:VAL:CG1 | 2.67 | 0.42 |
| 1:P7:53:LYS:HZ2 | 8:Q7:120:GLN:CD | 2.27 | 0.42 |
| 8:Q7:20:PRO:HG2 | 8:C7:101:VAL:CG2 | 2.50 | 0.42 |
| 8:S7:120:GLN:CD | 1:X7:53:LYS:NZ | 2.78 | 0.42 |
| 8:C7:95:GLY:HA3 | 8:C7:104:ILE:HD11 | 2.01 | 0.42 |
| 1:H7:72:MET:HE2 | 1:H7:72:MET:HB3 | 1.87 | 0.42 |
| 8:g7:161:GLN:HG2 | 1:v7:49:THR:CG2 | 2.50 | 0.42 |
| 8:W7:66:VAL:O | 8:W7:66:VAL:CG1 | 2.66 | 0.42 |
| 8:a7:56:ASP:OD1 | 11:a9:325:LEU:HB2 | 2.20 | 0.42 |
| 8:a7:67:SER:O | 8:a7:68:PRO:C | 2.63 | 0.42 |
| 8:c7:20:PRO:HG3 | 8:m7:151:PHE:O | 2.19 | 0.42 |
| 8:c7:49:ARG:CZ | 8:c7:140:LEU:HD22 | 2.49 | 0.42 |
| 8:c7:112:VAL:HG23 | 8:c7:115:MET:HE2 | 2.02 | 0.42 |
| 8:e7:22:GLU:O | 8:e7:26:ILE:HG13 | 2.20 | 0.42 |
| 2:C8:38:MET:HE3 | 3:D8:24:LEU:CD2 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:D8:2:GLN:HA | 3:D8:6:THR:HG21 | 2.00 | 0.42 |
| 8:o7:22:GLU:O | 8:o7:26:ILE:HG13 | 2.20 | 0.42 |
| 8:u7:22:GLU:O | 8:u7:26:ILE:HG13 | 2.20 | 0.42 |
| 8:u7:67:SER:O | 8:u7:68:PRO:C | 2.63 | 0.42 |
| 2:V8:38:MET:HE3 | 3:W8:24:LEU:CD2 | 2.49 | 0.42 |
| 2:X8:69:PRO:HB2 | 2:S9:42:ARG:HD2 | 2.02 | 0.42 |
| 12:H8:201:CYC:CBA | 11:a9:261:SER:OG | 2.66 | 0.42 |
| 3:J8:3:ASP:H | 3:J8:6:THR:HB | 1.85 | 0.42 |
| 4:M8:4:LEU:HD12 | 4:M8:4:LEU:C | 2.45 | 0.42 |
| 4:M8:23:PRO:HB2 | 4:M8:34:ASP:HB3 | 2.02 | 0.42 |
| 4:M8:140:ARG:HG2 | 4:M8:209:TYR:OH | 2.20 | 0.42 |
| 3:L9:24:LEU:CD2 | 2:K9:38:MET:HE3 | 2.50 | 0.42 |
| 4:M9:93:LEU:HA | 4:M9:93:LEU:HD12 | 1.66 | 0.42 |
| 2:O9:49:ASP:O | 2:O9:50:SER:C | 2.62 | 0.42 |
| 12:D9:202:CYC:HB | 12:D9:202:CYC:HMA3 | 1.84 | 0.42 |
| 2:K9:15:GLN:HA | 11:a9:393:ARG:HD3 | 2.01 | 0.42 |
| 2:K9:17:ARG:NH1 | 2:K9:17:ARG:CB | 2.73 | 0.42 |
| 2:G1:38:MET:HE3 | 3:H1:24:LEU:CD2 | 2.50 | 0.42 |
| 11:a9:801:ASN:ND2 | 11:a9:802:ARG:HD2 | 2.34 | 0.42 |
| 3:H1:3:ASP:H | 3:H1:6:THR:HB | 1.85 | 0.42 |
| 4:M1:28:HIS:HD2 | 4:M1:35:THR:CG2 | 2.33 | 0.42 |
| 4:M1:185:ALA:HA | 12:Z1:202:CYC:CGA | 2.50 | 0.42 |
| 2:U1:138:VAL:O | 2:U1:138:VAL:CG1 | 2.67 | 0.42 |
| 2:W1:138:VAL:O | 2:W1:138:VAL:CG1 | 2.67 | 0.42 |
| 12:W1:201:CYC:CMA | 12:W1:201:CYC:NB | 2.81 | 0.42 |
| 2:Y1:38:MET:HE3 | 3:Z1:24:LEU:CD2 | 2.50 | 0.42 |
| 3:D2:3:ASP:H | 3:D2:6:THR:HB | 1.85 | 0.42 |
| 2:EA:138:VAL:O | 2:EA:138:VAL:CG1 | 2.67 | 0.42 |
| 2:IA:98:VAL:HG21 | 3:JA:19:LEU:CD1 | 2.41 | 0.42 |
| 4:MA:232:VAL:HG11 | 3:XA:111:ASN:C | 2.40 | 0.42 |
| 3:RA:2:GLN:HA | 3:RA:6:THR:HG21 | 2.00 | 0.42 |
| 12:RA:202:CYC:CMD | 12:RA:202:CYC:NC | 2.76 | 0.42 |
| 3:VA:3:ASP:H | 3:VA:6:THR:HB | 1.85 | 0.42 |
| 12:O1:201:CYC:CMA | 12:O1:201:CYC:NB | 2.81 | 0.42 |
| 12:R1:201:CYC:O1D | 5:N1:50:LEU:CD2 | 2.66 | 0.42 |
| 3:H3:3:ASP:H | 3:H3:6:THR:HB | 1.85 | 0.42 |
| 3:J3:77:ARG:CD | 2:K3:111:ALA:CB | 2.98 | 0.42 |
| 6:M2:62:ARG:HH22 | 1:h7:58:LYS:N | 2.17 | 0.42 |
| 3:B3:124:THR:HB | 3:B3:171:ILE:O | 2.18 | 0.42 |
| 3:F3:65:ASP:OD1 | 3:F3:65:ASP:N | 2.47 | 0.42 |
| 12:Z3:202:CYC:HB | 12:Z3:202:CYC:HMA3 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:B4:97:LEU:HA | 3:B4:163:TYR:HE2 | 1.85 | 0.42 |
| 3:B4:113:LEU:HG | 3:B4:171:ILE:HG12 | 2.01 | 0.42 |
| 4:M3:246:ALA:HB2 | 3:X3:109:CYS:O | 2.20 | 0.42 |
| 12:U4:202:CYC:HB | 12:U4:202:CYC:HMA3 | 1.84 | 0.42 |
| 3:H4:108:ARG:NH2 | 11:aA:97:ALA:CB | 2.82 | 0.42 |
| 12:I4:201:CYC:CMA | 12:I4:201:CYC:NB | 2.82 | 0.42 |
| 4:M4:23:PRO:HB2 | 4:M4:34:ASP:HB3 | 2.02 | 0.42 |
| 3:Y4:102:ALA:HB1 | 3:Y4:106:GLU:H | 1.84 | 0.42 |
| 3:Y4:113:LEU:HD11 | 3:Y4:117:TYR:CD2 | 2.54 | 0.42 |
| 5:Z4:53:LEU:C | 5:Z4:53:LEU:CD2 | 2.92 | 0.42 |
| 5:Z4:60:ILE:HD13 | 5:Z4:60:ILE:HG21 | 1.74 | 0.42 |
| 1:B5:107:ARG:NH1 | 9:z5:21:ARG:HB2 | 2.34 | 0.42 |
| 8:E5:22:GLU:O | 8:E5:26:ILE:HG13 | 2.20 | 0.42 |
| 8:I5:105:GLU:HG2 | 8:I5:110:ILE:HG23 | 2.02 | 0.42 |
| 1:f5:18:TYR:CZ | 10:j5:165:ARG:CD | 3.01 | 0.42 |
| 1:R5:120:GLY:O | 10:k5:703:LEU:CD1 | 2.67 | 0.42 |
| 8:S5:67:SER:O | 8:S5:68:PRO:C | 2.63 | 0.42 |
| 8:Y5:66:VAL:O | 8:Y5:66:VAL:CG1 | 2.66 | 0.42 |
| 8:a5:25:ARG:H | 8:a5:25:ARG:HG3 | 1.62 | 0.42 |
| 3:J6:3:ASP:H | 3:J6:6:THR:HB | 1.85 | 0.42 |
| 6:M6:147:ASP:OD2 | 2:E6:15:GLN:NE2 | 2.53 | 0.42 |
| 8:A7:120:GLN:CD | 1:F7:53:LYS:NZ | 2.78 | 0.42 |
| 10:j5:526:MET:HE2 | 10:j5:683:ARG:HD2 | 2.01 | 0.42 |
| 10:j5:725:LEU:O | 8:K7:83:ARG:HD3 | 2.20 | 0.42 |
| 10:j5:853:LEU:O | 10:j5:853:LEU:CG | 2.68 | 0.42 |
| 10:j5:1008:PHE:CD1 | 1:v7:87:TYR:OH | 2.64 | 0.42 |
| 10:k5:144:ASN:OD1 | 10:k5:144:ASN:N | 2.50 | 0.42 |
| 10:k5:623:VAL:O | 10:k5:623:VAL:HG12 | 2.17 | 0.42 |
| 10:k5:759:THR:H | 10:k5:759:THR:HG22 | 1.58 | 0.42 |
| 10:k5:978:LEU:HD12 | 10:k5:978:LEU:HA | 1.88 | 0.42 |
| 10:k5:1025:LEU:CD2 | 10:k5:1035:PHE:CG | 2.74 | 0.42 |
| 10:k5:1064:LYS:O | 10:k5:1068:GLY:CA | 2.68 | 0.42 |
| 8:Q7:122:PRO:HD2 | 12:Q7:201:CYC:OC | 2.19 | 0.42 |
| 1:D7:75:THR:HB | 8:E7:112:VAL:CA | 2.50 | 0.42 |
| 12:D7:201:CYC:HMD1 | 12:D7:201:CYC:NC | 2.10 | 0.42 |
| 8:E7:67:SER:O | 8:E7:68:PRO:C | 2.63 | 0.42 |
| 8:E7:122:PRO:HD2 | 12:E7:201:CYC:OC | 2.19 | 0.42 |
| 8:M7:67:SER:O | 8:M7:68:PRO:C | 2.63 | 0.42 |
| 8:i7:141:LEU:HD12 | 8:i7:146:ALA:HA | 2.01 | 0.42 |
| 1:V7:72:MET:HE2 | 1:V7:72:MET:HB3 | 1.87 | 0.42 |
| 8:a7:62:ARG:HA | 11:a9:336:ILE:HG21 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:c7:13:ALA:CB | 9:x7:46:LYS:HE3 | 2.50 | 0.42 |
| 8:c7:112:VAL:C | 8:c7:115:MET:H | 2.28 | 0.42 |
| 2:E1:38:MET:HE3 | 3:F1:24:LEU:CD2 | 2.50 | 0.42 |
| 3:B8:125:ARG:HD2 | 3:W8:14:LEU:CD1 | 2.50 | 0.42 |
| 1:l7:72:MET:HE2 | 1:l7:72:MET:HB3 | 1.87 | 0.42 |
| 8:o7:94:TYR:CZ | 1:p7:17:LYS:O | 2.69 | 0.42 |
| 8:q7:67:SER:O | 8:q7:68:PRO:C | 2.63 | 0.42 |
| 8:s7:67:SER:O | 8:s7:68:PRO:C | 2.63 | 0.42 |
| 8:u7:76:LYS:O | 8:u7:80:LEU:HG | 2.19 | 0.42 |
| 8:u7:80:LEU:CD1 | 12:u7:201:CYC:C3D | 2.97 | 0.42 |
| 9:w7:11:ILE:HG21 | 9:w7:11:ILE:HD13 | 1.64 | 0.42 |
| 2:T8:38:MET:HE2 | 2:T8:38:MET:HB3 | 1.81 | 0.42 |
| 12:W8:202:CYC:HB | 12:W8:202:CYC:HMA3 | 1.83 | 0.42 |
| 12:X8:201:CYC:CMA | 12:X8:201:CYC:NB | 2.81 | 0.42 |
| 12:K8:201:CYC:CMA | 12:K8:201:CYC:NB | 2.81 | 0.42 |
| 2:N8:38:MET:HE2 | 2:N8:38:MET:HB3 | 1.81 | 0.42 |
| 3:L9:107:ASP:C | 3:L9:111:ASN:HB2 | 2.45 | 0.42 |
| 4:M9:140:ARG:NH1 | 4:M9:204:ILE:O | 2.52 | 0.42 |
| 4:M9:188:LEU:HG | 3:V9:84:ARG:NH1 | 2.33 | 0.42 |
| 2:O9:30:ARG:NH1 | 3:P9:5:PHE:CE1 | 2.88 | 0.42 |
| 3:B9:14:LEU:HD13 | 3:X9:125:ARG:CD | 2.47 | 0.42 |
| 3:H9:127:VAL:HA | 12:H9:202:CYC:HBC3 | 2.02 | 0.42 |
| 12:J9:201:CYC:NC | 12:J9:201:CYC:HMD3 | 2.35 | 0.42 |
| 12:X9:202:CYC:HB | 12:X9:202:CYC:HMA3 | 1.83 | 0.42 |
| 2:Y9:38:MET:HE3 | 3:Z9:24:LEU:CD2 | 2.50 | 0.42 |
| 11:a9:388:VAL:O | 11:a9:392:ILE:HD12 | 2.20 | 0.42 |
| 11:a9:526:GLN:H | 11:a9:526:GLN:HG2 | 1.53 | 0.42 |
| 11:a9:584:ARG:O | 11:a9:588:VAL:N | 2.51 | 0.42 |
| 11:a9:643:LEU:HD11 | 11:a9:766:ASN:CA | 2.50 | 0.42 |
| 11:aA:92:LYS:HA | 11:aA:92:LYS:HD3 | 1.54 | 0.42 |
| 11:aA:283:GLN:CG | 11:aA:284:PRO:HD3 | 2.48 | 0.42 |
| 2:K1:38:MET:HE3 | 3:L1:24:LEU:CD2 | 2.50 | 0.42 |
| 4:M1:211:GLN:O | 5:N1:28:HIS:NE2 | 2.45 | 0.42 |
| 3:X1:81:ALA:HA | 3:X1:84:ARG:CZ | 2.49 | 0.42 |
| 3:Z1:3:ASP:H | 3:Z1:6:THR:HB | 1.84 | 0.42 |
| 2:E2:38:MET:HE3 | 3:F2:24:LEU:CD2 | 2.50 | 0.42 |
| 3:DA:111:ASN:ND2 | 4:MA:73:ASP:HA | 2.31 | 0.42 |
| 12:DA:202:CYC:HB | 12:DA:202:CYC:HMA3 | 1.84 | 0.42 |
| 3:FA:148:VAL:HG11 | 12:F9:302:CYC:C1D | 2.49 | 0.42 |
| 2:IA:19:LEU:CD1 | 3:JA:41:VAL:CG1 | 2.98 | 0.42 |
| 3:LA:3:ASP:H | 3:LA:6:THR:HB | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:MA:262:ASP:OD1 | 4:MA:263:PRO:CD | 2.68 | 0.42 |
| 2:OA:30:ARG:NH1 | 3:PA:5:PHE:CE1 | 2.88 | 0.42 |
| 2:SA:38:MET:C | 2:X4:69:PRO:HG3 | 2.37 | 0.42 |
| 12:VA:202:CYC:CMD | 12:VA:202:CYC:NC | 2.75 | 0.42 |
| 2:WA:99:ALA:HB2 | 3:XA:9:ILE:HD13 | 2.00 | 0.42 |
| 2:O1:34:ALA:HB3 | 3:P1:31:VAL:CG1 | 2.39 | 0.42 |
| 2:S1:38:MET:HE3 | 3:T1:24:LEU:CD2 | 2.50 | 0.42 |
| 2:G3:38:MET:HE3 | 3:H3:24:LEU:CD2 | 2.50 | 0.42 |
| 12:G3:201:CYC:CMA | 12:G3:201:CYC:NB | 2.82 | 0.42 |
| 2:K3:138:VAL:O | 2:K3:138:VAL:CG1 | 2.67 | 0.42 |
| 12:G2:201:CYC:CBB | 3:L2:74:TYR:CZ | 3.02 | 0.42 |
| 3:J2:3:ASP:H | 3:J2:6:THR:HB | 1.85 | 0.42 |
| 7:N2:4:ASN:O | 7:N2:5:VAL:C | 2.61 | 0.42 |
| 3:D3:3:ASP:H | 3:D3:6:THR:HB | 1.85 | 0.42 |
| 3:L3:3:ASP:H | 3:L3:6:THR:HB | 1.85 | 0.42 |
| 3:X3:81:ALA:HA | 3:X3:84:ARG:CZ | 2.49 | 0.42 |
| 3:U4:3:ASP:H | 3:U4:6:THR:HB | 1.85 | 0.42 |
| 2:K4:38:MET:HE3 | 3:L4:24:LEU:CD2 | 2.50 | 0.42 |
| 4:M4:132:LEU:HD12 | 4:M4:137:ILE:HD12 | 2.01 | 0.42 |
| 4:M4:225:LYS:N | 12:M4:301:CYC:O2A | 2.10 | 0.42 |
| 2:R4:38:MET:HE2 | 2:R4:38:MET:HB3 | 1.81 | 0.42 |
| 2:R4:138:VAL:O | 2:R4:138:VAL:CG1 | 2.67 | 0.42 |
| 8:K5:116:TYR:HB3 | 8:K5:123:ILE:CG1 | 2.49 | 0.42 |
| 12:K5:201:CYC:HBB2 | 1:J5:73:TYR:HE1 | 1.85 | 0.42 |
| 8:O5:2:SER:HA | 8:O5:100:ASP:HB3 | 2.01 | 0.42 |
| 5:Z4:31:TRP:CB | 5:Z4:32:PRO:HD2 | 2.32 | 0.42 |
| 8:A5:22:GLU:O | 8:A5:26:ILE:HG13 | 2.20 | 0.42 |
| 8:A5:88:TYR:CZ | 12:A5:201:CYC:CMB | 3.03 | 0.42 |
| 8:A5:121:THR:HG22 | 12:A5:201:CYC:HMC3 | 2.01 | 0.42 |
| 1:B5:10:ASN:OD1 | 10:k5:557:VAL:HG23 | 2.13 | 0.42 |
| 8:C5:67:SER:O | 8:C5:68:PRO:C | 2.63 | 0.42 |
| 8:G5:22:GLU:O | 8:G5:26:ILE:HG13 | 2.20 | 0.42 |
| 8:G5:67:SER:O | 8:G5:68:PRO:C | 2.63 | 0.42 |
| 8:e5:5:THR:C | 8:e5:7:ALA:N | 2.78 | 0.42 |
| 8:S5:90:ARG:CD | 1:T5:18:TYR:N | 2.83 | 0.42 |
| 8:S5:105:GLU:HG2 | 8:S5:110:ILE:HG23 | 2.02 | 0.42 |
| 8:U5:67:SER:O | 8:U5:68:PRO:C | 2.63 | 0.42 |
| 8:U5:105:GLU:HG2 | 8:U5:110:ILE:HG23 | 2.02 | 0.42 |
| 1:b5:30:TYR:HH | 10:k5:47:PHE:HZ | 0.42 | 0.42 |
| 12:K6:201:CYC:CMA | 12:K6:201:CYC:NB | 2.81 | 0.42 |
| 3:L6:70:GLY:HA2 | 6:M6:67:GLY:CA | 2.45 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:A7:120:GLN:CG | 1:F7:53:LYS:NZ | 2.78 | 0.42 |
| 10:j5:558:VAL:O | 10:j5:560:VAL:N | 2.53 | 0.42 |
| 10:j5:739:VAL:O | 10:j5:739:VAL:HG12 | 2.18 | 0.42 |
| 10:j5:830:GLU:O | 10:j5:830:GLU:HG3 | 2.20 | 0.42 |
| 10:j5:922:LYS:HB2 | 10:j5:922:LYS:HE3 | 1.78 | 0.42 |
| 10:j5:942:LYS:HD2 | 10:j5:943:THR:HG22 | 2.02 | 0.42 |
| 10:j5:971:VAL:CG1 | 1:t7:76:ARG:NH2 | 2.83 | 0.42 |
| 10:j5:1052:PRO:HA | 1:r7:106:GLU:OE2 | 2.20 | 0.42 |
| 10:j5:1144:SER:CB | 1:r7:13:ASP:OD2 | 2.62 | 0.42 |
| 10:k5:277:ILE:HG12 | 10:k5:284:PRO:HB3 | 0.61 | 0.42 |
| 10:k5:393:MET:HA | 10:k5:394:PRO:HD3 | 1.68 | 0.42 |
| 10:k5:414:ILE:HD13 | 10:k5:414:ILE:HG21 | 1.73 | 0.42 |
| 10:k5:549:LYS:HG2 | 10:k5:551:MET:HB2 | 2.01 | 0.42 |
| 10:k5:1018:LEU:CA | 10:k5:1021:ALA:HB3 | 2.40 | 0.42 |
| 10:k5:1064:LYS:HD2 | 10:k5:1065:HIS:H | 1.82 | 0.42 |
| 10:k5:1118:THR:HG23 | 12:k5:1204:CYC:CMA | 2.49 | 0.42 |
| 12:B6:201:CYC:HB | 12:B6:201:CYC:HMA3 | 1.84 | 0.42 |
| 12:D6:202:CYC:HB | 12:D6:202:CYC:HMA3 | 1.84 | 0.42 |
| 8:O7:67:SER:O | 8:O7:68:PRO:C | 2.63 | 0.42 |
| 1:P7:76:ARG:HD3 | 8:Q7:110:ILE:CD1 | 2.50 | 0.42 |
| 12:P7:201:CYC:CBB | 9:z7:21:ARG:CG | 2.97 | 0.42 |
| 8:Q7:67:SER:O | 8:Q7:68:PRO:C | 2.63 | 0.42 |
| 8:S7:22:GLU:O | 8:S7:26:ILE:HG13 | 2.20 | 0.42 |
| 8:C7:67:SER:O | 8:C7:68:PRO:C | 2.63 | 0.42 |
| 1:H7:54:GLU:OE2 | 11:aA:563:PHE:CB | 2.63 | 0.42 |
| 1:H7:89:LEU:HB2 | 1:H7:133:MET:HE1 | 2.02 | 0.42 |
| 8:I7:2:SER:O | 8:I7:100:ASP:OD2 | 2.37 | 0.42 |
| 1:L7:8:VAL:HB | 1:L7:27:LEU:HD21 | 2.02 | 0.42 |
| 8:M7:105:GLU:HG2 | 8:M7:110:ILE:HG23 | 2.02 | 0.42 |
| 8:g7:67:SER:O | 8:g7:68:PRO:C | 2.63 | 0.42 |
| 8:i7:22:GLU:O | 8:i7:26:ILE:HG13 | 2.20 | 0.42 |
| 8:i7:47:ARG:CB | 1:j7:18:TYR:CZ | 3.01 | 0.42 |
| 8:k7:120:GLN:CD | 1:p7:53:LYS:NZ | 2.78 | 0.42 |
| 8:W7:105:GLU:HG2 | 8:W7:110:ILE:HG23 | 2.02 | 0.42 |
| 1:b7:37:ARG:HG2 | 1:b7:37:ARG:HH11 | 1.85 | 0.42 |
| 2:C8:138:VAL:O | 2:C8:138:VAL:CG1 | 2.67 | 0.42 |
| 8:u7:94:TYR:CZ | 1:v7:17:LYS:O | 2.69 | 0.42 |
| 2:T8:38:MET:HE3 | 3:U8:24:LEU:CD2 | 2.49 | 0.42 |
| 3:U8:3:ASP:H | 3:U8:6:THR:HB | 1.85 | 0.42 |
| 3:F8:3:ASP:H | 3:F8:6:THR:HB | 1.85 | 0.42 |
| 3:F8:108:ARG:HE | 4:M8:9:GLN:HA | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:H8:14:LEU:HD13 | 11:a9:85:ALA:CB | 2.48 | 0.42 |
| 4:M8:87:ILE:HD13 | 3:Y8:77:ARG:HG3 | 0.43 | 0.42 |
| 4:M8:132:LEU:HD12 | 4:M8:137:ILE:HD12 | 2.01 | 0.42 |
| 4:M8:184:ILE:HA | 4:M8:184:ILE:HD13 | 1.65 | 0.42 |
| 4:M8:222:ARG:HH11 | 4:M8:222:ARG:CG | 2.13 | 0.42 |
| 3:F1:113:LEU:HD13 | 4:M1:38:PRO:HB3 | 2.01 | 0.42 |
| 4:M9:23:PRO:HB2 | 4:M9:34:ASP:HB3 | 2.02 | 0.42 |
| 4:M9:162:ASN:N | 12:V9:201:CYC:CBB | 2.61 | 0.42 |
| 2:C9:138:VAL:O | 2:C9:138:VAL:CG1 | 2.67 | 0.42 |
| 2:G9:38:MET:HE3 | 3:H9:24:LEU:CD2 | 2.50 | 0.42 |
| 2:I9:99:ALA:HB2 | 3:J9:9:ILE:HD13 | 2.00 | 0.42 |
| 2:I9:138:VAL:O | 2:I9:138:VAL:CG1 | 2.67 | 0.42 |
| 12:T9:302:CYC:HB | 12:T9:302:CYC:HMA3 | 1.83 | 0.42 |
| 11:a9:419:ARG:O | 11:a9:420:ASN:C | 2.58 | 0.42 |
| 11:a9:579:PHE:O | 11:a9:580:THR:C | 2.57 | 0.42 |
| 11:aA:334:LYS:HE2 | 11:aA:334:LYS:HB2 | 1.89 | 0.42 |
| 11:aA:735:VAL:HG13 | 3:L1:84:ARG:HH12 | 1.85 | 0.42 |
| 5:N1:54:LEU:HB3 | 5:N1:55:PRO:HD3 | 2.02 | 0.42 |
| 3:B2:77:ARG:HA | 3:B2:77:ARG:HD2 | 1.59 | 0.42 |
| 2:C2:99:ALA:HB2 | 3:D2:9:ILE:HD13 | 2.00 | 0.42 |
| 3:BA:3:ASP:H | 3:BA:6:THR:HB | 1.84 | 0.41 |
| 12:BA:202:CYC:HB | 12:BA:202:CYC:HMA3 | 1.84 | 0.41 |
| 12:DA:201:CYC:HBB1 | 4:MA:6:THR:HG21 | 2.01 | 0.41 |
| 12:HA:201:CYC:HB | 12:HA:201:CYC:HMA3 | 1.83 | 0.41 |
| 2:IA:38:MET:HE3 | 3:JA:24:LEU:CD2 | 2.50 | 0.41 |
| 2:O1:30:ARG:NH1 | 3:P1:5:PHE:CE1 | 2.88 | 0.41 |
| 2:O1:49:ASP:O | 2:O1:50:SER:C | 2.62 | 0.41 |
| 3:P1:151:GLY:HA3 | 12:P1:202:CYC:CMD | 2.50 | 0.41 |
| 12:P1:201:CYC:HBA2 | 4:M1:134:ASN:HB2 | 2.00 | 0.41 |
| 2:G3:99:ALA:HB2 | 3:H3:9:ILE:HD13 | 2.00 | 0.41 |
| 2:G3:138:VAL:O | 2:G3:138:VAL:CG1 | 2.67 | 0.41 |
| 3:D3:116:THR:OG1 | 4:M3:69:ILE:HG13 | 2.20 | 0.41 |
| 3:B4:108:ARG:HA | 4:M4:61:ASN:HB2 | 1.99 | 0.41 |
| 4:M3:18:THR:C | 4:M3:19:MET:HG3 | 2.43 | 0.41 |
| 4:M3:28:HIS:CD2 | 4:M3:35:THR:HG23 | 2.55 | 0.41 |
| 4:M3:274:VAL:HG12 | 4:M3:274:VAL:OXT | 2.20 | 0.41 |
| 5:N3:16:PHE:CE1 | 3:R3:120:LEU:CD2 | 3.02 | 0.41 |
| 3:P3:3:ASP:H | 3:P3:6:THR:HB | 1.85 | 0.41 |
| 12:S3:201:CYC:CMA | 12:S3:201:CYC:NB | 2.81 | 0.41 |
| 3:T3:3:ASP:H | 3:T3:6:THR:HB | 1.85 | 0.41 |
| 2:W3:138:VAL:O | 2:W3:138:VAL:CG1 | 2.67 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:G4:201:CYC:CMA | 12:G4:201:CYC:NB | 2.82 | 0.41 |
| 4:M4:138:SER:HB3 | 12:Z4:301:CYC:HAB2 | 2.00 | 0.41 |
| 8:K5:102:THR:N | 8:K5:103:PRO:HD2 | 2.34 | 0.41 |
| 8:K5:110:ILE:HG21 | 8:K5:110:ILE:HD13 | 1.59 | 0.41 |
| 8:A5:88:TYR:OH | 12:A5:201:CYC:CMB | 2.68 | 0.41 |
| 1:H5:76:ARG:HG3 | 9:i5:14:LEU:O | 2.20 | 0.41 |
| 8:U5:2:SER:O | 8:U5:100:ASP:OD2 | 2.37 | 0.41 |
| 12:V5:201:CYC:HBB2 | 10:j5:623:VAL:CB | 2.49 | 0.41 |
| 12:V5:201:CYC:CMA | 12:V5:201:CYC:NB | 2.74 | 0.41 |
| 8:Y5:22:GLU:O | 8:Y5:26:ILE:HG13 | 2.20 | 0.41 |
| 8:Y5:67:SER:O | 8:Y5:68:PRO:C | 2.63 | 0.41 |
| 8:a5:67:SER:O | 8:a5:68:PRO:C | 2.63 | 0.41 |
| 10:j5:156:SER:HG | 12:j5:1201:CYC:HHD | 1.84 | 0.41 |
| 10:j5:194:CYS:CB | 12:j5:1201:CYC:CAC | 2.92 | 0.41 |
| 10:j5:284:PRO:HB2 | 10:j5:286:VAL:N | 2.34 | 0.41 |
| 10:j5:549:LYS:HG2 | 10:j5:551:MET:HB2 | 2.01 | 0.41 |
| 10:j5:623:VAL:O | 10:j5:623:VAL:HG12 | 2.17 | 0.41 |
| 10:j5:747:LYS:O | 10:j5:750:ARG:NH1 | 2.53 | 0.41 |
| 10:j5:872:TYR:HB3 | 9:w7:43:ARG:NH1 | 2.35 | 0.41 |
| 10:j5:1064:LYS:O | 10:j5:1065:HIS:C | 2.63 | 0.41 |
| 10:j5:1064:LYS:O | 10:j5:1068:GLY:CA | 2.67 | 0.41 |
| 10:k5:274:MET:HE2 | 10:k5:323:VAL:HG22 | 2.01 | 0.41 |
| 10:k5:277:ILE:CB | 10:k5:284:PRO:CA | 2.98 | 0.41 |
| 10:k5:306:GLU:CD | 10:k5:362:LYS:HZ3 | 2.21 | 0.41 |
| 10:k5:591:ILE:HD12 | 10:k5:591:ILE:HA | 1.62 | 0.41 |
| 10:k5:942:LYS:HD2 | 10:k5:943:THR:HG22 | 2.02 | 0.41 |
| 10:k5:1008:PHE:HD1 | 12:p7:201:CYC:CBB | 2.33 | 0.41 |
| 2:A6:38:MET:HE2 | 2:A6:38:MET:HB3 | 1.81 | 0.41 |
| 3:D1:3:ASP:H | 3:D1:6:THR:HB | 1.85 | 0.41 |
| 8:O7:66:VAL:O | 8:O7:66:VAL:CG1 | 2.66 | 0.41 |
| 1:R7:53:LYS:NZ | 8:M7:120:GLN:CD | 2.78 | 0.41 |
| 8:S7:105:GLU:HG2 | 8:S7:110:ILE:HG23 | 2.02 | 0.41 |
| 12:C7:201:CYC:HB | 12:C7:201:CYC:CMA | 2.21 | 0.41 |
| 8:I7:161:GLN:HG3 | 1:X7:49:THR:HG21 | 1.95 | 0.41 |
| 8:i7:112:VAL:HG23 | 8:i7:115:MET:HE2 | 2.02 | 0.41 |
| 1:T7:89:LEU:HB2 | 1:T7:133:MET:HE1 | 2.02 | 0.41 |
| 8:W7:121:THR:HG23 | 12:W7:201:CYC:NC | 2.35 | 0.41 |
| 1:b7:75:THR:HG21 | 8:c7:112:VAL:HB | 2.02 | 0.41 |
| 3:B8:112:GLY:HA3 | 4:M8:66:VAL:HG23 | 2.01 | 0.41 |
| 3:B8:116:THR:HG21 | 4:M8:56:MET:HB2 | 1.83 | 0.41 |
| 3:D8:3:ASP:H | 3:D8:6:THR:HB | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:u7:45:GLU:OE2 | 8:u7:45:GLU:CA | 2.68 | 0.41 |
| 1:v7:72:MET:HE2 | 1:v7:72:MET:HB3 | 1.87 | 0.41 |
| 9:y7:14:LEU:C | 9:y7:14:LEU:CD1 | 2.93 | 0.41 |
| 3:U8:151:GLY:HA3 | 12:U8:202:CYC:CMD | 2.51 | 0.41 |
| 12:U8:202:CYC:HMD3 | 12:U8:202:CYC:NC | 2.35 | 0.41 |
| 2:X8:69:PRO:HG3 | 2:S9:38:MET:C | 2.37 | 0.41 |
| 3:F8:84:ARG:HG3 | 11:a9:139:ILE:HG21 | 2.02 | 0.41 |
| 4:M8:100:SER:HA | 4:M8:103:GLN:HB2 | 2.00 | 0.41 |
| 4:M8:124:ARG:H | 4:M8:124:ARG:HG2 | 1.66 | 0.41 |
| 4:M8:225:LYS:CD | 3:Y8:81:ALA:CB | 2.98 | 0.41 |
| 4:M9:33:LEU:HD21 | 2:E9:115:GLU:OE2 | 2.11 | 0.41 |
| 4:M9:124:ARG:H | 4:M9:124:ARG:HG2 | 1.66 | 0.41 |
| 5:Z8:42:SER:CA | 12:Z8:301:CYC:CMA | 2.43 | 0.41 |
| 3:D9:3:ASP:H | 3:D9:6:THR:HB | 1.84 | 0.41 |
| 3:V9:108:ARG:HG2 | 3:V9:108:ARG:HH21 | 1.84 | 0.41 |
| 2:Y9:38:MET:HE2 | 2:Y9:38:MET:HB3 | 1.81 | 0.41 |
| 11:a9:89:ALA:CB | 11:a9:92:LYS:NZ | 2.81 | 0.41 |
| 11:a9:327:SER:OG | 11:a9:328:GLN:NE2 | 2.53 | 0.41 |
| 11:a9:465:TYR:CE2 | 11:a9:516:GLN:HA | 2.54 | 0.41 |
| 11:a9:763:PHE:CE1 | 11:a9:772:ARG:NH2 | 2.88 | 0.41 |
| 11:aA:250:ARG:HA | 11:aA:285:VAL:HG21 | 2.02 | 0.41 |
| 11:aA:389:GLN:NE2 | 11:aA:389:GLN:CA | 2.72 | 0.41 |
| 11:aA:412:VAL:O | 11:aA:415:GLU:OE1 | 2.38 | 0.41 |
| 11:aA:462:ARG:CG | 11:aA:462:ARG:NH1 | 2.71 | 0.41 |
| 4:M1:23:PRO:HB2 | 4:M1:34:ASP:HB3 | 2.02 | 0.41 |
| 4:M1:145:LEU:HD23 | 4:M1:145:LEU:HA | 1.89 | 0.41 |
| 1:A:16:GLY:HA2 | 8:a5:90:ARG:HH12 | 1.78 | 0.41 |
| 1:Z:118:SER:OG | 10:j5:9:SER:CB | 2.62 | 0.41 |
| 2:AA:2:LYS:HZ2 | 2:KA:17:ARG:NH2 | 2.18 | 0.41 |
| 3:FA:36:LYS:HE2 | 3:FA:156:LEU:HD13 | 2.03 | 0.41 |
| 2:GA:138:VAL:O | 2:GA:138:VAL:CG1 | 2.67 | 0.41 |
| 2:IA:4:VAL:HG21 | 2:IA:30:ARG:HB2 | 2.02 | 0.41 |
| 2:IA:8:VAL:CG1 | 2:IA:23:GLU:OE2 | 2.64 | 0.41 |
| 2:IA:37:SER:CB | 2:IA:97:LEU:CD1 | 2.97 | 0.41 |
| 4:MA:28:HIS:CD2 | 4:MA:35:THR:HG23 | 2.55 | 0.41 |
| 4:MA:263:PRO:C | 3:VA:119:ALA:HB2 | 2.43 | 0.41 |
| 3:R1:2:GLN:HA | 3:R1:6:THR:HG21 | 2.01 | 0.41 |
| 2:A1:63:PHE:O | 2:A1:66:LEU:CB | 2.68 | 0.41 |
| 12:H2:202:CYC:HB | 12:H2:202:CYC:HMA3 | 1.83 | 0.41 |
| 3:B4:86:MET:CG | 12:B4:202:CYC:CBC | 2.92 | 0.41 |
| 3:D4:150:ARG:NH1 | 2:C1:140:SER:HB3 | 2.33 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:L3:77:ARG:HD3 | 11:a9:824:VAL:OXT | 2.20 | 0.41 |
| 3:X3:3:ASP:H | 3:X3:6:THR:HB | 1.85 | 0.41 |
| 3:U4:151:GLY:HA3 | 12:U4:202:CYC:CMD | 2.51 | 0.41 |
| 3:W4:3:ASP:H | 3:W4:6:THR:HB | 1.85 | 0.41 |
| 2:G4:15:GLN:HE21 | 11:aA:120:ARG:NH1 | 2.17 | 0.41 |
| 3:J4:125:ARG:NH2 | 2:C2:68:GLN:HE21 | 2.18 | 0.41 |
| 4:M4:143:VAL:HG21 | 4:M4:219:PRO:CG | 2.50 | 0.41 |
| 4:M4:232:VAL:CG1 | 12:M4:301:CYC:HBB2 | 2.47 | 0.41 |
| 12:O4:202:CYC:HMD3 | 12:O4:202:CYC:NC | 2.35 | 0.41 |
| 1:L5:8:VAL:HB | 1:L5:27:LEU:HD21 | 2.02 | 0.41 |
| 8:M5:22:GLU:O | 8:M5:26:ILE:HG13 | 2.20 | 0.41 |
| 1:B5:140:LEU:HD11 | 8:W7:49:ARG:NH1 | 2.35 | 0.41 |
| 8:E5:64:ASP:HB2 | 8:Q5:64:ASP:HB2 | 2.03 | 0.41 |
| 8:I5:67:SER:O | 8:I5:68:PRO:C | 2.63 | 0.41 |
| 1:J5:118:SER:O | 9:i5:56:LEU:HD21 | 2.19 | 0.41 |
| 8:c5:22:GLU:O | 8:c5:26:ILE:HG13 | 2.20 | 0.41 |
| 8:e5:25:ARG:C | 8:e5:27:LYS:H | 2.27 | 0.41 |
| 8:e5:67:SER:O | 8:e5:68:PRO:C | 2.63 | 0.41 |
| 8:U5:95:GLY:HA3 | 8:U5:104:ILE:HD11 | 2.01 | 0.41 |
| 8:U5:130:VAL:CG1 | 8:U5:157:VAL:HG23 | 2.49 | 0.41 |
| 3:J6:65:ASP:OD1 | 3:J6:65:ASP:N | 2.47 | 0.41 |
| 3:L6:151:GLY:HA3 | 12:L6:202:CYC:CMD | 2.51 | 0.41 |
| 6:M6:83:ALA:HB1 | 6:M6:222:LYS:HE3 | 2.01 | 0.41 |
| 10:j5:387:VAL:O | 10:j5:394:PRO:HG3 | 2.05 | 0.41 |
| 10:j5:431:GLN:CA | 10:j5:431:GLN:HE21 | 2.33 | 0.41 |
| 10:j5:780:ILE:O | 10:j5:780:ILE:HG13 | 2.11 | 0.41 |
| 10:j5:953:LEU:HA | 10:j5:953:LEU:HD23 | 1.60 | 0.41 |
| 10:j5:1033:ARG:NH2 | 10:j5:1098:GLU:HG2 | 2.34 | 0.41 |
| 10:j5:1142:SER:O | 1:r7:10:ASN:ND2 | 2.53 | 0.41 |
| 10:k5:28:ILE:HD13 | 10:k5:28:ILE:HG21 | 1.59 | 0.41 |
| 10:k5:277:ILE:CA | 10:k5:284:PRO:HB3 | 2.49 | 0.41 |
| 10:k5:423:LEU:HD23 | 10:k5:423:LEU:HA | 1.75 | 0.41 |
| 10:k5:526:MET:HE2 | 10:k5:683:ARG:HD2 | 2.01 | 0.41 |
| 10:k5:783:TYR:OH | 1:F7:83:ARG:NE | 2.50 | 0.41 |
| 10:k5:802:VAL:O | 10:k5:802:VAL:CG1 | 2.69 | 0.41 |
| 2:A6:63:PHE:O | 2:A6:66:LEU:CB | 2.68 | 0.41 |
| 3:D1:116:THR:OG1 | 4:M1:69:ILE:HG13 | 2.20 | 0.41 |
| 1:B7:89:LEU:HB2 | 1:B7:133:MET:HE1 | 2.03 | 0.41 |
| 8:C7:2:SER:HA | 8:C7:100:ASP:HB3 | 2.01 | 0.41 |
| 1:F7:8:VAL:HB | 1:F7:27:LEU:HD21 | 2.02 | 0.41 |
| 8:K7:121:THR:HG23 | 12:K7:201:CYC:NC | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:g7:37:LEU:HD22 | 1:h7:24:LEU:CD2 | 2.46 | 0.41 |
| 8:g7:67:SER:HB3 | 8:g7:68:PRO:HD2 | 2.00 | 0.41 |
| 8:k7:105:GLU:HG2 | 8:k7:110:ILE:HG23 | 2.02 | 0.41 |
| 1:T7:72:MET:HE2 | 1:T7:72:MET:HB3 | 1.86 | 0.41 |
| 8:U7:15:ALA:CA | 1:V7:90:ARG:CZ | 2.98 | 0.41 |
| 8:a7:2:SER:HA | 8:a7:100:ASP:HB3 | 2.01 | 0.41 |
| 8:a7:6:LYS:NZ | 8:o7:16:ARG:HH22 | 2.15 | 0.41 |
| 3:B8:81:ALA:O | 12:B8:202:CYC:NC | 2.53 | 0.41 |
| 2:E8:38:MET:HE3 | 3:F8:24:LEU:CD2 | 2.50 | 0.41 |
| 8:q7:22:GLU:O | 8:q7:26:ILE:HG13 | 2.20 | 0.41 |
| 1:v7:8:VAL:HB | 1:v7:27:LEU:HD21 | 2.03 | 0.41 |
| 9:y7:40:GLU:OE2 | 9:y7:43:ARG:CD | 2.65 | 0.41 |
| 2:X8:38:MET:HE3 | 3:Y8:24:LEU:CD2 | 2.50 | 0.41 |
| 12:J8:202:CYC:HB | 12:J8:202:CYC:HMA3 | 1.84 | 0.41 |
| 2:K8:138:VAL:O | 2:K8:138:VAL:CG1 | 2.67 | 0.41 |
| 3:L8:117:TYR:HE1 | 12:a9:901:CYC:NA | 2.18 | 0.41 |
| 4:M8:104:ALA:HB2 | 2:P8:14:SER:H | 1.80 | 0.41 |
| 4:M8:274:VAL:OXT | 4:M8:274:VAL:HG12 | 2.21 | 0.41 |
| 3:O8:112:GLY:CA | 5:Z8:69:GLU:CA | 2.98 | 0.41 |
| 12:F1:201:CYC:CMA | 12:F1:201:CYC:HB | 2.25 | 0.41 |
| 4:M9:4:LEU:HD12 | 4:M9:4:LEU:C | 2.45 | 0.41 |
| 4:M9:70:SER:O | 4:M9:70:SER:OG | 2.35 | 0.41 |
| 5:Z8:1:MET:CA | 5:Z8:1:MET:CE | 2.85 | 0.41 |
| 2:I9:155:ASP:O | 2:I9:159:ASN:OD1 | 2.37 | 0.41 |
| 11:a9:629:LYS:NZ | 11:a9:629:LYS:CA | 2.72 | 0.41 |
| 11:aA:89:ALA:CA | 11:aA:92:LYS:HZ2 | 2.29 | 0.41 |
| 11:aA:351:THR:O | 11:aA:353:ALA:HA | 2.20 | 0.41 |
| 11:aA:379:LEU:HD12 | 11:aA:379:LEU:HA | 1.42 | 0.41 |
| 11:aA:813:PRO:CA | 3:L1:119:ALA:HB1 | 2.41 | 0.41 |
| 12:H1:202:CYC:HB | 12:H1:202:CYC:HMA3 | 1.84 | 0.41 |
| 4:M1:132:LEU:HD12 | 4:M1:137:ILE:HD12 | 2.01 | 0.41 |
| 2:AA:30:ARG:NH1 | 3:BA:5:PHE:CE1 | 2.88 | 0.41 |
| 3:BA:107:ASP:HB3 | 11:aA:382:ASN:HB3 | 2.02 | 0.41 |
| 3:DA:3:ASP:H | 3:DA:6:THR:HB | 1.84 | 0.41 |
| 3:DA:115:GLU:OE2 | 4:MA:76:ALA:C | 2.49 | 0.41 |
| 3:FA:145:PRO:HG3 | 12:F9:302:CYC:HMC3 | 1.91 | 0.41 |
| 2:IA:18:PHE:CE2 | 3:JA:48:ALA:HB2 | 2.55 | 0.41 |
| 2:IA:38:MET:HE2 | 2:IA:38:MET:HB3 | 1.81 | 0.41 |
| 2:KA:18:PHE:CE1 | 3:LA:90:LEU:CD2 | 3.03 | 0.41 |
| 4:MA:99:VAL:HG13 | 3:RA:77:ARG:HD2 | 2.01 | 0.41 |
| 12:PA:202:CYC:HB | 12:PA:202:CYC:HMA3 | 1.83 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:RA:151:GLY:HA3 | 12:RA:202:CYC:CMD | 2.51 | 0.41 |
| 2:UA:81:LYS:NZ | 12:UA:201:CYC:O1A | 2.51 | 0.41 |
| 3:H2:3:ASP:H | 3:H2:6:THR:HB | 1.85 | 0.41 |
| 2:C3:38:MET:HE3 | 3:D3:24:LEU:CD2 | 2.50 | 0.41 |
| 12:D3:201:CYC:HB | 12:D3:201:CYC:HMA3 | 1.84 | 0.41 |
| 2:A4:30:ARG:NH1 | 3:B4:5:PHE:CE1 | 2.88 | 0.41 |
| 2:A4:63:PHE:O | 2:A4:66:LEU:CB | 2.69 | 0.41 |
| 12:B4:202:CYC:OB | 4:M4:58:TYR:CD1 | 2.73 | 0.41 |
| 3:P3:151:GLY:HA3 | 12:P3:202:CYC:CMD | 2.50 | 0.41 |
| 2:W3:38:MET:HE3 | 3:X3:24:LEU:CD2 | 2.49 | 0.41 |
| 2:T4:38:MET:HE2 | 2:T4:38:MET:HB3 | 1.81 | 0.41 |
| 4:M4:28:HIS:CD2 | 4:M4:35:THR:HG23 | 2.55 | 0.41 |
| 4:M4:61:ASN:CG | 4:M4:62:LYS:HD3 | 2.46 | 0.41 |
| 4:M4:205:ASP:OD2 | 5:Z4:59:ARG:HG2 | 2.20 | 0.41 |
| 3:O4:112:GLY:CA | 5:Z4:69:GLU:C | 2.93 | 0.41 |
| 12:O4:202:CYC:HB | 12:O4:202:CYC:HMA3 | 1.84 | 0.41 |
| 1:L5:106:GLU:CG | 9:i5:58:THR:HG23 | 2.48 | 0.41 |
| 8:M5:107:ILE:HG21 | 1:N5:13:ASP:OD1 | 2.19 | 0.41 |
| 8:O5:67:SER:O | 8:O5:68:PRO:C | 2.63 | 0.41 |
| 12:Y4:201:CYC:HB | 12:Y4:201:CYC:HMA3 | 1.84 | 0.41 |
| 5:Z4:23:SER:HB2 | 5:Z4:25:THR:H | 1.84 | 0.41 |
| 8:C5:25:ARG:C | 8:C5:25:ARG:CD | 2.86 | 0.41 |
| 8:G5:5:THR:CG2 | 10:j5:559:THR:HG21 | 2.50 | 0.41 |
| 8:I5:8:ILE:O | 8:I5:8:ILE:HG22 | 2.20 | 0.41 |
| 8:I5:95:GLY:HA3 | 8:I5:104:ILE:HD11 | 2.01 | 0.41 |
| 8:I5:107:ILE:O | 12:I5:201:CYC:HAB2 | 2.20 | 0.41 |
| 12:J5:201:CYC:NB | 9:i5:38:PHE:CE2 | 2.88 | 0.41 |
| 8:c5:105:GLU:HG2 | 8:c5:110:ILE:HG23 | 2.02 | 0.41 |
| 12:f5:201:CYC:HC | 12:f5:201:CYC:CMD | 2.13 | 0.41 |
| 8:S5:15:ALA:HB2 | 10:j5:573:GLN:CD | 2.45 | 0.41 |
| 12:J6:201:CYC:HMD3 | 12:J6:201:CYC:NC | 2.34 | 0.41 |
| 7:N6:49:LEU:O | 7:N6:53:GLN:HB2 | 2.19 | 0.41 |
| 9:i5:8:THR:HB | 9:i5:53:SER:H | 1.85 | 0.41 |
| 9:i5:23:LEU:CA | 9:i5:25:ASN:H | 2.33 | 0.41 |
| 10:j5:195:SER:O | 10:j5:199:THR:CG2 | 2.63 | 0.41 |
| 10:j5:344:ARG:HH12 | 10:j5:349:GLN:HG3 | 1.86 | 0.41 |
| 10:j5:938:GLN:OE1 | 1:J7:28:LYS:HD3 | 2.06 | 0.41 |
| 10:k5:975:ARG:HD3 | 10:k5:1116:TYR:CE2 | 2.55 | 0.41 |
| 12:A6:201:CYC:CMA | 12:A6:201:CYC:NB | 2.82 | 0.41 |
| 8:O7:33:GLY:HA2 | 8:O7:36:ARG:HB2 | 2.01 | 0.41 |
| 8:Q7:22:GLU:O | 8:Q7:26:ILE:HG13 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:R7:8:VAL:HB | 1:R7:27:LEU:HD21 | 2.03 | 0.41 |
| 12:R7:201:CYC:HMD1 | 12:R7:201:CYC:NC | 2.09 | 0.41 |
| 8:S7:67:SER:O | 8:S7:68:PRO:C | 2.63 | 0.41 |
| 1:D7:72:MET:HB3 | 1:D7:72:MET:HE2 | 1.87 | 0.41 |
| 8:G7:64:ASP:HA | 8:G7:67:SER:HG | 1.85 | 0.41 |
| 1:J7:75:THR:HB | 8:K7:112:VAL:CA | 2.50 | 0.41 |
| 1:N7:89:LEU:HB2 | 1:N7:133:MET:HE1 | 2.02 | 0.41 |
| 8:W7:67:SER:O | 8:W7:68:PRO:C | 2.63 | 0.41 |
| 8:a7:33:GLY:HA2 | 8:a7:36:ARG:HB2 | 2.01 | 0.41 |
| 2:A8:30:ARG:NH1 | 3:B8:5:PHE:CE1 | 2.88 | 0.41 |
| 8:m7:105:GLU:HG2 | 8:m7:110:ILE:HG23 | 2.02 | 0.41 |
| 8:o7:45:GLU:OE2 | 8:o7:45:GLU:CA | 2.68 | 0.41 |
| 8:o7:77:MET:O | 12:o7:201:CYC:HMD3 | 2.20 | 0.41 |
| 9:z7:6:LYS:N | 9:z7:55:LYS:O | 2.45 | 0.41 |
| 9:z7:36:ASN:OD1 | 9:z7:36:ASN:N | 2.52 | 0.41 |
| 3:F8:84:ARG:CG | 11:a9:139:ILE:CG2 | 2.93 | 0.41 |
| 2:G8:38:MET:HE3 | 3:H8:24:LEU:CD2 | 2.49 | 0.41 |
| 3:H8:3:ASP:H | 3:H8:6:THR:HB | 1.85 | 0.41 |
| 3:H8:108:ARG:NH2 | 11:a9:97:ALA:CB | 2.83 | 0.41 |
| 3:H8:151:GLY:HA3 | 12:H8:202:CYC:CMD | 2.51 | 0.41 |
| 4:M8:93:LEU:O | 4:M8:94:TRP:C | 2.62 | 0.41 |
| 3:Q8:77:ARG:CA | 5:Z8:34:LEU:HD13 | 2.48 | 0.41 |
| 4:M9:99:VAL:HG13 | 3:R9:77:ARG:HD2 | 2.01 | 0.41 |
| 4:M9:163:ASN:CG | 12:V9:201:CYC:HMA3 | 2.41 | 0.41 |
| 4:M9:274:VAL:OXT | 4:M9:274:VAL:HG12 | 2.20 | 0.41 |
| 5:N9:56:GLU:OE2 | 5:N9:59:ARG:NH2 | 2.51 | 0.41 |
| 3:P9:3:ASP:H | 3:P9:6:THR:HB | 1.85 | 0.41 |
| 12:Y8:201:CYC:HMD3 | 12:Y8:201:CYC:NC | 2.35 | 0.41 |
| 12:Z9:201:CYC:HB | 12:Z9:201:CYC:HMA3 | 1.83 | 0.41 |
| 11:a9:812:ASP:HA | 11:a9:813:PRO:HD3 | 1.69 | 0.41 |
| 11:aA:328:GLN:NE2 | 11:aA:328:GLN:CA | 2.83 | 0.41 |
| 11:aA:388:VAL:O | 11:aA:392:ILE:HD12 | 2.20 | 0.41 |
| 11:aA:562:TYR:CD1 | 11:aA:562:TYR:C | 2.94 | 0.41 |
| 12:J1:201:CYC:HMD3 | 12:J1:201:CYC:NC | 2.34 | 0.41 |
| 5:N1:37:HIS:HD2 | 12:T1:301:CYC:CMA | 2.33 | 0.41 |
| 2:A2:138:VAL:O | 2:A2:138:VAL:CG1 | 2.67 | 0.41 |
| 3:BA:151:GLY:HA3 | 12:BA:202:CYC:CMD | 2.51 | 0.41 |
| 3:HA:151:GLY:HA3 | 12:HA:201:CYC:CMD | 2.51 | 0.41 |
| 12:LA:201:CYC:HB | 12:LA:201:CYC:HMA3 | 1.84 | 0.41 |
| 4:MA:184:ILE:HD13 | 4:MA:184:ILE:HA | 1.65 | 0.41 |
| 4:MA:271:ARG:HH21 | 4:MA:271:ARG:HD2 | 1.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:QA:29:GLY:CA | 2:UA:25:GLN:O | 2.68 | 0.41 |
| 2:O1:63:PHE:O | 2:O1:66:LEU:CB | 2.69 | 0.41 |
| 2:G2:116:VAL:CG2 | 3:L2:76:ASN:OD1 | 2.61 | 0.41 |
| 2:K2:38:MET:HE3 | 3:L2:24:LEU:CD2 | 2.50 | 0.41 |
| 3:L2:77:ARG:CZ | 6:M2:70:GLU:CG | 2.95 | 0.41 |
| 6:M2:19:ASP:HB2 | 8:Y5:48:GLU:HG2 | 2.01 | 0.41 |
| 6:M2:66:GLY:HA2 | 1:h7:125:ALA:N | 2.35 | 0.41 |
| 6:M2:83:ALA:HB1 | 6:M2:222:LYS:HE3 | 2.01 | 0.41 |
| 6:M2:130:ARG:HH11 | 12:F2:201:CYC:CGA | 2.33 | 0.41 |
| 7:N2:4:ASN:ND2 | 12:F2:201:CYC:HBB1 | 2.35 | 0.41 |
| 7:N2:16:PHE:CD2 | 7:N2:67:PRO:HA | 2.55 | 0.41 |
| 3:B1:65:ASP:OD1 | 3:B1:65:ASP:N | 2.47 | 0.41 |
| 3:S4:82:CYS:CA | 12:S4:202:CYC:CAC | 2.66 | 0.41 |
| 2:G4:53:LYS:CE | 11:aA:71:ILE:HG23 | 2.48 | 0.41 |
| 2:I4:14:SER:HB3 | 11:aA:170:PHE:HE2 | 1.85 | 0.41 |
| 12:J4:201:CYC:HMA1 | 11:aA:176:ASN:ND2 | 2.21 | 0.41 |
| 2:N4:63:PHE:O | 2:N4:66:LEU:CB | 2.68 | 0.41 |
| 2:N4:111:ALA:CB | 5:Z4:34:LEU:HD12 | 2.22 | 0.41 |
| 3:O4:104:VAL:HA | 5:Z4:61:LYS:HE3 | 2.00 | 0.41 |
| 12:O4:201:CYC:HBA2 | 5:Z4:50:LEU:CD1 | 2.36 | 0.41 |
| 3:Q4:77:ARG:CA | 5:Z4:34:LEU:HD13 | 2.50 | 0.41 |
| 8:K5:8:ILE:O | 8:K5:11:ALA:N | 2.51 | 0.41 |
| 8:K5:151:PHE:CE1 | 1:V5:42:ALA:CB | 3.04 | 0.41 |
| 8:M5:4:LEU:CD2 | 8:M5:26:ILE:HD13 | 2.47 | 0.41 |
| 8:M5:105:GLU:HG2 | 8:M5:110:ILE:HG23 | 2.02 | 0.41 |
| 3:Y4:89:ILE:CA | 3:Y4:92:TYR:CD2 | 2.68 | 0.41 |
| 3:Y4:119:ALA:C | 3:Y4:121:GLY:H | 2.27 | 0.41 |
| 5:Z4:38:GLU:HA | 5:Z4:39:PRO:HD2 | 1.75 | 0.41 |
| 1:B5:10:ASN:CG | 10:k5:557:VAL:CA | 2.93 | 0.41 |
| 8:E5:119:LEU:O | 8:E5:120:GLN:C | 2.64 | 0.41 |
| 8:I5:33:GLY:HA2 | 8:I5:36:ARG:HB2 | 2.01 | 0.41 |
| 1:J5:6:THR:HA | 1:J5:9:ILE:HB | 2.03 | 0.41 |
| 8:e5:9:VAL:O | 8:e5:9:VAL:HG13 | 2.20 | 0.41 |
| 8:Q5:8:ILE:CG2 | 1:R5:94:TYR:CB | 2.98 | 0.41 |
| 8:S5:66:VAL:HG11 | 8:E7:68:PRO:CG | 2.22 | 0.41 |
| 8:W5:8:ILE:CG2 | 1:X5:94:TYR:CB | 2.98 | 0.41 |
| 8:Y5:105:GLU:HG2 | 8:Y5:110:ILE:HG23 | 2.02 | 0.41 |
| 3:J6:24:LEU:CD2 | 2:I6:38:MET:HE3 | 2.50 | 0.41 |
| 6:M6:147:ASP:OD1 | 6:M6:147:ASP:N | 2.52 | 0.41 |
| 9:z5:6:LYS:NZ | 9:z5:29:THR:HG21 | 2.33 | 0.41 |
| 9:z5:23:LEU:CA | 9:z5:25:ASN:H | 2.33 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:i5:16:ARG:HE | 9:i5:16:ARG:HA | 1.82 | 0.41 |
| 10:j5:232:ARG:NH1 | 10:j5:232:ARG:CB | 2.82 | 0.41 |
| 10:j5:277:ILE:HA | 10:j5:284:PRO:HB3 | 2.02 | 0.41 |
| 10:j5:837:LEU:HD23 | 10:j5:837:LEU:HA | 1.81 | 0.41 |
| 10:j5:947:MET:HE3 | 10:j5:948:SER:HB3 | 2.03 | 0.41 |
| 10:j5:967:VAL:HG21 | 1:v7:10:ASN:OD1 | 2.20 | 0.41 |
| 10:k5:431:GLN:HA | 10:k5:431:GLN:HE21 | 1.84 | 0.41 |
| 10:k5:623:VAL:O | 10:k5:623:VAL:CG1 | 2.68 | 0.41 |
| 10:k5:889:LEU:HG | 1:D7:87:TYR:OH | 2.19 | 0.41 |
| 10:k5:900:LEU:HA | 10:k5:900:LEU:HD12 | 1.62 | 0.41 |
| 10:k5:1002:ARG:HA | 10:k5:1007:VAL:CG1 | 2.50 | 0.41 |
| 10:k5:1069:ARG:NE | 10:k5:1101:GLU:OE1 | 2.51 | 0.41 |
| 3:H6:3:ASP:H | 3:H6:6:THR:HB | 1.85 | 0.41 |
| 8:Q7:105:GLU:HG2 | 8:Q7:110:ILE:HG23 | 2.02 | 0.41 |
| 8:S7:64:ASP:OD2 | 8:I7:69:GLY:C | 2.63 | 0.41 |
| 1:D7:89:LEU:HB2 | 1:D7:133:MET:HE1 | 2.03 | 0.41 |
| 8:I7:6:LYS:HZ1 | 8:W7:19:SER:CB | 2.31 | 0.41 |
| 8:I7:15:ALA:CA | 1:J7:90:ARG:CZ | 2.98 | 0.41 |
| 8:i7:42:THR:HG21 | 8:i7:141:LEU:HD23 | 0.53 | 0.41 |
| 8:U7:52:LYS:HD2 | 11:a9:27:PHE:CD2 | 2.55 | 0.41 |
| 1:V7:76:ARG:HD3 | 8:W7:110:ILE:CD1 | 2.50 | 0.41 |
| 1:X7:8:VAL:HB | 1:X7:27:LEU:HD21 | 2.03 | 0.41 |
| 1:X7:89:LEU:HB2 | 1:X7:133:MET:HE1 | 2.03 | 0.41 |
| 8:Y7:67:SER:O | 8:Y7:68:PRO:C | 2.63 | 0.41 |
| 3:D8:151:GLY:HA3 | 12:D8:201:CYC:CMD | 2.51 | 0.41 |
| 1:l7:89:LEU:HB2 | 1:l7:133:MET:HE1 | 2.03 | 0.41 |
| 8:m7:7:ALA:HB1 | 8:m7:22:GLU:HB3 | 2.03 | 0.41 |
| 8:o7:67:SER:O | 8:o7:68:PRO:C | 2.63 | 0.41 |
| 12:r7:201:CYC:CMA | 12:r7:201:CYC:NB | 2.74 | 0.41 |
| 8:s7:18:LEU:CD1 | 1:t7:94:TYR:HE1 | 2.33 | 0.41 |
| 8:s7:33:GLY:HA2 | 8:s7:36:ARG:HB2 | 2.01 | 0.41 |
| 8:u7:105:GLU:HG2 | 8:u7:110:ILE:HG23 | 2.02 | 0.41 |
| 9:w7:15:LYS:CE | 9:w7:16:ARG:HD3 | 2.50 | 0.41 |
| 2:K8:38:MET:HE2 | 2:K8:38:MET:HB3 | 1.81 | 0.41 |
| 4:M8:129:GLU:CA | 4:M8:142:PHE:CZ | 3.03 | 0.41 |
| 4:M8:164:ARG:NH2 | 4:M8:168:LEU:HD21 | 2.36 | 0.41 |
| 4:M8:231:THR:H | 12:M8:301:CYC:CAB | 2.21 | 0.41 |
| 12:P8:201:CYC:CMA | 12:P8:201:CYC:NB | 2.82 | 0.41 |
| 3:F1:3:ASP:H | 3:F1:6:THR:HB | 1.85 | 0.41 |
| 12:F1:201:CYC:CAA | 4:M1:36:TYR:CE2 | 3.03 | 0.41 |
| 4:M9:6:THR:HG21 | 12:D9:201:CYC:HBB1 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M9:252:LEU:HD13 | 3:Z9:77:ARG:NH1 | 2.35 | 0.41 |
| 12:O9:201:CYC:CMA | 12:O9:201:CYC:NB | 2.82 | 0.41 |
| 12:Y8:201:CYC:CMD | 12:Y8:201:CYC:NC | 2.75 | 0.41 |
| 3:B9:151:GLY:HA3 | 12:B9:202:CYC:CMD | 2.51 | 0.41 |
| 2:C9:38:MET:HE3 | 3:D9:24:LEU:CD2 | 2.49 | 0.41 |
| 2:E9:38:MET:HE3 | 3:F9:24:LEU:CD2 | 2.50 | 0.41 |
| 12:G9:201:CYC:CMA | 12:G9:201:CYC:NB | 2.82 | 0.41 |
| 2:I9:98:VAL:HG21 | 3:J9:19:LEU:CD1 | 2.42 | 0.41 |
| 3:R9:3:ASP:H | 3:R9:6:THR:HB | 1.85 | 0.41 |
| 3:Z9:151:GLY:HA3 | 12:Z9:201:CYC:CMD | 2.51 | 0.41 |
| 11:a9:38:VAL:HA | 11:a9:39:PRO:HD3 | 1.85 | 0.41 |
| 11:a9:91:THR:C | 11:a9:92:LYS:HE3 | 2.40 | 0.41 |
| 11:a9:250:ARG:HA | 11:a9:285:VAL:HG21 | 2.02 | 0.41 |
| 11:a9:351:THR:O | 11:a9:353:ALA:HA | 2.20 | 0.41 |
| 11:a9:365:LYS:HD3 | 11:a9:365:LYS:HA | 1.35 | 0.41 |
| 11:a9:426:ARG:HD2 | 11:a9:490:ILE:HG23 | 1.99 | 0.41 |
| 11:aA:304:ALA:C | 11:aA:306:GLY:N | 2.78 | 0.41 |
| 11:aA:586:LEU:HD13 | 11:aA:586:LEU:HA | 1.43 | 0.41 |
| 11:aA:763:PHE:CE1 | 11:aA:772:ARG:NH2 | 2.88 | 0.41 |
| 4:M1:3:VAL:O | 4:M1:3:VAL:HG12 | 2.21 | 0.41 |
| 4:M1:102:VAL:O | 4:M1:102:VAL:CG1 | 2.69 | 0.41 |
| 4:M1:144:ARG:CZ | 5:N1:52:ARG:NH2 | 2.82 | 0.41 |
| 5:N1:56:GLU:OE2 | 5:N1:59:ARG:NH2 | 2.51 | 0.41 |
| 12:T1:301:CYC:HC | 12:T1:301:CYC:HMD3 | 1.82 | 0.41 |
| 3:B2:77:ARG:HD2 | 3:B2:77:ARG:O | 2.21 | 0.41 |
| 3:DA:151:GLY:HA3 | 12:DA:202:CYC:CMD | 2.51 | 0.41 |
| 3:JA:3:ASP:H | 3:JA:6:THR:HB | 1.84 | 0.41 |
| 4:MA:19:MET:HE2 | 4:MA:59:ILE:CD1 | 2.46 | 0.41 |
| 4:MA:102:VAL:O | 4:MA:102:VAL:CG1 | 2.69 | 0.41 |
| 4:MA:164:ARG:NH2 | 4:MA:168:LEU:HD21 | 2.36 | 0.41 |
| 4:MA:188:LEU:CG | 3:VA:84:ARG:CZ | 2.84 | 0.41 |
| 3:PA:151:GLY:HA3 | 12:PA:202:CYC:CMD | 2.51 | 0.41 |
| 12:PA:201:CYC:HB | 12:PA:201:CYC:CMA | 2.25 | 0.41 |
| 2:QA:68:GLN:CB | 2:QA:69:PRO:HD3 | 2.46 | 0.41 |
| 3:TA:25:ASN:OD1 | 2:X4:68:GLN:CB | 2.64 | 0.41 |
| 3:XA:3:ASP:H | 3:XA:6:THR:HB | 1.85 | 0.41 |
| 2:A1:34:ALA:HB3 | 3:B1:31:VAL:CG1 | 2.39 | 0.41 |
| 2:G2:38:MET:HE3 | 3:H2:24:LEU:CD2 | 2.49 | 0.41 |
| 3:L2:151:GLY:HA3 | 12:L2:202:CYC:CMD | 2.51 | 0.41 |
| 6:M2:57:GLU:OE2 | 8:i7:76:LYS:CE | 2.67 | 0.41 |
| 3:B4:86:MET:CA | 12:B4:202:CYC:CBC | 2.75 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 4:M3:262:ASP:OD1 | 4:M3:263:PRO:CD | 2.68 | 0.41 |
| 3:F4:107:ASP:OD1 | 3:F4:108:ARG:HG3 | 2.20 | 0.41 |
| 2:I4:111:ALA:HA | 11:aA:133:LEU:HD13 | 2.03 | 0.41 |
| 4:M4:184:ILE:HA | 4:M4:184:ILE:HD13 | 1.65 | 0.41 |
| 4:M4:190:ARG:HE | 4:M4:190:ARG:HB2 | 1.71 | 0.41 |
| 4:M4:228:SER:HA | 3:Y4:91:ARG:NH2 | 2.31 | 0.41 |
| 3:Q4:3:ASP:H | 3:Q4:6:THR:HB | 1.84 | 0.41 |
| 3:Q4:91:ARG:HH22 | 3:Q4:92:TYR:HB3 | 1.85 | 0.41 |
| 8:K5:22:GLU:O | 8:K5:26:ILE:HG13 | 2.20 | 0.41 |
| 8:M5:25:ARG:NE | 8:A5:25:ARG:NH2 | 2.59 | 0.41 |
| 8:A5:67:SER:O | 8:A5:68:PRO:C | 2.63 | 0.41 |
| 8:C5:8:ILE:O | 8:C5:8:ILE:CG2 | 2.67 | 0.41 |
| 8:c5:67:SER:O | 8:c5:68:PRO:C | 2.63 | 0.41 |
| 8:W5:105:GLU:HG2 | 8:W5:110:ILE:HG23 | 2.03 | 0.41 |
| 1:Z5:89:LEU:HB2 | 1:Z5:133:MET:HE1 | 2.03 | 0.41 |
| 1:b5:5:ILE:HD12 | 10:k5:46:PHE:HZ | 1.49 | 0.41 |
| 8:A7:22:GLU:O | 8:A7:26:ILE:HG13 | 2.20 | 0.41 |
| 10:j5:141:GLU:O | 10:j5:142:PRO:C | 2.59 | 0.41 |
| 10:j5:797:ASN:HB2 | 12:T7:201:CYC:HBA2 | 2.01 | 0.41 |
| 10:j5:1030:ILE:HD12 | 10:j5:1030:ILE:HA | 1.46 | 0.41 |
| 10:j5:1081:VAL:CG1 | 12:r7:201:CYC:HMA2 | 2.30 | 0.41 |
| 10:k5:853:LEU:O | 10:k5:853:LEU:CG | 2.68 | 0.41 |
| 10:k5:1005:LEU:HD13 | 10:k5:1016:LEU:HD22 | 2.01 | 0.41 |
| 10:k5:1052:PRO:O | 10:k5:1053:TYR:CD2 | 2.73 | 0.41 |
| 10:k5:1084:LEU:HD22 | 10:k5:1092:ALA:HB2 | 2.02 | 0.41 |
| 10:k5:1128:VAL:O | 10:k5:1128:VAL:CG1 | 2.68 | 0.41 |
| 10:k5:1153:VAL:HG11 | 1:p7:59:ALA:O | 2.20 | 0.41 |
| 12:I6:201:CYC:CMA | 12:I6:201:CYC:NB | 2.82 | 0.41 |
| 12:D1:201:CYC:HB | 12:D1:201:CYC:HMA3 | 1.84 | 0.41 |
| 8:O7:105:GLU:HG2 | 8:O7:110:ILE:HG23 | 2.02 | 0.41 |
| 1:F7:89:LEU:HB2 | 1:F7:133:MET:HE1 | 2.03 | 0.41 |
| 8:G7:67:SER:O | 8:G7:68:PRO:C | 2.63 | 0.41 |
| 8:I7:21:GLY:C | 8:I7:23:LEU:H | 2.29 | 0.41 |
| 1:J7:89:LEU:HB2 | 1:J7:133:MET:HE1 | 2.03 | 0.41 |
| 1:h7:75:THR:CG2 | 8:i7:112:VAL:HG23 | 2.47 | 0.41 |
| 8:i7:112:VAL:C | 8:i7:114:GLU:N | 2.76 | 0.41 |
| 1:Z7:89:LEU:HB2 | 1:Z7:133:MET:HE1 | 2.02 | 0.41 |
| 8:a7:37:LEU:HD11 | 1:b7:27:LEU:CB | 2.51 | 0.41 |
| 8:c7:42:THR:HG21 | 8:c7:141:LEU:HD23 | 0.53 | 0.41 |
| 8:c7:94:TYR:HB3 | 1:d7:9:ILE:HD13 | 2.03 | 0.41 |
| 8:m7:67:SER:O | 8:m7:68:PRO:C | 2.63 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:o7:105:GLU:HG2 | 8:o7:110:ILE:HG23 | 2.02 | 0.41 |
| 1:p7:136:VAL:HA | 11:a9:342:ARG:HH11 | 1.85 | 0.41 |
| 8:u7:17:TYR:CD2 | 1:v7:93:THR:HB | 2.53 | 0.41 |
| 9:x7:11:ILE:HD11 | 9:x7:28:PHE:HE1 | 1.86 | 0.41 |
| 9:x7:14:LEU:C | 9:x7:14:LEU:CD1 | 2.93 | 0.41 |
| 3:F8:111:ASN:OD1 | 3:F8:112:GLY:N | 2.52 | 0.41 |
| 4:M8:145:LEU:HA | 4:M8:145:LEU:HD23 | 1.88 | 0.41 |
| 12:O8:202:CYC:HB | 12:O8:202:CYC:HMA3 | 1.84 | 0.41 |
| 12:O8:202:CYC:NC | 12:O8:202:CYC:HMD3 | 2.35 | 0.41 |
| 3:F1:119:ALA:HB2 | 4:M1:41:ASN:ND2 | 2.34 | 0.41 |
| 2:O9:60:TYR:CZ | 2:O9:79:GLN:HG2 | 2.56 | 0.41 |
| 2:E9:102:THR:HG21 | 2:I9:20:ASN:HD22 | 1.85 | 0.41 |
| 2:I9:12:ALA:HB1 | 3:J9:95:TYR:CE1 | 2.56 | 0.41 |
| 3:J9:88:ILE:HG21 | 11:a9:512:TYR:CE2 | 2.56 | 0.41 |
| 11:a9:110:PHE:CD1 | 11:a9:115:VAL:CG2 | 3.04 | 0.41 |
| 11:a9:337:GLU:HG2 | 11:a9:339:GLU:HG2 | 2.03 | 0.41 |
| 11:a9:595:ARG:HA | 11:a9:595:ARG:HD2 | 1.75 | 0.41 |
| 11:aA:516:GLN:HG3 | 11:aA:516:GLN:O | 2.17 | 0.41 |
| 4:M1:28:HIS:CD2 | 4:M1:35:THR:HG23 | 2.55 | 0.41 |
| 4:M1:274:VAL:OXT | 4:M1:274:VAL:HG12 | 2.20 | 0.41 |
| 3:B2:77:ARG:O | 3:B2:77:ARG:CD | 2.69 | 0.41 |
| 3:B2:151:GLY:HA3 | 12:B2:201:CYC:CMD | 2.51 | 0.41 |
| 1:A:72:MET:HE2 | 1:A:72:MET:HB3 | 1.87 | 0.41 |
| 4:MA:52:LEU:O | 4:MA:52:LEU:CD2 | 2.69 | 0.41 |
| 4:MA:271:ARG:NH2 | 3:VA:78:ARG:NH1 | 2.68 | 0.41 |
| 4:MA:274:VAL:OXT | 3:VA:77:ARG:NH2 | 2.53 | 0.41 |
| 2:OA:60:TYR:CZ | 2:OA:79:GLN:HG2 | 2.56 | 0.41 |
| 3:RA:3:ASP:H | 3:RA:6:THR:HB | 1.85 | 0.41 |
| 12:VA:201:CYC:HC | 12:VA:201:CYC:HMD3 | 1.83 | 0.41 |
| 2:A1:30:ARG:NH1 | 3:B1:5:PHE:CE1 | 2.88 | 0.41 |
| 3:H2:151:GLY:HA3 | 12:H2:202:CYC:CMD | 2.51 | 0.41 |
| 2:A3:49:ASP:O | 2:A3:50:SER:C | 2.62 | 0.41 |
| 3:Z3:3:ASP:H | 3:Z3:6:THR:HB | 1.84 | 0.41 |
| 3:Z3:151:GLY:HA3 | 12:Z3:202:CYC:CMD | 2.51 | 0.41 |
| 5:N3:54:LEU:HB3 | 5:N3:55:PRO:HD3 | 2.02 | 0.41 |
| 2:O3:63:PHE:O | 2:O3:66:LEU:CB | 2.69 | 0.41 |
| 3:B1:151:GLY:HA3 | 12:B1:201:CYC:CMD | 2.51 | 0.41 |
| 2:I4:14:SER:CA | 11:aA:170:PHE:CE2 | 3.03 | 0.41 |
| 2:K4:38:MET:HE2 | 2:K4:38:MET:HB3 | 1.81 | 0.41 |
| 4:M4:3:VAL:HG12 | 4:M4:3:VAL:O | 2.20 | 0.41 |
| 4:M4:52:LEU:O | 4:M4:52:LEU:CD2 | 2.69 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 12:M4:301:CYC:HMD1 | 3:Y4:78:ARG:HG2 | 2.02 | 0.41 |
| 3:O4:3:ASP:H | 3:O4:6:THR:HB | 1.84 | 0.41 |
| 3:Q4:85:ASP:CB | 12:Z4:301:CYC:HBC1 | 2.50 | 0.41 |
| 12:N5:201:CYC:CMA | 12:N5:201:CYC:NB | 2.74 | 0.41 |
| 8:O5:6:LYS:NZ | 8:E5:22:GLU:OE2 | 2.52 | 0.41 |
| 5:Z4:54:LEU:HB3 | 5:Z4:55:PRO:HD3 | 2.02 | 0.41 |
| 8:A5:105:GLU:HG2 | 8:A5:110:ILE:HG23 | 2.02 | 0.41 |
| 8:A5:126:VAL:HG23 | 12:A5:201:CYC:HMC3 | 2.03 | 0.41 |
| 8:G5:12:ASP:OD2 | 1:H5:91:TYR:HE1 | 2.03 | 0.41 |
| 1:d5:62:TYR:HH | 12:e5:201:CYC:CGD | 2.33 | 0.41 |
| 1:f5:19:LEU:HD12 | 10:j5:172:LEU:HD12 | 1.80 | 0.41 |
| 8:Q5:105:GLU:HG2 | 8:Q5:110:ILE:HG23 | 2.02 | 0.41 |
| 1:R5:87:TYR:HE1 | 10:k5:521:GLY:HA3 | 1.86 | 0.41 |
| 1:Z5:64:ASP:CB | 10:k5:705:THR:HG21 | 2.45 | 0.41 |
| 6:M6:43:TRP:CE2 | 8:c7:56:ASP:OD2 | 2.73 | 0.41 |
| 10:j5:19:THR:O | 10:j5:21:MET:N | 2.53 | 0.41 |
| 10:j5:283:ARG:C | 10:j5:283:ARG:CD | 2.84 | 0.41 |
| 10:j5:868:ASP:HB3 | 9:w7:43:ARG:HD2 | 2.02 | 0.41 |
| 10:k5:277:ILE:HG21 | 10:k5:284:PRO:HD3 | 2.01 | 0.41 |
| 10:k5:837:LEU:HD23 | 10:k5:837:LEU:HA | 1.81 | 0.41 |
| 10:k5:1119:LEU:HD21 | 1:n7:87:TYR:CE1 | 2.55 | 0.41 |
| 3:B6:77:ARG:HD2 | 3:B6:77:ARG:HA | 1.59 | 0.41 |
| 8:O7:22:GLU:HA | 8:O7:25:ARG:CG | 2.49 | 0.41 |
| 8:O7:102:THR:CB | 8:O7:103:PRO:HD3 | 2.33 | 0.41 |
| 8:C7:105:GLU:HG2 | 8:C7:110:ILE:HG23 | 2.02 | 0.41 |
| 8:E7:121:THR:HG23 | 12:E7:201:CYC:NC | 2.35 | 0.41 |
| 1:L7:89:LEU:HB2 | 1:L7:133:MET:HE1 | 2.03 | 0.41 |
| 12:L7:201:CYC:HC | 12:L7:201:CYC:CMD | 2.13 | 0.41 |
| 12:B8:201:CYC:HB | 12:B8:201:CYC:HMA3 | 1.84 | 0.41 |
| 8:o7:23:LEU:HA | 1:p7:38:VAL:HG21 | 1.97 | 0.41 |
| 8:o7:66:VAL:O | 8:o7:66:VAL:CG1 | 2.66 | 0.41 |
| 1:r7:89:LEU:HB2 | 1:r7:133:MET:HE1 | 2.03 | 0.41 |
| 8:s7:15:ALA:CA | 1:t7:90:ARG:CZ | 2.98 | 0.41 |
| 1:t7:89:LEU:HB2 | 1:t7:133:MET:HE1 | 2.03 | 0.41 |
| 8:u7:27:LYS:CE | 1:v7:35:ALA:CA | 2.80 | 0.41 |
| 2:G8:138:VAL:O | 2:G8:138:VAL:CG1 | 2.67 | 0.41 |
| 2:I8:14:SER:HB3 | 11:a9:170:PHE:HE2 | 1.86 | 0.41 |
| 3:L8:151:GLY:HA3 | 12:L8:201:CYC:CMD | 2.51 | 0.41 |
| 4:M8:61:ASN:CG | 4:M8:62:LYS:HD3 | 2.45 | 0.41 |
| 4:M8:201:ASP:OD2 | 5:Z8:56:GLU:CD | 2.63 | 0.41 |
| 2:N8:60:TYR:CZ | 2:N8:79:GLN:HG2 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:Q8:84:ARG:CG | 5:Z8:31:TRP:CE2 | 2.73 | 0.41 |
| 3:L9:3:ASP:H | 3:L9:6:THR:HB | 1.85 | 0.41 |
| 3:L9:113:LEU:O | 3:L9:113:LEU:CD1 | 2.69 | 0.41 |
| 3:L9:151:GLY:HA3 | 12:L9:201:CYC:CMD | 2.51 | 0.41 |
| 12:L9:201:CYC:HB | 12:L9:201:CYC:HMA3 | 1.84 | 0.41 |
| 4:M9:13:LYS:HD2 | 4:M9:13:LYS:HA | 1.86 | 0.41 |
| 4:M9:35:THR:CB | 3:B9:84:ARG:CZ | 2.99 | 0.41 |
| 4:M9:118:TYR:CD1 | 3:Z9:84:ARG:NH2 | 2.89 | 0.41 |
| 5:Z8:38:GLU:C | 12:Z8:301:CYC:CMB | 2.94 | 0.41 |
| 2:A9:25:GLN:HG3 | 2:K9:33:ARG:HG2 | 1.99 | 0.41 |
| 3:B9:3:ASP:H | 3:B9:6:THR:HB | 1.84 | 0.41 |
| 2:I9:18:PHE:CE2 | 3:J9:48:ALA:HB2 | 2.55 | 0.41 |
| 3:T9:151:GLY:HA3 | 12:T9:302:CYC:CMD | 2.51 | 0.41 |
| 11:a9:95:ILE:O | 11:a9:95:ILE:CG2 | 2.69 | 0.41 |
| 11:a9:308:LEU:HD23 | 11:a9:312:ASP:HB3 | 2.02 | 0.41 |
| 11:a9:370:ALA:CB | 11:a9:531:ASP:OD2 | 2.69 | 0.41 |
| 11:a9:412:VAL:O | 11:a9:415:GLU:OE1 | 2.38 | 0.41 |
| 11:a9:800:THR:O | 11:a9:800:THR:OG1 | 2.32 | 0.41 |
| 11:aA:275:THR:O | 11:aA:276:SER:C | 2.63 | 0.41 |
| 11:aA:308:LEU:HD23 | 11:aA:312:ASP:HB3 | 2.02 | 0.41 |
| 11:aA:327:SER:OG | 11:aA:328:GLN:NE2 | 2.53 | 0.41 |
| 11:aA:425:VAL:HG21 | 11:aA:502:ASN:C | 2.46 | 0.41 |
| 4:M1:57:THR:O | 4:M1:57:THR:HG22 | 2.19 | 0.41 |
| 4:M1:163:ASN:ND2 | 12:Z1:202:CYC:CMA | 2.83 | 0.41 |
| 4:M1:246:ALA:HB2 | 3:X1:109:CYS:O | 2.20 | 0.41 |
| 3:V1:3:ASP:H | 3:V1:6:THR:HB | 1.84 | 0.41 |
| 3:B2:3:ASP:H | 3:B2:6:THR:HB | 1.85 | 0.41 |
| 12:D2:202:CYC:HMD3 | 12:D2:202:CYC:NC | 2.35 | 0.41 |
| 4:MA:4:LEU:HD12 | 4:MA:4:LEU:C | 2.45 | 0.41 |
| 4:MA:188:LEU:HG | 3:VA:84:ARG:NH1 | 2.33 | 0.41 |
| 5:NA:50:LEU:CD1 | 12:TA:301:CYC:O1D | 2.69 | 0.41 |
| 12:VA:202:CYC:HB | 12:VA:202:CYC:HMA3 | 1.84 | 0.41 |
| 3:R1:151:GLY:HA3 | 12:R1:202:CYC:CMD | 2.51 | 0.41 |
| 3:H3:151:GLY:HA3 | 12:H3:201:CYC:CMD | 2.51 | 0.41 |
| 2:G2:38:MET:HE2 | 2:G2:38:MET:HB3 | 1.81 | 0.41 |
| 6:M2:34:ARG:CD | 8:O5:52:LYS:CD | 2.96 | 0.41 |
| 3:B3:111:ASN:HD21 | 4:M3:73:ASP:HA | 1.85 | 0.41 |
| 3:B3:125:ARG:HD2 | 3:X3:14:LEU:HD11 | 2.03 | 0.41 |
| 3:F3:113:LEU:HD13 | 4:M3:38:PRO:HB3 | 2.02 | 0.41 |
| 12:F3:202:CYC:HMD3 | 12:F3:202:CYC:NC | 2.35 | 0.41 |
| 12:Z3:201:CYC:CGA | 4:M3:185:ALA:HA | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:L3:65:ASP:OD1 | 3:L3:65:ASP:N | 2.47 | 0.41 |
| 4:M3:21:LEU:C | 4:M3:21:LEU:CD1 | 2.94 | 0.41 |
| 4:M3:132:LEU:HD12 | 4:M3:137:ILE:HD12 | 2.01 | 0.41 |
| 3:W4:151:GLY:HA3 | 12:W4:202:CYC:CMD | 2.51 | 0.41 |
| 3:H4:1:MET:H2 | 11:aA:96:THR:HG21 | 1.85 | 0.41 |
| 3:H4:151:GLY:HA3 | 12:H4:202:CYC:CMD | 2.51 | 0.41 |
| 3:L4:151:GLY:HA3 | 12:L4:201:CYC:CMD | 2.51 | 0.41 |
| 4:M4:4:LEU:HD12 | 4:M4:4:LEU:C | 2.45 | 0.41 |
| 4:M4:21:LEU:C | 4:M4:21:LEU:CD1 | 2.94 | 0.41 |
| 4:M4:100:SER:N | 3:Q4:1:MET:HE3 | 2.03 | 0.41 |
| 4:M4:164:ARG:NH2 | 4:M4:168:LEU:HD21 | 2.36 | 0.41 |
| 12:M4:301:CYC:C2B | 3:Y4:88:ILE:HD11 | 2.51 | 0.41 |
| 2:N4:30:ARG:NH1 | 3:O4:5:PHE:CE1 | 2.88 | 0.41 |
| 2:N4:49:ASP:O | 2:N4:50:SER:C | 2.62 | 0.41 |
| 12:N4:201:CYC:CMA | 12:N4:201:CYC:NB | 2.82 | 0.41 |
| 3:Q4:85:ASP:CB | 12:Z4:301:CYC:HBC3 | 2.41 | 0.41 |
| 12:Q4:201:CYC:HB | 12:Q4:201:CYC:HMA3 | 1.83 | 0.41 |
| 8:K5:67:SER:O | 8:K5:68:PRO:C | 2.63 | 0.41 |
| 8:M5:66:VAL:CG1 | 8:M5:66:VAL:O | 2.66 | 0.41 |
| 8:M5:67:SER:O | 8:M5:68:PRO:C | 2.63 | 0.41 |
| 12:N5:201:CYC:OB | 10:k5:482:GLN:HB2 | 2.20 | 0.41 |
| 8:O5:24:ASP:O | 8:O5:25:ARG:C | 2.64 | 0.41 |
| 3:Y4:3:ASP:H | 3:Y4:6:THR:HB | 1.85 | 0.41 |
| 1:D5:6:THR:HA | 1:D5:9:ILE:HB | 2.03 | 0.41 |
| 1:F5:72:MET:HB3 | 1:F5:72:MET:HE2 | 1.87 | 0.41 |
| 8:G5:105:GLU:HG2 | 8:G5:110:ILE:HG23 | 2.03 | 0.41 |
| 1:H5:51:ILE:HG22 | 1:H5:133:MET:CE | 2.51 | 0.41 |
| 8:I5:27:LYS:CA | 8:I5:30:VAL:CG2 | 2.79 | 0.41 |
| 1:J5:51:ILE:HG22 | 1:J5:133:MET:CE | 2.51 | 0.41 |
| 1:d5:89:LEU:HB2 | 1:d5:133:MET:HE1 | 2.03 | 0.41 |
| 8:W5:121:THR:HG23 | 12:W5:201:CYC:NC | 2.35 | 0.41 |
| 8:Y5:120:GLN:CG | 1:b5:53:LYS:NZ | 2.78 | 0.41 |
| 2:K6:38:MET:HE3 | 3:L6:24:LEU:CD2 | 2.50 | 0.41 |
| 6:M6:251:LYS:NZ | 3:H6:120:LEU:C | 2.77 | 0.41 |
| 6:M6:273:PHE:CD1 | 1:d7:128:GLY:HA2 | 2.55 | 0.41 |
| 9:z5:8:THR:HB | 9:z5:53:SER:H | 1.85 | 0.41 |
| 9:i5:45:GLN:HG2 | 9:i5:45:GLN:H | 1.66 | 0.41 |
| 10:j5:298:ARG:HD3 | 10:j5:308:ASP:OD2 | 2.21 | 0.41 |
| 10:j5:440:TYR:N | 10:j5:440:TYR:CD1 | 2.84 | 0.41 |
| 10:j5:559:THR:HG22 | 10:j5:560:VAL:N | 2.36 | 0.41 |
| 10:j5:568:ILE:O | 10:j5:568:ILE:CG2 | 2.66 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:j5:631:HIS:HB2 | 10:j5:664:MET:HE1 | 2.01 | 0.41 |
| 10:j5:1052:PRO:O | 10:j5:1053:TYR:CD2 | 2.74 | 0.41 |
| 10:j5:1069:ARG:NE | 10:j5:1101:GLU:OE1 | 2.51 | 0.41 |
| 10:k5:264:LEU:O | 10:k5:264:LEU:CD2 | 2.69 | 0.41 |
| 8:O7:15:ALA:CA | 1:P7:90:ARG:CZ | 2.98 | 0.41 |
| 1:H7:136:VAL:CB | 11:aA:563:PHE:CZ | 3.03 | 0.41 |
| 8:I7:18:LEU:CD1 | 1:J7:94:TYR:HE1 | 2.34 | 0.41 |
| 8:I7:67:SER:O | 8:I7:68:PRO:C | 2.63 | 0.41 |
| 8:g7:25:ARG:HH21 | 8:u7:25:ARG:HD2 | 1.85 | 0.41 |
| 1:V7:89:LEU:HB2 | 1:V7:133:MET:HE1 | 2.03 | 0.41 |
| 8:c7:25:ARG:NH2 | 8:m7:6:LYS:HZ2 | 2.06 | 0.41 |
| 8:c7:112:VAL:C | 8:c7:114:GLU:N | 2.76 | 0.41 |
| 12:c7:201:CYC:HB | 12:c7:201:CYC:CMA | 2.21 | 0.41 |
| 3:B8:120:LEU:HD21 | 4:M8:52:LEU:CB | 2.42 | 0.41 |
| 12:E8:201:CYC:CMA | 12:E8:201:CYC:NB | 2.81 | 0.41 |
| 8:q7:120:GLN:CD | 1:v7:53:LYS:NZ | 2.78 | 0.41 |
| 9:z7:44:ILE:HD13 | 9:z7:44:ILE:HG21 | 1.83 | 0.41 |
| 9:w7:16:ARG:NH2 | 9:w7:18:ARG:HG3 | 2.36 | 0.41 |
| 3:W8:151:GLY:HA3 | 12:W8:202:CYC:CMD | 2.51 | 0.41 |
| 2:X8:16:GLY:O | 4:M8:228:SER:CB | 2.66 | 0.41 |
| 3:F8:110:LEU:O | 4:M8:6:THR:N | 2.33 | 0.41 |
| 4:M8:58:TYR:CA | 4:M8:61:ASN:ND2 | 2.83 | 0.41 |
| 2:N8:63:PHE:O | 2:N8:66:LEU:CB | 2.68 | 0.41 |
| 5:N9:4:LEU:HD11 | 3:R9:111:ASN:HD22 | 1.83 | 0.41 |
| 5:N9:54:LEU:O | 5:N9:54:LEU:HG | 2.21 | 0.41 |
| 2:A9:63:PHE:O | 2:A9:66:LEU:CB | 2.69 | 0.41 |
| 3:H9:151:GLY:HA3 | 12:H9:201:CYC:CMD | 2.51 | 0.41 |
| 12:H9:201:CYC:HB | 12:H9:201:CYC:HMA3 | 1.83 | 0.41 |
| 2:K9:19:LEU:HD23 | 2:K9:19:LEU:HA | 1.75 | 0.41 |
| 11:aA:392:ILE:O | 11:aA:392:ILE:HG22 | 2.19 | 0.41 |
| 11:aA:415:GLU:CD | 11:aA:415:GLU:N | 2.72 | 0.41 |
| 11:aA:595:ARG:HA | 11:aA:595:ARG:HD2 | 1.75 | 0.41 |
| 3:L1:3:ASP:H | 3:L1:6:THR:HB | 1.85 | 0.41 |
| 3:L1:151:GLY:HA3 | 12:L1:201:CYC:CMD | 2.51 | 0.41 |
| 12:L1:201:CYC:HB | 12:L1:201:CYC:HMA3 | 1.84 | 0.41 |
| 4:M1:132:LEU:CD1 | 4:M1:142:PHE:CB | 2.95 | 0.41 |
| 5:N1:68:LEU:HA | 5:N1:68:LEU:HD23 | 1.81 | 0.41 |
| 3:T1:3:ASP:H | 3:T1:6:THR:HB | 1.85 | 0.41 |
| 12:A2:201:CYC:CMA | 12:A2:201:CYC:NB | 2.82 | 0.41 |
| 1:Z:89:LEU:HB2 | 1:Z:133:MET:HE1 | 2.03 | 0.41 |
| 2:EA:38:MET:HE3 | 3:FA:24:LEU:CD2 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:IA:1:MET:HE2 | 2:IA:108:TYR:CE1 | 2.45 | 0.41 |
| 3:JA:116:THR:HA | 11:aA:521:PHE:CD1 | 2.56 | 0.41 |
| 3:LA:97:LEU:HD11 | 3:LA:156:LEU:HD22 | 2.03 | 0.41 |
| 3:LA:107:ASP:C | 3:LA:111:ASN:HB2 | 2.45 | 0.41 |
| 3:LA:113:LEU:O | 3:LA:113:LEU:CD1 | 2.69 | 0.41 |
| 4:MA:274:VAL:OXT | 4:MA:274:VAL:HG12 | 2.20 | 0.41 |
| 3:J3:111:ASN:ND2 | 11:a9:631:GLY:HA2 | 2.35 | 0.41 |
| 3:J3:151:GLY:HA3 | 12:J3:201:CYC:CMD | 2.51 | 0.41 |
| 6:M2:283:VAL:CG1 | 6:M2:284:SER:N | 2.83 | 0.41 |
| 3:D3:151:GLY:HA3 | 12:D3:201:CYC:CMD | 2.51 | 0.41 |
| 12:A4:201:CYC:CMA | 12:A4:201:CYC:NB | 2.82 | 0.41 |
| 3:J4:151:GLY:HA3 | 12:J4:202:CYC:CMD | 2.51 | 0.41 |
| 4:M4:13:LYS:HD2 | 4:M4:13:LYS:HA | 1.86 | 0.41 |
| 4:M4:53:LEU:O | 4:M4:53:LEU:CD1 | 2.69 | 0.41 |
| 4:M4:59:ILE:HD13 | 4:M4:59:ILE:HG21 | 1.67 | 0.41 |
| 4:M4:233:GLU:HG3 | 3:Y4:112:GLY:N | 2.36 | 0.41 |
| 3:Q4:84:ARG:HE | 5:Z4:29:HIS:CD2 | 2.39 | 0.41 |
| 3:Y4:89:ILE:CG1 | 3:Y4:92:TYR:CZ | 3.04 | 0.41 |
| 5:Z4:38:GLU:CG | 12:Z4:301:CYC:HMB2 | 2.50 | 0.41 |
| 1:B5:89:LEU:HB2 | 1:B5:133:MET:HE1 | 2.02 | 0.41 |
| 8:E5:67:SER:O | 8:E5:68:PRO:C | 2.63 | 0.41 |
| 8:c5:52:LYS:HG2 | 6:M6:15:ILE:HG12 | 2.02 | 0.41 |
| 8:e5:2:SER:HA | 8:e5:100:ASP:HB3 | 2.01 | 0.41 |
| 8:e5:33:GLY:HA2 | 8:e5:36:ARG:HB2 | 2.01 | 0.41 |
| 8:W5:119:LEU:O | 8:W5:120:GLN:C | 2.64 | 0.41 |
| 1:Z5:66:THR:OG1 | 12:a5:201:CYC:O2A | 2.26 | 0.41 |
| 8:a5:5:THR:C | 8:a5:7:ALA:N | 2.78 | 0.41 |
| 9:z5:8:THR:O | 9:z5:51:VAL:HA | 2.21 | 0.41 |
| 9:i5:8:THR:O | 9:i5:51:VAL:HA | 2.21 | 0.41 |
| 10:j5:87:ARG:O | 10:j5:89:LYS:N | 2.54 | 0.41 |
| 10:j5:802:VAL:O | 10:j5:802:VAL:CG1 | 2.69 | 0.41 |
| 10:j5:827:LYS:O | 10:j5:827:LYS:CG | 2.68 | 0.41 |
| 10:j5:900:LEU:HA | 10:j5:900:LEU:HD12 | 1.62 | 0.41 |
| 10:j5:953:LEU:CD1 | 8:u7:48:GLU:OE1 | 2.68 | 0.41 |
| 10:j5:1150:TYR:CD2 | 1:v7:70:GLY:HA2 | 2.56 | 0.41 |
| 10:k5:288:LEU:HA | 10:k5:288:LEU:HD23 | 1.77 | 0.41 |
| 10:k5:305:PHE:O | 10:k5:307:ARG:NH2 | 2.54 | 0.41 |
| 10:k5:1077:ILE:HG22 | 12:k5:1203:CYC:HBA2 | 1.99 | 0.41 |
| 3:D6:151:GLY:HA3 | 12:D6:202:CYC:CMD | 2.51 | 0.41 |
| 3:H6:151:GLY:HA3 | 12:H6:202:CYC:CMD | 2.51 | 0.41 |
| 3:D1:151:GLY:HA3 | 12:D1:201:CYC:CMD | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:P7:51:ILE:HG22 | 1:P7:133:MET:CE | 2.51 | 0.41 |
| 1:P7:89:LEU:HB2 | 1:P7:133:MET:HE1 | 2.03 | 0.41 |
| 1:B7:65:LEU:HB3 | 1:B7:72:MET:HE3 | 2.03 | 0.41 |
| 8:C7:18:LEU:CD1 | 1:D7:94:TYR:HE1 | 2.34 | 0.41 |
| 1:J7:51:ILE:HG22 | 1:J7:133:MET:CE | 2.51 | 0.41 |
| 8:g7:105:GLU:HG2 | 8:g7:110:ILE:HG23 | 2.02 | 0.41 |
| 8:i7:112:VAL:C | 8:i7:115:MET:H | 2.28 | 0.41 |
| 8:i7:137:ALA:O | 8:i7:139:SER:N | 2.54 | 0.41 |
| 1:V7:75:THR:HB | 8:W7:112:VAL:CA | 2.50 | 0.41 |
| 8:Y7:22:GLU:O | 8:Y7:26:ILE:HG13 | 2.20 | 0.41 |
| 1:Z7:51:ILE:HG22 | 1:Z7:133:MET:CE | 2.51 | 0.41 |
| 1:b7:89:LEU:HB2 | 1:b7:133:MET:HE1 | 2.03 | 0.41 |
| 3:B8:116:THR:HG21 | 4:M8:53:LEU:HA | 1.91 | 0.41 |
| 3:B8:151:GLY:HA3 | 12:B8:201:CYC:CMD | 2.51 | 0.41 |
| 1:l7:51:ILE:HG22 | 1:l7:133:MET:CE | 2.51 | 0.41 |
| 8:m7:15:ALA:CA | 1:n7:90:ARG:CZ | 2.98 | 0.41 |
| 8:q7:68:PRO:CB | 11:aA:334:LYS:HZ2 | 2.32 | 0.41 |
| 1:r7:51:ILE:HG22 | 1:r7:133:MET:CE | 2.51 | 0.41 |
| 1:r7:65:LEU:HB3 | 1:r7:72:MET:HE3 | 2.03 | 0.41 |
| 1:t7:51:ILE:HG22 | 1:t7:133:MET:CE | 2.51 | 0.41 |
| 9:w7:10:CYS:O | 9:w7:10:CYS:SG | 2.78 | 0.41 |
| 9:w7:16:ARG:O | 9:w7:16:ARG:CG | 2.69 | 0.41 |
| 9:x7:32:VAL:CG2 | 9:x7:33:PRO:HD2 | 2.51 | 0.41 |
| 3:F8:1:MET:H3 | 4:M8:10:ARG:CB | 2.19 | 0.41 |
| 2:G8:53:LYS:CE | 11:a9:71:ILE:HG23 | 2.49 | 0.41 |
| 4:M9:52:LEU:O | 4:M9:52:LEU:CD2 | 2.69 | 0.41 |
| 5:N9:14:LYS:HD3 | 5:N9:14:LYS:N | 2.32 | 0.41 |
| 5:N9:23:SER:C | 5:N9:25:THR:N | 2.74 | 0.41 |
| 5:N9:50:LEU:HD11 | 3:T9:77:ARG:NH1 | 2.36 | 0.41 |
| 3:Y8:106:GLU:HA | 3:Y8:110:LEU:HD12 | 2.03 | 0.41 |
| 5:Z8:29:HIS:ND1 | 5:Z8:31:TRP:N | 2.68 | 0.41 |
| 5:Z8:54:LEU:HB3 | 5:Z8:55:PRO:HD3 | 2.02 | 0.41 |
| 2:A9:49:ASP:O | 2:A9:50:SER:C | 2.62 | 0.41 |
| 2:K9:22:THR:O | 2:K9:22:THR:HG22 | 2.19 | 0.41 |
| 11:a9:328:GLN:NE2 | 11:a9:328:GLN:CA | 2.83 | 0.41 |
| 11:a9:352:PRO:HB2 | 11:a9:354:VAL:N | 2.36 | 0.41 |
| 11:aA:31:SER:OG | 11:aA:34:ILE:CG2 | 2.68 | 0.41 |
| 11:aA:302:ASN:O | 11:aA:303:GLY:C | 2.63 | 0.41 |
| 11:aA:337:GLU:HG2 | 11:aA:339:GLU:HG2 | 2.03 | 0.41 |
| 11:aA:629:LYS:HA | 11:aA:629:LYS:HZ2 | 1.81 | 0.41 |
| 11:aA:816:LEU:O | 11:aA:816:LEU:CD2 | 2.69 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 3:Z1:151:GLY:HA3 | 12:Z1:201:CYC:CMD | 2.51 | 0.41 |
| 2:A2:30:ARG:NH1 | 3:B2:5:PHE:CE1 | 2.88 | 0.41 |
| 2:A2:60:TYR:CZ | 2:A2:79:GLN:HG2 | 2.56 | 0.41 |
| 2:A2:63:PHE:O | 2:A2:66:LEU:CB | 2.69 | 0.41 |
| 12:C2:201:CYC:CMA | 12:C2:201:CYC:NB | 2.81 | 0.41 |
| 1:A:66:THR:HG21 | 12:k5:1201:CYC:HBA2 | 2.03 | 0.41 |
| 2:AA:63:PHE:O | 2:AA:66:LEU:CB | 2.69 | 0.41 |
| 3:BA:14:LEU:HD11 | 3:XA:125:ARG:CD | 2.51 | 0.41 |
| 2:EA:102:THR:HG21 | 2:IA:20:ASN:HD22 | 1.85 | 0.41 |
| 2:KA:90:LEU:O | 2:KA:94:THR:HG23 | 2.21 | 0.41 |
| 4:MA:70:SER:O | 4:MA:70:SER:OG | 2.35 | 0.41 |
| 4:MA:78:GLY:HA3 | 4:MA:79:PRO:HD2 | 1.81 | 0.41 |
| 4:MA:222:ARG:NH1 | 4:MA:222:ARG:CG | 2.72 | 0.41 |
| 5:NA:60:ILE:HD13 | 5:NA:60:ILE:HG21 | 1.74 | 0.41 |
| 3:PA:3:ASP:H | 3:PA:6:THR:HB | 1.85 | 0.41 |
| 3:TA:3:ASP:H | 3:TA:6:THR:HB | 1.84 | 0.41 |
| 3:TA:151:GLY:HA3 | 12:TA:302:CYC:CMD | 2.51 | 0.41 |
| 3:VA:151:GLY:HA3 | 12:VA:202:CYC:CMD | 2.51 | 0.41 |
| 3:H3:125:ARG:HH22 | 8:k7:41:GLN:NE2 | 2.18 | 0.41 |
| 3:J3:120:LEU:CD2 | 11:a9:800:THR:HG23 | 2.42 | 0.41 |
| 3:J2:108:ARG:CZ | 6:M2:155:ASN:CA | 2.99 | 0.41 |
| 6:M2:271:VAL:HG21 | 1:j7:127:VAL:HB | 2.02 | 0.41 |
| 7:N2:2:TYR:CD1 | 7:N2:2:TYR:N | 2.73 | 0.41 |
| 12:A3:201:CYC:CMA | 12:A3:201:CYC:NB | 2.82 | 0.41 |
| 3:F3:119:ALA:HB2 | 4:M3:41:ASN:ND2 | 2.34 | 0.41 |
| 12:F3:201:CYC:CAA | 4:M3:36:TYR:CE2 | 3.03 | 0.41 |
| 2:A4:19:LEU:HD13 | 3:B4:98:LEU:HD22 | 2.03 | 0.41 |
| 3:B4:125:ARG:HD2 | 3:W4:14:LEU:CD1 | 2.50 | 0.41 |
| 3:B4:151:GLY:HA3 | 12:B4:201:CYC:CMD | 2.51 | 0.41 |
| 12:B4:202:CYC:O2D | 4:M4:50:ASP:CA | 2.68 | 0.41 |
| 4:M3:23:PRO:HB2 | 4:M3:34:ASP:HB3 | 2.02 | 0.41 |
| 4:M3:164:ARG:NH2 | 4:M3:168:LEU:HD21 | 2.36 | 0.41 |
| 4:M3:218:VAL:HG23 | 4:M3:218:VAL:H | 1.66 | 0.41 |
| 5:N3:39:PRO:CA | 3:T3:116:THR:OG1 | 2.69 | 0.41 |
| 2:O3:28:ASN:HB2 | 12:P3:202:CYC:OB | 2.21 | 0.41 |
| 2:O3:60:TYR:CZ | 2:O3:79:GLN:HG2 | 2.56 | 0.41 |
| 3:V3:151:GLY:HA3 | 12:V3:202:CYC:CMD | 2.51 | 0.41 |
| 3:X3:151:GLY:HA3 | 12:X3:202:CYC:CMD | 2.51 | 0.41 |
| 3:S4:120:LEU:CD1 | 12:S4:202:CYC:HBD1 | 2.51 | 0.41 |
| 2:T4:90:LEU:O | 2:T4:94:THR:HG23 | 2.21 | 0.41 |
| 3:F4:84:ARG:HG3 | 11:aA:139:ILE:HG21 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F4:151:GLY:HA3 | 12:F4:201:CYC:CMD | 2.51 | 0.41 |
| 4:M4:94:TRP:HB3 | 3:Q4:88:ILE:CG1 | 2.51 | 0.41 |
| 4:M4:171:LYS:HE2 | 4:M4:221:TYR:OH | 2.21 | 0.41 |
| 4:M4:226:SER:HB2 | 3:Y4:85:ASP:CG | 2.23 | 0.41 |
| 4:M4:274:VAL:HG12 | 4:M4:274:VAL:OXT | 2.21 | 0.41 |
| 2:N4:60:TYR:CD2 | 2:N4:67:THR:CG2 | 3.04 | 0.41 |
| 2:N4:90:LEU:O | 2:N4:94:THR:HG23 | 2.21 | 0.41 |
| 3:Q4:117:TYR:CD1 | 5:Z4:39:PRO:HB2 | 2.56 | 0.41 |
| 3:Q4:151:GLY:HA3 | 12:Q4:201:CYC:CMD | 2.51 | 0.41 |
| 8:K5:115:MET:O | 8:K5:119:LEU:HG | 2.21 | 0.41 |
| 1:L5:72:MET:HB3 | 1:L5:72:MET:HE2 | 1.87 | 0.41 |
| 8:M5:14:GLU:HG2 | 10:k5:538:PHE:HZ | 1.82 | 0.41 |
| 8:O5:24:ASP:C | 8:O5:26:ILE:N | 2.79 | 0.41 |
| 8:O5:33:GLY:HA2 | 8:O5:36:ARG:HB2 | 2.01 | 0.41 |
| 3:Y4:89:ILE:HG21 | 3:Y4:92:TYR:OH | 2.01 | 0.41 |
| 5:Z4:53:LEU:HA | 5:Z4:53:LEU:HD23 | 1.88 | 0.41 |
| 1:B5:51:ILE:HG22 | 1:B5:133:MET:CE | 2.51 | 0.41 |
| 8:C5:8:ILE:O | 8:C5:8:ILE:HG22 | 2.20 | 0.41 |
| 8:C5:9:VAL:O | 8:C5:9:VAL:HG13 | 2.20 | 0.41 |
| 8:C5:18:LEU:HD12 | 8:C5:18:LEU:N | 2.36 | 0.41 |
| 8:C5:105:GLU:HG2 | 8:C5:110:ILE:HG23 | 2.02 | 0.41 |
| 1:F5:8:VAL:HB | 1:F5:27:LEU:HD21 | 2.02 | 0.41 |
| 8:G5:88:TYR:OH | 12:G5:201:CYC:CMB | 2.68 | 0.41 |
| 8:G5:88:TYR:CZ | 12:G5:201:CYC:CMB | 3.03 | 0.41 |
| 8:I5:2:SER:HA | 8:I5:100:ASP:HB3 | 2.01 | 0.41 |
| 8:c5:14:GLU:HG2 | 10:j5:399:TYR:HE2 | 1.86 | 0.41 |
| 1:d5:51:ILE:HG22 | 1:d5:133:MET:CE | 2.51 | 0.41 |
| 8:e5:95:GLY:HA3 | 8:e5:104:ILE:HD11 | 2.01 | 0.41 |
| 1:P5:87:TYR:OH | 10:k5:649:PHE:CE1 | 2.57 | 0.41 |
| 8:U5:13:ALA:O | 10:j5:656:GLY:HA3 | 2.21 | 0.41 |
| 8:W5:8:ILE:O | 8:W5:11:ALA:N | 2.51 | 0.41 |
| 8:W5:22:GLU:O | 8:W5:26:ILE:HG13 | 2.20 | 0.41 |
| 1:Z5:51:ILE:HG22 | 1:Z5:133:MET:CE | 2.51 | 0.41 |
| 8:a5:105:GLU:HG2 | 8:a5:110:ILE:HG23 | 2.02 | 0.41 |
| 3:J6:108:ARG:CZ | 6:M6:155:ASN:CA | 2.99 | 0.41 |
| 2:K6:14:SER:HA | 6:M6:226:ASN:CB | 2.38 | 0.41 |
| 7:N6:16:PHE:CD2 | 7:N6:67:PRO:HA | 2.55 | 0.41 |
| 9:i5:16:ARG:NH2 | 10:j5:527:SER:HB2 | 2.35 | 0.41 |
| 9:i5:24:GLN:HE21 | 9:i5:24:GLN:HB3 | 1.57 | 0.41 |
| 10:j5:352:ILE:CG2 | 10:j5:353:ASN:N | 2.84 | 0.41 |
| 10:j5:538:PHE:HB3 | 10:j5:567:LEU:CD2 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:j5:975:ARG:HD3 | 10:j5:1116:TYR:CE2 | 2.56 | 0.41 |
| 10:k5:17:PHE:CD1 | 10:k5:19:THR:CG2 | 3.02 | 0.41 |
| 10:k5:204:LEU:HD23 | 10:k5:204:LEU:HA | 1.90 | 0.41 |
| 10:k5:388:ARG:HA | 10:k5:394:PRO:CG | 2.46 | 0.41 |
| 10:k5:406:ILE:O | 10:k5:406:ILE:HG22 | 2.20 | 0.41 |
| 10:k5:631:HIS:CA | 10:k5:664:MET:HE1 | 2.50 | 0.41 |
| 10:k5:722:ILE:HD13 | 10:k5:722:ILE:HG21 | 1.79 | 0.41 |
| 10:k5:830:GLU:O | 10:k5:830:GLU:HG3 | 2.20 | 0.41 |
| 10:k5:867:VAL:O | 10:k5:867:VAL:HG13 | 2.21 | 0.41 |
| 10:k5:919:ILE:H | 10:k5:919:ILE:HG12 | 1.62 | 0.41 |
| 10:k5:942:LYS:HE2 | 10:k5:942:LYS:HB3 | 1.79 | 0.41 |
| 10:k5:970:GLY:H | 1:n7:77:ARG:HH22 | 1.55 | 0.41 |
| 10:k5:1071:PRO:CD | 10:k5:1071:PRO:O | 2.65 | 0.41 |
| 2:A6:60:TYR:CZ | 2:A6:79:GLN:HG2 | 2.56 | 0.41 |
| 3:D6:3:ASP:H | 3:D6:6:THR:HB | 1.85 | 0.41 |
| 3:F6:151:GLY:HA3 | 12:F6:202:CYC:CMD | 2.51 | 0.41 |
| 12:P7:201:CYC:HBB1 | 9:z7:21:ARG:HG3 | 2.02 | 0.41 |
| 12:Q7:201:CYC:HB | 12:Q7:201:CYC:CMA | 2.21 | 0.41 |
| 1:B7:51:ILE:HG22 | 1:B7:133:MET:CE | 2.51 | 0.41 |
| 8:C7:15:ALA:CA | 1:D7:90:ARG:CZ | 2.98 | 0.41 |
| 1:D7:51:ILE:HG22 | 1:D7:133:MET:CE | 2.51 | 0.41 |
| 8:E7:105:GLU:HG2 | 8:E7:110:ILE:HG23 | 2.02 | 0.41 |
| 12:F7:201:CYC:HC | 12:F7:201:CYC:CMD | 2.13 | 0.41 |
| 8:G7:4:LEU:CD2 | 8:G7:26:ILE:HD13 | 2.47 | 0.41 |
| 8:G7:22:GLU:O | 8:G7:26:ILE:HG13 | 2.20 | 0.41 |
| 8:G7:105:GLU:HG2 | 8:G7:110:ILE:HG23 | 2.02 | 0.41 |
| 12:J7:201:CYC:HC | 12:J7:201:CYC:CMD | 2.14 | 0.41 |
| 1:L7:65:LEU:HB3 | 1:L7:72:MET:HE3 | 2.03 | 0.41 |
| 8:M7:4:LEU:CD2 | 8:M7:26:ILE:HD13 | 2.47 | 0.41 |
| 8:g7:36:ARG:NH1 | 8:u7:24:ASP:OD2 | 2.54 | 0.41 |
| 8:g7:37:LEU:HD11 | 1:h7:27:LEU:CB | 2.51 | 0.41 |
| 1:h7:37:ARG:HG2 | 1:h7:37:ARG:HH11 | 1.85 | 0.41 |
| 8:i7:12:ASP:CG | 9:y7:46:LYS:HZ1 | 2.21 | 0.41 |
| 8:i7:67:SER:O | 8:i7:68:PRO:C | 2.63 | 0.41 |
| 8:i7:159:ALA:C | 8:i7:161:GLN:H | 2.29 | 0.41 |
| 1:T7:51:ILE:HG22 | 1:T7:133:MET:CE | 2.51 | 0.41 |
| 8:U7:67:SER:O | 8:U7:68:PRO:C | 2.63 | 0.41 |
| 12:V7:201:CYC:CBB | 9:w7:21:ARG:HA | 2.49 | 0.41 |
| 1:Z7:72:MET:HE2 | 1:Z7:72:MET:HB3 | 1.87 | 0.41 |
| 8:a7:105:GLU:HG2 | 8:a7:110:ILE:HG23 | 2.02 | 0.41 |
| 8:c7:105:GLU:HG2 | 8:c7:110:ILE:HG23 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:d7:89:LEU:HB2 | 1:d7:133:MET:HE1 | 2.03 | 0.41 |
| 8:e7:105:GLU:HG2 | 8:e7:110:ILE:HG23 | 2.02 | 0.41 |
| 1:f7:51:ILE:HG22 | 1:f7:133:MET:CE | 2.51 | 0.41 |
| 1:f7:65:LEU:HB3 | 1:f7:72:MET:HE3 | 2.03 | 0.41 |
| 2:E1:90:LEU:O | 2:E1:94:THR:HG23 | 2.21 | 0.41 |
| 2:A8:60:TYR:CD2 | 2:A8:67:THR:CG2 | 3.04 | 0.41 |
| 2:A8:63:PHE:O | 2:A8:66:LEU:CB | 2.69 | 0.41 |
| 2:E8:1:MET:C | 4:M8:10:ARG:NH2 | 2.79 | 0.41 |
| 8:m7:18:LEU:CD1 | 1:n7:94:TYR:HE1 | 2.33 | 0.41 |
| 1:n7:89:LEU:HB2 | 1:n7:133:MET:HE1 | 2.03 | 0.41 |
| 1:p7:65:LEU:HB3 | 1:p7:72:MET:HE3 | 2.03 | 0.41 |
| 1:v7:51:ILE:HG22 | 1:v7:133:MET:CE | 2.51 | 0.41 |
| 9:z7:15:LYS:O | 9:z7:15:LYS:CG | 2.69 | 0.41 |
| 9:y7:18:ARG:HE | 9:y7:18:ARG:HB2 | 1.68 | 0.41 |
| 9:y7:30:LYS:O | 9:y7:30:LYS:CG | 2.69 | 0.41 |
| 3:F8:108:ARG:NE | 4:M8:9:GLN:HB3 | 2.36 | 0.41 |
| 2:G8:90:LEU:O | 2:G8:94:THR:HG23 | 2.21 | 0.41 |
| 3:J8:151:GLY:HA3 | 12:J8:202:CYC:CMD | 2.51 | 0.41 |
| 2:K8:90:LEU:O | 2:K8:94:THR:HG23 | 2.21 | 0.41 |
| 4:M8:59:ILE:HD13 | 4:M8:59:ILE:HG21 | 1.67 | 0.41 |
| 4:M8:98:ASP:N | 3:Q8:108:ARG:HB2 | 2.36 | 0.41 |
| 4:M8:262:ASP:OD1 | 4:M8:263:PRO:CD | 2.68 | 0.41 |
| 12:M8:302:CYC:CAC | 3:S8:78:ARG:HA | 2.39 | 0.41 |
| 3:O8:104:VAL:CB | 5:Z8:61:LYS:HE3 | 2.46 | 0.41 |
| 3:O8:107:ASP:O | 5:Z8:66:ARG:HA | 2.21 | 0.41 |
| 3:O8:116:THR:N | 5:Z8:70:ILE:CG2 | 2.84 | 0.41 |
| 3:Q8:78:ARG:CD | 12:Z8:301:CYC:HMD3 | 2.50 | 0.41 |
| 3:Q8:151:GLY:HA3 | 12:Q8:201:CYC:CMD | 2.51 | 0.41 |
| 3:L9:90:LEU:CD2 | 2:K9:18:PHE:CE1 | 3.03 | 0.41 |
| 4:M9:164:ARG:NH2 | 4:M9:168:LEU:HD21 | 2.36 | 0.41 |
| 4:M9:176:ARG:HG3 | 4:M9:176:ARG:NH1 | 2.36 | 0.41 |
| 4:M9:262:ASP:OD1 | 4:M9:263:PRO:CD | 2.68 | 0.41 |
| 5:N9:50:LEU:CD1 | 12:T9:301:CYC:O1D | 2.69 | 0.41 |
| 2:O9:60:TYR:CD2 | 2:O9:67:THR:CG2 | 3.04 | 0.41 |
| 2:O9:63:PHE:O | 2:O9:66:LEU:CB | 2.68 | 0.41 |
| 12:P9:202:CYC:HB | 12:P9:202:CYC:HMA3 | 1.83 | 0.41 |
| 3:Y8:3:ASP:H | 3:Y8:6:THR:HB | 1.85 | 0.41 |
| 12:Y8:201:CYC:HB | 12:Y8:201:CYC:HMA3 | 1.84 | 0.41 |
| 5:Z8:37:HIS:HB2 | 12:Z8:301:CYC:C2B | 2.50 | 0.41 |
| 2:A9:30:ARG:NH1 | 3:B9:5:PHE:CE1 | 2.88 | 0.41 |
| 3:F9:36:LYS:HE2 | 3:F9:156:LEU:HD13 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:J9:116:THR:HA | 11:a9:521:PHE:CD1 | 2.55 | 0.41 |
| 3:R9:151:GLY:HA3 | 12:R9:202:CYC:CMD | 2.51 | 0.41 |
| 3:V9:151:GLY:HA3 | 12:V9:202:CYC:CMD | 2.51 | 0.41 |
| 12:W9:201:CYC:CMA | 12:W9:201:CYC:NB | 2.81 | 0.41 |
| 11:a9:60:GLY:HA2 | 11:a9:64:ARG:HE | 1.86 | 0.41 |
| 11:a9:293:LEU:O | 11:a9:294:THR:C | 2.64 | 0.41 |
| 11:a9:308:LEU:O | 11:a9:309:ALA:C | 2.62 | 0.41 |
| 11:a9:550:PHE:HD1 | 11:a9:550:PHE:HA | 1.70 | 0.41 |
| 11:aA:20:PRO:HB2 | 11:aA:21:THR:H | 1.64 | 0.41 |
| 11:aA:48:LEU:C | 11:aA:48:LEU:CD1 | 2.84 | 0.41 |
| 11:aA:62:MET:O | 11:aA:64:ARG:N | 2.50 | 0.41 |
| 11:aA:110:PHE:CD1 | 11:aA:115:VAL:CG2 | 3.04 | 0.41 |
| 11:aA:308:LEU:O | 11:aA:309:ALA:C | 2.62 | 0.41 |
| 11:aA:399:ILE:O | 11:aA:399:ILE:CG2 | 2.69 | 0.41 |
| 11:aA:467:GLN:HE22 | 11:aA:553:SER:HB3 | 1.86 | 0.41 |
| 11:aA:643:LEU:H | 11:aA:643:LEU:CD1 | 2.04 | 0.41 |
| 3:H1:151:GLY:HA3 | 12:H1:202:CYC:CMD | 2.51 | 0.41 |
| 3:J1:151:GLY:HA3 | 12:J1:201:CYC:CMD | 2.51 | 0.41 |
| 4:M1:13:LYS:HD2 | 4:M1:13:LYS:HA | 1.86 | 0.41 |
| 4:M1:21:LEU:C | 4:M1:21:LEU:CD1 | 2.94 | 0.41 |
| 4:M1:144:ARG:NH2 | 5:N1:52:ARG:CZ | 2.82 | 0.41 |
| 4:M1:144:ARG:HH21 | 5:N1:52:ARG:NH2 | 2.09 | 0.41 |
| 4:M1:158:PHE:CZ | 2:Y1:10:ALA:HB1 | 2.56 | 0.41 |
| 4:M1:188:LEU:HD22 | 12:Z1:202:CYC:NB | 2.33 | 0.41 |
| 4:M1:250:THR:O | 4:M1:250:THR:HG22 | 2.19 | 0.41 |
| 5:N1:14:LYS:HE3 | 5:N1:50:LEU:HD23 | 2.02 | 0.41 |
| 5:N1:39:PRO:HA | 3:T1:116:THR:OG1 | 2.20 | 0.41 |
| 3:V1:151:GLY:HA3 | 12:V1:202:CYC:CMD | 2.51 | 0.41 |
| 2:A2:60:TYR:CD2 | 2:A2:67:THR:CG2 | 3.04 | 0.41 |
| 3:F2:78:ARG:O | 12:F2:201:CYC:HMD1 | 2.21 | 0.41 |
| 2:EA:115:GLU:OE2 | 4:MA:33:LEU:HD21 | 2.11 | 0.41 |
| 3:HA:66:LEU:CD2 | 12:HA:202:CYC:HMC1 | 2.51 | 0.41 |
| 2:IA:12:ALA:HB1 | 3:JA:95:TYR:CE1 | 2.56 | 0.41 |
| 12:IA:201:CYC:CMA | 12:IA:201:CYC:NB | 2.81 | 0.41 |
| 3:JA:151:GLY:HA3 | 12:JA:201:CYC:CMD | 2.51 | 0.41 |
| 5:NA:34:LEU:HB3 | 3:PA:84:ARG:HH11 | 1.86 | 0.41 |
| 2:QA:33:ARG:NH1 | 12:VA:202:CYC:NB | 2.69 | 0.41 |
| 3:XA:151:GLY:HA3 | 12:XA:202:CYC:CMD | 2.51 | 0.41 |
| 2:YA:90:LEU:O | 2:YA:94:THR:HG23 | 2.21 | 0.41 |
| 2:A3:34:ALA:HB3 | 3:B3:31:VAL:CG1 | 2.39 | 0.41 |
| 2:A3:60:TYR:CZ | 2:A3:79:GLN:HG2 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:A4:28:ASN:HB2 | 12:B4:201:CYC:OB | 2.21 | 0.41 |
| 2:A4:60:TYR:CD2 | 2:A4:67:THR:CG2 | 3.04 | 0.41 |
| 3:B4:108:ARG:CA | 4:M4:61:ASN:HB2 | 2.51 | 0.41 |
| 3:L3:108:ARG:O | 11:a9:712:ASN:CG | 2.52 | 0.41 |
| 4:M3:13:LYS:HA | 4:M3:13:LYS:HD2 | 1.86 | 0.41 |
| 4:M3:52:LEU:O | 4:M3:52:LEU:CD2 | 2.69 | 0.41 |
| 5:N3:26:LEU:HD23 | 5:N3:27:ALA:HB3 | 2.03 | 0.41 |
| 2:S3:38:MET:HE2 | 2:S3:38:MET:HB3 | 1.81 | 0.41 |
| 2:Y3:38:MET:HB3 | 2:Y3:38:MET:HE2 | 1.81 | 0.41 |
| 3:J4:108:ARG:HH22 | 11:aA:171:ARG:CG | 2.32 | 0.41 |
| 4:M4:98:ASP:O | 3:Q4:104:VAL:HB | 2.20 | 0.41 |
| 12:M4:301:CYC:HAB2 | 3:Y4:92:TYR:CE2 | 2.55 | 0.41 |
| 8:K5:20:PRO:CA | 8:U5:151:PHE:HB3 | 2.51 | 0.41 |
| 1:B5:110:ASN:CG | 10:k5:547:ARG:HD3 | 2.46 | 0.41 |
| 8:C5:107:ILE:O | 12:C5:201:CYC:HAB2 | 2.20 | 0.41 |
| 1:D5:73:TYR:HE1 | 12:E5:201:CYC:HBB2 | 1.85 | 0.41 |
| 8:G5:106:GLU:OE1 | 10:j5:557:VAL:CG2 | 2.68 | 0.41 |
| 1:H5:89:LEU:HB2 | 1:H5:133:MET:HE1 | 2.02 | 0.41 |
| 1:J5:89:LEU:HB2 | 1:J5:133:MET:HE1 | 2.03 | 0.41 |
| 2:C1:90:LEU:O | 2:C1:94:THR:HG23 | 2.21 | 0.41 |
| 1:d5:65:LEU:HB3 | 1:d5:72:MET:HE3 | 2.03 | 0.41 |
| 1:P5:155:TYR:CE2 | 1:b5:113:LYS:HD2 | 2.56 | 0.41 |
| 1:R5:89:LEU:HB2 | 1:R5:133:MET:HE1 | 2.03 | 0.41 |
| 1:R5:110:ASN:OD1 | 10:k5:466:LEU:C | 2.63 | 0.41 |
| 8:S5:90:ARG:NH1 | 1:T5:16:GLY:CA | 2.81 | 0.41 |
| 1:X5:89:LEU:HB2 | 1:X5:133:MET:HE1 | 2.03 | 0.41 |
| 1:b5:8:VAL:HB | 1:b5:27:LEU:HD21 | 2.03 | 0.41 |
| 1:b5:51:ILE:HG22 | 1:b5:133:MET:CE | 2.51 | 0.41 |
| 10:j5:154:GLN:H | 10:j5:154:GLN:HG3 | 1.71 | 0.41 |
| 10:j5:277:ILE:HG21 | 10:j5:284:PRO:HD3 | 2.01 | 0.41 |
| 10:j5:357:LEU:HG | 10:j5:382:ILE:HD11 | 2.03 | 0.41 |
| 10:j5:388:ARG:CZ | 10:j5:388:ARG:CB | 2.87 | 0.41 |
| 10:j5:1045:TYR:OH | 10:j5:1062:LEU:HD22 | 2.13 | 0.41 |
| 10:j5:1084:LEU:HD22 | 10:j5:1092:ALA:HB2 | 2.02 | 0.41 |
| 10:k5:156:SER:OG | 12:k5:1201:CYC:CAC | 2.66 | 0.41 |
| 10:k5:221:LYS:C | 10:k5:221:LYS:HZ1 | 2.23 | 0.41 |
| 10:k5:245:ILE:H | 10:k5:245:ILE:HG12 | 1.45 | 0.41 |
| 10:k5:462:TYR:HD1 | 10:k5:462:TYR:HA | 1.63 | 0.41 |
| 10:k5:512:ASN:HD22 | 10:k5:682:GLU:HG2 | 1.86 | 0.41 |
| 10:k5:947:MET:HE3 | 10:k5:948:SER:HB3 | 2.02 | 0.41 |
| 10:k5:1019:SER:O | 10:k5:1020:GLU:CB | 2.60 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:I6:90:LEU:O | 2:I6:94:THR:HG23 | 2.21 | 0.41 |
| 8:Q7:119:LEU:O | 8:Q7:120:GLN:C | 2.64 | 0.41 |
| 1:R7:51:ILE:HG22 | 1:R7:133:MET:CE | 2.51 | 0.41 |
| 1:D7:74:THR:HA | 8:E7:107:ILE:O | 2.21 | 0.41 |
| 8:I7:105:GLU:HG2 | 8:I7:110:ILE:HG23 | 2.02 | 0.41 |
| 8:K7:22:GLU:O | 8:K7:26:ILE:HG13 | 2.20 | 0.41 |
| 1:L7:51:ILE:HG22 | 1:L7:133:MET:CE | 2.51 | 0.41 |
| 8:g7:95:GLY:HA3 | 8:g7:104:ILE:HD11 | 2.02 | 0.41 |
| 8:i7:112:VAL:O | 8:i7:116:TYR:N | 2.41 | 0.41 |
| 1:j7:75:THR:HB | 8:e7:112:VAL:HA | 2.03 | 0.41 |
| 1:T7:65:LEU:HB3 | 1:T7:72:MET:HE3 | 2.03 | 0.41 |
| 1:d7:51:ILE:HG22 | 1:d7:133:MET:CE | 2.51 | 0.41 |
| 2:E8:90:LEU:O | 2:E8:94:THR:HG23 | 2.21 | 0.41 |
| 8:m7:18:LEU:CD1 | 1:n7:94:TYR:CE1 | 3.04 | 0.41 |
| 8:o7:90:ARG:CG | 1:p7:18:TYR:CD1 | 3.04 | 0.41 |
| 8:u7:2:SER:CB | 1:v7:5:ILE:CB | 2.90 | 0.41 |
| 8:u7:77:MET:O | 12:u7:201:CYC:HMD3 | 2.20 | 0.41 |
| 9:x7:15:LYS:O | 9:x7:15:LYS:CG | 2.69 | 0.41 |
| 9:y7:32:VAL:CG2 | 9:y7:33:PRO:HD2 | 2.51 | 0.41 |
| 2:X8:90:LEU:O | 2:X8:94:THR:HG23 | 2.21 | 0.41 |
| 2:I8:38:MET:HE2 | 2:I8:38:MET:HB3 | 1.81 | 0.41 |
| 4:M8:230:GLN:C | 12:M8:301:CYC:OB | 2.63 | 0.41 |
| 12:M8:302:CYC:C4C | 3:S8:78:ARG:HG2 | 2.52 | 0.41 |
| 3:O8:119:ALA:CB | 5:Z8:72:GLU:CB | 2.78 | 0.41 |
| 3:O8:151:GLY:HA3 | 12:O8:202:CYC:CMD | 2.51 | 0.41 |
| 4:M9:145:LEU:HD23 | 4:M9:145:LEU:HA | 1.89 | 0.41 |
| 4:M9:192:GLN:NE2 | 3:V9:87:GLU:CD | 2.79 | 0.41 |
| 4:M9:232:VAL:H | 4:M9:232:VAL:HG12 | 1.57 | 0.41 |
| 3:P9:151:GLY:HA3 | 12:P9:202:CYC:CMD | 2.51 | 0.41 |
| 5:Z8:22:LEU:HD13 | 12:Z8:301:CYC:OB | 2.00 | 0.41 |
| 5:Z8:54:LEU:O | 5:Z8:54:LEU:HG | 2.21 | 0.41 |
| 2:A9:38:MET:HE2 | 2:A9:38:MET:HB3 | 1.81 | 0.41 |
| 2:A9:60:TYR:CZ | 2:A9:79:GLN:HG2 | 2.56 | 0.41 |
| 2:E9:90:LEU:O | 2:E9:94:THR:HG23 | 2.21 | 0.41 |
| 2:I9:4:VAL:HG21 | 2:I9:30:ARG:HB2 | 2.02 | 0.41 |
| 2:K9:17:ARG:HB3 | 2:K9:17:ARG:HH11 | 1.81 | 0.41 |
| 3:X9:151:GLY:HA3 | 12:X9:202:CYC:CMD | 2.51 | 0.41 |
| 11:a9:20:PRO:HB2 | 11:a9:21:THR:H | 1.64 | 0.41 |
| 11:a9:239:TYR:CE1 | 12:a9:901:CYC:C3A | 2.99 | 0.41 |
| 11:a9:418:LEU:HD12 | 11:a9:418:LEU:HA | 1.96 | 0.41 |
| 11:a9:476:ARG:HE | 11:a9:476:ARG:HB2 | 1.70 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:aA:54:ARG:HH11 | 11:aA:609:LEU:C | 2.29 | 0.41 |
| 11:aA:351:THR:O | 11:aA:351:THR:OG1 | 2.31 | 0.41 |
| 11:aA:418:LEU:CD1 | 11:aA:428:PHE:HB2 | 2.44 | 0.41 |
| 11:aA:430:ARG:O | 11:aA:430:ARG:CG | 2.69 | 0.41 |
| 11:aA:708:HIS:HA | 3:L1:108:ARG:CZ | 2.48 | 0.41 |
| 11:aA:710:THR:C | 3:L1:107:ASP:O | 2.64 | 0.41 |
| 11:aA:804:ARG:HH21 | 3:J1:121:GLY:CA | 2.21 | 0.41 |
| 4:M1:139:VAL:O | 4:M1:139:VAL:CG1 | 2.69 | 0.41 |
| 5:N1:26:LEU:HD23 | 5:N1:27:ALA:HB3 | 2.03 | 0.41 |
| 1:Z:73:TYR:OH | 10:j5:162:TRP:CZ2 | 2.73 | 0.40 |
| 2:AA:28:ASN:HB2 | 12:BA:202:CYC:OB | 2.21 | 0.40 |
| 3:HA:87:GLU:HB3 | 11:aA:478:HIS:HE1 | 1.86 | 0.40 |
| 4:MA:95:ALA:CB | 5:NA:38:GLU:OE1 | 2.69 | 0.40 |
| 4:MA:204:ILE:O | 4:MA:204:ILE:CG2 | 2.69 | 0.40 |
| 2:SA:90:LEU:O | 2:SA:94:THR:HG23 | 2.22 | 0.40 |
| 2:UA:90:LEU:O | 2:UA:94:THR:HG23 | 2.22 | 0.40 |
| 3:ZA:3:ASP:H | 3:ZA:6:THR:HB | 1.85 | 0.40 |
| 3:P1:3:ASP:H | 3:P1:6:THR:HB | 1.85 | 0.40 |
| 2:Q1:38:MET:HE2 | 2:Q1:38:MET:HB3 | 1.81 | 0.40 |
| 2:I3:38:MET:HE2 | 2:I3:38:MET:HB3 | 1.81 | 0.40 |
| 2:G2:90:LEU:O | 2:G2:94:THR:HG23 | 2.21 | 0.40 |
| 2:K2:14:SER:HA | 6:M2:226:ASN:CB | 2.38 | 0.40 |
| 2:K2:90:LEU:O | 2:K2:94:THR:HG23 | 2.21 | 0.40 |
| 3:L2:78:ARG:HH22 | 6:M2:70:GLU:CA | 2.34 | 0.40 |
| 3:L2:125:ARG:HD2 | 1:h7:69:GLY:CA | 2.51 | 0.40 |
| 3:D4:151:GLY:HA3 | 12:D4:201:CYC:CMD | 2.51 | 0.40 |
| 3:L3:151:GLY:HA3 | 12:L3:201:CYC:CMD | 2.51 | 0.40 |
| 4:M3:77:LEU:H | 4:M3:77:LEU:HG | 1.63 | 0.40 |
| 4:M3:245:ASP:O | 12:X3:201:CYC:HBB3 | 2.19 | 0.40 |
| 3:B1:111:ASN:HD21 | 4:M1:73:ASP:HA | 1.85 | 0.40 |
| 3:B1:125:ARG:HD2 | 3:X1:14:LEU:HD11 | 2.03 | 0.40 |
| 2:V4:90:LEU:O | 2:V4:94:THR:HG23 | 2.21 | 0.40 |
| 3:F4:115:GLU:CD | 4:M4:3:VAL:HG13 | 2.43 | 0.40 |
| 4:M4:57:THR:O | 4:M4:57:THR:HG22 | 2.19 | 0.40 |
| 4:M4:139:VAL:O | 4:M4:139:VAL:CG1 | 2.69 | 0.40 |
| 4:M4:190:ARG:HH12 | 4:M4:202:SER:HB2 | 1.68 | 0.40 |
| 1:L5:51:ILE:HG22 | 1:L5:133:MET:CE | 2.51 | 0.40 |
| 1:L5:89:LEU:HB2 | 1:L5:133:MET:HE1 | 2.03 | 0.40 |
| 12:L5:201:CYC:HC | 12:L5:201:CYC:CMD | 2.13 | 0.40 |
| 5:Z4:37:HIS:CE1 | 12:Z4:301:CYC:C4D | 3.04 | 0.40 |
| 8:C5:33:GLY:HA2 | 8:C5:36:ARG:HB2 | 2.01 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:I5:9:VAL:O | 8:I5:9:VAL:HG13 | 2.20 | 0.40 |
| 8:I5:18:LEU:HD12 | 8:I5:18:LEU:N | 2.35 | 0.40 |
| 8:e5:8:ILE:HG21 | 8:e5:8:ILE:HD13 | 1.72 | 0.40 |
| 8:e5:34:GLU:OE1 | 8:e5:38:ARG:NH1 | 2.54 | 0.40 |
| 1:V5:65:LEU:HB3 | 1:V5:72:MET:HE3 | 2.03 | 0.40 |
| 1:X5:8:VAL:HB | 1:X5:27:LEU:HD21 | 2.03 | 0.40 |
| 3:L6:65:ASP:OD2 | 1:b7:64:ASP:OD2 | 2.40 | 0.40 |
| 3:L6:78:ARG:HH22 | 6:M6:70:GLU:CA | 2.34 | 0.40 |
| 8:A7:105:GLU:HG2 | 8:A7:110:ILE:HG23 | 2.02 | 0.40 |
| 9:z5:24:GLN:HE21 | 9:z5:24:GLN:HB3 | 1.56 | 0.40 |
| 10:j5:959:PHE:CD2 | 1:t7:67:ARG:NH1 | 2.88 | 0.40 |
| 10:j5:1025:LEU:HA | 10:j5:1030:ILE:HG23 | 1.94 | 0.40 |
| 10:k5:278:TYR:HE2 | 10:k5:287:ASN:CG | 2.30 | 0.40 |
| 10:k5:298:ARG:HD3 | 10:k5:308:ASP:OD2 | 2.21 | 0.40 |
| 10:k5:669:GLU:O | 10:k5:669:GLU:CG | 2.69 | 0.40 |
| 10:k5:879:ASP:O | 10:k5:879:ASP:CG | 2.64 | 0.40 |
| 10:k5:1034:GLU:OE2 | 10:k5:1037:ARG:NH2 | 2.39 | 0.40 |
| 10:k5:1043:GLU:CD | 8:Y7:14:GLU:CG | 2.94 | 0.40 |
| 10:k5:1146:THR:O | 10:k5:1146:THR:CG2 | 2.69 | 0.40 |
| 3:B6:77:ARG:HD2 | 3:B6:77:ARG:O | 2.21 | 0.40 |
| 8:K7:105:GLU:HG2 | 8:K7:110:ILE:HG23 | 2.02 | 0.40 |
| 8:i7:105:GLU:HG2 | 8:i7:110:ILE:HG23 | 2.02 | 0.40 |
| 1:V7:74:THR:HA | 8:W7:107:ILE:O | 2.21 | 0.40 |
| 1:X7:65:LEU:HB3 | 1:X7:72:MET:HE3 | 2.03 | 0.40 |
| 1:Z7:65:LEU:HB3 | 1:Z7:72:MET:HE3 | 2.03 | 0.40 |
| 1:d7:8:VAL:HB | 1:d7:27:LEU:HD21 | 2.03 | 0.40 |
| 1:l7:65:LEU:HB3 | 1:l7:72:MET:HE3 | 2.03 | 0.40 |
| 8:o7:39:ILE:HD11 | 8:o7:145:ASP:CG | 2.45 | 0.40 |
| 1:p7:51:ILE:HG22 | 1:p7:133:MET:CE | 2.51 | 0.40 |
| 8:u7:38:ARG:HH11 | 8:u7:38:ARG:HD3 | 1.76 | 0.40 |
| 8:u7:98:ALA:CB | 1:v7:9:ILE:HD11 | 2.38 | 0.40 |
| 9:z7:16:ARG:O | 9:z7:16:ARG:CG | 2.69 | 0.40 |
| 9:z7:21:ARG:O | 9:z7:23:LEU:N | 2.54 | 0.40 |
| 9:x7:52:LEU:HD23 | 9:x7:52:LEU:N | 2.36 | 0.40 |
| 9:y7:12:PRO:O | 9:y7:12:PRO:CD | 2.69 | 0.40 |
| 3:U8:108:ARG:HB3 | 4:M8:246:ALA:CB | 2.44 | 0.40 |
| 3:L8:69:PRO:C | 3:L8:71:GLY:N | 2.75 | 0.40 |
| 3:L9:84:ARG:NH2 | 11:a9:405:ILE:O | 2.54 | 0.40 |
| 4:M9:21:LEU:C | 4:M9:21:LEU:CD1 | 2.94 | 0.40 |
| 4:M9:85:VAL:O | 4:M9:85:VAL:CG1 | 2.67 | 0.40 |
| 4:M9:95:ALA:CB | 5:N9:38:GLU:OE1 | 2.69 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:M9:120:LEU:HD23 | 4:M9:120:LEU:HA | 1.89 | 0.40 |
| 4:M9:171:LYS:HE2 | 4:M9:221:TYR:OH | 2.21 | 0.40 |
| 4:M9:273:ILE:HG22 | 2:W9:107:ASP:O | 2.20 | 0.40 |
| 3:Y8:89:ILE:CG1 | 3:Y8:92:TYR:CZ | 3.04 | 0.40 |
| 5:Z8:60:ILE:HD13 | 5:Z8:60:ILE:HG21 | 1.74 | 0.40 |
| 12:B9:202:CYC:HB | 12:B9:202:CYC:HMA3 | 1.84 | 0.40 |
| 3:D9:151:GLY:HA3 | 12:D9:202:CYC:CMD | 2.51 | 0.40 |
| 3:F9:36:LYS:C | 3:F9:156:LEU:CD2 | 2.92 | 0.40 |
| 11:a9:427:GLU:HG3 | 11:a9:430:ARG:HD2 | 2.03 | 0.40 |
| 11:a9:816:LEU:O | 11:a9:816:LEU:CD2 | 2.69 | 0.40 |
| 11:aA:368:ILE:HG21 | 11:aA:368:ILE:HD13 | 1.68 | 0.40 |
| 11:aA:371:VAL:HG21 | 11:aA:507:PHE:CD2 | 2.56 | 0.40 |
| 11:aA:427:GLU:HG3 | 11:aA:430:ARG:HD2 | 2.03 | 0.40 |
| 11:aA:486:ILE:HA | 11:aA:486:ILE:HD13 | 1.79 | 0.40 |
| 11:aA:643:LEU:HD11 | 11:aA:766:ASN:CA | 2.49 | 0.40 |
| 4:M1:28:HIS:CE1 | 4:M1:37:GLU:OE1 | 2.74 | 0.40 |
| 4:M1:164:ARG:NH2 | 4:M1:168:LEU:HD21 | 2.36 | 0.40 |
| 2:U1:90:LEU:O | 2:U1:94:THR:HG23 | 2.21 | 0.40 |
| 2:A2:90:LEU:O | 2:A2:94:THR:HG23 | 2.21 | 0.40 |
| 3:F2:126:SER:HB2 | 12:F2:201:CYC:HMC1 | 2.03 | 0.40 |
| 1:A:89:LEU:HB2 | 1:A:133:MET:HE1 | 2.03 | 0.40 |
| 12:A:201:CYC:HC | 12:A:201:CYC:CMD | 2.14 | 0.40 |
| 1:Z:27:LEU:CD1 | 8:e5:37:LEU:HD21 | 2.51 | 0.40 |
| 1:Z:51:ILE:HG22 | 1:Z:133:MET:CE | 2.51 | 0.40 |
| 2:AA:60:TYR:CD2 | 2:AA:67:THR:CG2 | 3.04 | 0.40 |
| 3:FA:111:ASN:OD1 | 4:MA:65:ARG:NH1 | 2.54 | 0.40 |
| 3:JA:88:ILE:HD13 | 11:aA:512:TYR:CD1 | 2.49 | 0.40 |
| 3:LA:151:GLY:HA3 | 12:LA:201:CYC:CMD | 2.51 | 0.40 |
| 4:MA:1:MET:HE1 | 4:MA:45:VAL:HG13 | 1.92 | 0.40 |
| 4:MA:33:LEU:O | 4:MA:33:LEU:CD1 | 2.70 | 0.40 |
| 2:SA:42:ARG:HD2 | 2:X4:69:PRO:HB2 | 2.02 | 0.40 |
| 3:TA:24:LEU:CB | 2:X4:68:GLN:HG3 | 2.43 | 0.40 |
| 2:A1:25:GLN:HG3 | 2:K1:33:ARG:HG2 | 1.99 | 0.40 |
| 2:K3:33:ARG:HG2 | 2:A3:25:GLN:HG3 | 1.99 | 0.40 |
| 12:H2:202:CYC:HMD3 | 12:H2:202:CYC:NC | 2.34 | 0.40 |
| 2:A3:28:ASN:HB2 | 12:B3:201:CYC:OB | 2.22 | 0.40 |
| 3:B3:151:GLY:HA3 | 12:B3:201:CYC:CMD | 2.51 | 0.40 |
| 2:E3:90:LEU:O | 2:E3:94:THR:HG23 | 2.21 | 0.40 |
| 3:F3:151:GLY:HA3 | 12:F3:202:CYC:CMD | 2.51 | 0.40 |
| 3:B4:113:LEU:CB | 4:M4:60:LYS:HE2 | 2.51 | 0.40 |
| 3:D4:3:ASP:H | 3:D4:6:THR:HB | 1.85 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:N3:39:PRO:HA | 3:T3:116:THR:OG1 | 2.20 | 0.40 |
| 2:U3:99:ALA:HB2 | 3:V3:9:ILE:HD13 | 2.00 | 0.40 |
| 3:S4:151:GLY:HA3 | 12:S4:201:CYC:CMD | 2.51 | 0.40 |
| 3:F4:113:LEU:CA | 4:M4:5:THR:CB | 2.97 | 0.40 |
| 2:G4:53:LYS:CE | 11:aA:71:ILE:CG2 | 2.99 | 0.40 |
| 4:M4:7:SER:C | 4:M4:14:LEU:HD13 | 2.08 | 0.40 |
| 4:M4:33:LEU:O | 4:M4:33:LEU:CD1 | 2.70 | 0.40 |
| 3:O4:151:GLY:HA3 | 12:O4:202:CYC:CMD | 2.51 | 0.40 |
| 2:P4:90:LEU:O | 2:P4:94:THR:HG23 | 2.21 | 0.40 |
| 8:K5:20:PRO:CG | 8:U5:151:PHE:C | 2.92 | 0.40 |
| 1:N5:89:LEU:HB2 | 1:N5:133:MET:HE1 | 2.03 | 0.40 |
| 3:Y4:113:LEU:CD1 | 3:Y4:117:TYR:HB2 | 2.51 | 0.40 |
| 5:Z4:41:GLN:CB | 12:Z4:301:CYC:NB | 2.81 | 0.40 |
| 8:A5:118:SER:CB | 1:F5:82:ILE:HD13 | 2.48 | 0.40 |
| 1:D5:19:LEU:HD22 | 1:D5:23:ALA:HB1 | 2.03 | 0.40 |
| 1:D5:76:ARG:HH12 | 9:z5:67:VAL:CB | 2.34 | 0.40 |
| 8:E5:116:TYR:HD1 | 8:E5:116:TYR:HA | 1.59 | 0.40 |
| 12:F5:201:CYC:O2A | 10:k5:591:ILE:CG1 | 2.53 | 0.40 |
| 8:G5:4:LEU:CD2 | 8:G5:26:ILE:HD13 | 2.47 | 0.40 |
| 1:H5:65:LEU:HB3 | 1:H5:72:MET:HE3 | 2.03 | 0.40 |
| 1:d5:75:THR:HB | 8:e5:111:GLY:C | 2.46 | 0.40 |
| 12:d5:201:CYC:OB | 10:j5:379:PHE:HE1 | 2.04 | 0.40 |
| 8:S5:4:LEU:CD2 | 8:S5:26:ILE:HD13 | 2.47 | 0.40 |
| 1:T5:65:LEU:HB3 | 1:T5:72:MET:HE3 | 2.03 | 0.40 |
| 1:V5:89:LEU:HB2 | 1:V5:133:MET:HE1 | 2.03 | 0.40 |
| 1:Z5:75:THR:HB | 8:a5:111:GLY:C | 2.46 | 0.40 |
| 8:a5:9:VAL:O | 8:a5:9:VAL:HG13 | 2.20 | 0.40 |
| 10:j5:190:LEU:HD13 | 12:j5:1201:CYC:NC | 2.36 | 0.40 |
| 10:j5:406:ILE:O | 10:j5:406:ILE:HG22 | 2.20 | 0.40 |
| 10:j5:462:TYR:HD1 | 10:j5:462:TYR:HA | 1.63 | 0.40 |
| 10:j5:867:VAL:O | 10:j5:867:VAL:HG13 | 2.21 | 0.40 |
| 10:j5:1047:LYS:O | 10:j5:1051:GLU:HB2 | 2.12 | 0.40 |
| 10:k5:762:GLU:OE2 | 10:k5:762:GLU:CA | 2.69 | 0.40 |
| 10:k5:827:LYS:O | 10:k5:827:LYS:CG | 2.68 | 0.40 |
| 10:k5:1140:TRP:CD1 | 10:k5:1140:TRP:H | 2.39 | 0.40 |
| 2:A6:60:TYR:CD2 | 2:A6:67:THR:CG2 | 3.04 | 0.40 |
| 2:A6:90:LEU:O | 2:A6:94:THR:HG23 | 2.21 | 0.40 |
| 3:B6:151:GLY:HA3 | 12:B6:201:CYC:CMD | 2.51 | 0.40 |
| 1:D7:65:LEU:HB3 | 1:D7:72:MET:HE3 | 2.03 | 0.40 |
| 1:F7:51:ILE:HG22 | 1:F7:133:MET:CE | 2.51 | 0.40 |
| 8:G7:52:LYS:HG3 | 11:a9:586:LEU:HD21 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:H7:65:LEU:HB3 | 1:H7:72:MET:HE3 | 2.03 | 0.40 |
| 8:I7:18:LEU:CD1 | 1:J7:94:TYR:CE1 | 3.04 | 0.40 |
| 1:N7:51:ILE:HG22 | 1:N7:133:MET:CE | 2.51 | 0.40 |
| 8:g7:11:ALA:C | 8:g7:13:ALA:N | 2.75 | 0.40 |
| 1:h7:24:LEU:CD2 | 1:h7:24:LEU:O | 2.70 | 0.40 |
| 8:i7:42:THR:HB | 8:i7:141:LEU:CD2 | 2.51 | 0.40 |
| 8:Y7:111:GLY:HA3 | 1:d7:75:THR:O | 2.22 | 0.40 |
| 1:Z7:67:ARG:NH1 | 11:a9:307:ARG:HD3 | 2.37 | 0.40 |
| 8:c7:8:ILE:O | 8:c7:11:ALA:N | 2.50 | 0.40 |
| 8:c7:11:ALA:O | 1:d7:94:TYR:OH | 2.32 | 0.40 |
| 12:B8:202:CYC:OB | 4:M8:58:TYR:CD1 | 2.73 | 0.40 |
| 8:q7:105:GLU:HG2 | 8:q7:110:ILE:HG23 | 2.02 | 0.40 |
| 1:v7:62:TYR:CE1 | 11:aA:602:PRO:CG | 2.87 | 0.40 |
| 1:v7:65:LEU:HB3 | 1:v7:72:MET:HE3 | 2.03 | 0.40 |
| 9:z7:16:ARG:NH2 | 9:z7:18:ARG:HG3 | 2.36 | 0.40 |
| 9:w7:5:PHE:CE2 | 9:w7:37:TRP:HD1 | 2.38 | 0.40 |
| 12:T8:201:CYC:CMA | 12:T8:201:CYC:NB | 2.81 | 0.40 |
| 4:M8:236:ASN:HB2 | 3:Y8:116:THR:HG21 | 2.03 | 0.40 |
| 12:M8:302:CYC:C1C | 3:S8:78:ARG:HG2 | 2.47 | 0.40 |
| 2:N8:10:ALA:O | 5:Z8:62:ARG:NH2 | 2.54 | 0.40 |
| 2:N8:60:TYR:CD2 | 2:N8:67:THR:CG2 | 3.04 | 0.40 |
| 2:P8:90:LEU:O | 2:P8:94:THR:HG23 | 2.21 | 0.40 |
| 3:Q8:81:ALA:HB2 | 5:Z8:36:THR:OG1 | 2.21 | 0.40 |
| 3:Q8:110:LEU:HD11 | 3:Q8:166:LYS:HB3 | 2.02 | 0.40 |
| 2:R8:90:LEU:O | 2:R8:94:THR:HG23 | 2.22 | 0.40 |
| 2:O9:25:GLN:HG3 | 2:Y9:33:ARG:HG2 | 1.99 | 0.40 |
| 2:A9:60:TYR:CD2 | 2:A9:67:THR:CG2 | 3.04 | 0.40 |
| 3:H9:72:ASN:HB3 | 12:H9:202:CYC:OC | 2.21 | 0.40 |
| 11:a9:51:SER:C | 11:a9:53:VAL:N | 2.74 | 0.40 |
| 11:a9:283:GLN:CG | 11:a9:284:PRO:HD3 | 2.48 | 0.40 |
| 11:a9:346:TYR:O | 11:a9:346:TYR:HD1 | 2.04 | 0.40 |
| 11:a9:379:LEU:HD12 | 11:a9:379:LEU:HA | 1.43 | 0.40 |
| 11:a9:415:GLU:OE1 | 11:a9:415:GLU:N | 2.55 | 0.40 |
| 11:a9:425:VAL:HG21 | 11:a9:502:ASN:C | 2.46 | 0.40 |
| 11:a9:607:MET:HE3 | 11:a9:609:LEU:HD12 | 2.03 | 0.40 |
| 11:aA:371:VAL:HG21 | 11:aA:507:PHE:HD2 | 1.86 | 0.40 |
| 11:aA:373:PRO:O | 11:aA:373:PRO:CG | 2.69 | 0.40 |
| 11:aA:403:THR:CG2 | 11:aA:536:THR:HG21 | 2.31 | 0.40 |
| 2:I1:90:LEU:O | 2:I1:94:THR:HG23 | 2.21 | 0.40 |
| 4:M1:52:LEU:O | 4:M1:52:LEU:CD2 | 2.69 | 0.40 |
| 5:N1:31:TRP:CZ3 | 12:T1:301:CYC:HAB1 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:Z:73:TYR:CD1 | 10:j5:162:TRP:CH2 | 3.04 | 0.40 |
| 2:GA:90:LEU:O | 2:GA:94:THR:HG23 | 2.22 | 0.40 |
| 3:HA:84:ARG:HD2 | 11:aA:478:HIS:HB2 | 0.90 | 0.40 |
| 3:HA:113:LEU:HD13 | 12:HA:202:CYC:CMB | 2.47 | 0.40 |
| 4:MA:118:TYR:CD1 | 3:ZA:84:ARG:NH2 | 2.89 | 0.40 |
| 4:MA:210:ILE:O | 4:MA:210:ILE:CG2 | 2.69 | 0.40 |
| 5:NA:26:LEU:HD23 | 5:NA:27:ALA:HB3 | 2.03 | 0.40 |
| 12:RA:202:CYC:HMD3 | 12:RA:202:CYC:NC | 2.35 | 0.40 |
| 3:J2:151:GLY:HA3 | 12:J2:201:CYC:CMD | 2.51 | 0.40 |
| 3:L2:74:TYR:N | 3:L2:75:PRO:CD | 2.85 | 0.40 |
| 6:M2:97:GLU:OE2 | 2:C2:1:MET:HA | 2.21 | 0.40 |
| 7:N2:29:LEU:HD23 | 2:A2:112:GLY:HA2 | 2.03 | 0.40 |
| 4:M3:102:VAL:O | 4:M3:102:VAL:CG1 | 2.69 | 0.40 |
| 5:N3:31:TRP:CZ3 | 12:T3:301:CYC:HAB1 | 2.56 | 0.40 |
| 5:N3:54:LEU:O | 5:N3:54:LEU:HG | 2.21 | 0.40 |
| 2:O3:25:GLN:HG3 | 2:Y3:33:ARG:HG2 | 1.99 | 0.40 |
| 2:O3:60:TYR:CD2 | 2:O3:67:THR:CG2 | 3.04 | 0.40 |
| 3:B1:115:GLU:OE2 | 4:M1:78:GLY:HA2 | 2.21 | 0.40 |
| 12:F4:202:CYC:HMA1 | 11:aA:144:LEU:HD23 | 2.03 | 0.40 |
| 4:M4:37:GLU:OE1 | 11:aA:229:ASN:ND2 | 2.54 | 0.40 |
| 4:M4:250:THR:O | 4:M4:250:THR:HG22 | 2.19 | 0.40 |
| 2:N4:28:ASN:HB2 | 12:O4:202:CYC:OB | 2.21 | 0.40 |
| 5:Z4:54:LEU:O | 5:Z4:54:LEU:HG | 2.21 | 0.40 |
| 8:E5:63:PRO:C | 8:E5:65:VAL:N | 2.80 | 0.40 |
| 8:E5:106:GLU:OE1 | 9:z5:66:GLY:N | 2.52 | 0.40 |
| 1:H5:2:GLN:OE1 | 10:j5:551:MET:SD | 2.79 | 0.40 |
| 1:J5:65:LEU:HB3 | 1:J5:72:MET:HE3 | 2.03 | 0.40 |
| 1:f5:34:GLY:C | 10:j5:47:PHE:HD2 | 2.28 | 0.40 |
| 1:P5:65:LEU:HB3 | 1:P5:72:MET:HE3 | 2.04 | 0.40 |
| 8:Q5:161:GLN:H | 8:Q5:161:GLN:HG2 | 1.67 | 0.40 |
| 1:R5:106:GLU:HG3 | 10:k5:505:VAL:N | 2.35 | 0.40 |
| 8:S5:22:GLU:O | 8:S5:26:ILE:HG13 | 2.20 | 0.40 |
| 8:U5:19:SER:O | 8:U5:20:PRO:C | 2.64 | 0.40 |
| 1:b5:114:GLU:CA | 10:k5:491:THR:CG2 | 2.99 | 0.40 |
| 8:A7:67:SER:O | 8:A7:68:PRO:C | 2.63 | 0.40 |
| 9:i5:58:THR:CG2 | 9:i5:58:THR:O | 2.69 | 0.40 |
| 10:j5:278:TYR:HE2 | 10:j5:287:ASN:CG | 2.30 | 0.40 |
| 10:j5:481:ILE:H | 10:j5:481:ILE:HG12 | 1.67 | 0.40 |
| 10:j5:767:LEU:HA | 10:j5:767:LEU:HD23 | 1.91 | 0.40 |
| 10:j5:920:ARG:HE | 10:j5:920:ARG:HB3 | 1.59 | 0.40 |
| 10:j5:995:VAL:O | 10:j5:995:VAL:HG12 | 2.19 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:k5:665:LEU:HD12 | 10:k5:665:LEU:HA | 1.83 | 0.40 |
| 10:k5:780:ILE:O | 10:k5:780:ILE:HG13 | 2.11 | 0.40 |
| 10:k5:783:TYR:CE1 | 1:F7:83:ARG:HD3 | 2.56 | 0.40 |
| 10:k5:853:LEU:O | 10:k5:853:LEU:CD1 | 2.69 | 0.40 |
| 10:k5:867:VAL:O | 10:k5:867:VAL:CG1 | 2.67 | 0.40 |
| 10:k5:1150:TYR:CZ | 11:a9:38:VAL:HG13 | 2.57 | 0.40 |
| 3:B6:77:ARG:O | 3:B6:77:ARG:CD | 2.69 | 0.40 |
| 2:G6:90:LEU:O | 2:G6:94:THR:HG23 | 2.21 | 0.40 |
| 3:D1:68:ARG:NH2 | 3:X1:68:ARG:HH12 | 2.19 | 0.40 |
| 1:H7:51:ILE:HG22 | 1:H7:133:MET:CE | 2.51 | 0.40 |
| 8:g7:2:SER:HA | 8:g7:100:ASP:HB3 | 2.01 | 0.40 |
| 8:k7:22:GLU:O | 8:k7:26:ILE:HG13 | 2.20 | 0.40 |
| 8:U7:18:LEU:CD1 | 1:V7:94:TYR:HE1 | 2.34 | 0.40 |
| 8:W7:22:GLU:O | 8:W7:26:ILE:HG13 | 2.20 | 0.40 |
| 8:Y7:112:VAL:HA | 1:d7:75:THR:HB | 2.03 | 0.40 |
| 1:b7:74:THR:HA | 8:c7:107:ILE:O | 2.21 | 0.40 |
| 12:b7:201:CYC:C4B | 9:x7:23:LEU:HB2 | 2.51 | 0.40 |
| 2:A8:28:ASN:HB2 | 12:B8:201:CYC:OB | 2.21 | 0.40 |
| 2:A8:94:THR:O | 2:A8:98:VAL:HG23 | 2.22 | 0.40 |
| 3:B8:109:CYS:C | 4:M8:60:LYS:HZ3 | 2.29 | 0.40 |
| 12:B8:202:CYC:O2D | 4:M8:50:ASP:CA | 2.68 | 0.40 |
| 8:o7:43:LEU:HA | 8:o7:43:LEU:HD12 | 1.84 | 0.40 |
| 1:p7:8:VAL:HB | 1:p7:27:LEU:HD21 | 2.03 | 0.40 |
| 9:z7:18:ARG:HE | 9:z7:18:ARG:HB2 | 1.77 | 0.40 |
| 2:T8:90:LEU:O | 2:T8:94:THR:HG23 | 2.21 | 0.40 |
| 2:X8:69:PRO:HB3 | 2:S9:39:GLU:CB | 2.52 | 0.40 |
| 3:F8:151:GLY:HA3 | 12:F8:201:CYC:CMD | 2.51 | 0.40 |
| 3:H8:14:LEU:HD22 | 11:a9:85:ALA:CA | 2.27 | 0.40 |
| 4:M8:23:PRO:CD | 4:M8:23:PRO:O | 2.70 | 0.40 |
| 4:M8:150:GLU:O | 4:M8:154:GLU:HB3 | 2.21 | 0.40 |
| 12:Q8:201:CYC:HB | 12:Q8:201:CYC:HMA3 | 1.83 | 0.40 |
| 3:F1:151:GLY:HA3 | 12:F1:202:CYC:CMD | 2.51 | 0.40 |
| 12:F1:201:CYC:CBA | 4:M1:36:TYR:CD2 | 3.04 | 0.40 |
| 3:L9:97:LEU:HD11 | 3:L9:156:LEU:HD22 | 2.03 | 0.40 |
| 4:M9:28:HIS:HD2 | 4:M9:35:THR:HG23 | 1.87 | 0.40 |
| 4:M9:36:TYR:CE2 | 12:B9:201:CYC:HBA2 | 2.57 | 0.40 |
| 5:N9:28:HIS:CD2 | 5:N9:28:HIS:H | 2.38 | 0.40 |
| 5:N9:54:LEU:CD2 | 3:T9:84:ARG:NH1 | 2.67 | 0.40 |
| 2:O9:59:VAL:O | 2:O9:66:LEU:CD1 | 2.62 | 0.40 |
| 2:Q9:94:THR:O | 2:Q9:98:VAL:HG23 | 2.21 | 0.40 |
| 5:Z8:19:THR:HA | 5:Z8:44:TYR:O | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:F9:302:CYC:HMD3 | 12:F9:302:CYC:NC | 2.35 | 0.40 |
| 12:F9:303:CYC:HB | 12:F9:303:CYC:HMA3 | 1.84 | 0.40 |
| 3:H9:78:ARG:CD | 12:H9:202:CYC:HAD1 | 2.51 | 0.40 |
| 11:a9:355:GLU:OE1 | 11:a9:355:GLU:CA | 2.69 | 0.40 |
| 11:a9:430:ARG:HH22 | 11:a9:491:ASP:HB2 | 1.86 | 0.40 |
| 11:aA:370:ALA:CB | 11:aA:531:ASP:OD2 | 2.69 | 0.40 |
| 4:M1:171:LYS:HE2 | 4:M1:221:TYR:OH | 2.21 | 0.40 |
| 2:W1:94:THR:O | 2:W1:98:VAL:HG23 | 2.22 | 0.40 |
| 1:A:65:LEU:HB3 | 1:A:72:MET:HE3 | 2.03 | 0.40 |
| 2:AA:90:LEU:O | 2:AA:94:THR:HG23 | 2.21 | 0.40 |
| 2:IA:90:LEU:O | 2:IA:94:THR:HG23 | 2.21 | 0.40 |
| 4:MA:29:PRO:CG | 11:aA:378:GLU:CD | 2.91 | 0.40 |
| 4:MA:140:ARG:NH1 | 4:MA:204:ILE:O | 2.52 | 0.40 |
| 5:NA:56:GLU:OE2 | 5:NA:59:ARG:NH2 | 2.51 | 0.40 |
| 2:OA:63:PHE:O | 2:OA:66:LEU:CB | 2.68 | 0.40 |
| 2:A1:60:TYR:CD2 | 2:A1:67:THR:CG2 | 3.04 | 0.40 |
| 2:I3:94:THR:O | 2:I3:98:VAL:HG23 | 2.22 | 0.40 |
| 2:A3:60:TYR:CD2 | 2:A3:67:THR:CG2 | 3.04 | 0.40 |
| 2:A3:63:PHE:O | 2:A3:66:LEU:CB | 2.68 | 0.40 |
| 3:B3:115:GLU:OE2 | 4:M3:78:GLY:HA2 | 2.21 | 0.40 |
| 2:C4:90:LEU:O | 2:C4:94:THR:HG23 | 2.21 | 0.40 |
| 4:M3:56:MET:HB3 | 4:M3:56:MET:HE2 | 1.75 | 0.40 |
| 2:T4:94:THR:O | 2:T4:98:VAL:HG23 | 2.22 | 0.40 |
| 3:H4:3:ASP:H | 3:H4:6:THR:HB | 1.85 | 0.40 |
| 3:H4:14:LEU:HD13 | 11:aA:85:ALA:CB | 2.47 | 0.40 |
| 4:M4:150:GLU:O | 4:M4:154:GLU:HB3 | 2.21 | 0.40 |
| 3:O4:107:ASP:HB3 | 5:Z4:66:ARG:CA | 2.46 | 0.40 |
| 2:P4:19:LEU:HD11 | 3:Q4:95:TYR:HD1 | 1.77 | 0.40 |
| 3:Q4:93:VAL:HG11 | 3:Q4:164:PHE:CG | 2.57 | 0.40 |
| 1:L5:14:VAL:HG12 | 9:i5:64:ASN:HD21 | 1.85 | 0.40 |
| 5:Z4:28:HIS:HB3 | 5:Z4:35:ASP:C | 2.46 | 0.40 |
| 8:E5:115:MET:O | 8:E5:119:LEU:HG | 2.21 | 0.40 |
| 1:F5:65:LEU:HB3 | 1:F5:72:MET:HE3 | 2.03 | 0.40 |
| 2:C1:94:THR:O | 2:C1:98:VAL:HG23 | 2.22 | 0.40 |
| 8:c5:114:GLU:OE2 | 10:j5:312:TYR:C | 2.64 | 0.40 |
| 8:e5:34:GLU:O | 8:e5:38:ARG:HG3 | 2.20 | 0.40 |
| 8:e5:105:GLU:HG2 | 8:e5:110:ILE:HG23 | 2.02 | 0.40 |
| 1:R5:65:LEU:HB3 | 1:R5:72:MET:HE3 | 2.03 | 0.40 |
| 1:R5:106:GLU:CG | 10:k5:505:VAL:N | 2.83 | 0.40 |
| 12:R5:201:CYC:HBB1 | 10:k5:520:ARG:CZ | 2.51 | 0.40 |
| 8:S5:115:MET:SD | 1:X5:75:THR:HG22 | 2.62 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 12:T5:201:CYC:HC | 12:T5:201:CYC:CMD | 2.14 | 0.40 |
| 1:b5:89:LEU:HB2 | 1:b5:133:MET:HE1 | 2.03 | 0.40 |
| 6:M6:53:LEU:CG | 8:c7:80:LEU:HD21 | 2.51 | 0.40 |
| 10:j5:26:ASN:ND2 | 10:j5:267:ASP:CG | 2.79 | 0.40 |
| 10:j5:292:GLU:OE1 | 10:j5:292:GLU:HA | 2.21 | 0.40 |
| 10:j5:611:GLU:OE1 | 10:j5:611:GLU:CA | 2.67 | 0.40 |
| 10:j5:1077:ILE:HG22 | 12:r7:201:CYC:CBA | 2.52 | 0.40 |
| 10:j5:1150:TYR:HD2 | 1:v7:70:GLY:HA2 | 1.87 | 0.40 |
| 10:k5:190:LEU:CD2 | 10:k5:194:CYS:SG | 3.08 | 0.40 |
| 10:k5:232:ARG:NH1 | 10:k5:232:ARG:CB | 2.82 | 0.40 |
| 10:k5:806:VAL:O | 10:k5:806:VAL:HG12 | 2.20 | 0.40 |
| 10:k5:1069:ARG:HD3 | 10:k5:1115:ARG:NH1 | 2.34 | 0.40 |
| 10:k5:1070:ALA:CB | 10:k5:1071:PRO:CD | 2.97 | 0.40 |
| 2:E6:90:LEU:O | 2:E6:94:THR:HG23 | 2.22 | 0.40 |
| 8:S7:49:ARG:HB2 | 11:aA:550:PHE:CZ | 2.56 | 0.40 |
| 8:C7:18:LEU:CD1 | 1:D7:94:TYR:CE1 | 3.04 | 0.40 |
| 8:E7:22:GLU:O | 8:E7:26:ILE:HG13 | 2.20 | 0.40 |
| 1:H7:76:ARG:HB2 | 8:I7:110:ILE:HG13 | 2.04 | 0.40 |
| 8:I7:27:LYS:C | 8:I7:30:VAL:HG22 | 2.47 | 0.40 |
| 8:M7:22:GLU:O | 8:M7:26:ILE:HG13 | 2.20 | 0.40 |
| 1:N7:65:LEU:HB3 | 1:N7:72:MET:HE3 | 2.03 | 0.40 |
| 8:i7:50:ILE:CG2 | 8:i7:133:MET:HG2 | 2.38 | 0.40 |
| 1:T7:76:ARG:HB2 | 8:U7:110:ILE:HG13 | 2.04 | 0.40 |
| 12:V7:201:CYC:HMD1 | 12:V7:201:CYC:NC | 2.09 | 0.40 |
| 8:c7:137:ALA:O | 8:c7:139:SER:N | 2.54 | 0.40 |
| 1:d7:107:ARG:HA | 9:x7:45:GLN:HB3 | 2.04 | 0.40 |
| 1:f7:67:ARG:NH1 | 11:aA:307:ARG:HD3 | 2.36 | 0.40 |
| 2:E1:94:THR:O | 2:E1:98:VAL:HG23 | 2.22 | 0.40 |
| 8:o7:17:TYR:CD2 | 1:p7:93:THR:HB | 2.53 | 0.40 |
| 8:s7:105:GLU:HG2 | 8:s7:110:ILE:HG23 | 2.02 | 0.40 |
| 8:u7:90:ARG:CG | 1:v7:18:TYR:CD1 | 3.04 | 0.40 |
| 9:x7:14:LEU:O | 9:x7:14:LEU:CD1 | 2.70 | 0.40 |
| 2:X8:94:THR:O | 2:X8:98:VAL:HG23 | 2.22 | 0.40 |
| 3:H8:1:MET:N | 11:a9:96:THR:HG21 | 2.33 | 0.40 |
| 4:M8:33:LEU:O | 4:M8:33:LEU:CD1 | 2.70 | 0.40 |
| 4:M8:132:LEU:HD13 | 4:M8:142:PHE:CB | 2.51 | 0.40 |
| 4:M8:140:ARG:NH2 | 4:M8:210:ILE:CG1 | 2.77 | 0.40 |
| 3:Q8:122:THR:HG21 | 12:Z8:301:CYC:CMC | 2.50 | 0.40 |
| 3:S8:151:GLY:HA3 | 12:S8:201:CYC:CMD | 2.51 | 0.40 |
| 4:M9:18:THR:C | 4:M9:19:MET:HG3 | 2.43 | 0.40 |
| 4:M9:53:LEU:HD12 | 12:F9:301:CYC:C4B | 2.19 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:M9:57:THR:O | 4:M9:57:THR:HG22 | 2.19 | 0.40 |
| 2:O9:94:THR:O | 2:O9:98:VAL:HG23 | 2.22 | 0.40 |
| 2:G9:38:MET:HE2 | 2:G9:38:MET:HB3 | 1.81 | 0.40 |
| 2:K9:90:LEU:O | 2:K9:94:THR:HG23 | 2.21 | 0.40 |
| 11:a9:684:ASN:CG | 11:a9:686:SER:HG | 2.30 | 0.40 |
| 11:aA:68:THR:O | 11:aA:69:ARG:CG | 2.70 | 0.40 |
| 4:M1:28:HIS:HD2 | 4:M1:35:THR:HG23 | 1.87 | 0.40 |
| 4:M1:53:LEU:O | 4:M1:53:LEU:CD1 | 2.69 | 0.40 |
| 4:M1:134:ASN:CG | 5:N1:1:MET:N | 2.79 | 0.40 |
| 5:N1:28:HIS:CD2 | 5:N1:28:HIS:H | 2.38 | 0.40 |
| 5:N1:54:LEU:O | 5:N1:54:LEU:HG | 2.21 | 0.40 |
| 2:E2:90:LEU:O | 2:E2:94:THR:HG23 | 2.22 | 0.40 |
| 1:A:13:ASP:OD2 | 8:a5:107:ILE:CD1 | 2.69 | 0.40 |
| 3:JA:88:ILE:HG21 | 11:aA:512:TYR:CE2 | 2.56 | 0.40 |
| 4:MA:252:LEU:HD13 | 3:ZA:77:ARG:NH1 | 2.35 | 0.40 |
| 5:NA:40:SER:O | 5:NA:40:SER:OG | 2.30 | 0.40 |
| 2:QA:29:GLY:N | 2:UA:29:GLY:HA3 | 2.37 | 0.40 |
| 12:QA:201:CYC:CMA | 3:TA:79:MET:HE3 | 2.49 | 0.40 |
| 2:UA:94:THR:O | 2:UA:98:VAL:HG23 | 2.22 | 0.40 |
| 2:YA:94:THR:O | 2:YA:98:VAL:HG23 | 2.22 | 0.40 |
| 2:O1:60:TYR:CD2 | 2:O1:67:THR:CG2 | 3.04 | 0.40 |
| 3:J3:3:ASP:H | 3:J3:6:THR:HB | 1.85 | 0.40 |
| 2:K3:94:THR:O | 2:K3:98:VAL:HG23 | 2.22 | 0.40 |
| 6:M2:36:ILE:HG23 | 6:M2:43:TRP:HB3 | 2.03 | 0.40 |
| 2:A4:25:GLN:HG3 | 2:K4:33:ARG:HG2 | 1.99 | 0.40 |
| 2:A4:60:TYR:CZ | 2:A4:79:GLN:HG2 | 2.56 | 0.40 |
| 2:A4:90:LEU:O | 2:A4:94:THR:HG23 | 2.22 | 0.40 |
| 3:B4:82:CYS:CB | 12:B4:202:CYC:H2C | 2.50 | 0.40 |
| 12:B4:202:CYC:CMA | 12:B4:202:CYC:HB | 2.25 | 0.40 |
| 5:N3:13:SER:HB3 | 5:N3:14:LYS:H | 1.55 | 0.40 |
| 12:T3:301:CYC:HB | 12:T3:301:CYC:CMA | 2.25 | 0.40 |
| 2:K4:90:LEU:O | 2:K4:94:THR:HG23 | 2.21 | 0.40 |
| 4:M4:70:SER:O | 4:M4:70:SER:OG | 2.36 | 0.40 |
| 4:M4:101:ASP:OD1 | 2:P4:13:ASP:OD1 | 2.39 | 0.40 |
| 3:Y4:101:ASP:HB3 | 3:Y4:103:SER:OG | 2.21 | 0.40 |
| 3:Y4:102:ALA:O | 3:Y4:106:GLU:N | 2.55 | 0.40 |
| 8:A5:64:ASP:O | 8:A5:65:VAL:C | 2.61 | 0.40 |
| 1:B5:107:ARG:HD2 | 9:z5:21:ARG:HD3 | 2.03 | 0.40 |
| 1:D5:9:ILE:HD13 | 1:D5:9:ILE:HG21 | 1.66 | 0.40 |
| 1:D5:51:ILE:HG22 | 1:D5:133:MET:CE | 2.51 | 0.40 |
| 1:F5:51:ILE:HG22 | 1:F5:133:MET:CE | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 8:G5:119:LEU:CD1 | 12:G5:201:CYC:HAA2 | 2.52 | 0.40 |
| 8:I5:107:ILE:HG22 | 12:I5:201:CYC:HBB1 | 2.04 | 0.40 |
| 1:J5:76:ARG:HH12 | 9:i5:67:VAL:CG1 | 2.34 | 0.40 |
| 8:Q5:102:THR:N | 8:Q5:103:PRO:HD2 | 2.37 | 0.40 |
| 1:T5:89:LEU:HB2 | 1:T5:133:MET:HE1 | 2.03 | 0.40 |
| 12:V5:201:CYC:HMD1 | 12:V5:201:CYC:NC | 2.10 | 0.40 |
| 1:b5:65:LEU:HB3 | 1:b5:72:MET:HE3 | 2.03 | 0.40 |
| 2:K6:94:THR:O | 2:K6:98:VAL:HG23 | 2.22 | 0.40 |
| 7:N6:29:LEU:HD23 | 2:A6:112:GLY:HA2 | 2.03 | 0.40 |
| 10:j5:264:LEU:CD2 | 10:j5:264:LEU:O | 2.69 | 0.40 |
| 10:j5:301:TYR:CE1 | 10:j5:337:LEU:HD21 | 2.56 | 0.40 |
| 10:j5:349:GLN:CB | 10:j5:350:PRO:HD3 | 2.52 | 0.40 |
| 10:j5:512:ASN:HD22 | 10:j5:682:GLU:HG2 | 1.86 | 0.40 |
| 10:j5:699:SER:O | 10:j5:699:SER:OG | 2.38 | 0.40 |
| 10:j5:1067:LEU:HD22 | 10:j5:1067:LEU:HA | 1.70 | 0.40 |
| 10:j5:1144:SER:OG | 1:v7:74:THR:HG21 | 2.21 | 0.40 |
| 10:k5:221:LYS:NZ | 10:k5:221:LYS:CA | 2.85 | 0.40 |
| 10:k5:357:LEU:HG | 10:k5:382:ILE:HD11 | 2.03 | 0.40 |
| 10:k5:953:LEU:HD23 | 10:k5:953:LEU:HA | 1.60 | 0.40 |
| 10:k5:1008:PHE:CE1 | 1:p7:87:TYR:HH | 1.78 | 0.40 |
| 10:k5:1118:THR:OG1 | 12:k5:1204:CYC:CGA | 2.67 | 0.40 |
| 10:k5:1134:GLU:O | 10:k5:1134:GLU:CG | 2.69 | 0.40 |
| 1:P7:65:LEU:HB3 | 1:P7:72:MET:HE3 | 2.03 | 0.40 |
| 1:R7:87:TYR:CE2 | 9:z7:38:PHE:HE1 | 2.38 | 0.40 |
| 8:i7:47:ARG:NE | 1:j7:18:TYR:CG | 2.86 | 0.40 |
| 8:i7:152:TYR:CE2 | 8:s7:20:PRO:HB3 | 2.57 | 0.40 |
| 1:j7:51:ILE:HG22 | 1:j7:133:MET:CE | 2.51 | 0.40 |
| 1:j7:75:THR:O | 8:e7:111:GLY:HA3 | 2.22 | 0.40 |
| 1:j7:89:LEU:HB2 | 1:j7:133:MET:HE1 | 2.03 | 0.40 |
| 1:j7:119:LEU:HD21 | 9:y7:5:PHE:CZ | 2.57 | 0.40 |
| 1:V7:51:ILE:HG22 | 1:V7:133:MET:CE | 2.51 | 0.40 |
| 1:X7:51:ILE:HG22 | 1:X7:133:MET:CE | 2.51 | 0.40 |
| 12:b7:201:CYC:OB | 9:x7:23:LEU:N | 2.55 | 0.40 |
| 8:c7:92:VAL:HG22 | 8:c7:156:LEU:HG | 2.03 | 0.40 |
| 1:f7:89:LEU:HB2 | 1:f7:133:MET:HE1 | 2.02 | 0.40 |
| 2:C8:38:MET:HE2 | 2:C8:38:MET:HB3 | 1.81 | 0.40 |
| 8:m7:27:LYS:C | 8:m7:30:VAL:HG22 | 2.47 | 0.40 |
| 1:n7:51:ILE:HG22 | 1:n7:133:MET:CE | 2.51 | 0.40 |
| 8:o7:98:ALA:CB | 1:p7:9:ILE:HD11 | 2.38 | 0.40 |
| 8:s7:18:LEU:CD1 | 1:t7:94:TYR:CE1 | 3.04 | 0.40 |
| 8:u7:39:ILE:HD11 | 8:u7:145:ASP:CG | 2.46 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:u7:71:ASN:HB3 | 12:u7:201:CYC:OC | 2.22 | 0.40 |
| 9:x7:5:PHE:HD1 | 9:x7:55:LYS:O | 2.05 | 0.40 |
| 2:X8:69:PRO:CG | 2:S9:39:GLU:HA | 2.50 | 0.40 |
| 4:M8:87:ILE:HD12 | 3:Y8:77:ARG:CD | 2.51 | 0.40 |
| 4:M8:140:ARG:O | 4:M8:143:VAL:CB | 2.65 | 0.40 |
| 4:M8:141:GLU:HA | 4:M8:144:ARG:HB2 | 2.03 | 0.40 |
| 2:N8:90:LEU:O | 2:N8:94:THR:HG23 | 2.21 | 0.40 |
| 12:N8:201:CYC:NB | 3:Q8:76:ASN:OD1 | 2.54 | 0.40 |
| 4:M9:204:ILE:O | 4:M9:204:ILE:CG2 | 2.69 | 0.40 |
| 5:N9:26:LEU:CD2 | 5:N9:26:LEU:O | 2.70 | 0.40 |
| 5:N9:34:LEU:HD22 | 5:N9:34:LEU:HA | 1.71 | 0.40 |
| 5:N9:61:LYS:HD2 | 12:T9:301:CYC:HBB3 | 1.98 | 0.40 |
| 5:N9:72:GLU:CG | 3:T9:119:ALA:O | 2.58 | 0.40 |
| 3:Y8:89:ILE:CA | 3:Y8:92:TYR:CD2 | 2.68 | 0.40 |
| 2:K9:94:THR:O | 2:K9:98:VAL:HG23 | 2.22 | 0.40 |
| 2:W9:94:THR:O | 2:W9:98:VAL:HG23 | 2.22 | 0.40 |
| 2:Y9:94:THR:O | 2:Y9:98:VAL:HG23 | 2.22 | 0.40 |
| 2:G1:94:THR:O | 2:G1:98:VAL:HG23 | 2.22 | 0.40 |
| 2:G1:107:ASP:O | 3:L1:77:ARG:NE | 2.55 | 0.40 |
| 11:a9:31:SER:OG | 11:a9:34:ILE:CG2 | 2.68 | 0.40 |
| 11:a9:399:ILE:O | 11:a9:399:ILE:CG2 | 2.69 | 0.40 |
| 11:a9:556:LEU:HD22 | 11:a9:556:LEU:HA | 1.92 | 0.40 |
| 11:aA:95:ILE:HD13 | 11:aA:237:PHE:CD2 | 2.57 | 0.40 |
| 11:aA:352:PRO:HB2 | 11:aA:354:VAL:N | 2.36 | 0.40 |
| 11:aA:430:ARG:HH22 | 11:aA:491:ASP:HB2 | 1.86 | 0.40 |
| 2:K1:94:THR:O | 2:K1:98:VAL:HG23 | 2.22 | 0.40 |
| 4:M1:33:LEU:O | 4:M1:33:LEU:CD1 | 2.70 | 0.40 |
| 4:M1:274:VAL:HG22 | 3:Z1:77:ARG:HB2 | 2.04 | 0.40 |
| 5:N1:26:LEU:CD2 | 5:N1:26:LEU:O | 2.70 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1 | A | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | B5 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | B7 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | D5 | 158/161 (98%) | 145 (92%) | 9 (6%) | 4 (2%) | 4 | 17 |
| 1 | D7 | 158/161 (98%) | 149 (94%) | 6 (4%) | 3 (2%) | 6 | 23 |
| 1 | F5 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | F7 | 158/161 (98%) | 151 (96%) | 5 (3%) | 2 (1%) | 10 | 32 |
| 1 | H5 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | H7 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | J5 | 158/161 (98%) | 145 (92%) | 9 (6%) | 4 (2%) | 4 | 17 |
| 1 | J7 | 158/161 (98%) | 149 (94%) | 6 (4%) | 3 (2%) | 6 | 23 |
| 1 | L5 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | L7 | 158/161 (98%) | 151 (96%) | 5 (3%) | 2 (1%) | 10 | 32 |
| 1 | N5 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | N7 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | P5 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | P7 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | R5 | 158/161 (98%) | 151 (96%) | 5 (3%) | 2 (1%) | 10 | 32 |
| 1 | R7 | 158/161 (98%) | 151 (96%) | 5 (3%) | 2 (1%) | 10 | 32 |
| 1 | T5 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | T7 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | V5 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | V7 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | X5 | 158/161 (98%) | 151 (96%) | 5 (3%) | 2 (1%) | 10 | 32 |
| 1 | X7 | 158/161 (98%) | 151 (96%) | 5 (3%) | 2 (1%) | 10 | 32 |
| 1 | Z | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | Z5 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | Z7 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | b5 | 158/161 (98%) | 151 (96%) | 5 (3%) | 2 (1%) | 10 | 32 |
| 1 | b7 | 158/161 (98%) | 150 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 1 | d5 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | d7 | 158/161 (98%) | 151 (96%) | 5 (3%) | 2 (1%) | 10 | 32 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | f5 | 158/161 (98%) | 151 (96%) | 5 (3%) | 2 (1%) | 10 | 32 |
| 1 | f7 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | h7 | 158/161 (98%) | 150 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 1 | j7 | 158/161 (98%) | 151 (96%) | 5 (3%) | 2 (1%) | 10 | 32 |
| 1 | l7 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | n7 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | p7 | 158/161 (98%) | 151 (96%) | 5 (3%) | 2 (1%) | 10 | 32 |
| 1 | r7 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | t7 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 1 | v7 | 158/161 (98%) | 151 (96%) | 5 (3%) | 2 (1%) | 10 | 32 |
| 2 | A1 | 160/162 (99%) | 155 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | A2 | 160/162 (99%) | 155 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | A3 | 160/162 (99%) | 155 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | A4 | 160/162 (99%) | 155 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | A6 | 160/162 (99%) | 155 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | A8 | 160/162 (99%) | 155 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | A9 | 160/162 (99%) | 155 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | AA | 160/162 (99%) | 155 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | C1 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | C2 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | C3 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | C4 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | C6 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | C8 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | C9 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | CA | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | E1 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | E2 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | E3 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | E4 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | E6 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2 | E8 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | E9 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | EA | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | G1 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | G2 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | G3 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | G4 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | G6 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | G8 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | G9 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | GA | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | I1 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | I2 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | I3 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | I4 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | I6 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | I8 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | I9 | 160/162 (99%) | 153 (96%) | 6 (4%) | 1 (1%) | 22 | 51 |
| 2 | IA | 160/162 (99%) | 153 (96%) | 6 (4%) | 1 (1%) | 22 | 51 |
| 2 | K1 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | K2 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | K3 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | K4 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | K6 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | K8 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | K9 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | KA | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | N4 | 160/162 (99%) | 155 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | N8 | 160/162 (99%) | 154 (96%) | 5 (3%) | 1 (1%) | 22 | 51 |
| 2 | O1 | 160/162 (99%) | 155 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | O3 | 160/162 (99%) | 155 (97%) | 5 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2 | O9 | 160/162 (99%) | 155 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | OA | 160/162 (99%) | 155 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | P4 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | P8 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | Q1 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | Q3 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | Q9 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | QA | 160/162 (99%) | 156 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | R4 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | R8 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | S1 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | S3 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | S9 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | SA | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | T4 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | T8 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | U1 | 160/162 (99%) | 157 (98%) | 3 (2%) | 0 | 100 | 100 |
| 2 | U3 | 160/162 (99%) | 157 (98%) | 2 (1%) | 1 (1%) | 22 | 51 |
| 2 | U9 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | UA | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | V4 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | V8 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | W1 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | W3 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | W9 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | WA | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | X4 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | X8 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | Y1 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | Y3 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | Y9 | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2 | YA | 160/162 (99%) | 158 (99%) | 2 (1%) | 0 | 100 | 100 |
| 3 | B1 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | B2 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | B3 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | B4 | 170/172 (99%) | 159 (94%) | 9 (5%) | 2 (1%) | 11 | 34 |
| 3 | B6 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | B8 | 170/172 (99%) | 160 (94%) | 9 (5%) | 1 (1%) | 22 | 51 |
| 3 | B9 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | BA | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | D1 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | D2 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | D3 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | D4 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | D6 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | D8 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | D9 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | DA | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | F1 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | F2 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | F3 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | F4 | 170/172 (99%) | 158 (93%) | 7 (4%) | 5 (3%) | 3 | 13 |
| 3 | F6 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | F8 | 170/172 (99%) | 159 (94%) | 7 (4%) | 4 (2%) | 5 | 18 |
| 3 | F9 | 170/172 (99%) | 160 (94%) | 8 (5%) | 2 (1%) | 11 | 34 |
| 3 | FA | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | H1 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | H2 | 170/172 (99%) | 161 (95%) | 8 (5%) | 1 (1%) | 22 | 51 |
| 3 | H3 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | H4 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | H6 | 170/172 (99%) | 161 (95%) | 8 (5%) | 1 (1%) | 22 | 51 |
| 3 | H8 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 3 | H9 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | HA | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | J1 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | J2 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | J3 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | J4 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | J6 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | J8 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | J9 | 170/172 (99%) | 163 (96%) | 5 (3%) | 2 (1%) | 11 | 34 |
| 3 | JA | 170/172 (99%) | 163 (96%) | 5 (3%) | 2 (1%) | 11 | 34 |
| 3 | L1 | 170/172 (99%) | 161 (95%) | 7 (4%) | 2 (1%) | 11 | 34 |
| 3 | L2 | 170/172 (99%) | 163 (96%) | 6 (4%) | 1 (1%) | 22 | 51 |
| 3 | L3 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | L4 | 170/172 (99%) | 158 (93%) | 7 (4%) | 5 (3%) | 3 | 13 |
| 3 | L6 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | L8 | 170/172 (99%) | 159 (94%) | 7 (4%) | 4 (2%) | 5 | 18 |
| 3 | L9 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | LA | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | O4 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | O8 | 170/172 (99%) | 162 (95%) | 6 (4%) | 2 (1%) | 11 | 34 |
| 3 | P1 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | P3 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | P9 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | PA | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | Q4 | 170/172 (99%) | 156 (92%) | 11 (6%) | 3 (2%) | 7 | 24 |
| 3 | Q8 | 170/172 (99%) | 156 (92%) | 12 (7%) | 2 (1%) | 11 | 34 |
| 3 | R1 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | R3 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | R9 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | RA | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | S4 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 3 | S8 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | T1 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | T3 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | T9 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | TA | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | U4 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | U8 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | V1 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | V3 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | V9 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | VA | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | W4 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | W8 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | X1 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | X3 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | X9 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | XA | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | Y4 | 170/172 (99%) | 153 (90%) | 15 (9%) | 2 (1%) | 11 | 34 |
| 3 | Y8 | 170/172 (99%) | 155 (91%) | 14 (8%) | 1 (1%) | 22 | 51 |
| 3 | Z1 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | Z3 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | Z9 | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 3 | ZA | 170/172 (99%) | 162 (95%) | 7 (4%) | 1 (1%) | 22 | 51 |
| 4 | M1 | 272/274 (99%) | 253 (93%) | 10 (4%) | 9 (3%) | 3 | 11 |
| 4 | M3 | 272/274 (99%) | 253 (93%) | 10 (4%) | 9 (3%) | 3 | 11 |
| 4 | M4 | 272/274 (99%) | 251 (92%) | 10 (4%) | 11 (4%) | 2 | 8 |
| 4 | M8 | 272/274 (99%) | 245 (90%) | 11 (4%) | 16 (6%) | 1 | 4 |
| 4 | M9 | 272/274 (99%) | 253 (93%) | 10 (4%) | 9 (3%) | 3 | 11 |
| 4 | MA | 272/274 (99%) | 253 (93%) | 10 (4%) | 9 (3%) | 3 | 11 |
| 5 | N1 | 72/275 (26%) | 65 (90%) | 5 (7%) | 2 (3%) | 4 | 14 |
| 5 | N3 | 72/275 (26%) | 65 (90%) | 5 (7%) | 2 (3%) | 4 | 14 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 5 | N9 | 72/275 (26%) | 65 (90%) | 5 (7%) | 2 (3%) | 4 | 14 |
| 5 | NA | 72/275 (26%) | 65 (90%) | 5 (7%) | 2 (3%) | 4 | 14 |
| 5 | Z4 | 72/275 (26%) | 59 (82%) | 7 (10%) | 6 (8%) | 0 | 1 |
| 5 | Z8 | 72/275 (26%) | 65 (90%) | 5 (7%) | 2 (3%) | 4 | 14 |
| 6 | M2 | 277/729 (38%) | 246 (89%) | 30 (11%) | 1 (0%) | 30 | 61 |
| 6 | M6 | 277/729 (38%) | 246 (89%) | 30 (11%) | 1 (0%) | 30 | 61 |
| 7 | N2 | 68/70 (97%) | 54 (79%) | 13 (19%) | 1 (2%) | 8 | 29 |
| 7 | N6 | 68/70 (97%) | 54 (79%) | 13 (19%) | 1 (2%) | 8 | 29 |
| 8 | A5 | 158/161 (98%) | 154 (98%) | 3 (2%) | 1 (1%) | 22 | 51 |
| 8 | A7 | 158/161 (98%) | 154 (98%) | 3 (2%) | 1 (1%) | 22 | 51 |
| 8 | C5 | 158/161 (98%) | 145 (92%) | 9 (6%) | 4 (2%) | 4 | 17 |
| 8 | C7 | 158/161 (98%) | 154 (98%) | 2 (1%) | 2 (1%) | 10 | 32 |
| 8 | E5 | 158/161 (98%) | 152 (96%) | 3 (2%) | 3 (2%) | 6 | 23 |
| 8 | E7 | 158/161 (98%) | 151 (96%) | 5 (3%) | 2 (1%) | 10 | 32 |
| 8 | G5 | 158/161 (98%) | 154 (98%) | 3 (2%) | 1 (1%) | 22 | 51 |
| 8 | G7 | 158/161 (98%) | 154 (98%) | 3 (2%) | 1 (1%) | 22 | 51 |
| 8 | I5 | 158/161 (98%) | 145 (92%) | 9 (6%) | 4 (2%) | 4 | 17 |
| 8 | I7 | 158/161 (98%) | 154 (98%) | 2 (1%) | 2 (1%) | 10 | 32 |
| 8 | K5 | 158/161 (98%) | 152 (96%) | 3 (2%) | 3 (2%) | 6 | 23 |
| 8 | K7 | 158/161 (98%) | 151 (96%) | 5 (3%) | 2 (1%) | 10 | 32 |
| 8 | M5 | 158/161 (98%) | 154 (98%) | 3 (2%) | 1 (1%) | 22 | 51 |
| 8 | M7 | 158/161 (98%) | 154 (98%) | 3 (2%) | 1 (1%) | 22 | 51 |
| 8 | O5 | 158/161 (98%) | 148 (94%) | 6 (4%) | 4 (2%) | 4 | 17 |
| 8 | O7 | 158/161 (98%) | 151 (96%) | 2 (1%) | 5 (3%) | 3 | 12 |
| 8 | Q5 | 158/161 (98%) | 150 (95%) | 5 (3%) | 3 (2%) | 6 | 23 |
| 8 | Q7 | 158/161 (98%) | 151 (96%) | 5 (3%) | 2 (1%) | 10 | 32 |
| 8 | S5 | 158/161 (98%) | 154 (98%) | 3 (2%) | 1 (1%) | 22 | 51 |
| 8 | S7 | 158/161 (98%) | 154 (98%) | 3 (2%) | 1 (1%) | 22 | 51 |
| 8 | U5 | 158/161 (98%) | 151 (96%) | 3 (2%) | 4 (2%) | 4 | 17 |
| 8 | U7 | 158/161 (98%) | 151 (96%) | 3 (2%) | 4 (2%) | 4 | 17 |
| 8 | W5 | 158/161 (98%) | 150 (95%) | 5 (3%) | 3 (2%) | 6 | 23 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|----------|-------------|----|
| 8 | W7 | 158/161 (98%) | 151 (96%) | 5 (3%) | 2 (1%) | 10 | 32 |
| 8 | Y5 | 158/161 (98%) | 154 (98%) | 3 (2%) | 1 (1%) | 22 | 51 |
| 8 | Y7 | 158/161 (98%) | 154 (98%) | 3 (2%) | 1 (1%) | 22 | 51 |
| 8 | a5 | 158/161 (98%) | 149 (94%) | 5 (3%) | 4 (2%) | 4 | 17 |
| 8 | a7 | 158/161 (98%) | 152 (96%) | 4 (2%) | 2 (1%) | 10 | 32 |
| 8 | c5 | 158/161 (98%) | 154 (98%) | 3 (2%) | 1 (1%) | 22 | 51 |
| 8 | c7 | 158/161 (98%) | 149 (94%) | 7 (4%) | 2 (1%) | 10 | 32 |
| 8 | e5 | 158/161 (98%) | 149 (94%) | 5 (3%) | 4 (2%) | 4 | 17 |
| 8 | e7 | 158/161 (98%) | 154 (98%) | 3 (2%) | 1 (1%) | 22 | 51 |
| 8 | g7 | 158/161 (98%) | 152 (96%) | 4 (2%) | 2 (1%) | 10 | 32 |
| 8 | i7 | 158/161 (98%) | 149 (94%) | 7 (4%) | 2 (1%) | 10 | 32 |
| 8 | k7 | 158/161 (98%) | 154 (98%) | 3 (2%) | 1 (1%) | 22 | 51 |
| 8 | m7 | 158/161 (98%) | 150 (95%) | 4 (2%) | 4 (2%) | 4 | 17 |
| 8 | o7 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 8 | q7 | 158/161 (98%) | 154 (98%) | 3 (2%) | 1 (1%) | 22 | 51 |
| 8 | s7 | 158/161 (98%) | 152 (96%) | 3 (2%) | 3 (2%) | 6 | 23 |
| 8 | u7 | 158/161 (98%) | 150 (95%) | 6 (4%) | 2 (1%) | 10 | 32 |
| 9 | i5 | 66/68 (97%) | 61 (92%) | 3 (4%) | 2 (3%) | 3 | 13 |
| 9 | w7 | 66/68 (97%) | 55 (83%) | 8 (12%) | 3 (4%) | 2 | 7 |
| 9 | x7 | 66/68 (97%) | 53 (80%) | 11 (17%) | 2 (3%) | 3 | 13 |
| 9 | y7 | 66/68 (97%) | 53 (80%) | 11 (17%) | 2 (3%) | 3 | 13 |
| 9 | z5 | 66/68 (97%) | 61 (92%) | 3 (4%) | 2 (3%) | 3 | 13 |
| 9 | z7 | 66/68 (97%) | 55 (83%) | 8 (12%) | 3 (4%) | 2 | 7 |
| 10 | j5 | 1104/1155 (96%) | 967 (88%) | 88 (8%) | 49 (4%) | 2 | 7 |
| 10 | k5 | 1104/1155 (96%) | 966 (88%) | 88 (8%) | 50 (4%) | 2 | 7 |
| 11 | a9 | 796/824 (97%) | 691 (87%) | 70 (9%) | 35 (4%) | 2 | 7 |
| 11 | aA | 796/824 (97%) | 688 (86%) | 70 (9%) | 38 (5%) | 2 | 6 |
| All | All | 47626/50516 (94%) | 45281 (95%) | 1786 (4%) | 559 (1%) | 14 | 34 |

All (559) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | FA | 145 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | JA | 21 | GLU |
| 4 | MA | 2 | ASN |
| 4 | MA | 78 | GLY |
| 4 | MA | 79 | PRO |
| 4 | MA | 99 | VAL |
| 4 | MA | 250 | THR |
| 4 | M3 | 2 | ASN |
| 4 | M3 | 78 | GLY |
| 4 | M3 | 79 | PRO |
| 4 | M3 | 99 | VAL |
| 4 | M3 | 250 | THR |
| 3 | F4 | 111 | ASN |
| 3 | L4 | 66 | LEU |
| 3 | L4 | 69 | PRO |
| 4 | M4 | 2 | ASN |
| 4 | M4 | 78 | GLY |
| 4 | M4 | 79 | PRO |
| 4 | M4 | 136 | SER |
| 4 | M4 | 250 | THR |
| 8 | K5 | 64 | ASP |
| 8 | O5 | 25 | ARG |
| 8 | O5 | 102 | THR |
| 3 | Y4 | 109 | CYS |
| 5 | Z4 | 28 | HIS |
| 8 | C5 | 28 | SER |
| 8 | C5 | 102 | THR |
| 1 | D5 | 21 | GLY |
| 8 | E5 | 64 | ASP |
| 8 | I5 | 28 | SER |
| 8 | I5 | 102 | THR |
| 1 | J5 | 21 | GLY |
| 8 | e5 | 102 | THR |
| 8 | Q5 | 64 | ASP |
| 8 | U5 | 102 | THR |
| 8 | W5 | 64 | ASP |
| 8 | a5 | 102 | THR |
| 10 | j5 | 20 | VAL |
| 10 | j5 | 50 | GLY |
| 10 | j5 | 236 | ALA |
| 10 | j5 | 267 | ASP |
| 10 | j5 | 277 | ILE |
| 10 | j5 | 286 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 10 | j5 | 387 | VAL |
| 10 | j5 | 392 | SER |
| 10 | j5 | 394 | PRO |
| 10 | j5 | 543 | ASN |
| 10 | j5 | 549 | LYS |
| 10 | j5 | 559 | THR |
| 10 | j5 | 736 | GLU |
| 10 | j5 | 744 | PRO |
| 10 | j5 | 880 | THR |
| 10 | j5 | 973 | THR |
| 10 | j5 | 984 | ILE |
| 10 | j5 | 1011 | ILE |
| 10 | j5 | 1016 | LEU |
| 10 | j5 | 1052 | PRO |
| 10 | j5 | 1055 | SER |
| 10 | j5 | 1056 | PRO |
| 10 | k5 | 20 | VAL |
| 10 | k5 | 50 | GLY |
| 10 | k5 | 236 | ALA |
| 10 | k5 | 267 | ASP |
| 10 | k5 | 277 | ILE |
| 10 | k5 | 286 | VAL |
| 10 | k5 | 387 | VAL |
| 10 | k5 | 392 | SER |
| 10 | k5 | 394 | PRO |
| 10 | k5 | 543 | ASN |
| 10 | k5 | 549 | LYS |
| 10 | k5 | 736 | GLU |
| 10 | k5 | 744 | PRO |
| 10 | k5 | 880 | THR |
| 10 | k5 | 973 | THR |
| 10 | k5 | 984 | ILE |
| 10 | k5 | 1011 | ILE |
| 10 | k5 | 1016 | LEU |
| 10 | k5 | 1052 | PRO |
| 10 | k5 | 1055 | SER |
| 10 | k5 | 1056 | PRO |
| 8 | O7 | 20 | PRO |
| 8 | O7 | 22 | GLU |
| 8 | O7 | 102 | THR |
| 8 | Q7 | 64 | ASP |
| 8 | C7 | 102 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D7 | 68 | PRO |
| 8 | E7 | 64 | ASP |
| 8 | I7 | 102 | THR |
| 1 | J7 | 68 | PRO |
| 8 | K7 | 64 | ASP |
| 8 | g7 | 102 | THR |
| 8 | i7 | 64 | ASP |
| 8 | U7 | 102 | THR |
| 8 | W7 | 64 | ASP |
| 8 | a7 | 102 | THR |
| 8 | c7 | 64 | ASP |
| 8 | m7 | 102 | THR |
| 8 | o7 | 64 | ASP |
| 8 | s7 | 20 | PRO |
| 8 | s7 | 102 | THR |
| 8 | u7 | 64 | ASP |
| 9 | z7 | 22 | GLU |
| 9 | z7 | 37 | TRP |
| 9 | w7 | 22 | GLU |
| 9 | w7 | 37 | TRP |
| 9 | x7 | 63 | ALA |
| 9 | y7 | 63 | ALA |
| 3 | F8 | 110 | LEU |
| 3 | L8 | 69 | PRO |
| 4 | M8 | 2 | ASN |
| 4 | M8 | 78 | GLY |
| 4 | M8 | 79 | PRO |
| 4 | M8 | 97 | ALA |
| 4 | M8 | 99 | VAL |
| 4 | M8 | 136 | SER |
| 4 | M8 | 211 | GLN |
| 4 | M8 | 226 | SER |
| 4 | M8 | 231 | THR |
| 4 | M8 | 250 | THR |
| 2 | N8 | 111 | ALA |
| 3 | Q8 | 109 | CYS |
| 4 | M9 | 2 | ASN |
| 4 | M9 | 78 | GLY |
| 4 | M9 | 79 | PRO |
| 4 | M9 | 99 | VAL |
| 4 | M9 | 250 | THR |
| 3 | F9 | 145 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | J9 | 21 | GLU |
| 11 | a9 | 62 | MET |
| 11 | a9 | 71 | ILE |
| 11 | a9 | 84 | THR |
| 11 | a9 | 86 | ASP |
| 11 | a9 | 90 | GLN |
| 11 | a9 | 93 | LEU |
| 11 | a9 | 99 | ALA |
| 11 | a9 | 352 | PRO |
| 11 | a9 | 358 | PRO |
| 11 | a9 | 589 | THR |
| 11 | a9 | 590 | PRO |
| 11 | a9 | 598 | SER |
| 11 | a9 | 599 | PRO |
| 11 | a9 | 604 | ALA |
| 11 | a9 | 608 | PRO |
| 11 | a9 | 619 | ARG |
| 11 | a9 | 821 | ARG |
| 11 | aA | 62 | MET |
| 11 | aA | 71 | ILE |
| 11 | aA | 84 | THR |
| 11 | aA | 86 | ASP |
| 11 | aA | 90 | GLN |
| 11 | aA | 93 | LEU |
| 11 | aA | 99 | ALA |
| 11 | aA | 291 | TYR |
| 11 | aA | 352 | PRO |
| 11 | aA | 358 | PRO |
| 11 | aA | 556 | LEU |
| 11 | aA | 589 | THR |
| 11 | aA | 590 | PRO |
| 11 | aA | 598 | SER |
| 11 | aA | 599 | PRO |
| 11 | aA | 604 | ALA |
| 11 | aA | 608 | PRO |
| 11 | aA | 619 | ARG |
| 11 | aA | 821 | ARG |
| 3 | L1 | 78 | ARG |
| 4 | M1 | 2 | ASN |
| 4 | M1 | 78 | GLY |
| 4 | M1 | 79 | PRO |
| 4 | M1 | 99 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 4 | M1 | 250 | THR |
| 2 | IA | 19 | LEU |
| 4 | MA | 34 | ASP |
| 6 | M2 | 260 | THR |
| 7 | N2 | 4 | ASN |
| 3 | B4 | 113 | LEU |
| 4 | M3 | 34 | ASP |
| 2 | U3 | 47 | ASN |
| 3 | F4 | 112 | GLY |
| 3 | L4 | 70 | GLY |
| 3 | L4 | 71 | GLY |
| 4 | M4 | 34 | ASP |
| 3 | Q4 | 97 | LEU |
| 3 | Q4 | 117 | TYR |
| 5 | Z4 | 27 | ALA |
| 5 | Z4 | 39 | PRO |
| 5 | Z4 | 40 | SER |
| 8 | C5 | 25 | ARG |
| 8 | I5 | 25 | ARG |
| 8 | Q5 | 160 | MET |
| 8 | W5 | 160 | MET |
| 6 | M6 | 260 | THR |
| 7 | N6 | 4 | ASN |
| 10 | j5 | 269 | LEU |
| 10 | j5 | 386 | ILE |
| 10 | j5 | 487 | PHE |
| 10 | j5 | 588 | VAL |
| 10 | j5 | 636 | GLY |
| 10 | j5 | 702 | VAL |
| 10 | j5 | 920 | ARG |
| 10 | j5 | 1138 | GLN |
| 10 | k5 | 269 | LEU |
| 10 | k5 | 386 | ILE |
| 10 | k5 | 487 | PHE |
| 10 | k5 | 588 | VAL |
| 10 | k5 | 636 | GLY |
| 10 | k5 | 702 | VAL |
| 10 | k5 | 920 | ARG |
| 10 | k5 | 1138 | GLN |
| 8 | O7 | 21 | GLY |
| 3 | F8 | 113 | LEU |
| 3 | L8 | 70 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | L8 | 71 | GLY |
| 4 | M8 | 34 | ASP |
| 4 | M9 | 24 | ALA |
| 4 | M9 | 34 | ASP |
| 2 | I9 | 19 | LEU |
| 11 | a9 | 267 | GLN |
| 11 | a9 | 291 | TYR |
| 11 | a9 | 354 | VAL |
| 11 | a9 | 355 | GLU |
| 11 | a9 | 600 | THR |
| 11 | a9 | 603 | THR |
| 11 | a9 | 645 | PRO |
| 11 | aA | 267 | GLN |
| 11 | aA | 354 | VAL |
| 11 | aA | 355 | GLU |
| 11 | aA | 600 | THR |
| 11 | aA | 603 | THR |
| 11 | aA | 645 | PRO |
| 4 | M1 | 34 | ASP |
| 4 | MA | 24 | ALA |
| 4 | MA | 26 | SER |
| 5 | NA | 2 | SER |
| 4 | M3 | 24 | ALA |
| 4 | M3 | 26 | SER |
| 5 | N3 | 2 | SER |
| 3 | F4 | 110 | LEU |
| 4 | M4 | 7 | SER |
| 4 | M4 | 24 | ALA |
| 4 | M4 | 26 | SER |
| 8 | O5 | 77 | MET |
| 5 | Z4 | 2 | SER |
| 1 | D5 | 40 | ALA |
| 1 | J5 | 40 | ALA |
| 8 | e5 | 12 | ASP |
| 8 | U5 | 77 | MET |
| 8 | a5 | 12 | ASP |
| 9 | z5 | 12 | PRO |
| 9 | i5 | 12 | PRO |
| 10 | j5 | 218 | ALA |
| 10 | j5 | 548 | SER |
| 10 | j5 | 562 | GLY |
| 10 | j5 | 1054 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 10 | j5 | 1121 | ALA |
| 10 | j5 | 1133 | GLU |
| 10 | k5 | 218 | ALA |
| 10 | k5 | 548 | SER |
| 10 | k5 | 562 | GLY |
| 10 | k5 | 1054 | SER |
| 10 | k5 | 1133 | GLU |
| 8 | U7 | 23 | LEU |
| 9 | x7 | 12 | PRO |
| 9 | y7 | 12 | PRO |
| 3 | F8 | 111 | ASN |
| 4 | M8 | 7 | SER |
| 4 | M8 | 24 | ALA |
| 4 | M8 | 26 | SER |
| 4 | M8 | 98 | ASP |
| 4 | M9 | 26 | SER |
| 5 | N9 | 2 | SER |
| 5 | Z8 | 2 | SER |
| 11 | a9 | 83 | ALA |
| 11 | aA | 83 | ALA |
| 11 | aA | 305 | ALA |
| 4 | M1 | 24 | ALA |
| 4 | M1 | 26 | SER |
| 5 | N1 | 2 | SER |
| 4 | MA | 259 | ARG |
| 4 | M3 | 259 | ARG |
| 3 | F4 | 113 | LEU |
| 4 | M4 | 259 | ARG |
| 8 | U5 | 20 | PRO |
| 10 | j5 | 490 | SER |
| 10 | j5 | 530 | ALA |
| 10 | j5 | 544 | VAL |
| 10 | j5 | 1077 | ILE |
| 10 | k5 | 490 | SER |
| 10 | k5 | 530 | ALA |
| 10 | k5 | 544 | VAL |
| 10 | k5 | 1077 | ILE |
| 10 | k5 | 1121 | ALA |
| 8 | m7 | 20 | PRO |
| 8 | m7 | 22 | GLU |
| 9 | z7 | 57 | PHE |
| 9 | w7 | 57 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | M8 | 259 | ARG |
| 3 | O8 | 109 | CYS |
| 4 | M9 | 259 | ARG |
| 11 | a9 | 26 | PRO |
| 11 | a9 | 38 | VAL |
| 11 | a9 | 280 | ASP |
| 11 | a9 | 284 | PRO |
| 11 | aA | 38 | VAL |
| 11 | aA | 65 | LEU |
| 11 | aA | 280 | ASP |
| 11 | aA | 284 | PRO |
| 11 | aA | 295 | ARG |
| 4 | M1 | 259 | ARG |
| 1 | A | 48 | ALA |
| 1 | A | 74 | THR |
| 1 | Z | 48 | ALA |
| 1 | Z | 74 | THR |
| 3 | BA | 145 | PRO |
| 3 | DA | 145 | PRO |
| 3 | HA | 145 | PRO |
| 3 | JA | 145 | PRO |
| 3 | LA | 145 | PRO |
| 3 | PA | 145 | PRO |
| 3 | RA | 145 | PRO |
| 3 | TA | 145 | PRO |
| 3 | VA | 145 | PRO |
| 3 | XA | 145 | PRO |
| 3 | ZA | 145 | PRO |
| 3 | P1 | 145 | PRO |
| 3 | R1 | 145 | PRO |
| 3 | H3 | 145 | PRO |
| 3 | J3 | 145 | PRO |
| 3 | H2 | 145 | PRO |
| 3 | J2 | 145 | PRO |
| 3 | L2 | 145 | PRO |
| 3 | B3 | 145 | PRO |
| 3 | D3 | 145 | PRO |
| 3 | F3 | 145 | PRO |
| 3 | Z3 | 145 | PRO |
| 3 | B4 | 145 | PRO |
| 3 | D4 | 145 | PRO |
| 3 | L3 | 145 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | P3 | 145 | PRO |
| 3 | R3 | 145 | PRO |
| 3 | T3 | 145 | PRO |
| 3 | V3 | 145 | PRO |
| 3 | X3 | 145 | PRO |
| 3 | B1 | 145 | PRO |
| 3 | S4 | 145 | PRO |
| 3 | U4 | 145 | PRO |
| 3 | W4 | 145 | PRO |
| 3 | F4 | 145 | PRO |
| 3 | H4 | 145 | PRO |
| 3 | J4 | 145 | PRO |
| 3 | L4 | 145 | PRO |
| 3 | O4 | 145 | PRO |
| 3 | Q4 | 145 | PRO |
| 1 | L5 | 48 | ALA |
| 1 | L5 | 74 | THR |
| 1 | N5 | 48 | ALA |
| 1 | N5 | 74 | THR |
| 3 | Y4 | 145 | PRO |
| 5 | Z4 | 37 | HIS |
| 1 | B5 | 48 | ALA |
| 1 | B5 | 74 | THR |
| 1 | D5 | 48 | ALA |
| 1 | D5 | 74 | THR |
| 1 | F5 | 48 | ALA |
| 1 | F5 | 74 | THR |
| 1 | H5 | 48 | ALA |
| 1 | H5 | 74 | THR |
| 1 | J5 | 48 | ALA |
| 1 | J5 | 74 | THR |
| 1 | d5 | 48 | ALA |
| 1 | d5 | 74 | THR |
| 8 | e5 | 26 | ILE |
| 1 | f5 | 48 | ALA |
| 1 | f5 | 74 | THR |
| 1 | P5 | 48 | ALA |
| 1 | P5 | 74 | THR |
| 1 | R5 | 48 | ALA |
| 1 | R5 | 74 | THR |
| 1 | T5 | 48 | ALA |
| 1 | T5 | 74 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | V5 | 48 | ALA |
| 1 | V5 | 74 | THR |
| 1 | X5 | 48 | ALA |
| 1 | X5 | 74 | THR |
| 1 | Z5 | 48 | ALA |
| 1 | Z5 | 74 | THR |
| 1 | b5 | 48 | ALA |
| 1 | b5 | 74 | THR |
| 3 | J6 | 145 | PRO |
| 3 | L6 | 145 | PRO |
| 9 | z5 | 17 | VAL |
| 9 | i5 | 17 | VAL |
| 10 | j5 | 3 | ILE |
| 10 | j5 | 34 | TYR |
| 10 | j5 | 729 | ILE |
| 10 | j5 | 760 | ASP |
| 10 | k5 | 3 | ILE |
| 10 | k5 | 34 | TYR |
| 10 | k5 | 729 | ILE |
| 10 | k5 | 760 | ASP |
| 10 | k5 | 1107 | ASN |
| 3 | B6 | 145 | PRO |
| 3 | D6 | 145 | PRO |
| 3 | F6 | 145 | PRO |
| 3 | H6 | 145 | PRO |
| 3 | D1 | 145 | PRO |
| 1 | P7 | 48 | ALA |
| 1 | P7 | 74 | THR |
| 1 | R7 | 48 | ALA |
| 1 | R7 | 74 | THR |
| 1 | B7 | 48 | ALA |
| 1 | B7 | 74 | THR |
| 1 | D7 | 48 | ALA |
| 1 | D7 | 74 | THR |
| 1 | F7 | 48 | ALA |
| 1 | F7 | 74 | THR |
| 1 | H7 | 48 | ALA |
| 1 | H7 | 74 | THR |
| 1 | J7 | 48 | ALA |
| 1 | J7 | 74 | THR |
| 1 | L7 | 48 | ALA |
| 1 | L7 | 74 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N7 | 48 | ALA |
| 1 | N7 | 74 | THR |
| 1 | h7 | 74 | THR |
| 1 | j7 | 48 | ALA |
| 1 | j7 | 74 | THR |
| 1 | T7 | 48 | ALA |
| 1 | T7 | 74 | THR |
| 1 | V7 | 48 | ALA |
| 1 | V7 | 74 | THR |
| 1 | X7 | 48 | ALA |
| 1 | X7 | 74 | THR |
| 1 | Z7 | 48 | ALA |
| 1 | Z7 | 74 | THR |
| 1 | b7 | 74 | THR |
| 1 | d7 | 48 | ALA |
| 1 | d7 | 74 | THR |
| 1 | f7 | 48 | ALA |
| 1 | f7 | 74 | THR |
| 3 | B8 | 145 | PRO |
| 3 | D8 | 145 | PRO |
| 1 | l7 | 48 | ALA |
| 1 | l7 | 74 | THR |
| 1 | n7 | 48 | ALA |
| 1 | n7 | 74 | THR |
| 1 | p7 | 48 | ALA |
| 1 | p7 | 74 | THR |
| 1 | r7 | 48 | ALA |
| 1 | r7 | 74 | THR |
| 1 | t7 | 48 | ALA |
| 1 | t7 | 74 | THR |
| 1 | v7 | 48 | ALA |
| 1 | v7 | 74 | THR |
| 3 | U8 | 145 | PRO |
| 3 | W8 | 145 | PRO |
| 3 | F8 | 145 | PRO |
| 3 | H8 | 145 | PRO |
| 3 | J8 | 145 | PRO |
| 3 | L8 | 145 | PRO |
| 3 | O8 | 145 | PRO |
| 3 | Q8 | 145 | PRO |
| 3 | S8 | 145 | PRO |
| 3 | F1 | 145 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | L9 | 145 | PRO |
| 3 | P9 | 145 | PRO |
| 3 | Y8 | 145 | PRO |
| 3 | B9 | 145 | PRO |
| 3 | D9 | 145 | PRO |
| 3 | F9 | 149 | THR |
| 3 | H9 | 145 | PRO |
| 3 | J9 | 145 | PRO |
| 3 | R9 | 145 | PRO |
| 3 | T9 | 145 | PRO |
| 3 | V9 | 145 | PRO |
| 3 | X9 | 145 | PRO |
| 3 | Z9 | 145 | PRO |
| 11 | a9 | 65 | LEU |
| 11 | a9 | 336 | ILE |
| 11 | a9 | 342 | ARG |
| 11 | aA | 26 | PRO |
| 11 | aA | 336 | ILE |
| 11 | aA | 342 | ARG |
| 3 | H1 | 145 | PRO |
| 3 | J1 | 145 | PRO |
| 3 | L1 | 145 | PRO |
| 3 | T1 | 145 | PRO |
| 3 | V1 | 145 | PRO |
| 3 | X1 | 145 | PRO |
| 3 | Z1 | 145 | PRO |
| 3 | B2 | 145 | PRO |
| 3 | D2 | 145 | PRO |
| 3 | F2 | 145 | PRO |
| 4 | M4 | 99 | VAL |
| 10 | j5 | 276 | ALA |
| 10 | j5 | 413 | SER |
| 10 | j5 | 912 | VAL |
| 10 | j5 | 1013 | PRO |
| 10 | k5 | 276 | ALA |
| 10 | k5 | 413 | SER |
| 10 | k5 | 912 | VAL |
| 10 | k5 | 1013 | PRO |
| 8 | U7 | 20 | PRO |
| 11 | a9 | 256 | SER |
| 11 | aA | 256 | SER |
| 8 | a5 | 26 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | k5 | 558 | VAL |
| 5 | NA | 23 | SER |
| 5 | N3 | 23 | SER |
| 8 | K5 | 68 | PRO |
| 8 | M5 | 68 | PRO |
| 8 | O5 | 68 | PRO |
| 8 | A5 | 68 | PRO |
| 8 | C5 | 68 | PRO |
| 8 | E5 | 68 | PRO |
| 8 | G5 | 68 | PRO |
| 8 | I5 | 68 | PRO |
| 8 | e5 | 68 | PRO |
| 8 | Q5 | 68 | PRO |
| 8 | U5 | 68 | PRO |
| 8 | W5 | 68 | PRO |
| 8 | Y5 | 68 | PRO |
| 8 | a5 | 68 | PRO |
| 8 | A7 | 68 | PRO |
| 10 | j5 | 705 | THR |
| 10 | k5 | 705 | THR |
| 8 | O7 | 68 | PRO |
| 8 | Q7 | 68 | PRO |
| 8 | S7 | 68 | PRO |
| 8 | C7 | 68 | PRO |
| 8 | E7 | 68 | PRO |
| 8 | I7 | 68 | PRO |
| 8 | K7 | 68 | PRO |
| 8 | M7 | 68 | PRO |
| 8 | g7 | 68 | PRO |
| 8 | i7 | 68 | PRO |
| 8 | U7 | 68 | PRO |
| 8 | W7 | 68 | PRO |
| 8 | Y7 | 68 | PRO |
| 8 | a7 | 68 | PRO |
| 8 | c7 | 68 | PRO |
| 8 | e7 | 68 | PRO |
| 8 | m7 | 68 | PRO |
| 8 | s7 | 68 | PRO |
| 5 | N9 | 23 | SER |
| 5 | N1 | 23 | SER |
| 8 | K5 | 108 | GLY |
| 8 | E5 | 108 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | c5 | 68 | PRO |
| 8 | S5 | 68 | PRO |
| 8 | G7 | 68 | PRO |
| 8 | k7 | 68 | PRO |
| 8 | o7 | 68 | PRO |
| 8 | q7 | 68 | PRO |
| 8 | u7 | 68 | PRO |
| 5 | Z8 | 23 | SER |
| 11 | a9 | 301 | GLY |
| 11 | a9 | 543 | GLN |
| 11 | aA | 543 | GLN |
| 11 | aA | 296 | VAL |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | A | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | B5 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | B7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | D5 | 121/121 (100%) | 114 (94%) | 7 (6%) | 17 | 45 |
| 1 | D7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | F5 | 121/121 (100%) | 118 (98%) | 3 (2%) | 42 | 75 |
| 1 | F7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | H5 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | H7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | J5 | 121/121 (100%) | 114 (94%) | 7 (6%) | 17 | 45 |
| 1 | J7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | L5 | 121/121 (100%) | 118 (98%) | 3 (2%) | 42 | 75 |
| 1 | L7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | N5 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | N7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | P5 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | P7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | R5 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | R7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | T5 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | T7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | V5 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | V7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | X5 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | X7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | Z | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | Z5 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | Z7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | b5 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | b7 | 121/121 (100%) | 114 (94%) | 7 (6%) | 17 | 45 |
| 1 | d5 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | d7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | f5 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | f7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | h7 | 121/121 (100%) | 114 (94%) | 7 (6%) | 17 | 45 |
| 1 | j7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | l7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | n7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | p7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | r7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | t7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 1 | v7 | 121/121 (100%) | 119 (98%) | 2 (2%) | 56 | 84 |
| 2 | A1 | 130/130 (100%) | 125 (96%) | 5 (4%) | 28 | 62 |
| 2 | A2 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | A3 | 130/130 (100%) | 123 (95%) | 7 (5%) | 18 | 48 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | A4 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | A6 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | A8 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | A9 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | AA | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | C1 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | C2 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | C3 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | C4 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | C6 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | C8 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | C9 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | CA | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | E1 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | E2 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | E3 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | E4 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | E6 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | E8 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | E9 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | EA | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | G1 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | G2 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | G3 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | G4 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | G6 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | G8 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | G9 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | GA | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | I1 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | I2 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | I3 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | I4 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | I6 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | I8 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | I9 | 130/130 (100%) | 125 (96%) | 5 (4%) | 28 | 62 |
| 2 | IA | 130/130 (100%) | 125 (96%) | 5 (4%) | 28 | 62 |
| 2 | K1 | 130/130 (100%) | 125 (96%) | 5 (4%) | 28 | 62 |
| 2 | K2 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | K3 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | K4 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | K6 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | K8 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | K9 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | KA | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | N4 | 130/130 (100%) | 125 (96%) | 5 (4%) | 28 | 62 |
| 2 | N8 | 130/130 (100%) | 125 (96%) | 5 (4%) | 28 | 62 |
| 2 | O1 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | O3 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | O9 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | OA | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | P4 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | P8 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | Q1 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | Q3 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | Q9 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | QA | 130/130 (100%) | 123 (95%) | 7 (5%) | 18 | 48 |
| 2 | R4 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | R8 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | S1 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | S3 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | S9 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | SA | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | T4 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | T8 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | U1 | 130/130 (100%) | 122 (94%) | 8 (6%) | 15 | 43 |
| 2 | U3 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | U9 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | UA | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | V4 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | V8 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | W1 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | W3 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | W9 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | WA | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | X4 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | X8 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | Y1 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | Y3 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | Y9 | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 2 | YA | 130/130 (100%) | 124 (95%) | 6 (5%) | 23 | 55 |
| 3 | B1 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | B2 | 134/134 (100%) | 130 (97%) | 4 (3%) | 36 | 70 |
| 3 | B3 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | B4 | 134/134 (100%) | 128 (96%) | 6 (4%) | 23 | 55 |
| 3 | B6 | 134/134 (100%) | 130 (97%) | 4 (3%) | 36 | 70 |
| 3 | B8 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | B9 | 134/134 (100%) | 132 (98%) | 2 (2%) | 60 | 86 |
| 3 | BA | 134/134 (100%) | 132 (98%) | 2 (2%) | 60 | 86 |
| 3 | D1 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | D2 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | D3 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | D4 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3 | D6 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | D8 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | D9 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | DA | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | F1 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | F2 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | F3 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | F4 | 134/134 (100%) | 130 (97%) | 4 (3%) | 36 | 70 |
| 3 | F6 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | F8 | 134/134 (100%) | 129 (96%) | 5 (4%) | 29 | 63 |
| 3 | F9 | 134/134 (100%) | 129 (96%) | 5 (4%) | 29 | 63 |
| 3 | FA | 134/134 (100%) | 129 (96%) | 5 (4%) | 29 | 63 |
| 3 | H1 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | H2 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | H3 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | H4 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | H6 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | H8 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | H9 | 134/134 (100%) | 130 (97%) | 4 (3%) | 36 | 70 |
| 3 | HA | 134/134 (100%) | 130 (97%) | 4 (3%) | 36 | 70 |
| 3 | J1 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | J2 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | J3 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | J4 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | J6 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | J8 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | J9 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | JA | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | L1 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | L2 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | L3 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3 | L4 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | L6 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | L8 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | L9 | 134/134 (100%) | 124 (92%) | 10 (8%) | 11 | 33 |
| 3 | LA | 134/134 (100%) | 124 (92%) | 10 (8%) | 11 | 33 |
| 3 | O4 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | O8 | 134/134 (100%) | 130 (97%) | 4 (3%) | 36 | 70 |
| 3 | P1 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | P3 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | P9 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | PA | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | Q4 | 134/134 (100%) | 129 (96%) | 5 (4%) | 29 | 63 |
| 3 | Q8 | 134/134 (100%) | 127 (95%) | 7 (5%) | 19 | 50 |
| 3 | R1 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | R3 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | R9 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | RA | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | S4 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | S8 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | T1 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | T3 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | T9 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | TA | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | U4 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | U8 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | V1 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | V3 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | V9 | 134/134 (100%) | 130 (97%) | 4 (3%) | 36 | 70 |
| 3 | VA | 134/134 (100%) | 130 (97%) | 4 (3%) | 36 | 70 |
| 3 | W4 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | W8 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3 | X1 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | X3 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | X9 | 134/134 (100%) | 132 (98%) | 2 (2%) | 60 | 86 |
| 3 | XA | 134/134 (100%) | 132 (98%) | 2 (2%) | 60 | 86 |
| 3 | Y4 | 134/134 (100%) | 129 (96%) | 5 (4%) | 29 | 63 |
| 3 | Y8 | 134/134 (100%) | 128 (96%) | 6 (4%) | 23 | 55 |
| 3 | Z1 | 134/134 (100%) | 130 (97%) | 4 (3%) | 36 | 70 |
| 3 | Z3 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | Z9 | 134/134 (100%) | 131 (98%) | 3 (2%) | 47 | 79 |
| 3 | ZA | 134/134 (100%) | 130 (97%) | 4 (3%) | 36 | 70 |
| 4 | M1 | 235/238 (99%) | 182 (77%) | 53 (23%) | 1 | 2 |
| 4 | M3 | 235/238 (99%) | 182 (77%) | 53 (23%) | 1 | 2 |
| 4 | M4 | 235/238 (99%) | 181 (77%) | 54 (23%) | 0 | 2 |
| 4 | M8 | 235/238 (99%) | 182 (77%) | 53 (23%) | 1 | 2 |
| 4 | M9 | 235/238 (99%) | 182 (77%) | 53 (23%) | 1 | 2 |
| 4 | MA | 235/238 (99%) | 182 (77%) | 53 (23%) | 1 | 2 |
| 5 | N1 | 66/240 (28%) | 40 (61%) | 26 (39%) | 0 | 0 |
| 5 | N3 | 66/240 (28%) | 40 (61%) | 26 (39%) | 0 | 0 |
| 5 | N9 | 66/240 (28%) | 39 (59%) | 27 (41%) | 0 | 0 |
| 5 | NA | 66/240 (28%) | 39 (59%) | 27 (41%) | 0 | 0 |
| 5 | Z4 | 66/240 (28%) | 43 (65%) | 23 (35%) | 0 | 0 |
| 5 | Z8 | 66/240 (28%) | 46 (70%) | 20 (30%) | 0 | 0 |
| 6 | M2 | 230/603 (38%) | 228 (99%) | 2 (1%) | 75 | 92 |
| 6 | M6 | 230/603 (38%) | 228 (99%) | 2 (1%) | 75 | 92 |
| 7 | N2 | 61/62 (98%) | 57 (93%) | 4 (7%) | 14 | 39 |
| 7 | N6 | 61/62 (98%) | 57 (93%) | 4 (7%) | 14 | 39 |
| 8 | A5 | 127/128 (99%) | 120 (94%) | 7 (6%) | 18 | 47 |
| 8 | A7 | 127/128 (99%) | 122 (96%) | 5 (4%) | 27 | 61 |
| 8 | C5 | 127/128 (99%) | 120 (94%) | 7 (6%) | 18 | 47 |
| 8 | C7 | 127/128 (99%) | 124 (98%) | 3 (2%) | 44 | 77 |
| 8 | E5 | 127/128 (99%) | 115 (91%) | 12 (9%) | 7 | 23 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 8 | E7 | 127/128 (99%) | 122 (96%) | 5 (4%) | 27 | 61 |
| 8 | G5 | 127/128 (99%) | 120 (94%) | 7 (6%) | 18 | 47 |
| 8 | G7 | 127/128 (99%) | 122 (96%) | 5 (4%) | 27 | 61 |
| 8 | I5 | 127/128 (99%) | 120 (94%) | 7 (6%) | 18 | 47 |
| 8 | I7 | 127/128 (99%) | 124 (98%) | 3 (2%) | 44 | 77 |
| 8 | K5 | 127/128 (99%) | 115 (91%) | 12 (9%) | 7 | 23 |
| 8 | K7 | 127/128 (99%) | 122 (96%) | 5 (4%) | 27 | 61 |
| 8 | M5 | 127/128 (99%) | 121 (95%) | 6 (5%) | 22 | 54 |
| 8 | M7 | 127/128 (99%) | 121 (95%) | 6 (5%) | 22 | 54 |
| 8 | O5 | 127/128 (99%) | 123 (97%) | 4 (3%) | 35 | 69 |
| 8 | O7 | 127/128 (99%) | 124 (98%) | 3 (2%) | 44 | 77 |
| 8 | Q5 | 127/128 (99%) | 121 (95%) | 6 (5%) | 22 | 54 |
| 8 | Q7 | 127/128 (99%) | 122 (96%) | 5 (4%) | 27 | 61 |
| 8 | S5 | 127/128 (99%) | 121 (95%) | 6 (5%) | 22 | 54 |
| 8 | S7 | 127/128 (99%) | 121 (95%) | 6 (5%) | 22 | 54 |
| 8 | U5 | 127/128 (99%) | 122 (96%) | 5 (4%) | 27 | 61 |
| 8 | U7 | 127/128 (99%) | 123 (97%) | 4 (3%) | 35 | 69 |
| 8 | W5 | 127/128 (99%) | 121 (95%) | 6 (5%) | 22 | 54 |
| 8 | W7 | 127/128 (99%) | 122 (96%) | 5 (4%) | 27 | 61 |
| 8 | Y5 | 127/128 (99%) | 121 (95%) | 6 (5%) | 22 | 54 |
| 8 | Y7 | 127/128 (99%) | 121 (95%) | 6 (5%) | 22 | 54 |
| 8 | a5 | 127/128 (99%) | 120 (94%) | 7 (6%) | 18 | 47 |
| 8 | a7 | 127/128 (99%) | 125 (98%) | 2 (2%) | 58 | 85 |
| 8 | c5 | 127/128 (99%) | 121 (95%) | 6 (5%) | 22 | 54 |
| 8 | c7 | 127/128 (99%) | 116 (91%) | 11 (9%) | 8 | 26 |
| 8 | e5 | 127/128 (99%) | 120 (94%) | 7 (6%) | 18 | 47 |
| 8 | e7 | 127/128 (99%) | 121 (95%) | 6 (5%) | 22 | 54 |
| 8 | g7 | 127/128 (99%) | 125 (98%) | 2 (2%) | 58 | 85 |
| 8 | i7 | 127/128 (99%) | 116 (91%) | 11 (9%) | 8 | 26 |
| 8 | k7 | 127/128 (99%) | 122 (96%) | 5 (4%) | 27 | 61 |
| 8 | m7 | 127/128 (99%) | 123 (97%) | 4 (3%) | 35 | 69 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|-------------|----|
| 8 | o7 | 127/128 (99%) | 117 (92%) | 10 (8%) | 10 | 30 |
| 8 | q7 | 127/128 (99%) | 121 (95%) | 6 (5%) | 22 | 54 |
| 8 | s7 | 127/128 (99%) | 123 (97%) | 4 (3%) | 35 | 69 |
| 8 | u7 | 127/128 (99%) | 117 (92%) | 10 (8%) | 10 | 30 |
| 9 | i5 | 57/57 (100%) | 48 (84%) | 9 (16%) | 2 | 7 |
| 9 | w7 | 57/57 (100%) | 42 (74%) | 15 (26%) | 0 | 1 |
| 9 | x7 | 57/57 (100%) | 40 (70%) | 17 (30%) | 0 | 1 |
| 9 | y7 | 57/57 (100%) | 40 (70%) | 17 (30%) | 0 | 1 |
| 9 | z5 | 57/57 (100%) | 48 (84%) | 9 (16%) | 2 | 7 |
| 9 | z7 | 57/57 (100%) | 42 (74%) | 15 (26%) | 0 | 1 |
| 10 | j5 | 941/977 (96%) | 716 (76%) | 225 (24%) | 0 | 2 |
| 10 | k5 | 941/977 (96%) | 717 (76%) | 224 (24%) | 0 | 2 |
| 11 | a9 | 652/670 (97%) | 525 (80%) | 127 (20%) | 1 | 3 |
| 11 | aA | 652/670 (97%) | 522 (80%) | 130 (20%) | 1 | 3 |
| All | All | 38254/40212 (95%) | 35843 (94%) | 2411 (6%) | 17 | 42 |

All (2411) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 32 | THR |
| 1 | A | 157 | SER |
| 1 | Z | 32 | THR |
| 1 | Z | 157 | SER |
| 2 | AA | 17 | ARG |
| 2 | AA | 25 | GLN |
| 2 | AA | 30 | ARG |
| 2 | AA | 45 | THR |
| 2 | AA | 115 | GLU |
| 2 | AA | 123 | SER |
| 3 | BA | 67 | ILE |
| 3 | BA | 144 | SER |
| 2 | CA | 17 | ARG |
| 2 | CA | 25 | GLN |
| 2 | CA | 30 | ARG |
| 2 | CA | 45 | THR |
| 2 | CA | 115 | GLU |
| 2 | CA | 123 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | DA | 6 | THR |
| 3 | DA | 65 | ASP |
| 3 | DA | 144 | SER |
| 2 | EA | 17 | ARG |
| 2 | EA | 25 | GLN |
| 2 | EA | 30 | ARG |
| 2 | EA | 45 | THR |
| 2 | EA | 115 | GLU |
| 2 | EA | 123 | SER |
| 3 | FA | 6 | THR |
| 3 | FA | 65 | ASP |
| 3 | FA | 146 | SER |
| 3 | FA | 156 | LEU |
| 3 | FA | 158 | ASN |
| 2 | GA | 17 | ARG |
| 2 | GA | 25 | GLN |
| 2 | GA | 30 | ARG |
| 2 | GA | 45 | THR |
| 2 | GA | 115 | GLU |
| 2 | GA | 123 | SER |
| 3 | HA | 6 | THR |
| 3 | HA | 65 | ASP |
| 3 | HA | 108 | ARG |
| 3 | HA | 144 | SER |
| 2 | IA | 25 | GLN |
| 2 | IA | 30 | ARG |
| 2 | IA | 45 | THR |
| 2 | IA | 115 | GLU |
| 2 | IA | 123 | SER |
| 3 | JA | 6 | THR |
| 3 | JA | 65 | ASP |
| 3 | JA | 144 | SER |
| 2 | KA | 17 | ARG |
| 2 | KA | 23 | GLU |
| 2 | KA | 30 | ARG |
| 2 | KA | 45 | THR |
| 2 | KA | 115 | GLU |
| 2 | KA | 123 | SER |
| 3 | LA | 6 | THR |
| 3 | LA | 65 | ASP |
| 3 | LA | 84 | ARG |
| 3 | LA | 88 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | LA | 94 | SER |
| 3 | LA | 97 | LEU |
| 3 | LA | 98 | LEU |
| 3 | LA | 115 | GLU |
| 3 | LA | 116 | THR |
| 3 | LA | 144 | SER |
| 4 | MA | 4 | LEU |
| 4 | MA | 13 | LYS |
| 4 | MA | 19 | MET |
| 4 | MA | 25 | LEU |
| 4 | MA | 33 | LEU |
| 4 | MA | 44 | SER |
| 4 | MA | 45 | VAL |
| 4 | MA | 50 | ASP |
| 4 | MA | 51 | ARG |
| 4 | MA | 52 | LEU |
| 4 | MA | 65 | ARG |
| 4 | MA | 68 | ASP |
| 4 | MA | 69 | ILE |
| 4 | MA | 73 | ASP |
| 4 | MA | 74 | LEU |
| 4 | MA | 77 | LEU |
| 4 | MA | 79 | PRO |
| 4 | MA | 87 | ILE |
| 4 | MA | 92 | GLU |
| 4 | MA | 100 | SER |
| 4 | MA | 101 | ASP |
| 4 | MA | 113 | ILE |
| 4 | MA | 123 | GLU |
| 4 | MA | 124 | ARG |
| 4 | MA | 125 | LEU |
| 4 | MA | 130 | SER |
| 4 | MA | 132 | LEU |
| 4 | MA | 137 | ILE |
| 4 | MA | 141 | GLU |
| 4 | MA | 146 | LEU |
| 4 | MA | 151 | LEU |
| 4 | MA | 155 | ARG |
| 4 | MA | 162 | ASN |
| 4 | MA | 166 | THR |
| 4 | MA | 167 | GLU |
| 4 | MA | 176 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | MA | 184 | ILE |
| 4 | MA | 189 | ASP |
| 4 | MA | 200 | ILE |
| 4 | MA | 202 | SER |
| 4 | MA | 211 | GLN |
| 4 | MA | 227 | GLN |
| 4 | MA | 230 | GLN |
| 4 | MA | 232 | VAL |
| 4 | MA | 241 | LEU |
| 4 | MA | 251 | ASN |
| 4 | MA | 255 | GLN |
| 4 | MA | 257 | GLN |
| 4 | MA | 261 | VAL |
| 4 | MA | 266 | LEU |
| 4 | MA | 271 | ARG |
| 4 | MA | 273 | ILE |
| 4 | MA | 274 | VAL |
| 5 | NA | 4 | LEU |
| 5 | NA | 7 | ASP |
| 5 | NA | 8 | ASN |
| 5 | NA | 9 | GLN |
| 5 | NA | 13 | SER |
| 5 | NA | 14 | LYS |
| 5 | NA | 15 | LEU |
| 5 | NA | 17 | LYS |
| 5 | NA | 18 | ILE |
| 5 | NA | 20 | ILE |
| 5 | NA | 22 | LEU |
| 5 | NA | 26 | LEU |
| 5 | NA | 30 | PRO |
| 5 | NA | 34 | LEU |
| 5 | NA | 41 | GLN |
| 5 | NA | 46 | THR |
| 5 | NA | 50 | LEU |
| 5 | NA | 51 | GLU |
| 5 | NA | 53 | LEU |
| 5 | NA | 55 | PRO |
| 5 | NA | 59 | ARG |
| 5 | NA | 60 | ILE |
| 5 | NA | 66 | ARG |
| 5 | NA | 67 | ILE |
| 5 | NA | 69 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | NA | 70 | ILE |
| 5 | NA | 74 | GLU |
| 2 | OA | 17 | ARG |
| 2 | OA | 25 | GLN |
| 2 | OA | 30 | ARG |
| 2 | OA | 45 | THR |
| 2 | OA | 115 | GLU |
| 2 | OA | 123 | SER |
| 3 | PA | 6 | THR |
| 3 | PA | 65 | ASP |
| 3 | PA | 144 | SER |
| 2 | QA | 17 | ARG |
| 2 | QA | 25 | GLN |
| 2 | QA | 30 | ARG |
| 2 | QA | 45 | THR |
| 2 | QA | 68 | GLN |
| 2 | QA | 115 | GLU |
| 2 | QA | 123 | SER |
| 3 | RA | 6 | THR |
| 3 | RA | 65 | ASP |
| 3 | RA | 144 | SER |
| 2 | SA | 17 | ARG |
| 2 | SA | 25 | GLN |
| 2 | SA | 30 | ARG |
| 2 | SA | 45 | THR |
| 2 | SA | 115 | GLU |
| 2 | SA | 123 | SER |
| 3 | TA | 6 | THR |
| 3 | TA | 65 | ASP |
| 3 | TA | 144 | SER |
| 2 | UA | 17 | ARG |
| 2 | UA | 25 | GLN |
| 2 | UA | 30 | ARG |
| 2 | UA | 45 | THR |
| 2 | UA | 115 | GLU |
| 2 | UA | 123 | SER |
| 3 | VA | 6 | THR |
| 3 | VA | 65 | ASP |
| 3 | VA | 108 | ARG |
| 3 | VA | 144 | SER |
| 2 | WA | 17 | ARG |
| 2 | WA | 25 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | WA | 30 | ARG |
| 2 | WA | 45 | THR |
| 2 | WA | 115 | GLU |
| 2 | WA | 123 | SER |
| 3 | XA | 65 | ASP |
| 3 | XA | 144 | SER |
| 2 | YA | 17 | ARG |
| 2 | YA | 25 | GLN |
| 2 | YA | 30 | ARG |
| 2 | YA | 45 | THR |
| 2 | YA | 115 | GLU |
| 2 | YA | 123 | SER |
| 3 | ZA | 6 | THR |
| 3 | ZA | 65 | ASP |
| 3 | ZA | 84 | ARG |
| 3 | ZA | 144 | SER |
| 2 | O1 | 17 | ARG |
| 2 | O1 | 25 | GLN |
| 2 | O1 | 30 | ARG |
| 2 | O1 | 45 | THR |
| 2 | O1 | 115 | GLU |
| 2 | O1 | 123 | SER |
| 3 | P1 | 6 | THR |
| 3 | P1 | 65 | ASP |
| 3 | P1 | 144 | SER |
| 2 | Q1 | 17 | ARG |
| 2 | Q1 | 25 | GLN |
| 2 | Q1 | 30 | ARG |
| 2 | Q1 | 45 | THR |
| 2 | Q1 | 115 | GLU |
| 2 | Q1 | 123 | SER |
| 3 | R1 | 6 | THR |
| 3 | R1 | 65 | ASP |
| 3 | R1 | 144 | SER |
| 2 | S1 | 17 | ARG |
| 2 | S1 | 25 | GLN |
| 2 | S1 | 30 | ARG |
| 2 | S1 | 45 | THR |
| 2 | S1 | 115 | GLU |
| 2 | S1 | 123 | SER |
| 2 | A1 | 25 | GLN |
| 2 | A1 | 45 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A1 | 57 | GLN |
| 2 | A1 | 115 | GLU |
| 2 | A1 | 123 | SER |
| 2 | G3 | 17 | ARG |
| 2 | G3 | 25 | GLN |
| 2 | G3 | 30 | ARG |
| 2 | G3 | 45 | THR |
| 2 | G3 | 115 | GLU |
| 2 | G3 | 123 | SER |
| 3 | H3 | 6 | THR |
| 3 | H3 | 65 | ASP |
| 3 | H3 | 144 | SER |
| 2 | I3 | 17 | ARG |
| 2 | I3 | 25 | GLN |
| 2 | I3 | 30 | ARG |
| 2 | I3 | 45 | THR |
| 2 | I3 | 115 | GLU |
| 2 | I3 | 123 | SER |
| 3 | J3 | 6 | THR |
| 3 | J3 | 65 | ASP |
| 3 | J3 | 144 | SER |
| 2 | K3 | 17 | ARG |
| 2 | K3 | 25 | GLN |
| 2 | K3 | 30 | ARG |
| 2 | K3 | 45 | THR |
| 2 | K3 | 115 | GLU |
| 2 | K3 | 123 | SER |
| 2 | G2 | 17 | ARG |
| 2 | G2 | 25 | GLN |
| 2 | G2 | 30 | ARG |
| 2 | G2 | 45 | THR |
| 2 | G2 | 115 | GLU |
| 2 | G2 | 123 | SER |
| 3 | H2 | 6 | THR |
| 3 | H2 | 65 | ASP |
| 3 | H2 | 144 | SER |
| 2 | I2 | 17 | ARG |
| 2 | I2 | 25 | GLN |
| 2 | I2 | 30 | ARG |
| 2 | I2 | 45 | THR |
| 2 | I2 | 115 | GLU |
| 2 | I2 | 123 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | J2 | 6 | THR |
| 3 | J2 | 65 | ASP |
| 3 | J2 | 144 | SER |
| 2 | K2 | 17 | ARG |
| 2 | K2 | 25 | GLN |
| 2 | K2 | 30 | ARG |
| 2 | K2 | 45 | THR |
| 2 | K2 | 115 | GLU |
| 2 | K2 | 123 | SER |
| 3 | L2 | 6 | THR |
| 3 | L2 | 65 | ASP |
| 3 | L2 | 144 | SER |
| 6 | M2 | 256 | THR |
| 6 | M2 | 258 | VAL |
| 7 | N2 | 1 | MET |
| 7 | N2 | 2 | TYR |
| 7 | N2 | 5 | VAL |
| 7 | N2 | 49 | LEU |
| 2 | A3 | 2 | LYS |
| 2 | A3 | 17 | ARG |
| 2 | A3 | 25 | GLN |
| 2 | A3 | 30 | ARG |
| 2 | A3 | 45 | THR |
| 2 | A3 | 115 | GLU |
| 2 | A3 | 123 | SER |
| 3 | B3 | 6 | THR |
| 3 | B3 | 65 | ASP |
| 3 | B3 | 144 | SER |
| 2 | C3 | 17 | ARG |
| 2 | C3 | 25 | GLN |
| 2 | C3 | 30 | ARG |
| 2 | C3 | 45 | THR |
| 2 | C3 | 115 | GLU |
| 2 | C3 | 123 | SER |
| 3 | D3 | 6 | THR |
| 3 | D3 | 65 | ASP |
| 3 | D3 | 144 | SER |
| 2 | E3 | 17 | ARG |
| 2 | E3 | 25 | GLN |
| 2 | E3 | 30 | ARG |
| 2 | E3 | 45 | THR |
| 2 | E3 | 115 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | E3 | 123 | SER |
| 3 | F3 | 6 | THR |
| 3 | F3 | 65 | ASP |
| 3 | F3 | 144 | SER |
| 3 | Z3 | 2 | GLN |
| 3 | Z3 | 65 | ASP |
| 3 | Z3 | 144 | SER |
| 2 | A4 | 17 | ARG |
| 2 | A4 | 25 | GLN |
| 2 | A4 | 30 | ARG |
| 2 | A4 | 45 | THR |
| 2 | A4 | 115 | GLU |
| 2 | A4 | 123 | SER |
| 3 | B4 | 6 | THR |
| 3 | B4 | 65 | ASP |
| 3 | B4 | 110 | LEU |
| 3 | B4 | 111 | ASN |
| 3 | B4 | 113 | LEU |
| 3 | B4 | 144 | SER |
| 2 | C4 | 17 | ARG |
| 2 | C4 | 25 | GLN |
| 2 | C4 | 30 | ARG |
| 2 | C4 | 45 | THR |
| 2 | C4 | 115 | GLU |
| 2 | C4 | 123 | SER |
| 3 | D4 | 6 | THR |
| 3 | D4 | 65 | ASP |
| 3 | D4 | 144 | SER |
| 3 | L3 | 6 | THR |
| 3 | L3 | 65 | ASP |
| 3 | L3 | 144 | SER |
| 4 | M3 | 4 | LEU |
| 4 | M3 | 13 | LYS |
| 4 | M3 | 19 | MET |
| 4 | M3 | 25 | LEU |
| 4 | M3 | 33 | LEU |
| 4 | M3 | 44 | SER |
| 4 | M3 | 45 | VAL |
| 4 | M3 | 50 | ASP |
| 4 | M3 | 51 | ARG |
| 4 | M3 | 52 | LEU |
| 4 | M3 | 65 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | M3 | 68 | ASP |
| 4 | M3 | 69 | ILE |
| 4 | M3 | 73 | ASP |
| 4 | M3 | 74 | LEU |
| 4 | M3 | 77 | LEU |
| 4 | M3 | 79 | PRO |
| 4 | M3 | 87 | ILE |
| 4 | M3 | 92 | GLU |
| 4 | M3 | 100 | SER |
| 4 | M3 | 101 | ASP |
| 4 | M3 | 113 | ILE |
| 4 | M3 | 123 | GLU |
| 4 | M3 | 124 | ARG |
| 4 | M3 | 125 | LEU |
| 4 | M3 | 130 | SER |
| 4 | M3 | 132 | LEU |
| 4 | M3 | 137 | ILE |
| 4 | M3 | 141 | GLU |
| 4 | M3 | 146 | LEU |
| 4 | M3 | 151 | LEU |
| 4 | M3 | 155 | ARG |
| 4 | M3 | 162 | ASN |
| 4 | M3 | 166 | THR |
| 4 | M3 | 167 | GLU |
| 4 | M3 | 176 | ARG |
| 4 | M3 | 184 | ILE |
| 4 | M3 | 189 | ASP |
| 4 | M3 | 200 | ILE |
| 4 | M3 | 202 | SER |
| 4 | M3 | 211 | GLN |
| 4 | M3 | 227 | GLN |
| 4 | M3 | 230 | GLN |
| 4 | M3 | 232 | VAL |
| 4 | M3 | 241 | LEU |
| 4 | M3 | 251 | ASN |
| 4 | M3 | 255 | GLN |
| 4 | M3 | 257 | GLN |
| 4 | M3 | 261 | VAL |
| 4 | M3 | 266 | LEU |
| 4 | M3 | 271 | ARG |
| 4 | M3 | 273 | ILE |
| 4 | M3 | 274 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | N3 | 4 | LEU |
| 5 | N3 | 7 | ASP |
| 5 | N3 | 8 | ASN |
| 5 | N3 | 13 | SER |
| 5 | N3 | 14 | LYS |
| 5 | N3 | 15 | LEU |
| 5 | N3 | 17 | LYS |
| 5 | N3 | 18 | ILE |
| 5 | N3 | 20 | ILE |
| 5 | N3 | 22 | LEU |
| 5 | N3 | 26 | LEU |
| 5 | N3 | 30 | PRO |
| 5 | N3 | 34 | LEU |
| 5 | N3 | 41 | GLN |
| 5 | N3 | 46 | THR |
| 5 | N3 | 50 | LEU |
| 5 | N3 | 51 | GLU |
| 5 | N3 | 53 | LEU |
| 5 | N3 | 55 | PRO |
| 5 | N3 | 59 | ARG |
| 5 | N3 | 60 | ILE |
| 5 | N3 | 66 | ARG |
| 5 | N3 | 67 | ILE |
| 5 | N3 | 69 | GLU |
| 5 | N3 | 70 | ILE |
| 5 | N3 | 74 | GLU |
| 2 | O3 | 17 | ARG |
| 2 | O3 | 25 | GLN |
| 2 | O3 | 30 | ARG |
| 2 | O3 | 45 | THR |
| 2 | O3 | 115 | GLU |
| 2 | O3 | 123 | SER |
| 3 | P3 | 6 | THR |
| 3 | P3 | 65 | ASP |
| 3 | P3 | 144 | SER |
| 2 | Q3 | 17 | ARG |
| 2 | Q3 | 25 | GLN |
| 2 | Q3 | 30 | ARG |
| 2 | Q3 | 45 | THR |
| 2 | Q3 | 115 | GLU |
| 2 | Q3 | 123 | SER |
| 3 | R3 | 6 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | R3 | 65 | ASP |
| 3 | R3 | 144 | SER |
| 2 | S3 | 17 | ARG |
| 2 | S3 | 25 | GLN |
| 2 | S3 | 30 | ARG |
| 2 | S3 | 45 | THR |
| 2 | S3 | 115 | GLU |
| 2 | S3 | 123 | SER |
| 3 | T3 | 6 | THR |
| 3 | T3 | 65 | ASP |
| 3 | T3 | 144 | SER |
| 2 | U3 | 17 | ARG |
| 2 | U3 | 25 | GLN |
| 2 | U3 | 30 | ARG |
| 2 | U3 | 45 | THR |
| 2 | U3 | 115 | GLU |
| 2 | U3 | 123 | SER |
| 3 | V3 | 6 | THR |
| 3 | V3 | 65 | ASP |
| 3 | V3 | 144 | SER |
| 2 | W3 | 17 | ARG |
| 2 | W3 | 25 | GLN |
| 2 | W3 | 30 | ARG |
| 2 | W3 | 45 | THR |
| 2 | W3 | 115 | GLU |
| 2 | W3 | 123 | SER |
| 3 | X3 | 6 | THR |
| 3 | X3 | 65 | ASP |
| 3 | X3 | 144 | SER |
| 2 | Y3 | 17 | ARG |
| 2 | Y3 | 25 | GLN |
| 2 | Y3 | 30 | ARG |
| 2 | Y3 | 45 | THR |
| 2 | Y3 | 115 | GLU |
| 2 | Y3 | 123 | SER |
| 3 | B1 | 6 | THR |
| 3 | B1 | 65 | ASP |
| 3 | B1 | 144 | SER |
| 3 | S4 | 6 | THR |
| 3 | S4 | 65 | ASP |
| 3 | S4 | 144 | SER |
| 2 | T4 | 17 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | T4 | 25 | GLN |
| 2 | T4 | 30 | ARG |
| 2 | T4 | 45 | THR |
| 2 | T4 | 115 | GLU |
| 2 | T4 | 123 | SER |
| 3 | U4 | 6 | THR |
| 3 | U4 | 65 | ASP |
| 3 | U4 | 144 | SER |
| 2 | V4 | 17 | ARG |
| 2 | V4 | 25 | GLN |
| 2 | V4 | 30 | ARG |
| 2 | V4 | 45 | THR |
| 2 | V4 | 115 | GLU |
| 2 | V4 | 123 | SER |
| 3 | W4 | 6 | THR |
| 3 | W4 | 65 | ASP |
| 3 | W4 | 144 | SER |
| 2 | E4 | 17 | ARG |
| 2 | E4 | 25 | GLN |
| 2 | E4 | 30 | ARG |
| 2 | E4 | 45 | THR |
| 2 | E4 | 115 | GLU |
| 2 | E4 | 123 | SER |
| 3 | F4 | 6 | THR |
| 3 | F4 | 65 | ASP |
| 3 | F4 | 110 | LEU |
| 3 | F4 | 144 | SER |
| 2 | G4 | 17 | ARG |
| 2 | G4 | 25 | GLN |
| 2 | G4 | 30 | ARG |
| 2 | G4 | 45 | THR |
| 2 | G4 | 115 | GLU |
| 2 | G4 | 123 | SER |
| 3 | H4 | 6 | THR |
| 3 | H4 | 65 | ASP |
| 3 | H4 | 144 | SER |
| 2 | I4 | 17 | ARG |
| 2 | I4 | 25 | GLN |
| 2 | I4 | 30 | ARG |
| 2 | I4 | 45 | THR |
| 2 | I4 | 115 | GLU |
| 2 | I4 | 123 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | J4 | 6 | THR |
| 3 | J4 | 65 | ASP |
| 3 | J4 | 144 | SER |
| 2 | K4 | 17 | ARG |
| 2 | K4 | 25 | GLN |
| 2 | K4 | 30 | ARG |
| 2 | K4 | 45 | THR |
| 2 | K4 | 115 | GLU |
| 2 | K4 | 123 | SER |
| 3 | L4 | 6 | THR |
| 3 | L4 | 65 | ASP |
| 3 | L4 | 144 | SER |
| 4 | M4 | 4 | LEU |
| 4 | M4 | 7 | SER |
| 4 | M4 | 13 | LYS |
| 4 | M4 | 19 | MET |
| 4 | M4 | 25 | LEU |
| 4 | M4 | 33 | LEU |
| 4 | M4 | 44 | SER |
| 4 | M4 | 45 | VAL |
| 4 | M4 | 50 | ASP |
| 4 | M4 | 51 | ARG |
| 4 | M4 | 52 | LEU |
| 4 | M4 | 65 | ARG |
| 4 | M4 | 68 | ASP |
| 4 | M4 | 69 | ILE |
| 4 | M4 | 73 | ASP |
| 4 | M4 | 74 | LEU |
| 4 | M4 | 77 | LEU |
| 4 | M4 | 79 | PRO |
| 4 | M4 | 87 | ILE |
| 4 | M4 | 96 | LYS |
| 4 | M4 | 100 | SER |
| 4 | M4 | 101 | ASP |
| 4 | M4 | 113 | ILE |
| 4 | M4 | 123 | GLU |
| 4 | M4 | 124 | ARG |
| 4 | M4 | 125 | LEU |
| 4 | M4 | 130 | SER |
| 4 | M4 | 132 | LEU |
| 4 | M4 | 137 | ILE |
| 4 | M4 | 142 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | M4 | 143 | VAL |
| 4 | M4 | 146 | LEU |
| 4 | M4 | 151 | LEU |
| 4 | M4 | 155 | ARG |
| 4 | M4 | 162 | ASN |
| 4 | M4 | 166 | THR |
| 4 | M4 | 167 | GLU |
| 4 | M4 | 176 | ARG |
| 4 | M4 | 184 | ILE |
| 4 | M4 | 189 | ASP |
| 4 | M4 | 200 | ILE |
| 4 | M4 | 202 | SER |
| 4 | M4 | 227 | GLN |
| 4 | M4 | 230 | GLN |
| 4 | M4 | 232 | VAL |
| 4 | M4 | 241 | LEU |
| 4 | M4 | 251 | ASN |
| 4 | M4 | 255 | GLN |
| 4 | M4 | 257 | GLN |
| 4 | M4 | 261 | VAL |
| 4 | M4 | 266 | LEU |
| 4 | M4 | 271 | ARG |
| 4 | M4 | 273 | ILE |
| 4 | M4 | 274 | VAL |
| 2 | N4 | 17 | ARG |
| 2 | N4 | 25 | GLN |
| 2 | N4 | 30 | ARG |
| 2 | N4 | 45 | THR |
| 2 | N4 | 123 | SER |
| 3 | O4 | 6 | THR |
| 3 | O4 | 65 | ASP |
| 3 | O4 | 144 | SER |
| 2 | P4 | 17 | ARG |
| 2 | P4 | 25 | GLN |
| 2 | P4 | 30 | ARG |
| 2 | P4 | 45 | THR |
| 2 | P4 | 115 | GLU |
| 2 | P4 | 123 | SER |
| 3 | Q4 | 6 | THR |
| 3 | Q4 | 65 | ASP |
| 3 | Q4 | 85 | ASP |
| 3 | Q4 | 113 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | Q4 | 144 | SER |
| 2 | R4 | 17 | ARG |
| 2 | R4 | 25 | GLN |
| 2 | R4 | 30 | ARG |
| 2 | R4 | 45 | THR |
| 2 | R4 | 115 | GLU |
| 2 | R4 | 123 | SER |
| 8 | K5 | 34 | GLU |
| 8 | K5 | 43 | LEU |
| 8 | K5 | 58 | LEU |
| 8 | K5 | 78 | THR |
| 8 | K5 | 91 | LEU |
| 8 | K5 | 96 | ILE |
| 8 | K5 | 97 | VAL |
| 8 | K5 | 102 | THR |
| 8 | K5 | 105 | GLU |
| 8 | K5 | 109 | ILE |
| 8 | K5 | 110 | ILE |
| 8 | K5 | 138 | THR |
| 1 | L5 | 3 | ASP |
| 1 | L5 | 32 | THR |
| 1 | L5 | 157 | SER |
| 8 | M5 | 34 | GLU |
| 8 | M5 | 43 | LEU |
| 8 | M5 | 52 | LYS |
| 8 | M5 | 91 | LEU |
| 8 | M5 | 102 | THR |
| 8 | M5 | 138 | THR |
| 1 | N5 | 32 | THR |
| 1 | N5 | 157 | SER |
| 8 | O5 | 20 | PRO |
| 8 | O5 | 76 | LYS |
| 8 | O5 | 91 | LEU |
| 8 | O5 | 138 | THR |
| 2 | X4 | 17 | ARG |
| 2 | X4 | 25 | GLN |
| 2 | X4 | 30 | ARG |
| 2 | X4 | 45 | THR |
| 2 | X4 | 115 | GLU |
| 2 | X4 | 123 | SER |
| 3 | Y4 | 6 | THR |
| 3 | Y4 | 65 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | Y4 | 101 | ASP |
| 3 | Y4 | 113 | LEU |
| 3 | Y4 | 144 | SER |
| 5 | Z4 | 8 | ASN |
| 5 | Z4 | 13 | SER |
| 5 | Z4 | 14 | LYS |
| 5 | Z4 | 15 | LEU |
| 5 | Z4 | 17 | LYS |
| 5 | Z4 | 18 | ILE |
| 5 | Z4 | 20 | ILE |
| 5 | Z4 | 22 | LEU |
| 5 | Z4 | 36 | THR |
| 5 | Z4 | 37 | HIS |
| 5 | Z4 | 38 | GLU |
| 5 | Z4 | 46 | THR |
| 5 | Z4 | 50 | LEU |
| 5 | Z4 | 51 | GLU |
| 5 | Z4 | 53 | LEU |
| 5 | Z4 | 55 | PRO |
| 5 | Z4 | 59 | ARG |
| 5 | Z4 | 60 | ILE |
| 5 | Z4 | 66 | ARG |
| 5 | Z4 | 67 | ILE |
| 5 | Z4 | 69 | GLU |
| 5 | Z4 | 70 | ILE |
| 5 | Z4 | 74 | GLU |
| 8 | A5 | 34 | GLU |
| 8 | A5 | 43 | LEU |
| 8 | A5 | 48 | GLU |
| 8 | A5 | 52 | LYS |
| 8 | A5 | 91 | LEU |
| 8 | A5 | 102 | THR |
| 8 | A5 | 138 | THR |
| 1 | B5 | 32 | THR |
| 1 | B5 | 157 | SER |
| 8 | C5 | 4 | LEU |
| 8 | C5 | 5 | THR |
| 8 | C5 | 9 | VAL |
| 8 | C5 | 16 | ARG |
| 8 | C5 | 25 | ARG |
| 8 | C5 | 91 | LEU |
| 8 | C5 | 138 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D5 | 1 | MET |
| 1 | D5 | 3 | ASP |
| 1 | D5 | 8 | VAL |
| 1 | D5 | 11 | ASN |
| 1 | D5 | 14 | VAL |
| 1 | D5 | 32 | THR |
| 1 | D5 | 157 | SER |
| 8 | E5 | 34 | GLU |
| 8 | E5 | 43 | LEU |
| 8 | E5 | 58 | LEU |
| 8 | E5 | 78 | THR |
| 8 | E5 | 91 | LEU |
| 8 | E5 | 96 | ILE |
| 8 | E5 | 97 | VAL |
| 8 | E5 | 102 | THR |
| 8 | E5 | 105 | GLU |
| 8 | E5 | 109 | ILE |
| 8 | E5 | 110 | ILE |
| 8 | E5 | 138 | THR |
| 1 | F5 | 3 | ASP |
| 1 | F5 | 32 | THR |
| 1 | F5 | 157 | SER |
| 8 | G5 | 34 | GLU |
| 8 | G5 | 43 | LEU |
| 8 | G5 | 48 | GLU |
| 8 | G5 | 52 | LYS |
| 8 | G5 | 91 | LEU |
| 8 | G5 | 102 | THR |
| 8 | G5 | 138 | THR |
| 1 | H5 | 32 | THR |
| 1 | H5 | 157 | SER |
| 8 | I5 | 4 | LEU |
| 8 | I5 | 5 | THR |
| 8 | I5 | 9 | VAL |
| 8 | I5 | 16 | ARG |
| 8 | I5 | 25 | ARG |
| 8 | I5 | 91 | LEU |
| 8 | I5 | 138 | THR |
| 1 | J5 | 1 | MET |
| 1 | J5 | 3 | ASP |
| 1 | J5 | 8 | VAL |
| 1 | J5 | 11 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J5 | 14 | VAL |
| 1 | J5 | 32 | THR |
| 1 | J5 | 157 | SER |
| 2 | C1 | 17 | ARG |
| 2 | C1 | 25 | GLN |
| 2 | C1 | 30 | ARG |
| 2 | C1 | 45 | THR |
| 2 | C1 | 115 | GLU |
| 2 | C1 | 123 | SER |
| 8 | c5 | 34 | GLU |
| 8 | c5 | 43 | LEU |
| 8 | c5 | 52 | LYS |
| 8 | c5 | 91 | LEU |
| 8 | c5 | 102 | THR |
| 8 | c5 | 138 | THR |
| 1 | d5 | 32 | THR |
| 1 | d5 | 157 | SER |
| 8 | e5 | 9 | VAL |
| 8 | e5 | 18 | LEU |
| 8 | e5 | 20 | PRO |
| 8 | e5 | 25 | ARG |
| 8 | e5 | 26 | ILE |
| 8 | e5 | 91 | LEU |
| 8 | e5 | 138 | THR |
| 1 | f5 | 32 | THR |
| 1 | f5 | 157 | SER |
| 1 | P5 | 32 | THR |
| 1 | P5 | 157 | SER |
| 8 | Q5 | 34 | GLU |
| 8 | Q5 | 43 | LEU |
| 8 | Q5 | 91 | LEU |
| 8 | Q5 | 102 | THR |
| 8 | Q5 | 138 | THR |
| 8 | Q5 | 161 | GLN |
| 1 | R5 | 32 | THR |
| 1 | R5 | 157 | SER |
| 8 | S5 | 34 | GLU |
| 8 | S5 | 43 | LEU |
| 8 | S5 | 52 | LYS |
| 8 | S5 | 91 | LEU |
| 8 | S5 | 102 | THR |
| 8 | S5 | 138 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | T5 | 32 | THR |
| 1 | T5 | 157 | SER |
| 8 | U5 | 20 | PRO |
| 8 | U5 | 22 | GLU |
| 8 | U5 | 76 | LYS |
| 8 | U5 | 91 | LEU |
| 8 | U5 | 138 | THR |
| 1 | V5 | 32 | THR |
| 1 | V5 | 157 | SER |
| 8 | W5 | 34 | GLU |
| 8 | W5 | 43 | LEU |
| 8 | W5 | 91 | LEU |
| 8 | W5 | 102 | THR |
| 8 | W5 | 138 | THR |
| 8 | W5 | 161 | GLN |
| 1 | X5 | 32 | THR |
| 1 | X5 | 157 | SER |
| 8 | Y5 | 34 | GLU |
| 8 | Y5 | 43 | LEU |
| 8 | Y5 | 52 | LYS |
| 8 | Y5 | 91 | LEU |
| 8 | Y5 | 102 | THR |
| 8 | Y5 | 138 | THR |
| 1 | Z5 | 32 | THR |
| 1 | Z5 | 157 | SER |
| 8 | a5 | 9 | VAL |
| 8 | a5 | 18 | LEU |
| 8 | a5 | 20 | PRO |
| 8 | a5 | 25 | ARG |
| 8 | a5 | 26 | ILE |
| 8 | a5 | 91 | LEU |
| 8 | a5 | 138 | THR |
| 1 | b5 | 32 | THR |
| 1 | b5 | 157 | SER |
| 3 | J6 | 6 | THR |
| 3 | J6 | 65 | ASP |
| 3 | J6 | 144 | SER |
| 2 | K6 | 17 | ARG |
| 2 | K6 | 25 | GLN |
| 2 | K6 | 30 | ARG |
| 2 | K6 | 45 | THR |
| 2 | K6 | 115 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | K6 | 123 | SER |
| 3 | L6 | 6 | THR |
| 3 | L6 | 65 | ASP |
| 3 | L6 | 144 | SER |
| 6 | M6 | 256 | THR |
| 6 | M6 | 258 | VAL |
| 7 | N6 | 1 | MET |
| 7 | N6 | 2 | TYR |
| 7 | N6 | 5 | VAL |
| 7 | N6 | 49 | LEU |
| 8 | A7 | 34 | GLU |
| 8 | A7 | 43 | LEU |
| 8 | A7 | 91 | LEU |
| 8 | A7 | 102 | THR |
| 8 | A7 | 138 | THR |
| 9 | z5 | 14 | LEU |
| 9 | z5 | 17 | VAL |
| 9 | z5 | 22 | GLU |
| 9 | z5 | 24 | GLN |
| 9 | z5 | 39 | THR |
| 9 | z5 | 43 | ARG |
| 9 | z5 | 45 | GLN |
| 9 | z5 | 56 | LEU |
| 9 | z5 | 60 | VAL |
| 9 | i5 | 14 | LEU |
| 9 | i5 | 17 | VAL |
| 9 | i5 | 22 | GLU |
| 9 | i5 | 24 | GLN |
| 9 | i5 | 39 | THR |
| 9 | i5 | 43 | ARG |
| 9 | i5 | 45 | GLN |
| 9 | i5 | 56 | LEU |
| 9 | i5 | 60 | VAL |
| 10 | j5 | 9 | SER |
| 10 | j5 | 15 | ARG |
| 10 | j5 | 16 | LEU |
| 10 | j5 | 19 | THR |
| 10 | j5 | 21 | MET |
| 10 | j5 | 24 | THR |
| 10 | j5 | 29 | ASN |
| 10 | j5 | 33 | ARG |
| 10 | j5 | 35 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | j5 | 39 | GLU |
| 10 | j5 | 51 | GLN |
| 10 | j5 | 57 | VAL |
| 10 | j5 | 61 | THR |
| 10 | j5 | 66 | MET |
| 10 | j5 | 74 | ARG |
| 10 | j5 | 80 | SER |
| 10 | j5 | 87 | ARG |
| 10 | j5 | 88 | GLN |
| 10 | j5 | 136 | VAL |
| 10 | j5 | 140 | PHE |
| 10 | j5 | 147 | ARG |
| 10 | j5 | 155 | LYS |
| 10 | j5 | 156 | SER |
| 10 | j5 | 157 | ILE |
| 10 | j5 | 178 | ILE |
| 10 | j5 | 179 | LEU |
| 10 | j5 | 180 | GLU |
| 10 | j5 | 182 | ASN |
| 10 | j5 | 184 | LEU |
| 10 | j5 | 186 | LEU |
| 10 | j5 | 191 | GLU |
| 10 | j5 | 192 | LYS |
| 10 | j5 | 197 | SER |
| 10 | j5 | 199 | THR |
| 10 | j5 | 200 | ILE |
| 10 | j5 | 201 | VAL |
| 10 | j5 | 208 | LYS |
| 10 | j5 | 209 | ASN |
| 10 | j5 | 217 | GLU |
| 10 | j5 | 221 | LYS |
| 10 | j5 | 224 | SER |
| 10 | j5 | 225 | SER |
| 10 | j5 | 227 | ILE |
| 10 | j5 | 232 | ARG |
| 10 | j5 | 235 | ASP |
| 10 | j5 | 238 | ARG |
| 10 | j5 | 240 | ASP |
| 10 | j5 | 245 | ILE |
| 10 | j5 | 246 | VAL |
| 10 | j5 | 252 | ASP |
| 10 | j5 | 253 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | j5 | 256 | LEU |
| 10 | j5 | 261 | ILE |
| 10 | j5 | 263 | LYS |
| 10 | j5 | 264 | LEU |
| 10 | j5 | 270 | THR |
| 10 | j5 | 275 | THR |
| 10 | j5 | 277 | ILE |
| 10 | j5 | 283 | ARG |
| 10 | j5 | 287 | ASN |
| 10 | j5 | 292 | GLU |
| 10 | j5 | 294 | GLU |
| 10 | j5 | 297 | VAL |
| 10 | j5 | 298 | ARG |
| 10 | j5 | 325 | ASN |
| 10 | j5 | 327 | GLU |
| 10 | j5 | 328 | ILE |
| 10 | j5 | 349 | GLN |
| 10 | j5 | 362 | LYS |
| 10 | j5 | 367 | ARG |
| 10 | j5 | 370 | GLU |
| 10 | j5 | 372 | ARG |
| 10 | j5 | 381 | ILE |
| 10 | j5 | 382 | ILE |
| 10 | j5 | 383 | SER |
| 10 | j5 | 388 | ARG |
| 10 | j5 | 393 | MET |
| 10 | j5 | 414 | ILE |
| 10 | j5 | 421 | PRO |
| 10 | j5 | 423 | LEU |
| 10 | j5 | 449 | ARG |
| 10 | j5 | 471 | PRO |
| 10 | j5 | 476 | ASN |
| 10 | j5 | 488 | LYS |
| 10 | j5 | 489 | ASN |
| 10 | j5 | 490 | SER |
| 10 | j5 | 491 | THR |
| 10 | j5 | 492 | ILE |
| 10 | j5 | 493 | ASN |
| 10 | j5 | 497 | ARG |
| 10 | j5 | 501 | ILE |
| 10 | j5 | 507 | ARG |
| 10 | j5 | 517 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | j5 | 520 | ARG |
| 10 | j5 | 527 | SER |
| 10 | j5 | 532 | THR |
| 10 | j5 | 535 | PRO |
| 10 | j5 | 539 | LYS |
| 10 | j5 | 541 | THR |
| 10 | j5 | 544 | VAL |
| 10 | j5 | 547 | ARG |
| 10 | j5 | 548 | SER |
| 10 | j5 | 549 | LYS |
| 10 | j5 | 552 | VAL |
| 10 | j5 | 557 | VAL |
| 10 | j5 | 560 | VAL |
| 10 | j5 | 567 | LEU |
| 10 | j5 | 569 | THR |
| 10 | j5 | 574 | GLN |
| 10 | j5 | 578 | ARG |
| 10 | j5 | 585 | ARG |
| 10 | j5 | 586 | LEU |
| 10 | j5 | 588 | VAL |
| 10 | j5 | 591 | ILE |
| 10 | j5 | 593 | LEU |
| 10 | j5 | 602 | GLU |
| 10 | j5 | 612 | ILE |
| 10 | j5 | 615 | LYS |
| 10 | j5 | 619 | GLU |
| 10 | j5 | 633 | ARG |
| 10 | j5 | 642 | ARG |
| 10 | j5 | 651 | ILE |
| 10 | j5 | 665 | LEU |
| 10 | j5 | 676 | GLU |
| 10 | j5 | 690 | LEU |
| 10 | j5 | 703 | LEU |
| 10 | j5 | 704 | THR |
| 10 | j5 | 710 | THR |
| 10 | j5 | 718 | MET |
| 10 | j5 | 723 | GLN |
| 10 | j5 | 724 | GLU |
| 10 | j5 | 725 | LEU |
| 10 | j5 | 727 | THR |
| 10 | j5 | 728 | PRO |
| 10 | j5 | 736 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | j5 | 737 | MET |
| 10 | j5 | 743 | VAL |
| 10 | j5 | 744 | PRO |
| 10 | j5 | 747 | LYS |
| 10 | j5 | 752 | VAL |
| 10 | j5 | 754 | LYS |
| 10 | j5 | 755 | GLN |
| 10 | j5 | 759 | THR |
| 10 | j5 | 760 | ASP |
| 10 | j5 | 761 | ARG |
| 10 | j5 | 762 | GLU |
| 10 | j5 | 767 | LEU |
| 10 | j5 | 769 | THR |
| 10 | j5 | 780 | ILE |
| 10 | j5 | 795 | LEU |
| 10 | j5 | 804 | GLU |
| 10 | j5 | 809 | LEU |
| 10 | j5 | 822 | ARG |
| 10 | j5 | 826 | THR |
| 10 | j5 | 834 | LYS |
| 10 | j5 | 847 | LEU |
| 10 | j5 | 854 | LEU |
| 10 | j5 | 859 | ILE |
| 10 | j5 | 867 | VAL |
| 10 | j5 | 870 | GLU |
| 10 | j5 | 882 | PRO |
| 10 | j5 | 883 | SER |
| 10 | j5 | 893 | ASN |
| 10 | j5 | 899 | GLU |
| 10 | j5 | 900 | LEU |
| 10 | j5 | 902 | ASN |
| 10 | j5 | 906 | ARG |
| 10 | j5 | 909 | ASP |
| 10 | j5 | 911 | LEU |
| 10 | j5 | 919 | ILE |
| 10 | j5 | 922 | LYS |
| 10 | j5 | 923 | MET |
| 10 | j5 | 925 | ILE |
| 10 | j5 | 931 | VAL |
| 10 | j5 | 935 | LEU |
| 10 | j5 | 937 | GLU |
| 10 | j5 | 941 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 10 | j5 | 942 | LYS |
| 10 | j5 | 943 | THR |
| 10 | j5 | 946 | ASP |
| 10 | j5 | 949 | ARG |
| 10 | j5 | 951 | MET |
| 10 | j5 | 963 | ASP |
| 10 | j5 | 966 | SER |
| 10 | j5 | 967 | VAL |
| 10 | j5 | 969 | VAL |
| 10 | j5 | 974 | LEU |
| 10 | j5 | 976 | ARG |
| 10 | j5 | 977 | GLN |
| 10 | j5 | 978 | LEU |
| 10 | j5 | 979 | GLU |
| 10 | j5 | 984 | ILE |
| 10 | j5 | 989 | THR |
| 10 | j5 | 990 | ARG |
| 10 | j5 | 991 | SER |
| 10 | j5 | 992 | GLU |
| 10 | j5 | 993 | LYS |
| 10 | j5 | 1011 | ILE |
| 10 | j5 | 1014 | SER |
| 10 | j5 | 1015 | TYR |
| 10 | j5 | 1017 | ARG |
| 10 | j5 | 1019 | SER |
| 10 | j5 | 1054 | SER |
| 10 | j5 | 1064 | LYS |
| 10 | j5 | 1067 | LEU |
| 10 | j5 | 1069 | ARG |
| 10 | j5 | 1086 | THR |
| 10 | j5 | 1089 | LEU |
| 10 | j5 | 1096 | ILE |
| 10 | j5 | 1100 | PRO |
| 10 | j5 | 1101 | GLU |
| 10 | j5 | 1103 | LEU |
| 10 | j5 | 1105 | ILE |
| 10 | j5 | 1110 | ILE |
| 10 | j5 | 1114 | ARG |
| 10 | j5 | 1120 | PRO |
| 10 | j5 | 1125 | ARG |
| 10 | j5 | 1134 | GLU |
| 10 | j5 | 1136 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 10 | j5 | 1144 | SER |
| 10 | j5 | 1147 | TYR |
| 10 | j5 | 1148 | THR |
| 10 | j5 | 1150 | TYR |
| 10 | j5 | 1152 | TYR |
| 10 | j5 | 1155 | ARG |
| 10 | k5 | 9 | SER |
| 10 | k5 | 15 | ARG |
| 10 | k5 | 16 | LEU |
| 10 | k5 | 19 | THR |
| 10 | k5 | 21 | MET |
| 10 | k5 | 24 | THR |
| 10 | k5 | 29 | ASN |
| 10 | k5 | 33 | ARG |
| 10 | k5 | 35 | PRO |
| 10 | k5 | 39 | GLU |
| 10 | k5 | 51 | GLN |
| 10 | k5 | 57 | VAL |
| 10 | k5 | 61 | THR |
| 10 | k5 | 66 | MET |
| 10 | k5 | 74 | ARG |
| 10 | k5 | 80 | SER |
| 10 | k5 | 87 | ARG |
| 10 | k5 | 88 | GLN |
| 10 | k5 | 136 | VAL |
| 10 | k5 | 140 | PHE |
| 10 | k5 | 147 | ARG |
| 10 | k5 | 155 | LYS |
| 10 | k5 | 156 | SER |
| 10 | k5 | 157 | ILE |
| 10 | k5 | 178 | ILE |
| 10 | k5 | 179 | LEU |
| 10 | k5 | 180 | GLU |
| 10 | k5 | 182 | ASN |
| 10 | k5 | 184 | LEU |
| 10 | k5 | 186 | LEU |
| 10 | k5 | 191 | GLU |
| 10 | k5 | 192 | LYS |
| 10 | k5 | 197 | SER |
| 10 | k5 | 199 | THR |
| 10 | k5 | 200 | ILE |
| 10 | k5 | 201 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | k5 | 208 | LYS |
| 10 | k5 | 209 | ASN |
| 10 | k5 | 217 | GLU |
| 10 | k5 | 221 | LYS |
| 10 | k5 | 224 | SER |
| 10 | k5 | 225 | SER |
| 10 | k5 | 227 | ILE |
| 10 | k5 | 232 | ARG |
| 10 | k5 | 235 | ASP |
| 10 | k5 | 238 | ARG |
| 10 | k5 | 240 | ASP |
| 10 | k5 | 245 | ILE |
| 10 | k5 | 246 | VAL |
| 10 | k5 | 252 | ASP |
| 10 | k5 | 253 | ARG |
| 10 | k5 | 256 | LEU |
| 10 | k5 | 261 | ILE |
| 10 | k5 | 263 | LYS |
| 10 | k5 | 264 | LEU |
| 10 | k5 | 270 | THR |
| 10 | k5 | 275 | THR |
| 10 | k5 | 277 | ILE |
| 10 | k5 | 283 | ARG |
| 10 | k5 | 287 | ASN |
| 10 | k5 | 292 | GLU |
| 10 | k5 | 294 | GLU |
| 10 | k5 | 297 | VAL |
| 10 | k5 | 298 | ARG |
| 10 | k5 | 325 | ASN |
| 10 | k5 | 327 | GLU |
| 10 | k5 | 328 | ILE |
| 10 | k5 | 349 | GLN |
| 10 | k5 | 362 | LYS |
| 10 | k5 | 367 | ARG |
| 10 | k5 | 370 | GLU |
| 10 | k5 | 372 | ARG |
| 10 | k5 | 381 | ILE |
| 10 | k5 | 382 | ILE |
| 10 | k5 | 383 | SER |
| 10 | k5 | 388 | ARG |
| 10 | k5 | 393 | MET |
| 10 | k5 | 414 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | k5 | 421 | PRO |
| 10 | k5 | 423 | LEU |
| 10 | k5 | 449 | ARG |
| 10 | k5 | 471 | PRO |
| 10 | k5 | 476 | ASN |
| 10 | k5 | 488 | LYS |
| 10 | k5 | 489 | ASN |
| 10 | k5 | 490 | SER |
| 10 | k5 | 491 | THR |
| 10 | k5 | 492 | ILE |
| 10 | k5 | 493 | ASN |
| 10 | k5 | 497 | ARG |
| 10 | k5 | 501 | ILE |
| 10 | k5 | 507 | ARG |
| 10 | k5 | 517 | SER |
| 10 | k5 | 520 | ARG |
| 10 | k5 | 527 | SER |
| 10 | k5 | 532 | THR |
| 10 | k5 | 535 | PRO |
| 10 | k5 | 539 | LYS |
| 10 | k5 | 541 | THR |
| 10 | k5 | 544 | VAL |
| 10 | k5 | 547 | ARG |
| 10 | k5 | 548 | SER |
| 10 | k5 | 549 | LYS |
| 10 | k5 | 552 | VAL |
| 10 | k5 | 559 | THR |
| 10 | k5 | 567 | LEU |
| 10 | k5 | 569 | THR |
| 10 | k5 | 574 | GLN |
| 10 | k5 | 578 | ARG |
| 10 | k5 | 585 | ARG |
| 10 | k5 | 586 | LEU |
| 10 | k5 | 588 | VAL |
| 10 | k5 | 591 | ILE |
| 10 | k5 | 593 | LEU |
| 10 | k5 | 602 | GLU |
| 10 | k5 | 612 | ILE |
| 10 | k5 | 615 | LYS |
| 10 | k5 | 619 | GLU |
| 10 | k5 | 633 | ARG |
| 10 | k5 | 642 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | k5 | 651 | ILE |
| 10 | k5 | 665 | LEU |
| 10 | k5 | 676 | GLU |
| 10 | k5 | 690 | LEU |
| 10 | k5 | 703 | LEU |
| 10 | k5 | 704 | THR |
| 10 | k5 | 710 | THR |
| 10 | k5 | 718 | MET |
| 10 | k5 | 723 | GLN |
| 10 | k5 | 724 | GLU |
| 10 | k5 | 725 | LEU |
| 10 | k5 | 727 | THR |
| 10 | k5 | 728 | PRO |
| 10 | k5 | 736 | GLU |
| 10 | k5 | 737 | MET |
| 10 | k5 | 743 | VAL |
| 10 | k5 | 744 | PRO |
| 10 | k5 | 747 | LYS |
| 10 | k5 | 752 | VAL |
| 10 | k5 | 754 | LYS |
| 10 | k5 | 755 | GLN |
| 10 | k5 | 759 | THR |
| 10 | k5 | 760 | ASP |
| 10 | k5 | 761 | ARG |
| 10 | k5 | 762 | GLU |
| 10 | k5 | 767 | LEU |
| 10 | k5 | 769 | THR |
| 10 | k5 | 780 | ILE |
| 10 | k5 | 795 | LEU |
| 10 | k5 | 804 | GLU |
| 10 | k5 | 809 | LEU |
| 10 | k5 | 822 | ARG |
| 10 | k5 | 826 | THR |
| 10 | k5 | 834 | LYS |
| 10 | k5 | 847 | LEU |
| 10 | k5 | 854 | LEU |
| 10 | k5 | 859 | ILE |
| 10 | k5 | 867 | VAL |
| 10 | k5 | 870 | GLU |
| 10 | k5 | 882 | PRO |
| 10 | k5 | 883 | SER |
| 10 | k5 | 893 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 10 | k5 | 899 | GLU |
| 10 | k5 | 900 | LEU |
| 10 | k5 | 902 | ASN |
| 10 | k5 | 906 | ARG |
| 10 | k5 | 909 | ASP |
| 10 | k5 | 910 | SER |
| 10 | k5 | 911 | LEU |
| 10 | k5 | 919 | ILE |
| 10 | k5 | 922 | LYS |
| 10 | k5 | 923 | MET |
| 10 | k5 | 925 | ILE |
| 10 | k5 | 931 | VAL |
| 10 | k5 | 935 | LEU |
| 10 | k5 | 937 | GLU |
| 10 | k5 | 941 | THR |
| 10 | k5 | 942 | LYS |
| 10 | k5 | 943 | THR |
| 10 | k5 | 946 | ASP |
| 10 | k5 | 949 | ARG |
| 10 | k5 | 951 | MET |
| 10 | k5 | 963 | ASP |
| 10 | k5 | 966 | SER |
| 10 | k5 | 967 | VAL |
| 10 | k5 | 969 | VAL |
| 10 | k5 | 974 | LEU |
| 10 | k5 | 976 | ARG |
| 10 | k5 | 977 | GLN |
| 10 | k5 | 978 | LEU |
| 10 | k5 | 979 | GLU |
| 10 | k5 | 984 | ILE |
| 10 | k5 | 989 | THR |
| 10 | k5 | 990 | ARG |
| 10 | k5 | 991 | SER |
| 10 | k5 | 992 | GLU |
| 10 | k5 | 993 | LYS |
| 10 | k5 | 1011 | ILE |
| 10 | k5 | 1014 | SER |
| 10 | k5 | 1015 | TYR |
| 10 | k5 | 1017 | ARG |
| 10 | k5 | 1019 | SER |
| 10 | k5 | 1054 | SER |
| 10 | k5 | 1064 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 10 | k5 | 1067 | LEU |
| 10 | k5 | 1069 | ARG |
| 10 | k5 | 1086 | THR |
| 10 | k5 | 1089 | LEU |
| 10 | k5 | 1096 | ILE |
| 10 | k5 | 1100 | PRO |
| 10 | k5 | 1101 | GLU |
| 10 | k5 | 1103 | LEU |
| 10 | k5 | 1105 | ILE |
| 10 | k5 | 1114 | ARG |
| 10 | k5 | 1120 | PRO |
| 10 | k5 | 1125 | ARG |
| 10 | k5 | 1134 | GLU |
| 10 | k5 | 1136 | ILE |
| 10 | k5 | 1144 | SER |
| 10 | k5 | 1147 | TYR |
| 10 | k5 | 1148 | THR |
| 10 | k5 | 1150 | TYR |
| 10 | k5 | 1152 | TYR |
| 10 | k5 | 1155 | ARG |
| 2 | A6 | 17 | ARG |
| 2 | A6 | 25 | GLN |
| 2 | A6 | 30 | ARG |
| 2 | A6 | 45 | THR |
| 2 | A6 | 115 | GLU |
| 2 | A6 | 123 | SER |
| 3 | B6 | 6 | THR |
| 3 | B6 | 65 | ASP |
| 3 | B6 | 77 | ARG |
| 3 | B6 | 144 | SER |
| 2 | C6 | 17 | ARG |
| 2 | C6 | 25 | GLN |
| 2 | C6 | 30 | ARG |
| 2 | C6 | 45 | THR |
| 2 | C6 | 115 | GLU |
| 2 | C6 | 123 | SER |
| 3 | D6 | 6 | THR |
| 3 | D6 | 65 | ASP |
| 3 | D6 | 144 | SER |
| 2 | E6 | 17 | ARG |
| 2 | E6 | 25 | GLN |
| 2 | E6 | 30 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | E6 | 45 | THR |
| 2 | E6 | 115 | GLU |
| 2 | E6 | 123 | SER |
| 3 | F6 | 6 | THR |
| 3 | F6 | 65 | ASP |
| 3 | F6 | 144 | SER |
| 2 | G6 | 17 | ARG |
| 2 | G6 | 25 | GLN |
| 2 | G6 | 30 | ARG |
| 2 | G6 | 45 | THR |
| 2 | G6 | 115 | GLU |
| 2 | G6 | 123 | SER |
| 3 | H6 | 6 | THR |
| 3 | H6 | 65 | ASP |
| 3 | H6 | 144 | SER |
| 2 | I6 | 17 | ARG |
| 2 | I6 | 25 | GLN |
| 2 | I6 | 30 | ARG |
| 2 | I6 | 45 | THR |
| 2 | I6 | 115 | GLU |
| 2 | I6 | 123 | SER |
| 3 | D1 | 6 | THR |
| 3 | D1 | 65 | ASP |
| 3 | D1 | 144 | SER |
| 8 | O7 | 20 | PRO |
| 8 | O7 | 91 | LEU |
| 8 | O7 | 138 | THR |
| 1 | P7 | 32 | THR |
| 1 | P7 | 157 | SER |
| 8 | Q7 | 34 | GLU |
| 8 | Q7 | 43 | LEU |
| 8 | Q7 | 91 | LEU |
| 8 | Q7 | 102 | THR |
| 8 | Q7 | 138 | THR |
| 1 | R7 | 32 | THR |
| 1 | R7 | 157 | SER |
| 8 | S7 | 34 | GLU |
| 8 | S7 | 43 | LEU |
| 8 | S7 | 52 | LYS |
| 8 | S7 | 91 | LEU |
| 8 | S7 | 102 | THR |
| 8 | S7 | 138 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B7 | 32 | THR |
| 1 | B7 | 157 | SER |
| 8 | C7 | 19 | SER |
| 8 | C7 | 91 | LEU |
| 8 | C7 | 138 | THR |
| 1 | D7 | 32 | THR |
| 1 | D7 | 157 | SER |
| 8 | E7 | 34 | GLU |
| 8 | E7 | 43 | LEU |
| 8 | E7 | 91 | LEU |
| 8 | E7 | 102 | THR |
| 8 | E7 | 138 | THR |
| 1 | F7 | 32 | THR |
| 1 | F7 | 157 | SER |
| 8 | G7 | 34 | GLU |
| 8 | G7 | 43 | LEU |
| 8 | G7 | 91 | LEU |
| 8 | G7 | 102 | THR |
| 8 | G7 | 138 | THR |
| 1 | H7 | 32 | THR |
| 1 | H7 | 157 | SER |
| 8 | I7 | 19 | SER |
| 8 | I7 | 91 | LEU |
| 8 | I7 | 138 | THR |
| 1 | J7 | 32 | THR |
| 1 | J7 | 157 | SER |
| 8 | K7 | 34 | GLU |
| 8 | K7 | 43 | LEU |
| 8 | K7 | 91 | LEU |
| 8 | K7 | 102 | THR |
| 8 | K7 | 138 | THR |
| 1 | L7 | 32 | THR |
| 1 | L7 | 157 | SER |
| 8 | M7 | 34 | GLU |
| 8 | M7 | 43 | LEU |
| 8 | M7 | 52 | LYS |
| 8 | M7 | 91 | LEU |
| 8 | M7 | 102 | THR |
| 8 | M7 | 138 | THR |
| 1 | N7 | 32 | THR |
| 1 | N7 | 157 | SER |
| 8 | g7 | 91 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | g7 | 138 | THR |
| 1 | h7 | 28 | LYS |
| 1 | h7 | 32 | THR |
| 1 | h7 | 39 | ARG |
| 1 | h7 | 44 | ILE |
| 1 | h7 | 49 | THR |
| 1 | h7 | 58 | LYS |
| 1 | h7 | 157 | SER |
| 8 | i7 | 34 | GLU |
| 8 | i7 | 43 | LEU |
| 8 | i7 | 91 | LEU |
| 8 | i7 | 102 | THR |
| 8 | i7 | 114 | GLU |
| 8 | i7 | 121 | THR |
| 8 | i7 | 123 | ILE |
| 8 | i7 | 128 | GLU |
| 8 | i7 | 131 | ARG |
| 8 | i7 | 138 | THR |
| 8 | i7 | 142 | SER |
| 1 | j7 | 32 | THR |
| 1 | j7 | 157 | SER |
| 8 | k7 | 34 | GLU |
| 8 | k7 | 43 | LEU |
| 8 | k7 | 91 | LEU |
| 8 | k7 | 102 | THR |
| 8 | k7 | 138 | THR |
| 1 | T7 | 32 | THR |
| 1 | T7 | 157 | SER |
| 8 | U7 | 19 | SER |
| 8 | U7 | 20 | PRO |
| 8 | U7 | 91 | LEU |
| 8 | U7 | 138 | THR |
| 1 | V7 | 32 | THR |
| 1 | V7 | 157 | SER |
| 8 | W7 | 34 | GLU |
| 8 | W7 | 43 | LEU |
| 8 | W7 | 91 | LEU |
| 8 | W7 | 102 | THR |
| 8 | W7 | 138 | THR |
| 1 | X7 | 32 | THR |
| 1 | X7 | 157 | SER |
| 8 | Y7 | 34 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | Y7 | 43 | LEU |
| 8 | Y7 | 52 | LYS |
| 8 | Y7 | 91 | LEU |
| 8 | Y7 | 102 | THR |
| 8 | Y7 | 138 | THR |
| 1 | Z7 | 32 | THR |
| 1 | Z7 | 157 | SER |
| 8 | a7 | 91 | LEU |
| 8 | a7 | 138 | THR |
| 1 | b7 | 28 | LYS |
| 1 | b7 | 32 | THR |
| 1 | b7 | 39 | ARG |
| 1 | b7 | 44 | ILE |
| 1 | b7 | 49 | THR |
| 1 | b7 | 58 | LYS |
| 1 | b7 | 157 | SER |
| 8 | c7 | 34 | GLU |
| 8 | c7 | 43 | LEU |
| 8 | c7 | 91 | LEU |
| 8 | c7 | 102 | THR |
| 8 | c7 | 114 | GLU |
| 8 | c7 | 121 | THR |
| 8 | c7 | 123 | ILE |
| 8 | c7 | 128 | GLU |
| 8 | c7 | 131 | ARG |
| 8 | c7 | 138 | THR |
| 8 | c7 | 142 | SER |
| 1 | d7 | 32 | THR |
| 1 | d7 | 157 | SER |
| 8 | e7 | 34 | GLU |
| 8 | e7 | 43 | LEU |
| 8 | e7 | 52 | LYS |
| 8 | e7 | 91 | LEU |
| 8 | e7 | 102 | THR |
| 8 | e7 | 138 | THR |
| 1 | f7 | 32 | THR |
| 1 | f7 | 157 | SER |
| 2 | E1 | 17 | ARG |
| 2 | E1 | 25 | GLN |
| 2 | E1 | 30 | ARG |
| 2 | E1 | 45 | THR |
| 2 | E1 | 115 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | E1 | 123 | SER |
| 2 | A8 | 17 | ARG |
| 2 | A8 | 25 | GLN |
| 2 | A8 | 30 | ARG |
| 2 | A8 | 45 | THR |
| 2 | A8 | 115 | GLU |
| 2 | A8 | 123 | SER |
| 3 | B8 | 6 | THR |
| 3 | B8 | 65 | ASP |
| 3 | B8 | 144 | SER |
| 2 | C8 | 17 | ARG |
| 2 | C8 | 25 | GLN |
| 2 | C8 | 30 | ARG |
| 2 | C8 | 45 | THR |
| 2 | C8 | 115 | GLU |
| 2 | C8 | 123 | SER |
| 3 | D8 | 6 | THR |
| 3 | D8 | 65 | ASP |
| 3 | D8 | 144 | SER |
| 2 | E8 | 17 | ARG |
| 2 | E8 | 25 | GLN |
| 2 | E8 | 30 | ARG |
| 2 | E8 | 45 | THR |
| 2 | E8 | 115 | GLU |
| 2 | E8 | 123 | SER |
| 1 | l7 | 32 | THR |
| 1 | l7 | 157 | SER |
| 8 | m7 | 20 | PRO |
| 8 | m7 | 22 | GLU |
| 8 | m7 | 91 | LEU |
| 8 | m7 | 138 | THR |
| 1 | n7 | 32 | THR |
| 1 | n7 | 157 | SER |
| 8 | o7 | 34 | GLU |
| 8 | o7 | 42 | THR |
| 8 | o7 | 45 | GLU |
| 8 | o7 | 47 | ARG |
| 8 | o7 | 49 | ARG |
| 8 | o7 | 58 | LEU |
| 8 | o7 | 82 | LEU |
| 8 | o7 | 91 | LEU |
| 8 | o7 | 102 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | o7 | 138 | THR |
| 1 | p7 | 32 | THR |
| 1 | p7 | 157 | SER |
| 8 | q7 | 34 | GLU |
| 8 | q7 | 43 | LEU |
| 8 | q7 | 52 | LYS |
| 8 | q7 | 91 | LEU |
| 8 | q7 | 102 | THR |
| 8 | q7 | 138 | THR |
| 1 | r7 | 32 | THR |
| 1 | r7 | 157 | SER |
| 8 | s7 | 19 | SER |
| 8 | s7 | 20 | PRO |
| 8 | s7 | 91 | LEU |
| 8 | s7 | 138 | THR |
| 1 | t7 | 32 | THR |
| 1 | t7 | 157 | SER |
| 8 | u7 | 34 | GLU |
| 8 | u7 | 42 | THR |
| 8 | u7 | 45 | GLU |
| 8 | u7 | 47 | ARG |
| 8 | u7 | 49 | ARG |
| 8 | u7 | 58 | LEU |
| 8 | u7 | 82 | LEU |
| 8 | u7 | 91 | LEU |
| 8 | u7 | 102 | THR |
| 8 | u7 | 138 | THR |
| 1 | v7 | 32 | THR |
| 1 | v7 | 157 | SER |
| 9 | z7 | 6 | LYS |
| 9 | z7 | 7 | VAL |
| 9 | z7 | 16 | ARG |
| 9 | z7 | 17 | VAL |
| 9 | z7 | 19 | THR |
| 9 | z7 | 21 | ARG |
| 9 | z7 | 26 | THR |
| 9 | z7 | 39 | THR |
| 9 | z7 | 40 | GLU |
| 9 | z7 | 41 | GLN |
| 9 | z7 | 51 | VAL |
| 9 | z7 | 52 | LEU |
| 9 | z7 | 55 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | z7 | 56 | LEU |
| 9 | z7 | 65 | THR |
| 9 | w7 | 6 | LYS |
| 9 | w7 | 7 | VAL |
| 9 | w7 | 16 | ARG |
| 9 | w7 | 17 | VAL |
| 9 | w7 | 19 | THR |
| 9 | w7 | 21 | ARG |
| 9 | w7 | 26 | THR |
| 9 | w7 | 39 | THR |
| 9 | w7 | 40 | GLU |
| 9 | w7 | 41 | GLN |
| 9 | w7 | 51 | VAL |
| 9 | w7 | 52 | LEU |
| 9 | w7 | 55 | LYS |
| 9 | w7 | 56 | LEU |
| 9 | w7 | 65 | THR |
| 9 | x7 | 11 | ILE |
| 9 | x7 | 14 | LEU |
| 9 | x7 | 21 | ARG |
| 9 | x7 | 22 | GLU |
| 9 | x7 | 23 | LEU |
| 9 | x7 | 29 | THR |
| 9 | x7 | 31 | LEU |
| 9 | x7 | 41 | GLN |
| 9 | x7 | 42 | GLN |
| 9 | x7 | 43 | ARG |
| 9 | x7 | 44 | ILE |
| 9 | x7 | 52 | LEU |
| 9 | x7 | 56 | LEU |
| 9 | x7 | 58 | THR |
| 9 | x7 | 61 | GLN |
| 9 | x7 | 64 | ASN |
| 9 | x7 | 65 | THR |
| 9 | y7 | 11 | ILE |
| 9 | y7 | 14 | LEU |
| 9 | y7 | 21 | ARG |
| 9 | y7 | 22 | GLU |
| 9 | y7 | 23 | LEU |
| 9 | y7 | 29 | THR |
| 9 | y7 | 31 | LEU |
| 9 | y7 | 41 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | y7 | 42 | GLN |
| 9 | y7 | 43 | ARG |
| 9 | y7 | 44 | ILE |
| 9 | y7 | 52 | LEU |
| 9 | y7 | 56 | LEU |
| 9 | y7 | 58 | THR |
| 9 | y7 | 61 | GLN |
| 9 | y7 | 64 | ASN |
| 9 | y7 | 65 | THR |
| 2 | T8 | 17 | ARG |
| 2 | T8 | 25 | GLN |
| 2 | T8 | 30 | ARG |
| 2 | T8 | 45 | THR |
| 2 | T8 | 115 | GLU |
| 2 | T8 | 123 | SER |
| 3 | U8 | 6 | THR |
| 3 | U8 | 65 | ASP |
| 3 | U8 | 144 | SER |
| 2 | V8 | 17 | ARG |
| 2 | V8 | 25 | GLN |
| 2 | V8 | 30 | ARG |
| 2 | V8 | 45 | THR |
| 2 | V8 | 115 | GLU |
| 2 | V8 | 123 | SER |
| 3 | W8 | 6 | THR |
| 3 | W8 | 65 | ASP |
| 3 | W8 | 144 | SER |
| 2 | X8 | 17 | ARG |
| 2 | X8 | 25 | GLN |
| 2 | X8 | 30 | ARG |
| 2 | X8 | 45 | THR |
| 2 | X8 | 115 | GLU |
| 2 | X8 | 123 | SER |
| 3 | F8 | 6 | THR |
| 3 | F8 | 65 | ASP |
| 3 | F8 | 111 | ASN |
| 3 | F8 | 113 | LEU |
| 3 | F8 | 144 | SER |
| 2 | G8 | 17 | ARG |
| 2 | G8 | 25 | GLN |
| 2 | G8 | 30 | ARG |
| 2 | G8 | 45 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | G8 | 115 | GLU |
| 2 | G8 | 123 | SER |
| 3 | H8 | 6 | THR |
| 3 | H8 | 65 | ASP |
| 3 | H8 | 144 | SER |
| 2 | I8 | 17 | ARG |
| 2 | I8 | 25 | GLN |
| 2 | I8 | 30 | ARG |
| 2 | I8 | 45 | THR |
| 2 | I8 | 115 | GLU |
| 2 | I8 | 123 | SER |
| 3 | J8 | 6 | THR |
| 3 | J8 | 65 | ASP |
| 3 | J8 | 144 | SER |
| 2 | K8 | 17 | ARG |
| 2 | K8 | 25 | GLN |
| 2 | K8 | 30 | ARG |
| 2 | K8 | 45 | THR |
| 2 | K8 | 115 | GLU |
| 2 | K8 | 123 | SER |
| 3 | L8 | 6 | THR |
| 3 | L8 | 65 | ASP |
| 3 | L8 | 144 | SER |
| 4 | M8 | 4 | LEU |
| 4 | M8 | 7 | SER |
| 4 | M8 | 13 | LYS |
| 4 | M8 | 19 | MET |
| 4 | M8 | 25 | LEU |
| 4 | M8 | 33 | LEU |
| 4 | M8 | 44 | SER |
| 4 | M8 | 45 | VAL |
| 4 | M8 | 50 | ASP |
| 4 | M8 | 51 | ARG |
| 4 | M8 | 52 | LEU |
| 4 | M8 | 65 | ARG |
| 4 | M8 | 68 | ASP |
| 4 | M8 | 69 | ILE |
| 4 | M8 | 73 | ASP |
| 4 | M8 | 74 | LEU |
| 4 | M8 | 77 | LEU |
| 4 | M8 | 79 | PRO |
| 4 | M8 | 87 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | M8 | 96 | LYS |
| 4 | M8 | 98 | ASP |
| 4 | M8 | 113 | ILE |
| 4 | M8 | 123 | GLU |
| 4 | M8 | 124 | ARG |
| 4 | M8 | 125 | LEU |
| 4 | M8 | 130 | SER |
| 4 | M8 | 132 | LEU |
| 4 | M8 | 137 | ILE |
| 4 | M8 | 139 | VAL |
| 4 | M8 | 146 | LEU |
| 4 | M8 | 151 | LEU |
| 4 | M8 | 155 | ARG |
| 4 | M8 | 162 | ASN |
| 4 | M8 | 166 | THR |
| 4 | M8 | 167 | GLU |
| 4 | M8 | 176 | ARG |
| 4 | M8 | 184 | ILE |
| 4 | M8 | 189 | ASP |
| 4 | M8 | 200 | ILE |
| 4 | M8 | 202 | SER |
| 4 | M8 | 211 | GLN |
| 4 | M8 | 227 | GLN |
| 4 | M8 | 231 | THR |
| 4 | M8 | 232 | VAL |
| 4 | M8 | 241 | LEU |
| 4 | M8 | 251 | ASN |
| 4 | M8 | 255 | GLN |
| 4 | M8 | 257 | GLN |
| 4 | M8 | 261 | VAL |
| 4 | M8 | 266 | LEU |
| 4 | M8 | 271 | ARG |
| 4 | M8 | 273 | ILE |
| 4 | M8 | 274 | VAL |
| 2 | N8 | 17 | ARG |
| 2 | N8 | 25 | GLN |
| 2 | N8 | 30 | ARG |
| 2 | N8 | 45 | THR |
| 2 | N8 | 123 | SER |
| 3 | O8 | 6 | THR |
| 3 | O8 | 65 | ASP |
| 3 | O8 | 109 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | O8 | 144 | SER |
| 2 | P8 | 17 | ARG |
| 2 | P8 | 25 | GLN |
| 2 | P8 | 30 | ARG |
| 2 | P8 | 45 | THR |
| 2 | P8 | 115 | GLU |
| 2 | P8 | 123 | SER |
| 3 | Q8 | 6 | THR |
| 3 | Q8 | 65 | ASP |
| 3 | Q8 | 104 | VAL |
| 3 | Q8 | 105 | LEU |
| 3 | Q8 | 109 | CYS |
| 3 | Q8 | 113 | LEU |
| 3 | Q8 | 144 | SER |
| 2 | R8 | 17 | ARG |
| 2 | R8 | 25 | GLN |
| 2 | R8 | 30 | ARG |
| 2 | R8 | 45 | THR |
| 2 | R8 | 115 | GLU |
| 2 | R8 | 123 | SER |
| 3 | S8 | 6 | THR |
| 3 | S8 | 65 | ASP |
| 3 | S8 | 144 | SER |
| 3 | F1 | 6 | THR |
| 3 | F1 | 65 | ASP |
| 3 | F1 | 144 | SER |
| 3 | L9 | 6 | THR |
| 3 | L9 | 65 | ASP |
| 3 | L9 | 84 | ARG |
| 3 | L9 | 88 | ILE |
| 3 | L9 | 94 | SER |
| 3 | L9 | 97 | LEU |
| 3 | L9 | 98 | LEU |
| 3 | L9 | 115 | GLU |
| 3 | L9 | 116 | THR |
| 3 | L9 | 144 | SER |
| 4 | M9 | 4 | LEU |
| 4 | M9 | 13 | LYS |
| 4 | M9 | 19 | MET |
| 4 | M9 | 25 | LEU |
| 4 | M9 | 33 | LEU |
| 4 | M9 | 44 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | M9 | 45 | VAL |
| 4 | M9 | 50 | ASP |
| 4 | M9 | 51 | ARG |
| 4 | M9 | 52 | LEU |
| 4 | M9 | 65 | ARG |
| 4 | M9 | 68 | ASP |
| 4 | M9 | 69 | ILE |
| 4 | M9 | 73 | ASP |
| 4 | M9 | 74 | LEU |
| 4 | M9 | 77 | LEU |
| 4 | M9 | 79 | PRO |
| 4 | M9 | 87 | ILE |
| 4 | M9 | 92 | GLU |
| 4 | M9 | 100 | SER |
| 4 | M9 | 101 | ASP |
| 4 | M9 | 113 | ILE |
| 4 | M9 | 123 | GLU |
| 4 | M9 | 124 | ARG |
| 4 | M9 | 125 | LEU |
| 4 | M9 | 130 | SER |
| 4 | M9 | 132 | LEU |
| 4 | M9 | 137 | ILE |
| 4 | M9 | 141 | GLU |
| 4 | M9 | 146 | LEU |
| 4 | M9 | 151 | LEU |
| 4 | M9 | 155 | ARG |
| 4 | M9 | 162 | ASN |
| 4 | M9 | 166 | THR |
| 4 | M9 | 167 | GLU |
| 4 | M9 | 176 | ARG |
| 4 | M9 | 184 | ILE |
| 4 | M9 | 189 | ASP |
| 4 | M9 | 200 | ILE |
| 4 | M9 | 202 | SER |
| 4 | M9 | 211 | GLN |
| 4 | M9 | 227 | GLN |
| 4 | M9 | 230 | GLN |
| 4 | M9 | 232 | VAL |
| 4 | M9 | 241 | LEU |
| 4 | M9 | 251 | ASN |
| 4 | M9 | 255 | GLN |
| 4 | M9 | 257 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | M9 | 261 | VAL |
| 4 | M9 | 266 | LEU |
| 4 | M9 | 271 | ARG |
| 4 | M9 | 273 | ILE |
| 4 | M9 | 274 | VAL |
| 5 | N9 | 4 | LEU |
| 5 | N9 | 7 | ASP |
| 5 | N9 | 8 | ASN |
| 5 | N9 | 9 | GLN |
| 5 | N9 | 13 | SER |
| 5 | N9 | 14 | LYS |
| 5 | N9 | 15 | LEU |
| 5 | N9 | 17 | LYS |
| 5 | N9 | 18 | ILE |
| 5 | N9 | 20 | ILE |
| 5 | N9 | 22 | LEU |
| 5 | N9 | 26 | LEU |
| 5 | N9 | 30 | PRO |
| 5 | N9 | 34 | LEU |
| 5 | N9 | 41 | GLN |
| 5 | N9 | 46 | THR |
| 5 | N9 | 50 | LEU |
| 5 | N9 | 51 | GLU |
| 5 | N9 | 53 | LEU |
| 5 | N9 | 55 | PRO |
| 5 | N9 | 59 | ARG |
| 5 | N9 | 60 | ILE |
| 5 | N9 | 66 | ARG |
| 5 | N9 | 67 | ILE |
| 5 | N9 | 69 | GLU |
| 5 | N9 | 70 | ILE |
| 5 | N9 | 74 | GLU |
| 2 | O9 | 17 | ARG |
| 2 | O9 | 25 | GLN |
| 2 | O9 | 30 | ARG |
| 2 | O9 | 45 | THR |
| 2 | O9 | 115 | GLU |
| 2 | O9 | 123 | SER |
| 3 | P9 | 6 | THR |
| 3 | P9 | 65 | ASP |
| 3 | P9 | 144 | SER |
| 2 | Q9 | 17 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | Q9 | 25 | GLN |
| 2 | Q9 | 30 | ARG |
| 2 | Q9 | 45 | THR |
| 2 | Q9 | 115 | GLU |
| 2 | Q9 | 123 | SER |
| 3 | Y8 | 6 | THR |
| 3 | Y8 | 65 | ASP |
| 3 | Y8 | 105 | LEU |
| 3 | Y8 | 115 | GLU |
| 3 | Y8 | 118 | VAL |
| 3 | Y8 | 144 | SER |
| 5 | Z8 | 13 | SER |
| 5 | Z8 | 14 | LYS |
| 5 | Z8 | 15 | LEU |
| 5 | Z8 | 17 | LYS |
| 5 | Z8 | 18 | ILE |
| 5 | Z8 | 20 | ILE |
| 5 | Z8 | 22 | LEU |
| 5 | Z8 | 26 | LEU |
| 5 | Z8 | 30 | PRO |
| 5 | Z8 | 50 | LEU |
| 5 | Z8 | 51 | GLU |
| 5 | Z8 | 53 | LEU |
| 5 | Z8 | 55 | PRO |
| 5 | Z8 | 59 | ARG |
| 5 | Z8 | 60 | ILE |
| 5 | Z8 | 66 | ARG |
| 5 | Z8 | 67 | ILE |
| 5 | Z8 | 69 | GLU |
| 5 | Z8 | 70 | ILE |
| 5 | Z8 | 74 | GLU |
| 2 | A9 | 17 | ARG |
| 2 | A9 | 25 | GLN |
| 2 | A9 | 30 | ARG |
| 2 | A9 | 45 | THR |
| 2 | A9 | 115 | GLU |
| 2 | A9 | 123 | SER |
| 3 | B9 | 67 | ILE |
| 3 | B9 | 144 | SER |
| 2 | C9 | 17 | ARG |
| 2 | C9 | 25 | GLN |
| 2 | C9 | 30 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C9 | 45 | THR |
| 2 | C9 | 115 | GLU |
| 2 | C9 | 123 | SER |
| 3 | D9 | 6 | THR |
| 3 | D9 | 65 | ASP |
| 3 | D9 | 144 | SER |
| 2 | E9 | 17 | ARG |
| 2 | E9 | 25 | GLN |
| 2 | E9 | 30 | ARG |
| 2 | E9 | 45 | THR |
| 2 | E9 | 115 | GLU |
| 2 | E9 | 123 | SER |
| 3 | F9 | 6 | THR |
| 3 | F9 | 65 | ASP |
| 3 | F9 | 144 | SER |
| 3 | F9 | 146 | SER |
| 3 | F9 | 156 | LEU |
| 2 | G9 | 17 | ARG |
| 2 | G9 | 25 | GLN |
| 2 | G9 | 30 | ARG |
| 2 | G9 | 45 | THR |
| 2 | G9 | 115 | GLU |
| 2 | G9 | 123 | SER |
| 3 | H9 | 6 | THR |
| 3 | H9 | 65 | ASP |
| 3 | H9 | 108 | ARG |
| 3 | H9 | 144 | SER |
| 2 | I9 | 25 | GLN |
| 2 | I9 | 30 | ARG |
| 2 | I9 | 45 | THR |
| 2 | I9 | 115 | GLU |
| 2 | I9 | 123 | SER |
| 3 | J9 | 6 | THR |
| 3 | J9 | 65 | ASP |
| 3 | J9 | 144 | SER |
| 2 | K9 | 17 | ARG |
| 2 | K9 | 23 | GLU |
| 2 | K9 | 30 | ARG |
| 2 | K9 | 45 | THR |
| 2 | K9 | 115 | GLU |
| 2 | K9 | 123 | SER |
| 3 | R9 | 6 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | R9 | 65 | ASP |
| 3 | R9 | 144 | SER |
| 2 | S9 | 17 | ARG |
| 2 | S9 | 25 | GLN |
| 2 | S9 | 30 | ARG |
| 2 | S9 | 45 | THR |
| 2 | S9 | 115 | GLU |
| 2 | S9 | 123 | SER |
| 3 | T9 | 6 | THR |
| 3 | T9 | 65 | ASP |
| 3 | T9 | 144 | SER |
| 2 | U9 | 17 | ARG |
| 2 | U9 | 25 | GLN |
| 2 | U9 | 30 | ARG |
| 2 | U9 | 45 | THR |
| 2 | U9 | 115 | GLU |
| 2 | U9 | 123 | SER |
| 3 | V9 | 6 | THR |
| 3 | V9 | 65 | ASP |
| 3 | V9 | 108 | ARG |
| 3 | V9 | 144 | SER |
| 2 | W9 | 17 | ARG |
| 2 | W9 | 25 | GLN |
| 2 | W9 | 30 | ARG |
| 2 | W9 | 45 | THR |
| 2 | W9 | 115 | GLU |
| 2 | W9 | 123 | SER |
| 3 | X9 | 65 | ASP |
| 3 | X9 | 144 | SER |
| 2 | Y9 | 17 | ARG |
| 2 | Y9 | 25 | GLN |
| 2 | Y9 | 30 | ARG |
| 2 | Y9 | 45 | THR |
| 2 | Y9 | 115 | GLU |
| 2 | Y9 | 123 | SER |
| 3 | Z9 | 65 | ASP |
| 3 | Z9 | 84 | ARG |
| 3 | Z9 | 144 | SER |
| 2 | G1 | 17 | ARG |
| 2 | G1 | 25 | GLN |
| 2 | G1 | 30 | ARG |
| 2 | G1 | 45 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | G1 | 115 | GLU |
| 2 | G1 | 123 | SER |
| 11 | a9 | 21 | THR |
| 11 | a9 | 29 | ARG |
| 11 | a9 | 31 | SER |
| 11 | a9 | 32 | ARG |
| 11 | a9 | 33 | MET |
| 11 | a9 | 34 | ILE |
| 11 | a9 | 35 | ARG |
| 11 | a9 | 38 | VAL |
| 11 | a9 | 40 | GLU |
| 11 | a9 | 42 | ARG |
| 11 | a9 | 48 | LEU |
| 11 | a9 | 52 | MET |
| 11 | a9 | 62 | MET |
| 11 | a9 | 64 | ARG |
| 11 | a9 | 71 | ILE |
| 11 | a9 | 73 | TYR |
| 11 | a9 | 86 | ASP |
| 11 | a9 | 92 | LYS |
| 11 | a9 | 93 | LEU |
| 11 | a9 | 95 | ILE |
| 11 | a9 | 106 | LEU |
| 11 | a9 | 111 | THR |
| 11 | a9 | 173 | THR |
| 11 | a9 | 258 | ASP |
| 11 | a9 | 266 | ASN |
| 11 | a9 | 276 | SER |
| 11 | a9 | 278 | LEU |
| 11 | a9 | 280 | ASP |
| 11 | a9 | 285 | VAL |
| 11 | a9 | 286 | ARG |
| 11 | a9 | 288 | ARG |
| 11 | a9 | 289 | THR |
| 11 | a9 | 290 | ASP |
| 11 | a9 | 294 | THR |
| 11 | a9 | 307 | ARG |
| 11 | a9 | 312 | ASP |
| 11 | a9 | 313 | GLU |
| 11 | a9 | 314 | SER |
| 11 | a9 | 315 | LEU |
| 11 | a9 | 319 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | a9 | 323 | ARG |
| 11 | a9 | 325 | LEU |
| 11 | a9 | 328 | GLN |
| 11 | a9 | 332 | SER |
| 11 | a9 | 333 | GLN |
| 11 | a9 | 337 | GLU |
| 11 | a9 | 338 | VAL |
| 11 | a9 | 348 | GLN |
| 11 | a9 | 350 | LEU |
| 11 | a9 | 354 | VAL |
| 11 | a9 | 355 | GLU |
| 11 | a9 | 357 | THR |
| 11 | a9 | 358 | PRO |
| 11 | a9 | 363 | GLN |
| 11 | a9 | 365 | LYS |
| 11 | a9 | 366 | LEU |
| 11 | a9 | 375 | GLN |
| 11 | a9 | 379 | LEU |
| 11 | a9 | 387 | GLU |
| 11 | a9 | 388 | VAL |
| 11 | a9 | 399 | ILE |
| 11 | a9 | 405 | ILE |
| 11 | a9 | 411 | VAL |
| 11 | a9 | 415 | GLU |
| 11 | a9 | 416 | SER |
| 11 | a9 | 419 | ARG |
| 11 | a9 | 426 | ARG |
| 11 | a9 | 427 | GLU |
| 11 | a9 | 431 | LEU |
| 11 | a9 | 437 | LEU |
| 11 | a9 | 439 | ARG |
| 11 | a9 | 445 | THR |
| 11 | a9 | 454 | LEU |
| 11 | a9 | 455 | ASN |
| 11 | a9 | 460 | LEU |
| 11 | a9 | 462 | ARG |
| 11 | a9 | 470 | ILE |
| 11 | a9 | 479 | LYS |
| 11 | a9 | 490 | ILE |
| 11 | a9 | 498 | VAL |
| 11 | a9 | 508 | ARG |
| 11 | a9 | 519 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | a9 | 522 | ASP |
| 11 | a9 | 526 | GLN |
| 11 | a9 | 531 | ASP |
| 11 | a9 | 538 | ARG |
| 11 | a9 | 543 | GLN |
| 11 | a9 | 549 | THR |
| 11 | a9 | 556 | LEU |
| 11 | a9 | 559 | THR |
| 11 | a9 | 562 | TYR |
| 11 | a9 | 574 | ASP |
| 11 | a9 | 576 | LEU |
| 11 | a9 | 580 | THR |
| 11 | a9 | 585 | GLU |
| 11 | a9 | 586 | LEU |
| 11 | a9 | 591 | VAL |
| 11 | a9 | 594 | ARG |
| 11 | a9 | 597 | THR |
| 11 | a9 | 600 | THR |
| 11 | a9 | 602 | PRO |
| 11 | a9 | 603 | THR |
| 11 | a9 | 605 | PRO |
| 11 | a9 | 607 | MET |
| 11 | a9 | 609 | LEU |
| 11 | a9 | 615 | ARG |
| 11 | a9 | 619 | ARG |
| 11 | a9 | 621 | THR |
| 11 | a9 | 623 | ASP |
| 11 | a9 | 628 | THR |
| 11 | a9 | 629 | LYS |
| 11 | a9 | 630 | LEU |
| 11 | a9 | 632 | ILE |
| 11 | a9 | 635 | VAL |
| 11 | a9 | 637 | PRO |
| 11 | a9 | 639 | GLN |
| 11 | a9 | 641 | VAL |
| 11 | a9 | 643 | LEU |
| 11 | a9 | 730 | ASN |
| 11 | a9 | 778 | THR |
| 11 | a9 | 795 | ASP |
| 11 | a9 | 801 | ASN |
| 11 | a9 | 802 | ARG |
| 11 | a9 | 814 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | a9 | 816 | LEU |
| 11 | a9 | 818 | ARG |
| 11 | a9 | 823 | ILE |
| 11 | aA | 21 | THR |
| 11 | aA | 29 | ARG |
| 11 | aA | 31 | SER |
| 11 | aA | 32 | ARG |
| 11 | aA | 33 | MET |
| 11 | aA | 34 | ILE |
| 11 | aA | 35 | ARG |
| 11 | aA | 38 | VAL |
| 11 | aA | 40 | GLU |
| 11 | aA | 42 | ARG |
| 11 | aA | 48 | LEU |
| 11 | aA | 52 | MET |
| 11 | aA | 62 | MET |
| 11 | aA | 64 | ARG |
| 11 | aA | 71 | ILE |
| 11 | aA | 73 | TYR |
| 11 | aA | 86 | ASP |
| 11 | aA | 92 | LYS |
| 11 | aA | 93 | LEU |
| 11 | aA | 95 | ILE |
| 11 | aA | 106 | LEU |
| 11 | aA | 111 | THR |
| 11 | aA | 173 | THR |
| 11 | aA | 258 | ASP |
| 11 | aA | 266 | ASN |
| 11 | aA | 276 | SER |
| 11 | aA | 278 | LEU |
| 11 | aA | 280 | ASP |
| 11 | aA | 285 | VAL |
| 11 | aA | 286 | ARG |
| 11 | aA | 288 | ARG |
| 11 | aA | 289 | THR |
| 11 | aA | 290 | ASP |
| 11 | aA | 297 | ASP |
| 11 | aA | 302 | ASN |
| 11 | aA | 307 | ARG |
| 11 | aA | 312 | ASP |
| 11 | aA | 313 | GLU |
| 11 | aA | 314 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | aA | 315 | LEU |
| 11 | aA | 319 | LEU |
| 11 | aA | 323 | ARG |
| 11 | aA | 325 | LEU |
| 11 | aA | 328 | GLN |
| 11 | aA | 332 | SER |
| 11 | aA | 333 | GLN |
| 11 | aA | 337 | GLU |
| 11 | aA | 338 | VAL |
| 11 | aA | 348 | GLN |
| 11 | aA | 350 | LEU |
| 11 | aA | 354 | VAL |
| 11 | aA | 355 | GLU |
| 11 | aA | 357 | THR |
| 11 | aA | 358 | PRO |
| 11 | aA | 363 | GLN |
| 11 | aA | 365 | LYS |
| 11 | aA | 366 | LEU |
| 11 | aA | 375 | GLN |
| 11 | aA | 379 | LEU |
| 11 | aA | 387 | GLU |
| 11 | aA | 388 | VAL |
| 11 | aA | 399 | ILE |
| 11 | aA | 405 | ILE |
| 11 | aA | 411 | VAL |
| 11 | aA | 415 | GLU |
| 11 | aA | 416 | SER |
| 11 | aA | 419 | ARG |
| 11 | aA | 426 | ARG |
| 11 | aA | 427 | GLU |
| 11 | aA | 431 | LEU |
| 11 | aA | 437 | LEU |
| 11 | aA | 439 | ARG |
| 11 | aA | 445 | THR |
| 11 | aA | 454 | LEU |
| 11 | aA | 455 | ASN |
| 11 | aA | 460 | LEU |
| 11 | aA | 462 | ARG |
| 11 | aA | 470 | ILE |
| 11 | aA | 479 | LYS |
| 11 | aA | 490 | ILE |
| 11 | aA | 498 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | aA | 508 | ARG |
| 11 | aA | 519 | ARG |
| 11 | aA | 522 | ASP |
| 11 | aA | 526 | GLN |
| 11 | aA | 531 | ASP |
| 11 | aA | 538 | ARG |
| 11 | aA | 543 | GLN |
| 11 | aA | 549 | THR |
| 11 | aA | 553 | SER |
| 11 | aA | 554 | ARG |
| 11 | aA | 556 | LEU |
| 11 | aA | 559 | THR |
| 11 | aA | 562 | TYR |
| 11 | aA | 574 | ASP |
| 11 | aA | 576 | LEU |
| 11 | aA | 580 | THR |
| 11 | aA | 585 | GLU |
| 11 | aA | 586 | LEU |
| 11 | aA | 591 | VAL |
| 11 | aA | 594 | ARG |
| 11 | aA | 597 | THR |
| 11 | aA | 600 | THR |
| 11 | aA | 602 | PRO |
| 11 | aA | 603 | THR |
| 11 | aA | 605 | PRO |
| 11 | aA | 607 | MET |
| 11 | aA | 609 | LEU |
| 11 | aA | 615 | ARG |
| 11 | aA | 619 | ARG |
| 11 | aA | 621 | THR |
| 11 | aA | 623 | ASP |
| 11 | aA | 628 | THR |
| 11 | aA | 629 | LYS |
| 11 | aA | 630 | LEU |
| 11 | aA | 632 | ILE |
| 11 | aA | 635 | VAL |
| 11 | aA | 637 | PRO |
| 11 | aA | 639 | GLN |
| 11 | aA | 641 | VAL |
| 11 | aA | 643 | LEU |
| 11 | aA | 730 | ASN |
| 11 | aA | 778 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | aA | 795 | ASP |
| 11 | aA | 801 | ASN |
| 11 | aA | 814 | GLN |
| 11 | aA | 816 | LEU |
| 11 | aA | 818 | ARG |
| 11 | aA | 823 | ILE |
| 11 | aA | 824 | VAL |
| 3 | H1 | 6 | THR |
| 3 | H1 | 65 | ASP |
| 3 | H1 | 144 | SER |
| 2 | I1 | 17 | ARG |
| 2 | I1 | 25 | GLN |
| 2 | I1 | 30 | ARG |
| 2 | I1 | 45 | THR |
| 2 | I1 | 115 | GLU |
| 2 | I1 | 123 | SER |
| 3 | J1 | 6 | THR |
| 3 | J1 | 65 | ASP |
| 3 | J1 | 144 | SER |
| 2 | K1 | 17 | ARG |
| 2 | K1 | 25 | GLN |
| 2 | K1 | 30 | ARG |
| 2 | K1 | 45 | THR |
| 2 | K1 | 123 | SER |
| 3 | L1 | 6 | THR |
| 3 | L1 | 65 | ASP |
| 3 | L1 | 144 | SER |
| 4 | M1 | 4 | LEU |
| 4 | M1 | 13 | LYS |
| 4 | M1 | 19 | MET |
| 4 | M1 | 25 | LEU |
| 4 | M1 | 33 | LEU |
| 4 | M1 | 44 | SER |
| 4 | M1 | 45 | VAL |
| 4 | M1 | 50 | ASP |
| 4 | M1 | 51 | ARG |
| 4 | M1 | 52 | LEU |
| 4 | M1 | 65 | ARG |
| 4 | M1 | 68 | ASP |
| 4 | M1 | 69 | ILE |
| 4 | M1 | 73 | ASP |
| 4 | M1 | 74 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | M1 | 77 | LEU |
| 4 | M1 | 79 | PRO |
| 4 | M1 | 87 | ILE |
| 4 | M1 | 92 | GLU |
| 4 | M1 | 100 | SER |
| 4 | M1 | 101 | ASP |
| 4 | M1 | 113 | ILE |
| 4 | M1 | 123 | GLU |
| 4 | M1 | 124 | ARG |
| 4 | M1 | 125 | LEU |
| 4 | M1 | 130 | SER |
| 4 | M1 | 132 | LEU |
| 4 | M1 | 137 | ILE |
| 4 | M1 | 141 | GLU |
| 4 | M1 | 146 | LEU |
| 4 | M1 | 151 | LEU |
| 4 | M1 | 155 | ARG |
| 4 | M1 | 162 | ASN |
| 4 | M1 | 166 | THR |
| 4 | M1 | 167 | GLU |
| 4 | M1 | 176 | ARG |
| 4 | M1 | 184 | ILE |
| 4 | M1 | 189 | ASP |
| 4 | M1 | 200 | ILE |
| 4 | M1 | 202 | SER |
| 4 | M1 | 211 | GLN |
| 4 | M1 | 227 | GLN |
| 4 | M1 | 230 | GLN |
| 4 | M1 | 232 | VAL |
| 4 | M1 | 241 | LEU |
| 4 | M1 | 251 | ASN |
| 4 | M1 | 255 | GLN |
| 4 | M1 | 257 | GLN |
| 4 | M1 | 261 | VAL |
| 4 | M1 | 266 | LEU |
| 4 | M1 | 271 | ARG |
| 4 | M1 | 273 | ILE |
| 4 | M1 | 274 | VAL |
| 5 | N1 | 4 | LEU |
| 5 | N1 | 7 | ASP |
| 5 | N1 | 8 | ASN |
| 5 | N1 | 13 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | N1 | 14 | LYS |
| 5 | N1 | 15 | LEU |
| 5 | N1 | 17 | LYS |
| 5 | N1 | 18 | ILE |
| 5 | N1 | 20 | ILE |
| 5 | N1 | 22 | LEU |
| 5 | N1 | 26 | LEU |
| 5 | N1 | 30 | PRO |
| 5 | N1 | 34 | LEU |
| 5 | N1 | 41 | GLN |
| 5 | N1 | 46 | THR |
| 5 | N1 | 50 | LEU |
| 5 | N1 | 51 | GLU |
| 5 | N1 | 53 | LEU |
| 5 | N1 | 55 | PRO |
| 5 | N1 | 59 | ARG |
| 5 | N1 | 60 | ILE |
| 5 | N1 | 66 | ARG |
| 5 | N1 | 67 | ILE |
| 5 | N1 | 69 | GLU |
| 5 | N1 | 70 | ILE |
| 5 | N1 | 74 | GLU |
| 3 | T1 | 6 | THR |
| 3 | T1 | 65 | ASP |
| 3 | T1 | 144 | SER |
| 2 | U1 | 17 | ARG |
| 2 | U1 | 25 | GLN |
| 2 | U1 | 30 | ARG |
| 2 | U1 | 45 | THR |
| 2 | U1 | 46 | SER |
| 2 | U1 | 47 | ASN |
| 2 | U1 | 115 | GLU |
| 2 | U1 | 123 | SER |
| 3 | V1 | 6 | THR |
| 3 | V1 | 65 | ASP |
| 3 | V1 | 144 | SER |
| 2 | W1 | 17 | ARG |
| 2 | W1 | 25 | GLN |
| 2 | W1 | 30 | ARG |
| 2 | W1 | 45 | THR |
| 2 | W1 | 115 | GLU |
| 2 | W1 | 123 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | X1 | 6 | THR |
| 3 | X1 | 65 | ASP |
| 3 | X1 | 144 | SER |
| 2 | Y1 | 17 | ARG |
| 2 | Y1 | 25 | GLN |
| 2 | Y1 | 30 | ARG |
| 2 | Y1 | 45 | THR |
| 2 | Y1 | 115 | GLU |
| 2 | Y1 | 123 | SER |
| 3 | Z1 | 6 | THR |
| 3 | Z1 | 57 | HIS |
| 3 | Z1 | 65 | ASP |
| 3 | Z1 | 144 | SER |
| 2 | A2 | 17 | ARG |
| 2 | A2 | 25 | GLN |
| 2 | A2 | 30 | ARG |
| 2 | A2 | 45 | THR |
| 2 | A2 | 115 | GLU |
| 2 | A2 | 123 | SER |
| 3 | B2 | 6 | THR |
| 3 | B2 | 65 | ASP |
| 3 | B2 | 77 | ARG |
| 3 | B2 | 144 | SER |
| 2 | C2 | 17 | ARG |
| 2 | C2 | 25 | GLN |
| 2 | C2 | 30 | ARG |
| 2 | C2 | 45 | THR |
| 2 | C2 | 115 | GLU |
| 2 | C2 | 123 | SER |
| 3 | D2 | 6 | THR |
| 3 | D2 | 65 | ASP |
| 3 | D2 | 144 | SER |
| 2 | E2 | 17 | ARG |
| 2 | E2 | 25 | GLN |
| 2 | E2 | 30 | ARG |
| 2 | E2 | 45 | THR |
| 2 | E2 | 115 | GLU |
| 2 | E2 | 123 | SER |
| 3 | F2 | 6 | THR |
| 3 | F2 | 65 | ASP |
| 3 | F2 | 144 | SER |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (542)

such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 11 | ASN |
| 1 | A | 110 | ASN |
| 1 | Z | 11 | ASN |
| 2 | AA | 88 | HIS |
| 2 | AA | 145 | GLN |
| 3 | BA | 2 | GLN |
| 2 | CA | 88 | HIS |
| 3 | DA | 2 | GLN |
| 2 | EA | 21 | ASN |
| 2 | EA | 88 | HIS |
| 3 | FA | 2 | GLN |
| 3 | FA | 47 | ASN |
| 2 | GA | 88 | HIS |
| 3 | HA | 2 | GLN |
| 2 | IA | 15 | GLN |
| 2 | IA | 25 | GLN |
| 2 | IA | 88 | HIS |
| 3 | JA | 2 | GLN |
| 2 | KA | 88 | HIS |
| 3 | LA | 2 | GLN |
| 4 | MA | 40 | GLN |
| 4 | MA | 41 | ASN |
| 4 | MA | 163 | ASN |
| 4 | MA | 172 | HIS |
| 4 | MA | 216 | ASN |
| 4 | MA | 227 | GLN |
| 4 | MA | 251 | ASN |
| 4 | MA | 257 | GLN |
| 5 | NA | 29 | HIS |
| 5 | NA | 37 | HIS |
| 5 | NA | 41 | GLN |
| 2 | OA | 88 | HIS |
| 2 | OA | 145 | GLN |
| 3 | PA | 2 | GLN |
| 3 | PA | 111 | ASN |
| 2 | QA | 25 | GLN |
| 3 | RA | 2 | GLN |
| 3 | RA | 111 | ASN |
| 2 | SA | 88 | HIS |
| 3 | TA | 2 | GLN |
| 3 | TA | 57 | HIS |
| 3 | TA | 76 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | UA | 28 | ASN |
| 2 | UA | 88 | HIS |
| 3 | VA | 2 | GLN |
| 2 | WA | 88 | HIS |
| 3 | XA | 2 | GLN |
| 2 | YA | 88 | HIS |
| 3 | ZA | 2 | GLN |
| 3 | ZA | 111 | ASN |
| 2 | O1 | 145 | GLN |
| 3 | P1 | 2 | GLN |
| 3 | P1 | 111 | ASN |
| 2 | Q1 | 88 | HIS |
| 3 | R1 | 2 | GLN |
| 3 | R1 | 111 | ASN |
| 2 | S1 | 88 | HIS |
| 2 | A1 | 88 | HIS |
| 2 | A1 | 145 | GLN |
| 2 | G3 | 88 | HIS |
| 3 | H3 | 2 | GLN |
| 3 | H3 | 111 | ASN |
| 2 | I3 | 88 | HIS |
| 3 | J3 | 2 | GLN |
| 3 | J3 | 111 | ASN |
| 2 | K3 | 88 | HIS |
| 2 | G2 | 88 | HIS |
| 3 | H2 | 2 | GLN |
| 2 | I2 | 88 | HIS |
| 3 | J2 | 2 | GLN |
| 2 | K2 | 88 | HIS |
| 3 | L2 | 2 | GLN |
| 3 | L2 | 132 | GLN |
| 6 | M2 | 74 | GLN |
| 6 | M2 | 160 | ASN |
| 6 | M2 | 178 | HIS |
| 6 | M2 | 227 | GLN |
| 7 | N2 | 53 | GLN |
| 2 | A3 | 145 | GLN |
| 3 | B3 | 2 | GLN |
| 2 | C3 | 88 | HIS |
| 3 | D3 | 2 | GLN |
| 2 | E3 | 88 | HIS |
| 3 | F3 | 2 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | Z3 | 2 | GLN |
| 2 | A4 | 88 | HIS |
| 2 | A4 | 145 | GLN |
| 3 | B4 | 2 | GLN |
| 3 | B4 | 111 | ASN |
| 2 | C4 | 88 | HIS |
| 3 | D4 | 2 | GLN |
| 3 | L3 | 2 | GLN |
| 3 | L3 | 111 | ASN |
| 4 | M3 | 27 | HIS |
| 4 | M3 | 40 | GLN |
| 4 | M3 | 41 | ASN |
| 4 | M3 | 163 | ASN |
| 4 | M3 | 172 | HIS |
| 4 | M3 | 181 | GLN |
| 4 | M3 | 216 | ASN |
| 4 | M3 | 227 | GLN |
| 4 | M3 | 251 | ASN |
| 4 | M3 | 257 | GLN |
| 5 | N3 | 9 | GLN |
| 5 | N3 | 29 | HIS |
| 5 | N3 | 37 | HIS |
| 5 | N3 | 41 | GLN |
| 2 | O3 | 88 | HIS |
| 2 | O3 | 145 | GLN |
| 3 | P3 | 2 | GLN |
| 3 | P3 | 111 | ASN |
| 2 | Q3 | 88 | HIS |
| 3 | R3 | 2 | GLN |
| 3 | R3 | 111 | ASN |
| 2 | S3 | 88 | HIS |
| 3 | T3 | 2 | GLN |
| 2 | U3 | 88 | HIS |
| 3 | V3 | 2 | GLN |
| 3 | V3 | 111 | ASN |
| 2 | W3 | 88 | HIS |
| 3 | X3 | 2 | GLN |
| 3 | X3 | 111 | ASN |
| 2 | Y3 | 88 | HIS |
| 3 | B1 | 2 | GLN |
| 3 | B1 | 111 | ASN |
| 3 | S4 | 2 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | S4 | 72 | ASN |
| 2 | T4 | 88 | HIS |
| 3 | U4 | 2 | GLN |
| 2 | V4 | 88 | HIS |
| 2 | E4 | 88 | HIS |
| 3 | F4 | 2 | GLN |
| 2 | G4 | 15 | GLN |
| 2 | G4 | 88 | HIS |
| 3 | H4 | 2 | GLN |
| 2 | I4 | 88 | HIS |
| 3 | J4 | 2 | GLN |
| 2 | K4 | 88 | HIS |
| 3 | L4 | 2 | GLN |
| 4 | M4 | 9 | GLN |
| 4 | M4 | 28 | HIS |
| 4 | M4 | 40 | GLN |
| 4 | M4 | 172 | HIS |
| 4 | M4 | 180 | ASN |
| 4 | M4 | 227 | GLN |
| 4 | M4 | 251 | ASN |
| 4 | M4 | 257 | GLN |
| 2 | N4 | 88 | HIS |
| 2 | N4 | 145 | GLN |
| 3 | O4 | 2 | GLN |
| 2 | P4 | 88 | HIS |
| 3 | Q4 | 2 | GLN |
| 3 | Q4 | 29 | ASN |
| 3 | Q4 | 111 | ASN |
| 2 | R4 | 88 | HIS |
| 8 | K5 | 57 | GLN |
| 1 | L5 | 10 | ASN |
| 1 | L5 | 11 | ASN |
| 1 | L5 | 110 | ASN |
| 1 | N5 | 11 | ASN |
| 1 | N5 | 110 | ASN |
| 8 | O5 | 10 | ASN |
| 8 | O5 | 57 | GLN |
| 8 | O5 | 120 | GLN |
| 8 | O5 | 161 | GLN |
| 2 | X4 | 57 | GLN |
| 2 | X4 | 88 | HIS |
| 5 | Z4 | 9 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | Z4 | 28 | HIS |
| 5 | Z4 | 63 | ASN |
| 8 | A5 | 57 | GLN |
| 1 | B5 | 11 | ASN |
| 8 | C5 | 57 | GLN |
| 1 | D5 | 11 | ASN |
| 1 | D5 | 15 | GLN |
| 8 | E5 | 57 | GLN |
| 8 | E5 | 161 | GLN |
| 1 | F5 | 10 | ASN |
| 1 | F5 | 11 | ASN |
| 1 | F5 | 110 | ASN |
| 8 | G5 | 57 | GLN |
| 1 | H5 | 15 | GLN |
| 8 | I5 | 57 | GLN |
| 1 | J5 | 11 | ASN |
| 1 | J5 | 15 | GLN |
| 2 | C1 | 88 | HIS |
| 1 | d5 | 11 | ASN |
| 1 | d5 | 110 | ASN |
| 8 | e5 | 57 | GLN |
| 1 | f5 | 11 | ASN |
| 1 | f5 | 110 | ASN |
| 1 | P5 | 11 | ASN |
| 8 | Q5 | 57 | GLN |
| 8 | Q5 | 161 | GLN |
| 1 | T5 | 11 | ASN |
| 1 | T5 | 110 | ASN |
| 8 | U5 | 57 | GLN |
| 8 | U5 | 120 | GLN |
| 1 | V5 | 11 | ASN |
| 8 | W5 | 57 | GLN |
| 8 | W5 | 161 | GLN |
| 1 | X5 | 11 | ASN |
| 1 | Z5 | 11 | ASN |
| 1 | Z5 | 110 | ASN |
| 8 | a5 | 57 | GLN |
| 1 | b5 | 11 | ASN |
| 1 | b5 | 110 | ASN |
| 3 | J6 | 2 | GLN |
| 2 | K6 | 88 | HIS |
| 3 | L6 | 2 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | L6 | 132 | GLN |
| 6 | M6 | 74 | GLN |
| 6 | M6 | 160 | ASN |
| 6 | M6 | 178 | HIS |
| 6 | M6 | 227 | GLN |
| 7 | N6 | 53 | GLN |
| 9 | z5 | 24 | GLN |
| 9 | z5 | 42 | GLN |
| 9 | z5 | 45 | GLN |
| 9 | z5 | 64 | ASN |
| 9 | i5 | 24 | GLN |
| 9 | i5 | 42 | GLN |
| 9 | i5 | 45 | GLN |
| 9 | i5 | 64 | ASN |
| 10 | j5 | 26 | ASN |
| 10 | j5 | 42 | GLN |
| 10 | j5 | 45 | GLN |
| 10 | j5 | 182 | ASN |
| 10 | j5 | 287 | ASN |
| 10 | j5 | 353 | ASN |
| 10 | j5 | 376 | GLN |
| 10 | j5 | 431 | GLN |
| 10 | j5 | 469 | GLN |
| 10 | j5 | 470 | HIS |
| 10 | j5 | 482 | GLN |
| 10 | j5 | 489 | ASN |
| 10 | j5 | 574 | GLN |
| 10 | j5 | 584 | GLN |
| 10 | j5 | 631 | HIS |
| 10 | j5 | 723 | GLN |
| 10 | j5 | 755 | GLN |
| 10 | j5 | 774 | GLN |
| 10 | j5 | 818 | GLN |
| 10 | j5 | 820 | HIS |
| 10 | j5 | 844 | GLN |
| 10 | j5 | 885 | GLN |
| 10 | j5 | 893 | ASN |
| 10 | j5 | 932 | GLN |
| 10 | j5 | 965 | GLN |
| 10 | j5 | 977 | GLN |
| 10 | j5 | 1044 | ASN |
| 10 | j5 | 1065 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 10 | j5 | 1151 | GLN |
| 10 | k5 | 26 | ASN |
| 10 | k5 | 42 | GLN |
| 10 | k5 | 45 | GLN |
| 10 | k5 | 182 | ASN |
| 10 | k5 | 287 | ASN |
| 10 | k5 | 353 | ASN |
| 10 | k5 | 376 | GLN |
| 10 | k5 | 431 | GLN |
| 10 | k5 | 469 | GLN |
| 10 | k5 | 470 | HIS |
| 10 | k5 | 489 | ASN |
| 10 | k5 | 553 | GLN |
| 10 | k5 | 574 | GLN |
| 10 | k5 | 584 | GLN |
| 10 | k5 | 631 | HIS |
| 10 | k5 | 723 | GLN |
| 10 | k5 | 730 | ASN |
| 10 | k5 | 755 | GLN |
| 10 | k5 | 774 | GLN |
| 10 | k5 | 818 | GLN |
| 10 | k5 | 844 | GLN |
| 10 | k5 | 885 | GLN |
| 10 | k5 | 893 | ASN |
| 10 | k5 | 932 | GLN |
| 10 | k5 | 977 | GLN |
| 10 | k5 | 1044 | ASN |
| 10 | k5 | 1065 | HIS |
| 10 | k5 | 1151 | GLN |
| 2 | A6 | 88 | HIS |
| 2 | A6 | 145 | GLN |
| 3 | B6 | 2 | GLN |
| 2 | C6 | 88 | HIS |
| 3 | D6 | 2 | GLN |
| 2 | E6 | 15 | GLN |
| 2 | E6 | 88 | HIS |
| 3 | F6 | 2 | GLN |
| 2 | G6 | 88 | HIS |
| 3 | H6 | 2 | GLN |
| 2 | I6 | 88 | HIS |
| 3 | D1 | 2 | GLN |
| 8 | O7 | 57 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | O7 | 161 | GLN |
| 1 | P7 | 11 | ASN |
| 8 | Q7 | 41 | GLN |
| 8 | Q7 | 57 | GLN |
| 1 | R7 | 11 | ASN |
| 8 | S7 | 10 | ASN |
| 8 | S7 | 41 | GLN |
| 8 | S7 | 60 | GLN |
| 1 | B7 | 11 | ASN |
| 8 | C7 | 57 | GLN |
| 1 | D7 | 11 | ASN |
| 1 | D7 | 117 | ASN |
| 8 | E7 | 57 | GLN |
| 8 | G7 | 161 | GLN |
| 1 | H7 | 11 | ASN |
| 8 | I7 | 57 | GLN |
| 1 | J7 | 11 | ASN |
| 8 | K7 | 57 | GLN |
| 1 | L7 | 11 | ASN |
| 8 | M7 | 41 | GLN |
| 8 | M7 | 60 | GLN |
| 1 | N7 | 11 | ASN |
| 1 | N7 | 110 | ASN |
| 8 | g7 | 57 | GLN |
| 1 | h7 | 11 | ASN |
| 1 | j7 | 11 | ASN |
| 1 | j7 | 110 | ASN |
| 8 | k7 | 41 | GLN |
| 1 | T7 | 11 | ASN |
| 1 | T7 | 110 | ASN |
| 8 | U7 | 57 | GLN |
| 1 | V7 | 11 | ASN |
| 8 | W7 | 41 | GLN |
| 8 | W7 | 57 | GLN |
| 1 | X7 | 11 | ASN |
| 1 | Z7 | 11 | ASN |
| 1 | Z7 | 110 | ASN |
| 8 | a7 | 57 | GLN |
| 1 | b7 | 11 | ASN |
| 1 | d7 | 11 | ASN |
| 1 | d7 | 110 | ASN |
| 1 | f7 | 11 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | f7 | 110 | ASN |
| 2 | E1 | 88 | HIS |
| 2 | A8 | 88 | HIS |
| 2 | A8 | 145 | GLN |
| 3 | B8 | 2 | GLN |
| 2 | C8 | 88 | HIS |
| 3 | D8 | 2 | GLN |
| 2 | E8 | 88 | HIS |
| 1 | l7 | 11 | ASN |
| 8 | m7 | 57 | GLN |
| 1 | n7 | 11 | ASN |
| 8 | o7 | 10 | ASN |
| 1 | p7 | 11 | ASN |
| 1 | p7 | 15 | GLN |
| 8 | q7 | 41 | GLN |
| 1 | r7 | 11 | ASN |
| 8 | s7 | 57 | GLN |
| 8 | s7 | 161 | GLN |
| 1 | t7 | 10 | ASN |
| 1 | t7 | 11 | ASN |
| 8 | u7 | 10 | ASN |
| 1 | v7 | 11 | ASN |
| 1 | v7 | 15 | GLN |
| 9 | z7 | 25 | ASN |
| 9 | z7 | 42 | GLN |
| 9 | z7 | 45 | GLN |
| 9 | z7 | 61 | GLN |
| 9 | w7 | 42 | GLN |
| 9 | w7 | 45 | GLN |
| 9 | w7 | 64 | ASN |
| 9 | x7 | 24 | GLN |
| 9 | x7 | 36 | ASN |
| 9 | x7 | 41 | GLN |
| 9 | x7 | 45 | GLN |
| 9 | x7 | 64 | ASN |
| 9 | y7 | 24 | GLN |
| 9 | y7 | 36 | ASN |
| 9 | y7 | 45 | GLN |
| 2 | T8 | 88 | HIS |
| 3 | U8 | 2 | GLN |
| 2 | V8 | 88 | HIS |
| 3 | W8 | 2 | GLN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | X8 | 57 | GLN |
| 2 | X8 | 88 | HIS |
| 3 | F8 | 2 | GLN |
| 2 | G8 | 15 | GLN |
| 2 | G8 | 88 | HIS |
| 3 | H8 | 2 | GLN |
| 2 | I8 | 88 | HIS |
| 3 | J8 | 2 | GLN |
| 2 | K8 | 88 | HIS |
| 3 | L8 | 2 | GLN |
| 4 | M8 | 28 | HIS |
| 4 | M8 | 40 | GLN |
| 4 | M8 | 103 | GLN |
| 4 | M8 | 172 | HIS |
| 4 | M8 | 211 | GLN |
| 4 | M8 | 227 | GLN |
| 4 | M8 | 230 | GLN |
| 4 | M8 | 251 | ASN |
| 4 | M8 | 257 | GLN |
| 2 | N8 | 88 | HIS |
| 2 | N8 | 145 | GLN |
| 3 | O8 | 2 | GLN |
| 2 | P8 | 88 | HIS |
| 3 | Q8 | 2 | GLN |
| 2 | R8 | 88 | HIS |
| 3 | S8 | 2 | GLN |
| 3 | F1 | 2 | GLN |
| 3 | L9 | 2 | GLN |
| 4 | M9 | 27 | HIS |
| 4 | M9 | 40 | GLN |
| 4 | M9 | 41 | ASN |
| 4 | M9 | 163 | ASN |
| 4 | M9 | 172 | HIS |
| 4 | M9 | 216 | ASN |
| 4 | M9 | 227 | GLN |
| 4 | M9 | 251 | ASN |
| 4 | M9 | 255 | GLN |
| 4 | M9 | 257 | GLN |
| 5 | N9 | 29 | HIS |
| 5 | N9 | 37 | HIS |
| 5 | N9 | 41 | GLN |
| 2 | O9 | 88 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | O9 | 145 | GLN |
| 3 | P9 | 2 | GLN |
| 3 | P9 | 111 | ASN |
| 2 | Q9 | 68 | GLN |
| 2 | Q9 | 88 | HIS |
| 3 | Y8 | 2 | GLN |
| 5 | Z8 | 8 | ASN |
| 5 | Z8 | 37 | HIS |
| 2 | A9 | 88 | HIS |
| 2 | A9 | 145 | GLN |
| 3 | B9 | 2 | GLN |
| 2 | C9 | 88 | HIS |
| 3 | D9 | 2 | GLN |
| 2 | E9 | 88 | HIS |
| 3 | F9 | 2 | GLN |
| 3 | F9 | 47 | ASN |
| 2 | G9 | 88 | HIS |
| 3 | H9 | 2 | GLN |
| 2 | I9 | 15 | GLN |
| 2 | I9 | 25 | GLN |
| 2 | I9 | 88 | HIS |
| 3 | J9 | 2 | GLN |
| 2 | K9 | 88 | HIS |
| 3 | R9 | 2 | GLN |
| 3 | R9 | 111 | ASN |
| 2 | S9 | 88 | HIS |
| 3 | T9 | 2 | GLN |
| 2 | U9 | 88 | HIS |
| 3 | V9 | 2 | GLN |
| 2 | W9 | 88 | HIS |
| 3 | X9 | 2 | GLN |
| 2 | Y9 | 88 | HIS |
| 3 | Z9 | 2 | GLN |
| 3 | Z9 | 111 | ASN |
| 2 | G1 | 88 | HIS |
| 11 | a9 | 82 | GLN |
| 11 | a9 | 140 | GLN |
| 11 | a9 | 176 | ASN |
| 11 | a9 | 200 | HIS |
| 11 | a9 | 266 | ASN |
| 11 | a9 | 268 | ASN |
| 11 | a9 | 328 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | a9 | 329 | ASN |
| 11 | a9 | 348 | GLN |
| 11 | a9 | 363 | GLN |
| 11 | a9 | 382 | ASN |
| 11 | a9 | 389 | GLN |
| 11 | a9 | 448 | ASN |
| 11 | a9 | 449 | ASN |
| 11 | a9 | 473 | HIS |
| 11 | a9 | 523 | GLN |
| 11 | a9 | 639 | GLN |
| 11 | a9 | 662 | GLN |
| 11 | a9 | 677 | GLN |
| 11 | a9 | 780 | GLN |
| 11 | aA | 140 | GLN |
| 11 | aA | 176 | ASN |
| 11 | aA | 200 | HIS |
| 11 | aA | 229 | ASN |
| 11 | aA | 266 | ASN |
| 11 | aA | 268 | ASN |
| 11 | aA | 302 | ASN |
| 11 | aA | 328 | GLN |
| 11 | aA | 329 | ASN |
| 11 | aA | 348 | GLN |
| 11 | aA | 363 | GLN |
| 11 | aA | 382 | ASN |
| 11 | aA | 389 | GLN |
| 11 | aA | 448 | ASN |
| 11 | aA | 449 | ASN |
| 11 | aA | 467 | GLN |
| 11 | aA | 473 | HIS |
| 11 | aA | 478 | HIS |
| 11 | aA | 523 | GLN |
| 11 | aA | 567 | GLN |
| 11 | aA | 639 | GLN |
| 11 | aA | 662 | GLN |
| 11 | aA | 677 | GLN |
| 11 | aA | 684 | ASN |
| 11 | aA | 766 | ASN |
| 11 | aA | 780 | GLN |
| 11 | aA | 803 | ASN |
| 3 | H1 | 2 | GLN |
| 3 | H1 | 111 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | I1 | 88 | HIS |
| 3 | J1 | 2 | GLN |
| 3 | J1 | 111 | ASN |
| 2 | K1 | 88 | HIS |
| 3 | L1 | 2 | GLN |
| 3 | L1 | 111 | ASN |
| 4 | M1 | 40 | GLN |
| 4 | M1 | 41 | ASN |
| 4 | M1 | 61 | ASN |
| 4 | M1 | 163 | ASN |
| 4 | M1 | 172 | HIS |
| 4 | M1 | 181 | GLN |
| 4 | M1 | 216 | ASN |
| 4 | M1 | 227 | GLN |
| 4 | M1 | 251 | ASN |
| 4 | M1 | 257 | GLN |
| 5 | N1 | 29 | HIS |
| 5 | N1 | 37 | HIS |
| 5 | N1 | 41 | GLN |
| 3 | T1 | 2 | GLN |
| 2 | U1 | 88 | HIS |
| 3 | V1 | 2 | GLN |
| 3 | V1 | 111 | ASN |
| 2 | W1 | 88 | HIS |
| 3 | X1 | 2 | GLN |
| 3 | X1 | 111 | ASN |
| 2 | Y1 | 88 | HIS |
| 3 | Z1 | 2 | GLN |
| 2 | A2 | 88 | HIS |
| 2 | A2 | 145 | GLN |
| 3 | B2 | 2 | GLN |
| 2 | C2 | 68 | GLN |
| 2 | C2 | 88 | HIS |
| 3 | D2 | 2 | GLN |
| 2 | E2 | 15 | GLN |
| 2 | E2 | 88 | HIS |
| 3 | F2 | 2 | GLN |
| 3 | F2 | 72 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

42 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 1 | MEN | N5 | 71 | 1 | 7,8,9 | 0.37 | 0 | 6,9,11 | 0.61 | 0 |
| 1 | MEN | J7 | 71 | 1 | 7,8,9 | 0.37 | 0 | 6,9,11 | 0.63 | 0 |
| 1 | MEN | b5 | 71 | 1 | 7,8,9 | 0.32 | 0 | 6,9,11 | 0.59 | 0 |
| 1 | MEN | Z7 | 71 | 1 | 7,8,9 | 0.36 | 0 | 6,9,11 | 0.62 | 0 |
| 1 | MEN | j7 | 71 | 1 | 7,8,9 | 0.34 | 0 | 6,9,11 | 0.63 | 0 |
| 1 | MEN | f5 | 71 | 1 | 7,8,9 | 0.32 | 0 | 6,9,11 | 0.60 | 0 |
| 1 | MEN | A | 71 | 1 | 7,8,9 | 0.36 | 0 | 6,9,11 | 0.60 | 0 |
| 1 | MEN | V5 | 71 | 1 | 7,8,9 | 0.37 | 0 | 6,9,11 | 0.61 | 0 |
| 1 | MEN | R5 | 71 | 1 | 7,8,9 | 0.35 | 0 | 6,9,11 | 0.61 | 0 |
| 1 | MEN | Z | 71 | 1 | 7,8,9 | 0.35 | 0 | 6,9,11 | 0.59 | 0 |
| 1 | MEN | L7 | 71 | 1 | 7,8,9 | 0.35 | 0 | 6,9,11 | 0.60 | 0 |
| 1 | MEN | d5 | 71 | 1 | 7,8,9 | 0.35 | 0 | 6,9,11 | 0.60 | 0 |
| 1 | MEN | d7 | 71 | 1 | 7,8,9 | 0.36 | 0 | 6,9,11 | 0.63 | 0 |
| 1 | MEN | n7 | 71 | 1 | 7,8,9 | 0.36 | 0 | 6,9,11 | 0.61 | 0 |
| 1 | MEN | N7 | 71 | 1 | 7,8,9 | 0.36 | 0 | 6,9,11 | 0.63 | 0 |
| 1 | MEN | P5 | 71 | 1 | 7,8,9 | 0.36 | 0 | 6,9,11 | 0.63 | 0 |
| 1 | MEN | P7 | 71 | 1 | 7,8,9 | 0.36 | 0 | 6,9,11 | 0.61 | 0 |
| 1 | MEN | D5 | 71 | 1 | 7,8,9 | 0.37 | 0 | 6,9,11 | 0.63 | 0 |
| 1 | MEN | R7 | 71 | 1 | 7,8,9 | 0.36 | 0 | 6,9,11 | 0.60 | 0 |
| 1 | MEN | l7 | 71 | 1 | 7,8,9 | 0.35 | 0 | 6,9,11 | 0.60 | 0 |
| 1 | MEN | B5 | 71 | 1 | 7,8,9 | 0.36 | 0 | 6,9,11 | 0.64 | 0 |
| 1 | MEN | X7 | 71 | 1 | 7,8,9 | 0.36 | 0 | 6,9,11 | 0.63 | 0 |
| 1 | MEN | v7 | 71 | 1 | 7,8,9 | 0.34 | 0 | 6,9,11 | 0.61 | 0 |
| 1 | MEN | B7 | 71 | 1 | 7,8,9 | 0.36 | 0 | 6,9,11 | 0.62 | 0 |
| 1 | MEN | Z5 | 71 | 1 | 7,8,9 | 0.35 | 0 | 6,9,11 | 0.60 | 0 |
| 1 | MEN | f7 | 71 | 1 | 7,8,9 | 0.37 | 0 | 6,9,11 | 0.62 | 0 |
| 1 | MEN | F5 | 71 | 1 | 7,8,9 | 0.35 | 0 | 6,9,11 | 0.64 | 0 |
| 1 | MEN | H5 | 71 | 1 | 7,8,9 | 0.37 | 0 | 6,9,11 | 0.63 | 0 |
| 1 | MEN | D7 | 71 | 1 | 7,8,9 | 0.36 | 0 | 6,9,11 | 0.64 | 0 |
| 1 | MEN | V7 | 71 | 1 | 7,8,9 | 0.34 | 0 | 6,9,11 | 0.62 | 0 |
| 1 | MEN | T5 | 71 | 1 | 7,8,9 | 0.38 | 0 | 6,9,11 | 0.60 | 0 |
| 1 | MEN | X5 | 71 | 1 | 7,8,9 | 0.36 | 0 | 6,9,11 | 0.62 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MEN | b7 | 71 | 1 | 7,8,9 | 0.33 | 0 | 6,9,11 | 0.62 | 0 |
| 1 | MEN | L5 | 71 | 1 | 7,8,9 | 0.33 | 0 | 6,9,11 | 0.63 | 0 |
| 1 | MEN | h7 | 71 | 1 | 7,8,9 | 0.33 | 0 | 6,9,11 | 0.63 | 0 |
| 1 | MEN | F7 | 71 | 1 | 7,8,9 | 0.34 | 0 | 6,9,11 | 0.60 | 0 |
| 1 | MEN | p7 | 71 | 1 | 7,8,9 | 0.35 | 0 | 6,9,11 | 0.60 | 0 |
| 1 | MEN | r7 | 71 | 1 | 7,8,9 | 0.35 | 0 | 6,9,11 | 0.62 | 0 |
| 1 | MEN | H7 | 71 | 1 | 7,8,9 | 0.37 | 0 | 6,9,11 | 0.61 | 0 |
| 1 | MEN | J5 | 71 | 1 | 7,8,9 | 0.37 | 0 | 6,9,11 | 0.65 | 0 |
| 1 | MEN | T7 | 71 | 1 | 7,8,9 | 0.36 | 0 | 6,9,11 | 0.60 | 0 |
| 1 | MEN | t7 | 71 | 1 | 7,8,9 | 0.35 | 0 | 6,9,11 | 0.61 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MEN | N5 | 71 | 1 | - | 0/7/8/10 | - |
| 1 | MEN | J7 | 71 | 1 | - | 0/7/8/10 | - |
| 1 | MEN | b5 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | Z7 | 71 | 1 | - | 0/7/8/10 | - |
| 1 | MEN | j7 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | f5 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | A | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | V5 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | R5 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | Z | 71 | 1 | - | 0/7/8/10 | - |
| 1 | MEN | L7 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | d5 | 71 | 1 | - | 0/7/8/10 | - |
| 1 | MEN | d7 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | n7 | 71 | 1 | - | 0/7/8/10 | - |
| 1 | MEN | N7 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | P5 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | P7 | 71 | 1 | - | 0/7/8/10 | - |
| 1 | MEN | D5 | 71 | 1 | - | 0/7/8/10 | - |
| 1 | MEN | R7 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | l7 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | B5 | 71 | 1 | - | 0/7/8/10 | - |
| 1 | MEN | X7 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | v7 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | B7 | 71 | 1 | - | 0/7/8/10 | - |
| 1 | MEN | Z5 | 71 | 1 | - | 0/7/8/10 | - |
| 1 | MEN | f7 | 71 | 1 | - | 0/7/8/10 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MEN | F5 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | H5 | 71 | 1 | - | 0/7/8/10 | - |
| 1 | MEN | D7 | 71 | 1 | - | 0/7/8/10 | - |
| 1 | MEN | V7 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | T5 | 71 | 1 | - | 0/7/8/10 | - |
| 1 | MEN | X5 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | b7 | 71 | 1 | - | 0/7/8/10 | - |
| 1 | MEN | L5 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | h7 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | F7 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | p7 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | r7 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | H7 | 71 | 1 | - | 0/7/8/10 | - |
| 1 | MEN | J5 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | T7 | 71 | 1 | - | 1/7/8/10 | - |
| 1 | MEN | t7 | 71 | 1 | - | 0/7/8/10 | - |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | A | 71 | MEN | CA-CB-CG-OD1 |
| 1 | L5 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | F5 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | J5 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | f5 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | P5 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | R5 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | V5 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | X5 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | b5 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | R7 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | F7 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | L7 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | N7 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | h7 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | j7 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | T7 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | V7 | 71 | MEN | CA-CB-CG-OD1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | X7 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | d7 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | l7 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | p7 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | r7 | 71 | MEN | CA-CB-CG-OD1 |
| 1 | v7 | 71 | MEN | CA-CB-CG-OD1 |

There are no ring outliers.

42 monomers are involved in 62 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | N5 | 71 | MEN | 1 | 0 |
| 1 | J7 | 71 | MEN | 1 | 0 |
| 1 | b5 | 71 | MEN | 1 | 0 |
| 1 | Z7 | 71 | MEN | 1 | 0 |
| 1 | j7 | 71 | MEN | 1 | 0 |
| 1 | f5 | 71 | MEN | 1 | 0 |
| 1 | A | 71 | MEN | 1 | 0 |
| 1 | V5 | 71 | MEN | 1 | 0 |
| 1 | R5 | 71 | MEN | 1 | 0 |
| 1 | Z | 71 | MEN | 1 | 0 |
| 1 | L7 | 71 | MEN | 1 | 0 |
| 1 | d5 | 71 | MEN | 1 | 0 |
| 1 | d7 | 71 | MEN | 1 | 0 |
| 1 | n7 | 71 | MEN | 1 | 0 |
| 1 | N7 | 71 | MEN | 1 | 0 |
| 1 | P5 | 71 | MEN | 1 | 0 |
| 1 | P7 | 71 | MEN | 1 | 0 |
| 1 | D5 | 71 | MEN | 9 | 0 |
| 1 | R7 | 71 | MEN | 1 | 0 |
| 1 | l7 | 71 | MEN | 1 | 0 |
| 1 | B5 | 71 | MEN | 1 | 0 |
| 1 | X7 | 71 | MEN | 1 | 0 |
| 1 | v7 | 71 | MEN | 6 | 0 |
| 1 | B7 | 71 | MEN | 1 | 0 |
| 1 | Z5 | 71 | MEN | 1 | 0 |
| 1 | f7 | 71 | MEN | 1 | 0 |
| 1 | F5 | 71 | MEN | 1 | 0 |
| 1 | H5 | 71 | MEN | 1 | 0 |
| 1 | D7 | 71 | MEN | 1 | 0 |
| 1 | V7 | 71 | MEN | 1 | 0 |
| 1 | T5 | 71 | MEN | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | X5 | 71 | MEN | 1 | 0 |
| 1 | b7 | 71 | MEN | 1 | 0 |
| 1 | L5 | 71 | MEN | 1 | 0 |
| 1 | h7 | 71 | MEN | 1 | 0 |
| 1 | F7 | 71 | MEN | 1 | 0 |
| 1 | p7 | 71 | MEN | 1 | 0 |
| 1 | r7 | 71 | MEN | 1 | 0 |
| 1 | H7 | 71 | MEN | 1 | 0 |
| 1 | J5 | 71 | MEN | 8 | 0 |
| 1 | T7 | 71 | MEN | 1 | 0 |
| 1 | t7 | 71 | MEN | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

336 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 12 | CYC | I8 | 201 | - | 42,46,46 | 3.21 | 13 (30%) | 50,67,67 | 2.88 | 23 (46%) |
| 12 | CYC | P8 | 201 | - | 42,46,46 | 3.14 | 13 (30%) | 50,67,67 | 2.87 | 22 (44%) |
| 12 | CYC | PA | 202 | - | 42,46,46 | 2.99 | 11 (26%) | 50,67,67 | 2.95 | 19 (38%) |
| 12 | CYC | J6 | 201 | - | 42,46,46 | 2.98 | 10 (23%) | 50,67,67 | 2.94 | 20 (40%) |
| 12 | CYC | D4 | 201 | - | 42,46,46 | 2.96 | 11 (26%) | 50,67,67 | 2.94 | 20 (40%) |
| 12 | CYC | j7 | 201 | - | 42,46,46 | 3.28 | 14 (33%) | 50,67,67 | 2.75 | 20 (40%) |
| 12 | CYC | X7 | 201 | - | 42,46,46 | 3.27 | 14 (33%) | 50,67,67 | 2.74 | 20 (40%) |
| 12 | CYC | P1 | 202 | - | 42,46,46 | 2.97 | 10 (23%) | 50,67,67 | 2.96 | 20 (40%) |
| 12 | CYC | a9 | 901 | - | 42,46,46 | 3.29 | 16 (38%) | 50,67,67 | 2.92 | 21 (42%) |
| 12 | CYC | E1 | 201 | - | 42,46,46 | 3.16 | 13 (30%) | 50,67,67 | 2.88 | 23 (46%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 12 | CYC | E3 | 201 | - | 42,46,46 | 3.16 | 13 (30%) | 50,67,67 | 2.88 | 23 (46%) |
| 12 | CYC | E8 | 201 | - | 42,46,46 | 3.17 | 13 (30%) | 50,67,67 | 2.90 | 23 (46%) |
| 12 | CYC | EA | 201 | - | 42,46,46 | 3.16 | 13 (30%) | 50,67,67 | 2.90 | 23 (46%) |
| 12 | CYC | c5 | 201 | - | 42,46,46 | 3.28 | 12 (28%) | 50,67,67 | 3.02 | 19 (38%) |
| 12 | CYC | HA | 201 | - | 42,46,46 | 2.97 | 11 (26%) | 50,67,67 | 2.92 | 20 (40%) |
| 12 | CYC | T8 | 201 | - | 42,46,46 | 3.19 | 12 (28%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | P9 | 201 | - | 42,46,46 | 3.28 | 16 (38%) | 50,67,67 | 2.95 | 23 (46%) |
| 12 | CYC | D5 | 201 | - | 42,46,46 | 3.29 | 13 (30%) | 50,67,67 | 2.74 | 19 (38%) |
| 12 | CYC | A2 | 201 | - | 42,46,46 | 3.19 | 13 (30%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | T4 | 201 | - | 42,46,46 | 3.19 | 12 (28%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | G6 | 201 | - | 42,46,46 | 3.16 | 13 (30%) | 50,67,67 | 2.88 | 23 (46%) |
| 12 | CYC | TA | 302 | - | 42,46,46 | 3.00 | 11 (26%) | 50,67,67 | 2.92 | 19 (38%) |
| 12 | CYC | Y3 | 201 | - | 42,46,46 | 3.16 | 12 (28%) | 50,67,67 | 2.88 | 23 (46%) |
| 12 | CYC | S4 | 201 | - | 42,46,46 | 3.00 | 9 (21%) | 50,67,67 | 2.94 | 20 (40%) |
| 12 | CYC | C3 | 201 | - | 42,46,46 | 3.19 | 12 (28%) | 50,67,67 | 2.88 | 23 (46%) |
| 12 | CYC | B9 | 202 | - | 42,46,46 | 2.95 | 11 (26%) | 50,67,67 | 2.95 | 20 (40%) |
| 12 | CYC | BA | 202 | - | 42,46,46 | 2.95 | 11 (26%) | 50,67,67 | 2.95 | 20 (40%) |
| 12 | CYC | V1 | 202 | - | 42,46,46 | 2.97 | 11 (26%) | 50,67,67 | 2.93 | 20 (40%) |
| 12 | CYC | U4 | 201 | - | 42,46,46 | 3.29 | 15 (35%) | 50,67,67 | 2.93 | 23 (46%) |
| 12 | CYC | LA | 202 | - | 42,46,46 | 3.32 | 16 (38%) | 50,67,67 | 2.94 | 22 (44%) |
| 12 | CYC | SA | 201 | - | 42,46,46 | 3.18 | 13 (30%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | M4 | 301 | - | 42,46,46 | 3.31 | 16 (38%) | 50,67,67 | 2.90 | 22 (44%) |
| 12 | CYC | v7 | 201 | - | 42,46,46 | 3.27 | 13 (30%) | 50,67,67 | 2.74 | 20 (40%) |
| 12 | CYC | C6 | 201 | - | 42,46,46 | 3.15 | 13 (30%) | 50,67,67 | 2.89 | 22 (44%) |
| 12 | CYC | L6 | 202 | - | 42,46,46 | 2.99 | 10 (23%) | 50,67,67 | 2.94 | 20 (40%) |
| 12 | CYC | B1 | 202 | - | 42,46,46 | 3.29 | 16 (38%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | P1 | 201 | - | 42,46,46 | 3.28 | 16 (38%) | 50,67,67 | 2.90 | 22 (44%) |
| 12 | CYC | X8 | 201 | - | 42,46,46 | 3.19 | 12 (28%) | 50,67,67 | 2.90 | 23 (46%) |
| 12 | CYC | G4 | 201 | - | 42,46,46 | 3.18 | 13 (30%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | B5 | 201 | - | 42,46,46 | 3.30 | 14 (33%) | 50,67,67 | 2.73 | 19 (38%) |
| 12 | CYC | K4 | 201 | - | 42,46,46 | 3.17 | 13 (30%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | Z5 | 201 | - | 42,46,46 | 3.25 | 14 (33%) | 50,67,67 | 2.72 | 19 (38%) |
| 12 | CYC | Z1 | 202 | - | 42,46,46 | 3.32 | 16 (38%) | 50,67,67 | 2.93 | 23 (46%) |
| 12 | CYC | L3 | 202 | - | 42,46,46 | 3.31 | 16 (38%) | 50,67,67 | 2.91 | 21 (42%) |
| 12 | CYC | E5 | 201 | - | 42,46,46 | 3.27 | 12 (28%) | 50,67,67 | 3.02 | 20 (40%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 12 | CYC | D6 | 201 | - | 42,46,46 | 3.27 | 16 (38%) | 50,67,67 | 2.89 | 20 (40%) |
| 12 | CYC | V1 | 201 | - | 42,46,46 | 3.33 | 16 (38%) | 50,67,67 | 2.93 | 21 (42%) |
| 12 | CYC | F3 | 201 | - | 42,46,46 | 3.32 | 16 (38%) | 50,67,67 | 2.92 | 22 (44%) |
| 12 | CYC | k5 | 1204 | - | 42,46,46 | 3.27 | 13 (30%) | 50,67,67 | 2.72 | 19 (38%) |
| 12 | CYC | A1 | 201 | - | 42,46,46 | 3.20 | 12 (28%) | 50,67,67 | 2.90 | 23 (46%) |
| 12 | CYC | JA | 201 | - | 42,46,46 | 2.99 | 11 (26%) | 50,67,67 | 2.95 | 20 (40%) |
| 12 | CYC | I5 | 201 | - | 42,46,46 | 3.27 | 12 (28%) | 50,67,67 | 3.01 | 19 (38%) |
| 12 | CYC | Q5 | 201 | - | 42,46,46 | 3.30 | 12 (28%) | 50,67,67 | 3.01 | 19 (38%) |
| 12 | CYC | R8 | 201 | - | 42,46,46 | 3.15 | 12 (28%) | 50,67,67 | 2.90 | 23 (46%) |
| 12 | CYC | V9 | 201 | - | 42,46,46 | 3.29 | 16 (38%) | 50,67,67 | 2.95 | 22 (44%) |
| 12 | CYC | V7 | 201 | - | 42,46,46 | 3.30 | 13 (30%) | 50,67,67 | 2.74 | 19 (38%) |
| 12 | CYC | g7 | 201 | - | 42,46,46 | 3.29 | 12 (28%) | 50,67,67 | 3.05 | 19 (38%) |
| 12 | CYC | R9 | 202 | - | 42,46,46 | 2.97 | 11 (26%) | 50,67,67 | 2.93 | 20 (40%) |
| 12 | CYC | OA | 201 | - | 42,46,46 | 3.20 | 13 (30%) | 50,67,67 | 2.88 | 23 (46%) |
| 12 | CYC | M8 | 302 | - | 42,46,46 | 3.28 | 16 (38%) | 50,67,67 | 2.93 | 20 (40%) |
| 12 | CYC | D8 | 202 | - | 42,46,46 | 3.31 | 16 (38%) | 50,67,67 | 2.91 | 24 (48%) |
| 12 | CYC | T3 | 301 | - | 42,46,46 | 3.28 | 16 (38%) | 50,67,67 | 2.91 | 21 (42%) |
| 12 | CYC | F6 | 201 | - | 42,46,46 | 3.27 | 16 (38%) | 50,67,67 | 2.92 | 22 (44%) |
| 12 | CYC | G3 | 201 | - | 42,46,46 | 3.15 | 13 (30%) | 50,67,67 | 2.88 | 23 (46%) |
| 12 | CYC | o7 | 201 | - | 42,46,46 | 3.28 | 12 (28%) | 50,67,67 | 3.01 | 19 (38%) |
| 12 | CYC | XA | 202 | - | 42,46,46 | 2.98 | 10 (23%) | 50,67,67 | 2.95 | 20 (40%) |
| 12 | CYC | H9 | 201 | - | 42,46,46 | 2.96 | 11 (26%) | 50,67,67 | 2.92 | 20 (40%) |
| 12 | CYC | J7 | 201 | - | 42,46,46 | 3.27 | 13 (30%) | 50,67,67 | 2.74 | 20 (40%) |
| 12 | CYC | I9 | 201 | - | 42,46,46 | 3.14 | 12 (28%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | K9 | 201 | - | 42,46,46 | 3.16 | 13 (30%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | ZA | 202 | - | 42,46,46 | 3.29 | 16 (38%) | 50,67,67 | 2.95 | 21 (42%) |
| 12 | CYC | J9 | 201 | - | 42,46,46 | 2.99 | 11 (26%) | 50,67,67 | 2.95 | 20 (40%) |
| 12 | CYC | BA | 201 | - | 42,46,46 | 3.30 | 16 (38%) | 50,67,67 | 2.92 | 24 (48%) |
| 12 | CYC | N4 | 201 | - | 42,46,46 | 3.19 | 12 (28%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | S3 | 201 | - | 42,46,46 | 3.15 | 12 (28%) | 50,67,67 | 2.89 | 22 (44%) |
| 12 | CYC | H8 | 202 | - | 42,46,46 | 2.97 | 10 (23%) | 50,67,67 | 2.92 | 20 (40%) |
| 12 | CYC | M8 | 301 | - | 42,46,46 | 3.30 | 16 (38%) | 50,67,67 | 2.89 | 22 (44%) |
| 12 | CYC | F8 | 201 | - | 42,46,46 | 2.98 | 11 (26%) | 50,67,67 | 2.93 | 19 (38%) |
| 12 | CYC | R3 | 201 | - | 42,46,46 | 3.29 | 16 (38%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | N2 | 101 | - | 42,46,46 | 3.28 | 16 (38%) | 50,67,67 | 2.93 | 20 (40%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 12 | CYC | K1 | 201 | - | 42,46,46 | 3.16 | 12 (28%) | 50,67,67 | 2.90 | 23 (46%) |
| 12 | CYC | F3 | 202 | - | 42,46,46 | 2.99 | 11 (26%) | 50,67,67 | 2.92 | 20 (40%) |
| 12 | CYC | k5 | 1202 | - | 42,46,46 | 3.32 | 14 (33%) | 50,67,67 | 2.74 | 20 (40%) |
| 12 | CYC | JA | 202 | - | 42,46,46 | 3.32 | 16 (38%) | 50,67,67 | 2.92 | 21 (42%) |
| 12 | CYC | ZA | 201 | - | 42,46,46 | 2.97 | 10 (23%) | 50,67,67 | 2.93 | 19 (38%) |
| 12 | CYC | IA | 201 | - | 42,46,46 | 3.14 | 12 (28%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | A3 | 201 | - | 42,46,46 | 3.20 | 12 (28%) | 50,67,67 | 2.90 | 23 (46%) |
| 12 | CYC | a7 | 201 | - | 42,46,46 | 3.29 | 12 (28%) | 50,67,67 | 3.04 | 19 (38%) |
| 12 | CYC | D2 | 202 | - | 42,46,46 | 2.99 | 11 (26%) | 50,67,67 | 2.93 | 19 (38%) |
| 12 | CYC | L2 | 202 | - | 42,46,46 | 2.97 | 10 (23%) | 50,67,67 | 2.93 | 20 (40%) |
| 12 | CYC | V3 | 202 | - | 42,46,46 | 2.97 | 11 (26%) | 50,67,67 | 2.93 | 20 (40%) |
| 12 | CYC | S9 | 201 | - | 42,46,46 | 3.18 | 13 (30%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | K5 | 201 | - | 42,46,46 | 3.27 | 12 (28%) | 50,67,67 | 3.03 | 20 (40%) |
| 12 | CYC | N8 | 201 | - | 42,46,46 | 3.19 | 12 (28%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | U1 | 201 | - | 42,46,46 | 3.17 | 13 (30%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | U9 | 201 | - | 42,46,46 | 3.18 | 13 (30%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | P3 | 202 | - | 42,46,46 | 2.97 | 10 (23%) | 50,67,67 | 2.96 | 20 (40%) |
| 12 | CYC | Y8 | 201 | - | 42,46,46 | 2.96 | 11 (26%) | 50,67,67 | 2.97 | 20 (40%) |
| 12 | CYC | XA | 201 | - | 42,46,46 | 3.33 | 16 (38%) | 50,67,67 | 2.94 | 20 (40%) |
| 12 | CYC | R4 | 201 | - | 42,46,46 | 3.15 | 12 (28%) | 50,67,67 | 2.90 | 23 (46%) |
| 12 | CYC | D7 | 201 | - | 42,46,46 | 3.27 | 13 (30%) | 50,67,67 | 2.74 | 19 (38%) |
| 12 | CYC | LA | 201 | - | 42,46,46 | 2.95 | 10 (23%) | 50,67,67 | 2.94 | 19 (38%) |
| 12 | CYC | HA | 202 | - | 42,46,46 | 3.32 | 16 (38%) | 50,67,67 | 2.90 | 19 (38%) |
| 12 | CYC | QA | 201 | - | 42,46,46 | 3.17 | 13 (30%) | 50,67,67 | 2.88 | 22 (44%) |
| 12 | CYC | k5 | 1201 | - | 42,46,46 | 3.60 | 13 (30%) | 50,67,67 | 2.93 | 21 (42%) |
| 12 | CYC | B9 | 201 | - | 42,46,46 | 3.30 | 16 (38%) | 50,67,67 | 2.92 | 24 (48%) |
| 12 | CYC | J1 | 201 | - | 42,46,46 | 2.95 | 11 (26%) | 50,67,67 | 2.92 | 20 (40%) |
| 12 | CYC | DA | 202 | - | 42,46,46 | 2.96 | 10 (23%) | 50,67,67 | 2.92 | 19 (38%) |
| 12 | CYC | F2 | 202 | - | 42,46,46 | 3.00 | 11 (26%) | 50,67,67 | 2.91 | 19 (38%) |
| 12 | CYC | E9 | 201 | - | 42,46,46 | 3.16 | 13 (30%) | 50,67,67 | 2.90 | 23 (46%) |
| 12 | CYC | X1 | 201 | - | 42,46,46 | 3.31 | 16 (38%) | 50,67,67 | 2.93 | 24 (48%) |
| 12 | CYC | e7 | 201 | - | 42,46,46 | 3.29 | 12 (28%) | 50,67,67 | 2.98 | 19 (38%) |
| 12 | CYC | J9 | 202 | - | 42,46,46 | 3.32 | 16 (38%) | 50,67,67 | 2.92 | 21 (42%) |
| 12 | CYC | H1 | 202 | - | 42,46,46 | 2.97 | 12 (28%) | 50,67,67 | 2.93 | 20 (40%) |
| 12 | CYC | Z8 | 301 | - | 42,46,46 | 3.30 | 16 (38%) | 50,67,67 | 2.90 | 23 (46%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 12 | CYC | J3 | 201 | - | 42,46,46 | 2.95 | 11 (26%) | 50,67,67 | 2.92 | 20 (40%) |
| 12 | CYC | Q9 | 201 | - | 42,46,46 | 3.17 | 13 (30%) | 50,67,67 | 2.88 | 23 (46%) |
| 12 | CYC | s7 | 201 | - | 42,46,46 | 3.26 | 12 (28%) | 50,67,67 | 3.00 | 19 (38%) |
| 12 | CYC | O7 | 201 | - | 42,46,46 | 3.26 | 12 (28%) | 50,67,67 | 3.01 | 19 (38%) |
| 12 | CYC | j5 | 1202 | - | 42,46,46 | 3.28 | 13 (30%) | 50,67,67 | 2.72 | 19 (38%) |
| 12 | CYC | Y9 | 201 | - | 42,46,46 | 3.15 | 13 (30%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | W3 | 201 | - | 42,46,46 | 3.19 | 13 (30%) | 50,67,67 | 2.85 | 24 (48%) |
| 12 | CYC | E7 | 201 | - | 42,46,46 | 3.30 | 12 (28%) | 50,67,67 | 3.02 | 19 (38%) |
| 12 | CYC | C4 | 201 | - | 42,46,46 | 3.13 | 13 (30%) | 50,67,67 | 2.89 | 22 (44%) |
| 12 | CYC | W5 | 201 | - | 42,46,46 | 3.29 | 12 (28%) | 50,67,67 | 3.01 | 19 (38%) |
| 12 | CYC | Z1 | 201 | - | 42,46,46 | 2.98 | 11 (26%) | 50,67,67 | 2.92 | 21 (42%) |
| 12 | CYC | Z4 | 301 | - | 42,46,46 | 3.31 | 16 (38%) | 50,67,67 | 2.90 | 22 (44%) |
| 12 | CYC | A7 | 201 | - | 42,46,46 | 3.24 | 12 (28%) | 50,67,67 | 3.00 | 19 (38%) |
| 12 | CYC | I2 | 201 | - | 42,46,46 | 3.18 | 13 (30%) | 50,67,67 | 2.88 | 23 (46%) |
| 12 | CYC | d5 | 201 | - | 42,46,46 | 3.27 | 14 (33%) | 50,67,67 | 2.73 | 19 (38%) |
| 12 | CYC | W7 | 201 | - | 42,46,46 | 3.29 | 12 (28%) | 50,67,67 | 3.02 | 20 (40%) |
| 12 | CYC | J2 | 202 | - | 42,46,46 | 3.30 | 16 (38%) | 50,67,67 | 2.94 | 21 (42%) |
| 12 | CYC | h7 | 201 | - | 42,46,46 | 3.29 | 14 (33%) | 50,67,67 | 2.72 | 20 (40%) |
| 12 | CYC | H1 | 201 | - | 42,46,46 | 3.27 | 16 (38%) | 50,67,67 | 2.92 | 22 (44%) |
| 12 | CYC | O1 | 201 | - | 42,46,46 | 3.23 | 12 (28%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | L5 | 201 | - | 42,46,46 | 3.28 | 14 (33%) | 50,67,67 | 2.75 | 20 (40%) |
| 12 | CYC | N5 | 201 | - | 42,46,46 | 3.30 | 14 (33%) | 50,67,67 | 2.74 | 19 (38%) |
| 12 | CYC | J4 | 202 | - | 42,46,46 | 3.01 | 11 (26%) | 50,67,67 | 2.95 | 21 (42%) |
| 12 | CYC | S5 | 201 | - | 42,46,46 | 3.23 | 12 (28%) | 50,67,67 | 2.98 | 19 (38%) |
| 12 | CYC | i7 | 201 | - | 42,46,46 | 3.29 | 12 (28%) | 50,67,67 | 3.05 | 20 (40%) |
| 12 | CYC | Z9 | 202 | - | 42,46,46 | 3.29 | 16 (38%) | 50,67,67 | 2.95 | 21 (42%) |
| 12 | CYC | FA | 301 | - | 42,46,46 | 3.27 | 16 (38%) | 50,67,67 | 2.91 | 22 (44%) |
| 12 | CYC | WA | 201 | - | 42,46,46 | 3.17 | 12 (28%) | 50,67,67 | 2.87 | 23 (46%) |
| 12 | CYC | J2 | 201 | - | 42,46,46 | 2.97 | 10 (23%) | 50,67,67 | 2.95 | 20 (40%) |
| 12 | CYC | B8 | 201 | - | 42,46,46 | 2.96 | 10 (23%) | 50,67,67 | 2.98 | 19 (38%) |
| 12 | CYC | DA | 201 | - | 42,46,46 | 3.25 | 16 (38%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | P5 | 201 | - | 42,46,46 | 3.30 | 13 (30%) | 50,67,67 | 2.73 | 20 (40%) |
| 12 | CYC | V4 | 201 | - | 42,46,46 | 3.18 | 13 (30%) | 50,67,67 | 2.88 | 23 (46%) |
| 12 | CYC | I4 | 201 | - | 42,46,46 | 3.21 | 13 (30%) | 50,67,67 | 2.88 | 23 (46%) |
| 12 | CYC | O8 | 202 | - | 42,46,46 | 2.94 | 10 (23%) | 50,67,67 | 2.96 | 19 (38%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 12 | CYC | B2 | 201 | - | 42,46,46 | 2.96 | 11 (26%) | 50,67,67 | 2.95 | 19 (38%) |
| 12 | CYC | L2 | 201 | - | 42,46,46 | 3.33 | 16 (38%) | 50,67,67 | 2.93 | 21 (42%) |
| 12 | CYC | k7 | 201 | - | 42,46,46 | 3.27 | 12 (28%) | 50,67,67 | 2.99 | 19 (38%) |
| 12 | CYC | D9 | 201 | - | 42,46,46 | 3.25 | 16 (38%) | 50,67,67 | 2.90 | 22 (44%) |
| 12 | CYC | c7 | 201 | - | 42,46,46 | 3.30 | 12 (28%) | 50,67,67 | 3.03 | 20 (40%) |
| 12 | CYC | E6 | 201 | - | 42,46,46 | 3.17 | 13 (30%) | 50,67,67 | 2.90 | 23 (46%) |
| 12 | CYC | F1 | 202 | - | 42,46,46 | 2.99 | 11 (26%) | 50,67,67 | 2.92 | 20 (40%) |
| 12 | CYC | L8 | 201 | - | 42,46,46 | 2.95 | 11 (26%) | 50,67,67 | 2.95 | 19 (38%) |
| 12 | CYC | L4 | 201 | - | 42,46,46 | 2.95 | 11 (26%) | 50,67,67 | 2.94 | 19 (38%) |
| 12 | CYC | R1 | 202 | - | 42,46,46 | 2.97 | 11 (26%) | 50,67,67 | 2.93 | 20 (40%) |
| 12 | CYC | A5 | 201 | - | 42,46,46 | 3.25 | 12 (28%) | 50,67,67 | 3.00 | 19 (38%) |
| 12 | CYC | N6 | 101 | - | 42,46,46 | 3.28 | 16 (38%) | 50,67,67 | 2.93 | 21 (42%) |
| 12 | CYC | W8 | 202 | - | 42,46,46 | 2.99 | 10 (23%) | 50,67,67 | 2.95 | 21 (42%) |
| 12 | CYC | T9 | 302 | - | 42,46,46 | 3.01 | 11 (26%) | 50,67,67 | 2.93 | 19 (38%) |
| 12 | CYC | C1 | 201 | - | 42,46,46 | 3.19 | 12 (28%) | 50,67,67 | 2.88 | 23 (46%) |
| 12 | CYC | F1 | 201 | - | 42,46,46 | 3.32 | 16 (38%) | 50,67,67 | 2.91 | 22 (44%) |
| 12 | CYC | f7 | 201 | - | 42,46,46 | 3.31 | 14 (33%) | 50,67,67 | 2.74 | 20 (40%) |
| 12 | CYC | L1 | 201 | - | 42,46,46 | 2.95 | 11 (26%) | 50,67,67 | 2.94 | 20 (40%) |
| 12 | CYC | aA | 901 | - | 42,46,46 | 3.32 | 16 (38%) | 50,67,67 | 2.93 | 23 (46%) |
| 12 | CYC | Y4 | 201 | - | 42,46,46 | 2.95 | 11 (26%) | 50,67,67 | 2.97 | 20 (40%) |
| 12 | CYC | L9 | 202 | - | 42,46,46 | 3.32 | 16 (38%) | 50,67,67 | 2.94 | 21 (42%) |
| 12 | CYC | H5 | 201 | - | 42,46,46 | 3.29 | 14 (33%) | 50,67,67 | 2.73 | 19 (38%) |
| 12 | CYC | I1 | 201 | - | 42,46,46 | 3.17 | 13 (30%) | 50,67,67 | 2.90 | 22 (44%) |
| 12 | CYC | S7 | 201 | - | 42,46,46 | 3.24 | 12 (28%) | 50,67,67 | 2.98 | 19 (38%) |
| 12 | CYC | G8 | 201 | - | 42,46,46 | 3.18 | 13 (30%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | M7 | 201 | - | 42,46,46 | 3.26 | 12 (28%) | 50,67,67 | 3.01 | 19 (38%) |
| 12 | CYC | R7 | 201 | - | 42,46,46 | 3.28 | 14 (33%) | 50,67,67 | 2.74 | 20 (40%) |
| 12 | CYC | p7 | 201 | - | 42,46,46 | 3.28 | 13 (30%) | 50,67,67 | 2.75 | 20 (40%) |
| 12 | CYC | Q1 | 201 | - | 42,46,46 | 3.17 | 13 (30%) | 50,67,67 | 2.87 | 22 (44%) |
| 12 | CYC | B8 | 202 | - | 42,46,46 | 3.30 | 16 (38%) | 50,67,67 | 2.90 | 22 (44%) |
| 12 | CYC | m7 | 201 | - | 42,46,46 | 3.26 | 12 (28%) | 50,67,67 | 3.01 | 19 (38%) |
| 12 | CYC | A6 | 201 | - | 42,46,46 | 3.19 | 13 (30%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | J4 | 201 | - | 42,46,46 | 3.32 | 16 (38%) | 50,67,67 | 2.93 | 21 (42%) |
| 12 | CYC | J8 | 202 | - | 42,46,46 | 3.01 | 11 (26%) | 50,67,67 | 2.96 | 21 (42%) |
| 12 | CYC | R9 | 201 | - | 42,46,46 | 3.32 | 16 (38%) | 50,67,67 | 2.90 | 19 (38%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 12 | CYC | P7 | 201 | - | 42,46,46 | 3.28 | 13 (30%) | 50,67,67 | 2.73 | 20 (40%) |
| 12 | CYC | L3 | 201 | - | 42,46,46 | 2.95 | 11 (26%) | 50,67,67 | 2.94 | 19 (38%) |
| 12 | CYC | D8 | 201 | - | 42,46,46 | 2.96 | 11 (26%) | 50,67,67 | 2.94 | 20 (40%) |
| 12 | CYC | B1 | 201 | - | 42,46,46 | 2.98 | 11 (26%) | 50,67,67 | 2.96 | 20 (40%) |
| 12 | CYC | N7 | 201 | - | 42,46,46 | 3.29 | 13 (30%) | 50,67,67 | 2.72 | 19 (38%) |
| 12 | CYC | L4 | 202 | - | 42,46,46 | 3.29 | 16 (38%) | 50,67,67 | 2.92 | 21 (42%) |
| 12 | CYC | U8 | 202 | - | 42,46,46 | 2.96 | 11 (26%) | 50,67,67 | 2.91 | 20 (40%) |
| 12 | CYC | H3 | 202 | - | 42,46,46 | 3.27 | 16 (38%) | 50,67,67 | 2.92 | 22 (44%) |
| 12 | CYC | Z3 | 202 | - | 42,46,46 | 2.98 | 11 (26%) | 50,67,67 | 2.93 | 21 (42%) |
| 12 | CYC | L6 | 201 | - | 42,46,46 | 3.33 | 16 (38%) | 50,67,67 | 2.93 | 21 (42%) |
| 12 | CYC | B3 | 202 | - | 42,46,46 | 3.30 | 16 (38%) | 50,67,67 | 2.91 | 24 (48%) |
| 12 | CYC | S1 | 201 | - | 42,46,46 | 3.15 | 13 (30%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | W4 | 202 | - | 42,46,46 | 2.99 | 10 (23%) | 50,67,67 | 2.96 | 21 (42%) |
| 12 | CYC | f5 | 201 | - | 42,46,46 | 3.26 | 13 (30%) | 50,67,67 | 2.74 | 20 (40%) |
| 12 | CYC | E4 | 201 | - | 42,46,46 | 3.17 | 13 (30%) | 50,67,67 | 2.90 | 23 (46%) |
| 12 | CYC | b7 | 201 | - | 42,46,46 | 3.29 | 14 (33%) | 50,67,67 | 2.73 | 20 (40%) |
| 12 | CYC | K8 | 201 | - | 42,46,46 | 3.17 | 13 (30%) | 50,67,67 | 2.90 | 23 (46%) |
| 12 | CYC | W4 | 201 | - | 42,46,46 | 3.28 | 15 (35%) | 50,67,67 | 2.90 | 22 (44%) |
| 12 | CYC | Y7 | 201 | - | 42,46,46 | 3.28 | 12 (28%) | 50,67,67 | 2.98 | 19 (38%) |
| 12 | CYC | J8 | 201 | - | 42,46,46 | 3.32 | 16 (38%) | 50,67,67 | 2.93 | 21 (42%) |
| 12 | CYC | F9 | 301 | - | 42,46,46 | 3.28 | 16 (38%) | 50,67,67 | 2.91 | 22 (44%) |
| 12 | CYC | P4 | 201 | - | 42,46,46 | 3.14 | 13 (30%) | 50,67,67 | 2.87 | 22 (44%) |
| 12 | CYC | G5 | 201 | - | 42,46,46 | 3.25 | 12 (28%) | 50,67,67 | 3.01 | 19 (38%) |
| 12 | CYC | Z3 | 201 | - | 42,46,46 | 3.32 | 16 (38%) | 50,67,67 | 2.93 | 23 (46%) |
| 12 | CYC | M5 | 201 | - | 42,46,46 | 3.23 | 12 (28%) | 50,67,67 | 2.98 | 19 (38%) |
| 12 | CYC | O9 | 201 | - | 42,46,46 | 3.20 | 13 (30%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | u7 | 201 | - | 42,46,46 | 3.28 | 12 (28%) | 50,67,67 | 3.01 | 19 (38%) |
| 12 | CYC | F4 | 202 | - | 42,46,46 | 3.28 | 17 (40%) | 50,67,67 | 2.94 | 22 (44%) |
| 12 | CYC | B7 | 201 | - | 42,46,46 | 3.30 | 14 (33%) | 50,67,67 | 2.73 | 19 (38%) |
| 12 | CYC | e5 | 201 | - | 42,46,46 | 3.29 | 12 (28%) | 50,67,67 | 3.01 | 20 (40%) |
| 12 | CYC | r7 | 201 | - | 42,46,46 | 3.30 | 14 (33%) | 50,67,67 | 2.73 | 19 (38%) |
| 12 | CYC | A4 | 201 | - | 42,46,46 | 3.19 | 13 (30%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | I3 | 201 | - | 42,46,46 | 3.17 | 13 (30%) | 50,67,67 | 2.90 | 22 (44%) |
| 12 | CYC | D1 | 202 | - | 42,46,46 | 3.31 | 16 (38%) | 50,67,67 | 2.92 | 23 (46%) |
| 12 | CYC | X5 | 201 | - | 42,46,46 | 3.28 | 15 (35%) | 50,67,67 | 2.75 | 20 (40%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 12 | CYC | Y5 | 201 | - | 42,46,46 | 3.28 | 12 (28%) | 50,67,67 | 3.03 | 19 (38%) |
| 12 | CYC | F5 | 201 | - | 42,46,46 | 3.29 | 14 (33%) | 50,67,67 | 2.75 | 20 (40%) |
| 12 | CYC | KA | 201 | - | 42,46,46 | 3.16 | 13 (30%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | P3 | 201 | - | 42,46,46 | 3.28 | 16 (38%) | 50,67,67 | 2.90 | 22 (44%) |
| 12 | CYC | D4 | 202 | - | 42,46,46 | 3.31 | 16 (38%) | 50,67,67 | 2.91 | 24 (48%) |
| 12 | CYC | K2 | 201 | - | 42,46,46 | 3.15 | 12 (28%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | X3 | 202 | - | 42,46,46 | 2.97 | 11 (26%) | 50,67,67 | 2.93 | 20 (40%) |
| 12 | CYC | R1 | 201 | - | 42,46,46 | 3.29 | 16 (38%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | C8 | 201 | - | 42,46,46 | 3.13 | 13 (30%) | 50,67,67 | 2.89 | 22 (44%) |
| 12 | CYC | q7 | 201 | - | 42,46,46 | 3.26 | 12 (28%) | 50,67,67 | 2.99 | 19 (38%) |
| 12 | CYC | D2 | 201 | - | 42,46,46 | 3.27 | 16 (38%) | 50,67,67 | 2.89 | 20 (40%) |
| 12 | CYC | H3 | 201 | - | 42,46,46 | 2.97 | 12 (28%) | 50,67,67 | 2.92 | 20 (40%) |
| 12 | CYC | W8 | 201 | - | 42,46,46 | 3.28 | 15 (35%) | 50,67,67 | 2.90 | 22 (44%) |
| 12 | CYC | H4 | 202 | - | 42,46,46 | 2.97 | 10 (23%) | 50,67,67 | 2.92 | 20 (40%) |
| 12 | CYC | Q4 | 201 | - | 42,46,46 | 2.97 | 11 (26%) | 50,67,67 | 2.95 | 20 (40%) |
| 12 | CYC | H8 | 201 | - | 42,46,46 | 3.33 | 16 (38%) | 50,67,67 | 2.92 | 23 (46%) |
| 12 | CYC | F2 | 201 | - | 42,46,46 | 3.29 | 16 (38%) | 50,67,67 | 2.91 | 20 (40%) |
| 12 | CYC | D1 | 201 | - | 42,46,46 | 2.97 | 11 (26%) | 50,67,67 | 2.93 | 20 (40%) |
| 12 | CYC | P9 | 202 | - | 42,46,46 | 2.99 | 11 (26%) | 50,67,67 | 2.95 | 19 (38%) |
| 12 | CYC | V3 | 201 | - | 42,46,46 | 3.32 | 16 (38%) | 50,67,67 | 2.93 | 20 (40%) |
| 12 | CYC | a5 | 201 | - | 42,46,46 | 3.29 | 12 (28%) | 50,67,67 | 3.02 | 19 (38%) |
| 12 | CYC | U7 | 201 | - | 42,46,46 | 3.25 | 12 (28%) | 50,67,67 | 3.02 | 19 (38%) |
| 12 | CYC | B4 | 201 | - | 42,46,46 | 2.97 | 10 (23%) | 50,67,67 | 2.98 | 20 (40%) |
| 12 | CYC | F9 | 302 | - | 42,46,46 | 2.95 | 10 (23%) | 50,67,67 | 2.94 | 20 (40%) |
| 12 | CYC | I6 | 201 | - | 42,46,46 | 3.19 | 13 (30%) | 50,67,67 | 2.88 | 23 (46%) |
| 12 | CYC | R5 | 201 | - | 42,46,46 | 3.27 | 14 (33%) | 50,67,67 | 2.75 | 20 (40%) |
| 12 | CYC | X3 | 201 | - | 42,46,46 | 3.31 | 16 (38%) | 50,67,67 | 2.93 | 24 (48%) |
| 12 | CYC | G2 | 201 | - | 42,46,46 | 3.17 | 12 (28%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | L9 | 201 | - | 42,46,46 | 2.95 | 10 (23%) | 50,67,67 | 2.94 | 19 (38%) |
| 12 | CYC | F7 | 201 | - | 42,46,46 | 3.28 | 14 (33%) | 50,67,67 | 2.75 | 20 (40%) |
| 12 | CYC | G9 | 201 | - | 42,46,46 | 3.17 | 13 (30%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | O3 | 201 | - | 42,46,46 | 3.23 | 12 (28%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | C9 | 201 | - | 42,46,46 | 3.16 | 12 (28%) | 50,67,67 | 2.89 | 24 (48%) |
| 12 | CYC | Q7 | 201 | - | 42,46,46 | 3.28 | 12 (28%) | 50,67,67 | 3.03 | 20 (40%) |
| 12 | CYC | H4 | 201 | - | 42,46,46 | 3.33 | 16 (38%) | 50,67,67 | 2.92 | 23 (46%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 12 | CYC | K3 | 201 | - | 42,46,46 | 3.16 | 12 (28%) | 50,67,67 | 2.90 | 23 (46%) |
| 12 | CYC | X9 | 201 | - | 42,46,46 | 3.32 | 16 (38%) | 50,67,67 | 2.94 | 20 (40%) |
| 12 | CYC | E2 | 201 | - | 42,46,46 | 3.18 | 14 (33%) | 50,67,67 | 2.90 | 23 (46%) |
| 12 | CYC | T5 | 201 | - | 42,46,46 | 3.31 | 14 (33%) | 50,67,67 | 2.74 | 19 (38%) |
| 12 | CYC | G1 | 201 | - | 42,46,46 | 3.16 | 13 (30%) | 50,67,67 | 2.88 | 23 (46%) |
| 12 | CYC | k5 | 1203 | - | 42,46,46 | 3.30 | 15 (35%) | 50,67,67 | 2.73 | 20 (40%) |
| 12 | CYC | W1 | 201 | - | 42,46,46 | 3.19 | 13 (30%) | 50,67,67 | 2.86 | 24 (48%) |
| 12 | CYC | C5 | 201 | - | 42,46,46 | 3.27 | 12 (28%) | 50,67,67 | 3.01 | 19 (38%) |
| 12 | CYC | K6 | 201 | - | 42,46,46 | 3.16 | 12 (28%) | 50,67,67 | 2.90 | 23 (46%) |
| 12 | CYC | F9 | 303 | - | 42,46,46 | 2.95 | 9 (21%) | 50,67,67 | 2.94 | 20 (40%) |
| 12 | CYC | B6 | 201 | - | 42,46,46 | 2.97 | 11 (26%) | 50,67,67 | 2.95 | 19 (38%) |
| 12 | CYC | YA | 201 | - | 42,46,46 | 3.15 | 13 (30%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | H6 | 202 | - | 42,46,46 | 2.95 | 10 (23%) | 50,67,67 | 2.93 | 20 (40%) |
| 12 | CYC | A9 | 201 | - | 42,46,46 | 3.18 | 13 (30%) | 50,67,67 | 2.86 | 23 (46%) |
| 12 | CYC | D9 | 202 | - | 42,46,46 | 2.96 | 10 (23%) | 50,67,67 | 2.92 | 19 (38%) |
| 12 | CYC | A8 | 201 | - | 42,46,46 | 3.19 | 13 (30%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | T7 | 201 | - | 42,46,46 | 3.27 | 14 (33%) | 50,67,67 | 2.74 | 20 (40%) |
| 12 | CYC | T3 | 302 | - | 42,46,46 | 2.98 | 11 (26%) | 50,67,67 | 2.94 | 20 (40%) |
| 12 | CYC | B3 | 201 | - | 42,46,46 | 2.98 | 11 (26%) | 50,67,67 | 2.95 | 20 (40%) |
| 12 | CYC | RA | 201 | - | 42,46,46 | 3.32 | 16 (38%) | 50,67,67 | 2.89 | 19 (38%) |
| 12 | CYC | H9 | 202 | - | 42,46,46 | 3.31 | 16 (38%) | 50,67,67 | 2.90 | 19 (38%) |
| 12 | CYC | D6 | 202 | - | 42,46,46 | 2.99 | 11 (26%) | 50,67,67 | 2.93 | 19 (38%) |
| 12 | CYC | U3 | 201 | - | 42,46,46 | 3.17 | 13 (30%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | T1 | 301 | - | 42,46,46 | 3.28 | 16 (38%) | 50,67,67 | 2.91 | 21 (42%) |
| 12 | CYC | b5 | 201 | - | 42,46,46 | 3.25 | 13 (30%) | 50,67,67 | 2.74 | 20 (40%) |
| 12 | CYC | J5 | 201 | - | 42,46,46 | 3.29 | 13 (30%) | 50,67,67 | 2.75 | 19 (38%) |
| 12 | CYC | Y1 | 201 | - | 42,46,46 | 3.16 | 12 (28%) | 50,67,67 | 2.88 | 23 (46%) |
| 12 | CYC | J6 | 202 | - | 42,46,46 | 3.28 | 16 (38%) | 50,67,67 | 2.93 | 20 (40%) |
| 12 | CYC | U5 | 201 | - | 42,46,46 | 3.27 | 12 (28%) | 50,67,67 | 3.03 | 19 (38%) |
| 12 | CYC | V9 | 202 | - | 42,46,46 | 2.95 | 11 (26%) | 50,67,67 | 2.94 | 19 (38%) |
| 12 | CYC | V5 | 201 | - | 42,46,46 | 3.29 | 13 (30%) | 50,67,67 | 2.73 | 20 (40%) |
| 12 | CYC | j5 | 1201 | - | 42,46,46 | 3.60 | 13 (30%) | 50,67,67 | 2.94 | 21 (42%) |
| 12 | CYC | X4 | 201 | - | 42,46,46 | 3.19 | 12 (28%) | 50,67,67 | 2.90 | 23 (46%) |
| 12 | CYC | C7 | 201 | - | 42,46,46 | 3.27 | 12 (28%) | 50,67,67 | 3.01 | 20 (40%) |
| 12 | CYC | F6 | 202 | - | 42,46,46 | 3.00 | 11 (26%) | 50,67,67 | 2.92 | 19 (38%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 12 | CYC | F4 | 201 | - | 42,46,46 | 2.98 | 11 (26%) | 50,67,67 | 2.93 | 19 (38%) |
| 12 | CYC | V8 | 201 | - | 42,46,46 | 3.17 | 13 (30%) | 50,67,67 | 2.88 | 23 (46%) |
| 12 | CYC | T1 | 302 | - | 42,46,46 | 2.98 | 11 (26%) | 50,67,67 | 2.94 | 20 (40%) |
| 12 | CYC | A | 201 | - | 42,46,46 | 3.29 | 13 (30%) | 50,67,67 | 2.74 | 20 (40%) |
| 12 | CYC | S8 | 201 | - | 42,46,46 | 3.00 | 9 (21%) | 50,67,67 | 2.94 | 20 (40%) |
| 12 | CYC | J3 | 202 | - | 42,46,46 | 3.32 | 16 (38%) | 50,67,67 | 2.92 | 23 (46%) |
| 12 | CYC | Z9 | 201 | - | 42,46,46 | 2.97 | 10 (23%) | 50,67,67 | 2.93 | 19 (38%) |
| 12 | CYC | O8 | 201 | - | 42,46,46 | 3.26 | 15 (35%) | 50,67,67 | 2.91 | 22 (44%) |
| 12 | CYC | Q3 | 201 | - | 42,46,46 | 3.17 | 13 (30%) | 50,67,67 | 2.87 | 22 (44%) |
| 12 | CYC | GA | 201 | - | 42,46,46 | 3.17 | 13 (30%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | VA | 202 | - | 42,46,46 | 2.96 | 11 (26%) | 50,67,67 | 2.94 | 19 (38%) |
| 12 | CYC | RA | 202 | - | 42,46,46 | 2.97 | 11 (26%) | 50,67,67 | 2.93 | 20 (40%) |
| 12 | CYC | Q8 | 201 | - | 42,46,46 | 2.97 | 11 (26%) | 50,67,67 | 2.95 | 20 (40%) |
| 12 | CYC | F8 | 202 | - | 42,46,46 | 3.28 | 17 (40%) | 50,67,67 | 2.94 | 22 (44%) |
| 12 | CYC | R3 | 202 | - | 42,46,46 | 2.97 | 11 (26%) | 50,67,67 | 2.93 | 20 (40%) |
| 12 | CYC | D3 | 202 | - | 42,46,46 | 3.31 | 16 (38%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | O5 | 201 | - | 42,46,46 | 3.26 | 12 (28%) | 50,67,67 | 3.02 | 19 (38%) |
| 12 | CYC | O4 | 202 | - | 42,46,46 | 2.94 | 10 (23%) | 50,67,67 | 2.96 | 19 (38%) |
| 12 | CYC | H6 | 201 | - | 42,46,46 | 3.30 | 16 (38%) | 50,67,67 | 2.91 | 21 (42%) |
| 12 | CYC | aA | 902 | - | 42,46,46 | 3.31 | 16 (38%) | 50,67,67 | 2.91 | 21 (42%) |
| 12 | CYC | TA | 301 | - | 42,46,46 | 3.29 | 16 (38%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | U8 | 201 | - | 42,46,46 | 3.29 | 15 (35%) | 50,67,67 | 2.93 | 23 (46%) |
| 12 | CYC | L7 | 201 | - | 42,46,46 | 3.28 | 14 (33%) | 50,67,67 | 2.75 | 20 (40%) |
| 12 | CYC | I7 | 201 | - | 42,46,46 | 3.27 | 12 (28%) | 50,67,67 | 3.02 | 20 (40%) |
| 12 | CYC | VA | 201 | - | 42,46,46 | 3.29 | 16 (38%) | 50,67,67 | 2.96 | 22 (44%) |
| 12 | CYC | AA | 201 | - | 42,46,46 | 3.18 | 13 (30%) | 50,67,67 | 2.86 | 23 (46%) |
| 12 | CYC | D3 | 201 | - | 42,46,46 | 2.97 | 11 (26%) | 50,67,67 | 2.93 | 20 (40%) |
| 12 | CYC | H7 | 201 | - | 42,46,46 | 3.30 | 14 (33%) | 50,67,67 | 2.74 | 20 (40%) |
| 12 | CYC | X9 | 202 | - | 42,46,46 | 2.97 | 10 (23%) | 50,67,67 | 2.95 | 20 (40%) |
| 12 | CYC | G7 | 201 | - | 42,46,46 | 3.25 | 12 (28%) | 50,67,67 | 3.00 | 19 (38%) |
| 12 | CYC | O4 | 201 | - | 42,46,46 | 3.26 | 15 (35%) | 50,67,67 | 2.91 | 22 (44%) |
| 12 | CYC | U4 | 202 | - | 42,46,46 | 2.97 | 11 (26%) | 50,67,67 | 2.91 | 20 (40%) |
| 12 | CYC | d7 | 201 | - | 42,46,46 | 3.29 | 14 (33%) | 50,67,67 | 2.75 | 20 (40%) |
| 12 | CYC | CA | 201 | - | 42,46,46 | 3.16 | 12 (28%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | PA | 201 | - | 42,46,46 | 3.29 | 16 (38%) | 50,67,67 | 2.95 | 23 (46%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 12 | CYC | UA | 201 | - | 42,46,46 | 3.18 | 13 (30%) | 50,67,67 | 2.89 | 23 (46%) |
| 12 | CYC | H2 | 202 | - | 42,46,46 | 2.95 | 10 (23%) | 50,67,67 | 2.92 | 20 (40%) |
| 12 | CYC | C2 | 201 | - | 42,46,46 | 3.13 | 13 (30%) | 50,67,67 | 2.89 | 22 (44%) |
| 12 | CYC | K7 | 201 | - | 42,46,46 | 3.30 | 12 (28%) | 50,67,67 | 3.02 | 19 (38%) |
| 12 | CYC | X1 | 202 | - | 42,46,46 | 2.97 | 11 (26%) | 50,67,67 | 2.93 | 20 (40%) |
| 12 | CYC | W9 | 201 | - | 42,46,46 | 3.17 | 12 (28%) | 50,67,67 | 2.87 | 23 (46%) |
| 12 | CYC | S4 | 202 | - | 42,46,46 | 3.31 | 16 (38%) | 50,67,67 | 2.95 | 21 (42%) |
| 12 | CYC | T9 | 301 | - | 42,46,46 | 3.29 | 16 (38%) | 50,67,67 | 2.91 | 23 (46%) |
| 12 | CYC | H2 | 201 | - | 42,46,46 | 3.31 | 16 (38%) | 50,67,67 | 2.90 | 22 (44%) |
| 12 | CYC | B4 | 202 | - | 42,46,46 | 3.31 | 16 (38%) | 50,67,67 | 2.92 | 23 (46%) |
| 12 | CYC | Z | 201 | - | 42,46,46 | 3.29 | 13 (30%) | 50,67,67 | 2.74 | 20 (40%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 12 | CYC | I8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | P8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | PA | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | J6 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | D4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | j7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | X7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | P1 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | a9 | 901 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | E1 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | E3 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | E8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | EA | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | c5 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | HA | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | T8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | P9 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | D5 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-------------|---------|
| 12 | CYC | A2 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | T4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | G6 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | TA | 302 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | Y3 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | S4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | C3 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | B9 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | BA | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | V1 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | U4 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | LA | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | SA | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | M4 | 301 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | v7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | C6 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | L6 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | B1 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | P1 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | X8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | G4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | B5 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | K4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | Z5 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | Z1 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | L3 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | E5 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | D6 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | V1 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | F3 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | k5 | 1204 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | A1 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | JA | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | I5 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-------------|---------|
| 12 | CYC | Q5 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | R8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | V9 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | V7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | g7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | R9 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | OA | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | M8 | 302 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | D8 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | T3 | 301 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | F6 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | G3 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | o7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | XA | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | H9 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | J7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | I9 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | K9 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | ZA | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | J9 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | BA | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | N4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | S3 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | H8 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | M8 | 301 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | F8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | R3 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | N2 | 101 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | K1 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | F3 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | k5 | 1202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | JA | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | ZA | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | IA | 201 | - | - | 10/25/74/74 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-------------|---------|
| 12 | CYC | A3 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | a7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | D2 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | L2 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | V3 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | S9 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | K5 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | N8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | U1 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | U9 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | P3 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | Y8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | XA | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | R4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | D7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | LA | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | HA | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | QA | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | k5 | 1201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | B9 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | J1 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | DA | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | F2 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | E9 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | X1 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | e7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | J9 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | H1 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | Z8 | 301 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | J3 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | Q9 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | s7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | O7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | j5 | 1202 | - | - | 10/25/74/74 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 12 | CYC | Y9 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | W3 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | E7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | C4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | W5 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | Z1 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | Z4 | 301 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | A7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | I2 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | d5 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | W7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | J2 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | h7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | H1 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | O1 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | L5 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | N5 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | J4 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | S5 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | i7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | Z9 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | FA | 301 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | WA | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | J2 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | B8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | DA | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | P5 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | V4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | I4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | O8 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | B2 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | L2 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | k7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | D9 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 12 | CYC | c7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | E6 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | F1 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | L8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | L4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | R1 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | A5 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | N6 | 101 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | W8 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | T9 | 302 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | C1 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | F1 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | f7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | L1 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | aA | 901 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | Y4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | L9 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | H5 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | I1 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | S7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | G8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | M7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | R7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | p7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | Q1 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | B8 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | m7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | A6 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | J4 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | J8 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | R9 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | P7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | L3 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | D8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 12 | CYC | B1 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | N7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | L4 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | U8 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | H3 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | Z3 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | L6 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | B3 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | S1 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | W4 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | f5 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | E4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | b7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | K8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | W4 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | Y7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | J8 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | F9 | 301 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | P4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | G5 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | Z3 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | M5 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | O9 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | u7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | F4 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | B7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | e5 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | r7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | A4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | I3 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | D1 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | X5 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | Y5 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | F5 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 12 | CYC | KA | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | P3 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | D4 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | K2 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | X3 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | R1 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | C8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | q7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | D2 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | H3 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | W8 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | H4 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | Q4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | H8 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | F2 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | D1 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | P9 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | V3 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | a5 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | U7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | B4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | F9 | 302 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | I6 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | R5 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | X3 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | G2 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | L9 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | F7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | G9 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | O3 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | C9 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | Q7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | H4 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | K3 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-------------|---------|
| 12 | CYC | X9 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | E2 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | T5 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | G1 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | k5 | 1203 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | W1 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | C5 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | K6 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | F9 | 303 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | B6 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | YA | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | H6 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | A9 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | D9 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | A8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | T7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | T3 | 302 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | B3 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | RA | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | H9 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | D6 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | U3 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | T1 | 301 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | b5 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | J5 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | Y1 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | J6 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | U5 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | V9 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | V5 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | j5 | 1201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | X4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | C7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | F6 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 12 | CYC | F4 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | V8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | T1 | 302 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | A | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | S8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | J3 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | Z9 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | O8 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | Q3 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | GA | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | VA | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | RA | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | Q8 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | F8 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | R3 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | D3 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | O5 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | O4 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | H6 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | aA | 902 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | TA | 301 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | U8 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | L7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | I7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | VA | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | AA | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | D3 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | H7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | X9 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | G7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | O4 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | U4 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | d7 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | CA | 201 | - | - | 10/25/74/74 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 12 | CYC | PA | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | UA | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | H2 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | C2 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | K7 | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 12 | CYC | X1 | 202 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | W9 | 201 | - | - | 10/25/74/74 | 0/4/4/4 |
| 12 | CYC | S4 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | T9 | 301 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | H2 | 201 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | B4 | 202 | - | - | 6/25/74/74 | 0/4/4/4 |
| 12 | CYC | Z | 201 | - | - | 10/25/74/74 | 0/4/4/4 |

All (4379) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | k5 | 1201 | CYC | CHA-C1A | 18.03 | 1.50 | 1.35 |
| 12 | j5 | 1201 | CYC | CHA-C1A | 17.99 | 1.50 | 1.35 |
| 12 | L2 | 201 | CYC | CHA-C1A | 17.22 | 1.49 | 1.35 |
| 12 | L6 | 201 | CYC | CHA-C1A | 17.22 | 1.49 | 1.35 |
| 12 | V1 | 201 | CYC | CHA-C1A | 17.18 | 1.49 | 1.35 |
| 12 | HA | 202 | CYC | CHA-C1A | 17.15 | 1.49 | 1.35 |
| 12 | H4 | 201 | CYC | CHA-C1A | 17.14 | 1.49 | 1.35 |
| 12 | H8 | 201 | CYC | CHA-C1A | 17.14 | 1.49 | 1.35 |
| 12 | F3 | 201 | CYC | CHA-C1A | 17.14 | 1.49 | 1.35 |
| 12 | XA | 201 | CYC | CHA-C1A | 17.12 | 1.49 | 1.35 |
| 12 | X9 | 201 | CYC | CHA-C1A | 17.12 | 1.49 | 1.35 |
| 12 | JA | 202 | CYC | CHA-C1A | 17.11 | 1.49 | 1.35 |
| 12 | J3 | 202 | CYC | CHA-C1A | 17.11 | 1.49 | 1.35 |
| 12 | J9 | 202 | CYC | CHA-C1A | 17.11 | 1.49 | 1.35 |
| 12 | aA | 901 | CYC | CHA-C1A | 17.11 | 1.49 | 1.35 |
| 12 | V3 | 201 | CYC | CHA-C1A | 17.10 | 1.49 | 1.35 |
| 12 | F1 | 201 | CYC | CHA-C1A | 17.09 | 1.49 | 1.35 |
| 12 | H9 | 202 | CYC | CHA-C1A | 17.08 | 1.49 | 1.35 |
| 12 | Z3 | 201 | CYC | CHA-C1A | 17.08 | 1.49 | 1.35 |
| 12 | Z1 | 202 | CYC | CHA-C1A | 17.08 | 1.49 | 1.35 |
| 12 | RA | 201 | CYC | CHA-C1A | 17.03 | 1.49 | 1.35 |
| 12 | R9 | 201 | CYC | CHA-C1A | 17.03 | 1.49 | 1.35 |
| 12 | J4 | 201 | CYC | CHA-C1A | 17.03 | 1.49 | 1.35 |
| 12 | J8 | 201 | CYC | CHA-C1A | 17.03 | 1.49 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | LA | 202 | CYC | CHA-C1A | 17.02 | 1.49 | 1.35 |
| 12 | L9 | 202 | CYC | CHA-C1A | 17.02 | 1.49 | 1.35 |
| 12 | H2 | 201 | CYC | CHA-C1A | 17.01 | 1.49 | 1.35 |
| 12 | H6 | 201 | CYC | CHA-C1A | 16.99 | 1.49 | 1.35 |
| 12 | M4 | 301 | CYC | CHA-C1A | 16.99 | 1.49 | 1.35 |
| 12 | B4 | 202 | CYC | CHA-C1A | 16.99 | 1.49 | 1.35 |
| 12 | L3 | 202 | CYC | CHA-C1A | 16.99 | 1.49 | 1.35 |
| 12 | aA | 902 | CYC | CHA-C1A | 16.99 | 1.49 | 1.35 |
| 12 | M8 | 301 | CYC | CHA-C1A | 16.97 | 1.49 | 1.35 |
| 12 | D3 | 202 | CYC | CHA-C1A | 16.97 | 1.49 | 1.35 |
| 12 | D1 | 202 | CYC | CHA-C1A | 16.97 | 1.49 | 1.35 |
| 12 | E7 | 201 | CYC | CHA-C1A | 16.96 | 1.49 | 1.35 |
| 12 | B8 | 202 | CYC | CHA-C1A | 16.95 | 1.49 | 1.35 |
| 12 | TA | 301 | CYC | CHA-C1A | 16.95 | 1.49 | 1.35 |
| 12 | T9 | 301 | CYC | CHA-C1A | 16.95 | 1.49 | 1.35 |
| 12 | c7 | 201 | CYC | CHA-C1A | 16.94 | 1.49 | 1.35 |
| 12 | B3 | 202 | CYC | CHA-C1A | 16.94 | 1.49 | 1.35 |
| 12 | K7 | 201 | CYC | CHA-C1A | 16.94 | 1.49 | 1.35 |
| 12 | Q5 | 201 | CYC | CHA-C1A | 16.94 | 1.49 | 1.35 |
| 12 | Z8 | 301 | CYC | CHA-C1A | 16.92 | 1.49 | 1.35 |
| 12 | e7 | 201 | CYC | CHA-C1A | 16.92 | 1.49 | 1.35 |
| 12 | Z4 | 301 | CYC | CHA-C1A | 16.91 | 1.49 | 1.35 |
| 12 | S4 | 202 | CYC | CHA-C1A | 16.90 | 1.49 | 1.35 |
| 12 | X3 | 201 | CYC | CHA-C1A | 16.90 | 1.49 | 1.35 |
| 12 | X1 | 201 | CYC | CHA-C1A | 16.90 | 1.49 | 1.35 |
| 12 | W5 | 201 | CYC | CHA-C1A | 16.89 | 1.49 | 1.35 |
| 12 | BA | 201 | CYC | CHA-C1A | 16.89 | 1.49 | 1.35 |
| 12 | B9 | 201 | CYC | CHA-C1A | 16.89 | 1.49 | 1.35 |
| 12 | a5 | 201 | CYC | CHA-C1A | 16.89 | 1.49 | 1.35 |
| 12 | B1 | 202 | CYC | CHA-C1A | 16.88 | 1.49 | 1.35 |
| 12 | a9 | 901 | CYC | CHA-C1A | 16.88 | 1.49 | 1.35 |
| 12 | Y7 | 201 | CYC | CHA-C1A | 16.88 | 1.49 | 1.35 |
| 12 | L4 | 202 | CYC | CHA-C1A | 16.87 | 1.49 | 1.35 |
| 12 | J2 | 202 | CYC | CHA-C1A | 16.87 | 1.49 | 1.35 |
| 12 | e5 | 201 | CYC | CHA-C1A | 16.86 | 1.49 | 1.35 |
| 12 | c5 | 201 | CYC | CHA-C1A | 16.85 | 1.49 | 1.35 |
| 12 | R1 | 201 | CYC | CHA-C1A | 16.85 | 1.49 | 1.35 |
| 12 | R3 | 201 | CYC | CHA-C1A | 16.85 | 1.49 | 1.35 |
| 12 | D4 | 202 | CYC | CHA-C1A | 16.85 | 1.49 | 1.35 |
| 12 | D8 | 202 | CYC | CHA-C1A | 16.85 | 1.49 | 1.35 |
| 12 | W7 | 201 | CYC | CHA-C1A | 16.84 | 1.49 | 1.35 |
| 12 | F9 | 301 | CYC | CHA-C1A | 16.83 | 1.49 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | F2 | 201 | CYC | CHA-C1A | 16.83 | 1.49 | 1.35 |
| 12 | a7 | 201 | CYC | CHA-C1A | 16.83 | 1.49 | 1.35 |
| 12 | VA | 201 | CYC | CHA-C1A | 16.83 | 1.49 | 1.35 |
| 12 | V9 | 201 | CYC | CHA-C1A | 16.83 | 1.49 | 1.35 |
| 12 | g7 | 201 | CYC | CHA-C1A | 16.83 | 1.49 | 1.35 |
| 12 | i7 | 201 | CYC | CHA-C1A | 16.81 | 1.49 | 1.35 |
| 12 | U4 | 201 | CYC | CHA-C1A | 16.81 | 1.49 | 1.35 |
| 12 | U8 | 201 | CYC | CHA-C1A | 16.81 | 1.49 | 1.35 |
| 12 | P1 | 201 | CYC | CHA-C1A | 16.79 | 1.49 | 1.35 |
| 12 | P3 | 201 | CYC | CHA-C1A | 16.79 | 1.49 | 1.35 |
| 12 | N2 | 101 | CYC | CHA-C1A | 16.79 | 1.49 | 1.35 |
| 12 | N6 | 101 | CYC | CHA-C1A | 16.79 | 1.49 | 1.35 |
| 12 | u7 | 201 | CYC | CHA-C1A | 16.77 | 1.49 | 1.35 |
| 12 | PA | 201 | CYC | CHA-C1A | 16.76 | 1.49 | 1.35 |
| 12 | P9 | 201 | CYC | CHA-C1A | 16.76 | 1.49 | 1.35 |
| 12 | Y5 | 201 | CYC | CHA-C1A | 16.76 | 1.49 | 1.35 |
| 12 | FA | 301 | CYC | CHA-C1A | 16.75 | 1.49 | 1.35 |
| 12 | W4 | 201 | CYC | CHA-C1A | 16.75 | 1.49 | 1.35 |
| 12 | W8 | 201 | CYC | CHA-C1A | 16.75 | 1.49 | 1.35 |
| 12 | o7 | 201 | CYC | CHA-C1A | 16.75 | 1.49 | 1.35 |
| 12 | Q7 | 201 | CYC | CHA-C1A | 16.75 | 1.49 | 1.35 |
| 12 | F4 | 202 | CYC | CHA-C1A | 16.74 | 1.49 | 1.35 |
| 12 | F8 | 202 | CYC | CHA-C1A | 16.74 | 1.49 | 1.35 |
| 12 | T3 | 301 | CYC | CHA-C1A | 16.74 | 1.49 | 1.35 |
| 12 | C5 | 201 | CYC | CHA-C1A | 16.74 | 1.49 | 1.35 |
| 12 | I7 | 201 | CYC | CHA-C1A | 16.74 | 1.49 | 1.35 |
| 12 | T1 | 301 | CYC | CHA-C1A | 16.74 | 1.49 | 1.35 |
| 12 | M8 | 302 | CYC | CHA-C1A | 16.73 | 1.49 | 1.35 |
| 12 | ZA | 202 | CYC | CHA-C1A | 16.72 | 1.49 | 1.35 |
| 12 | Z9 | 202 | CYC | CHA-C1A | 16.72 | 1.49 | 1.35 |
| 12 | k7 | 201 | CYC | CHA-C1A | 16.72 | 1.49 | 1.35 |
| 12 | J6 | 202 | CYC | CHA-C1A | 16.71 | 1.49 | 1.35 |
| 12 | E5 | 201 | CYC | CHA-C1A | 16.71 | 1.49 | 1.35 |
| 12 | O4 | 201 | CYC | CHA-C1A | 16.70 | 1.49 | 1.35 |
| 12 | O8 | 201 | CYC | CHA-C1A | 16.70 | 1.49 | 1.35 |
| 12 | U5 | 201 | CYC | CHA-C1A | 16.69 | 1.49 | 1.35 |
| 12 | K5 | 201 | CYC | CHA-C1A | 16.69 | 1.49 | 1.35 |
| 12 | C7 | 201 | CYC | CHA-C1A | 16.69 | 1.49 | 1.35 |
| 12 | F6 | 201 | CYC | CHA-C1A | 16.68 | 1.49 | 1.35 |
| 12 | m7 | 201 | CYC | CHA-C1A | 16.67 | 1.49 | 1.35 |
| 12 | I5 | 201 | CYC | CHA-C1A | 16.67 | 1.49 | 1.35 |
| 12 | s7 | 201 | CYC | CHA-C1A | 16.67 | 1.49 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | q7 | 201 | CYC | CHA-C1A | 16.66 | 1.49 | 1.35 |
| 12 | H3 | 202 | CYC | CHA-C1A | 16.65 | 1.49 | 1.35 |
| 12 | D6 | 201 | CYC | CHA-C1A | 16.65 | 1.49 | 1.35 |
| 12 | H1 | 201 | CYC | CHA-C1A | 16.64 | 1.49 | 1.35 |
| 12 | A5 | 201 | CYC | CHA-C1A | 16.64 | 1.49 | 1.35 |
| 12 | M7 | 201 | CYC | CHA-C1A | 16.64 | 1.49 | 1.35 |
| 12 | D2 | 201 | CYC | CHA-C1A | 16.63 | 1.49 | 1.35 |
| 12 | O5 | 201 | CYC | CHA-C1A | 16.62 | 1.49 | 1.35 |
| 12 | G5 | 201 | CYC | CHA-C1A | 16.61 | 1.49 | 1.35 |
| 12 | O7 | 201 | CYC | CHA-C1A | 16.59 | 1.49 | 1.35 |
| 12 | S7 | 201 | CYC | CHA-C1A | 16.59 | 1.49 | 1.35 |
| 12 | G7 | 201 | CYC | CHA-C1A | 16.57 | 1.49 | 1.35 |
| 12 | U7 | 201 | CYC | CHA-C1A | 16.54 | 1.48 | 1.35 |
| 12 | A7 | 201 | CYC | CHA-C1A | 16.53 | 1.48 | 1.35 |
| 12 | M5 | 201 | CYC | CHA-C1A | 16.51 | 1.48 | 1.35 |
| 12 | DA | 201 | CYC | CHA-C1A | 16.48 | 1.48 | 1.35 |
| 12 | D9 | 201 | CYC | CHA-C1A | 16.48 | 1.48 | 1.35 |
| 12 | S5 | 201 | CYC | CHA-C1A | 16.47 | 1.48 | 1.35 |
| 12 | k5 | 1202 | CYC | CHA-C1A | 16.42 | 1.48 | 1.35 |
| 12 | T5 | 201 | CYC | CHA-C1A | 16.40 | 1.48 | 1.35 |
| 12 | f7 | 201 | CYC | CHA-C1A | 16.38 | 1.48 | 1.35 |
| 12 | B7 | 201 | CYC | CHA-C1A | 16.34 | 1.48 | 1.35 |
| 12 | r7 | 201 | CYC | CHA-C1A | 16.33 | 1.48 | 1.35 |
| 12 | H7 | 201 | CYC | CHA-C1A | 16.32 | 1.48 | 1.35 |
| 12 | V7 | 201 | CYC | CHA-C1A | 16.31 | 1.48 | 1.35 |
| 12 | P5 | 201 | CYC | CHA-C1A | 16.31 | 1.48 | 1.35 |
| 12 | N5 | 201 | CYC | CHA-C1A | 16.29 | 1.48 | 1.35 |
| 12 | k5 | 1203 | CYC | CHA-C1A | 16.29 | 1.48 | 1.35 |
| 12 | A | 201 | CYC | CHA-C1A | 16.28 | 1.48 | 1.35 |
| 12 | N7 | 201 | CYC | CHA-C1A | 16.26 | 1.48 | 1.35 |
| 12 | Z | 201 | CYC | CHA-C1A | 16.22 | 1.48 | 1.35 |
| 12 | V5 | 201 | CYC | CHA-C1A | 16.22 | 1.48 | 1.35 |
| 12 | d7 | 201 | CYC | CHA-C1A | 16.16 | 1.48 | 1.35 |
| 12 | O1 | 201 | CYC | CHA-C1A | 16.16 | 1.48 | 1.35 |
| 12 | O3 | 201 | CYC | CHA-C1A | 16.16 | 1.48 | 1.35 |
| 12 | J5 | 201 | CYC | CHA-C1A | 16.15 | 1.48 | 1.35 |
| 12 | P7 | 201 | CYC | CHA-C1A | 16.15 | 1.48 | 1.35 |
| 12 | D5 | 201 | CYC | CHA-C1A | 16.14 | 1.48 | 1.35 |
| 12 | B5 | 201 | CYC | CHA-C1A | 16.14 | 1.48 | 1.35 |
| 12 | b7 | 201 | CYC | CHA-C1A | 16.14 | 1.48 | 1.35 |
| 12 | F5 | 201 | CYC | CHA-C1A | 16.14 | 1.48 | 1.35 |
| 12 | j5 | 1202 | CYC | CHA-C1A | 16.13 | 1.48 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | h7 | 201 | CYC | CHA-C1A | 16.13 | 1.48 | 1.35 |
| 12 | H5 | 201 | CYC | CHA-C1A | 16.10 | 1.48 | 1.35 |
| 12 | p7 | 201 | CYC | CHA-C1A | 16.10 | 1.48 | 1.35 |
| 12 | j7 | 201 | CYC | CHA-C1A | 16.09 | 1.48 | 1.35 |
| 12 | R7 | 201 | CYC | CHA-C1A | 16.09 | 1.48 | 1.35 |
| 12 | v7 | 201 | CYC | CHA-C1A | 16.08 | 1.48 | 1.35 |
| 12 | k5 | 1204 | CYC | CHA-C1A | 16.08 | 1.48 | 1.35 |
| 12 | F7 | 201 | CYC | CHA-C1A | 16.08 | 1.48 | 1.35 |
| 12 | L7 | 201 | CYC | CHA-C1A | 16.07 | 1.48 | 1.35 |
| 12 | X5 | 201 | CYC | CHA-C1A | 16.06 | 1.48 | 1.35 |
| 12 | L5 | 201 | CYC | CHA-C1A | 16.06 | 1.48 | 1.35 |
| 12 | I4 | 201 | CYC | CHA-C1A | 16.06 | 1.48 | 1.35 |
| 12 | I8 | 201 | CYC | CHA-C1A | 16.06 | 1.48 | 1.35 |
| 12 | d5 | 201 | CYC | CHA-C1A | 16.04 | 1.48 | 1.35 |
| 12 | R5 | 201 | CYC | CHA-C1A | 16.04 | 1.48 | 1.35 |
| 12 | T7 | 201 | CYC | CHA-C1A | 16.02 | 1.48 | 1.35 |
| 12 | X7 | 201 | CYC | CHA-C1A | 16.01 | 1.48 | 1.35 |
| 12 | D7 | 201 | CYC | CHA-C1A | 16.00 | 1.48 | 1.35 |
| 12 | C3 | 201 | CYC | CHA-C1A | 15.97 | 1.48 | 1.35 |
| 12 | C1 | 201 | CYC | CHA-C1A | 15.97 | 1.48 | 1.35 |
| 12 | OA | 201 | CYC | CHA-C1A | 15.96 | 1.48 | 1.35 |
| 12 | O9 | 201 | CYC | CHA-C1A | 15.96 | 1.48 | 1.35 |
| 12 | W3 | 201 | CYC | CHA-C1A | 15.96 | 1.48 | 1.35 |
| 12 | W1 | 201 | CYC | CHA-C1A | 15.96 | 1.48 | 1.35 |
| 12 | T4 | 201 | CYC | CHA-C1A | 15.95 | 1.48 | 1.35 |
| 12 | T8 | 201 | CYC | CHA-C1A | 15.95 | 1.48 | 1.35 |
| 12 | A3 | 201 | CYC | CHA-C1A | 15.94 | 1.48 | 1.35 |
| 12 | I6 | 201 | CYC | CHA-C1A | 15.94 | 1.48 | 1.35 |
| 12 | A1 | 201 | CYC | CHA-C1A | 15.92 | 1.48 | 1.35 |
| 12 | J7 | 201 | CYC | CHA-C1A | 15.92 | 1.48 | 1.35 |
| 12 | X4 | 201 | CYC | CHA-C1A | 15.92 | 1.48 | 1.35 |
| 12 | X8 | 201 | CYC | CHA-C1A | 15.92 | 1.48 | 1.35 |
| 12 | A6 | 201 | CYC | CHA-C1A | 15.91 | 1.48 | 1.35 |
| 12 | A2 | 201 | CYC | CHA-C1A | 15.91 | 1.48 | 1.35 |
| 12 | b5 | 201 | CYC | CHA-C1A | 15.90 | 1.48 | 1.35 |
| 12 | SA | 201 | CYC | CHA-C1A | 15.89 | 1.48 | 1.35 |
| 12 | S9 | 201 | CYC | CHA-C1A | 15.89 | 1.48 | 1.35 |
| 12 | f5 | 201 | CYC | CHA-C1A | 15.89 | 1.48 | 1.35 |
| 12 | N4 | 201 | CYC | CHA-C1A | 15.88 | 1.48 | 1.35 |
| 12 | N8 | 201 | CYC | CHA-C1A | 15.88 | 1.48 | 1.35 |
| 12 | AA | 201 | CYC | CHA-C1A | 15.87 | 1.48 | 1.35 |
| 12 | A9 | 201 | CYC | CHA-C1A | 15.87 | 1.48 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | I2 | 201 | CYC | CHA-C1A | 15.86 | 1.48 | 1.35 |
| 12 | Z5 | 201 | CYC | CHA-C1A | 15.86 | 1.48 | 1.35 |
| 12 | V4 | 201 | CYC | CHA-C1A | 15.84 | 1.48 | 1.35 |
| 12 | V8 | 201 | CYC | CHA-C1A | 15.84 | 1.48 | 1.35 |
| 12 | Q1 | 201 | CYC | CHA-C1A | 15.83 | 1.48 | 1.35 |
| 12 | Q3 | 201 | CYC | CHA-C1A | 15.83 | 1.48 | 1.35 |
| 12 | UA | 201 | CYC | CHA-C1A | 15.82 | 1.48 | 1.35 |
| 12 | U9 | 201 | CYC | CHA-C1A | 15.82 | 1.48 | 1.35 |
| 12 | A4 | 201 | CYC | CHA-C1A | 15.81 | 1.48 | 1.35 |
| 12 | A8 | 201 | CYC | CHA-C1A | 15.81 | 1.48 | 1.35 |
| 12 | G4 | 201 | CYC | CHA-C1A | 15.80 | 1.48 | 1.35 |
| 12 | G8 | 201 | CYC | CHA-C1A | 15.80 | 1.48 | 1.35 |
| 12 | Q9 | 201 | CYC | CHA-C1A | 15.77 | 1.48 | 1.35 |
| 12 | E2 | 201 | CYC | CHA-C1A | 15.77 | 1.48 | 1.35 |
| 12 | WA | 201 | CYC | CHA-C1A | 15.77 | 1.48 | 1.35 |
| 12 | U3 | 201 | CYC | CHA-C1A | 15.77 | 1.48 | 1.35 |
| 12 | W9 | 201 | CYC | CHA-C1A | 15.77 | 1.48 | 1.35 |
| 12 | U1 | 201 | CYC | CHA-C1A | 15.77 | 1.48 | 1.35 |
| 12 | QA | 201 | CYC | CHA-C1A | 15.75 | 1.48 | 1.35 |
| 12 | E4 | 201 | CYC | CHA-C1A | 15.73 | 1.48 | 1.35 |
| 12 | E8 | 201 | CYC | CHA-C1A | 15.73 | 1.48 | 1.35 |
| 12 | GA | 201 | CYC | CHA-C1A | 15.71 | 1.48 | 1.35 |
| 12 | G9 | 201 | CYC | CHA-C1A | 15.71 | 1.48 | 1.35 |
| 12 | G2 | 201 | CYC | CHA-C1A | 15.71 | 1.48 | 1.35 |
| 12 | G6 | 201 | CYC | CHA-C1A | 15.71 | 1.48 | 1.35 |
| 12 | CA | 201 | CYC | CHA-C1A | 15.70 | 1.48 | 1.35 |
| 12 | Y3 | 201 | CYC | CHA-C1A | 15.69 | 1.48 | 1.35 |
| 12 | E6 | 201 | CYC | CHA-C1A | 15.69 | 1.48 | 1.35 |
| 12 | Y1 | 201 | CYC | CHA-C1A | 15.69 | 1.48 | 1.35 |
| 12 | E3 | 201 | CYC | CHA-C1A | 15.68 | 1.48 | 1.35 |
| 12 | E1 | 201 | CYC | CHA-C1A | 15.68 | 1.48 | 1.35 |
| 12 | I3 | 201 | CYC | CHA-C1A | 15.68 | 1.48 | 1.35 |
| 12 | I1 | 201 | CYC | CHA-C1A | 15.68 | 1.48 | 1.35 |
| 12 | C9 | 201 | CYC | CHA-C1A | 15.68 | 1.48 | 1.35 |
| 12 | K4 | 201 | CYC | CHA-C1A | 15.66 | 1.48 | 1.35 |
| 12 | K8 | 201 | CYC | CHA-C1A | 15.66 | 1.48 | 1.35 |
| 12 | KA | 201 | CYC | CHA-C1A | 15.65 | 1.48 | 1.35 |
| 12 | K9 | 201 | CYC | CHA-C1A | 15.65 | 1.48 | 1.35 |
| 12 | K6 | 201 | CYC | CHA-C1A | 15.64 | 1.48 | 1.35 |
| 12 | K3 | 201 | CYC | CHA-C1A | 15.64 | 1.48 | 1.35 |
| 12 | K1 | 201 | CYC | CHA-C1A | 15.64 | 1.48 | 1.35 |
| 12 | IA | 201 | CYC | CHA-C1A | 15.63 | 1.48 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | I9 | 201 | CYC | CHA-C1A | 15.63 | 1.48 | 1.35 |
| 12 | EA | 201 | CYC | CHA-C1A | 15.57 | 1.48 | 1.35 |
| 12 | G3 | 201 | CYC | CHA-C1A | 15.57 | 1.48 | 1.35 |
| 12 | E9 | 201 | CYC | CHA-C1A | 15.57 | 1.48 | 1.35 |
| 12 | G1 | 201 | CYC | CHA-C1A | 15.57 | 1.48 | 1.35 |
| 12 | YA | 201 | CYC | CHA-C1A | 15.56 | 1.48 | 1.35 |
| 12 | Y9 | 201 | CYC | CHA-C1A | 15.56 | 1.48 | 1.35 |
| 12 | S1 | 201 | CYC | CHA-C1A | 15.56 | 1.48 | 1.35 |
| 12 | S3 | 201 | CYC | CHA-C1A | 15.56 | 1.48 | 1.35 |
| 12 | C6 | 201 | CYC | CHA-C1A | 15.56 | 1.48 | 1.35 |
| 12 | R4 | 201 | CYC | CHA-C1A | 15.51 | 1.48 | 1.35 |
| 12 | R8 | 201 | CYC | CHA-C1A | 15.51 | 1.48 | 1.35 |
| 12 | K2 | 201 | CYC | CHA-C1A | 15.50 | 1.48 | 1.35 |
| 12 | P4 | 201 | CYC | CHA-C1A | 15.50 | 1.48 | 1.35 |
| 12 | P8 | 201 | CYC | CHA-C1A | 15.50 | 1.48 | 1.35 |
| 12 | C4 | 201 | CYC | CHA-C1A | 15.45 | 1.48 | 1.35 |
| 12 | C8 | 201 | CYC | CHA-C1A | 15.45 | 1.48 | 1.35 |
| 12 | C2 | 201 | CYC | CHA-C1A | 15.44 | 1.48 | 1.35 |
| 12 | F2 | 202 | CYC | CHA-C1A | 15.07 | 1.47 | 1.35 |
| 12 | F6 | 202 | CYC | CHA-C1A | 15.01 | 1.47 | 1.35 |
| 12 | TA | 302 | CYC | CHA-C1A | 14.96 | 1.47 | 1.35 |
| 12 | T9 | 302 | CYC | CHA-C1A | 14.96 | 1.47 | 1.35 |
| 12 | S4 | 201 | CYC | CHA-C1A | 14.94 | 1.47 | 1.35 |
| 12 | S8 | 201 | CYC | CHA-C1A | 14.94 | 1.47 | 1.35 |
| 12 | D2 | 202 | CYC | CHA-C1A | 14.93 | 1.47 | 1.35 |
| 12 | F3 | 202 | CYC | CHA-C1A | 14.92 | 1.47 | 1.35 |
| 12 | F1 | 202 | CYC | CHA-C1A | 14.92 | 1.47 | 1.35 |
| 12 | L6 | 202 | CYC | CHA-C1A | 14.90 | 1.47 | 1.35 |
| 12 | D6 | 202 | CYC | CHA-C1A | 14.90 | 1.47 | 1.35 |
| 12 | J4 | 202 | CYC | CHA-C1A | 14.88 | 1.47 | 1.35 |
| 12 | J8 | 202 | CYC | CHA-C1A | 14.88 | 1.47 | 1.35 |
| 12 | JA | 201 | CYC | CHA-C1A | 14.87 | 1.47 | 1.35 |
| 12 | J9 | 201 | CYC | CHA-C1A | 14.87 | 1.47 | 1.35 |
| 12 | PA | 202 | CYC | CHA-C1A | 14.84 | 1.47 | 1.35 |
| 12 | P9 | 202 | CYC | CHA-C1A | 14.84 | 1.47 | 1.35 |
| 12 | ZA | 201 | CYC | CHA-C1A | 14.77 | 1.47 | 1.35 |
| 12 | L2 | 202 | CYC | CHA-C1A | 14.77 | 1.47 | 1.35 |
| 12 | Z9 | 201 | CYC | CHA-C1A | 14.77 | 1.47 | 1.35 |
| 12 | F4 | 201 | CYC | CHA-C1A | 14.76 | 1.47 | 1.35 |
| 12 | F8 | 201 | CYC | CHA-C1A | 14.76 | 1.47 | 1.35 |
| 12 | T3 | 302 | CYC | CHA-C1A | 14.75 | 1.47 | 1.35 |
| 12 | T1 | 302 | CYC | CHA-C1A | 14.75 | 1.47 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | W4 | 202 | CYC | CHA-C1A | 14.74 | 1.47 | 1.35 |
| 12 | W8 | 202 | CYC | CHA-C1A | 14.74 | 1.47 | 1.35 |
| 12 | X3 | 202 | CYC | CHA-C1A | 14.74 | 1.47 | 1.35 |
| 12 | X1 | 202 | CYC | CHA-C1A | 14.74 | 1.47 | 1.35 |
| 12 | RA | 202 | CYC | CHA-C1A | 14.73 | 1.47 | 1.35 |
| 12 | R9 | 202 | CYC | CHA-C1A | 14.73 | 1.47 | 1.35 |
| 12 | B3 | 201 | CYC | CHA-C1A | 14.73 | 1.47 | 1.35 |
| 12 | B1 | 201 | CYC | CHA-C1A | 14.73 | 1.47 | 1.35 |
| 12 | HA | 201 | CYC | CHA-C1A | 14.71 | 1.47 | 1.35 |
| 12 | D3 | 201 | CYC | CHA-C1A | 14.71 | 1.47 | 1.35 |
| 12 | D1 | 201 | CYC | CHA-C1A | 14.71 | 1.47 | 1.35 |
| 12 | J6 | 201 | CYC | CHA-C1A | 14.68 | 1.47 | 1.35 |
| 12 | Z3 | 202 | CYC | CHA-C1A | 14.67 | 1.47 | 1.35 |
| 12 | Z1 | 201 | CYC | CHA-C1A | 14.67 | 1.47 | 1.35 |
| 12 | Q8 | 201 | CYC | CHA-C1A | 14.67 | 1.47 | 1.35 |
| 12 | XA | 202 | CYC | CHA-C1A | 14.66 | 1.47 | 1.35 |
| 12 | R1 | 202 | CYC | CHA-C1A | 14.65 | 1.47 | 1.35 |
| 12 | R3 | 202 | CYC | CHA-C1A | 14.65 | 1.47 | 1.35 |
| 12 | U4 | 202 | CYC | CHA-C1A | 14.64 | 1.47 | 1.35 |
| 12 | H9 | 201 | CYC | CHA-C1A | 14.64 | 1.47 | 1.35 |
| 12 | H3 | 201 | CYC | CHA-C1A | 14.62 | 1.47 | 1.35 |
| 12 | H1 | 202 | CYC | CHA-C1A | 14.62 | 1.47 | 1.35 |
| 12 | J2 | 201 | CYC | CHA-C1A | 14.62 | 1.47 | 1.35 |
| 12 | U8 | 202 | CYC | CHA-C1A | 14.61 | 1.47 | 1.35 |
| 12 | J3 | 201 | CYC | CHA-C1A | 14.61 | 1.47 | 1.35 |
| 12 | Q4 | 201 | CYC | CHA-C1A | 14.61 | 1.47 | 1.35 |
| 12 | J1 | 201 | CYC | CHA-C1A | 14.61 | 1.47 | 1.35 |
| 12 | VA | 202 | CYC | CHA-C1A | 14.61 | 1.47 | 1.35 |
| 12 | X9 | 202 | CYC | CHA-C1A | 14.61 | 1.47 | 1.35 |
| 12 | V3 | 202 | CYC | CHA-C1A | 14.60 | 1.47 | 1.35 |
| 12 | V1 | 202 | CYC | CHA-C1A | 14.60 | 1.47 | 1.35 |
| 12 | H4 | 202 | CYC | CHA-C1A | 14.59 | 1.47 | 1.35 |
| 12 | H8 | 202 | CYC | CHA-C1A | 14.59 | 1.47 | 1.35 |
| 12 | P1 | 202 | CYC | CHA-C1A | 14.58 | 1.47 | 1.35 |
| 12 | P3 | 202 | CYC | CHA-C1A | 14.58 | 1.47 | 1.35 |
| 12 | D4 | 201 | CYC | CHA-C1A | 14.57 | 1.47 | 1.35 |
| 12 | D8 | 201 | CYC | CHA-C1A | 14.57 | 1.47 | 1.35 |
| 12 | B6 | 201 | CYC | CHA-C1A | 14.56 | 1.47 | 1.35 |
| 12 | B4 | 201 | CYC | CHA-C1A | 14.56 | 1.47 | 1.35 |
| 12 | B8 | 201 | CYC | CHA-C1A | 14.56 | 1.47 | 1.35 |
| 12 | DA | 202 | CYC | CHA-C1A | 14.56 | 1.47 | 1.35 |
| 12 | D9 | 202 | CYC | CHA-C1A | 14.56 | 1.47 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | V9 | 202 | CYC | CHA-C1A | 14.54 | 1.47 | 1.35 |
| 12 | LA | 201 | CYC | CHA-C1A | 14.53 | 1.47 | 1.35 |
| 12 | L9 | 201 | CYC | CHA-C1A | 14.53 | 1.47 | 1.35 |
| 12 | L3 | 201 | CYC | CHA-C1A | 14.52 | 1.47 | 1.35 |
| 12 | L1 | 201 | CYC | CHA-C1A | 14.52 | 1.47 | 1.35 |
| 12 | H2 | 202 | CYC | CHA-C1A | 14.50 | 1.47 | 1.35 |
| 12 | H6 | 202 | CYC | CHA-C1A | 14.50 | 1.47 | 1.35 |
| 12 | F9 | 303 | CYC | CHA-C1A | 14.49 | 1.47 | 1.35 |
| 12 | F9 | 302 | CYC | CHA-C1A | 14.48 | 1.47 | 1.35 |
| 12 | B2 | 201 | CYC | CHA-C1A | 14.47 | 1.47 | 1.35 |
| 12 | L4 | 201 | CYC | CHA-C1A | 14.44 | 1.47 | 1.35 |
| 12 | L8 | 201 | CYC | CHA-C1A | 14.44 | 1.47 | 1.35 |
| 12 | O4 | 202 | CYC | CHA-C1A | 14.42 | 1.47 | 1.35 |
| 12 | O8 | 202 | CYC | CHA-C1A | 14.42 | 1.47 | 1.35 |
| 12 | BA | 202 | CYC | CHA-C1A | 14.42 | 1.47 | 1.35 |
| 12 | B9 | 202 | CYC | CHA-C1A | 14.42 | 1.47 | 1.35 |
| 12 | Y4 | 201 | CYC | CHA-C1A | 14.40 | 1.47 | 1.35 |
| 12 | Y8 | 201 | CYC | CHA-C1A | 14.40 | 1.47 | 1.35 |
| 12 | F7 | 201 | CYC | C3B-C2B | 6.16 | 1.49 | 1.36 |
| 12 | p7 | 201 | CYC | C3B-C2B | 6.15 | 1.49 | 1.36 |
| 12 | F5 | 201 | CYC | C3B-C2B | 6.14 | 1.49 | 1.36 |
| 12 | V7 | 201 | CYC | C3B-C2B | 6.14 | 1.49 | 1.36 |
| 12 | J5 | 201 | CYC | C3B-C2B | 6.14 | 1.49 | 1.36 |
| 12 | f5 | 201 | CYC | C3B-C2B | 6.13 | 1.49 | 1.36 |
| 12 | L5 | 201 | CYC | C3B-C2B | 6.13 | 1.49 | 1.36 |
| 12 | L7 | 201 | CYC | C3B-C2B | 6.13 | 1.49 | 1.36 |
| 12 | v7 | 201 | CYC | C3B-C2B | 6.11 | 1.49 | 1.36 |
| 12 | D5 | 201 | CYC | C3B-C2B | 6.11 | 1.49 | 1.36 |
| 12 | R5 | 201 | CYC | C3B-C2B | 6.11 | 1.49 | 1.36 |
| 12 | H7 | 201 | CYC | C3B-C2B | 6.10 | 1.49 | 1.36 |
| 12 | b7 | 201 | CYC | C3B-C2B | 6.10 | 1.49 | 1.36 |
| 12 | k5 | 1204 | CYC | C3B-C2B | 6.09 | 1.49 | 1.36 |
| 12 | T5 | 201 | CYC | C3B-C2B | 6.09 | 1.49 | 1.36 |
| 12 | X5 | 201 | CYC | C3B-C2B | 6.09 | 1.49 | 1.36 |
| 12 | T7 | 201 | CYC | C3B-C2B | 6.09 | 1.49 | 1.36 |
| 12 | N7 | 201 | CYC | C3B-C2B | 6.08 | 1.49 | 1.36 |
| 12 | k5 | 1202 | CYC | C3B-C2B | 6.08 | 1.49 | 1.36 |
| 12 | h7 | 201 | CYC | C3B-C2B | 6.07 | 1.49 | 1.36 |
| 12 | D7 | 201 | CYC | C3B-C2B | 6.07 | 1.49 | 1.36 |
| 12 | Z | 201 | CYC | C3B-C2B | 6.07 | 1.49 | 1.36 |
| 12 | B5 | 201 | CYC | C3B-C2B | 6.06 | 1.49 | 1.36 |
| 12 | b5 | 201 | CYC | C3B-C2B | 6.06 | 1.49 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 12 | f7 | 201 | CYC | C3B-C2B | 6.06 | 1.49 | 1.36 |
| 12 | R7 | 201 | CYC | C3B-C2B | 6.06 | 1.49 | 1.36 |
| 12 | j5 | 1202 | CYC | C3B-C2B | 6.06 | 1.49 | 1.36 |
| 12 | B7 | 201 | CYC | C3B-C2B | 6.06 | 1.49 | 1.36 |
| 12 | N5 | 201 | CYC | C3B-C2B | 6.06 | 1.49 | 1.36 |
| 12 | r7 | 201 | CYC | C3B-C2B | 6.05 | 1.49 | 1.36 |
| 12 | A | 201 | CYC | C3B-C2B | 6.05 | 1.49 | 1.36 |
| 12 | j7 | 201 | CYC | C3B-C2B | 6.05 | 1.49 | 1.36 |
| 12 | H5 | 201 | CYC | C3B-C2B | 6.05 | 1.49 | 1.36 |
| 12 | X7 | 201 | CYC | C3B-C2B | 6.04 | 1.49 | 1.36 |
| 12 | J7 | 201 | CYC | C3B-C2B | 6.03 | 1.49 | 1.36 |
| 12 | k5 | 1203 | CYC | C3B-C2B | 6.03 | 1.49 | 1.36 |
| 12 | Z5 | 201 | CYC | C3B-C2B | 6.02 | 1.49 | 1.36 |
| 12 | d5 | 201 | CYC | C3B-C2B | 6.01 | 1.49 | 1.36 |
| 12 | P7 | 201 | CYC | C3B-C2B | 6.01 | 1.49 | 1.36 |
| 12 | d7 | 201 | CYC | C3B-C2B | 5.98 | 1.49 | 1.36 |
| 12 | V5 | 201 | CYC | C3B-C2B | 5.97 | 1.49 | 1.36 |
| 12 | P5 | 201 | CYC | C3B-C2B | 5.96 | 1.49 | 1.36 |
| 12 | X7 | 201 | CYC | C2A-C3A | 5.64 | 1.48 | 1.36 |
| 12 | k5 | 1202 | CYC | C2A-C3A | 5.64 | 1.48 | 1.36 |
| 12 | j5 | 1201 | CYC | CHB-C1B | 5.63 | 1.51 | 1.38 |
| 12 | f7 | 201 | CYC | C2A-C3A | 5.61 | 1.48 | 1.36 |
| 12 | P5 | 201 | CYC | C2A-C3A | 5.61 | 1.48 | 1.36 |
| 12 | V5 | 201 | CYC | C2A-C3A | 5.61 | 1.48 | 1.36 |
| 12 | j5 | 1201 | CYC | C2A-C3A | 5.60 | 1.48 | 1.36 |
| 12 | R7 | 201 | CYC | C2A-C3A | 5.59 | 1.48 | 1.36 |
| 12 | k5 | 1201 | CYC | C2A-C3A | 5.59 | 1.48 | 1.36 |
| 12 | J7 | 201 | CYC | C2A-C3A | 5.58 | 1.48 | 1.36 |
| 12 | d7 | 201 | CYC | C2A-C3A | 5.57 | 1.48 | 1.36 |
| 12 | b7 | 201 | CYC | C2A-C3A | 5.57 | 1.48 | 1.36 |
| 12 | X5 | 201 | CYC | C2A-C3A | 5.56 | 1.48 | 1.36 |
| 12 | k5 | 1201 | CYC | CHB-C1B | 5.56 | 1.51 | 1.38 |
| 12 | h7 | 201 | CYC | C2A-C3A | 5.56 | 1.48 | 1.36 |
| 12 | p7 | 201 | CYC | C2A-C3A | 5.56 | 1.48 | 1.36 |
| 12 | f5 | 201 | CYC | C2A-C3A | 5.55 | 1.48 | 1.36 |
| 12 | R5 | 201 | CYC | C2A-C3A | 5.55 | 1.48 | 1.36 |
| 12 | b5 | 201 | CYC | C2A-C3A | 5.54 | 1.48 | 1.36 |
| 12 | j7 | 201 | CYC | C2A-C3A | 5.54 | 1.48 | 1.36 |
| 12 | F5 | 201 | CYC | C2A-C3A | 5.54 | 1.48 | 1.36 |
| 12 | L7 | 201 | CYC | C2A-C3A | 5.53 | 1.48 | 1.36 |
| 12 | F7 | 201 | CYC | C2A-C3A | 5.53 | 1.48 | 1.36 |
| 12 | A | 201 | CYC | C2A-C3A | 5.53 | 1.48 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 12 | O7 | 201 | CYC | C2A-C3A | 5.53 | 1.48 | 1.36 |
| 12 | a7 | 201 | CYC | C2A-C3A | 5.52 | 1.48 | 1.36 |
| 12 | v7 | 201 | CYC | C2A-C3A | 5.52 | 1.48 | 1.36 |
| 12 | H7 | 201 | CYC | C2A-C3A | 5.51 | 1.48 | 1.36 |
| 12 | B7 | 201 | CYC | C2A-C3A | 5.51 | 1.48 | 1.36 |
| 12 | D7 | 201 | CYC | C2A-C3A | 5.51 | 1.48 | 1.36 |
| 12 | J5 | 201 | CYC | C2A-C3A | 5.50 | 1.48 | 1.36 |
| 12 | I7 | 201 | CYC | C2A-C3A | 5.50 | 1.48 | 1.36 |
| 12 | k5 | 1203 | CYC | C2A-C3A | 5.50 | 1.48 | 1.36 |
| 12 | r7 | 201 | CYC | C2A-C3A | 5.50 | 1.48 | 1.36 |
| 12 | H5 | 201 | CYC | C2A-C3A | 5.50 | 1.48 | 1.36 |
| 12 | Z | 201 | CYC | C2A-C3A | 5.49 | 1.48 | 1.36 |
| 12 | D5 | 201 | CYC | C2A-C3A | 5.49 | 1.48 | 1.36 |
| 12 | L5 | 201 | CYC | C2A-C3A | 5.49 | 1.48 | 1.36 |
| 12 | C7 | 201 | CYC | C2A-C3A | 5.49 | 1.48 | 1.36 |
| 12 | G2 | 201 | CYC | C2A-C3A | 5.48 | 1.48 | 1.36 |
| 12 | K8 | 201 | CYC | C2A-C3A | 5.48 | 1.48 | 1.36 |
| 12 | N7 | 201 | CYC | C2A-C3A | 5.48 | 1.48 | 1.36 |
| 12 | A7 | 201 | CYC | C2A-C3A | 5.48 | 1.48 | 1.36 |
| 12 | G7 | 201 | CYC | C2A-C3A | 5.47 | 1.48 | 1.36 |
| 12 | g7 | 201 | CYC | C2A-C3A | 5.47 | 1.48 | 1.36 |
| 12 | K7 | 201 | CYC | C2A-C3A | 5.47 | 1.48 | 1.36 |
| 12 | V7 | 201 | CYC | C2A-C3A | 5.47 | 1.48 | 1.36 |
| 12 | B5 | 201 | CYC | C2A-C3A | 5.46 | 1.48 | 1.36 |
| 12 | k5 | 1204 | CYC | C2A-C3A | 5.46 | 1.48 | 1.36 |
| 12 | j5 | 1202 | CYC | C2A-C3A | 5.46 | 1.48 | 1.36 |
| 12 | R4 | 201 | CYC | C2A-C3A | 5.46 | 1.48 | 1.36 |
| 12 | R8 | 201 | CYC | C2A-C3A | 5.46 | 1.48 | 1.36 |
| 12 | T7 | 201 | CYC | C2A-C3A | 5.45 | 1.48 | 1.36 |
| 12 | U7 | 201 | CYC | C2A-C3A | 5.45 | 1.48 | 1.36 |
| 12 | I5 | 201 | CYC | C2A-C3A | 5.45 | 1.48 | 1.36 |
| 12 | E5 | 201 | CYC | C2A-C3A | 5.45 | 1.48 | 1.36 |
| 12 | s7 | 201 | CYC | C2A-C3A | 5.45 | 1.48 | 1.36 |
| 12 | E7 | 201 | CYC | C2A-C3A | 5.44 | 1.48 | 1.36 |
| 12 | k7 | 201 | CYC | C2A-C3A | 5.44 | 1.48 | 1.36 |
| 12 | K4 | 201 | CYC | C2A-C3A | 5.44 | 1.48 | 1.36 |
| 12 | C5 | 201 | CYC | C2A-C3A | 5.43 | 1.48 | 1.36 |
| 12 | T5 | 201 | CYC | C2A-C3A | 5.43 | 1.48 | 1.36 |
| 12 | m7 | 201 | CYC | C2A-C3A | 5.43 | 1.48 | 1.36 |
| 12 | i7 | 201 | CYC | C2A-C3A | 5.42 | 1.48 | 1.36 |
| 12 | N5 | 201 | CYC | C2A-C3A | 5.42 | 1.48 | 1.36 |
| 12 | G6 | 201 | CYC | C2A-C3A | 5.42 | 1.48 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | e7 | 201 | CYC | C2A-C3A | 5.42 | 1.48 | 1.36 |
| 12 | K2 | 201 | CYC | C2A-C3A | 5.42 | 1.48 | 1.36 |
| 12 | K6 | 201 | CYC | C2A-C3A | 5.42 | 1.48 | 1.36 |
| 12 | O5 | 201 | CYC | C2A-C3A | 5.42 | 1.48 | 1.36 |
| 12 | c5 | 201 | CYC | C2A-C3A | 5.42 | 1.48 | 1.36 |
| 12 | P7 | 201 | CYC | C2A-C3A | 5.42 | 1.48 | 1.36 |
| 12 | C3 | 201 | CYC | C2A-C3A | 5.41 | 1.48 | 1.36 |
| 12 | G5 | 201 | CYC | C2A-C3A | 5.41 | 1.48 | 1.36 |
| 12 | C1 | 201 | CYC | C2A-C3A | 5.41 | 1.48 | 1.36 |
| 12 | Q5 | 201 | CYC | C2A-C3A | 5.41 | 1.48 | 1.36 |
| 12 | d5 | 201 | CYC | C2A-C3A | 5.41 | 1.48 | 1.36 |
| 12 | Y7 | 201 | CYC | C2A-C3A | 5.41 | 1.48 | 1.36 |
| 12 | q7 | 201 | CYC | C2A-C3A | 5.41 | 1.48 | 1.36 |
| 12 | a5 | 201 | CYC | C2A-C3A | 5.40 | 1.48 | 1.36 |
| 12 | Z5 | 201 | CYC | C2A-C3A | 5.40 | 1.48 | 1.36 |
| 12 | K5 | 201 | CYC | C2A-C3A | 5.40 | 1.48 | 1.36 |
| 12 | e5 | 201 | CYC | C2A-C3A | 5.40 | 1.48 | 1.36 |
| 12 | W7 | 201 | CYC | C2A-C3A | 5.40 | 1.48 | 1.36 |
| 12 | c7 | 201 | CYC | C2A-C3A | 5.40 | 1.48 | 1.36 |
| 12 | W5 | 201 | CYC | C2A-C3A | 5.39 | 1.48 | 1.36 |
| 12 | S1 | 201 | CYC | C2A-C3A | 5.39 | 1.48 | 1.36 |
| 12 | S3 | 201 | CYC | C2A-C3A | 5.39 | 1.48 | 1.36 |
| 12 | Y5 | 201 | CYC | C2A-C3A | 5.39 | 1.48 | 1.36 |
| 12 | u7 | 201 | CYC | C2A-C3A | 5.39 | 1.48 | 1.36 |
| 12 | A5 | 201 | CYC | C2A-C3A | 5.39 | 1.48 | 1.36 |
| 12 | I1 | 201 | CYC | C2A-C3A | 5.38 | 1.48 | 1.36 |
| 12 | N4 | 201 | CYC | C2A-C3A | 5.38 | 1.48 | 1.36 |
| 12 | P4 | 201 | CYC | C2A-C3A | 5.38 | 1.48 | 1.36 |
| 12 | P8 | 201 | CYC | C2A-C3A | 5.38 | 1.48 | 1.36 |
| 12 | I3 | 201 | CYC | C2A-C3A | 5.38 | 1.48 | 1.36 |
| 12 | WA | 201 | CYC | C2A-C3A | 5.38 | 1.48 | 1.36 |
| 12 | W9 | 201 | CYC | C2A-C3A | 5.38 | 1.48 | 1.36 |
| 12 | U5 | 201 | CYC | C2A-C3A | 5.38 | 1.48 | 1.36 |
| 12 | O1 | 201 | CYC | C2A-C3A | 5.37 | 1.48 | 1.36 |
| 12 | O3 | 201 | CYC | C2A-C3A | 5.37 | 1.48 | 1.36 |
| 12 | U9 | 201 | CYC | C2A-C3A | 5.37 | 1.48 | 1.36 |
| 12 | UA | 201 | CYC | C2A-C3A | 5.37 | 1.48 | 1.36 |
| 12 | C6 | 201 | CYC | C2A-C3A | 5.37 | 1.48 | 1.36 |
| 12 | o7 | 201 | CYC | C2A-C3A | 5.37 | 1.48 | 1.36 |
| 12 | Q7 | 201 | CYC | C2A-C3A | 5.37 | 1.48 | 1.36 |
| 12 | X4 | 201 | CYC | C2A-C3A | 5.37 | 1.48 | 1.36 |
| 12 | X8 | 201 | CYC | C2A-C3A | 5.37 | 1.48 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | CA | 201 | CYC | C2A-C3A | 5.36 | 1.48 | 1.36 |
| 12 | M7 | 201 | CYC | C2A-C3A | 5.36 | 1.48 | 1.36 |
| 12 | C9 | 201 | CYC | C2A-C3A | 5.36 | 1.48 | 1.36 |
| 12 | G1 | 201 | CYC | C2A-C3A | 5.36 | 1.48 | 1.36 |
| 12 | V4 | 201 | CYC | C2A-C3A | 5.36 | 1.48 | 1.36 |
| 12 | V8 | 201 | CYC | C2A-C3A | 5.36 | 1.48 | 1.36 |
| 12 | K3 | 201 | CYC | C2A-C3A | 5.35 | 1.48 | 1.36 |
| 12 | AA | 201 | CYC | C2A-C3A | 5.35 | 1.48 | 1.36 |
| 12 | A9 | 201 | CYC | C2A-C3A | 5.35 | 1.48 | 1.36 |
| 12 | M5 | 201 | CYC | C2A-C3A | 5.35 | 1.48 | 1.36 |
| 12 | E6 | 201 | CYC | C2A-C3A | 5.35 | 1.48 | 1.36 |
| 12 | N8 | 201 | CYC | C2A-C3A | 5.34 | 1.48 | 1.36 |
| 12 | W3 | 201 | CYC | C2A-C3A | 5.34 | 1.48 | 1.36 |
| 12 | T4 | 201 | CYC | C2A-C3A | 5.34 | 1.48 | 1.36 |
| 12 | T8 | 201 | CYC | C2A-C3A | 5.34 | 1.48 | 1.36 |
| 12 | G3 | 201 | CYC | C2A-C3A | 5.34 | 1.48 | 1.36 |
| 12 | K1 | 201 | CYC | C2A-C3A | 5.34 | 1.48 | 1.36 |
| 12 | W1 | 201 | CYC | C2A-C3A | 5.33 | 1.48 | 1.36 |
| 12 | C2 | 201 | CYC | C2A-C3A | 5.33 | 1.48 | 1.36 |
| 12 | E4 | 201 | CYC | C2A-C3A | 5.33 | 1.48 | 1.36 |
| 12 | E8 | 201 | CYC | C2A-C3A | 5.33 | 1.48 | 1.36 |
| 12 | IA | 201 | CYC | C2A-C3A | 5.33 | 1.48 | 1.36 |
| 12 | G4 | 201 | CYC | C2A-C3A | 5.33 | 1.48 | 1.36 |
| 12 | G8 | 201 | CYC | C2A-C3A | 5.33 | 1.48 | 1.36 |
| 12 | I9 | 201 | CYC | C2A-C3A | 5.33 | 1.48 | 1.36 |
| 12 | Q1 | 201 | CYC | C2A-C3A | 5.33 | 1.48 | 1.36 |
| 12 | Q3 | 201 | CYC | C2A-C3A | 5.33 | 1.48 | 1.36 |
| 12 | S7 | 201 | CYC | C2A-C3A | 5.33 | 1.48 | 1.36 |
| 12 | A1 | 201 | CYC | C2A-C3A | 5.33 | 1.48 | 1.36 |
| 12 | A3 | 201 | CYC | C2A-C3A | 5.33 | 1.48 | 1.36 |
| 12 | E2 | 201 | CYC | C2A-C3A | 5.33 | 1.48 | 1.36 |
| 12 | QA | 201 | CYC | C2A-C3A | 5.32 | 1.48 | 1.36 |
| 12 | S5 | 201 | CYC | C2A-C3A | 5.32 | 1.48 | 1.36 |
| 12 | O9 | 201 | CYC | C2A-C3A | 5.32 | 1.48 | 1.36 |
| 12 | GA | 201 | CYC | C2A-C3A | 5.32 | 1.48 | 1.36 |
| 12 | G9 | 201 | CYC | C2A-C3A | 5.32 | 1.48 | 1.36 |
| 12 | EA | 201 | CYC | C2A-C3A | 5.31 | 1.48 | 1.36 |
| 12 | X3 | 201 | CYC | C2A-C3A | 5.31 | 1.48 | 1.36 |
| 12 | E9 | 201 | CYC | C2A-C3A | 5.31 | 1.48 | 1.36 |
| 12 | X1 | 201 | CYC | C2A-C3A | 5.31 | 1.48 | 1.36 |
| 12 | E3 | 201 | CYC | C2A-C3A | 5.31 | 1.48 | 1.36 |
| 12 | E1 | 201 | CYC | C2A-C3A | 5.31 | 1.48 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | XA | 201 | CYC | C3B-C2B | 5.31 | 1.48 | 1.36 |
| 12 | R9 | 201 | CYC | C2A-C3A | 5.31 | 1.48 | 1.36 |
| 12 | I5 | 201 | CYC | C3B-C2B | 5.31 | 1.48 | 1.36 |
| 12 | KA | 201 | CYC | C2A-C3A | 5.31 | 1.48 | 1.36 |
| 12 | K9 | 201 | CYC | C2A-C3A | 5.31 | 1.48 | 1.36 |
| 12 | Q9 | 201 | CYC | C2A-C3A | 5.30 | 1.48 | 1.36 |
| 12 | YA | 201 | CYC | C2A-C3A | 5.30 | 1.48 | 1.36 |
| 12 | Y9 | 201 | CYC | C2A-C3A | 5.30 | 1.48 | 1.36 |
| 12 | g7 | 201 | CYC | C3B-C2B | 5.30 | 1.48 | 1.36 |
| 12 | D4 | 202 | CYC | C2A-C3A | 5.29 | 1.48 | 1.36 |
| 12 | D8 | 202 | CYC | C2A-C3A | 5.29 | 1.48 | 1.36 |
| 12 | J2 | 201 | CYC | C2A-C3A | 5.29 | 1.48 | 1.36 |
| 12 | H2 | 202 | CYC | C2A-C3A | 5.28 | 1.48 | 1.36 |
| 12 | H6 | 202 | CYC | C2A-C3A | 5.28 | 1.48 | 1.36 |
| 12 | I4 | 201 | CYC | C2A-C3A | 5.28 | 1.48 | 1.36 |
| 12 | I8 | 201 | CYC | C2A-C3A | 5.28 | 1.48 | 1.36 |
| 12 | OA | 201 | CYC | C2A-C3A | 5.28 | 1.48 | 1.36 |
| 12 | C5 | 201 | CYC | C3B-C2B | 5.28 | 1.48 | 1.36 |
| 12 | LA | 202 | CYC | C2A-C3A | 5.28 | 1.48 | 1.36 |
| 12 | L9 | 202 | CYC | C2A-C3A | 5.28 | 1.48 | 1.36 |
| 12 | C4 | 201 | CYC | C2A-C3A | 5.28 | 1.47 | 1.36 |
| 12 | C8 | 201 | CYC | C2A-C3A | 5.28 | 1.47 | 1.36 |
| 12 | X9 | 201 | CYC | C3B-C2B | 5.28 | 1.47 | 1.36 |
| 12 | BA | 202 | CYC | C2A-C3A | 5.28 | 1.47 | 1.36 |
| 12 | a7 | 201 | CYC | C3B-C2B | 5.28 | 1.47 | 1.36 |
| 12 | B9 | 202 | CYC | C2A-C3A | 5.28 | 1.47 | 1.36 |
| 12 | J6 | 201 | CYC | C2A-C3A | 5.27 | 1.47 | 1.36 |
| 12 | A2 | 201 | CYC | C2A-C3A | 5.27 | 1.47 | 1.36 |
| 12 | A6 | 201 | CYC | C2A-C3A | 5.27 | 1.47 | 1.36 |
| 12 | VA | 201 | CYC | C3B-C2B | 5.27 | 1.47 | 1.36 |
| 12 | V9 | 201 | CYC | C3B-C2B | 5.27 | 1.47 | 1.36 |
| 12 | ZA | 202 | CYC | C3B-C2B | 5.27 | 1.47 | 1.36 |
| 12 | Y3 | 201 | CYC | C2A-C3A | 5.27 | 1.47 | 1.36 |
| 12 | Z9 | 202 | CYC | C3B-C2B | 5.27 | 1.47 | 1.36 |
| 12 | Y1 | 201 | CYC | C2A-C3A | 5.27 | 1.47 | 1.36 |
| 12 | RA | 201 | CYC | C2A-C3A | 5.27 | 1.47 | 1.36 |
| 12 | I6 | 201 | CYC | C2A-C3A | 5.27 | 1.47 | 1.36 |
| 12 | A4 | 201 | CYC | C2A-C3A | 5.26 | 1.47 | 1.36 |
| 12 | A8 | 201 | CYC | C2A-C3A | 5.26 | 1.47 | 1.36 |
| 12 | O4 | 202 | CYC | C2A-C3A | 5.26 | 1.47 | 1.36 |
| 12 | O8 | 202 | CYC | C2A-C3A | 5.26 | 1.47 | 1.36 |
| 12 | P1 | 202 | CYC | C2A-C3A | 5.26 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | P3 | 202 | CYC | C2A-C3A | 5.26 | 1.47 | 1.36 |
| 12 | SA | 201 | CYC | C2A-C3A | 5.26 | 1.47 | 1.36 |
| 12 | S9 | 201 | CYC | C2A-C3A | 5.26 | 1.47 | 1.36 |
| 12 | Z4 | 301 | CYC | C3B-C2B | 5.26 | 1.47 | 1.36 |
| 12 | PA | 201 | CYC | C2A-C3A | 5.25 | 1.47 | 1.36 |
| 12 | I2 | 201 | CYC | C2A-C3A | 5.25 | 1.47 | 1.36 |
| 12 | W4 | 202 | CYC | C2A-C3A | 5.25 | 1.47 | 1.36 |
| 12 | W8 | 202 | CYC | C2A-C3A | 5.25 | 1.47 | 1.36 |
| 12 | M7 | 201 | CYC | C3B-C2B | 5.25 | 1.47 | 1.36 |
| 12 | T9 | 302 | CYC | C3B-C2B | 5.24 | 1.47 | 1.36 |
| 12 | D3 | 202 | CYC | C2A-C3A | 5.24 | 1.47 | 1.36 |
| 12 | D1 | 202 | CYC | C2A-C3A | 5.24 | 1.47 | 1.36 |
| 12 | O1 | 201 | CYC | C3B-C2B | 5.24 | 1.47 | 1.36 |
| 12 | O3 | 201 | CYC | C3B-C2B | 5.24 | 1.47 | 1.36 |
| 12 | P9 | 201 | CYC | C2A-C3A | 5.24 | 1.47 | 1.36 |
| 12 | TA | 301 | CYC | C2A-C3A | 5.24 | 1.47 | 1.36 |
| 12 | T9 | 301 | CYC | C2A-C3A | 5.24 | 1.47 | 1.36 |
| 12 | D2 | 201 | CYC | C2A-C3A | 5.24 | 1.47 | 1.36 |
| 12 | S5 | 201 | CYC | C3B-C2B | 5.24 | 1.47 | 1.36 |
| 12 | m7 | 201 | CYC | C3B-C2B | 5.23 | 1.47 | 1.36 |
| 12 | L4 | 202 | CYC | C2A-C3A | 5.23 | 1.47 | 1.36 |
| 12 | J4 | 201 | CYC | C2A-C3A | 5.23 | 1.47 | 1.36 |
| 12 | N2 | 101 | CYC | C2A-C3A | 5.23 | 1.47 | 1.36 |
| 12 | N6 | 101 | CYC | C2A-C3A | 5.23 | 1.47 | 1.36 |
| 12 | N2 | 101 | CYC | C3B-C2B | 5.23 | 1.47 | 1.36 |
| 12 | J3 | 202 | CYC | C3B-C2B | 5.23 | 1.47 | 1.36 |
| 12 | aA | 901 | CYC | C3B-C2B | 5.23 | 1.47 | 1.36 |
| 12 | J8 | 201 | CYC | C2A-C3A | 5.23 | 1.47 | 1.36 |
| 12 | B4 | 202 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |
| 12 | DA | 201 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |
| 12 | TA | 302 | CYC | C3B-C2B | 5.22 | 1.47 | 1.36 |
| 12 | D9 | 201 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |
| 12 | BA | 201 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |
| 12 | B9 | 201 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |
| 12 | VA | 201 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |
| 12 | D4 | 202 | CYC | C3B-C2B | 5.22 | 1.47 | 1.36 |
| 12 | V9 | 201 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |
| 12 | L3 | 202 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |
| 12 | Z3 | 201 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |
| 12 | F9 | 302 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |
| 12 | Z1 | 202 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |
| 12 | D6 | 201 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | s7 | 201 | CYC | C3B-C2B | 5.22 | 1.47 | 1.36 |
| 12 | O4 | 201 | CYC | C3B-C2B | 5.22 | 1.47 | 1.36 |
| 12 | O8 | 201 | CYC | C3B-C2B | 5.22 | 1.47 | 1.36 |
| 12 | H2 | 201 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |
| 12 | U3 | 201 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |
| 12 | H4 | 202 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |
| 12 | H8 | 202 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |
| 12 | U1 | 201 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |
| 12 | S4 | 202 | CYC | C2A-C3A | 5.22 | 1.47 | 1.36 |
| 12 | U7 | 201 | CYC | C3B-C2B | 5.22 | 1.47 | 1.36 |
| 12 | o7 | 201 | CYC | C3B-C2B | 5.22 | 1.47 | 1.36 |
| 12 | FA | 301 | CYC | C2A-C3A | 5.21 | 1.47 | 1.36 |
| 12 | F9 | 301 | CYC | C2A-C3A | 5.21 | 1.47 | 1.36 |
| 12 | LA | 202 | CYC | C3B-C2B | 5.21 | 1.47 | 1.36 |
| 12 | O7 | 201 | CYC | C3B-C2B | 5.21 | 1.47 | 1.36 |
| 12 | L9 | 202 | CYC | C3B-C2B | 5.21 | 1.47 | 1.36 |
| 12 | aA | 902 | CYC | C2A-C3A | 5.21 | 1.47 | 1.36 |
| 12 | i7 | 201 | CYC | C3B-C2B | 5.21 | 1.47 | 1.36 |
| 12 | B3 | 202 | CYC | C2A-C3A | 5.21 | 1.47 | 1.36 |
| 12 | e5 | 201 | CYC | C3B-C2B | 5.21 | 1.47 | 1.36 |
| 12 | F9 | 303 | CYC | C2A-C3A | 5.21 | 1.47 | 1.36 |
| 12 | a9 | 901 | CYC | C2A-C3A | 5.21 | 1.47 | 1.36 |
| 12 | Z8 | 301 | CYC | C3B-C2B | 5.20 | 1.47 | 1.36 |
| 12 | F6 | 201 | CYC | C3B-C2B | 5.20 | 1.47 | 1.36 |
| 12 | X9 | 202 | CYC | C2A-C3A | 5.20 | 1.47 | 1.36 |
| 12 | H6 | 201 | CYC | C2A-C3A | 5.20 | 1.47 | 1.36 |
| 12 | aA | 901 | CYC | C2A-C3A | 5.20 | 1.47 | 1.36 |
| 12 | B1 | 202 | CYC | C2A-C3A | 5.20 | 1.47 | 1.36 |
| 12 | N6 | 101 | CYC | C3B-C2B | 5.20 | 1.47 | 1.36 |
| 12 | K5 | 201 | CYC | C3B-C2B | 5.20 | 1.47 | 1.36 |
| 12 | XA | 202 | CYC | C2A-C3A | 5.20 | 1.47 | 1.36 |
| 12 | B4 | 201 | CYC | C2A-C3A | 5.20 | 1.47 | 1.36 |
| 12 | B8 | 201 | CYC | C2A-C3A | 5.20 | 1.47 | 1.36 |
| 12 | D8 | 202 | CYC | C3B-C2B | 5.20 | 1.47 | 1.36 |
| 12 | V3 | 202 | CYC | C2A-C3A | 5.20 | 1.47 | 1.36 |
| 12 | B8 | 202 | CYC | C2A-C3A | 5.20 | 1.47 | 1.36 |
| 12 | V1 | 202 | CYC | C2A-C3A | 5.20 | 1.47 | 1.36 |
| 12 | F3 | 201 | CYC | C3B-C2B | 5.20 | 1.47 | 1.36 |
| 12 | F1 | 201 | CYC | C3B-C2B | 5.20 | 1.47 | 1.36 |
| 12 | J3 | 202 | CYC | C2A-C3A | 5.20 | 1.47 | 1.36 |
| 12 | PA | 201 | CYC | C3B-C2B | 5.19 | 1.47 | 1.36 |
| 12 | P9 | 201 | CYC | C3B-C2B | 5.19 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | F4 | 202 | CYC | C2A-C3A | 5.19 | 1.47 | 1.36 |
| 12 | F8 | 202 | CYC | C2A-C3A | 5.19 | 1.47 | 1.36 |
| 12 | M8 | 302 | CYC | C2A-C3A | 5.19 | 1.47 | 1.36 |
| 12 | Z4 | 301 | CYC | C2A-C3A | 5.19 | 1.47 | 1.36 |
| 12 | R7 | 201 | CYC | CHB-C1B | 5.19 | 1.50 | 1.38 |
| 12 | KA | 201 | CYC | C3B-C2B | 5.19 | 1.47 | 1.36 |
| 12 | K9 | 201 | CYC | C3B-C2B | 5.19 | 1.47 | 1.36 |
| 12 | B3 | 201 | CYC | C2A-C3A | 5.19 | 1.47 | 1.36 |
| 12 | B1 | 201 | CYC | C2A-C3A | 5.19 | 1.47 | 1.36 |
| 12 | W4 | 201 | CYC | C2A-C3A | 5.19 | 1.47 | 1.36 |
| 12 | J4 | 202 | CYC | C2A-C3A | 5.19 | 1.47 | 1.36 |
| 12 | W8 | 201 | CYC | C2A-C3A | 5.19 | 1.47 | 1.36 |
| 12 | J8 | 202 | CYC | C2A-C3A | 5.19 | 1.47 | 1.36 |
| 12 | GA | 201 | CYC | C3B-C2B | 5.18 | 1.47 | 1.36 |
| 12 | G9 | 201 | CYC | C3B-C2B | 5.18 | 1.47 | 1.36 |
| 12 | Q5 | 201 | CYC | C3B-C2B | 5.18 | 1.47 | 1.36 |
| 12 | L2 | 201 | CYC | C2A-C3A | 5.18 | 1.47 | 1.36 |
| 12 | L6 | 201 | CYC | C2A-C3A | 5.18 | 1.47 | 1.36 |
| 12 | S4 | 202 | CYC | C3B-C2B | 5.18 | 1.47 | 1.36 |
| 12 | X3 | 202 | CYC | C2A-C3A | 5.18 | 1.47 | 1.36 |
| 12 | W5 | 201 | CYC | C3B-C2B | 5.18 | 1.47 | 1.36 |
| 12 | u7 | 201 | CYC | C3B-C2B | 5.18 | 1.47 | 1.36 |
| 12 | X1 | 202 | CYC | C2A-C3A | 5.18 | 1.47 | 1.36 |
| 12 | B2 | 201 | CYC | C2A-C3A | 5.18 | 1.47 | 1.36 |
| 12 | a5 | 201 | CYC | C3B-C2B | 5.18 | 1.47 | 1.36 |
| 12 | L3 | 201 | CYC | C2A-C3A | 5.18 | 1.47 | 1.36 |
| 12 | L1 | 201 | CYC | C2A-C3A | 5.18 | 1.47 | 1.36 |
| 12 | I7 | 201 | CYC | C3B-C2B | 5.18 | 1.47 | 1.36 |
| 12 | J2 | 202 | CYC | C3B-C2B | 5.18 | 1.47 | 1.36 |
| 12 | E5 | 201 | CYC | C3B-C2B | 5.18 | 1.47 | 1.36 |
| 12 | W7 | 201 | CYC | C3B-C2B | 5.18 | 1.47 | 1.36 |
| 12 | U5 | 201 | CYC | C3B-C2B | 5.18 | 1.47 | 1.36 |
| 12 | H4 | 201 | CYC | C3B-C2B | 5.17 | 1.47 | 1.36 |
| 12 | C6 | 201 | CYC | C3B-C2B | 5.17 | 1.47 | 1.36 |
| 12 | i7 | 201 | CYC | CHB-C1B | 5.17 | 1.50 | 1.38 |
| 12 | TA | 302 | CYC | C2A-C3A | 5.17 | 1.47 | 1.36 |
| 12 | T9 | 302 | CYC | C2A-C3A | 5.17 | 1.47 | 1.36 |
| 12 | M4 | 301 | CYC | C2A-C3A | 5.17 | 1.47 | 1.36 |
| 12 | H9 | 202 | CYC | C3B-C2B | 5.17 | 1.47 | 1.36 |
| 12 | D3 | 202 | CYC | C3B-C2B | 5.17 | 1.47 | 1.36 |
| 12 | D1 | 202 | CYC | C3B-C2B | 5.17 | 1.47 | 1.36 |
| 12 | O5 | 201 | CYC | C3B-C2B | 5.17 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | E9 | 201 | CYC | C3B-C2B | 5.17 | 1.47 | 1.36 |
| 12 | B6 | 201 | CYC | C2A-C3A | 5.17 | 1.47 | 1.36 |
| 12 | V3 | 201 | CYC | C2A-C3A | 5.17 | 1.47 | 1.36 |
| 12 | V1 | 201 | CYC | C2A-C3A | 5.17 | 1.47 | 1.36 |
| 12 | K2 | 201 | CYC | C3B-C2B | 5.17 | 1.47 | 1.36 |
| 12 | H4 | 201 | CYC | C2A-C3A | 5.17 | 1.47 | 1.36 |
| 12 | K6 | 201 | CYC | C3B-C2B | 5.17 | 1.47 | 1.36 |
| 12 | H8 | 201 | CYC | C2A-C3A | 5.17 | 1.47 | 1.36 |
| 12 | JA | 201 | CYC | C2A-C3A | 5.16 | 1.47 | 1.36 |
| 12 | R4 | 201 | CYC | C3B-C2B | 5.16 | 1.47 | 1.36 |
| 12 | M5 | 201 | CYC | C3B-C2B | 5.16 | 1.47 | 1.36 |
| 12 | R8 | 201 | CYC | C3B-C2B | 5.16 | 1.47 | 1.36 |
| 12 | J9 | 201 | CYC | C2A-C3A | 5.16 | 1.47 | 1.36 |
| 12 | J2 | 202 | CYC | C2A-C3A | 5.16 | 1.47 | 1.36 |
| 12 | T3 | 302 | CYC | C2A-C3A | 5.16 | 1.47 | 1.36 |
| 12 | J6 | 202 | CYC | C2A-C3A | 5.16 | 1.47 | 1.36 |
| 12 | Q7 | 201 | CYC | C3B-C2B | 5.16 | 1.47 | 1.36 |
| 12 | T1 | 302 | CYC | C2A-C3A | 5.16 | 1.47 | 1.36 |
| 12 | X3 | 201 | CYC | C3B-C2B | 5.16 | 1.47 | 1.36 |
| 12 | O4 | 201 | CYC | C2A-C3A | 5.16 | 1.47 | 1.36 |
| 12 | O8 | 201 | CYC | C2A-C3A | 5.16 | 1.47 | 1.36 |
| 12 | E6 | 201 | CYC | C3B-C2B | 5.16 | 1.47 | 1.36 |
| 12 | E2 | 201 | CYC | C3B-C2B | 5.16 | 1.47 | 1.36 |
| 12 | Z8 | 301 | CYC | C2A-C3A | 5.16 | 1.47 | 1.36 |
| 12 | p7 | 201 | CYC | CHB-C1B | 5.16 | 1.50 | 1.38 |
| 12 | XA | 201 | CYC | C2A-C3A | 5.16 | 1.47 | 1.36 |
| 12 | X9 | 201 | CYC | C2A-C3A | 5.16 | 1.47 | 1.36 |
| 12 | PA | 202 | CYC | C2A-C3A | 5.16 | 1.47 | 1.36 |
| 12 | P9 | 202 | CYC | C2A-C3A | 5.16 | 1.47 | 1.36 |
| 12 | C4 | 201 | CYC | C3B-C2B | 5.16 | 1.47 | 1.36 |
| 12 | R3 | 201 | CYC | C3B-C2B | 5.16 | 1.47 | 1.36 |
| 12 | Y5 | 201 | CYC | C3B-C2B | 5.16 | 1.47 | 1.36 |
| 12 | C8 | 201 | CYC | C3B-C2B | 5.16 | 1.47 | 1.36 |
| 12 | H3 | 202 | CYC | C3B-C2B | 5.16 | 1.47 | 1.36 |
| 12 | D2 | 201 | CYC | C3B-C2B | 5.16 | 1.47 | 1.36 |
| 12 | U5 | 201 | CYC | CHB-C1B | 5.15 | 1.50 | 1.38 |
| 12 | P1 | 201 | CYC | C2A-C3A | 5.15 | 1.47 | 1.36 |
| 12 | P3 | 201 | CYC | C2A-C3A | 5.15 | 1.47 | 1.36 |
| 12 | F4 | 201 | CYC | C2A-C3A | 5.15 | 1.47 | 1.36 |
| 12 | F8 | 201 | CYC | C2A-C3A | 5.15 | 1.47 | 1.36 |
| 12 | j7 | 201 | CYC | CHB-C1B | 5.15 | 1.50 | 1.38 |
| 12 | R1 | 201 | CYC | C2A-C3A | 5.15 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | R3 | 201 | CYC | C2A-C3A | 5.15 | 1.47 | 1.36 |
| 12 | M8 | 302 | CYC | C3B-C2B | 5.15 | 1.47 | 1.36 |
| 12 | J6 | 202 | CYC | C3B-C2B | 5.15 | 1.47 | 1.36 |
| 12 | R1 | 201 | CYC | C3B-C2B | 5.15 | 1.47 | 1.36 |
| 12 | H1 | 202 | CYC | C2A-C3A | 5.15 | 1.47 | 1.36 |
| 12 | D4 | 201 | CYC | C3B-C2B | 5.15 | 1.47 | 1.36 |
| 12 | D8 | 201 | CYC | C3B-C2B | 5.15 | 1.47 | 1.36 |
| 12 | C7 | 201 | CYC | C3B-C2B | 5.15 | 1.47 | 1.36 |
| 12 | A1 | 201 | CYC | C3B-C2B | 5.15 | 1.47 | 1.36 |
| 12 | A3 | 201 | CYC | C3B-C2B | 5.15 | 1.47 | 1.36 |
| 12 | O5 | 201 | CYC | CHB-C1B | 5.15 | 1.50 | 1.38 |
| 12 | d7 | 201 | CYC | CHB-C1B | 5.15 | 1.50 | 1.38 |
| 12 | a9 | 901 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | c7 | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | JA | 202 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | J9 | 202 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | H6 | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | S8 | 201 | CYC | C2A-C3A | 5.14 | 1.47 | 1.36 |
| 12 | TA | 301 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | S4 | 201 | CYC | C2A-C3A | 5.14 | 1.47 | 1.36 |
| 12 | N4 | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | N8 | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | T9 | 301 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | DA | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | D9 | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | J2 | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | Z3 | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | J6 | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | Z1 | 202 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | B1 | 202 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | F6 | 202 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | F8 | 202 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | A2 | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | H8 | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | EA | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | RA | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | I3 | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | V3 | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | R9 | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | I1 | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | V1 | 201 | CYC | C3B-C2B | 5.14 | 1.47 | 1.36 |
| 12 | E4 | 201 | CYC | C3B-C2B | 5.13 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | E8 | 201 | CYC | C3B-C2B | 5.13 | 1.47 | 1.36 |
| 12 | C2 | 201 | CYC | C3B-C2B | 5.13 | 1.47 | 1.36 |
| 12 | HA | 202 | CYC | C3B-C2B | 5.13 | 1.47 | 1.36 |
| 12 | X7 | 201 | CYC | CHB-C1B | 5.13 | 1.50 | 1.38 |
| 12 | X4 | 201 | CYC | C3B-C2B | 5.13 | 1.47 | 1.36 |
| 12 | X8 | 201 | CYC | C3B-C2B | 5.13 | 1.47 | 1.36 |
| 12 | H3 | 201 | CYC | C2A-C3A | 5.13 | 1.47 | 1.36 |
| 12 | G5 | 201 | CYC | C3B-C2B | 5.13 | 1.47 | 1.36 |
| 12 | R1 | 202 | CYC | C2A-C3A | 5.13 | 1.47 | 1.36 |
| 12 | R3 | 202 | CYC | C2A-C3A | 5.13 | 1.47 | 1.36 |
| 12 | A6 | 201 | CYC | C3B-C2B | 5.13 | 1.47 | 1.36 |
| 12 | v7 | 201 | CYC | CHB-C1B | 5.13 | 1.50 | 1.38 |
| 12 | JA | 202 | CYC | C2A-C3A | 5.13 | 1.47 | 1.36 |
| 12 | J9 | 202 | CYC | C2A-C3A | 5.13 | 1.47 | 1.36 |
| 12 | ZA | 202 | CYC | C2A-C3A | 5.13 | 1.47 | 1.36 |
| 12 | Y4 | 201 | CYC | C2A-C3A | 5.13 | 1.47 | 1.36 |
| 12 | G7 | 201 | CYC | C3B-C2B | 5.13 | 1.47 | 1.36 |
| 12 | Y8 | 201 | CYC | C2A-C3A | 5.13 | 1.47 | 1.36 |
| 12 | Z9 | 202 | CYC | C2A-C3A | 5.13 | 1.47 | 1.36 |
| 12 | A4 | 201 | CYC | C3B-C2B | 5.13 | 1.47 | 1.36 |
| 12 | A8 | 201 | CYC | C3B-C2B | 5.13 | 1.47 | 1.36 |
| 12 | B3 | 202 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |
| 12 | Q4 | 201 | CYC | C2A-C3A | 5.12 | 1.47 | 1.36 |
| 12 | J4 | 202 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |
| 12 | F6 | 201 | CYC | C2A-C3A | 5.12 | 1.47 | 1.36 |
| 12 | J8 | 202 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |
| 12 | J3 | 201 | CYC | C2A-C3A | 5.12 | 1.47 | 1.36 |
| 12 | J1 | 201 | CYC | C2A-C3A | 5.12 | 1.47 | 1.36 |
| 12 | X5 | 201 | CYC | CHB-C1B | 5.12 | 1.50 | 1.38 |
| 12 | E7 | 201 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |
| 12 | X1 | 201 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |
| 12 | D6 | 201 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |
| 12 | W4 | 201 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |
| 12 | A5 | 201 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |
| 12 | W8 | 201 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |
| 12 | B4 | 202 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |
| 12 | FA | 301 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |
| 12 | U4 | 201 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |
| 12 | L4 | 202 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |
| 12 | U8 | 201 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |
| 12 | F9 | 301 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |
| 12 | XA | 202 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | X9 | 202 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |
| 12 | H1 | 201 | CYC | C3B-C2B | 5.12 | 1.47 | 1.36 |
| 12 | M8 | 301 | CYC | C2A-C3A | 5.12 | 1.47 | 1.36 |
| 12 | Q8 | 201 | CYC | C2A-C3A | 5.11 | 1.47 | 1.36 |
| 12 | F9 | 302 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | Y7 | 201 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | J5 | 201 | CYC | CHB-C1B | 5.11 | 1.50 | 1.38 |
| 12 | T3 | 301 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | T1 | 301 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | c5 | 201 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | R5 | 201 | CYC | CHB-C1B | 5.11 | 1.50 | 1.38 |
| 12 | U4 | 201 | CYC | C2A-C3A | 5.11 | 1.47 | 1.36 |
| 12 | U8 | 201 | CYC | C2A-C3A | 5.11 | 1.47 | 1.36 |
| 12 | H9 | 202 | CYC | C2A-C3A | 5.11 | 1.47 | 1.36 |
| 12 | j5 | 1201 | CYC | C1C-NC | -5.11 | 1.31 | 1.37 |
| 12 | D3 | 201 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | D1 | 201 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | f7 | 201 | CYC | CHB-C1B | 5.11 | 1.50 | 1.38 |
| 12 | A7 | 201 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | e7 | 201 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | k7 | 201 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | HA | 202 | CYC | C2A-C3A | 5.11 | 1.47 | 1.36 |
| 12 | B4 | 201 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | B8 | 201 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | B8 | 202 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | L3 | 202 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | F4 | 202 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | H2 | 201 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | HA | 201 | CYC | C2A-C3A | 5.11 | 1.47 | 1.36 |
| 12 | H9 | 201 | CYC | C2A-C3A | 5.11 | 1.47 | 1.36 |
| 12 | CA | 201 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | LA | 201 | CYC | C2A-C3A | 5.11 | 1.47 | 1.36 |
| 12 | G4 | 201 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | G8 | 201 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | L9 | 201 | CYC | C2A-C3A | 5.11 | 1.47 | 1.36 |
| 12 | C9 | 201 | CYC | C3B-C2B | 5.11 | 1.47 | 1.36 |
| 12 | T3 | 302 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | T1 | 302 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | B5 | 201 | CYC | CHB-C1B | 5.10 | 1.50 | 1.38 |
| 12 | RA | 202 | CYC | C2A-C3A | 5.10 | 1.47 | 1.36 |
| 12 | Q9 | 201 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | R9 | 202 | CYC | C2A-C3A | 5.10 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 12 | D5 | 201 | CYC | CHB-C1B | 5.10 | 1.50 | 1.38 |
| 12 | aA | 902 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | J4 | 201 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | L6 | 201 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | J8 | 201 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | Y9 | 201 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | F2 | 201 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | h7 | 201 | CYC | CHB-C1B | 5.10 | 1.50 | 1.38 |
| 12 | K7 | 201 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | U3 | 201 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | Y4 | 201 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | Y8 | 201 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | U1 | 201 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | I5 | 201 | CYC | CHB-C1B | 5.10 | 1.50 | 1.38 |
| 12 | RA | 202 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | L2 | 201 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | R9 | 202 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | K8 | 201 | CYC | C3B-C2B | 5.10 | 1.47 | 1.36 |
| 12 | Y5 | 201 | CYC | CHB-C1B | 5.09 | 1.50 | 1.38 |
| 12 | C5 | 201 | CYC | CHB-C1B | 5.09 | 1.50 | 1.38 |
| 12 | W5 | 201 | CYC | CHB-C1B | 5.09 | 1.50 | 1.38 |
| 12 | F3 | 201 | CYC | C2A-C3A | 5.09 | 1.47 | 1.36 |
| 12 | F1 | 201 | CYC | C2A-C3A | 5.09 | 1.47 | 1.36 |
| 12 | U4 | 202 | CYC | C2A-C3A | 5.09 | 1.47 | 1.36 |
| 12 | o7 | 201 | CYC | CHB-C1B | 5.09 | 1.50 | 1.38 |
| 12 | Z3 | 202 | CYC | C2A-C3A | 5.09 | 1.47 | 1.36 |
| 12 | Z1 | 201 | CYC | C2A-C3A | 5.09 | 1.47 | 1.36 |
| 12 | b7 | 201 | CYC | CHB-C1B | 5.09 | 1.50 | 1.38 |
| 12 | ZA | 201 | CYC | C2A-C3A | 5.09 | 1.47 | 1.36 |
| 12 | Z9 | 201 | CYC | C2A-C3A | 5.09 | 1.47 | 1.36 |
| 12 | f5 | 201 | CYC | CHB-C1B | 5.09 | 1.50 | 1.38 |
| 12 | k5 | 1202 | CYC | CHB-C1B | 5.09 | 1.50 | 1.38 |
| 12 | O9 | 201 | CYC | C3B-C2B | 5.09 | 1.47 | 1.36 |
| 12 | C7 | 201 | CYC | CHB-C1B | 5.09 | 1.50 | 1.38 |
| 12 | QA | 201 | CYC | C3B-C2B | 5.08 | 1.47 | 1.36 |
| 12 | u7 | 201 | CYC | CHB-C1B | 5.08 | 1.50 | 1.38 |
| 12 | L4 | 201 | CYC | C2A-C3A | 5.08 | 1.47 | 1.36 |
| 12 | L8 | 201 | CYC | C2A-C3A | 5.08 | 1.47 | 1.36 |
| 12 | Q5 | 201 | CYC | CHB-C1B | 5.08 | 1.50 | 1.38 |
| 12 | YA | 201 | CYC | C3B-C2B | 5.08 | 1.47 | 1.36 |
| 12 | b5 | 201 | CYC | CHB-C1B | 5.08 | 1.50 | 1.38 |
| 12 | D9 | 202 | CYC | C2A-C3A | 5.08 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | F5 | 201 | CYC | CHB-C1B | 5.08 | 1.50 | 1.38 |
| 12 | I7 | 201 | CYC | CHB-C1B | 5.08 | 1.50 | 1.38 |
| 12 | c7 | 201 | CYC | CHB-C1B | 5.08 | 1.50 | 1.38 |
| 12 | Q4 | 201 | CYC | C3B-C2B | 5.08 | 1.47 | 1.36 |
| 12 | k5 | 1201 | CYC | C1C-NC | -5.08 | 1.31 | 1.37 |
| 12 | N5 | 201 | CYC | CHB-C1B | 5.08 | 1.50 | 1.38 |
| 12 | IA | 201 | CYC | C3B-C2B | 5.08 | 1.47 | 1.36 |
| 12 | I9 | 201 | CYC | C3B-C2B | 5.08 | 1.47 | 1.36 |
| 12 | a5 | 201 | CYC | CHB-C1B | 5.08 | 1.50 | 1.38 |
| 12 | B6 | 201 | CYC | C3B-C2B | 5.08 | 1.47 | 1.36 |
| 12 | B2 | 201 | CYC | C3B-C2B | 5.08 | 1.47 | 1.36 |
| 12 | F7 | 201 | CYC | CHB-C1B | 5.07 | 1.50 | 1.38 |
| 12 | W7 | 201 | CYC | CHB-C1B | 5.07 | 1.50 | 1.38 |
| 12 | V3 | 202 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | k5 | 1201 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | V1 | 202 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | DA | 202 | CYC | C2A-C3A | 5.07 | 1.47 | 1.36 |
| 12 | K3 | 201 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | K1 | 201 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | T4 | 201 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | T8 | 201 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | SA | 201 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | VA | 202 | CYC | C2A-C3A | 5.07 | 1.47 | 1.36 |
| 12 | S9 | 201 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | V9 | 202 | CYC | C2A-C3A | 5.07 | 1.47 | 1.36 |
| 12 | F4 | 201 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | F8 | 201 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | DA | 202 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | Q8 | 201 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | D9 | 202 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | BA | 201 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | B9 | 201 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | q7 | 201 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | OA | 201 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | R1 | 202 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | L2 | 202 | CYC | C2A-C3A | 5.07 | 1.47 | 1.36 |
| 12 | R3 | 202 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | K4 | 201 | CYC | C3B-C2B | 5.07 | 1.47 | 1.36 |
| 12 | c5 | 201 | CYC | CHB-C1B | 5.07 | 1.50 | 1.38 |
| 12 | G2 | 201 | CYC | C3B-C2B | 5.06 | 1.47 | 1.36 |
| 12 | F9 | 303 | CYC | C3B-C2B | 5.06 | 1.47 | 1.36 |
| 12 | B7 | 201 | CYC | CHB-C1B | 5.06 | 1.50 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 12 | H3 | 202 | CYC | C2A-C3A | 5.06 | 1.47 | 1.36 |
| 12 | T3 | 301 | CYC | C2A-C3A | 5.06 | 1.47 | 1.36 |
| 12 | Y3 | 201 | CYC | C3B-C2B | 5.06 | 1.47 | 1.36 |
| 12 | T1 | 301 | CYC | C2A-C3A | 5.06 | 1.47 | 1.36 |
| 12 | Y1 | 201 | CYC | C3B-C2B | 5.06 | 1.47 | 1.36 |
| 12 | D4 | 201 | CYC | C2A-C3A | 5.06 | 1.47 | 1.36 |
| 12 | D8 | 201 | CYC | C2A-C3A | 5.06 | 1.47 | 1.36 |
| 12 | e5 | 201 | CYC | CHB-C1B | 5.06 | 1.50 | 1.38 |
| 12 | L7 | 201 | CYC | CHB-C1B | 5.06 | 1.50 | 1.38 |
| 12 | U8 | 202 | CYC | C2A-C3A | 5.06 | 1.47 | 1.36 |
| 12 | UA | 201 | CYC | C3B-C2B | 5.06 | 1.47 | 1.36 |
| 12 | U9 | 201 | CYC | C3B-C2B | 5.06 | 1.47 | 1.36 |
| 12 | F2 | 202 | CYC | C3B-C2B | 5.06 | 1.47 | 1.36 |
| 12 | H6 | 202 | CYC | C3B-C2B | 5.06 | 1.47 | 1.36 |
| 12 | Q7 | 201 | CYC | CHB-C1B | 5.06 | 1.50 | 1.38 |
| 12 | P5 | 201 | CYC | CHB-C1B | 5.05 | 1.50 | 1.38 |
| 12 | a7 | 201 | CYC | CHB-C1B | 5.05 | 1.50 | 1.38 |
| 12 | H5 | 201 | CYC | CHB-C1B | 5.05 | 1.50 | 1.38 |
| 12 | V7 | 201 | CYC | CHB-C1B | 5.05 | 1.50 | 1.38 |
| 12 | F2 | 202 | CYC | C2A-C3A | 5.05 | 1.47 | 1.36 |
| 12 | P4 | 201 | CYC | C3B-C2B | 5.05 | 1.47 | 1.36 |
| 12 | H7 | 201 | CYC | CHB-C1B | 5.05 | 1.50 | 1.38 |
| 12 | G3 | 201 | CYC | C3B-C2B | 5.05 | 1.47 | 1.36 |
| 12 | I2 | 201 | CYC | C3B-C2B | 5.05 | 1.47 | 1.36 |
| 12 | M4 | 301 | CYC | C3B-C2B | 5.05 | 1.47 | 1.36 |
| 12 | G1 | 201 | CYC | C3B-C2B | 5.05 | 1.47 | 1.36 |
| 12 | V5 | 201 | CYC | CHB-C1B | 5.05 | 1.50 | 1.38 |
| 12 | BA | 202 | CYC | C3B-C2B | 5.05 | 1.47 | 1.36 |
| 12 | B9 | 202 | CYC | C3B-C2B | 5.05 | 1.47 | 1.36 |
| 12 | VA | 202 | CYC | C3B-C2B | 5.05 | 1.47 | 1.36 |
| 12 | r7 | 201 | CYC | CHB-C1B | 5.05 | 1.50 | 1.38 |
| 12 | H1 | 201 | CYC | C2A-C3A | 5.05 | 1.47 | 1.36 |
| 12 | k5 | 1203 | CYC | CHB-C1B | 5.05 | 1.50 | 1.38 |
| 12 | k5 | 1204 | CYC | CHB-C1B | 5.05 | 1.50 | 1.38 |
| 12 | L6 | 202 | CYC | C2A-C3A | 5.05 | 1.47 | 1.36 |
| 12 | G6 | 201 | CYC | C3B-C2B | 5.05 | 1.47 | 1.36 |
| 12 | WA | 201 | CYC | C3B-C2B | 5.04 | 1.47 | 1.36 |
| 12 | C1 | 201 | CYC | C3B-C2B | 5.04 | 1.47 | 1.36 |
| 12 | W9 | 201 | CYC | C3B-C2B | 5.04 | 1.47 | 1.36 |
| 12 | d5 | 201 | CYC | CHB-C1B | 5.04 | 1.50 | 1.38 |
| 12 | F6 | 202 | CYC | C2A-C3A | 5.04 | 1.47 | 1.36 |
| 12 | j5 | 1202 | CYC | CHB-C1B | 5.04 | 1.50 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 12 | F3 | 202 | CYC | C3B-C2B | 5.04 | 1.47 | 1.36 |
| 12 | I4 | 201 | CYC | C3B-C2B | 5.04 | 1.47 | 1.36 |
| 12 | I8 | 201 | CYC | C3B-C2B | 5.04 | 1.47 | 1.36 |
| 12 | F1 | 202 | CYC | C3B-C2B | 5.04 | 1.47 | 1.36 |
| 12 | L5 | 201 | CYC | CHB-C1B | 5.04 | 1.50 | 1.38 |
| 12 | Z5 | 201 | CYC | CHB-C1B | 5.04 | 1.50 | 1.38 |
| 12 | F2 | 201 | CYC | C2A-C3A | 5.04 | 1.47 | 1.36 |
| 12 | ZA | 201 | CYC | C3B-C2B | 5.04 | 1.47 | 1.36 |
| 12 | Z9 | 201 | CYC | C3B-C2B | 5.04 | 1.47 | 1.36 |
| 12 | H9 | 201 | CYC | C3B-C2B | 5.04 | 1.47 | 1.36 |
| 12 | J7 | 201 | CYC | CHB-C1B | 5.03 | 1.50 | 1.38 |
| 12 | Q1 | 201 | CYC | C3B-C2B | 5.03 | 1.47 | 1.36 |
| 12 | Q3 | 201 | CYC | C3B-C2B | 5.03 | 1.47 | 1.36 |
| 12 | g7 | 201 | CYC | CHB-C1B | 5.03 | 1.50 | 1.38 |
| 12 | j5 | 1201 | CYC | C3B-C2B | 5.03 | 1.47 | 1.36 |
| 12 | F3 | 202 | CYC | C2A-C3A | 5.03 | 1.47 | 1.36 |
| 12 | F1 | 202 | CYC | C2A-C3A | 5.03 | 1.47 | 1.36 |
| 12 | T5 | 201 | CYC | CHB-C1B | 5.03 | 1.50 | 1.38 |
| 12 | I6 | 201 | CYC | C3B-C2B | 5.03 | 1.47 | 1.36 |
| 12 | H2 | 202 | CYC | C3B-C2B | 5.03 | 1.47 | 1.36 |
| 12 | Z3 | 202 | CYC | C3B-C2B | 5.03 | 1.47 | 1.36 |
| 12 | Z1 | 201 | CYC | C3B-C2B | 5.03 | 1.47 | 1.36 |
| 12 | U4 | 202 | CYC | C3B-C2B | 5.03 | 1.47 | 1.36 |
| 12 | O7 | 201 | CYC | CHB-C1B | 5.03 | 1.50 | 1.38 |
| 12 | J9 | 201 | CYC | C3B-C2B | 5.03 | 1.47 | 1.36 |
| 12 | S7 | 201 | CYC | C3B-C2B | 5.02 | 1.47 | 1.36 |
| 12 | U7 | 201 | CYC | CHB-C1B | 5.02 | 1.50 | 1.38 |
| 12 | P1 | 201 | CYC | C3B-C2B | 5.02 | 1.47 | 1.36 |
| 12 | P3 | 201 | CYC | C3B-C2B | 5.02 | 1.47 | 1.36 |
| 12 | N7 | 201 | CYC | CHB-C1B | 5.02 | 1.50 | 1.38 |
| 12 | X3 | 202 | CYC | C3B-C2B | 5.02 | 1.47 | 1.36 |
| 12 | X1 | 202 | CYC | C3B-C2B | 5.02 | 1.47 | 1.36 |
| 12 | D2 | 202 | CYC | C3B-C2B | 5.02 | 1.47 | 1.36 |
| 12 | T7 | 201 | CYC | CHB-C1B | 5.02 | 1.50 | 1.38 |
| 12 | JA | 201 | CYC | C3B-C2B | 5.02 | 1.47 | 1.36 |
| 12 | HA | 201 | CYC | C3B-C2B | 5.02 | 1.47 | 1.36 |
| 12 | P8 | 201 | CYC | C3B-C2B | 5.02 | 1.47 | 1.36 |
| 12 | AA | 201 | CYC | C3B-C2B | 5.02 | 1.47 | 1.36 |
| 12 | A9 | 201 | CYC | C3B-C2B | 5.02 | 1.47 | 1.36 |
| 12 | A | 201 | CYC | CHB-C1B | 5.01 | 1.50 | 1.38 |
| 12 | A7 | 201 | CYC | CHB-C1B | 5.01 | 1.50 | 1.38 |
| 12 | B3 | 201 | CYC | C3B-C2B | 5.01 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | B1 | 201 | CYC | C3B-C2B | 5.01 | 1.47 | 1.36 |
| 12 | L6 | 202 | CYC | C3B-C2B | 5.01 | 1.47 | 1.36 |
| 12 | PA | 202 | CYC | C3B-C2B | 5.01 | 1.47 | 1.36 |
| 12 | P9 | 202 | CYC | C3B-C2B | 5.01 | 1.47 | 1.36 |
| 12 | V9 | 202 | CYC | C3B-C2B | 5.01 | 1.47 | 1.36 |
| 12 | C3 | 201 | CYC | C3B-C2B | 5.00 | 1.47 | 1.36 |
| 12 | D6 | 202 | CYC | C2A-C3A | 5.00 | 1.47 | 1.36 |
| 12 | D2 | 202 | CYC | C2A-C3A | 5.00 | 1.47 | 1.36 |
| 12 | U8 | 202 | CYC | C3B-C2B | 5.00 | 1.47 | 1.36 |
| 12 | D6 | 202 | CYC | C3B-C2B | 5.00 | 1.47 | 1.36 |
| 12 | W4 | 202 | CYC | C3B-C2B | 5.00 | 1.47 | 1.36 |
| 12 | W8 | 202 | CYC | C3B-C2B | 5.00 | 1.47 | 1.36 |
| 12 | L2 | 202 | CYC | C3B-C2B | 5.00 | 1.47 | 1.36 |
| 12 | D3 | 201 | CYC | C2A-C3A | 5.00 | 1.47 | 1.36 |
| 12 | D1 | 201 | CYC | C2A-C3A | 5.00 | 1.47 | 1.36 |
| 12 | E3 | 201 | CYC | C3B-C2B | 5.00 | 1.47 | 1.36 |
| 12 | V4 | 201 | CYC | C3B-C2B | 5.00 | 1.47 | 1.36 |
| 12 | E1 | 201 | CYC | C3B-C2B | 5.00 | 1.47 | 1.36 |
| 12 | V8 | 201 | CYC | C3B-C2B | 5.00 | 1.47 | 1.36 |
| 12 | q7 | 201 | CYC | CHB-C1B | 5.00 | 1.49 | 1.38 |
| 12 | D7 | 201 | CYC | CHB-C1B | 4.99 | 1.49 | 1.38 |
| 12 | Z | 201 | CYC | CHB-C1B | 4.99 | 1.49 | 1.38 |
| 12 | J3 | 201 | CYC | C3B-C2B | 4.99 | 1.47 | 1.36 |
| 12 | J1 | 201 | CYC | C3B-C2B | 4.99 | 1.47 | 1.36 |
| 12 | S4 | 201 | CYC | C3B-C2B | 4.99 | 1.47 | 1.36 |
| 12 | L4 | 201 | CYC | C3B-C2B | 4.99 | 1.47 | 1.36 |
| 12 | S8 | 201 | CYC | C3B-C2B | 4.99 | 1.47 | 1.36 |
| 12 | L9 | 201 | CYC | C3B-C2B | 4.99 | 1.47 | 1.36 |
| 12 | P7 | 201 | CYC | CHB-C1B | 4.98 | 1.49 | 1.38 |
| 12 | W3 | 201 | CYC | C3B-C2B | 4.98 | 1.47 | 1.36 |
| 12 | W1 | 201 | CYC | C3B-C2B | 4.98 | 1.47 | 1.36 |
| 12 | K5 | 201 | CYC | CHB-C1B | 4.98 | 1.49 | 1.38 |
| 12 | S1 | 201 | CYC | C3B-C2B | 4.98 | 1.47 | 1.36 |
| 12 | S3 | 201 | CYC | C3B-C2B | 4.98 | 1.47 | 1.36 |
| 12 | L8 | 201 | CYC | C3B-C2B | 4.98 | 1.47 | 1.36 |
| 12 | e7 | 201 | CYC | CHB-C1B | 4.98 | 1.49 | 1.38 |
| 12 | H3 | 201 | CYC | C3B-C2B | 4.98 | 1.47 | 1.36 |
| 12 | G5 | 201 | CYC | CHB-C1B | 4.98 | 1.49 | 1.38 |
| 12 | E7 | 201 | CYC | CHB-C1B | 4.97 | 1.49 | 1.38 |
| 12 | E5 | 201 | CYC | CHB-C1B | 4.97 | 1.49 | 1.38 |
| 12 | LA | 201 | CYC | C3B-C2B | 4.97 | 1.47 | 1.36 |
| 12 | H4 | 202 | CYC | C3B-C2B | 4.97 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | H8 | 202 | CYC | C3B-C2B | 4.97 | 1.47 | 1.36 |
| 12 | P1 | 202 | CYC | C3B-C2B | 4.97 | 1.47 | 1.36 |
| 12 | P3 | 202 | CYC | C3B-C2B | 4.97 | 1.47 | 1.36 |
| 12 | M8 | 301 | CYC | C3B-C2B | 4.97 | 1.47 | 1.36 |
| 12 | m7 | 201 | CYC | CHB-C1B | 4.97 | 1.49 | 1.38 |
| 12 | H1 | 202 | CYC | C3B-C2B | 4.97 | 1.47 | 1.36 |
| 12 | O4 | 202 | CYC | C3B-C2B | 4.96 | 1.47 | 1.36 |
| 12 | O8 | 202 | CYC | C3B-C2B | 4.96 | 1.47 | 1.36 |
| 12 | K7 | 201 | CYC | CHB-C1B | 4.96 | 1.49 | 1.38 |
| 12 | k7 | 201 | CYC | CHB-C1B | 4.96 | 1.49 | 1.38 |
| 12 | s7 | 201 | CYC | CHB-C1B | 4.95 | 1.49 | 1.38 |
| 12 | Y7 | 201 | CYC | CHB-C1B | 4.94 | 1.49 | 1.38 |
| 12 | G7 | 201 | CYC | CHB-C1B | 4.94 | 1.49 | 1.38 |
| 12 | M5 | 201 | CYC | CHB-C1B | 4.93 | 1.49 | 1.38 |
| 12 | M7 | 201 | CYC | CHB-C1B | 4.93 | 1.49 | 1.38 |
| 12 | A5 | 201 | CYC | CHB-C1B | 4.93 | 1.49 | 1.38 |
| 12 | S7 | 201 | CYC | CHB-C1B | 4.93 | 1.49 | 1.38 |
| 12 | L3 | 201 | CYC | C3B-C2B | 4.92 | 1.47 | 1.36 |
| 12 | L1 | 201 | CYC | C3B-C2B | 4.92 | 1.47 | 1.36 |
| 12 | S5 | 201 | CYC | CHB-C1B | 4.91 | 1.49 | 1.38 |
| 12 | C1 | 201 | CYC | CHB-C1B | 4.88 | 1.49 | 1.38 |
| 12 | YA | 201 | CYC | CHB-C1B | 4.86 | 1.49 | 1.38 |
| 12 | Y9 | 201 | CYC | CHB-C1B | 4.86 | 1.49 | 1.38 |
| 12 | C3 | 201 | CYC | CHB-C1B | 4.86 | 1.49 | 1.38 |
| 12 | X4 | 201 | CYC | CHB-C1B | 4.86 | 1.49 | 1.38 |
| 12 | OA | 201 | CYC | CHB-C1B | 4.85 | 1.49 | 1.38 |
| 12 | O9 | 201 | CYC | CHB-C1B | 4.85 | 1.49 | 1.38 |
| 12 | X8 | 201 | CYC | CHB-C1B | 4.83 | 1.49 | 1.38 |
| 12 | Q1 | 201 | CYC | CHB-C1B | 4.83 | 1.49 | 1.38 |
| 12 | Q3 | 201 | CYC | CHB-C1B | 4.83 | 1.49 | 1.38 |
| 12 | I4 | 201 | CYC | CHB-C1B | 4.83 | 1.49 | 1.38 |
| 12 | I8 | 201 | CYC | CHB-C1B | 4.83 | 1.49 | 1.38 |
| 12 | A2 | 201 | CYC | CHB-C1B | 4.83 | 1.49 | 1.38 |
| 12 | CA | 201 | CYC | CHB-C1B | 4.83 | 1.49 | 1.38 |
| 12 | O1 | 201 | CYC | CHB-C1B | 4.82 | 1.49 | 1.38 |
| 12 | O3 | 201 | CYC | CHB-C1B | 4.82 | 1.49 | 1.38 |
| 12 | I6 | 201 | CYC | CHB-C1B | 4.81 | 1.49 | 1.38 |
| 12 | C9 | 201 | CYC | CHB-C1B | 4.81 | 1.49 | 1.38 |
| 12 | Q9 | 201 | CYC | CHB-C1B | 4.80 | 1.49 | 1.38 |
| 12 | A1 | 201 | CYC | CHB-C1B | 4.80 | 1.49 | 1.38 |
| 12 | A3 | 201 | CYC | CHB-C1B | 4.80 | 1.49 | 1.38 |
| 12 | QA | 201 | CYC | CHB-C1B | 4.80 | 1.49 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | C2 | 201 | CYC | CHB-C1B | 4.80 | 1.49 | 1.38 |
| 12 | K3 | 201 | CYC | CHB-C1B | 4.80 | 1.49 | 1.38 |
| 12 | K1 | 201 | CYC | CHB-C1B | 4.80 | 1.49 | 1.38 |
| 12 | IA | 201 | CYC | CHB-C1B | 4.79 | 1.49 | 1.38 |
| 12 | I9 | 201 | CYC | CHB-C1B | 4.79 | 1.49 | 1.38 |
| 12 | K4 | 201 | CYC | CHB-C1B | 4.79 | 1.49 | 1.38 |
| 12 | K8 | 201 | CYC | CHB-C1B | 4.79 | 1.49 | 1.38 |
| 12 | K2 | 201 | CYC | CHB-C1B | 4.78 | 1.49 | 1.38 |
| 12 | UA | 201 | CYC | CHB-C1B | 4.78 | 1.49 | 1.38 |
| 12 | U9 | 201 | CYC | CHB-C1B | 4.78 | 1.49 | 1.38 |
| 12 | C6 | 201 | CYC | CHB-C1B | 4.78 | 1.49 | 1.38 |
| 12 | A4 | 201 | CYC | CHB-C1B | 4.77 | 1.49 | 1.38 |
| 12 | A8 | 201 | CYC | CHB-C1B | 4.77 | 1.49 | 1.38 |
| 12 | EA | 201 | CYC | CHB-C1B | 4.77 | 1.49 | 1.38 |
| 12 | E9 | 201 | CYC | CHB-C1B | 4.77 | 1.49 | 1.38 |
| 12 | T4 | 201 | CYC | CHB-C1B | 4.77 | 1.49 | 1.38 |
| 12 | T8 | 201 | CYC | CHB-C1B | 4.77 | 1.49 | 1.38 |
| 12 | G3 | 201 | CYC | CHB-C1B | 4.77 | 1.49 | 1.38 |
| 12 | G1 | 201 | CYC | CHB-C1B | 4.77 | 1.49 | 1.38 |
| 12 | A6 | 201 | CYC | CHB-C1B | 4.77 | 1.49 | 1.38 |
| 12 | KA | 201 | CYC | CHB-C1B | 4.77 | 1.49 | 1.38 |
| 12 | K9 | 201 | CYC | CHB-C1B | 4.77 | 1.49 | 1.38 |
| 12 | V4 | 201 | CYC | CHB-C1B | 4.77 | 1.49 | 1.38 |
| 12 | V8 | 201 | CYC | CHB-C1B | 4.77 | 1.49 | 1.38 |
| 12 | I2 | 201 | CYC | CHB-C1B | 4.76 | 1.49 | 1.38 |
| 12 | GA | 201 | CYC | CHB-C1B | 4.76 | 1.49 | 1.38 |
| 12 | G9 | 201 | CYC | CHB-C1B | 4.76 | 1.49 | 1.38 |
| 12 | W3 | 201 | CYC | CHB-C1B | 4.76 | 1.49 | 1.38 |
| 12 | W1 | 201 | CYC | CHB-C1B | 4.76 | 1.49 | 1.38 |
| 12 | WA | 201 | CYC | CHB-C1B | 4.76 | 1.49 | 1.38 |
| 12 | W9 | 201 | CYC | CHB-C1B | 4.76 | 1.49 | 1.38 |
| 12 | G2 | 201 | CYC | CHB-C1B | 4.75 | 1.49 | 1.38 |
| 12 | E4 | 201 | CYC | CHB-C1B | 4.75 | 1.49 | 1.38 |
| 12 | E8 | 201 | CYC | CHB-C1B | 4.75 | 1.49 | 1.38 |
| 12 | K6 | 201 | CYC | CHB-C1B | 4.75 | 1.49 | 1.38 |
| 12 | P4 | 201 | CYC | CHB-C1B | 4.75 | 1.49 | 1.38 |
| 12 | P8 | 201 | CYC | CHB-C1B | 4.75 | 1.49 | 1.38 |
| 12 | I3 | 201 | CYC | CHB-C1B | 4.75 | 1.49 | 1.38 |
| 12 | I1 | 201 | CYC | CHB-C1B | 4.75 | 1.49 | 1.38 |
| 12 | G6 | 201 | CYC | CHB-C1B | 4.74 | 1.49 | 1.38 |
| 12 | U3 | 201 | CYC | CHB-C1B | 4.74 | 1.49 | 1.38 |
| 12 | U1 | 201 | CYC | CHB-C1B | 4.74 | 1.49 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | C4 | 201 | CYC | CHB-C1B | 4.74 | 1.49 | 1.38 |
| 12 | C8 | 201 | CYC | CHB-C1B | 4.74 | 1.49 | 1.38 |
| 12 | AA | 201 | CYC | CHB-C1B | 4.73 | 1.49 | 1.38 |
| 12 | A9 | 201 | CYC | CHB-C1B | 4.73 | 1.49 | 1.38 |
| 12 | S1 | 201 | CYC | CHB-C1B | 4.73 | 1.49 | 1.38 |
| 12 | S3 | 201 | CYC | CHB-C1B | 4.73 | 1.49 | 1.38 |
| 12 | R4 | 201 | CYC | CHB-C1B | 4.73 | 1.49 | 1.38 |
| 12 | R8 | 201 | CYC | CHB-C1B | 4.73 | 1.49 | 1.38 |
| 12 | N4 | 201 | CYC | CHB-C1B | 4.72 | 1.49 | 1.38 |
| 12 | N8 | 201 | CYC | CHB-C1B | 4.72 | 1.49 | 1.38 |
| 12 | Y3 | 201 | CYC | CHB-C1B | 4.72 | 1.49 | 1.38 |
| 12 | E6 | 201 | CYC | CHB-C1B | 4.72 | 1.49 | 1.38 |
| 12 | Y1 | 201 | CYC | CHB-C1B | 4.72 | 1.49 | 1.38 |
| 12 | SA | 201 | CYC | CHB-C1B | 4.71 | 1.49 | 1.38 |
| 12 | S9 | 201 | CYC | CHB-C1B | 4.71 | 1.49 | 1.38 |
| 12 | E2 | 201 | CYC | CHB-C1B | 4.70 | 1.49 | 1.38 |
| 12 | E3 | 201 | CYC | CHB-C1B | 4.70 | 1.49 | 1.38 |
| 12 | E1 | 201 | CYC | CHB-C1B | 4.70 | 1.49 | 1.38 |
| 12 | G4 | 201 | CYC | CHB-C1B | 4.67 | 1.49 | 1.38 |
| 12 | G8 | 201 | CYC | CHB-C1B | 4.67 | 1.49 | 1.38 |
| 12 | k5 | 1201 | CYC | C2C-C1C | -4.67 | 1.47 | 1.52 |
| 12 | j5 | 1201 | CYC | C2C-C1C | -4.66 | 1.47 | 1.52 |
| 12 | Y8 | 201 | CYC | CHB-C1B | 4.57 | 1.48 | 1.38 |
| 12 | Y4 | 201 | CYC | CHB-C1B | 4.54 | 1.48 | 1.38 |
| 12 | U4 | 202 | CYC | CHB-C1B | 4.51 | 1.48 | 1.38 |
| 12 | U8 | 202 | CYC | CHB-C1B | 4.51 | 1.48 | 1.38 |
| 12 | V3 | 202 | CYC | CHB-C1B | 4.48 | 1.48 | 1.38 |
| 12 | F4 | 201 | CYC | CHB-C1B | 4.47 | 1.48 | 1.38 |
| 12 | F8 | 201 | CYC | CHB-C1B | 4.47 | 1.48 | 1.38 |
| 12 | H3 | 201 | CYC | CHB-C1B | 4.47 | 1.48 | 1.38 |
| 12 | H1 | 202 | CYC | CHB-C1B | 4.47 | 1.48 | 1.38 |
| 12 | W8 | 202 | CYC | CHB-C1B | 4.47 | 1.48 | 1.38 |
| 12 | B4 | 201 | CYC | CHB-C1B | 4.47 | 1.48 | 1.38 |
| 12 | B8 | 201 | CYC | CHB-C1B | 4.47 | 1.48 | 1.38 |
| 12 | P1 | 202 | CYC | CHB-C1B | 4.45 | 1.48 | 1.38 |
| 12 | P3 | 202 | CYC | CHB-C1B | 4.45 | 1.48 | 1.38 |
| 12 | V1 | 202 | CYC | CHB-C1B | 4.45 | 1.48 | 1.38 |
| 12 | JA | 201 | CYC | CHB-C1B | 4.45 | 1.48 | 1.38 |
| 12 | J9 | 201 | CYC | CHB-C1B | 4.45 | 1.48 | 1.38 |
| 12 | Z3 | 202 | CYC | CHB-C1B | 4.45 | 1.48 | 1.38 |
| 12 | Z1 | 201 | CYC | CHB-C1B | 4.45 | 1.48 | 1.38 |
| 12 | W4 | 202 | CYC | CHB-C1B | 4.45 | 1.48 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | L3 | 201 | CYC | CHB-C1B | 4.44 | 1.48 | 1.38 |
| 12 | L1 | 201 | CYC | CHB-C1B | 4.44 | 1.48 | 1.38 |
| 12 | BA | 202 | CYC | CHB-C1B | 4.44 | 1.48 | 1.38 |
| 12 | B9 | 202 | CYC | CHB-C1B | 4.44 | 1.48 | 1.38 |
| 12 | B6 | 201 | CYC | CHB-C1B | 4.44 | 1.48 | 1.38 |
| 12 | J4 | 202 | CYC | CHB-C1B | 4.43 | 1.48 | 1.38 |
| 12 | J8 | 202 | CYC | CHB-C1B | 4.43 | 1.48 | 1.38 |
| 12 | S4 | 201 | CYC | CHB-C1B | 4.43 | 1.48 | 1.38 |
| 12 | S8 | 201 | CYC | CHB-C1B | 4.43 | 1.48 | 1.38 |
| 12 | H4 | 202 | CYC | CHB-C1B | 4.42 | 1.48 | 1.38 |
| 12 | H8 | 202 | CYC | CHB-C1B | 4.42 | 1.48 | 1.38 |
| 12 | J2 | 202 | CYC | CHB-C1B | 4.42 | 1.48 | 1.38 |
| 12 | L6 | 202 | CYC | CHB-C1B | 4.42 | 1.48 | 1.38 |
| 12 | B2 | 201 | CYC | CHB-C1B | 4.42 | 1.48 | 1.38 |
| 12 | B1 | 202 | CYC | CHB-C1B | 4.42 | 1.48 | 1.38 |
| 12 | a9 | 901 | CYC | CHB-C1B | 4.41 | 1.48 | 1.38 |
| 12 | L4 | 201 | CYC | CHB-C1B | 4.40 | 1.48 | 1.38 |
| 12 | L8 | 201 | CYC | CHB-C1B | 4.40 | 1.48 | 1.38 |
| 12 | X3 | 202 | CYC | CHB-C1B | 4.40 | 1.48 | 1.38 |
| 12 | X1 | 202 | CYC | CHB-C1B | 4.40 | 1.48 | 1.38 |
| 12 | VA | 202 | CYC | CHB-C1B | 4.40 | 1.48 | 1.38 |
| 12 | V9 | 202 | CYC | CHB-C1B | 4.40 | 1.48 | 1.38 |
| 12 | R1 | 202 | CYC | CHB-C1B | 4.40 | 1.48 | 1.38 |
| 12 | R3 | 202 | CYC | CHB-C1B | 4.40 | 1.48 | 1.38 |
| 12 | F3 | 201 | CYC | CHB-C1B | 4.40 | 1.48 | 1.38 |
| 12 | F1 | 201 | CYC | CHB-C1B | 4.40 | 1.48 | 1.38 |
| 12 | LA | 201 | CYC | CHB-C1B | 4.39 | 1.48 | 1.38 |
| 12 | L9 | 201 | CYC | CHB-C1B | 4.39 | 1.48 | 1.38 |
| 12 | L2 | 202 | CYC | CHB-C1B | 4.39 | 1.48 | 1.38 |
| 12 | B3 | 202 | CYC | CHB-C1B | 4.39 | 1.48 | 1.38 |
| 12 | P1 | 201 | CYC | CHB-C1B | 4.39 | 1.48 | 1.38 |
| 12 | P3 | 201 | CYC | CHB-C1B | 4.39 | 1.48 | 1.38 |
| 12 | J3 | 201 | CYC | CHB-C1B | 4.39 | 1.48 | 1.38 |
| 12 | H2 | 202 | CYC | CHB-C1B | 4.39 | 1.48 | 1.38 |
| 12 | H6 | 202 | CYC | CHB-C1B | 4.39 | 1.48 | 1.38 |
| 12 | J1 | 201 | CYC | CHB-C1B | 4.39 | 1.48 | 1.38 |
| 12 | PA | 202 | CYC | CHB-C1B | 4.39 | 1.48 | 1.38 |
| 12 | P9 | 202 | CYC | CHB-C1B | 4.39 | 1.48 | 1.38 |
| 12 | B3 | 201 | CYC | CHB-C1B | 4.39 | 1.48 | 1.38 |
| 12 | B1 | 201 | CYC | CHB-C1B | 4.39 | 1.48 | 1.38 |
| 12 | L4 | 202 | CYC | CHB-C1B | 4.39 | 1.48 | 1.38 |
| 12 | F4 | 202 | CYC | CHB-C1B | 4.38 | 1.48 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | F9 | 303 | CYC | CHB-C1B | 4.38 | 1.48 | 1.38 |
| 12 | H9 | 202 | CYC | CHB-C1B | 4.38 | 1.48 | 1.38 |
| 12 | DA | 202 | CYC | CHB-C1B | 4.38 | 1.48 | 1.38 |
| 12 | D9 | 202 | CYC | CHB-C1B | 4.38 | 1.48 | 1.38 |
| 12 | D4 | 201 | CYC | CHB-C1B | 4.37 | 1.48 | 1.38 |
| 12 | D8 | 201 | CYC | CHB-C1B | 4.37 | 1.48 | 1.38 |
| 12 | F3 | 202 | CYC | CHB-C1B | 4.37 | 1.48 | 1.38 |
| 12 | F1 | 202 | CYC | CHB-C1B | 4.37 | 1.48 | 1.38 |
| 12 | U4 | 201 | CYC | CHB-C1B | 4.37 | 1.48 | 1.38 |
| 12 | U8 | 201 | CYC | CHB-C1B | 4.37 | 1.48 | 1.38 |
| 12 | J6 | 202 | CYC | CHB-C1B | 4.37 | 1.48 | 1.38 |
| 12 | D3 | 201 | CYC | CHB-C1B | 4.37 | 1.48 | 1.38 |
| 12 | M4 | 301 | CYC | CHB-C1B | 4.37 | 1.48 | 1.38 |
| 12 | F9 | 302 | CYC | CHB-C1B | 4.37 | 1.48 | 1.38 |
| 12 | Q4 | 201 | CYC | CHB-C1B | 4.37 | 1.48 | 1.38 |
| 12 | Z4 | 301 | CYC | CHB-C1B | 4.36 | 1.48 | 1.38 |
| 12 | Q8 | 201 | CYC | CHB-C1B | 4.36 | 1.48 | 1.38 |
| 12 | W4 | 201 | CYC | CHB-C1B | 4.36 | 1.48 | 1.38 |
| 12 | W8 | 201 | CYC | CHB-C1B | 4.36 | 1.48 | 1.38 |
| 12 | HA | 202 | CYC | CHB-C1B | 4.36 | 1.48 | 1.38 |
| 12 | F8 | 202 | CYC | CHB-C1B | 4.35 | 1.48 | 1.38 |
| 12 | F6 | 201 | CYC | CHB-C1B | 4.35 | 1.48 | 1.38 |
| 12 | ZA | 201 | CYC | CHB-C1B | 4.35 | 1.48 | 1.38 |
| 12 | Z9 | 201 | CYC | CHB-C1B | 4.35 | 1.48 | 1.38 |
| 12 | J6 | 201 | CYC | CHB-C1B | 4.35 | 1.48 | 1.38 |
| 12 | XA | 202 | CYC | CHB-C1B | 4.35 | 1.48 | 1.38 |
| 12 | X9 | 202 | CYC | CHB-C1B | 4.35 | 1.48 | 1.38 |
| 12 | D1 | 201 | CYC | CHB-C1B | 4.35 | 1.48 | 1.38 |
| 12 | T3 | 301 | CYC | CHB-C1B | 4.34 | 1.48 | 1.38 |
| 12 | T1 | 301 | CYC | CHB-C1B | 4.34 | 1.48 | 1.38 |
| 12 | R1 | 201 | CYC | CHB-C1B | 4.34 | 1.48 | 1.38 |
| 12 | R3 | 201 | CYC | CHB-C1B | 4.34 | 1.48 | 1.38 |
| 12 | F2 | 201 | CYC | CHB-C1B | 4.34 | 1.48 | 1.38 |
| 12 | Z3 | 201 | CYC | CHB-C1B | 4.34 | 1.48 | 1.38 |
| 12 | Z1 | 202 | CYC | CHB-C1B | 4.34 | 1.48 | 1.38 |
| 12 | F6 | 202 | CYC | CHB-C1B | 4.34 | 1.48 | 1.38 |
| 12 | aA | 902 | CYC | CHB-C1B | 4.34 | 1.48 | 1.38 |
| 12 | TA | 302 | CYC | CHB-C1B | 4.34 | 1.48 | 1.38 |
| 12 | RA | 202 | CYC | CHB-C1B | 4.33 | 1.48 | 1.38 |
| 12 | R9 | 202 | CYC | CHB-C1B | 4.33 | 1.48 | 1.38 |
| 12 | H4 | 201 | CYC | CHB-C1B | 4.33 | 1.48 | 1.38 |
| 12 | H8 | 201 | CYC | CHB-C1B | 4.33 | 1.48 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | H2 | 201 | CYC | CHB-C1B | 4.33 | 1.48 | 1.38 |
| 12 | H6 | 201 | CYC | CHB-C1B | 4.33 | 1.48 | 1.38 |
| 12 | J2 | 201 | CYC | CHB-C1B | 4.33 | 1.48 | 1.38 |
| 12 | D6 | 202 | CYC | CHB-C1B | 4.33 | 1.48 | 1.38 |
| 12 | D2 | 202 | CYC | CHB-C1B | 4.33 | 1.48 | 1.38 |
| 12 | J4 | 201 | CYC | CHB-C1B | 4.33 | 1.48 | 1.38 |
| 12 | J8 | 201 | CYC | CHB-C1B | 4.33 | 1.48 | 1.38 |
| 12 | L6 | 201 | CYC | CHB-C1B | 4.33 | 1.48 | 1.38 |
| 12 | M8 | 301 | CYC | CHB-C1B | 4.32 | 1.48 | 1.38 |
| 12 | TA | 301 | CYC | CHB-C1B | 4.32 | 1.48 | 1.38 |
| 12 | T9 | 301 | CYC | CHB-C1B | 4.32 | 1.48 | 1.38 |
| 12 | Z8 | 301 | CYC | CHB-C1B | 4.32 | 1.48 | 1.38 |
| 12 | B4 | 202 | CYC | CHB-C1B | 4.32 | 1.48 | 1.38 |
| 12 | HA | 201 | CYC | CHB-C1B | 4.32 | 1.48 | 1.38 |
| 12 | O4 | 201 | CYC | CHB-C1B | 4.32 | 1.48 | 1.38 |
| 12 | O8 | 201 | CYC | CHB-C1B | 4.32 | 1.48 | 1.38 |
| 12 | H9 | 201 | CYC | CHB-C1B | 4.32 | 1.48 | 1.38 |
| 12 | T9 | 302 | CYC | CHB-C1B | 4.32 | 1.48 | 1.38 |
| 12 | FA | 301 | CYC | CHB-C1B | 4.32 | 1.48 | 1.38 |
| 12 | F9 | 301 | CYC | CHB-C1B | 4.32 | 1.48 | 1.38 |
| 12 | PA | 201 | CYC | CHB-C1B | 4.31 | 1.48 | 1.38 |
| 12 | P9 | 201 | CYC | CHB-C1B | 4.31 | 1.48 | 1.38 |
| 12 | R9 | 201 | CYC | CHB-C1B | 4.31 | 1.48 | 1.38 |
| 12 | ZA | 202 | CYC | CHB-C1B | 4.31 | 1.48 | 1.38 |
| 12 | D4 | 202 | CYC | CHB-C1B | 4.31 | 1.48 | 1.38 |
| 12 | D8 | 202 | CYC | CHB-C1B | 4.31 | 1.48 | 1.38 |
| 12 | F2 | 202 | CYC | CHB-C1B | 4.31 | 1.48 | 1.38 |
| 12 | L3 | 202 | CYC | CHB-C1B | 4.31 | 1.48 | 1.38 |
| 12 | N2 | 101 | CYC | CHB-C1B | 4.31 | 1.48 | 1.38 |
| 12 | O4 | 202 | CYC | CHB-C1B | 4.31 | 1.48 | 1.38 |
| 12 | N6 | 101 | CYC | CHB-C1B | 4.31 | 1.48 | 1.38 |
| 12 | O8 | 202 | CYC | CHB-C1B | 4.31 | 1.48 | 1.38 |
| 12 | LA | 202 | CYC | CHB-C1B | 4.30 | 1.48 | 1.38 |
| 12 | L9 | 202 | CYC | CHB-C1B | 4.30 | 1.48 | 1.38 |
| 12 | H1 | 201 | CYC | CHB-C1B | 4.30 | 1.48 | 1.38 |
| 12 | B8 | 202 | CYC | CHB-C1B | 4.30 | 1.48 | 1.38 |
| 12 | BA | 201 | CYC | CHB-C1B | 4.30 | 1.48 | 1.38 |
| 12 | B9 | 201 | CYC | CHB-C1B | 4.30 | 1.48 | 1.38 |
| 12 | X3 | 201 | CYC | CHB-C1B | 4.30 | 1.48 | 1.38 |
| 12 | X1 | 201 | CYC | CHB-C1B | 4.30 | 1.48 | 1.38 |
| 12 | S4 | 202 | CYC | CHB-C1B | 4.29 | 1.48 | 1.38 |
| 12 | RA | 201 | CYC | CHB-C1B | 4.29 | 1.48 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | L2 | 201 | CYC | CHB-C1B | 4.29 | 1.48 | 1.38 |
| 12 | H3 | 202 | CYC | CHB-C1B | 4.29 | 1.48 | 1.38 |
| 12 | JA | 202 | CYC | CHB-C1B | 4.28 | 1.48 | 1.38 |
| 12 | J9 | 202 | CYC | CHB-C1B | 4.28 | 1.48 | 1.38 |
| 12 | DA | 201 | CYC | CHB-C1B | 4.28 | 1.48 | 1.38 |
| 12 | D9 | 201 | CYC | CHB-C1B | 4.28 | 1.48 | 1.38 |
| 12 | T3 | 302 | CYC | CHB-C1B | 4.28 | 1.48 | 1.38 |
| 12 | T1 | 302 | CYC | CHB-C1B | 4.28 | 1.48 | 1.38 |
| 12 | Z9 | 202 | CYC | CHB-C1B | 4.28 | 1.48 | 1.38 |
| 12 | D6 | 201 | CYC | CHB-C1B | 4.28 | 1.48 | 1.38 |
| 12 | XA | 201 | CYC | CHB-C1B | 4.26 | 1.48 | 1.38 |
| 12 | M8 | 302 | CYC | CHB-C1B | 4.26 | 1.48 | 1.38 |
| 12 | V3 | 201 | CYC | CHB-C1B | 4.25 | 1.48 | 1.38 |
| 12 | VA | 201 | CYC | CHB-C1B | 4.24 | 1.48 | 1.38 |
| 12 | aA | 901 | CYC | CHB-C1B | 4.24 | 1.48 | 1.38 |
| 12 | V1 | 201 | CYC | CHB-C1B | 4.23 | 1.48 | 1.38 |
| 12 | D3 | 202 | CYC | CHB-C1B | 4.23 | 1.48 | 1.38 |
| 12 | D1 | 202 | CYC | CHB-C1B | 4.23 | 1.48 | 1.38 |
| 12 | J3 | 202 | CYC | CHB-C1B | 4.23 | 1.48 | 1.38 |
| 12 | X9 | 201 | CYC | CHB-C1B | 4.23 | 1.48 | 1.38 |
| 12 | D2 | 201 | CYC | CHB-C1B | 4.22 | 1.48 | 1.38 |
| 12 | V9 | 201 | CYC | CHB-C1B | 4.20 | 1.48 | 1.38 |
| 12 | G8 | 201 | CYC | CHB-C4A | 4.15 | 1.50 | 1.40 |
| 12 | K3 | 201 | CYC | CHB-C4A | 4.14 | 1.50 | 1.40 |
| 12 | K1 | 201 | CYC | CHB-C4A | 4.14 | 1.50 | 1.40 |
| 12 | G4 | 201 | CYC | CHB-C4A | 4.13 | 1.50 | 1.40 |
| 12 | K4 | 201 | CYC | CHB-C4A | 4.13 | 1.50 | 1.40 |
| 12 | K8 | 201 | CYC | CHB-C4A | 4.13 | 1.50 | 1.40 |
| 12 | YA | 201 | CYC | CHB-C4A | 4.12 | 1.50 | 1.40 |
| 12 | Y9 | 201 | CYC | CHB-C4A | 4.12 | 1.50 | 1.40 |
| 12 | U1 | 201 | CYC | CHB-C4A | 4.12 | 1.50 | 1.40 |
| 12 | A1 | 201 | CYC | CHB-C4A | 4.11 | 1.50 | 1.40 |
| 12 | A3 | 201 | CYC | CHB-C4A | 4.11 | 1.50 | 1.40 |
| 12 | Y3 | 201 | CYC | CHB-C4A | 4.11 | 1.50 | 1.40 |
| 12 | Y1 | 201 | CYC | CHB-C4A | 4.11 | 1.50 | 1.40 |
| 12 | N4 | 201 | CYC | CHB-C4A | 4.11 | 1.50 | 1.40 |
| 12 | N8 | 201 | CYC | CHB-C4A | 4.11 | 1.50 | 1.40 |
| 12 | K2 | 201 | CYC | CHB-C4A | 4.11 | 1.50 | 1.40 |
| 12 | K6 | 201 | CYC | CHB-C4A | 4.11 | 1.50 | 1.40 |
| 12 | U3 | 201 | CYC | CHB-C4A | 4.10 | 1.50 | 1.40 |
| 12 | G3 | 201 | CYC | CHB-C4A | 4.10 | 1.50 | 1.40 |
| 12 | G1 | 201 | CYC | CHB-C4A | 4.10 | 1.50 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 12 | C9 | 201 | CYC | CHB-C4A | 4.10 | 1.50 | 1.40 |
| 12 | T4 | 201 | CYC | CHB-C4A | 4.09 | 1.50 | 1.40 |
| 12 | T8 | 201 | CYC | CHB-C4A | 4.09 | 1.50 | 1.40 |
| 12 | S1 | 201 | CYC | CHB-C4A | 4.09 | 1.50 | 1.40 |
| 12 | S3 | 201 | CYC | CHB-C4A | 4.09 | 1.50 | 1.40 |
| 12 | KA | 201 | CYC | CHB-C4A | 4.08 | 1.50 | 1.40 |
| 12 | K9 | 201 | CYC | CHB-C4A | 4.08 | 1.50 | 1.40 |
| 12 | E4 | 201 | CYC | CHB-C4A | 4.08 | 1.50 | 1.40 |
| 12 | E8 | 201 | CYC | CHB-C4A | 4.08 | 1.50 | 1.40 |
| 12 | AA | 201 | CYC | CHB-C4A | 4.08 | 1.50 | 1.40 |
| 12 | CA | 201 | CYC | CHB-C4A | 4.07 | 1.50 | 1.40 |
| 12 | SA | 201 | CYC | CHB-C4A | 4.07 | 1.50 | 1.40 |
| 12 | S9 | 201 | CYC | CHB-C4A | 4.07 | 1.50 | 1.40 |
| 12 | R4 | 201 | CYC | CHB-C4A | 4.07 | 1.49 | 1.40 |
| 12 | E2 | 201 | CYC | CHB-C4A | 4.07 | 1.49 | 1.40 |
| 12 | Q9 | 201 | CYC | CHB-C4A | 4.07 | 1.49 | 1.40 |
| 12 | O1 | 201 | CYC | CHB-C4A | 4.06 | 1.49 | 1.40 |
| 12 | O3 | 201 | CYC | CHB-C4A | 4.06 | 1.49 | 1.40 |
| 12 | j5 | 1201 | CYC | CHB-C4A | 4.06 | 1.49 | 1.40 |
| 12 | k5 | 1201 | CYC | CHB-C4A | 4.06 | 1.49 | 1.40 |
| 12 | UA | 201 | CYC | CHB-C4A | 4.06 | 1.49 | 1.40 |
| 12 | U9 | 201 | CYC | CHB-C4A | 4.06 | 1.49 | 1.40 |
| 12 | E6 | 201 | CYC | CHB-C4A | 4.05 | 1.49 | 1.40 |
| 12 | QA | 201 | CYC | CHB-C4A | 4.05 | 1.49 | 1.40 |
| 12 | R8 | 201 | CYC | CHB-C4A | 4.05 | 1.49 | 1.40 |
| 12 | A6 | 201 | CYC | CHB-C4A | 4.05 | 1.49 | 1.40 |
| 12 | A9 | 201 | CYC | CHB-C4A | 4.05 | 1.49 | 1.40 |
| 12 | G2 | 201 | CYC | CHB-C4A | 4.04 | 1.49 | 1.40 |
| 12 | C2 | 201 | CYC | CHB-C4A | 4.04 | 1.49 | 1.40 |
| 12 | A4 | 201 | CYC | CHB-C4A | 4.04 | 1.49 | 1.40 |
| 12 | A8 | 201 | CYC | CHB-C4A | 4.04 | 1.49 | 1.40 |
| 12 | E3 | 201 | CYC | CHB-C4A | 4.02 | 1.49 | 1.40 |
| 12 | E1 | 201 | CYC | CHB-C4A | 4.02 | 1.49 | 1.40 |
| 12 | C6 | 201 | CYC | CHB-C4A | 4.02 | 1.49 | 1.40 |
| 12 | GA | 201 | CYC | CHB-C4A | 4.02 | 1.49 | 1.40 |
| 12 | IA | 201 | CYC | CHB-C4A | 4.02 | 1.49 | 1.40 |
| 12 | I9 | 201 | CYC | CHB-C4A | 4.02 | 1.49 | 1.40 |
| 12 | G6 | 201 | CYC | CHB-C4A | 4.02 | 1.49 | 1.40 |
| 12 | A2 | 201 | CYC | CHB-C4A | 4.01 | 1.49 | 1.40 |
| 12 | C8 | 201 | CYC | CHB-C4A | 4.00 | 1.49 | 1.40 |
| 12 | P4 | 201 | CYC | CHB-C4A | 4.00 | 1.49 | 1.40 |
| 12 | P8 | 201 | CYC | CHB-C4A | 4.00 | 1.49 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 12 | j5 | 1202 | CYC | CHB-C4A | 3.99 | 1.49 | 1.40 |
| 12 | Z | 201 | CYC | CHB-C4A | 3.99 | 1.49 | 1.40 |
| 12 | OA | 201 | CYC | CHB-C4A | 3.99 | 1.49 | 1.40 |
| 12 | O9 | 201 | CYC | CHB-C4A | 3.99 | 1.49 | 1.40 |
| 12 | G9 | 201 | CYC | CHB-C4A | 3.99 | 1.49 | 1.40 |
| 12 | P7 | 201 | CYC | CHB-C4A | 3.99 | 1.49 | 1.40 |
| 12 | k5 | 1204 | CYC | CHB-C4A | 3.99 | 1.49 | 1.40 |
| 12 | C4 | 201 | CYC | CHB-C4A | 3.99 | 1.49 | 1.40 |
| 12 | X4 | 201 | CYC | CHB-C4A | 3.98 | 1.49 | 1.40 |
| 12 | X8 | 201 | CYC | CHB-C4A | 3.98 | 1.49 | 1.40 |
| 12 | A | 201 | CYC | CHB-C4A | 3.98 | 1.49 | 1.40 |
| 12 | V7 | 201 | CYC | CHB-C4A | 3.98 | 1.49 | 1.40 |
| 12 | Q1 | 201 | CYC | CHB-C4A | 3.97 | 1.49 | 1.40 |
| 12 | Q3 | 201 | CYC | CHB-C4A | 3.97 | 1.49 | 1.40 |
| 12 | V4 | 201 | CYC | CHB-C4A | 3.97 | 1.49 | 1.40 |
| 12 | V8 | 201 | CYC | CHB-C4A | 3.97 | 1.49 | 1.40 |
| 12 | P5 | 201 | CYC | CHB-C4A | 3.96 | 1.49 | 1.40 |
| 12 | C3 | 201 | CYC | CHB-C4A | 3.96 | 1.49 | 1.40 |
| 12 | D7 | 201 | CYC | CHB-C4A | 3.96 | 1.49 | 1.40 |
| 12 | J7 | 201 | CYC | CHB-C4A | 3.96 | 1.49 | 1.40 |
| 12 | WA | 201 | CYC | CHB-C4A | 3.96 | 1.49 | 1.40 |
| 12 | W9 | 201 | CYC | CHB-C4A | 3.96 | 1.49 | 1.40 |
| 12 | E9 | 201 | CYC | CHB-C4A | 3.95 | 1.49 | 1.40 |
| 12 | C1 | 201 | CYC | CHB-C4A | 3.94 | 1.49 | 1.40 |
| 12 | v7 | 201 | CYC | CHB-C4A | 3.94 | 1.49 | 1.40 |
| 12 | EA | 201 | CYC | CHB-C4A | 3.94 | 1.49 | 1.40 |
| 12 | I6 | 201 | CYC | CHB-C4A | 3.94 | 1.49 | 1.40 |
| 12 | V5 | 201 | CYC | CHB-C4A | 3.93 | 1.49 | 1.40 |
| 12 | I3 | 201 | CYC | CHB-C4A | 3.93 | 1.49 | 1.40 |
| 12 | I1 | 201 | CYC | CHB-C4A | 3.93 | 1.49 | 1.40 |
| 12 | D5 | 201 | CYC | CHB-C4A | 3.92 | 1.49 | 1.40 |
| 12 | H5 | 201 | CYC | CHB-C4A | 3.92 | 1.49 | 1.40 |
| 12 | B5 | 201 | CYC | CHB-C4A | 3.92 | 1.49 | 1.40 |
| 12 | W3 | 201 | CYC | CHB-C4A | 3.90 | 1.49 | 1.40 |
| 12 | F7 | 201 | CYC | CHB-C4A | 3.90 | 1.49 | 1.40 |
| 12 | p7 | 201 | CYC | CHB-C4A | 3.90 | 1.49 | 1.40 |
| 12 | H7 | 201 | CYC | CHB-C4A | 3.90 | 1.49 | 1.40 |
| 12 | h7 | 201 | CYC | CHB-C4A | 3.89 | 1.49 | 1.40 |
| 12 | W1 | 201 | CYC | CHB-C4A | 3.89 | 1.49 | 1.40 |
| 12 | T5 | 201 | CYC | CHB-C4A | 3.89 | 1.49 | 1.40 |
| 12 | b7 | 201 | CYC | CHB-C4A | 3.89 | 1.49 | 1.40 |
| 12 | J5 | 201 | CYC | CHB-C4A | 3.88 | 1.49 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 12 | L7 | 201 | CYC | CHB-C4A | 3.88 | 1.49 | 1.40 |
| 12 | X7 | 201 | CYC | CHB-C4A | 3.87 | 1.49 | 1.40 |
| 12 | F5 | 201 | CYC | CHB-C4A | 3.87 | 1.49 | 1.40 |
| 12 | k5 | 1203 | CYC | CHB-C4A | 3.86 | 1.49 | 1.40 |
| 12 | N7 | 201 | CYC | CHB-C4A | 3.86 | 1.49 | 1.40 |
| 12 | L5 | 201 | CYC | CHB-C4A | 3.86 | 1.49 | 1.40 |
| 12 | N5 | 201 | CYC | CHB-C4A | 3.86 | 1.49 | 1.40 |
| 12 | I4 | 201 | CYC | CHB-C4A | 3.86 | 1.49 | 1.40 |
| 12 | b5 | 201 | CYC | CHB-C4A | 3.86 | 1.49 | 1.40 |
| 12 | I8 | 201 | CYC | CHB-C4A | 3.86 | 1.49 | 1.40 |
| 12 | d7 | 201 | CYC | CHB-C4A | 3.86 | 1.49 | 1.40 |
| 12 | B7 | 201 | CYC | CHB-C4A | 3.85 | 1.49 | 1.40 |
| 12 | k5 | 1202 | CYC | CHB-C4A | 3.85 | 1.49 | 1.40 |
| 12 | T7 | 201 | CYC | CHB-C4A | 3.85 | 1.49 | 1.40 |
| 12 | f7 | 201 | CYC | CHB-C4A | 3.85 | 1.49 | 1.40 |
| 12 | I2 | 201 | CYC | CHB-C4A | 3.85 | 1.49 | 1.40 |
| 12 | f5 | 201 | CYC | CHB-C4A | 3.84 | 1.49 | 1.40 |
| 12 | R5 | 201 | CYC | CHB-C4A | 3.84 | 1.49 | 1.40 |
| 12 | r7 | 201 | CYC | CHB-C4A | 3.84 | 1.49 | 1.40 |
| 12 | X5 | 201 | CYC | CHB-C4A | 3.83 | 1.49 | 1.40 |
| 12 | j7 | 201 | CYC | CHB-C4A | 3.82 | 1.49 | 1.40 |
| 12 | R7 | 201 | CYC | CHB-C4A | 3.82 | 1.49 | 1.40 |
| 12 | Z5 | 201 | CYC | CHB-C4A | 3.76 | 1.49 | 1.40 |
| 12 | d5 | 201 | CYC | CHB-C4A | 3.75 | 1.49 | 1.40 |
| 12 | E7 | 201 | CYC | CHB-C4A | 3.75 | 1.49 | 1.40 |
| 12 | K7 | 201 | CYC | CHB-C4A | 3.73 | 1.49 | 1.40 |
| 12 | A5 | 201 | CYC | CHB-C4A | 3.71 | 1.49 | 1.40 |
| 12 | G7 | 201 | CYC | CHB-C4A | 3.71 | 1.49 | 1.40 |
| 12 | S7 | 201 | CYC | CHB-C4A | 3.69 | 1.49 | 1.40 |
| 12 | O7 | 201 | CYC | CHB-C4A | 3.68 | 1.49 | 1.40 |
| 12 | C7 | 201 | CYC | CHB-C4A | 3.68 | 1.49 | 1.40 |
| 12 | U5 | 201 | CYC | CHB-C4A | 3.67 | 1.49 | 1.40 |
| 12 | E5 | 201 | CYC | CHB-C4A | 3.66 | 1.49 | 1.40 |
| 12 | k7 | 201 | CYC | CHB-C4A | 3.66 | 1.49 | 1.40 |
| 12 | G5 | 201 | CYC | CHB-C4A | 3.66 | 1.49 | 1.40 |
| 12 | I7 | 201 | CYC | CHB-C4A | 3.66 | 1.49 | 1.40 |
| 12 | K5 | 201 | CYC | CHB-C4A | 3.65 | 1.49 | 1.40 |
| 12 | M7 | 201 | CYC | CHB-C4A | 3.65 | 1.49 | 1.40 |
| 12 | S5 | 201 | CYC | CHB-C4A | 3.65 | 1.49 | 1.40 |
| 12 | A7 | 201 | CYC | CHB-C4A | 3.64 | 1.49 | 1.40 |
| 12 | q7 | 201 | CYC | CHB-C4A | 3.64 | 1.49 | 1.40 |
| 12 | g7 | 201 | CYC | CHB-C4A | 3.64 | 1.48 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | a7 | 201 | CYC | CHB-C4A | 3.64 | 1.48 | 1.40 |
| 12 | O5 | 201 | CYC | CHB-C4A | 3.64 | 1.48 | 1.40 |
| 12 | W5 | 201 | CYC | CHB-C4A | 3.64 | 1.48 | 1.40 |
| 12 | Y5 | 201 | CYC | CHB-C4A | 3.64 | 1.48 | 1.40 |
| 12 | Y7 | 201 | CYC | CHB-C4A | 3.63 | 1.48 | 1.40 |
| 12 | u7 | 201 | CYC | CHB-C4A | 3.63 | 1.48 | 1.40 |
| 12 | e7 | 201 | CYC | CHB-C4A | 3.63 | 1.48 | 1.40 |
| 12 | U7 | 201 | CYC | CHB-C4A | 3.63 | 1.48 | 1.40 |
| 12 | Q7 | 201 | CYC | CHB-C4A | 3.62 | 1.48 | 1.40 |
| 12 | o7 | 201 | CYC | CHB-C4A | 3.61 | 1.48 | 1.40 |
| 12 | Q5 | 201 | CYC | CHB-C4A | 3.61 | 1.48 | 1.40 |
| 12 | M5 | 201 | CYC | CHB-C4A | 3.61 | 1.48 | 1.40 |
| 12 | i7 | 201 | CYC | CHB-C4A | 3.61 | 1.48 | 1.40 |
| 12 | m7 | 201 | CYC | CHB-C4A | 3.61 | 1.48 | 1.40 |
| 12 | s7 | 201 | CYC | CHB-C4A | 3.61 | 1.48 | 1.40 |
| 12 | c7 | 201 | CYC | CHB-C4A | 3.61 | 1.48 | 1.40 |
| 12 | E5 | 201 | CYC | C3D-C2D | 3.60 | 1.48 | 1.37 |
| 12 | F3 | 202 | CYC | CHB-C4A | 3.60 | 1.48 | 1.40 |
| 12 | F1 | 202 | CYC | CHB-C4A | 3.60 | 1.48 | 1.40 |
| 12 | e5 | 201 | CYC | CHB-C4A | 3.60 | 1.48 | 1.40 |
| 12 | a5 | 201 | CYC | CHB-C4A | 3.59 | 1.48 | 1.40 |
| 12 | c5 | 201 | CYC | CHB-C4A | 3.59 | 1.48 | 1.40 |
| 12 | I5 | 201 | CYC | CHB-C4A | 3.59 | 1.48 | 1.40 |
| 12 | K5 | 201 | CYC | C3D-C2D | 3.59 | 1.48 | 1.37 |
| 12 | XA | 202 | CYC | CHB-C4A | 3.59 | 1.48 | 1.40 |
| 12 | X9 | 202 | CYC | CHB-C4A | 3.59 | 1.48 | 1.40 |
| 12 | W7 | 201 | CYC | CHB-C4A | 3.58 | 1.48 | 1.40 |
| 12 | B2 | 201 | CYC | CHB-C4A | 3.58 | 1.48 | 1.40 |
| 12 | D2 | 201 | CYC | C3D-C2D | 3.57 | 1.48 | 1.37 |
| 12 | D6 | 201 | CYC | C3D-C2D | 3.57 | 1.48 | 1.37 |
| 12 | L2 | 202 | CYC | CHB-C4A | 3.57 | 1.48 | 1.40 |
| 12 | C5 | 201 | CYC | CHB-C4A | 3.57 | 1.48 | 1.40 |
| 12 | O4 | 202 | CYC | CHB-C4A | 3.56 | 1.48 | 1.40 |
| 12 | O8 | 202 | CYC | CHB-C4A | 3.56 | 1.48 | 1.40 |
| 12 | T3 | 302 | CYC | CHB-C4A | 3.56 | 1.48 | 1.40 |
| 12 | T1 | 302 | CYC | CHB-C4A | 3.56 | 1.48 | 1.40 |
| 12 | u7 | 201 | CYC | C3D-C2D | 3.56 | 1.48 | 1.37 |
| 12 | S4 | 201 | CYC | CHB-C4A | 3.56 | 1.48 | 1.40 |
| 12 | S8 | 201 | CYC | CHB-C4A | 3.56 | 1.48 | 1.40 |
| 12 | Q7 | 201 | CYC | C3D-C2D | 3.55 | 1.48 | 1.37 |
| 12 | U7 | 201 | CYC | C3D-C2D | 3.54 | 1.48 | 1.37 |
| 12 | B3 | 201 | CYC | CHB-C4A | 3.54 | 1.48 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 12 | B1 | 201 | CYC | CHB-C4A | 3.54 | 1.48 | 1.40 |
| 12 | H4 | 201 | CYC | C3D-C2D | 3.54 | 1.48 | 1.37 |
| 12 | H8 | 201 | CYC | C3D-C2D | 3.54 | 1.48 | 1.37 |
| 12 | LA | 201 | CYC | CHB-C4A | 3.54 | 1.48 | 1.40 |
| 12 | W7 | 201 | CYC | C3D-C2D | 3.54 | 1.48 | 1.37 |
| 12 | L6 | 202 | CYC | CHB-C4A | 3.54 | 1.48 | 1.40 |
| 12 | i7 | 201 | CYC | C3D-C2D | 3.54 | 1.48 | 1.37 |
| 12 | Q4 | 201 | CYC | CHB-C4A | 3.54 | 1.48 | 1.40 |
| 12 | PA | 202 | CYC | CHB-C4A | 3.53 | 1.48 | 1.40 |
| 12 | P9 | 202 | CYC | CHB-C4A | 3.53 | 1.48 | 1.40 |
| 12 | B6 | 201 | CYC | CHB-C4A | 3.53 | 1.48 | 1.40 |
| 12 | Q8 | 201 | CYC | CHB-C4A | 3.53 | 1.48 | 1.40 |
| 12 | HA | 201 | CYC | CHB-C4A | 3.53 | 1.48 | 1.40 |
| 12 | H9 | 201 | CYC | CHB-C4A | 3.53 | 1.48 | 1.40 |
| 12 | J4 | 202 | CYC | CHB-C4A | 3.52 | 1.48 | 1.40 |
| 12 | J8 | 202 | CYC | CHB-C4A | 3.52 | 1.48 | 1.40 |
| 12 | H3 | 201 | CYC | CHB-C4A | 3.52 | 1.48 | 1.40 |
| 12 | H1 | 202 | CYC | CHB-C4A | 3.52 | 1.48 | 1.40 |
| 12 | Q5 | 201 | CYC | C3D-C2D | 3.52 | 1.48 | 1.37 |
| 12 | L9 | 201 | CYC | CHB-C4A | 3.52 | 1.48 | 1.40 |
| 12 | R1 | 202 | CYC | CHB-C4A | 3.52 | 1.48 | 1.40 |
| 12 | e7 | 201 | CYC | C3D-C2D | 3.52 | 1.48 | 1.37 |
| 12 | D2 | 202 | CYC | CHB-C4A | 3.52 | 1.48 | 1.40 |
| 12 | T3 | 301 | CYC | C3D-C2D | 3.51 | 1.48 | 1.37 |
| 12 | T1 | 301 | CYC | C3D-C2D | 3.51 | 1.48 | 1.37 |
| 12 | F9 | 301 | CYC | C3D-C2D | 3.51 | 1.48 | 1.37 |
| 12 | c7 | 201 | CYC | C3D-C2D | 3.51 | 1.48 | 1.37 |
| 12 | W5 | 201 | CYC | C3D-C2D | 3.51 | 1.48 | 1.37 |
| 12 | O7 | 201 | CYC | C3D-C2D | 3.51 | 1.48 | 1.37 |
| 12 | M7 | 201 | CYC | C3D-C2D | 3.51 | 1.48 | 1.37 |
| 12 | F9 | 303 | CYC | CHB-C4A | 3.51 | 1.48 | 1.40 |
| 12 | ZA | 202 | CYC | C3D-C2D | 3.51 | 1.48 | 1.37 |
| 12 | Z9 | 202 | CYC | C3D-C2D | 3.51 | 1.48 | 1.37 |
| 12 | R3 | 202 | CYC | CHB-C4A | 3.51 | 1.48 | 1.40 |
| 12 | F4 | 201 | CYC | CHB-C4A | 3.51 | 1.48 | 1.40 |
| 12 | F8 | 201 | CYC | CHB-C4A | 3.51 | 1.48 | 1.40 |
| 12 | b5 | 201 | CYC | C3D-C2D | 3.51 | 1.48 | 1.37 |
| 12 | D6 | 202 | CYC | CHB-C4A | 3.51 | 1.48 | 1.40 |
| 12 | A5 | 201 | CYC | C3D-C2D | 3.50 | 1.48 | 1.37 |
| 12 | VA | 202 | CYC | CHB-C4A | 3.50 | 1.48 | 1.40 |
| 12 | V9 | 202 | CYC | CHB-C4A | 3.50 | 1.48 | 1.40 |
| 12 | L4 | 201 | CYC | CHB-C4A | 3.50 | 1.48 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | L8 | 201 | CYC | CHB-C4A | 3.50 | 1.48 | 1.40 |
| 12 | P1 | 202 | CYC | CHB-C4A | 3.50 | 1.48 | 1.40 |
| 12 | P3 | 202 | CYC | CHB-C4A | 3.50 | 1.48 | 1.40 |
| 12 | F9 | 302 | CYC | CHB-C4A | 3.50 | 1.48 | 1.40 |
| 12 | Y4 | 201 | CYC | CHB-C4A | 3.50 | 1.48 | 1.40 |
| 12 | Y8 | 201 | CYC | CHB-C4A | 3.50 | 1.48 | 1.40 |
| 12 | V5 | 201 | CYC | C3D-C2D | 3.49 | 1.48 | 1.37 |
| 12 | H4 | 202 | CYC | CHB-C4A | 3.49 | 1.48 | 1.40 |
| 12 | H8 | 202 | CYC | CHB-C4A | 3.49 | 1.48 | 1.40 |
| 12 | Z | 201 | CYC | C3D-C2D | 3.49 | 1.48 | 1.37 |
| 12 | Z3 | 201 | CYC | C3D-C2D | 3.49 | 1.48 | 1.37 |
| 12 | Z1 | 202 | CYC | C3D-C2D | 3.49 | 1.48 | 1.37 |
| 12 | G5 | 201 | CYC | C3D-C2D | 3.49 | 1.48 | 1.37 |
| 12 | k7 | 201 | CYC | C3D-C2D | 3.49 | 1.48 | 1.37 |
| 12 | A7 | 201 | CYC | C3D-C2D | 3.49 | 1.48 | 1.37 |
| 12 | Y7 | 201 | CYC | C3D-C2D | 3.49 | 1.48 | 1.37 |
| 12 | A | 201 | CYC | C3D-C2D | 3.49 | 1.48 | 1.37 |
| 12 | B4 | 201 | CYC | CHB-C4A | 3.49 | 1.48 | 1.40 |
| 12 | B8 | 201 | CYC | CHB-C4A | 3.49 | 1.48 | 1.40 |
| 12 | d7 | 201 | CYC | C3D-C2D | 3.49 | 1.48 | 1.37 |
| 12 | T7 | 201 | CYC | C1C-NC | -3.49 | 1.33 | 1.37 |
| 12 | M5 | 201 | CYC | C3D-C2D | 3.49 | 1.48 | 1.37 |
| 12 | F8 | 202 | CYC | C3D-C2D | 3.49 | 1.48 | 1.37 |
| 12 | D4 | 201 | CYC | CHB-C4A | 3.49 | 1.48 | 1.40 |
| 12 | D8 | 201 | CYC | CHB-C4A | 3.49 | 1.48 | 1.40 |
| 12 | FA | 301 | CYC | C3D-C2D | 3.49 | 1.48 | 1.37 |
| 12 | XA | 201 | CYC | C3D-C2D | 3.49 | 1.48 | 1.37 |
| 12 | X9 | 201 | CYC | C3D-C2D | 3.49 | 1.48 | 1.37 |
| 12 | E7 | 201 | CYC | C3D-C2D | 3.48 | 1.48 | 1.37 |
| 12 | H2 | 202 | CYC | CHB-C4A | 3.48 | 1.48 | 1.40 |
| 12 | H6 | 202 | CYC | CHB-C4A | 3.48 | 1.48 | 1.40 |
| 12 | K7 | 201 | CYC | C3D-C2D | 3.48 | 1.48 | 1.37 |
| 12 | L3 | 201 | CYC | CHB-C4A | 3.48 | 1.48 | 1.40 |
| 12 | L1 | 201 | CYC | CHB-C4A | 3.48 | 1.48 | 1.40 |
| 12 | f5 | 201 | CYC | C3D-C2D | 3.48 | 1.48 | 1.37 |
| 12 | o7 | 201 | CYC | C3D-C2D | 3.48 | 1.48 | 1.37 |
| 12 | JA | 201 | CYC | CHB-C4A | 3.48 | 1.48 | 1.40 |
| 12 | J9 | 201 | CYC | CHB-C4A | 3.48 | 1.48 | 1.40 |
| 12 | c5 | 201 | CYC | C3D-C2D | 3.48 | 1.48 | 1.37 |
| 12 | F4 | 202 | CYC | C3D-C2D | 3.48 | 1.48 | 1.37 |
| 12 | H5 | 201 | CYC | C3D-C2D | 3.48 | 1.48 | 1.37 |
| 12 | Z4 | 301 | CYC | C3D-C2D | 3.47 | 1.48 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | D3 | 202 | CYC | C3D-C2D | 3.47 | 1.48 | 1.37 |
| 12 | D1 | 202 | CYC | C3D-C2D | 3.47 | 1.48 | 1.37 |
| 12 | L3 | 202 | CYC | C3D-C2D | 3.47 | 1.48 | 1.37 |
| 12 | J3 | 201 | CYC | CHB-C4A | 3.47 | 1.48 | 1.40 |
| 12 | J1 | 201 | CYC | CHB-C4A | 3.47 | 1.48 | 1.40 |
| 12 | U4 | 201 | CYC | C2C-C1C | -3.47 | 1.49 | 1.52 |
| 12 | U8 | 201 | CYC | C2C-C1C | -3.47 | 1.49 | 1.52 |
| 12 | PA | 201 | CYC | C3D-C2D | 3.47 | 1.47 | 1.37 |
| 12 | P9 | 201 | CYC | C3D-C2D | 3.47 | 1.47 | 1.37 |
| 12 | J4 | 201 | CYC | C3D-C2D | 3.47 | 1.47 | 1.37 |
| 12 | a7 | 201 | CYC | C3D-C2D | 3.47 | 1.47 | 1.37 |
| 12 | J8 | 201 | CYC | C3D-C2D | 3.47 | 1.47 | 1.37 |
| 12 | X7 | 201 | CYC | C3D-C2D | 3.47 | 1.47 | 1.37 |
| 12 | P5 | 201 | CYC | C3D-C2D | 3.47 | 1.47 | 1.37 |
| 12 | BA | 202 | CYC | CHB-C4A | 3.47 | 1.48 | 1.40 |
| 12 | B9 | 202 | CYC | CHB-C4A | 3.47 | 1.48 | 1.40 |
| 12 | X3 | 201 | CYC | C3D-C2D | 3.47 | 1.47 | 1.37 |
| 12 | Z5 | 201 | CYC | C3D-C2D | 3.47 | 1.47 | 1.37 |
| 12 | X1 | 201 | CYC | C3D-C2D | 3.47 | 1.47 | 1.37 |
| 12 | j7 | 201 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | f7 | 201 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | RA | 201 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | S7 | 201 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | R9 | 201 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | T9 | 302 | CYC | CHB-C4A | 3.46 | 1.48 | 1.40 |
| 12 | G7 | 201 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | DA | 201 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | D9 | 201 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | J2 | 201 | CYC | CHB-C4A | 3.46 | 1.48 | 1.40 |
| 12 | J6 | 201 | CYC | CHB-C4A | 3.46 | 1.48 | 1.40 |
| 12 | R7 | 201 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | Y5 | 201 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | q7 | 201 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | B5 | 201 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | V3 | 202 | CYC | CHB-C4A | 3.46 | 1.48 | 1.40 |
| 12 | V1 | 202 | CYC | CHB-C4A | 3.46 | 1.48 | 1.40 |
| 12 | X3 | 202 | CYC | CHB-C4A | 3.46 | 1.48 | 1.40 |
| 12 | X1 | 202 | CYC | CHB-C4A | 3.46 | 1.48 | 1.40 |
| 12 | VA | 201 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | J3 | 202 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | V9 | 201 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | aA | 901 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | S4 | 202 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | I7 | 201 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | RA | 202 | CYC | CHB-C4A | 3.46 | 1.48 | 1.40 |
| 12 | R9 | 202 | CYC | CHB-C4A | 3.46 | 1.48 | 1.40 |
| 12 | TA | 301 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | T9 | 301 | CYC | C3D-C2D | 3.46 | 1.47 | 1.37 |
| 12 | D3 | 201 | CYC | CHB-C4A | 3.45 | 1.48 | 1.40 |
| 12 | D1 | 201 | CYC | CHB-C4A | 3.45 | 1.48 | 1.40 |
| 12 | W4 | 202 | CYC | CHB-C4A | 3.45 | 1.48 | 1.40 |
| 12 | W8 | 202 | CYC | CHB-C4A | 3.45 | 1.48 | 1.40 |
| 12 | B8 | 202 | CYC | C3D-C2D | 3.45 | 1.47 | 1.37 |
| 12 | U4 | 202 | CYC | CHB-C4A | 3.45 | 1.48 | 1.40 |
| 12 | U8 | 202 | CYC | CHB-C4A | 3.45 | 1.48 | 1.40 |
| 12 | D5 | 201 | CYC | C3D-C2D | 3.45 | 1.47 | 1.37 |
| 12 | H2 | 201 | CYC | C3D-C2D | 3.45 | 1.47 | 1.37 |
| 12 | H6 | 201 | CYC | C3D-C2D | 3.45 | 1.47 | 1.37 |
| 12 | M8 | 301 | CYC | C3D-C2D | 3.45 | 1.47 | 1.37 |
| 12 | J5 | 201 | CYC | C3D-C2D | 3.45 | 1.47 | 1.37 |
| 12 | S5 | 201 | CYC | C3D-C2D | 3.45 | 1.47 | 1.37 |
| 12 | B4 | 202 | CYC | C3D-C2D | 3.45 | 1.47 | 1.37 |
| 12 | L6 | 201 | CYC | C3D-C2D | 3.45 | 1.47 | 1.37 |
| 12 | e5 | 201 | CYC | C3D-C2D | 3.45 | 1.47 | 1.37 |
| 12 | P7 | 201 | CYC | C3D-C2D | 3.45 | 1.47 | 1.37 |
| 12 | k5 | 1202 | CYC | C1C-NC | -3.45 | 1.33 | 1.37 |
| 12 | f7 | 201 | CYC | C1C-NC | -3.45 | 1.33 | 1.37 |
| 12 | LA | 202 | CYC | C3D-C2D | 3.45 | 1.47 | 1.37 |
| 12 | L9 | 202 | CYC | C3D-C2D | 3.45 | 1.47 | 1.37 |
| 12 | aA | 902 | CYC | C3D-C2D | 3.45 | 1.47 | 1.37 |
| 12 | k5 | 1202 | CYC | C3D-C2D | 3.45 | 1.47 | 1.37 |
| 12 | O5 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | T5 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | N5 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | P1 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | L2 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | P3 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | g7 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | M8 | 302 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | F2 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | V7 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | s7 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | L7 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | M4 | 301 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 12 | D4 | 202 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | D8 | 202 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | V3 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | V1 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | W4 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | U5 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | W8 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | F6 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | m7 | 201 | CYC | C3D-C2D | 3.44 | 1.47 | 1.37 |
| 12 | D9 | 202 | CYC | CHB-C4A | 3.43 | 1.48 | 1.40 |
| 12 | H3 | 202 | CYC | C3D-C2D | 3.43 | 1.47 | 1.37 |
| 12 | L5 | 201 | CYC | C3D-C2D | 3.43 | 1.47 | 1.37 |
| 12 | BA | 201 | CYC | C3D-C2D | 3.43 | 1.47 | 1.37 |
| 12 | C7 | 201 | CYC | C3D-C2D | 3.43 | 1.47 | 1.37 |
| 12 | B9 | 201 | CYC | C3D-C2D | 3.43 | 1.47 | 1.37 |
| 12 | d5 | 201 | CYC | C3D-C2D | 3.43 | 1.47 | 1.37 |
| 12 | DA | 202 | CYC | CHB-C4A | 3.43 | 1.48 | 1.40 |
| 12 | F7 | 201 | CYC | C3D-C2D | 3.43 | 1.47 | 1.37 |
| 12 | F6 | 202 | CYC | CHB-C4A | 3.43 | 1.48 | 1.40 |
| 12 | F2 | 202 | CYC | CHB-C4A | 3.43 | 1.48 | 1.40 |
| 12 | j5 | 1202 | CYC | C3D-C2D | 3.43 | 1.47 | 1.37 |
| 12 | Z8 | 301 | CYC | C3D-C2D | 3.43 | 1.47 | 1.37 |
| 12 | T7 | 201 | CYC | C3D-C2D | 3.43 | 1.47 | 1.37 |
| 12 | F5 | 201 | CYC | C3D-C2D | 3.42 | 1.47 | 1.37 |
| 12 | TA | 302 | CYC | CHB-C4A | 3.42 | 1.48 | 1.40 |
| 12 | R1 | 201 | CYC | C3D-C2D | 3.42 | 1.47 | 1.37 |
| 12 | R3 | 201 | CYC | C3D-C2D | 3.42 | 1.47 | 1.37 |
| 12 | ZA | 201 | CYC | CHB-C4A | 3.42 | 1.48 | 1.40 |
| 12 | Z9 | 201 | CYC | CHB-C4A | 3.42 | 1.48 | 1.40 |
| 12 | H1 | 201 | CYC | C3D-C2D | 3.42 | 1.47 | 1.37 |
| 12 | X5 | 201 | CYC | C3D-C2D | 3.42 | 1.47 | 1.37 |
| 12 | p7 | 201 | CYC | C3D-C2D | 3.42 | 1.47 | 1.37 |
| 12 | D7 | 201 | CYC | C3D-C2D | 3.42 | 1.47 | 1.37 |
| 12 | J7 | 201 | CYC | C3D-C2D | 3.42 | 1.47 | 1.37 |
| 12 | a5 | 201 | CYC | C3D-C2D | 3.42 | 1.47 | 1.37 |
| 12 | J2 | 202 | CYC | C3D-C2D | 3.41 | 1.47 | 1.37 |
| 12 | k5 | 1203 | CYC | C3D-C2D | 3.41 | 1.47 | 1.37 |
| 12 | v7 | 201 | CYC | C3D-C2D | 3.41 | 1.47 | 1.37 |
| 12 | r7 | 201 | CYC | C3D-C2D | 3.41 | 1.47 | 1.37 |
| 12 | H9 | 202 | CYC | C3D-C2D | 3.41 | 1.47 | 1.37 |
| 12 | H7 | 201 | CYC | C3D-C2D | 3.41 | 1.47 | 1.37 |
| 12 | HA | 202 | CYC | C3D-C2D | 3.40 | 1.47 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | L4 | 202 | CYC | C3D-C2D | 3.40 | 1.47 | 1.37 |
| 12 | JA | 202 | CYC | C3D-C2D | 3.40 | 1.47 | 1.37 |
| 12 | J9 | 202 | CYC | C3D-C2D | 3.40 | 1.47 | 1.37 |
| 12 | B1 | 202 | CYC | C3D-C2D | 3.40 | 1.47 | 1.37 |
| 12 | BA | 201 | CYC | CHB-C4A | 3.40 | 1.48 | 1.40 |
| 12 | B9 | 201 | CYC | CHB-C4A | 3.40 | 1.48 | 1.40 |
| 12 | N6 | 101 | CYC | C3D-C2D | 3.40 | 1.47 | 1.37 |
| 12 | B7 | 201 | CYC | C3D-C2D | 3.40 | 1.47 | 1.37 |
| 12 | h7 | 201 | CYC | C3D-C2D | 3.39 | 1.47 | 1.37 |
| 12 | F3 | 201 | CYC | C3D-C2D | 3.39 | 1.47 | 1.37 |
| 12 | F1 | 201 | CYC | C3D-C2D | 3.39 | 1.47 | 1.37 |
| 12 | k5 | 1204 | CYC | C3D-C2D | 3.39 | 1.47 | 1.37 |
| 12 | N2 | 101 | CYC | C3D-C2D | 3.39 | 1.47 | 1.37 |
| 12 | B3 | 202 | CYC | C3D-C2D | 3.39 | 1.47 | 1.37 |
| 12 | R5 | 201 | CYC | C3D-C2D | 3.39 | 1.47 | 1.37 |
| 12 | U4 | 201 | CYC | C3D-C2D | 3.39 | 1.47 | 1.37 |
| 12 | U8 | 201 | CYC | C3D-C2D | 3.39 | 1.47 | 1.37 |
| 12 | C5 | 201 | CYC | C3D-C2D | 3.39 | 1.47 | 1.37 |
| 12 | Z3 | 202 | CYC | CHB-C4A | 3.39 | 1.48 | 1.40 |
| 12 | Z1 | 201 | CYC | CHB-C4A | 3.39 | 1.48 | 1.40 |
| 12 | D6 | 201 | CYC | C2C-C1C | -3.39 | 1.49 | 1.52 |
| 12 | I5 | 201 | CYC | C3D-C2D | 3.39 | 1.47 | 1.37 |
| 12 | D4 | 202 | CYC | C2C-C1C | -3.39 | 1.49 | 1.52 |
| 12 | D8 | 202 | CYC | C2C-C1C | -3.39 | 1.49 | 1.52 |
| 12 | J6 | 202 | CYC | C3D-C2D | 3.38 | 1.47 | 1.37 |
| 12 | a9 | 901 | CYC | C3D-C2D | 3.38 | 1.47 | 1.37 |
| 12 | b7 | 201 | CYC | C3D-C2D | 3.38 | 1.47 | 1.37 |
| 12 | j5 | 1201 | CYC | C3D-C2D | 3.38 | 1.47 | 1.37 |
| 12 | N7 | 201 | CYC | C3D-C2D | 3.37 | 1.47 | 1.37 |
| 12 | k5 | 1201 | CYC | C3D-C2D | 3.36 | 1.47 | 1.37 |
| 12 | D2 | 201 | CYC | C2C-C1C | -3.36 | 1.49 | 1.52 |
| 12 | H1 | 201 | CYC | CHB-C4A | 3.36 | 1.48 | 1.40 |
| 12 | PA | 201 | CYC | CHB-C4A | 3.36 | 1.48 | 1.40 |
| 12 | P9 | 201 | CYC | CHB-C4A | 3.36 | 1.48 | 1.40 |
| 12 | H3 | 202 | CYC | CHB-C4A | 3.36 | 1.48 | 1.40 |
| 12 | D7 | 201 | CYC | C1C-NC | -3.35 | 1.33 | 1.37 |
| 12 | O4 | 201 | CYC | C3D-C2D | 3.35 | 1.47 | 1.37 |
| 12 | O8 | 201 | CYC | C3D-C2D | 3.35 | 1.47 | 1.37 |
| 12 | J7 | 201 | CYC | C1C-NC | -3.34 | 1.33 | 1.37 |
| 12 | V3 | 201 | CYC | CHB-C4A | 3.34 | 1.48 | 1.40 |
| 12 | V1 | 201 | CYC | CHB-C4A | 3.34 | 1.48 | 1.40 |
| 12 | B5 | 201 | CYC | C1C-NC | -3.34 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | Z3 | 201 | CYC | CHB-C4A | 3.33 | 1.48 | 1.40 |
| 12 | Z1 | 202 | CYC | CHB-C4A | 3.33 | 1.48 | 1.40 |
| 12 | T5 | 201 | CYC | C1C-NC | -3.33 | 1.33 | 1.37 |
| 12 | F2 | 201 | CYC | CHB-C4A | 3.32 | 1.48 | 1.40 |
| 12 | ZA | 202 | CYC | CHB-C4A | 3.32 | 1.48 | 1.40 |
| 12 | Z9 | 202 | CYC | CHB-C4A | 3.32 | 1.48 | 1.40 |
| 12 | H5 | 201 | CYC | C1C-NC | -3.32 | 1.33 | 1.37 |
| 12 | D3 | 202 | CYC | CHB-C4A | 3.32 | 1.48 | 1.40 |
| 12 | D1 | 202 | CYC | CHB-C4A | 3.32 | 1.48 | 1.40 |
| 12 | X9 | 201 | CYC | CHB-C4A | 3.31 | 1.48 | 1.40 |
| 12 | DA | 201 | CYC | CHB-C4A | 3.31 | 1.48 | 1.40 |
| 12 | D9 | 201 | CYC | CHB-C4A | 3.31 | 1.48 | 1.40 |
| 12 | D4 | 202 | CYC | CHB-C4A | 3.30 | 1.48 | 1.40 |
| 12 | D8 | 202 | CYC | CHB-C4A | 3.30 | 1.48 | 1.40 |
| 12 | J3 | 202 | CYC | CHB-C4A | 3.29 | 1.48 | 1.40 |
| 12 | aA | 901 | CYC | CHB-C4A | 3.29 | 1.48 | 1.40 |
| 12 | VA | 201 | CYC | CHB-C4A | 3.29 | 1.48 | 1.40 |
| 12 | V9 | 201 | CYC | CHB-C4A | 3.29 | 1.48 | 1.40 |
| 12 | N2 | 101 | CYC | CHB-C4A | 3.28 | 1.48 | 1.40 |
| 12 | N6 | 101 | CYC | CHB-C4A | 3.28 | 1.48 | 1.40 |
| 12 | XA | 201 | CYC | CHB-C4A | 3.28 | 1.48 | 1.40 |
| 12 | R1 | 201 | CYC | CHB-C4A | 3.28 | 1.48 | 1.40 |
| 12 | R3 | 201 | CYC | CHB-C4A | 3.28 | 1.48 | 1.40 |
| 12 | N5 | 201 | CYC | C1C-NC | -3.28 | 1.33 | 1.37 |
| 12 | O4 | 201 | CYC | CHB-C4A | 3.28 | 1.48 | 1.40 |
| 12 | O8 | 201 | CYC | CHB-C4A | 3.28 | 1.48 | 1.40 |
| 12 | Z3 | 202 | CYC | C1C-NC | -3.28 | 1.33 | 1.37 |
| 12 | Z1 | 201 | CYC | C1C-NC | -3.28 | 1.33 | 1.37 |
| 12 | r7 | 201 | CYC | C1C-NC | -3.27 | 1.33 | 1.37 |
| 12 | W4 | 201 | CYC | CHB-C4A | 3.27 | 1.48 | 1.40 |
| 12 | W8 | 201 | CYC | CHB-C4A | 3.27 | 1.48 | 1.40 |
| 12 | d5 | 201 | CYC | C1C-NC | -3.27 | 1.33 | 1.37 |
| 12 | LA | 202 | CYC | CHB-C4A | 3.27 | 1.48 | 1.40 |
| 12 | L9 | 202 | CYC | CHB-C4A | 3.27 | 1.48 | 1.40 |
| 12 | N7 | 201 | CYC | C1C-NC | -3.27 | 1.33 | 1.37 |
| 12 | F6 | 201 | CYC | CHB-C4A | 3.27 | 1.48 | 1.40 |
| 12 | J6 | 202 | CYC | CHB-C4A | 3.26 | 1.48 | 1.40 |
| 12 | Z | 201 | CYC | C1C-NC | -3.26 | 1.33 | 1.37 |
| 12 | FA | 301 | CYC | CHB-C4A | 3.26 | 1.48 | 1.40 |
| 12 | F9 | 301 | CYC | CHB-C4A | 3.26 | 1.48 | 1.40 |
| 12 | F7 | 201 | CYC | C1C-NC | -3.26 | 1.33 | 1.37 |
| 12 | J2 | 202 | CYC | CHB-C4A | 3.26 | 1.48 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | JA | 202 | CYC | CHB-C4A | 3.25 | 1.48 | 1.40 |
| 12 | J9 | 202 | CYC | CHB-C4A | 3.25 | 1.48 | 1.40 |
| 12 | A | 201 | CYC | C1C-NC | -3.25 | 1.33 | 1.37 |
| 12 | L7 | 201 | CYC | C1C-NC | -3.25 | 1.33 | 1.37 |
| 12 | L2 | 201 | CYC | CHB-C4A | 3.25 | 1.48 | 1.40 |
| 12 | h7 | 201 | CYC | C1C-NC | -3.25 | 1.33 | 1.37 |
| 12 | M8 | 302 | CYC | CHB-C4A | 3.25 | 1.48 | 1.40 |
| 12 | U4 | 201 | CYC | CHB-C4A | 3.25 | 1.48 | 1.40 |
| 12 | U8 | 201 | CYC | CHB-C4A | 3.25 | 1.48 | 1.40 |
| 12 | TA | 301 | CYC | CHB-C4A | 3.25 | 1.48 | 1.40 |
| 12 | L3 | 202 | CYC | CHB-C4A | 3.25 | 1.48 | 1.40 |
| 12 | T9 | 301 | CYC | CHB-C4A | 3.25 | 1.48 | 1.40 |
| 12 | aA | 902 | CYC | CHB-C4A | 3.25 | 1.48 | 1.40 |
| 12 | L6 | 201 | CYC | CHB-C4A | 3.25 | 1.48 | 1.40 |
| 12 | H4 | 201 | CYC | CHB-C4A | 3.24 | 1.48 | 1.40 |
| 12 | H8 | 201 | CYC | CHB-C4A | 3.24 | 1.48 | 1.40 |
| 12 | B3 | 202 | CYC | CHB-C4A | 3.24 | 1.48 | 1.40 |
| 12 | F4 | 202 | CYC | CHB-C4A | 3.24 | 1.48 | 1.40 |
| 12 | F8 | 202 | CYC | CHB-C4A | 3.24 | 1.48 | 1.40 |
| 12 | DA | 201 | CYC | C2C-C1C | -3.24 | 1.49 | 1.52 |
| 12 | D9 | 201 | CYC | C2C-C1C | -3.24 | 1.49 | 1.52 |
| 12 | B1 | 202 | CYC | CHB-C4A | 3.24 | 1.48 | 1.40 |
| 12 | B8 | 202 | CYC | C2C-C1C | -3.24 | 1.49 | 1.52 |
| 12 | M8 | 301 | CYC | CHB-C4A | 3.24 | 1.48 | 1.40 |
| 12 | M4 | 301 | CYC | CHB-C4A | 3.24 | 1.48 | 1.40 |
| 12 | D2 | 202 | CYC | C3D-C2D | 3.24 | 1.47 | 1.37 |
| 12 | DA | 202 | CYC | C1C-NC | -3.23 | 1.33 | 1.37 |
| 12 | D9 | 202 | CYC | C1C-NC | -3.23 | 1.33 | 1.37 |
| 12 | H2 | 201 | CYC | CHB-C4A | 3.23 | 1.48 | 1.40 |
| 12 | T3 | 301 | CYC | CHB-C4A | 3.23 | 1.48 | 1.40 |
| 12 | T1 | 301 | CYC | CHB-C4A | 3.23 | 1.48 | 1.40 |
| 12 | X3 | 201 | CYC | CHB-C4A | 3.23 | 1.48 | 1.40 |
| 12 | X1 | 201 | CYC | CHB-C4A | 3.23 | 1.48 | 1.40 |
| 12 | S4 | 202 | CYC | CHB-C4A | 3.23 | 1.48 | 1.40 |
| 12 | Z4 | 301 | CYC | C2C-C1C | -3.23 | 1.49 | 1.52 |
| 12 | B8 | 202 | CYC | CHB-C4A | 3.23 | 1.48 | 1.40 |
| 12 | EA | 201 | CYC | C3D-C2D | 3.23 | 1.47 | 1.37 |
| 12 | E9 | 201 | CYC | C3D-C2D | 3.23 | 1.47 | 1.37 |
| 12 | B4 | 202 | CYC | CHB-C4A | 3.23 | 1.48 | 1.40 |
| 12 | L5 | 201 | CYC | C1C-NC | -3.22 | 1.33 | 1.37 |
| 12 | H6 | 201 | CYC | CHB-C4A | 3.22 | 1.48 | 1.40 |
| 12 | RA | 201 | CYC | CHB-C4A | 3.21 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | R9 | 201 | CYC | CHB-C4A | 3.21 | 1.47 | 1.40 |
| 12 | L2 | 202 | CYC | C1C-NC | -3.21 | 1.33 | 1.37 |
| 12 | B7 | 201 | CYC | C1C-NC | -3.21 | 1.33 | 1.37 |
| 12 | Z3 | 202 | CYC | C3D-C2D | 3.21 | 1.47 | 1.37 |
| 12 | Z1 | 201 | CYC | C3D-C2D | 3.21 | 1.47 | 1.37 |
| 12 | J4 | 201 | CYC | CHB-C4A | 3.21 | 1.47 | 1.40 |
| 12 | J8 | 201 | CYC | CHB-C4A | 3.21 | 1.47 | 1.40 |
| 12 | P1 | 202 | CYC | OB-C4B | 3.21 | 1.29 | 1.23 |
| 12 | P3 | 202 | CYC | OB-C4B | 3.21 | 1.29 | 1.23 |
| 12 | HA | 202 | CYC | CHB-C4A | 3.21 | 1.47 | 1.40 |
| 12 | k5 | 1203 | CYC | C1C-NC | -3.21 | 1.33 | 1.37 |
| 12 | R7 | 201 | CYC | C1C-NC | -3.21 | 1.33 | 1.37 |
| 12 | Z8 | 301 | CYC | C2C-C1C | -3.20 | 1.49 | 1.52 |
| 12 | W4 | 202 | CYC | C1C-NC | -3.20 | 1.33 | 1.37 |
| 12 | W8 | 202 | CYC | C1C-NC | -3.20 | 1.33 | 1.37 |
| 12 | Z8 | 301 | CYC | CHB-C4A | 3.20 | 1.47 | 1.40 |
| 12 | F5 | 201 | CYC | C1C-NC | -3.20 | 1.33 | 1.37 |
| 12 | R4 | 201 | CYC | C3D-C2D | 3.20 | 1.47 | 1.37 |
| 12 | R8 | 201 | CYC | C3D-C2D | 3.20 | 1.47 | 1.37 |
| 12 | P1 | 202 | CYC | C1C-NC | -3.20 | 1.33 | 1.37 |
| 12 | P7 | 201 | CYC | C1C-NC | -3.20 | 1.33 | 1.37 |
| 12 | D2 | 201 | CYC | CHB-C4A | 3.19 | 1.47 | 1.40 |
| 12 | D9 | 202 | CYC | OB-C4B | 3.19 | 1.29 | 1.23 |
| 12 | H9 | 202 | CYC | CHB-C4A | 3.19 | 1.47 | 1.40 |
| 12 | D6 | 202 | CYC | C3D-C2D | 3.19 | 1.47 | 1.37 |
| 12 | H3 | 201 | CYC | C3D-C2D | 3.19 | 1.47 | 1.37 |
| 12 | H1 | 202 | CYC | C3D-C2D | 3.19 | 1.47 | 1.37 |
| 12 | JA | 201 | CYC | OB-C4B | 3.19 | 1.29 | 1.23 |
| 12 | J9 | 201 | CYC | OB-C4B | 3.19 | 1.29 | 1.23 |
| 12 | Q4 | 201 | CYC | C3D-C2D | 3.19 | 1.47 | 1.37 |
| 12 | D9 | 202 | CYC | C3D-C2D | 3.18 | 1.47 | 1.37 |
| 12 | L9 | 201 | CYC | C3D-C2D | 3.18 | 1.47 | 1.37 |
| 12 | F3 | 201 | CYC | CHB-C4A | 3.18 | 1.47 | 1.40 |
| 12 | F1 | 201 | CYC | CHB-C4A | 3.18 | 1.47 | 1.40 |
| 12 | Z5 | 201 | CYC | C1C-NC | -3.18 | 1.33 | 1.37 |
| 12 | H7 | 201 | CYC | C1C-NC | -3.18 | 1.33 | 1.37 |
| 12 | D4 | 201 | CYC | C3D-C2D | 3.18 | 1.47 | 1.37 |
| 12 | D8 | 201 | CYC | C3D-C2D | 3.18 | 1.47 | 1.37 |
| 12 | D3 | 201 | CYC | C1C-NC | -3.18 | 1.33 | 1.37 |
| 12 | D1 | 201 | CYC | C1C-NC | -3.18 | 1.33 | 1.37 |
| 12 | Q8 | 201 | CYC | C3D-C2D | 3.18 | 1.47 | 1.37 |
| 12 | b7 | 201 | CYC | C1C-NC | -3.18 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | E6 | 201 | CYC | C3D-C2D | 3.18 | 1.47 | 1.37 |
| 12 | BA | 202 | CYC | OB-C4B | 3.18 | 1.29 | 1.23 |
| 12 | B9 | 202 | CYC | OB-C4B | 3.18 | 1.29 | 1.23 |
| 12 | O4 | 202 | CYC | OB-C4B | 3.18 | 1.29 | 1.23 |
| 12 | O8 | 202 | CYC | OB-C4B | 3.18 | 1.29 | 1.23 |
| 12 | J4 | 202 | CYC | C1C-NC | -3.18 | 1.33 | 1.37 |
| 12 | J8 | 202 | CYC | C1C-NC | -3.18 | 1.33 | 1.37 |
| 12 | VA | 202 | CYC | C3D-C2D | 3.18 | 1.47 | 1.37 |
| 12 | V9 | 202 | CYC | C3D-C2D | 3.18 | 1.47 | 1.37 |
| 12 | LA | 201 | CYC | C1C-NC | -3.18 | 1.33 | 1.37 |
| 12 | L9 | 201 | CYC | C1C-NC | -3.18 | 1.33 | 1.37 |
| 12 | Y8 | 201 | CYC | C3D-C2D | 3.17 | 1.47 | 1.37 |
| 12 | d7 | 201 | CYC | C1C-NC | -3.17 | 1.33 | 1.37 |
| 12 | Y3 | 201 | CYC | C3D-C2D | 3.17 | 1.47 | 1.37 |
| 12 | Y1 | 201 | CYC | C3D-C2D | 3.17 | 1.47 | 1.37 |
| 12 | S1 | 201 | CYC | C3D-C2D | 3.17 | 1.47 | 1.37 |
| 12 | S3 | 201 | CYC | C3D-C2D | 3.17 | 1.47 | 1.37 |
| 12 | B4 | 201 | CYC | OB-C4B | 3.17 | 1.29 | 1.23 |
| 12 | B8 | 201 | CYC | OB-C4B | 3.17 | 1.29 | 1.23 |
| 12 | E2 | 201 | CYC | C3D-C2D | 3.17 | 1.47 | 1.37 |
| 12 | H4 | 202 | CYC | C3D-C2D | 3.17 | 1.47 | 1.37 |
| 12 | L6 | 202 | CYC | C1C-NC | -3.17 | 1.33 | 1.37 |
| 12 | LA | 201 | CYC | C3D-C2D | 3.17 | 1.47 | 1.37 |
| 12 | j7 | 201 | CYC | C1C-NC | -3.17 | 1.33 | 1.37 |
| 12 | C3 | 201 | CYC | C3D-C2D | 3.17 | 1.47 | 1.37 |
| 12 | C1 | 201 | CYC | C3D-C2D | 3.17 | 1.47 | 1.37 |
| 12 | DA | 202 | CYC | C3D-C2D | 3.17 | 1.47 | 1.37 |
| 12 | RA | 202 | CYC | C1C-NC | -3.17 | 1.33 | 1.37 |
| 12 | R9 | 202 | CYC | C1C-NC | -3.17 | 1.33 | 1.37 |
| 12 | I2 | 201 | CYC | OB-C4B | 3.17 | 1.29 | 1.23 |
| 12 | D3 | 201 | CYC | C3D-C2D | 3.17 | 1.47 | 1.37 |
| 12 | D1 | 201 | CYC | C3D-C2D | 3.17 | 1.47 | 1.37 |
| 12 | D6 | 201 | CYC | CHB-C4A | 3.17 | 1.47 | 1.40 |
| 12 | P3 | 202 | CYC | C1C-NC | -3.17 | 1.33 | 1.37 |
| 12 | K4 | 201 | CYC | C3D-C2D | 3.16 | 1.47 | 1.37 |
| 12 | K8 | 201 | CYC | C3D-C2D | 3.16 | 1.47 | 1.37 |
| 12 | A1 | 201 | CYC | C3D-C2D | 3.16 | 1.47 | 1.37 |
| 12 | A3 | 201 | CYC | C3D-C2D | 3.16 | 1.47 | 1.37 |
| 12 | XA | 202 | CYC | OB-C4B | 3.16 | 1.29 | 1.23 |
| 12 | X9 | 202 | CYC | OB-C4B | 3.16 | 1.29 | 1.23 |
| 12 | L4 | 201 | CYC | C1C-NC | -3.16 | 1.33 | 1.37 |
| 12 | L8 | 201 | CYC | C1C-NC | -3.16 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | DA | 202 | CYC | OB-C4B | 3.16 | 1.29 | 1.23 |
| 12 | P1 | 201 | CYC | CHB-C4A | 3.16 | 1.47 | 1.40 |
| 12 | P3 | 201 | CYC | CHB-C4A | 3.16 | 1.47 | 1.40 |
| 12 | TA | 302 | CYC | C3D-C2D | 3.16 | 1.47 | 1.37 |
| 12 | T9 | 302 | CYC | C3D-C2D | 3.16 | 1.47 | 1.37 |
| 12 | Z4 | 301 | CYC | CHB-C4A | 3.16 | 1.47 | 1.40 |
| 12 | IA | 201 | CYC | C3D-C2D | 3.16 | 1.47 | 1.37 |
| 12 | I9 | 201 | CYC | C3D-C2D | 3.16 | 1.47 | 1.37 |
| 12 | Y4 | 201 | CYC | OB-C4B | 3.15 | 1.29 | 1.23 |
| 12 | Q8 | 201 | CYC | OB-C4B | 3.15 | 1.29 | 1.23 |
| 12 | Y8 | 201 | CYC | OB-C4B | 3.15 | 1.29 | 1.23 |
| 12 | E4 | 201 | CYC | C3D-C2D | 3.15 | 1.47 | 1.37 |
| 12 | E8 | 201 | CYC | C3D-C2D | 3.15 | 1.47 | 1.37 |
| 12 | Y4 | 201 | CYC | C3D-C2D | 3.15 | 1.47 | 1.37 |
| 12 | p7 | 201 | CYC | C1C-NC | -3.15 | 1.33 | 1.37 |
| 12 | PA | 202 | CYC | C3D-C2D | 3.15 | 1.47 | 1.37 |
| 12 | P9 | 202 | CYC | C3D-C2D | 3.15 | 1.47 | 1.37 |
| 12 | j5 | 1202 | CYC | C1C-NC | -3.15 | 1.33 | 1.37 |
| 12 | SA | 201 | CYC | C3D-C2D | 3.15 | 1.47 | 1.37 |
| 12 | S9 | 201 | CYC | C3D-C2D | 3.15 | 1.47 | 1.37 |
| 12 | G3 | 201 | CYC | C3D-C2D | 3.15 | 1.47 | 1.37 |
| 12 | G1 | 201 | CYC | C3D-C2D | 3.15 | 1.47 | 1.37 |
| 12 | H8 | 202 | CYC | C3D-C2D | 3.15 | 1.47 | 1.37 |
| 12 | B3 | 201 | CYC | C3D-C2D | 3.15 | 1.47 | 1.37 |
| 12 | B1 | 201 | CYC | C3D-C2D | 3.15 | 1.47 | 1.37 |
| 12 | P1 | 201 | CYC | C2C-C1C | -3.14 | 1.49 | 1.52 |
| 12 | P3 | 201 | CYC | C2C-C1C | -3.14 | 1.49 | 1.52 |
| 12 | U4 | 202 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | U8 | 202 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | N4 | 201 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | N8 | 201 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | J8 | 201 | CYC | C2C-C1C | -3.14 | 1.49 | 1.52 |
| 12 | d5 | 201 | CYC | C2C-C1C | -3.14 | 1.49 | 1.52 |
| 12 | D4 | 201 | CYC | OB-C4B | 3.14 | 1.29 | 1.23 |
| 12 | I6 | 201 | CYC | OB-C4B | 3.14 | 1.29 | 1.23 |
| 12 | D8 | 201 | CYC | OB-C4B | 3.14 | 1.29 | 1.23 |
| 12 | A4 | 201 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | A8 | 201 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | U4 | 202 | CYC | C1C-NC | -3.14 | 1.33 | 1.37 |
| 12 | U8 | 202 | CYC | C1C-NC | -3.14 | 1.33 | 1.37 |
| 12 | CA | 201 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | C9 | 201 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | L4 | 202 | CYC | CHB-C4A | 3.14 | 1.47 | 1.40 |
| 12 | W3 | 201 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | W1 | 201 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | f5 | 201 | CYC | C1C-NC | -3.14 | 1.33 | 1.37 |
| 12 | ZA | 202 | CYC | C2C-C1C | -3.14 | 1.49 | 1.52 |
| 12 | Z9 | 202 | CYC | C2C-C1C | -3.14 | 1.49 | 1.52 |
| 12 | F4 | 201 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | F8 | 201 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | V3 | 202 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | V1 | 202 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | I3 | 201 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | I1 | 201 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | E3 | 201 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | G8 | 201 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | BA | 202 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | B9 | 202 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | H2 | 202 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | H6 | 202 | CYC | C3D-C2D | 3.14 | 1.47 | 1.37 |
| 12 | XA | 202 | CYC | C1C-NC | -3.13 | 1.33 | 1.37 |
| 12 | X9 | 202 | CYC | C1C-NC | -3.13 | 1.33 | 1.37 |
| 12 | YA | 201 | CYC | C3D-C2D | 3.13 | 1.47 | 1.37 |
| 12 | Y9 | 201 | CYC | C3D-C2D | 3.13 | 1.47 | 1.37 |
| 12 | J6 | 202 | CYC | C2C-C1C | -3.13 | 1.49 | 1.52 |
| 12 | B6 | 201 | CYC | C3D-C2D | 3.13 | 1.47 | 1.37 |
| 12 | D4 | 201 | CYC | C1C-NC | -3.13 | 1.33 | 1.37 |
| 12 | a9 | 901 | CYC | CHB-C4A | 3.13 | 1.47 | 1.40 |
| 12 | S4 | 201 | CYC | OB-C4B | 3.13 | 1.29 | 1.23 |
| 12 | S8 | 201 | CYC | OB-C4B | 3.13 | 1.29 | 1.23 |
| 12 | Q3 | 201 | CYC | C3D-C2D | 3.13 | 1.46 | 1.37 |
| 12 | X9 | 202 | CYC | C3D-C2D | 3.13 | 1.46 | 1.37 |
| 12 | B2 | 201 | CYC | C3D-C2D | 3.13 | 1.46 | 1.37 |
| 12 | K3 | 201 | CYC | C3D-C2D | 3.13 | 1.46 | 1.37 |
| 12 | K1 | 201 | CYC | C3D-C2D | 3.13 | 1.46 | 1.37 |
| 12 | R1 | 202 | CYC | C3D-C2D | 3.13 | 1.46 | 1.37 |
| 12 | R3 | 202 | CYC | C3D-C2D | 3.13 | 1.46 | 1.37 |
| 12 | L3 | 201 | CYC | C1C-NC | -3.13 | 1.33 | 1.37 |
| 12 | L1 | 201 | CYC | C1C-NC | -3.13 | 1.33 | 1.37 |
| 12 | W4 | 201 | CYC | C2C-C1C | -3.12 | 1.49 | 1.52 |
| 12 | W8 | 201 | CYC | C2C-C1C | -3.12 | 1.49 | 1.52 |
| 12 | Q4 | 201 | CYC | OB-C4B | 3.12 | 1.29 | 1.23 |
| 12 | J4 | 201 | CYC | C2C-C1C | -3.12 | 1.49 | 1.52 |
| 12 | WA | 201 | CYC | C3D-C2D | 3.12 | 1.46 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | W9 | 201 | CYC | C3D-C2D | 3.12 | 1.46 | 1.37 |
| 12 | D6 | 202 | CYC | OB-C4B | 3.12 | 1.29 | 1.23 |
| 12 | D2 | 202 | CYC | OB-C4B | 3.12 | 1.29 | 1.23 |
| 12 | v7 | 201 | CYC | C1C-NC | -3.12 | 1.33 | 1.37 |
| 12 | D5 | 201 | CYC | C1C-NC | -3.12 | 1.33 | 1.37 |
| 12 | F2 | 202 | CYC | C3D-C2D | 3.12 | 1.46 | 1.37 |
| 12 | W4 | 202 | CYC | C3D-C2D | 3.12 | 1.46 | 1.37 |
| 12 | W8 | 202 | CYC | C3D-C2D | 3.12 | 1.46 | 1.37 |
| 12 | U3 | 201 | CYC | C3D-C2D | 3.12 | 1.46 | 1.37 |
| 12 | U1 | 201 | CYC | C3D-C2D | 3.12 | 1.46 | 1.37 |
| 12 | E1 | 201 | CYC | C3D-C2D | 3.12 | 1.46 | 1.37 |
| 12 | RA | 202 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | R9 | 202 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | XA | 202 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | B1 | 202 | CYC | C2C-C1C | -3.11 | 1.49 | 1.52 |
| 12 | Y4 | 201 | CYC | C1C-NC | -3.11 | 1.33 | 1.37 |
| 12 | Y8 | 201 | CYC | C1C-NC | -3.11 | 1.33 | 1.37 |
| 12 | UA | 201 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | U9 | 201 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | G4 | 201 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | Q1 | 201 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | X3 | 202 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | A6 | 201 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | K9 | 201 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | X1 | 202 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | A2 | 201 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | b5 | 201 | CYC | C1C-NC | -3.11 | 1.33 | 1.37 |
| 12 | Z5 | 201 | CYC | C2C-C1C | -3.11 | 1.49 | 1.52 |
| 12 | B4 | 201 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | I4 | 201 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | I8 | 201 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | PA | 202 | CYC | OB-C4B | 3.11 | 1.29 | 1.23 |
| 12 | T3 | 302 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | T4 | 201 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | T8 | 201 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | T1 | 302 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | K2 | 201 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | O1 | 201 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | O3 | 201 | CYC | C3D-C2D | 3.11 | 1.46 | 1.37 |
| 12 | B4 | 202 | CYC | C2C-C1C | -3.10 | 1.49 | 1.52 |
| 12 | B8 | 201 | CYC | C3D-C2D | 3.10 | 1.46 | 1.37 |
| 12 | KA | 201 | CYC | C3D-C2D | 3.10 | 1.46 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | O4 | 202 | CYC | C3D-C2D | 3.10 | 1.46 | 1.37 |
| 12 | O8 | 202 | CYC | C3D-C2D | 3.10 | 1.46 | 1.37 |
| 12 | F9 | 302 | CYC | C3D-C2D | 3.10 | 1.46 | 1.37 |
| 12 | K6 | 201 | CYC | C3D-C2D | 3.10 | 1.46 | 1.37 |
| 12 | J4 | 202 | CYC | C3D-C2D | 3.10 | 1.46 | 1.37 |
| 12 | J8 | 202 | CYC | C3D-C2D | 3.10 | 1.46 | 1.37 |
| 12 | B6 | 201 | CYC | OB-C4B | 3.10 | 1.29 | 1.23 |
| 12 | L8 | 201 | CYC | OB-C4B | 3.10 | 1.29 | 1.23 |
| 12 | H2 | 202 | CYC | C1C-NC | -3.09 | 1.33 | 1.37 |
| 12 | H6 | 202 | CYC | C1C-NC | -3.09 | 1.33 | 1.37 |
| 12 | BA | 202 | CYC | C1C-NC | -3.09 | 1.33 | 1.37 |
| 12 | B9 | 202 | CYC | C1C-NC | -3.09 | 1.33 | 1.37 |
| 12 | D3 | 201 | CYC | OB-C4B | 3.09 | 1.29 | 1.23 |
| 12 | D1 | 201 | CYC | OB-C4B | 3.09 | 1.29 | 1.23 |
| 12 | O4 | 202 | CYC | C1C-NC | -3.09 | 1.33 | 1.37 |
| 12 | O8 | 202 | CYC | C1C-NC | -3.09 | 1.33 | 1.37 |
| 12 | S4 | 202 | CYC | C2C-C1C | -3.09 | 1.49 | 1.52 |
| 12 | H3 | 201 | CYC | C1C-NC | -3.09 | 1.33 | 1.37 |
| 12 | H1 | 202 | CYC | C1C-NC | -3.09 | 1.33 | 1.37 |
| 12 | PA | 201 | CYC | C2C-C1C | -3.09 | 1.49 | 1.52 |
| 12 | V9 | 202 | CYC | C1C-NC | -3.09 | 1.33 | 1.37 |
| 12 | E6 | 201 | CYC | OB-C4B | 3.09 | 1.29 | 1.23 |
| 12 | E2 | 201 | CYC | OB-C4B | 3.09 | 1.29 | 1.23 |
| 12 | ZA | 201 | CYC | C1C-NC | -3.09 | 1.33 | 1.37 |
| 12 | H4 | 202 | CYC | C1C-NC | -3.09 | 1.33 | 1.37 |
| 12 | H8 | 202 | CYC | C1C-NC | -3.09 | 1.33 | 1.37 |
| 12 | L3 | 202 | CYC | C2C-C1C | -3.09 | 1.49 | 1.52 |
| 12 | aA | 902 | CYC | C2C-C1C | -3.09 | 1.49 | 1.52 |
| 12 | B4 | 201 | CYC | C1C-NC | -3.09 | 1.33 | 1.37 |
| 12 | B8 | 201 | CYC | C1C-NC | -3.09 | 1.33 | 1.37 |
| 12 | J6 | 201 | CYC | C3D-C2D | 3.09 | 1.46 | 1.37 |
| 12 | M8 | 302 | CYC | C2C-C1C | -3.09 | 1.49 | 1.52 |
| 12 | J6 | 201 | CYC | C1C-NC | -3.08 | 1.33 | 1.37 |
| 12 | D8 | 201 | CYC | C1C-NC | -3.08 | 1.33 | 1.37 |
| 12 | Z9 | 201 | CYC | C1C-NC | -3.08 | 1.33 | 1.37 |
| 12 | B2 | 201 | CYC | C1C-NC | -3.08 | 1.33 | 1.37 |
| 12 | F9 | 303 | CYC | C3D-C2D | 3.08 | 1.46 | 1.37 |
| 12 | I2 | 201 | CYC | C3D-C2D | 3.08 | 1.46 | 1.37 |
| 12 | LA | 202 | CYC | C2C-C1C | -3.08 | 1.49 | 1.52 |
| 12 | H2 | 201 | CYC | C2C-C1C | -3.08 | 1.49 | 1.52 |
| 12 | D3 | 202 | CYC | C2C-C1C | -3.08 | 1.49 | 1.52 |
| 12 | D1 | 202 | CYC | C2C-C1C | -3.08 | 1.49 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | L9 | 202 | CYC | C2C-C1C | -3.08 | 1.49 | 1.52 |
| 12 | D6 | 202 | CYC | C1C-NC | -3.08 | 1.33 | 1.37 |
| 12 | X4 | 201 | CYC | C3D-C2D | 3.08 | 1.46 | 1.37 |
| 12 | X8 | 201 | CYC | C3D-C2D | 3.08 | 1.46 | 1.37 |
| 12 | C2 | 201 | CYC | C3D-C2D | 3.08 | 1.46 | 1.37 |
| 12 | V7 | 201 | CYC | C1C-NC | -3.08 | 1.33 | 1.37 |
| 12 | F6 | 202 | CYC | C3D-C2D | 3.08 | 1.46 | 1.37 |
| 12 | I3 | 201 | CYC | OB-C4B | 3.08 | 1.29 | 1.23 |
| 12 | F9 | 303 | CYC | OB-C4B | 3.08 | 1.29 | 1.23 |
| 12 | I1 | 201 | CYC | OB-C4B | 3.08 | 1.29 | 1.23 |
| 12 | P1 | 202 | CYC | C3D-C2D | 3.08 | 1.46 | 1.37 |
| 12 | G2 | 201 | CYC | C3D-C2D | 3.08 | 1.46 | 1.37 |
| 12 | G6 | 201 | CYC | C3D-C2D | 3.08 | 1.46 | 1.37 |
| 12 | L3 | 201 | CYC | C3D-C2D | 3.08 | 1.46 | 1.37 |
| 12 | L1 | 201 | CYC | C3D-C2D | 3.08 | 1.46 | 1.37 |
| 12 | B3 | 201 | CYC | OB-C4B | 3.08 | 1.29 | 1.23 |
| 12 | L3 | 201 | CYC | OB-C4B | 3.08 | 1.29 | 1.23 |
| 12 | B1 | 201 | CYC | OB-C4B | 3.08 | 1.29 | 1.23 |
| 12 | L1 | 201 | CYC | OB-C4B | 3.08 | 1.29 | 1.23 |
| 12 | I6 | 201 | CYC | C3D-C2D | 3.08 | 1.46 | 1.37 |
| 12 | ZA | 201 | CYC | C3D-C2D | 3.08 | 1.46 | 1.37 |
| 12 | Z9 | 201 | CYC | C3D-C2D | 3.08 | 1.46 | 1.37 |
| 12 | H4 | 202 | CYC | OB-C4B | 3.08 | 1.29 | 1.23 |
| 12 | H8 | 202 | CYC | OB-C4B | 3.08 | 1.29 | 1.23 |
| 12 | F9 | 302 | CYC | OB-C4B | 3.08 | 1.29 | 1.23 |
| 12 | W4 | 202 | CYC | OB-C4B | 3.08 | 1.29 | 1.23 |
| 12 | W8 | 202 | CYC | OB-C4B | 3.08 | 1.29 | 1.23 |
| 12 | L2 | 202 | CYC | C3D-C2D | 3.08 | 1.46 | 1.37 |
| 12 | L6 | 202 | CYC | C3D-C2D | 3.08 | 1.46 | 1.37 |
| 12 | X5 | 201 | CYC | C1C-NC | -3.08 | 1.33 | 1.37 |
| 12 | J2 | 202 | CYC | C2C-C1C | -3.08 | 1.49 | 1.52 |
| 12 | YA | 201 | CYC | OB-C4B | 3.07 | 1.29 | 1.23 |
| 12 | Y9 | 201 | CYC | OB-C4B | 3.07 | 1.29 | 1.23 |
| 12 | B3 | 202 | CYC | C2C-C1C | -3.07 | 1.49 | 1.52 |
| 12 | V3 | 202 | CYC | OB-C4B | 3.07 | 1.29 | 1.23 |
| 12 | V1 | 202 | CYC | OB-C4B | 3.07 | 1.29 | 1.23 |
| 12 | HA | 201 | CYC | C3D-C2D | 3.07 | 1.46 | 1.37 |
| 12 | H9 | 201 | CYC | C3D-C2D | 3.07 | 1.46 | 1.37 |
| 12 | O4 | 201 | CYC | C2C-C1C | -3.07 | 1.49 | 1.52 |
| 12 | N6 | 101 | CYC | C2C-C1C | -3.07 | 1.49 | 1.52 |
| 12 | O8 | 201 | CYC | C2C-C1C | -3.07 | 1.49 | 1.52 |
| 12 | P4 | 201 | CYC | C3D-C2D | 3.07 | 1.46 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | P8 | 201 | CYC | C3D-C2D | 3.07 | 1.46 | 1.37 |
| 12 | L4 | 201 | CYC | C3D-C2D | 3.07 | 1.46 | 1.37 |
| 12 | L8 | 201 | CYC | C3D-C2D | 3.07 | 1.46 | 1.37 |
| 12 | Z8 | 301 | CYC | C1C-NC | -3.07 | 1.33 | 1.37 |
| 12 | Q8 | 201 | CYC | C1C-NC | -3.07 | 1.33 | 1.37 |
| 12 | J2 | 201 | CYC | C3D-C2D | 3.07 | 1.46 | 1.37 |
| 12 | J5 | 201 | CYC | C1C-NC | -3.07 | 1.33 | 1.37 |
| 12 | G3 | 201 | CYC | OB-C4B | 3.07 | 1.29 | 1.23 |
| 12 | G1 | 201 | CYC | OB-C4B | 3.07 | 1.29 | 1.23 |
| 12 | JA | 201 | CYC | C3D-C2D | 3.06 | 1.46 | 1.37 |
| 12 | J9 | 201 | CYC | C3D-C2D | 3.06 | 1.46 | 1.37 |
| 12 | R1 | 202 | CYC | C1C-NC | -3.06 | 1.33 | 1.37 |
| 12 | R3 | 202 | CYC | C1C-NC | -3.06 | 1.33 | 1.37 |
| 12 | F1 | 202 | CYC | C3D-C2D | 3.06 | 1.46 | 1.37 |
| 12 | L4 | 201 | CYC | OB-C4B | 3.06 | 1.29 | 1.23 |
| 12 | P5 | 201 | CYC | C1C-NC | -3.06 | 1.33 | 1.37 |
| 12 | P9 | 202 | CYC | OB-C4B | 3.06 | 1.29 | 1.23 |
| 12 | GA | 201 | CYC | OB-C4B | 3.06 | 1.29 | 1.23 |
| 12 | G9 | 201 | CYC | OB-C4B | 3.06 | 1.29 | 1.23 |
| 12 | P3 | 202 | CYC | C3D-C2D | 3.06 | 1.46 | 1.37 |
| 12 | VA | 202 | CYC | C1C-NC | -3.06 | 1.33 | 1.37 |
| 12 | Q4 | 201 | CYC | C1C-NC | -3.06 | 1.33 | 1.37 |
| 12 | C4 | 201 | CYC | C3D-C2D | 3.06 | 1.46 | 1.37 |
| 12 | C8 | 201 | CYC | C3D-C2D | 3.06 | 1.46 | 1.37 |
| 12 | C6 | 201 | CYC | C3D-C2D | 3.06 | 1.46 | 1.37 |
| 12 | J4 | 202 | CYC | OB-C4B | 3.06 | 1.29 | 1.23 |
| 12 | J8 | 202 | CYC | OB-C4B | 3.06 | 1.29 | 1.23 |
| 12 | J2 | 201 | CYC | C1C-NC | -3.06 | 1.33 | 1.37 |
| 12 | F6 | 202 | CYC | OB-C4B | 3.06 | 1.29 | 1.23 |
| 12 | AA | 201 | CYC | C3D-C2D | 3.06 | 1.46 | 1.37 |
| 12 | A9 | 201 | CYC | C3D-C2D | 3.06 | 1.46 | 1.37 |
| 12 | Q9 | 201 | CYC | C3D-C2D | 3.06 | 1.46 | 1.37 |
| 12 | V5 | 201 | CYC | C1C-NC | -3.05 | 1.33 | 1.37 |
| 12 | S4 | 201 | CYC | C3D-C2D | 3.05 | 1.46 | 1.37 |
| 12 | S8 | 201 | CYC | C3D-C2D | 3.05 | 1.46 | 1.37 |
| 12 | KA | 201 | CYC | OB-C4B | 3.05 | 1.29 | 1.23 |
| 12 | K9 | 201 | CYC | OB-C4B | 3.05 | 1.29 | 1.23 |
| 12 | B5 | 201 | CYC | C2C-C1C | -3.05 | 1.49 | 1.52 |
| 12 | GA | 201 | CYC | C3D-C2D | 3.05 | 1.46 | 1.37 |
| 12 | G9 | 201 | CYC | C3D-C2D | 3.05 | 1.46 | 1.37 |
| 12 | HA | 201 | CYC | C1C-NC | -3.05 | 1.33 | 1.37 |
| 12 | k5 | 1204 | CYC | C1C-NC | -3.05 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | H9 | 201 | CYC | C1C-NC | -3.05 | 1.33 | 1.37 |
| 12 | F4 | 201 | CYC | OB-C4B | 3.05 | 1.29 | 1.23 |
| 12 | B6 | 201 | CYC | C1C-NC | -3.05 | 1.33 | 1.37 |
| 12 | F3 | 202 | CYC | C3D-C2D | 3.04 | 1.46 | 1.37 |
| 12 | Z3 | 202 | CYC | OB-C4B | 3.04 | 1.29 | 1.23 |
| 12 | Z1 | 201 | CYC | OB-C4B | 3.04 | 1.29 | 1.23 |
| 12 | F8 | 201 | CYC | OB-C4B | 3.04 | 1.29 | 1.23 |
| 12 | J2 | 201 | CYC | OB-C4B | 3.04 | 1.29 | 1.23 |
| 12 | J1 | 201 | CYC | C1C-NC | -3.04 | 1.33 | 1.37 |
| 12 | F2 | 202 | CYC | OB-C4B | 3.04 | 1.29 | 1.23 |
| 12 | J3 | 201 | CYC | C3D-C2D | 3.04 | 1.46 | 1.37 |
| 12 | J1 | 201 | CYC | C3D-C2D | 3.04 | 1.46 | 1.37 |
| 12 | P7 | 201 | CYC | C2C-C1C | -3.04 | 1.49 | 1.52 |
| 12 | OA | 201 | CYC | C3D-C2D | 3.04 | 1.46 | 1.37 |
| 12 | O9 | 201 | CYC | C3D-C2D | 3.04 | 1.46 | 1.37 |
| 12 | R5 | 201 | CYC | C1C-NC | -3.03 | 1.33 | 1.37 |
| 12 | X7 | 201 | CYC | C1C-NC | -3.03 | 1.33 | 1.37 |
| 12 | RA | 201 | CYC | C2C-C1C | -3.03 | 1.49 | 1.52 |
| 12 | H5 | 201 | CYC | C2C-C1C | -3.03 | 1.49 | 1.52 |
| 12 | R9 | 201 | CYC | C2C-C1C | -3.03 | 1.49 | 1.52 |
| 12 | J7 | 201 | CYC | C2C-C1C | -3.03 | 1.49 | 1.52 |
| 12 | K3 | 201 | CYC | OB-C4B | 3.03 | 1.29 | 1.23 |
| 12 | K1 | 201 | CYC | OB-C4B | 3.03 | 1.29 | 1.23 |
| 12 | H2 | 202 | CYC | OB-C4B | 3.03 | 1.29 | 1.23 |
| 12 | T3 | 302 | CYC | OB-C4B | 3.03 | 1.29 | 1.23 |
| 12 | D7 | 201 | CYC | C2C-C1C | -3.03 | 1.49 | 1.52 |
| 12 | E8 | 201 | CYC | OB-C4B | 3.03 | 1.29 | 1.23 |
| 12 | QA | 201 | CYC | C3D-C2D | 3.03 | 1.46 | 1.37 |
| 12 | V3 | 202 | CYC | C1C-NC | -3.03 | 1.33 | 1.37 |
| 12 | F9 | 302 | CYC | C1C-NC | -3.03 | 1.33 | 1.37 |
| 12 | V1 | 202 | CYC | C1C-NC | -3.03 | 1.33 | 1.37 |
| 12 | B2 | 201 | CYC | OB-C4B | 3.03 | 1.29 | 1.23 |
| 12 | W9 | 201 | CYC | OB-C4B | 3.02 | 1.29 | 1.23 |
| 12 | T1 | 302 | CYC | OB-C4B | 3.02 | 1.29 | 1.23 |
| 12 | EA | 201 | CYC | OB-C4B | 3.02 | 1.29 | 1.23 |
| 12 | E9 | 201 | CYC | OB-C4B | 3.02 | 1.29 | 1.23 |
| 12 | S4 | 201 | CYC | C1C-NC | -3.02 | 1.33 | 1.37 |
| 12 | S8 | 201 | CYC | C1C-NC | -3.02 | 1.33 | 1.37 |
| 12 | G4 | 201 | CYC | OB-C4B | 3.01 | 1.29 | 1.23 |
| 12 | G8 | 201 | CYC | OB-C4B | 3.01 | 1.29 | 1.23 |
| 12 | VA | 202 | CYC | OB-C4B | 3.01 | 1.29 | 1.23 |
| 12 | V9 | 202 | CYC | OB-C4B | 3.01 | 1.29 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | D2 | 202 | CYC | C1C-NC | -3.01 | 1.33 | 1.37 |
| 12 | J3 | 202 | CYC | C2C-C1C | -3.01 | 1.49 | 1.52 |
| 12 | aA | 901 | CYC | C2C-C1C | -3.01 | 1.49 | 1.52 |
| 12 | T4 | 201 | CYC | OB-C4B | 3.01 | 1.29 | 1.23 |
| 12 | T8 | 201 | CYC | OB-C4B | 3.01 | 1.29 | 1.23 |
| 12 | I4 | 201 | CYC | OB-C4B | 3.01 | 1.29 | 1.23 |
| 12 | X4 | 201 | CYC | OB-C4B | 3.01 | 1.29 | 1.23 |
| 12 | H6 | 202 | CYC | OB-C4B | 3.01 | 1.29 | 1.23 |
| 12 | X8 | 201 | CYC | OB-C4B | 3.01 | 1.29 | 1.23 |
| 12 | I8 | 201 | CYC | OB-C4B | 3.01 | 1.29 | 1.23 |
| 12 | H3 | 201 | CYC | OB-C4B | 3.01 | 1.29 | 1.23 |
| 12 | H1 | 202 | CYC | OB-C4B | 3.01 | 1.29 | 1.23 |
| 12 | T3 | 301 | CYC | C2C-C1C | -3.01 | 1.49 | 1.52 |
| 12 | T1 | 301 | CYC | C2C-C1C | -3.01 | 1.49 | 1.52 |
| 12 | N8 | 201 | CYC | OB-C4B | 3.00 | 1.29 | 1.23 |
| 12 | F2 | 201 | CYC | C1C-NC | -3.00 | 1.33 | 1.37 |
| 12 | HA | 201 | CYC | OB-C4B | 3.00 | 1.29 | 1.23 |
| 12 | H9 | 201 | CYC | OB-C4B | 3.00 | 1.29 | 1.23 |
| 12 | J3 | 201 | CYC | C1C-NC | -3.00 | 1.33 | 1.37 |
| 12 | J6 | 201 | CYC | OB-C4B | 3.00 | 1.29 | 1.23 |
| 12 | V4 | 201 | CYC | C3D-C2D | 3.00 | 1.46 | 1.37 |
| 12 | SA | 201 | CYC | OB-C4B | 3.00 | 1.29 | 1.23 |
| 12 | S9 | 201 | CYC | OB-C4B | 3.00 | 1.29 | 1.23 |
| 12 | P9 | 201 | CYC | C2C-C1C | -2.99 | 1.49 | 1.52 |
| 12 | WA | 201 | CYC | OB-C4B | 2.99 | 1.29 | 1.23 |
| 12 | C6 | 201 | CYC | OB-C4B | 2.99 | 1.29 | 1.23 |
| 12 | E3 | 201 | CYC | OB-C4B | 2.99 | 1.29 | 1.23 |
| 12 | E1 | 201 | CYC | OB-C4B | 2.99 | 1.29 | 1.23 |
| 12 | Z4 | 301 | CYC | C1C-NC | -2.99 | 1.33 | 1.37 |
| 12 | RA | 202 | CYC | OB-C4B | 2.99 | 1.29 | 1.23 |
| 12 | R9 | 202 | CYC | OB-C4B | 2.99 | 1.29 | 1.23 |
| 12 | E4 | 201 | CYC | OB-C4B | 2.99 | 1.29 | 1.23 |
| 12 | R4 | 201 | CYC | OB-C4B | 2.99 | 1.29 | 1.23 |
| 12 | R8 | 201 | CYC | OB-C4B | 2.99 | 1.29 | 1.23 |
| 12 | V8 | 201 | CYC | C3D-C2D | 2.98 | 1.46 | 1.37 |
| 12 | BA | 201 | CYC | C2C-C1C | -2.98 | 1.49 | 1.52 |
| 12 | B9 | 201 | CYC | C2C-C1C | -2.98 | 1.49 | 1.52 |
| 12 | F9 | 303 | CYC | C1C-NC | -2.98 | 1.33 | 1.37 |
| 12 | IA | 201 | CYC | OB-C4B | 2.98 | 1.29 | 1.23 |
| 12 | I9 | 201 | CYC | OB-C4B | 2.98 | 1.29 | 1.23 |
| 12 | M8 | 301 | CYC | C2C-C1C | -2.98 | 1.49 | 1.52 |
| 12 | JA | 202 | CYC | C1C-NC | -2.98 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | J9 | 202 | CYC | C1C-NC | -2.98 | 1.33 | 1.37 |
| 12 | T1 | 302 | CYC | C1C-NC | -2.98 | 1.33 | 1.37 |
| 12 | M4 | 301 | CYC | C2C-C1C | -2.98 | 1.49 | 1.52 |
| 12 | H9 | 202 | CYC | C2C-C1C | -2.98 | 1.49 | 1.52 |
| 12 | TA | 302 | CYC | C1C-NC | -2.98 | 1.33 | 1.37 |
| 12 | T9 | 302 | CYC | C1C-NC | -2.98 | 1.33 | 1.37 |
| 12 | J3 | 201 | CYC | OB-C4B | 2.97 | 1.29 | 1.23 |
| 12 | U3 | 201 | CYC | OB-C4B | 2.97 | 1.29 | 1.23 |
| 12 | N4 | 201 | CYC | OB-C4B | 2.97 | 1.29 | 1.23 |
| 12 | J1 | 201 | CYC | OB-C4B | 2.97 | 1.29 | 1.23 |
| 12 | U1 | 201 | CYC | OB-C4B | 2.97 | 1.29 | 1.23 |
| 12 | ZA | 202 | CYC | C1C-NC | -2.97 | 1.33 | 1.37 |
| 12 | Z9 | 202 | CYC | C1C-NC | -2.97 | 1.33 | 1.37 |
| 12 | B3 | 201 | CYC | C1C-NC | -2.97 | 1.33 | 1.37 |
| 12 | X3 | 202 | CYC | C1C-NC | -2.97 | 1.33 | 1.37 |
| 12 | B1 | 201 | CYC | C1C-NC | -2.97 | 1.33 | 1.37 |
| 12 | F4 | 201 | CYC | C1C-NC | -2.97 | 1.33 | 1.37 |
| 12 | F8 | 201 | CYC | C1C-NC | -2.97 | 1.33 | 1.37 |
| 12 | X1 | 202 | CYC | C1C-NC | -2.97 | 1.33 | 1.37 |
| 12 | R1 | 202 | CYC | OB-C4B | 2.97 | 1.29 | 1.23 |
| 12 | R3 | 202 | CYC | OB-C4B | 2.97 | 1.29 | 1.23 |
| 12 | h7 | 201 | CYC | C2C-C1C | -2.97 | 1.49 | 1.52 |
| 12 | S1 | 201 | CYC | OB-C4B | 2.97 | 1.29 | 1.23 |
| 12 | S3 | 201 | CYC | OB-C4B | 2.97 | 1.29 | 1.23 |
| 12 | K4 | 201 | CYC | OB-C4B | 2.97 | 1.29 | 1.23 |
| 12 | K8 | 201 | CYC | OB-C4B | 2.97 | 1.29 | 1.23 |
| 12 | BA | 201 | CYC | C1C-NC | -2.97 | 1.33 | 1.37 |
| 12 | B9 | 201 | CYC | C1C-NC | -2.97 | 1.33 | 1.37 |
| 12 | b7 | 201 | CYC | C2C-C1C | -2.97 | 1.49 | 1.52 |
| 12 | F3 | 202 | CYC | OB-C4B | 2.97 | 1.29 | 1.23 |
| 12 | F1 | 202 | CYC | OB-C4B | 2.97 | 1.29 | 1.23 |
| 12 | LA | 201 | CYC | OB-C4B | 2.97 | 1.29 | 1.23 |
| 12 | L9 | 201 | CYC | OB-C4B | 2.97 | 1.29 | 1.23 |
| 12 | HA | 202 | CYC | C1C-NC | -2.97 | 1.33 | 1.37 |
| 12 | X3 | 202 | CYC | OB-C4B | 2.97 | 1.29 | 1.23 |
| 12 | X1 | 202 | CYC | OB-C4B | 2.97 | 1.29 | 1.23 |
| 12 | H3 | 202 | CYC | C1C-NC | -2.97 | 1.33 | 1.37 |
| 12 | H6 | 201 | CYC | C1C-NC | -2.97 | 1.33 | 1.37 |
| 12 | H4 | 201 | CYC | C2C-C1C | -2.96 | 1.49 | 1.52 |
| 12 | H8 | 201 | CYC | C2C-C1C | -2.96 | 1.49 | 1.52 |
| 12 | C4 | 201 | CYC | OB-C4B | 2.96 | 1.29 | 1.23 |
| 12 | C8 | 201 | CYC | OB-C4B | 2.96 | 1.29 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | M8 | 301 | CYC | C1C-NC | -2.96 | 1.33 | 1.37 |
| 12 | H7 | 201 | CYC | C2C-C1C | -2.96 | 1.49 | 1.52 |
| 12 | A1 | 201 | CYC | OB-C4B | 2.96 | 1.29 | 1.23 |
| 12 | A3 | 201 | CYC | OB-C4B | 2.96 | 1.29 | 1.23 |
| 12 | O1 | 201 | CYC | OB-C4B | 2.96 | 1.29 | 1.23 |
| 12 | O3 | 201 | CYC | OB-C4B | 2.96 | 1.29 | 1.23 |
| 12 | X3 | 201 | CYC | C2C-C1C | -2.96 | 1.49 | 1.52 |
| 12 | X1 | 201 | CYC | C2C-C1C | -2.96 | 1.49 | 1.52 |
| 12 | C2 | 201 | CYC | OB-C4B | 2.96 | 1.29 | 1.23 |
| 12 | N2 | 101 | CYC | C2C-C1C | -2.96 | 1.49 | 1.52 |
| 12 | J4 | 201 | CYC | C1C-NC | -2.96 | 1.33 | 1.37 |
| 12 | J8 | 201 | CYC | C1C-NC | -2.96 | 1.33 | 1.37 |
| 12 | A4 | 201 | CYC | OB-C4B | 2.95 | 1.29 | 1.23 |
| 12 | A8 | 201 | CYC | OB-C4B | 2.95 | 1.29 | 1.23 |
| 12 | V4 | 201 | CYC | OB-C4B | 2.95 | 1.29 | 1.23 |
| 12 | V8 | 201 | CYC | OB-C4B | 2.95 | 1.29 | 1.23 |
| 12 | UA | 201 | CYC | OB-C4B | 2.95 | 1.29 | 1.23 |
| 12 | U9 | 201 | CYC | OB-C4B | 2.95 | 1.29 | 1.23 |
| 12 | HA | 202 | CYC | C2C-C1C | -2.95 | 1.49 | 1.52 |
| 12 | a9 | 901 | CYC | C2C-C1C | -2.95 | 1.49 | 1.52 |
| 12 | TA | 302 | CYC | OB-C4B | 2.95 | 1.29 | 1.23 |
| 12 | T9 | 302 | CYC | OB-C4B | 2.95 | 1.29 | 1.23 |
| 12 | T3 | 302 | CYC | C1C-NC | -2.95 | 1.33 | 1.37 |
| 12 | J5 | 201 | CYC | C2C-C1C | -2.95 | 1.49 | 1.52 |
| 12 | H1 | 201 | CYC | C2C-C1C | -2.95 | 1.49 | 1.52 |
| 12 | d5 | 201 | CYC | C1B-C2B | 2.94 | 1.50 | 1.45 |
| 12 | QA | 201 | CYC | OB-C4B | 2.94 | 1.29 | 1.23 |
| 12 | JA | 201 | CYC | C1C-NC | -2.94 | 1.33 | 1.37 |
| 12 | Z5 | 201 | CYC | C1B-C2B | 2.94 | 1.50 | 1.45 |
| 12 | D5 | 201 | CYC | C2C-C1C | -2.94 | 1.49 | 1.52 |
| 12 | EA | 201 | CYC | C2C-C1C | -2.94 | 1.49 | 1.52 |
| 12 | j5 | 1202 | CYC | C2C-C1C | -2.94 | 1.49 | 1.52 |
| 12 | E9 | 201 | CYC | C2C-C1C | -2.94 | 1.49 | 1.52 |
| 12 | L2 | 201 | CYC | C2C-C1C | -2.94 | 1.49 | 1.52 |
| 12 | B7 | 201 | CYC | C2C-C1C | -2.94 | 1.49 | 1.52 |
| 12 | X5 | 201 | CYC | C1B-C2B | 2.94 | 1.50 | 1.45 |
| 12 | H1 | 201 | CYC | C1C-NC | -2.94 | 1.33 | 1.37 |
| 12 | P4 | 201 | CYC | OB-C4B | 2.93 | 1.29 | 1.23 |
| 12 | P8 | 201 | CYC | OB-C4B | 2.93 | 1.29 | 1.23 |
| 12 | Z3 | 201 | CYC | C2C-C1C | -2.93 | 1.49 | 1.52 |
| 12 | Z1 | 202 | CYC | C2C-C1C | -2.93 | 1.49 | 1.52 |
| 12 | Y3 | 201 | CYC | OB-C4B | 2.93 | 1.29 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | Y1 | 201 | CYC | OB-C4B | 2.93 | 1.29 | 1.23 |
| 12 | J3 | 202 | CYC | C1C-NC | -2.93 | 1.33 | 1.37 |
| 12 | aA | 901 | CYC | C1C-NC | -2.93 | 1.33 | 1.37 |
| 12 | XA | 201 | CYC | C2C-C1C | -2.93 | 1.49 | 1.52 |
| 12 | JA | 202 | CYC | C2C-C1C | -2.93 | 1.49 | 1.52 |
| 12 | J9 | 202 | CYC | C2C-C1C | -2.93 | 1.49 | 1.52 |
| 12 | f5 | 201 | CYC | C2C-C1C | -2.93 | 1.49 | 1.52 |
| 12 | U4 | 202 | CYC | OB-C4B | 2.92 | 1.29 | 1.23 |
| 12 | U8 | 202 | CYC | OB-C4B | 2.92 | 1.29 | 1.23 |
| 12 | H9 | 202 | CYC | C1C-NC | -2.92 | 1.33 | 1.37 |
| 12 | PA | 202 | CYC | C1C-NC | -2.92 | 1.33 | 1.37 |
| 12 | F3 | 202 | CYC | C1C-NC | -2.92 | 1.33 | 1.37 |
| 12 | F1 | 202 | CYC | C1C-NC | -2.92 | 1.33 | 1.37 |
| 12 | P9 | 202 | CYC | C1C-NC | -2.92 | 1.33 | 1.37 |
| 12 | d7 | 201 | CYC | C2C-C1C | -2.92 | 1.49 | 1.52 |
| 12 | H4 | 201 | CYC | C1C-NC | -2.92 | 1.33 | 1.37 |
| 12 | W3 | 201 | CYC | OB-C4B | 2.92 | 1.29 | 1.23 |
| 12 | W1 | 201 | CYC | OB-C4B | 2.92 | 1.29 | 1.23 |
| 12 | K2 | 201 | CYC | OB-C4B | 2.92 | 1.29 | 1.23 |
| 12 | K6 | 201 | CYC | OB-C4B | 2.92 | 1.29 | 1.23 |
| 12 | LA | 202 | CYC | C1C-NC | -2.92 | 1.33 | 1.37 |
| 12 | L9 | 202 | CYC | C1C-NC | -2.92 | 1.33 | 1.37 |
| 12 | A2 | 201 | CYC | OB-C4B | 2.91 | 1.29 | 1.23 |
| 12 | B5 | 201 | CYC | C1B-C2B | 2.91 | 1.50 | 1.45 |
| 12 | F5 | 201 | CYC | C2C-C1C | -2.91 | 1.49 | 1.52 |
| 12 | ZA | 201 | CYC | OB-C4B | 2.91 | 1.29 | 1.23 |
| 12 | Z9 | 201 | CYC | OB-C4B | 2.91 | 1.29 | 1.23 |
| 12 | J6 | 202 | CYC | C1C-NC | -2.91 | 1.33 | 1.37 |
| 12 | VA | 201 | CYC | C1C-NC | -2.91 | 1.33 | 1.37 |
| 12 | V9 | 201 | CYC | C1C-NC | -2.91 | 1.33 | 1.37 |
| 12 | A6 | 201 | CYC | OB-C4B | 2.91 | 1.29 | 1.23 |
| 12 | k5 | 1204 | CYC | C2C-C1C | -2.91 | 1.49 | 1.52 |
| 12 | b5 | 201 | CYC | C2C-C1C | -2.91 | 1.49 | 1.52 |
| 12 | T5 | 201 | CYC | C1B-C2B | 2.91 | 1.50 | 1.45 |
| 12 | Z | 201 | CYC | C2C-C1C | -2.91 | 1.49 | 1.52 |
| 12 | H2 | 201 | CYC | C1C-NC | -2.91 | 1.33 | 1.37 |
| 12 | H3 | 202 | CYC | C2C-C1C | -2.90 | 1.49 | 1.52 |
| 12 | G2 | 201 | CYC | OB-C4B | 2.90 | 1.29 | 1.23 |
| 12 | X7 | 201 | CYC | C2C-C1C | -2.90 | 1.49 | 1.52 |
| 12 | Q9 | 201 | CYC | OB-C4B | 2.90 | 1.29 | 1.23 |
| 12 | L4 | 202 | CYC | C2C-C1C | -2.90 | 1.49 | 1.52 |
| 12 | F6 | 201 | CYC | C1C-NC | -2.90 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | J9 | 201 | CYC | C1C-NC | -2.90 | 1.33 | 1.37 |
| 12 | XA | 201 | CYC | C1C-NC | -2.90 | 1.33 | 1.37 |
| 12 | X9 | 201 | CYC | C1C-NC | -2.90 | 1.33 | 1.37 |
| 12 | V7 | 201 | CYC | C2C-C1C | -2.89 | 1.49 | 1.52 |
| 12 | M4 | 301 | CYC | C1C-NC | -2.89 | 1.33 | 1.37 |
| 12 | AA | 201 | CYC | OB-C4B | 2.89 | 1.29 | 1.23 |
| 12 | A9 | 201 | CYC | OB-C4B | 2.89 | 1.29 | 1.23 |
| 12 | OA | 201 | CYC | OB-C4B | 2.89 | 1.29 | 1.23 |
| 12 | O9 | 201 | CYC | OB-C4B | 2.89 | 1.29 | 1.23 |
| 12 | N7 | 201 | CYC | C2C-C1C | -2.89 | 1.49 | 1.52 |
| 12 | R1 | 201 | CYC | C2C-C1C | -2.88 | 1.49 | 1.52 |
| 12 | R3 | 201 | CYC | C2C-C1C | -2.88 | 1.49 | 1.52 |
| 12 | F4 | 202 | CYC | C2C-C1C | -2.88 | 1.49 | 1.52 |
| 12 | F8 | 202 | CYC | C2C-C1C | -2.88 | 1.49 | 1.52 |
| 12 | H6 | 201 | CYC | C2C-C1C | -2.88 | 1.49 | 1.52 |
| 12 | N2 | 101 | CYC | C1C-NC | -2.88 | 1.33 | 1.37 |
| 12 | D4 | 202 | CYC | C1C-NC | -2.88 | 1.33 | 1.37 |
| 12 | D8 | 202 | CYC | C1C-NC | -2.88 | 1.33 | 1.37 |
| 12 | H5 | 201 | CYC | C1B-C2B | 2.88 | 1.50 | 1.45 |
| 12 | R5 | 201 | CYC | C1B-C2B | 2.88 | 1.50 | 1.45 |
| 12 | H8 | 201 | CYC | C1C-NC | -2.87 | 1.33 | 1.37 |
| 12 | G6 | 201 | CYC | OB-C4B | 2.87 | 1.29 | 1.23 |
| 12 | J2 | 202 | CYC | C1C-NC | -2.87 | 1.33 | 1.37 |
| 12 | U4 | 201 | CYC | C1C-NC | -2.87 | 1.33 | 1.37 |
| 12 | D6 | 201 | CYC | C1C-NC | -2.87 | 1.33 | 1.37 |
| 12 | U8 | 201 | CYC | C1C-NC | -2.87 | 1.33 | 1.37 |
| 12 | j7 | 201 | CYC | C2C-C1C | -2.87 | 1.49 | 1.52 |
| 12 | N5 | 201 | CYC | C1B-C2B | 2.87 | 1.50 | 1.45 |
| 12 | A | 201 | CYC | C2C-C1C | -2.87 | 1.49 | 1.52 |
| 12 | b5 | 201 | CYC | C1B-C2B | 2.86 | 1.50 | 1.45 |
| 12 | C3 | 201 | CYC | OB-C4B | 2.86 | 1.29 | 1.23 |
| 12 | C1 | 201 | CYC | OB-C4B | 2.86 | 1.29 | 1.23 |
| 12 | L6 | 202 | CYC | OB-C4B | 2.86 | 1.29 | 1.23 |
| 12 | G2 | 201 | CYC | C2C-C1C | -2.86 | 1.49 | 1.52 |
| 12 | L5 | 201 | CYC | C2C-C1C | -2.86 | 1.49 | 1.52 |
| 12 | k5 | 1203 | CYC | C2C-C1C | -2.86 | 1.49 | 1.52 |
| 12 | k5 | 1203 | CYC | C1B-C2B | 2.86 | 1.50 | 1.45 |
| 12 | N7 | 201 | CYC | C1B-C2B | 2.86 | 1.50 | 1.45 |
| 12 | PA | 201 | CYC | C1C-NC | -2.86 | 1.33 | 1.37 |
| 12 | S4 | 202 | CYC | C1C-NC | -2.86 | 1.33 | 1.37 |
| 12 | P9 | 201 | CYC | C1C-NC | -2.86 | 1.33 | 1.37 |
| 12 | T7 | 201 | CYC | C1B-C2B | 2.85 | 1.50 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | RA | 201 | CYC | C1C-NC | -2.85 | 1.33 | 1.37 |
| 12 | R9 | 201 | CYC | C1C-NC | -2.85 | 1.33 | 1.37 |
| 12 | L7 | 201 | CYC | C1B-C2B | 2.85 | 1.50 | 1.45 |
| 12 | L6 | 201 | CYC | C2C-C1C | -2.85 | 1.49 | 1.52 |
| 12 | f5 | 201 | CYC | C1B-C2B | 2.85 | 1.50 | 1.45 |
| 12 | L2 | 202 | CYC | OB-C4B | 2.85 | 1.29 | 1.23 |
| 12 | X9 | 201 | CYC | C2C-C1C | -2.85 | 1.49 | 1.52 |
| 12 | T3 | 301 | CYC | C1C-NC | -2.85 | 1.33 | 1.37 |
| 12 | T1 | 301 | CYC | C1C-NC | -2.85 | 1.33 | 1.37 |
| 12 | R3 | 201 | CYC | C1C-NC | -2.85 | 1.33 | 1.37 |
| 12 | Q1 | 201 | CYC | OB-C4B | 2.84 | 1.29 | 1.23 |
| 12 | Q3 | 201 | CYC | OB-C4B | 2.84 | 1.29 | 1.23 |
| 12 | L4 | 202 | CYC | C1C-NC | -2.84 | 1.33 | 1.37 |
| 12 | CA | 201 | CYC | OB-C4B | 2.84 | 1.29 | 1.23 |
| 12 | C9 | 201 | CYC | OB-C4B | 2.84 | 1.29 | 1.23 |
| 12 | D2 | 201 | CYC | C1C-NC | -2.84 | 1.33 | 1.37 |
| 12 | V3 | 201 | CYC | C1C-NC | -2.84 | 1.33 | 1.37 |
| 12 | V1 | 201 | CYC | C1C-NC | -2.84 | 1.33 | 1.37 |
| 12 | V3 | 201 | CYC | C2C-C1C | -2.84 | 1.49 | 1.52 |
| 12 | V1 | 201 | CYC | C2C-C1C | -2.84 | 1.49 | 1.52 |
| 12 | VA | 201 | CYC | C2C-C1C | -2.84 | 1.49 | 1.52 |
| 12 | V9 | 201 | CYC | C2C-C1C | -2.84 | 1.49 | 1.52 |
| 12 | L5 | 201 | CYC | C1B-C2B | 2.84 | 1.50 | 1.45 |
| 12 | k5 | 1201 | CYC | C1B-C2B | 2.83 | 1.50 | 1.45 |
| 12 | r7 | 201 | CYC | C2C-C1C | -2.83 | 1.49 | 1.52 |
| 12 | D9 | 201 | CYC | C1C-NC | -2.83 | 1.33 | 1.37 |
| 12 | F7 | 201 | CYC | C1B-C2B | 2.83 | 1.50 | 1.45 |
| 12 | C6 | 201 | CYC | C2C-C1C | -2.83 | 1.49 | 1.52 |
| 12 | v7 | 201 | CYC | C1B-C2B | 2.83 | 1.50 | 1.45 |
| 12 | p7 | 201 | CYC | C2C-C1C | -2.83 | 1.49 | 1.52 |
| 12 | R1 | 201 | CYC | C1C-NC | -2.83 | 1.33 | 1.37 |
| 12 | a9 | 901 | CYC | C1C-NC | -2.83 | 1.33 | 1.37 |
| 12 | L2 | 201 | CYC | C1C-NC | -2.83 | 1.33 | 1.37 |
| 12 | L6 | 201 | CYC | C1C-NC | -2.83 | 1.33 | 1.37 |
| 12 | F4 | 202 | CYC | C1C-NC | -2.83 | 1.33 | 1.37 |
| 12 | F8 | 202 | CYC | C1C-NC | -2.83 | 1.33 | 1.37 |
| 12 | T5 | 201 | CYC | C2C-C1C | -2.83 | 1.49 | 1.52 |
| 12 | G6 | 201 | CYC | C2C-C1C | -2.82 | 1.49 | 1.52 |
| 12 | H7 | 201 | CYC | C1B-C2B | 2.82 | 1.50 | 1.45 |
| 12 | N6 | 101 | CYC | C1C-NC | -2.82 | 1.34 | 1.37 |
| 12 | r7 | 201 | CYC | C1B-C2B | 2.81 | 1.50 | 1.45 |
| 12 | T7 | 201 | CYC | C2C-C1C | -2.81 | 1.49 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | Z3 | 201 | CYC | C1C-NC | -2.81 | 1.34 | 1.37 |
| 12 | Z1 | 202 | CYC | C1C-NC | -2.81 | 1.34 | 1.37 |
| 12 | R7 | 201 | CYC | C1B-C2B | 2.81 | 1.50 | 1.45 |
| 12 | j5 | 1202 | CYC | C1B-C2B | 2.80 | 1.50 | 1.45 |
| 12 | V5 | 201 | CYC | C1B-C2B | 2.80 | 1.50 | 1.45 |
| 12 | k5 | 1204 | CYC | C1B-C2B | 2.80 | 1.50 | 1.45 |
| 12 | B1 | 202 | CYC | C1C-NC | -2.80 | 1.34 | 1.37 |
| 12 | F2 | 202 | CYC | C1C-NC | -2.80 | 1.34 | 1.37 |
| 12 | E3 | 201 | CYC | C2C-C1C | -2.80 | 1.49 | 1.52 |
| 12 | E1 | 201 | CYC | C2C-C1C | -2.80 | 1.49 | 1.52 |
| 12 | N5 | 201 | CYC | C2C-C1C | -2.80 | 1.49 | 1.52 |
| 12 | X3 | 201 | CYC | C1C-NC | -2.80 | 1.34 | 1.37 |
| 12 | X1 | 201 | CYC | C1C-NC | -2.80 | 1.34 | 1.37 |
| 12 | WA | 201 | CYC | C2C-C1C | -2.79 | 1.49 | 1.52 |
| 12 | W9 | 201 | CYC | C2C-C1C | -2.79 | 1.49 | 1.52 |
| 12 | k5 | 1202 | CYC | C1B-C2B | 2.79 | 1.50 | 1.45 |
| 12 | DA | 201 | CYC | C1C-NC | -2.79 | 1.34 | 1.37 |
| 12 | D7 | 201 | CYC | C1B-C2B | 2.79 | 1.50 | 1.45 |
| 12 | P5 | 201 | CYC | C1B-C2B | 2.79 | 1.50 | 1.45 |
| 12 | j5 | 1201 | CYC | C1B-C2B | 2.79 | 1.50 | 1.45 |
| 12 | I2 | 201 | CYC | C2C-C1C | -2.79 | 1.49 | 1.52 |
| 12 | B3 | 202 | CYC | C1C-NC | -2.79 | 1.34 | 1.37 |
| 12 | R5 | 201 | CYC | C2C-C1C | -2.78 | 1.49 | 1.52 |
| 12 | d7 | 201 | CYC | C1B-C2B | 2.78 | 1.50 | 1.45 |
| 12 | p7 | 201 | CYC | C1B-C2B | 2.78 | 1.50 | 1.45 |
| 12 | P7 | 201 | CYC | C1B-C2B | 2.78 | 1.50 | 1.45 |
| 12 | F3 | 201 | CYC | C2C-C1C | -2.78 | 1.49 | 1.52 |
| 12 | F1 | 201 | CYC | C2C-C1C | -2.78 | 1.49 | 1.52 |
| 12 | B7 | 201 | CYC | C1B-C2B | 2.78 | 1.50 | 1.45 |
| 12 | D3 | 202 | CYC | C1C-NC | -2.78 | 1.34 | 1.37 |
| 12 | F2 | 201 | CYC | C2C-C1C | -2.78 | 1.49 | 1.52 |
| 12 | J7 | 201 | CYC | C1B-C2B | 2.78 | 1.50 | 1.45 |
| 12 | R7 | 201 | CYC | C2C-C1C | -2.78 | 1.49 | 1.52 |
| 12 | X5 | 201 | CYC | C2C-C1C | -2.77 | 1.49 | 1.52 |
| 12 | f7 | 201 | CYC | C1B-C2B | 2.77 | 1.50 | 1.45 |
| 12 | M8 | 302 | CYC | C1C-NC | -2.77 | 1.34 | 1.37 |
| 12 | F3 | 201 | CYC | C1C-NC | -2.77 | 1.34 | 1.37 |
| 12 | F1 | 201 | CYC | C1C-NC | -2.77 | 1.34 | 1.37 |
| 12 | F5 | 201 | CYC | C1B-C2B | 2.77 | 1.50 | 1.45 |
| 12 | k5 | 1202 | CYC | C2C-C1C | -2.77 | 1.49 | 1.52 |
| 12 | W4 | 201 | CYC | C1C-NC | -2.77 | 1.34 | 1.37 |
| 12 | W8 | 201 | CYC | C1C-NC | -2.77 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | I6 | 201 | CYC | C2C-C1C | -2.76 | 1.49 | 1.52 |
| 12 | B8 | 202 | CYC | C1C-NC | -2.76 | 1.34 | 1.37 |
| 12 | X7 | 201 | CYC | C1B-C2B | 2.76 | 1.50 | 1.45 |
| 12 | C2 | 201 | CYC | C2C-C1C | -2.75 | 1.49 | 1.52 |
| 12 | b7 | 201 | CYC | C1B-C2B | 2.75 | 1.50 | 1.45 |
| 12 | L3 | 202 | CYC | C1C-NC | -2.75 | 1.34 | 1.37 |
| 12 | aA | 902 | CYC | C1C-NC | -2.75 | 1.34 | 1.37 |
| 12 | D5 | 201 | CYC | C1B-C2B | 2.74 | 1.50 | 1.45 |
| 12 | U7 | 201 | CYC | C1C-NC | -2.74 | 1.34 | 1.37 |
| 12 | P1 | 201 | CYC | C1C-NC | -2.74 | 1.34 | 1.37 |
| 12 | P3 | 201 | CYC | C1C-NC | -2.74 | 1.34 | 1.37 |
| 12 | O4 | 201 | CYC | C1C-NC | -2.74 | 1.34 | 1.37 |
| 12 | O8 | 201 | CYC | C1C-NC | -2.74 | 1.34 | 1.37 |
| 12 | k7 | 201 | CYC | C1C-NC | -2.74 | 1.34 | 1.37 |
| 12 | f7 | 201 | CYC | C2C-C1C | -2.74 | 1.49 | 1.52 |
| 12 | L7 | 201 | CYC | C2C-C1C | -2.74 | 1.49 | 1.52 |
| 12 | a7 | 201 | CYC | C1C-NC | -2.74 | 1.34 | 1.37 |
| 12 | j7 | 201 | CYC | C1B-C2B | 2.74 | 1.50 | 1.45 |
| 12 | W7 | 201 | CYC | C1C-NC | -2.74 | 1.34 | 1.37 |
| 12 | U5 | 201 | CYC | C1C-NC | -2.74 | 1.34 | 1.37 |
| 12 | D1 | 202 | CYC | C1C-NC | -2.73 | 1.34 | 1.37 |
| 12 | v7 | 201 | CYC | C2C-C1C | -2.73 | 1.49 | 1.52 |
| 12 | Q9 | 201 | CYC | C2C-C1C | -2.73 | 1.49 | 1.52 |
| 12 | h7 | 201 | CYC | C1B-C2B | 2.73 | 1.50 | 1.45 |
| 12 | B4 | 202 | CYC | C1C-NC | -2.73 | 1.34 | 1.37 |
| 12 | A4 | 201 | CYC | C2C-C1C | -2.73 | 1.49 | 1.52 |
| 12 | A8 | 201 | CYC | C2C-C1C | -2.73 | 1.49 | 1.52 |
| 12 | g7 | 201 | CYC | C1C-NC | -2.72 | 1.34 | 1.37 |
| 12 | s7 | 201 | CYC | C1C-NC | -2.72 | 1.34 | 1.37 |
| 12 | c7 | 201 | CYC | C1C-NC | -2.72 | 1.34 | 1.37 |
| 12 | SA | 201 | CYC | C2C-C1C | -2.72 | 1.49 | 1.52 |
| 12 | V5 | 201 | CYC | C2C-C1C | -2.72 | 1.49 | 1.52 |
| 12 | S9 | 201 | CYC | C2C-C1C | -2.72 | 1.49 | 1.52 |
| 12 | G3 | 201 | CYC | C2C-C1C | -2.72 | 1.49 | 1.52 |
| 12 | G1 | 201 | CYC | C2C-C1C | -2.72 | 1.49 | 1.52 |
| 12 | QA | 201 | CYC | C2C-C1C | -2.71 | 1.49 | 1.52 |
| 12 | J5 | 201 | CYC | C1B-C2B | 2.71 | 1.50 | 1.45 |
| 12 | F6 | 202 | CYC | C1C-NC | -2.71 | 1.34 | 1.37 |
| 12 | Q7 | 201 | CYC | C1C-NC | -2.71 | 1.34 | 1.37 |
| 12 | GA | 201 | CYC | C2C-C1C | -2.70 | 1.49 | 1.52 |
| 12 | G9 | 201 | CYC | C2C-C1C | -2.70 | 1.49 | 1.52 |
| 12 | FA | 301 | CYC | C1C-NC | -2.70 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | F9 | 301 | CYC | C1C-NC | -2.70 | 1.34 | 1.37 |
| 12 | q7 | 201 | CYC | C1C-NC | -2.70 | 1.34 | 1.37 |
| 12 | K5 | 201 | CYC | C1C-NC | -2.70 | 1.34 | 1.37 |
| 12 | F6 | 201 | CYC | C2C-C1C | -2.69 | 1.49 | 1.52 |
| 12 | G4 | 201 | CYC | C2C-C1C | -2.69 | 1.49 | 1.52 |
| 12 | G8 | 201 | CYC | C2C-C1C | -2.69 | 1.49 | 1.52 |
| 12 | o7 | 201 | CYC | C1C-NC | -2.69 | 1.34 | 1.37 |
| 12 | UA | 201 | CYC | C2C-C1C | -2.69 | 1.49 | 1.52 |
| 12 | U9 | 201 | CYC | C2C-C1C | -2.69 | 1.49 | 1.52 |
| 12 | E5 | 201 | CYC | C1C-NC | -2.69 | 1.34 | 1.37 |
| 12 | N4 | 201 | CYC | C2C-C1C | -2.68 | 1.49 | 1.52 |
| 12 | N8 | 201 | CYC | C2C-C1C | -2.68 | 1.49 | 1.52 |
| 12 | F7 | 201 | CYC | C2C-C1C | -2.68 | 1.49 | 1.52 |
| 12 | Z | 201 | CYC | C1B-C2B | 2.68 | 1.49 | 1.45 |
| 12 | V7 | 201 | CYC | C1B-C2B | 2.68 | 1.49 | 1.45 |
| 12 | P4 | 201 | CYC | C2C-C1C | -2.68 | 1.49 | 1.52 |
| 12 | P8 | 201 | CYC | C2C-C1C | -2.68 | 1.49 | 1.52 |
| 12 | u7 | 201 | CYC | C1C-NC | -2.68 | 1.34 | 1.37 |
| 12 | A2 | 201 | CYC | C1B-NB | -2.67 | 1.33 | 1.37 |
| 12 | P5 | 201 | CYC | C2C-C1C | -2.67 | 1.49 | 1.52 |
| 12 | TA | 301 | CYC | C2C-C1C | -2.67 | 1.49 | 1.52 |
| 12 | X4 | 201 | CYC | C2C-C1C | -2.67 | 1.49 | 1.52 |
| 12 | X8 | 201 | CYC | C2C-C1C | -2.67 | 1.49 | 1.52 |
| 12 | T9 | 301 | CYC | C2C-C1C | -2.67 | 1.49 | 1.52 |
| 12 | Y5 | 201 | CYC | OB-C4B | 2.67 | 1.28 | 1.23 |
| 12 | m7 | 201 | CYC | C1C-NC | -2.67 | 1.34 | 1.37 |
| 12 | e5 | 201 | CYC | OB-C4B | 2.67 | 1.28 | 1.23 |
| 12 | A | 201 | CYC | C1B-C2B | 2.66 | 1.49 | 1.45 |
| 12 | FA | 301 | CYC | C2C-C1C | -2.66 | 1.49 | 1.52 |
| 12 | F9 | 301 | CYC | C2C-C1C | -2.66 | 1.49 | 1.52 |
| 12 | Q5 | 201 | CYC | C1C-NC | -2.66 | 1.34 | 1.37 |
| 12 | g7 | 201 | CYC | OB-C4B | 2.66 | 1.28 | 1.23 |
| 12 | a5 | 201 | CYC | OB-C4B | 2.65 | 1.28 | 1.23 |
| 12 | S7 | 201 | CYC | C1C-NC | -2.65 | 1.34 | 1.37 |
| 12 | i7 | 201 | CYC | C1C-NC | -2.65 | 1.34 | 1.37 |
| 12 | I3 | 201 | CYC | C2C-C1C | -2.65 | 1.49 | 1.52 |
| 12 | I1 | 201 | CYC | C2C-C1C | -2.65 | 1.49 | 1.52 |
| 12 | W5 | 201 | CYC | C1C-NC | -2.64 | 1.34 | 1.37 |
| 12 | V4 | 201 | CYC | C2C-C1C | -2.64 | 1.49 | 1.52 |
| 12 | V8 | 201 | CYC | C2C-C1C | -2.64 | 1.49 | 1.52 |
| 12 | OA | 201 | CYC | C2C-C1C | -2.64 | 1.49 | 1.52 |
| 12 | C4 | 201 | CYC | C2C-C1C | -2.64 | 1.49 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | W3 | 201 | CYC | C2C-C1C | -2.64 | 1.49 | 1.52 |
| 12 | C8 | 201 | CYC | C2C-C1C | -2.64 | 1.49 | 1.52 |
| 12 | K7 | 201 | CYC | C1C-NC | -2.64 | 1.34 | 1.37 |
| 12 | O7 | 201 | CYC | C1C-NC | -2.64 | 1.34 | 1.37 |
| 12 | TA | 301 | CYC | C1C-NC | -2.64 | 1.34 | 1.37 |
| 12 | O5 | 201 | CYC | C1C-NC | -2.64 | 1.34 | 1.37 |
| 12 | T9 | 301 | CYC | C1C-NC | -2.64 | 1.34 | 1.37 |
| 12 | S5 | 201 | CYC | C1B-C2B | 2.64 | 1.49 | 1.45 |
| 12 | U7 | 201 | CYC | OB-C4B | 2.64 | 1.28 | 1.23 |
| 12 | a7 | 201 | CYC | OB-C4B | 2.63 | 1.28 | 1.23 |
| 12 | c5 | 201 | CYC | OB-C4B | 2.63 | 1.28 | 1.23 |
| 12 | C3 | 201 | CYC | C2C-C1C | -2.63 | 1.49 | 1.52 |
| 12 | C1 | 201 | CYC | C2C-C1C | -2.63 | 1.49 | 1.52 |
| 12 | A6 | 201 | CYC | C1B-NB | -2.63 | 1.33 | 1.37 |
| 12 | Y7 | 201 | CYC | C1B-C2B | 2.62 | 1.49 | 1.45 |
| 12 | S1 | 201 | CYC | C2C-C1C | -2.62 | 1.49 | 1.52 |
| 12 | S3 | 201 | CYC | C2C-C1C | -2.62 | 1.49 | 1.52 |
| 12 | AA | 201 | CYC | C2C-C1C | -2.62 | 1.49 | 1.52 |
| 12 | A9 | 201 | CYC | C2C-C1C | -2.62 | 1.49 | 1.52 |
| 12 | O9 | 201 | CYC | C2C-C1C | -2.62 | 1.49 | 1.52 |
| 12 | M5 | 201 | CYC | C1B-C2B | 2.62 | 1.49 | 1.45 |
| 12 | E6 | 201 | CYC | C2C-C1C | -2.61 | 1.49 | 1.52 |
| 12 | E2 | 201 | CYC | C2C-C1C | -2.61 | 1.49 | 1.52 |
| 12 | m7 | 201 | CYC | OB-C4B | 2.61 | 1.28 | 1.23 |
| 12 | C7 | 201 | CYC | C1C-NC | -2.61 | 1.34 | 1.37 |
| 12 | U5 | 201 | CYC | OB-C4B | 2.61 | 1.28 | 1.23 |
| 12 | O9 | 201 | CYC | C1B-NB | -2.61 | 1.33 | 1.37 |
| 12 | O7 | 201 | CYC | OB-C4B | 2.60 | 1.28 | 1.23 |
| 12 | G5 | 201 | CYC | OB-C4B | 2.60 | 1.28 | 1.23 |
| 12 | K7 | 201 | CYC | C1B-C2B | 2.60 | 1.49 | 1.45 |
| 12 | A2 | 201 | CYC | C2C-C1C | -2.60 | 1.49 | 1.52 |
| 12 | M7 | 201 | CYC | C1B-C2B | 2.60 | 1.49 | 1.45 |
| 12 | O1 | 201 | CYC | C2C-C1C | -2.59 | 1.49 | 1.52 |
| 12 | O3 | 201 | CYC | C2C-C1C | -2.59 | 1.49 | 1.52 |
| 12 | U3 | 201 | CYC | C2C-C1C | -2.59 | 1.49 | 1.52 |
| 12 | I4 | 201 | CYC | C2C-C1C | -2.59 | 1.49 | 1.52 |
| 12 | I8 | 201 | CYC | C2C-C1C | -2.59 | 1.49 | 1.52 |
| 12 | U1 | 201 | CYC | C2C-C1C | -2.59 | 1.49 | 1.52 |
| 12 | A4 | 201 | CYC | C1B-NB | -2.59 | 1.33 | 1.37 |
| 12 | A8 | 201 | CYC | C1B-NB | -2.59 | 1.33 | 1.37 |
| 12 | Y3 | 201 | CYC | C2C-C1C | -2.59 | 1.49 | 1.52 |
| 12 | Y1 | 201 | CYC | C2C-C1C | -2.59 | 1.49 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | k7 | 201 | CYC | C1B-C2B | 2.59 | 1.49 | 1.45 |
| 12 | L5 | 201 | CYC | C1D-CHD | 2.59 | 1.51 | 1.41 |
| 12 | L5 | 201 | CYC | OB-C4B | 2.58 | 1.28 | 1.23 |
| 12 | Y5 | 201 | CYC | C1C-NC | -2.58 | 1.34 | 1.37 |
| 12 | A5 | 201 | CYC | C1B-C2B | 2.58 | 1.49 | 1.45 |
| 12 | C7 | 201 | CYC | OB-C4B | 2.58 | 1.28 | 1.23 |
| 12 | e7 | 201 | CYC | C1B-C2B | 2.58 | 1.49 | 1.45 |
| 12 | O5 | 201 | CYC | OB-C4B | 2.58 | 1.28 | 1.23 |
| 12 | OA | 201 | CYC | C1B-NB | -2.58 | 1.33 | 1.37 |
| 12 | K7 | 201 | CYC | OB-C4B | 2.58 | 1.28 | 1.23 |
| 12 | G5 | 201 | CYC | C1C-NC | -2.58 | 1.34 | 1.37 |
| 12 | A5 | 201 | CYC | C1C-NC | -2.57 | 1.34 | 1.37 |
| 12 | K2 | 201 | CYC | C2C-C1C | -2.57 | 1.49 | 1.52 |
| 12 | K6 | 201 | CYC | C2C-C1C | -2.57 | 1.49 | 1.52 |
| 12 | a5 | 201 | CYC | C1C-NC | -2.57 | 1.34 | 1.37 |
| 12 | E7 | 201 | CYC | C1C-NC | -2.57 | 1.34 | 1.37 |
| 12 | C5 | 201 | CYC | OB-C4B | 2.57 | 1.28 | 1.23 |
| 12 | i7 | 201 | CYC | OB-C4B | 2.57 | 1.28 | 1.23 |
| 12 | P5 | 201 | CYC | C1D-CHD | 2.57 | 1.51 | 1.41 |
| 12 | C5 | 201 | CYC | C1C-NC | -2.57 | 1.34 | 1.37 |
| 12 | c5 | 201 | CYC | C1C-NC | -2.57 | 1.34 | 1.37 |
| 12 | V5 | 201 | CYC | C1D-CHD | 2.57 | 1.51 | 1.41 |
| 12 | Z5 | 201 | CYC | OB-C4B | 2.57 | 1.28 | 1.23 |
| 12 | j7 | 201 | CYC | OB-C4B | 2.57 | 1.28 | 1.23 |
| 12 | h7 | 201 | CYC | C1D-CHD | 2.57 | 1.51 | 1.41 |
| 12 | ZA | 202 | CYC | C4C-NC | -2.57 | 1.32 | 1.37 |
| 12 | Z9 | 202 | CYC | C4C-NC | -2.57 | 1.32 | 1.37 |
| 12 | I7 | 201 | CYC | OB-C4B | 2.56 | 1.28 | 1.23 |
| 12 | KA | 201 | CYC | C2C-C1C | -2.56 | 1.49 | 1.52 |
| 12 | K9 | 201 | CYC | C2C-C1C | -2.56 | 1.49 | 1.52 |
| 12 | W1 | 201 | CYC | C2C-C1C | -2.56 | 1.49 | 1.52 |
| 12 | H7 | 201 | CYC | C1D-CHD | 2.56 | 1.51 | 1.41 |
| 12 | F6 | 201 | CYC | C4C-NC | -2.56 | 1.32 | 1.37 |
| 12 | e5 | 201 | CYC | C1C-NC | -2.56 | 1.34 | 1.37 |
| 12 | FA | 301 | CYC | C4C-NC | -2.56 | 1.32 | 1.37 |
| 12 | F9 | 301 | CYC | C4C-NC | -2.56 | 1.32 | 1.37 |
| 12 | E7 | 201 | CYC | C1B-C2B | 2.56 | 1.49 | 1.45 |
| 12 | S5 | 201 | CYC | C1C-NC | -2.56 | 1.34 | 1.37 |
| 12 | W7 | 201 | CYC | OB-C4B | 2.56 | 1.28 | 1.23 |
| 12 | H5 | 201 | CYC | C1D-CHD | 2.56 | 1.51 | 1.41 |
| 12 | T7 | 201 | CYC | C1D-CHD | 2.56 | 1.51 | 1.41 |
| 12 | B5 | 201 | CYC | C1D-CHD | 2.55 | 1.51 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | E4 | 201 | CYC | C2C-C1C | -2.55 | 1.49 | 1.52 |
| 12 | Q7 | 201 | CYC | OB-C4B | 2.55 | 1.28 | 1.23 |
| 12 | B7 | 201 | CYC | C1D-CHD | 2.55 | 1.51 | 1.41 |
| 12 | U3 | 201 | CYC | C1B-NB | -2.55 | 1.33 | 1.37 |
| 12 | U1 | 201 | CYC | C1B-NB | -2.55 | 1.33 | 1.37 |
| 12 | E5 | 201 | CYC | OB-C4B | 2.55 | 1.28 | 1.23 |
| 12 | d7 | 201 | CYC | OB-C4B | 2.55 | 1.28 | 1.23 |
| 12 | Q7 | 201 | CYC | C1B-C2B | 2.55 | 1.49 | 1.45 |
| 12 | E7 | 201 | CYC | OB-C4B | 2.55 | 1.28 | 1.23 |
| 12 | s7 | 201 | CYC | OB-C4B | 2.55 | 1.28 | 1.23 |
| 12 | F5 | 201 | CYC | C1D-CHD | 2.55 | 1.51 | 1.41 |
| 12 | P1 | 201 | CYC | C4C-NC | -2.54 | 1.32 | 1.37 |
| 12 | P3 | 201 | CYC | C4C-NC | -2.54 | 1.32 | 1.37 |
| 12 | J7 | 201 | CYC | C1D-CHD | 2.54 | 1.51 | 1.41 |
| 12 | J5 | 201 | CYC | OB-C4B | 2.54 | 1.28 | 1.23 |
| 12 | RA | 201 | CYC | C4C-NC | -2.54 | 1.32 | 1.37 |
| 12 | R9 | 201 | CYC | C4C-NC | -2.54 | 1.32 | 1.37 |
| 12 | N7 | 201 | CYC | C1D-CHD | 2.54 | 1.51 | 1.41 |
| 12 | Y7 | 201 | CYC | C1C-NC | -2.54 | 1.34 | 1.37 |
| 12 | YA | 201 | CYC | C2C-C1C | -2.54 | 1.49 | 1.52 |
| 12 | Y9 | 201 | CYC | C2C-C1C | -2.54 | 1.49 | 1.52 |
| 12 | e7 | 201 | CYC | C1C-NC | -2.54 | 1.34 | 1.37 |
| 12 | S1 | 201 | CYC | C1B-C2B | 2.54 | 1.49 | 1.45 |
| 12 | S3 | 201 | CYC | C1B-C2B | 2.54 | 1.49 | 1.45 |
| 12 | S7 | 201 | CYC | C1B-C2B | 2.54 | 1.49 | 1.45 |
| 12 | V7 | 201 | CYC | C1D-CHD | 2.54 | 1.51 | 1.41 |
| 12 | b7 | 201 | CYC | C1D-CHD | 2.54 | 1.50 | 1.41 |
| 12 | f7 | 201 | CYC | C1D-CHD | 2.53 | 1.50 | 1.41 |
| 12 | A5 | 201 | CYC | OB-C4B | 2.53 | 1.28 | 1.23 |
| 12 | F2 | 201 | CYC | C4C-NC | -2.53 | 1.32 | 1.37 |
| 12 | Z5 | 201 | CYC | C1D-CHD | 2.53 | 1.50 | 1.41 |
| 12 | G5 | 201 | CYC | C1B-C2B | 2.53 | 1.49 | 1.45 |
| 12 | M5 | 201 | CYC | C1C-NC | -2.53 | 1.34 | 1.37 |
| 12 | N5 | 201 | CYC | C1D-CHD | 2.53 | 1.50 | 1.41 |
| 12 | d5 | 201 | CYC | C1D-CHD | 2.53 | 1.50 | 1.41 |
| 12 | G7 | 201 | CYC | C1B-C2B | 2.53 | 1.49 | 1.45 |
| 12 | I7 | 201 | CYC | C1C-NC | -2.53 | 1.34 | 1.37 |
| 12 | I5 | 201 | CYC | OB-C4B | 2.53 | 1.28 | 1.23 |
| 12 | T4 | 201 | CYC | C2C-C1C | -2.53 | 1.49 | 1.52 |
| 12 | T8 | 201 | CYC | C2C-C1C | -2.53 | 1.49 | 1.52 |
| 12 | L3 | 202 | CYC | C4C-NC | -2.53 | 1.32 | 1.37 |
| 12 | aA | 902 | CYC | C4C-NC | -2.53 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | v7 | 201 | CYC | C1D-CHD | 2.53 | 1.50 | 1.41 |
| 12 | k5 | 1204 | CYC | C1D-CHD | 2.53 | 1.50 | 1.41 |
| 12 | D7 | 201 | CYC | C1D-CHD | 2.53 | 1.50 | 1.41 |
| 12 | D8 | 202 | CYC | C4C-NC | -2.53 | 1.32 | 1.37 |
| 12 | P7 | 201 | CYC | C1D-CHD | 2.53 | 1.50 | 1.41 |
| 12 | A6 | 201 | CYC | C2C-C1C | -2.53 | 1.49 | 1.52 |
| 12 | D5 | 201 | CYC | C1D-CHD | 2.53 | 1.50 | 1.41 |
| 12 | O1 | 201 | CYC | C1B-NB | -2.53 | 1.33 | 1.37 |
| 12 | O3 | 201 | CYC | C1B-NB | -2.53 | 1.33 | 1.37 |
| 12 | I6 | 201 | CYC | C1B-NB | -2.53 | 1.33 | 1.37 |
| 12 | B5 | 201 | CYC | OB-C4B | 2.53 | 1.28 | 1.23 |
| 12 | E8 | 201 | CYC | C2C-C1C | -2.53 | 1.49 | 1.52 |
| 12 | I4 | 201 | CYC | C1B-NB | -2.52 | 1.33 | 1.37 |
| 12 | I8 | 201 | CYC | C1B-NB | -2.52 | 1.33 | 1.37 |
| 12 | J5 | 201 | CYC | C1D-CHD | 2.52 | 1.50 | 1.41 |
| 12 | X5 | 201 | CYC | OB-C4B | 2.52 | 1.28 | 1.23 |
| 12 | T5 | 201 | CYC | C1D-CHD | 2.52 | 1.50 | 1.41 |
| 12 | j5 | 1202 | CYC | C1D-CHD | 2.52 | 1.50 | 1.41 |
| 12 | F5 | 201 | CYC | OB-C4B | 2.52 | 1.28 | 1.23 |
| 12 | e5 | 201 | CYC | C1B-C2B | 2.52 | 1.49 | 1.45 |
| 12 | I5 | 201 | CYC | C1C-NC | -2.52 | 1.34 | 1.37 |
| 12 | Y7 | 201 | CYC | OB-C4B | 2.52 | 1.28 | 1.23 |
| 12 | M7 | 201 | CYC | C1C-NC | -2.52 | 1.34 | 1.37 |
| 12 | J7 | 201 | CYC | OB-C4B | 2.51 | 1.28 | 1.23 |
| 12 | Y3 | 201 | CYC | C1B-NB | -2.51 | 1.33 | 1.37 |
| 12 | Y1 | 201 | CYC | C1B-NB | -2.51 | 1.33 | 1.37 |
| 12 | E5 | 201 | CYC | C1B-C2B | 2.51 | 1.49 | 1.45 |
| 12 | GA | 201 | CYC | C1B-NB | -2.51 | 1.33 | 1.37 |
| 12 | UA | 201 | CYC | C1B-NB | -2.51 | 1.33 | 1.37 |
| 12 | K2 | 201 | CYC | C1B-NB | -2.51 | 1.33 | 1.37 |
| 12 | G9 | 201 | CYC | C1B-NB | -2.51 | 1.33 | 1.37 |
| 12 | U9 | 201 | CYC | C1B-NB | -2.51 | 1.33 | 1.37 |
| 12 | Y4 | 201 | CYC | C1D-CHD | 2.51 | 1.50 | 1.41 |
| 12 | k5 | 1202 | CYC | C1D-CHD | 2.51 | 1.50 | 1.41 |
| 12 | k5 | 1203 | CYC | OB-C4B | 2.51 | 1.28 | 1.23 |
| 12 | EA | 201 | CYC | C1B-C2B | 2.51 | 1.49 | 1.45 |
| 12 | E9 | 201 | CYC | C1B-C2B | 2.51 | 1.49 | 1.45 |
| 12 | Z4 | 301 | CYC | C4C-NC | -2.51 | 1.32 | 1.37 |
| 12 | p7 | 201 | CYC | C1D-CHD | 2.51 | 1.50 | 1.41 |
| 12 | c7 | 201 | CYC | C1B-C2B | 2.51 | 1.49 | 1.45 |
| 12 | I2 | 201 | CYC | C1B-NB | -2.51 | 1.33 | 1.37 |
| 12 | R4 | 201 | CYC | C2C-C1C | -2.51 | 1.49 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | R8 | 201 | CYC | C2C-C1C | -2.51 | 1.49 | 1.52 |
| 12 | D5 | 201 | CYC | OB-C4B | 2.51 | 1.28 | 1.23 |
| 12 | C6 | 201 | CYC | C1B-C2B | 2.51 | 1.49 | 1.45 |
| 12 | K5 | 201 | CYC | OB-C4B | 2.51 | 1.28 | 1.23 |
| 12 | D4 | 202 | CYC | C4C-NC | -2.51 | 1.32 | 1.37 |
| 12 | T7 | 201 | CYC | OB-C4B | 2.51 | 1.28 | 1.23 |
| 12 | CA | 201 | CYC | C2C-C1C | -2.51 | 1.49 | 1.52 |
| 12 | c7 | 201 | CYC | OB-C4B | 2.51 | 1.28 | 1.23 |
| 12 | N7 | 201 | CYC | OB-C4B | 2.50 | 1.28 | 1.23 |
| 12 | YA | 201 | CYC | C1B-NB | -2.50 | 1.33 | 1.37 |
| 12 | Y9 | 201 | CYC | C1B-NB | -2.50 | 1.33 | 1.37 |
| 12 | d5 | 201 | CYC | OB-C4B | 2.50 | 1.28 | 1.23 |
| 12 | W4 | 202 | CYC | C1D-CHD | 2.50 | 1.50 | 1.41 |
| 12 | W8 | 202 | CYC | C1D-CHD | 2.50 | 1.50 | 1.41 |
| 12 | A7 | 201 | CYC | C1B-C2B | 2.50 | 1.49 | 1.45 |
| 12 | R7 | 201 | CYC | OB-C4B | 2.50 | 1.28 | 1.23 |
| 12 | q7 | 201 | CYC | C1B-C2B | 2.50 | 1.49 | 1.45 |
| 12 | G7 | 201 | CYC | OB-C4B | 2.50 | 1.28 | 1.23 |
| 12 | D7 | 201 | CYC | OB-C4B | 2.50 | 1.28 | 1.23 |
| 12 | j5 | 1201 | CYC | OB-C4B | 2.50 | 1.28 | 1.23 |
| 12 | X5 | 201 | CYC | C1D-CHD | 2.50 | 1.50 | 1.41 |
| 12 | C9 | 201 | CYC | C2C-C1C | -2.50 | 1.49 | 1.52 |
| 12 | Y8 | 201 | CYC | C1D-CHD | 2.50 | 1.50 | 1.41 |
| 12 | r7 | 201 | CYC | C1D-CHD | 2.50 | 1.50 | 1.41 |
| 12 | P7 | 201 | CYC | C1A-C2A | 2.50 | 1.49 | 1.45 |
| 12 | G1 | 201 | CYC | C1B-NB | -2.50 | 1.33 | 1.37 |
| 12 | K3 | 201 | CYC | C1B-NB | -2.50 | 1.33 | 1.37 |
| 12 | K1 | 201 | CYC | C1B-NB | -2.50 | 1.33 | 1.37 |
| 12 | S4 | 202 | CYC | C1B-C2B | 2.50 | 1.49 | 1.45 |
| 12 | a5 | 201 | CYC | C1B-C2B | 2.50 | 1.49 | 1.45 |
| 12 | B4 | 202 | CYC | C1B-C2B | 2.50 | 1.49 | 1.45 |
| 12 | PA | 201 | CYC | C4C-NC | -2.50 | 1.32 | 1.37 |
| 12 | P9 | 201 | CYC | C4C-NC | -2.50 | 1.32 | 1.37 |
| 12 | Q5 | 201 | CYC | C2C-C1C | -2.50 | 1.49 | 1.52 |
| 12 | I4 | 201 | CYC | C1B-C2B | 2.50 | 1.49 | 1.45 |
| 12 | I8 | 201 | CYC | C1B-C2B | 2.50 | 1.49 | 1.45 |
| 12 | JA | 201 | CYC | C1D-CHD | 2.49 | 1.50 | 1.41 |
| 12 | J9 | 201 | CYC | C1D-CHD | 2.49 | 1.50 | 1.41 |
| 12 | q7 | 201 | CYC | OB-C4B | 2.49 | 1.28 | 1.23 |
| 12 | p7 | 201 | CYC | OB-C4B | 2.49 | 1.28 | 1.23 |
| 12 | C3 | 201 | CYC | C1B-NB | -2.49 | 1.33 | 1.37 |
| 12 | C1 | 201 | CYC | C1B-NB | -2.49 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | r7 | 201 | CYC | OB-C4B | 2.49 | 1.28 | 1.23 |
| 12 | DA | 201 | CYC | C4C-NC | -2.49 | 1.32 | 1.37 |
| 12 | M8 | 301 | CYC | C4C-NC | -2.49 | 1.32 | 1.37 |
| 12 | D9 | 201 | CYC | C4C-NC | -2.49 | 1.32 | 1.37 |
| 12 | R5 | 201 | CYC | C1D-CHD | 2.49 | 1.50 | 1.41 |
| 12 | k5 | 1203 | CYC | C1D-CHD | 2.49 | 1.50 | 1.41 |
| 12 | j7 | 201 | CYC | C1D-CHD | 2.49 | 1.50 | 1.41 |
| 12 | P7 | 201 | CYC | OB-C4B | 2.49 | 1.28 | 1.23 |
| 12 | K4 | 201 | CYC | C2C-C1C | -2.49 | 1.49 | 1.52 |
| 12 | K8 | 201 | CYC | C2C-C1C | -2.49 | 1.49 | 1.52 |
| 12 | N8 | 201 | CYC | C1B-NB | -2.49 | 1.33 | 1.37 |
| 12 | A4 | 201 | CYC | C1B-C2B | 2.49 | 1.49 | 1.45 |
| 12 | A8 | 201 | CYC | C1B-C2B | 2.49 | 1.49 | 1.45 |
| 12 | J2 | 201 | CYC | C1D-CHD | 2.49 | 1.50 | 1.41 |
| 12 | J6 | 201 | CYC | C1D-CHD | 2.49 | 1.50 | 1.41 |
| 12 | A7 | 201 | CYC | OB-C4B | 2.49 | 1.28 | 1.23 |
| 12 | F7 | 201 | CYC | C1D-CHD | 2.49 | 1.50 | 1.41 |
| 12 | k5 | 1201 | CYC | OB-C4B | 2.49 | 1.28 | 1.23 |
| 12 | v7 | 201 | CYC | OB-C4B | 2.49 | 1.28 | 1.23 |
| 12 | V5 | 201 | CYC | OB-C4B | 2.48 | 1.28 | 1.23 |
| 12 | Z3 | 201 | CYC | C4C-NC | -2.48 | 1.32 | 1.37 |
| 12 | Z1 | 202 | CYC | C4C-NC | -2.48 | 1.32 | 1.37 |
| 12 | e7 | 201 | CYC | OB-C4B | 2.48 | 1.28 | 1.23 |
| 12 | A | 201 | CYC | C1D-CHD | 2.48 | 1.50 | 1.41 |
| 12 | g7 | 201 | CYC | C1B-C2B | 2.48 | 1.49 | 1.45 |
| 12 | KA | 201 | CYC | C1B-NB | -2.48 | 1.33 | 1.37 |
| 12 | K9 | 201 | CYC | C1B-NB | -2.48 | 1.33 | 1.37 |
| 12 | K3 | 201 | CYC | C1B-C2B | 2.48 | 1.49 | 1.45 |
| 12 | K1 | 201 | CYC | C1B-C2B | 2.48 | 1.49 | 1.45 |
| 12 | M7 | 201 | CYC | OB-C4B | 2.48 | 1.28 | 1.23 |
| 12 | D6 | 202 | CYC | C1D-CHD | 2.48 | 1.50 | 1.41 |
| 12 | D2 | 202 | CYC | C1D-CHD | 2.48 | 1.50 | 1.41 |
| 12 | R1 | 202 | CYC | C1D-CHD | 2.48 | 1.50 | 1.41 |
| 12 | R3 | 202 | CYC | C1D-CHD | 2.48 | 1.50 | 1.41 |
| 12 | L7 | 201 | CYC | C1D-CHD | 2.48 | 1.50 | 1.41 |
| 12 | D3 | 202 | CYC | C1B-C2B | 2.48 | 1.49 | 1.45 |
| 12 | D1 | 202 | CYC | C1B-C2B | 2.48 | 1.49 | 1.45 |
| 12 | L4 | 202 | CYC | C4C-NC | -2.48 | 1.32 | 1.37 |
| 12 | OA | 201 | CYC | C1C-NC | -2.48 | 1.34 | 1.37 |
| 12 | O9 | 201 | CYC | C1C-NC | -2.48 | 1.34 | 1.37 |
| 12 | P5 | 201 | CYC | OB-C4B | 2.48 | 1.28 | 1.23 |
| 12 | L4 | 201 | CYC | C1D-CHD | 2.48 | 1.50 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | L8 | 201 | CYC | C1D-CHD | 2.48 | 1.50 | 1.41 |
| 12 | Z | 201 | CYC | C1D-CHD | 2.48 | 1.50 | 1.41 |
| 12 | B3 | 201 | CYC | C1D-CHD | 2.48 | 1.50 | 1.41 |
| 12 | B1 | 201 | CYC | C1D-CHD | 2.48 | 1.50 | 1.41 |
| 12 | X7 | 201 | CYC | OB-C4B | 2.48 | 1.28 | 1.23 |
| 12 | G7 | 201 | CYC | C1C-NC | -2.48 | 1.34 | 1.37 |
| 12 | S4 | 201 | CYC | C1D-CHD | 2.48 | 1.50 | 1.41 |
| 12 | S8 | 201 | CYC | C1D-CHD | 2.48 | 1.50 | 1.41 |
| 12 | i7 | 201 | CYC | C1B-C2B | 2.48 | 1.49 | 1.45 |
| 12 | o7 | 201 | CYC | OB-C4B | 2.48 | 1.28 | 1.23 |
| 12 | AA | 201 | CYC | C1B-NB | -2.48 | 1.33 | 1.37 |
| 12 | A9 | 201 | CYC | C1B-NB | -2.48 | 1.33 | 1.37 |
| 12 | F3 | 201 | CYC | C4C-NC | -2.47 | 1.32 | 1.37 |
| 12 | F1 | 201 | CYC | C4C-NC | -2.47 | 1.32 | 1.37 |
| 12 | Q1 | 201 | CYC | C2C-C1C | -2.47 | 1.49 | 1.52 |
| 12 | Q3 | 201 | CYC | C2C-C1C | -2.47 | 1.49 | 1.52 |
| 12 | o7 | 201 | CYC | C2C-C1C | -2.47 | 1.49 | 1.52 |
| 12 | N4 | 201 | CYC | C1B-NB | -2.47 | 1.33 | 1.37 |
| 12 | R5 | 201 | CYC | OB-C4B | 2.47 | 1.28 | 1.23 |
| 12 | a7 | 201 | CYC | C1B-C2B | 2.47 | 1.49 | 1.45 |
| 12 | a9 | 901 | CYC | C4C-NC | -2.47 | 1.32 | 1.37 |
| 12 | S1 | 201 | CYC | C1B-NB | -2.47 | 1.33 | 1.37 |
| 12 | S3 | 201 | CYC | C1B-NB | -2.47 | 1.33 | 1.37 |
| 12 | C2 | 201 | CYC | C1B-C2B | 2.47 | 1.49 | 1.45 |
| 12 | A | 201 | CYC | OB-C4B | 2.47 | 1.28 | 1.23 |
| 12 | m7 | 201 | CYC | C1B-C2B | 2.47 | 1.49 | 1.45 |
| 12 | d7 | 201 | CYC | C1D-CHD | 2.47 | 1.50 | 1.41 |
| 12 | Y3 | 201 | CYC | C1B-C2B | 2.47 | 1.49 | 1.45 |
| 12 | s7 | 201 | CYC | C1B-C2B | 2.47 | 1.49 | 1.45 |
| 12 | Y1 | 201 | CYC | C1B-C2B | 2.47 | 1.49 | 1.45 |
| 12 | H5 | 201 | CYC | OB-C4B | 2.47 | 1.28 | 1.23 |
| 12 | A6 | 201 | CYC | C1B-C2B | 2.47 | 1.49 | 1.45 |
| 12 | M8 | 302 | CYC | C4C-NC | -2.47 | 1.32 | 1.37 |
| 12 | D2 | 201 | CYC | C1B-C2B | 2.47 | 1.49 | 1.45 |
| 12 | W1 | 201 | CYC | C1B-NB | -2.47 | 1.33 | 1.37 |
| 12 | Z8 | 301 | CYC | C4C-NC | -2.46 | 1.32 | 1.37 |
| 12 | L3 | 201 | CYC | C1D-CHD | 2.46 | 1.50 | 1.41 |
| 12 | L1 | 201 | CYC | C1D-CHD | 2.46 | 1.50 | 1.41 |
| 12 | L6 | 202 | CYC | C1D-CHD | 2.46 | 1.50 | 1.41 |
| 12 | F2 | 201 | CYC | C1B-C2B | 2.46 | 1.49 | 1.45 |
| 12 | X7 | 201 | CYC | C1D-CHD | 2.46 | 1.50 | 1.41 |
| 12 | DA | 201 | CYC | C1B-C2B | 2.46 | 1.49 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | W5 | 201 | CYC | C2C-C1C | -2.46 | 1.49 | 1.52 |
| 12 | Q7 | 201 | CYC | C2C-C1C | -2.46 | 1.49 | 1.52 |
| 12 | O8 | 202 | CYC | C1D-CHD | 2.46 | 1.50 | 1.41 |
| 12 | A1 | 201 | CYC | C1B-NB | -2.46 | 1.33 | 1.37 |
| 12 | A3 | 201 | CYC | C1B-NB | -2.46 | 1.33 | 1.37 |
| 12 | JA | 202 | CYC | C1B-C2B | 2.46 | 1.49 | 1.45 |
| 12 | J9 | 202 | CYC | C1B-C2B | 2.46 | 1.49 | 1.45 |
| 12 | S7 | 201 | CYC | OB-C4B | 2.46 | 1.28 | 1.23 |
| 12 | W5 | 201 | CYC | C1B-C2B | 2.46 | 1.49 | 1.45 |
| 12 | K6 | 201 | CYC | C1B-NB | -2.46 | 1.33 | 1.37 |
| 12 | f5 | 201 | CYC | C1D-CHD | 2.46 | 1.50 | 1.41 |
| 12 | K5 | 201 | CYC | C1B-C2B | 2.46 | 1.49 | 1.45 |
| 12 | L7 | 201 | CYC | OB-C4B | 2.46 | 1.28 | 1.23 |
| 12 | CA | 201 | CYC | C1B-NB | -2.46 | 1.33 | 1.37 |
| 12 | C9 | 201 | CYC | C1B-NB | -2.46 | 1.33 | 1.37 |
| 12 | J4 | 202 | CYC | C1D-CHD | 2.46 | 1.50 | 1.41 |
| 12 | J8 | 202 | CYC | C1D-CHD | 2.46 | 1.50 | 1.41 |
| 12 | J3 | 201 | CYC | C1D-CHD | 2.46 | 1.50 | 1.41 |
| 12 | J1 | 201 | CYC | C1D-CHD | 2.46 | 1.50 | 1.41 |
| 12 | DA | 202 | CYC | C1D-CHD | 2.46 | 1.50 | 1.41 |
| 12 | D9 | 202 | CYC | C1D-CHD | 2.46 | 1.50 | 1.41 |
| 12 | D6 | 201 | CYC | C1B-C2B | 2.46 | 1.49 | 1.45 |
| 12 | B8 | 202 | CYC | C1B-C2B | 2.46 | 1.49 | 1.45 |
| 12 | M8 | 302 | CYC | C1B-C2B | 2.46 | 1.49 | 1.45 |
| 12 | TA | 301 | CYC | C4C-NC | -2.45 | 1.32 | 1.37 |
| 12 | T9 | 301 | CYC | C4C-NC | -2.45 | 1.32 | 1.37 |
| 12 | Z3 | 202 | CYC | C1D-CHD | 2.45 | 1.50 | 1.41 |
| 12 | Z1 | 201 | CYC | C1D-CHD | 2.45 | 1.50 | 1.41 |
| 12 | k7 | 201 | CYC | OB-C4B | 2.45 | 1.28 | 1.23 |
| 12 | o7 | 201 | CYC | C1B-C2B | 2.45 | 1.49 | 1.45 |
| 12 | c7 | 201 | CYC | C2C-C1C | -2.45 | 1.49 | 1.52 |
| 12 | W5 | 201 | CYC | OB-C4B | 2.45 | 1.28 | 1.23 |
| 12 | A7 | 201 | CYC | C1C-NC | -2.45 | 1.34 | 1.37 |
| 12 | V7 | 201 | CYC | OB-C4B | 2.45 | 1.28 | 1.23 |
| 12 | Q5 | 201 | CYC | C1B-C2B | 2.45 | 1.49 | 1.45 |
| 12 | S4 | 202 | CYC | C4C-NC | -2.45 | 1.32 | 1.37 |
| 12 | b5 | 201 | CYC | C1D-CHD | 2.45 | 1.50 | 1.41 |
| 12 | B5 | 201 | CYC | C1A-C2A | 2.45 | 1.49 | 1.45 |
| 12 | L2 | 202 | CYC | C1D-CHD | 2.45 | 1.50 | 1.41 |
| 12 | T3 | 302 | CYC | C1D-CHD | 2.45 | 1.50 | 1.41 |
| 12 | T1 | 302 | CYC | C1D-CHD | 2.45 | 1.50 | 1.41 |
| 12 | W7 | 201 | CYC | C2C-C1C | -2.45 | 1.49 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | u7 | 201 | CYC | C1B-C2B | 2.45 | 1.49 | 1.45 |
| 12 | L2 | 201 | CYC | C4C-NC | -2.45 | 1.32 | 1.37 |
| 12 | Q5 | 201 | CYC | OB-C4B | 2.45 | 1.28 | 1.23 |
| 12 | G3 | 201 | CYC | C1B-NB | -2.45 | 1.33 | 1.37 |
| 12 | K2 | 201 | CYC | C1B-C2B | 2.45 | 1.49 | 1.45 |
| 12 | Z | 201 | CYC | OB-C4B | 2.45 | 1.28 | 1.23 |
| 12 | B7 | 201 | CYC | OB-C4B | 2.45 | 1.28 | 1.23 |
| 12 | f7 | 201 | CYC | OB-C4B | 2.45 | 1.28 | 1.23 |
| 12 | LA | 201 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | XA | 202 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | L9 | 201 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | X9 | 202 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | G4 | 201 | CYC | C1B-NB | -2.44 | 1.33 | 1.37 |
| 12 | G8 | 201 | CYC | C1B-NB | -2.44 | 1.33 | 1.37 |
| 12 | R7 | 201 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | D9 | 201 | CYC | C1B-C2B | 2.44 | 1.49 | 1.45 |
| 12 | D3 | 201 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | Q4 | 201 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | D1 | 201 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | O4 | 201 | CYC | C4C-NC | -2.44 | 1.32 | 1.37 |
| 12 | O8 | 201 | CYC | C4C-NC | -2.44 | 1.32 | 1.37 |
| 12 | X3 | 201 | CYC | C1B-C2B | 2.44 | 1.49 | 1.45 |
| 12 | X1 | 201 | CYC | C1B-C2B | 2.44 | 1.49 | 1.45 |
| 12 | F1 | 202 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | O4 | 202 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | ZA | 201 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | Z9 | 201 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | F6 | 201 | CYC | C1B-C2B | 2.44 | 1.49 | 1.45 |
| 12 | K6 | 201 | CYC | C1B-C2B | 2.44 | 1.49 | 1.45 |
| 12 | J5 | 201 | CYC | C4C-NC | -2.44 | 1.32 | 1.37 |
| 12 | b5 | 201 | CYC | OB-C4B | 2.44 | 1.28 | 1.23 |
| 12 | k5 | 1202 | CYC | OB-C4B | 2.44 | 1.28 | 1.23 |
| 12 | BA | 202 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | PA | 202 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | P9 | 202 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | B9 | 202 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | P1 | 202 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | P3 | 202 | CYC | C1D-CHD | 2.44 | 1.50 | 1.41 |
| 12 | b7 | 201 | CYC | OB-C4B | 2.44 | 1.28 | 1.23 |
| 12 | EA | 201 | CYC | C1B-NB | -2.44 | 1.33 | 1.37 |
| 12 | E8 | 201 | CYC | C1B-NB | -2.44 | 1.33 | 1.37 |
| 12 | C5 | 201 | CYC | C1B-C2B | 2.44 | 1.49 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | R1 | 201 | CYC | C4C-NC | -2.44 | 1.32 | 1.37 |
| 12 | R3 | 201 | CYC | C4C-NC | -2.44 | 1.32 | 1.37 |
| 12 | M4 | 301 | CYC | C4C-NC | -2.44 | 1.32 | 1.37 |
| 12 | H7 | 201 | CYC | OB-C4B | 2.44 | 1.28 | 1.23 |
| 12 | HA | 201 | CYC | C1D-CHD | 2.43 | 1.50 | 1.41 |
| 12 | H9 | 201 | CYC | C1D-CHD | 2.43 | 1.50 | 1.41 |
| 12 | F4 | 201 | CYC | C1D-CHD | 2.43 | 1.50 | 1.41 |
| 12 | F8 | 201 | CYC | C1D-CHD | 2.43 | 1.50 | 1.41 |
| 12 | V3 | 201 | CYC | C4C-NC | -2.43 | 1.32 | 1.37 |
| 12 | V1 | 201 | CYC | C4C-NC | -2.43 | 1.32 | 1.37 |
| 12 | W3 | 201 | CYC | C1B-C2B | 2.43 | 1.49 | 1.45 |
| 12 | V4 | 201 | CYC | C1B-C2B | 2.43 | 1.49 | 1.45 |
| 12 | W1 | 201 | CYC | C1B-C2B | 2.43 | 1.49 | 1.45 |
| 12 | j5 | 1202 | CYC | OB-C4B | 2.43 | 1.28 | 1.23 |
| 12 | E9 | 201 | CYC | C1B-NB | -2.43 | 1.33 | 1.37 |
| 12 | K8 | 201 | CYC | C1B-NB | -2.43 | 1.33 | 1.37 |
| 12 | Q8 | 201 | CYC | C1D-CHD | 2.43 | 1.50 | 1.41 |
| 12 | T3 | 301 | CYC | C1B-C2B | 2.43 | 1.49 | 1.45 |
| 12 | T1 | 301 | CYC | C1B-C2B | 2.43 | 1.49 | 1.45 |
| 12 | k5 | 1204 | CYC | C4C-NC | -2.43 | 1.32 | 1.37 |
| 12 | W3 | 201 | CYC | C1B-NB | -2.43 | 1.33 | 1.37 |
| 12 | D5 | 201 | CYC | C4C-NC | -2.43 | 1.32 | 1.37 |
| 12 | V1 | 202 | CYC | C1D-CHD | 2.43 | 1.50 | 1.41 |
| 12 | TA | 302 | CYC | C1D-CHD | 2.43 | 1.50 | 1.41 |
| 12 | T9 | 302 | CYC | C1D-CHD | 2.43 | 1.50 | 1.41 |
| 12 | G2 | 201 | CYC | C1B-NB | -2.43 | 1.33 | 1.37 |
| 12 | X3 | 201 | CYC | C4C-NC | -2.43 | 1.32 | 1.37 |
| 12 | W4 | 201 | CYC | C4C-NC | -2.43 | 1.32 | 1.37 |
| 12 | W8 | 201 | CYC | C4C-NC | -2.43 | 1.32 | 1.37 |
| 12 | X1 | 201 | CYC | C4C-NC | -2.43 | 1.32 | 1.37 |
| 12 | S1 | 201 | CYC | C1C-NC | -2.43 | 1.34 | 1.37 |
| 12 | S3 | 201 | CYC | C1C-NC | -2.43 | 1.34 | 1.37 |
| 12 | D6 | 201 | CYC | C4C-NC | -2.43 | 1.32 | 1.37 |
| 12 | K4 | 201 | CYC | C1B-NB | -2.43 | 1.33 | 1.37 |
| 12 | F4 | 202 | CYC | C4C-NC | -2.42 | 1.32 | 1.37 |
| 12 | F8 | 202 | CYC | C4C-NC | -2.42 | 1.32 | 1.37 |
| 12 | F7 | 201 | CYC | OB-C4B | 2.42 | 1.28 | 1.23 |
| 12 | V3 | 202 | CYC | C1D-CHD | 2.42 | 1.50 | 1.41 |
| 12 | B6 | 201 | CYC | C1D-CHD | 2.42 | 1.50 | 1.41 |
| 12 | WA | 201 | CYC | C1B-NB | -2.42 | 1.33 | 1.37 |
| 12 | UA | 201 | CYC | C1B-C2B | 2.42 | 1.49 | 1.45 |
| 12 | U9 | 201 | CYC | C1B-C2B | 2.42 | 1.49 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | X3 | 202 | CYC | C1D-CHD | 2.42 | 1.50 | 1.41 |
| 12 | X1 | 202 | CYC | C1D-CHD | 2.42 | 1.50 | 1.41 |
| 12 | u7 | 201 | CYC | OB-C4B | 2.42 | 1.28 | 1.23 |
| 12 | I7 | 201 | CYC | C1B-C2B | 2.42 | 1.49 | 1.45 |
| 12 | VA | 202 | CYC | C1D-CHD | 2.42 | 1.50 | 1.41 |
| 12 | V9 | 202 | CYC | C1D-CHD | 2.42 | 1.50 | 1.41 |
| 12 | G1 | 201 | CYC | C1B-C2B | 2.42 | 1.49 | 1.45 |
| 12 | F3 | 202 | CYC | C1D-CHD | 2.42 | 1.50 | 1.41 |
| 12 | H4 | 202 | CYC | C1D-CHD | 2.42 | 1.50 | 1.41 |
| 12 | H8 | 202 | CYC | C1D-CHD | 2.42 | 1.50 | 1.41 |
| 12 | I5 | 201 | CYC | C1B-C2B | 2.42 | 1.49 | 1.45 |
| 12 | D4 | 201 | CYC | C1D-CHD | 2.42 | 1.50 | 1.41 |
| 12 | D8 | 201 | CYC | C1D-CHD | 2.42 | 1.50 | 1.41 |
| 12 | B4 | 202 | CYC | C4C-NC | -2.42 | 1.32 | 1.37 |
| 12 | V4 | 201 | CYC | C1B-NB | -2.42 | 1.33 | 1.37 |
| 12 | BA | 201 | CYC | C4C-NC | -2.42 | 1.32 | 1.37 |
| 12 | B9 | 201 | CYC | C4C-NC | -2.42 | 1.32 | 1.37 |
| 12 | B3 | 202 | CYC | C4C-NC | -2.42 | 1.32 | 1.37 |
| 12 | Q1 | 201 | CYC | C1B-NB | -2.42 | 1.33 | 1.37 |
| 12 | Q3 | 201 | CYC | C1B-NB | -2.42 | 1.33 | 1.37 |
| 12 | P8 | 201 | CYC | C1B-C2B | 2.42 | 1.49 | 1.45 |
| 12 | LA | 202 | CYC | C4C-NC | -2.42 | 1.32 | 1.37 |
| 12 | L9 | 202 | CYC | C4C-NC | -2.42 | 1.32 | 1.37 |
| 12 | G4 | 201 | CYC | C1B-C2B | 2.42 | 1.49 | 1.45 |
| 12 | G8 | 201 | CYC | C1B-C2B | 2.42 | 1.49 | 1.45 |
| 12 | j5 | 1201 | CYC | C4B-NB | -2.42 | 1.32 | 1.38 |
| 12 | P4 | 201 | CYC | C1B-NB | -2.42 | 1.33 | 1.37 |
| 12 | P8 | 201 | CYC | C1B-NB | -2.42 | 1.33 | 1.37 |
| 12 | j5 | 1202 | CYC | C1A-C2A | 2.42 | 1.49 | 1.45 |
| 12 | E4 | 201 | CYC | C1B-NB | -2.41 | 1.33 | 1.37 |
| 12 | T3 | 301 | CYC | C4C-NC | -2.41 | 1.32 | 1.37 |
| 12 | T1 | 301 | CYC | C4C-NC | -2.41 | 1.32 | 1.37 |
| 12 | AA | 201 | CYC | C1B-C2B | 2.41 | 1.49 | 1.45 |
| 12 | C7 | 201 | CYC | C1B-C2B | 2.41 | 1.49 | 1.45 |
| 12 | A9 | 201 | CYC | C1B-C2B | 2.41 | 1.49 | 1.45 |
| 12 | F6 | 202 | CYC | C1D-CHD | 2.41 | 1.50 | 1.41 |
| 12 | F2 | 202 | CYC | C1D-CHD | 2.41 | 1.50 | 1.41 |
| 12 | RA | 202 | CYC | C1D-CHD | 2.41 | 1.50 | 1.41 |
| 12 | R9 | 202 | CYC | C1D-CHD | 2.41 | 1.50 | 1.41 |
| 12 | A2 | 201 | CYC | C1B-C2B | 2.41 | 1.49 | 1.45 |
| 12 | B8 | 202 | CYC | C4C-NC | -2.41 | 1.32 | 1.37 |
| 12 | c5 | 201 | CYC | C1B-C2B | 2.41 | 1.49 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | D2 | 201 | CYC | C4C-NC | -2.41 | 1.32 | 1.37 |
| 12 | U5 | 201 | CYC | C1B-C2B | 2.41 | 1.49 | 1.45 |
| 12 | L6 | 201 | CYC | C4C-NC | -2.41 | 1.32 | 1.37 |
| 12 | VA | 201 | CYC | C4C-NC | -2.41 | 1.32 | 1.37 |
| 12 | V9 | 201 | CYC | C4C-NC | -2.41 | 1.32 | 1.37 |
| 12 | D3 | 202 | CYC | C4C-NC | -2.41 | 1.32 | 1.37 |
| 12 | D1 | 202 | CYC | C4C-NC | -2.41 | 1.32 | 1.37 |
| 12 | A1 | 201 | CYC | C1C-NC | -2.41 | 1.34 | 1.37 |
| 12 | A3 | 201 | CYC | C1C-NC | -2.41 | 1.34 | 1.37 |
| 12 | OA | 201 | CYC | C1B-C2B | 2.41 | 1.49 | 1.45 |
| 12 | C4 | 201 | CYC | C1B-C2B | 2.41 | 1.49 | 1.45 |
| 12 | C8 | 201 | CYC | C1B-C2B | 2.41 | 1.49 | 1.45 |
| 12 | O9 | 201 | CYC | C1B-C2B | 2.41 | 1.49 | 1.45 |
| 12 | WA | 201 | CYC | C1B-C2B | 2.41 | 1.49 | 1.45 |
| 12 | W9 | 201 | CYC | C1B-C2B | 2.41 | 1.49 | 1.45 |
| 12 | H5 | 201 | CYC | C1A-C2A | 2.41 | 1.49 | 1.45 |
| 12 | V8 | 201 | CYC | C1B-C2B | 2.41 | 1.49 | 1.45 |
| 12 | O1 | 201 | CYC | C1B-C2B | 2.41 | 1.49 | 1.45 |
| 12 | O3 | 201 | CYC | C1B-C2B | 2.41 | 1.49 | 1.45 |
| 12 | QA | 201 | CYC | C1B-NB | -2.41 | 1.33 | 1.37 |
| 12 | h7 | 201 | CYC | C1A-C2A | 2.41 | 1.49 | 1.45 |
| 12 | b7 | 201 | CYC | C1A-C2A | 2.41 | 1.49 | 1.45 |
| 12 | N5 | 201 | CYC | OB-C4B | 2.41 | 1.28 | 1.23 |
| 12 | O7 | 201 | CYC | C1B-C2B | 2.41 | 1.49 | 1.45 |
| 12 | h7 | 201 | CYC | OB-C4B | 2.40 | 1.28 | 1.23 |
| 12 | B2 | 201 | CYC | C1D-CHD | 2.40 | 1.50 | 1.41 |
| 12 | XA | 201 | CYC | C4C-NC | -2.40 | 1.32 | 1.37 |
| 12 | X9 | 201 | CYC | C4C-NC | -2.40 | 1.32 | 1.37 |
| 12 | H1 | 201 | CYC | OB-C4B | 2.40 | 1.28 | 1.23 |
| 12 | I2 | 201 | CYC | C1B-C2B | 2.40 | 1.49 | 1.45 |
| 12 | Q9 | 201 | CYC | C1B-NB | -2.40 | 1.33 | 1.37 |
| 12 | D5 | 201 | CYC | C1A-C2A | 2.40 | 1.49 | 1.45 |
| 12 | FA | 301 | CYC | C1B-C2B | 2.40 | 1.49 | 1.45 |
| 12 | F9 | 301 | CYC | C1B-C2B | 2.40 | 1.49 | 1.45 |
| 12 | E3 | 201 | CYC | C1B-NB | -2.40 | 1.33 | 1.37 |
| 12 | E1 | 201 | CYC | C1B-NB | -2.40 | 1.33 | 1.37 |
| 12 | M5 | 201 | CYC | OB-C4B | 2.40 | 1.28 | 1.23 |
| 12 | N6 | 101 | CYC | C4C-NC | -2.40 | 1.32 | 1.37 |
| 12 | T5 | 201 | CYC | OB-C4B | 2.40 | 1.28 | 1.23 |
| 12 | Y5 | 201 | CYC | C1B-C2B | 2.40 | 1.49 | 1.45 |
| 12 | H3 | 202 | CYC | OB-C4B | 2.40 | 1.28 | 1.23 |
| 12 | J3 | 202 | CYC | C4C-NC | -2.40 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | aA | 901 | CYC | C4C-NC | -2.40 | 1.32 | 1.37 |
| 12 | X4 | 201 | CYC | C1B-NB | -2.40 | 1.33 | 1.37 |
| 12 | X8 | 201 | CYC | C1B-NB | -2.40 | 1.33 | 1.37 |
| 12 | O5 | 201 | CYC | C1B-C2B | 2.39 | 1.49 | 1.45 |
| 12 | S5 | 201 | CYC | OB-C4B | 2.39 | 1.28 | 1.23 |
| 12 | k5 | 1204 | CYC | OB-C4B | 2.39 | 1.28 | 1.23 |
| 12 | G6 | 201 | CYC | C1B-NB | -2.39 | 1.33 | 1.37 |
| 12 | B4 | 201 | CYC | C1D-CHD | 2.39 | 1.50 | 1.41 |
| 12 | B8 | 201 | CYC | C1D-CHD | 2.39 | 1.50 | 1.41 |
| 12 | R1 | 201 | CYC | C1B-C2B | 2.39 | 1.49 | 1.45 |
| 12 | R3 | 201 | CYC | C1B-C2B | 2.39 | 1.49 | 1.45 |
| 12 | k5 | 1204 | CYC | C1A-C2A | 2.39 | 1.49 | 1.45 |
| 12 | J6 | 202 | CYC | C4C-NC | -2.39 | 1.32 | 1.37 |
| 12 | G3 | 201 | CYC | C1B-C2B | 2.39 | 1.49 | 1.45 |
| 12 | W9 | 201 | CYC | C1B-NB | -2.39 | 1.33 | 1.37 |
| 12 | V8 | 201 | CYC | C1B-NB | -2.39 | 1.33 | 1.37 |
| 12 | L3 | 202 | CYC | C1B-C2B | 2.38 | 1.49 | 1.45 |
| 12 | IA | 201 | CYC | C2C-C1C | -2.38 | 1.50 | 1.52 |
| 12 | K3 | 201 | CYC | C2C-C1C | -2.38 | 1.50 | 1.52 |
| 12 | I9 | 201 | CYC | C2C-C1C | -2.38 | 1.50 | 1.52 |
| 12 | u7 | 201 | CYC | C2C-C1C | -2.38 | 1.50 | 1.52 |
| 12 | Q1 | 201 | CYC | C1B-C2B | 2.38 | 1.49 | 1.45 |
| 12 | Q3 | 201 | CYC | C1B-C2B | 2.38 | 1.49 | 1.45 |
| 12 | J5 | 201 | CYC | C1A-C2A | 2.38 | 1.49 | 1.45 |
| 12 | KA | 201 | CYC | C1B-C2B | 2.38 | 1.49 | 1.45 |
| 12 | K9 | 201 | CYC | C1B-C2B | 2.38 | 1.49 | 1.45 |
| 12 | LA | 202 | CYC | OB-C4B | 2.38 | 1.28 | 1.23 |
| 12 | L9 | 202 | CYC | OB-C4B | 2.38 | 1.28 | 1.23 |
| 12 | J7 | 201 | CYC | C1A-C2A | 2.38 | 1.49 | 1.45 |
| 12 | H6 | 202 | CYC | C1D-CHD | 2.38 | 1.50 | 1.41 |
| 12 | F9 | 302 | CYC | C1D-CHD | 2.38 | 1.50 | 1.41 |
| 12 | J4 | 201 | CYC | C4C-NC | -2.38 | 1.32 | 1.37 |
| 12 | J8 | 201 | CYC | C4C-NC | -2.38 | 1.32 | 1.37 |
| 12 | TA | 301 | CYC | C1B-C2B | 2.38 | 1.49 | 1.45 |
| 12 | T9 | 301 | CYC | C1B-C2B | 2.38 | 1.49 | 1.45 |
| 12 | T4 | 201 | CYC | C1B-NB | -2.38 | 1.33 | 1.37 |
| 12 | T8 | 201 | CYC | C1B-NB | -2.38 | 1.33 | 1.37 |
| 12 | H3 | 201 | CYC | C1D-CHD | 2.38 | 1.50 | 1.41 |
| 12 | H1 | 202 | CYC | C1D-CHD | 2.38 | 1.50 | 1.41 |
| 12 | N4 | 201 | CYC | C1B-C2B | 2.37 | 1.49 | 1.45 |
| 12 | N8 | 201 | CYC | C1B-C2B | 2.37 | 1.49 | 1.45 |
| 12 | B1 | 202 | CYC | C4C-NC | -2.37 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | VA | 201 | CYC | OB-C4B | 2.37 | 1.28 | 1.23 |
| 12 | V9 | 201 | CYC | OB-C4B | 2.37 | 1.28 | 1.23 |
| 12 | E3 | 201 | CYC | C1B-C2B | 2.37 | 1.49 | 1.45 |
| 12 | E1 | 201 | CYC | C1B-C2B | 2.37 | 1.49 | 1.45 |
| 12 | Y5 | 201 | CYC | C2C-C1C | -2.37 | 1.50 | 1.52 |
| 12 | H9 | 202 | CYC | C4C-NC | -2.37 | 1.32 | 1.37 |
| 12 | R4 | 201 | CYC | C1B-NB | -2.37 | 1.33 | 1.37 |
| 12 | R8 | 201 | CYC | C1B-NB | -2.37 | 1.33 | 1.37 |
| 12 | j5 | 1201 | CYC | C1D-CHD | 2.37 | 1.50 | 1.41 |
| 12 | J2 | 202 | CYC | C4C-NC | -2.37 | 1.32 | 1.37 |
| 12 | V7 | 201 | CYC | C1A-C2A | 2.37 | 1.49 | 1.45 |
| 12 | IA | 201 | CYC | C1B-C2B | 2.37 | 1.49 | 1.45 |
| 12 | I9 | 201 | CYC | C1B-C2B | 2.37 | 1.49 | 1.45 |
| 12 | C2 | 201 | CYC | C1B-NB | -2.37 | 1.33 | 1.37 |
| 12 | RA | 201 | CYC | C1B-C2B | 2.37 | 1.49 | 1.45 |
| 12 | R9 | 201 | CYC | C1B-C2B | 2.37 | 1.49 | 1.45 |
| 12 | T5 | 201 | CYC | C4C-NC | -2.37 | 1.32 | 1.37 |
| 12 | P4 | 201 | CYC | C1B-C2B | 2.37 | 1.49 | 1.45 |
| 12 | H1 | 201 | CYC | C4C-NC | -2.37 | 1.32 | 1.37 |
| 12 | U4 | 202 | CYC | C1D-CHD | 2.37 | 1.50 | 1.41 |
| 12 | U8 | 202 | CYC | C1D-CHD | 2.37 | 1.50 | 1.41 |
| 12 | F9 | 303 | CYC | C1D-CHD | 2.36 | 1.50 | 1.41 |
| 12 | V7 | 201 | CYC | C4C-NC | -2.36 | 1.32 | 1.37 |
| 12 | B4 | 202 | CYC | C1D-CHD | 2.36 | 1.50 | 1.41 |
| 12 | W7 | 201 | CYC | C1B-C2B | 2.36 | 1.49 | 1.45 |
| 12 | k5 | 1201 | CYC | C4B-NB | -2.36 | 1.33 | 1.38 |
| 12 | j5 | 1202 | CYC | C4C-NC | -2.36 | 1.32 | 1.37 |
| 12 | k5 | 1201 | CYC | C1D-CHD | 2.36 | 1.50 | 1.41 |
| 12 | IA | 201 | CYC | C1B-NB | -2.36 | 1.33 | 1.37 |
| 12 | I9 | 201 | CYC | C1B-NB | -2.36 | 1.33 | 1.37 |
| 12 | I6 | 201 | CYC | C1B-C2B | 2.36 | 1.49 | 1.45 |
| 12 | V3 | 201 | CYC | C1D-CHD | 2.36 | 1.50 | 1.41 |
| 12 | X3 | 201 | CYC | C1D-CHD | 2.36 | 1.50 | 1.41 |
| 12 | X1 | 201 | CYC | C1D-CHD | 2.36 | 1.50 | 1.41 |
| 12 | J4 | 201 | CYC | OB-C4B | 2.36 | 1.28 | 1.23 |
| 12 | J8 | 201 | CYC | OB-C4B | 2.36 | 1.28 | 1.23 |
| 12 | U3 | 201 | CYC | C1B-C2B | 2.36 | 1.49 | 1.45 |
| 12 | R4 | 201 | CYC | C1B-C2B | 2.36 | 1.49 | 1.45 |
| 12 | R8 | 201 | CYC | C1B-C2B | 2.36 | 1.49 | 1.45 |
| 12 | U1 | 201 | CYC | C1B-C2B | 2.36 | 1.49 | 1.45 |
| 12 | N5 | 201 | CYC | C4C-NC | -2.36 | 1.32 | 1.37 |
| 12 | K1 | 201 | CYC | C2C-C1C | -2.36 | 1.50 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | T7 | 201 | CYC | C1A-C2A | 2.36 | 1.49 | 1.45 |
| 12 | f5 | 201 | CYC | OB-C4B | 2.35 | 1.28 | 1.23 |
| 12 | D8 | 202 | CYC | C4B-NB | -2.35 | 1.33 | 1.38 |
| 12 | E7 | 201 | CYC | C2C-C1C | -2.35 | 1.50 | 1.52 |
| 12 | Z8 | 301 | CYC | C1D-CHD | 2.35 | 1.50 | 1.41 |
| 12 | V1 | 201 | CYC | C1D-CHD | 2.35 | 1.50 | 1.41 |
| 12 | HA | 202 | CYC | C4C-NC | -2.35 | 1.32 | 1.37 |
| 12 | I3 | 201 | CYC | C1B-C2B | 2.35 | 1.49 | 1.45 |
| 12 | T4 | 201 | CYC | C1B-C2B | 2.35 | 1.49 | 1.45 |
| 12 | T8 | 201 | CYC | C1B-C2B | 2.35 | 1.49 | 1.45 |
| 12 | I1 | 201 | CYC | C1B-C2B | 2.35 | 1.49 | 1.45 |
| 12 | W4 | 201 | CYC | C1B-C2B | 2.35 | 1.49 | 1.45 |
| 12 | W8 | 201 | CYC | C1B-C2B | 2.35 | 1.49 | 1.45 |
| 12 | D2 | 201 | CYC | C4B-NB | -2.35 | 1.33 | 1.38 |
| 12 | I3 | 201 | CYC | C1B-NB | -2.35 | 1.33 | 1.37 |
| 12 | I1 | 201 | CYC | C1B-NB | -2.35 | 1.33 | 1.37 |
| 12 | B8 | 202 | CYC | C1D-CHD | 2.35 | 1.50 | 1.41 |
| 12 | P1 | 201 | CYC | C1B-C2B | 2.35 | 1.49 | 1.45 |
| 12 | P3 | 201 | CYC | C1B-C2B | 2.35 | 1.49 | 1.45 |
| 12 | O4 | 201 | CYC | C1D-CHD | 2.35 | 1.50 | 1.41 |
| 12 | O8 | 201 | CYC | C1D-CHD | 2.35 | 1.50 | 1.41 |
| 12 | C6 | 201 | CYC | C1B-NB | -2.35 | 1.33 | 1.37 |
| 12 | H2 | 202 | CYC | C1D-CHD | 2.35 | 1.50 | 1.41 |
| 12 | i7 | 201 | CYC | C2C-C1C | -2.35 | 1.50 | 1.52 |
| 12 | D7 | 201 | CYC | C1A-C2A | 2.35 | 1.49 | 1.45 |
| 12 | U4 | 201 | CYC | OB-C4B | 2.34 | 1.28 | 1.23 |
| 12 | U8 | 201 | CYC | OB-C4B | 2.34 | 1.28 | 1.23 |
| 12 | H1 | 201 | CYC | C1D-CHD | 2.34 | 1.50 | 1.41 |
| 12 | aA | 902 | CYC | C1B-C2B | 2.34 | 1.49 | 1.45 |
| 12 | HA | 202 | CYC | OB-C4B | 2.34 | 1.28 | 1.23 |
| 12 | b5 | 201 | CYC | C4C-NC | -2.34 | 1.32 | 1.37 |
| 12 | CA | 201 | CYC | C1B-C2B | 2.34 | 1.49 | 1.45 |
| 12 | J3 | 202 | CYC | C1B-C2B | 2.34 | 1.49 | 1.45 |
| 12 | M4 | 301 | CYC | C1B-C2B | 2.34 | 1.49 | 1.45 |
| 12 | C9 | 201 | CYC | C1B-C2B | 2.34 | 1.49 | 1.45 |
| 12 | aA | 901 | CYC | C1B-C2B | 2.34 | 1.49 | 1.45 |
| 12 | P1 | 201 | CYC | C1D-CHD | 2.34 | 1.50 | 1.41 |
| 12 | P3 | 201 | CYC | C1D-CHD | 2.34 | 1.50 | 1.41 |
| 12 | A | 201 | CYC | C4C-NC | -2.34 | 1.32 | 1.37 |
| 12 | U4 | 201 | CYC | C1D-CHD | 2.34 | 1.50 | 1.41 |
| 12 | U8 | 201 | CYC | C1D-CHD | 2.34 | 1.50 | 1.41 |
| 12 | X4 | 201 | CYC | C1B-C2B | 2.34 | 1.49 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | X8 | 201 | CYC | C1B-C2B | 2.34 | 1.49 | 1.45 |
| 12 | GA | 201 | CYC | C1C-NC | -2.34 | 1.34 | 1.37 |
| 12 | G9 | 201 | CYC | C1C-NC | -2.34 | 1.34 | 1.37 |
| 12 | S4 | 202 | CYC | OB-C4B | 2.34 | 1.28 | 1.23 |
| 12 | H9 | 202 | CYC | OB-C4B | 2.34 | 1.28 | 1.23 |
| 12 | A1 | 201 | CYC | C2C-C1C | -2.34 | 1.50 | 1.52 |
| 12 | A3 | 201 | CYC | C2C-C1C | -2.34 | 1.50 | 1.52 |
| 12 | JA | 202 | CYC | OB-C4B | 2.34 | 1.28 | 1.23 |
| 12 | J9 | 202 | CYC | OB-C4B | 2.34 | 1.28 | 1.23 |
| 12 | VA | 201 | CYC | C4B-NB | -2.34 | 1.33 | 1.38 |
| 12 | E2 | 201 | CYC | C1B-C2B | 2.34 | 1.49 | 1.45 |
| 12 | N2 | 101 | CYC | C4C-NC | -2.34 | 1.32 | 1.37 |
| 12 | D4 | 202 | CYC | C1B-C2B | 2.34 | 1.49 | 1.45 |
| 12 | D8 | 202 | CYC | C1B-C2B | 2.34 | 1.49 | 1.45 |
| 12 | PA | 201 | CYC | C1D-CHD | 2.33 | 1.50 | 1.41 |
| 12 | P9 | 201 | CYC | C1D-CHD | 2.33 | 1.50 | 1.41 |
| 12 | V9 | 201 | CYC | C4B-NB | -2.33 | 1.33 | 1.38 |
| 12 | U4 | 201 | CYC | C1B-C2B | 2.33 | 1.49 | 1.45 |
| 12 | U8 | 201 | CYC | C1B-C2B | 2.33 | 1.49 | 1.45 |
| 12 | H3 | 202 | CYC | C1D-CHD | 2.33 | 1.50 | 1.41 |
| 12 | X3 | 201 | CYC | OB-C4B | 2.33 | 1.28 | 1.23 |
| 12 | X1 | 201 | CYC | OB-C4B | 2.33 | 1.28 | 1.23 |
| 12 | R5 | 201 | CYC | C1A-C2A | 2.33 | 1.49 | 1.45 |
| 12 | f5 | 201 | CYC | C4C-NC | -2.33 | 1.32 | 1.37 |
| 12 | Z4 | 301 | CYC | C1D-CHD | 2.33 | 1.50 | 1.41 |
| 12 | N2 | 101 | CYC | C1D-CHD | 2.33 | 1.50 | 1.41 |
| 12 | O4 | 201 | CYC | C1B-C2B | 2.33 | 1.49 | 1.45 |
| 12 | O8 | 201 | CYC | C1B-C2B | 2.33 | 1.49 | 1.45 |
| 12 | L2 | 201 | CYC | C1D-CHD | 2.33 | 1.50 | 1.41 |
| 12 | D4 | 202 | CYC | C4B-NB | -2.33 | 1.33 | 1.38 |
| 12 | XA | 201 | CYC | OB-C4B | 2.33 | 1.28 | 1.23 |
| 12 | X9 | 201 | CYC | OB-C4B | 2.33 | 1.28 | 1.23 |
| 12 | Z | 201 | CYC | C4C-NC | -2.33 | 1.32 | 1.37 |
| 12 | PA | 201 | CYC | C1B-C2B | 2.33 | 1.49 | 1.45 |
| 12 | P9 | 201 | CYC | C1B-C2B | 2.33 | 1.49 | 1.45 |
| 12 | G2 | 201 | CYC | C1B-C2B | 2.33 | 1.49 | 1.45 |
| 12 | U7 | 201 | CYC | C1B-C2B | 2.33 | 1.49 | 1.45 |
| 12 | L2 | 201 | CYC | C1B-C2B | 2.33 | 1.49 | 1.45 |
| 12 | L5 | 201 | CYC | C1A-C2A | 2.33 | 1.49 | 1.45 |
| 12 | H3 | 202 | CYC | C4C-NC | -2.32 | 1.32 | 1.37 |
| 12 | B9 | 201 | CYC | OB-C4B | 2.32 | 1.28 | 1.23 |
| 12 | G7 | 201 | CYC | C2C-C1C | -2.32 | 1.50 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | U4 | 201 | CYC | C4C-NC | -2.32 | 1.32 | 1.37 |
| 12 | U8 | 201 | CYC | C4C-NC | -2.32 | 1.32 | 1.37 |
| 12 | BA | 201 | CYC | C1D-CHD | 2.32 | 1.50 | 1.41 |
| 12 | B9 | 201 | CYC | C1D-CHD | 2.32 | 1.50 | 1.41 |
| 12 | V5 | 201 | CYC | C1A-C2A | 2.32 | 1.49 | 1.45 |
| 12 | N2 | 101 | CYC | C1B-C2B | 2.32 | 1.49 | 1.45 |
| 12 | ZA | 202 | CYC | C1B-C2B | 2.32 | 1.49 | 1.45 |
| 12 | E6 | 201 | CYC | C1B-C2B | 2.32 | 1.49 | 1.45 |
| 12 | Q9 | 201 | CYC | C1B-C2B | 2.32 | 1.49 | 1.45 |
| 12 | Z9 | 202 | CYC | C1B-C2B | 2.32 | 1.49 | 1.45 |
| 12 | L6 | 201 | CYC | C1B-C2B | 2.32 | 1.49 | 1.45 |
| 12 | X7 | 201 | CYC | C1A-C2A | 2.32 | 1.49 | 1.45 |
| 12 | L6 | 201 | CYC | C1D-CHD | 2.32 | 1.50 | 1.41 |
| 12 | B1 | 202 | CYC | C1D-CHD | 2.32 | 1.50 | 1.41 |
| 12 | S5 | 201 | CYC | C2C-C1C | -2.32 | 1.50 | 1.52 |
| 12 | E2 | 201 | CYC | C1B-NB | -2.32 | 1.33 | 1.37 |
| 12 | FA | 301 | CYC | C1D-CHD | 2.32 | 1.50 | 1.41 |
| 12 | F9 | 301 | CYC | C1D-CHD | 2.32 | 1.50 | 1.41 |
| 12 | A2 | 201 | CYC | C1C-NC | -2.32 | 1.34 | 1.37 |
| 12 | F5 | 201 | CYC | C1A-C2A | 2.32 | 1.49 | 1.45 |
| 12 | A1 | 201 | CYC | C1B-C2B | 2.32 | 1.49 | 1.45 |
| 12 | A3 | 201 | CYC | C1B-C2B | 2.32 | 1.49 | 1.45 |
| 12 | D3 | 202 | CYC | C1D-CHD | 2.32 | 1.50 | 1.41 |
| 12 | D1 | 202 | CYC | C1D-CHD | 2.32 | 1.50 | 1.41 |
| 12 | R9 | 201 | CYC | C1D-CHD | 2.32 | 1.50 | 1.41 |
| 12 | ZA | 202 | CYC | OB-C4B | 2.32 | 1.28 | 1.23 |
| 12 | V3 | 201 | CYC | OB-C4B | 2.32 | 1.28 | 1.23 |
| 12 | Z9 | 202 | CYC | OB-C4B | 2.32 | 1.28 | 1.23 |
| 12 | V1 | 201 | CYC | OB-C4B | 2.32 | 1.28 | 1.23 |
| 12 | J3 | 202 | CYC | C1D-CHD | 2.32 | 1.50 | 1.41 |
| 12 | aA | 901 | CYC | C1D-CHD | 2.32 | 1.50 | 1.41 |
| 12 | b7 | 201 | CYC | C4C-NC | -2.31 | 1.32 | 1.37 |
| 12 | U9 | 201 | CYC | C1C-NC | -2.31 | 1.34 | 1.37 |
| 12 | h7 | 201 | CYC | C4C-NC | -2.31 | 1.32 | 1.37 |
| 12 | N7 | 201 | CYC | C1A-C2A | 2.31 | 1.49 | 1.45 |
| 12 | P5 | 201 | CYC | C1A-C2A | 2.31 | 1.49 | 1.45 |
| 12 | D6 | 201 | CYC | C4B-NB | -2.31 | 1.33 | 1.38 |
| 12 | r7 | 201 | CYC | C4C-NC | -2.31 | 1.32 | 1.37 |
| 12 | D2 | 201 | CYC | C1D-CHD | 2.31 | 1.50 | 1.41 |
| 12 | H8 | 201 | CYC | C4B-NB | -2.31 | 1.33 | 1.38 |
| 12 | F3 | 201 | CYC | C1B-C2B | 2.31 | 1.49 | 1.45 |
| 12 | F1 | 201 | CYC | C1B-C2B | 2.31 | 1.49 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | X9 | 201 | CYC | C1B-C2B | 2.31 | 1.49 | 1.45 |
| 12 | a5 | 201 | CYC | C2C-C1C | -2.31 | 1.50 | 1.52 |
| 12 | VA | 201 | CYC | C1B-C2B | 2.31 | 1.49 | 1.45 |
| 12 | V9 | 201 | CYC | C1B-C2B | 2.31 | 1.49 | 1.45 |
| 12 | G6 | 201 | CYC | C1B-C2B | 2.31 | 1.49 | 1.45 |
| 12 | N6 | 101 | CYC | C1D-CHD | 2.31 | 1.50 | 1.41 |
| 12 | QA | 201 | CYC | C1B-C2B | 2.30 | 1.49 | 1.45 |
| 12 | J6 | 202 | CYC | C1B-C2B | 2.30 | 1.49 | 1.45 |
| 12 | UA | 201 | CYC | C1C-NC | -2.30 | 1.34 | 1.37 |
| 12 | K7 | 201 | CYC | C2C-C1C | -2.30 | 1.50 | 1.52 |
| 12 | Z5 | 201 | CYC | C1A-C2A | 2.30 | 1.49 | 1.45 |
| 12 | D7 | 201 | CYC | C4C-NC | -2.30 | 1.32 | 1.37 |
| 12 | L2 | 201 | CYC | C1A-NA | -2.30 | 1.33 | 1.38 |
| 12 | L6 | 201 | CYC | C1A-NA | -2.30 | 1.33 | 1.38 |
| 12 | H6 | 201 | CYC | C4C-NC | -2.30 | 1.32 | 1.37 |
| 12 | XA | 201 | CYC | C1D-CHD | 2.30 | 1.50 | 1.41 |
| 12 | B3 | 202 | CYC | C1D-CHD | 2.30 | 1.50 | 1.41 |
| 12 | X9 | 201 | CYC | C1D-CHD | 2.30 | 1.50 | 1.41 |
| 12 | JA | 202 | CYC | C4C-NC | -2.30 | 1.32 | 1.37 |
| 12 | J9 | 202 | CYC | C4C-NC | -2.30 | 1.32 | 1.37 |
| 12 | C3 | 201 | CYC | C1B-C2B | 2.30 | 1.49 | 1.45 |
| 12 | H2 | 201 | CYC | C4C-NC | -2.30 | 1.32 | 1.37 |
| 12 | D4 | 202 | CYC | C1D-CHD | 2.30 | 1.50 | 1.41 |
| 12 | D8 | 202 | CYC | C1D-CHD | 2.30 | 1.50 | 1.41 |
| 12 | Z3 | 201 | CYC | OB-C4B | 2.30 | 1.28 | 1.23 |
| 12 | Z1 | 202 | CYC | OB-C4B | 2.30 | 1.28 | 1.23 |
| 12 | X5 | 201 | CYC | C1A-C2A | 2.30 | 1.49 | 1.45 |
| 12 | F4 | 202 | CYC | C1D-CHD | 2.30 | 1.50 | 1.41 |
| 12 | F8 | 202 | CYC | C1D-CHD | 2.30 | 1.50 | 1.41 |
| 12 | W4 | 201 | CYC | OB-C4B | 2.30 | 1.28 | 1.23 |
| 12 | W8 | 201 | CYC | OB-C4B | 2.30 | 1.28 | 1.23 |
| 12 | BA | 201 | CYC | OB-C4B | 2.30 | 1.28 | 1.23 |
| 12 | F3 | 201 | CYC | C1D-CHD | 2.30 | 1.50 | 1.41 |
| 12 | F1 | 201 | CYC | C1D-CHD | 2.30 | 1.50 | 1.41 |
| 12 | YA | 201 | CYC | C1B-C2B | 2.30 | 1.49 | 1.45 |
| 12 | Y9 | 201 | CYC | C1B-C2B | 2.30 | 1.49 | 1.45 |
| 12 | P7 | 201 | CYC | C4C-NC | -2.30 | 1.32 | 1.37 |
| 12 | L4 | 202 | CYC | C1B-C2B | 2.30 | 1.49 | 1.45 |
| 12 | F2 | 201 | CYC | C1D-CHD | 2.30 | 1.50 | 1.41 |
| 12 | RA | 201 | CYC | C1D-CHD | 2.30 | 1.50 | 1.41 |
| 12 | B3 | 202 | CYC | OB-C4B | 2.30 | 1.28 | 1.23 |
| 12 | N2 | 101 | CYC | OB-C4B | 2.30 | 1.28 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | N6 | 101 | CYC | OB-C4B | 2.30 | 1.28 | 1.23 |
| 12 | O1 | 201 | CYC | C1C-NC | -2.30 | 1.34 | 1.37 |
| 12 | O3 | 201 | CYC | C1C-NC | -2.30 | 1.34 | 1.37 |
| 12 | F4 | 202 | CYC | C1B-C2B | 2.29 | 1.49 | 1.45 |
| 12 | F8 | 202 | CYC | C1B-C2B | 2.29 | 1.49 | 1.45 |
| 12 | G2 | 201 | CYC | C1C-NC | -2.29 | 1.34 | 1.37 |
| 12 | G6 | 201 | CYC | C1C-NC | -2.29 | 1.34 | 1.37 |
| 12 | JA | 202 | CYC | C1D-CHD | 2.29 | 1.50 | 1.41 |
| 12 | J9 | 202 | CYC | C1D-CHD | 2.29 | 1.50 | 1.41 |
| 12 | J2 | 202 | CYC | OB-C4B | 2.29 | 1.27 | 1.23 |
| 12 | J6 | 202 | CYC | OB-C4B | 2.29 | 1.27 | 1.23 |
| 12 | C4 | 201 | CYC | C1B-NB | -2.29 | 1.34 | 1.37 |
| 12 | C8 | 201 | CYC | C1B-NB | -2.29 | 1.34 | 1.37 |
| 12 | K3 | 201 | CYC | C1C-NC | -2.29 | 1.34 | 1.37 |
| 12 | K1 | 201 | CYC | C1C-NC | -2.29 | 1.34 | 1.37 |
| 12 | H2 | 201 | CYC | OB-C4B | 2.29 | 1.27 | 1.23 |
| 12 | H8 | 201 | CYC | C4C-NC | -2.29 | 1.32 | 1.37 |
| 12 | L4 | 202 | CYC | OB-C4B | 2.29 | 1.27 | 1.23 |
| 12 | W8 | 201 | CYC | C1D-CHD | 2.29 | 1.50 | 1.41 |
| 12 | K4 | 201 | CYC | C1B-C2B | 2.29 | 1.49 | 1.45 |
| 12 | K8 | 201 | CYC | C1B-C2B | 2.29 | 1.49 | 1.45 |
| 12 | e7 | 201 | CYC | C2C-C1C | -2.29 | 1.50 | 1.52 |
| 12 | f5 | 201 | CYC | C1A-C2A | 2.29 | 1.49 | 1.45 |
| 12 | C4 | 201 | CYC | C1D-CHD | 2.29 | 1.50 | 1.41 |
| 12 | C8 | 201 | CYC | C1D-CHD | 2.29 | 1.50 | 1.41 |
| 12 | E4 | 201 | CYC | C1C-NC | -2.29 | 1.34 | 1.37 |
| 12 | E8 | 201 | CYC | C1C-NC | -2.29 | 1.34 | 1.37 |
| 12 | Y7 | 201 | CYC | C2C-C1C | -2.29 | 1.50 | 1.52 |
| 12 | a9 | 901 | CYC | C1B-C2B | 2.29 | 1.49 | 1.45 |
| 12 | B3 | 202 | CYC | C1B-C2B | 2.29 | 1.49 | 1.45 |
| 12 | B1 | 202 | CYC | C1B-C2B | 2.29 | 1.49 | 1.45 |
| 12 | J4 | 201 | CYC | C1B-C2B | 2.29 | 1.49 | 1.45 |
| 12 | J8 | 201 | CYC | C1B-C2B | 2.29 | 1.49 | 1.45 |
| 12 | F4 | 202 | CYC | C4B-NB | -2.29 | 1.33 | 1.38 |
| 12 | F8 | 202 | CYC | C4B-NB | -2.29 | 1.33 | 1.38 |
| 12 | B1 | 202 | CYC | OB-C4B | 2.29 | 1.27 | 1.23 |
| 12 | M8 | 302 | CYC | OB-C4B | 2.29 | 1.27 | 1.23 |
| 12 | R1 | 201 | CYC | C1D-CHD | 2.29 | 1.50 | 1.41 |
| 12 | R3 | 201 | CYC | C1D-CHD | 2.29 | 1.50 | 1.41 |
| 12 | Z4 | 301 | CYC | C1B-C2B | 2.29 | 1.49 | 1.45 |
| 12 | H7 | 201 | CYC | C4C-NC | -2.29 | 1.32 | 1.37 |
| 12 | Z9 | 202 | CYC | C1D-CHD | 2.29 | 1.50 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | A7 | 201 | CYC | C2C-C1C | -2.29 | 1.50 | 1.52 |
| 12 | B7 | 201 | CYC | C4C-NC | -2.29 | 1.32 | 1.37 |
| 12 | d7 | 201 | CYC | C4C-NC | -2.29 | 1.32 | 1.37 |
| 12 | J7 | 201 | CYC | C4C-NC | -2.29 | 1.32 | 1.37 |
| 12 | RA | 202 | CYC | C1B-C2B | 2.29 | 1.49 | 1.45 |
| 12 | R9 | 202 | CYC | C1B-C2B | 2.29 | 1.49 | 1.45 |
| 12 | H4 | 201 | CYC | C4B-NB | -2.29 | 1.33 | 1.38 |
| 12 | S7 | 201 | CYC | C2C-C1C | -2.29 | 1.50 | 1.52 |
| 12 | E4 | 201 | CYC | C1B-C2B | 2.29 | 1.49 | 1.45 |
| 12 | E3 | 201 | CYC | C1C-NC | -2.29 | 1.34 | 1.37 |
| 12 | E1 | 201 | CYC | C1C-NC | -2.29 | 1.34 | 1.37 |
| 12 | DA | 201 | CYC | C4B-NB | -2.29 | 1.33 | 1.38 |
| 12 | aA | 901 | CYC | C4B-NB | -2.29 | 1.33 | 1.38 |
| 12 | ZA | 202 | CYC | C1D-CHD | 2.29 | 1.50 | 1.41 |
| 12 | PA | 201 | CYC | OB-C4B | 2.28 | 1.27 | 1.23 |
| 12 | P9 | 201 | CYC | OB-C4B | 2.28 | 1.27 | 1.23 |
| 12 | LA | 202 | CYC | C1D-CHD | 2.28 | 1.50 | 1.41 |
| 12 | L9 | 202 | CYC | C1D-CHD | 2.28 | 1.50 | 1.41 |
| 12 | S4 | 202 | CYC | C4B-NB | -2.28 | 1.33 | 1.38 |
| 12 | P5 | 201 | CYC | C4C-NC | -2.28 | 1.32 | 1.37 |
| 12 | W4 | 201 | CYC | C1D-CHD | 2.28 | 1.50 | 1.41 |
| 12 | N4 | 201 | CYC | C1D-CHD | 2.28 | 1.50 | 1.41 |
| 12 | N8 | 201 | CYC | C1D-CHD | 2.28 | 1.50 | 1.41 |
| 12 | D6 | 201 | CYC | C1D-CHD | 2.28 | 1.50 | 1.41 |
| 12 | R1 | 201 | CYC | OB-C4B | 2.28 | 1.27 | 1.23 |
| 12 | R3 | 201 | CYC | OB-C4B | 2.28 | 1.27 | 1.23 |
| 12 | T3 | 301 | CYC | C1D-CHD | 2.28 | 1.50 | 1.41 |
| 12 | T1 | 301 | CYC | C1D-CHD | 2.28 | 1.50 | 1.41 |
| 12 | E6 | 201 | CYC | C1B-NB | -2.28 | 1.34 | 1.37 |
| 12 | V5 | 201 | CYC | C4C-NC | -2.28 | 1.32 | 1.37 |
| 12 | b5 | 201 | CYC | C1A-C2A | 2.28 | 1.49 | 1.45 |
| 12 | L3 | 202 | CYC | C1D-CHD | 2.28 | 1.50 | 1.41 |
| 12 | aA | 902 | CYC | C1D-CHD | 2.28 | 1.50 | 1.41 |
| 12 | Z3 | 201 | CYC | C1D-CHD | 2.28 | 1.50 | 1.41 |
| 12 | Z1 | 202 | CYC | C1D-CHD | 2.28 | 1.50 | 1.41 |
| 12 | VA | 201 | CYC | C1D-CHD | 2.28 | 1.49 | 1.41 |
| 12 | V9 | 201 | CYC | C1D-CHD | 2.28 | 1.49 | 1.41 |
| 12 | W8 | 201 | CYC | C4B-NB | -2.28 | 1.33 | 1.38 |
| 12 | M8 | 301 | CYC | C1B-C2B | 2.28 | 1.49 | 1.45 |
| 12 | OA | 201 | CYC | C1D-CHD | 2.28 | 1.49 | 1.41 |
| 12 | D9 | 201 | CYC | C4B-NB | -2.28 | 1.33 | 1.38 |
| 12 | E5 | 201 | CYC | C2C-C1C | -2.28 | 1.50 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | V3 | 201 | CYC | C4B-NB | -2.28 | 1.33 | 1.38 |
| 12 | V1 | 201 | CYC | C4B-NB | -2.28 | 1.33 | 1.38 |
| 12 | K4 | 201 | CYC | C1D-CHD | 2.28 | 1.49 | 1.41 |
| 12 | K8 | 201 | CYC | C1D-CHD | 2.28 | 1.49 | 1.41 |
| 12 | M8 | 302 | CYC | C4B-NB | -2.28 | 1.33 | 1.38 |
| 12 | M7 | 201 | CYC | C2C-C1C | -2.28 | 1.50 | 1.52 |
| 12 | QA | 201 | CYC | C1D-CHD | 2.28 | 1.49 | 1.41 |
| 12 | H4 | 201 | CYC | C1D-CHD | 2.28 | 1.49 | 1.41 |
| 12 | H8 | 201 | CYC | C1D-CHD | 2.28 | 1.49 | 1.41 |
| 12 | C1 | 201 | CYC | C1B-C2B | 2.28 | 1.49 | 1.45 |
| 12 | H2 | 201 | CYC | C1D-CHD | 2.28 | 1.49 | 1.41 |
| 12 | H4 | 201 | CYC | C4C-NC | -2.28 | 1.32 | 1.37 |
| 12 | a7 | 201 | CYC | C2C-C1C | -2.28 | 1.50 | 1.52 |
| 12 | F6 | 201 | CYC | C1D-CHD | 2.27 | 1.49 | 1.41 |
| 12 | a9 | 901 | CYC | C1D-CHD | 2.27 | 1.49 | 1.41 |
| 12 | M8 | 302 | CYC | C1D-CHD | 2.27 | 1.49 | 1.41 |
| 12 | LA | 202 | CYC | C1B-C2B | 2.27 | 1.49 | 1.45 |
| 12 | O9 | 201 | CYC | C1D-CHD | 2.27 | 1.49 | 1.41 |
| 12 | I3 | 201 | CYC | C1C-NC | -2.27 | 1.34 | 1.37 |
| 12 | I1 | 201 | CYC | C1C-NC | -2.27 | 1.34 | 1.37 |
| 12 | R4 | 201 | CYC | C1D-CHD | 2.27 | 1.49 | 1.41 |
| 12 | R8 | 201 | CYC | C1D-CHD | 2.27 | 1.49 | 1.41 |
| 12 | L3 | 202 | CYC | OB-C4B | 2.27 | 1.27 | 1.23 |
| 12 | aA | 902 | CYC | OB-C4B | 2.27 | 1.27 | 1.23 |
| 12 | X3 | 201 | CYC | C4B-NB | -2.27 | 1.33 | 1.38 |
| 12 | X1 | 201 | CYC | C4B-NB | -2.27 | 1.33 | 1.38 |
| 12 | XA | 201 | CYC | C1B-C2B | 2.27 | 1.49 | 1.45 |
| 12 | j7 | 201 | CYC | C4C-NC | -2.27 | 1.32 | 1.37 |
| 12 | K2 | 201 | CYC | C1D-CHD | 2.27 | 1.49 | 1.41 |
| 12 | K6 | 201 | CYC | C1D-CHD | 2.27 | 1.49 | 1.41 |
| 12 | S4 | 202 | CYC | C1D-CHD | 2.27 | 1.49 | 1.41 |
| 12 | U5 | 201 | CYC | C4D-CHA | 2.27 | 1.49 | 1.41 |
| 12 | k5 | 1203 | CYC | C1A-C2A | 2.27 | 1.49 | 1.45 |
| 12 | A1 | 201 | CYC | C1D-CHD | 2.27 | 1.49 | 1.41 |
| 12 | A3 | 201 | CYC | C1D-CHD | 2.27 | 1.49 | 1.41 |
| 12 | R7 | 201 | CYC | C4C-NC | -2.27 | 1.32 | 1.37 |
| 12 | a9 | 901 | CYC | OB-C4B | 2.27 | 1.27 | 1.23 |
| 12 | M8 | 301 | CYC | OB-C4B | 2.27 | 1.27 | 1.23 |
| 12 | N6 | 101 | CYC | C1B-C2B | 2.27 | 1.49 | 1.45 |
| 12 | Z3 | 201 | CYC | C1B-C2B | 2.27 | 1.49 | 1.45 |
| 12 | H6 | 201 | CYC | C1D-CHD | 2.27 | 1.49 | 1.41 |
| 12 | F4 | 202 | CYC | OB-C4B | 2.27 | 1.27 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | H4 | 201 | CYC | OB-C4B | 2.27 | 1.27 | 1.23 |
| 12 | H8 | 201 | CYC | OB-C4B | 2.27 | 1.27 | 1.23 |
| 12 | M8 | 301 | CYC | C1D-CHD | 2.27 | 1.49 | 1.41 |
| 12 | Z1 | 202 | CYC | C1B-C2B | 2.26 | 1.49 | 1.45 |
| 12 | YA | 201 | CYC | C1D-CHD | 2.26 | 1.49 | 1.41 |
| 12 | Y9 | 201 | CYC | C1D-CHD | 2.26 | 1.49 | 1.41 |
| 12 | J6 | 202 | CYC | C4B-NB | -2.26 | 1.33 | 1.38 |
| 12 | K5 | 201 | CYC | C2C-C1C | -2.26 | 1.50 | 1.52 |
| 12 | c5 | 201 | CYC | C2C-C1C | -2.26 | 1.50 | 1.52 |
| 12 | M4 | 301 | CYC | C1D-CHD | 2.26 | 1.49 | 1.41 |
| 12 | Q9 | 201 | CYC | C1D-CHD | 2.26 | 1.49 | 1.41 |
| 12 | L4 | 202 | CYC | C1D-CHD | 2.26 | 1.49 | 1.41 |
| 12 | M8 | 301 | CYC | C1A-NA | -2.26 | 1.33 | 1.38 |
| 12 | k5 | 1203 | CYC | C4C-NC | -2.26 | 1.32 | 1.37 |
| 12 | J2 | 202 | CYC | C1D-CHD | 2.26 | 1.49 | 1.41 |
| 12 | J6 | 202 | CYC | C1D-CHD | 2.26 | 1.49 | 1.41 |
| 12 | E8 | 201 | CYC | C1B-C2B | 2.26 | 1.49 | 1.45 |
| 12 | J4 | 201 | CYC | C4B-NB | -2.26 | 1.33 | 1.38 |
| 12 | J8 | 201 | CYC | C4B-NB | -2.26 | 1.33 | 1.38 |
| 12 | H5 | 201 | CYC | C4C-NC | -2.26 | 1.32 | 1.37 |
| 12 | N5 | 201 | CYC | C1A-C2A | 2.26 | 1.49 | 1.45 |
| 12 | C4 | 201 | CYC | C1C-NC | -2.26 | 1.34 | 1.37 |
| 12 | P4 | 201 | CYC | C1C-NC | -2.26 | 1.34 | 1.37 |
| 12 | C8 | 201 | CYC | C1C-NC | -2.26 | 1.34 | 1.37 |
| 12 | P8 | 201 | CYC | C1C-NC | -2.26 | 1.34 | 1.37 |
| 12 | B5 | 201 | CYC | C4C-NC | -2.26 | 1.32 | 1.37 |
| 12 | P1 | 201 | CYC | O2D-CGD | -2.26 | 1.23 | 1.30 |
| 12 | P3 | 201 | CYC | O2D-CGD | -2.26 | 1.23 | 1.30 |
| 12 | Q1 | 201 | CYC | C1D-CHD | 2.26 | 1.49 | 1.41 |
| 12 | Q3 | 201 | CYC | C1D-CHD | 2.26 | 1.49 | 1.41 |
| 12 | K4 | 201 | CYC | C1C-NC | -2.26 | 1.34 | 1.37 |
| 12 | K8 | 201 | CYC | C1C-NC | -2.26 | 1.34 | 1.37 |
| 12 | H6 | 201 | CYC | OB-C4B | 2.26 | 1.27 | 1.23 |
| 12 | AA | 201 | CYC | C1D-CHD | 2.25 | 1.49 | 1.41 |
| 12 | J4 | 201 | CYC | C1D-CHD | 2.25 | 1.49 | 1.41 |
| 12 | A9 | 201 | CYC | C1D-CHD | 2.25 | 1.49 | 1.41 |
| 12 | X7 | 201 | CYC | C4C-NC | -2.25 | 1.32 | 1.37 |
| 12 | L9 | 202 | CYC | C1B-C2B | 2.25 | 1.49 | 1.45 |
| 12 | G3 | 201 | CYC | C1D-CHD | 2.25 | 1.49 | 1.41 |
| 12 | G1 | 201 | CYC | C1D-CHD | 2.25 | 1.49 | 1.41 |
| 12 | A6 | 201 | CYC | C1C-NC | -2.25 | 1.34 | 1.37 |
| 12 | O5 | 201 | CYC | C4D-CHA | 2.25 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | H3 | 202 | CYC | C1B-C2B | 2.25 | 1.49 | 1.45 |
| 12 | I5 | 201 | CYC | C2C-C1C | -2.25 | 1.50 | 1.52 |
| 12 | O1 | 201 | CYC | C1D-CHD | 2.25 | 1.49 | 1.41 |
| 12 | H1 | 201 | CYC | C1B-C2B | 2.25 | 1.49 | 1.45 |
| 12 | F6 | 201 | CYC | C4B-NB | -2.25 | 1.33 | 1.38 |
| 12 | H9 | 202 | CYC | C4B-NB | -2.25 | 1.33 | 1.38 |
| 12 | O7 | 201 | CYC | C2C-C1C | -2.25 | 1.50 | 1.52 |
| 12 | C6 | 201 | CYC | C1D-CHD | 2.25 | 1.49 | 1.41 |
| 12 | P8 | 201 | CYC | C1D-CHD | 2.25 | 1.49 | 1.41 |
| 12 | G4 | 201 | CYC | C1D-CHD | 2.25 | 1.49 | 1.41 |
| 12 | G8 | 201 | CYC | C1D-CHD | 2.25 | 1.49 | 1.41 |
| 12 | j7 | 201 | CYC | C1A-C2A | 2.25 | 1.49 | 1.45 |
| 12 | W4 | 201 | CYC | C4B-NB | -2.25 | 1.33 | 1.38 |
| 12 | C2 | 201 | CYC | C1D-CHD | 2.25 | 1.49 | 1.41 |
| 12 | J3 | 202 | CYC | C4B-NB | -2.25 | 1.33 | 1.38 |
| 12 | F8 | 202 | CYC | OB-C4B | 2.25 | 1.27 | 1.23 |
| 12 | Z8 | 301 | CYC | C1B-C2B | 2.25 | 1.49 | 1.45 |
| 12 | T9 | 301 | CYC | C1D-CHD | 2.25 | 1.49 | 1.41 |
| 12 | d5 | 201 | CYC | C1A-C2A | 2.25 | 1.49 | 1.45 |
| 12 | A4 | 201 | CYC | C1C-NC | -2.25 | 1.34 | 1.37 |
| 12 | A8 | 201 | CYC | C1C-NC | -2.25 | 1.34 | 1.37 |
| 12 | TA | 301 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | J8 | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | SA | 201 | CYC | C1B-C2B | 2.24 | 1.49 | 1.45 |
| 12 | S9 | 201 | CYC | C1B-C2B | 2.24 | 1.49 | 1.45 |
| 12 | SA | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | S9 | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | L7 | 201 | CYC | C4C-NC | -2.24 | 1.32 | 1.37 |
| 12 | KA | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | K9 | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | M4 | 301 | CYC | C1A-NA | -2.24 | 1.33 | 1.38 |
| 12 | V4 | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | V8 | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | s7 | 201 | CYC | C2C-C1C | -2.24 | 1.50 | 1.52 |
| 12 | E2 | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | J2 | 202 | CYC | C1B-C2B | 2.24 | 1.49 | 1.45 |
| 12 | Z5 | 201 | CYC | C4C-NC | -2.24 | 1.32 | 1.37 |
| 12 | IA | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | W3 | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | X4 | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | G5 | 201 | CYC | C4D-CHA | 2.24 | 1.49 | 1.41 |
| 12 | X8 | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | I9 | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | W1 | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | E5 | 201 | CYC | C4D-CHA | 2.24 | 1.49 | 1.41 |
| 12 | C5 | 201 | CYC | C2C-C1C | -2.24 | 1.50 | 1.52 |
| 12 | F7 | 201 | CYC | C4C-NC | -2.24 | 1.32 | 1.37 |
| 12 | O3 | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | e5 | 201 | CYC | C2C-C1C | -2.24 | 1.50 | 1.52 |
| 12 | DA | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | A4 | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | A8 | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | D9 | 201 | CYC | C1D-CHD | 2.24 | 1.49 | 1.41 |
| 12 | U3 | 201 | CYC | C1D-CHD | 2.23 | 1.49 | 1.41 |
| 12 | U1 | 201 | CYC | C1D-CHD | 2.23 | 1.49 | 1.41 |
| 12 | E6 | 201 | CYC | C1D-CHD | 2.23 | 1.49 | 1.41 |
| 12 | H9 | 202 | CYC | C1D-CHD | 2.23 | 1.49 | 1.41 |
| 12 | EA | 201 | CYC | C1D-CHD | 2.23 | 1.49 | 1.41 |
| 12 | P4 | 201 | CYC | C1D-CHD | 2.23 | 1.49 | 1.41 |
| 12 | E9 | 201 | CYC | C1D-CHD | 2.23 | 1.49 | 1.41 |
| 12 | O4 | 201 | CYC | OB-C4B | 2.23 | 1.27 | 1.23 |
| 12 | O8 | 201 | CYC | OB-C4B | 2.23 | 1.27 | 1.23 |
| 12 | GA | 201 | CYC | C1D-CHD | 2.23 | 1.49 | 1.41 |
| 12 | G9 | 201 | CYC | C1D-CHD | 2.23 | 1.49 | 1.41 |
| 12 | KA | 201 | CYC | C1C-NC | -2.23 | 1.34 | 1.37 |
| 12 | K9 | 201 | CYC | C1C-NC | -2.23 | 1.34 | 1.37 |
| 12 | U7 | 201 | CYC | C4D-CHA | 2.23 | 1.49 | 1.41 |
| 12 | D3 | 202 | CYC | OB-C4B | 2.23 | 1.27 | 1.23 |
| 12 | D1 | 202 | CYC | OB-C4B | 2.23 | 1.27 | 1.23 |
| 12 | HA | 202 | CYC | C1D-CHD | 2.23 | 1.49 | 1.41 |
| 12 | I3 | 201 | CYC | C1D-CHD | 2.23 | 1.49 | 1.41 |
| 12 | I1 | 201 | CYC | C1D-CHD | 2.23 | 1.49 | 1.41 |
| 12 | N7 | 201 | CYC | C4C-NC | -2.23 | 1.32 | 1.37 |
| 12 | U9 | 201 | CYC | C1D-CHD | 2.23 | 1.49 | 1.41 |
| 12 | A5 | 201 | CYC | C4D-CHA | 2.23 | 1.49 | 1.41 |
| 12 | C5 | 201 | CYC | C4D-CHA | 2.23 | 1.49 | 1.41 |
| 12 | G2 | 201 | CYC | C1D-CHD | 2.23 | 1.49 | 1.41 |
| 12 | F7 | 201 | CYC | C1A-C2A | 2.23 | 1.49 | 1.45 |
| 12 | P1 | 201 | CYC | OB-C4B | 2.23 | 1.27 | 1.23 |
| 12 | P3 | 201 | CYC | OB-C4B | 2.23 | 1.27 | 1.23 |
| 12 | Z8 | 301 | CYC | O2D-CGD | -2.23 | 1.23 | 1.30 |
| 12 | DA | 201 | CYC | C4D-CHA | 2.23 | 1.49 | 1.41 |
| 12 | D9 | 201 | CYC | C4D-CHA | 2.23 | 1.49 | 1.41 |
| 12 | J2 | 202 | CYC | C4B-NB | -2.23 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | D3 | 202 | CYC | O2D-CGD | -2.23 | 1.23 | 1.30 |
| 12 | D1 | 202 | CYC | O2D-CGD | -2.23 | 1.23 | 1.30 |
| 12 | M4 | 301 | CYC | OB-C4B | 2.23 | 1.27 | 1.23 |
| 12 | BA | 201 | CYC | C1B-C2B | 2.23 | 1.49 | 1.45 |
| 12 | B9 | 201 | CYC | C1B-C2B | 2.23 | 1.49 | 1.45 |
| 12 | A6 | 201 | CYC | C1D-CHD | 2.23 | 1.49 | 1.41 |
| 12 | T7 | 201 | CYC | C4C-NC | -2.23 | 1.32 | 1.37 |
| 12 | FA | 301 | CYC | C4B-NB | -2.22 | 1.33 | 1.38 |
| 12 | F9 | 301 | CYC | C4B-NB | -2.22 | 1.33 | 1.38 |
| 12 | F2 | 201 | CYC | O2D-CGD | -2.22 | 1.23 | 1.30 |
| 12 | C1 | 201 | CYC | C1D-CHD | 2.22 | 1.49 | 1.41 |
| 12 | M4 | 301 | CYC | C4B-NB | -2.22 | 1.33 | 1.38 |
| 12 | HA | 202 | CYC | C1B-C2B | 2.22 | 1.49 | 1.45 |
| 12 | o7 | 201 | CYC | C4D-CHA | 2.22 | 1.49 | 1.41 |
| 12 | m7 | 201 | CYC | C2C-C1C | -2.22 | 1.50 | 1.52 |
| 12 | GA | 201 | CYC | C1B-C2B | 2.22 | 1.49 | 1.45 |
| 12 | G9 | 201 | CYC | C1B-C2B | 2.22 | 1.49 | 1.45 |
| 12 | T3 | 301 | CYC | C4B-NB | -2.22 | 1.33 | 1.38 |
| 12 | T1 | 301 | CYC | C4B-NB | -2.22 | 1.33 | 1.38 |
| 12 | Z3 | 201 | CYC | C1A-NA | -2.22 | 1.33 | 1.38 |
| 12 | Z1 | 202 | CYC | C1A-NA | -2.22 | 1.33 | 1.38 |
| 12 | I5 | 201 | CYC | C4D-CHA | 2.22 | 1.49 | 1.41 |
| 12 | U7 | 201 | CYC | C2C-C1C | -2.22 | 1.50 | 1.52 |
| 12 | L7 | 201 | CYC | C1A-C2A | 2.22 | 1.49 | 1.45 |
| 12 | CA | 201 | CYC | C1D-CHD | 2.22 | 1.49 | 1.41 |
| 12 | T4 | 201 | CYC | C1D-CHD | 2.22 | 1.49 | 1.41 |
| 12 | T8 | 201 | CYC | C1D-CHD | 2.22 | 1.49 | 1.41 |
| 12 | p7 | 201 | CYC | C1A-C2A | 2.22 | 1.49 | 1.45 |
| 12 | q7 | 201 | CYC | C4D-CHA | 2.22 | 1.49 | 1.41 |
| 12 | B3 | 202 | CYC | O2D-CGD | -2.22 | 1.23 | 1.30 |
| 12 | FA | 301 | CYC | OB-C4B | 2.22 | 1.27 | 1.23 |
| 12 | F9 | 301 | CYC | OB-C4B | 2.22 | 1.27 | 1.23 |
| 12 | LA | 202 | CYC | C1A-NA | -2.22 | 1.33 | 1.38 |
| 12 | L9 | 202 | CYC | C1A-NA | -2.22 | 1.33 | 1.38 |
| 12 | UA | 201 | CYC | C1D-CHD | 2.22 | 1.49 | 1.41 |
| 12 | DA | 202 | CYC | C1B-C2B | 2.22 | 1.49 | 1.45 |
| 12 | D9 | 202 | CYC | C1B-C2B | 2.22 | 1.49 | 1.45 |
| 12 | K5 | 201 | CYC | C4D-CHA | 2.22 | 1.49 | 1.41 |
| 12 | WA | 201 | CYC | C1D-CHD | 2.22 | 1.49 | 1.41 |
| 12 | C3 | 201 | CYC | C1D-CHD | 2.22 | 1.49 | 1.41 |
| 12 | W9 | 201 | CYC | C1D-CHD | 2.22 | 1.49 | 1.41 |
| 12 | G6 | 201 | CYC | C1D-CHD | 2.22 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | G1 | 201 | CYC | C1C-NC | -2.22 | 1.34 | 1.37 |
| 12 | a5 | 201 | CYC | C4D-CHA | 2.22 | 1.49 | 1.41 |
| 12 | F2 | 201 | CYC | C1A-NA | -2.22 | 1.33 | 1.38 |
| 12 | R1 | 201 | CYC | C4B-NB | -2.22 | 1.33 | 1.38 |
| 12 | R3 | 201 | CYC | C4B-NB | -2.22 | 1.33 | 1.38 |
| 12 | N2 | 101 | CYC | C4B-NB | -2.21 | 1.33 | 1.38 |
| 12 | Z4 | 301 | CYC | C4B-NB | -2.21 | 1.33 | 1.38 |
| 12 | N6 | 101 | CYC | C4B-NB | -2.21 | 1.33 | 1.38 |
| 12 | B4 | 202 | CYC | OB-C4B | 2.21 | 1.27 | 1.23 |
| 12 | K7 | 201 | CYC | C4D-CHA | 2.21 | 1.49 | 1.41 |
| 12 | B8 | 202 | CYC | OB-C4B | 2.21 | 1.27 | 1.23 |
| 12 | K3 | 201 | CYC | C1D-CHD | 2.21 | 1.49 | 1.41 |
| 12 | A7 | 201 | CYC | C4D-CHA | 2.21 | 1.49 | 1.41 |
| 12 | K1 | 201 | CYC | C1D-CHD | 2.21 | 1.49 | 1.41 |
| 12 | V3 | 201 | CYC | C1B-C2B | 2.21 | 1.49 | 1.45 |
| 12 | V1 | 201 | CYC | C1B-C2B | 2.21 | 1.49 | 1.45 |
| 12 | I6 | 201 | CYC | C1D-CHD | 2.21 | 1.49 | 1.41 |
| 12 | T3 | 302 | CYC | C1B-C2B | 2.21 | 1.49 | 1.45 |
| 12 | H4 | 201 | CYC | C1B-C2B | 2.21 | 1.49 | 1.45 |
| 12 | H8 | 201 | CYC | C1B-C2B | 2.21 | 1.49 | 1.45 |
| 12 | T1 | 302 | CYC | C1B-C2B | 2.21 | 1.49 | 1.45 |
| 12 | a9 | 901 | CYC | C1A-NA | -2.21 | 1.33 | 1.38 |
| 12 | D4 | 202 | CYC | OB-C4B | 2.21 | 1.27 | 1.23 |
| 12 | D8 | 202 | CYC | OB-C4B | 2.21 | 1.27 | 1.23 |
| 12 | L3 | 202 | CYC | C4B-NB | -2.21 | 1.33 | 1.38 |
| 12 | aA | 902 | CYC | C4B-NB | -2.21 | 1.33 | 1.38 |
| 12 | L2 | 201 | CYC | OB-C4B | 2.21 | 1.27 | 1.23 |
| 12 | L6 | 201 | CYC | OB-C4B | 2.21 | 1.27 | 1.23 |
| 12 | I7 | 201 | CYC | C2C-C1C | -2.21 | 1.50 | 1.52 |
| 12 | g7 | 201 | CYC | C2C-C1C | -2.21 | 1.50 | 1.52 |
| 12 | H2 | 201 | CYC | C4B-NB | -2.21 | 1.33 | 1.38 |
| 12 | B1 | 202 | CYC | C4B-NB | -2.21 | 1.33 | 1.38 |
| 12 | F5 | 201 | CYC | C4C-NC | -2.21 | 1.32 | 1.37 |
| 12 | RA | 201 | CYC | OB-C4B | 2.21 | 1.27 | 1.23 |
| 12 | R9 | 201 | CYC | OB-C4B | 2.21 | 1.27 | 1.23 |
| 12 | A2 | 201 | CYC | C1D-CHD | 2.21 | 1.49 | 1.41 |
| 12 | I2 | 201 | CYC | C1D-CHD | 2.21 | 1.49 | 1.41 |
| 12 | TA | 301 | CYC | C4B-NB | -2.21 | 1.33 | 1.38 |
| 12 | T9 | 301 | CYC | C4B-NB | -2.21 | 1.33 | 1.38 |
| 12 | C9 | 201 | CYC | C1D-CHD | 2.21 | 1.49 | 1.41 |
| 12 | F6 | 201 | CYC | O2D-CGD | -2.21 | 1.23 | 1.30 |
| 12 | e5 | 201 | CYC | C4D-CHA | 2.21 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | W5 | 201 | CYC | C4D-CHA | 2.21 | 1.49 | 1.41 |
| 12 | T5 | 201 | CYC | C1A-C2A | 2.21 | 1.49 | 1.45 |
| 12 | F2 | 201 | CYC | C4B-NB | -2.20 | 1.33 | 1.38 |
| 12 | G4 | 201 | CYC | C1C-NC | -2.20 | 1.34 | 1.37 |
| 12 | G8 | 201 | CYC | C1C-NC | -2.20 | 1.34 | 1.37 |
| 12 | r7 | 201 | CYC | C1A-C2A | 2.20 | 1.49 | 1.45 |
| 12 | M4 | 301 | CYC | C4D-CHA | 2.20 | 1.49 | 1.41 |
| 12 | RA | 201 | CYC | C1A-NA | -2.20 | 1.33 | 1.38 |
| 12 | R9 | 201 | CYC | C1A-NA | -2.20 | 1.33 | 1.38 |
| 12 | C7 | 201 | CYC | C4D-CHA | 2.20 | 1.49 | 1.41 |
| 12 | D2 | 202 | CYC | C1B-C2B | 2.20 | 1.49 | 1.45 |
| 12 | L2 | 201 | CYC | C4B-NB | -2.20 | 1.33 | 1.38 |
| 12 | O4 | 201 | CYC | C4B-NB | -2.20 | 1.33 | 1.38 |
| 12 | L6 | 201 | CYC | C4B-NB | -2.20 | 1.33 | 1.38 |
| 12 | O8 | 201 | CYC | C4B-NB | -2.20 | 1.33 | 1.38 |
| 12 | g7 | 201 | CYC | C4D-CHA | 2.20 | 1.49 | 1.41 |
| 12 | BA | 201 | CYC | C4B-NB | -2.20 | 1.33 | 1.38 |
| 12 | B9 | 201 | CYC | C4B-NB | -2.20 | 1.33 | 1.38 |
| 12 | Y3 | 201 | CYC | C1D-CHD | 2.20 | 1.49 | 1.41 |
| 12 | Y1 | 201 | CYC | C1D-CHD | 2.20 | 1.49 | 1.41 |
| 12 | A5 | 201 | CYC | C2C-C1C | -2.20 | 1.50 | 1.52 |
| 12 | u7 | 201 | CYC | C4D-CHA | 2.20 | 1.49 | 1.41 |
| 12 | k7 | 201 | CYC | C4D-CHA | 2.20 | 1.49 | 1.41 |
| 12 | H3 | 202 | CYC | O2D-CGD | -2.20 | 1.23 | 1.30 |
| 12 | H2 | 201 | CYC | C1B-C2B | 2.20 | 1.49 | 1.45 |
| 12 | H6 | 201 | CYC | C1B-C2B | 2.20 | 1.49 | 1.45 |
| 12 | L5 | 201 | CYC | C4C-NC | -2.20 | 1.32 | 1.37 |
| 12 | Q5 | 201 | CYC | C4D-CHA | 2.20 | 1.49 | 1.41 |
| 12 | G7 | 201 | CYC | C4D-CHA | 2.20 | 1.49 | 1.41 |
| 12 | B3 | 202 | CYC | C4B-NB | -2.20 | 1.33 | 1.38 |
| 12 | Q7 | 201 | CYC | C4D-CHA | 2.20 | 1.49 | 1.41 |
| 12 | D6 | 202 | CYC | C1B-C2B | 2.20 | 1.49 | 1.45 |
| 12 | WA | 201 | CYC | C1C-NC | -2.20 | 1.34 | 1.37 |
| 12 | N4 | 201 | CYC | C1C-NC | -2.20 | 1.34 | 1.37 |
| 12 | N8 | 201 | CYC | C1C-NC | -2.20 | 1.34 | 1.37 |
| 12 | W9 | 201 | CYC | C1C-NC | -2.20 | 1.34 | 1.37 |
| 12 | G5 | 201 | CYC | C2C-C1C | -2.20 | 1.50 | 1.52 |
| 12 | F6 | 201 | CYC | OB-C4B | 2.20 | 1.27 | 1.23 |
| 12 | S1 | 201 | CYC | C1D-CHD | 2.20 | 1.49 | 1.41 |
| 12 | E4 | 201 | CYC | C1D-CHD | 2.19 | 1.49 | 1.41 |
| 12 | E8 | 201 | CYC | C1D-CHD | 2.19 | 1.49 | 1.41 |
| 12 | Z4 | 301 | CYC | O2D-CGD | -2.19 | 1.23 | 1.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | H3 | 201 | CYC | C1B-C2B | 2.19 | 1.49 | 1.45 |
| 12 | H1 | 202 | CYC | C1B-C2B | 2.19 | 1.49 | 1.45 |
| 12 | M8 | 301 | CYC | C4D-CHA | 2.19 | 1.49 | 1.41 |
| 12 | F2 | 201 | CYC | OB-C4B | 2.19 | 1.27 | 1.23 |
| 12 | k5 | 1202 | CYC | C4C-NC | -2.19 | 1.32 | 1.37 |
| 12 | J3 | 202 | CYC | OB-C4B | 2.19 | 1.27 | 1.23 |
| 12 | aA | 901 | CYC | OB-C4B | 2.19 | 1.27 | 1.23 |
| 12 | U4 | 201 | CYC | C4B-NB | -2.19 | 1.33 | 1.38 |
| 12 | U8 | 201 | CYC | C4B-NB | -2.19 | 1.33 | 1.38 |
| 12 | L4 | 202 | CYC | C1A-NA | -2.19 | 1.33 | 1.38 |
| 12 | R1 | 201 | CYC | O2D-CGD | -2.19 | 1.23 | 1.30 |
| 12 | R3 | 201 | CYC | O2D-CGD | -2.19 | 1.23 | 1.30 |
| 12 | H1 | 201 | CYC | O2D-CGD | -2.19 | 1.23 | 1.30 |
| 12 | LA | 202 | CYC | C4B-NB | -2.19 | 1.33 | 1.38 |
| 12 | T3 | 301 | CYC | OB-C4B | 2.19 | 1.27 | 1.23 |
| 12 | T1 | 301 | CYC | OB-C4B | 2.19 | 1.27 | 1.23 |
| 12 | B1 | 202 | CYC | O2D-CGD | -2.19 | 1.23 | 1.30 |
| 12 | R5 | 201 | CYC | C4C-NC | -2.19 | 1.32 | 1.37 |
| 12 | E7 | 201 | CYC | C4D-CHA | 2.19 | 1.49 | 1.41 |
| 12 | K2 | 201 | CYC | C1C-NC | -2.19 | 1.34 | 1.37 |
| 12 | P1 | 201 | CYC | C4B-NB | -2.19 | 1.33 | 1.38 |
| 12 | P3 | 201 | CYC | C4B-NB | -2.19 | 1.33 | 1.38 |
| 12 | M8 | 301 | CYC | C4B-NB | -2.19 | 1.33 | 1.38 |
| 12 | S3 | 201 | CYC | C1D-CHD | 2.19 | 1.49 | 1.41 |
| 12 | I4 | 201 | CYC | C1D-CHD | 2.19 | 1.49 | 1.41 |
| 12 | I8 | 201 | CYC | C1D-CHD | 2.19 | 1.49 | 1.41 |
| 12 | L9 | 202 | CYC | C4B-NB | -2.19 | 1.33 | 1.38 |
| 12 | Y3 | 201 | CYC | C1C-NC | -2.18 | 1.34 | 1.37 |
| 12 | Y1 | 201 | CYC | C1C-NC | -2.18 | 1.34 | 1.37 |
| 12 | I7 | 201 | CYC | C4D-CHA | 2.18 | 1.49 | 1.41 |
| 12 | M5 | 201 | CYC | C2C-C1C | -2.18 | 1.50 | 1.52 |
| 12 | G3 | 201 | CYC | C1C-NC | -2.18 | 1.34 | 1.37 |
| 12 | I4 | 201 | CYC | C1C-NC | -2.18 | 1.34 | 1.37 |
| 12 | I8 | 201 | CYC | C1C-NC | -2.18 | 1.34 | 1.37 |
| 12 | D2 | 201 | CYC | OB-C4B | 2.18 | 1.27 | 1.23 |
| 12 | C7 | 201 | CYC | C2C-C1C | -2.18 | 1.50 | 1.52 |
| 12 | O7 | 201 | CYC | C4D-CHA | 2.18 | 1.49 | 1.41 |
| 12 | a7 | 201 | CYC | C4D-CHA | 2.18 | 1.49 | 1.41 |
| 12 | R1 | 201 | CYC | C4D-CHA | 2.18 | 1.49 | 1.41 |
| 12 | R3 | 201 | CYC | C4D-CHA | 2.18 | 1.49 | 1.41 |
| 12 | S7 | 201 | CYC | C4D-CHA | 2.18 | 1.49 | 1.41 |
| 12 | HA | 202 | CYC | C4B-NB | -2.18 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | RA | 201 | CYC | C4B-NB | -2.18 | 1.33 | 1.38 |
| 12 | D1 | 202 | CYC | C4B-NB | -2.18 | 1.33 | 1.38 |
| 12 | R9 | 201 | CYC | C4B-NB | -2.18 | 1.33 | 1.38 |
| 12 | R1 | 201 | CYC | C1A-NA | -2.18 | 1.33 | 1.38 |
| 12 | R3 | 201 | CYC | C1A-NA | -2.18 | 1.33 | 1.38 |
| 12 | V3 | 201 | CYC | O2D-CGD | -2.18 | 1.23 | 1.30 |
| 12 | V1 | 201 | CYC | O2D-CGD | -2.18 | 1.23 | 1.30 |
| 12 | Z8 | 301 | CYC | C4D-CHA | 2.18 | 1.49 | 1.41 |
| 12 | W4 | 201 | CYC | O2D-CGD | -2.18 | 1.23 | 1.30 |
| 12 | W8 | 201 | CYC | O2D-CGD | -2.18 | 1.23 | 1.30 |
| 12 | J2 | 201 | CYC | C1B-C2B | 2.18 | 1.49 | 1.45 |
| 12 | E1 | 201 | CYC | C1D-CHD | 2.18 | 1.49 | 1.41 |
| 12 | d7 | 201 | CYC | C1A-C2A | 2.18 | 1.49 | 1.45 |
| 12 | D4 | 202 | CYC | O2D-CGD | -2.18 | 1.23 | 1.30 |
| 12 | D8 | 202 | CYC | O2D-CGD | -2.18 | 1.23 | 1.30 |
| 12 | XA | 201 | CYC | C4B-NB | -2.18 | 1.33 | 1.38 |
| 12 | X9 | 201 | CYC | C4B-NB | -2.18 | 1.33 | 1.38 |
| 12 | W7 | 201 | CYC | C4D-CHA | 2.18 | 1.49 | 1.41 |
| 12 | X5 | 201 | CYC | C4C-NC | -2.18 | 1.32 | 1.37 |
| 12 | LA | 202 | CYC | O2D-CGD | -2.18 | 1.23 | 1.30 |
| 12 | L9 | 202 | CYC | O2D-CGD | -2.18 | 1.23 | 1.30 |
| 12 | B8 | 202 | CYC | O2D-CGD | -2.18 | 1.23 | 1.30 |
| 12 | H4 | 201 | CYC | O2D-CGD | -2.18 | 1.23 | 1.30 |
| 12 | H8 | 201 | CYC | O2D-CGD | -2.18 | 1.23 | 1.30 |
| 12 | DA | 201 | CYC | OB-C4B | 2.17 | 1.27 | 1.23 |
| 12 | D9 | 201 | CYC | OB-C4B | 2.17 | 1.27 | 1.23 |
| 12 | R9 | 201 | CYC | O2D-CGD | -2.17 | 1.23 | 1.30 |
| 12 | PA | 202 | CYC | C1B-C2B | 2.17 | 1.49 | 1.45 |
| 12 | P9 | 202 | CYC | C1B-C2B | 2.17 | 1.49 | 1.45 |
| 12 | H6 | 201 | CYC | C4B-NB | -2.17 | 1.33 | 1.38 |
| 12 | e7 | 201 | CYC | C4D-CHA | 2.17 | 1.49 | 1.41 |
| 12 | S5 | 201 | CYC | C4D-CHA | 2.17 | 1.49 | 1.41 |
| 12 | Z | 201 | CYC | C1A-C2A | 2.17 | 1.49 | 1.45 |
| 12 | T3 | 301 | CYC | C1A-NA | -2.17 | 1.33 | 1.38 |
| 12 | T1 | 301 | CYC | C1A-NA | -2.17 | 1.33 | 1.38 |
| 12 | TA | 301 | CYC | OB-C4B | 2.17 | 1.27 | 1.23 |
| 12 | T9 | 301 | CYC | OB-C4B | 2.17 | 1.27 | 1.23 |
| 12 | d5 | 201 | CYC | C4C-NC | -2.17 | 1.32 | 1.37 |
| 12 | f7 | 201 | CYC | C4C-NC | -2.17 | 1.32 | 1.37 |
| 12 | T4 | 201 | CYC | C1C-NC | -2.17 | 1.34 | 1.37 |
| 12 | T8 | 201 | CYC | C1C-NC | -2.17 | 1.34 | 1.37 |
| 12 | RA | 201 | CYC | O2D-CGD | -2.17 | 1.23 | 1.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | N2 | 101 | CYC | C4D-CHA | 2.17 | 1.49 | 1.41 |
| 12 | E3 | 201 | CYC | C1D-CHD | 2.17 | 1.49 | 1.41 |
| 12 | D3 | 202 | CYC | C4B-NB | -2.17 | 1.33 | 1.38 |
| 12 | E6 | 201 | CYC | C1C-NC | -2.17 | 1.34 | 1.37 |
| 12 | E2 | 201 | CYC | C1C-NC | -2.17 | 1.34 | 1.37 |
| 12 | HA | 201 | CYC | C1B-C2B | 2.17 | 1.49 | 1.45 |
| 12 | H9 | 201 | CYC | C1B-C2B | 2.17 | 1.49 | 1.45 |
| 12 | F3 | 201 | CYC | O2D-CGD | -2.17 | 1.23 | 1.30 |
| 12 | F1 | 201 | CYC | O2D-CGD | -2.17 | 1.23 | 1.30 |
| 12 | J3 | 202 | CYC | C1A-NA | -2.17 | 1.33 | 1.38 |
| 12 | aA | 901 | CYC | C1A-NA | -2.17 | 1.33 | 1.38 |
| 12 | Y9 | 201 | CYC | C1C-NC | -2.17 | 1.34 | 1.37 |
| 12 | B4 | 202 | CYC | O2D-CGD | -2.17 | 1.23 | 1.30 |
| 12 | N2 | 101 | CYC | O2D-CGD | -2.16 | 1.23 | 1.30 |
| 12 | N6 | 101 | CYC | C4D-CHA | 2.16 | 1.49 | 1.41 |
| 12 | Z3 | 201 | CYC | C4B-NB | -2.16 | 1.33 | 1.38 |
| 12 | Z1 | 202 | CYC | C4B-NB | -2.16 | 1.33 | 1.38 |
| 12 | V3 | 202 | CYC | C1B-C2B | 2.16 | 1.49 | 1.45 |
| 12 | V1 | 202 | CYC | C1B-C2B | 2.16 | 1.49 | 1.45 |
| 12 | L4 | 202 | CYC | C4B-NB | -2.16 | 1.33 | 1.38 |
| 12 | H1 | 201 | CYC | C4B-NB | -2.16 | 1.33 | 1.38 |
| 12 | HA | 202 | CYC | C1A-NA | -2.16 | 1.33 | 1.38 |
| 12 | V4 | 201 | CYC | C1A-C2A | 2.16 | 1.49 | 1.45 |
| 12 | V8 | 201 | CYC | C1A-C2A | 2.16 | 1.49 | 1.45 |
| 12 | LA | 201 | CYC | C1B-C2B | 2.16 | 1.49 | 1.45 |
| 12 | L9 | 201 | CYC | C1B-C2B | 2.16 | 1.49 | 1.45 |
| 12 | m7 | 201 | CYC | C4D-CHA | 2.16 | 1.49 | 1.41 |
| 12 | A | 201 | CYC | C1A-C2A | 2.16 | 1.49 | 1.45 |
| 12 | H7 | 201 | CYC | C1A-C2A | 2.16 | 1.49 | 1.45 |
| 12 | F3 | 201 | CYC | OB-C4B | 2.16 | 1.27 | 1.23 |
| 12 | F1 | 201 | CYC | OB-C4B | 2.16 | 1.27 | 1.23 |
| 12 | P1 | 201 | CYC | C4D-CHA | 2.16 | 1.49 | 1.41 |
| 12 | P3 | 201 | CYC | C4D-CHA | 2.16 | 1.49 | 1.41 |
| 12 | Y7 | 201 | CYC | C4D-CHA | 2.16 | 1.49 | 1.41 |
| 12 | H3 | 202 | CYC | C4B-NB | -2.16 | 1.33 | 1.38 |
| 12 | U3 | 201 | CYC | C1C-NC | -2.16 | 1.34 | 1.37 |
| 12 | U1 | 201 | CYC | C1C-NC | -2.16 | 1.34 | 1.37 |
| 12 | a9 | 901 | CYC | O2D-CGD | -2.16 | 1.23 | 1.30 |
| 12 | AA | 201 | CYC | C1C-NC | -2.16 | 1.34 | 1.37 |
| 12 | A9 | 201 | CYC | C1C-NC | -2.16 | 1.34 | 1.37 |
| 12 | M7 | 201 | CYC | C4D-CHA | 2.16 | 1.49 | 1.41 |
| 12 | Z4 | 301 | CYC | OB-C4B | 2.15 | 1.27 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | Z8 | 301 | CYC | C4B-NB | -2.15 | 1.33 | 1.38 |
| 12 | F2 | 201 | CYC | C4D-CHA | 2.15 | 1.49 | 1.41 |
| 12 | D3 | 201 | CYC | C1B-C2B | 2.15 | 1.49 | 1.45 |
| 12 | D1 | 201 | CYC | C1B-C2B | 2.15 | 1.49 | 1.45 |
| 12 | SA | 201 | CYC | C1B-NB | -2.15 | 1.34 | 1.37 |
| 12 | S9 | 201 | CYC | C1B-NB | -2.15 | 1.34 | 1.37 |
| 12 | D6 | 201 | CYC | C4D-CHA | 2.15 | 1.49 | 1.41 |
| 12 | D2 | 201 | CYC | C4D-CHA | 2.15 | 1.49 | 1.41 |
| 12 | L6 | 201 | CYC | O2D-CGD | -2.15 | 1.23 | 1.30 |
| 12 | W3 | 201 | CYC | C1C-NC | -2.15 | 1.34 | 1.37 |
| 12 | W1 | 201 | CYC | C1C-NC | -2.15 | 1.34 | 1.37 |
| 12 | M5 | 201 | CYC | C4D-CHA | 2.15 | 1.49 | 1.41 |
| 12 | X3 | 202 | CYC | C4C-NC | -2.15 | 1.32 | 1.37 |
| 12 | X1 | 202 | CYC | C4C-NC | -2.15 | 1.32 | 1.37 |
| 12 | L4 | 202 | CYC | O2D-CGD | -2.15 | 1.23 | 1.30 |
| 12 | D3 | 202 | CYC | C4D-CHA | 2.15 | 1.49 | 1.41 |
| 12 | D1 | 202 | CYC | C4D-CHA | 2.15 | 1.49 | 1.41 |
| 12 | v7 | 201 | CYC | C4C-NC | -2.15 | 1.32 | 1.37 |
| 12 | R7 | 201 | CYC | C1A-C2A | 2.15 | 1.49 | 1.45 |
| 12 | a9 | 901 | CYC | C4B-NB | -2.15 | 1.33 | 1.38 |
| 12 | J6 | 201 | CYC | C1B-C2B | 2.15 | 1.49 | 1.45 |
| 12 | B7 | 201 | CYC | C1A-C2A | 2.15 | 1.49 | 1.45 |
| 12 | B1 | 202 | CYC | C4D-CHA | 2.15 | 1.49 | 1.41 |
| 12 | g7 | 201 | CYC | C1D-CHD | 2.15 | 1.49 | 1.41 |
| 12 | Z3 | 201 | CYC | O2D-CGD | -2.15 | 1.23 | 1.30 |
| 12 | Z1 | 202 | CYC | O2D-CGD | -2.15 | 1.23 | 1.30 |
| 12 | U4 | 201 | CYC | O2D-CGD | -2.15 | 1.23 | 1.30 |
| 12 | U8 | 201 | CYC | O2D-CGD | -2.15 | 1.23 | 1.30 |
| 12 | D2 | 201 | CYC | O2D-CGD | -2.15 | 1.23 | 1.30 |
| 12 | LA | 202 | CYC | C4D-CHA | 2.15 | 1.49 | 1.41 |
| 12 | L9 | 202 | CYC | C4D-CHA | 2.15 | 1.49 | 1.41 |
| 12 | N6 | 101 | CYC | O2D-CGD | -2.15 | 1.23 | 1.30 |
| 12 | Q1 | 201 | CYC | C1C-NC | -2.15 | 1.34 | 1.37 |
| 12 | Q3 | 201 | CYC | C1C-NC | -2.15 | 1.34 | 1.37 |
| 12 | P9 | 201 | CYC | C1A-NA | -2.15 | 1.34 | 1.38 |
| 12 | X3 | 201 | CYC | O2D-CGD | -2.15 | 1.23 | 1.30 |
| 12 | F4 | 202 | CYC | O2D-CGD | -2.15 | 1.23 | 1.30 |
| 12 | F8 | 202 | CYC | O2D-CGD | -2.15 | 1.23 | 1.30 |
| 12 | X1 | 201 | CYC | O2D-CGD | -2.15 | 1.23 | 1.30 |
| 12 | Z4 | 301 | CYC | C4D-CHA | 2.15 | 1.49 | 1.41 |
| 12 | H9 | 202 | CYC | C1B-C2B | 2.15 | 1.49 | 1.45 |
| 12 | F3 | 201 | CYC | C1A-NA | -2.15 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | F1 | 201 | CYC | C1A-NA | -2.15 | 1.34 | 1.38 |
| 12 | p7 | 201 | CYC | C4C-NC | -2.15 | 1.32 | 1.37 |
| 12 | F3 | 201 | CYC | C4B-NB | -2.15 | 1.33 | 1.38 |
| 12 | F1 | 201 | CYC | C4B-NB | -2.15 | 1.33 | 1.38 |
| 12 | TA | 301 | CYC | O2D-CGD | -2.14 | 1.23 | 1.30 |
| 12 | T9 | 301 | CYC | O2D-CGD | -2.14 | 1.23 | 1.30 |
| 12 | s7 | 201 | CYC | C4D-CHA | 2.14 | 1.49 | 1.41 |
| 12 | JA | 202 | CYC | C4B-NB | -2.14 | 1.33 | 1.38 |
| 12 | J9 | 202 | CYC | C4B-NB | -2.14 | 1.33 | 1.38 |
| 12 | v7 | 201 | CYC | C1A-C2A | 2.14 | 1.49 | 1.45 |
| 12 | B3 | 202 | CYC | C4D-CHA | 2.14 | 1.49 | 1.41 |
| 12 | H6 | 201 | CYC | C1A-NA | -2.14 | 1.34 | 1.38 |
| 12 | PA | 201 | CYC | O2D-CGD | -2.14 | 1.23 | 1.30 |
| 12 | P9 | 201 | CYC | O2D-CGD | -2.14 | 1.23 | 1.30 |
| 12 | H4 | 202 | CYC | C1B-C2B | 2.14 | 1.49 | 1.45 |
| 12 | H8 | 202 | CYC | C1B-C2B | 2.14 | 1.49 | 1.45 |
| 12 | L3 | 202 | CYC | O2D-CGD | -2.14 | 1.23 | 1.30 |
| 12 | aA | 902 | CYC | O2D-CGD | -2.14 | 1.23 | 1.30 |
| 12 | O4 | 201 | CYC | O2D-CGD | -2.14 | 1.23 | 1.30 |
| 12 | O8 | 201 | CYC | O2D-CGD | -2.14 | 1.23 | 1.30 |
| 12 | BA | 201 | CYC | O2D-CGD | -2.14 | 1.23 | 1.30 |
| 12 | B9 | 201 | CYC | O2D-CGD | -2.14 | 1.23 | 1.30 |
| 12 | T3 | 301 | CYC | O2D-CGD | -2.14 | 1.23 | 1.30 |
| 12 | T1 | 301 | CYC | O2D-CGD | -2.14 | 1.23 | 1.30 |
| 12 | O5 | 201 | CYC | C2C-C1C | -2.14 | 1.50 | 1.52 |
| 12 | U4 | 201 | CYC | C4D-CHA | 2.14 | 1.49 | 1.41 |
| 12 | U8 | 201 | CYC | C4D-CHA | 2.14 | 1.49 | 1.41 |
| 12 | H1 | 201 | CYC | C4D-CHA | 2.14 | 1.49 | 1.41 |
| 12 | W4 | 201 | CYC | C4D-CHA | 2.14 | 1.49 | 1.41 |
| 12 | W8 | 201 | CYC | C4D-CHA | 2.14 | 1.49 | 1.41 |
| 12 | FA | 301 | CYC | O2D-CGD | -2.14 | 1.23 | 1.30 |
| 12 | F9 | 301 | CYC | O2D-CGD | -2.14 | 1.23 | 1.30 |
| 12 | L3 | 201 | CYC | C4C-NC | -2.14 | 1.32 | 1.37 |
| 12 | D6 | 201 | CYC | O2D-CGD | -2.14 | 1.23 | 1.30 |
| 12 | V4 | 201 | CYC | C1C-NC | -2.14 | 1.34 | 1.37 |
| 12 | V8 | 201 | CYC | C1C-NC | -2.14 | 1.34 | 1.37 |
| 12 | ZA | 202 | CYC | C4B-NB | -2.14 | 1.33 | 1.38 |
| 12 | Z9 | 202 | CYC | C4B-NB | -2.14 | 1.33 | 1.38 |
| 12 | C2 | 201 | CYC | C1A-C2A | 2.14 | 1.49 | 1.45 |
| 12 | T3 | 301 | CYC | C4D-CHA | 2.14 | 1.49 | 1.41 |
| 12 | T1 | 301 | CYC | C4D-CHA | 2.14 | 1.49 | 1.41 |
| 12 | H2 | 201 | CYC | O2D-CGD | -2.14 | 1.23 | 1.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | XA | 202 | CYC | C4C-NC | -2.14 | 1.32 | 1.37 |
| 12 | X9 | 202 | CYC | C4C-NC | -2.14 | 1.32 | 1.37 |
| 12 | B8 | 202 | CYC | C4D-CHA | 2.14 | 1.49 | 1.41 |
| 12 | D3 | 202 | CYC | C1A-NA | -2.14 | 1.34 | 1.38 |
| 12 | D1 | 202 | CYC | C1A-NA | -2.14 | 1.34 | 1.38 |
| 12 | C2 | 201 | CYC | C1C-NC | -2.14 | 1.34 | 1.37 |
| 12 | H3 | 202 | CYC | C4D-CHA | 2.13 | 1.49 | 1.41 |
| 12 | E7 | 201 | CYC | C1D-CHD | 2.13 | 1.49 | 1.41 |
| 12 | M8 | 301 | CYC | O2D-CGD | -2.13 | 1.23 | 1.30 |
| 12 | VA | 201 | CYC | C4D-CHA | 2.13 | 1.49 | 1.41 |
| 12 | V9 | 201 | CYC | C4D-CHA | 2.13 | 1.49 | 1.41 |
| 12 | C7 | 201 | CYC | C1D-CHD | 2.13 | 1.49 | 1.41 |
| 12 | B4 | 202 | CYC | C4B-NB | -2.13 | 1.33 | 1.38 |
| 12 | F6 | 201 | CYC | C1A-NA | -2.13 | 1.34 | 1.38 |
| 12 | H2 | 201 | CYC | C4D-CHA | 2.13 | 1.49 | 1.41 |
| 12 | PA | 201 | CYC | C4B-NB | -2.13 | 1.33 | 1.38 |
| 12 | P9 | 201 | CYC | C4B-NB | -2.13 | 1.33 | 1.38 |
| 12 | D6 | 201 | CYC | OB-C4B | 2.13 | 1.27 | 1.23 |
| 12 | L2 | 201 | CYC | O2D-CGD | -2.13 | 1.23 | 1.30 |
| 12 | J4 | 201 | CYC | O2D-CGD | -2.13 | 1.23 | 1.30 |
| 12 | J8 | 201 | CYC | O2D-CGD | -2.13 | 1.23 | 1.30 |
| 12 | a7 | 201 | CYC | C1D-CHD | 2.13 | 1.49 | 1.41 |
| 12 | F3 | 202 | CYC | C1B-C2B | 2.13 | 1.48 | 1.45 |
| 12 | F1 | 202 | CYC | C1B-C2B | 2.13 | 1.48 | 1.45 |
| 12 | TA | 301 | CYC | C1A-NA | -2.13 | 1.34 | 1.38 |
| 12 | T9 | 301 | CYC | C1A-NA | -2.13 | 1.34 | 1.38 |
| 12 | S5 | 201 | CYC | C1D-CHD | 2.13 | 1.49 | 1.41 |
| 12 | q7 | 201 | CYC | C2C-C1C | -2.13 | 1.50 | 1.52 |
| 12 | L4 | 201 | CYC | C1B-C2B | 2.13 | 1.48 | 1.45 |
| 12 | L8 | 201 | CYC | C1B-C2B | 2.13 | 1.48 | 1.45 |
| 12 | f7 | 201 | CYC | C1A-C2A | 2.13 | 1.49 | 1.45 |
| 12 | Q5 | 201 | CYC | C1D-CHD | 2.13 | 1.49 | 1.41 |
| 12 | PA | 201 | CYC | C1A-NA | -2.13 | 1.34 | 1.38 |
| 12 | JA | 202 | CYC | O2D-CGD | -2.13 | 1.23 | 1.30 |
| 12 | J9 | 202 | CYC | O2D-CGD | -2.13 | 1.23 | 1.30 |
| 12 | L6 | 202 | CYC | C1B-C2B | 2.13 | 1.48 | 1.45 |
| 12 | R4 | 201 | CYC | C1C-NC | -2.12 | 1.34 | 1.37 |
| 12 | V3 | 201 | CYC | C1A-NA | -2.12 | 1.34 | 1.38 |
| 12 | V1 | 201 | CYC | C1A-NA | -2.12 | 1.34 | 1.38 |
| 12 | YA | 201 | CYC | C1C-NC | -2.12 | 1.34 | 1.37 |
| 12 | H9 | 202 | CYC | O2D-CGD | -2.12 | 1.23 | 1.30 |
| 12 | TA | 302 | CYC | C1B-C2B | 2.12 | 1.48 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | T9 | 302 | CYC | C1B-C2B | 2.12 | 1.48 | 1.45 |
| 12 | B8 | 202 | CYC | C4B-NB | -2.12 | 1.33 | 1.38 |
| 12 | U5 | 201 | CYC | C2C-C1C | -2.12 | 1.50 | 1.52 |
| 12 | HA | 202 | CYC | O2D-CGD | -2.12 | 1.23 | 1.30 |
| 12 | O4 | 201 | CYC | C4D-CHA | 2.12 | 1.49 | 1.41 |
| 12 | O8 | 201 | CYC | C4D-CHA | 2.12 | 1.49 | 1.41 |
| 12 | BA | 201 | CYC | C4D-CHA | 2.12 | 1.49 | 1.41 |
| 12 | i7 | 201 | CYC | C4D-CHA | 2.12 | 1.49 | 1.41 |
| 12 | B9 | 201 | CYC | C4D-CHA | 2.12 | 1.49 | 1.41 |
| 12 | H6 | 201 | CYC | C4D-CHA | 2.12 | 1.49 | 1.41 |
| 12 | Y5 | 201 | CYC | C4D-CHA | 2.12 | 1.49 | 1.41 |
| 12 | F3 | 201 | CYC | C4D-CHA | 2.12 | 1.49 | 1.41 |
| 12 | F1 | 201 | CYC | C4D-CHA | 2.12 | 1.49 | 1.41 |
| 12 | M8 | 302 | CYC | O2D-CGD | -2.12 | 1.23 | 1.30 |
| 12 | FA | 301 | CYC | C4D-CHA | 2.12 | 1.49 | 1.41 |
| 12 | RA | 201 | CYC | C4D-CHA | 2.12 | 1.49 | 1.41 |
| 12 | c5 | 201 | CYC | C4D-CHA | 2.12 | 1.49 | 1.41 |
| 12 | F9 | 301 | CYC | C4D-CHA | 2.12 | 1.49 | 1.41 |
| 12 | R9 | 201 | CYC | C4D-CHA | 2.12 | 1.49 | 1.41 |
| 12 | aA | 902 | CYC | C1A-NA | -2.12 | 1.34 | 1.38 |
| 12 | H4 | 201 | CYC | C4D-CHA | 2.12 | 1.49 | 1.41 |
| 12 | H8 | 201 | CYC | C4D-CHA | 2.12 | 1.49 | 1.41 |
| 12 | C3 | 201 | CYC | C1C-NC | -2.12 | 1.34 | 1.37 |
| 12 | C1 | 201 | CYC | C1C-NC | -2.12 | 1.34 | 1.37 |
| 12 | H6 | 201 | CYC | O2D-CGD | -2.12 | 1.23 | 1.30 |
| 12 | J4 | 202 | CYC | C1B-C2B | 2.12 | 1.48 | 1.45 |
| 12 | J8 | 202 | CYC | C1B-C2B | 2.12 | 1.48 | 1.45 |
| 12 | H9 | 202 | CYC | C1A-NA | -2.12 | 1.34 | 1.38 |
| 12 | PA | 202 | CYC | C4C-NC | -2.12 | 1.32 | 1.37 |
| 12 | P9 | 202 | CYC | C4C-NC | -2.12 | 1.32 | 1.37 |
| 12 | SA | 201 | CYC | C1C-NC | -2.12 | 1.34 | 1.37 |
| 12 | S9 | 201 | CYC | C1C-NC | -2.12 | 1.34 | 1.37 |
| 12 | XA | 201 | CYC | O2D-CGD | -2.11 | 1.23 | 1.30 |
| 12 | X9 | 201 | CYC | O2D-CGD | -2.11 | 1.23 | 1.30 |
| 12 | H3 | 201 | CYC | C2C-C1C | -2.11 | 1.50 | 1.52 |
| 12 | H1 | 202 | CYC | C2C-C1C | -2.11 | 1.50 | 1.52 |
| 12 | L1 | 201 | CYC | C4C-NC | -2.11 | 1.32 | 1.37 |
| 12 | B3 | 202 | CYC | C1A-NA | -2.11 | 1.34 | 1.38 |
| 12 | U4 | 202 | CYC | C1B-C2B | 2.11 | 1.48 | 1.45 |
| 12 | U8 | 202 | CYC | C1B-C2B | 2.11 | 1.48 | 1.45 |
| 12 | o7 | 201 | CYC | C1D-CHD | 2.11 | 1.49 | 1.41 |
| 12 | H9 | 202 | CYC | C4D-CHA | 2.11 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | K7 | 201 | CYC | C1D-CHD | 2.11 | 1.49 | 1.41 |
| 12 | EA | 201 | CYC | C1A-C2A | 2.11 | 1.49 | 1.45 |
| 12 | SA | 201 | CYC | C1A-C2A | 2.11 | 1.49 | 1.45 |
| 12 | S9 | 201 | CYC | C1A-C2A | 2.11 | 1.49 | 1.45 |
| 12 | U5 | 201 | CYC | C1D-CHD | 2.11 | 1.49 | 1.41 |
| 12 | M4 | 301 | CYC | O2D-CGD | -2.11 | 1.23 | 1.30 |
| 12 | PA | 201 | CYC | C4D-CHA | 2.11 | 1.49 | 1.41 |
| 12 | P9 | 201 | CYC | C4D-CHA | 2.11 | 1.49 | 1.41 |
| 12 | Z3 | 202 | CYC | C1B-C2B | 2.11 | 1.48 | 1.45 |
| 12 | Z1 | 201 | CYC | C1B-C2B | 2.11 | 1.48 | 1.45 |
| 12 | E9 | 201 | CYC | C1A-C2A | 2.11 | 1.49 | 1.45 |
| 12 | L4 | 202 | CYC | C4D-CHA | 2.11 | 1.49 | 1.41 |
| 12 | J2 | 202 | CYC | O2D-CGD | -2.11 | 1.23 | 1.30 |
| 12 | J6 | 202 | CYC | O2D-CGD | -2.11 | 1.23 | 1.30 |
| 12 | G3 | 201 | CYC | C1A-C2A | 2.11 | 1.49 | 1.45 |
| 12 | G1 | 201 | CYC | C1A-C2A | 2.11 | 1.49 | 1.45 |
| 12 | J9 | 202 | CYC | C4D-CHA | 2.11 | 1.49 | 1.41 |
| 12 | IA | 201 | CYC | C1C-NC | -2.11 | 1.34 | 1.37 |
| 12 | I2 | 201 | CYC | C1C-NC | -2.11 | 1.34 | 1.37 |
| 12 | I6 | 201 | CYC | C1C-NC | -2.11 | 1.34 | 1.37 |
| 12 | I9 | 201 | CYC | C1C-NC | -2.11 | 1.34 | 1.37 |
| 12 | R1 | 202 | CYC | C4C-NC | -2.11 | 1.32 | 1.37 |
| 12 | R3 | 202 | CYC | C4C-NC | -2.11 | 1.32 | 1.37 |
| 12 | B4 | 202 | CYC | C4D-CHA | 2.11 | 1.49 | 1.41 |
| 12 | HA | 202 | CYC | C4D-CHA | 2.11 | 1.49 | 1.41 |
| 12 | E5 | 201 | CYC | C1D-CHD | 2.11 | 1.49 | 1.41 |
| 12 | I7 | 201 | CYC | C1D-CHD | 2.11 | 1.49 | 1.41 |
| 12 | Z3 | 201 | CYC | C4D-CHA | 2.11 | 1.49 | 1.41 |
| 12 | Z1 | 202 | CYC | C4D-CHA | 2.11 | 1.49 | 1.41 |
| 12 | k7 | 201 | CYC | C2C-C1C | -2.11 | 1.50 | 1.52 |
| 12 | K5 | 201 | CYC | C1D-CHD | 2.11 | 1.49 | 1.41 |
| 12 | BA | 202 | CYC | C1B-C2B | 2.11 | 1.48 | 1.45 |
| 12 | a9 | 901 | CYC | C4D-CHA | 2.11 | 1.49 | 1.41 |
| 12 | F2 | 202 | CYC | C1B-C2B | 2.11 | 1.48 | 1.45 |
| 12 | XA | 201 | CYC | C4D-CHA | 2.10 | 1.49 | 1.41 |
| 12 | k7 | 201 | CYC | C1D-CHD | 2.10 | 1.49 | 1.41 |
| 12 | X9 | 201 | CYC | C4D-CHA | 2.10 | 1.49 | 1.41 |
| 12 | K6 | 201 | CYC | C1C-NC | -2.10 | 1.34 | 1.37 |
| 12 | q7 | 201 | CYC | C1D-CHD | 2.10 | 1.49 | 1.41 |
| 12 | k5 | 1202 | CYC | C1A-C2A | 2.10 | 1.49 | 1.45 |
| 12 | R8 | 201 | CYC | C1C-NC | -2.10 | 1.34 | 1.37 |
| 12 | VA | 201 | CYC | C1A-NA | -2.10 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | H4 | 201 | CYC | C1A-NA | -2.10 | 1.34 | 1.38 |
| 12 | H8 | 201 | CYC | C1A-NA | -2.10 | 1.34 | 1.38 |
| 12 | V9 | 201 | CYC | C1A-NA | -2.10 | 1.34 | 1.38 |
| 12 | X3 | 201 | CYC | C4D-CHA | 2.10 | 1.49 | 1.41 |
| 12 | X1 | 201 | CYC | C4D-CHA | 2.10 | 1.49 | 1.41 |
| 12 | B9 | 202 | CYC | C1B-C2B | 2.10 | 1.48 | 1.45 |
| 12 | D4 | 202 | CYC | C4D-CHA | 2.10 | 1.49 | 1.41 |
| 12 | D8 | 202 | CYC | C4D-CHA | 2.10 | 1.49 | 1.41 |
| 12 | e5 | 201 | CYC | C1D-CHD | 2.10 | 1.49 | 1.41 |
| 12 | a5 | 201 | CYC | C1D-CHD | 2.10 | 1.49 | 1.41 |
| 12 | I1 | 201 | CYC | C1A-C2A | 2.10 | 1.49 | 1.45 |
| 12 | B8 | 202 | CYC | C1A-NA | -2.10 | 1.34 | 1.38 |
| 12 | AA | 201 | CYC | C1A-C2A | 2.10 | 1.49 | 1.45 |
| 12 | A9 | 201 | CYC | C1A-C2A | 2.10 | 1.49 | 1.45 |
| 12 | L3 | 202 | CYC | C4D-CHA | 2.10 | 1.49 | 1.41 |
| 12 | F6 | 201 | CYC | C4D-CHA | 2.10 | 1.49 | 1.41 |
| 12 | aA | 902 | CYC | C4D-CHA | 2.10 | 1.49 | 1.41 |
| 12 | P1 | 201 | CYC | C1A-NA | -2.10 | 1.34 | 1.38 |
| 12 | P3 | 201 | CYC | C1A-NA | -2.10 | 1.34 | 1.38 |
| 12 | EA | 201 | CYC | C1C-NC | -2.10 | 1.34 | 1.37 |
| 12 | E9 | 201 | CYC | C1C-NC | -2.10 | 1.34 | 1.37 |
| 12 | ZA | 201 | CYC | C1B-C2B | 2.10 | 1.48 | 1.45 |
| 12 | B4 | 201 | CYC | C1B-C2B | 2.10 | 1.48 | 1.45 |
| 12 | B8 | 201 | CYC | C1B-C2B | 2.10 | 1.48 | 1.45 |
| 12 | Z9 | 201 | CYC | C1B-C2B | 2.10 | 1.48 | 1.45 |
| 12 | J4 | 201 | CYC | C4D-CHA | 2.10 | 1.49 | 1.41 |
| 12 | J8 | 201 | CYC | C4D-CHA | 2.10 | 1.49 | 1.41 |
| 12 | ZA | 202 | CYC | O2D-CGD | -2.10 | 1.23 | 1.30 |
| 12 | S4 | 202 | CYC | O2D-CGD | -2.10 | 1.23 | 1.30 |
| 12 | Z9 | 202 | CYC | O2D-CGD | -2.10 | 1.23 | 1.30 |
| 12 | JA | 202 | CYC | C4D-CHA | 2.10 | 1.49 | 1.41 |
| 12 | W5 | 201 | CYC | C1D-CHD | 2.10 | 1.49 | 1.41 |
| 12 | c7 | 201 | CYC | C4D-CHA | 2.10 | 1.49 | 1.41 |
| 12 | A7 | 201 | CYC | C1D-CHD | 2.10 | 1.49 | 1.41 |
| 12 | G7 | 201 | CYC | C1D-CHD | 2.10 | 1.49 | 1.41 |
| 12 | X3 | 201 | CYC | C1A-NA | -2.10 | 1.34 | 1.38 |
| 12 | X1 | 201 | CYC | C1A-NA | -2.10 | 1.34 | 1.38 |
| 12 | B6 | 201 | CYC | C1B-C2B | 2.10 | 1.48 | 1.45 |
| 12 | B2 | 201 | CYC | C1B-C2B | 2.10 | 1.48 | 1.45 |
| 12 | V3 | 201 | CYC | C4D-CHA | 2.10 | 1.49 | 1.41 |
| 12 | V1 | 201 | CYC | C4D-CHA | 2.10 | 1.49 | 1.41 |
| 12 | J3 | 202 | CYC | C4D-CHA | 2.10 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | aA | 901 | CYC | C4D-CHA | 2.10 | 1.49 | 1.41 |
| 12 | L2 | 201 | CYC | C4D-CHA | 2.09 | 1.49 | 1.41 |
| 12 | L6 | 201 | CYC | C4D-CHA | 2.09 | 1.49 | 1.41 |
| 12 | M8 | 302 | CYC | C4D-CHA | 2.09 | 1.49 | 1.41 |
| 12 | P1 | 202 | CYC | C1B-C2B | 2.09 | 1.48 | 1.45 |
| 12 | P3 | 202 | CYC | C1B-C2B | 2.09 | 1.48 | 1.45 |
| 12 | J2 | 202 | CYC | C4D-CHA | 2.09 | 1.49 | 1.41 |
| 12 | J6 | 202 | CYC | C4D-CHA | 2.09 | 1.49 | 1.41 |
| 12 | J2 | 202 | CYC | C1A-NA | -2.09 | 1.34 | 1.38 |
| 12 | F6 | 202 | CYC | C4C-NC | -2.09 | 1.33 | 1.37 |
| 12 | W7 | 201 | CYC | C1D-CHD | 2.09 | 1.49 | 1.41 |
| 12 | TA | 301 | CYC | C4D-CHA | 2.09 | 1.49 | 1.41 |
| 12 | T9 | 301 | CYC | C4D-CHA | 2.09 | 1.49 | 1.41 |
| 12 | VA | 201 | CYC | O2D-CGD | -2.09 | 1.23 | 1.30 |
| 12 | V9 | 201 | CYC | O2D-CGD | -2.09 | 1.23 | 1.30 |
| 12 | D4 | 202 | CYC | C1A-NA | -2.09 | 1.34 | 1.38 |
| 12 | D8 | 202 | CYC | C1A-NA | -2.09 | 1.34 | 1.38 |
| 12 | L2 | 202 | CYC | C1B-C2B | 2.09 | 1.48 | 1.45 |
| 12 | U4 | 202 | CYC | C4C-NC | -2.09 | 1.33 | 1.37 |
| 12 | U8 | 202 | CYC | C4C-NC | -2.09 | 1.33 | 1.37 |
| 12 | c5 | 201 | CYC | C1D-CHD | 2.09 | 1.49 | 1.41 |
| 12 | Q7 | 201 | CYC | C1D-CHD | 2.09 | 1.49 | 1.41 |
| 12 | F6 | 202 | CYC | C1B-C2B | 2.09 | 1.48 | 1.45 |
| 12 | ZA | 202 | CYC | C1A-NA | -2.09 | 1.34 | 1.38 |
| 12 | Z9 | 202 | CYC | C1A-NA | -2.09 | 1.34 | 1.38 |
| 12 | H3 | 201 | CYC | C4C-NC | -2.09 | 1.33 | 1.37 |
| 12 | H1 | 202 | CYC | C4C-NC | -2.09 | 1.33 | 1.37 |
| 12 | Z5 | 201 | CYC | C4D-CHA | 2.09 | 1.49 | 1.41 |
| 12 | CA | 201 | CYC | C1C-NC | -2.09 | 1.34 | 1.37 |
| 12 | C9 | 201 | CYC | C1C-NC | -2.09 | 1.34 | 1.37 |
| 12 | J3 | 202 | CYC | O2D-CGD | -2.08 | 1.23 | 1.30 |
| 12 | aA | 901 | CYC | O2D-CGD | -2.08 | 1.23 | 1.30 |
| 12 | ZA | 202 | CYC | C4D-CHA | 2.08 | 1.49 | 1.41 |
| 12 | u7 | 201 | CYC | C1D-CHD | 2.08 | 1.49 | 1.41 |
| 12 | Z9 | 202 | CYC | C4D-CHA | 2.08 | 1.49 | 1.41 |
| 12 | Y5 | 201 | CYC | C1D-CHD | 2.08 | 1.49 | 1.41 |
| 12 | F4 | 202 | CYC | C4D-CHA | 2.08 | 1.49 | 1.41 |
| 12 | G5 | 201 | CYC | C1D-CHD | 2.08 | 1.49 | 1.41 |
| 12 | F8 | 202 | CYC | C4D-CHA | 2.08 | 1.49 | 1.41 |
| 12 | UA | 201 | CYC | C1A-C2A | 2.08 | 1.49 | 1.45 |
| 12 | U9 | 201 | CYC | C1A-C2A | 2.08 | 1.49 | 1.45 |
| 12 | DA | 201 | CYC | O2D-CGD | -2.08 | 1.23 | 1.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | D9 | 201 | CYC | O2D-CGD | -2.08 | 1.23 | 1.30 |
| 12 | M5 | 201 | CYC | C1D-CHD | 2.08 | 1.49 | 1.41 |
| 12 | s7 | 201 | CYC | C1D-CHD | 2.08 | 1.49 | 1.41 |
| 12 | KA | 201 | CYC | C1A-C2A | 2.08 | 1.49 | 1.45 |
| 12 | K9 | 201 | CYC | C1A-C2A | 2.08 | 1.49 | 1.45 |
| 12 | H3 | 202 | CYC | C1A-NA | -2.08 | 1.34 | 1.38 |
| 12 | C6 | 201 | CYC | C1C-NC | -2.08 | 1.34 | 1.37 |
| 12 | C4 | 201 | CYC | C1A-C2A | 2.08 | 1.49 | 1.45 |
| 12 | C8 | 201 | CYC | C1A-C2A | 2.08 | 1.49 | 1.45 |
| 12 | L3 | 202 | CYC | C1A-NA | -2.08 | 1.34 | 1.38 |
| 12 | O7 | 201 | CYC | C1D-CHD | 2.08 | 1.49 | 1.41 |
| 12 | L4 | 201 | CYC | C4C-NC | -2.08 | 1.33 | 1.37 |
| 12 | L8 | 201 | CYC | C4C-NC | -2.08 | 1.33 | 1.37 |
| 12 | M8 | 302 | CYC | C1A-NA | -2.08 | 1.34 | 1.38 |
| 12 | I5 | 201 | CYC | C1D-CHD | 2.08 | 1.49 | 1.41 |
| 12 | JA | 202 | CYC | C1A-NA | -2.07 | 1.34 | 1.38 |
| 12 | J9 | 202 | CYC | C1A-NA | -2.07 | 1.34 | 1.38 |
| 12 | B1 | 202 | CYC | C1A-NA | -2.07 | 1.34 | 1.38 |
| 12 | J6 | 202 | CYC | C1A-NA | -2.07 | 1.34 | 1.38 |
| 12 | JA | 201 | CYC | C1B-C2B | 2.07 | 1.48 | 1.45 |
| 12 | J9 | 201 | CYC | C1B-C2B | 2.07 | 1.48 | 1.45 |
| 12 | U3 | 201 | CYC | C1A-C2A | 2.07 | 1.49 | 1.45 |
| 12 | U1 | 201 | CYC | C1A-C2A | 2.07 | 1.49 | 1.45 |
| 12 | d5 | 201 | CYC | C4D-CHA | 2.07 | 1.49 | 1.41 |
| 12 | O5 | 201 | CYC | C1D-CHD | 2.07 | 1.49 | 1.41 |
| 12 | BA | 201 | CYC | C1A-NA | -2.07 | 1.34 | 1.38 |
| 12 | B9 | 201 | CYC | C1A-NA | -2.07 | 1.34 | 1.38 |
| 12 | i7 | 201 | CYC | C1D-CHD | 2.07 | 1.49 | 1.41 |
| 12 | C5 | 201 | CYC | C1D-CHD | 2.07 | 1.49 | 1.41 |
| 12 | H2 | 202 | CYC | C1B-C2B | 2.07 | 1.48 | 1.45 |
| 12 | VA | 202 | CYC | C4C-NC | -2.07 | 1.33 | 1.37 |
| 12 | Z8 | 301 | CYC | OB-C4B | 2.07 | 1.27 | 1.23 |
| 12 | B4 | 202 | CYC | C1A-NA | -2.07 | 1.34 | 1.38 |
| 12 | Z8 | 301 | CYC | C1A-NA | -2.07 | 1.34 | 1.38 |
| 12 | S4 | 202 | CYC | C1A-NA | -2.07 | 1.34 | 1.38 |
| 12 | I3 | 201 | CYC | C1A-C2A | 2.07 | 1.49 | 1.45 |
| 12 | J4 | 202 | CYC | C4C-NC | -2.07 | 1.33 | 1.37 |
| 12 | J8 | 202 | CYC | C4C-NC | -2.07 | 1.33 | 1.37 |
| 12 | F4 | 202 | CYC | C1B-NB | -2.07 | 1.34 | 1.37 |
| 12 | F8 | 202 | CYC | C1B-NB | -2.07 | 1.34 | 1.37 |
| 12 | S4 | 202 | CYC | C4D-CHA | 2.07 | 1.49 | 1.41 |
| 12 | S7 | 201 | CYC | C1D-CHD | 2.06 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | D2 | 202 | CYC | C4C-NC | -2.06 | 1.33 | 1.37 |
| 12 | X3 | 202 | CYC | C1B-C2B | 2.06 | 1.48 | 1.45 |
| 12 | X1 | 202 | CYC | C1B-C2B | 2.06 | 1.48 | 1.45 |
| 12 | A5 | 201 | CYC | C1D-CHD | 2.06 | 1.49 | 1.41 |
| 12 | Q8 | 201 | CYC | C1B-C2B | 2.06 | 1.48 | 1.45 |
| 12 | H2 | 201 | CYC | C1A-NA | -2.06 | 1.34 | 1.38 |
| 12 | D6 | 201 | CYC | C1A-NA | -2.06 | 1.34 | 1.38 |
| 12 | D2 | 201 | CYC | C1A-NA | -2.06 | 1.34 | 1.38 |
| 12 | m7 | 201 | CYC | C1D-CHD | 2.06 | 1.49 | 1.41 |
| 12 | GA | 201 | CYC | C1A-C2A | 2.06 | 1.49 | 1.45 |
| 12 | G9 | 201 | CYC | C1A-C2A | 2.06 | 1.49 | 1.45 |
| 12 | XA | 201 | CYC | C1A-NA | -2.06 | 1.34 | 1.38 |
| 12 | X9 | 201 | CYC | C1A-NA | -2.06 | 1.34 | 1.38 |
| 12 | J8 | 201 | CYC | C1A-NA | -2.06 | 1.34 | 1.38 |
| 12 | C6 | 201 | CYC | C1A-C2A | 2.06 | 1.49 | 1.45 |
| 12 | L7 | 201 | CYC | C4D-CHA | 2.06 | 1.49 | 1.41 |
| 12 | A4 | 201 | CYC | C1A-C2A | 2.06 | 1.49 | 1.45 |
| 12 | A8 | 201 | CYC | C1A-C2A | 2.06 | 1.49 | 1.45 |
| 12 | Z4 | 301 | CYC | C1A-NA | -2.06 | 1.34 | 1.38 |
| 12 | H1 | 201 | CYC | C1A-NA | -2.06 | 1.34 | 1.38 |
| 12 | VA | 202 | CYC | C1B-C2B | 2.06 | 1.48 | 1.45 |
| 12 | F4 | 201 | CYC | C1B-C2B | 2.06 | 1.48 | 1.45 |
| 12 | F8 | 201 | CYC | C1B-C2B | 2.06 | 1.48 | 1.45 |
| 12 | V9 | 202 | CYC | C1B-C2B | 2.06 | 1.48 | 1.45 |
| 12 | DA | 201 | CYC | C1A-NA | -2.05 | 1.34 | 1.38 |
| 12 | D9 | 201 | CYC | C1A-NA | -2.05 | 1.34 | 1.38 |
| 12 | J3 | 201 | CYC | C1B-C2B | 2.05 | 1.48 | 1.45 |
| 12 | W4 | 202 | CYC | C1B-C2B | 2.05 | 1.48 | 1.45 |
| 12 | W8 | 202 | CYC | C1B-C2B | 2.05 | 1.48 | 1.45 |
| 12 | R1 | 202 | CYC | C1B-C2B | 2.05 | 1.48 | 1.45 |
| 12 | R3 | 202 | CYC | C1B-C2B | 2.05 | 1.48 | 1.45 |
| 12 | P4 | 201 | CYC | C1A-C2A | 2.05 | 1.49 | 1.45 |
| 12 | P8 | 201 | CYC | C1A-C2A | 2.05 | 1.49 | 1.45 |
| 12 | F7 | 201 | CYC | C4D-CHA | 2.05 | 1.49 | 1.41 |
| 12 | M7 | 201 | CYC | C1D-CHD | 2.05 | 1.49 | 1.41 |
| 12 | YA | 201 | CYC | C1A-C2A | 2.05 | 1.49 | 1.45 |
| 12 | Y9 | 201 | CYC | C1A-C2A | 2.05 | 1.49 | 1.45 |
| 12 | J1 | 201 | CYC | C1B-C2B | 2.05 | 1.48 | 1.45 |
| 12 | J4 | 201 | CYC | C1A-NA | -2.05 | 1.34 | 1.38 |
| 12 | J3 | 201 | CYC | C4C-NC | -2.05 | 1.33 | 1.37 |
| 12 | Z3 | 202 | CYC | C4C-NC | -2.05 | 1.33 | 1.37 |
| 12 | V9 | 202 | CYC | C4C-NC | -2.05 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12 | J1 | 201 | CYC | C4C-NC | -2.05 | 1.33 | 1.37 |
| 12 | Z1 | 201 | CYC | C4C-NC | -2.05 | 1.33 | 1.37 |
| 12 | U7 | 201 | CYC | C1D-CHD | 2.05 | 1.49 | 1.41 |
| 12 | Q4 | 201 | CYC | C4C-NC | -2.05 | 1.33 | 1.37 |
| 12 | W3 | 201 | CYC | C1A-C2A | 2.05 | 1.49 | 1.45 |
| 12 | W1 | 201 | CYC | C1A-C2A | 2.05 | 1.49 | 1.45 |
| 12 | I4 | 201 | CYC | C1A-C2A | 2.05 | 1.49 | 1.45 |
| 12 | I8 | 201 | CYC | C1A-C2A | 2.05 | 1.49 | 1.45 |
| 12 | B6 | 201 | CYC | C4C-NC | -2.05 | 1.33 | 1.37 |
| 12 | B2 | 201 | CYC | C4C-NC | -2.05 | 1.33 | 1.37 |
| 12 | O4 | 202 | CYC | C1B-C2B | 2.05 | 1.48 | 1.45 |
| 12 | Q4 | 201 | CYC | C1B-C2B | 2.05 | 1.48 | 1.45 |
| 12 | O8 | 202 | CYC | C1B-C2B | 2.05 | 1.48 | 1.45 |
| 12 | d7 | 201 | CYC | C4D-CHA | 2.04 | 1.49 | 1.41 |
| 12 | c7 | 201 | CYC | C1D-CHD | 2.04 | 1.49 | 1.41 |
| 12 | N2 | 101 | CYC | C1A-NA | -2.04 | 1.34 | 1.38 |
| 12 | N6 | 101 | CYC | C1A-NA | -2.04 | 1.34 | 1.38 |
| 12 | B3 | 201 | CYC | C1B-C2B | 2.04 | 1.48 | 1.45 |
| 12 | B1 | 201 | CYC | C1B-C2B | 2.04 | 1.48 | 1.45 |
| 12 | HA | 201 | CYC | C4C-NC | -2.04 | 1.33 | 1.37 |
| 12 | B3 | 201 | CYC | C4C-NC | -2.04 | 1.33 | 1.37 |
| 12 | D4 | 201 | CYC | C1B-C2B | 2.04 | 1.48 | 1.45 |
| 12 | D8 | 201 | CYC | C1B-C2B | 2.04 | 1.48 | 1.45 |
| 12 | H9 | 201 | CYC | C4C-NC | -2.04 | 1.33 | 1.37 |
| 12 | TA | 302 | CYC | C4C-NC | -2.04 | 1.33 | 1.37 |
| 12 | T9 | 302 | CYC | C4C-NC | -2.04 | 1.33 | 1.37 |
| 12 | F9 | 301 | CYC | C1A-NA | -2.04 | 1.34 | 1.38 |
| 12 | R7 | 201 | CYC | C4D-CHA | 2.04 | 1.49 | 1.41 |
| 12 | BA | 202 | CYC | C4C-NC | -2.04 | 1.33 | 1.37 |
| 12 | B9 | 202 | CYC | C4C-NC | -2.04 | 1.33 | 1.37 |
| 12 | X5 | 201 | CYC | C4A-C3A | 2.04 | 1.50 | 1.45 |
| 12 | FA | 301 | CYC | C1A-NA | -2.04 | 1.34 | 1.38 |
| 12 | JA | 201 | CYC | C4C-NC | -2.04 | 1.33 | 1.37 |
| 12 | F4 | 201 | CYC | C4C-NC | -2.04 | 1.33 | 1.37 |
| 12 | F8 | 201 | CYC | C4C-NC | -2.04 | 1.33 | 1.37 |
| 12 | J9 | 201 | CYC | C4C-NC | -2.04 | 1.33 | 1.37 |
| 12 | S1 | 201 | CYC | C1A-C2A | 2.04 | 1.49 | 1.45 |
| 12 | N5 | 201 | CYC | C4D-CHA | 2.04 | 1.49 | 1.41 |
| 12 | Q9 | 201 | CYC | C1A-C2A | 2.04 | 1.49 | 1.45 |
| 12 | e7 | 201 | CYC | C1D-CHD | 2.03 | 1.49 | 1.41 |
| 12 | X8 | 201 | CYC | C1C-NC | -2.03 | 1.35 | 1.37 |
| 12 | j7 | 201 | CYC | C4D-CHA | 2.03 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | E2 | 201 | CYC | C1A-C2A | 2.03 | 1.48 | 1.45 |
| 12 | T3 | 302 | CYC | C4C-NC | -2.03 | 1.33 | 1.37 |
| 12 | T1 | 302 | CYC | C4C-NC | -2.03 | 1.33 | 1.37 |
| 12 | F3 | 202 | CYC | C4C-NC | -2.03 | 1.33 | 1.37 |
| 12 | F1 | 202 | CYC | C4C-NC | -2.03 | 1.33 | 1.37 |
| 12 | B7 | 201 | CYC | C4D-CHA | 2.03 | 1.49 | 1.41 |
| 12 | T5 | 201 | CYC | C4D-CHA | 2.03 | 1.49 | 1.41 |
| 12 | H5 | 201 | CYC | C4D-CHA | 2.03 | 1.49 | 1.41 |
| 12 | Y7 | 201 | CYC | C1D-CHD | 2.03 | 1.49 | 1.41 |
| 12 | RA | 202 | CYC | C4C-NC | -2.03 | 1.33 | 1.37 |
| 12 | R9 | 202 | CYC | C4C-NC | -2.03 | 1.33 | 1.37 |
| 12 | F2 | 202 | CYC | C4C-NC | -2.03 | 1.33 | 1.37 |
| 12 | X7 | 201 | CYC | C4D-CHA | 2.03 | 1.49 | 1.41 |
| 12 | Q9 | 201 | CYC | C1C-NC | -2.03 | 1.35 | 1.37 |
| 12 | K4 | 201 | CYC | C1A-C2A | 2.03 | 1.48 | 1.45 |
| 12 | Q8 | 201 | CYC | C4C-NC | -2.03 | 1.33 | 1.37 |
| 12 | QA | 201 | CYC | C1A-C2A | 2.02 | 1.48 | 1.45 |
| 12 | QA | 201 | CYC | C1C-NC | -2.02 | 1.35 | 1.37 |
| 12 | F9 | 302 | CYC | C2C-C1C | -2.02 | 1.50 | 1.52 |
| 12 | E4 | 201 | CYC | C1A-C2A | 2.02 | 1.48 | 1.45 |
| 12 | E8 | 201 | CYC | C1A-C2A | 2.02 | 1.48 | 1.45 |
| 12 | T7 | 201 | CYC | C4D-CHA | 2.02 | 1.48 | 1.41 |
| 12 | L5 | 201 | CYC | C4D-CHA | 2.02 | 1.48 | 1.41 |
| 12 | H6 | 202 | CYC | C1B-C2B | 2.02 | 1.48 | 1.45 |
| 12 | R5 | 201 | CYC | C4A-C3A | 2.02 | 1.50 | 1.45 |
| 12 | D3 | 201 | CYC | C4C-NC | -2.02 | 1.33 | 1.37 |
| 12 | X5 | 201 | CYC | C4D-CHA | 2.02 | 1.48 | 1.41 |
| 12 | k5 | 1203 | CYC | C4D-CHA | 2.02 | 1.48 | 1.41 |
| 12 | j5 | 1201 | CYC | C4A-C3A | 2.02 | 1.50 | 1.45 |
| 12 | I2 | 201 | CYC | C1A-C2A | 2.02 | 1.48 | 1.45 |
| 12 | b7 | 201 | CYC | C4A-C3A | 2.02 | 1.50 | 1.45 |
| 12 | E6 | 201 | CYC | O2D-CGD | -2.01 | 1.24 | 1.30 |
| 12 | V3 | 202 | CYC | C4C-NC | -2.01 | 1.33 | 1.37 |
| 12 | V1 | 202 | CYC | C4C-NC | -2.01 | 1.33 | 1.37 |
| 12 | K8 | 201 | CYC | C1A-C2A | 2.01 | 1.48 | 1.45 |
| 12 | h7 | 201 | CYC | C4A-C3A | 2.01 | 1.50 | 1.45 |
| 12 | Y4 | 201 | CYC | C1B-C2B | 2.01 | 1.48 | 1.45 |
| 12 | Y8 | 201 | CYC | C1B-C2B | 2.01 | 1.48 | 1.45 |
| 12 | Y4 | 201 | CYC | C4C-NC | -2.01 | 1.33 | 1.37 |
| 12 | Y8 | 201 | CYC | C4C-NC | -2.01 | 1.33 | 1.37 |
| 12 | G4 | 201 | CYC | C1A-C2A | 2.01 | 1.48 | 1.45 |
| 12 | G8 | 201 | CYC | C1A-C2A | 2.01 | 1.48 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12 | A6 | 201 | CYC | C1A-C2A | 2.01 | 1.48 | 1.45 |
| 12 | A2 | 201 | CYC | C1A-C2A | 2.01 | 1.48 | 1.45 |
| 12 | D1 | 201 | CYC | C4C-NC | -2.01 | 1.33 | 1.37 |
| 12 | B5 | 201 | CYC | C4D-CHA | 2.01 | 1.48 | 1.41 |
| 12 | G6 | 201 | CYC | C4D-CHA | 2.01 | 1.48 | 1.41 |
| 12 | H7 | 201 | CYC | C4D-CHA | 2.01 | 1.48 | 1.41 |
| 12 | L3 | 201 | CYC | C1B-C2B | 2.01 | 1.48 | 1.45 |
| 12 | L1 | 201 | CYC | C1B-C2B | 2.01 | 1.48 | 1.45 |
| 12 | k5 | 1201 | CYC | C4A-C3A | 2.01 | 1.50 | 1.45 |
| 12 | E3 | 201 | CYC | C1A-C2A | 2.01 | 1.48 | 1.45 |
| 12 | E1 | 201 | CYC | C1A-C2A | 2.01 | 1.48 | 1.45 |
| 12 | D6 | 202 | CYC | C4C-NC | -2.01 | 1.33 | 1.37 |
| 12 | E2 | 201 | CYC | O2D-CGD | -2.01 | 1.24 | 1.30 |
| 12 | f7 | 201 | CYC | C4A-C3A | 2.01 | 1.50 | 1.45 |
| 12 | I6 | 201 | CYC | C1A-C2A | 2.01 | 1.48 | 1.45 |
| 12 | B1 | 201 | CYC | C4C-NC | -2.01 | 1.33 | 1.37 |
| 12 | D4 | 201 | CYC | C4C-NC | -2.01 | 1.33 | 1.37 |
| 12 | D8 | 201 | CYC | C4C-NC | -2.01 | 1.33 | 1.37 |
| 12 | F5 | 201 | CYC | C4D-CHA | 2.01 | 1.48 | 1.41 |
| 12 | OA | 201 | CYC | C1A-C2A | 2.00 | 1.48 | 1.45 |
| 12 | O9 | 201 | CYC | C1A-C2A | 2.00 | 1.48 | 1.45 |
| 12 | r7 | 201 | CYC | C4D-CHA | 2.00 | 1.48 | 1.41 |
| 12 | Q1 | 201 | CYC | C1A-C2A | 2.00 | 1.48 | 1.45 |
| 12 | Q3 | 201 | CYC | C1A-C2A | 2.00 | 1.48 | 1.45 |
| 12 | k5 | 1202 | CYC | C4D-CHA | 2.00 | 1.48 | 1.41 |
| 12 | F4 | 202 | CYC | C1A-NA | -2.00 | 1.34 | 1.38 |
| 12 | F8 | 202 | CYC | C1A-NA | -2.00 | 1.34 | 1.38 |
| 12 | X4 | 201 | CYC | C1C-NC | -2.00 | 1.35 | 1.37 |
| 12 | k5 | 1203 | CYC | C4A-C3A | 2.00 | 1.50 | 1.45 |

All (7051) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 12 | i7 | 201 | CYC | C3B-C4B-NB | 12.21 | 116.64 | 106.78 |
| 12 | g7 | 201 | CYC | C3B-C4B-NB | 12.16 | 116.60 | 106.78 |
| 12 | K5 | 201 | CYC | C3B-C4B-NB | 12.15 | 116.59 | 106.78 |
| 12 | Q7 | 201 | CYC | C3B-C4B-NB | 12.14 | 116.59 | 106.78 |
| 12 | a7 | 201 | CYC | C3B-C4B-NB | 12.11 | 116.56 | 106.78 |
| 12 | Y5 | 201 | CYC | C3B-C4B-NB | 12.11 | 116.56 | 106.78 |
| 12 | E5 | 201 | CYC | C3B-C4B-NB | 12.10 | 116.55 | 106.78 |
| 12 | c7 | 201 | CYC | C3B-C4B-NB | 12.09 | 116.55 | 106.78 |
| 12 | G5 | 201 | CYC | C3B-C4B-NB | 12.09 | 116.55 | 106.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 12 | K7 | 201 | CYC | C3B-C4B-NB | 12.07 | 116.53 | 106.78 |
| 12 | E7 | 201 | CYC | C3B-C4B-NB | 12.07 | 116.53 | 106.78 |
| 12 | m7 | 201 | CYC | C3B-C4B-NB | 12.06 | 116.53 | 106.78 |
| 12 | a5 | 201 | CYC | C3B-C4B-NB | 12.04 | 116.50 | 106.78 |
| 12 | e5 | 201 | CYC | C3B-C4B-NB | 12.04 | 116.50 | 106.78 |
| 12 | c5 | 201 | CYC | C3B-C4B-NB | 12.04 | 116.50 | 106.78 |
| 12 | U7 | 201 | CYC | C3B-C4B-NB | 12.04 | 116.50 | 106.78 |
| 12 | G7 | 201 | CYC | C3B-C4B-NB | 12.03 | 116.50 | 106.78 |
| 12 | W7 | 201 | CYC | C3B-C4B-NB | 12.03 | 116.50 | 106.78 |
| 12 | A7 | 201 | CYC | C3B-C4B-NB | 12.02 | 116.49 | 106.78 |
| 12 | A5 | 201 | CYC | C3B-C4B-NB | 12.02 | 116.49 | 106.78 |
| 12 | u7 | 201 | CYC | C3B-C4B-NB | 12.02 | 116.49 | 106.78 |
| 12 | o7 | 201 | CYC | C3B-C4B-NB | 12.01 | 116.48 | 106.78 |
| 12 | O5 | 201 | CYC | C3B-C4B-NB | 12.01 | 116.48 | 106.78 |
| 12 | U5 | 201 | CYC | C3B-C4B-NB | 12.01 | 116.48 | 106.78 |
| 12 | C7 | 201 | CYC | C3B-C4B-NB | 11.99 | 116.47 | 106.78 |
| 12 | I7 | 201 | CYC | C3B-C4B-NB | 11.99 | 116.47 | 106.78 |
| 12 | Q5 | 201 | CYC | C3B-C4B-NB | 11.98 | 116.46 | 106.78 |
| 12 | O7 | 201 | CYC | C3B-C4B-NB | 11.98 | 116.46 | 106.78 |
| 12 | W5 | 201 | CYC | C3B-C4B-NB | 11.97 | 116.45 | 106.78 |
| 12 | s7 | 201 | CYC | C3B-C4B-NB | 11.96 | 116.44 | 106.78 |
| 12 | M7 | 201 | CYC | C3B-C4B-NB | 11.95 | 116.43 | 106.78 |
| 12 | C5 | 201 | CYC | C3B-C4B-NB | 11.93 | 116.42 | 106.78 |
| 12 | I5 | 201 | CYC | C3B-C4B-NB | 11.90 | 116.39 | 106.78 |
| 12 | q7 | 201 | CYC | C3B-C4B-NB | 11.87 | 116.37 | 106.78 |
| 12 | S5 | 201 | CYC | C3B-C4B-NB | 11.86 | 116.36 | 106.78 |
| 12 | Y7 | 201 | CYC | C3B-C4B-NB | 11.84 | 116.35 | 106.78 |
| 12 | k7 | 201 | CYC | C3B-C4B-NB | 11.84 | 116.34 | 106.78 |
| 12 | M5 | 201 | CYC | C3B-C4B-NB | 11.81 | 116.32 | 106.78 |
| 12 | e7 | 201 | CYC | C3B-C4B-NB | 11.81 | 116.32 | 106.78 |
| 12 | S7 | 201 | CYC | C3B-C4B-NB | 11.79 | 116.31 | 106.78 |
| 12 | S4 | 202 | CYC | C3B-C4B-NB | 11.52 | 116.08 | 106.78 |
| 12 | VA | 201 | CYC | C3B-C4B-NB | 11.50 | 116.07 | 106.78 |
| 12 | V9 | 201 | CYC | C3B-C4B-NB | 11.46 | 116.04 | 106.78 |
| 12 | J2 | 202 | CYC | C3B-C4B-NB | 11.45 | 116.03 | 106.78 |
| 12 | LA | 202 | CYC | C3B-C4B-NB | 11.45 | 116.03 | 106.78 |
| 12 | PA | 201 | CYC | C3B-C4B-NB | 11.45 | 116.03 | 106.78 |
| 12 | P9 | 201 | CYC | C3B-C4B-NB | 11.45 | 116.03 | 106.78 |
| 12 | ZA | 202 | CYC | C3B-C4B-NB | 11.44 | 116.02 | 106.78 |
| 12 | Z9 | 202 | CYC | C3B-C4B-NB | 11.44 | 116.02 | 106.78 |
| 12 | M8 | 302 | CYC | C3B-C4B-NB | 11.42 | 116.01 | 106.78 |
| 12 | J6 | 202 | CYC | C3B-C4B-NB | 11.42 | 116.00 | 106.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 12 | N2 | 101 | CYC | C3B-C4B-NB | 11.41 | 116.00 | 106.78 |
| 12 | L9 | 202 | CYC | C3B-C4B-NB | 11.41 | 116.00 | 106.78 |
| 12 | XA | 201 | CYC | C3B-C4B-NB | 11.40 | 115.99 | 106.78 |
| 12 | X9 | 201 | CYC | C3B-C4B-NB | 11.40 | 115.99 | 106.78 |
| 12 | N6 | 101 | CYC | C3B-C4B-NB | 11.40 | 115.99 | 106.78 |
| 12 | J4 | 201 | CYC | C3B-C4B-NB | 11.39 | 115.98 | 106.78 |
| 12 | J8 | 201 | CYC | C3B-C4B-NB | 11.39 | 115.98 | 106.78 |
| 12 | X3 | 201 | CYC | C3B-C4B-NB | 11.39 | 115.98 | 106.78 |
| 12 | X1 | 201 | CYC | C3B-C4B-NB | 11.39 | 115.98 | 106.78 |
| 12 | U4 | 201 | CYC | C3B-C4B-NB | 11.39 | 115.98 | 106.78 |
| 12 | U8 | 201 | CYC | C3B-C4B-NB | 11.39 | 115.98 | 106.78 |
| 12 | J3 | 202 | CYC | C3B-C4B-NB | 11.37 | 115.97 | 106.78 |
| 12 | L2 | 201 | CYC | C3B-C4B-NB | 11.37 | 115.97 | 106.78 |
| 12 | aA | 901 | CYC | C3B-C4B-NB | 11.37 | 115.97 | 106.78 |
| 12 | L6 | 201 | CYC | C3B-C4B-NB | 11.37 | 115.96 | 106.78 |
| 12 | DA | 201 | CYC | C3B-C4B-NB | 11.35 | 115.94 | 106.78 |
| 12 | JA | 202 | CYC | C3B-C4B-NB | 11.35 | 115.94 | 106.78 |
| 12 | J9 | 202 | CYC | C3B-C4B-NB | 11.35 | 115.94 | 106.78 |
| 12 | D1 | 202 | CYC | C3B-C4B-NB | 11.34 | 115.94 | 106.78 |
| 12 | F6 | 201 | CYC | C3B-C4B-NB | 11.33 | 115.93 | 106.78 |
| 12 | V3 | 201 | CYC | C3B-C4B-NB | 11.32 | 115.93 | 106.78 |
| 12 | V1 | 201 | CYC | C3B-C4B-NB | 11.32 | 115.93 | 106.78 |
| 12 | H1 | 201 | CYC | C3B-C4B-NB | 11.31 | 115.91 | 106.78 |
| 12 | Z3 | 201 | CYC | C3B-C4B-NB | 11.31 | 115.91 | 106.78 |
| 12 | D9 | 201 | CYC | C3B-C4B-NB | 11.30 | 115.91 | 106.78 |
| 12 | T3 | 301 | CYC | C3B-C4B-NB | 11.30 | 115.91 | 106.78 |
| 12 | T1 | 301 | CYC | C3B-C4B-NB | 11.30 | 115.91 | 106.78 |
| 12 | F4 | 202 | CYC | C3B-C4B-NB | 11.29 | 115.90 | 106.78 |
| 12 | F8 | 202 | CYC | C3B-C4B-NB | 11.29 | 115.90 | 106.78 |
| 12 | H3 | 202 | CYC | C3B-C4B-NB | 11.29 | 115.90 | 106.78 |
| 12 | B4 | 202 | CYC | C3B-C4B-NB | 11.29 | 115.90 | 106.78 |
| 12 | Z1 | 202 | CYC | C3B-C4B-NB | 11.28 | 115.89 | 106.78 |
| 12 | B3 | 202 | CYC | C3B-C4B-NB | 11.27 | 115.89 | 106.78 |
| 12 | F2 | 201 | CYC | C3B-C4B-NB | 11.27 | 115.89 | 106.78 |
| 12 | D3 | 202 | CYC | C3B-C4B-NB | 11.27 | 115.88 | 106.78 |
| 12 | H6 | 201 | CYC | C3B-C4B-NB | 11.27 | 115.88 | 106.78 |
| 12 | B1 | 202 | CYC | C3B-C4B-NB | 11.27 | 115.88 | 106.78 |
| 12 | R1 | 201 | CYC | C3B-C4B-NB | 11.26 | 115.88 | 106.78 |
| 12 | R3 | 201 | CYC | C3B-C4B-NB | 11.26 | 115.88 | 106.78 |
| 12 | BA | 201 | CYC | C3B-C4B-NB | 11.25 | 115.86 | 106.78 |
| 12 | B9 | 201 | CYC | C3B-C4B-NB | 11.25 | 115.86 | 106.78 |
| 12 | O4 | 201 | CYC | C3B-C4B-NB | 11.24 | 115.86 | 106.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 12 | O8 | 201 | CYC | C3B-C4B-NB | 11.24 | 115.86 | 106.78 |
| 12 | F3 | 201 | CYC | C3B-C4B-NB | 11.23 | 115.85 | 106.78 |
| 12 | F1 | 201 | CYC | C3B-C4B-NB | 11.23 | 115.85 | 106.78 |
| 12 | H8 | 201 | CYC | C3B-C4B-NB | 11.23 | 115.85 | 106.78 |
| 12 | L4 | 202 | CYC | C3B-C4B-NB | 11.22 | 115.84 | 106.78 |
| 12 | L3 | 202 | CYC | C3B-C4B-NB | 11.21 | 115.84 | 106.78 |
| 12 | aA | 902 | CYC | C3B-C4B-NB | 11.21 | 115.84 | 106.78 |
| 12 | J5 | 201 | CYC | C3B-C4B-NB | 11.21 | 115.83 | 106.78 |
| 12 | L5 | 201 | CYC | C3B-C4B-NB | 11.21 | 115.83 | 106.78 |
| 12 | H2 | 201 | CYC | C3B-C4B-NB | 11.20 | 115.83 | 106.78 |
| 12 | D8 | 202 | CYC | C3B-C4B-NB | 11.20 | 115.83 | 106.78 |
| 12 | X5 | 201 | CYC | C3B-C4B-NB | 11.20 | 115.83 | 106.78 |
| 12 | HA | 202 | CYC | C3B-C4B-NB | 11.19 | 115.82 | 106.78 |
| 12 | a9 | 901 | CYC | C3B-C4B-NB | 11.19 | 115.82 | 106.78 |
| 12 | P1 | 201 | CYC | C3B-C4B-NB | 11.19 | 115.82 | 106.78 |
| 12 | P3 | 201 | CYC | C3B-C4B-NB | 11.19 | 115.82 | 106.78 |
| 12 | H4 | 201 | CYC | C3B-C4B-NB | 11.19 | 115.82 | 106.78 |
| 12 | B8 | 202 | CYC | C3B-C4B-NB | 11.19 | 115.82 | 106.78 |
| 12 | FA | 301 | CYC | C3B-C4B-NB | 11.19 | 115.82 | 106.78 |
| 12 | F9 | 301 | CYC | C3B-C4B-NB | 11.19 | 115.82 | 106.78 |
| 12 | R5 | 201 | CYC | C3B-C4B-NB | 11.18 | 115.81 | 106.78 |
| 12 | D2 | 201 | CYC | C3B-C4B-NB | 11.18 | 115.81 | 106.78 |
| 12 | D4 | 202 | CYC | C3B-C4B-NB | 11.17 | 115.80 | 106.78 |
| 12 | F5 | 201 | CYC | C3B-C4B-NB | 11.17 | 115.80 | 106.78 |
| 12 | J7 | 201 | CYC | C3B-C4B-NB | 11.17 | 115.80 | 106.78 |
| 12 | p7 | 201 | CYC | C3B-C4B-NB | 11.17 | 115.80 | 106.78 |
| 12 | H9 | 202 | CYC | C3B-C4B-NB | 11.17 | 115.80 | 106.78 |
| 12 | W8 | 201 | CYC | C3B-C4B-NB | 11.16 | 115.80 | 106.78 |
| 12 | d7 | 201 | CYC | C3B-C4B-NB | 11.16 | 115.79 | 106.78 |
| 12 | TA | 301 | CYC | C3B-C4B-NB | 11.15 | 115.79 | 106.78 |
| 12 | T9 | 301 | CYC | C3B-C4B-NB | 11.15 | 115.79 | 106.78 |
| 12 | Z4 | 301 | CYC | C3B-C4B-NB | 11.15 | 115.78 | 106.78 |
| 12 | M4 | 301 | CYC | C3B-C4B-NB | 11.14 | 115.78 | 106.78 |
| 12 | F7 | 201 | CYC | C3B-C4B-NB | 11.13 | 115.77 | 106.78 |
| 12 | Z8 | 301 | CYC | C3B-C4B-NB | 11.13 | 115.77 | 106.78 |
| 12 | Y4 | 201 | CYC | C3B-C4B-NB | 11.13 | 115.77 | 106.78 |
| 12 | Y8 | 201 | CYC | C3B-C4B-NB | 11.13 | 115.77 | 106.78 |
| 12 | L7 | 201 | CYC | C3B-C4B-NB | 11.13 | 115.77 | 106.78 |
| 12 | D7 | 201 | CYC | C3B-C4B-NB | 11.12 | 115.76 | 106.78 |
| 12 | j7 | 201 | CYC | C3B-C4B-NB | 11.12 | 115.76 | 106.78 |
| 12 | X7 | 201 | CYC | C3B-C4B-NB | 11.11 | 115.75 | 106.78 |
| 12 | Z | 201 | CYC | C3B-C4B-NB | 11.11 | 115.75 | 106.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 12 | W4 | 201 | CYC | C3B-C4B-NB | 11.11 | 115.75 | 106.78 |
| 12 | T5 | 201 | CYC | C3B-C4B-NB | 11.11 | 115.75 | 106.78 |
| 12 | N5 | 201 | CYC | C3B-C4B-NB | 11.10 | 115.75 | 106.78 |
| 12 | D6 | 201 | CYC | C3B-C4B-NB | 11.10 | 115.75 | 106.78 |
| 12 | RA | 201 | CYC | C3B-C4B-NB | 11.10 | 115.75 | 106.78 |
| 12 | R9 | 201 | CYC | C3B-C4B-NB | 11.10 | 115.75 | 106.78 |
| 12 | D5 | 201 | CYC | C3B-C4B-NB | 11.10 | 115.75 | 106.78 |
| 12 | v7 | 201 | CYC | C3B-C4B-NB | 11.10 | 115.75 | 106.78 |
| 12 | d5 | 201 | CYC | C3B-C4B-NB | 11.10 | 115.74 | 106.78 |
| 12 | B4 | 201 | CYC | C3B-C4B-NB | 11.09 | 115.74 | 106.78 |
| 12 | B8 | 201 | CYC | C3B-C4B-NB | 11.09 | 115.74 | 106.78 |
| 12 | V7 | 201 | CYC | C3B-C4B-NB | 11.08 | 115.73 | 106.78 |
| 12 | T7 | 201 | CYC | C3B-C4B-NB | 11.08 | 115.73 | 106.78 |
| 12 | R7 | 201 | CYC | C3B-C4B-NB | 11.08 | 115.73 | 106.78 |
| 12 | f5 | 201 | CYC | C3B-C4B-NB | 11.08 | 115.73 | 106.78 |
| 12 | A | 201 | CYC | C3B-C4B-NB | 11.08 | 115.73 | 106.78 |
| 12 | b7 | 201 | CYC | C3B-C4B-NB | 11.08 | 115.73 | 106.78 |
| 12 | b5 | 201 | CYC | C3B-C4B-NB | 11.07 | 115.72 | 106.78 |
| 12 | k5 | 1203 | CYC | C3B-C4B-NB | 11.06 | 115.72 | 106.78 |
| 12 | H7 | 201 | CYC | C3B-C4B-NB | 11.06 | 115.72 | 106.78 |
| 12 | Z5 | 201 | CYC | C3B-C4B-NB | 11.06 | 115.71 | 106.78 |
| 12 | M8 | 301 | CYC | C3B-C4B-NB | 11.05 | 115.71 | 106.78 |
| 12 | V5 | 201 | CYC | C3B-C4B-NB | 11.05 | 115.70 | 106.78 |
| 12 | B7 | 201 | CYC | C3B-C4B-NB | 11.05 | 115.70 | 106.78 |
| 12 | r7 | 201 | CYC | C3B-C4B-NB | 11.04 | 115.70 | 106.78 |
| 12 | P7 | 201 | CYC | C3B-C4B-NB | 11.03 | 115.69 | 106.78 |
| 12 | B3 | 201 | CYC | C3B-C4B-NB | 11.02 | 115.68 | 106.78 |
| 12 | B1 | 201 | CYC | C3B-C4B-NB | 11.02 | 115.68 | 106.78 |
| 12 | H5 | 201 | CYC | C3B-C4B-NB | 11.01 | 115.67 | 106.78 |
| 12 | B6 | 201 | CYC | C3B-C4B-NB | 11.00 | 115.67 | 106.78 |
| 12 | B5 | 201 | CYC | C3B-C4B-NB | 11.00 | 115.67 | 106.78 |
| 12 | P5 | 201 | CYC | C3B-C4B-NB | 11.00 | 115.66 | 106.78 |
| 12 | O4 | 202 | CYC | C3B-C4B-NB | 11.00 | 115.66 | 106.78 |
| 12 | O8 | 202 | CYC | C3B-C4B-NB | 11.00 | 115.66 | 106.78 |
| 12 | D6 | 202 | CYC | C3B-C4B-NB | 10.99 | 115.66 | 106.78 |
| 12 | J8 | 202 | CYC | C3B-C4B-NB | 10.99 | 115.66 | 106.78 |
| 12 | L8 | 201 | CYC | C3B-C4B-NB | 10.99 | 115.66 | 106.78 |
| 12 | F9 | 302 | CYC | C3B-C4B-NB | 10.99 | 115.66 | 106.78 |
| 12 | k5 | 1204 | CYC | C3B-C4B-NB | 10.98 | 115.65 | 106.78 |
| 12 | S4 | 201 | CYC | C3B-C4B-NB | 10.98 | 115.65 | 106.78 |
| 12 | S8 | 201 | CYC | C3B-C4B-NB | 10.98 | 115.65 | 106.78 |
| 12 | k5 | 1202 | CYC | C3B-C4B-NB | 10.98 | 115.65 | 106.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 12 | F6 | 202 | CYC | C3B-C4B-NB | 10.98 | 115.65 | 106.78 |
| 12 | N7 | 201 | CYC | C3B-C4B-NB | 10.98 | 115.65 | 106.78 |
| 12 | BA | 202 | CYC | C3B-C4B-NB | 10.98 | 115.64 | 106.78 |
| 12 | B9 | 202 | CYC | C3B-C4B-NB | 10.98 | 115.64 | 106.78 |
| 12 | D2 | 202 | CYC | C3B-C4B-NB | 10.97 | 115.64 | 106.78 |
| 12 | Q4 | 201 | CYC | C3B-C4B-NB | 10.97 | 115.64 | 106.78 |
| 12 | B2 | 201 | CYC | C3B-C4B-NB | 10.97 | 115.64 | 106.78 |
| 12 | h7 | 201 | CYC | C3B-C4B-NB | 10.96 | 115.64 | 106.78 |
| 12 | VA | 202 | CYC | C3B-C4B-NB | 10.96 | 115.64 | 106.78 |
| 12 | V9 | 202 | CYC | C3B-C4B-NB | 10.96 | 115.64 | 106.78 |
| 12 | j5 | 1202 | CYC | C3B-C4B-NB | 10.96 | 115.63 | 106.78 |
| 12 | L4 | 201 | CYC | C3B-C4B-NB | 10.96 | 115.63 | 106.78 |
| 12 | J2 | 201 | CYC | C3B-C4B-NB | 10.96 | 115.63 | 106.78 |
| 12 | Q8 | 201 | CYC | C3B-C4B-NB | 10.96 | 115.63 | 106.78 |
| 12 | JA | 201 | CYC | C3B-C4B-NB | 10.95 | 115.63 | 106.78 |
| 12 | XA | 202 | CYC | C3B-C4B-NB | 10.95 | 115.63 | 106.78 |
| 12 | X9 | 202 | CYC | C3B-C4B-NB | 10.95 | 115.63 | 106.78 |
| 12 | P1 | 202 | CYC | C3B-C4B-NB | 10.94 | 115.62 | 106.78 |
| 12 | P3 | 202 | CYC | C3B-C4B-NB | 10.94 | 115.62 | 106.78 |
| 12 | f7 | 201 | CYC | C3B-C4B-NB | 10.94 | 115.62 | 106.78 |
| 12 | F9 | 303 | CYC | C3B-C4B-NB | 10.94 | 115.62 | 106.78 |
| 12 | PA | 202 | CYC | C3B-C4B-NB | 10.93 | 115.61 | 106.78 |
| 12 | D4 | 201 | CYC | C3B-C4B-NB | 10.93 | 115.61 | 106.78 |
| 12 | D8 | 201 | CYC | C3B-C4B-NB | 10.93 | 115.61 | 106.78 |
| 12 | P9 | 202 | CYC | C3B-C4B-NB | 10.93 | 115.61 | 106.78 |
| 12 | W4 | 202 | CYC | C3B-C4B-NB | 10.93 | 115.61 | 106.78 |
| 12 | W8 | 202 | CYC | C3B-C4B-NB | 10.93 | 115.61 | 106.78 |
| 12 | L3 | 201 | CYC | C3B-C4B-NB | 10.92 | 115.60 | 106.78 |
| 12 | L1 | 201 | CYC | C3B-C4B-NB | 10.92 | 115.60 | 106.78 |
| 12 | J4 | 202 | CYC | C3B-C4B-NB | 10.92 | 115.60 | 106.78 |
| 12 | J9 | 201 | CYC | C3B-C4B-NB | 10.91 | 115.59 | 106.78 |
| 12 | T3 | 302 | CYC | C3B-C4B-NB | 10.90 | 115.59 | 106.78 |
| 12 | T9 | 302 | CYC | C3B-C4B-NB | 10.90 | 115.59 | 106.78 |
| 12 | T1 | 302 | CYC | C3B-C4B-NB | 10.90 | 115.59 | 106.78 |
| 12 | F2 | 202 | CYC | C3B-C4B-NB | 10.90 | 115.59 | 106.78 |
| 12 | L6 | 202 | CYC | C3B-C4B-NB | 10.90 | 115.58 | 106.78 |
| 12 | J6 | 201 | CYC | C3B-C4B-NB | 10.89 | 115.58 | 106.78 |
| 12 | TA | 302 | CYC | C3B-C4B-NB | 10.89 | 115.57 | 106.78 |
| 12 | D3 | 201 | CYC | C3B-C4B-NB | 10.87 | 115.56 | 106.78 |
| 12 | D1 | 201 | CYC | C3B-C4B-NB | 10.87 | 115.56 | 106.78 |
| 12 | L2 | 202 | CYC | C3B-C4B-NB | 10.87 | 115.56 | 106.78 |
| 12 | L9 | 201 | CYC | C3B-C4B-NB | 10.85 | 115.54 | 106.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 12 | V3 | 202 | CYC | C3B-C4B-NB | 10.85 | 115.54 | 106.78 |
| 12 | V1 | 202 | CYC | C3B-C4B-NB | 10.85 | 115.54 | 106.78 |
| 12 | R1 | 202 | CYC | C3B-C4B-NB | 10.84 | 115.54 | 106.78 |
| 12 | R3 | 202 | CYC | C3B-C4B-NB | 10.84 | 115.54 | 106.78 |
| 12 | F4 | 201 | CYC | C3B-C4B-NB | 10.84 | 115.54 | 106.78 |
| 12 | F8 | 201 | CYC | C3B-C4B-NB | 10.84 | 115.54 | 106.78 |
| 12 | ZA | 201 | CYC | C3B-C4B-NB | 10.84 | 115.54 | 106.78 |
| 12 | Z9 | 201 | CYC | C3B-C4B-NB | 10.84 | 115.54 | 106.78 |
| 12 | LA | 201 | CYC | C3B-C4B-NB | 10.82 | 115.52 | 106.78 |
| 12 | D9 | 202 | CYC | C3B-C4B-NB | 10.82 | 115.52 | 106.78 |
| 12 | DA | 202 | CYC | C3B-C4B-NB | 10.81 | 115.52 | 106.78 |
| 12 | HA | 201 | CYC | C3B-C4B-NB | 10.79 | 115.50 | 106.78 |
| 12 | X3 | 202 | CYC | C3B-C4B-NB | 10.78 | 115.49 | 106.78 |
| 12 | X1 | 202 | CYC | C3B-C4B-NB | 10.78 | 115.49 | 106.78 |
| 12 | H3 | 201 | CYC | C3B-C4B-NB | 10.77 | 115.48 | 106.78 |
| 12 | H1 | 202 | CYC | C3B-C4B-NB | 10.77 | 115.48 | 106.78 |
| 12 | Z3 | 202 | CYC | C3B-C4B-NB | 10.77 | 115.48 | 106.78 |
| 12 | H4 | 202 | CYC | C3B-C4B-NB | 10.77 | 115.48 | 106.78 |
| 12 | H8 | 202 | CYC | C3B-C4B-NB | 10.77 | 115.48 | 106.78 |
| 12 | Z1 | 201 | CYC | C3B-C4B-NB | 10.77 | 115.48 | 106.78 |
| 12 | H9 | 201 | CYC | C3B-C4B-NB | 10.76 | 115.47 | 106.78 |
| 12 | RA | 202 | CYC | C3B-C4B-NB | 10.75 | 115.46 | 106.78 |
| 12 | R9 | 202 | CYC | C3B-C4B-NB | 10.75 | 115.46 | 106.78 |
| 12 | H6 | 202 | CYC | C3B-C4B-NB | 10.73 | 115.45 | 106.78 |
| 12 | J1 | 201 | CYC | C3B-C4B-NB | 10.73 | 115.45 | 106.78 |
| 12 | H2 | 202 | CYC | C3B-C4B-NB | 10.70 | 115.42 | 106.78 |
| 12 | J3 | 201 | CYC | C3B-C4B-NB | 10.70 | 115.42 | 106.78 |
| 12 | U8 | 202 | CYC | C3B-C4B-NB | 10.69 | 115.41 | 106.78 |
| 12 | F3 | 202 | CYC | C3B-C4B-NB | 10.66 | 115.39 | 106.78 |
| 12 | F1 | 202 | CYC | C3B-C4B-NB | 10.66 | 115.39 | 106.78 |
| 12 | U4 | 202 | CYC | C3B-C4B-NB | 10.64 | 115.37 | 106.78 |
| 12 | KA | 201 | CYC | C3B-C4B-NB | 10.59 | 115.33 | 106.78 |
| 12 | K9 | 201 | CYC | C3B-C4B-NB | 10.59 | 115.33 | 106.78 |
| 12 | I3 | 201 | CYC | C3B-C4B-NB | 10.56 | 115.31 | 106.78 |
| 12 | T4 | 201 | CYC | C3B-C4B-NB | 10.56 | 115.31 | 106.78 |
| 12 | T8 | 201 | CYC | C3B-C4B-NB | 10.56 | 115.31 | 106.78 |
| 12 | I1 | 201 | CYC | C3B-C4B-NB | 10.56 | 115.31 | 106.78 |
| 12 | E6 | 201 | CYC | C3B-C4B-NB | 10.55 | 115.30 | 106.78 |
| 12 | E2 | 201 | CYC | C3B-C4B-NB | 10.55 | 115.30 | 106.78 |
| 12 | YA | 201 | CYC | C3B-C4B-NB | 10.54 | 115.30 | 106.78 |
| 12 | SA | 201 | CYC | C3B-C4B-NB | 10.54 | 115.29 | 106.78 |
| 12 | S9 | 201 | CYC | C3B-C4B-NB | 10.54 | 115.29 | 106.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 12 | EA | 201 | CYC | C3B-C4B-NB | 10.52 | 115.27 | 106.78 |
| 12 | E9 | 201 | CYC | C3B-C4B-NB | 10.52 | 115.27 | 106.78 |
| 12 | K3 | 201 | CYC | C3B-C4B-NB | 10.51 | 115.27 | 106.78 |
| 12 | K1 | 201 | CYC | C3B-C4B-NB | 10.51 | 115.27 | 106.78 |
| 12 | Y9 | 201 | CYC | C3B-C4B-NB | 10.50 | 115.26 | 106.78 |
| 12 | I2 | 201 | CYC | C3B-C4B-NB | 10.49 | 115.25 | 106.78 |
| 12 | S1 | 201 | CYC | C3B-C4B-NB | 10.49 | 115.25 | 106.78 |
| 12 | S3 | 201 | CYC | C3B-C4B-NB | 10.49 | 115.25 | 106.78 |
| 12 | R4 | 201 | CYC | C3B-C4B-NB | 10.48 | 115.25 | 106.78 |
| 12 | X4 | 201 | CYC | C3B-C4B-NB | 10.48 | 115.25 | 106.78 |
| 12 | X8 | 201 | CYC | C3B-C4B-NB | 10.48 | 115.25 | 106.78 |
| 12 | R8 | 201 | CYC | C3B-C4B-NB | 10.48 | 115.25 | 106.78 |
| 12 | E8 | 201 | CYC | C3B-C4B-NB | 10.47 | 115.24 | 106.78 |
| 12 | G4 | 201 | CYC | C3B-C4B-NB | 10.47 | 115.24 | 106.78 |
| 12 | G8 | 201 | CYC | C3B-C4B-NB | 10.47 | 115.24 | 106.78 |
| 12 | C4 | 201 | CYC | C3B-C4B-NB | 10.47 | 115.23 | 106.78 |
| 12 | C8 | 201 | CYC | C3B-C4B-NB | 10.47 | 115.23 | 106.78 |
| 12 | C6 | 201 | CYC | C3B-C4B-NB | 10.46 | 115.23 | 106.78 |
| 12 | G2 | 201 | CYC | C3B-C4B-NB | 10.45 | 115.22 | 106.78 |
| 12 | K2 | 201 | CYC | C3B-C4B-NB | 10.44 | 115.22 | 106.78 |
| 12 | K6 | 201 | CYC | C3B-C4B-NB | 10.44 | 115.22 | 106.78 |
| 12 | G6 | 201 | CYC | C3B-C4B-NB | 10.44 | 115.21 | 106.78 |
| 12 | I6 | 201 | CYC | C3B-C4B-NB | 10.43 | 115.21 | 106.78 |
| 12 | C2 | 201 | CYC | C3B-C4B-NB | 10.43 | 115.20 | 106.78 |
| 12 | IA | 201 | CYC | C3B-C4B-NB | 10.42 | 115.19 | 106.78 |
| 12 | I9 | 201 | CYC | C3B-C4B-NB | 10.42 | 115.19 | 106.78 |
| 12 | j5 | 1201 | CYC | C3B-C4B-NB | 10.42 | 115.19 | 106.78 |
| 12 | O1 | 201 | CYC | C3B-C4B-NB | 10.41 | 115.19 | 106.78 |
| 12 | O3 | 201 | CYC | C3B-C4B-NB | 10.41 | 115.19 | 106.78 |
| 12 | E4 | 201 | CYC | C3B-C4B-NB | 10.41 | 115.19 | 106.78 |
| 12 | E3 | 201 | CYC | C3B-C4B-NB | 10.40 | 115.18 | 106.78 |
| 12 | E1 | 201 | CYC | C3B-C4B-NB | 10.40 | 115.18 | 106.78 |
| 12 | K8 | 201 | CYC | C3B-C4B-NB | 10.40 | 115.18 | 106.78 |
| 12 | A8 | 201 | CYC | C3B-C4B-NB | 10.39 | 115.17 | 106.78 |
| 12 | A4 | 201 | CYC | C3B-C4B-NB | 10.38 | 115.17 | 106.78 |
| 12 | A1 | 201 | CYC | C3B-C4B-NB | 10.38 | 115.16 | 106.78 |
| 12 | A3 | 201 | CYC | C3B-C4B-NB | 10.38 | 115.16 | 106.78 |
| 12 | Q9 | 201 | CYC | C3B-C4B-NB | 10.37 | 115.16 | 106.78 |
| 12 | GA | 201 | CYC | C3B-C4B-NB | 10.37 | 115.15 | 106.78 |
| 12 | I4 | 201 | CYC | C3B-C4B-NB | 10.37 | 115.15 | 106.78 |
| 12 | I8 | 201 | CYC | C3B-C4B-NB | 10.37 | 115.15 | 106.78 |
| 12 | G9 | 201 | CYC | C3B-C4B-NB | 10.37 | 115.15 | 106.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 12 | V8 | 201 | CYC | C3B-C4B-NB | 10.36 | 115.15 | 106.78 |
| 12 | QA | 201 | CYC | C3B-C4B-NB | 10.36 | 115.15 | 106.78 |
| 12 | G3 | 201 | CYC | C3B-C4B-NB | 10.36 | 115.15 | 106.78 |
| 12 | G1 | 201 | CYC | C3B-C4B-NB | 10.36 | 115.15 | 106.78 |
| 12 | U3 | 201 | CYC | C3B-C4B-NB | 10.36 | 115.15 | 106.78 |
| 12 | U1 | 201 | CYC | C3B-C4B-NB | 10.36 | 115.15 | 106.78 |
| 12 | K4 | 201 | CYC | C3B-C4B-NB | 10.34 | 115.13 | 106.78 |
| 12 | UA | 201 | CYC | C3B-C4B-NB | 10.33 | 115.12 | 106.78 |
| 12 | U9 | 201 | CYC | C3B-C4B-NB | 10.33 | 115.12 | 106.78 |
| 12 | A6 | 201 | CYC | C3B-C4B-NB | 10.32 | 115.12 | 106.78 |
| 12 | Y3 | 201 | CYC | C3B-C4B-NB | 10.32 | 115.12 | 106.78 |
| 12 | Y1 | 201 | CYC | C3B-C4B-NB | 10.32 | 115.12 | 106.78 |
| 12 | V4 | 201 | CYC | C3B-C4B-NB | 10.32 | 115.12 | 106.78 |
| 12 | O9 | 201 | CYC | C3B-C4B-NB | 10.30 | 115.10 | 106.78 |
| 12 | N4 | 201 | CYC | C3B-C4B-NB | 10.30 | 115.10 | 106.78 |
| 12 | P4 | 201 | CYC | C3B-C4B-NB | 10.29 | 115.09 | 106.78 |
| 12 | P8 | 201 | CYC | C3B-C4B-NB | 10.29 | 115.09 | 106.78 |
| 12 | W9 | 201 | CYC | C3B-C4B-NB | 10.29 | 115.09 | 106.78 |
| 12 | OA | 201 | CYC | C3B-C4B-NB | 10.29 | 115.09 | 106.78 |
| 12 | A2 | 201 | CYC | C3B-C4B-NB | 10.29 | 115.09 | 106.78 |
| 12 | CA | 201 | CYC | C3B-C4B-NB | 10.28 | 115.08 | 106.78 |
| 12 | C9 | 201 | CYC | C3B-C4B-NB | 10.28 | 115.08 | 106.78 |
| 12 | N8 | 201 | CYC | C3B-C4B-NB | 10.27 | 115.08 | 106.78 |
| 12 | k5 | 1201 | CYC | C3B-C4B-NB | 10.26 | 115.07 | 106.78 |
| 12 | WA | 201 | CYC | C3B-C4B-NB | 10.26 | 115.07 | 106.78 |
| 12 | AA | 201 | CYC | C3B-C4B-NB | 10.25 | 115.06 | 106.78 |
| 12 | A9 | 201 | CYC | C3B-C4B-NB | 10.25 | 115.06 | 106.78 |
| 12 | W1 | 201 | CYC | C3B-C4B-NB | 10.24 | 115.05 | 106.78 |
| 12 | C3 | 201 | CYC | C3B-C4B-NB | 10.23 | 115.04 | 106.78 |
| 12 | C1 | 201 | CYC | C3B-C4B-NB | 10.23 | 115.04 | 106.78 |
| 12 | Q1 | 201 | CYC | C3B-C4B-NB | 10.22 | 115.04 | 106.78 |
| 12 | Q3 | 201 | CYC | C3B-C4B-NB | 10.22 | 115.04 | 106.78 |
| 12 | W3 | 201 | CYC | C3B-C4B-NB | 10.21 | 115.03 | 106.78 |
| 12 | B4 | 201 | CYC | OB-C4B-C3B | -7.99 | 119.36 | 128.04 |
| 12 | B8 | 201 | CYC | OB-C4B-C3B | -7.99 | 119.36 | 128.04 |
| 12 | O4 | 202 | CYC | OB-C4B-C3B | -7.92 | 119.44 | 128.04 |
| 12 | O8 | 202 | CYC | OB-C4B-C3B | -7.92 | 119.44 | 128.04 |
| 12 | F4 | 201 | CYC | OB-C4B-C3B | -7.91 | 119.45 | 128.04 |
| 12 | F9 | 303 | CYC | OB-C4B-C3B | -7.88 | 119.48 | 128.04 |
| 12 | BA | 202 | CYC | OB-C4B-C3B | -7.88 | 119.49 | 128.04 |
| 12 | B9 | 202 | CYC | OB-C4B-C3B | -7.88 | 119.49 | 128.04 |
| 12 | F9 | 302 | CYC | OB-C4B-C3B | -7.88 | 119.49 | 128.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 12 | F8 | 201 | CYC | OB-C4B-C3B | -7.87 | 119.49 | 128.04 |
| 12 | F2 | 202 | CYC | OB-C4B-C3B | -7.87 | 119.50 | 128.04 |
| 12 | Y4 | 201 | CYC | OB-C4B-C3B | -7.87 | 119.50 | 128.04 |
| 12 | Y8 | 201 | CYC | OB-C4B-C3B | -7.87 | 119.50 | 128.04 |
| 12 | L6 | 202 | CYC | OB-C4B-C3B | -7.87 | 119.50 | 128.04 |
| 12 | L8 | 201 | CYC | OB-C4B-C3B | -7.85 | 119.52 | 128.04 |
| 12 | RA | 202 | CYC | OB-C4B-C3B | -7.84 | 119.53 | 128.04 |
| 12 | R9 | 202 | CYC | OB-C4B-C3B | -7.84 | 119.53 | 128.04 |
| 12 | ZA | 201 | CYC | OB-C4B-C3B | -7.84 | 119.53 | 128.04 |
| 12 | Z9 | 201 | CYC | OB-C4B-C3B | -7.84 | 119.53 | 128.04 |
| 12 | D4 | 201 | CYC | OB-C4B-C3B | -7.84 | 119.53 | 128.04 |
| 12 | X3 | 202 | CYC | OB-C4B-C3B | -7.84 | 119.53 | 128.04 |
| 12 | D8 | 201 | CYC | OB-C4B-C3B | -7.84 | 119.53 | 128.04 |
| 12 | X1 | 202 | CYC | OB-C4B-C3B | -7.84 | 119.53 | 128.04 |
| 12 | F6 | 202 | CYC | OB-C4B-C3B | -7.83 | 119.54 | 128.04 |
| 12 | B6 | 201 | CYC | OB-C4B-C3B | -7.83 | 119.54 | 128.04 |
| 12 | D6 | 202 | CYC | OB-C4B-C3B | -7.83 | 119.54 | 128.04 |
| 12 | D2 | 202 | CYC | OB-C4B-C3B | -7.83 | 119.54 | 128.04 |
| 12 | L4 | 201 | CYC | OB-C4B-C3B | -7.83 | 119.54 | 128.04 |
| 12 | B2 | 201 | CYC | OB-C4B-C3B | -7.83 | 119.54 | 128.04 |
| 12 | J8 | 202 | CYC | OB-C4B-C3B | -7.82 | 119.56 | 128.04 |
| 12 | R1 | 202 | CYC | OB-C4B-C3B | -7.82 | 119.56 | 128.04 |
| 12 | R3 | 202 | CYC | OB-C4B-C3B | -7.82 | 119.56 | 128.04 |
| 12 | B3 | 201 | CYC | OB-C4B-C3B | -7.81 | 119.56 | 128.04 |
| 12 | B1 | 201 | CYC | OB-C4B-C3B | -7.81 | 119.56 | 128.04 |
| 12 | L2 | 202 | CYC | OB-C4B-C3B | -7.81 | 119.56 | 128.04 |
| 12 | T3 | 302 | CYC | OB-C4B-C3B | -7.81 | 119.56 | 128.04 |
| 12 | P1 | 202 | CYC | OB-C4B-C3B | -7.81 | 119.57 | 128.04 |
| 12 | P3 | 202 | CYC | OB-C4B-C3B | -7.81 | 119.57 | 128.04 |
| 12 | Q8 | 201 | CYC | OB-C4B-C3B | -7.80 | 119.58 | 128.04 |
| 12 | J4 | 202 | CYC | OB-C4B-C3B | -7.80 | 119.58 | 128.04 |
| 12 | JA | 201 | CYC | OB-C4B-C3B | -7.79 | 119.58 | 128.04 |
| 12 | J9 | 201 | CYC | OB-C4B-C3B | -7.79 | 119.58 | 128.04 |
| 12 | D3 | 201 | CYC | OB-C4B-C3B | -7.79 | 119.58 | 128.04 |
| 12 | D1 | 201 | CYC | OB-C4B-C3B | -7.79 | 119.58 | 128.04 |
| 12 | T1 | 302 | CYC | OB-C4B-C3B | -7.79 | 119.58 | 128.04 |
| 12 | L3 | 201 | CYC | OB-C4B-C3B | -7.79 | 119.59 | 128.04 |
| 12 | L1 | 201 | CYC | OB-C4B-C3B | -7.79 | 119.59 | 128.04 |
| 12 | J2 | 201 | CYC | OB-C4B-C3B | -7.78 | 119.59 | 128.04 |
| 12 | W4 | 202 | CYC | OB-C4B-C3B | -7.78 | 119.59 | 128.04 |
| 12 | W8 | 202 | CYC | OB-C4B-C3B | -7.78 | 119.59 | 128.04 |
| 12 | F3 | 202 | CYC | OB-C4B-C3B | -7.78 | 119.60 | 128.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 12 | F1 | 202 | CYC | OB-C4B-C3B | -7.78 | 119.60 | 128.04 |
| 12 | Q4 | 201 | CYC | OB-C4B-C3B | -7.77 | 119.61 | 128.04 |
| 12 | P9 | 202 | CYC | OB-C4B-C3B | -7.77 | 119.61 | 128.04 |
| 12 | PA | 202 | CYC | OB-C4B-C3B | -7.76 | 119.62 | 128.04 |
| 12 | VA | 202 | CYC | OB-C4B-C3B | -7.76 | 119.62 | 128.04 |
| 12 | V9 | 202 | CYC | OB-C4B-C3B | -7.76 | 119.62 | 128.04 |
| 12 | H4 | 202 | CYC | OB-C4B-C3B | -7.75 | 119.63 | 128.04 |
| 12 | H8 | 202 | CYC | OB-C4B-C3B | -7.75 | 119.63 | 128.04 |
| 12 | D9 | 202 | CYC | OB-C4B-C3B | -7.75 | 119.63 | 128.04 |
| 12 | S4 | 201 | CYC | OB-C4B-C3B | -7.74 | 119.64 | 128.04 |
| 12 | S8 | 201 | CYC | OB-C4B-C3B | -7.74 | 119.64 | 128.04 |
| 12 | J6 | 201 | CYC | OB-C4B-C3B | -7.73 | 119.65 | 128.04 |
| 12 | DA | 202 | CYC | OB-C4B-C3B | -7.73 | 119.65 | 128.04 |
| 12 | HA | 201 | CYC | OB-C4B-C3B | -7.73 | 119.66 | 128.04 |
| 12 | H9 | 201 | CYC | OB-C4B-C3B | -7.73 | 119.66 | 128.04 |
| 12 | T9 | 302 | CYC | OB-C4B-C3B | -7.72 | 119.66 | 128.04 |
| 12 | Z3 | 202 | CYC | OB-C4B-C3B | -7.72 | 119.67 | 128.04 |
| 12 | Z1 | 201 | CYC | OB-C4B-C3B | -7.72 | 119.67 | 128.04 |
| 12 | XA | 202 | CYC | OB-C4B-C3B | -7.71 | 119.67 | 128.04 |
| 12 | X9 | 202 | CYC | OB-C4B-C3B | -7.71 | 119.67 | 128.04 |
| 12 | LA | 201 | CYC | OB-C4B-C3B | -7.71 | 119.67 | 128.04 |
| 12 | L9 | 201 | CYC | OB-C4B-C3B | -7.71 | 119.67 | 128.04 |
| 12 | H3 | 201 | CYC | OB-C4B-C3B | -7.71 | 119.67 | 128.04 |
| 12 | H1 | 202 | CYC | OB-C4B-C3B | -7.71 | 119.67 | 128.04 |
| 12 | TA | 302 | CYC | OB-C4B-C3B | -7.70 | 119.68 | 128.04 |
| 12 | J3 | 201 | CYC | OB-C4B-C3B | -7.66 | 119.73 | 128.04 |
| 12 | J1 | 201 | CYC | OB-C4B-C3B | -7.66 | 119.73 | 128.04 |
| 12 | V3 | 202 | CYC | OB-C4B-C3B | -7.66 | 119.73 | 128.04 |
| 12 | V1 | 202 | CYC | OB-C4B-C3B | -7.66 | 119.73 | 128.04 |
| 12 | H6 | 202 | CYC | OB-C4B-C3B | -7.65 | 119.73 | 128.04 |
| 12 | U4 | 202 | CYC | OB-C4B-C3B | -7.63 | 119.76 | 128.04 |
| 12 | U8 | 202 | CYC | OB-C4B-C3B | -7.63 | 119.76 | 128.04 |
| 12 | H2 | 202 | CYC | OB-C4B-C3B | -7.61 | 119.78 | 128.04 |
| 12 | m7 | 201 | CYC | OB-C4B-C3B | -7.19 | 120.23 | 128.04 |
| 12 | g7 | 201 | CYC | OB-C4B-C3B | -7.14 | 120.29 | 128.04 |
| 12 | s7 | 201 | CYC | OB-C4B-C3B | -7.13 | 120.30 | 128.04 |
| 12 | a7 | 201 | CYC | OB-C4B-C3B | -7.10 | 120.33 | 128.04 |
| 12 | I5 | 201 | CYC | OB-C4B-C3B | -7.09 | 120.35 | 128.04 |
| 12 | C5 | 201 | CYC | OB-C4B-C3B | -7.09 | 120.35 | 128.04 |
| 12 | U7 | 201 | CYC | OB-C4B-C3B | -7.08 | 120.36 | 128.04 |
| 12 | I7 | 201 | CYC | OB-C4B-C3B | -7.07 | 120.36 | 128.04 |
| 12 | O5 | 201 | CYC | OB-C4B-C3B | -7.07 | 120.37 | 128.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | U5 | 201 | CYC | OB-C4B-C3B | -7.05 | 120.39 | 128.04 |
| 12 | C7 | 201 | CYC | OB-C4B-C3B | -7.04 | 120.40 | 128.04 |
| 12 | Q5 | 201 | CYC | OB-C4B-C3B | -7.03 | 120.41 | 128.04 |
| 12 | i7 | 201 | CYC | OB-C4B-C3B | -7.03 | 120.41 | 128.04 |
| 12 | O7 | 201 | CYC | OB-C4B-C3B | -7.02 | 120.42 | 128.04 |
| 12 | u7 | 201 | CYC | OB-C4B-C3B | -7.00 | 120.44 | 128.04 |
| 12 | a5 | 201 | CYC | OB-C4B-C3B | -7.00 | 120.44 | 128.04 |
| 12 | e5 | 201 | CYC | OB-C4B-C3B | -6.99 | 120.45 | 128.04 |
| 12 | Q7 | 201 | CYC | OB-C4B-C3B | -6.98 | 120.46 | 128.04 |
| 12 | c7 | 201 | CYC | OB-C4B-C3B | -6.97 | 120.48 | 128.04 |
| 12 | A2 | 201 | CYC | CAB-C3B-C4B | 6.96 | 132.37 | 121.38 |
| 12 | o7 | 201 | CYC | OB-C4B-C3B | -6.96 | 120.49 | 128.04 |
| 12 | Y5 | 201 | CYC | OB-C4B-C3B | -6.95 | 120.50 | 128.04 |
| 12 | W5 | 201 | CYC | OB-C4B-C3B | -6.95 | 120.50 | 128.04 |
| 12 | E8 | 201 | CYC | CAB-C3B-C4B | 6.94 | 132.34 | 121.38 |
| 12 | W7 | 201 | CYC | OB-C4B-C3B | -6.94 | 120.51 | 128.04 |
| 12 | A4 | 201 | CYC | CAB-C3B-C4B | 6.94 | 132.34 | 121.38 |
| 12 | O1 | 201 | CYC | CAB-C3B-C4B | 6.94 | 132.34 | 121.38 |
| 12 | O3 | 201 | CYC | CAB-C3B-C4B | 6.94 | 132.34 | 121.38 |
| 12 | A6 | 201 | CYC | CAB-C3B-C4B | 6.93 | 132.33 | 121.38 |
| 12 | j5 | 1201 | CYC | CHB-C4A-NA | -6.93 | 110.43 | 124.93 |
| 12 | A8 | 201 | CYC | CAB-C3B-C4B | 6.93 | 132.32 | 121.38 |
| 12 | k5 | 1201 | CYC | CHB-C4A-NA | -6.93 | 110.44 | 124.93 |
| 12 | K5 | 201 | CYC | OB-C4B-C3B | -6.92 | 120.53 | 128.04 |
| 12 | E7 | 201 | CYC | OB-C4B-C3B | -6.92 | 120.53 | 128.04 |
| 12 | KA | 201 | CYC | CAB-C3B-C4B | 6.91 | 132.29 | 121.38 |
| 12 | E4 | 201 | CYC | CAB-C3B-C4B | 6.91 | 132.29 | 121.38 |
| 12 | K9 | 201 | CYC | CAB-C3B-C4B | 6.91 | 132.29 | 121.38 |
| 12 | K3 | 201 | CYC | CAB-C3B-C4B | 6.91 | 132.29 | 121.38 |
| 12 | K1 | 201 | CYC | CAB-C3B-C4B | 6.91 | 132.29 | 121.38 |
| 12 | c5 | 201 | CYC | OB-C4B-C3B | -6.91 | 120.55 | 128.04 |
| 12 | M7 | 201 | CYC | OB-C4B-C3B | -6.91 | 120.55 | 128.04 |
| 12 | C4 | 201 | CYC | CAB-C3B-C4B | 6.90 | 132.28 | 121.38 |
| 12 | C8 | 201 | CYC | CAB-C3B-C4B | 6.90 | 132.28 | 121.38 |
| 12 | YA | 201 | CYC | CAB-C3B-C4B | 6.90 | 132.28 | 121.38 |
| 12 | Y9 | 201 | CYC | CAB-C3B-C4B | 6.90 | 132.28 | 121.38 |
| 12 | EA | 201 | CYC | CAB-C3B-C4B | 6.90 | 132.28 | 121.38 |
| 12 | GA | 201 | CYC | CAB-C3B-C4B | 6.90 | 132.28 | 121.38 |
| 12 | E9 | 201 | CYC | CAB-C3B-C4B | 6.90 | 132.28 | 121.38 |
| 12 | G9 | 201 | CYC | CAB-C3B-C4B | 6.90 | 132.28 | 121.38 |
| 12 | U3 | 201 | CYC | CAB-C3B-C4B | 6.89 | 132.27 | 121.38 |
| 12 | U1 | 201 | CYC | CAB-C3B-C4B | 6.89 | 132.27 | 121.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | K7 | 201 | CYC | OB-C4B-C3B | -6.89 | 120.56 | 128.04 |
| 12 | I3 | 201 | CYC | CAB-C3B-C4B | 6.89 | 132.27 | 121.38 |
| 12 | E5 | 201 | CYC | OB-C4B-C3B | -6.89 | 120.56 | 128.04 |
| 12 | G4 | 201 | CYC | CAB-C3B-C4B | 6.89 | 132.26 | 121.38 |
| 12 | R4 | 201 | CYC | CAB-C3B-C4B | 6.89 | 132.26 | 121.38 |
| 12 | G8 | 201 | CYC | CAB-C3B-C4B | 6.89 | 132.26 | 121.38 |
| 12 | R8 | 201 | CYC | CAB-C3B-C4B | 6.89 | 132.26 | 121.38 |
| 12 | T4 | 201 | CYC | CAB-C3B-C4B | 6.89 | 132.25 | 121.38 |
| 12 | T8 | 201 | CYC | CAB-C3B-C4B | 6.89 | 132.25 | 121.38 |
| 12 | A1 | 201 | CYC | CAB-C3B-C4B | 6.88 | 132.25 | 121.38 |
| 12 | A3 | 201 | CYC | CAB-C3B-C4B | 6.88 | 132.25 | 121.38 |
| 12 | E6 | 201 | CYC | CAB-C3B-C4B | 6.88 | 132.25 | 121.38 |
| 12 | E2 | 201 | CYC | CAB-C3B-C4B | 6.88 | 132.25 | 121.38 |
| 12 | C2 | 201 | CYC | CAB-C3B-C4B | 6.88 | 132.25 | 121.38 |
| 12 | I1 | 201 | CYC | CAB-C3B-C4B | 6.88 | 132.24 | 121.38 |
| 12 | UA | 201 | CYC | CAB-C3B-C4B | 6.87 | 132.24 | 121.38 |
| 12 | U9 | 201 | CYC | CAB-C3B-C4B | 6.87 | 132.24 | 121.38 |
| 12 | K6 | 201 | CYC | CAB-C3B-C4B | 6.87 | 132.23 | 121.38 |
| 12 | C6 | 201 | CYC | CAB-C3B-C4B | 6.87 | 132.23 | 121.38 |
| 12 | P4 | 201 | CYC | CAB-C3B-C4B | 6.87 | 132.23 | 121.38 |
| 12 | P8 | 201 | CYC | CAB-C3B-C4B | 6.87 | 132.23 | 121.38 |
| 12 | K2 | 201 | CYC | CAB-C3B-C4B | 6.87 | 132.23 | 121.38 |
| 12 | Y3 | 201 | CYC | CAB-C3B-C4B | 6.87 | 132.23 | 121.38 |
| 12 | Y1 | 201 | CYC | CAB-C3B-C4B | 6.87 | 132.23 | 121.38 |
| 12 | I9 | 201 | CYC | CAB-C3B-C4B | 6.86 | 132.22 | 121.38 |
| 12 | S7 | 201 | CYC | OB-C4B-C3B | -6.86 | 120.59 | 128.04 |
| 12 | WA | 201 | CYC | CAB-C3B-C4B | 6.86 | 132.22 | 121.38 |
| 12 | W9 | 201 | CYC | CAB-C3B-C4B | 6.86 | 132.22 | 121.38 |
| 12 | V8 | 201 | CYC | CAB-C3B-C4B | 6.86 | 132.22 | 121.38 |
| 12 | SA | 201 | CYC | CAB-C3B-C4B | 6.86 | 132.21 | 121.38 |
| 12 | S9 | 201 | CYC | CAB-C3B-C4B | 6.86 | 132.21 | 121.38 |
| 12 | N4 | 201 | CYC | CAB-C3B-C4B | 6.86 | 132.21 | 121.38 |
| 12 | K8 | 201 | CYC | CAB-C3B-C4B | 6.85 | 132.20 | 121.38 |
| 12 | X4 | 201 | CYC | CAB-C3B-C4B | 6.85 | 132.20 | 121.38 |
| 12 | X8 | 201 | CYC | CAB-C3B-C4B | 6.85 | 132.20 | 121.38 |
| 12 | Q9 | 201 | CYC | CAB-C3B-C4B | 6.85 | 132.19 | 121.38 |
| 12 | A7 | 201 | CYC | OB-C4B-C3B | -6.84 | 120.61 | 128.04 |
| 12 | G7 | 201 | CYC | OB-C4B-C3B | -6.84 | 120.61 | 128.04 |
| 12 | IA | 201 | CYC | CAB-C3B-C4B | 6.84 | 132.19 | 121.38 |
| 12 | N8 | 201 | CYC | CAB-C3B-C4B | 6.84 | 132.19 | 121.38 |
| 12 | QA | 201 | CYC | CAB-C3B-C4B | 6.84 | 132.19 | 121.38 |
| 12 | G5 | 201 | CYC | OB-C4B-C3B | -6.84 | 120.62 | 128.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | V4 | 201 | CYC | CAB-C3B-C4B | 6.84 | 132.18 | 121.38 |
| 12 | G2 | 201 | CYC | CAB-C3B-C4B | 6.84 | 132.18 | 121.38 |
| 12 | A5 | 201 | CYC | OB-C4B-C3B | -6.84 | 120.62 | 128.04 |
| 12 | E3 | 201 | CYC | CAB-C3B-C4B | 6.84 | 132.18 | 121.38 |
| 12 | E1 | 201 | CYC | CAB-C3B-C4B | 6.84 | 132.18 | 121.38 |
| 12 | O9 | 201 | CYC | CAB-C3B-C4B | 6.83 | 132.17 | 121.38 |
| 12 | I2 | 201 | CYC | CAB-C3B-C4B | 6.83 | 132.17 | 121.38 |
| 12 | I4 | 201 | CYC | CAB-C3B-C4B | 6.83 | 132.17 | 121.38 |
| 12 | I8 | 201 | CYC | CAB-C3B-C4B | 6.83 | 132.17 | 121.38 |
| 12 | G3 | 201 | CYC | CAB-C3B-C4B | 6.83 | 132.17 | 121.38 |
| 12 | G1 | 201 | CYC | CAB-C3B-C4B | 6.83 | 132.17 | 121.38 |
| 12 | Y7 | 201 | CYC | OB-C4B-C3B | -6.83 | 120.63 | 128.04 |
| 12 | K4 | 201 | CYC | CAB-C3B-C4B | 6.82 | 132.15 | 121.38 |
| 12 | Q1 | 201 | CYC | CAB-C3B-C4B | 6.82 | 132.15 | 121.38 |
| 12 | Q3 | 201 | CYC | CAB-C3B-C4B | 6.82 | 132.15 | 121.38 |
| 12 | G6 | 201 | CYC | CAB-C3B-C4B | 6.82 | 132.15 | 121.38 |
| 12 | OA | 201 | CYC | CAB-C3B-C4B | 6.81 | 132.14 | 121.38 |
| 12 | S5 | 201 | CYC | OB-C4B-C3B | -6.81 | 120.65 | 128.04 |
| 12 | S1 | 201 | CYC | CAB-C3B-C4B | 6.81 | 132.13 | 121.38 |
| 12 | S3 | 201 | CYC | CAB-C3B-C4B | 6.81 | 132.13 | 121.38 |
| 12 | AA | 201 | CYC | CAB-C3B-C4B | 6.80 | 132.12 | 121.38 |
| 12 | A9 | 201 | CYC | CAB-C3B-C4B | 6.80 | 132.12 | 121.38 |
| 12 | k7 | 201 | CYC | OB-C4B-C3B | -6.80 | 120.66 | 128.04 |
| 12 | CA | 201 | CYC | CAB-C3B-C4B | 6.80 | 132.12 | 121.38 |
| 12 | C9 | 201 | CYC | CAB-C3B-C4B | 6.80 | 132.12 | 121.38 |
| 12 | e7 | 201 | CYC | OB-C4B-C3B | -6.80 | 120.67 | 128.04 |
| 12 | I6 | 201 | CYC | CAB-C3B-C4B | 6.79 | 132.11 | 121.38 |
| 12 | M5 | 201 | CYC | OB-C4B-C3B | -6.79 | 120.67 | 128.04 |
| 12 | W1 | 201 | CYC | CAB-C3B-C4B | 6.77 | 132.08 | 121.38 |
| 12 | q7 | 201 | CYC | OB-C4B-C3B | -6.77 | 120.69 | 128.04 |
| 12 | C3 | 201 | CYC | CAB-C3B-C4B | 6.77 | 132.07 | 121.38 |
| 12 | C1 | 201 | CYC | CAB-C3B-C4B | 6.77 | 132.07 | 121.38 |
| 12 | W3 | 201 | CYC | CAB-C3B-C4B | 6.74 | 132.03 | 121.38 |
| 12 | L2 | 201 | CYC | OB-C4B-C3B | -6.28 | 121.23 | 128.04 |
| 12 | L6 | 201 | CYC | OB-C4B-C3B | -6.27 | 121.23 | 128.04 |
| 12 | aA | 901 | CYC | OB-C4B-C3B | -6.20 | 121.31 | 128.04 |
| 12 | F8 | 202 | CYC | OB-C4B-C3B | -6.19 | 121.32 | 128.04 |
| 12 | J4 | 201 | CYC | OB-C4B-C3B | -6.19 | 121.32 | 128.04 |
| 12 | J8 | 201 | CYC | OB-C4B-C3B | -6.19 | 121.32 | 128.04 |
| 12 | TA | 301 | CYC | OB-C4B-C3B | -6.18 | 121.33 | 128.04 |
| 12 | T9 | 301 | CYC | OB-C4B-C3B | -6.18 | 121.33 | 128.04 |
| 12 | J3 | 202 | CYC | OB-C4B-C3B | -6.18 | 121.33 | 128.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 12 | F2 | 201 | CYC | OB-C4B-C3B | -6.17 | 121.34 | 128.04 |
| 12 | J2 | 202 | CYC | OB-C4B-C3B | -6.16 | 121.35 | 128.04 |
| 12 | J6 | 202 | CYC | OB-C4B-C3B | -6.16 | 121.36 | 128.04 |
| 12 | F4 | 202 | CYC | OB-C4B-C3B | -6.16 | 121.36 | 128.04 |
| 12 | S4 | 202 | CYC | OB-C4B-C3B | -6.15 | 121.36 | 128.04 |
| 12 | M8 | 302 | CYC | OB-C4B-C3B | -6.15 | 121.36 | 128.04 |
| 12 | ZA | 202 | CYC | OB-C4B-C3B | -6.15 | 121.37 | 128.04 |
| 12 | Z9 | 202 | CYC | OB-C4B-C3B | -6.15 | 121.37 | 128.04 |
| 12 | DA | 201 | CYC | OB-C4B-C3B | -6.15 | 121.37 | 128.04 |
| 12 | D9 | 201 | CYC | OB-C4B-C3B | -6.15 | 121.37 | 128.04 |
| 12 | W8 | 201 | CYC | OB-C4B-C3B | -6.14 | 121.37 | 128.04 |
| 12 | F6 | 201 | CYC | OB-C4B-C3B | -6.14 | 121.38 | 128.04 |
| 12 | VA | 201 | CYC | OB-C4B-C3B | -6.13 | 121.39 | 128.04 |
| 12 | D2 | 201 | CYC | OB-C4B-C3B | -6.13 | 121.39 | 128.04 |
| 12 | XA | 201 | CYC | OB-C4B-C3B | -6.12 | 121.39 | 128.04 |
| 12 | X9 | 201 | CYC | OB-C4B-C3B | -6.12 | 121.39 | 128.04 |
| 12 | L4 | 202 | CYC | OB-C4B-C3B | -6.12 | 121.39 | 128.04 |
| 12 | V9 | 201 | CYC | OB-C4B-C3B | -6.12 | 121.40 | 128.04 |
| 12 | W4 | 201 | CYC | OB-C4B-C3B | -6.12 | 121.40 | 128.04 |
| 12 | T3 | 301 | CYC | OB-C4B-C3B | -6.12 | 121.40 | 128.04 |
| 12 | T1 | 301 | CYC | OB-C4B-C3B | -6.12 | 121.40 | 128.04 |
| 12 | a9 | 901 | CYC | OB-C4B-C3B | -6.10 | 121.42 | 128.04 |
| 12 | V3 | 201 | CYC | OB-C4B-C3B | -6.09 | 121.43 | 128.04 |
| 12 | V1 | 201 | CYC | OB-C4B-C3B | -6.09 | 121.43 | 128.04 |
| 12 | F3 | 201 | CYC | OB-C4B-C3B | -6.09 | 121.43 | 128.04 |
| 12 | F1 | 201 | CYC | OB-C4B-C3B | -6.09 | 121.43 | 128.04 |
| 12 | X3 | 201 | CYC | OB-C4B-C3B | -6.09 | 121.43 | 128.04 |
| 12 | X1 | 201 | CYC | OB-C4B-C3B | -6.09 | 121.43 | 128.04 |
| 12 | Z3 | 201 | CYC | OB-C4B-C3B | -6.09 | 121.43 | 128.04 |
| 12 | D4 | 202 | CYC | OB-C4B-C3B | -6.09 | 121.43 | 128.04 |
| 12 | D8 | 202 | CYC | OB-C4B-C3B | -6.09 | 121.43 | 128.04 |
| 12 | H6 | 201 | CYC | OB-C4B-C3B | -6.09 | 121.44 | 128.04 |
| 12 | LA | 202 | CYC | OB-C4B-C3B | -6.08 | 121.44 | 128.04 |
| 12 | L9 | 202 | CYC | OB-C4B-C3B | -6.08 | 121.44 | 128.04 |
| 12 | RA | 201 | CYC | OB-C4B-C3B | -6.07 | 121.45 | 128.04 |
| 12 | R9 | 201 | CYC | OB-C4B-C3B | -6.07 | 121.45 | 128.04 |
| 12 | j7 | 201 | CYC | OB-C4B-C3B | -6.07 | 121.45 | 128.04 |
| 12 | M4 | 301 | CYC | OB-C4B-C3B | -6.07 | 121.45 | 128.04 |
| 12 | Z1 | 202 | CYC | OB-C4B-C3B | -6.07 | 121.45 | 128.04 |
| 12 | U4 | 201 | CYC | OB-C4B-C3B | -6.07 | 121.46 | 128.04 |
| 12 | U8 | 201 | CYC | OB-C4B-C3B | -6.07 | 121.46 | 128.04 |
| 12 | f5 | 201 | CYC | OB-C4B-C3B | -6.06 | 121.46 | 128.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 12 | Z4 | 301 | CYC | OB-C4B-C3B | -6.06 | 121.46 | 128.04 |
| 12 | H4 | 201 | CYC | OB-C4B-C3B | -6.05 | 121.47 | 128.04 |
| 12 | H8 | 201 | CYC | OB-C4B-C3B | -6.05 | 121.47 | 128.04 |
| 12 | D1 | 202 | CYC | OB-C4B-C3B | -6.05 | 121.47 | 128.04 |
| 12 | b5 | 201 | CYC | OB-C4B-C3B | -6.05 | 121.47 | 128.04 |
| 12 | H2 | 201 | CYC | OB-C4B-C3B | -6.04 | 121.48 | 128.04 |
| 12 | L3 | 202 | CYC | OB-C4B-C3B | -6.04 | 121.48 | 128.04 |
| 12 | aA | 902 | CYC | OB-C4B-C3B | -6.04 | 121.48 | 128.04 |
| 12 | L5 | 201 | CYC | OB-C4B-C3B | -6.04 | 121.48 | 128.04 |
| 12 | d7 | 201 | CYC | OB-C4B-C3B | -6.04 | 121.49 | 128.04 |
| 12 | F5 | 201 | CYC | OB-C4B-C3B | -6.04 | 121.49 | 128.04 |
| 12 | R1 | 201 | CYC | OB-C4B-C3B | -6.03 | 121.49 | 128.04 |
| 12 | R3 | 201 | CYC | OB-C4B-C3B | -6.03 | 121.49 | 128.04 |
| 12 | Z8 | 301 | CYC | OB-C4B-C3B | -6.03 | 121.49 | 128.04 |
| 12 | D3 | 202 | CYC | OB-C4B-C3B | -6.03 | 121.50 | 128.04 |
| 12 | F7 | 201 | CYC | OB-C4B-C3B | -6.03 | 121.50 | 128.04 |
| 12 | H1 | 201 | CYC | OB-C4B-C3B | -6.02 | 121.50 | 128.04 |
| 12 | JA | 202 | CYC | OB-C4B-C3B | -6.02 | 121.51 | 128.04 |
| 12 | L7 | 201 | CYC | OB-C4B-C3B | -6.02 | 121.51 | 128.04 |
| 12 | J9 | 202 | CYC | OB-C4B-C3B | -6.02 | 121.51 | 128.04 |
| 12 | H3 | 202 | CYC | OB-C4B-C3B | -6.02 | 121.51 | 128.04 |
| 12 | FA | 301 | CYC | OB-C4B-C3B | -6.01 | 121.51 | 128.04 |
| 12 | F9 | 301 | CYC | OB-C4B-C3B | -6.01 | 121.51 | 128.04 |
| 12 | PA | 201 | CYC | OB-C4B-C3B | -6.01 | 121.52 | 128.04 |
| 12 | P9 | 201 | CYC | OB-C4B-C3B | -6.01 | 121.52 | 128.04 |
| 12 | X5 | 201 | CYC | OB-C4B-C3B | -6.01 | 121.52 | 128.04 |
| 12 | Z5 | 201 | CYC | OB-C4B-C3B | -6.01 | 121.52 | 128.04 |
| 12 | N2 | 101 | CYC | OB-C4B-C3B | -6.01 | 121.52 | 128.04 |
| 12 | H9 | 202 | CYC | OB-C4B-C3B | -6.01 | 121.52 | 128.04 |
| 12 | D6 | 201 | CYC | OB-C4B-C3B | -6.00 | 121.53 | 128.04 |
| 12 | O4 | 201 | CYC | OB-C4B-C3B | -6.00 | 121.53 | 128.04 |
| 12 | O8 | 201 | CYC | OB-C4B-C3B | -6.00 | 121.53 | 128.04 |
| 12 | N6 | 101 | CYC | OB-C4B-C3B | -6.00 | 121.53 | 128.04 |
| 12 | H5 | 201 | CYC | OB-C4B-C3B | -5.99 | 121.54 | 128.04 |
| 12 | B5 | 201 | CYC | OB-C4B-C3B | -5.98 | 121.55 | 128.04 |
| 12 | N5 | 201 | CYC | OB-C4B-C3B | -5.98 | 121.55 | 128.04 |
| 12 | H7 | 201 | CYC | OB-C4B-C3B | -5.98 | 121.55 | 128.04 |
| 12 | T7 | 201 | CYC | OB-C4B-C3B | -5.98 | 121.55 | 128.04 |
| 12 | HA | 202 | CYC | OB-C4B-C3B | -5.97 | 121.56 | 128.04 |
| 12 | B9 | 201 | CYC | OB-C4B-C3B | -5.97 | 121.56 | 128.04 |
| 12 | T5 | 201 | CYC | OB-C4B-C3B | -5.97 | 121.57 | 128.04 |
| 12 | BA | 201 | CYC | OB-C4B-C3B | -5.96 | 121.57 | 128.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 12 | R7 | 201 | CYC | OB-C4B-C3B | -5.96 | 121.57 | 128.04 |
| 12 | r7 | 201 | CYC | OB-C4B-C3B | -5.96 | 121.57 | 128.04 |
| 12 | d5 | 201 | CYC | OB-C4B-C3B | -5.95 | 121.58 | 128.04 |
| 12 | R5 | 201 | CYC | OB-C4B-C3B | -5.95 | 121.58 | 128.04 |
| 12 | p7 | 201 | CYC | OB-C4B-C3B | -5.95 | 121.58 | 128.04 |
| 12 | B3 | 202 | CYC | OB-C4B-C3B | -5.95 | 121.58 | 128.04 |
| 12 | P1 | 201 | CYC | OB-C4B-C3B | -5.95 | 121.59 | 128.04 |
| 12 | P3 | 201 | CYC | OB-C4B-C3B | -5.95 | 121.59 | 128.04 |
| 12 | J5 | 201 | CYC | OB-C4B-C3B | -5.95 | 121.59 | 128.04 |
| 12 | k5 | 1203 | CYC | OB-C4B-C3B | -5.94 | 121.59 | 128.04 |
| 12 | V7 | 201 | CYC | OB-C4B-C3B | -5.94 | 121.59 | 128.04 |
| 12 | B7 | 201 | CYC | OB-C4B-C3B | -5.93 | 121.60 | 128.04 |
| 12 | M8 | 301 | CYC | OB-C4B-C3B | -5.93 | 121.61 | 128.04 |
| 12 | X7 | 201 | CYC | OB-C4B-C3B | -5.92 | 121.62 | 128.04 |
| 12 | v7 | 201 | CYC | OB-C4B-C3B | -5.92 | 121.62 | 128.04 |
| 12 | V5 | 201 | CYC | OB-C4B-C3B | -5.91 | 121.62 | 128.04 |
| 12 | B1 | 202 | CYC | OB-C4B-C3B | -5.91 | 121.62 | 128.04 |
| 12 | B4 | 202 | CYC | OB-C4B-C3B | -5.90 | 121.64 | 128.04 |
| 12 | P5 | 201 | CYC | OB-C4B-C3B | -5.90 | 121.64 | 128.04 |
| 12 | D5 | 201 | CYC | OB-C4B-C3B | -5.89 | 121.65 | 128.04 |
| 12 | P7 | 201 | CYC | OB-C4B-C3B | -5.89 | 121.65 | 128.04 |
| 12 | Z | 201 | CYC | OB-C4B-C3B | -5.88 | 121.66 | 128.04 |
| 12 | A | 201 | CYC | OB-C4B-C3B | -5.88 | 121.66 | 128.04 |
| 12 | b7 | 201 | CYC | OB-C4B-C3B | -5.83 | 121.71 | 128.04 |
| 12 | k5 | 1202 | CYC | OB-C4B-C3B | -5.81 | 121.74 | 128.04 |
| 12 | B8 | 202 | CYC | OB-C4B-C3B | -5.81 | 121.74 | 128.04 |
| 12 | f7 | 201 | CYC | OB-C4B-C3B | -5.80 | 121.75 | 128.04 |
| 12 | j5 | 1202 | CYC | OB-C4B-C3B | -5.80 | 121.75 | 128.04 |
| 12 | N7 | 201 | CYC | OB-C4B-C3B | -5.79 | 121.76 | 128.04 |
| 12 | h7 | 201 | CYC | OB-C4B-C3B | -5.77 | 121.78 | 128.04 |
| 12 | k5 | 1204 | CYC | OB-C4B-C3B | -5.75 | 121.80 | 128.04 |
| 12 | D7 | 201 | CYC | OB-C4B-C3B | -5.74 | 121.81 | 128.04 |
| 12 | J7 | 201 | CYC | OB-C4B-C3B | -5.72 | 121.84 | 128.04 |
| 12 | U5 | 201 | CYC | CHB-C4A-NA | -5.33 | 113.78 | 124.93 |
| 12 | Q5 | 201 | CYC | CHB-C4A-NA | -5.30 | 113.84 | 124.93 |
| 12 | i7 | 201 | CYC | CHB-C4A-NA | -5.30 | 113.85 | 124.93 |
| 12 | E7 | 201 | CYC | CHB-C4A-NA | -5.30 | 113.85 | 124.93 |
| 12 | I7 | 201 | CYC | CHB-C4A-NA | -5.29 | 113.86 | 124.93 |
| 12 | W5 | 201 | CYC | CHB-C4A-NA | -5.29 | 113.86 | 124.93 |
| 12 | C7 | 201 | CYC | CHB-C4A-NA | -5.29 | 113.87 | 124.93 |
| 12 | O5 | 201 | CYC | CHB-C4A-NA | -5.29 | 113.87 | 124.93 |
| 12 | K7 | 201 | CYC | CHB-C4A-NA | -5.28 | 113.89 | 124.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | a5 | 201 | CYC | CHB-C4A-NA | -5.28 | 113.89 | 124.93 |
| 12 | L5 | 201 | CYC | CAB-C3B-C4B | 5.27 | 129.70 | 121.38 |
| 12 | Q7 | 201 | CYC | CHB-C4A-NA | -5.27 | 113.92 | 124.93 |
| 12 | R5 | 201 | CYC | CAB-C3B-C4B | 5.27 | 129.70 | 121.38 |
| 12 | e5 | 201 | CYC | CHB-C4A-NA | -5.26 | 113.93 | 124.93 |
| 12 | c7 | 201 | CYC | CHB-C4A-NA | -5.26 | 113.93 | 124.93 |
| 12 | k5 | 1201 | CYC | CHD-C4C-NC | 5.25 | 131.45 | 125.20 |
| 12 | s7 | 201 | CYC | CHB-C4A-NA | -5.25 | 113.95 | 124.93 |
| 12 | T5 | 201 | CYC | CAB-C3B-C4B | 5.25 | 129.66 | 121.38 |
| 12 | A5 | 201 | CYC | CHB-C4A-NA | -5.24 | 113.96 | 124.93 |
| 12 | j5 | 1201 | CYC | CHD-C4C-NC | 5.24 | 131.44 | 125.20 |
| 12 | S7 | 201 | CYC | CHB-C4A-NA | -5.24 | 113.96 | 124.93 |
| 12 | J5 | 201 | CYC | CAB-C3B-C4B | 5.24 | 129.66 | 121.38 |
| 12 | U7 | 201 | CYC | CHB-C4A-NA | -5.24 | 113.97 | 124.93 |
| 12 | F5 | 201 | CYC | CAB-C3B-C4B | 5.24 | 129.66 | 121.38 |
| 12 | F7 | 201 | CYC | CAB-C3B-C4B | 5.24 | 129.65 | 121.38 |
| 12 | G5 | 201 | CYC | CHB-C4A-NA | -5.24 | 113.97 | 124.93 |
| 12 | u7 | 201 | CYC | CHB-C4A-NA | -5.24 | 113.98 | 124.93 |
| 12 | W7 | 201 | CYC | CHB-C4A-NA | -5.24 | 113.98 | 124.93 |
| 12 | k7 | 201 | CYC | CHB-C4A-NA | -5.23 | 113.98 | 124.93 |
| 12 | I5 | 201 | CYC | CHB-C4A-NA | -5.23 | 113.99 | 124.93 |
| 12 | Y5 | 201 | CYC | CHB-C4A-NA | -5.23 | 113.99 | 124.93 |
| 12 | O7 | 201 | CYC | CHB-C4A-NA | -5.23 | 114.00 | 124.93 |
| 12 | X5 | 201 | CYC | CAB-C3B-C4B | 5.23 | 129.63 | 121.38 |
| 12 | G7 | 201 | CYC | CHB-C4A-NA | -5.23 | 114.00 | 124.93 |
| 12 | f5 | 201 | CYC | CAB-C3B-C4B | 5.23 | 129.63 | 121.38 |
| 12 | j5 | 1201 | CYC | OB-C4B-C3B | -5.22 | 122.37 | 128.04 |
| 12 | o7 | 201 | CYC | CHB-C4A-NA | -5.22 | 114.00 | 124.93 |
| 12 | m7 | 201 | CYC | CHB-C4A-NA | -5.22 | 114.00 | 124.93 |
| 12 | A7 | 201 | CYC | CHB-C4A-NA | -5.22 | 114.01 | 124.93 |
| 12 | C5 | 201 | CYC | CHB-C4A-NA | -5.22 | 114.01 | 124.93 |
| 12 | a7 | 201 | CYC | CHB-C4A-NA | -5.22 | 114.02 | 124.93 |
| 12 | e7 | 201 | CYC | CHB-C4A-NA | -5.22 | 114.02 | 124.93 |
| 12 | M7 | 201 | CYC | CHB-C4A-NA | -5.21 | 114.03 | 124.93 |
| 12 | p7 | 201 | CYC | CAB-C3B-C4B | 5.21 | 129.61 | 121.38 |
| 12 | E5 | 201 | CYC | CHB-C4A-NA | -5.21 | 114.04 | 124.93 |
| 12 | V7 | 201 | CYC | CAB-C3B-C4B | 5.21 | 129.60 | 121.38 |
| 12 | c5 | 201 | CYC | CHB-C4A-NA | -5.21 | 114.04 | 124.93 |
| 12 | q7 | 201 | CYC | CHB-C4A-NA | -5.21 | 114.04 | 124.93 |
| 12 | N5 | 201 | CYC | CAB-C3B-C4B | 5.21 | 129.60 | 121.38 |
| 12 | H7 | 201 | CYC | CAB-C3B-C4B | 5.20 | 129.60 | 121.38 |
| 12 | S5 | 201 | CYC | CHB-C4A-NA | -5.20 | 114.05 | 124.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | g7 | 201 | CYC | CHB-C4A-NA | -5.20 | 114.05 | 124.93 |
| 12 | r7 | 201 | CYC | CAB-C3B-C4B | 5.20 | 129.60 | 121.38 |
| 12 | k5 | 1204 | CYC | CAB-C3B-C4B | 5.20 | 129.59 | 121.38 |
| 12 | X7 | 201 | CYC | CAB-C3B-C4B | 5.20 | 129.59 | 121.38 |
| 12 | K5 | 201 | CYC | CHB-C4A-NA | -5.20 | 114.06 | 124.93 |
| 12 | b5 | 201 | CYC | CAB-C3B-C4B | 5.20 | 129.59 | 121.38 |
| 12 | Y7 | 201 | CYC | CHB-C4A-NA | -5.19 | 114.07 | 124.93 |
| 12 | v7 | 201 | CYC | CAB-C3B-C4B | 5.19 | 129.58 | 121.38 |
| 12 | d5 | 201 | CYC | CAB-C3B-C4B | 5.19 | 129.58 | 121.38 |
| 12 | Z5 | 201 | CYC | CAB-C3B-C4B | 5.19 | 129.58 | 121.38 |
| 12 | B5 | 201 | CYC | CAB-C3B-C4B | 5.19 | 129.58 | 121.38 |
| 12 | j5 | 1202 | CYC | CAB-C3B-C4B | 5.19 | 129.58 | 121.38 |
| 12 | L7 | 201 | CYC | CAB-C3B-C4B | 5.19 | 129.57 | 121.38 |
| 12 | H5 | 201 | CYC | CAB-C3B-C4B | 5.18 | 129.57 | 121.38 |
| 12 | M5 | 201 | CYC | CHB-C4A-NA | -5.18 | 114.09 | 124.93 |
| 12 | T7 | 201 | CYC | CAB-C3B-C4B | 5.18 | 129.56 | 121.38 |
| 12 | P7 | 201 | CYC | CAB-C3B-C4B | 5.18 | 129.56 | 121.38 |
| 12 | R7 | 201 | CYC | CAB-C3B-C4B | 5.18 | 129.56 | 121.38 |
| 12 | f7 | 201 | CYC | CAB-C3B-C4B | 5.17 | 129.54 | 121.38 |
| 12 | D5 | 201 | CYC | CAB-C3B-C4B | 5.17 | 129.54 | 121.38 |
| 12 | k5 | 1203 | CYC | CAB-C3B-C4B | 5.17 | 129.54 | 121.38 |
| 12 | j7 | 201 | CYC | CAB-C3B-C4B | 5.16 | 129.53 | 121.38 |
| 12 | V5 | 201 | CYC | CAB-C3B-C4B | 5.16 | 129.53 | 121.38 |
| 12 | J7 | 201 | CYC | CAB-C3B-C4B | 5.16 | 129.53 | 121.38 |
| 12 | b7 | 201 | CYC | CAB-C3B-C4B | 5.15 | 129.52 | 121.38 |
| 12 | k5 | 1202 | CYC | CAB-C3B-C4B | 5.15 | 129.51 | 121.38 |
| 12 | B7 | 201 | CYC | CAB-C3B-C4B | 5.15 | 129.51 | 121.38 |
| 12 | P5 | 201 | CYC | CAB-C3B-C4B | 5.15 | 129.51 | 121.38 |
| 12 | D7 | 201 | CYC | CAB-C3B-C4B | 5.14 | 129.50 | 121.38 |
| 12 | k5 | 1201 | CYC | OB-C4B-C3B | -5.14 | 122.46 | 128.04 |
| 12 | d7 | 201 | CYC | CAB-C3B-C4B | 5.13 | 129.49 | 121.38 |
| 12 | Z | 201 | CYC | CAB-C3B-C4B | 5.13 | 129.48 | 121.38 |
| 12 | A | 201 | CYC | CAB-C3B-C4B | 5.13 | 129.48 | 121.38 |
| 12 | h7 | 201 | CYC | CAB-C3B-C4B | 5.13 | 129.48 | 121.38 |
| 12 | N7 | 201 | CYC | CAB-C3B-C4B | 5.12 | 129.46 | 121.38 |
| 12 | k5 | 1201 | CYC | CMB-C2B-C1B | 5.05 | 130.48 | 124.17 |
| 12 | j5 | 1201 | CYC | CMB-C2B-C1B | 5.02 | 130.43 | 124.17 |
| 12 | k7 | 201 | CYC | OC-C1C-C2C | -5.01 | 122.19 | 126.17 |
| 12 | N4 | 201 | CYC | CAA-CBA-CGA | -5.01 | 102.82 | 113.60 |
| 12 | N8 | 201 | CYC | CAA-CBA-CGA | -5.01 | 102.82 | 113.60 |
| 12 | G4 | 201 | CYC | CAA-CBA-CGA | -5.00 | 102.84 | 113.60 |
| 12 | G8 | 201 | CYC | CAA-CBA-CGA | -5.00 | 102.84 | 113.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | Y4 | 201 | CYC | C1B-NB-C4B | -5.00 | 104.31 | 110.67 |
| 12 | Y8 | 201 | CYC | C1B-NB-C4B | -5.00 | 104.31 | 110.67 |
| 12 | g7 | 201 | CYC | OC-C1C-C2C | -4.99 | 122.21 | 126.17 |
| 12 | k5 | 1201 | CYC | CHB-C4A-C3A | 4.99 | 137.72 | 124.90 |
| 12 | EA | 201 | CYC | CAA-CBA-CGA | -4.99 | 102.88 | 113.60 |
| 12 | E9 | 201 | CYC | CAA-CBA-CGA | -4.99 | 102.88 | 113.60 |
| 12 | A2 | 201 | CYC | CAA-CBA-CGA | -4.98 | 102.89 | 113.60 |
| 12 | V4 | 201 | CYC | CAA-CBA-CGA | -4.98 | 102.89 | 113.60 |
| 12 | A6 | 201 | CYC | CAA-CBA-CGA | -4.98 | 102.89 | 113.60 |
| 12 | V8 | 201 | CYC | CAA-CBA-CGA | -4.98 | 102.89 | 113.60 |
| 12 | G3 | 201 | CYC | CAA-CBA-CGA | -4.98 | 102.89 | 113.60 |
| 12 | G1 | 201 | CYC | CAA-CBA-CGA | -4.98 | 102.89 | 113.60 |
| 12 | j5 | 1201 | CYC | CHB-C4A-C3A | 4.98 | 137.70 | 124.90 |
| 12 | C3 | 201 | CYC | CAA-CBA-CGA | -4.97 | 102.91 | 113.60 |
| 12 | C1 | 201 | CYC | CAA-CBA-CGA | -4.97 | 102.91 | 113.60 |
| 12 | GA | 201 | CYC | CAA-CBA-CGA | -4.97 | 102.91 | 113.60 |
| 12 | OA | 201 | CYC | CAA-CBA-CGA | -4.97 | 102.91 | 113.60 |
| 12 | X8 | 201 | CYC | CAA-CBA-CGA | -4.97 | 102.91 | 113.60 |
| 12 | O9 | 201 | CYC | CAA-CBA-CGA | -4.97 | 102.91 | 113.60 |
| 12 | G9 | 201 | CYC | CAA-CBA-CGA | -4.97 | 102.91 | 113.60 |
| 12 | E4 | 201 | CYC | CAA-CBA-CGA | -4.97 | 102.91 | 113.60 |
| 12 | E8 | 201 | CYC | CAA-CBA-CGA | -4.97 | 102.91 | 113.60 |
| 12 | O1 | 201 | CYC | CAA-CBA-CGA | -4.97 | 102.91 | 113.60 |
| 12 | S1 | 201 | CYC | CAA-CBA-CGA | -4.97 | 102.91 | 113.60 |
| 12 | O3 | 201 | CYC | CAA-CBA-CGA | -4.97 | 102.91 | 113.60 |
| 12 | WA | 201 | CYC | CAA-CBA-CGA | -4.97 | 102.92 | 113.60 |
| 12 | W9 | 201 | CYC | CAA-CBA-CGA | -4.97 | 102.92 | 113.60 |
| 12 | P4 | 201 | CYC | CAA-CBA-CGA | -4.97 | 102.92 | 113.60 |
| 12 | P8 | 201 | CYC | CAA-CBA-CGA | -4.97 | 102.92 | 113.60 |
| 12 | E3 | 201 | CYC | CAA-CBA-CGA | -4.95 | 102.94 | 113.60 |
| 12 | E1 | 201 | CYC | CAA-CBA-CGA | -4.95 | 102.94 | 113.60 |
| 12 | I1 | 201 | CYC | CAA-CBA-CGA | -4.95 | 102.94 | 113.60 |
| 12 | X4 | 201 | CYC | CAA-CBA-CGA | -4.95 | 102.95 | 113.60 |
| 12 | I3 | 201 | CYC | CAA-CBA-CGA | -4.95 | 102.95 | 113.60 |
| 12 | S3 | 201 | CYC | CAA-CBA-CGA | -4.95 | 102.95 | 113.60 |
| 12 | Q1 | 201 | CYC | CAA-CBA-CGA | -4.95 | 102.95 | 113.60 |
| 12 | G2 | 201 | CYC | CAA-CBA-CGA | -4.95 | 102.95 | 113.60 |
| 12 | Q3 | 201 | CYC | CAA-CBA-CGA | -4.95 | 102.95 | 113.60 |
| 12 | W3 | 201 | CYC | CAA-CBA-CGA | -4.95 | 102.95 | 113.60 |
| 12 | S9 | 201 | CYC | CAA-CBA-CGA | -4.95 | 102.95 | 113.60 |
| 12 | W1 | 201 | CYC | CAA-CBA-CGA | -4.95 | 102.95 | 113.60 |
| 12 | G6 | 201 | CYC | CAA-CBA-CGA | -4.95 | 102.95 | 113.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | q7 | 201 | CYC | OC-C1C-C2C | -4.95 | 122.24 | 126.17 |
| 12 | YA | 201 | CYC | CAA-CBA-CGA | -4.94 | 102.97 | 113.60 |
| 12 | Y9 | 201 | CYC | CAA-CBA-CGA | -4.94 | 102.97 | 113.60 |
| 12 | E6 | 201 | CYC | CAA-CBA-CGA | -4.94 | 102.97 | 113.60 |
| 12 | C8 | 201 | CYC | CAA-CBA-CGA | -4.94 | 102.97 | 113.60 |
| 12 | CA | 201 | CYC | CAA-CBA-CGA | -4.94 | 102.97 | 113.60 |
| 12 | C9 | 201 | CYC | CAA-CBA-CGA | -4.94 | 102.97 | 113.60 |
| 12 | IA | 201 | CYC | CAA-CBA-CGA | -4.94 | 102.98 | 113.60 |
| 12 | UA | 201 | CYC | CAA-CBA-CGA | -4.94 | 102.98 | 113.60 |
| 12 | I9 | 201 | CYC | CAA-CBA-CGA | -4.94 | 102.98 | 113.60 |
| 12 | U9 | 201 | CYC | CAA-CBA-CGA | -4.94 | 102.98 | 113.60 |
| 12 | C4 | 201 | CYC | CAA-CBA-CGA | -4.94 | 102.98 | 113.60 |
| 12 | SA | 201 | CYC | CAA-CBA-CGA | -4.93 | 102.98 | 113.60 |
| 12 | E2 | 201 | CYC | CAA-CBA-CGA | -4.93 | 102.99 | 113.60 |
| 12 | K2 | 201 | CYC | CAA-CBA-CGA | -4.93 | 102.99 | 113.60 |
| 12 | A4 | 201 | CYC | CAA-CBA-CGA | -4.93 | 102.99 | 113.60 |
| 12 | A8 | 201 | CYC | CAA-CBA-CGA | -4.93 | 102.99 | 113.60 |
| 12 | K6 | 201 | CYC | CAA-CBA-CGA | -4.93 | 102.99 | 113.60 |
| 12 | c7 | 201 | CYC | OC-C1C-C2C | -4.93 | 122.25 | 126.17 |
| 12 | U3 | 201 | CYC | CAA-CBA-CGA | -4.93 | 103.00 | 113.60 |
| 12 | U1 | 201 | CYC | CAA-CBA-CGA | -4.93 | 103.00 | 113.60 |
| 12 | T8 | 201 | CYC | CAA-CBA-CGA | -4.93 | 103.00 | 113.60 |
| 12 | I4 | 201 | CYC | CAA-CBA-CGA | -4.93 | 103.00 | 113.60 |
| 12 | K4 | 201 | CYC | CAA-CBA-CGA | -4.93 | 103.00 | 113.60 |
| 12 | I8 | 201 | CYC | CAA-CBA-CGA | -4.93 | 103.00 | 113.60 |
| 12 | K8 | 201 | CYC | CAA-CBA-CGA | -4.93 | 103.00 | 113.60 |
| 12 | R8 | 201 | CYC | CAA-CBA-CGA | -4.92 | 103.01 | 113.60 |
| 12 | C2 | 201 | CYC | CAA-CBA-CGA | -4.92 | 103.01 | 113.60 |
| 12 | A1 | 201 | CYC | CAA-CBA-CGA | -4.92 | 103.02 | 113.60 |
| 12 | A3 | 201 | CYC | CAA-CBA-CGA | -4.92 | 103.02 | 113.60 |
| 12 | O4 | 202 | CYC | C1B-NB-C4B | -4.91 | 104.41 | 110.67 |
| 12 | O8 | 202 | CYC | C1B-NB-C4B | -4.91 | 104.41 | 110.67 |
| 12 | A9 | 201 | CYC | CAA-CBA-CGA | -4.91 | 103.03 | 113.60 |
| 12 | T4 | 201 | CYC | CAA-CBA-CGA | -4.91 | 103.04 | 113.60 |
| 12 | VA | 202 | CYC | C1B-NB-C4B | -4.91 | 104.42 | 110.67 |
| 12 | V9 | 202 | CYC | C1B-NB-C4B | -4.91 | 104.42 | 110.67 |
| 12 | Y4 | 201 | CYC | C2B-C1B-NB | 4.91 | 114.17 | 106.99 |
| 12 | Y8 | 201 | CYC | C2B-C1B-NB | 4.91 | 114.17 | 106.99 |
| 12 | R4 | 201 | CYC | CAA-CBA-CGA | -4.91 | 103.05 | 113.60 |
| 12 | a7 | 201 | CYC | OC-C1C-C2C | -4.90 | 122.27 | 126.17 |
| 12 | i7 | 201 | CYC | CMA-C3A-C4A | 4.90 | 132.62 | 125.06 |
| 12 | W4 | 202 | CYC | C1B-NB-C4B | -4.90 | 104.43 | 110.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | W8 | 202 | CYC | C1B-NB-C4B | -4.90 | 104.43 | 110.67 |
| 12 | KA | 201 | CYC | CAA-CBA-CGA | -4.90 | 103.05 | 113.60 |
| 12 | I6 | 201 | CYC | CAA-CBA-CGA | -4.90 | 103.05 | 113.60 |
| 12 | K9 | 201 | CYC | CAA-CBA-CGA | -4.90 | 103.05 | 113.60 |
| 12 | Q9 | 201 | CYC | CAA-CBA-CGA | -4.90 | 103.06 | 113.60 |
| 12 | Y1 | 201 | CYC | CAA-CBA-CGA | -4.90 | 103.06 | 113.60 |
| 12 | AA | 201 | CYC | CAA-CBA-CGA | -4.90 | 103.06 | 113.60 |
| 12 | I2 | 201 | CYC | CAA-CBA-CGA | -4.90 | 103.06 | 113.60 |
| 12 | QA | 201 | CYC | CAA-CBA-CGA | -4.90 | 103.06 | 113.60 |
| 12 | K7 | 201 | CYC | CMA-C3A-C4A | 4.90 | 132.61 | 125.06 |
| 12 | C6 | 201 | CYC | CAA-CBA-CGA | -4.90 | 103.06 | 113.60 |
| 12 | XA | 202 | CYC | C1B-NB-C4B | -4.89 | 104.44 | 110.67 |
| 12 | X9 | 202 | CYC | C1B-NB-C4B | -4.89 | 104.44 | 110.67 |
| 12 | I7 | 201 | CYC | CMA-C3A-C4A | 4.89 | 132.60 | 125.06 |
| 12 | S4 | 201 | CYC | C1B-NB-C4B | -4.89 | 104.44 | 110.67 |
| 12 | S8 | 201 | CYC | C1B-NB-C4B | -4.89 | 104.44 | 110.67 |
| 12 | O7 | 201 | CYC | CMA-C3A-C4A | 4.89 | 132.59 | 125.06 |
| 12 | Y3 | 201 | CYC | CAA-CBA-CGA | -4.89 | 103.09 | 113.60 |
| 12 | L9 | 201 | CYC | C1B-NB-C4B | -4.89 | 104.45 | 110.67 |
| 12 | Q4 | 201 | CYC | C1B-NB-C4B | -4.88 | 104.45 | 110.67 |
| 12 | L3 | 201 | CYC | C1B-NB-C4B | -4.88 | 104.46 | 110.67 |
| 12 | L1 | 201 | CYC | C1B-NB-C4B | -4.88 | 104.46 | 110.67 |
| 12 | C7 | 201 | CYC | CMA-C3A-C4A | 4.87 | 132.57 | 125.06 |
| 12 | K3 | 201 | CYC | CAA-CBA-CGA | -4.87 | 103.12 | 113.60 |
| 12 | K1 | 201 | CYC | CAA-CBA-CGA | -4.87 | 103.12 | 113.60 |
| 12 | E7 | 201 | CYC | CMA-C3A-C4A | 4.87 | 132.56 | 125.06 |
| 12 | i7 | 201 | CYC | OC-C1C-C2C | -4.87 | 122.30 | 126.17 |
| 12 | g7 | 201 | CYC | CMA-C3A-C4A | 4.87 | 132.56 | 125.06 |
| 12 | c5 | 201 | CYC | CMA-C3A-C4A | 4.87 | 132.56 | 125.06 |
| 12 | W7 | 201 | CYC | CMA-C3A-C4A | 4.87 | 132.56 | 125.06 |
| 12 | LA | 201 | CYC | C1B-NB-C4B | -4.87 | 104.47 | 110.67 |
| 12 | u7 | 201 | CYC | CMA-C3A-C4A | 4.86 | 132.55 | 125.06 |
| 12 | PA | 202 | CYC | C1B-NB-C4B | -4.86 | 104.48 | 110.67 |
| 12 | P9 | 202 | CYC | C1B-NB-C4B | -4.86 | 104.48 | 110.67 |
| 12 | A7 | 201 | CYC | CMA-C3A-C4A | 4.85 | 132.54 | 125.06 |
| 12 | a7 | 201 | CYC | CMA-C3A-C4A | 4.85 | 132.54 | 125.06 |
| 12 | B3 | 201 | CYC | C1B-NB-C4B | -4.85 | 104.49 | 110.67 |
| 12 | B1 | 201 | CYC | C1B-NB-C4B | -4.85 | 104.49 | 110.67 |
| 12 | G7 | 201 | CYC | CMA-C3A-C4A | 4.85 | 132.53 | 125.06 |
| 12 | Q8 | 201 | CYC | C1B-NB-C4B | -4.85 | 104.49 | 110.67 |
| 12 | J8 | 202 | CYC | C1B-NB-C4B | -4.85 | 104.50 | 110.67 |
| 12 | U7 | 201 | CYC | CMA-C3A-C4A | 4.85 | 132.53 | 125.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | J1 | 201 | CYC | C1B-NB-C4B | -4.85 | 104.50 | 110.67 |
| 12 | Q7 | 201 | CYC | OC-C1C-C2C | -4.84 | 122.32 | 126.17 |
| 12 | M7 | 201 | CYC | OC-C1C-C2C | -4.84 | 122.32 | 126.17 |
| 12 | B4 | 201 | CYC | C1B-NB-C4B | -4.84 | 104.50 | 110.67 |
| 12 | B8 | 201 | CYC | C1B-NB-C4B | -4.84 | 104.50 | 110.67 |
| 12 | J4 | 202 | CYC | C2B-C1B-NB | 4.84 | 114.08 | 106.99 |
| 12 | J8 | 202 | CYC | C2B-C1B-NB | 4.84 | 114.08 | 106.99 |
| 12 | E5 | 201 | CYC | CMA-C3A-C4A | 4.84 | 132.52 | 125.06 |
| 12 | S5 | 201 | CYC | OC-C1C-C2C | -4.84 | 122.32 | 126.17 |
| 12 | c7 | 201 | CYC | CMA-C3A-C4A | 4.84 | 132.51 | 125.06 |
| 12 | JA | 201 | CYC | C1B-NB-C4B | -4.84 | 104.51 | 110.67 |
| 12 | L2 | 201 | CYC | CHA-C1A-NA | -4.84 | 122.12 | 128.83 |
| 12 | L6 | 201 | CYC | CHA-C1A-NA | -4.84 | 122.12 | 128.83 |
| 12 | Q7 | 201 | CYC | CMA-C3A-C4A | 4.84 | 132.51 | 125.06 |
| 12 | G5 | 201 | CYC | CMA-C3A-C4A | 4.83 | 132.51 | 125.06 |
| 12 | M5 | 201 | CYC | OC-C1C-C2C | -4.83 | 122.33 | 126.17 |
| 12 | o7 | 201 | CYC | CMA-C3A-C4A | 4.83 | 132.50 | 125.06 |
| 12 | U5 | 201 | CYC | CMA-C3A-C4A | 4.83 | 132.50 | 125.06 |
| 12 | Y5 | 201 | CYC | CMA-C3A-C4A | 4.83 | 132.50 | 125.06 |
| 12 | L6 | 202 | CYC | C1B-NB-C4B | -4.83 | 104.52 | 110.67 |
| 12 | H2 | 202 | CYC | C2B-C1B-NB | 4.83 | 114.06 | 106.99 |
| 12 | J3 | 201 | CYC | C1B-NB-C4B | -4.83 | 104.52 | 110.67 |
| 12 | O5 | 201 | CYC | CMA-C3A-C4A | 4.83 | 132.50 | 125.06 |
| 12 | L8 | 201 | CYC | C1B-NB-C4B | -4.82 | 104.53 | 110.67 |
| 12 | H6 | 202 | CYC | C2B-C1B-NB | 4.82 | 114.05 | 106.99 |
| 12 | J4 | 202 | CYC | C1B-NB-C4B | -4.82 | 104.53 | 110.67 |
| 12 | H2 | 202 | CYC | C1B-NB-C4B | -4.82 | 104.53 | 110.67 |
| 12 | D4 | 201 | CYC | C1B-NB-C4B | -4.82 | 104.53 | 110.67 |
| 12 | H6 | 202 | CYC | C1B-NB-C4B | -4.82 | 104.53 | 110.67 |
| 12 | D8 | 201 | CYC | C1B-NB-C4B | -4.82 | 104.53 | 110.67 |
| 12 | m7 | 201 | CYC | CMA-C3A-C4A | 4.82 | 132.48 | 125.06 |
| 12 | XA | 202 | CYC | C2B-C1B-NB | 4.81 | 114.04 | 106.99 |
| 12 | X9 | 202 | CYC | C2B-C1B-NB | 4.81 | 114.04 | 106.99 |
| 12 | M7 | 201 | CYC | CMA-C3A-C4A | 4.81 | 132.48 | 125.06 |
| 12 | k7 | 201 | CYC | CMA-C3A-C4A | 4.81 | 132.48 | 125.06 |
| 12 | J9 | 201 | CYC | C1B-NB-C4B | -4.81 | 104.54 | 110.67 |
| 12 | M5 | 201 | CYC | CMA-C3A-C4A | 4.81 | 132.47 | 125.06 |
| 12 | Q5 | 201 | CYC | CMA-C3A-C4A | 4.81 | 132.47 | 125.06 |
| 12 | L4 | 201 | CYC | C1B-NB-C4B | -4.81 | 104.55 | 110.67 |
| 12 | W5 | 201 | CYC | CMA-C3A-C4A | 4.81 | 132.47 | 125.06 |
| 12 | FA | 301 | CYC | CHA-C1A-NA | -4.81 | 122.16 | 128.83 |
| 12 | A5 | 201 | CYC | CMA-C3A-C4A | 4.80 | 132.46 | 125.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | F9 | 301 | CYC | CHA-C1A-NA | -4.80 | 122.16 | 128.83 |
| 12 | L2 | 202 | CYC | C1B-NB-C4B | -4.80 | 104.56 | 110.67 |
| 12 | B4 | 202 | CYC | CHA-C1A-NA | -4.80 | 122.17 | 128.83 |
| 12 | q7 | 201 | CYC | CMA-C3A-C4A | 4.80 | 132.46 | 125.06 |
| 12 | B8 | 202 | CYC | CHA-C1A-NA | -4.80 | 122.17 | 128.83 |
| 12 | X3 | 202 | CYC | C1B-NB-C4B | -4.80 | 104.56 | 110.67 |
| 12 | X1 | 202 | CYC | C1B-NB-C4B | -4.80 | 104.56 | 110.67 |
| 12 | S5 | 201 | CYC | CMA-C3A-C4A | 4.80 | 132.45 | 125.06 |
| 12 | J6 | 201 | CYC | C1B-NB-C4B | -4.80 | 104.56 | 110.67 |
| 12 | VA | 202 | CYC | C2B-C1B-NB | 4.80 | 114.01 | 106.99 |
| 12 | J1 | 201 | CYC | C2B-C1B-NB | 4.80 | 114.01 | 106.99 |
| 12 | O4 | 201 | CYC | CHA-C1A-NA | -4.80 | 122.17 | 128.83 |
| 12 | O8 | 201 | CYC | CHA-C1A-NA | -4.80 | 122.17 | 128.83 |
| 12 | c5 | 201 | CYC | OC-C1C-C2C | -4.80 | 122.36 | 126.17 |
| 12 | X3 | 202 | CYC | C2B-C1B-NB | 4.80 | 114.01 | 106.99 |
| 12 | W4 | 202 | CYC | C2B-C1B-NB | 4.80 | 114.01 | 106.99 |
| 12 | W8 | 202 | CYC | C2B-C1B-NB | 4.80 | 114.01 | 106.99 |
| 12 | X1 | 202 | CYC | C2B-C1B-NB | 4.80 | 114.01 | 106.99 |
| 12 | P1 | 201 | CYC | CHA-C1A-NA | -4.79 | 122.18 | 128.83 |
| 12 | P3 | 201 | CYC | CHA-C1A-NA | -4.79 | 122.18 | 128.83 |
| 12 | P1 | 202 | CYC | C1B-NB-C4B | -4.79 | 104.57 | 110.67 |
| 12 | P3 | 202 | CYC | C1B-NB-C4B | -4.79 | 104.57 | 110.67 |
| 12 | BA | 202 | CYC | C1B-NB-C4B | -4.79 | 104.57 | 110.67 |
| 12 | L4 | 202 | CYC | CHA-C1A-NA | -4.79 | 122.18 | 128.83 |
| 12 | J2 | 201 | CYC | C1B-NB-C4B | -4.79 | 104.57 | 110.67 |
| 12 | e5 | 201 | CYC | OC-C1C-C2C | -4.79 | 122.36 | 126.17 |
| 12 | I5 | 201 | CYC | CMA-C3A-C4A | 4.79 | 132.44 | 125.06 |
| 12 | B6 | 201 | CYC | C1B-NB-C4B | -4.79 | 104.57 | 110.67 |
| 12 | B9 | 202 | CYC | C1B-NB-C4B | -4.79 | 104.57 | 110.67 |
| 12 | C5 | 201 | CYC | CMA-C3A-C4A | 4.79 | 132.44 | 125.06 |
| 12 | Q4 | 201 | CYC | C2B-C1B-NB | 4.79 | 114.00 | 106.99 |
| 12 | Z8 | 301 | CYC | CHA-C1A-NA | -4.79 | 122.19 | 128.83 |
| 12 | Y5 | 201 | CYC | OC-C1C-C2C | -4.78 | 122.37 | 126.17 |
| 12 | W7 | 201 | CYC | OC-C1C-C2C | -4.78 | 122.37 | 126.17 |
| 12 | Y7 | 201 | CYC | CMA-C3A-C4A | 4.78 | 132.43 | 125.06 |
| 12 | s7 | 201 | CYC | CMA-C3A-C4A | 4.78 | 132.43 | 125.06 |
| 12 | U5 | 201 | CYC | OC-C1C-C2C | -4.78 | 122.37 | 126.17 |
| 12 | U4 | 202 | CYC | C2B-C1B-NB | 4.78 | 113.99 | 106.99 |
| 12 | U8 | 202 | CYC | C2B-C1B-NB | 4.78 | 113.99 | 106.99 |
| 12 | K5 | 201 | CYC | CMA-C3A-C4A | 4.78 | 132.43 | 125.06 |
| 12 | H4 | 201 | CYC | CHA-C1A-NA | -4.78 | 122.19 | 128.83 |
| 12 | H8 | 201 | CYC | CHA-C1A-NA | -4.78 | 122.19 | 128.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | H1 | 202 | CYC | C1B-NB-C4B | -4.78 | 104.58 | 110.67 |
| 12 | BA | 201 | CYC | CHA-C1A-NA | -4.78 | 122.20 | 128.83 |
| 12 | B9 | 201 | CYC | CHA-C1A-NA | -4.78 | 122.20 | 128.83 |
| 12 | D3 | 201 | CYC | C1B-NB-C4B | -4.78 | 104.58 | 110.67 |
| 12 | D1 | 201 | CYC | C1B-NB-C4B | -4.78 | 104.58 | 110.67 |
| 12 | K5 | 201 | CYC | OC-C1C-C2C | -4.78 | 122.37 | 126.17 |
| 12 | B2 | 201 | CYC | C1B-NB-C4B | -4.78 | 104.59 | 110.67 |
| 12 | PA | 201 | CYC | CHA-C1A-NA | -4.78 | 122.20 | 128.83 |
| 12 | J3 | 201 | CYC | C2B-C1B-NB | 4.78 | 113.98 | 106.99 |
| 12 | S7 | 201 | CYC | CMA-C3A-C4A | 4.78 | 132.42 | 125.06 |
| 12 | V9 | 202 | CYC | C2B-C1B-NB | 4.78 | 113.98 | 106.99 |
| 12 | a9 | 901 | CYC | CHA-C1A-NA | -4.77 | 122.20 | 128.83 |
| 12 | P9 | 201 | CYC | CHA-C1A-NA | -4.77 | 122.20 | 128.83 |
| 12 | e7 | 201 | CYC | CMA-C3A-C4A | 4.77 | 132.41 | 125.06 |
| 12 | LA | 201 | CYC | C2B-C1B-NB | 4.77 | 113.97 | 106.99 |
| 12 | L9 | 201 | CYC | C2B-C1B-NB | 4.77 | 113.97 | 106.99 |
| 12 | H1 | 202 | CYC | C2B-C1B-NB | 4.77 | 113.97 | 106.99 |
| 12 | B4 | 201 | CYC | C2B-C1B-NB | 4.77 | 113.97 | 106.99 |
| 12 | B8 | 201 | CYC | C2B-C1B-NB | 4.77 | 113.97 | 106.99 |
| 12 | a5 | 201 | CYC | CMA-C3A-C4A | 4.77 | 132.41 | 125.06 |
| 12 | JA | 201 | CYC | C2B-C1B-NB | 4.77 | 113.97 | 106.99 |
| 12 | J9 | 201 | CYC | C2B-C1B-NB | 4.77 | 113.97 | 106.99 |
| 12 | D4 | 201 | CYC | C2B-C1B-NB | 4.77 | 113.96 | 106.99 |
| 12 | D8 | 201 | CYC | C2B-C1B-NB | 4.77 | 113.96 | 106.99 |
| 12 | ZA | 202 | CYC | C1B-C2B-C3B | -4.76 | 102.90 | 107.87 |
| 12 | Z9 | 202 | CYC | C1B-C2B-C3B | -4.76 | 102.90 | 107.87 |
| 12 | D2 | 201 | CYC | CHA-C1A-NA | -4.76 | 122.22 | 128.83 |
| 12 | U8 | 202 | CYC | C1B-NB-C4B | -4.76 | 104.61 | 110.67 |
| 12 | PA | 202 | CYC | C2B-C1B-NB | 4.76 | 113.96 | 106.99 |
| 12 | P9 | 202 | CYC | C2B-C1B-NB | 4.76 | 113.96 | 106.99 |
| 12 | V1 | 201 | CYC | CHA-C1A-NA | -4.76 | 122.22 | 128.83 |
| 12 | K7 | 201 | CYC | OC-C1C-C2C | -4.76 | 122.39 | 126.17 |
| 12 | XA | 201 | CYC | C1B-C2B-C3B | -4.76 | 102.91 | 107.87 |
| 12 | ZA | 201 | CYC | C1B-NB-C4B | -4.76 | 104.61 | 110.67 |
| 12 | Z9 | 201 | CYC | C1B-NB-C4B | -4.76 | 104.61 | 110.67 |
| 12 | S7 | 201 | CYC | OC-C1C-C2C | -4.76 | 122.39 | 126.17 |
| 12 | J6 | 201 | CYC | C2B-C1B-NB | 4.76 | 113.95 | 106.99 |
| 12 | Q8 | 201 | CYC | C2B-C1B-NB | 4.76 | 113.95 | 106.99 |
| 12 | X9 | 201 | CYC | C1B-C2B-C3B | -4.75 | 102.91 | 107.87 |
| 12 | R1 | 202 | CYC | C1B-NB-C4B | -4.75 | 104.62 | 110.67 |
| 12 | R3 | 202 | CYC | C1B-NB-C4B | -4.75 | 104.62 | 110.67 |
| 12 | Z3 | 202 | CYC | C2B-C1B-NB | 4.75 | 113.94 | 106.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | Z1 | 201 | CYC | C2B-C1B-NB | 4.75 | 113.94 | 106.99 |
| 12 | e5 | 201 | CYC | CMA-C3A-C4A | 4.75 | 132.38 | 125.06 |
| 12 | Z4 | 301 | CYC | CHA-C1A-NA | -4.75 | 122.24 | 128.83 |
| 12 | U4 | 201 | CYC | CHA-C1A-NA | -4.75 | 122.24 | 128.83 |
| 12 | U8 | 201 | CYC | CHA-C1A-NA | -4.75 | 122.24 | 128.83 |
| 12 | E5 | 201 | CYC | OC-C1C-C2C | -4.75 | 122.40 | 126.17 |
| 12 | TA | 302 | CYC | C1B-NB-C4B | -4.75 | 104.62 | 110.67 |
| 12 | H3 | 201 | CYC | C1B-NB-C4B | -4.75 | 104.62 | 110.67 |
| 12 | T9 | 302 | CYC | C1B-NB-C4B | -4.75 | 104.62 | 110.67 |
| 12 | L6 | 202 | CYC | C2B-C1B-NB | 4.75 | 113.94 | 106.99 |
| 12 | J2 | 202 | CYC | C1B-C2B-C3B | -4.75 | 102.92 | 107.87 |
| 12 | HA | 201 | CYC | C1B-NB-C4B | -4.75 | 104.63 | 110.67 |
| 12 | V3 | 201 | CYC | CHA-C1A-NA | -4.75 | 122.24 | 128.83 |
| 12 | F3 | 202 | CYC | C2B-C1B-NB | 4.75 | 113.94 | 106.99 |
| 12 | F1 | 202 | CYC | C2B-C1B-NB | 4.75 | 113.94 | 106.99 |
| 12 | F9 | 303 | CYC | C1B-NB-C4B | -4.74 | 104.63 | 110.67 |
| 12 | H3 | 201 | CYC | C2B-C1B-NB | 4.74 | 113.93 | 106.99 |
| 12 | L3 | 202 | CYC | C1B-C2B-C3B | -4.74 | 102.92 | 107.87 |
| 12 | V3 | 202 | CYC | C2B-C1B-NB | 4.74 | 113.92 | 106.99 |
| 12 | V1 | 202 | CYC | C2B-C1B-NB | 4.74 | 113.92 | 106.99 |
| 12 | D6 | 201 | CYC | CHA-C1A-NA | -4.74 | 122.26 | 128.83 |
| 12 | L3 | 201 | CYC | C2B-C1B-NB | 4.74 | 113.92 | 106.99 |
| 12 | L1 | 201 | CYC | C2B-C1B-NB | 4.74 | 113.92 | 106.99 |
| 12 | Z3 | 201 | CYC | CHA-C1A-NA | -4.73 | 122.26 | 128.83 |
| 12 | Z1 | 202 | CYC | CHA-C1A-NA | -4.73 | 122.26 | 128.83 |
| 12 | H4 | 202 | CYC | C1B-NB-C4B | -4.73 | 104.64 | 110.67 |
| 12 | H8 | 202 | CYC | C1B-NB-C4B | -4.73 | 104.64 | 110.67 |
| 12 | F4 | 202 | CYC | CHA-C1A-NA | -4.73 | 122.26 | 128.83 |
| 12 | F8 | 202 | CYC | CHA-C1A-NA | -4.73 | 122.26 | 128.83 |
| 12 | j5 | 1201 | CYC | CMA-C3A-C4A | 4.73 | 132.35 | 125.06 |
| 12 | D3 | 201 | CYC | C2B-C1B-NB | 4.73 | 113.92 | 106.99 |
| 12 | D1 | 201 | CYC | C2B-C1B-NB | 4.73 | 113.92 | 106.99 |
| 12 | U4 | 202 | CYC | C1B-NB-C4B | -4.73 | 104.64 | 110.67 |
| 12 | M8 | 301 | CYC | CHA-C1A-NA | -4.73 | 122.27 | 128.83 |
| 12 | B3 | 201 | CYC | C2B-C1B-NB | 4.73 | 113.91 | 106.99 |
| 12 | B1 | 201 | CYC | C2B-C1B-NB | 4.73 | 113.91 | 106.99 |
| 12 | H9 | 201 | CYC | C1B-NB-C4B | -4.73 | 104.65 | 110.67 |
| 12 | J6 | 202 | CYC | C1B-C2B-C3B | -4.73 | 102.94 | 107.87 |
| 12 | J2 | 201 | CYC | C2B-C1B-NB | 4.73 | 113.91 | 106.99 |
| 12 | F9 | 302 | CYC | C1B-NB-C4B | -4.73 | 104.65 | 110.67 |
| 12 | U7 | 201 | CYC | OC-C1C-C2C | -4.73 | 122.42 | 126.17 |
| 12 | S4 | 202 | CYC | C1B-C2B-C3B | -4.72 | 102.94 | 107.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | F8 | 202 | CYC | C1B-C2B-C3B | -4.72 | 102.94 | 107.87 |
| 12 | RA | 202 | CYC | C2B-C1B-NB | 4.72 | 113.90 | 106.99 |
| 12 | R9 | 202 | CYC | C2B-C1B-NB | 4.72 | 113.90 | 106.99 |
| 12 | YA | 201 | CYC | OB-C4B-C3B | -4.72 | 122.92 | 128.04 |
| 12 | C6 | 201 | CYC | OB-C4B-C3B | -4.72 | 122.92 | 128.04 |
| 12 | Y9 | 201 | CYC | OB-C4B-C3B | -4.72 | 122.92 | 128.04 |
| 12 | D4 | 202 | CYC | C1B-C2B-C3B | -4.72 | 102.94 | 107.87 |
| 12 | V3 | 202 | CYC | C1B-NB-C4B | -4.72 | 104.66 | 110.67 |
| 12 | V1 | 202 | CYC | C1B-NB-C4B | -4.72 | 104.66 | 110.67 |
| 12 | X1 | 201 | CYC | C1B-C2B-C3B | -4.72 | 102.95 | 107.87 |
| 12 | S4 | 201 | CYC | C2B-C1B-NB | 4.72 | 113.90 | 106.99 |
| 12 | S8 | 201 | CYC | C2B-C1B-NB | 4.72 | 113.90 | 106.99 |
| 12 | M8 | 302 | CYC | CHA-C1A-NA | -4.72 | 122.28 | 128.83 |
| 12 | XA | 201 | CYC | CHA-C1A-NA | -4.72 | 122.28 | 128.83 |
| 12 | X9 | 201 | CYC | CHA-C1A-NA | -4.72 | 122.28 | 128.83 |
| 12 | VA | 201 | CYC | OC-C1C-C2C | -4.72 | 122.42 | 126.17 |
| 12 | V9 | 201 | CYC | OC-C1C-C2C | -4.72 | 122.42 | 126.17 |
| 12 | EA | 201 | CYC | OB-C4B-C3B | -4.72 | 122.92 | 128.04 |
| 12 | E9 | 201 | CYC | OB-C4B-C3B | -4.72 | 122.92 | 128.04 |
| 12 | J4 | 201 | CYC | CHA-C1A-NA | -4.72 | 122.28 | 128.83 |
| 12 | W4 | 201 | CYC | C1B-C2B-C3B | -4.72 | 102.95 | 107.87 |
| 12 | W8 | 201 | CYC | C1B-C2B-C3B | -4.72 | 102.95 | 107.87 |
| 12 | G5 | 201 | CYC | OC-C1C-C2C | -4.72 | 122.42 | 126.17 |
| 12 | O4 | 202 | CYC | C2B-C1B-NB | 4.72 | 113.89 | 106.99 |
| 12 | O8 | 202 | CYC | C2B-C1B-NB | 4.72 | 113.89 | 106.99 |
| 12 | u7 | 201 | CYC | OC-C1C-C2C | -4.72 | 122.42 | 126.17 |
| 12 | D4 | 202 | CYC | CHA-C1A-NA | -4.71 | 122.29 | 128.83 |
| 12 | D8 | 202 | CYC | CHA-C1A-NA | -4.71 | 122.29 | 128.83 |
| 12 | L2 | 202 | CYC | C2B-C1B-NB | 4.71 | 113.89 | 106.99 |
| 12 | X3 | 201 | CYC | C1B-C2B-C3B | -4.71 | 102.95 | 107.87 |
| 12 | i7 | 201 | CYC | C1B-NB-C4B | -4.71 | 104.67 | 110.67 |
| 12 | Z3 | 202 | CYC | C1B-NB-C4B | -4.71 | 104.67 | 110.67 |
| 12 | Z1 | 201 | CYC | C1B-NB-C4B | -4.71 | 104.67 | 110.67 |
| 12 | VA | 201 | CYC | CHA-C1A-NA | -4.71 | 122.29 | 128.83 |
| 12 | J8 | 201 | CYC | CHA-C1A-NA | -4.71 | 122.29 | 128.83 |
| 12 | V9 | 201 | CYC | CHA-C1A-NA | -4.71 | 122.29 | 128.83 |
| 12 | P1 | 202 | CYC | C2B-C1B-NB | 4.71 | 113.89 | 106.99 |
| 12 | P3 | 202 | CYC | C2B-C1B-NB | 4.71 | 113.89 | 106.99 |
| 12 | N2 | 101 | CYC | CHA-C1A-NA | -4.71 | 122.30 | 128.83 |
| 12 | N6 | 101 | CYC | CHA-C1A-NA | -4.71 | 122.30 | 128.83 |
| 12 | L8 | 201 | CYC | C2B-C1B-NB | 4.71 | 113.88 | 106.99 |
| 12 | Z4 | 301 | CYC | C1B-C2B-C3B | -4.71 | 102.96 | 107.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | I7 | 201 | CYC | OC-C1C-C2C | -4.71 | 122.43 | 126.17 |
| 12 | ZA | 201 | CYC | C2B-C1B-NB | 4.71 | 113.88 | 106.99 |
| 12 | R1 | 202 | CYC | C2B-C1B-NB | 4.71 | 113.88 | 106.99 |
| 12 | R3 | 202 | CYC | C2B-C1B-NB | 4.71 | 113.88 | 106.99 |
| 12 | Z9 | 201 | CYC | C2B-C1B-NB | 4.71 | 113.88 | 106.99 |
| 12 | K5 | 201 | CYC | C1B-NB-C4B | -4.71 | 104.68 | 110.67 |
| 12 | D6 | 201 | CYC | C1B-C2B-C3B | -4.71 | 102.96 | 107.87 |
| 12 | C2 | 201 | CYC | OB-C4B-C3B | -4.71 | 122.93 | 128.04 |
| 12 | F4 | 202 | CYC | OC-C1C-C2C | -4.71 | 122.43 | 126.17 |
| 12 | a5 | 201 | CYC | OC-C1C-C2C | -4.71 | 122.43 | 126.17 |
| 12 | F8 | 202 | CYC | OC-C1C-C2C | -4.71 | 122.43 | 126.17 |
| 12 | aA | 902 | CYC | C1B-C2B-C3B | -4.70 | 102.96 | 107.87 |
| 12 | M4 | 301 | CYC | CHA-C1A-NA | -4.70 | 122.30 | 128.83 |
| 12 | H3 | 202 | CYC | CHA-C1A-NA | -4.70 | 122.30 | 128.83 |
| 12 | D6 | 202 | CYC | C1B-NB-C4B | -4.70 | 104.68 | 110.67 |
| 12 | T3 | 302 | CYC | C1B-NB-C4B | -4.70 | 104.68 | 110.67 |
| 12 | T1 | 302 | CYC | C1B-NB-C4B | -4.70 | 104.68 | 110.67 |
| 12 | HA | 201 | CYC | C2B-C1B-NB | 4.70 | 113.87 | 106.99 |
| 12 | H9 | 201 | CYC | C2B-C1B-NB | 4.70 | 113.87 | 106.99 |
| 12 | E8 | 201 | CYC | OB-C4B-C3B | -4.70 | 122.94 | 128.04 |
| 12 | BA | 202 | CYC | C2B-C1B-NB | 4.70 | 113.87 | 106.99 |
| 12 | ZA | 202 | CYC | C2B-C1B-NB | 4.70 | 113.87 | 106.99 |
| 12 | Z9 | 202 | CYC | C2B-C1B-NB | 4.70 | 113.87 | 106.99 |
| 12 | C7 | 201 | CYC | OC-C1C-C2C | -4.70 | 122.44 | 126.17 |
| 12 | H1 | 201 | CYC | CHA-C1A-NA | -4.70 | 122.31 | 128.83 |
| 12 | H4 | 202 | CYC | C2B-C1B-NB | 4.70 | 113.87 | 106.99 |
| 12 | H8 | 202 | CYC | C2B-C1B-NB | 4.70 | 113.87 | 106.99 |
| 12 | F6 | 202 | CYC | C1B-NB-C4B | -4.70 | 104.69 | 110.67 |
| 12 | DA | 201 | CYC | CHA-C1A-NA | -4.70 | 122.31 | 128.83 |
| 12 | D9 | 201 | CYC | CHA-C1A-NA | -4.70 | 122.31 | 128.83 |
| 12 | J2 | 202 | CYC | C2B-C1B-NB | 4.70 | 113.87 | 106.99 |
| 12 | U3 | 201 | CYC | OB-C4B-C3B | -4.70 | 122.94 | 128.04 |
| 12 | U1 | 201 | CYC | OB-C4B-C3B | -4.70 | 122.94 | 128.04 |
| 12 | L3 | 202 | CYC | CHA-C1A-NA | -4.70 | 122.31 | 128.83 |
| 12 | F6 | 201 | CYC | CHA-C1A-NA | -4.70 | 122.31 | 128.83 |
| 12 | H3 | 202 | CYC | C1B-C2B-C3B | -4.70 | 102.97 | 107.87 |
| 12 | N2 | 101 | CYC | C1B-C2B-C3B | -4.70 | 102.97 | 107.87 |
| 12 | k5 | 1201 | CYC | CMA-C3A-C4A | 4.70 | 132.29 | 125.06 |
| 12 | F3 | 201 | CYC | C1B-C2B-C3B | -4.69 | 102.97 | 107.87 |
| 12 | F1 | 201 | CYC | C1B-C2B-C3B | -4.69 | 102.97 | 107.87 |
| 12 | L4 | 201 | CYC | C2B-C1B-NB | 4.69 | 113.86 | 106.99 |
| 12 | I2 | 201 | CYC | OB-C4B-C3B | -4.69 | 122.95 | 128.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | GA | 201 | CYC | OB-C4B-C3B | -4.69 | 122.95 | 128.04 |
| 12 | G9 | 201 | CYC | OB-C4B-C3B | -4.69 | 122.95 | 128.04 |
| 12 | O4 | 201 | CYC | C1B-C2B-C3B | -4.69 | 102.97 | 107.87 |
| 12 | O8 | 201 | CYC | C1B-C2B-C3B | -4.69 | 102.97 | 107.87 |
| 12 | C5 | 201 | CYC | OC-C1C-C2C | -4.69 | 122.44 | 126.17 |
| 12 | D2 | 202 | CYC | C1B-NB-C4B | -4.69 | 104.70 | 110.67 |
| 12 | B2 | 201 | CYC | C2B-C1B-NB | 4.69 | 113.86 | 106.99 |
| 12 | F4 | 202 | CYC | C1B-C2B-C3B | -4.69 | 102.98 | 107.87 |
| 12 | LA | 202 | CYC | C1B-C2B-C3B | -4.69 | 102.98 | 107.87 |
| 12 | m7 | 201 | CYC | CAB-C3B-C4B | 4.69 | 128.78 | 121.38 |
| 12 | F3 | 202 | CYC | C1B-NB-C4B | -4.69 | 104.70 | 110.67 |
| 12 | F1 | 202 | CYC | C1B-NB-C4B | -4.69 | 104.70 | 110.67 |
| 12 | TA | 301 | CYC | CHA-C1A-NA | -4.69 | 122.32 | 128.83 |
| 12 | T9 | 301 | CYC | CHA-C1A-NA | -4.69 | 122.32 | 128.83 |
| 12 | B9 | 202 | CYC | C2B-C1B-NB | 4.69 | 113.85 | 106.99 |
| 12 | F8 | 202 | CYC | C2B-C1B-NB | 4.69 | 113.85 | 106.99 |
| 12 | B4 | 202 | CYC | C1B-C2B-C3B | -4.69 | 102.98 | 107.87 |
| 12 | E7 | 201 | CYC | OC-C1C-C2C | -4.68 | 122.45 | 126.17 |
| 12 | o7 | 201 | CYC | OC-C1C-C2C | -4.68 | 122.45 | 126.17 |
| 12 | TA | 302 | CYC | C2B-C1B-NB | 4.68 | 113.84 | 106.99 |
| 12 | T9 | 302 | CYC | C2B-C1B-NB | 4.68 | 113.84 | 106.99 |
| 12 | aA | 902 | CYC | CHA-C1A-NA | -4.68 | 122.33 | 128.83 |
| 12 | F2 | 202 | CYC | C1B-NB-C4B | -4.68 | 104.71 | 110.67 |
| 12 | B6 | 201 | CYC | C2B-C1B-NB | 4.68 | 113.84 | 106.99 |
| 12 | S4 | 202 | CYC | CHA-C1A-NA | -4.68 | 122.33 | 128.83 |
| 12 | P1 | 201 | CYC | C1B-C2B-C3B | -4.68 | 102.99 | 107.87 |
| 12 | P3 | 201 | CYC | C1B-C2B-C3B | -4.68 | 102.99 | 107.87 |
| 12 | D8 | 202 | CYC | C1B-C2B-C3B | -4.68 | 102.99 | 107.87 |
| 12 | PA | 201 | CYC | C1B-C2B-C3B | -4.68 | 102.99 | 107.87 |
| 12 | P9 | 201 | CYC | C1B-C2B-C3B | -4.68 | 102.99 | 107.87 |
| 12 | F9 | 303 | CYC | C2B-C1B-NB | 4.68 | 113.84 | 106.99 |
| 12 | ZA | 202 | CYC | CHA-C1A-NA | -4.68 | 122.34 | 128.83 |
| 12 | Z9 | 202 | CYC | CHA-C1A-NA | -4.68 | 122.34 | 128.83 |
| 12 | A4 | 201 | CYC | OB-C4B-C3B | -4.68 | 122.96 | 128.04 |
| 12 | VA | 201 | CYC | C1B-C2B-C3B | -4.68 | 102.99 | 107.87 |
| 12 | V9 | 201 | CYC | C1B-C2B-C3B | -4.68 | 102.99 | 107.87 |
| 12 | A5 | 201 | CYC | OC-C1C-C2C | -4.68 | 122.45 | 126.17 |
| 12 | F4 | 201 | CYC | C1B-NB-C4B | -4.68 | 104.71 | 110.67 |
| 12 | c7 | 201 | CYC | C1B-NB-C4B | -4.68 | 104.71 | 110.67 |
| 12 | F8 | 201 | CYC | C1B-NB-C4B | -4.68 | 104.71 | 110.67 |
| 12 | G6 | 201 | CYC | OB-C4B-C3B | -4.68 | 122.97 | 128.04 |
| 12 | H1 | 201 | CYC | C1B-C2B-C3B | -4.68 | 102.99 | 107.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | PA | 201 | CYC | C2B-C1B-NB | 4.67 | 113.83 | 106.99 |
| 12 | F4 | 201 | CYC | C2B-C1B-NB | 4.67 | 113.83 | 106.99 |
| 12 | F8 | 201 | CYC | C2B-C1B-NB | 4.67 | 113.83 | 106.99 |
| 12 | P9 | 201 | CYC | C2B-C1B-NB | 4.67 | 113.83 | 106.99 |
| 12 | B8 | 202 | CYC | C1B-C2B-C3B | -4.67 | 102.99 | 107.87 |
| 12 | D2 | 201 | CYC | C1B-C2B-C3B | -4.67 | 102.99 | 107.87 |
| 12 | A2 | 201 | CYC | OB-C4B-C3B | -4.67 | 122.97 | 128.04 |
| 12 | B1 | 202 | CYC | CHA-C1A-NA | -4.67 | 122.35 | 128.83 |
| 12 | LA | 202 | CYC | CHA-C1A-NA | -4.67 | 122.35 | 128.83 |
| 12 | L9 | 202 | CYC | CHA-C1A-NA | -4.67 | 122.35 | 128.83 |
| 12 | E4 | 201 | CYC | OB-C4B-C3B | -4.67 | 122.97 | 128.04 |
| 12 | W5 | 201 | CYC | OC-C1C-C2C | -4.67 | 122.46 | 126.17 |
| 12 | G4 | 201 | CYC | OB-C4B-C3B | -4.67 | 122.97 | 128.04 |
| 12 | G8 | 201 | CYC | OB-C4B-C3B | -4.67 | 122.97 | 128.04 |
| 12 | F4 | 202 | CYC | C2B-C1B-NB | 4.67 | 113.82 | 106.99 |
| 12 | M8 | 302 | CYC | C1B-C2B-C3B | -4.67 | 103.00 | 107.87 |
| 12 | R1 | 201 | CYC | CHA-C1A-NA | -4.67 | 122.35 | 128.83 |
| 12 | R3 | 201 | CYC | CHA-C1A-NA | -4.67 | 122.35 | 128.83 |
| 12 | L9 | 202 | CYC | C1B-C2B-C3B | -4.67 | 103.00 | 107.87 |
| 12 | AA | 201 | CYC | OB-C4B-C3B | -4.67 | 122.98 | 128.04 |
| 12 | A9 | 201 | CYC | OB-C4B-C3B | -4.67 | 122.98 | 128.04 |
| 12 | F3 | 201 | CYC | C2B-C1B-NB | 4.67 | 113.82 | 106.99 |
| 12 | F1 | 201 | CYC | C2B-C1B-NB | 4.67 | 113.82 | 106.99 |
| 12 | G2 | 201 | CYC | OB-C4B-C3B | -4.67 | 122.98 | 128.04 |
| 12 | V3 | 201 | CYC | C1B-C2B-C3B | -4.66 | 103.00 | 107.87 |
| 12 | V1 | 201 | CYC | C1B-C2B-C3B | -4.66 | 103.00 | 107.87 |
| 12 | N4 | 201 | CYC | OB-C4B-C3B | -4.66 | 122.98 | 128.04 |
| 12 | A8 | 201 | CYC | OB-C4B-C3B | -4.66 | 122.98 | 128.04 |
| 12 | a9 | 901 | CYC | C2B-C1B-NB | 4.66 | 113.81 | 106.99 |
| 12 | J3 | 202 | CYC | CHA-C1A-NA | -4.66 | 122.36 | 128.83 |
| 12 | aA | 901 | CYC | CHA-C1A-NA | -4.66 | 122.36 | 128.83 |
| 12 | F3 | 201 | CYC | CHA-C1A-NA | -4.66 | 122.36 | 128.83 |
| 12 | Q7 | 201 | CYC | CAB-C3B-C4B | 4.66 | 128.74 | 121.38 |
| 12 | JA | 202 | CYC | CHA-C1A-NA | -4.66 | 122.36 | 128.83 |
| 12 | J9 | 202 | CYC | CHA-C1A-NA | -4.66 | 122.36 | 128.83 |
| 12 | Z1 | 202 | CYC | C2B-C1B-NB | 4.66 | 113.81 | 106.99 |
| 12 | G5 | 201 | CYC | C1B-NB-C4B | -4.66 | 104.74 | 110.67 |
| 12 | T3 | 301 | CYC | C1B-C2B-C3B | -4.66 | 103.01 | 107.87 |
| 12 | T1 | 301 | CYC | C1B-C2B-C3B | -4.66 | 103.01 | 107.87 |
| 12 | QA | 201 | CYC | OB-C4B-C3B | -4.66 | 122.99 | 128.04 |
| 12 | RA | 202 | CYC | C1B-NB-C4B | -4.66 | 104.74 | 110.67 |
| 12 | R9 | 202 | CYC | C1B-NB-C4B | -4.66 | 104.74 | 110.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | M8 | 301 | CYC | OC-C1C-C2C | -4.66 | 122.47 | 126.17 |
| 12 | N8 | 201 | CYC | OB-C4B-C3B | -4.66 | 122.99 | 128.04 |
| 12 | H6 | 201 | CYC | CHA-C1A-NA | -4.65 | 122.37 | 128.83 |
| 12 | R3 | 201 | CYC | C1B-C2B-C3B | -4.65 | 103.01 | 107.87 |
| 12 | H9 | 202 | CYC | C1B-C2B-C3B | -4.65 | 103.01 | 107.87 |
| 12 | W7 | 201 | CYC | C1B-NB-C4B | -4.65 | 104.74 | 110.67 |
| 12 | a9 | 901 | CYC | C1B-C2B-C3B | -4.65 | 103.02 | 107.87 |
| 12 | Y7 | 201 | CYC | OC-C1C-C2C | -4.65 | 122.47 | 126.17 |
| 12 | I3 | 201 | CYC | OB-C4B-C3B | -4.65 | 122.99 | 128.04 |
| 12 | H1 | 201 | CYC | C2B-C1B-NB | 4.65 | 113.80 | 106.99 |
| 12 | D3 | 202 | CYC | CHA-C1A-NA | -4.65 | 122.38 | 128.83 |
| 12 | D1 | 202 | CYC | CHA-C1A-NA | -4.65 | 122.38 | 128.83 |
| 12 | K7 | 201 | CYC | C1B-NB-C4B | -4.65 | 104.75 | 110.67 |
| 12 | E5 | 201 | CYC | C1B-NB-C4B | -4.65 | 104.75 | 110.67 |
| 12 | O7 | 201 | CYC | OC-C1C-C2C | -4.65 | 122.48 | 126.17 |
| 12 | Q9 | 201 | CYC | OB-C4B-C3B | -4.65 | 123.00 | 128.04 |
| 12 | B1 | 202 | CYC | C1B-C2B-C3B | -4.65 | 103.02 | 107.87 |
| 12 | I5 | 201 | CYC | OC-C1C-C2C | -4.65 | 122.48 | 126.17 |
| 12 | RA | 201 | CYC | CHA-C1A-NA | -4.65 | 122.38 | 128.83 |
| 12 | R9 | 201 | CYC | CHA-C1A-NA | -4.65 | 122.38 | 128.83 |
| 12 | HA | 202 | CYC | C1B-C2B-C3B | -4.65 | 103.02 | 107.87 |
| 12 | XA | 201 | CYC | C2B-C1B-NB | 4.65 | 113.79 | 106.99 |
| 12 | H3 | 202 | CYC | C2B-C1B-NB | 4.65 | 113.79 | 106.99 |
| 12 | Z4 | 301 | CYC | C2B-C1B-NB | 4.64 | 113.79 | 106.99 |
| 12 | F9 | 302 | CYC | C2B-C1B-NB | 4.64 | 113.79 | 106.99 |
| 12 | JA | 202 | CYC | C1B-C2B-C3B | -4.64 | 103.02 | 107.87 |
| 12 | J9 | 202 | CYC | C1B-C2B-C3B | -4.64 | 103.02 | 107.87 |
| 12 | F6 | 201 | CYC | C1B-C2B-C3B | -4.64 | 103.03 | 107.87 |
| 12 | Z3 | 201 | CYC | C2B-C1B-NB | 4.64 | 113.79 | 106.99 |
| 12 | H2 | 201 | CYC | CHA-C1A-NA | -4.64 | 122.39 | 128.83 |
| 12 | J6 | 202 | CYC | C2B-C1B-NB | 4.64 | 113.78 | 106.99 |
| 12 | J2 | 202 | CYC | CHA-C1A-NA | -4.64 | 122.39 | 128.83 |
| 12 | KA | 201 | CYC | OB-C4B-C3B | -4.64 | 123.00 | 128.04 |
| 12 | K9 | 201 | CYC | OB-C4B-C3B | -4.64 | 123.00 | 128.04 |
| 12 | Z8 | 301 | CYC | OC-C1C-C2C | -4.64 | 122.48 | 126.17 |
| 12 | O1 | 201 | CYC | OB-C4B-C3B | -4.64 | 123.00 | 128.04 |
| 12 | O3 | 201 | CYC | OB-C4B-C3B | -4.64 | 123.00 | 128.04 |
| 12 | FA | 301 | CYC | OC-C1C-C2C | -4.64 | 122.48 | 126.17 |
| 12 | O5 | 201 | CYC | OC-C1C-C2C | -4.64 | 122.48 | 126.17 |
| 12 | F9 | 301 | CYC | OC-C1C-C2C | -4.64 | 122.48 | 126.17 |
| 12 | F1 | 201 | CYC | CHA-C1A-NA | -4.64 | 122.39 | 128.83 |
| 12 | C4 | 201 | CYC | OB-C4B-C3B | -4.64 | 123.01 | 128.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | C8 | 201 | CYC | OB-C4B-C3B | -4.64 | 123.01 | 128.04 |
| 12 | B3 | 202 | CYC | CHA-C1A-NA | -4.64 | 122.39 | 128.83 |
| 12 | HA | 202 | CYC | CHA-C1A-NA | -4.64 | 122.39 | 128.83 |
| 12 | T3 | 301 | CYC | CHA-C1A-NA | -4.64 | 122.39 | 128.83 |
| 12 | T1 | 301 | CYC | CHA-C1A-NA | -4.64 | 122.39 | 128.83 |
| 12 | C5 | 201 | CYC | CAB-C3B-C4B | 4.64 | 128.70 | 121.38 |
| 12 | FA | 301 | CYC | C1B-C2B-C3B | -4.64 | 103.03 | 107.87 |
| 12 | F9 | 301 | CYC | C1B-C2B-C3B | -4.64 | 103.03 | 107.87 |
| 12 | UA | 201 | CYC | OB-C4B-C3B | -4.64 | 123.01 | 128.04 |
| 12 | U9 | 201 | CYC | OB-C4B-C3B | -4.64 | 123.01 | 128.04 |
| 12 | K3 | 201 | CYC | OB-C4B-C3B | -4.64 | 123.01 | 128.04 |
| 12 | K1 | 201 | CYC | OB-C4B-C3B | -4.64 | 123.01 | 128.04 |
| 12 | JA | 202 | CYC | OC-C1C-C2C | -4.63 | 122.49 | 126.17 |
| 12 | J9 | 202 | CYC | OC-C1C-C2C | -4.63 | 122.49 | 126.17 |
| 12 | Y5 | 201 | CYC | C1B-NB-C4B | -4.63 | 104.77 | 110.67 |
| 12 | H9 | 202 | CYC | CHA-C1A-NA | -4.63 | 122.40 | 128.83 |
| 12 | F2 | 201 | CYC | CHA-C1A-NA | -4.63 | 122.40 | 128.83 |
| 12 | N6 | 101 | CYC | C1B-C2B-C3B | -4.63 | 103.04 | 107.87 |
| 12 | R4 | 201 | CYC | OB-C4B-C3B | -4.63 | 123.01 | 128.04 |
| 12 | R8 | 201 | CYC | OB-C4B-C3B | -4.63 | 123.01 | 128.04 |
| 12 | E7 | 201 | CYC | C1B-NB-C4B | -4.63 | 104.77 | 110.67 |
| 12 | I1 | 201 | CYC | OB-C4B-C3B | -4.63 | 123.01 | 128.04 |
| 12 | L6 | 201 | CYC | C2B-C1B-NB | 4.63 | 113.77 | 106.99 |
| 12 | RA | 201 | CYC | OC-C1C-C2C | -4.63 | 122.49 | 126.17 |
| 12 | R9 | 201 | CYC | OC-C1C-C2C | -4.63 | 122.49 | 126.17 |
| 12 | L4 | 202 | CYC | C2B-C1B-NB | 4.63 | 113.77 | 106.99 |
| 12 | X9 | 201 | CYC | C2B-C1B-NB | 4.63 | 113.77 | 106.99 |
| 12 | Q5 | 201 | CYC | OC-C1C-C2C | -4.63 | 122.49 | 126.17 |
| 12 | P9 | 201 | CYC | OC-C1C-C2C | -4.63 | 122.49 | 126.17 |
| 12 | TA | 301 | CYC | C1B-C2B-C3B | -4.63 | 103.04 | 107.87 |
| 12 | T9 | 301 | CYC | C1B-C2B-C3B | -4.63 | 103.04 | 107.87 |
| 12 | i7 | 201 | CYC | CAB-C3B-C4B | 4.63 | 128.69 | 121.38 |
| 12 | A1 | 201 | CYC | OB-C4B-C3B | -4.63 | 123.02 | 128.04 |
| 12 | A3 | 201 | CYC | OB-C4B-C3B | -4.63 | 123.02 | 128.04 |
| 12 | R1 | 201 | CYC | C1B-C2B-C3B | -4.63 | 103.04 | 107.87 |
| 12 | LA | 202 | CYC | C2B-C1B-NB | 4.63 | 113.76 | 106.99 |
| 12 | F6 | 202 | CYC | C2B-C1B-NB | 4.63 | 113.76 | 106.99 |
| 12 | U5 | 201 | CYC | C1B-NB-C4B | -4.62 | 104.78 | 110.67 |
| 12 | F2 | 201 | CYC | OC-C1C-C2C | -4.62 | 122.50 | 126.17 |
| 12 | T4 | 201 | CYC | OB-C4B-C3B | -4.62 | 123.02 | 128.04 |
| 12 | T8 | 201 | CYC | OB-C4B-C3B | -4.62 | 123.02 | 128.04 |
| 12 | Y5 | 201 | CYC | CAB-C3B-C4B | 4.62 | 128.68 | 121.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | K8 | 201 | CYC | OB-C4B-C3B | -4.62 | 123.02 | 128.04 |
| 12 | Q5 | 201 | CYC | CAB-C3B-C4B | 4.62 | 128.68 | 121.38 |
| 12 | X3 | 201 | CYC | CHA-C1A-NA | -4.62 | 122.42 | 128.83 |
| 12 | X1 | 201 | CYC | CHA-C1A-NA | -4.62 | 122.42 | 128.83 |
| 12 | c5 | 201 | CYC | C1B-NB-C4B | -4.62 | 104.78 | 110.67 |
| 12 | P1 | 201 | CYC | C2B-C1B-NB | 4.62 | 113.75 | 106.99 |
| 12 | P3 | 201 | CYC | C2B-C1B-NB | 4.62 | 113.75 | 106.99 |
| 12 | o7 | 201 | CYC | CAB-C3B-C4B | 4.62 | 128.68 | 121.38 |
| 12 | B3 | 202 | CYC | C1B-C2B-C3B | -4.62 | 103.05 | 107.87 |
| 12 | s7 | 201 | CYC | CAB-C3B-C4B | 4.62 | 128.68 | 121.38 |
| 12 | DA | 201 | CYC | C1B-C2B-C3B | -4.62 | 103.05 | 107.87 |
| 12 | Z1 | 202 | CYC | C1B-C2B-C3B | -4.62 | 103.05 | 107.87 |
| 12 | I4 | 201 | CYC | OB-C4B-C3B | -4.62 | 123.03 | 128.04 |
| 12 | I8 | 201 | CYC | OB-C4B-C3B | -4.62 | 123.03 | 128.04 |
| 12 | U4 | 201 | CYC | C2B-C1B-NB | 4.62 | 113.75 | 106.99 |
| 12 | U8 | 201 | CYC | C2B-C1B-NB | 4.62 | 113.75 | 106.99 |
| 12 | g7 | 201 | CYC | CAB-C3B-C4B | 4.62 | 128.67 | 121.38 |
| 12 | V8 | 201 | CYC | OB-C4B-C3B | -4.62 | 123.03 | 128.04 |
| 12 | O4 | 201 | CYC | C2B-C1B-NB | 4.62 | 113.75 | 106.99 |
| 12 | O8 | 201 | CYC | C2B-C1B-NB | 4.62 | 113.75 | 106.99 |
| 12 | K2 | 201 | CYC | OB-C4B-C3B | -4.62 | 123.03 | 128.04 |
| 12 | K6 | 201 | CYC | OB-C4B-C3B | -4.62 | 123.03 | 128.04 |
| 12 | W4 | 201 | CYC | CHA-C1A-NA | -4.62 | 122.42 | 128.83 |
| 12 | W8 | 201 | CYC | CHA-C1A-NA | -4.62 | 122.42 | 128.83 |
| 12 | I6 | 201 | CYC | OB-C4B-C3B | -4.62 | 123.03 | 128.04 |
| 12 | M7 | 201 | CYC | CAB-C3B-C4B | 4.62 | 128.67 | 121.38 |
| 12 | J4 | 201 | CYC | C1B-C2B-C3B | -4.62 | 103.06 | 107.87 |
| 12 | J8 | 201 | CYC | C1B-C2B-C3B | -4.62 | 103.06 | 107.87 |
| 12 | O5 | 201 | CYC | C1B-NB-C4B | -4.61 | 104.79 | 110.67 |
| 12 | L4 | 202 | CYC | C1B-C2B-C3B | -4.61 | 103.06 | 107.87 |
| 12 | G3 | 201 | CYC | OB-C4B-C3B | -4.61 | 123.03 | 128.04 |
| 12 | G1 | 201 | CYC | OB-C4B-C3B | -4.61 | 123.03 | 128.04 |
| 12 | A7 | 201 | CYC | C1B-NB-C4B | -4.61 | 104.80 | 110.67 |
| 12 | L9 | 202 | CYC | C2B-C1B-NB | 4.61 | 113.74 | 106.99 |
| 12 | F2 | 201 | CYC | C1B-C2B-C3B | -4.61 | 103.06 | 107.87 |
| 12 | I5 | 201 | CYC | CAB-C3B-C4B | 4.61 | 128.66 | 121.38 |
| 12 | X4 | 201 | CYC | OB-C4B-C3B | -4.61 | 123.04 | 128.04 |
| 12 | X8 | 201 | CYC | OB-C4B-C3B | -4.61 | 123.04 | 128.04 |
| 12 | U7 | 201 | CYC | CAB-C3B-C4B | 4.61 | 128.66 | 121.38 |
| 12 | T3 | 302 | CYC | C2B-C1B-NB | 4.61 | 113.73 | 106.99 |
| 12 | T1 | 302 | CYC | C2B-C1B-NB | 4.61 | 113.73 | 106.99 |
| 12 | U4 | 201 | CYC | C1B-C2B-C3B | -4.61 | 103.06 | 107.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | U8 | 201 | CYC | C1B-C2B-C3B | -4.61 | 103.06 | 107.87 |
| 12 | N2 | 101 | CYC | C2B-C1B-NB | 4.61 | 113.73 | 106.99 |
| 12 | A6 | 201 | CYC | OB-C4B-C3B | -4.60 | 123.04 | 128.04 |
| 12 | BA | 201 | CYC | C2B-C1B-NB | 4.60 | 113.73 | 106.99 |
| 12 | B9 | 201 | CYC | C2B-C1B-NB | 4.60 | 113.73 | 106.99 |
| 12 | TA | 301 | CYC | OC-C1C-C2C | -4.60 | 122.51 | 126.17 |
| 12 | T9 | 301 | CYC | OC-C1C-C2C | -4.60 | 122.51 | 126.17 |
| 12 | A5 | 201 | CYC | C1B-NB-C4B | -4.60 | 104.81 | 110.67 |
| 12 | u7 | 201 | CYC | CAB-C3B-C4B | 4.60 | 128.65 | 121.38 |
| 12 | CA | 201 | CYC | OB-C4B-C3B | -4.60 | 123.05 | 128.04 |
| 12 | C9 | 201 | CYC | OB-C4B-C3B | -4.60 | 123.05 | 128.04 |
| 12 | V3 | 201 | CYC | C2B-C1B-NB | 4.60 | 113.73 | 106.99 |
| 12 | V1 | 201 | CYC | C2B-C1B-NB | 4.60 | 113.73 | 106.99 |
| 12 | RA | 201 | CYC | C1B-C2B-C3B | -4.60 | 103.07 | 107.87 |
| 12 | R9 | 201 | CYC | C1B-C2B-C3B | -4.60 | 103.07 | 107.87 |
| 12 | F2 | 202 | CYC | C2B-C1B-NB | 4.60 | 113.72 | 106.99 |
| 12 | U7 | 201 | CYC | C1B-NB-C4B | -4.60 | 104.81 | 110.67 |
| 12 | W5 | 201 | CYC | CAB-C3B-C4B | 4.60 | 128.64 | 121.38 |
| 12 | G7 | 201 | CYC | CAB-C3B-C4B | 4.60 | 128.64 | 121.38 |
| 12 | S1 | 201 | CYC | OB-C4B-C3B | -4.60 | 123.05 | 128.04 |
| 12 | S3 | 201 | CYC | OB-C4B-C3B | -4.60 | 123.05 | 128.04 |
| 12 | H9 | 202 | CYC | C2B-C1B-NB | 4.60 | 113.72 | 106.99 |
| 12 | J3 | 202 | CYC | C1B-C2B-C3B | -4.60 | 103.07 | 107.87 |
| 12 | Z3 | 201 | CYC | C1B-C2B-C3B | -4.60 | 103.07 | 107.87 |
| 12 | H4 | 201 | CYC | C1B-C2B-C3B | -4.60 | 103.07 | 107.87 |
| 12 | aA | 901 | CYC | C1B-C2B-C3B | -4.60 | 103.07 | 107.87 |
| 12 | Q7 | 201 | CYC | C1B-NB-C4B | -4.60 | 104.82 | 110.67 |
| 12 | e5 | 201 | CYC | CAB-C3B-C4B | 4.60 | 128.64 | 121.38 |
| 12 | O7 | 201 | CYC | C1B-NB-C4B | -4.60 | 104.82 | 110.67 |
| 12 | DA | 202 | CYC | C1B-NB-C4B | -4.59 | 104.82 | 110.67 |
| 12 | J4 | 201 | CYC | C2B-C1B-NB | 4.59 | 113.71 | 106.99 |
| 12 | J8 | 201 | CYC | C2B-C1B-NB | 4.59 | 113.71 | 106.99 |
| 12 | Y3 | 201 | CYC | OB-C4B-C3B | -4.59 | 123.06 | 128.04 |
| 12 | Y1 | 201 | CYC | OB-C4B-C3B | -4.59 | 123.06 | 128.04 |
| 12 | a5 | 201 | CYC | CAB-C3B-C4B | 4.59 | 128.63 | 121.38 |
| 12 | N6 | 101 | CYC | C2B-C1B-NB | 4.59 | 113.71 | 106.99 |
| 12 | J6 | 202 | CYC | CHA-C1A-NA | -4.59 | 122.46 | 128.83 |
| 12 | D9 | 201 | CYC | C1B-C2B-C3B | -4.59 | 103.08 | 107.87 |
| 12 | L2 | 201 | CYC | C2B-C1B-NB | 4.59 | 113.71 | 106.99 |
| 12 | L3 | 202 | CYC | C2B-C1B-NB | 4.59 | 113.71 | 106.99 |
| 12 | W4 | 201 | CYC | C2B-C1B-NB | 4.59 | 113.71 | 106.99 |
| 12 | W8 | 201 | CYC | C2B-C1B-NB | 4.59 | 113.71 | 106.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | W5 | 201 | CYC | C1B-NB-C4B | -4.59 | 104.82 | 110.67 |
| 12 | R3 | 201 | CYC | C2B-C1B-NB | 4.59 | 113.71 | 106.99 |
| 12 | a7 | 201 | CYC | C1B-NB-C4B | -4.59 | 104.83 | 110.67 |
| 12 | H4 | 201 | CYC | OC-C1C-C2C | -4.59 | 122.52 | 126.17 |
| 12 | e7 | 201 | CYC | OC-C1C-C2C | -4.59 | 122.52 | 126.17 |
| 12 | H8 | 201 | CYC | OC-C1C-C2C | -4.59 | 122.52 | 126.17 |
| 12 | H8 | 201 | CYC | C1B-C2B-C3B | -4.59 | 103.08 | 107.87 |
| 12 | Z8 | 301 | CYC | C1B-C2B-C3B | -4.59 | 103.08 | 107.87 |
| 12 | D3 | 202 | CYC | C1B-C2B-C3B | -4.59 | 103.08 | 107.87 |
| 12 | M4 | 301 | CYC | C1B-C2B-C3B | -4.59 | 103.08 | 107.87 |
| 12 | D1 | 202 | CYC | C1B-C2B-C3B | -4.59 | 103.08 | 107.87 |
| 12 | O5 | 201 | CYC | CAB-C3B-C4B | 4.59 | 128.62 | 121.38 |
| 12 | U5 | 201 | CYC | CAB-C3B-C4B | 4.59 | 128.62 | 121.38 |
| 12 | V4 | 201 | CYC | OB-C4B-C3B | -4.59 | 123.06 | 128.04 |
| 12 | HA | 202 | CYC | C2B-C1B-NB | 4.58 | 113.70 | 106.99 |
| 12 | Z8 | 301 | CYC | C2B-C1B-NB | 4.58 | 113.70 | 106.99 |
| 12 | aA | 902 | CYC | C2B-C1B-NB | 4.58 | 113.70 | 106.99 |
| 12 | G7 | 201 | CYC | C1B-NB-C4B | -4.58 | 104.83 | 110.67 |
| 12 | B4 | 202 | CYC | OC-C1C-C2C | -4.58 | 122.53 | 126.17 |
| 12 | H6 | 201 | CYC | C2B-C1B-NB | 4.58 | 113.70 | 106.99 |
| 12 | X1 | 201 | CYC | C2B-C1B-NB | 4.58 | 113.70 | 106.99 |
| 12 | PA | 201 | CYC | OC-C1C-C2C | -4.58 | 122.53 | 126.17 |
| 12 | S4 | 202 | CYC | C2B-C1B-NB | 4.58 | 113.70 | 106.99 |
| 12 | S5 | 201 | CYC | CAB-C3B-C4B | 4.58 | 128.62 | 121.38 |
| 12 | J3 | 202 | CYC | C2B-C1B-NB | 4.58 | 113.69 | 106.99 |
| 12 | B1 | 202 | CYC | C2B-C1B-NB | 4.58 | 113.69 | 106.99 |
| 12 | aA | 901 | CYC | C2B-C1B-NB | 4.58 | 113.69 | 106.99 |
| 12 | B3 | 202 | CYC | C2B-C1B-NB | 4.58 | 113.69 | 106.99 |
| 12 | D2 | 202 | CYC | C2B-C1B-NB | 4.58 | 113.69 | 106.99 |
| 12 | HA | 202 | CYC | OC-C1C-C2C | -4.58 | 122.53 | 126.17 |
| 12 | H9 | 202 | CYC | OC-C1C-C2C | -4.58 | 122.53 | 126.17 |
| 12 | D9 | 202 | CYC | C1B-NB-C4B | -4.58 | 104.84 | 110.67 |
| 12 | PA | 201 | CYC | C1B-NB-C4B | -4.58 | 104.84 | 110.67 |
| 12 | g7 | 201 | CYC | C1B-NB-C4B | -4.58 | 104.84 | 110.67 |
| 12 | P9 | 201 | CYC | C1B-NB-C4B | -4.58 | 104.84 | 110.67 |
| 12 | K4 | 201 | CYC | OB-C4B-C3B | -4.58 | 123.07 | 128.04 |
| 12 | a7 | 201 | CYC | CAB-C3B-C4B | 4.58 | 128.61 | 121.38 |
| 12 | R1 | 201 | CYC | C2B-C1B-NB | 4.58 | 113.69 | 106.99 |
| 12 | G7 | 201 | CYC | OC-C1C-C2C | -4.57 | 122.54 | 126.17 |
| 12 | M8 | 302 | CYC | OC-C1C-C2C | -4.57 | 122.54 | 126.17 |
| 12 | BA | 201 | CYC | C1B-C2B-C3B | -4.57 | 103.10 | 107.87 |
| 12 | B9 | 201 | CYC | C1B-C2B-C3B | -4.57 | 103.10 | 107.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | D4 | 202 | CYC | C2B-C1B-NB | 4.57 | 113.68 | 106.99 |
| 12 | c5 | 201 | CYC | CAB-C3B-C4B | 4.57 | 128.60 | 121.38 |
| 12 | T3 | 301 | CYC | C2B-C1B-NB | 4.57 | 113.68 | 106.99 |
| 12 | T1 | 301 | CYC | C2B-C1B-NB | 4.57 | 113.68 | 106.99 |
| 12 | D3 | 202 | CYC | OC-C1C-C2C | -4.57 | 122.54 | 126.17 |
| 12 | D1 | 202 | CYC | OC-C1C-C2C | -4.57 | 122.54 | 126.17 |
| 12 | A7 | 201 | CYC | CAB-C3B-C4B | 4.57 | 128.60 | 121.38 |
| 12 | I7 | 201 | CYC | CAB-C3B-C4B | 4.57 | 128.59 | 121.38 |
| 12 | IA | 201 | CYC | OB-C4B-C3B | -4.57 | 123.08 | 128.04 |
| 12 | I9 | 201 | CYC | OB-C4B-C3B | -4.57 | 123.08 | 128.04 |
| 12 | TA | 301 | CYC | C2B-C1B-NB | 4.57 | 113.68 | 106.99 |
| 12 | T9 | 301 | CYC | C2B-C1B-NB | 4.57 | 113.68 | 106.99 |
| 12 | ZA | 202 | CYC | OC-C1C-C2C | -4.57 | 122.54 | 126.17 |
| 12 | B8 | 202 | CYC | OC-C1C-C2C | -4.57 | 122.54 | 126.17 |
| 12 | Z9 | 202 | CYC | OC-C1C-C2C | -4.57 | 122.54 | 126.17 |
| 12 | B4 | 202 | CYC | C2B-C1B-NB | 4.57 | 113.67 | 106.99 |
| 12 | H2 | 201 | CYC | C1B-C2B-C3B | -4.57 | 103.11 | 107.87 |
| 12 | D6 | 202 | CYC | C2B-C1B-NB | 4.57 | 113.67 | 106.99 |
| 12 | L4 | 202 | CYC | OC-C1C-C2C | -4.57 | 122.54 | 126.17 |
| 12 | F6 | 201 | CYC | OC-C1C-C2C | -4.57 | 122.54 | 126.17 |
| 12 | H6 | 201 | CYC | C1B-C2B-C3B | -4.57 | 103.11 | 107.87 |
| 12 | I7 | 201 | CYC | C1B-NB-C4B | -4.56 | 104.86 | 110.67 |
| 12 | W7 | 201 | CYC | CAB-C3B-C4B | 4.56 | 128.59 | 121.38 |
| 12 | X3 | 201 | CYC | C2B-C1B-NB | 4.56 | 113.67 | 106.99 |
| 12 | C7 | 201 | CYC | CAB-C3B-C4B | 4.56 | 128.59 | 121.38 |
| 12 | e7 | 201 | CYC | CAB-C3B-C4B | 4.56 | 128.59 | 121.38 |
| 12 | E6 | 201 | CYC | OB-C4B-C3B | -4.56 | 123.09 | 128.04 |
| 12 | E2 | 201 | CYC | OB-C4B-C3B | -4.56 | 123.09 | 128.04 |
| 12 | O9 | 201 | CYC | OB-C4B-C3B | -4.56 | 123.09 | 128.04 |
| 12 | VA | 201 | CYC | C2B-C1B-NB | 4.56 | 113.66 | 106.99 |
| 12 | V9 | 201 | CYC | C2B-C1B-NB | 4.56 | 113.66 | 106.99 |
| 12 | E7 | 201 | CYC | CAB-C3B-C4B | 4.56 | 128.58 | 121.38 |
| 12 | H2 | 201 | CYC | C2B-C1B-NB | 4.56 | 113.66 | 106.99 |
| 12 | M4 | 301 | CYC | OC-C1C-C2C | -4.56 | 122.55 | 126.17 |
| 12 | M4 | 301 | CYC | C2B-C1B-NB | 4.56 | 113.66 | 106.99 |
| 12 | k7 | 201 | CYC | CAB-C3B-C4B | 4.56 | 128.57 | 121.38 |
| 12 | M8 | 301 | CYC | C2B-C1B-NB | 4.56 | 113.66 | 106.99 |
| 12 | Y7 | 201 | CYC | CAB-C3B-C4B | 4.55 | 128.57 | 121.38 |
| 12 | L6 | 201 | CYC | C1B-C2B-C3B | -4.55 | 103.12 | 107.87 |
| 12 | M8 | 301 | CYC | C1B-C2B-C3B | -4.55 | 103.12 | 107.87 |
| 12 | B8 | 202 | CYC | C2B-C1B-NB | 4.55 | 113.66 | 106.99 |
| 12 | u7 | 201 | CYC | C1B-NB-C4B | -4.55 | 104.87 | 110.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | C7 | 201 | CYC | C1B-NB-C4B | -4.55 | 104.87 | 110.67 |
| 12 | M5 | 201 | CYC | CAB-C3B-C4B | 4.55 | 128.57 | 121.38 |
| 12 | A7 | 201 | CYC | OC-C1C-C2C | -4.55 | 122.55 | 126.17 |
| 12 | O7 | 201 | CYC | CAB-C3B-C4B | 4.55 | 128.57 | 121.38 |
| 12 | K7 | 201 | CYC | CAB-C3B-C4B | 4.55 | 128.56 | 121.38 |
| 12 | H4 | 201 | CYC | C2B-C1B-NB | 4.55 | 113.64 | 106.99 |
| 12 | D8 | 202 | CYC | C2B-C1B-NB | 4.55 | 113.64 | 106.99 |
| 12 | H8 | 201 | CYC | C2B-C1B-NB | 4.55 | 113.64 | 106.99 |
| 12 | e5 | 201 | CYC | C1B-NB-C4B | -4.54 | 104.89 | 110.67 |
| 12 | SA | 201 | CYC | OB-C4B-C3B | -4.54 | 123.11 | 128.04 |
| 12 | S9 | 201 | CYC | OB-C4B-C3B | -4.54 | 123.11 | 128.04 |
| 12 | P4 | 201 | CYC | OB-C4B-C3B | -4.54 | 123.11 | 128.04 |
| 12 | P8 | 201 | CYC | OB-C4B-C3B | -4.54 | 123.11 | 128.04 |
| 12 | H6 | 201 | CYC | OC-C1C-C2C | -4.54 | 122.56 | 126.17 |
| 12 | M8 | 302 | CYC | C2B-C1B-NB | 4.54 | 113.63 | 106.99 |
| 12 | B3 | 202 | CYC | OC-C1C-C2C | -4.54 | 122.56 | 126.17 |
| 12 | c7 | 201 | CYC | CAB-C3B-C4B | 4.54 | 128.55 | 121.38 |
| 12 | DA | 202 | CYC | C2B-C1B-NB | 4.54 | 113.63 | 106.99 |
| 12 | a5 | 201 | CYC | C1B-NB-C4B | -4.54 | 104.89 | 110.67 |
| 12 | o7 | 201 | CYC | C1B-NB-C4B | -4.54 | 104.89 | 110.67 |
| 12 | BA | 201 | CYC | OC-C1C-C2C | -4.54 | 122.57 | 126.17 |
| 12 | B9 | 201 | CYC | OC-C1C-C2C | -4.54 | 122.57 | 126.17 |
| 12 | G5 | 201 | CYC | CAB-C3B-C4B | 4.54 | 128.54 | 121.38 |
| 12 | Q5 | 201 | CYC | C1B-NB-C4B | -4.54 | 104.89 | 110.67 |
| 12 | FA | 301 | CYC | C2B-C1B-NB | 4.53 | 113.63 | 106.99 |
| 12 | F9 | 301 | CYC | C2B-C1B-NB | 4.53 | 113.63 | 106.99 |
| 12 | T3 | 301 | CYC | OC-C1C-C2C | -4.53 | 122.57 | 126.17 |
| 12 | T1 | 301 | CYC | OC-C1C-C2C | -4.53 | 122.57 | 126.17 |
| 12 | J2 | 202 | CYC | C1B-NB-C4B | -4.53 | 104.90 | 110.67 |
| 12 | C5 | 201 | CYC | C1B-NB-C4B | -4.53 | 104.90 | 110.67 |
| 12 | q7 | 201 | CYC | CAB-C3B-C4B | 4.53 | 128.53 | 121.38 |
| 12 | A5 | 201 | CYC | CAB-C3B-C4B | 4.53 | 128.53 | 121.38 |
| 12 | OA | 201 | CYC | OB-C4B-C3B | -4.53 | 123.13 | 128.04 |
| 12 | a9 | 901 | CYC | OC-C1C-C2C | -4.53 | 122.57 | 126.17 |
| 12 | C3 | 201 | CYC | OB-C4B-C3B | -4.53 | 123.13 | 128.04 |
| 12 | C1 | 201 | CYC | OB-C4B-C3B | -4.53 | 123.13 | 128.04 |
| 12 | S7 | 201 | CYC | CAB-C3B-C4B | 4.53 | 128.53 | 121.38 |
| 12 | K5 | 201 | CYC | CAB-C3B-C4B | 4.52 | 128.53 | 121.38 |
| 12 | X9 | 201 | CYC | OC-C1C-C2C | -4.52 | 122.58 | 126.17 |
| 12 | J4 | 201 | CYC | OC-C1C-C2C | -4.52 | 122.58 | 126.17 |
| 12 | RA | 201 | CYC | C2B-C1B-NB | 4.52 | 113.61 | 106.99 |
| 12 | R9 | 201 | CYC | C2B-C1B-NB | 4.52 | 113.61 | 106.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | D1 | 202 | CYC | C2B-C1B-NB | 4.52 | 113.61 | 106.99 |
| 12 | D9 | 202 | CYC | C2B-C1B-NB | 4.52 | 113.60 | 106.99 |
| 12 | ZA | 202 | CYC | C1B-NB-C4B | -4.51 | 104.92 | 110.67 |
| 12 | Z9 | 202 | CYC | C1B-NB-C4B | -4.51 | 104.92 | 110.67 |
| 12 | JA | 202 | CYC | C2B-C1B-NB | 4.51 | 113.60 | 106.99 |
| 12 | J9 | 202 | CYC | C2B-C1B-NB | 4.51 | 113.60 | 106.99 |
| 12 | Q1 | 201 | CYC | OB-C4B-C3B | -4.51 | 123.14 | 128.04 |
| 12 | Q3 | 201 | CYC | OB-C4B-C3B | -4.51 | 123.14 | 128.04 |
| 12 | I5 | 201 | CYC | C1B-NB-C4B | -4.51 | 104.92 | 110.67 |
| 12 | XA | 201 | CYC | OC-C1C-C2C | -4.51 | 122.58 | 126.17 |
| 12 | s7 | 201 | CYC | OC-C1C-C2C | -4.51 | 122.58 | 126.17 |
| 12 | R1 | 201 | CYC | OC-C1C-C2C | -4.51 | 122.59 | 126.17 |
| 12 | F3 | 201 | CYC | OC-C1C-C2C | -4.51 | 122.59 | 126.17 |
| 12 | R3 | 201 | CYC | OC-C1C-C2C | -4.51 | 122.59 | 126.17 |
| 12 | S4 | 202 | CYC | OC-C1C-C2C | -4.51 | 122.59 | 126.17 |
| 12 | E5 | 201 | CYC | CAB-C3B-C4B | 4.51 | 128.50 | 121.38 |
| 12 | M7 | 201 | CYC | C1B-NB-C4B | -4.51 | 104.93 | 110.67 |
| 12 | D3 | 202 | CYC | C2B-C1B-NB | 4.50 | 113.58 | 106.99 |
| 12 | G5 | 201 | CYC | CHD-C4C-NC | 4.50 | 130.56 | 125.20 |
| 12 | LA | 202 | CYC | C1B-NB-C4B | -4.50 | 104.94 | 110.67 |
| 12 | E3 | 201 | CYC | OB-C4B-C3B | -4.50 | 123.16 | 128.04 |
| 12 | E1 | 201 | CYC | OB-C4B-C3B | -4.50 | 123.16 | 128.04 |
| 12 | F6 | 201 | CYC | C2B-C1B-NB | 4.50 | 113.58 | 106.99 |
| 12 | A5 | 201 | CYC | CHD-C4C-NC | 4.50 | 130.55 | 125.20 |
| 12 | m7 | 201 | CYC | C1B-NB-C4B | -4.50 | 104.95 | 110.67 |
| 12 | W1 | 201 | CYC | OB-C4B-C3B | -4.49 | 123.16 | 128.04 |
| 12 | L2 | 201 | CYC | C1B-C2B-C3B | -4.49 | 103.18 | 107.87 |
| 12 | N2 | 101 | CYC | OC-C1C-C2C | -4.49 | 122.60 | 126.17 |
| 12 | J8 | 201 | CYC | OC-C1C-C2C | -4.49 | 122.60 | 126.17 |
| 12 | J3 | 202 | CYC | OC-C1C-C2C | -4.49 | 122.60 | 126.17 |
| 12 | aA | 901 | CYC | OC-C1C-C2C | -4.49 | 122.60 | 126.17 |
| 12 | F2 | 201 | CYC | C2B-C1B-NB | 4.49 | 113.55 | 106.99 |
| 12 | N2 | 101 | CYC | C1B-NB-C4B | -4.48 | 104.96 | 110.67 |
| 12 | N6 | 101 | CYC | C1B-NB-C4B | -4.48 | 104.96 | 110.67 |
| 12 | B1 | 202 | CYC | OC-C1C-C2C | -4.48 | 122.61 | 126.17 |
| 12 | DA | 201 | CYC | C2B-C1B-NB | 4.48 | 113.55 | 106.99 |
| 12 | Z4 | 301 | CYC | OC-C1C-C2C | -4.48 | 122.61 | 126.17 |
| 12 | m7 | 201 | CYC | OC-C1C-C2C | -4.48 | 122.61 | 126.17 |
| 12 | F1 | 201 | CYC | OC-C1C-C2C | -4.48 | 122.61 | 126.17 |
| 12 | L6 | 201 | CYC | C1B-NB-C4B | -4.48 | 104.97 | 110.67 |
| 12 | H1 | 201 | CYC | C1B-NB-C4B | -4.48 | 104.97 | 110.67 |
| 12 | L9 | 202 | CYC | C1B-NB-C4B | -4.48 | 104.97 | 110.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | Z3 | 201 | CYC | C1B-NB-C4B | -4.48 | 104.97 | 110.67 |
| 12 | Z1 | 202 | CYC | C1B-NB-C4B | -4.48 | 104.97 | 110.67 |
| 12 | J6 | 202 | CYC | C1B-NB-C4B | -4.47 | 104.98 | 110.67 |
| 12 | W3 | 201 | CYC | OB-C4B-C3B | -4.47 | 123.19 | 128.04 |
| 12 | Z3 | 201 | CYC | OC-C1C-C2C | -4.46 | 122.62 | 126.17 |
| 12 | Z1 | 202 | CYC | OC-C1C-C2C | -4.46 | 122.62 | 126.17 |
| 12 | L2 | 201 | CYC | C1B-NB-C4B | -4.46 | 104.98 | 110.67 |
| 12 | e7 | 201 | CYC | C1B-NB-C4B | -4.46 | 104.98 | 110.67 |
| 12 | q7 | 201 | CYC | C1B-NB-C4B | -4.46 | 104.98 | 110.67 |
| 12 | aA | 902 | CYC | OC-C1C-C2C | -4.46 | 122.62 | 126.17 |
| 12 | D9 | 201 | CYC | C2B-C1B-NB | 4.46 | 113.52 | 106.99 |
| 12 | P1 | 201 | CYC | OC-C1C-C2C | -4.46 | 122.63 | 126.17 |
| 12 | P3 | 201 | CYC | OC-C1C-C2C | -4.46 | 122.63 | 126.17 |
| 12 | Y5 | 201 | CYC | CHD-C4C-NC | 4.46 | 130.51 | 125.20 |
| 12 | H2 | 201 | CYC | OC-C1C-C2C | -4.46 | 122.63 | 126.17 |
| 12 | U4 | 201 | CYC | OC-C1C-C2C | -4.46 | 122.63 | 126.17 |
| 12 | U8 | 201 | CYC | OC-C1C-C2C | -4.46 | 122.63 | 126.17 |
| 12 | U4 | 201 | CYC | C1B-NB-C4B | -4.46 | 104.99 | 110.67 |
| 12 | U8 | 201 | CYC | C1B-NB-C4B | -4.46 | 104.99 | 110.67 |
| 12 | BA | 201 | CYC | C1B-NB-C4B | -4.46 | 104.99 | 110.67 |
| 12 | B9 | 201 | CYC | C1B-NB-C4B | -4.46 | 104.99 | 110.67 |
| 12 | D6 | 201 | CYC | C2B-C1B-NB | 4.46 | 113.51 | 106.99 |
| 12 | k5 | 1201 | CYC | C4D-CHA-C1A | 4.46 | 134.13 | 128.81 |
| 12 | XA | 201 | CYC | C1B-NB-C4B | -4.45 | 105.00 | 110.67 |
| 12 | X9 | 201 | CYC | C1B-NB-C4B | -4.45 | 105.00 | 110.67 |
| 12 | WA | 201 | CYC | OB-C4B-C3B | -4.45 | 123.21 | 128.04 |
| 12 | H3 | 202 | CYC | C1B-NB-C4B | -4.45 | 105.00 | 110.67 |
| 12 | S7 | 201 | CYC | C1B-NB-C4B | -4.45 | 105.00 | 110.67 |
| 12 | LA | 202 | CYC | OC-C1C-C2C | -4.45 | 122.64 | 126.17 |
| 12 | L9 | 202 | CYC | OC-C1C-C2C | -4.45 | 122.64 | 126.17 |
| 12 | P1 | 201 | CYC | C1B-NB-C4B | -4.45 | 105.01 | 110.67 |
| 12 | P3 | 201 | CYC | C1B-NB-C4B | -4.45 | 105.01 | 110.67 |
| 12 | s7 | 201 | CYC | C1B-NB-C4B | -4.45 | 105.01 | 110.67 |
| 12 | N6 | 101 | CYC | OC-C1C-C2C | -4.44 | 122.64 | 126.17 |
| 12 | K5 | 201 | CYC | CHD-C4C-NC | 4.44 | 130.49 | 125.20 |
| 12 | W9 | 201 | CYC | OB-C4B-C3B | -4.44 | 123.22 | 128.04 |
| 12 | Y7 | 201 | CYC | C1B-NB-C4B | -4.44 | 105.01 | 110.67 |
| 12 | P1 | 202 | CYC | CHB-C4A-NA | -4.44 | 115.64 | 124.93 |
| 12 | P3 | 202 | CYC | CHB-C4A-NA | -4.44 | 115.64 | 124.93 |
| 12 | M5 | 201 | CYC | C1B-NB-C4B | -4.44 | 105.01 | 110.67 |
| 12 | D4 | 202 | CYC | OC-C1C-C2C | -4.44 | 122.64 | 126.17 |
| 12 | D8 | 202 | CYC | OC-C1C-C2C | -4.44 | 122.64 | 126.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | D2 | 202 | CYC | CHB-C4A-NA | -4.44 | 115.64 | 124.93 |
| 12 | PA | 202 | CYC | CHB-C4A-NA | -4.44 | 115.65 | 124.93 |
| 12 | P9 | 202 | CYC | CHB-C4A-NA | -4.44 | 115.65 | 124.93 |
| 12 | O4 | 201 | CYC | OC-C1C-C2C | -4.44 | 122.65 | 126.17 |
| 12 | O8 | 201 | CYC | OC-C1C-C2C | -4.44 | 122.65 | 126.17 |
| 12 | L4 | 202 | CYC | C1B-NB-C4B | -4.44 | 105.02 | 110.67 |
| 12 | S4 | 202 | CYC | C1B-NB-C4B | -4.43 | 105.03 | 110.67 |
| 12 | c5 | 201 | CYC | CHD-C4C-NC | 4.43 | 130.47 | 125.20 |
| 12 | a9 | 901 | CYC | C1B-NB-C4B | -4.43 | 105.03 | 110.67 |
| 12 | W7 | 201 | CYC | CHD-C4C-NC | 4.43 | 130.47 | 125.20 |
| 12 | Q7 | 201 | CYC | CHD-C4C-NC | 4.43 | 130.47 | 125.20 |
| 12 | L3 | 202 | CYC | OC-C1C-C2C | -4.43 | 122.65 | 126.17 |
| 12 | D6 | 201 | CYC | OC-C1C-C2C | -4.43 | 122.65 | 126.17 |
| 12 | E5 | 201 | CYC | CHD-C4C-NC | 4.42 | 130.47 | 125.20 |
| 12 | H3 | 202 | CYC | OC-C1C-C2C | -4.42 | 122.66 | 126.17 |
| 12 | J4 | 201 | CYC | C1B-NB-C4B | -4.42 | 105.04 | 110.67 |
| 12 | J8 | 201 | CYC | C1B-NB-C4B | -4.42 | 105.04 | 110.67 |
| 12 | D2 | 201 | CYC | C2B-C1B-NB | 4.42 | 113.46 | 106.99 |
| 12 | N4 | 201 | CYC | CBD-CAD-C3D | -4.42 | 105.08 | 112.62 |
| 12 | N8 | 201 | CYC | CBD-CAD-C3D | -4.42 | 105.08 | 112.62 |
| 12 | B3 | 202 | CYC | C1B-NB-C4B | -4.42 | 105.04 | 110.67 |
| 12 | F3 | 201 | CYC | C1B-NB-C4B | -4.42 | 105.04 | 110.67 |
| 12 | F1 | 201 | CYC | C1B-NB-C4B | -4.42 | 105.04 | 110.67 |
| 12 | D6 | 202 | CYC | CHB-C4A-NA | -4.42 | 115.69 | 124.93 |
| 12 | B4 | 202 | CYC | C1B-NB-C4B | -4.41 | 105.05 | 110.67 |
| 12 | H6 | 201 | CYC | C1B-NB-C4B | -4.41 | 105.05 | 110.67 |
| 12 | S7 | 201 | CYC | CHD-C4C-NC | 4.41 | 130.45 | 125.20 |
| 12 | T4 | 201 | CYC | CBD-CAD-C3D | -4.41 | 105.09 | 112.62 |
| 12 | T8 | 201 | CYC | CBD-CAD-C3D | -4.41 | 105.09 | 112.62 |
| 12 | F4 | 201 | CYC | CHB-C4A-NA | -4.41 | 115.70 | 124.93 |
| 12 | F8 | 201 | CYC | CHB-C4A-NA | -4.41 | 115.70 | 124.93 |
| 12 | u7 | 201 | CYC | CHD-C4C-NC | 4.41 | 130.45 | 125.20 |
| 12 | X1 | 201 | CYC | C1B-NB-C4B | -4.41 | 105.06 | 110.67 |
| 12 | T3 | 302 | CYC | CHB-C4A-NA | -4.41 | 115.71 | 124.93 |
| 12 | T1 | 302 | CYC | CHB-C4A-NA | -4.41 | 115.71 | 124.93 |
| 12 | k7 | 201 | CYC | C1B-NB-C4B | -4.41 | 105.06 | 110.67 |
| 12 | S5 | 201 | CYC | C1B-NB-C4B | -4.41 | 105.06 | 110.67 |
| 12 | j5 | 1201 | CYC | C4D-CHA-C1A | 4.40 | 134.07 | 128.81 |
| 12 | B1 | 202 | CYC | C1B-NB-C4B | -4.40 | 105.06 | 110.67 |
| 12 | L9 | 201 | CYC | CHB-C4A-NA | -4.40 | 115.72 | 124.93 |
| 12 | BA | 202 | CYC | CHB-C4A-NA | -4.40 | 115.73 | 124.93 |
| 12 | Y4 | 201 | CYC | CHB-C4A-NA | -4.40 | 115.73 | 124.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | Y8 | 201 | CYC | CHB-C4A-NA | -4.40 | 115.73 | 124.93 |
| 12 | B9 | 202 | CYC | CHB-C4A-NA | -4.40 | 115.73 | 124.93 |
| 12 | F4 | 202 | CYC | C1B-NB-C4B | -4.40 | 105.07 | 110.67 |
| 12 | F8 | 202 | CYC | C1B-NB-C4B | -4.40 | 105.07 | 110.67 |
| 12 | V3 | 201 | CYC | C1B-NB-C4B | -4.40 | 105.07 | 110.67 |
| 12 | V1 | 201 | CYC | C1B-NB-C4B | -4.40 | 105.07 | 110.67 |
| 12 | UA | 201 | CYC | CBD-CAD-C3D | -4.40 | 105.12 | 112.62 |
| 12 | G2 | 201 | CYC | CBD-CAD-C3D | -4.40 | 105.12 | 112.62 |
| 12 | U9 | 201 | CYC | CBD-CAD-C3D | -4.40 | 105.12 | 112.62 |
| 12 | k7 | 201 | CYC | CHD-C4C-NC | 4.40 | 130.43 | 125.20 |
| 12 | GA | 201 | CYC | CMB-C2B-C1B | 4.39 | 129.66 | 124.17 |
| 12 | G9 | 201 | CYC | CMB-C2B-C1B | 4.39 | 129.66 | 124.17 |
| 12 | LA | 201 | CYC | CHB-C4A-NA | -4.39 | 115.74 | 124.93 |
| 12 | i7 | 201 | CYC | CHD-C4C-NC | 4.39 | 130.43 | 125.20 |
| 12 | O4 | 201 | CYC | C1B-NB-C4B | -4.39 | 105.07 | 110.67 |
| 12 | O8 | 201 | CYC | C1B-NB-C4B | -4.39 | 105.07 | 110.67 |
| 12 | Q5 | 201 | CYC | CHD-C4C-NC | 4.39 | 130.43 | 125.20 |
| 12 | o7 | 201 | CYC | CHD-C4C-NC | 4.39 | 130.43 | 125.20 |
| 12 | M8 | 302 | CYC | C1B-NB-C4B | -4.39 | 105.08 | 110.67 |
| 12 | K7 | 201 | CYC | CHD-C4C-NC | 4.39 | 130.43 | 125.20 |
| 12 | S1 | 201 | CYC | CBD-CAD-C3D | -4.39 | 105.13 | 112.62 |
| 12 | S3 | 201 | CYC | CBD-CAD-C3D | -4.39 | 105.13 | 112.62 |
| 12 | L3 | 202 | CYC | C1B-NB-C4B | -4.39 | 105.08 | 110.67 |
| 12 | B8 | 202 | CYC | C1B-NB-C4B | -4.39 | 105.08 | 110.67 |
| 12 | aA | 902 | CYC | C1B-NB-C4B | -4.39 | 105.08 | 110.67 |
| 12 | A4 | 201 | CYC | CBD-CAD-C3D | -4.39 | 105.13 | 112.62 |
| 12 | A8 | 201 | CYC | CBD-CAD-C3D | -4.39 | 105.13 | 112.62 |
| 12 | U7 | 201 | CYC | CHD-C4C-NC | 4.39 | 130.42 | 125.20 |
| 12 | c7 | 201 | CYC | CHD-C4C-NC | 4.39 | 130.42 | 125.20 |
| 12 | W4 | 201 | CYC | OC-C1C-C2C | -4.39 | 122.69 | 126.17 |
| 12 | W8 | 201 | CYC | OC-C1C-C2C | -4.39 | 122.69 | 126.17 |
| 12 | JA | 202 | CYC | C1B-NB-C4B | -4.39 | 105.08 | 110.67 |
| 12 | J9 | 202 | CYC | C1B-NB-C4B | -4.39 | 105.08 | 110.67 |
| 12 | D3 | 201 | CYC | CHB-C4A-NA | -4.39 | 115.76 | 124.93 |
| 12 | D1 | 201 | CYC | CHB-C4A-NA | -4.39 | 115.76 | 124.93 |
| 12 | HA | 202 | CYC | C1B-NB-C4B | -4.39 | 105.08 | 110.67 |
| 12 | X3 | 201 | CYC | C1B-NB-C4B | -4.39 | 105.08 | 110.67 |
| 12 | H1 | 201 | CYC | OC-C1C-C2C | -4.39 | 122.69 | 126.17 |
| 12 | J3 | 202 | CYC | C1B-NB-C4B | -4.38 | 105.09 | 110.67 |
| 12 | A1 | 201 | CYC | CBD-CAD-C3D | -4.38 | 105.14 | 112.62 |
| 12 | A3 | 201 | CYC | CBD-CAD-C3D | -4.38 | 105.14 | 112.62 |
| 12 | S4 | 201 | CYC | CHB-C4A-NA | -4.38 | 115.77 | 124.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | G6 | 201 | CYC | CBD-CAD-C3D | -4.38 | 105.15 | 112.62 |
| 12 | A6 | 201 | CYC | CBD-CAD-C3D | -4.38 | 105.15 | 112.62 |
| 12 | CA | 201 | CYC | CBD-CAD-C3D | -4.38 | 105.15 | 112.62 |
| 12 | C9 | 201 | CYC | CBD-CAD-C3D | -4.38 | 105.15 | 112.62 |
| 12 | DA | 202 | CYC | CHB-C4A-NA | -4.38 | 115.77 | 124.93 |
| 12 | P4 | 201 | CYC | CBD-CAD-C3D | -4.38 | 105.15 | 112.62 |
| 12 | P8 | 201 | CYC | CBD-CAD-C3D | -4.38 | 105.15 | 112.62 |
| 12 | VA | 201 | CYC | C1B-NB-C4B | -4.38 | 105.10 | 110.67 |
| 12 | e7 | 201 | CYC | CHD-C4C-NC | 4.38 | 130.41 | 125.20 |
| 12 | D9 | 202 | CYC | CHB-C4A-NA | -4.38 | 115.78 | 124.93 |
| 12 | I4 | 201 | CYC | CBD-CAD-C3D | -4.38 | 105.15 | 112.62 |
| 12 | I8 | 201 | CYC | CBD-CAD-C3D | -4.38 | 105.15 | 112.62 |
| 12 | V3 | 202 | CYC | CHB-C4A-NA | -4.37 | 115.78 | 124.93 |
| 12 | V1 | 202 | CYC | CHB-C4A-NA | -4.37 | 115.78 | 124.93 |
| 12 | T3 | 301 | CYC | C1B-NB-C4B | -4.37 | 105.10 | 110.67 |
| 12 | T1 | 301 | CYC | C1B-NB-C4B | -4.37 | 105.10 | 110.67 |
| 12 | R3 | 202 | CYC | CHB-C4A-NA | -4.37 | 115.78 | 124.93 |
| 12 | O4 | 202 | CYC | CHB-C4A-NA | -4.37 | 115.78 | 124.93 |
| 12 | O8 | 202 | CYC | CHB-C4A-NA | -4.37 | 115.78 | 124.93 |
| 12 | C4 | 201 | CYC | CBD-CAD-C3D | -4.37 | 105.16 | 112.62 |
| 12 | C8 | 201 | CYC | CBD-CAD-C3D | -4.37 | 105.16 | 112.62 |
| 12 | JA | 201 | CYC | CHB-C4A-NA | -4.37 | 115.78 | 124.93 |
| 12 | J9 | 201 | CYC | CHB-C4A-NA | -4.37 | 115.78 | 124.93 |
| 12 | Y3 | 201 | CYC | CBD-CAD-C3D | -4.37 | 105.16 | 112.62 |
| 12 | E7 | 201 | CYC | CHD-C4C-NC | 4.37 | 130.40 | 125.20 |
| 12 | W5 | 201 | CYC | CHD-C4C-NC | 4.37 | 130.40 | 125.20 |
| 12 | L6 | 201 | CYC | OC-C1C-C2C | -4.37 | 122.70 | 126.17 |
| 12 | S8 | 201 | CYC | CHB-C4A-NA | -4.37 | 115.79 | 124.93 |
| 12 | R3 | 201 | CYC | C1B-NB-C4B | -4.37 | 105.11 | 110.67 |
| 12 | Q1 | 201 | CYC | CBD-CAD-C3D | -4.37 | 105.17 | 112.62 |
| 12 | Q3 | 201 | CYC | CBD-CAD-C3D | -4.37 | 105.17 | 112.62 |
| 12 | S9 | 201 | CYC | CBD-CAD-C3D | -4.37 | 105.17 | 112.62 |
| 12 | H2 | 201 | CYC | C1B-NB-C4B | -4.37 | 105.11 | 110.67 |
| 12 | aA | 901 | CYC | C1B-NB-C4B | -4.37 | 105.11 | 110.67 |
| 12 | K2 | 201 | CYC | CMB-C2B-C1B | 4.37 | 129.62 | 124.17 |
| 12 | U4 | 202 | CYC | CHB-C4A-NA | -4.37 | 115.80 | 124.93 |
| 12 | U8 | 202 | CYC | CHB-C4A-NA | -4.37 | 115.80 | 124.93 |
| 12 | EA | 201 | CYC | CBD-CAD-C3D | -4.36 | 105.17 | 112.62 |
| 12 | E9 | 201 | CYC | CBD-CAD-C3D | -4.36 | 105.17 | 112.62 |
| 12 | L8 | 201 | CYC | CHB-C4A-NA | -4.36 | 115.80 | 124.93 |
| 12 | E3 | 201 | CYC | CBD-CAD-C3D | -4.36 | 105.17 | 112.62 |
| 12 | E1 | 201 | CYC | CBD-CAD-C3D | -4.36 | 105.17 | 112.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | V3 | 201 | CYC | OC-C1C-C2C | -4.36 | 122.70 | 126.17 |
| 12 | V1 | 201 | CYC | OC-C1C-C2C | -4.36 | 122.70 | 126.17 |
| 12 | B3 | 201 | CYC | CHB-C4A-NA | -4.36 | 115.81 | 124.93 |
| 12 | B1 | 201 | CYC | CHB-C4A-NA | -4.36 | 115.81 | 124.93 |
| 12 | V9 | 201 | CYC | C1B-NB-C4B | -4.36 | 105.12 | 110.67 |
| 12 | K3 | 201 | CYC | CBD-CAD-C3D | -4.36 | 105.18 | 112.62 |
| 12 | K1 | 201 | CYC | CBD-CAD-C3D | -4.36 | 105.18 | 112.62 |
| 12 | G3 | 201 | CYC | CBD-CAD-C3D | -4.36 | 105.18 | 112.62 |
| 12 | G1 | 201 | CYC | CBD-CAD-C3D | -4.36 | 105.18 | 112.62 |
| 12 | R1 | 202 | CYC | CHB-C4A-NA | -4.36 | 115.82 | 124.93 |
| 12 | D1 | 202 | CYC | C1B-NB-C4B | -4.36 | 105.12 | 110.67 |
| 12 | B4 | 201 | CYC | CHB-C4A-NA | -4.36 | 115.82 | 124.93 |
| 12 | Y9 | 201 | CYC | CMB-C2B-C1B | 4.36 | 129.61 | 124.17 |
| 12 | A2 | 201 | CYC | CMB-C2B-C1B | 4.36 | 129.61 | 124.17 |
| 12 | Q8 | 201 | CYC | CHB-C4A-NA | -4.36 | 115.82 | 124.93 |
| 12 | Y7 | 201 | CYC | CHD-C4C-NC | 4.35 | 130.38 | 125.20 |
| 12 | Q4 | 201 | CYC | CHB-C4A-NA | -4.35 | 115.82 | 124.93 |
| 12 | Y1 | 201 | CYC | CBD-CAD-C3D | -4.35 | 105.19 | 112.62 |
| 12 | M4 | 301 | CYC | C1B-NB-C4B | -4.35 | 105.12 | 110.67 |
| 12 | H9 | 202 | CYC | C1B-NB-C4B | -4.35 | 105.12 | 110.67 |
| 12 | B2 | 201 | CYC | CHB-C4A-NA | -4.35 | 115.83 | 124.93 |
| 12 | GA | 201 | CYC | CBD-CAD-C3D | -4.35 | 105.19 | 112.62 |
| 12 | G9 | 201 | CYC | CBD-CAD-C3D | -4.35 | 105.19 | 112.62 |
| 12 | C2 | 201 | CYC | CBD-CAD-C3D | -4.35 | 105.19 | 112.62 |
| 12 | s7 | 201 | CYC | CHD-C4C-NC | 4.35 | 130.38 | 125.20 |
| 12 | M8 | 301 | CYC | C1B-NB-C4B | -4.35 | 105.13 | 110.67 |
| 12 | O7 | 201 | CYC | CHD-C4C-NC | 4.35 | 130.38 | 125.20 |
| 12 | R1 | 201 | CYC | C1B-NB-C4B | -4.35 | 105.13 | 110.67 |
| 12 | DA | 201 | CYC | OC-C1C-C2C | -4.35 | 122.71 | 126.17 |
| 12 | D9 | 201 | CYC | OC-C1C-C2C | -4.35 | 122.71 | 126.17 |
| 12 | AA | 201 | CYC | CBD-CAD-C3D | -4.35 | 105.20 | 112.62 |
| 12 | A9 | 201 | CYC | CBD-CAD-C3D | -4.35 | 105.20 | 112.62 |
| 12 | XA | 202 | CYC | CHB-C4A-NA | -4.35 | 115.83 | 124.93 |
| 12 | A6 | 201 | CYC | CMB-C2B-C1B | 4.35 | 129.60 | 124.17 |
| 12 | S5 | 201 | CYC | CHD-C4C-NC | 4.35 | 130.38 | 125.20 |
| 12 | D2 | 201 | CYC | OC-C1C-C2C | -4.35 | 122.72 | 126.17 |
| 12 | J3 | 201 | CYC | CHB-C4A-NA | -4.35 | 115.84 | 124.93 |
| 12 | SA | 201 | CYC | CBD-CAD-C3D | -4.35 | 105.20 | 112.62 |
| 12 | A2 | 201 | CYC | CBD-CAD-C3D | -4.35 | 105.20 | 112.62 |
| 12 | H2 | 202 | CYC | CHB-C4A-NA | -4.35 | 115.84 | 124.93 |
| 12 | O1 | 201 | CYC | CBD-CAD-C3D | -4.35 | 105.20 | 112.62 |
| 12 | O3 | 201 | CYC | CBD-CAD-C3D | -4.35 | 105.20 | 112.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | B6 | 201 | CYC | CHB-C4A-NA | -4.35 | 115.84 | 124.93 |
| 12 | X1 | 202 | CYC | CHB-C4A-NA | -4.35 | 115.84 | 124.93 |
| 12 | L4 | 201 | CYC | CHB-C4A-NA | -4.34 | 115.84 | 124.93 |
| 12 | C3 | 201 | CYC | CBD-CAD-C3D | -4.34 | 105.21 | 112.62 |
| 12 | C1 | 201 | CYC | CBD-CAD-C3D | -4.34 | 105.21 | 112.62 |
| 12 | I5 | 201 | CYC | C2B-C1B-NB | 4.34 | 113.35 | 106.99 |
| 12 | F9 | 302 | CYC | CHB-C4A-NA | -4.34 | 115.84 | 124.93 |
| 12 | C6 | 201 | CYC | CBD-CAD-C3D | -4.34 | 105.21 | 112.62 |
| 12 | q7 | 201 | CYC | CHD-C4C-NC | 4.34 | 130.37 | 125.20 |
| 12 | YA | 201 | CYC | CBD-CAD-C3D | -4.34 | 105.21 | 112.62 |
| 12 | E6 | 201 | CYC | CBD-CAD-C3D | -4.34 | 105.21 | 112.62 |
| 12 | Y9 | 201 | CYC | CBD-CAD-C3D | -4.34 | 105.21 | 112.62 |
| 12 | E2 | 201 | CYC | CBD-CAD-C3D | -4.34 | 105.21 | 112.62 |
| 12 | J4 | 202 | CYC | CHB-C4A-NA | -4.34 | 115.85 | 124.93 |
| 12 | J8 | 202 | CYC | CHB-C4A-NA | -4.34 | 115.85 | 124.93 |
| 12 | J1 | 201 | CYC | CHB-C4A-NA | -4.34 | 115.85 | 124.93 |
| 12 | B8 | 201 | CYC | CHB-C4A-NA | -4.34 | 115.85 | 124.93 |
| 12 | F9 | 303 | CYC | CHB-C4A-NA | -4.34 | 115.86 | 124.93 |
| 12 | T9 | 302 | CYC | CHB-C4A-NA | -4.34 | 115.86 | 124.93 |
| 12 | L2 | 201 | CYC | OC-C1C-C2C | -4.34 | 122.72 | 126.17 |
| 12 | X3 | 201 | CYC | OC-C1C-C2C | -4.34 | 122.72 | 126.17 |
| 12 | X1 | 201 | CYC | OC-C1C-C2C | -4.34 | 122.72 | 126.17 |
| 12 | K6 | 201 | CYC | CMB-C2B-C1B | 4.34 | 129.58 | 124.17 |
| 12 | F3 | 202 | CYC | CHB-C4A-NA | -4.34 | 115.86 | 124.93 |
| 12 | F1 | 202 | CYC | CHB-C4A-NA | -4.34 | 115.86 | 124.93 |
| 12 | X3 | 202 | CYC | CHB-C4A-NA | -4.34 | 115.86 | 124.93 |
| 12 | L3 | 201 | CYC | CHB-C4A-NA | -4.34 | 115.86 | 124.93 |
| 12 | L1 | 201 | CYC | CHB-C4A-NA | -4.34 | 115.86 | 124.93 |
| 12 | OA | 201 | CYC | CBD-CAD-C3D | -4.34 | 105.22 | 112.62 |
| 12 | O9 | 201 | CYC | CBD-CAD-C3D | -4.34 | 105.22 | 112.62 |
| 12 | H3 | 201 | CYC | CHB-C4A-NA | -4.34 | 115.86 | 124.93 |
| 12 | H1 | 202 | CYC | CHB-C4A-NA | -4.34 | 115.86 | 124.93 |
| 12 | X9 | 202 | CYC | CHB-C4A-NA | -4.33 | 115.86 | 124.93 |
| 12 | R4 | 201 | CYC | CMB-C2B-C1B | 4.33 | 129.58 | 124.17 |
| 12 | R8 | 201 | CYC | CMB-C2B-C1B | 4.33 | 129.58 | 124.17 |
| 12 | QA | 201 | CYC | CBD-CAD-C3D | -4.33 | 105.22 | 112.62 |
| 12 | L2 | 202 | CYC | CHB-C4A-NA | -4.33 | 115.87 | 124.93 |
| 12 | m7 | 201 | CYC | CHD-C4C-NC | 4.33 | 130.36 | 125.20 |
| 12 | I1 | 201 | CYC | CBD-CAD-C3D | -4.33 | 105.23 | 112.62 |
| 12 | H8 | 202 | CYC | CHB-C4A-NA | -4.33 | 115.87 | 124.93 |
| 12 | C7 | 201 | CYC | CHD-C4C-NC | 4.33 | 130.35 | 125.20 |
| 12 | X4 | 201 | CYC | CMB-C2B-C1B | 4.33 | 129.57 | 124.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | X8 | 201 | CYC | CMB-C2B-C1B | 4.33 | 129.57 | 124.17 |
| 12 | H6 | 202 | CYC | CHB-C4A-NA | -4.33 | 115.88 | 124.93 |
| 12 | Z8 | 301 | CYC | C1B-NB-C4B | -4.33 | 105.16 | 110.67 |
| 12 | RA | 202 | CYC | CHB-C4A-NA | -4.33 | 115.88 | 124.93 |
| 12 | D4 | 201 | CYC | CHB-C4A-NA | -4.33 | 115.88 | 124.93 |
| 12 | D8 | 201 | CYC | CHB-C4A-NA | -4.33 | 115.88 | 124.93 |
| 12 | R9 | 202 | CYC | CHB-C4A-NA | -4.33 | 115.88 | 124.93 |
| 12 | YA | 201 | CYC | CMB-C2B-C1B | 4.33 | 129.57 | 124.17 |
| 12 | W9 | 201 | CYC | CBD-CAD-C3D | -4.33 | 105.24 | 112.62 |
| 12 | Q9 | 201 | CYC | CBD-CAD-C3D | -4.33 | 105.24 | 112.62 |
| 12 | KA | 201 | CYC | CBD-CAD-C3D | -4.32 | 105.24 | 112.62 |
| 12 | K9 | 201 | CYC | CBD-CAD-C3D | -4.32 | 105.24 | 112.62 |
| 12 | Z4 | 301 | CYC | C1B-NB-C4B | -4.32 | 105.16 | 110.67 |
| 12 | U3 | 201 | CYC | CBD-CAD-C3D | -4.32 | 105.24 | 112.62 |
| 12 | U1 | 201 | CYC | CBD-CAD-C3D | -4.32 | 105.24 | 112.62 |
| 12 | U5 | 201 | CYC | C2B-C1B-NB | 4.32 | 113.32 | 106.99 |
| 12 | E4 | 201 | CYC | CBD-CAD-C3D | -4.32 | 105.24 | 112.62 |
| 12 | E8 | 201 | CYC | CBD-CAD-C3D | -4.32 | 105.24 | 112.62 |
| 12 | U5 | 201 | CYC | CHD-C4C-NC | 4.32 | 130.34 | 125.20 |
| 12 | C5 | 201 | CYC | C2B-C1B-NB | 4.32 | 113.31 | 106.99 |
| 12 | L6 | 202 | CYC | CHB-C4A-NA | -4.32 | 115.89 | 124.93 |
| 12 | J6 | 202 | CYC | OC-C1C-C2C | -4.32 | 122.74 | 126.17 |
| 12 | W1 | 201 | CYC | CBD-CAD-C3D | -4.32 | 105.25 | 112.62 |
| 12 | O5 | 201 | CYC | CHD-C4C-NC | 4.32 | 130.34 | 125.20 |
| 12 | IA | 201 | CYC | CBD-CAD-C3D | -4.32 | 105.25 | 112.62 |
| 12 | I9 | 201 | CYC | CBD-CAD-C3D | -4.32 | 105.25 | 112.62 |
| 12 | N4 | 201 | CYC | CMB-C2B-C1B | 4.32 | 129.56 | 124.17 |
| 12 | N8 | 201 | CYC | CMB-C2B-C1B | 4.32 | 129.56 | 124.17 |
| 12 | I3 | 201 | CYC | CBD-CAD-C3D | -4.32 | 105.25 | 112.62 |
| 12 | TA | 302 | CYC | CHB-C4A-NA | -4.32 | 115.90 | 124.93 |
| 12 | F2 | 201 | CYC | C1B-NB-C4B | -4.32 | 105.17 | 110.67 |
| 12 | K8 | 201 | CYC | CBD-CAD-C3D | -4.32 | 105.25 | 112.62 |
| 12 | DA | 201 | CYC | C1B-NB-C4B | -4.32 | 105.17 | 110.67 |
| 12 | W8 | 201 | CYC | C1B-NB-C4B | -4.32 | 105.17 | 110.67 |
| 12 | H4 | 202 | CYC | CHB-C4A-NA | -4.32 | 115.91 | 124.93 |
| 12 | C1 | 201 | CYC | CMB-C2B-C1B | 4.31 | 129.56 | 124.17 |
| 12 | A7 | 201 | CYC | CHD-C4C-NC | 4.31 | 130.34 | 125.20 |
| 12 | J6 | 201 | CYC | CHB-C4A-NA | -4.31 | 115.91 | 124.93 |
| 12 | X4 | 201 | CYC | CBD-CAD-C3D | -4.31 | 105.26 | 112.62 |
| 12 | X8 | 201 | CYC | CBD-CAD-C3D | -4.31 | 105.26 | 112.62 |
| 12 | D3 | 202 | CYC | C1B-NB-C4B | -4.31 | 105.18 | 110.67 |
| 12 | H8 | 201 | CYC | C1B-NB-C4B | -4.31 | 105.18 | 110.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | W3 | 201 | CYC | CBD-CAD-C3D | -4.31 | 105.27 | 112.62 |
| 12 | K4 | 201 | CYC | CBD-CAD-C3D | -4.31 | 105.27 | 112.62 |
| 12 | I2 | 201 | CYC | CBD-CAD-C3D | -4.31 | 105.27 | 112.62 |
| 12 | I6 | 201 | CYC | CBD-CAD-C3D | -4.31 | 105.27 | 112.62 |
| 12 | J2 | 201 | CYC | CHB-C4A-NA | -4.31 | 115.92 | 124.93 |
| 12 | WA | 201 | CYC | CBD-CAD-C3D | -4.31 | 105.27 | 112.62 |
| 12 | F6 | 202 | CYC | CHB-C4A-NA | -4.30 | 115.93 | 124.93 |
| 12 | F2 | 202 | CYC | CHB-C4A-NA | -4.30 | 115.93 | 124.93 |
| 12 | W4 | 201 | CYC | C1B-NB-C4B | -4.30 | 105.19 | 110.67 |
| 12 | HA | 201 | CYC | CHB-C4A-NA | -4.30 | 115.94 | 124.93 |
| 12 | W4 | 202 | CYC | CHB-C4A-NA | -4.30 | 115.94 | 124.93 |
| 12 | H9 | 201 | CYC | CHB-C4A-NA | -4.30 | 115.94 | 124.93 |
| 12 | M5 | 201 | CYC | CHD-C4C-NC | 4.30 | 130.32 | 125.20 |
| 12 | A1 | 201 | CYC | CMB-C2B-C1B | 4.30 | 129.54 | 124.17 |
| 12 | A3 | 201 | CYC | CMB-C2B-C1B | 4.30 | 129.54 | 124.17 |
| 12 | O5 | 201 | CYC | C2B-C1B-NB | 4.30 | 113.28 | 106.99 |
| 12 | FA | 301 | CYC | C1B-NB-C4B | -4.30 | 105.20 | 110.67 |
| 12 | F9 | 301 | CYC | C1B-NB-C4B | -4.30 | 105.20 | 110.67 |
| 12 | W8 | 202 | CYC | CHB-C4A-NA | -4.29 | 115.95 | 124.93 |
| 12 | F6 | 201 | CYC | C1B-NB-C4B | -4.29 | 105.20 | 110.67 |
| 12 | TA | 301 | CYC | C1B-NB-C4B | -4.29 | 105.20 | 110.67 |
| 12 | T9 | 301 | CYC | C1B-NB-C4B | -4.29 | 105.20 | 110.67 |
| 12 | G7 | 201 | CYC | CHD-C4C-NC | 4.29 | 130.31 | 125.20 |
| 12 | RA | 201 | CYC | C1B-NB-C4B | -4.29 | 105.20 | 110.67 |
| 12 | R9 | 201 | CYC | C1B-NB-C4B | -4.29 | 105.20 | 110.67 |
| 12 | C3 | 201 | CYC | CMB-C2B-C1B | 4.29 | 129.53 | 124.17 |
| 12 | VA | 202 | CYC | CHB-C4A-NA | -4.29 | 115.96 | 124.93 |
| 12 | ZA | 201 | CYC | CHB-C4A-NA | -4.29 | 115.96 | 124.93 |
| 12 | V9 | 202 | CYC | CHB-C4A-NA | -4.29 | 115.96 | 124.93 |
| 12 | Z9 | 201 | CYC | CHB-C4A-NA | -4.29 | 115.96 | 124.93 |
| 12 | H4 | 201 | CYC | C1B-NB-C4B | -4.29 | 105.21 | 110.67 |
| 12 | V4 | 201 | CYC | CBD-CAD-C3D | -4.29 | 105.30 | 112.62 |
| 12 | V8 | 201 | CYC | CBD-CAD-C3D | -4.29 | 105.30 | 112.62 |
| 12 | D9 | 201 | CYC | C1B-NB-C4B | -4.29 | 105.21 | 110.67 |
| 12 | I3 | 201 | CYC | CMB-C2B-C1B | 4.29 | 129.52 | 124.17 |
| 12 | I1 | 201 | CYC | CMB-C2B-C1B | 4.29 | 129.52 | 124.17 |
| 12 | O1 | 201 | CYC | CMB-C2B-C1B | 4.29 | 129.52 | 124.17 |
| 12 | O3 | 201 | CYC | CMB-C2B-C1B | 4.29 | 129.52 | 124.17 |
| 12 | R4 | 201 | CYC | CBD-CAD-C3D | -4.29 | 105.31 | 112.62 |
| 12 | R8 | 201 | CYC | CBD-CAD-C3D | -4.29 | 105.31 | 112.62 |
| 12 | Z3 | 202 | CYC | CHB-C4A-NA | -4.28 | 115.98 | 124.93 |
| 12 | Z1 | 201 | CYC | CHB-C4A-NA | -4.28 | 115.98 | 124.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | EA | 201 | CYC | CMB-C2B-C1B | 4.28 | 129.51 | 124.17 |
| 12 | E9 | 201 | CYC | CMB-C2B-C1B | 4.28 | 129.51 | 124.17 |
| 12 | M7 | 201 | CYC | CHD-C4C-NC | 4.28 | 130.29 | 125.20 |
| 12 | C9 | 201 | CYC | CMB-C2B-C1B | 4.27 | 129.50 | 124.17 |
| 12 | I7 | 201 | CYC | CHD-C4C-NC | 4.27 | 130.28 | 125.20 |
| 12 | E2 | 201 | CYC | CMB-C2B-C1B | 4.27 | 129.50 | 124.17 |
| 12 | J2 | 202 | CYC | OC-C1C-C2C | -4.27 | 122.78 | 126.17 |
| 12 | Y3 | 201 | CYC | CMB-C2B-C1B | 4.27 | 129.49 | 124.17 |
| 12 | Y1 | 201 | CYC | CMB-C2B-C1B | 4.27 | 129.49 | 124.17 |
| 12 | j5 | 1201 | CYC | CAB-C3B-C4B | 4.26 | 128.11 | 121.38 |
| 12 | T4 | 201 | CYC | CMB-C2B-C1B | 4.26 | 129.49 | 124.17 |
| 12 | T8 | 201 | CYC | CMB-C2B-C1B | 4.26 | 129.49 | 124.17 |
| 12 | G4 | 201 | CYC | CBD-CAD-C3D | -4.26 | 105.35 | 112.62 |
| 12 | G8 | 201 | CYC | CBD-CAD-C3D | -4.26 | 105.35 | 112.62 |
| 12 | U3 | 201 | CYC | CMB-C2B-C1B | 4.26 | 129.49 | 124.17 |
| 12 | U1 | 201 | CYC | CMB-C2B-C1B | 4.26 | 129.49 | 124.17 |
| 12 | K2 | 201 | CYC | CBD-CAD-C3D | -4.26 | 105.35 | 112.62 |
| 12 | IA | 201 | CYC | CMB-C2B-C1B | 4.26 | 129.49 | 124.17 |
| 12 | I9 | 201 | CYC | CMB-C2B-C1B | 4.26 | 129.49 | 124.17 |
| 12 | H1 | 202 | CYC | CMA-C3A-C4A | 4.26 | 131.62 | 125.06 |
| 12 | a7 | 201 | CYC | C2B-C1B-NB | 4.26 | 113.22 | 106.99 |
| 12 | CA | 201 | CYC | CMB-C2B-C1B | 4.26 | 129.48 | 124.17 |
| 12 | i7 | 201 | CYC | C2B-C1B-NB | 4.26 | 113.22 | 106.99 |
| 12 | H6 | 202 | CYC | CMA-C3A-C4A | 4.26 | 131.62 | 125.06 |
| 12 | C6 | 201 | CYC | CMB-C2B-C1B | 4.26 | 129.48 | 124.17 |
| 12 | g7 | 201 | CYC | C2B-C1B-NB | 4.25 | 113.22 | 106.99 |
| 12 | G1 | 201 | CYC | CMB-C2B-C1B | 4.25 | 129.48 | 124.17 |
| 12 | BA | 202 | CYC | CMA-C3A-C4A | 4.25 | 131.61 | 125.06 |
| 12 | B9 | 202 | CYC | CMA-C3A-C4A | 4.25 | 131.61 | 125.06 |
| 12 | E4 | 201 | CYC | CMB-C2B-C1B | 4.25 | 129.48 | 124.17 |
| 12 | a7 | 201 | CYC | CHD-C4C-NC | 4.25 | 130.26 | 125.20 |
| 12 | D4 | 202 | CYC | C1B-NB-C4B | -4.25 | 105.26 | 110.67 |
| 12 | a5 | 201 | CYC | CHD-C4C-NC | 4.25 | 130.26 | 125.20 |
| 12 | O7 | 201 | CYC | C2B-C1B-NB | 4.25 | 113.21 | 106.99 |
| 12 | I6 | 201 | CYC | CMB-C2B-C1B | 4.25 | 129.47 | 124.17 |
| 12 | KA | 201 | CYC | CMB-C2B-C1B | 4.24 | 129.47 | 124.17 |
| 12 | K9 | 201 | CYC | CMB-C2B-C1B | 4.24 | 129.47 | 124.17 |
| 12 | C2 | 201 | CYC | CMB-C2B-C1B | 4.24 | 129.47 | 124.17 |
| 12 | U7 | 201 | CYC | C2B-C1B-NB | 4.24 | 113.20 | 106.99 |
| 12 | A6 | 201 | CYC | OC-C1C-NC | 4.24 | 130.08 | 124.94 |
| 12 | D8 | 202 | CYC | C1B-NB-C4B | -4.24 | 105.27 | 110.67 |
| 12 | W7 | 201 | CYC | C2B-C1B-NB | 4.24 | 113.20 | 106.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | A4 | 201 | CYC | CMB-C2B-C1B | 4.24 | 129.46 | 124.17 |
| 12 | A8 | 201 | CYC | CMB-C2B-C1B | 4.24 | 129.46 | 124.17 |
| 12 | UA | 201 | CYC | CMB-C2B-C1B | 4.24 | 129.46 | 124.17 |
| 12 | U9 | 201 | CYC | CMB-C2B-C1B | 4.24 | 129.46 | 124.17 |
| 12 | K6 | 201 | CYC | CBD-CAD-C3D | -4.24 | 105.39 | 112.62 |
| 12 | b5 | 201 | CYC | CHA-C1A-NA | -4.24 | 122.95 | 128.83 |
| 12 | OA | 201 | CYC | CMB-C2B-C1B | 4.23 | 129.46 | 124.17 |
| 12 | O9 | 201 | CYC | CMB-C2B-C1B | 4.23 | 129.46 | 124.17 |
| 12 | H2 | 202 | CYC | CMA-C3A-C4A | 4.23 | 131.59 | 125.06 |
| 12 | C5 | 201 | CYC | CHD-C4C-NC | 4.23 | 130.24 | 125.20 |
| 12 | H3 | 201 | CYC | CMA-C3A-C4A | 4.23 | 131.58 | 125.06 |
| 12 | X9 | 202 | CYC | CMA-C3A-C4A | 4.23 | 131.58 | 125.06 |
| 12 | G3 | 201 | CYC | CMB-C2B-C1B | 4.23 | 129.45 | 124.17 |
| 12 | v7 | 201 | CYC | CHA-C1A-NA | -4.23 | 122.96 | 128.83 |
| 12 | E8 | 201 | CYC | CMB-C2B-C1B | 4.23 | 129.45 | 124.17 |
| 12 | E6 | 201 | CYC | CMB-C2B-C1B | 4.23 | 129.45 | 124.17 |
| 12 | K5 | 201 | CYC | C2B-C1B-NB | 4.23 | 113.18 | 106.99 |
| 12 | H4 | 202 | CYC | CMA-C3A-C4A | 4.23 | 131.57 | 125.06 |
| 12 | H8 | 202 | CYC | CMA-C3A-C4A | 4.23 | 131.57 | 125.06 |
| 12 | QA | 201 | CYC | CMB-C2B-C1B | 4.23 | 129.44 | 124.17 |
| 12 | I2 | 201 | CYC | CMB-C2B-C1B | 4.23 | 129.44 | 124.17 |
| 12 | c7 | 201 | CYC | C2B-C1B-NB | 4.22 | 113.17 | 106.99 |
| 12 | T3 | 302 | CYC | CMA-C3A-C4A | 4.22 | 131.56 | 125.06 |
| 12 | T1 | 302 | CYC | CMA-C3A-C4A | 4.22 | 131.56 | 125.06 |
| 12 | W5 | 201 | CYC | C2B-C1B-NB | 4.22 | 113.17 | 106.99 |
| 12 | Q9 | 201 | CYC | CMB-C2B-C1B | 4.22 | 129.44 | 124.17 |
| 12 | G4 | 201 | CYC | CMB-C2B-C1B | 4.22 | 129.44 | 124.17 |
| 12 | I4 | 201 | CYC | CMB-C2B-C1B | 4.22 | 129.44 | 124.17 |
| 12 | I8 | 201 | CYC | CMB-C2B-C1B | 4.22 | 129.44 | 124.17 |
| 12 | B4 | 201 | CYC | CMA-C3A-C4A | 4.22 | 131.56 | 125.06 |
| 12 | B8 | 201 | CYC | CMA-C3A-C4A | 4.22 | 131.56 | 125.06 |
| 12 | E5 | 201 | CYC | C2B-C1B-NB | 4.22 | 113.16 | 106.99 |
| 12 | e5 | 201 | CYC | C2B-C1B-NB | 4.21 | 113.16 | 106.99 |
| 12 | F9 | 303 | CYC | CMA-C3A-C4A | 4.21 | 131.55 | 125.06 |
| 12 | k5 | 1201 | CYC | CAB-C3B-C4B | 4.21 | 128.03 | 121.38 |
| 12 | XA | 202 | CYC | CMA-C3A-C4A | 4.21 | 131.55 | 125.06 |
| 12 | I7 | 201 | CYC | C2B-C1B-NB | 4.21 | 113.15 | 106.99 |
| 12 | K8 | 201 | CYC | CMB-C2B-C1B | 4.21 | 129.42 | 124.17 |
| 12 | D6 | 201 | CYC | C1B-NB-C4B | -4.21 | 105.31 | 110.67 |
| 12 | a5 | 201 | CYC | C2B-C1B-NB | 4.21 | 113.14 | 106.99 |
| 12 | K4 | 201 | CYC | CMB-C2B-C1B | 4.20 | 129.41 | 124.17 |
| 12 | F9 | 302 | CYC | CMA-C3A-C4A | 4.20 | 131.53 | 125.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | A2 | 201 | CYC | OC-C1C-NC | 4.20 | 130.03 | 124.94 |
| 12 | G8 | 201 | CYC | CMB-C2B-C1B | 4.20 | 129.41 | 124.17 |
| 12 | V3 | 202 | CYC | CMA-C3A-C4A | 4.20 | 131.53 | 125.06 |
| 12 | V1 | 202 | CYC | CMA-C3A-C4A | 4.20 | 131.53 | 125.06 |
| 12 | I5 | 201 | CYC | CHD-C4C-NC | 4.20 | 130.20 | 125.20 |
| 12 | K1 | 201 | CYC | CMB-C2B-C1B | 4.20 | 129.41 | 124.17 |
| 12 | PA | 202 | CYC | CMA-C3A-C4A | 4.19 | 131.52 | 125.06 |
| 12 | E7 | 201 | CYC | C2B-C1B-NB | 4.19 | 113.13 | 106.99 |
| 12 | Y5 | 201 | CYC | C2B-C1B-NB | 4.19 | 113.12 | 106.99 |
| 12 | e5 | 201 | CYC | CHD-C4C-NC | 4.19 | 130.19 | 125.20 |
| 12 | A | 201 | CYC | CHA-C1A-NA | -4.19 | 123.02 | 128.83 |
| 12 | O4 | 202 | CYC | CMA-C3A-C4A | 4.19 | 131.52 | 125.06 |
| 12 | O8 | 202 | CYC | CMA-C3A-C4A | 4.19 | 131.52 | 125.06 |
| 12 | p7 | 201 | CYC | CHA-C1A-NA | -4.19 | 123.02 | 128.83 |
| 12 | o7 | 201 | CYC | C2B-C1B-NB | 4.19 | 113.12 | 106.99 |
| 12 | D2 | 201 | CYC | C1B-NB-C4B | -4.19 | 105.34 | 110.67 |
| 12 | T5 | 201 | CYC | CHA-C1A-NA | -4.19 | 123.02 | 128.83 |
| 12 | A7 | 201 | CYC | C2B-C1B-NB | 4.18 | 113.11 | 106.99 |
| 12 | P9 | 202 | CYC | CMA-C3A-C4A | 4.18 | 131.51 | 125.06 |
| 12 | SA | 201 | CYC | CMB-C2B-C1B | 4.18 | 129.39 | 124.17 |
| 12 | S9 | 201 | CYC | CMB-C2B-C1B | 4.18 | 129.39 | 124.17 |
| 12 | k5 | 1204 | CYC | CHA-C1A-NA | -4.18 | 123.02 | 128.83 |
| 12 | B1 | 202 | CYC | C4A-C3A-C2A | -4.18 | 101.70 | 106.51 |
| 12 | c5 | 201 | CYC | C2B-C1B-NB | 4.18 | 113.11 | 106.99 |
| 12 | PA | 201 | CYC | CMA-C3A-C4A | 4.18 | 131.50 | 125.06 |
| 12 | P9 | 201 | CYC | CMA-C3A-C4A | 4.18 | 131.50 | 125.06 |
| 12 | K7 | 201 | CYC | C2B-C1B-NB | 4.18 | 113.11 | 106.99 |
| 12 | W4 | 202 | CYC | CMA-C3A-C4A | 4.18 | 131.50 | 125.06 |
| 12 | W8 | 202 | CYC | CMA-C3A-C4A | 4.18 | 131.50 | 125.06 |
| 12 | C7 | 201 | CYC | C2B-C1B-NB | 4.18 | 113.11 | 106.99 |
| 12 | B3 | 201 | CYC | CMA-C3A-C4A | 4.18 | 131.50 | 125.06 |
| 12 | B1 | 201 | CYC | CMA-C3A-C4A | 4.18 | 131.50 | 125.06 |
| 12 | u7 | 201 | CYC | C2B-C1B-NB | 4.18 | 113.10 | 106.99 |
| 12 | B3 | 202 | CYC | C4A-C3A-C2A | -4.17 | 101.72 | 106.51 |
| 12 | H7 | 201 | CYC | CHA-C1A-NA | -4.17 | 123.04 | 128.83 |
| 12 | j7 | 201 | CYC | CHA-C1A-NA | -4.17 | 123.04 | 128.83 |
| 12 | g7 | 201 | CYC | CHD-C4C-NC | 4.17 | 130.17 | 125.20 |
| 12 | K3 | 201 | CYC | CMB-C2B-C1B | 4.17 | 129.38 | 124.17 |
| 12 | B6 | 201 | CYC | CMA-C3A-C4A | 4.17 | 131.49 | 125.06 |
| 12 | J4 | 202 | CYC | CMA-C3A-C4A | 4.17 | 131.49 | 125.06 |
| 12 | J8 | 202 | CYC | CMA-C3A-C4A | 4.17 | 131.49 | 125.06 |
| 12 | Q5 | 201 | CYC | C2B-C1B-NB | 4.17 | 113.09 | 106.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | Q7 | 201 | CYC | C2B-C1B-NB | 4.17 | 113.09 | 106.99 |
| 12 | S4 | 201 | CYC | CMA-C3A-C4A | 4.17 | 131.49 | 125.06 |
| 12 | S8 | 201 | CYC | CMA-C3A-C4A | 4.17 | 131.49 | 125.06 |
| 12 | Q1 | 201 | CYC | CMB-C2B-C1B | 4.17 | 129.37 | 124.17 |
| 12 | Q3 | 201 | CYC | CMB-C2B-C1B | 4.17 | 129.37 | 124.17 |
| 12 | d7 | 201 | CYC | CHA-C1A-NA | -4.17 | 123.04 | 128.83 |
| 12 | J2 | 201 | CYC | CMA-C3A-C4A | 4.17 | 131.48 | 125.06 |
| 12 | R1 | 202 | CYC | CMA-C3A-C4A | 4.17 | 131.48 | 125.06 |
| 12 | R3 | 202 | CYC | CMA-C3A-C4A | 4.17 | 131.48 | 125.06 |
| 12 | f5 | 201 | CYC | CHA-C1A-NA | -4.17 | 123.05 | 128.83 |
| 12 | P1 | 202 | CYC | CMA-C3A-C4A | 4.17 | 131.48 | 125.06 |
| 12 | P3 | 202 | CYC | CMA-C3A-C4A | 4.17 | 131.48 | 125.06 |
| 12 | Z | 201 | CYC | CHA-C1A-NA | -4.17 | 123.05 | 128.83 |
| 12 | D1 | 202 | CYC | C4A-C3A-C2A | -4.17 | 101.72 | 106.51 |
| 12 | L8 | 201 | CYC | CMA-C3A-C4A | 4.16 | 131.48 | 125.06 |
| 12 | X3 | 201 | CYC | CMA-C3A-C4A | 4.16 | 131.47 | 125.06 |
| 12 | j5 | 1202 | CYC | CHA-C1A-NA | -4.16 | 123.05 | 128.83 |
| 12 | D3 | 202 | CYC | C4A-C3A-C2A | -4.16 | 101.73 | 106.51 |
| 12 | f7 | 201 | CYC | CHA-C1A-NA | -4.16 | 123.06 | 128.83 |
| 12 | aA | 902 | CYC | CMA-C3A-C4A | 4.16 | 131.47 | 125.06 |
| 12 | L4 | 201 | CYC | CMA-C3A-C4A | 4.16 | 131.47 | 125.06 |
| 12 | M7 | 201 | CYC | C2B-C1B-NB | 4.16 | 113.08 | 106.99 |
| 12 | G5 | 201 | CYC | C2B-C1B-NB | 4.16 | 113.08 | 106.99 |
| 12 | m7 | 201 | CYC | C2B-C1B-NB | 4.16 | 113.08 | 106.99 |
| 12 | L3 | 202 | CYC | CMA-C3A-C4A | 4.16 | 131.47 | 125.06 |
| 12 | B2 | 201 | CYC | CMA-C3A-C4A | 4.16 | 131.47 | 125.06 |
| 12 | J6 | 202 | CYC | C4A-C3A-C2A | -4.16 | 101.73 | 106.51 |
| 12 | r7 | 201 | CYC | CHA-C1A-NA | -4.16 | 123.06 | 128.83 |
| 12 | L2 | 201 | CYC | CMA-C3A-C4A | 4.16 | 131.46 | 125.06 |
| 12 | RA | 202 | CYC | CMA-C3A-C4A | 4.15 | 131.46 | 125.06 |
| 12 | R9 | 202 | CYC | CMA-C3A-C4A | 4.15 | 131.46 | 125.06 |
| 12 | E3 | 201 | CYC | CMB-C2B-C1B | 4.15 | 129.35 | 124.17 |
| 12 | E1 | 201 | CYC | CMB-C2B-C1B | 4.15 | 129.35 | 124.17 |
| 12 | R7 | 201 | CYC | CHA-C1A-NA | -4.15 | 123.07 | 128.83 |
| 12 | F4 | 201 | CYC | CMA-C3A-C4A | 4.15 | 131.46 | 125.06 |
| 12 | Q4 | 201 | CYC | CMA-C3A-C4A | 4.15 | 131.46 | 125.06 |
| 12 | F8 | 201 | CYC | CMA-C3A-C4A | 4.15 | 131.46 | 125.06 |
| 12 | U4 | 201 | CYC | C4A-C3A-C2A | -4.15 | 101.74 | 106.51 |
| 12 | U8 | 201 | CYC | C4A-C3A-C2A | -4.15 | 101.74 | 106.51 |
| 12 | OA | 201 | CYC | OC-C1C-NC | 4.15 | 129.97 | 124.94 |
| 12 | O9 | 201 | CYC | OC-C1C-NC | 4.15 | 129.97 | 124.94 |
| 12 | C4 | 201 | CYC | CMB-C2B-C1B | 4.15 | 129.35 | 124.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | C8 | 201 | CYC | CMB-C2B-C1B | 4.15 | 129.35 | 124.17 |
| 12 | J6 | 201 | CYC | CMA-C3A-C4A | 4.15 | 131.46 | 125.06 |
| 12 | Q8 | 201 | CYC | CMA-C3A-C4A | 4.15 | 131.46 | 125.06 |
| 12 | P5 | 201 | CYC | CHA-C1A-NA | -4.15 | 123.07 | 128.83 |
| 12 | D4 | 201 | CYC | CMA-C3A-C4A | 4.15 | 131.45 | 125.06 |
| 12 | D8 | 201 | CYC | CMA-C3A-C4A | 4.15 | 131.45 | 125.06 |
| 12 | J3 | 201 | CYC | CMA-C3A-C4A | 4.15 | 131.45 | 125.06 |
| 12 | J1 | 201 | CYC | CMA-C3A-C4A | 4.15 | 131.45 | 125.06 |
| 12 | X7 | 201 | CYC | CHA-C1A-NA | -4.15 | 123.08 | 128.83 |
| 12 | V7 | 201 | CYC | CHA-C1A-NA | -4.15 | 123.08 | 128.83 |
| 12 | TA | 301 | CYC | C4A-C3A-C2A | -4.14 | 101.75 | 106.51 |
| 12 | T9 | 301 | CYC | C4A-C3A-C2A | -4.14 | 101.75 | 106.51 |
| 12 | R9 | 201 | CYC | C4A-C3A-C2A | -4.14 | 101.75 | 106.51 |
| 12 | B7 | 201 | CYC | CHA-C1A-NA | -4.14 | 123.08 | 128.83 |
| 12 | F7 | 201 | CYC | CHA-C1A-NA | -4.14 | 123.08 | 128.83 |
| 12 | k5 | 1202 | CYC | CHA-C1A-NA | -4.14 | 123.08 | 128.83 |
| 12 | CA | 201 | CYC | OC-C1C-NC | 4.14 | 129.96 | 124.94 |
| 12 | C9 | 201 | CYC | OC-C1C-NC | 4.14 | 129.96 | 124.94 |
| 12 | LA | 201 | CYC | CMA-C3A-C4A | 4.14 | 131.44 | 125.06 |
| 12 | L9 | 201 | CYC | CMA-C3A-C4A | 4.14 | 131.44 | 125.06 |
| 12 | DA | 202 | CYC | CMA-C3A-C4A | 4.14 | 131.44 | 125.06 |
| 12 | L6 | 201 | CYC | CMA-C3A-C4A | 4.14 | 131.44 | 125.06 |
| 12 | B1 | 202 | CYC | CMA-C3A-C4A | 4.14 | 131.44 | 125.06 |
| 12 | J2 | 202 | CYC | C4A-C3A-C2A | -4.14 | 101.75 | 106.51 |
| 12 | B3 | 202 | CYC | CMA-C3A-C4A | 4.14 | 131.44 | 125.06 |
| 12 | WA | 201 | CYC | CMB-C2B-C1B | 4.14 | 129.34 | 124.17 |
| 12 | W9 | 201 | CYC | CMB-C2B-C1B | 4.14 | 129.34 | 124.17 |
| 12 | VA | 201 | CYC | CMA-C3A-C4A | 4.14 | 131.44 | 125.06 |
| 12 | V9 | 201 | CYC | CMA-C3A-C4A | 4.14 | 131.44 | 125.06 |
| 12 | K4 | 201 | CYC | OC-C1C-NC | 4.14 | 129.95 | 124.94 |
| 12 | K8 | 201 | CYC | OC-C1C-NC | 4.14 | 129.95 | 124.94 |
| 12 | TA | 302 | CYC | CMA-C3A-C4A | 4.14 | 131.44 | 125.06 |
| 12 | T9 | 302 | CYC | CMA-C3A-C4A | 4.14 | 131.44 | 125.06 |
| 12 | HA | 201 | CYC | CMA-C3A-C4A | 4.14 | 131.43 | 125.06 |
| 12 | H9 | 201 | CYC | CMA-C3A-C4A | 4.14 | 131.43 | 125.06 |
| 12 | U4 | 202 | CYC | CMA-C3A-C4A | 4.14 | 131.43 | 125.06 |
| 12 | U8 | 202 | CYC | CMA-C3A-C4A | 4.14 | 131.43 | 125.06 |
| 12 | P9 | 201 | CYC | C4A-C3A-C2A | -4.14 | 101.76 | 106.51 |
| 12 | G6 | 201 | CYC | CMB-C2B-C1B | 4.13 | 129.33 | 124.17 |
| 12 | F5 | 201 | CYC | CHA-C1A-NA | -4.13 | 123.09 | 128.83 |
| 12 | e7 | 201 | CYC | C2B-C1B-NB | 4.13 | 113.04 | 106.99 |
| 12 | Z3 | 201 | CYC | CMA-C3A-C4A | 4.13 | 131.43 | 125.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | L3 | 201 | CYC | CMA-C3A-C4A | 4.13 | 131.43 | 125.06 |
| 12 | F6 | 202 | CYC | CMA-C3A-C4A | 4.13 | 131.43 | 125.06 |
| 12 | L1 | 201 | CYC | CMA-C3A-C4A | 4.13 | 131.43 | 125.06 |
| 12 | Z1 | 202 | CYC | CMA-C3A-C4A | 4.13 | 131.43 | 125.06 |
| 12 | V4 | 201 | CYC | CMB-C2B-C1B | 4.13 | 129.33 | 124.17 |
| 12 | b7 | 201 | CYC | CHA-C1A-NA | -4.13 | 123.09 | 128.83 |
| 12 | N5 | 201 | CYC | CHA-C1A-NA | -4.13 | 123.10 | 128.83 |
| 12 | B4 | 202 | CYC | C4A-C3A-C2A | -4.13 | 101.77 | 106.51 |
| 12 | F3 | 202 | CYC | CMA-C3A-C4A | 4.13 | 131.42 | 125.06 |
| 12 | G7 | 201 | CYC | C2B-C1B-NB | 4.13 | 113.03 | 106.99 |
| 12 | L2 | 201 | CYC | C4A-C3A-C2A | -4.13 | 101.77 | 106.51 |
| 12 | D9 | 202 | CYC | CMA-C3A-C4A | 4.13 | 131.42 | 125.06 |
| 12 | X1 | 201 | CYC | CMA-C3A-C4A | 4.12 | 131.42 | 125.06 |
| 12 | L5 | 201 | CYC | CHA-C1A-NA | -4.12 | 123.11 | 128.83 |
| 12 | k5 | 1203 | CYC | CHA-C1A-NA | -4.12 | 123.11 | 128.83 |
| 12 | A5 | 201 | CYC | C2B-C1B-NB | 4.12 | 113.03 | 106.99 |
| 12 | K2 | 201 | CYC | OC-C1C-NC | 4.12 | 129.94 | 124.94 |
| 12 | PA | 201 | CYC | C4A-C3A-C2A | -4.12 | 101.77 | 106.51 |
| 12 | Y4 | 201 | CYC | CMA-C3A-C4A | 4.12 | 131.41 | 125.06 |
| 12 | Z3 | 202 | CYC | CMA-C3A-C4A | 4.12 | 131.41 | 125.06 |
| 12 | G2 | 201 | CYC | CMB-C2B-C1B | 4.12 | 129.31 | 124.17 |
| 12 | L7 | 201 | CYC | CHA-C1A-NA | -4.12 | 123.11 | 128.83 |
| 12 | L2 | 202 | CYC | CMA-C3A-C4A | 4.12 | 131.41 | 125.06 |
| 12 | s7 | 201 | CYC | C2B-C1B-NB | 4.12 | 113.02 | 106.99 |
| 12 | RA | 201 | CYC | C4A-C3A-C2A | -4.12 | 101.78 | 106.51 |
| 12 | Y8 | 201 | CYC | CMA-C3A-C4A | 4.12 | 131.40 | 125.06 |
| 12 | U4 | 201 | CYC | CMA-C3A-C4A | 4.11 | 131.40 | 125.06 |
| 12 | U8 | 201 | CYC | CMA-C3A-C4A | 4.11 | 131.40 | 125.06 |
| 12 | B8 | 202 | CYC | C4A-C3A-C2A | -4.11 | 101.78 | 106.51 |
| 12 | VA | 202 | CYC | CMA-C3A-C4A | 4.11 | 131.40 | 125.06 |
| 12 | V9 | 202 | CYC | CMA-C3A-C4A | 4.11 | 131.40 | 125.06 |
| 12 | D7 | 201 | CYC | CHA-C1A-NA | -4.11 | 123.12 | 128.83 |
| 12 | X3 | 202 | CYC | CMA-C3A-C4A | 4.11 | 131.40 | 125.06 |
| 12 | X1 | 202 | CYC | CMA-C3A-C4A | 4.11 | 131.40 | 125.06 |
| 12 | Y7 | 201 | CYC | C2B-C1B-NB | 4.11 | 113.01 | 106.99 |
| 12 | V8 | 201 | CYC | CMB-C2B-C1B | 4.11 | 129.30 | 124.17 |
| 12 | L6 | 202 | CYC | CMA-C3A-C4A | 4.11 | 131.39 | 125.06 |
| 12 | AA | 201 | CYC | CMB-C2B-C1B | 4.11 | 129.30 | 124.17 |
| 12 | A9 | 201 | CYC | CMB-C2B-C1B | 4.11 | 129.30 | 124.17 |
| 12 | R1 | 201 | CYC | C4A-C3A-C2A | -4.11 | 101.79 | 106.51 |
| 12 | F1 | 202 | CYC | CMA-C3A-C4A | 4.11 | 131.39 | 125.06 |
| 12 | JA | 201 | CYC | CMA-C3A-C4A | 4.11 | 131.39 | 125.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | J9 | 201 | CYC | CMA-C3A-C4A | 4.11 | 131.39 | 125.06 |
| 12 | S4 | 202 | CYC | C4A-C3A-C2A | -4.11 | 101.79 | 106.51 |
| 12 | Z1 | 201 | CYC | CMA-C3A-C4A | 4.11 | 131.39 | 125.06 |
| 12 | D1 | 202 | CYC | CMA-C3A-C4A | 4.11 | 131.39 | 125.06 |
| 12 | D3 | 202 | CYC | CMA-C3A-C4A | 4.10 | 131.38 | 125.06 |
| 12 | F2 | 202 | CYC | CMA-C3A-C4A | 4.10 | 131.38 | 125.06 |
| 12 | R3 | 201 | CYC | C4A-C3A-C2A | -4.10 | 101.80 | 106.51 |
| 12 | W1 | 201 | CYC | OC-C1C-NC | 4.10 | 129.91 | 124.94 |
| 12 | LA | 202 | CYC | CMA-C3A-C4A | 4.10 | 131.38 | 125.06 |
| 12 | TA | 301 | CYC | CMA-C3A-C4A | 4.10 | 131.38 | 125.06 |
| 12 | L9 | 202 | CYC | CMA-C3A-C4A | 4.10 | 131.38 | 125.06 |
| 12 | T9 | 301 | CYC | CMA-C3A-C4A | 4.10 | 131.38 | 125.06 |
| 12 | V4 | 201 | CYC | OC-C1C-NC | 4.10 | 129.91 | 124.94 |
| 12 | V8 | 201 | CYC | OC-C1C-NC | 4.10 | 129.91 | 124.94 |
| 12 | L6 | 201 | CYC | C4A-C3A-C2A | -4.10 | 101.80 | 106.51 |
| 12 | aA | 902 | CYC | C4A-C3A-C2A | -4.10 | 101.80 | 106.51 |
| 12 | W3 | 201 | CYC | CMB-C2B-C1B | 4.10 | 129.28 | 124.17 |
| 12 | W1 | 201 | CYC | CMB-C2B-C1B | 4.10 | 129.28 | 124.17 |
| 12 | V5 | 201 | CYC | CHA-C1A-NA | -4.10 | 123.15 | 128.83 |
| 12 | N6 | 101 | CYC | CMA-C3A-C4A | 4.09 | 131.37 | 125.06 |
| 12 | X3 | 201 | CYC | C4A-C3A-C2A | -4.09 | 101.81 | 106.51 |
| 12 | U4 | 202 | CYC | C1B-C2B-C3B | -4.09 | 103.60 | 107.87 |
| 12 | P4 | 201 | CYC | CMB-C2B-C1B | 4.09 | 129.28 | 124.17 |
| 12 | E4 | 201 | CYC | OC-C1C-NC | 4.09 | 129.90 | 124.94 |
| 12 | E8 | 201 | CYC | OC-C1C-NC | 4.09 | 129.90 | 124.94 |
| 12 | M5 | 201 | CYC | C2B-C1B-NB | 4.09 | 112.98 | 106.99 |
| 12 | d5 | 201 | CYC | CHA-C1A-NA | -4.09 | 123.15 | 128.83 |
| 12 | X1 | 201 | CYC | C4A-C3A-C2A | -4.09 | 101.81 | 106.51 |
| 12 | O1 | 201 | CYC | OC-C1C-NC | 4.09 | 129.89 | 124.94 |
| 12 | O3 | 201 | CYC | OC-C1C-NC | 4.09 | 129.89 | 124.94 |
| 12 | LA | 202 | CYC | C4A-C3A-C2A | -4.09 | 101.81 | 106.51 |
| 12 | L9 | 202 | CYC | C4A-C3A-C2A | -4.09 | 101.81 | 106.51 |
| 12 | R9 | 201 | CYC | CMA-C3A-C4A | 4.09 | 131.36 | 125.06 |
| 12 | B5 | 201 | CYC | CHA-C1A-NA | -4.09 | 123.16 | 128.83 |
| 12 | M4 | 301 | CYC | C4A-C3A-C2A | -4.08 | 101.82 | 106.51 |
| 12 | L3 | 202 | CYC | C4A-C3A-C2A | -4.08 | 101.82 | 106.51 |
| 12 | J7 | 201 | CYC | CHA-C1A-NA | -4.08 | 123.17 | 128.83 |
| 12 | h7 | 201 | CYC | CHA-C1A-NA | -4.08 | 123.17 | 128.83 |
| 12 | K3 | 201 | CYC | OC-C1C-NC | 4.08 | 129.88 | 124.94 |
| 12 | W3 | 201 | CYC | OC-C1C-NC | 4.08 | 129.88 | 124.94 |
| 12 | K1 | 201 | CYC | OC-C1C-NC | 4.08 | 129.88 | 124.94 |
| 12 | ZA | 202 | CYC | CMA-C3A-C4A | 4.08 | 131.34 | 125.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | Z9 | 202 | CYC | CMA-C3A-C4A | 4.08 | 131.34 | 125.06 |
| 12 | DA | 201 | CYC | CMA-C3A-C4A | 4.08 | 131.34 | 125.06 |
| 12 | ZA | 201 | CYC | CMA-C3A-C4A | 4.08 | 131.34 | 125.06 |
| 12 | D9 | 201 | CYC | CMA-C3A-C4A | 4.08 | 131.34 | 125.06 |
| 12 | Z9 | 201 | CYC | CMA-C3A-C4A | 4.08 | 131.34 | 125.06 |
| 12 | W4 | 201 | CYC | CMA-C3A-C4A | 4.08 | 131.34 | 125.06 |
| 12 | W8 | 201 | CYC | CMA-C3A-C4A | 4.08 | 131.34 | 125.06 |
| 12 | N7 | 201 | CYC | CHA-C1A-NA | -4.08 | 123.17 | 128.83 |
| 12 | R5 | 201 | CYC | CHA-C1A-NA | -4.08 | 123.17 | 128.83 |
| 12 | J6 | 202 | CYC | CMA-C3A-C4A | 4.08 | 131.34 | 125.06 |
| 12 | X5 | 201 | CYC | CHA-C1A-NA | -4.08 | 123.17 | 128.83 |
| 12 | A4 | 201 | CYC | OC-C1C-NC | 4.07 | 129.88 | 124.94 |
| 12 | A8 | 201 | CYC | OC-C1C-NC | 4.07 | 129.88 | 124.94 |
| 12 | P8 | 201 | CYC | CMB-C2B-C1B | 4.07 | 129.25 | 124.17 |
| 12 | H5 | 201 | CYC | CHA-C1A-NA | -4.07 | 123.18 | 128.83 |
| 12 | H4 | 201 | CYC | C4A-C3A-C2A | -4.07 | 101.83 | 106.51 |
| 12 | H8 | 201 | CYC | C4A-C3A-C2A | -4.07 | 101.83 | 106.51 |
| 12 | S1 | 201 | CYC | CMB-C2B-C1B | 4.07 | 129.25 | 124.17 |
| 12 | P7 | 201 | CYC | CHA-C1A-NA | -4.07 | 123.18 | 128.83 |
| 12 | AA | 201 | CYC | OC-C1C-NC | 4.07 | 129.87 | 124.94 |
| 12 | A9 | 201 | CYC | OC-C1C-NC | 4.07 | 129.87 | 124.94 |
| 12 | BA | 201 | CYC | C4A-C3A-C2A | -4.07 | 101.83 | 106.51 |
| 12 | D2 | 201 | CYC | C4A-C3A-C2A | -4.07 | 101.83 | 106.51 |
| 12 | J2 | 202 | CYC | CMA-C3A-C4A | 4.07 | 131.33 | 125.06 |
| 12 | D4 | 202 | CYC | CMA-C3A-C4A | 4.07 | 131.33 | 125.06 |
| 12 | D8 | 202 | CYC | CMA-C3A-C4A | 4.07 | 131.33 | 125.06 |
| 12 | H3 | 202 | CYC | CMA-C3A-C4A | 4.07 | 131.33 | 125.06 |
| 12 | N2 | 101 | CYC | CMA-C3A-C4A | 4.07 | 131.33 | 125.06 |
| 12 | B9 | 201 | CYC | C4A-C3A-C2A | -4.07 | 101.84 | 106.51 |
| 12 | H1 | 201 | CYC | CMA-C3A-C4A | 4.07 | 131.33 | 125.06 |
| 12 | C3 | 201 | CYC | OC-C1C-NC | 4.07 | 129.87 | 124.94 |
| 12 | RA | 201 | CYC | CMA-C3A-C4A | 4.06 | 131.32 | 125.06 |
| 12 | U8 | 202 | CYC | C1B-C2B-C3B | -4.06 | 103.63 | 107.87 |
| 12 | K6 | 201 | CYC | OC-C1C-NC | 4.06 | 129.86 | 124.94 |
| 12 | H2 | 201 | CYC | CMA-C3A-C4A | 4.06 | 131.32 | 125.06 |
| 12 | J8 | 201 | CYC | C4A-C3A-C2A | -4.06 | 101.84 | 106.51 |
| 12 | T7 | 201 | CYC | CHA-C1A-NA | -4.06 | 123.20 | 128.83 |
| 12 | E3 | 201 | CYC | OC-C1C-NC | 4.06 | 129.85 | 124.94 |
| 12 | E1 | 201 | CYC | OC-C1C-NC | 4.06 | 129.85 | 124.94 |
| 12 | DA | 201 | CYC | C4A-C3A-C2A | -4.06 | 101.85 | 106.51 |
| 12 | D9 | 201 | CYC | C4A-C3A-C2A | -4.06 | 101.85 | 106.51 |
| 12 | BA | 201 | CYC | CMA-C3A-C4A | 4.06 | 131.31 | 125.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | q7 | 201 | CYC | C2B-C1B-NB | 4.06 | 112.93 | 106.99 |
| 12 | B9 | 201 | CYC | CMA-C3A-C4A | 4.06 | 131.31 | 125.06 |
| 12 | C1 | 201 | CYC | OC-C1C-NC | 4.05 | 129.85 | 124.94 |
| 12 | A1 | 201 | CYC | OC-C1C-NC | 4.05 | 129.85 | 124.94 |
| 12 | A3 | 201 | CYC | OC-C1C-NC | 4.05 | 129.85 | 124.94 |
| 12 | Z3 | 201 | CYC | C4A-C3A-C2A | -4.05 | 101.85 | 106.51 |
| 12 | Z1 | 202 | CYC | C4A-C3A-C2A | -4.05 | 101.85 | 106.51 |
| 12 | S5 | 201 | CYC | C2B-C1B-NB | 4.05 | 112.92 | 106.99 |
| 12 | J4 | 201 | CYC | C4A-C3A-C2A | -4.05 | 101.86 | 106.51 |
| 12 | V3 | 201 | CYC | C4A-C3A-C2A | -4.05 | 101.86 | 106.51 |
| 12 | V1 | 201 | CYC | C4A-C3A-C2A | -4.05 | 101.86 | 106.51 |
| 12 | D5 | 201 | CYC | CHA-C1A-NA | -4.05 | 123.21 | 128.83 |
| 12 | U3 | 201 | CYC | OC-C1C-NC | 4.05 | 129.85 | 124.94 |
| 12 | U1 | 201 | CYC | OC-C1C-NC | 4.05 | 129.85 | 124.94 |
| 12 | FA | 301 | CYC | CMA-C3A-C4A | 4.05 | 131.30 | 125.06 |
| 12 | F9 | 301 | CYC | CMA-C3A-C4A | 4.05 | 131.30 | 125.06 |
| 12 | JA | 202 | CYC | C4A-C3A-C2A | -4.05 | 101.86 | 106.51 |
| 12 | J9 | 202 | CYC | C4A-C3A-C2A | -4.05 | 101.86 | 106.51 |
| 12 | T4 | 201 | CYC | OC-C1C-NC | 4.05 | 129.84 | 124.94 |
| 12 | T8 | 201 | CYC | OC-C1C-NC | 4.05 | 129.84 | 124.94 |
| 12 | D6 | 202 | CYC | CMA-C3A-C4A | 4.04 | 131.29 | 125.06 |
| 12 | Y3 | 201 | CYC | OC-C1C-NC | 4.04 | 129.84 | 124.94 |
| 12 | Y1 | 201 | CYC | OC-C1C-NC | 4.04 | 129.84 | 124.94 |
| 12 | S3 | 201 | CYC | CMB-C2B-C1B | 4.04 | 129.22 | 124.17 |
| 12 | P1 | 201 | CYC | CMA-C3A-C4A | 4.04 | 131.29 | 125.06 |
| 12 | P3 | 201 | CYC | CMA-C3A-C4A | 4.04 | 131.29 | 125.06 |
| 12 | O4 | 201 | CYC | CMA-C3A-C4A | 4.04 | 131.29 | 125.06 |
| 12 | O8 | 201 | CYC | CMA-C3A-C4A | 4.04 | 131.29 | 125.06 |
| 12 | N4 | 201 | CYC | OC-C1C-NC | 4.04 | 129.84 | 124.94 |
| 12 | P4 | 201 | CYC | OC-C1C-NC | 4.04 | 129.84 | 124.94 |
| 12 | N8 | 201 | CYC | OC-C1C-NC | 4.04 | 129.84 | 124.94 |
| 12 | P8 | 201 | CYC | OC-C1C-NC | 4.04 | 129.84 | 124.94 |
| 12 | D3 | 201 | CYC | CMA-C3A-C4A | 4.04 | 131.29 | 125.06 |
| 12 | D1 | 201 | CYC | CMA-C3A-C4A | 4.04 | 131.29 | 125.06 |
| 12 | M8 | 302 | CYC | C4A-C3A-C2A | -4.04 | 101.87 | 106.51 |
| 12 | D2 | 202 | CYC | CMA-C3A-C4A | 4.04 | 131.28 | 125.06 |
| 12 | X4 | 201 | CYC | CHA-C1A-NA | -4.04 | 123.23 | 128.83 |
| 12 | X8 | 201 | CYC | CHA-C1A-NA | -4.04 | 123.23 | 128.83 |
| 12 | H2 | 202 | CYC | C1B-C2B-C3B | -4.04 | 103.66 | 107.87 |
| 12 | H6 | 201 | CYC | CMA-C3A-C4A | 4.04 | 131.28 | 125.06 |
| 12 | J5 | 201 | CYC | CHA-C1A-NA | -4.03 | 123.23 | 128.83 |
| 12 | B4 | 202 | CYC | CMA-C3A-C4A | 4.03 | 131.28 | 125.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | RA | 202 | CYC | C1B-C2B-C3B | -4.03 | 103.66 | 107.87 |
| 12 | R9 | 202 | CYC | C1B-C2B-C3B | -4.03 | 103.66 | 107.87 |
| 12 | XA | 201 | CYC | CMA-C3A-C4A | 4.03 | 131.27 | 125.06 |
| 12 | X9 | 201 | CYC | CMA-C3A-C4A | 4.03 | 131.27 | 125.06 |
| 12 | k7 | 201 | CYC | C2B-C1B-NB | 4.03 | 112.89 | 106.99 |
| 12 | aA | 901 | CYC | C4A-C3A-C2A | -4.03 | 101.88 | 106.51 |
| 12 | aA | 901 | CYC | CMA-C3A-C4A | 4.03 | 131.27 | 125.06 |
| 12 | J3 | 202 | CYC | CMA-C3A-C4A | 4.03 | 131.27 | 125.06 |
| 12 | P1 | 201 | CYC | C4A-C3A-C2A | -4.03 | 101.88 | 106.51 |
| 12 | D4 | 202 | CYC | C4A-C3A-C2A | -4.03 | 101.88 | 106.51 |
| 12 | P3 | 201 | CYC | C4A-C3A-C2A | -4.03 | 101.88 | 106.51 |
| 12 | D8 | 202 | CYC | C4A-C3A-C2A | -4.03 | 101.88 | 106.51 |
| 12 | F6 | 201 | CYC | CMA-C3A-C4A | 4.03 | 131.26 | 125.06 |
| 12 | V3 | 202 | CYC | C1B-C2B-C3B | -4.03 | 103.67 | 107.87 |
| 12 | V1 | 202 | CYC | C1B-C2B-C3B | -4.03 | 103.67 | 107.87 |
| 12 | H4 | 201 | CYC | CMA-C3A-C4A | 4.03 | 131.26 | 125.06 |
| 12 | H8 | 201 | CYC | CMA-C3A-C4A | 4.03 | 131.26 | 125.06 |
| 12 | H9 | 201 | CYC | C1B-C2B-C3B | -4.02 | 103.67 | 107.87 |
| 12 | JA | 202 | CYC | CMA-C3A-C4A | 4.02 | 131.26 | 125.06 |
| 12 | J9 | 202 | CYC | CMA-C3A-C4A | 4.02 | 131.26 | 125.06 |
| 12 | V1 | 201 | CYC | CMA-C3A-C4A | 4.02 | 131.26 | 125.06 |
| 12 | S7 | 201 | CYC | C2B-C1B-NB | 4.02 | 112.88 | 106.99 |
| 12 | R1 | 201 | CYC | CMA-C3A-C4A | 4.02 | 131.26 | 125.06 |
| 12 | R3 | 201 | CYC | CMA-C3A-C4A | 4.02 | 131.26 | 125.06 |
| 12 | I6 | 201 | CYC | OC-C1C-NC | 4.02 | 129.81 | 124.94 |
| 12 | H3 | 202 | CYC | C4A-C3A-C2A | -4.02 | 101.89 | 106.51 |
| 12 | H6 | 201 | CYC | C4A-C3A-C2A | -4.02 | 101.89 | 106.51 |
| 12 | N2 | 101 | CYC | C4A-C3A-C2A | -4.02 | 101.89 | 106.51 |
| 12 | N6 | 101 | CYC | C4A-C3A-C2A | -4.02 | 101.89 | 106.51 |
| 12 | S1 | 201 | CYC | OC-C1C-NC | 4.02 | 129.81 | 124.94 |
| 12 | S3 | 201 | CYC | OC-C1C-NC | 4.02 | 129.81 | 124.94 |
| 12 | I4 | 201 | CYC | OC-C1C-NC | 4.02 | 129.81 | 124.94 |
| 12 | I8 | 201 | CYC | OC-C1C-NC | 4.02 | 129.81 | 124.94 |
| 12 | E6 | 201 | CYC | CHA-C1A-NA | -4.02 | 123.25 | 128.83 |
| 12 | HA | 202 | CYC | CMA-C3A-C4A | 4.02 | 131.25 | 125.06 |
| 12 | B8 | 202 | CYC | CMA-C3A-C4A | 4.02 | 131.25 | 125.06 |
| 12 | Q1 | 201 | CYC | OC-C1C-NC | 4.02 | 129.81 | 124.94 |
| 12 | Q3 | 201 | CYC | OC-C1C-NC | 4.02 | 129.81 | 124.94 |
| 12 | H2 | 201 | CYC | C4A-C3A-C2A | -4.02 | 101.90 | 106.51 |
| 12 | H9 | 202 | CYC | CMA-C3A-C4A | 4.02 | 131.25 | 125.06 |
| 12 | H1 | 201 | CYC | C4A-C3A-C2A | -4.01 | 101.90 | 106.51 |
| 12 | HA | 201 | CYC | C1B-C2B-C3B | -4.01 | 103.68 | 107.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | VA | 201 | CYC | C4A-C3A-C2A | -4.01 | 101.90 | 106.51 |
| 12 | V9 | 201 | CYC | C4A-C3A-C2A | -4.01 | 101.90 | 106.51 |
| 12 | J4 | 201 | CYC | CMA-C3A-C4A | 4.01 | 131.24 | 125.06 |
| 12 | J8 | 201 | CYC | CMA-C3A-C4A | 4.01 | 131.24 | 125.06 |
| 12 | L4 | 202 | CYC | CMA-C3A-C4A | 4.01 | 131.24 | 125.06 |
| 12 | ZA | 202 | CYC | C4A-C3A-C2A | -4.01 | 101.90 | 106.51 |
| 12 | Z9 | 202 | CYC | C4A-C3A-C2A | -4.01 | 101.90 | 106.51 |
| 12 | J6 | 201 | CYC | C1B-C2B-C3B | -4.01 | 103.69 | 107.87 |
| 12 | H1 | 202 | CYC | C1B-C2B-C3B | -4.01 | 103.69 | 107.87 |
| 12 | R4 | 201 | CYC | OC-C1C-NC | 4.01 | 129.80 | 124.94 |
| 12 | XA | 201 | CYC | C4A-C3A-C2A | -4.01 | 101.91 | 106.51 |
| 12 | X9 | 201 | CYC | C4A-C3A-C2A | -4.01 | 101.91 | 106.51 |
| 12 | E2 | 201 | CYC | CHA-C1A-NA | -4.01 | 123.27 | 128.83 |
| 12 | I3 | 201 | CYC | OC-C1C-NC | 4.00 | 129.79 | 124.94 |
| 12 | U9 | 201 | CYC | OC-C1C-NC | 4.00 | 129.79 | 124.94 |
| 12 | I1 | 201 | CYC | OC-C1C-NC | 4.00 | 129.79 | 124.94 |
| 12 | F4 | 202 | CYC | C4A-C3A-C2A | -4.00 | 101.91 | 106.51 |
| 12 | F8 | 202 | CYC | C4A-C3A-C2A | -4.00 | 101.91 | 106.51 |
| 12 | Z5 | 201 | CYC | CHA-C1A-NA | -4.00 | 123.28 | 128.83 |
| 12 | D6 | 201 | CYC | C4A-C3A-C2A | -4.00 | 101.91 | 106.51 |
| 12 | V3 | 201 | CYC | CMA-C3A-C4A | 4.00 | 131.22 | 125.06 |
| 12 | IA | 201 | CYC | OC-C1C-NC | 4.00 | 129.78 | 124.94 |
| 12 | E6 | 201 | CYC | OC-C1C-NC | 4.00 | 129.78 | 124.94 |
| 12 | I9 | 201 | CYC | OC-C1C-NC | 4.00 | 129.78 | 124.94 |
| 12 | W4 | 201 | CYC | C4A-C3A-C2A | -4.00 | 101.92 | 106.51 |
| 12 | W8 | 201 | CYC | C4A-C3A-C2A | -4.00 | 101.92 | 106.51 |
| 12 | IA | 201 | CYC | CHA-C1A-NA | -4.00 | 123.28 | 128.83 |
| 12 | I9 | 201 | CYC | CHA-C1A-NA | -4.00 | 123.28 | 128.83 |
| 12 | J3 | 202 | CYC | C4A-C3A-C2A | -4.00 | 101.92 | 106.51 |
| 12 | F3 | 202 | CYC | CHA-C1A-NA | -4.00 | 123.28 | 128.83 |
| 12 | M4 | 301 | CYC | CMA-C3A-C4A | 4.00 | 131.22 | 125.06 |
| 12 | J2 | 201 | CYC | C1B-C2B-C3B | -3.99 | 103.70 | 107.87 |
| 12 | L4 | 202 | CYC | C4A-C3A-C2A | -3.99 | 101.92 | 106.51 |
| 12 | B4 | 201 | CYC | C1B-C2B-C3B | -3.99 | 103.70 | 107.87 |
| 12 | B8 | 201 | CYC | C1B-C2B-C3B | -3.99 | 103.70 | 107.87 |
| 12 | C3 | 201 | CYC | CHA-C1A-NA | -3.99 | 123.29 | 128.83 |
| 12 | C1 | 201 | CYC | CHA-C1A-NA | -3.99 | 123.29 | 128.83 |
| 12 | F3 | 202 | CYC | C1B-C2B-C3B | -3.99 | 103.71 | 107.87 |
| 12 | F1 | 202 | CYC | C1B-C2B-C3B | -3.99 | 103.71 | 107.87 |
| 12 | J9 | 201 | CYC | C1B-C2B-C3B | -3.99 | 103.71 | 107.87 |
| 12 | F3 | 201 | CYC | C4A-C3A-C2A | -3.99 | 101.93 | 106.51 |
| 12 | F1 | 201 | CYC | C4A-C3A-C2A | -3.99 | 101.93 | 106.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | FA | 301 | CYC | C4A-C3A-C2A | -3.99 | 101.93 | 106.51 |
| 12 | F9 | 301 | CYC | C4A-C3A-C2A | -3.99 | 101.93 | 106.51 |
| 12 | G2 | 201 | CYC | OC-C1C-NC | 3.99 | 129.77 | 124.94 |
| 12 | F6 | 201 | CYC | C4A-C3A-C2A | -3.99 | 101.93 | 106.51 |
| 12 | F3 | 201 | CYC | CMA-C3A-C4A | 3.99 | 131.20 | 125.06 |
| 12 | F1 | 201 | CYC | CMA-C3A-C4A | 3.99 | 131.20 | 125.06 |
| 12 | F8 | 202 | CYC | CMA-C3A-C4A | 3.99 | 131.20 | 125.06 |
| 12 | a9 | 901 | CYC | CMA-C3A-C4A | 3.99 | 131.20 | 125.06 |
| 12 | I2 | 201 | CYC | OC-C1C-NC | 3.99 | 129.77 | 124.94 |
| 12 | H6 | 202 | CYC | C1B-C2B-C3B | -3.99 | 103.71 | 107.87 |
| 12 | WA | 201 | CYC | OC-C1C-NC | 3.98 | 129.76 | 124.94 |
| 12 | W9 | 201 | CYC | OC-C1C-NC | 3.98 | 129.76 | 124.94 |
| 12 | UA | 201 | CYC | OC-C1C-NC | 3.98 | 129.76 | 124.94 |
| 12 | F4 | 202 | CYC | CMA-C3A-C4A | 3.98 | 131.19 | 125.06 |
| 12 | C4 | 201 | CYC | OC-C1C-NC | 3.98 | 129.76 | 124.94 |
| 12 | C8 | 201 | CYC | OC-C1C-NC | 3.98 | 129.76 | 124.94 |
| 12 | R8 | 201 | CYC | OC-C1C-NC | 3.98 | 129.76 | 124.94 |
| 12 | SA | 201 | CYC | OC-C1C-NC | 3.98 | 129.76 | 124.94 |
| 12 | S9 | 201 | CYC | OC-C1C-NC | 3.98 | 129.76 | 124.94 |
| 12 | a9 | 901 | CYC | C4A-C3A-C2A | -3.98 | 101.94 | 106.51 |
| 12 | VA | 202 | CYC | C1B-C2B-C3B | -3.98 | 103.72 | 107.87 |
| 12 | S4 | 202 | CYC | CMA-C3A-C4A | 3.98 | 131.19 | 125.06 |
| 12 | E2 | 201 | CYC | OC-C1C-NC | 3.98 | 129.76 | 124.94 |
| 12 | D6 | 201 | CYC | CMA-C3A-C4A | 3.97 | 131.19 | 125.06 |
| 12 | F2 | 201 | CYC | CMA-C3A-C4A | 3.97 | 131.19 | 125.06 |
| 12 | YA | 201 | CYC | OC-C1C-NC | 3.97 | 129.75 | 124.94 |
| 12 | H3 | 201 | CYC | C1B-C2B-C3B | -3.97 | 103.72 | 107.87 |
| 12 | Z3 | 202 | CYC | C1B-C2B-C3B | -3.97 | 103.72 | 107.87 |
| 12 | Z1 | 201 | CYC | C1B-C2B-C3B | -3.97 | 103.72 | 107.87 |
| 12 | Z4 | 301 | CYC | CMA-C3A-C4A | 3.97 | 131.18 | 125.06 |
| 12 | G1 | 201 | CYC | OC-C1C-NC | 3.97 | 129.75 | 124.94 |
| 12 | QA | 201 | CYC | OC-C1C-NC | 3.97 | 129.75 | 124.94 |
| 12 | Z4 | 301 | CYC | C4A-C3A-C2A | -3.97 | 101.95 | 106.51 |
| 12 | Z8 | 301 | CYC | CMA-C3A-C4A | 3.97 | 131.18 | 125.06 |
| 12 | G4 | 201 | CYC | OC-C1C-NC | 3.97 | 129.75 | 124.94 |
| 12 | T3 | 301 | CYC | CMA-C3A-C4A | 3.97 | 131.18 | 125.06 |
| 12 | T1 | 301 | CYC | CMA-C3A-C4A | 3.97 | 131.18 | 125.06 |
| 12 | M8 | 301 | CYC | CMA-C3A-C4A | 3.97 | 131.17 | 125.06 |
| 12 | C6 | 201 | CYC | OC-C1C-NC | 3.97 | 129.75 | 124.94 |
| 12 | G6 | 201 | CYC | OC-C1C-NC | 3.97 | 129.75 | 124.94 |
| 12 | S3 | 201 | CYC | CHA-C1A-NA | -3.97 | 123.33 | 128.83 |
| 12 | F1 | 202 | CYC | CHA-C1A-NA | -3.97 | 123.33 | 128.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | Y9 | 201 | CYC | OC-C1C-NC | 3.97 | 129.75 | 124.94 |
| 12 | X1 | 202 | CYC | CHA-C1A-NA | -3.96 | 123.33 | 128.83 |
| 12 | M8 | 301 | CYC | C4A-C3A-C2A | -3.96 | 101.96 | 106.51 |
| 12 | KA | 201 | CYC | OC-C1C-NC | 3.96 | 129.74 | 124.94 |
| 12 | K9 | 201 | CYC | OC-C1C-NC | 3.96 | 129.74 | 124.94 |
| 12 | PA | 202 | CYC | C1B-C2B-C3B | -3.96 | 103.73 | 107.87 |
| 12 | P9 | 202 | CYC | C1B-C2B-C3B | -3.96 | 103.73 | 107.87 |
| 12 | B3 | 201 | CYC | CHA-C1A-NA | -3.96 | 123.33 | 128.83 |
| 12 | B1 | 201 | CYC | CHA-C1A-NA | -3.96 | 123.33 | 128.83 |
| 12 | J1 | 201 | CYC | C1B-C2B-C3B | -3.96 | 103.74 | 107.87 |
| 12 | Q9 | 201 | CYC | OC-C1C-NC | 3.96 | 129.74 | 124.94 |
| 12 | C9 | 201 | CYC | CHA-C1A-NA | -3.96 | 123.33 | 128.83 |
| 12 | JA | 201 | CYC | C1B-C2B-C3B | -3.96 | 103.74 | 107.87 |
| 12 | F6 | 202 | CYC | CHA-C1A-NA | -3.96 | 123.33 | 128.83 |
| 12 | B8 | 201 | CYC | CAB-C3B-C4B | 3.96 | 127.63 | 121.38 |
| 12 | Y4 | 201 | CYC | C1B-C2B-C3B | -3.96 | 103.74 | 107.87 |
| 12 | Y8 | 201 | CYC | C1B-C2B-C3B | -3.96 | 103.74 | 107.87 |
| 12 | S1 | 201 | CYC | CHA-C1A-NA | -3.96 | 123.34 | 128.83 |
| 12 | H4 | 202 | CYC | C1B-C2B-C3B | -3.96 | 103.74 | 107.87 |
| 12 | H8 | 202 | CYC | C1B-C2B-C3B | -3.96 | 103.74 | 107.87 |
| 12 | O1 | 201 | CYC | CHA-C1A-NA | -3.96 | 123.34 | 128.83 |
| 12 | O3 | 201 | CYC | CHA-C1A-NA | -3.96 | 123.34 | 128.83 |
| 12 | GA | 201 | CYC | OC-C1C-NC | 3.95 | 129.73 | 124.94 |
| 12 | G9 | 201 | CYC | OC-C1C-NC | 3.95 | 129.73 | 124.94 |
| 12 | D2 | 201 | CYC | CMA-C3A-C4A | 3.95 | 131.15 | 125.06 |
| 12 | CA | 201 | CYC | CHA-C1A-NA | -3.95 | 123.34 | 128.83 |
| 12 | C2 | 201 | CYC | OC-C1C-NC | 3.95 | 129.73 | 124.94 |
| 12 | SA | 201 | CYC | CHA-C1A-NA | -3.95 | 123.34 | 128.83 |
| 12 | S9 | 201 | CYC | CHA-C1A-NA | -3.95 | 123.34 | 128.83 |
| 12 | F2 | 202 | CYC | CHA-C1A-NA | -3.95 | 123.35 | 128.83 |
| 12 | X3 | 202 | CYC | CHA-C1A-NA | -3.95 | 123.35 | 128.83 |
| 12 | J4 | 202 | CYC | C1B-C2B-C3B | -3.95 | 103.75 | 107.87 |
| 12 | J8 | 202 | CYC | C1B-C2B-C3B | -3.95 | 103.75 | 107.87 |
| 12 | M8 | 302 | CYC | CMA-C3A-C4A | 3.95 | 131.15 | 125.06 |
| 12 | Z8 | 301 | CYC | C4A-C3A-C2A | -3.95 | 101.97 | 106.51 |
| 12 | B4 | 201 | CYC | CAB-C3B-C4B | 3.95 | 127.61 | 121.38 |
| 12 | EA | 201 | CYC | OC-C1C-NC | 3.94 | 129.72 | 124.94 |
| 12 | E9 | 201 | CYC | OC-C1C-NC | 3.94 | 129.72 | 124.94 |
| 12 | k5 | 1202 | CYC | OC-C1C-C2C | -3.94 | 123.04 | 126.17 |
| 12 | G3 | 201 | CYC | OC-C1C-NC | 3.94 | 129.72 | 124.94 |
| 12 | G8 | 201 | CYC | OC-C1C-NC | 3.94 | 129.71 | 124.94 |
| 12 | X8 | 201 | CYC | OC-C1C-NC | 3.94 | 129.71 | 124.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | V9 | 202 | CYC | C1B-C2B-C3B | -3.94 | 103.76 | 107.87 |
| 12 | H9 | 202 | CYC | C4A-C3A-C2A | -3.94 | 101.99 | 106.51 |
| 12 | R4 | 201 | CYC | CHA-C1A-NA | -3.93 | 123.37 | 128.83 |
| 12 | R8 | 201 | CYC | CHA-C1A-NA | -3.93 | 123.37 | 128.83 |
| 12 | J3 | 201 | CYC | C1B-C2B-C3B | -3.93 | 103.77 | 107.87 |
| 12 | DA | 202 | CYC | CHA-C1A-NA | -3.93 | 123.37 | 128.83 |
| 12 | D9 | 202 | CYC | CHA-C1A-NA | -3.93 | 123.37 | 128.83 |
| 12 | E4 | 201 | CYC | CHA-C1A-NA | -3.93 | 123.38 | 128.83 |
| 12 | Q8 | 201 | CYC | CHA-C1A-NA | -3.93 | 123.38 | 128.83 |
| 12 | S4 | 201 | CYC | CHA-C1A-NA | -3.93 | 123.38 | 128.83 |
| 12 | S8 | 201 | CYC | CHA-C1A-NA | -3.93 | 123.38 | 128.83 |
| 12 | L9 | 201 | CYC | CHA-C1A-NA | -3.93 | 123.38 | 128.83 |
| 12 | O4 | 201 | CYC | C4A-C3A-C2A | -3.93 | 102.00 | 106.51 |
| 12 | O8 | 201 | CYC | C4A-C3A-C2A | -3.93 | 102.00 | 106.51 |
| 12 | I6 | 201 | CYC | CHA-C1A-NA | -3.93 | 123.38 | 128.83 |
| 12 | LA | 201 | CYC | C1B-C2B-C3B | -3.93 | 103.77 | 107.87 |
| 12 | R1 | 202 | CYC | C1B-C2B-C3B | -3.93 | 103.77 | 107.87 |
| 12 | R3 | 202 | CYC | C1B-C2B-C3B | -3.93 | 103.77 | 107.87 |
| 12 | d5 | 201 | CYC | OC-C1C-C2C | -3.93 | 123.05 | 126.17 |
| 12 | TA | 302 | CYC | CHA-C1A-NA | -3.92 | 123.38 | 128.83 |
| 12 | T9 | 302 | CYC | CHA-C1A-NA | -3.92 | 123.38 | 128.83 |
| 12 | F4 | 201 | CYC | CAB-C3B-C4B | 3.92 | 127.57 | 121.38 |
| 12 | A1 | 201 | CYC | CHA-C1A-NA | -3.92 | 123.39 | 128.83 |
| 12 | J3 | 201 | CYC | CHA-C1A-NA | -3.92 | 123.39 | 128.83 |
| 12 | J1 | 201 | CYC | CHA-C1A-NA | -3.92 | 123.39 | 128.83 |
| 12 | KA | 201 | CYC | CHA-C1A-NA | -3.92 | 123.39 | 128.83 |
| 12 | K9 | 201 | CYC | CHA-C1A-NA | -3.92 | 123.39 | 128.83 |
| 12 | XA | 202 | CYC | CHA-C1A-NA | -3.92 | 123.39 | 128.83 |
| 12 | X4 | 201 | CYC | OC-C1C-NC | 3.91 | 129.68 | 124.94 |
| 12 | T4 | 201 | CYC | CHA-C1A-NA | -3.91 | 123.40 | 128.83 |
| 12 | T8 | 201 | CYC | CHA-C1A-NA | -3.91 | 123.40 | 128.83 |
| 12 | HA | 202 | CYC | C4A-C3A-C2A | -3.91 | 102.02 | 106.51 |
| 12 | A6 | 201 | CYC | CHA-C1A-NA | -3.91 | 123.40 | 128.83 |
| 12 | A2 | 201 | CYC | CHA-C1A-NA | -3.91 | 123.40 | 128.83 |
| 12 | Q4 | 201 | CYC | CHA-C1A-NA | -3.91 | 123.40 | 128.83 |
| 12 | F8 | 201 | CYC | CAB-C3B-C4B | 3.91 | 127.55 | 121.38 |
| 12 | YA | 201 | CYC | CHA-C1A-NA | -3.91 | 123.41 | 128.83 |
| 12 | Y9 | 201 | CYC | CHA-C1A-NA | -3.91 | 123.41 | 128.83 |
| 12 | LA | 201 | CYC | CHA-C1A-NA | -3.91 | 123.41 | 128.83 |
| 12 | E8 | 201 | CYC | CHA-C1A-NA | -3.90 | 123.41 | 128.83 |
| 12 | JA | 201 | CYC | CHA-C1A-NA | -3.90 | 123.41 | 128.83 |
| 12 | J9 | 201 | CYC | CHA-C1A-NA | -3.90 | 123.41 | 128.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | QA | 201 | CYC | CHA-C1A-NA | -3.90 | 123.41 | 128.83 |
| 12 | T7 | 201 | CYC | OC-C1C-C2C | -3.90 | 123.07 | 126.17 |
| 12 | XA | 202 | CYC | C1B-C2B-C3B | -3.90 | 103.80 | 107.87 |
| 12 | X9 | 202 | CYC | C1B-C2B-C3B | -3.90 | 103.80 | 107.87 |
| 12 | A3 | 201 | CYC | CHA-C1A-NA | -3.90 | 123.42 | 128.83 |
| 12 | BA | 202 | CYC | C1B-C2B-C3B | -3.90 | 103.80 | 107.87 |
| 12 | X9 | 202 | CYC | CHA-C1A-NA | -3.90 | 123.42 | 128.83 |
| 12 | L6 | 202 | CYC | C1B-C2B-C3B | -3.90 | 103.80 | 107.87 |
| 12 | B4 | 201 | CYC | CHA-C1A-NA | -3.90 | 123.42 | 128.83 |
| 12 | Y3 | 201 | CYC | CHA-C1A-NA | -3.90 | 123.42 | 128.83 |
| 12 | B8 | 201 | CYC | CHA-C1A-NA | -3.90 | 123.42 | 128.83 |
| 12 | Q9 | 201 | CYC | CHA-C1A-NA | -3.90 | 123.42 | 128.83 |
| 12 | Y1 | 201 | CYC | CHA-C1A-NA | -3.90 | 123.42 | 128.83 |
| 12 | B2 | 201 | CYC | CAB-C3B-C4B | 3.90 | 127.53 | 121.38 |
| 12 | C4 | 201 | CYC | CHA-C1A-NA | -3.90 | 123.42 | 128.83 |
| 12 | C8 | 201 | CYC | CHA-C1A-NA | -3.90 | 123.42 | 128.83 |
| 12 | L9 | 201 | CYC | C1B-C2B-C3B | -3.90 | 103.81 | 107.87 |
| 12 | W4 | 202 | CYC | C1B-C2B-C3B | -3.89 | 103.81 | 107.87 |
| 12 | W8 | 202 | CYC | C1B-C2B-C3B | -3.89 | 103.81 | 107.87 |
| 12 | C6 | 201 | CYC | CHA-C1A-NA | -3.89 | 123.42 | 128.83 |
| 12 | F9 | 303 | CYC | CHA-C1A-NA | -3.89 | 123.42 | 128.83 |
| 12 | K3 | 201 | CYC | CHA-C1A-NA | -3.89 | 123.43 | 128.83 |
| 12 | T3 | 302 | CYC | CHA-C1A-NA | -3.89 | 123.43 | 128.83 |
| 12 | T1 | 302 | CYC | CHA-C1A-NA | -3.89 | 123.43 | 128.83 |
| 12 | F4 | 201 | CYC | CHA-C1A-NA | -3.89 | 123.43 | 128.83 |
| 12 | N4 | 201 | CYC | CHA-C1A-NA | -3.89 | 123.43 | 128.83 |
| 12 | F8 | 201 | CYC | CHA-C1A-NA | -3.89 | 123.43 | 128.83 |
| 12 | K1 | 201 | CYC | CHA-C1A-NA | -3.89 | 123.43 | 128.83 |
| 12 | E3 | 201 | CYC | CHA-C1A-NA | -3.89 | 123.43 | 128.83 |
| 12 | E1 | 201 | CYC | CHA-C1A-NA | -3.89 | 123.43 | 128.83 |
| 12 | B3 | 201 | CYC | CAB-C3B-C4B | 3.89 | 127.52 | 121.38 |
| 12 | B1 | 201 | CYC | CAB-C3B-C4B | 3.89 | 127.52 | 121.38 |
| 12 | T9 | 302 | CYC | CAB-C3B-C4B | 3.89 | 127.52 | 121.38 |
| 12 | P1 | 202 | CYC | C1B-C2B-C3B | -3.89 | 103.81 | 107.87 |
| 12 | P3 | 202 | CYC | C1B-C2B-C3B | -3.89 | 103.81 | 107.87 |
| 12 | WA | 201 | CYC | CHA-C1A-NA | -3.89 | 123.43 | 128.83 |
| 12 | B9 | 202 | CYC | C1B-C2B-C3B | -3.89 | 103.81 | 107.87 |
| 12 | I2 | 201 | CYC | CHA-C1A-NA | -3.89 | 123.44 | 128.83 |
| 12 | W9 | 201 | CYC | CHA-C1A-NA | -3.89 | 123.44 | 128.83 |
| 12 | C2 | 201 | CYC | CHA-C1A-NA | -3.89 | 123.44 | 128.83 |
| 12 | B6 | 201 | CYC | CAB-C3B-C4B | 3.89 | 127.52 | 121.38 |
| 12 | EA | 201 | CYC | CHA-C1A-NA | -3.89 | 123.44 | 128.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | L6 | 202 | CYC | CHA-C1A-NA | -3.89 | 123.44 | 128.83 |
| 12 | E9 | 201 | CYC | CHA-C1A-NA | -3.89 | 123.44 | 128.83 |
| 12 | j7 | 201 | CYC | OC-C1C-C2C | -3.89 | 123.08 | 126.17 |
| 12 | f7 | 201 | CYC | OC-C1C-C2C | -3.89 | 123.08 | 126.17 |
| 12 | W4 | 202 | CYC | CHA-C1A-NA | -3.89 | 123.44 | 128.83 |
| 12 | W8 | 202 | CYC | CHA-C1A-NA | -3.89 | 123.44 | 128.83 |
| 12 | L8 | 201 | CYC | C1B-C2B-C3B | -3.88 | 103.82 | 107.87 |
| 12 | UA | 201 | CYC | CHA-C1A-NA | -3.88 | 123.44 | 128.83 |
| 12 | U9 | 201 | CYC | CHA-C1A-NA | -3.88 | 123.44 | 128.83 |
| 12 | D6 | 202 | CYC | CAB-C3B-C4B | 3.88 | 127.51 | 121.38 |
| 12 | D2 | 202 | CYC | CAB-C3B-C4B | 3.88 | 127.51 | 121.38 |
| 12 | Q1 | 201 | CYC | CHA-C1A-NA | -3.88 | 123.44 | 128.83 |
| 12 | Q3 | 201 | CYC | CHA-C1A-NA | -3.88 | 123.44 | 128.83 |
| 12 | R3 | 202 | CYC | CHA-C1A-NA | -3.88 | 123.44 | 128.83 |
| 12 | K4 | 201 | CYC | CHA-C1A-NA | -3.88 | 123.44 | 128.83 |
| 12 | K8 | 201 | CYC | CHA-C1A-NA | -3.88 | 123.44 | 128.83 |
| 12 | B6 | 201 | CYC | C1B-C2B-C3B | -3.88 | 103.82 | 107.87 |
| 12 | B2 | 201 | CYC | C1B-C2B-C3B | -3.88 | 103.82 | 107.87 |
| 12 | Q4 | 201 | CYC | C1B-C2B-C3B | -3.88 | 103.82 | 107.87 |
| 12 | TA | 302 | CYC | CAB-C3B-C4B | 3.88 | 127.51 | 121.38 |
| 12 | BA | 202 | CYC | CAB-C3B-C4B | 3.88 | 127.51 | 121.38 |
| 12 | B9 | 202 | CYC | CAB-C3B-C4B | 3.88 | 127.51 | 121.38 |
| 12 | L4 | 201 | CYC | C1B-C2B-C3B | -3.88 | 103.82 | 107.87 |
| 12 | I4 | 201 | CYC | CHA-C1A-NA | -3.88 | 123.45 | 128.83 |
| 12 | I8 | 201 | CYC | CHA-C1A-NA | -3.88 | 123.45 | 128.83 |
| 12 | OA | 201 | CYC | OC-C1C-C2C | -3.88 | 123.09 | 126.17 |
| 12 | T5 | 201 | CYC | OC-C1C-C2C | -3.88 | 123.09 | 126.17 |
| 12 | N8 | 201 | CYC | CHA-C1A-NA | -3.88 | 123.45 | 128.83 |
| 12 | F6 | 202 | CYC | CAB-C3B-C4B | 3.88 | 127.50 | 121.38 |
| 12 | RA | 202 | CYC | CHA-C1A-NA | -3.88 | 123.45 | 128.83 |
| 12 | R9 | 202 | CYC | CHA-C1A-NA | -3.88 | 123.45 | 128.83 |
| 12 | B3 | 201 | CYC | C1B-C2B-C3B | -3.88 | 103.83 | 107.87 |
| 12 | B1 | 201 | CYC | C1B-C2B-C3B | -3.88 | 103.83 | 107.87 |
| 12 | PA | 202 | CYC | CHA-C1A-NA | -3.87 | 123.45 | 128.83 |
| 12 | P1 | 202 | CYC | CHA-C1A-NA | -3.87 | 123.45 | 128.83 |
| 12 | P3 | 202 | CYC | CHA-C1A-NA | -3.87 | 123.45 | 128.83 |
| 12 | H4 | 202 | CYC | CHA-C1A-NA | -3.87 | 123.45 | 128.83 |
| 12 | H8 | 202 | CYC | CHA-C1A-NA | -3.87 | 123.45 | 128.83 |
| 12 | P9 | 202 | CYC | CHA-C1A-NA | -3.87 | 123.45 | 128.83 |
| 12 | F2 | 201 | CYC | C4A-C3A-C2A | -3.87 | 102.06 | 106.51 |
| 12 | R1 | 202 | CYC | CHA-C1A-NA | -3.87 | 123.45 | 128.83 |
| 12 | H2 | 202 | CYC | CHA-C1A-NA | -3.87 | 123.45 | 128.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | Q8 | 201 | CYC | CAB-C3B-C4B | 3.87 | 127.50 | 121.38 |
| 12 | T3 | 301 | CYC | C4A-C3A-C2A | -3.87 | 102.06 | 106.51 |
| 12 | T1 | 301 | CYC | C4A-C3A-C2A | -3.87 | 102.06 | 106.51 |
| 12 | O4 | 202 | CYC | CHA-C1A-NA | -3.87 | 123.46 | 128.83 |
| 12 | O8 | 202 | CYC | CHA-C1A-NA | -3.87 | 123.46 | 128.83 |
| 12 | D2 | 202 | CYC | CHA-C1A-NA | -3.87 | 123.46 | 128.83 |
| 12 | Q4 | 201 | CYC | CAB-C3B-C4B | 3.87 | 127.49 | 121.38 |
| 12 | ZA | 201 | CYC | C1B-C2B-C3B | -3.87 | 103.83 | 107.87 |
| 12 | Z9 | 201 | CYC | C1B-C2B-C3B | -3.87 | 103.83 | 107.87 |
| 12 | K6 | 201 | CYC | CHA-C1A-NA | -3.87 | 123.46 | 128.83 |
| 12 | W3 | 201 | CYC | CHA-C1A-NA | -3.87 | 123.46 | 128.83 |
| 12 | W1 | 201 | CYC | CHA-C1A-NA | -3.87 | 123.46 | 128.83 |
| 12 | H6 | 202 | CYC | CHA-C1A-NA | -3.87 | 123.47 | 128.83 |
| 12 | D4 | 201 | CYC | CAB-C3B-C4B | 3.86 | 127.48 | 121.38 |
| 12 | T3 | 302 | CYC | CAB-C3B-C4B | 3.86 | 127.48 | 121.38 |
| 12 | D8 | 201 | CYC | CAB-C3B-C4B | 3.86 | 127.48 | 121.38 |
| 12 | T1 | 302 | CYC | CAB-C3B-C4B | 3.86 | 127.48 | 121.38 |
| 12 | D3 | 201 | CYC | CHA-C1A-NA | -3.86 | 123.47 | 128.83 |
| 12 | D1 | 201 | CYC | CHA-C1A-NA | -3.86 | 123.47 | 128.83 |
| 12 | X3 | 202 | CYC | C1B-C2B-C3B | -3.86 | 103.84 | 107.87 |
| 12 | T9 | 302 | CYC | C1B-C2B-C3B | -3.86 | 103.84 | 107.87 |
| 12 | X1 | 202 | CYC | C1B-C2B-C3B | -3.86 | 103.84 | 107.87 |
| 12 | Z3 | 202 | CYC | CHA-C1A-NA | -3.86 | 123.47 | 128.83 |
| 12 | Q8 | 201 | CYC | C1B-C2B-C3B | -3.86 | 103.84 | 107.87 |
| 12 | D4 | 201 | CYC | C1B-C2B-C3B | -3.86 | 103.84 | 107.87 |
| 12 | L3 | 201 | CYC | C1B-C2B-C3B | -3.86 | 103.84 | 107.87 |
| 12 | D8 | 201 | CYC | C1B-C2B-C3B | -3.86 | 103.84 | 107.87 |
| 12 | L1 | 201 | CYC | C1B-C2B-C3B | -3.86 | 103.84 | 107.87 |
| 12 | L4 | 201 | CYC | CHA-C1A-NA | -3.86 | 123.47 | 128.83 |
| 12 | L8 | 201 | CYC | CHA-C1A-NA | -3.86 | 123.47 | 128.83 |
| 12 | B5 | 201 | CYC | OC-C1C-C2C | -3.86 | 123.10 | 126.17 |
| 12 | J2 | 201 | CYC | CAB-C3B-C4B | 3.86 | 127.47 | 121.38 |
| 12 | L2 | 202 | CYC | C1B-C2B-C3B | -3.86 | 103.85 | 107.87 |
| 12 | D3 | 201 | CYC | C1B-C2B-C3B | -3.86 | 103.85 | 107.87 |
| 12 | D1 | 201 | CYC | C1B-C2B-C3B | -3.86 | 103.85 | 107.87 |
| 12 | H3 | 201 | CYC | CHA-C1A-NA | -3.86 | 123.48 | 128.83 |
| 12 | F9 | 302 | CYC | CHA-C1A-NA | -3.86 | 123.48 | 128.83 |
| 12 | H1 | 202 | CYC | CHA-C1A-NA | -3.86 | 123.48 | 128.83 |
| 12 | ZA | 201 | CYC | CHA-C1A-NA | -3.86 | 123.48 | 128.83 |
| 12 | Z9 | 201 | CYC | CHA-C1A-NA | -3.86 | 123.48 | 128.83 |
| 12 | TA | 302 | CYC | C1B-C2B-C3B | -3.86 | 103.85 | 107.87 |
| 12 | F9 | 302 | CYC | CAB-C3B-C4B | 3.85 | 127.47 | 121.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | r7 | 201 | CYC | OC-C1C-C2C | -3.85 | 123.11 | 126.17 |
| 12 | OA | 201 | CYC | CHA-C1A-NA | -3.85 | 123.48 | 128.83 |
| 12 | GA | 201 | CYC | CHA-C1A-NA | -3.85 | 123.48 | 128.83 |
| 12 | G9 | 201 | CYC | CHA-C1A-NA | -3.85 | 123.48 | 128.83 |
| 12 | V9 | 202 | CYC | CHA-C1A-NA | -3.85 | 123.48 | 128.83 |
| 12 | HA | 201 | CYC | CHA-C1A-NA | -3.85 | 123.49 | 128.83 |
| 12 | K2 | 201 | CYC | CHA-C1A-NA | -3.85 | 123.49 | 128.83 |
| 12 | J8 | 202 | CYC | CAB-C3B-C4B | 3.85 | 127.46 | 121.38 |
| 12 | L8 | 201 | CYC | CAB-C3B-C4B | 3.85 | 127.45 | 121.38 |
| 12 | L3 | 201 | CYC | CHA-C1A-NA | -3.85 | 123.49 | 128.83 |
| 12 | L1 | 201 | CYC | CHA-C1A-NA | -3.85 | 123.49 | 128.83 |
| 12 | D2 | 202 | CYC | C1B-C2B-C3B | -3.85 | 103.86 | 107.87 |
| 12 | g7 | 201 | CYC | C4A-C3A-C2A | -3.85 | 102.09 | 106.51 |
| 12 | i7 | 201 | CYC | C4A-C3A-C2A | -3.85 | 102.09 | 106.51 |
| 12 | J6 | 201 | CYC | CHA-C1A-NA | -3.84 | 123.49 | 128.83 |
| 12 | T4 | 201 | CYC | OC-C1C-C2C | -3.84 | 123.12 | 126.17 |
| 12 | P7 | 201 | CYC | OC-C1C-C2C | -3.84 | 123.12 | 126.17 |
| 12 | T8 | 201 | CYC | OC-C1C-C2C | -3.84 | 123.12 | 126.17 |
| 12 | O9 | 201 | CYC | OC-C1C-C2C | -3.84 | 123.12 | 126.17 |
| 12 | RA | 202 | CYC | CAB-C3B-C4B | 3.84 | 127.45 | 121.38 |
| 12 | R9 | 202 | CYC | CAB-C3B-C4B | 3.84 | 127.45 | 121.38 |
| 12 | O4 | 202 | CYC | C1B-C2B-C3B | -3.84 | 103.86 | 107.87 |
| 12 | O8 | 202 | CYC | C1B-C2B-C3B | -3.84 | 103.86 | 107.87 |
| 12 | H5 | 201 | CYC | OC-C1C-C2C | -3.84 | 123.12 | 126.17 |
| 12 | F2 | 202 | CYC | CAB-C3B-C4B | 3.84 | 127.44 | 121.38 |
| 12 | Z1 | 201 | CYC | CHA-C1A-NA | -3.84 | 123.50 | 128.83 |
| 12 | U3 | 201 | CYC | CHA-C1A-NA | -3.84 | 123.50 | 128.83 |
| 12 | U1 | 201 | CYC | CHA-C1A-NA | -3.84 | 123.50 | 128.83 |
| 12 | O4 | 202 | CYC | CAB-C3B-C4B | 3.84 | 127.44 | 121.38 |
| 12 | O8 | 202 | CYC | CAB-C3B-C4B | 3.84 | 127.44 | 121.38 |
| 12 | F7 | 201 | CYC | OC-C1C-C2C | -3.84 | 123.12 | 126.17 |
| 12 | T3 | 302 | CYC | C1B-C2B-C3B | -3.84 | 103.87 | 107.87 |
| 12 | T1 | 302 | CYC | C1B-C2B-C3B | -3.84 | 103.87 | 107.87 |
| 12 | D4 | 201 | CYC | CHA-C1A-NA | -3.83 | 123.51 | 128.83 |
| 12 | D8 | 201 | CYC | CHA-C1A-NA | -3.83 | 123.51 | 128.83 |
| 12 | L4 | 201 | CYC | CAB-C3B-C4B | 3.83 | 127.43 | 121.38 |
| 12 | JA | 201 | CYC | CAB-C3B-C4B | 3.83 | 127.43 | 121.38 |
| 12 | J9 | 201 | CYC | CAB-C3B-C4B | 3.83 | 127.43 | 121.38 |
| 12 | XA | 202 | CYC | CAB-C3B-C4B | 3.83 | 127.43 | 121.38 |
| 12 | X9 | 202 | CYC | CAB-C3B-C4B | 3.83 | 127.43 | 121.38 |
| 12 | J4 | 202 | CYC | CHA-C1A-NA | -3.83 | 123.51 | 128.83 |
| 12 | J8 | 202 | CYC | CHA-C1A-NA | -3.83 | 123.51 | 128.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | VA | 202 | CYC | CAB-C3B-C4B | 3.83 | 127.43 | 121.38 |
| 12 | BA | 202 | CYC | CHA-C1A-NA | -3.83 | 123.51 | 128.83 |
| 12 | B9 | 202 | CYC | CHA-C1A-NA | -3.83 | 123.51 | 128.83 |
| 12 | Y4 | 201 | CYC | CAB-C3B-C4B | 3.83 | 127.43 | 121.38 |
| 12 | Y8 | 201 | CYC | CAB-C3B-C4B | 3.83 | 127.43 | 121.38 |
| 12 | VA | 202 | CYC | CHA-C1A-NA | -3.83 | 123.52 | 128.83 |
| 12 | P4 | 201 | CYC | CHA-C1A-NA | -3.83 | 123.52 | 128.83 |
| 12 | P8 | 201 | CYC | CHA-C1A-NA | -3.83 | 123.52 | 128.83 |
| 12 | V4 | 201 | CYC | CHA-C1A-NA | -3.83 | 123.52 | 128.83 |
| 12 | d7 | 201 | CYC | OC-C1C-C2C | -3.83 | 123.13 | 126.17 |
| 12 | J6 | 201 | CYC | CAB-C3B-C4B | 3.83 | 127.42 | 121.38 |
| 12 | V3 | 202 | CYC | CHA-C1A-NA | -3.82 | 123.52 | 128.83 |
| 12 | O9 | 201 | CYC | CHA-C1A-NA | -3.82 | 123.52 | 128.83 |
| 12 | V1 | 202 | CYC | CHA-C1A-NA | -3.82 | 123.52 | 128.83 |
| 12 | L2 | 202 | CYC | CHA-C1A-NA | -3.82 | 123.52 | 128.83 |
| 12 | D6 | 202 | CYC | C1B-C2B-C3B | -3.82 | 103.88 | 107.87 |
| 12 | F9 | 303 | CYC | CAB-C3B-C4B | 3.82 | 127.42 | 121.38 |
| 12 | G2 | 201 | CYC | CHA-C1A-NA | -3.82 | 123.53 | 128.83 |
| 12 | G6 | 201 | CYC | CHA-C1A-NA | -3.82 | 123.53 | 128.83 |
| 12 | H9 | 201 | CYC | CHA-C1A-NA | -3.82 | 123.53 | 128.83 |
| 12 | P1 | 202 | CYC | CAB-C3B-C4B | 3.82 | 127.41 | 121.38 |
| 12 | P3 | 202 | CYC | CAB-C3B-C4B | 3.82 | 127.41 | 121.38 |
| 12 | DA | 202 | CYC | CAB-C3B-C4B | 3.82 | 127.41 | 121.38 |
| 12 | D9 | 202 | CYC | CAB-C3B-C4B | 3.82 | 127.41 | 121.38 |
| 12 | D6 | 202 | CYC | CHA-C1A-NA | -3.82 | 123.53 | 128.83 |
| 12 | P9 | 202 | CYC | CAB-C3B-C4B | 3.82 | 127.41 | 121.38 |
| 12 | YA | 201 | CYC | C2B-C1B-NB | 3.82 | 112.58 | 106.99 |
| 12 | Y9 | 201 | CYC | C2B-C1B-NB | 3.82 | 112.58 | 106.99 |
| 12 | c7 | 201 | CYC | C4A-C3A-C2A | -3.82 | 102.13 | 106.51 |
| 12 | N5 | 201 | CYC | OC-C1C-C2C | -3.82 | 123.14 | 126.17 |
| 12 | G3 | 201 | CYC | CHA-C1A-NA | -3.81 | 123.53 | 128.83 |
| 12 | A4 | 201 | CYC | CHA-C1A-NA | -3.81 | 123.53 | 128.83 |
| 12 | A8 | 201 | CYC | CHA-C1A-NA | -3.81 | 123.53 | 128.83 |
| 12 | G1 | 201 | CYC | CHA-C1A-NA | -3.81 | 123.53 | 128.83 |
| 12 | U4 | 202 | CYC | CHA-C1A-NA | -3.81 | 123.54 | 128.83 |
| 12 | G4 | 201 | CYC | CHA-C1A-NA | -3.81 | 123.54 | 128.83 |
| 12 | G8 | 201 | CYC | CHA-C1A-NA | -3.81 | 123.54 | 128.83 |
| 12 | J4 | 202 | CYC | CAB-C3B-C4B | 3.81 | 127.40 | 121.38 |
| 12 | V9 | 202 | CYC | CAB-C3B-C4B | 3.81 | 127.40 | 121.38 |
| 12 | L2 | 202 | CYC | CAB-C3B-C4B | 3.81 | 127.40 | 121.38 |
| 12 | R1 | 202 | CYC | CAB-C3B-C4B | 3.81 | 127.39 | 121.38 |
| 12 | R3 | 202 | CYC | CAB-C3B-C4B | 3.81 | 127.39 | 121.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | L3 | 201 | CYC | CAB-C3B-C4B | 3.81 | 127.39 | 121.38 |
| 12 | L1 | 201 | CYC | CAB-C3B-C4B | 3.81 | 127.39 | 121.38 |
| 12 | J2 | 201 | CYC | CHA-C1A-NA | -3.81 | 123.55 | 128.83 |
| 12 | GA | 201 | CYC | C2B-C1B-NB | 3.81 | 112.56 | 106.99 |
| 12 | G9 | 201 | CYC | C2B-C1B-NB | 3.81 | 112.56 | 106.99 |
| 12 | a7 | 201 | CYC | C4A-C3A-C2A | -3.80 | 102.14 | 106.51 |
| 12 | L6 | 202 | CYC | CAB-C3B-C4B | 3.80 | 127.39 | 121.38 |
| 12 | V8 | 201 | CYC | CHA-C1A-NA | -3.80 | 123.55 | 128.83 |
| 12 | B6 | 201 | CYC | CHA-C1A-NA | -3.80 | 123.55 | 128.83 |
| 12 | F2 | 201 | CYC | CHB-C4A-NA | -3.80 | 116.98 | 124.93 |
| 12 | A6 | 201 | CYC | OC-C1C-C2C | -3.80 | 123.15 | 126.17 |
| 12 | D3 | 201 | CYC | CAB-C3B-C4B | 3.80 | 127.37 | 121.38 |
| 12 | D1 | 201 | CYC | CAB-C3B-C4B | 3.80 | 127.37 | 121.38 |
| 12 | PA | 202 | CYC | CAB-C3B-C4B | 3.80 | 127.37 | 121.38 |
| 12 | R4 | 201 | CYC | C2B-C1B-NB | 3.80 | 112.54 | 106.99 |
| 12 | R8 | 201 | CYC | C2B-C1B-NB | 3.80 | 112.54 | 106.99 |
| 12 | k5 | 1203 | CYC | OC-C1C-C2C | -3.79 | 123.16 | 126.17 |
| 12 | X3 | 202 | CYC | CAB-C3B-C4B | 3.79 | 127.37 | 121.38 |
| 12 | X1 | 202 | CYC | CAB-C3B-C4B | 3.79 | 127.37 | 121.38 |
| 12 | I3 | 201 | CYC | CHA-C1A-NA | -3.79 | 123.56 | 128.83 |
| 12 | I1 | 201 | CYC | CHA-C1A-NA | -3.79 | 123.56 | 128.83 |
| 12 | L5 | 201 | CYC | OC-C1C-C2C | -3.79 | 123.16 | 126.17 |
| 12 | V3 | 202 | CYC | CAB-C3B-C4B | 3.79 | 127.37 | 121.38 |
| 12 | V1 | 202 | CYC | CAB-C3B-C4B | 3.79 | 127.37 | 121.38 |
| 12 | Y4 | 201 | CYC | CHA-C1A-NA | -3.79 | 123.57 | 128.83 |
| 12 | U8 | 202 | CYC | CHA-C1A-NA | -3.79 | 123.57 | 128.83 |
| 12 | Y8 | 201 | CYC | CHA-C1A-NA | -3.79 | 123.57 | 128.83 |
| 12 | DA | 202 | CYC | C1B-C2B-C3B | -3.79 | 103.92 | 107.87 |
| 12 | D9 | 202 | CYC | C1B-C2B-C3B | -3.79 | 103.92 | 107.87 |
| 12 | ZA | 201 | CYC | CAB-C3B-C4B | 3.79 | 127.36 | 121.38 |
| 12 | Z9 | 201 | CYC | CAB-C3B-C4B | 3.79 | 127.36 | 121.38 |
| 12 | O4 | 201 | CYC | CHB-C4A-NA | -3.79 | 117.01 | 124.93 |
| 12 | A | 201 | CYC | OC-C1C-C2C | -3.79 | 123.16 | 126.17 |
| 12 | D4 | 202 | CYC | CHB-C4A-NA | -3.79 | 117.01 | 124.93 |
| 12 | D8 | 202 | CYC | CHB-C4A-NA | -3.79 | 117.01 | 124.93 |
| 12 | HA | 201 | CYC | CAB-C3B-C4B | 3.79 | 127.36 | 121.38 |
| 12 | H9 | 201 | CYC | CAB-C3B-C4B | 3.79 | 127.36 | 121.38 |
| 12 | AA | 201 | CYC | CHA-C1A-NA | -3.79 | 123.58 | 128.83 |
| 12 | A9 | 201 | CYC | CHA-C1A-NA | -3.79 | 123.58 | 128.83 |
| 12 | O8 | 201 | CYC | CHB-C4A-NA | -3.79 | 117.01 | 124.93 |
| 12 | Z | 201 | CYC | OC-C1C-C2C | -3.79 | 123.16 | 126.17 |
| 12 | L7 | 201 | CYC | OC-C1C-C2C | -3.79 | 123.16 | 126.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | B2 | 201 | CYC | CHA-C1A-NA | -3.79 | 123.58 | 128.83 |
| 12 | Z5 | 201 | CYC | OC-C1C-C2C | -3.78 | 123.16 | 126.17 |
| 12 | j5 | 1202 | CYC | OC-C1C-C2C | -3.78 | 123.17 | 126.17 |
| 12 | H6 | 202 | CYC | CAB-C3B-C4B | 3.78 | 127.35 | 121.38 |
| 12 | B1 | 202 | CYC | CHB-C4A-NA | -3.78 | 117.02 | 124.93 |
| 12 | W4 | 202 | CYC | CAB-C3B-C4B | 3.78 | 127.35 | 121.38 |
| 12 | W8 | 202 | CYC | CAB-C3B-C4B | 3.78 | 127.35 | 121.38 |
| 12 | H4 | 201 | CYC | CHB-C4A-NA | -3.78 | 117.03 | 124.93 |
| 12 | F6 | 201 | CYC | CHB-C4A-NA | -3.78 | 117.03 | 124.93 |
| 12 | H8 | 201 | CYC | CHB-C4A-NA | -3.78 | 117.03 | 124.93 |
| 12 | A2 | 201 | CYC | C2B-C1B-NB | 3.78 | 112.52 | 106.99 |
| 12 | Z3 | 202 | CYC | CAB-C3B-C4B | 3.77 | 127.34 | 121.38 |
| 12 | Z1 | 201 | CYC | CAB-C3B-C4B | 3.77 | 127.34 | 121.38 |
| 12 | b5 | 201 | CYC | OC-C1C-C2C | -3.77 | 123.17 | 126.17 |
| 12 | H4 | 202 | CYC | CAB-C3B-C4B | 3.77 | 127.33 | 121.38 |
| 12 | H8 | 202 | CYC | CAB-C3B-C4B | 3.77 | 127.33 | 121.38 |
| 12 | X3 | 201 | CYC | CHB-C4A-NA | -3.77 | 117.05 | 124.93 |
| 12 | X1 | 201 | CYC | CHB-C4A-NA | -3.77 | 117.05 | 124.93 |
| 12 | U4 | 201 | CYC | CHB-C4A-NA | -3.77 | 117.05 | 124.93 |
| 12 | U8 | 201 | CYC | CHB-C4A-NA | -3.77 | 117.05 | 124.93 |
| 12 | H1 | 201 | CYC | CHB-C4A-NA | -3.77 | 117.06 | 124.93 |
| 12 | O7 | 201 | CYC | C4A-C3A-C2A | -3.76 | 102.19 | 106.51 |
| 12 | JA | 202 | CYC | CHB-C4A-NA | -3.76 | 117.06 | 124.93 |
| 12 | J9 | 202 | CYC | CHB-C4A-NA | -3.76 | 117.06 | 124.93 |
| 12 | S4 | 201 | CYC | CAB-C3B-C4B | 3.76 | 127.32 | 121.38 |
| 12 | S8 | 201 | CYC | CAB-C3B-C4B | 3.76 | 127.32 | 121.38 |
| 12 | f5 | 201 | CYC | OC-C1C-C2C | -3.76 | 123.18 | 126.17 |
| 12 | R7 | 201 | CYC | OC-C1C-C2C | -3.76 | 123.18 | 126.17 |
| 12 | H3 | 202 | CYC | CHB-C4A-NA | -3.76 | 117.06 | 124.93 |
| 12 | V7 | 201 | CYC | OC-C1C-C2C | -3.76 | 123.18 | 126.17 |
| 12 | D3 | 202 | CYC | CHB-C4A-NA | -3.76 | 117.07 | 124.93 |
| 12 | D1 | 202 | CYC | CHB-C4A-NA | -3.76 | 117.07 | 124.93 |
| 12 | H2 | 202 | CYC | CAB-C3B-C4B | 3.76 | 127.32 | 121.38 |
| 12 | A4 | 201 | CYC | OC-C1C-C2C | -3.76 | 123.18 | 126.17 |
| 12 | A8 | 201 | CYC | OC-C1C-C2C | -3.76 | 123.18 | 126.17 |
| 12 | W4 | 201 | CYC | CHB-C4A-NA | -3.76 | 117.07 | 124.93 |
| 12 | W8 | 201 | CYC | CHB-C4A-NA | -3.76 | 117.07 | 124.93 |
| 12 | EA | 201 | CYC | C2B-C1B-NB | 3.76 | 112.49 | 106.99 |
| 12 | R3 | 201 | CYC | CHB-C4A-NA | -3.76 | 117.07 | 124.93 |
| 12 | c5 | 201 | CYC | C4A-C3A-C2A | -3.76 | 102.19 | 106.51 |
| 12 | Y5 | 201 | CYC | C4A-C3A-C2A | -3.76 | 102.19 | 106.51 |
| 12 | LA | 201 | CYC | CAB-C3B-C4B | 3.76 | 127.31 | 121.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | L9 | 201 | CYC | CAB-C3B-C4B | 3.76 | 127.31 | 121.38 |
| 12 | G5 | 201 | CYC | C4A-C3A-C2A | -3.76 | 102.19 | 106.51 |
| 12 | F4 | 201 | CYC | C1B-C2B-C3B | -3.76 | 103.95 | 107.87 |
| 12 | F8 | 201 | CYC | C1B-C2B-C3B | -3.76 | 103.95 | 107.87 |
| 12 | DA | 201 | CYC | CHB-C4A-NA | -3.76 | 117.08 | 124.93 |
| 12 | D9 | 201 | CYC | CHB-C4A-NA | -3.76 | 117.08 | 124.93 |
| 12 | R1 | 201 | CYC | CHB-C4A-NA | -3.75 | 117.08 | 124.93 |
| 12 | D5 | 201 | CYC | C2B-C1B-NB | 3.75 | 112.48 | 106.99 |
| 12 | E2 | 201 | CYC | C2B-C1B-NB | 3.75 | 112.48 | 106.99 |
| 12 | T3 | 301 | CYC | CHB-C4A-NA | -3.75 | 117.09 | 124.93 |
| 12 | T1 | 301 | CYC | CHB-C4A-NA | -3.75 | 117.09 | 124.93 |
| 12 | B4 | 202 | CYC | CHB-C4A-NA | -3.75 | 117.09 | 124.93 |
| 12 | A5 | 201 | CYC | C4A-C3A-C2A | -3.75 | 102.20 | 106.51 |
| 12 | B3 | 202 | CYC | CHB-C4A-NA | -3.75 | 117.09 | 124.93 |
| 12 | J5 | 201 | CYC | C2B-C1B-NB | 3.75 | 112.48 | 106.99 |
| 12 | F3 | 202 | CYC | CAB-C3B-C4B | 3.75 | 127.30 | 121.38 |
| 12 | F1 | 202 | CYC | CAB-C3B-C4B | 3.75 | 127.30 | 121.38 |
| 12 | TA | 301 | CYC | CHB-C4A-NA | -3.75 | 117.09 | 124.93 |
| 12 | T9 | 301 | CYC | CHB-C4A-NA | -3.75 | 117.09 | 124.93 |
| 12 | F6 | 202 | CYC | C1B-C2B-C3B | -3.75 | 103.96 | 107.87 |
| 12 | K7 | 201 | CYC | C4A-C3A-C2A | -3.75 | 102.21 | 106.51 |
| 12 | KA | 201 | CYC | C2B-C1B-NB | 3.75 | 112.47 | 106.99 |
| 12 | K9 | 201 | CYC | C2B-C1B-NB | 3.75 | 112.47 | 106.99 |
| 12 | J7 | 201 | CYC | OC-C1C-C2C | -3.75 | 123.19 | 126.17 |
| 12 | K3 | 201 | CYC | OC-C1C-C2C | -3.74 | 123.20 | 126.17 |
| 12 | a5 | 201 | CYC | C4A-C3A-C2A | -3.74 | 102.21 | 106.51 |
| 12 | XA | 201 | CYC | CHB-C4A-NA | -3.74 | 117.11 | 124.93 |
| 12 | E6 | 201 | CYC | C2B-C1B-NB | 3.74 | 112.46 | 106.99 |
| 12 | A2 | 201 | CYC | OC-C1C-C2C | -3.74 | 123.20 | 126.17 |
| 12 | A7 | 201 | CYC | C4A-C3A-C2A | -3.74 | 102.22 | 106.51 |
| 12 | VA | 201 | CYC | CMB-C2B-C1B | 3.74 | 128.83 | 124.17 |
| 12 | V9 | 201 | CYC | CMB-C2B-C1B | 3.74 | 128.83 | 124.17 |
| 12 | E8 | 201 | CYC | C2B-C1B-NB | 3.74 | 112.46 | 106.99 |
| 12 | J3 | 202 | CYC | CHB-C4A-NA | -3.73 | 117.12 | 124.93 |
| 12 | aA | 901 | CYC | CHB-C4A-NA | -3.73 | 117.12 | 124.93 |
| 12 | A6 | 201 | CYC | C2B-C1B-NB | 3.73 | 112.45 | 106.99 |
| 12 | G4 | 201 | CYC | OC-C1C-C2C | -3.73 | 123.20 | 126.17 |
| 12 | V3 | 201 | CYC | CHB-C4A-NA | -3.73 | 117.12 | 124.93 |
| 12 | V1 | 201 | CYC | CHB-C4A-NA | -3.73 | 117.12 | 124.93 |
| 12 | p7 | 201 | CYC | C2B-C1B-NB | 3.73 | 112.45 | 106.99 |
| 12 | H2 | 201 | CYC | CHB-C4A-NA | -3.73 | 117.12 | 124.93 |
| 12 | B8 | 202 | CYC | CHB-C4A-NA | -3.73 | 117.12 | 124.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | H3 | 201 | CYC | CAB-C3B-C4B | 3.73 | 127.27 | 121.38 |
| 12 | H1 | 202 | CYC | CAB-C3B-C4B | 3.73 | 127.27 | 121.38 |
| 12 | k5 | 1204 | CYC | OC-C1C-C2C | -3.73 | 123.21 | 126.17 |
| 12 | W7 | 201 | CYC | C4A-C3A-C2A | -3.73 | 102.22 | 106.51 |
| 12 | J6 | 202 | CYC | CHB-C4A-NA | -3.73 | 117.13 | 124.93 |
| 12 | E9 | 201 | CYC | C2B-C1B-NB | 3.73 | 112.45 | 106.99 |
| 12 | S7 | 201 | CYC | C4A-C3A-C2A | -3.73 | 102.23 | 106.51 |
| 12 | E4 | 201 | CYC | C2B-C1B-NB | 3.73 | 112.45 | 106.99 |
| 12 | U4 | 202 | CYC | CAB-C3B-C4B | 3.73 | 127.27 | 121.38 |
| 12 | U8 | 202 | CYC | CAB-C3B-C4B | 3.73 | 127.27 | 121.38 |
| 12 | BA | 201 | CYC | CHB-C4A-NA | -3.73 | 117.13 | 124.93 |
| 12 | B9 | 201 | CYC | CHB-C4A-NA | -3.73 | 117.13 | 124.93 |
| 12 | PA | 201 | CYC | CHB-C4A-NA | -3.73 | 117.14 | 124.93 |
| 12 | P9 | 201 | CYC | CHB-C4A-NA | -3.73 | 117.14 | 124.93 |
| 12 | C1 | 201 | CYC | C2B-C1B-NB | 3.73 | 112.44 | 106.99 |
| 12 | C2 | 201 | CYC | C2B-C1B-NB | 3.73 | 112.44 | 106.99 |
| 12 | X9 | 201 | CYC | CHB-C4A-NA | -3.73 | 117.14 | 124.93 |
| 12 | N4 | 201 | CYC | OC-C1C-C2C | -3.73 | 123.21 | 126.17 |
| 12 | N8 | 201 | CYC | OC-C1C-C2C | -3.73 | 123.21 | 126.17 |
| 12 | FA | 301 | CYC | CHB-C4A-NA | -3.73 | 117.14 | 124.93 |
| 12 | F9 | 301 | CYC | CHB-C4A-NA | -3.73 | 117.14 | 124.93 |
| 12 | VA | 201 | CYC | CHB-C4A-NA | -3.73 | 117.14 | 124.93 |
| 12 | J2 | 202 | CYC | CHB-C4A-NA | -3.73 | 117.14 | 124.93 |
| 12 | C7 | 201 | CYC | C4A-C3A-C2A | -3.72 | 102.23 | 106.51 |
| 12 | F3 | 201 | CYC | CHB-C4A-NA | -3.72 | 117.14 | 124.93 |
| 12 | F1 | 201 | CYC | CHB-C4A-NA | -3.72 | 117.14 | 124.93 |
| 12 | F9 | 303 | CYC | C1B-C2B-C3B | -3.72 | 103.99 | 107.87 |
| 12 | O1 | 201 | CYC | C2B-C1B-NB | 3.72 | 112.44 | 106.99 |
| 12 | O3 | 201 | CYC | C2B-C1B-NB | 3.72 | 112.44 | 106.99 |
| 12 | K2 | 201 | CYC | C2B-C1B-NB | 3.72 | 112.44 | 106.99 |
| 12 | S4 | 202 | CYC | CHB-C4A-NA | -3.72 | 117.15 | 124.93 |
| 12 | h7 | 201 | CYC | OC-C1C-C2C | -3.72 | 123.22 | 126.17 |
| 12 | D6 | 201 | CYC | CHB-C4A-NA | -3.72 | 117.15 | 124.93 |
| 12 | C4 | 201 | CYC | OC-C1C-C2C | -3.72 | 123.22 | 126.17 |
| 12 | C8 | 201 | CYC | OC-C1C-C2C | -3.72 | 123.22 | 126.17 |
| 12 | K4 | 201 | CYC | OC-C1C-C2C | -3.72 | 123.22 | 126.17 |
| 12 | K8 | 201 | CYC | OC-C1C-C2C | -3.72 | 123.22 | 126.17 |
| 12 | F4 | 202 | CYC | CHB-C4A-NA | -3.72 | 117.16 | 124.93 |
| 12 | F8 | 202 | CYC | CHB-C4A-NA | -3.72 | 117.16 | 124.93 |
| 12 | K8 | 201 | CYC | C2B-C1B-NB | 3.72 | 112.43 | 106.99 |
| 12 | F9 | 302 | CYC | C1B-C2B-C3B | -3.72 | 103.99 | 107.87 |
| 12 | U3 | 201 | CYC | OC-C1C-C2C | -3.72 | 123.22 | 126.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | U1 | 201 | CYC | OC-C1C-C2C | -3.72 | 123.22 | 126.17 |
| 12 | K3 | 201 | CYC | C2B-C1B-NB | 3.71 | 112.42 | 106.99 |
| 12 | O9 | 201 | CYC | C2B-C1B-NB | 3.71 | 112.42 | 106.99 |
| 12 | K1 | 201 | CYC | C2B-C1B-NB | 3.71 | 112.42 | 106.99 |
| 12 | N2 | 101 | CYC | CHB-C4A-NA | -3.71 | 117.17 | 124.93 |
| 12 | N6 | 101 | CYC | CHB-C4A-NA | -3.71 | 117.17 | 124.93 |
| 12 | G2 | 201 | CYC | OC-C1C-C2C | -3.71 | 123.22 | 126.17 |
| 12 | F5 | 201 | CYC | OC-C1C-C2C | -3.71 | 123.22 | 126.17 |
| 12 | D7 | 201 | CYC | OC-C1C-C2C | -3.71 | 123.22 | 126.17 |
| 12 | R5 | 201 | CYC | C2B-C1B-NB | 3.71 | 112.42 | 106.99 |
| 12 | G7 | 201 | CYC | C4A-C3A-C2A | -3.71 | 102.25 | 106.51 |
| 12 | A1 | 201 | CYC | C2B-C1B-NB | 3.71 | 112.42 | 106.99 |
| 12 | A3 | 201 | CYC | C2B-C1B-NB | 3.71 | 112.42 | 106.99 |
| 12 | E5 | 201 | CYC | C4A-C3A-C2A | -3.71 | 102.25 | 106.51 |
| 12 | V9 | 201 | CYC | CHB-C4A-NA | -3.71 | 117.17 | 124.93 |
| 12 | C3 | 201 | CYC | C2B-C1B-NB | 3.71 | 112.42 | 106.99 |
| 12 | k5 | 1202 | CYC | C2B-C1B-NB | 3.71 | 112.42 | 106.99 |
| 12 | C6 | 201 | CYC | C2B-C1B-NB | 3.71 | 112.41 | 106.99 |
| 12 | F8 | 202 | CYC | CMB-C2B-C1B | 3.71 | 128.79 | 124.17 |
| 12 | B7 | 201 | CYC | OC-C1C-C2C | -3.71 | 123.23 | 126.17 |
| 12 | M4 | 301 | CYC | CHB-C4A-NA | -3.71 | 117.18 | 124.93 |
| 12 | K5 | 201 | CYC | C4A-C3A-C2A | -3.71 | 102.25 | 106.51 |
| 12 | I7 | 201 | CYC | C4A-C3A-C2A | -3.71 | 102.25 | 106.51 |
| 12 | CA | 201 | CYC | C2B-C1B-NB | 3.70 | 112.41 | 106.99 |
| 12 | C9 | 201 | CYC | C2B-C1B-NB | 3.70 | 112.41 | 106.99 |
| 12 | M8 | 301 | CYC | CHB-C4A-NA | -3.70 | 117.18 | 124.93 |
| 12 | E7 | 201 | CYC | C4A-C3A-C2A | -3.70 | 102.25 | 106.51 |
| 12 | H6 | 201 | CYC | CHB-C4A-NA | -3.70 | 117.19 | 124.93 |
| 12 | M8 | 302 | CYC | CHB-C4A-NA | -3.70 | 117.19 | 124.93 |
| 12 | J3 | 201 | CYC | CAB-C3B-C4B | 3.70 | 127.23 | 121.38 |
| 12 | J1 | 201 | CYC | CAB-C3B-C4B | 3.70 | 127.23 | 121.38 |
| 12 | Z3 | 201 | CYC | CHB-C4A-NA | -3.70 | 117.19 | 124.93 |
| 12 | Z1 | 202 | CYC | CHB-C4A-NA | -3.70 | 117.19 | 124.93 |
| 12 | QA | 201 | CYC | C2B-C1B-NB | 3.70 | 112.41 | 106.99 |
| 12 | XA | 201 | CYC | CMB-C2B-C1B | 3.70 | 128.79 | 124.17 |
| 12 | e5 | 201 | CYC | C4A-C3A-C2A | -3.70 | 102.26 | 106.51 |
| 12 | f7 | 201 | CYC | C2B-C1B-NB | 3.70 | 112.41 | 106.99 |
| 12 | H9 | 202 | CYC | CHB-C4A-NA | -3.70 | 117.19 | 124.93 |
| 12 | Z4 | 301 | CYC | CMB-C2B-C1B | 3.70 | 128.79 | 124.17 |
| 12 | K1 | 201 | CYC | OC-C1C-C2C | -3.70 | 123.23 | 126.17 |
| 12 | Q9 | 201 | CYC | C2B-C1B-NB | 3.70 | 112.40 | 106.99 |
| 12 | F3 | 201 | CYC | CMB-C2B-C1B | 3.70 | 128.78 | 124.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | B1 | 202 | CYC | CMB-C2B-C1B | 3.70 | 128.78 | 124.17 |
| 12 | P1 | 201 | CYC | CHB-C4A-NA | -3.70 | 117.20 | 124.93 |
| 12 | P3 | 201 | CYC | CHB-C4A-NA | -3.70 | 117.20 | 124.93 |
| 12 | H7 | 201 | CYC | OC-C1C-C2C | -3.70 | 123.23 | 126.17 |
| 12 | N7 | 201 | CYC | OC-C1C-C2C | -3.70 | 123.23 | 126.17 |
| 12 | S5 | 201 | CYC | C4A-C3A-C2A | -3.69 | 102.27 | 106.51 |
| 12 | X4 | 201 | CYC | C2B-C1B-NB | 3.69 | 112.40 | 106.99 |
| 12 | X5 | 201 | CYC | C2B-C1B-NB | 3.69 | 112.40 | 106.99 |
| 12 | X8 | 201 | CYC | C2B-C1B-NB | 3.69 | 112.40 | 106.99 |
| 12 | E3 | 201 | CYC | OC-C1C-C2C | -3.69 | 123.24 | 126.17 |
| 12 | E1 | 201 | CYC | OC-C1C-C2C | -3.69 | 123.24 | 126.17 |
| 12 | SA | 201 | CYC | C2B-C1B-NB | 3.69 | 112.39 | 106.99 |
| 12 | S9 | 201 | CYC | C2B-C1B-NB | 3.69 | 112.39 | 106.99 |
| 12 | G8 | 201 | CYC | OC-C1C-C2C | -3.69 | 123.24 | 126.17 |
| 12 | G4 | 201 | CYC | C2B-C1B-NB | 3.69 | 112.39 | 106.99 |
| 12 | G8 | 201 | CYC | C2B-C1B-NB | 3.69 | 112.39 | 106.99 |
| 12 | ZA | 202 | CYC | CHB-C4A-NA | -3.69 | 117.21 | 124.93 |
| 12 | Z9 | 202 | CYC | CHB-C4A-NA | -3.69 | 117.21 | 124.93 |
| 12 | OA | 201 | CYC | C2B-C1B-NB | 3.69 | 112.39 | 106.99 |
| 12 | K6 | 201 | CYC | C2B-C1B-NB | 3.69 | 112.39 | 106.99 |
| 12 | IA | 201 | CYC | C2B-C1B-NB | 3.69 | 112.39 | 106.99 |
| 12 | I9 | 201 | CYC | C2B-C1B-NB | 3.69 | 112.39 | 106.99 |
| 12 | LA | 202 | CYC | CHB-C4A-NA | -3.69 | 117.22 | 124.93 |
| 12 | L9 | 202 | CYC | CHB-C4A-NA | -3.69 | 117.22 | 124.93 |
| 12 | K4 | 201 | CYC | C2B-C1B-NB | 3.69 | 112.39 | 106.99 |
| 12 | b7 | 201 | CYC | OC-C1C-C2C | -3.69 | 123.24 | 126.17 |
| 12 | D4 | 202 | CYC | CMB-C2B-C1B | 3.69 | 128.77 | 124.17 |
| 12 | D8 | 202 | CYC | CMB-C2B-C1B | 3.69 | 128.77 | 124.17 |
| 12 | G2 | 201 | CYC | C2B-C1B-NB | 3.69 | 112.39 | 106.99 |
| 12 | H9 | 202 | CYC | CMB-C2B-C1B | 3.69 | 128.77 | 124.17 |
| 12 | B3 | 202 | CYC | CMB-C2B-C1B | 3.69 | 128.77 | 124.17 |
| 12 | D2 | 201 | CYC | CHB-C4A-NA | -3.68 | 117.22 | 124.93 |
| 12 | N4 | 201 | CYC | C2B-C1B-NB | 3.68 | 112.38 | 106.99 |
| 12 | S1 | 201 | CYC | C2B-C1B-NB | 3.68 | 112.38 | 106.99 |
| 12 | S3 | 201 | CYC | C2B-C1B-NB | 3.68 | 112.38 | 106.99 |
| 12 | U3 | 201 | CYC | C2B-C1B-NB | 3.68 | 112.38 | 106.99 |
| 12 | v7 | 201 | CYC | C2B-C1B-NB | 3.68 | 112.38 | 106.99 |
| 12 | U1 | 201 | CYC | C2B-C1B-NB | 3.68 | 112.38 | 106.99 |
| 12 | A1 | 201 | CYC | OC-C1C-C2C | -3.68 | 123.25 | 126.17 |
| 12 | A3 | 201 | CYC | OC-C1C-C2C | -3.68 | 123.25 | 126.17 |
| 12 | F2 | 202 | CYC | C1B-C2B-C3B | -3.68 | 104.03 | 107.87 |
| 12 | V3 | 201 | CYC | CMB-C2B-C1B | 3.68 | 128.76 | 124.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | X9 | 201 | CYC | CMB-C2B-C1B | 3.68 | 128.76 | 124.17 |
| 12 | V1 | 201 | CYC | CMB-C2B-C1B | 3.68 | 128.76 | 124.17 |
| 12 | HA | 202 | CYC | CHB-C4A-NA | -3.68 | 117.23 | 124.93 |
| 12 | F1 | 201 | CYC | CMB-C2B-C1B | 3.68 | 128.76 | 124.17 |
| 12 | L6 | 201 | CYC | CHB-C4A-NA | -3.68 | 117.23 | 124.93 |
| 12 | a9 | 901 | CYC | CHB-C4A-NA | -3.68 | 117.24 | 124.93 |
| 12 | V5 | 201 | CYC | OC-C1C-C2C | -3.68 | 123.25 | 126.17 |
| 12 | I3 | 201 | CYC | C2B-C1B-NB | 3.68 | 112.37 | 106.99 |
| 12 | I1 | 201 | CYC | C2B-C1B-NB | 3.68 | 112.37 | 106.99 |
| 12 | T4 | 201 | CYC | C2B-C1B-NB | 3.68 | 112.37 | 106.99 |
| 12 | T8 | 201 | CYC | C2B-C1B-NB | 3.68 | 112.37 | 106.99 |
| 12 | RA | 201 | CYC | CHB-C4A-NA | -3.68 | 117.24 | 124.93 |
| 12 | R9 | 201 | CYC | CHB-C4A-NA | -3.68 | 117.24 | 124.93 |
| 12 | G6 | 201 | CYC | C2B-C1B-NB | 3.68 | 112.37 | 106.99 |
| 12 | O1 | 201 | CYC | OC-C1C-C2C | -3.68 | 123.25 | 126.17 |
| 12 | O3 | 201 | CYC | OC-C1C-C2C | -3.68 | 123.25 | 126.17 |
| 12 | O5 | 201 | CYC | C4A-C3A-C2A | -3.68 | 102.29 | 106.51 |
| 12 | s7 | 201 | CYC | C4A-C3A-C2A | -3.68 | 102.29 | 106.51 |
| 12 | Q1 | 201 | CYC | C2B-C1B-NB | 3.68 | 112.37 | 106.99 |
| 12 | Q3 | 201 | CYC | C2B-C1B-NB | 3.68 | 112.37 | 106.99 |
| 12 | R7 | 201 | CYC | C2B-C1B-NB | 3.68 | 112.37 | 106.99 |
| 12 | S4 | 201 | CYC | C1B-C2B-C3B | -3.67 | 104.04 | 107.87 |
| 12 | S8 | 201 | CYC | C1B-C2B-C3B | -3.67 | 104.04 | 107.87 |
| 12 | D5 | 201 | CYC | OC-C1C-C2C | -3.67 | 123.25 | 126.17 |
| 12 | L4 | 202 | CYC | CHB-C4A-NA | -3.67 | 117.25 | 124.93 |
| 12 | C3 | 201 | CYC | OC-C1C-C2C | -3.67 | 123.25 | 126.17 |
| 12 | UA | 201 | CYC | C2B-C1B-NB | 3.67 | 112.36 | 106.99 |
| 12 | U9 | 201 | CYC | C2B-C1B-NB | 3.67 | 112.36 | 106.99 |
| 12 | H4 | 201 | CYC | CMB-C2B-C1B | 3.67 | 128.75 | 124.17 |
| 12 | H8 | 201 | CYC | CMB-C2B-C1B | 3.67 | 128.75 | 124.17 |
| 12 | L3 | 202 | CYC | CHB-C4A-NA | -3.67 | 117.26 | 124.93 |
| 12 | aA | 902 | CYC | CHB-C4A-NA | -3.67 | 117.26 | 124.93 |
| 12 | b7 | 201 | CYC | C2B-C1B-NB | 3.67 | 112.36 | 106.99 |
| 12 | L2 | 201 | CYC | CHB-C4A-NA | -3.67 | 117.26 | 124.93 |
| 12 | D7 | 201 | CYC | C2B-C1B-NB | 3.66 | 112.35 | 106.99 |
| 12 | C5 | 201 | CYC | C4A-C3A-C2A | -3.66 | 102.30 | 106.51 |
| 12 | F4 | 202 | CYC | CMB-C2B-C1B | 3.66 | 128.74 | 124.17 |
| 12 | P5 | 201 | CYC | OC-C1C-C2C | -3.66 | 123.26 | 126.17 |
| 12 | m7 | 201 | CYC | C4A-C3A-C2A | -3.66 | 102.30 | 106.51 |
| 12 | Q5 | 201 | CYC | C4A-C3A-C2A | -3.66 | 102.30 | 106.51 |
| 12 | LA | 202 | CYC | CMB-C2B-C1B | 3.66 | 128.74 | 124.17 |
| 12 | H3 | 202 | CYC | CMB-C2B-C1B | 3.66 | 128.74 | 124.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | M7 | 201 | CYC | C4A-C3A-C2A | -3.66 | 102.31 | 106.51 |
| 12 | V7 | 201 | CYC | C2B-C1B-NB | 3.66 | 112.35 | 106.99 |
| 12 | N8 | 201 | CYC | C2B-C1B-NB | 3.66 | 112.34 | 106.99 |
| 12 | UA | 201 | CYC | OC-C1C-C2C | -3.66 | 123.27 | 126.17 |
| 12 | G6 | 201 | CYC | OC-C1C-C2C | -3.66 | 123.27 | 126.17 |
| 12 | U9 | 201 | CYC | OC-C1C-C2C | -3.66 | 123.27 | 126.17 |
| 12 | J5 | 201 | CYC | C1B-NB-C4B | -3.66 | 106.01 | 110.67 |
| 12 | C1 | 201 | CYC | OC-C1C-C2C | -3.66 | 123.27 | 126.17 |
| 12 | h7 | 201 | CYC | C2B-C1B-NB | 3.66 | 112.34 | 106.99 |
| 12 | H1 | 201 | CYC | CMB-C2B-C1B | 3.66 | 128.73 | 124.17 |
| 12 | V4 | 201 | CYC | OC-C1C-C2C | -3.65 | 123.27 | 126.17 |
| 12 | V8 | 201 | CYC | OC-C1C-C2C | -3.65 | 123.27 | 126.17 |
| 12 | Z4 | 301 | CYC | CHB-C4A-NA | -3.65 | 117.29 | 124.93 |
| 12 | Z8 | 301 | CYC | CHB-C4A-NA | -3.65 | 117.29 | 124.93 |
| 12 | Q7 | 201 | CYC | C4A-C3A-C2A | -3.65 | 102.31 | 106.51 |
| 12 | Z8 | 301 | CYC | CMB-C2B-C1B | 3.65 | 128.73 | 124.17 |
| 12 | J4 | 201 | CYC | CHB-C4A-NA | -3.65 | 117.30 | 124.93 |
| 12 | J8 | 201 | CYC | CHB-C4A-NA | -3.65 | 117.30 | 124.93 |
| 12 | R5 | 201 | CYC | OC-C1C-C2C | -3.65 | 123.27 | 126.17 |
| 12 | I6 | 201 | CYC | C2B-C1B-NB | 3.65 | 112.33 | 106.99 |
| 12 | L7 | 201 | CYC | C2B-C1B-NB | 3.65 | 112.33 | 106.99 |
| 12 | M5 | 201 | CYC | C4A-C3A-C2A | -3.65 | 102.32 | 106.51 |
| 12 | U7 | 201 | CYC | C4A-C3A-C2A | -3.65 | 102.32 | 106.51 |
| 12 | S1 | 201 | CYC | OC-C1C-C2C | -3.65 | 123.27 | 126.17 |
| 12 | S3 | 201 | CYC | OC-C1C-C2C | -3.65 | 123.27 | 126.17 |
| 12 | I4 | 201 | CYC | OC-C1C-C2C | -3.65 | 123.27 | 126.17 |
| 12 | I8 | 201 | CYC | OC-C1C-C2C | -3.65 | 123.27 | 126.17 |
| 12 | BA | 201 | CYC | CMB-C2B-C1B | 3.65 | 128.72 | 124.17 |
| 12 | B9 | 201 | CYC | CMB-C2B-C1B | 3.65 | 128.72 | 124.17 |
| 12 | Y3 | 201 | CYC | C2B-C1B-NB | 3.65 | 112.33 | 106.99 |
| 12 | Y1 | 201 | CYC | C2B-C1B-NB | 3.65 | 112.33 | 106.99 |
| 12 | W5 | 201 | CYC | C4A-C3A-C2A | -3.65 | 102.32 | 106.51 |
| 12 | N2 | 101 | CYC | CMB-C2B-C1B | 3.65 | 128.72 | 124.17 |
| 12 | U4 | 201 | CYC | CMB-C2B-C1B | 3.65 | 128.72 | 124.17 |
| 12 | U8 | 201 | CYC | CMB-C2B-C1B | 3.65 | 128.72 | 124.17 |
| 12 | F7 | 201 | CYC | C2B-C1B-NB | 3.65 | 112.33 | 106.99 |
| 12 | V8 | 201 | CYC | C2B-C1B-NB | 3.65 | 112.33 | 106.99 |
| 12 | Z | 201 | CYC | C2B-C1B-NB | 3.64 | 112.32 | 106.99 |
| 12 | L9 | 202 | CYC | CMB-C2B-C1B | 3.64 | 128.71 | 124.17 |
| 12 | U5 | 201 | CYC | C4A-C3A-C2A | -3.64 | 102.33 | 106.51 |
| 12 | E3 | 201 | CYC | C2B-C1B-NB | 3.64 | 112.32 | 106.99 |
| 12 | E1 | 201 | CYC | C2B-C1B-NB | 3.64 | 112.32 | 106.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | G1 | 201 | CYC | C2B-C1B-NB | 3.64 | 112.32 | 106.99 |
| 12 | J7 | 201 | CYC | C2B-C1B-NB | 3.64 | 112.31 | 106.99 |
| 12 | v7 | 201 | CYC | OC-C1C-C2C | -3.64 | 123.28 | 126.17 |
| 12 | I5 | 201 | CYC | C4A-C3A-C2A | -3.64 | 102.33 | 106.51 |
| 12 | P4 | 201 | CYC | C2B-C1B-NB | 3.64 | 112.31 | 106.99 |
| 12 | B7 | 201 | CYC | C2B-C1B-NB | 3.64 | 112.31 | 106.99 |
| 12 | A | 201 | CYC | C2B-C1B-NB | 3.63 | 112.31 | 106.99 |
| 12 | C2 | 201 | CYC | OC-C1C-C2C | -3.63 | 123.28 | 126.17 |
| 12 | f5 | 201 | CYC | C2B-C1B-NB | 3.63 | 112.31 | 106.99 |
| 12 | X5 | 201 | CYC | OC-C1C-C2C | -3.63 | 123.28 | 126.17 |
| 12 | V4 | 201 | CYC | C2B-C1B-NB | 3.63 | 112.31 | 106.99 |
| 12 | J3 | 202 | CYC | CMB-C2B-C1B | 3.63 | 128.70 | 124.17 |
| 12 | H6 | 201 | CYC | CMB-C2B-C1B | 3.63 | 128.70 | 124.17 |
| 12 | aA | 901 | CYC | CMB-C2B-C1B | 3.63 | 128.70 | 124.17 |
| 12 | b5 | 201 | CYC | C2B-C1B-NB | 3.63 | 112.31 | 106.99 |
| 12 | q7 | 201 | CYC | C4A-C3A-C2A | -3.63 | 102.34 | 106.51 |
| 12 | G3 | 201 | CYC | C2B-C1B-NB | 3.63 | 112.30 | 106.99 |
| 12 | N7 | 201 | CYC | C2B-C1B-NB | 3.63 | 112.30 | 106.99 |
| 12 | H2 | 201 | CYC | CMB-C2B-C1B | 3.63 | 128.70 | 124.17 |
| 12 | J5 | 201 | CYC | OC-C1C-C2C | -3.63 | 123.29 | 126.17 |
| 12 | H7 | 201 | CYC | C2B-C1B-NB | 3.63 | 112.30 | 106.99 |
| 12 | F3 | 202 | CYC | CHB-C1B-C2B | -3.63 | 119.76 | 126.95 |
| 12 | F1 | 202 | CYC | CHB-C1B-C2B | -3.63 | 119.76 | 126.95 |
| 12 | HA | 202 | CYC | CMB-C2B-C1B | 3.63 | 128.69 | 124.17 |
| 12 | R1 | 201 | CYC | CMB-C2B-C1B | 3.63 | 128.69 | 124.17 |
| 12 | R3 | 201 | CYC | CMB-C2B-C1B | 3.63 | 128.69 | 124.17 |
| 12 | C4 | 201 | CYC | C2B-C1B-NB | 3.63 | 112.30 | 106.99 |
| 12 | C8 | 201 | CYC | C2B-C1B-NB | 3.63 | 112.30 | 106.99 |
| 12 | N6 | 101 | CYC | CMB-C2B-C1B | 3.62 | 128.69 | 124.17 |
| 12 | p7 | 201 | CYC | OC-C1C-C2C | -3.62 | 123.29 | 126.17 |
| 12 | k5 | 1204 | CYC | C2B-C1B-NB | 3.62 | 112.29 | 106.99 |
| 12 | k7 | 201 | CYC | C4A-C3A-C2A | -3.62 | 102.35 | 106.51 |
| 12 | X7 | 201 | CYC | C2B-C1B-NB | 3.62 | 112.29 | 106.99 |
| 12 | W9 | 201 | CYC | C2B-C1B-NB | 3.62 | 112.29 | 106.99 |
| 12 | WA | 201 | CYC | C2B-C1B-NB | 3.62 | 112.29 | 106.99 |
| 12 | P8 | 201 | CYC | C2B-C1B-NB | 3.62 | 112.29 | 106.99 |
| 12 | J7 | 201 | CYC | C1B-NB-C4B | -3.62 | 106.06 | 110.67 |
| 12 | P7 | 201 | CYC | C2B-C1B-NB | 3.62 | 112.29 | 106.99 |
| 12 | X3 | 201 | CYC | CMB-C2B-C1B | 3.62 | 128.69 | 124.17 |
| 12 | X1 | 201 | CYC | CMB-C2B-C1B | 3.62 | 128.69 | 124.17 |
| 12 | E8 | 201 | CYC | OC-C1C-C2C | -3.62 | 123.30 | 126.17 |
| 12 | I4 | 201 | CYC | C2B-C1B-NB | 3.62 | 112.28 | 106.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | F5 | 201 | CYC | C2B-C1B-NB | 3.62 | 112.28 | 106.99 |
| 12 | I8 | 201 | CYC | C2B-C1B-NB | 3.62 | 112.28 | 106.99 |
| 12 | D5 | 201 | CYC | C1B-NB-C4B | -3.61 | 106.07 | 110.67 |
| 12 | Y3 | 201 | CYC | OC-C1C-C2C | -3.61 | 123.30 | 126.17 |
| 12 | Y1 | 201 | CYC | OC-C1C-C2C | -3.61 | 123.30 | 126.17 |
| 12 | ZA | 202 | CYC | CMB-C2B-C1B | 3.61 | 128.68 | 124.17 |
| 12 | Z9 | 202 | CYC | CMB-C2B-C1B | 3.61 | 128.68 | 124.17 |
| 12 | j7 | 201 | CYC | C2B-C1B-NB | 3.61 | 112.28 | 106.99 |
| 12 | X7 | 201 | CYC | OC-C1C-C2C | -3.61 | 123.30 | 126.17 |
| 12 | j5 | 1202 | CYC | C2B-C1B-NB | 3.61 | 112.28 | 106.99 |
| 12 | V3 | 202 | CYC | CHB-C1B-C2B | -3.61 | 119.79 | 126.95 |
| 12 | I6 | 201 | CYC | OC-C1C-C2C | -3.61 | 123.30 | 126.17 |
| 12 | N5 | 201 | CYC | C2B-C1B-NB | 3.61 | 112.27 | 106.99 |
| 12 | Y8 | 201 | CYC | CHB-C1B-C2B | -3.61 | 119.80 | 126.95 |
| 12 | Y4 | 201 | CYC | CHB-C1B-C2B | -3.61 | 119.80 | 126.95 |
| 12 | O4 | 201 | CYC | CMB-C2B-C1B | 3.61 | 128.67 | 124.17 |
| 12 | O8 | 201 | CYC | CMB-C2B-C1B | 3.61 | 128.67 | 124.17 |
| 12 | WA | 201 | CYC | OC-C1C-C2C | -3.61 | 123.31 | 126.17 |
| 12 | W9 | 201 | CYC | OC-C1C-C2C | -3.61 | 123.31 | 126.17 |
| 12 | I2 | 201 | CYC | C2B-C1B-NB | 3.61 | 112.27 | 106.99 |
| 12 | W1 | 201 | CYC | C2B-C1B-NB | 3.61 | 112.27 | 106.99 |
| 12 | I2 | 201 | CYC | OC-C1C-C2C | -3.60 | 123.31 | 126.17 |
| 12 | J2 | 202 | CYC | CMB-C2B-C1B | 3.60 | 128.67 | 124.17 |
| 12 | V1 | 202 | CYC | CHB-C1B-C2B | -3.60 | 119.81 | 126.95 |
| 12 | Z | 201 | CYC | C1B-NB-C4B | -3.60 | 106.08 | 110.67 |
| 12 | D7 | 201 | CYC | C1B-NB-C4B | -3.60 | 106.08 | 110.67 |
| 12 | P5 | 201 | CYC | C2B-C1B-NB | 3.60 | 112.26 | 106.99 |
| 12 | H3 | 201 | CYC | CHB-C1B-C2B | -3.60 | 119.82 | 126.95 |
| 12 | H1 | 202 | CYC | CHB-C1B-C2B | -3.60 | 119.82 | 126.95 |
| 12 | Y7 | 201 | CYC | C4A-C3A-C2A | -3.60 | 102.38 | 106.51 |
| 12 | I3 | 201 | CYC | OC-C1C-C2C | -3.60 | 123.31 | 126.17 |
| 12 | I1 | 201 | CYC | OC-C1C-C2C | -3.60 | 123.31 | 126.17 |
| 12 | T3 | 301 | CYC | CMB-C2B-C1B | 3.59 | 128.66 | 124.17 |
| 12 | T1 | 301 | CYC | CMB-C2B-C1B | 3.59 | 128.66 | 124.17 |
| 12 | W3 | 201 | CYC | C2B-C1B-NB | 3.59 | 112.25 | 106.99 |
| 12 | P4 | 201 | CYC | OC-C1C-C2C | -3.59 | 123.32 | 126.17 |
| 12 | P8 | 201 | CYC | OC-C1C-C2C | -3.59 | 123.32 | 126.17 |
| 12 | s7 | 201 | CYC | CHA-C1A-NA | -3.59 | 123.84 | 128.83 |
| 12 | u7 | 201 | CYC | C4A-C3A-C2A | -3.59 | 102.38 | 106.51 |
| 12 | FA | 301 | CYC | CMB-C2B-C1B | 3.59 | 128.65 | 124.17 |
| 12 | F9 | 301 | CYC | CMB-C2B-C1B | 3.59 | 128.65 | 124.17 |
| 12 | U4 | 202 | CYC | CHB-C1B-C2B | -3.59 | 119.84 | 126.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | U8 | 202 | CYC | CHB-C1B-C2B | -3.59 | 119.84 | 126.95 |
| 12 | d7 | 201 | CYC | C2B-C1B-NB | 3.59 | 112.24 | 106.99 |
| 12 | J4 | 202 | CYC | CHB-C1B-C2B | -3.59 | 119.84 | 126.95 |
| 12 | J8 | 202 | CYC | CHB-C1B-C2B | -3.59 | 119.84 | 126.95 |
| 12 | A4 | 201 | CYC | C2B-C1B-NB | 3.59 | 112.24 | 106.99 |
| 12 | A8 | 201 | CYC | C2B-C1B-NB | 3.59 | 112.24 | 106.99 |
| 12 | C6 | 201 | CYC | OC-C1C-C2C | -3.59 | 123.32 | 126.17 |
| 12 | K2 | 201 | CYC | OC-C1C-C2C | -3.59 | 123.32 | 126.17 |
| 12 | B5 | 201 | CYC | C2B-C1B-NB | 3.59 | 112.24 | 106.99 |
| 12 | J6 | 202 | CYC | CMB-C2B-C1B | 3.59 | 128.64 | 124.17 |
| 12 | A | 201 | CYC | C1B-NB-C4B | -3.59 | 106.10 | 110.67 |
| 12 | GA | 201 | CYC | OC-C1C-C2C | -3.58 | 123.32 | 126.17 |
| 12 | G9 | 201 | CYC | OC-C1C-C2C | -3.58 | 123.32 | 126.17 |
| 12 | L5 | 201 | CYC | C2B-C1B-NB | 3.58 | 112.23 | 106.99 |
| 12 | T5 | 201 | CYC | C2B-C1B-NB | 3.58 | 112.23 | 106.99 |
| 12 | QA | 201 | CYC | OC-C1C-C2C | -3.58 | 123.32 | 126.17 |
| 12 | E4 | 201 | CYC | OC-C1C-C2C | -3.58 | 123.33 | 126.17 |
| 12 | V5 | 201 | CYC | C2B-C1B-NB | 3.58 | 112.23 | 106.99 |
| 12 | W4 | 201 | CYC | CMB-C2B-C1B | 3.58 | 128.63 | 124.17 |
| 12 | W8 | 201 | CYC | CMB-C2B-C1B | 3.58 | 128.63 | 124.17 |
| 12 | G3 | 201 | CYC | OC-C1C-C2C | -3.58 | 123.33 | 126.17 |
| 12 | G1 | 201 | CYC | OC-C1C-C2C | -3.58 | 123.33 | 126.17 |
| 12 | Z1 | 202 | CYC | CMB-C2B-C1B | 3.58 | 128.63 | 124.17 |
| 12 | RA | 202 | CYC | CHB-C1B-C2B | -3.57 | 119.87 | 126.95 |
| 12 | H4 | 202 | CYC | CHB-C1B-C2B | -3.57 | 119.87 | 126.95 |
| 12 | H8 | 202 | CYC | CHB-C1B-C2B | -3.57 | 119.87 | 126.95 |
| 12 | R9 | 202 | CYC | CHB-C1B-C2B | -3.57 | 119.87 | 126.95 |
| 12 | TA | 301 | CYC | CMB-C2B-C1B | 3.57 | 128.63 | 124.17 |
| 12 | B8 | 202 | CYC | CMB-C2B-C1B | 3.57 | 128.63 | 124.17 |
| 12 | B4 | 202 | CYC | CMB-C2B-C1B | 3.57 | 128.63 | 124.17 |
| 12 | JA | 201 | CYC | CHB-C1B-C2B | -3.57 | 119.87 | 126.95 |
| 12 | J9 | 201 | CYC | CHB-C1B-C2B | -3.57 | 119.87 | 126.95 |
| 12 | Z3 | 202 | CYC | CHB-C1B-C2B | -3.57 | 119.87 | 126.95 |
| 12 | Z1 | 201 | CYC | CHB-C1B-C2B | -3.57 | 119.87 | 126.95 |
| 12 | I5 | 201 | CYC | C1B-C2B-C3B | -3.57 | 104.14 | 107.87 |
| 12 | o7 | 201 | CYC | C4A-C3A-C2A | -3.57 | 102.41 | 106.51 |
| 12 | H5 | 201 | CYC | C2B-C1B-NB | 3.57 | 112.21 | 106.99 |
| 12 | AA | 201 | CYC | C2B-C1B-NB | 3.57 | 112.21 | 106.99 |
| 12 | T7 | 201 | CYC | C2B-C1B-NB | 3.57 | 112.21 | 106.99 |
| 12 | A9 | 201 | CYC | C2B-C1B-NB | 3.57 | 112.21 | 106.99 |
| 12 | J2 | 201 | CYC | CHB-C1B-C2B | -3.57 | 119.88 | 126.95 |
| 12 | J6 | 201 | CYC | CHB-C1B-C2B | -3.57 | 119.88 | 126.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | CA | 201 | CYC | OC-C1C-C2C | -3.56 | 123.34 | 126.17 |
| 12 | r7 | 201 | CYC | C2B-C1B-NB | 3.56 | 112.20 | 106.99 |
| 12 | p7 | 201 | CYC | C1B-NB-C4B | -3.56 | 106.13 | 110.67 |
| 12 | D3 | 202 | CYC | CMB-C2B-C1B | 3.56 | 128.62 | 124.17 |
| 12 | D1 | 202 | CYC | CMB-C2B-C1B | 3.56 | 128.62 | 124.17 |
| 12 | PA | 201 | CYC | CMB-C2B-C1B | 3.56 | 128.62 | 124.17 |
| 12 | P9 | 201 | CYC | CMB-C2B-C1B | 3.56 | 128.62 | 124.17 |
| 12 | a5 | 201 | CYC | CHA-C1A-NA | -3.56 | 123.89 | 128.83 |
| 12 | C6 | 201 | CYC | CMA-C3A-C4A | 3.56 | 130.55 | 125.06 |
| 12 | P1 | 201 | CYC | CMB-C2B-C1B | 3.56 | 128.61 | 124.17 |
| 12 | T9 | 301 | CYC | CMB-C2B-C1B | 3.56 | 128.61 | 124.17 |
| 12 | k5 | 1203 | CYC | C2B-C1B-NB | 3.56 | 112.20 | 106.99 |
| 12 | Z3 | 201 | CYC | CMB-C2B-C1B | 3.56 | 128.61 | 124.17 |
| 12 | e7 | 201 | CYC | C4A-C3A-C2A | -3.56 | 102.42 | 106.51 |
| 12 | P3 | 201 | CYC | CMB-C2B-C1B | 3.55 | 128.60 | 124.17 |
| 12 | B2 | 201 | CYC | CHB-C1B-C2B | -3.55 | 119.91 | 126.95 |
| 12 | d7 | 201 | CYC | C1B-NB-C4B | -3.55 | 106.14 | 110.67 |
| 12 | HA | 201 | CYC | CHB-C1B-C2B | -3.55 | 119.91 | 126.95 |
| 12 | H9 | 201 | CYC | CHB-C1B-C2B | -3.55 | 119.91 | 126.95 |
| 12 | B4 | 201 | CYC | CHB-C1B-C2B | -3.55 | 119.91 | 126.95 |
| 12 | B8 | 201 | CYC | CHB-C1B-C2B | -3.55 | 119.91 | 126.95 |
| 12 | Y7 | 201 | CYC | CHA-C1A-NA | -3.55 | 123.90 | 128.83 |
| 12 | D2 | 201 | CYC | CMB-C2B-C1B | 3.55 | 128.60 | 124.17 |
| 12 | k5 | 1202 | CYC | C1B-NB-C4B | -3.55 | 106.15 | 110.67 |
| 12 | Y9 | 201 | CYC | OC-C1C-C2C | -3.55 | 123.35 | 126.17 |
| 12 | H2 | 202 | CYC | CHB-C1B-C2B | -3.55 | 119.92 | 126.95 |
| 12 | R5 | 201 | CYC | C1B-NB-C4B | -3.55 | 106.15 | 110.67 |
| 12 | K6 | 201 | CYC | OC-C1C-C2C | -3.55 | 123.35 | 126.17 |
| 12 | H6 | 202 | CYC | CHB-C1B-C2B | -3.55 | 119.92 | 126.95 |
| 12 | C5 | 201 | CYC | C1B-C2B-C3B | -3.55 | 104.17 | 107.87 |
| 12 | YA | 201 | CYC | OC-C1C-C2C | -3.54 | 123.36 | 126.17 |
| 12 | M7 | 201 | CYC | C1B-C2B-C3B | -3.54 | 104.17 | 107.87 |
| 12 | D6 | 201 | CYC | CMB-C2B-C1B | 3.54 | 128.59 | 124.17 |
| 12 | a9 | 901 | CYC | CMB-C2B-C1B | 3.54 | 128.58 | 124.17 |
| 12 | B6 | 201 | CYC | CHB-C1B-C2B | -3.54 | 119.94 | 126.95 |
| 12 | X5 | 201 | CYC | C1B-NB-C4B | -3.54 | 106.17 | 110.67 |
| 12 | Z5 | 201 | CYC | C2B-C1B-NB | 3.54 | 112.17 | 106.99 |
| 12 | XA | 202 | CYC | CHB-C1B-C2B | -3.54 | 119.94 | 126.95 |
| 12 | X9 | 202 | CYC | CHB-C1B-C2B | -3.54 | 119.94 | 126.95 |
| 12 | j7 | 201 | CYC | C1B-NB-C4B | -3.54 | 106.17 | 110.67 |
| 12 | ZA | 202 | CYC | CAB-C3B-C4B | 3.54 | 126.96 | 121.38 |
| 12 | Z9 | 202 | CYC | CAB-C3B-C4B | 3.54 | 126.96 | 121.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | i7 | 201 | CYC | C1B-C2B-C3B | -3.53 | 104.18 | 107.87 |
| 12 | XA | 201 | CYC | CAB-C3B-C4B | 3.53 | 126.96 | 121.38 |
| 12 | X9 | 201 | CYC | CAB-C3B-C4B | 3.53 | 126.96 | 121.38 |
| 12 | b7 | 201 | CYC | C1B-NB-C4B | -3.53 | 106.17 | 110.67 |
| 12 | aA | 902 | CYC | CMB-C2B-C1B | 3.53 | 128.58 | 124.17 |
| 12 | i7 | 201 | CYC | CHA-C1A-NA | -3.53 | 123.93 | 128.83 |
| 12 | W8 | 202 | CYC | CHB-C1B-C2B | -3.53 | 119.95 | 126.95 |
| 12 | C2 | 201 | CYC | CMA-C3A-C4A | 3.53 | 130.50 | 125.06 |
| 12 | U5 | 201 | CYC | C1B-C2B-C3B | -3.53 | 104.19 | 107.87 |
| 12 | W4 | 202 | CYC | CHB-C1B-C2B | -3.53 | 119.96 | 126.95 |
| 12 | d5 | 201 | CYC | C2B-C1B-NB | 3.53 | 112.15 | 106.99 |
| 12 | Q1 | 201 | CYC | OC-C1C-C2C | -3.53 | 123.37 | 126.17 |
| 12 | Q3 | 201 | CYC | OC-C1C-C2C | -3.53 | 123.37 | 126.17 |
| 12 | m7 | 201 | CYC | CHA-C1A-NA | -3.53 | 123.94 | 128.83 |
| 12 | V7 | 201 | CYC | C1B-NB-C4B | -3.53 | 106.18 | 110.67 |
| 12 | S4 | 202 | CYC | CAB-C3B-C4B | 3.53 | 126.95 | 121.38 |
| 12 | VA | 202 | CYC | CHB-C1B-C2B | -3.53 | 119.96 | 126.95 |
| 12 | f7 | 201 | CYC | C1B-NB-C4B | -3.53 | 106.18 | 110.67 |
| 12 | X3 | 202 | CYC | CHB-C1B-C2B | -3.52 | 119.96 | 126.95 |
| 12 | X1 | 202 | CYC | CHB-C1B-C2B | -3.52 | 119.96 | 126.95 |
| 12 | D3 | 201 | CYC | CHB-C1B-C2B | -3.52 | 119.97 | 126.95 |
| 12 | T3 | 302 | CYC | CHB-C1B-C2B | -3.52 | 119.97 | 126.95 |
| 12 | D1 | 201 | CYC | CHB-C1B-C2B | -3.52 | 119.97 | 126.95 |
| 12 | T1 | 302 | CYC | CHB-C1B-C2B | -3.52 | 119.97 | 126.95 |
| 12 | e7 | 201 | CYC | CHA-C1A-NA | -3.52 | 123.94 | 128.83 |
| 12 | F6 | 201 | CYC | CMB-C2B-C1B | 3.52 | 128.57 | 124.17 |
| 12 | T9 | 302 | CYC | CHB-C1B-C2B | -3.52 | 119.97 | 126.95 |
| 12 | J1 | 201 | CYC | CHB-C1B-C2B | -3.52 | 119.97 | 126.95 |
| 12 | X7 | 201 | CYC | C1B-NB-C4B | -3.52 | 106.18 | 110.67 |
| 12 | PA | 202 | CYC | CHB-C1B-C2B | -3.52 | 119.97 | 126.95 |
| 12 | P9 | 202 | CYC | CHB-C1B-C2B | -3.52 | 119.97 | 126.95 |
| 12 | N4 | 201 | CYC | CMA-C3A-C4A | 3.52 | 130.49 | 125.06 |
| 12 | S4 | 202 | CYC | CMB-C2B-C1B | 3.52 | 128.56 | 124.17 |
| 12 | J4 | 201 | CYC | CMB-C2B-C1B | 3.52 | 128.56 | 124.17 |
| 12 | J8 | 201 | CYC | CMB-C2B-C1B | 3.52 | 128.56 | 124.17 |
| 12 | E7 | 201 | CYC | CHA-C1A-NA | -3.52 | 123.94 | 128.83 |
| 12 | C9 | 201 | CYC | OC-C1C-C2C | -3.52 | 123.37 | 126.17 |
| 12 | LA | 201 | CYC | CHB-C1B-C2B | -3.52 | 119.97 | 126.95 |
| 12 | P1 | 202 | CYC | CHB-C1B-C2B | -3.52 | 119.97 | 126.95 |
| 12 | P3 | 202 | CYC | CHB-C1B-C2B | -3.52 | 119.97 | 126.95 |
| 12 | L9 | 201 | CYC | CHB-C1B-C2B | -3.52 | 119.97 | 126.95 |
| 12 | P5 | 201 | CYC | CHB-C4A-NA | -3.52 | 117.57 | 124.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | R7 | 201 | CYC | C1B-NB-C4B | -3.52 | 106.19 | 110.67 |
| 12 | B3 | 201 | CYC | CHB-C1B-C2B | -3.52 | 119.98 | 126.95 |
| 12 | B1 | 201 | CYC | CHB-C1B-C2B | -3.52 | 119.98 | 126.95 |
| 12 | N5 | 201 | CYC | C1B-NB-C4B | -3.52 | 106.19 | 110.67 |
| 12 | RA | 201 | CYC | CMB-C2B-C1B | 3.52 | 128.56 | 124.17 |
| 12 | R9 | 201 | CYC | CMB-C2B-C1B | 3.52 | 128.56 | 124.17 |
| 12 | A | 201 | CYC | CHB-C4A-NA | -3.52 | 117.58 | 124.93 |
| 12 | Z | 201 | CYC | CHB-C4A-NA | -3.52 | 117.58 | 124.93 |
| 12 | j5 | 1202 | CYC | CHB-C4A-NA | -3.52 | 117.58 | 124.93 |
| 12 | KA | 201 | CYC | OC-C1C-C2C | -3.52 | 123.38 | 126.17 |
| 12 | K9 | 201 | CYC | OC-C1C-C2C | -3.52 | 123.38 | 126.17 |
| 12 | L3 | 202 | CYC | CMB-C2B-C1B | 3.52 | 128.56 | 124.17 |
| 12 | A1 | 201 | CYC | CMA-C3A-C4A | 3.52 | 130.48 | 125.06 |
| 12 | A3 | 201 | CYC | CMA-C3A-C4A | 3.52 | 130.48 | 125.06 |
| 12 | YA | 201 | CYC | C1B-NB-C4B | -3.51 | 106.19 | 110.67 |
| 12 | Q7 | 201 | CYC | C1B-C2B-C3B | -3.51 | 104.20 | 107.87 |
| 12 | Q9 | 201 | CYC | OC-C1C-C2C | -3.51 | 123.38 | 126.17 |
| 12 | SA | 201 | CYC | C1B-NB-C4B | -3.51 | 106.19 | 110.67 |
| 12 | S9 | 201 | CYC | C1B-NB-C4B | -3.51 | 106.19 | 110.67 |
| 12 | J2 | 202 | CYC | CAB-C3B-C4B | 3.51 | 126.93 | 121.38 |
| 12 | BA | 202 | CYC | CHB-C1B-C2B | -3.51 | 119.99 | 126.95 |
| 12 | P7 | 201 | CYC | C1B-NB-C4B | -3.51 | 106.20 | 110.67 |
| 12 | D4 | 201 | CYC | CHB-C1B-C2B | -3.51 | 119.99 | 126.95 |
| 12 | D8 | 201 | CYC | CHB-C1B-C2B | -3.51 | 119.99 | 126.95 |
| 12 | F9 | 302 | CYC | CHB-C1B-C2B | -3.51 | 119.99 | 126.95 |
| 12 | V9 | 202 | CYC | CHB-C1B-C2B | -3.51 | 119.99 | 126.95 |
| 12 | F4 | 201 | CYC | CHB-C1B-C2B | -3.51 | 119.99 | 126.95 |
| 12 | F8 | 201 | CYC | CHB-C1B-C2B | -3.51 | 119.99 | 126.95 |
| 12 | J3 | 201 | CYC | CHB-C1B-C2B | -3.51 | 120.00 | 126.95 |
| 12 | e5 | 201 | CYC | CHA-C1A-NA | -3.51 | 123.96 | 128.83 |
| 12 | k5 | 1204 | CYC | CHB-C4A-NA | -3.51 | 117.59 | 124.93 |
| 12 | TA | 302 | CYC | CHB-C1B-C2B | -3.51 | 120.00 | 126.95 |
| 12 | S4 | 201 | CYC | CHB-C1B-C2B | -3.51 | 120.00 | 126.95 |
| 12 | S8 | 201 | CYC | CHB-C1B-C2B | -3.51 | 120.00 | 126.95 |
| 12 | F9 | 303 | CYC | CHB-C1B-C2B | -3.51 | 120.00 | 126.95 |
| 12 | B9 | 202 | CYC | CHB-C1B-C2B | -3.51 | 120.00 | 126.95 |
| 12 | I1 | 201 | CYC | CMA-C3A-C4A | 3.50 | 130.46 | 125.06 |
| 12 | V5 | 201 | CYC | CHB-C4A-NA | -3.50 | 117.61 | 124.93 |
| 12 | V7 | 201 | CYC | CHB-C4A-NA | -3.50 | 117.61 | 124.93 |
| 12 | L7 | 201 | CYC | C1B-NB-C4B | -3.50 | 106.21 | 110.67 |
| 12 | M7 | 201 | CYC | CHA-C1A-NA | -3.50 | 123.97 | 128.83 |
| 12 | v7 | 201 | CYC | C1B-NB-C4B | -3.50 | 106.21 | 110.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | W5 | 201 | CYC | CHA-C1A-NA | -3.50 | 123.97 | 128.83 |
| 12 | A7 | 201 | CYC | CHA-C1A-NA | -3.50 | 123.97 | 128.83 |
| 12 | F2 | 201 | CYC | CAB-C3B-C4B | 3.50 | 126.91 | 121.38 |
| 12 | UA | 201 | CYC | CMA-C3A-C4A | 3.50 | 130.46 | 125.06 |
| 12 | N8 | 201 | CYC | CMA-C3A-C4A | 3.50 | 130.46 | 125.06 |
| 12 | U9 | 201 | CYC | CMA-C3A-C4A | 3.50 | 130.46 | 125.06 |
| 12 | DA | 201 | CYC | CMB-C2B-C1B | 3.50 | 128.54 | 124.17 |
| 12 | X7 | 201 | CYC | CMA-C3A-C4A | 3.50 | 130.45 | 125.06 |
| 12 | I5 | 201 | CYC | CHA-C1A-NA | -3.50 | 123.97 | 128.83 |
| 12 | VA | 201 | CYC | CAB-C3B-C4B | 3.50 | 126.91 | 121.38 |
| 12 | G1 | 201 | CYC | CMA-C3A-C4A | 3.50 | 130.45 | 125.06 |
| 12 | L4 | 201 | CYC | CHB-C1B-C2B | -3.50 | 120.02 | 126.95 |
| 12 | L8 | 201 | CYC | CHB-C1B-C2B | -3.50 | 120.02 | 126.95 |
| 12 | V5 | 201 | CYC | C1B-NB-C4B | -3.50 | 106.22 | 110.67 |
| 12 | J5 | 201 | CYC | CHB-C4A-NA | -3.50 | 117.62 | 124.93 |
| 12 | F6 | 201 | CYC | CAB-C3B-C4B | 3.50 | 126.90 | 121.38 |
| 12 | F7 | 201 | CYC | C1B-NB-C4B | -3.50 | 106.22 | 110.67 |
| 12 | c7 | 201 | CYC | C1B-C2B-C3B | -3.50 | 104.22 | 107.87 |
| 12 | DA | 202 | CYC | OC-C1C-C2C | -3.50 | 123.39 | 126.17 |
| 12 | D9 | 202 | CYC | OC-C1C-C2C | -3.50 | 123.39 | 126.17 |
| 12 | W1 | 201 | CYC | OC-C1C-C2C | -3.50 | 123.39 | 126.17 |
| 12 | L2 | 202 | CYC | CHB-C1B-C2B | -3.50 | 120.02 | 126.95 |
| 12 | H5 | 201 | CYC | CMA-C3A-C4A | 3.49 | 130.45 | 125.06 |
| 12 | C5 | 201 | CYC | CHA-C1A-NA | -3.49 | 123.98 | 128.83 |
| 12 | L6 | 202 | CYC | CHB-C1B-C2B | -3.49 | 120.03 | 126.95 |
| 12 | I3 | 201 | CYC | CMA-C3A-C4A | 3.49 | 130.44 | 125.06 |
| 12 | K8 | 201 | CYC | CMA-C3A-C4A | 3.49 | 130.44 | 125.06 |
| 12 | P5 | 201 | CYC | C1B-NB-C4B | -3.49 | 106.22 | 110.67 |
| 12 | R1 | 202 | CYC | CHB-C1B-C2B | -3.49 | 120.03 | 126.95 |
| 12 | R3 | 202 | CYC | CHB-C1B-C2B | -3.49 | 120.03 | 126.95 |
| 12 | O3 | 201 | CYC | CMA-C3A-C4A | 3.49 | 130.44 | 125.06 |
| 12 | a7 | 201 | CYC | CHA-C1A-NA | -3.49 | 123.98 | 128.83 |
| 12 | J6 | 202 | CYC | CAB-C3B-C4B | 3.49 | 126.89 | 121.38 |
| 12 | G3 | 201 | CYC | CMA-C3A-C4A | 3.49 | 130.44 | 125.06 |
| 12 | S1 | 201 | CYC | CMA-C3A-C4A | 3.49 | 130.44 | 125.06 |
| 12 | S3 | 201 | CYC | CMA-C3A-C4A | 3.49 | 130.44 | 125.06 |
| 12 | N7 | 201 | CYC | CHB-C4A-NA | -3.49 | 117.63 | 124.93 |
| 12 | JA | 202 | CYC | CMB-C2B-C1B | 3.49 | 128.53 | 124.17 |
| 12 | J9 | 202 | CYC | CMB-C2B-C1B | 3.49 | 128.53 | 124.17 |
| 12 | k5 | 1204 | CYC | C1B-NB-C4B | -3.49 | 106.23 | 110.67 |
| 12 | h7 | 201 | CYC | C1B-NB-C4B | -3.49 | 106.23 | 110.67 |
| 12 | C7 | 201 | CYC | CHA-C1A-NA | -3.49 | 123.99 | 128.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | M8 | 302 | CYC | CAB-C3B-C4B | 3.49 | 126.89 | 121.38 |
| 12 | E6 | 201 | CYC | C1B-NB-C4B | -3.49 | 106.23 | 110.67 |
| 12 | D9 | 201 | CYC | CMB-C2B-C1B | 3.49 | 128.52 | 124.17 |
| 12 | V5 | 201 | CYC | CMA-C3A-C4A | 3.49 | 130.43 | 125.06 |
| 12 | W7 | 201 | CYC | CHA-C1A-NA | -3.49 | 123.99 | 128.83 |
| 12 | f7 | 201 | CYC | CHB-C4A-NA | -3.49 | 117.64 | 124.93 |
| 12 | S7 | 201 | CYC | CHA-C1A-NA | -3.49 | 123.99 | 128.83 |
| 12 | CA | 201 | CYC | CMA-C3A-C4A | 3.49 | 130.43 | 125.06 |
| 12 | C9 | 201 | CYC | CMA-C3A-C4A | 3.49 | 130.43 | 125.06 |
| 12 | E2 | 201 | CYC | C1B-NB-C4B | -3.49 | 106.23 | 110.67 |
| 12 | J7 | 201 | CYC | CHB-C4A-NA | -3.49 | 117.64 | 124.93 |
| 12 | O5 | 201 | CYC | C1B-C2B-C3B | -3.49 | 104.23 | 107.87 |
| 12 | T5 | 201 | CYC | C1B-NB-C4B | -3.48 | 106.23 | 110.67 |
| 12 | M8 | 302 | CYC | CMB-C2B-C1B | 3.48 | 128.52 | 124.17 |
| 12 | Q4 | 201 | CYC | CHB-C1B-C2B | -3.48 | 120.04 | 126.95 |
| 12 | B7 | 201 | CYC | C1B-NB-C4B | -3.48 | 106.23 | 110.67 |
| 12 | Y9 | 201 | CYC | C1B-NB-C4B | -3.48 | 106.23 | 110.67 |
| 12 | ZA | 201 | CYC | CHB-C1B-C2B | -3.48 | 120.05 | 126.95 |
| 12 | Z9 | 201 | CYC | CHB-C1B-C2B | -3.48 | 120.05 | 126.95 |
| 12 | D5 | 201 | CYC | CHB-C4A-NA | -3.48 | 117.64 | 124.93 |
| 12 | p7 | 201 | CYC | CHB-C4A-NA | -3.48 | 117.64 | 124.93 |
| 12 | O1 | 201 | CYC | CMA-C3A-C4A | 3.48 | 130.43 | 125.06 |
| 12 | L3 | 201 | CYC | CHB-C1B-C2B | -3.48 | 120.05 | 126.95 |
| 12 | L1 | 201 | CYC | CHB-C1B-C2B | -3.48 | 120.05 | 126.95 |
| 12 | DA | 202 | CYC | CHB-C1B-C2B | -3.48 | 120.05 | 126.95 |
| 12 | D9 | 202 | CYC | CHB-C1B-C2B | -3.48 | 120.05 | 126.95 |
| 12 | R7 | 201 | CYC | CMA-C3A-C4A | 3.48 | 130.43 | 125.06 |
| 12 | F5 | 201 | CYC | C1B-NB-C4B | -3.48 | 106.24 | 110.67 |
| 12 | b5 | 201 | CYC | CHB-C4A-NA | -3.48 | 117.65 | 124.93 |
| 12 | v7 | 201 | CYC | CHB-C4A-NA | -3.48 | 117.65 | 124.93 |
| 12 | V9 | 201 | CYC | CAB-C3B-C4B | 3.48 | 126.88 | 121.38 |
| 12 | P5 | 201 | CYC | CMA-C3A-C4A | 3.48 | 130.43 | 125.06 |
| 12 | b5 | 201 | CYC | C1B-NB-C4B | -3.48 | 106.24 | 110.67 |
| 12 | Z5 | 201 | CYC | CHB-C4A-NA | -3.48 | 117.65 | 124.93 |
| 12 | U4 | 201 | CYC | CAB-C3B-C4B | 3.48 | 126.88 | 121.38 |
| 12 | U8 | 201 | CYC | CAB-C3B-C4B | 3.48 | 126.88 | 121.38 |
| 12 | R5 | 201 | CYC | C1A-C2A-C3A | -3.48 | 102.93 | 106.78 |
| 12 | L4 | 202 | CYC | CMB-C2B-C1B | 3.48 | 128.51 | 124.17 |
| 12 | K7 | 201 | CYC | CHA-C1A-NA | -3.48 | 124.00 | 128.83 |
| 12 | d5 | 201 | CYC | CHB-C4A-NA | -3.48 | 117.66 | 124.93 |
| 12 | I7 | 201 | CYC | CHA-C1A-NA | -3.48 | 124.00 | 128.83 |
| 12 | X7 | 201 | CYC | CHB-C4A-NA | -3.48 | 117.66 | 124.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | F6 | 202 | CYC | CHB-C1B-C2B | -3.48 | 120.06 | 126.95 |
| 12 | k5 | 1202 | CYC | CHB-C4A-NA | -3.48 | 117.66 | 124.93 |
| 12 | D7 | 201 | CYC | CHB-C4A-NA | -3.48 | 117.66 | 124.93 |
| 12 | D2 | 202 | CYC | CHB-C1B-C2B | -3.48 | 120.06 | 126.95 |
| 12 | V4 | 201 | CYC | CMA-C3A-C4A | 3.48 | 130.42 | 125.06 |
| 12 | G4 | 201 | CYC | CMA-C3A-C4A | 3.48 | 130.42 | 125.06 |
| 12 | p7 | 201 | CYC | CMA-C3A-C4A | 3.48 | 130.42 | 125.06 |
| 12 | N5 | 201 | CYC | CHB-C4A-NA | -3.48 | 117.66 | 124.93 |
| 12 | R4 | 201 | CYC | OC-C1C-C2C | -3.47 | 123.41 | 126.17 |
| 12 | R8 | 201 | CYC | OC-C1C-C2C | -3.47 | 123.41 | 126.17 |
| 12 | K4 | 201 | CYC | CMA-C3A-C4A | 3.47 | 130.41 | 125.06 |
| 12 | e7 | 201 | CYC | C1B-C2B-C3B | -3.47 | 104.25 | 107.87 |
| 12 | c7 | 201 | CYC | CHA-C1A-NA | -3.47 | 124.01 | 128.83 |
| 12 | EA | 201 | CYC | OC-C1C-C2C | -3.47 | 123.41 | 126.17 |
| 12 | SA | 201 | CYC | OC-C1C-C2C | -3.47 | 123.41 | 126.17 |
| 12 | W4 | 202 | CYC | OC-C1C-C2C | -3.47 | 123.41 | 126.17 |
| 12 | W8 | 202 | CYC | OC-C1C-C2C | -3.47 | 123.41 | 126.17 |
| 12 | E9 | 201 | CYC | OC-C1C-C2C | -3.47 | 123.41 | 126.17 |
| 12 | S9 | 201 | CYC | OC-C1C-C2C | -3.47 | 123.41 | 126.17 |
| 12 | AA | 201 | CYC | CMA-C3A-C4A | 3.47 | 130.41 | 125.06 |
| 12 | A9 | 201 | CYC | CMA-C3A-C4A | 3.47 | 130.41 | 125.06 |
| 12 | O7 | 201 | CYC | C1B-C2B-C3B | -3.47 | 104.25 | 107.87 |
| 12 | a7 | 201 | CYC | C1B-C2B-C3B | -3.47 | 104.25 | 107.87 |
| 12 | A6 | 201 | CYC | CMA-C3A-C4A | 3.47 | 130.41 | 125.06 |
| 12 | P7 | 201 | CYC | CHB-C4A-NA | -3.47 | 117.67 | 124.93 |
| 12 | A7 | 201 | CYC | C1B-C2B-C3B | -3.47 | 104.25 | 107.87 |
| 12 | k5 | 1203 | CYC | CMA-C3A-C4A | 3.47 | 130.41 | 125.06 |
| 12 | A2 | 201 | CYC | CMA-C3A-C4A | 3.47 | 130.41 | 125.06 |
| 12 | Y7 | 201 | CYC | C1B-C2B-C3B | -3.47 | 104.25 | 107.87 |
| 12 | Q8 | 201 | CYC | CHB-C1B-C2B | -3.47 | 120.08 | 126.95 |
| 12 | AA | 201 | CYC | OC-C1C-C2C | -3.47 | 123.42 | 126.17 |
| 12 | J2 | 201 | CYC | OC-C1C-C2C | -3.47 | 123.42 | 126.17 |
| 12 | A9 | 201 | CYC | OC-C1C-C2C | -3.47 | 123.42 | 126.17 |
| 12 | D6 | 202 | CYC | CHB-C1B-C2B | -3.47 | 120.08 | 126.95 |
| 12 | G5 | 201 | CYC | C1B-C2B-C3B | -3.47 | 104.25 | 107.87 |
| 12 | j5 | 1202 | CYC | C1B-NB-C4B | -3.47 | 106.25 | 110.67 |
| 12 | N7 | 201 | CYC | C1B-NB-C4B | -3.47 | 106.25 | 110.67 |
| 12 | g7 | 201 | CYC | CHA-C1A-NA | -3.47 | 124.02 | 128.83 |
| 12 | A5 | 201 | CYC | C1B-C2B-C3B | -3.47 | 104.25 | 107.87 |
| 12 | T7 | 201 | CYC | CHB-C4A-NA | -3.47 | 117.68 | 124.93 |
| 12 | IA | 201 | CYC | OC-C1C-C2C | -3.47 | 123.42 | 126.17 |
| 12 | VA | 202 | CYC | OC-C1C-C2C | -3.47 | 123.42 | 126.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | P3 | 202 | CYC | OC-C1C-C2C | -3.47 | 123.42 | 126.17 |
| 12 | I9 | 201 | CYC | OC-C1C-C2C | -3.47 | 123.42 | 126.17 |
| 12 | V9 | 202 | CYC | OC-C1C-C2C | -3.47 | 123.42 | 126.17 |
| 12 | IA | 201 | CYC | CMA-C3A-C4A | 3.47 | 130.40 | 125.06 |
| 12 | I9 | 201 | CYC | CMA-C3A-C4A | 3.47 | 130.40 | 125.06 |
| 12 | PA | 201 | CYC | CAB-C3B-C4B | 3.47 | 126.85 | 121.38 |
| 12 | P9 | 201 | CYC | CAB-C3B-C4B | 3.47 | 126.85 | 121.38 |
| 12 | B7 | 201 | CYC | CHB-C4A-NA | -3.47 | 117.68 | 124.93 |
| 12 | P4 | 201 | CYC | CMA-C3A-C4A | 3.47 | 130.40 | 125.06 |
| 12 | P8 | 201 | CYC | CMA-C3A-C4A | 3.47 | 130.40 | 125.06 |
| 12 | F5 | 201 | CYC | CHB-C4A-NA | -3.46 | 117.69 | 124.93 |
| 12 | M4 | 301 | CYC | CMB-C2B-C1B | 3.46 | 128.49 | 124.17 |
| 12 | f5 | 201 | CYC | C1B-NB-C4B | -3.46 | 106.26 | 110.67 |
| 12 | G8 | 201 | CYC | CMA-C3A-C4A | 3.46 | 130.40 | 125.06 |
| 12 | W8 | 201 | CYC | CAB-C3B-C4B | 3.46 | 126.85 | 121.38 |
| 12 | O4 | 202 | CYC | CHB-C1B-C2B | -3.46 | 120.09 | 126.95 |
| 12 | O8 | 202 | CYC | CHB-C1B-C2B | -3.46 | 120.09 | 126.95 |
| 12 | QA | 201 | CYC | CMA-C3A-C4A | 3.46 | 130.40 | 125.06 |
| 12 | L5 | 201 | CYC | CHB-C4A-NA | -3.46 | 117.69 | 124.93 |
| 12 | ZA | 201 | CYC | OC-C1C-C2C | -3.46 | 123.42 | 126.17 |
| 12 | Z9 | 201 | CYC | OC-C1C-C2C | -3.46 | 123.42 | 126.17 |
| 12 | g7 | 201 | CYC | C1B-C2B-C3B | -3.46 | 104.26 | 107.87 |
| 12 | H7 | 201 | CYC | CHB-C4A-NA | -3.46 | 117.69 | 124.93 |
| 12 | k7 | 201 | CYC | CHA-C1A-NA | -3.46 | 124.03 | 128.83 |
| 12 | Y5 | 201 | CYC | CHA-C1A-NA | -3.46 | 124.03 | 128.83 |
| 12 | r7 | 201 | CYC | CHB-C4A-NA | -3.46 | 117.69 | 124.93 |
| 12 | T1 | 302 | CYC | OC-C1C-C2C | -3.46 | 123.42 | 126.17 |
| 12 | Q9 | 201 | CYC | CMA-C3A-C4A | 3.46 | 130.39 | 125.06 |
| 12 | r7 | 201 | CYC | CMA-C3A-C4A | 3.46 | 130.39 | 125.06 |
| 12 | L5 | 201 | CYC | C1B-NB-C4B | -3.45 | 106.27 | 110.67 |
| 12 | V3 | 201 | CYC | CAB-C3B-C4B | 3.45 | 126.83 | 121.38 |
| 12 | J4 | 201 | CYC | CAB-C3B-C4B | 3.45 | 126.83 | 121.38 |
| 12 | J8 | 201 | CYC | CAB-C3B-C4B | 3.45 | 126.83 | 121.38 |
| 12 | V1 | 201 | CYC | CAB-C3B-C4B | 3.45 | 126.83 | 121.38 |
| 12 | T8 | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.38 | 125.06 |
| 12 | U5 | 201 | CYC | CHA-C1A-NA | -3.45 | 124.03 | 128.83 |
| 12 | L6 | 201 | CYC | CMB-C2B-C1B | 3.45 | 128.48 | 124.17 |
| 12 | o7 | 201 | CYC | C1B-C2B-C3B | -3.45 | 104.27 | 107.87 |
| 12 | W3 | 201 | CYC | OC-C1C-C2C | -3.45 | 123.43 | 126.17 |
| 12 | X4 | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.38 | 125.06 |
| 12 | B5 | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.38 | 125.06 |
| 12 | WA | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.38 | 125.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | J7 | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.38 | 125.06 |
| 12 | H5 | 201 | CYC | CHB-C4A-NA | -3.45 | 117.71 | 124.93 |
| 12 | K2 | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.38 | 125.06 |
| 12 | K6 | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.38 | 125.06 |
| 12 | V8 | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.38 | 125.06 |
| 12 | T5 | 201 | CYC | CHB-C4A-NA | -3.45 | 117.71 | 124.93 |
| 12 | KA | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.38 | 125.06 |
| 12 | K9 | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.38 | 125.06 |
| 12 | d7 | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.38 | 125.06 |
| 12 | j7 | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.38 | 125.06 |
| 12 | H7 | 201 | CYC | C1B-NB-C4B | -3.45 | 106.28 | 110.67 |
| 12 | K3 | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.37 | 125.06 |
| 12 | O9 | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.37 | 125.06 |
| 12 | K1 | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.37 | 125.06 |
| 12 | B5 | 201 | CYC | CHB-C4A-NA | -3.45 | 117.72 | 124.93 |
| 12 | F5 | 201 | CYC | C1A-C2A-C3A | -3.45 | 102.97 | 106.78 |
| 12 | U3 | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.37 | 125.06 |
| 12 | W9 | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.37 | 125.06 |
| 12 | U1 | 201 | CYC | CMA-C3A-C4A | 3.45 | 130.37 | 125.06 |
| 12 | F2 | 202 | CYC | CHB-C1B-C2B | -3.45 | 120.12 | 126.95 |
| 12 | L2 | 201 | CYC | CMB-C2B-C1B | 3.45 | 128.47 | 124.17 |
| 12 | q7 | 201 | CYC | CHA-C1A-NA | -3.45 | 124.05 | 128.83 |
| 12 | e5 | 201 | CYC | C1B-C2B-C3B | -3.45 | 104.28 | 107.87 |
| 12 | S5 | 201 | CYC | C1B-C2B-C3B | -3.45 | 104.28 | 107.87 |
| 12 | C4 | 201 | CYC | CMA-C3A-C4A | 3.44 | 130.37 | 125.06 |
| 12 | r7 | 201 | CYC | C1B-NB-C4B | -3.44 | 106.28 | 110.67 |
| 12 | X7 | 201 | CYC | C1A-C2A-C3A | -3.44 | 102.97 | 106.78 |
| 12 | Y5 | 201 | CYC | C1B-C2B-C3B | -3.44 | 104.28 | 107.87 |
| 12 | T4 | 201 | CYC | CMA-C3A-C4A | 3.44 | 130.37 | 125.06 |
| 12 | O7 | 201 | CYC | CHA-C1A-NA | -3.44 | 124.05 | 128.83 |
| 12 | f5 | 201 | CYC | CHB-C4A-NA | -3.44 | 117.73 | 124.93 |
| 12 | R7 | 201 | CYC | CHB-C4A-NA | -3.44 | 117.73 | 124.93 |
| 12 | M8 | 301 | CYC | CMB-C2B-C1B | 3.44 | 128.47 | 124.17 |
| 12 | G2 | 201 | CYC | CMA-C3A-C4A | 3.44 | 130.36 | 125.06 |
| 12 | X8 | 201 | CYC | CMA-C3A-C4A | 3.44 | 130.36 | 125.06 |
| 12 | k5 | 1203 | CYC | C1B-NB-C4B | -3.44 | 106.29 | 110.67 |
| 12 | b7 | 201 | CYC | C1A-C2A-C3A | -3.44 | 102.97 | 106.78 |
| 12 | X4 | 201 | CYC | OC-C1C-C2C | -3.44 | 123.44 | 126.17 |
| 12 | X8 | 201 | CYC | OC-C1C-C2C | -3.44 | 123.44 | 126.17 |
| 12 | T7 | 201 | CYC | C1B-NB-C4B | -3.44 | 106.29 | 110.67 |
| 12 | LA | 202 | CYC | CAB-C3B-C4B | 3.44 | 126.81 | 121.38 |
| 12 | L9 | 202 | CYC | CAB-C3B-C4B | 3.44 | 126.81 | 121.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | a5 | 201 | CYC | C1B-C2B-C3B | -3.44 | 104.28 | 107.87 |
| 12 | R4 | 201 | CYC | C1B-NB-C4B | -3.44 | 106.29 | 110.67 |
| 12 | R8 | 201 | CYC | C1B-NB-C4B | -3.44 | 106.29 | 110.67 |
| 12 | P1 | 202 | CYC | OC-C1C-C2C | -3.44 | 123.44 | 126.17 |
| 12 | G7 | 201 | CYC | CHA-C1A-NA | -3.44 | 124.06 | 128.83 |
| 12 | D6 | 202 | CYC | OC-C1C-C2C | -3.44 | 123.44 | 126.17 |
| 12 | aA | 901 | CYC | CAB-C3B-C4B | 3.44 | 126.81 | 121.38 |
| 12 | KA | 201 | CYC | C1B-NB-C4B | -3.44 | 106.29 | 110.67 |
| 12 | H5 | 201 | CYC | C1B-NB-C4B | -3.44 | 106.29 | 110.67 |
| 12 | K9 | 201 | CYC | C1B-NB-C4B | -3.44 | 106.29 | 110.67 |
| 12 | B2 | 201 | CYC | OC-C1C-C2C | -3.44 | 123.44 | 126.17 |
| 12 | c5 | 201 | CYC | CHA-C1A-NA | -3.44 | 124.06 | 128.83 |
| 12 | Q7 | 201 | CYC | CHA-C1A-NA | -3.44 | 124.06 | 128.83 |
| 12 | D2 | 201 | CYC | CAB-C3B-C4B | 3.44 | 126.81 | 121.38 |
| 12 | OA | 201 | CYC | CMA-C3A-C4A | 3.44 | 130.36 | 125.06 |
| 12 | M5 | 201 | CYC | C1B-C2B-C3B | -3.44 | 104.28 | 107.87 |
| 12 | J6 | 201 | CYC | OC-C1C-C2C | -3.44 | 123.44 | 126.17 |
| 12 | L7 | 201 | CYC | CMA-C3A-C4A | 3.44 | 130.35 | 125.06 |
| 12 | F7 | 201 | CYC | CHB-C4A-NA | -3.44 | 117.75 | 124.93 |
| 12 | W4 | 201 | CYC | CAB-C3B-C4B | 3.44 | 126.80 | 121.38 |
| 12 | J3 | 202 | CYC | CAB-C3B-C4B | 3.43 | 126.80 | 121.38 |
| 12 | d5 | 201 | CYC | C1B-NB-C4B | -3.43 | 106.30 | 110.67 |
| 12 | d7 | 201 | CYC | CHB-C4A-NA | -3.43 | 117.75 | 124.93 |
| 12 | Q5 | 201 | CYC | CHA-C1A-NA | -3.43 | 124.06 | 128.83 |
| 12 | C8 | 201 | CYC | CMA-C3A-C4A | 3.43 | 130.35 | 125.06 |
| 12 | k5 | 1203 | CYC | CHB-C4A-NA | -3.43 | 117.75 | 124.93 |
| 12 | Q4 | 201 | CYC | OC-C1C-C2C | -3.43 | 123.44 | 126.17 |
| 12 | X5 | 201 | CYC | C1A-C2A-C3A | -3.43 | 102.98 | 106.78 |
| 12 | E5 | 201 | CYC | C1B-C2B-C3B | -3.43 | 104.29 | 107.87 |
| 12 | L7 | 201 | CYC | CHB-C4A-NA | -3.43 | 117.75 | 124.93 |
| 12 | C3 | 201 | CYC | CMA-C3A-C4A | 3.43 | 130.35 | 125.06 |
| 12 | C1 | 201 | CYC | CMA-C3A-C4A | 3.43 | 130.35 | 125.06 |
| 12 | Q8 | 201 | CYC | OC-C1C-C2C | -3.43 | 123.45 | 126.17 |
| 12 | W5 | 201 | CYC | C1B-C2B-C3B | -3.43 | 104.29 | 107.87 |
| 12 | j7 | 201 | CYC | CHB-C4A-NA | -3.43 | 117.76 | 124.93 |
| 12 | H6 | 201 | CYC | CAB-C3B-C4B | 3.43 | 126.79 | 121.38 |
| 12 | D4 | 201 | CYC | OC-C1C-C2C | -3.43 | 123.45 | 126.17 |
| 12 | D8 | 201 | CYC | OC-C1C-C2C | -3.43 | 123.45 | 126.17 |
| 12 | O5 | 201 | CYC | CHA-C1A-NA | -3.43 | 124.07 | 128.83 |
| 12 | A4 | 201 | CYC | CMA-C3A-C4A | 3.43 | 130.34 | 125.06 |
| 12 | A8 | 201 | CYC | CMA-C3A-C4A | 3.43 | 130.34 | 125.06 |
| 12 | T3 | 302 | CYC | OC-C1C-C2C | -3.43 | 123.45 | 126.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | E6 | 201 | CYC | OC-C1C-C2C | -3.43 | 123.45 | 126.17 |
| 12 | A5 | 201 | CYC | CHA-C1A-NA | -3.43 | 124.08 | 128.83 |
| 12 | W3 | 201 | CYC | CMA-C3A-C4A | 3.43 | 130.34 | 125.06 |
| 12 | G7 | 201 | CYC | C1B-C2B-C3B | -3.42 | 104.30 | 107.87 |
| 12 | H4 | 201 | CYC | CAB-C3B-C4B | 3.42 | 126.79 | 121.38 |
| 12 | L6 | 201 | CYC | CAB-C3B-C4B | 3.42 | 126.79 | 121.38 |
| 12 | H8 | 201 | CYC | CAB-C3B-C4B | 3.42 | 126.79 | 121.38 |
| 12 | S1 | 201 | CYC | C1B-NB-C4B | -3.42 | 106.31 | 110.67 |
| 12 | S3 | 201 | CYC | C1B-NB-C4B | -3.42 | 106.31 | 110.67 |
| 12 | G6 | 201 | CYC | C1B-NB-C4B | -3.42 | 106.31 | 110.67 |
| 12 | G6 | 201 | CYC | CMA-C3A-C4A | 3.42 | 130.34 | 125.06 |
| 12 | v7 | 201 | CYC | CMA-C3A-C4A | 3.42 | 130.34 | 125.06 |
| 12 | J3 | 201 | CYC | OC-C1C-C2C | -3.42 | 123.45 | 126.17 |
| 12 | J1 | 201 | CYC | OC-C1C-C2C | -3.42 | 123.45 | 126.17 |
| 12 | j7 | 201 | CYC | C1A-C2A-C3A | -3.42 | 103.00 | 106.78 |
| 12 | Z3 | 201 | CYC | CAB-C3B-C4B | 3.42 | 126.78 | 121.38 |
| 12 | W1 | 201 | CYC | CMA-C3A-C4A | 3.42 | 130.33 | 125.06 |
| 12 | XA | 202 | CYC | OC-C1C-C2C | -3.42 | 123.45 | 126.17 |
| 12 | X9 | 202 | CYC | OC-C1C-C2C | -3.42 | 123.45 | 126.17 |
| 12 | X5 | 201 | CYC | CHB-C4A-NA | -3.42 | 117.78 | 124.93 |
| 12 | F8 | 202 | CYC | CAB-C3B-C4B | 3.42 | 126.78 | 121.38 |
| 12 | H7 | 201 | CYC | CMA-C3A-C4A | 3.42 | 130.33 | 125.06 |
| 12 | G2 | 201 | CYC | C1B-NB-C4B | -3.42 | 106.31 | 110.67 |
| 12 | YA | 201 | CYC | CMA-C3A-C4A | 3.42 | 130.33 | 125.06 |
| 12 | Y9 | 201 | CYC | CMA-C3A-C4A | 3.42 | 130.33 | 125.06 |
| 12 | h7 | 201 | CYC | C1A-C2A-C3A | -3.42 | 103.00 | 106.78 |
| 12 | d7 | 201 | CYC | C1A-C2A-C3A | -3.42 | 103.00 | 106.78 |
| 12 | f7 | 201 | CYC | C1A-C2A-C3A | -3.42 | 103.00 | 106.78 |
| 12 | E5 | 201 | CYC | CHA-C1A-NA | -3.42 | 124.08 | 128.83 |
| 12 | u7 | 201 | CYC | CHA-C1A-NA | -3.42 | 124.09 | 128.83 |
| 12 | JA | 202 | CYC | CAB-C3B-C4B | 3.42 | 126.78 | 121.38 |
| 12 | J9 | 202 | CYC | CAB-C3B-C4B | 3.42 | 126.78 | 121.38 |
| 12 | K5 | 201 | CYC | C1B-C2B-C3B | -3.42 | 104.31 | 107.87 |
| 12 | K7 | 201 | CYC | C1B-C2B-C3B | -3.42 | 104.31 | 107.87 |
| 12 | D7 | 201 | CYC | CMA-C3A-C4A | 3.42 | 130.32 | 125.06 |
| 12 | E9 | 201 | CYC | CMA-C3A-C4A | 3.42 | 130.32 | 125.06 |
| 12 | DA | 201 | CYC | CAB-C3B-C4B | 3.41 | 126.77 | 121.38 |
| 12 | D9 | 201 | CYC | CAB-C3B-C4B | 3.41 | 126.77 | 121.38 |
| 12 | EA | 201 | CYC | C1B-NB-C4B | -3.41 | 106.32 | 110.67 |
| 12 | T4 | 201 | CYC | C1B-NB-C4B | -3.41 | 106.32 | 110.67 |
| 12 | Z5 | 201 | CYC | C1B-NB-C4B | -3.41 | 106.32 | 110.67 |
| 12 | T8 | 201 | CYC | C1B-NB-C4B | -3.41 | 106.32 | 110.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | N7 | 201 | CYC | C1A-C2A-C3A | -3.41 | 103.00 | 106.78 |
| 12 | c5 | 201 | CYC | C1B-C2B-C3B | -3.41 | 104.31 | 107.87 |
| 12 | K8 | 201 | CYC | C1B-NB-C4B | -3.41 | 106.32 | 110.67 |
| 12 | M5 | 201 | CYC | CHA-C1A-NA | -3.41 | 124.09 | 128.83 |
| 12 | m7 | 201 | CYC | C1B-C2B-C3B | -3.41 | 104.31 | 107.87 |
| 12 | T5 | 201 | CYC | C1A-C2A-C3A | -3.41 | 103.00 | 106.78 |
| 12 | F7 | 201 | CYC | CMA-C3A-C4A | 3.41 | 130.32 | 125.06 |
| 12 | K3 | 201 | CYC | C1B-NB-C4B | -3.41 | 106.32 | 110.67 |
| 12 | K1 | 201 | CYC | C1B-NB-C4B | -3.41 | 106.32 | 110.67 |
| 12 | k5 | 1202 | CYC | C1A-C2A-C3A | -3.41 | 103.01 | 106.78 |
| 12 | GA | 201 | CYC | CMA-C3A-C4A | 3.41 | 130.32 | 125.06 |
| 12 | G9 | 201 | CYC | CMA-C3A-C4A | 3.41 | 130.32 | 125.06 |
| 12 | H9 | 202 | CYC | CAB-C3B-C4B | 3.41 | 126.77 | 121.38 |
| 12 | L2 | 201 | CYC | CAB-C3B-C4B | 3.41 | 126.77 | 121.38 |
| 12 | E7 | 201 | CYC | C1B-C2B-C3B | -3.41 | 104.31 | 107.87 |
| 12 | j5 | 1202 | CYC | C1A-C2A-C3A | -3.41 | 103.01 | 106.78 |
| 12 | U7 | 201 | CYC | C1B-C2B-C3B | -3.41 | 104.31 | 107.87 |
| 12 | E4 | 201 | CYC | CMA-C3A-C4A | 3.41 | 130.31 | 125.06 |
| 12 | Z1 | 202 | CYC | CAB-C3B-C4B | 3.41 | 126.76 | 121.38 |
| 12 | I4 | 201 | CYC | CMA-C3A-C4A | 3.41 | 130.31 | 125.06 |
| 12 | E6 | 201 | CYC | CMA-C3A-C4A | 3.41 | 130.31 | 125.06 |
| 12 | I8 | 201 | CYC | CMA-C3A-C4A | 3.41 | 130.31 | 125.06 |
| 12 | P7 | 201 | CYC | C1A-C2A-C3A | -3.41 | 103.01 | 106.78 |
| 12 | H3 | 202 | CYC | CAB-C3B-C4B | 3.41 | 126.76 | 121.38 |
| 12 | T3 | 301 | CYC | CAB-C3B-C4B | 3.41 | 126.76 | 121.38 |
| 12 | T1 | 301 | CYC | CAB-C3B-C4B | 3.41 | 126.76 | 121.38 |
| 12 | f5 | 201 | CYC | CMA-C3A-C4A | 3.41 | 130.31 | 125.06 |
| 12 | k5 | 1204 | CYC | CMA-C3A-C4A | 3.41 | 130.31 | 125.06 |
| 12 | HA | 202 | CYC | CAB-C3B-C4B | 3.41 | 126.76 | 121.38 |
| 12 | R1 | 201 | CYC | CAB-C3B-C4B | 3.41 | 126.76 | 121.38 |
| 12 | R3 | 201 | CYC | CAB-C3B-C4B | 3.41 | 126.76 | 121.38 |
| 12 | F4 | 202 | CYC | CAB-C3B-C4B | 3.41 | 126.76 | 121.38 |
| 12 | o7 | 201 | CYC | CHA-C1A-NA | -3.40 | 124.10 | 128.83 |
| 12 | E8 | 201 | CYC | C1B-NB-C4B | -3.40 | 106.33 | 110.67 |
| 12 | E3 | 201 | CYC | CMA-C3A-C4A | 3.40 | 130.31 | 125.06 |
| 12 | E1 | 201 | CYC | CMA-C3A-C4A | 3.40 | 130.31 | 125.06 |
| 12 | I1 | 201 | CYC | C1B-NB-C4B | -3.40 | 106.33 | 110.67 |
| 12 | L3 | 202 | CYC | CAB-C3B-C4B | 3.40 | 126.75 | 121.38 |
| 12 | D6 | 201 | CYC | CAB-C3B-C4B | 3.40 | 126.75 | 121.38 |
| 12 | aA | 902 | CYC | CAB-C3B-C4B | 3.40 | 126.75 | 121.38 |
| 12 | N2 | 101 | CYC | CAB-C3B-C4B | 3.40 | 126.75 | 121.38 |
| 12 | U4 | 202 | CYC | OC-C1C-C2C | -3.40 | 123.47 | 126.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | U8 | 202 | CYC | OC-C1C-C2C | -3.40 | 123.47 | 126.17 |
| 12 | Q1 | 201 | CYC | CMA-C3A-C4A | 3.40 | 130.30 | 125.06 |
| 12 | Q3 | 201 | CYC | CMA-C3A-C4A | 3.40 | 130.30 | 125.06 |
| 12 | L5 | 201 | CYC | C1A-C2A-C3A | -3.40 | 103.02 | 106.78 |
| 12 | B7 | 201 | CYC | C1A-C2A-C3A | -3.40 | 103.02 | 106.78 |
| 12 | EA | 201 | CYC | CMA-C3A-C4A | 3.40 | 130.30 | 125.06 |
| 12 | O4 | 201 | CYC | CAB-C3B-C4B | 3.40 | 126.75 | 121.38 |
| 12 | O8 | 201 | CYC | CAB-C3B-C4B | 3.40 | 126.75 | 121.38 |
| 12 | B5 | 201 | CYC | C1B-NB-C4B | -3.40 | 106.34 | 110.67 |
| 12 | X3 | 201 | CYC | CAB-C3B-C4B | 3.40 | 126.75 | 121.38 |
| 12 | FA | 301 | CYC | CAB-C3B-C4B | 3.40 | 126.74 | 121.38 |
| 12 | F9 | 301 | CYC | CAB-C3B-C4B | 3.40 | 126.74 | 121.38 |
| 12 | V7 | 201 | CYC | CMA-C3A-C4A | 3.40 | 130.29 | 125.06 |
| 12 | S5 | 201 | CYC | CHA-C1A-NA | -3.40 | 124.11 | 128.83 |
| 12 | k5 | 1202 | CYC | C1B-C2B-C3B | -3.40 | 104.33 | 107.87 |
| 12 | H1 | 201 | CYC | CAB-C3B-C4B | 3.40 | 126.74 | 121.38 |
| 12 | L4 | 202 | CYC | CAB-C3B-C4B | 3.40 | 126.74 | 121.38 |
| 12 | k7 | 201 | CYC | C1B-C2B-C3B | -3.40 | 104.33 | 107.87 |
| 12 | q7 | 201 | CYC | C1B-C2B-C3B | -3.40 | 104.33 | 107.87 |
| 12 | Y3 | 201 | CYC | CMA-C3A-C4A | 3.39 | 130.29 | 125.06 |
| 12 | Y1 | 201 | CYC | CMA-C3A-C4A | 3.39 | 130.29 | 125.06 |
| 12 | f7 | 201 | CYC | CAA-CBA-CGA | -3.39 | 106.30 | 113.60 |
| 12 | N6 | 101 | CYC | CAB-C3B-C4B | 3.39 | 126.74 | 121.38 |
| 12 | D2 | 202 | CYC | OC-C1C-C2C | -3.39 | 123.47 | 126.17 |
| 12 | F7 | 201 | CYC | C1A-C2A-C3A | -3.39 | 103.03 | 106.78 |
| 12 | B7 | 201 | CYC | CMA-C3A-C4A | 3.39 | 130.29 | 125.06 |
| 12 | f7 | 201 | CYC | C1B-C2B-C3B | -3.39 | 104.33 | 107.87 |
| 12 | u7 | 201 | CYC | C1B-C2B-C3B | -3.39 | 104.33 | 107.87 |
| 12 | R4 | 201 | CYC | CMA-C3A-C4A | 3.39 | 130.29 | 125.06 |
| 12 | E2 | 201 | CYC | CMA-C3A-C4A | 3.39 | 130.29 | 125.06 |
| 12 | F2 | 201 | CYC | CMB-C2B-C1B | 3.39 | 128.40 | 124.17 |
| 12 | D5 | 201 | CYC | CMA-C3A-C4A | 3.39 | 130.28 | 125.06 |
| 12 | E3 | 201 | CYC | C1B-NB-C4B | -3.39 | 106.35 | 110.67 |
| 12 | E1 | 201 | CYC | C1B-NB-C4B | -3.39 | 106.35 | 110.67 |
| 12 | L5 | 201 | CYC | CAA-CBA-CGA | -3.39 | 106.31 | 113.60 |
| 12 | E2 | 201 | CYC | OC-C1C-C2C | -3.39 | 123.48 | 126.17 |
| 12 | I3 | 201 | CYC | C1B-NB-C4B | -3.39 | 106.36 | 110.67 |
| 12 | H2 | 202 | CYC | C4A-C3A-C2A | -3.39 | 102.62 | 106.51 |
| 12 | H6 | 202 | CYC | C4A-C3A-C2A | -3.39 | 102.62 | 106.51 |
| 12 | A | 201 | CYC | CMA-C3A-C4A | 3.39 | 130.28 | 125.06 |
| 12 | D4 | 202 | CYC | CAB-C3B-C4B | 3.39 | 126.73 | 121.38 |
| 12 | D8 | 202 | CYC | CAB-C3B-C4B | 3.39 | 126.73 | 121.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | R8 | 201 | CYC | CMA-C3A-C4A | 3.39 | 130.28 | 125.06 |
| 12 | B5 | 201 | CYC | C1A-C2A-C3A | -3.39 | 103.03 | 106.78 |
| 12 | K5 | 201 | CYC | CHA-C1A-NA | -3.39 | 124.13 | 128.83 |
| 12 | U7 | 201 | CYC | CHA-C1A-NA | -3.39 | 124.13 | 128.83 |
| 12 | Z4 | 301 | CYC | CAB-C3B-C4B | 3.39 | 126.73 | 121.38 |
| 12 | D1 | 202 | CYC | CAB-C3B-C4B | 3.39 | 126.72 | 121.38 |
| 12 | P7 | 201 | CYC | CMA-C3A-C4A | 3.38 | 130.28 | 125.06 |
| 12 | E8 | 201 | CYC | CMA-C3A-C4A | 3.38 | 130.28 | 125.06 |
| 12 | R5 | 201 | CYC | CHB-C4A-NA | -3.38 | 117.86 | 124.93 |
| 12 | V3 | 202 | CYC | C4A-C3A-C2A | -3.38 | 102.62 | 106.51 |
| 12 | V1 | 202 | CYC | C4A-C3A-C2A | -3.38 | 102.62 | 106.51 |
| 12 | F5 | 201 | CYC | CAA-CBA-CGA | -3.38 | 106.32 | 113.60 |
| 12 | D3 | 202 | CYC | CAB-C3B-C4B | 3.38 | 126.72 | 121.38 |
| 12 | j5 | 1202 | CYC | CMA-C3A-C4A | 3.38 | 130.27 | 125.06 |
| 12 | j5 | 1202 | CYC | CAA-CBA-CGA | -3.38 | 106.32 | 113.60 |
| 12 | X4 | 201 | CYC | C1B-NB-C4B | -3.38 | 106.36 | 110.67 |
| 12 | X8 | 201 | CYC | C1B-NB-C4B | -3.38 | 106.36 | 110.67 |
| 12 | P5 | 201 | CYC | C1A-C2A-C3A | -3.38 | 103.04 | 106.78 |
| 12 | H7 | 201 | CYC | C1A-C2A-C3A | -3.38 | 103.04 | 106.78 |
| 12 | RA | 202 | CYC | OC-C1C-C2C | -3.38 | 123.48 | 126.17 |
| 12 | R9 | 202 | CYC | OC-C1C-C2C | -3.38 | 123.48 | 126.17 |
| 12 | k5 | 1202 | CYC | CAA-CBA-CGA | -3.38 | 106.33 | 113.60 |
| 12 | TA | 301 | CYC | CAB-C3B-C4B | 3.38 | 126.72 | 121.38 |
| 12 | T9 | 301 | CYC | CAB-C3B-C4B | 3.38 | 126.72 | 121.38 |
| 12 | N5 | 201 | CYC | C1A-C2A-C3A | -3.38 | 103.04 | 106.78 |
| 12 | V7 | 201 | CYC | C1A-C2A-C3A | -3.38 | 103.04 | 106.78 |
| 12 | IA | 201 | CYC | C1B-NB-C4B | -3.38 | 106.36 | 110.67 |
| 12 | K4 | 201 | CYC | C1B-NB-C4B | -3.38 | 106.36 | 110.67 |
| 12 | I9 | 201 | CYC | C1B-NB-C4B | -3.38 | 106.36 | 110.67 |
| 12 | C2 | 201 | CYC | C1B-NB-C4B | -3.38 | 106.36 | 110.67 |
| 12 | E9 | 201 | CYC | C1B-NB-C4B | -3.38 | 106.37 | 110.67 |
| 12 | BA | 201 | CYC | CAB-C3B-C4B | 3.38 | 126.72 | 121.38 |
| 12 | B3 | 202 | CYC | CAB-C3B-C4B | 3.38 | 126.72 | 121.38 |
| 12 | B9 | 201 | CYC | CAB-C3B-C4B | 3.38 | 126.72 | 121.38 |
| 12 | p7 | 201 | CYC | C1B-C2B-C3B | -3.38 | 104.34 | 107.87 |
| 12 | B1 | 202 | CYC | CAB-C3B-C4B | 3.38 | 126.72 | 121.38 |
| 12 | R5 | 201 | CYC | CMA-C3A-C4A | 3.38 | 130.27 | 125.06 |
| 12 | J5 | 201 | CYC | C1A-C2A-C3A | -3.38 | 103.04 | 106.78 |
| 12 | X1 | 201 | CYC | CAB-C3B-C4B | 3.38 | 126.71 | 121.38 |
| 12 | k5 | 1204 | CYC | CAA-CBA-CGA | -3.38 | 106.33 | 113.60 |
| 12 | b7 | 201 | CYC | CMA-C3A-C4A | 3.38 | 130.26 | 125.06 |
| 12 | H2 | 201 | CYC | CAB-C3B-C4B | 3.38 | 126.71 | 121.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | a9 | 901 | CYC | CAB-C3B-C4B | 3.38 | 126.71 | 121.38 |
| 12 | E4 | 201 | CYC | C1B-NB-C4B | -3.37 | 106.37 | 110.67 |
| 12 | F1 | 201 | CYC | CAB-C3B-C4B | 3.37 | 126.71 | 121.38 |
| 12 | X5 | 201 | CYC | CMA-C3A-C4A | 3.37 | 130.26 | 125.06 |
| 12 | b5 | 201 | CYC | CMA-C3A-C4A | 3.37 | 130.25 | 125.06 |
| 12 | b7 | 201 | CYC | CHB-C4A-NA | -3.37 | 117.88 | 124.93 |
| 12 | J5 | 201 | CYC | CMA-C3A-C4A | 3.37 | 130.25 | 125.06 |
| 12 | BA | 202 | CYC | C4A-C3A-C2A | -3.37 | 102.64 | 106.51 |
| 12 | B9 | 202 | CYC | C4A-C3A-C2A | -3.37 | 102.64 | 106.51 |
| 12 | G5 | 201 | CYC | CHA-C1A-NA | -3.37 | 124.15 | 128.83 |
| 12 | B8 | 201 | CYC | OC-C1C-C2C | -3.37 | 123.49 | 126.17 |
| 12 | h7 | 201 | CYC | CMA-C3A-C4A | 3.37 | 130.25 | 125.06 |
| 12 | H1 | 202 | CYC | C4A-C3A-C2A | -3.37 | 102.64 | 106.51 |
| 12 | N5 | 201 | CYC | CAA-CBA-CGA | -3.37 | 106.35 | 113.60 |
| 12 | Z | 201 | CYC | CMA-C3A-C4A | 3.37 | 130.25 | 125.06 |
| 12 | h7 | 201 | CYC | CHB-C4A-NA | -3.37 | 117.89 | 124.93 |
| 12 | G4 | 201 | CYC | C1B-NB-C4B | -3.37 | 106.38 | 110.67 |
| 12 | G8 | 201 | CYC | C1B-NB-C4B | -3.37 | 106.38 | 110.67 |
| 12 | RA | 201 | CYC | CAB-C3B-C4B | 3.37 | 126.70 | 121.38 |
| 12 | R9 | 201 | CYC | CAB-C3B-C4B | 3.37 | 126.70 | 121.38 |
| 12 | H7 | 201 | CYC | CAA-CBA-CGA | -3.37 | 106.36 | 113.60 |
| 12 | PA | 202 | CYC | OC-C1C-C2C | -3.37 | 123.50 | 126.17 |
| 12 | P9 | 202 | CYC | OC-C1C-C2C | -3.37 | 123.50 | 126.17 |
| 12 | Q5 | 201 | CYC | C1B-C2B-C3B | -3.37 | 104.36 | 107.87 |
| 12 | v7 | 201 | CYC | C1B-C2B-C3B | -3.37 | 104.36 | 107.87 |
| 12 | N7 | 201 | CYC | CMA-C3A-C4A | 3.37 | 130.25 | 125.06 |
| 12 | HA | 201 | CYC | OC-C1C-C2C | -3.36 | 123.50 | 126.17 |
| 12 | H9 | 201 | CYC | OC-C1C-C2C | -3.36 | 123.50 | 126.17 |
| 12 | O4 | 202 | CYC | C4A-C3A-C2A | -3.36 | 102.64 | 106.51 |
| 12 | O8 | 202 | CYC | C4A-C3A-C2A | -3.36 | 102.64 | 106.51 |
| 12 | Z8 | 301 | CYC | CAB-C3B-C4B | 3.36 | 126.69 | 121.38 |
| 12 | D7 | 201 | CYC | CAA-CBA-CGA | -3.36 | 106.36 | 113.60 |
| 12 | SA | 201 | CYC | CMA-C3A-C4A | 3.36 | 130.24 | 125.06 |
| 12 | S9 | 201 | CYC | CMA-C3A-C4A | 3.36 | 130.24 | 125.06 |
| 12 | S7 | 201 | CYC | C1B-C2B-C3B | -3.36 | 104.36 | 107.87 |
| 12 | D5 | 201 | CYC | C1A-C2A-C3A | -3.36 | 103.06 | 106.78 |
| 12 | O4 | 202 | CYC | OC-C1C-C2C | -3.36 | 123.50 | 126.17 |
| 12 | L8 | 201 | CYC | OC-C1C-C2C | -3.36 | 123.50 | 126.17 |
| 12 | O8 | 202 | CYC | OC-C1C-C2C | -3.36 | 123.50 | 126.17 |
| 12 | B9 | 202 | CYC | OC-C1C-C2C | -3.36 | 123.50 | 126.17 |
| 12 | GA | 201 | CYC | C1B-NB-C4B | -3.36 | 106.39 | 110.67 |
| 12 | G9 | 201 | CYC | C1B-NB-C4B | -3.36 | 106.39 | 110.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | T7 | 201 | CYC | CMA-C3A-C4A | 3.36 | 130.24 | 125.06 |
| 12 | Z3 | 202 | CYC | OC-C1C-C2C | -3.36 | 123.50 | 126.17 |
| 12 | Z1 | 201 | CYC | OC-C1C-C2C | -3.36 | 123.50 | 126.17 |
| 12 | k5 | 1202 | CYC | CMA-C3A-C4A | 3.36 | 130.24 | 125.06 |
| 12 | L4 | 201 | CYC | C4A-C3A-C2A | -3.36 | 102.65 | 106.51 |
| 12 | L8 | 201 | CYC | C4A-C3A-C2A | -3.36 | 102.65 | 106.51 |
| 12 | LA | 201 | CYC | OC-C1C-C2C | -3.36 | 123.50 | 126.17 |
| 12 | L9 | 201 | CYC | OC-C1C-C2C | -3.36 | 123.50 | 126.17 |
| 12 | b5 | 201 | CYC | C1A-C2A-C3A | -3.36 | 103.07 | 106.78 |
| 12 | W7 | 201 | CYC | C1B-C2B-C3B | -3.36 | 104.37 | 107.87 |
| 12 | P5 | 201 | CYC | CAA-CBA-CGA | -3.36 | 106.38 | 113.60 |
| 12 | V5 | 201 | CYC | CAA-CBA-CGA | -3.36 | 106.38 | 113.60 |
| 12 | k5 | 1204 | CYC | C1A-C2A-C3A | -3.36 | 103.07 | 106.78 |
| 12 | L3 | 201 | CYC | OC-C1C-C2C | -3.36 | 123.50 | 126.17 |
| 12 | J4 | 202 | CYC | OC-C1C-C2C | -3.36 | 123.50 | 126.17 |
| 12 | J8 | 202 | CYC | OC-C1C-C2C | -3.36 | 123.50 | 126.17 |
| 12 | L1 | 201 | CYC | OC-C1C-C2C | -3.36 | 123.50 | 126.17 |
| 12 | N5 | 201 | CYC | CMA-C3A-C4A | 3.36 | 130.23 | 125.06 |
| 12 | F3 | 201 | CYC | CAB-C3B-C4B | 3.36 | 126.68 | 121.38 |
| 12 | B4 | 202 | CYC | CAB-C3B-C4B | 3.36 | 126.68 | 121.38 |
| 12 | D5 | 201 | CYC | CAA-CBA-CGA | -3.35 | 106.38 | 113.60 |
| 12 | J5 | 201 | CYC | CAA-CBA-CGA | -3.35 | 106.38 | 113.60 |
| 12 | T5 | 201 | CYC | CAA-CBA-CGA | -3.35 | 106.38 | 113.60 |
| 12 | J7 | 201 | CYC | CAA-CBA-CGA | -3.35 | 106.38 | 113.60 |
| 12 | R7 | 201 | CYC | C1A-C2A-C3A | -3.35 | 103.07 | 106.78 |
| 12 | s7 | 201 | CYC | C1B-C2B-C3B | -3.35 | 104.37 | 107.87 |
| 12 | V7 | 201 | CYC | CAA-CBA-CGA | -3.35 | 106.39 | 113.60 |
| 12 | T7 | 201 | CYC | C1A-C2A-C3A | -3.35 | 103.07 | 106.78 |
| 12 | I6 | 201 | CYC | CMA-C3A-C4A | 3.35 | 130.23 | 125.06 |
| 12 | H3 | 201 | CYC | OC-C1C-C2C | -3.35 | 123.51 | 126.17 |
| 12 | H1 | 202 | CYC | OC-C1C-C2C | -3.35 | 123.51 | 126.17 |
| 12 | N7 | 201 | CYC | C1B-C2B-C3B | -3.35 | 104.37 | 107.87 |
| 12 | V8 | 201 | CYC | C1B-NB-C4B | -3.35 | 106.40 | 110.67 |
| 12 | T5 | 201 | CYC | CMA-C3A-C4A | 3.35 | 130.22 | 125.06 |
| 12 | B6 | 201 | CYC | OC-C1C-C2C | -3.35 | 123.51 | 126.17 |
| 12 | X5 | 201 | CYC | C1B-C2B-C3B | -3.35 | 104.38 | 107.87 |
| 12 | k5 | 1201 | CYC | C1B-CHB-C4A | 3.35 | 136.26 | 128.08 |
| 12 | H3 | 201 | CYC | C4A-C3A-C2A | -3.35 | 102.67 | 106.51 |
| 12 | C6 | 201 | CYC | C1B-NB-C4B | -3.35 | 106.41 | 110.67 |
| 12 | I2 | 201 | CYC | CMA-C3A-C4A | 3.35 | 130.22 | 125.06 |
| 12 | K2 | 201 | CYC | C1B-NB-C4B | -3.34 | 106.41 | 110.67 |
| 12 | F5 | 201 | CYC | CMA-C3A-C4A | 3.34 | 130.21 | 125.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | p7 | 201 | CYC | C1A-C2A-C3A | -3.34 | 103.08 | 106.78 |
| 12 | C4 | 201 | CYC | C1B-NB-C4B | -3.34 | 106.41 | 110.67 |
| 12 | C8 | 201 | CYC | C1B-NB-C4B | -3.34 | 106.41 | 110.67 |
| 12 | Z | 201 | CYC | CAA-CBA-CGA | -3.34 | 106.41 | 113.60 |
| 12 | M4 | 301 | CYC | CAB-C3B-C4B | 3.34 | 126.66 | 121.38 |
| 12 | B4 | 201 | CYC | OC-C1C-C2C | -3.34 | 123.52 | 126.17 |
| 12 | j5 | 1201 | CYC | C1B-CHB-C4A | 3.34 | 136.24 | 128.08 |
| 12 | A | 201 | CYC | CAA-CBA-CGA | -3.34 | 106.41 | 113.60 |
| 12 | B4 | 201 | CYC | C4A-C3A-C2A | -3.34 | 102.67 | 106.51 |
| 12 | B8 | 201 | CYC | C4A-C3A-C2A | -3.34 | 102.67 | 106.51 |
| 12 | BA | 202 | CYC | OC-C1C-C2C | -3.34 | 123.52 | 126.17 |
| 12 | k5 | 1203 | CYC | CAA-CBA-CGA | -3.34 | 106.42 | 113.60 |
| 12 | k5 | 1204 | CYC | C1B-C2B-C3B | -3.34 | 104.39 | 107.87 |
| 12 | b7 | 201 | CYC | C1B-C2B-C3B | -3.34 | 104.39 | 107.87 |
| 12 | T3 | 302 | CYC | C4A-C3A-C2A | -3.34 | 102.67 | 106.51 |
| 12 | T1 | 302 | CYC | C4A-C3A-C2A | -3.34 | 102.67 | 106.51 |
| 12 | H5 | 201 | CYC | C1A-C2A-C3A | -3.34 | 103.09 | 106.78 |
| 12 | L7 | 201 | CYC | C1A-C2A-C3A | -3.34 | 103.09 | 106.78 |
| 12 | B7 | 201 | CYC | CAA-CBA-CGA | -3.34 | 106.42 | 113.60 |
| 12 | P7 | 201 | CYC | CAA-CBA-CGA | -3.34 | 106.42 | 113.60 |
| 12 | V5 | 201 | CYC | C1A-C2A-C3A | -3.34 | 103.09 | 106.78 |
| 12 | N7 | 201 | CYC | CAA-CBA-CGA | -3.34 | 106.42 | 113.60 |
| 12 | L4 | 201 | CYC | OC-C1C-C2C | -3.33 | 123.52 | 126.17 |
| 12 | K6 | 201 | CYC | C1B-NB-C4B | -3.33 | 106.42 | 110.67 |
| 12 | j5 | 1202 | CYC | C1B-C2B-C3B | -3.33 | 104.39 | 107.87 |
| 12 | F3 | 202 | CYC | C4A-C3A-C2A | -3.33 | 102.68 | 106.51 |
| 12 | W9 | 201 | CYC | C1B-NB-C4B | -3.33 | 106.43 | 110.67 |
| 12 | r7 | 201 | CYC | CAA-CBA-CGA | -3.33 | 106.43 | 113.60 |
| 12 | R5 | 201 | CYC | C1B-C2B-C3B | -3.33 | 104.39 | 107.87 |
| 12 | H7 | 201 | CYC | C1B-C2B-C3B | -3.33 | 104.39 | 107.87 |
| 12 | T7 | 201 | CYC | CAA-CBA-CGA | -3.33 | 106.44 | 113.60 |
| 12 | U4 | 202 | CYC | C4A-C3A-C2A | -3.33 | 102.68 | 106.51 |
| 12 | I7 | 201 | CYC | C1B-C2B-C3B | -3.33 | 104.40 | 107.87 |
| 12 | C3 | 201 | CYC | C1B-NB-C4B | -3.33 | 106.43 | 110.67 |
| 12 | C1 | 201 | CYC | C1B-NB-C4B | -3.33 | 106.43 | 110.67 |
| 12 | Q9 | 201 | CYC | C1B-NB-C4B | -3.33 | 106.43 | 110.67 |
| 12 | O1 | 201 | CYC | C1B-NB-C4B | -3.33 | 106.43 | 110.67 |
| 12 | O3 | 201 | CYC | C1B-NB-C4B | -3.33 | 106.43 | 110.67 |
| 12 | D5 | 201 | CYC | C1B-C2B-C3B | -3.33 | 104.40 | 107.87 |
| 12 | f5 | 201 | CYC | C1B-C2B-C3B | -3.33 | 104.40 | 107.87 |
| 12 | R7 | 201 | CYC | C1B-C2B-C3B | -3.33 | 104.40 | 107.87 |
| 12 | B8 | 202 | CYC | CAB-C3B-C4B | 3.33 | 126.63 | 121.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | P1 | 201 | CYC | CAB-C3B-C4B | 3.33 | 126.63 | 121.38 |
| 12 | P3 | 201 | CYC | CAB-C3B-C4B | 3.33 | 126.63 | 121.38 |
| 12 | J7 | 201 | CYC | C1A-C2A-C3A | -3.33 | 103.10 | 106.78 |
| 12 | d5 | 201 | CYC | CAA-CBA-CGA | -3.33 | 106.45 | 113.60 |
| 12 | d7 | 201 | CYC | CAA-CBA-CGA | -3.32 | 106.45 | 113.60 |
| 12 | f5 | 201 | CYC | CAA-CBA-CGA | -3.32 | 106.46 | 113.60 |
| 12 | v7 | 201 | CYC | CAA-CBA-CGA | -3.32 | 106.46 | 113.60 |
| 12 | QA | 201 | CYC | C1B-NB-C4B | -3.32 | 106.44 | 110.67 |
| 12 | JA | 201 | CYC | OC-C1C-C2C | -3.32 | 123.53 | 126.17 |
| 12 | J9 | 201 | CYC | OC-C1C-C2C | -3.32 | 123.53 | 126.17 |
| 12 | Z5 | 201 | CYC | CAA-CBA-CGA | -3.32 | 106.47 | 113.60 |
| 12 | C7 | 201 | CYC | C1B-C2B-C3B | -3.32 | 104.41 | 107.87 |
| 12 | S4 | 201 | CYC | C4A-C3A-C2A | -3.32 | 102.70 | 106.51 |
| 12 | D7 | 201 | CYC | C1B-C2B-C3B | -3.32 | 104.41 | 107.87 |
| 12 | A | 201 | CYC | C1A-C2A-C3A | -3.32 | 103.11 | 106.78 |
| 12 | I6 | 201 | CYC | C1B-NB-C4B | -3.32 | 106.45 | 110.67 |
| 12 | p7 | 201 | CYC | CAA-CBA-CGA | -3.32 | 106.47 | 113.60 |
| 12 | b7 | 201 | CYC | CAA-CBA-CGA | -3.31 | 106.47 | 113.60 |
| 12 | UA | 201 | CYC | C1B-NB-C4B | -3.31 | 106.45 | 110.67 |
| 12 | A1 | 201 | CYC | C1B-NB-C4B | -3.31 | 106.45 | 110.67 |
| 12 | A3 | 201 | CYC | C1B-NB-C4B | -3.31 | 106.45 | 110.67 |
| 12 | U9 | 201 | CYC | C1B-NB-C4B | -3.31 | 106.45 | 110.67 |
| 12 | B1 | 201 | CYC | OC-C1C-C2C | -3.31 | 123.54 | 126.17 |
| 12 | L3 | 201 | CYC | C4A-C3A-C2A | -3.31 | 102.70 | 106.51 |
| 12 | L1 | 201 | CYC | C4A-C3A-C2A | -3.31 | 102.70 | 106.51 |
| 12 | H5 | 201 | CYC | CAA-CBA-CGA | -3.31 | 106.47 | 113.60 |
| 12 | V4 | 201 | CYC | C1B-NB-C4B | -3.31 | 106.45 | 110.67 |
| 12 | D3 | 201 | CYC | OC-C1C-C2C | -3.31 | 123.54 | 126.17 |
| 12 | D1 | 201 | CYC | OC-C1C-C2C | -3.31 | 123.54 | 126.17 |
| 12 | U8 | 202 | CYC | C4A-C3A-C2A | -3.31 | 102.70 | 106.51 |
| 12 | O9 | 201 | CYC | C1B-NB-C4B | -3.31 | 106.45 | 110.67 |
| 12 | P4 | 201 | CYC | C1B-NB-C4B | -3.31 | 106.45 | 110.67 |
| 12 | P8 | 201 | CYC | C1B-NB-C4B | -3.31 | 106.45 | 110.67 |
| 12 | F7 | 201 | CYC | CAA-CBA-CGA | -3.31 | 106.48 | 113.60 |
| 12 | WA | 201 | CYC | C1B-NB-C4B | -3.31 | 106.45 | 110.67 |
| 12 | U3 | 201 | CYC | C1B-NB-C4B | -3.31 | 106.45 | 110.67 |
| 12 | U1 | 201 | CYC | C1B-NB-C4B | -3.31 | 106.45 | 110.67 |
| 12 | L6 | 202 | CYC | OC-C1C-C2C | -3.31 | 123.54 | 126.17 |
| 12 | A6 | 201 | CYC | C1B-NB-C4B | -3.31 | 106.45 | 110.67 |
| 12 | L5 | 201 | CYC | CMA-C3A-C4A | 3.31 | 130.16 | 125.06 |
| 12 | A2 | 201 | CYC | C1B-NB-C4B | -3.31 | 106.46 | 110.67 |
| 12 | T7 | 201 | CYC | C1B-C2B-C3B | -3.31 | 104.42 | 107.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | F1 | 202 | CYC | C4A-C3A-C2A | -3.31 | 102.71 | 106.51 |
| 12 | d5 | 201 | CYC | C1A-C2A-C3A | -3.31 | 103.12 | 106.78 |
| 12 | OA | 201 | CYC | C1B-NB-C4B | -3.31 | 106.46 | 110.67 |
| 12 | J5 | 201 | CYC | C1B-C2B-C3B | -3.31 | 104.42 | 107.87 |
| 12 | h7 | 201 | CYC | C1B-C2B-C3B | -3.31 | 104.42 | 107.87 |
| 12 | D7 | 201 | CYC | C1A-C2A-C3A | -3.30 | 103.13 | 106.78 |
| 12 | h7 | 201 | CYC | CAA-CBA-CGA | -3.30 | 106.50 | 113.60 |
| 12 | ZA | 201 | CYC | C4A-C3A-C2A | -3.30 | 102.72 | 106.51 |
| 12 | F9 | 303 | CYC | C4A-C3A-C2A | -3.30 | 102.72 | 106.51 |
| 12 | Z9 | 201 | CYC | C4A-C3A-C2A | -3.30 | 102.72 | 106.51 |
| 12 | b5 | 201 | CYC | CAA-CBA-CGA | -3.30 | 106.50 | 113.60 |
| 12 | F9 | 302 | CYC | C4A-C3A-C2A | -3.30 | 102.72 | 106.51 |
| 12 | B5 | 201 | CYC | C1B-C2B-C3B | -3.30 | 104.43 | 107.87 |
| 12 | R1 | 202 | CYC | C4A-C3A-C2A | -3.30 | 102.72 | 106.51 |
| 12 | R3 | 202 | CYC | C4A-C3A-C2A | -3.30 | 102.72 | 106.51 |
| 12 | W1 | 201 | CYC | C1B-NB-C4B | -3.30 | 106.47 | 110.67 |
| 12 | H6 | 202 | CYC | OC-C1C-C2C | -3.30 | 123.55 | 126.17 |
| 12 | B2 | 201 | CYC | C4A-C3A-C2A | -3.29 | 102.72 | 106.51 |
| 12 | S8 | 201 | CYC | C4A-C3A-C2A | -3.29 | 102.73 | 106.51 |
| 12 | Q1 | 201 | CYC | C1B-NB-C4B | -3.29 | 106.48 | 110.67 |
| 12 | Q3 | 201 | CYC | C1B-NB-C4B | -3.29 | 106.48 | 110.67 |
| 12 | b5 | 201 | CYC | C1B-C2B-C3B | -3.29 | 104.44 | 107.87 |
| 12 | B5 | 201 | CYC | CAA-CBA-CGA | -3.29 | 106.52 | 113.60 |
| 12 | B7 | 201 | CYC | C1B-C2B-C3B | -3.29 | 104.44 | 107.87 |
| 12 | F4 | 201 | CYC | C4A-C3A-C2A | -3.29 | 102.73 | 106.51 |
| 12 | F8 | 201 | CYC | C4A-C3A-C2A | -3.29 | 102.73 | 106.51 |
| 12 | v7 | 201 | CYC | C1A-C2A-C3A | -3.29 | 103.14 | 106.78 |
| 12 | L7 | 201 | CYC | CAA-CBA-CGA | -3.29 | 106.52 | 113.60 |
| 12 | R7 | 201 | CYC | CAA-CBA-CGA | -3.29 | 106.53 | 113.60 |
| 12 | HA | 201 | CYC | C4A-C3A-C2A | -3.29 | 102.73 | 106.51 |
| 12 | H9 | 201 | CYC | C4A-C3A-C2A | -3.29 | 102.73 | 106.51 |
| 12 | f7 | 201 | CYC | CMA-C3A-C4A | 3.29 | 130.12 | 125.06 |
| 12 | DA | 202 | CYC | C4A-C3A-C2A | -3.29 | 102.73 | 106.51 |
| 12 | X7 | 201 | CYC | CAA-CBA-CGA | -3.28 | 106.53 | 113.60 |
| 12 | V5 | 201 | CYC | C1B-C2B-C3B | -3.28 | 104.44 | 107.87 |
| 12 | Z5 | 201 | CYC | C1A-C2A-C3A | -3.28 | 103.15 | 106.78 |
| 12 | I2 | 201 | CYC | C1B-NB-C4B | -3.28 | 106.49 | 110.67 |
| 12 | L2 | 202 | CYC | OC-C1C-C2C | -3.28 | 123.56 | 126.17 |
| 12 | W3 | 201 | CYC | C1B-NB-C4B | -3.28 | 106.49 | 110.67 |
| 12 | CA | 201 | CYC | C1B-NB-C4B | -3.28 | 106.49 | 110.67 |
| 12 | C9 | 201 | CYC | C1B-NB-C4B | -3.28 | 106.49 | 110.67 |
| 12 | P1 | 202 | CYC | C4A-C3A-C2A | -3.28 | 102.74 | 106.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | P3 | 202 | CYC | C4A-C3A-C2A | -3.28 | 102.74 | 106.51 |
| 12 | W4 | 202 | CYC | C4A-C3A-C2A | -3.28 | 102.74 | 106.51 |
| 12 | W8 | 202 | CYC | C4A-C3A-C2A | -3.28 | 102.74 | 106.51 |
| 12 | f5 | 201 | CYC | C1A-C2A-C3A | -3.28 | 103.15 | 106.78 |
| 12 | V3 | 202 | CYC | OC-C1C-C2C | -3.28 | 123.57 | 126.17 |
| 12 | V1 | 202 | CYC | OC-C1C-C2C | -3.28 | 123.57 | 126.17 |
| 12 | Z | 201 | CYC | C1A-C2A-C3A | -3.28 | 103.16 | 106.78 |
| 12 | P5 | 201 | CYC | C1B-C2B-C3B | -3.28 | 104.45 | 107.87 |
| 12 | j7 | 201 | CYC | CAA-CBA-CGA | -3.28 | 106.56 | 113.60 |
| 12 | J3 | 201 | CYC | C4A-C3A-C2A | -3.27 | 102.75 | 106.51 |
| 12 | B6 | 201 | CYC | C4A-C3A-C2A | -3.27 | 102.75 | 106.51 |
| 12 | J1 | 201 | CYC | C4A-C3A-C2A | -3.27 | 102.75 | 106.51 |
| 12 | M8 | 301 | CYC | CAB-C3B-C4B | 3.27 | 126.55 | 121.38 |
| 12 | G3 | 201 | CYC | C1B-NB-C4B | -3.27 | 106.50 | 110.67 |
| 12 | Z5 | 201 | CYC | C1B-C2B-C3B | -3.27 | 104.45 | 107.87 |
| 12 | V4 | 201 | CYC | C1A-C2A-C3A | -3.27 | 103.16 | 106.78 |
| 12 | V8 | 201 | CYC | C1A-C2A-C3A | -3.27 | 103.16 | 106.78 |
| 12 | Z5 | 201 | CYC | CMA-C3A-C4A | 3.27 | 130.10 | 125.06 |
| 12 | T5 | 201 | CYC | C1B-C2B-C3B | -3.27 | 104.46 | 107.87 |
| 12 | X5 | 201 | CYC | CAA-CBA-CGA | -3.27 | 106.56 | 113.60 |
| 12 | d5 | 201 | CYC | C1B-C2B-C3B | -3.27 | 104.46 | 107.87 |
| 12 | P7 | 201 | CYC | C1B-C2B-C3B | -3.27 | 104.46 | 107.87 |
| 12 | LA | 201 | CYC | C4A-C3A-C2A | -3.27 | 102.76 | 106.51 |
| 12 | L9 | 201 | CYC | C4A-C3A-C2A | -3.27 | 102.76 | 106.51 |
| 12 | L7 | 201 | CYC | C1B-C2B-C3B | -3.27 | 104.46 | 107.87 |
| 12 | d5 | 201 | CYC | CMA-C3A-C4A | 3.26 | 130.09 | 125.06 |
| 12 | B3 | 201 | CYC | OC-C1C-C2C | -3.26 | 123.58 | 126.17 |
| 12 | X3 | 202 | CYC | OC-C1C-C2C | -3.26 | 123.58 | 126.17 |
| 12 | X1 | 202 | CYC | OC-C1C-C2C | -3.26 | 123.58 | 126.17 |
| 12 | G1 | 201 | CYC | C1B-NB-C4B | -3.26 | 106.51 | 110.67 |
| 12 | B3 | 201 | CYC | C4A-C3A-C2A | -3.26 | 102.76 | 106.51 |
| 12 | B1 | 201 | CYC | C4A-C3A-C2A | -3.26 | 102.76 | 106.51 |
| 12 | R1 | 202 | CYC | OC-C1C-C2C | -3.26 | 123.58 | 126.17 |
| 12 | R3 | 202 | CYC | OC-C1C-C2C | -3.26 | 123.58 | 126.17 |
| 12 | Y3 | 201 | CYC | C1B-NB-C4B | -3.26 | 106.51 | 110.67 |
| 12 | Y1 | 201 | CYC | C1B-NB-C4B | -3.26 | 106.51 | 110.67 |
| 12 | H2 | 202 | CYC | OC-C1C-C2C | -3.26 | 123.58 | 126.17 |
| 12 | VA | 202 | CYC | C4A-C3A-C2A | -3.26 | 102.76 | 106.51 |
| 12 | V9 | 202 | CYC | C4A-C3A-C2A | -3.26 | 102.76 | 106.51 |
| 12 | F7 | 201 | CYC | C1B-C2B-C3B | -3.26 | 104.47 | 107.87 |
| 12 | RA | 202 | CYC | C4A-C3A-C2A | -3.26 | 102.76 | 106.51 |
| 12 | R9 | 202 | CYC | C4A-C3A-C2A | -3.26 | 102.76 | 106.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | H5 | 201 | CYC | C1B-C2B-C3B | -3.26 | 104.47 | 107.87 |
| 12 | N4 | 201 | CYC | C1B-NB-C4B | -3.26 | 106.52 | 110.67 |
| 12 | k5 | 1203 | CYC | C1B-C2B-C3B | -3.26 | 104.47 | 107.87 |
| 12 | R5 | 201 | CYC | CAA-CBA-CGA | -3.26 | 106.59 | 113.60 |
| 12 | XA | 202 | CYC | C4A-C3A-C2A | -3.26 | 102.77 | 106.51 |
| 12 | X9 | 202 | CYC | C4A-C3A-C2A | -3.26 | 102.77 | 106.51 |
| 12 | Z3 | 202 | CYC | C4A-C3A-C2A | -3.26 | 102.77 | 106.51 |
| 12 | PA | 202 | CYC | C4A-C3A-C2A | -3.26 | 102.77 | 106.51 |
| 12 | P9 | 202 | CYC | C4A-C3A-C2A | -3.26 | 102.77 | 106.51 |
| 12 | D9 | 202 | CYC | C4A-C3A-C2A | -3.26 | 102.77 | 106.51 |
| 12 | J7 | 201 | CYC | C1B-C2B-C3B | -3.25 | 104.48 | 107.87 |
| 12 | r7 | 201 | CYC | C1A-C2A-C3A | -3.25 | 103.18 | 106.78 |
| 12 | H4 | 202 | CYC | C4A-C3A-C2A | -3.25 | 102.78 | 106.51 |
| 12 | H8 | 202 | CYC | C4A-C3A-C2A | -3.25 | 102.78 | 106.51 |
| 12 | L5 | 201 | CYC | C1B-C2B-C3B | -3.25 | 104.48 | 107.87 |
| 12 | r7 | 201 | CYC | C1B-C2B-C3B | -3.25 | 104.48 | 107.87 |
| 12 | J2 | 201 | CYC | C4A-C3A-C2A | -3.25 | 102.78 | 106.51 |
| 12 | Z | 201 | CYC | C1B-C2B-C3B | -3.25 | 104.48 | 107.87 |
| 12 | K6 | 201 | CYC | CMC-C2C-C1C | -3.24 | 105.41 | 112.40 |
| 12 | k5 | 1203 | CYC | C1A-C2A-C3A | -3.24 | 103.20 | 106.78 |
| 12 | I4 | 201 | CYC | C1B-NB-C4B | -3.24 | 106.54 | 110.67 |
| 12 | I8 | 201 | CYC | C1B-NB-C4B | -3.24 | 106.54 | 110.67 |
| 12 | N5 | 201 | CYC | C1B-C2B-C3B | -3.24 | 104.49 | 107.87 |
| 12 | H4 | 202 | CYC | OC-C1C-C2C | -3.24 | 123.60 | 126.17 |
| 12 | Y4 | 201 | CYC | OC-C1C-C2C | -3.24 | 123.60 | 126.17 |
| 12 | H8 | 202 | CYC | OC-C1C-C2C | -3.24 | 123.60 | 126.17 |
| 12 | Y8 | 201 | CYC | OC-C1C-C2C | -3.24 | 123.60 | 126.17 |
| 12 | F6 | 202 | CYC | C4A-C3A-C2A | -3.24 | 102.79 | 106.51 |
| 12 | Z1 | 201 | CYC | C4A-C3A-C2A | -3.24 | 102.79 | 106.51 |
| 12 | K2 | 201 | CYC | CMC-C2C-C1C | -3.24 | 105.43 | 112.40 |
| 12 | TA | 302 | CYC | C4A-C3A-C2A | -3.24 | 102.79 | 106.51 |
| 12 | T9 | 302 | CYC | C4A-C3A-C2A | -3.24 | 102.79 | 106.51 |
| 12 | j7 | 201 | CYC | C1B-C2B-C3B | -3.24 | 104.50 | 107.87 |
| 12 | YA | 201 | CYC | CMC-C2C-C1C | -3.23 | 105.43 | 112.40 |
| 12 | Y9 | 201 | CYC | CMC-C2C-C1C | -3.23 | 105.43 | 112.40 |
| 12 | A | 201 | CYC | C1B-C2B-C3B | -3.23 | 104.50 | 107.87 |
| 12 | SA | 201 | CYC | C1A-C2A-C3A | -3.23 | 103.21 | 106.78 |
| 12 | S9 | 201 | CYC | C1A-C2A-C3A | -3.23 | 103.21 | 106.78 |
| 12 | N8 | 201 | CYC | C1B-NB-C4B | -3.23 | 106.56 | 110.67 |
| 12 | D6 | 202 | CYC | C4A-C3A-C2A | -3.23 | 102.80 | 106.51 |
| 12 | T9 | 302 | CYC | C2A-C1A-NA | 3.23 | 114.74 | 110.05 |
| 12 | F5 | 201 | CYC | C1B-C2B-C3B | -3.23 | 104.50 | 107.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | F3 | 202 | CYC | OC-C1C-C2C | -3.23 | 123.61 | 126.17 |
| 12 | F1 | 202 | CYC | OC-C1C-C2C | -3.23 | 123.61 | 126.17 |
| 12 | T4 | 201 | CYC | CMC-C2C-C1C | -3.22 | 105.45 | 112.40 |
| 12 | T8 | 201 | CYC | CMC-C2C-C1C | -3.22 | 105.45 | 112.40 |
| 12 | D4 | 201 | CYC | C4A-C3A-C2A | -3.22 | 102.81 | 106.51 |
| 12 | J4 | 202 | CYC | C4A-C3A-C2A | -3.22 | 102.81 | 106.51 |
| 12 | D8 | 201 | CYC | C4A-C3A-C2A | -3.22 | 102.81 | 106.51 |
| 12 | J8 | 202 | CYC | C4A-C3A-C2A | -3.22 | 102.81 | 106.51 |
| 12 | WA | 201 | CYC | C1A-C2A-C3A | -3.22 | 103.22 | 106.78 |
| 12 | W9 | 201 | CYC | C1A-C2A-C3A | -3.22 | 103.22 | 106.78 |
| 12 | F3 | 202 | CYC | C2A-C1A-NA | 3.22 | 114.73 | 110.05 |
| 12 | V7 | 201 | CYC | C1B-C2B-C3B | -3.22 | 104.51 | 107.87 |
| 12 | D2 | 202 | CYC | C4A-C3A-C2A | -3.22 | 102.81 | 106.51 |
| 12 | D3 | 201 | CYC | C4A-C3A-C2A | -3.22 | 102.81 | 106.51 |
| 12 | D1 | 201 | CYC | C4A-C3A-C2A | -3.22 | 102.81 | 106.51 |
| 12 | AA | 201 | CYC | C1B-NB-C4B | -3.22 | 106.58 | 110.67 |
| 12 | A9 | 201 | CYC | C1B-NB-C4B | -3.22 | 106.58 | 110.67 |
| 12 | C4 | 201 | CYC | CMC-C2C-C1C | -3.21 | 105.47 | 112.40 |
| 12 | C8 | 201 | CYC | CMC-C2C-C1C | -3.21 | 105.47 | 112.40 |
| 12 | U9 | 201 | CYC | C1A-C2A-C3A | -3.21 | 103.23 | 106.78 |
| 12 | J6 | 201 | CYC | C4A-C3A-C2A | -3.21 | 102.82 | 106.51 |
| 12 | L6 | 202 | CYC | C4A-C3A-C2A | -3.21 | 102.82 | 106.51 |
| 12 | K1 | 201 | CYC | CMC-C2C-C1C | -3.21 | 105.48 | 112.40 |
| 12 | Q4 | 201 | CYC | C4A-C3A-C2A | -3.21 | 102.82 | 106.51 |
| 12 | IA | 201 | CYC | CMC-C2C-C1C | -3.21 | 105.49 | 112.40 |
| 12 | I9 | 201 | CYC | CMC-C2C-C1C | -3.21 | 105.49 | 112.40 |
| 12 | F2 | 202 | CYC | C4A-C3A-C2A | -3.20 | 102.83 | 106.51 |
| 12 | L2 | 202 | CYC | C4A-C3A-C2A | -3.20 | 102.83 | 106.51 |
| 12 | TA | 302 | CYC | C2A-C1A-NA | 3.20 | 114.71 | 110.05 |
| 12 | C3 | 201 | CYC | C1A-C2A-C3A | -3.20 | 103.24 | 106.78 |
| 12 | C1 | 201 | CYC | C1A-C2A-C3A | -3.20 | 103.24 | 106.78 |
| 12 | K3 | 201 | CYC | CMC-C2C-C1C | -3.20 | 105.50 | 112.40 |
| 12 | X7 | 201 | CYC | C1B-C2B-C3B | -3.20 | 104.53 | 107.87 |
| 12 | X8 | 201 | CYC | CMC-C2C-C1C | -3.20 | 105.51 | 112.40 |
| 12 | F9 | 302 | CYC | OC-C1C-C2C | -3.20 | 123.63 | 126.17 |
| 12 | d7 | 201 | CYC | C1B-C2B-C3B | -3.19 | 104.54 | 107.87 |
| 12 | T9 | 302 | CYC | OC-C1C-C2C | -3.19 | 123.63 | 126.17 |
| 12 | JA | 201 | CYC | C4A-C3A-C2A | -3.19 | 102.84 | 106.51 |
| 12 | J9 | 201 | CYC | C4A-C3A-C2A | -3.19 | 102.84 | 106.51 |
| 12 | F1 | 202 | CYC | C2A-C1A-NA | 3.19 | 114.69 | 110.05 |
| 12 | Y4 | 201 | CYC | C4A-C3A-C2A | -3.19 | 102.84 | 106.51 |
| 12 | Y8 | 201 | CYC | C4A-C3A-C2A | -3.19 | 102.84 | 106.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | AA | 201 | CYC | C1A-C2A-C3A | -3.19 | 103.25 | 106.78 |
| 12 | A9 | 201 | CYC | C1A-C2A-C3A | -3.19 | 103.25 | 106.78 |
| 12 | A8 | 201 | CYC | C1B-NB-C4B | -3.19 | 106.61 | 110.67 |
| 12 | C9 | 201 | CYC | CMC-C2C-C1C | -3.19 | 105.52 | 112.40 |
| 12 | X3 | 202 | CYC | C4A-C3A-C2A | -3.19 | 102.85 | 106.51 |
| 12 | X1 | 202 | CYC | C4A-C3A-C2A | -3.19 | 102.85 | 106.51 |
| 12 | UA | 201 | CYC | C1A-C2A-C3A | -3.19 | 103.25 | 106.78 |
| 12 | G4 | 201 | CYC | CMC-C2C-C1C | -3.19 | 105.53 | 112.40 |
| 12 | G8 | 201 | CYC | CMC-C2C-C1C | -3.19 | 105.53 | 112.40 |
| 12 | P4 | 201 | CYC | CMC-C2C-C1C | -3.19 | 105.53 | 112.40 |
| 12 | P8 | 201 | CYC | CMC-C2C-C1C | -3.19 | 105.53 | 112.40 |
| 12 | JA | 201 | CYC | C2A-C1A-NA | 3.19 | 114.68 | 110.05 |
| 12 | J9 | 201 | CYC | C2A-C1A-NA | 3.19 | 114.68 | 110.05 |
| 12 | E2 | 201 | CYC | C1A-C2A-C3A | -3.19 | 103.26 | 106.78 |
| 12 | Y3 | 201 | CYC | CMC-C2C-C1C | -3.18 | 105.54 | 112.40 |
| 12 | Y1 | 201 | CYC | CMC-C2C-C1C | -3.18 | 105.54 | 112.40 |
| 12 | KA | 201 | CYC | CMC-C2C-C1C | -3.18 | 105.54 | 112.40 |
| 12 | K9 | 201 | CYC | CMC-C2C-C1C | -3.18 | 105.54 | 112.40 |
| 12 | W1 | 201 | CYC | CMC-C2C-C1C | -3.18 | 105.54 | 112.40 |
| 12 | X4 | 201 | CYC | CMC-C2C-C1C | -3.18 | 105.54 | 112.40 |
| 12 | P1 | 202 | CYC | C2A-C1A-NA | 3.18 | 114.68 | 110.05 |
| 12 | P3 | 202 | CYC | C2A-C1A-NA | 3.18 | 114.68 | 110.05 |
| 12 | F4 | 201 | CYC | C2A-C1A-NA | 3.18 | 114.68 | 110.05 |
| 12 | F8 | 201 | CYC | C2A-C1A-NA | 3.18 | 114.68 | 110.05 |
| 12 | U3 | 201 | CYC | C1A-C2A-C3A | -3.18 | 103.26 | 106.78 |
| 12 | U1 | 201 | CYC | C1A-C2A-C3A | -3.18 | 103.26 | 106.78 |
| 12 | A1 | 201 | CYC | CMC-C2C-C1C | -3.18 | 105.55 | 112.40 |
| 12 | A3 | 201 | CYC | CMC-C2C-C1C | -3.18 | 105.55 | 112.40 |
| 12 | C3 | 201 | CYC | CMC-C2C-C1C | -3.18 | 105.55 | 112.40 |
| 12 | C1 | 201 | CYC | CMC-C2C-C1C | -3.18 | 105.55 | 112.40 |
| 12 | R8 | 201 | CYC | CMC-C2C-C1C | -3.18 | 105.55 | 112.40 |
| 12 | K4 | 201 | CYC | CMC-C2C-C1C | -3.18 | 105.55 | 112.40 |
| 12 | K8 | 201 | CYC | CMC-C2C-C1C | -3.18 | 105.55 | 112.40 |
| 12 | I4 | 201 | CYC | C1A-C2A-C3A | -3.18 | 103.27 | 106.78 |
| 12 | I8 | 201 | CYC | C1A-C2A-C3A | -3.18 | 103.27 | 106.78 |
| 12 | Q8 | 201 | CYC | C4A-C3A-C2A | -3.17 | 102.86 | 106.51 |
| 12 | C6 | 201 | CYC | CMC-C2C-C1C | -3.17 | 105.56 | 112.40 |
| 12 | A4 | 201 | CYC | C1B-NB-C4B | -3.17 | 106.63 | 110.67 |
| 12 | H8 | 201 | CYC | C2C-C1C-NC | 3.17 | 111.01 | 108.27 |
| 12 | GA | 201 | CYC | CMC-C2C-C1C | -3.17 | 105.56 | 112.40 |
| 12 | U5 | 201 | CYC | CHB-C4A-C3A | 3.17 | 133.06 | 124.90 |
| 12 | W3 | 201 | CYC | CMC-C2C-C1C | -3.17 | 105.57 | 112.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | T3 | 302 | CYC | C2A-C1A-NA | 3.17 | 114.66 | 110.05 |
| 12 | S4 | 201 | CYC | C2A-C1A-NA | 3.17 | 114.66 | 110.05 |
| 12 | S8 | 201 | CYC | C2A-C1A-NA | 3.17 | 114.66 | 110.05 |
| 12 | T1 | 302 | CYC | C2A-C1A-NA | 3.17 | 114.66 | 110.05 |
| 12 | I4 | 201 | CYC | CMC-C2C-C1C | -3.17 | 105.57 | 112.40 |
| 12 | I8 | 201 | CYC | CMC-C2C-C1C | -3.17 | 105.57 | 112.40 |
| 12 | W3 | 201 | CYC | C1A-C2A-C3A | -3.17 | 103.28 | 106.78 |
| 12 | CA | 201 | CYC | CMC-C2C-C1C | -3.17 | 105.57 | 112.40 |
| 12 | R4 | 201 | CYC | CMC-C2C-C1C | -3.17 | 105.57 | 112.40 |
| 12 | PA | 202 | CYC | C2A-C1A-NA | 3.17 | 114.66 | 110.05 |
| 12 | B3 | 201 | CYC | C2A-C1A-NA | 3.17 | 114.66 | 110.05 |
| 12 | B1 | 201 | CYC | C2A-C1A-NA | 3.17 | 114.66 | 110.05 |
| 12 | P9 | 202 | CYC | C2A-C1A-NA | 3.17 | 114.66 | 110.05 |
| 12 | X1 | 202 | CYC | C2A-C1A-NA | 3.17 | 114.66 | 110.05 |
| 12 | C2 | 201 | CYC | CMC-C2C-C1C | -3.17 | 105.58 | 112.40 |
| 12 | QA | 201 | CYC | C1A-C2A-C3A | -3.17 | 103.28 | 106.78 |
| 12 | Q1 | 201 | CYC | CMC-C2C-C1C | -3.17 | 105.58 | 112.40 |
| 12 | U3 | 201 | CYC | CMC-C2C-C1C | -3.16 | 105.58 | 112.40 |
| 12 | U1 | 201 | CYC | CMC-C2C-C1C | -3.16 | 105.58 | 112.40 |
| 12 | Q9 | 201 | CYC | C1A-C2A-C3A | -3.16 | 103.28 | 106.78 |
| 12 | TA | 302 | CYC | OC-C1C-C2C | -3.16 | 123.66 | 126.17 |
| 12 | G9 | 201 | CYC | CMC-C2C-C1C | -3.16 | 105.59 | 112.40 |
| 12 | F9 | 303 | CYC | OC-C1C-C2C | -3.16 | 123.66 | 126.17 |
| 12 | S8 | 201 | CYC | OC-C1C-C2C | -3.16 | 123.66 | 126.17 |
| 12 | W1 | 201 | CYC | C1A-C2A-C3A | -3.16 | 103.29 | 106.78 |
| 12 | Q3 | 201 | CYC | CMC-C2C-C1C | -3.16 | 105.60 | 112.40 |
| 12 | J4 | 202 | CYC | C2A-C1A-NA | 3.16 | 114.64 | 110.05 |
| 12 | J8 | 202 | CYC | C2A-C1A-NA | 3.16 | 114.64 | 110.05 |
| 12 | J6 | 201 | CYC | C2A-C1A-NA | 3.16 | 114.64 | 110.05 |
| 12 | S1 | 201 | CYC | CMC-C2C-C1C | -3.16 | 105.60 | 112.40 |
| 12 | S3 | 201 | CYC | CMC-C2C-C1C | -3.16 | 105.60 | 112.40 |
| 12 | L9 | 201 | CYC | C2A-C1A-NA | 3.16 | 114.64 | 110.05 |
| 12 | O5 | 201 | CYC | CHB-C4A-C3A | 3.15 | 133.01 | 124.90 |
| 12 | X3 | 202 | CYC | C2A-C1A-NA | 3.15 | 114.64 | 110.05 |
| 12 | G6 | 201 | CYC | CMC-C2C-C1C | -3.15 | 105.61 | 112.40 |
| 12 | O1 | 201 | CYC | C1A-C2A-C3A | -3.15 | 103.29 | 106.78 |
| 12 | O3 | 201 | CYC | C1A-C2A-C3A | -3.15 | 103.29 | 106.78 |
| 12 | e7 | 201 | CYC | CHB-C4A-C3A | 3.15 | 133.01 | 124.90 |
| 12 | Q1 | 201 | CYC | C1A-C2A-C3A | -3.15 | 103.30 | 106.78 |
| 12 | Q3 | 201 | CYC | C1A-C2A-C3A | -3.15 | 103.30 | 106.78 |
| 12 | E6 | 201 | CYC | C1A-C2A-C3A | -3.15 | 103.30 | 106.78 |
| 12 | q7 | 201 | CYC | CHB-C4A-C3A | 3.15 | 133.00 | 124.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | H4 | 201 | CYC | C2C-C1C-NC | 3.15 | 110.99 | 108.27 |
| 12 | s7 | 201 | CYC | CHB-C4A-C3A | 3.15 | 133.00 | 124.90 |
| 12 | A2 | 201 | CYC | CMC-C2C-C1C | -3.15 | 105.62 | 112.40 |
| 12 | W5 | 201 | CYC | CHB-C4A-C3A | 3.14 | 132.98 | 124.90 |
| 12 | e5 | 201 | CYC | CHB-C4A-C3A | 3.14 | 132.98 | 124.90 |
| 12 | k7 | 201 | CYC | CHB-C4A-C3A | 3.14 | 132.98 | 124.90 |
| 12 | F9 | 303 | CYC | C2A-C1A-NA | 3.14 | 114.62 | 110.05 |
| 12 | E4 | 201 | CYC | C1A-C2A-C3A | -3.14 | 103.31 | 106.78 |
| 12 | E8 | 201 | CYC | C1A-C2A-C3A | -3.14 | 103.31 | 106.78 |
| 12 | A6 | 201 | CYC | CMC-C2C-C1C | -3.14 | 105.63 | 112.40 |
| 12 | Q5 | 201 | CYC | CHB-C4A-C3A | 3.14 | 132.98 | 124.90 |
| 12 | UA | 201 | CYC | CMC-C2C-C1C | -3.14 | 105.63 | 112.40 |
| 12 | U9 | 201 | CYC | CMC-C2C-C1C | -3.14 | 105.63 | 112.40 |
| 12 | F9 | 302 | CYC | C2A-C1A-NA | 3.14 | 114.62 | 110.05 |
| 12 | G2 | 201 | CYC | CMC-C2C-C1C | -3.14 | 105.63 | 112.40 |
| 12 | Z3 | 202 | CYC | C2A-C1A-NA | 3.14 | 114.62 | 110.05 |
| 12 | WA | 201 | CYC | CMC-C2C-C1C | -3.14 | 105.64 | 112.40 |
| 12 | W9 | 201 | CYC | CMC-C2C-C1C | -3.14 | 105.64 | 112.40 |
| 12 | L6 | 202 | CYC | C2A-C1A-NA | 3.14 | 114.61 | 110.05 |
| 12 | F2 | 202 | CYC | C2A-C1A-NA | 3.14 | 114.61 | 110.05 |
| 12 | A6 | 201 | CYC | C1A-C2A-C3A | -3.14 | 103.31 | 106.78 |
| 12 | G3 | 201 | CYC | CMC-C2C-C1C | -3.14 | 105.64 | 112.40 |
| 12 | V4 | 201 | CYC | CMC-C2C-C1C | -3.14 | 105.64 | 112.40 |
| 12 | V8 | 201 | CYC | CMC-C2C-C1C | -3.14 | 105.64 | 112.40 |
| 12 | G1 | 201 | CYC | CMC-C2C-C1C | -3.14 | 105.64 | 112.40 |
| 12 | I3 | 201 | CYC | CMC-C2C-C1C | -3.14 | 105.64 | 112.40 |
| 12 | I1 | 201 | CYC | CMC-C2C-C1C | -3.14 | 105.64 | 112.40 |
| 12 | J2 | 201 | CYC | C2A-C1A-NA | 3.14 | 114.61 | 110.05 |
| 12 | P4 | 201 | CYC | C1A-C2A-C3A | -3.14 | 103.31 | 106.78 |
| 12 | P8 | 201 | CYC | C1A-C2A-C3A | -3.14 | 103.31 | 106.78 |
| 12 | R8 | 201 | CYC | C1A-C2A-C3A | -3.14 | 103.31 | 106.78 |
| 12 | OA | 201 | CYC | C1A-C2A-C3A | -3.13 | 103.31 | 106.78 |
| 12 | LA | 201 | CYC | C2A-C1A-NA | 3.13 | 114.61 | 110.05 |
| 12 | S4 | 201 | CYC | OC-C1C-C2C | -3.13 | 123.68 | 126.17 |
| 12 | SA | 201 | CYC | CMC-C2C-C1C | -3.13 | 105.65 | 112.40 |
| 12 | S9 | 201 | CYC | CMC-C2C-C1C | -3.13 | 105.65 | 112.40 |
| 12 | O9 | 201 | CYC | CMC-C2C-C1C | -3.13 | 105.65 | 112.40 |
| 12 | a9 | 901 | CYC | C2C-C1C-NC | 3.13 | 110.97 | 108.27 |
| 12 | a5 | 201 | CYC | CHB-C4A-C3A | 3.13 | 132.96 | 124.90 |
| 12 | O1 | 201 | CYC | CMC-C2C-C1C | -3.13 | 105.65 | 112.40 |
| 12 | O3 | 201 | CYC | CMC-C2C-C1C | -3.13 | 105.65 | 112.40 |
| 12 | N4 | 201 | CYC | CMC-C2C-C1C | -3.13 | 105.65 | 112.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | N8 | 201 | CYC | CMC-C2C-C1C | -3.13 | 105.65 | 112.40 |
| 12 | C4 | 201 | CYC | C1A-C2A-C3A | -3.13 | 103.32 | 106.78 |
| 12 | C8 | 201 | CYC | C1A-C2A-C3A | -3.13 | 103.32 | 106.78 |
| 12 | B4 | 201 | CYC | C2A-C1A-NA | 3.13 | 114.60 | 110.05 |
| 12 | I5 | 201 | CYC | CHB-C4A-C3A | 3.13 | 132.94 | 124.90 |
| 12 | Q8 | 201 | CYC | C2A-C1A-NA | 3.13 | 114.60 | 110.05 |
| 12 | F8 | 201 | CYC | OC-C1C-C2C | -3.13 | 123.69 | 126.17 |
| 12 | QA | 201 | CYC | CMC-C2C-C1C | -3.13 | 105.66 | 112.40 |
| 12 | EA | 201 | CYC | C1A-C2A-C3A | -3.13 | 103.32 | 106.78 |
| 12 | u7 | 201 | CYC | CHB-C4A-C3A | 3.13 | 132.94 | 124.90 |
| 12 | F6 | 202 | CYC | C2A-C1A-NA | 3.13 | 114.60 | 110.05 |
| 12 | C5 | 201 | CYC | CHB-C4A-C3A | 3.13 | 132.94 | 124.90 |
| 12 | O4 | 202 | CYC | C2A-C1A-NA | 3.13 | 114.60 | 110.05 |
| 12 | O8 | 202 | CYC | C2A-C1A-NA | 3.13 | 114.60 | 110.05 |
| 12 | E6 | 201 | CYC | CMC-C2C-C1C | -3.13 | 105.66 | 112.40 |
| 12 | E2 | 201 | CYC | CMC-C2C-C1C | -3.13 | 105.66 | 112.40 |
| 12 | K8 | 201 | CYC | C1A-C2A-C3A | -3.13 | 103.32 | 106.78 |
| 12 | G1 | 201 | CYC | C1A-C2A-C3A | -3.12 | 103.32 | 106.78 |
| 12 | m7 | 201 | CYC | CHB-C4A-C3A | 3.12 | 132.94 | 124.90 |
| 12 | AA | 201 | CYC | CMC-C2C-C1C | -3.12 | 105.67 | 112.40 |
| 12 | A9 | 201 | CYC | CMC-C2C-C1C | -3.12 | 105.67 | 112.40 |
| 12 | M5 | 201 | CYC | CHB-C4A-C3A | 3.12 | 132.93 | 124.90 |
| 12 | S7 | 201 | CYC | CHB-C4A-C3A | 3.12 | 132.93 | 124.90 |
| 12 | Y7 | 201 | CYC | CHB-C4A-C3A | 3.12 | 132.93 | 124.90 |
| 12 | o7 | 201 | CYC | CHB-C4A-C3A | 3.12 | 132.93 | 124.90 |
| 12 | OA | 201 | CYC | CMC-C2C-C1C | -3.12 | 105.67 | 112.40 |
| 12 | R4 | 201 | CYC | C1A-C2A-C3A | -3.12 | 103.33 | 106.78 |
| 12 | H8 | 202 | CYC | C2A-C1A-NA | 3.12 | 114.59 | 110.05 |
| 12 | R1 | 202 | CYC | C2A-C1A-NA | 3.12 | 114.59 | 110.05 |
| 12 | CA | 201 | CYC | C1A-C2A-C3A | -3.12 | 103.33 | 106.78 |
| 12 | IA | 201 | CYC | C1A-C2A-C3A | -3.12 | 103.33 | 106.78 |
| 12 | C9 | 201 | CYC | C1A-C2A-C3A | -3.12 | 103.33 | 106.78 |
| 12 | I9 | 201 | CYC | C1A-C2A-C3A | -3.12 | 103.33 | 106.78 |
| 12 | Z1 | 201 | CYC | C2A-C1A-NA | 3.12 | 114.58 | 110.05 |
| 12 | B8 | 201 | CYC | C2A-C1A-NA | 3.12 | 114.58 | 110.05 |
| 12 | W8 | 202 | CYC | C2A-C1A-NA | 3.12 | 114.58 | 110.05 |
| 12 | S5 | 201 | CYC | CHB-C4A-C3A | 3.12 | 132.91 | 124.90 |
| 12 | E8 | 201 | CYC | CMC-C2C-C1C | -3.12 | 105.69 | 112.40 |
| 12 | Q9 | 201 | CYC | CMC-C2C-C1C | -3.12 | 105.69 | 112.40 |
| 12 | O9 | 201 | CYC | C1A-C2A-C3A | -3.12 | 103.33 | 106.78 |
| 12 | A2 | 201 | CYC | C1A-C2A-C3A | -3.12 | 103.33 | 106.78 |
| 12 | W4 | 202 | CYC | C2A-C1A-NA | 3.12 | 114.58 | 110.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | C7 | 201 | CYC | CHB-C4A-C3A | 3.12 | 132.91 | 124.90 |
| 12 | C2 | 201 | CYC | C1A-C2A-C3A | -3.12 | 103.33 | 106.78 |
| 12 | R3 | 202 | CYC | C2A-C1A-NA | 3.11 | 114.58 | 110.05 |
| 12 | A4 | 201 | CYC | CMC-C2C-C1C | -3.11 | 105.69 | 112.40 |
| 12 | Y5 | 201 | CYC | CHB-C4A-C3A | 3.11 | 132.91 | 124.90 |
| 12 | A5 | 201 | CYC | CHB-C4A-C3A | 3.11 | 132.91 | 124.90 |
| 12 | G5 | 201 | CYC | CHB-C4A-C3A | 3.11 | 132.90 | 124.90 |
| 12 | K2 | 201 | CYC | C1A-C2A-C3A | -3.11 | 103.34 | 106.78 |
| 12 | I6 | 201 | CYC | C1A-C2A-C3A | -3.11 | 103.34 | 106.78 |
| 12 | M7 | 201 | CYC | CHB-C4A-C3A | 3.11 | 132.90 | 124.90 |
| 12 | XA | 202 | CYC | C2A-C1A-NA | 3.11 | 114.57 | 110.05 |
| 12 | I7 | 201 | CYC | CHB-C4A-C3A | 3.11 | 132.90 | 124.90 |
| 12 | A8 | 201 | CYC | CMC-C2C-C1C | -3.11 | 105.70 | 112.40 |
| 12 | K5 | 201 | CYC | CHB-C4A-C3A | 3.11 | 132.89 | 124.90 |
| 12 | K6 | 201 | CYC | C1A-C2A-C3A | -3.11 | 103.34 | 106.78 |
| 12 | I6 | 201 | CYC | CMC-C2C-C1C | -3.11 | 105.70 | 112.40 |
| 12 | F4 | 202 | CYC | C2C-C1C-NC | 3.11 | 110.95 | 108.27 |
| 12 | F8 | 202 | CYC | C2C-C1C-NC | 3.11 | 110.95 | 108.27 |
| 12 | E7 | 201 | CYC | CHB-C4A-C3A | 3.11 | 132.89 | 124.90 |
| 12 | i7 | 201 | CYC | CHB-C4A-C3A | 3.11 | 132.89 | 124.90 |
| 12 | E4 | 201 | CYC | CMC-C2C-C1C | -3.11 | 105.71 | 112.40 |
| 12 | BA | 202 | CYC | C2A-C1A-NA | 3.11 | 114.57 | 110.05 |
| 12 | B9 | 202 | CYC | C2A-C1A-NA | 3.11 | 114.57 | 110.05 |
| 12 | U7 | 201 | CYC | CHB-C4A-C3A | 3.11 | 132.88 | 124.90 |
| 12 | S1 | 201 | CYC | C1A-C2A-C3A | -3.11 | 103.35 | 106.78 |
| 12 | J3 | 201 | CYC | C2A-C1A-NA | 3.10 | 114.56 | 110.05 |
| 12 | H4 | 202 | CYC | C2A-C1A-NA | 3.10 | 114.56 | 110.05 |
| 12 | G3 | 201 | CYC | C1A-C2A-C3A | -3.10 | 103.35 | 106.78 |
| 12 | c7 | 201 | CYC | CHB-C4A-C3A | 3.10 | 132.88 | 124.90 |
| 12 | c5 | 201 | CYC | CHB-C4A-C3A | 3.10 | 132.88 | 124.90 |
| 12 | F4 | 201 | CYC | OC-C1C-C2C | -3.10 | 123.71 | 126.17 |
| 12 | E3 | 201 | CYC | C1A-C2A-C3A | -3.10 | 103.35 | 106.78 |
| 12 | E1 | 201 | CYC | C1A-C2A-C3A | -3.10 | 103.35 | 106.78 |
| 12 | Q7 | 201 | CYC | CHB-C4A-C3A | 3.10 | 132.88 | 124.90 |
| 12 | N4 | 201 | CYC | C1A-C2A-C3A | -3.10 | 103.35 | 106.78 |
| 12 | E3 | 201 | CYC | CMC-C2C-C1C | -3.10 | 105.72 | 112.40 |
| 12 | E1 | 201 | CYC | CMC-C2C-C1C | -3.10 | 105.72 | 112.40 |
| 12 | YA | 201 | CYC | C1A-C2A-C3A | -3.10 | 103.36 | 106.78 |
| 12 | A1 | 201 | CYC | C1A-C2A-C3A | -3.10 | 103.36 | 106.78 |
| 12 | A3 | 201 | CYC | C1A-C2A-C3A | -3.10 | 103.36 | 106.78 |
| 12 | Y9 | 201 | CYC | C1A-C2A-C3A | -3.10 | 103.36 | 106.78 |
| 12 | K4 | 201 | CYC | C1A-C2A-C3A | -3.10 | 103.36 | 106.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | C6 | 201 | CYC | C1A-C2A-C3A | -3.09 | 103.36 | 106.78 |
| 12 | E9 | 201 | CYC | C1A-C2A-C3A | -3.09 | 103.36 | 106.78 |
| 12 | I2 | 201 | CYC | CMC-C2C-C1C | -3.09 | 105.74 | 112.40 |
| 12 | X9 | 202 | CYC | C2A-C1A-NA | 3.09 | 114.55 | 110.05 |
| 12 | J1 | 201 | CYC | C2A-C1A-NA | 3.09 | 114.55 | 110.05 |
| 12 | H9 | 202 | CYC | C2C-C1C-NC | 3.09 | 110.94 | 108.27 |
| 12 | B6 | 201 | CYC | C2A-C1A-NA | 3.09 | 114.54 | 110.05 |
| 12 | A4 | 201 | CYC | C1A-C2A-C3A | -3.09 | 103.36 | 106.78 |
| 12 | A8 | 201 | CYC | C1A-C2A-C3A | -3.09 | 103.36 | 106.78 |
| 12 | K7 | 201 | CYC | CHB-C4A-C3A | 3.09 | 132.84 | 124.90 |
| 12 | L4 | 202 | CYC | C2C-C1C-NC | 3.09 | 110.94 | 108.27 |
| 12 | S3 | 201 | CYC | C1A-C2A-C3A | -3.09 | 103.36 | 106.78 |
| 12 | Q4 | 201 | CYC | C2A-C1A-NA | 3.09 | 114.54 | 110.05 |
| 12 | VA | 201 | CYC | C2C-C1C-NC | 3.09 | 110.93 | 108.27 |
| 12 | V9 | 201 | CYC | C2C-C1C-NC | 3.09 | 110.93 | 108.27 |
| 12 | B2 | 201 | CYC | C2A-C1A-NA | 3.08 | 114.53 | 110.05 |
| 12 | A7 | 201 | CYC | CHB-C4A-C3A | 3.08 | 132.83 | 124.90 |
| 12 | E5 | 201 | CYC | CHB-C4A-C3A | 3.08 | 132.83 | 124.90 |
| 12 | DA | 202 | CYC | C2A-C1A-NA | 3.08 | 114.53 | 110.05 |
| 12 | D9 | 202 | CYC | C2A-C1A-NA | 3.08 | 114.53 | 110.05 |
| 12 | GA | 201 | CYC | C1A-C2A-C3A | -3.08 | 103.37 | 106.78 |
| 12 | G9 | 201 | CYC | C1A-C2A-C3A | -3.08 | 103.37 | 106.78 |
| 12 | U4 | 201 | CYC | C2C-C1C-NC | 3.08 | 110.93 | 108.27 |
| 12 | U8 | 201 | CYC | C2C-C1C-NC | 3.08 | 110.93 | 108.27 |
| 12 | G7 | 201 | CYC | CHB-C4A-C3A | 3.08 | 132.82 | 124.90 |
| 12 | O7 | 201 | CYC | CHB-C4A-C3A | 3.08 | 132.82 | 124.90 |
| 12 | W7 | 201 | CYC | CHB-C4A-C3A | 3.08 | 132.82 | 124.90 |
| 12 | X4 | 201 | CYC | C1A-C2A-C3A | -3.08 | 103.38 | 106.78 |
| 12 | X8 | 201 | CYC | C1A-C2A-C3A | -3.08 | 103.38 | 106.78 |
| 12 | I1 | 201 | CYC | C1A-C2A-C3A | -3.08 | 103.38 | 106.78 |
| 12 | VA | 202 | CYC | C2A-C1A-NA | 3.07 | 114.52 | 110.05 |
| 12 | V9 | 202 | CYC | C2A-C1A-NA | 3.07 | 114.52 | 110.05 |
| 12 | HA | 202 | CYC | C2C-C1C-NC | 3.07 | 110.92 | 108.27 |
| 12 | H2 | 202 | CYC | C2A-C1A-NA | 3.07 | 114.52 | 110.05 |
| 12 | HA | 201 | CYC | C2A-C1A-NA | 3.07 | 114.51 | 110.05 |
| 12 | LA | 202 | CYC | C2C-C1C-NC | 3.07 | 110.92 | 108.27 |
| 12 | L9 | 202 | CYC | C2C-C1C-NC | 3.07 | 110.92 | 108.27 |
| 12 | G6 | 201 | CYC | C1A-C2A-C3A | -3.07 | 103.39 | 106.78 |
| 12 | H2 | 201 | CYC | C2C-C1C-NC | 3.07 | 110.92 | 108.27 |
| 12 | a7 | 201 | CYC | CHB-C4A-C3A | 3.06 | 132.78 | 124.90 |
| 12 | H6 | 202 | CYC | C2A-C1A-NA | 3.06 | 114.50 | 110.05 |
| 12 | L2 | 202 | CYC | C2A-C1A-NA | 3.06 | 114.50 | 110.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | D3 | 201 | CYC | C2A-C1A-NA | 3.06 | 114.50 | 110.05 |
| 12 | D1 | 201 | CYC | C2A-C1A-NA | 3.06 | 114.50 | 110.05 |
| 12 | G2 | 201 | CYC | C1A-C2A-C3A | -3.06 | 103.39 | 106.78 |
| 12 | I2 | 201 | CYC | C1A-C2A-C3A | -3.06 | 103.39 | 106.78 |
| 12 | j5 | 1201 | CYC | C2C-C1C-NC | 3.06 | 110.91 | 108.27 |
| 12 | D4 | 201 | CYC | C2A-C1A-NA | 3.06 | 114.50 | 110.05 |
| 12 | D8 | 201 | CYC | C2A-C1A-NA | 3.06 | 114.50 | 110.05 |
| 12 | L3 | 201 | CYC | C2A-C1A-NA | 3.06 | 114.50 | 110.05 |
| 12 | L1 | 201 | CYC | C2A-C1A-NA | 3.06 | 114.50 | 110.05 |
| 12 | D2 | 202 | CYC | CAC-C3C-C2C | -3.06 | 106.62 | 114.26 |
| 12 | EA | 201 | CYC | CMC-C2C-C1C | -3.06 | 105.81 | 112.40 |
| 12 | E9 | 201 | CYC | CMC-C2C-C1C | -3.06 | 105.81 | 112.40 |
| 12 | N8 | 201 | CYC | C1A-C2A-C3A | -3.06 | 103.40 | 106.78 |
| 12 | Y3 | 201 | CYC | C1A-C2A-C3A | -3.05 | 103.40 | 106.78 |
| 12 | Y1 | 201 | CYC | C1A-C2A-C3A | -3.05 | 103.40 | 106.78 |
| 12 | D6 | 202 | CYC | CAC-C3C-C2C | -3.05 | 106.63 | 114.26 |
| 12 | KA | 201 | CYC | C1A-C2A-C3A | -3.05 | 103.41 | 106.78 |
| 12 | K9 | 201 | CYC | C1A-C2A-C3A | -3.05 | 103.41 | 106.78 |
| 12 | H9 | 201 | CYC | C2A-C1A-NA | 3.05 | 114.48 | 110.05 |
| 12 | g7 | 201 | CYC | CHB-C4A-C3A | 3.05 | 132.74 | 124.90 |
| 12 | RA | 202 | CYC | C2A-C1A-NA | 3.05 | 114.48 | 110.05 |
| 12 | R9 | 202 | CYC | C2A-C1A-NA | 3.05 | 114.48 | 110.05 |
| 12 | H6 | 201 | CYC | C2C-C1C-NC | 3.05 | 110.90 | 108.27 |
| 12 | I3 | 201 | CYC | C1A-C2A-C3A | -3.05 | 103.41 | 106.78 |
| 12 | k5 | 1201 | CYC | C2C-C1C-NC | 3.04 | 110.90 | 108.27 |
| 12 | RA | 202 | CYC | CAC-C3C-C2C | -3.04 | 106.66 | 114.26 |
| 12 | R9 | 202 | CYC | CAC-C3C-C2C | -3.04 | 106.66 | 114.26 |
| 12 | B8 | 202 | CYC | C2C-C1C-NC | 3.04 | 110.89 | 108.27 |
| 12 | D2 | 202 | CYC | C2A-C1A-NA | 3.04 | 114.47 | 110.05 |
| 12 | V3 | 202 | CYC | C2A-C1A-NA | 3.04 | 114.47 | 110.05 |
| 12 | U4 | 202 | CYC | C2A-C1A-NA | 3.04 | 114.47 | 110.05 |
| 12 | V1 | 202 | CYC | C2A-C1A-NA | 3.04 | 114.47 | 110.05 |
| 12 | Q8 | 201 | CYC | CAC-C3C-C2C | -3.04 | 106.67 | 114.26 |
| 12 | BA | 202 | CYC | CAC-C3C-C2C | -3.04 | 106.67 | 114.26 |
| 12 | B9 | 202 | CYC | CAC-C3C-C2C | -3.04 | 106.67 | 114.26 |
| 12 | Q4 | 201 | CYC | CAC-C3C-C2C | -3.04 | 106.67 | 114.26 |
| 12 | EA | 201 | CYC | C1B-C2B-C3B | -3.04 | 104.70 | 107.87 |
| 12 | J6 | 201 | CYC | CAC-C3C-C2C | -3.04 | 106.67 | 114.26 |
| 12 | G4 | 201 | CYC | C1A-C2A-C3A | -3.03 | 103.43 | 106.78 |
| 12 | G8 | 201 | CYC | C1A-C2A-C3A | -3.03 | 103.43 | 106.78 |
| 12 | F2 | 202 | CYC | CAC-C3C-C2C | -3.03 | 106.68 | 114.26 |
| 12 | R4 | 201 | CYC | C1B-C2B-C3B | -3.03 | 104.71 | 107.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | R8 | 201 | CYC | C1B-C2B-C3B | -3.03 | 104.71 | 107.87 |
| 12 | Z3 | 202 | CYC | CAC-C3C-C2C | -3.03 | 106.69 | 114.26 |
| 12 | Z1 | 201 | CYC | CAC-C3C-C2C | -3.03 | 106.69 | 114.26 |
| 12 | J2 | 201 | CYC | CAC-C3C-C2C | -3.03 | 106.69 | 114.26 |
| 12 | Y4 | 201 | CYC | CAC-C3C-C2C | -3.03 | 106.69 | 114.26 |
| 12 | Y8 | 201 | CYC | CAC-C3C-C2C | -3.03 | 106.69 | 114.26 |
| 12 | T3 | 301 | CYC | C2C-C1C-NC | 3.03 | 110.89 | 108.27 |
| 12 | T1 | 301 | CYC | C2C-C1C-NC | 3.03 | 110.89 | 108.27 |
| 12 | H9 | 201 | CYC | CAC-C3C-C2C | -3.03 | 106.69 | 114.26 |
| 12 | D3 | 202 | CYC | C2C-C1C-NC | 3.03 | 110.88 | 108.27 |
| 12 | T4 | 201 | CYC | C1A-C2A-C3A | -3.03 | 103.43 | 106.78 |
| 12 | T8 | 201 | CYC | C1A-C2A-C3A | -3.03 | 103.43 | 106.78 |
| 12 | ZA | 202 | CYC | C2C-C1C-NC | 3.03 | 110.88 | 108.27 |
| 12 | Z9 | 202 | CYC | C2C-C1C-NC | 3.03 | 110.88 | 108.27 |
| 12 | Y4 | 201 | CYC | C2A-C1A-NA | 3.02 | 114.45 | 110.05 |
| 12 | Y8 | 201 | CYC | C2A-C1A-NA | 3.02 | 114.45 | 110.05 |
| 12 | D3 | 201 | CYC | CAC-C3C-C2C | -3.02 | 106.70 | 114.26 |
| 12 | D1 | 201 | CYC | CAC-C3C-C2C | -3.02 | 106.70 | 114.26 |
| 12 | ZA | 201 | CYC | CAC-C3C-C2C | -3.02 | 106.70 | 114.26 |
| 12 | S4 | 201 | CYC | CAC-C3C-C2C | -3.02 | 106.70 | 114.26 |
| 12 | S8 | 201 | CYC | CAC-C3C-C2C | -3.02 | 106.70 | 114.26 |
| 12 | U8 | 202 | CYC | C2A-C1A-NA | 3.02 | 114.45 | 110.05 |
| 12 | P1 | 202 | CYC | CAC-C3C-C2C | -3.02 | 106.71 | 114.26 |
| 12 | ZA | 201 | CYC | C2A-C1A-NA | 3.02 | 114.44 | 110.05 |
| 12 | f7 | 201 | CYC | C2A-C1A-NA | 3.02 | 114.44 | 110.05 |
| 12 | L8 | 201 | CYC | C2A-C1A-NA | 3.02 | 114.44 | 110.05 |
| 12 | Z9 | 201 | CYC | C2A-C1A-NA | 3.02 | 114.44 | 110.05 |
| 12 | F9 | 303 | CYC | CAC-C3C-C2C | -3.02 | 106.71 | 114.26 |
| 12 | F6 | 202 | CYC | CAC-C3C-C2C | -3.02 | 106.71 | 114.26 |
| 12 | H1 | 202 | CYC | C2A-C1A-NA | 3.02 | 114.44 | 110.05 |
| 12 | M8 | 302 | CYC | C2C-C1C-NC | 3.02 | 110.88 | 108.27 |
| 12 | F9 | 302 | CYC | CAC-C3C-C2C | -3.02 | 106.71 | 114.26 |
| 12 | PA | 202 | CYC | CAC-C3C-C2C | -3.02 | 106.71 | 114.26 |
| 12 | P3 | 202 | CYC | CAC-C3C-C2C | -3.02 | 106.71 | 114.26 |
| 12 | W4 | 202 | CYC | CAC-C3C-C2C | -3.02 | 106.71 | 114.26 |
| 12 | W8 | 202 | CYC | CAC-C3C-C2C | -3.02 | 106.71 | 114.26 |
| 12 | P9 | 202 | CYC | CAC-C3C-C2C | -3.02 | 106.71 | 114.26 |
| 12 | JA | 202 | CYC | C2C-C1C-NC | 3.02 | 110.88 | 108.27 |
| 12 | D4 | 202 | CYC | C2C-C1C-NC | 3.02 | 110.88 | 108.27 |
| 12 | D8 | 202 | CYC | C2C-C1C-NC | 3.02 | 110.88 | 108.27 |
| 12 | J9 | 202 | CYC | C2C-C1C-NC | 3.02 | 110.88 | 108.27 |
| 12 | H2 | 202 | CYC | CAC-C3C-C2C | -3.02 | 106.72 | 114.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | R1 | 202 | CYC | CAC-C3C-C2C | -3.02 | 106.72 | 114.26 |
| 12 | L2 | 202 | CYC | CAC-C3C-C2C | -3.02 | 106.72 | 114.26 |
| 12 | R3 | 202 | CYC | CAC-C3C-C2C | -3.02 | 106.72 | 114.26 |
| 12 | M8 | 301 | CYC | C2C-C1C-NC | 3.01 | 110.87 | 108.27 |
| 12 | HA | 201 | CYC | CAC-C3C-C2C | -3.01 | 106.73 | 114.26 |
| 12 | H3 | 201 | CYC | C2A-C1A-NA | 3.01 | 114.43 | 110.05 |
| 12 | P9 | 201 | CYC | C2C-C1C-NC | 3.01 | 110.87 | 108.27 |
| 12 | F4 | 201 | CYC | CAC-C3C-C2C | -3.01 | 106.73 | 114.26 |
| 12 | F8 | 201 | CYC | CAC-C3C-C2C | -3.01 | 106.73 | 114.26 |
| 12 | Z9 | 201 | CYC | CAC-C3C-C2C | -3.01 | 106.73 | 114.26 |
| 12 | PA | 201 | CYC | C2C-C1C-NC | 3.01 | 110.87 | 108.27 |
| 12 | DA | 202 | CYC | CAC-C3C-C2C | -3.01 | 106.73 | 114.26 |
| 12 | D9 | 202 | CYC | CAC-C3C-C2C | -3.01 | 106.73 | 114.26 |
| 12 | VA | 202 | CYC | CAC-C3C-C2C | -3.01 | 106.74 | 114.26 |
| 12 | K3 | 201 | CYC | C1A-C2A-C3A | -3.01 | 103.45 | 106.78 |
| 12 | D4 | 201 | CYC | CAC-C3C-C2C | -3.01 | 106.74 | 114.26 |
| 12 | L6 | 202 | CYC | CAC-C3C-C2C | -3.01 | 106.74 | 114.26 |
| 12 | D8 | 201 | CYC | CAC-C3C-C2C | -3.01 | 106.74 | 114.26 |
| 12 | B2 | 201 | CYC | CAC-C3C-C2C | -3.01 | 106.74 | 114.26 |
| 12 | J4 | 201 | CYC | C2C-C1C-NC | 3.01 | 110.87 | 108.27 |
| 12 | E9 | 201 | CYC | C1B-C2B-C3B | -3.01 | 104.73 | 107.87 |
| 12 | H6 | 202 | CYC | CAC-C3C-C2C | -3.01 | 106.75 | 114.26 |
| 12 | B6 | 201 | CYC | CAC-C3C-C2C | -3.01 | 106.75 | 114.26 |
| 12 | TA | 302 | CYC | CAC-C3C-C2C | -3.01 | 106.75 | 114.26 |
| 12 | T9 | 302 | CYC | CAC-C3C-C2C | -3.01 | 106.75 | 114.26 |
| 12 | V9 | 202 | CYC | CAC-C3C-C2C | -3.01 | 106.75 | 114.26 |
| 12 | V3 | 202 | CYC | CAC-C3C-C2C | -3.00 | 106.75 | 114.26 |
| 12 | V1 | 202 | CYC | CAC-C3C-C2C | -3.00 | 106.75 | 114.26 |
| 12 | H4 | 202 | CYC | CAC-C3C-C2C | -3.00 | 106.75 | 114.26 |
| 12 | H8 | 202 | CYC | CAC-C3C-C2C | -3.00 | 106.75 | 114.26 |
| 12 | k5 | 1202 | CYC | C2A-C1A-NA | 3.00 | 114.42 | 110.05 |
| 12 | L4 | 201 | CYC | CAC-C3C-C2C | -3.00 | 106.77 | 114.26 |
| 12 | L8 | 201 | CYC | CAC-C3C-C2C | -3.00 | 106.77 | 114.26 |
| 12 | L4 | 201 | CYC | C2A-C1A-NA | 3.00 | 114.41 | 110.05 |
| 12 | K1 | 201 | CYC | C1A-C2A-C3A | -3.00 | 103.46 | 106.78 |
| 12 | K2 | 201 | CYC | C1B-C2B-C3B | -3.00 | 104.74 | 107.87 |
| 12 | S4 | 202 | CYC | C2C-C1C-NC | 3.00 | 110.86 | 108.27 |
| 12 | XA | 202 | CYC | CAC-C3C-C2C | -3.00 | 106.77 | 114.26 |
| 12 | X9 | 202 | CYC | CAC-C3C-C2C | -3.00 | 106.77 | 114.26 |
| 12 | JA | 201 | CYC | CAC-C3C-C2C | -3.00 | 106.77 | 114.26 |
| 12 | T3 | 302 | CYC | CAC-C3C-C2C | -2.99 | 106.78 | 114.26 |
| 12 | T1 | 302 | CYC | CAC-C3C-C2C | -2.99 | 106.78 | 114.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | J9 | 201 | CYC | CAC-C3C-C2C | -2.99 | 106.78 | 114.26 |
| 12 | J4 | 202 | CYC | CAC-C3C-C2C | -2.99 | 106.78 | 114.26 |
| 12 | J8 | 202 | CYC | CAC-C3C-C2C | -2.99 | 106.78 | 114.26 |
| 12 | D1 | 202 | CYC | C2C-C1C-NC | 2.99 | 110.85 | 108.27 |
| 12 | J3 | 201 | CYC | CAC-C3C-C2C | -2.99 | 106.79 | 114.26 |
| 12 | J1 | 201 | CYC | CAC-C3C-C2C | -2.99 | 106.79 | 114.26 |
| 12 | D6 | 202 | CYC | C2A-C1A-NA | 2.99 | 114.39 | 110.05 |
| 12 | B1 | 201 | CYC | CAC-C3C-C2C | -2.99 | 106.80 | 114.26 |
| 12 | T5 | 201 | CYC | C2A-C1A-NA | 2.98 | 114.39 | 110.05 |
| 12 | F3 | 202 | CYC | CAC-C3C-C2C | -2.98 | 106.80 | 114.26 |
| 12 | F1 | 202 | CYC | CAC-C3C-C2C | -2.98 | 106.80 | 114.26 |
| 12 | d7 | 201 | CYC | C2A-C1A-NA | 2.98 | 114.39 | 110.05 |
| 12 | B4 | 201 | CYC | CAC-C3C-C2C | -2.98 | 106.81 | 114.26 |
| 12 | B8 | 201 | CYC | CAC-C3C-C2C | -2.98 | 106.81 | 114.26 |
| 12 | O1 | 201 | CYC | C1B-C2B-C3B | -2.98 | 104.76 | 107.87 |
| 12 | O3 | 201 | CYC | C1B-C2B-C3B | -2.98 | 104.76 | 107.87 |
| 12 | G1 | 201 | CYC | C1B-C2B-C3B | -2.98 | 104.76 | 107.87 |
| 12 | B7 | 201 | CYC | C2A-C1A-NA | 2.98 | 114.39 | 110.05 |
| 12 | X3 | 202 | CYC | CAC-C3C-C2C | -2.98 | 106.81 | 114.26 |
| 12 | X1 | 202 | CYC | CAC-C3C-C2C | -2.98 | 106.81 | 114.26 |
| 12 | J8 | 201 | CYC | C2C-C1C-NC | 2.98 | 110.84 | 108.27 |
| 12 | C6 | 201 | CYC | C1B-C2B-C3B | -2.98 | 104.76 | 107.87 |
| 12 | TA | 301 | CYC | C2C-C1C-NC | 2.98 | 110.84 | 108.27 |
| 12 | W4 | 201 | CYC | C2C-C1C-NC | 2.98 | 110.84 | 108.27 |
| 12 | W8 | 201 | CYC | C2C-C1C-NC | 2.98 | 110.84 | 108.27 |
| 12 | T9 | 301 | CYC | C2C-C1C-NC | 2.98 | 110.84 | 108.27 |
| 12 | O4 | 202 | CYC | CAC-C3C-C2C | -2.97 | 106.83 | 114.26 |
| 12 | O8 | 202 | CYC | CAC-C3C-C2C | -2.97 | 106.83 | 114.26 |
| 12 | LA | 201 | CYC | CAC-C3C-C2C | -2.97 | 106.83 | 114.26 |
| 12 | L9 | 201 | CYC | CAC-C3C-C2C | -2.97 | 106.83 | 114.26 |
| 12 | H3 | 201 | CYC | CAC-C3C-C2C | -2.97 | 106.83 | 114.26 |
| 12 | B3 | 201 | CYC | CAC-C3C-C2C | -2.97 | 106.83 | 114.26 |
| 12 | H1 | 202 | CYC | CAC-C3C-C2C | -2.97 | 106.83 | 114.26 |
| 12 | D9 | 201 | CYC | C2C-C1C-NC | 2.97 | 110.84 | 108.27 |
| 12 | L1 | 201 | CYC | CAC-C3C-C2C | -2.97 | 106.83 | 114.26 |
| 12 | E2 | 201 | CYC | C1B-C2B-C3B | -2.97 | 104.77 | 107.87 |
| 12 | C2 | 201 | CYC | C1B-C2B-C3B | -2.97 | 104.77 | 107.87 |
| 12 | H3 | 202 | CYC | C2C-C1C-NC | 2.96 | 110.83 | 108.27 |
| 12 | Y9 | 201 | CYC | C1B-C2B-C3B | -2.96 | 104.78 | 107.87 |
| 12 | P5 | 201 | CYC | C2A-C1A-NA | 2.96 | 114.36 | 110.05 |
| 12 | X7 | 201 | CYC | C2A-C1A-NA | 2.96 | 114.36 | 110.05 |
| 12 | K6 | 201 | CYC | C1B-C2B-C3B | -2.96 | 104.78 | 107.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | A2 | 201 | CYC | C1B-C2B-C3B | -2.96 | 104.78 | 107.87 |
| 12 | L3 | 201 | CYC | CAC-C3C-C2C | -2.96 | 106.86 | 114.26 |
| 12 | B4 | 202 | CYC | C2C-C1C-NC | 2.96 | 110.83 | 108.27 |
| 12 | H7 | 201 | CYC | C2A-C1A-NA | 2.96 | 114.36 | 110.05 |
| 12 | D6 | 201 | CYC | C2C-C1C-NC | 2.96 | 110.82 | 108.27 |
| 12 | G3 | 201 | CYC | C1B-C2B-C3B | -2.96 | 104.78 | 107.87 |
| 12 | M4 | 301 | CYC | C2C-C1C-NC | 2.96 | 110.82 | 108.27 |
| 12 | P8 | 201 | CYC | C1B-C2B-C3B | -2.96 | 104.79 | 107.87 |
| 12 | J4 | 202 | CYC | C1A-C2A-C3A | -2.96 | 103.51 | 106.78 |
| 12 | J8 | 202 | CYC | C1A-C2A-C3A | -2.96 | 103.51 | 106.78 |
| 12 | j5 | 1202 | CYC | C2A-C1A-NA | 2.95 | 114.35 | 110.05 |
| 12 | J6 | 201 | CYC | C1A-C2A-C3A | -2.95 | 103.51 | 106.78 |
| 12 | k5 | 1204 | CYC | C2A-C1A-NA | 2.95 | 114.35 | 110.05 |
| 12 | U4 | 202 | CYC | CAC-C3C-C2C | -2.95 | 106.88 | 114.26 |
| 12 | U8 | 202 | CYC | CAC-C3C-C2C | -2.95 | 106.88 | 114.26 |
| 12 | j7 | 201 | CYC | C2A-C1A-NA | 2.95 | 114.34 | 110.05 |
| 12 | P4 | 201 | CYC | C1B-C2B-C3B | -2.95 | 104.79 | 107.87 |
| 12 | E6 | 201 | CYC | C1B-C2B-C3B | -2.95 | 104.79 | 107.87 |
| 12 | CA | 201 | CYC | C1B-C2B-C3B | -2.95 | 104.79 | 107.87 |
| 12 | C9 | 201 | CYC | C1B-C2B-C3B | -2.95 | 104.79 | 107.87 |
| 12 | F2 | 202 | CYC | OC-C1C-C2C | -2.95 | 123.83 | 126.17 |
| 12 | F5 | 201 | CYC | C2A-C1A-NA | 2.95 | 114.34 | 110.05 |
| 12 | Q1 | 201 | CYC | C1B-C2B-C3B | -2.95 | 104.80 | 107.87 |
| 12 | Q3 | 201 | CYC | C1B-C2B-C3B | -2.95 | 104.80 | 107.87 |
| 12 | K3 | 201 | CYC | C1B-C2B-C3B | -2.95 | 104.80 | 107.87 |
| 12 | K1 | 201 | CYC | C1B-C2B-C3B | -2.95 | 104.80 | 107.87 |
| 12 | GA | 201 | CYC | C1B-C2B-C3B | -2.95 | 104.80 | 107.87 |
| 12 | S1 | 201 | CYC | C1B-C2B-C3B | -2.95 | 104.80 | 107.87 |
| 12 | S3 | 201 | CYC | C1B-C2B-C3B | -2.95 | 104.80 | 107.87 |
| 12 | G9 | 201 | CYC | C1B-C2B-C3B | -2.95 | 104.80 | 107.87 |
| 12 | L3 | 202 | CYC | C2C-C1C-NC | 2.95 | 110.81 | 108.27 |
| 12 | aA | 902 | CYC | C2C-C1C-NC | 2.95 | 110.81 | 108.27 |
| 12 | N5 | 201 | CYC | C2A-C1A-NA | 2.94 | 114.33 | 110.05 |
| 12 | A6 | 201 | CYC | C1B-C2B-C3B | -2.94 | 104.80 | 107.87 |
| 12 | F3 | 201 | CYC | C2C-C1C-NC | 2.94 | 110.81 | 108.27 |
| 12 | F1 | 201 | CYC | C2C-C1C-NC | 2.94 | 110.81 | 108.27 |
| 12 | R5 | 201 | CYC | C2A-C1A-NA | 2.94 | 114.33 | 110.05 |
| 12 | B3 | 202 | CYC | C2C-C1C-NC | 2.94 | 110.81 | 108.27 |
| 12 | B1 | 202 | CYC | C2C-C1C-NC | 2.94 | 110.81 | 108.27 |
| 12 | A1 | 201 | CYC | C1B-C2B-C3B | -2.94 | 104.80 | 107.87 |
| 12 | A3 | 201 | CYC | C1B-C2B-C3B | -2.94 | 104.80 | 107.87 |
| 12 | N4 | 201 | CYC | C1B-C2B-C3B | -2.94 | 104.80 | 107.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | N8 | 201 | CYC | C1B-C2B-C3B | -2.94 | 104.80 | 107.87 |
| 12 | L5 | 201 | CYC | C2A-C1A-NA | 2.94 | 114.32 | 110.05 |
| 12 | j5 | 1201 | CYC | OC-C1C-C2C | -2.94 | 123.84 | 126.17 |
| 12 | YA | 201 | CYC | C1B-C2B-C3B | -2.94 | 104.81 | 107.87 |
| 12 | J6 | 202 | CYC | C2C-C1C-NC | 2.93 | 110.80 | 108.27 |
| 12 | b7 | 201 | CYC | C2A-C1A-NA | 2.93 | 114.32 | 110.05 |
| 12 | X5 | 201 | CYC | C2A-C1A-NA | 2.93 | 114.32 | 110.05 |
| 12 | b5 | 201 | CYC | C2A-C1A-NA | 2.93 | 114.31 | 110.05 |
| 12 | R7 | 201 | CYC | C2A-C1A-NA | 2.93 | 114.31 | 110.05 |
| 12 | DA | 201 | CYC | C2C-C1C-NC | 2.93 | 110.80 | 108.27 |
| 12 | A | 201 | CYC | C2A-C1A-NA | 2.93 | 114.31 | 110.05 |
| 12 | J2 | 201 | CYC | C1A-C2A-C3A | -2.93 | 103.54 | 106.78 |
| 12 | D2 | 201 | CYC | C2C-C1C-NC | 2.93 | 110.80 | 108.27 |
| 12 | H8 | 202 | CYC | C1A-C2A-C3A | -2.93 | 103.54 | 106.78 |
| 12 | F7 | 201 | CYC | C2A-C1A-NA | 2.93 | 114.31 | 110.05 |
| 12 | G4 | 201 | CYC | C1B-C2B-C3B | -2.93 | 104.82 | 107.87 |
| 12 | G8 | 201 | CYC | C1B-C2B-C3B | -2.93 | 104.82 | 107.87 |
| 12 | X4 | 201 | CYC | C1B-C2B-C3B | -2.92 | 104.82 | 107.87 |
| 12 | X8 | 201 | CYC | C1B-C2B-C3B | -2.92 | 104.82 | 107.87 |
| 12 | K8 | 201 | CYC | C1B-C2B-C3B | -2.92 | 104.82 | 107.87 |
| 12 | T9 | 302 | CYC | C1A-C2A-C3A | -2.92 | 103.55 | 106.78 |
| 12 | Z3 | 201 | CYC | C2C-C1C-NC | 2.92 | 110.79 | 108.27 |
| 12 | Z1 | 202 | CYC | C2C-C1C-NC | 2.92 | 110.79 | 108.27 |
| 12 | j5 | 1201 | CYC | C4A-C3A-C2A | -2.92 | 103.16 | 106.51 |
| 12 | Y3 | 201 | CYC | C1B-C2B-C3B | -2.92 | 104.83 | 107.87 |
| 12 | Y1 | 201 | CYC | C1B-C2B-C3B | -2.92 | 104.83 | 107.87 |
| 12 | L7 | 201 | CYC | C2A-C1A-NA | 2.92 | 114.29 | 110.05 |
| 12 | F6 | 201 | CYC | C2C-C1C-NC | 2.91 | 110.78 | 108.27 |
| 12 | H1 | 201 | CYC | C2C-C1C-NC | 2.91 | 110.78 | 108.27 |
| 12 | p7 | 201 | CYC | C2A-C1A-NA | 2.91 | 114.28 | 110.05 |
| 12 | V7 | 201 | CYC | C2A-C1A-NA | 2.91 | 114.28 | 110.05 |
| 12 | H4 | 202 | CYC | C1A-C2A-C3A | -2.91 | 103.56 | 106.78 |
| 12 | J2 | 202 | CYC | C2C-C1C-NC | 2.91 | 110.78 | 108.27 |
| 12 | V5 | 201 | CYC | C2A-C1A-NA | 2.91 | 114.28 | 110.05 |
| 12 | h7 | 201 | CYC | C2A-C1A-NA | 2.91 | 114.28 | 110.05 |
| 12 | Z | 201 | CYC | C2A-C1A-NA | 2.91 | 114.28 | 110.05 |
| 12 | JA | 201 | CYC | C1A-C2A-C3A | -2.90 | 103.57 | 106.78 |
| 12 | J9 | 201 | CYC | C1A-C2A-C3A | -2.90 | 103.57 | 106.78 |
| 12 | KA | 201 | CYC | C1B-C2B-C3B | -2.90 | 104.84 | 107.87 |
| 12 | K9 | 201 | CYC | C1B-C2B-C3B | -2.90 | 104.84 | 107.87 |
| 12 | v7 | 201 | CYC | C2A-C1A-NA | 2.90 | 114.27 | 110.05 |
| 12 | W8 | 202 | CYC | C1A-C2A-C3A | -2.90 | 103.57 | 106.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | Z8 | 301 | CYC | C2C-C1C-NC | 2.90 | 110.77 | 108.27 |
| 12 | J5 | 201 | CYC | C2A-C1A-NA | 2.90 | 114.27 | 110.05 |
| 12 | W4 | 202 | CYC | C1A-C2A-C3A | -2.90 | 103.57 | 106.78 |
| 12 | I4 | 201 | CYC | C1B-C2B-C3B | -2.90 | 104.84 | 107.87 |
| 12 | I8 | 201 | CYC | C1B-C2B-C3B | -2.90 | 104.84 | 107.87 |
| 12 | T4 | 201 | CYC | C1B-C2B-C3B | -2.90 | 104.85 | 107.87 |
| 12 | T8 | 201 | CYC | C1B-C2B-C3B | -2.90 | 104.85 | 107.87 |
| 12 | X1 | 202 | CYC | C1A-C2A-C3A | -2.90 | 103.58 | 106.78 |
| 12 | r7 | 201 | CYC | C2A-C1A-NA | 2.90 | 114.27 | 110.05 |
| 12 | E3 | 201 | CYC | C1B-C2B-C3B | -2.90 | 104.85 | 107.87 |
| 12 | K4 | 201 | CYC | C1B-C2B-C3B | -2.90 | 104.85 | 107.87 |
| 12 | E1 | 201 | CYC | C1B-C2B-C3B | -2.90 | 104.85 | 107.87 |
| 12 | J3 | 202 | CYC | C2C-C1C-NC | 2.90 | 110.77 | 108.27 |
| 12 | aA | 901 | CYC | C2C-C1C-NC | 2.90 | 110.77 | 108.27 |
| 12 | X3 | 202 | CYC | C1A-C2A-C3A | -2.90 | 103.58 | 106.78 |
| 12 | F6 | 202 | CYC | OC-C1C-C2C | -2.90 | 123.87 | 126.17 |
| 12 | QA | 201 | CYC | C1B-C2B-C3B | -2.90 | 104.85 | 107.87 |
| 12 | G9 | 201 | CYC | CBC-CAC-C3C | -2.90 | 107.02 | 113.47 |
| 12 | Q9 | 201 | CYC | C1B-C2B-C3B | -2.89 | 104.85 | 107.87 |
| 12 | N7 | 201 | CYC | C2A-C1A-NA | 2.89 | 114.26 | 110.05 |
| 12 | GA | 201 | CYC | CBC-CAC-C3C | -2.89 | 107.02 | 113.47 |
| 12 | X9 | 201 | CYC | C2C-C1C-NC | 2.89 | 110.77 | 108.27 |
| 12 | P1 | 202 | CYC | C1A-C2A-C3A | -2.89 | 103.58 | 106.78 |
| 12 | P3 | 202 | CYC | C1A-C2A-C3A | -2.89 | 103.58 | 106.78 |
| 12 | Q8 | 201 | CYC | C1A-C2A-C3A | -2.89 | 103.58 | 106.78 |
| 12 | D7 | 201 | CYC | C2A-C1A-NA | 2.89 | 114.25 | 110.05 |
| 12 | TA | 302 | CYC | C1A-C2A-C3A | -2.89 | 103.58 | 106.78 |
| 12 | k5 | 1201 | CYC | OC-C1C-C2C | -2.89 | 123.88 | 126.17 |
| 12 | E6 | 201 | CYC | CBC-CAC-C3C | -2.89 | 107.03 | 113.47 |
| 12 | E2 | 201 | CYC | CBC-CAC-C3C | -2.89 | 107.03 | 113.47 |
| 12 | UA | 201 | CYC | C1B-C2B-C3B | -2.89 | 104.86 | 107.87 |
| 12 | U9 | 201 | CYC | C1B-C2B-C3B | -2.89 | 104.86 | 107.87 |
| 12 | O4 | 201 | CYC | C2C-C1C-NC | 2.88 | 110.76 | 108.27 |
| 12 | O8 | 201 | CYC | C2C-C1C-NC | 2.88 | 110.76 | 108.27 |
| 12 | A9 | 201 | CYC | CBC-CAC-C3C | -2.88 | 107.05 | 113.47 |
| 12 | XA | 201 | CYC | C2C-C1C-NC | 2.88 | 110.76 | 108.27 |
| 12 | Z4 | 301 | CYC | C2C-C1C-NC | 2.88 | 110.76 | 108.27 |
| 12 | F2 | 201 | CYC | C2C-C1C-NC | 2.88 | 110.76 | 108.27 |
| 12 | E4 | 201 | CYC | C1B-C2B-C3B | -2.88 | 104.86 | 107.87 |
| 12 | D5 | 201 | CYC | C2A-C1A-NA | 2.88 | 114.24 | 110.05 |
| 12 | f5 | 201 | CYC | C2A-C1A-NA | 2.88 | 114.24 | 110.05 |
| 12 | A2 | 201 | CYC | CHD-C4C-NC | 2.88 | 128.63 | 125.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | AA | 201 | CYC | CBC-CAC-C3C | -2.88 | 107.06 | 113.47 |
| 12 | BA | 201 | CYC | C2C-C1C-NC | 2.88 | 110.75 | 108.27 |
| 12 | B9 | 201 | CYC | C2C-C1C-NC | 2.88 | 110.75 | 108.27 |
| 12 | J7 | 201 | CYC | C2A-C1A-NA | 2.88 | 114.24 | 110.05 |
| 12 | I4 | 201 | CYC | CBC-CAC-C3C | -2.88 | 107.06 | 113.47 |
| 12 | I8 | 201 | CYC | CBC-CAC-C3C | -2.88 | 107.06 | 113.47 |
| 12 | k5 | 1203 | CYC | C2A-C1A-NA | 2.87 | 114.23 | 110.05 |
| 12 | O9 | 201 | CYC | C1B-C2B-C3B | -2.87 | 104.87 | 107.87 |
| 12 | L6 | 202 | CYC | C1A-C2A-C3A | -2.87 | 103.60 | 106.78 |
| 12 | d5 | 201 | CYC | C2A-C1A-NA | 2.87 | 114.23 | 110.05 |
| 12 | L2 | 202 | CYC | C1A-C2A-C3A | -2.87 | 103.61 | 106.78 |
| 12 | P1 | 201 | CYC | C2C-C1C-NC | 2.87 | 110.75 | 108.27 |
| 12 | P3 | 201 | CYC | C2C-C1C-NC | 2.87 | 110.75 | 108.27 |
| 12 | U3 | 201 | CYC | C1B-C2B-C3B | -2.87 | 104.88 | 107.87 |
| 12 | U1 | 201 | CYC | C1B-C2B-C3B | -2.87 | 104.88 | 107.87 |
| 12 | V3 | 201 | CYC | CHD-C4C-NC | 2.87 | 128.61 | 125.20 |
| 12 | V1 | 201 | CYC | CHD-C4C-NC | 2.87 | 128.61 | 125.20 |
| 12 | B6 | 201 | CYC | C1A-C2A-C3A | -2.87 | 103.61 | 106.78 |
| 12 | A4 | 201 | CYC | C1B-C2B-C3B | -2.86 | 104.88 | 107.87 |
| 12 | A8 | 201 | CYC | C1B-C2B-C3B | -2.86 | 104.88 | 107.87 |
| 12 | k5 | 1201 | CYC | C4A-C3A-C2A | -2.86 | 103.22 | 106.51 |
| 12 | B3 | 201 | CYC | C1A-C2A-C3A | -2.86 | 103.62 | 106.78 |
| 12 | B1 | 201 | CYC | C1A-C2A-C3A | -2.86 | 103.62 | 106.78 |
| 12 | P7 | 201 | CYC | C2A-C1A-NA | 2.86 | 114.21 | 110.05 |
| 12 | T7 | 201 | CYC | C2A-C1A-NA | 2.86 | 114.20 | 110.05 |
| 12 | S8 | 201 | CYC | C1A-C2A-C3A | -2.86 | 103.62 | 106.78 |
| 12 | E8 | 201 | CYC | C1B-C2B-C3B | -2.86 | 104.89 | 107.87 |
| 12 | OA | 201 | CYC | C1B-C2B-C3B | -2.86 | 104.89 | 107.87 |
| 12 | N2 | 101 | CYC | C2C-C1C-NC | 2.85 | 110.73 | 108.27 |
| 12 | T3 | 302 | CYC | C1A-C2A-C3A | -2.85 | 103.62 | 106.78 |
| 12 | T1 | 302 | CYC | C1A-C2A-C3A | -2.85 | 103.62 | 106.78 |
| 12 | F2 | 202 | CYC | C1A-C2A-C3A | -2.85 | 103.62 | 106.78 |
| 12 | C1 | 201 | CYC | C1B-C2B-C3B | -2.85 | 104.89 | 107.87 |
| 12 | F4 | 201 | CYC | C1A-C2A-C3A | -2.85 | 103.63 | 106.78 |
| 12 | F8 | 201 | CYC | C1A-C2A-C3A | -2.85 | 103.63 | 106.78 |
| 12 | L6 | 201 | CYC | C2C-C1C-NC | 2.85 | 110.73 | 108.27 |
| 12 | B2 | 201 | CYC | C1A-C2A-C3A | -2.85 | 103.63 | 106.78 |
| 12 | RA | 201 | CYC | C2C-C1C-NC | 2.85 | 110.73 | 108.27 |
| 12 | R9 | 201 | CYC | C2C-C1C-NC | 2.85 | 110.73 | 108.27 |
| 12 | R3 | 201 | CYC | C2C-C1C-NC | 2.85 | 110.73 | 108.27 |
| 12 | Q4 | 201 | CYC | C1A-C2A-C3A | -2.84 | 103.64 | 106.78 |
| 12 | A6 | 201 | CYC | CHD-C4C-NC | 2.84 | 128.59 | 125.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | R1 | 202 | CYC | C1A-C2A-C3A | -2.84 | 103.64 | 106.78 |
| 12 | J2 | 202 | CYC | CHD-C4C-NC | 2.84 | 128.59 | 125.20 |
| 12 | B5 | 201 | CYC | C2A-C1A-NA | 2.84 | 114.18 | 110.05 |
| 12 | L2 | 201 | CYC | C2C-C1C-NC | 2.84 | 110.72 | 108.27 |
| 12 | C4 | 201 | CYC | C1B-C2B-C3B | -2.84 | 104.91 | 107.87 |
| 12 | C8 | 201 | CYC | C1B-C2B-C3B | -2.84 | 104.91 | 107.87 |
| 12 | IA | 201 | CYC | C1B-C2B-C3B | -2.84 | 104.91 | 107.87 |
| 12 | I9 | 201 | CYC | C1B-C2B-C3B | -2.84 | 104.91 | 107.87 |
| 12 | N6 | 101 | CYC | C2C-C1C-NC | 2.84 | 110.72 | 108.27 |
| 12 | KA | 201 | CYC | CBC-CAC-C3C | -2.84 | 107.15 | 113.47 |
| 12 | K9 | 201 | CYC | CBC-CAC-C3C | -2.84 | 107.15 | 113.47 |
| 12 | LA | 201 | CYC | C1A-C2A-C3A | -2.84 | 103.64 | 106.78 |
| 12 | L9 | 201 | CYC | C1A-C2A-C3A | -2.84 | 103.64 | 106.78 |
| 12 | H5 | 201 | CYC | C2A-C1A-NA | 2.84 | 114.18 | 110.05 |
| 12 | PA | 202 | CYC | C1A-C2A-C3A | -2.84 | 103.64 | 106.78 |
| 12 | P9 | 202 | CYC | C1A-C2A-C3A | -2.84 | 103.64 | 106.78 |
| 12 | H1 | 201 | CYC | CHD-C4C-NC | 2.84 | 128.58 | 125.20 |
| 12 | Y3 | 201 | CYC | CBC-CAC-C3C | -2.84 | 107.15 | 113.47 |
| 12 | Y1 | 201 | CYC | CBC-CAC-C3C | -2.84 | 107.15 | 113.47 |
| 12 | X9 | 202 | CYC | C1A-C2A-C3A | -2.84 | 103.64 | 106.78 |
| 12 | C3 | 201 | CYC | C1B-C2B-C3B | -2.83 | 104.91 | 107.87 |
| 12 | V4 | 201 | CYC | C1B-C2B-C3B | -2.83 | 104.91 | 107.87 |
| 12 | D4 | 201 | CYC | C1A-C2A-C3A | -2.83 | 103.65 | 106.78 |
| 12 | D8 | 201 | CYC | C1A-C2A-C3A | -2.83 | 103.65 | 106.78 |
| 12 | S4 | 201 | CYC | C1A-C2A-C3A | -2.83 | 103.65 | 106.78 |
| 12 | XA | 202 | CYC | C1A-C2A-C3A | -2.83 | 103.65 | 106.78 |
| 12 | N7 | 201 | CYC | CMB-C2B-C1B | 2.83 | 127.70 | 124.17 |
| 12 | C9 | 201 | CYC | CBC-CAC-C3C | -2.83 | 107.17 | 113.47 |
| 12 | R3 | 202 | CYC | C1A-C2A-C3A | -2.83 | 103.66 | 106.78 |
| 12 | J6 | 202 | CYC | CHD-C4C-NC | 2.83 | 128.56 | 125.20 |
| 12 | F9 | 302 | CYC | C1A-C2A-C3A | -2.83 | 103.66 | 106.78 |
| 12 | P8 | 201 | CYC | CBC-CAC-C3C | -2.83 | 107.18 | 113.47 |
| 12 | G3 | 201 | CYC | CHD-C4C-NC | 2.83 | 128.56 | 125.20 |
| 12 | G1 | 201 | CYC | CHD-C4C-NC | 2.83 | 128.56 | 125.20 |
| 12 | SA | 201 | CYC | C1B-C2B-C3B | -2.82 | 104.92 | 107.87 |
| 12 | WA | 201 | CYC | C1B-C2B-C3B | -2.82 | 104.92 | 107.87 |
| 12 | S9 | 201 | CYC | C1B-C2B-C3B | -2.82 | 104.92 | 107.87 |
| 12 | W9 | 201 | CYC | C1B-C2B-C3B | -2.82 | 104.92 | 107.87 |
| 12 | IA | 201 | CYC | CBC-CAC-C3C | -2.82 | 107.18 | 113.47 |
| 12 | I9 | 201 | CYC | CBC-CAC-C3C | -2.82 | 107.18 | 113.47 |
| 12 | O4 | 202 | CYC | C1A-C2A-C3A | -2.82 | 103.66 | 106.78 |
| 12 | O8 | 202 | CYC | C1A-C2A-C3A | -2.82 | 103.66 | 106.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | V3 | 201 | CYC | C2C-C1C-NC | 2.82 | 110.71 | 108.27 |
| 12 | V1 | 201 | CYC | C2C-C1C-NC | 2.82 | 110.71 | 108.27 |
| 12 | E4 | 201 | CYC | CBC-CAC-C3C | -2.82 | 107.19 | 113.47 |
| 12 | E8 | 201 | CYC | CBC-CAC-C3C | -2.82 | 107.19 | 113.47 |
| 12 | BA | 201 | CYC | CHD-C4C-NC | 2.82 | 128.56 | 125.20 |
| 12 | B9 | 201 | CYC | CHD-C4C-NC | 2.82 | 128.56 | 125.20 |
| 12 | B4 | 201 | CYC | C1A-C2A-C3A | -2.82 | 103.66 | 106.78 |
| 12 | Y4 | 201 | CYC | C1A-C2A-C3A | -2.82 | 103.66 | 106.78 |
| 12 | Y8 | 201 | CYC | C1A-C2A-C3A | -2.82 | 103.66 | 106.78 |
| 12 | I3 | 201 | CYC | C1B-C2B-C3B | -2.82 | 104.93 | 107.87 |
| 12 | I1 | 201 | CYC | C1B-C2B-C3B | -2.82 | 104.93 | 107.87 |
| 12 | I3 | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.20 | 113.47 |
| 12 | T8 | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.20 | 113.47 |
| 12 | I1 | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.20 | 113.47 |
| 12 | Z5 | 201 | CYC | C2A-C1A-NA | 2.81 | 114.14 | 110.05 |
| 12 | CA | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.20 | 113.47 |
| 12 | OA | 201 | CYC | CHD-C4C-NC | 2.81 | 128.55 | 125.20 |
| 12 | P4 | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.21 | 113.47 |
| 12 | H3 | 202 | CYC | CHD-C4C-NC | 2.81 | 128.54 | 125.20 |
| 12 | D5 | 201 | CYC | CMB-C2B-C1B | 2.81 | 127.67 | 124.17 |
| 12 | K3 | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.22 | 113.47 |
| 12 | I6 | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.22 | 113.47 |
| 12 | K1 | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.22 | 113.47 |
| 12 | V8 | 201 | CYC | C1B-C2B-C3B | -2.81 | 104.94 | 107.87 |
| 12 | I2 | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.22 | 113.47 |
| 12 | T4 | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.22 | 113.47 |
| 12 | N4 | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.22 | 113.47 |
| 12 | R1 | 201 | CYC | C2C-C1C-NC | 2.81 | 110.69 | 108.27 |
| 12 | WA | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.22 | 113.47 |
| 12 | W9 | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.22 | 113.47 |
| 12 | K4 | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.22 | 113.47 |
| 12 | K8 | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.22 | 113.47 |
| 12 | SA | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.22 | 113.47 |
| 12 | S9 | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.22 | 113.47 |
| 12 | F9 | 303 | CYC | C1A-C2A-C3A | -2.81 | 103.68 | 106.78 |
| 12 | O9 | 201 | CYC | CHD-C4C-NC | 2.81 | 128.54 | 125.20 |
| 12 | R8 | 201 | CYC | CBC-CAC-C3C | -2.81 | 107.22 | 113.47 |
| 12 | F6 | 202 | CYC | C1A-C2A-C3A | -2.81 | 103.68 | 106.78 |
| 12 | p7 | 201 | CYC | CMB-C2B-C1B | 2.81 | 127.67 | 124.17 |
| 12 | UA | 201 | CYC | CHD-C4C-NC | 2.80 | 128.54 | 125.20 |
| 12 | U9 | 201 | CYC | CHD-C4C-NC | 2.80 | 128.54 | 125.20 |
| 12 | G3 | 201 | CYC | CBC-CAC-C3C | -2.80 | 107.22 | 113.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | G1 | 201 | CYC | CBC-CAC-C3C | -2.80 | 107.22 | 113.47 |
| 12 | W3 | 201 | CYC | C1B-C2B-C3B | -2.80 | 104.95 | 107.87 |
| 12 | W1 | 201 | CYC | C1B-C2B-C3B | -2.80 | 104.95 | 107.87 |
| 12 | h7 | 201 | CYC | CMB-C2B-C1B | 2.80 | 127.67 | 124.17 |
| 12 | J3 | 201 | CYC | C1A-C2A-C3A | -2.80 | 103.68 | 106.78 |
| 12 | K6 | 201 | CYC | CBC-CAC-C3C | -2.80 | 107.23 | 113.47 |
| 12 | b7 | 201 | CYC | CMB-C2B-C1B | 2.80 | 127.66 | 124.17 |
| 12 | C4 | 201 | CYC | CBC-CAC-C3C | -2.80 | 107.23 | 113.47 |
| 12 | C8 | 201 | CYC | CBC-CAC-C3C | -2.80 | 107.23 | 113.47 |
| 12 | B8 | 201 | CYC | C1A-C2A-C3A | -2.80 | 103.68 | 106.78 |
| 12 | F2 | 201 | CYC | CHD-C4C-NC | 2.80 | 128.53 | 125.20 |
| 12 | B7 | 201 | CYC | CMB-C2B-C1B | 2.80 | 127.66 | 124.17 |
| 12 | Q1 | 201 | CYC | CBC-CAC-C3C | -2.80 | 107.23 | 113.47 |
| 12 | Q3 | 201 | CYC | CBC-CAC-C3C | -2.80 | 107.23 | 113.47 |
| 12 | I6 | 201 | CYC | C1B-C2B-C3B | -2.80 | 104.95 | 107.87 |
| 12 | X3 | 201 | CYC | CHD-C4C-NC | 2.80 | 128.53 | 125.20 |
| 12 | X1 | 201 | CYC | CHD-C4C-NC | 2.80 | 128.53 | 125.20 |
| 12 | YA | 201 | CYC | CBC-CAC-C3C | -2.80 | 107.24 | 113.47 |
| 12 | Y9 | 201 | CYC | CBC-CAC-C3C | -2.80 | 107.24 | 113.47 |
| 12 | HA | 201 | CYC | C1A-C2A-C3A | -2.80 | 103.69 | 106.78 |
| 12 | H9 | 201 | CYC | C1A-C2A-C3A | -2.80 | 103.69 | 106.78 |
| 12 | J5 | 201 | CYC | CMB-C2B-C1B | 2.80 | 127.66 | 124.17 |
| 12 | Z3 | 202 | CYC | C1A-C2A-C3A | -2.80 | 103.69 | 106.78 |
| 12 | Z1 | 201 | CYC | C1A-C2A-C3A | -2.80 | 103.69 | 106.78 |
| 12 | S1 | 201 | CYC | CBC-CAC-C3C | -2.80 | 107.24 | 113.47 |
| 12 | S3 | 201 | CYC | CBC-CAC-C3C | -2.80 | 107.24 | 113.47 |
| 12 | UA | 201 | CYC | CBC-CAC-C3C | -2.80 | 107.24 | 113.47 |
| 12 | U9 | 201 | CYC | CBC-CAC-C3C | -2.80 | 107.24 | 113.47 |
| 12 | C6 | 201 | CYC | CBC-CAC-C3C | -2.79 | 107.25 | 113.47 |
| 12 | R4 | 201 | CYC | CBC-CAC-C3C | -2.79 | 107.25 | 113.47 |
| 12 | A6 | 201 | CYC | CBC-CAC-C3C | -2.79 | 107.25 | 113.47 |
| 12 | V4 | 201 | CYC | CBC-CAC-C3C | -2.79 | 107.25 | 113.47 |
| 12 | V8 | 201 | CYC | CBC-CAC-C3C | -2.79 | 107.25 | 113.47 |
| 12 | ZA | 202 | CYC | CHD-C4C-NC | 2.79 | 128.53 | 125.20 |
| 12 | Z9 | 202 | CYC | CHD-C4C-NC | 2.79 | 128.53 | 125.20 |
| 12 | N8 | 201 | CYC | CBC-CAC-C3C | -2.79 | 107.25 | 113.47 |
| 12 | X8 | 201 | CYC | CBC-CAC-C3C | -2.79 | 107.26 | 113.47 |
| 12 | H7 | 201 | CYC | CMB-C2B-C1B | 2.79 | 127.65 | 124.17 |
| 12 | j5 | 1202 | CYC | CHD-C4C-NC | 2.79 | 128.52 | 125.20 |
| 12 | F3 | 202 | CYC | C1A-C2A-C3A | -2.79 | 103.70 | 106.78 |
| 12 | F1 | 202 | CYC | C1A-C2A-C3A | -2.79 | 103.70 | 106.78 |
| 12 | f5 | 201 | CYC | CMB-C2B-C1B | 2.79 | 127.64 | 124.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | QA | 201 | CYC | CBC-CAC-C3C | -2.79 | 107.27 | 113.47 |
| 12 | U3 | 201 | CYC | CBC-CAC-C3C | -2.78 | 107.27 | 113.47 |
| 12 | U1 | 201 | CYC | CBC-CAC-C3C | -2.78 | 107.27 | 113.47 |
| 12 | J1 | 201 | CYC | C1A-C2A-C3A | -2.78 | 103.70 | 106.78 |
| 12 | C2 | 201 | CYC | CBC-CAC-C3C | -2.78 | 107.27 | 113.47 |
| 12 | v7 | 201 | CYC | CMB-C2B-C1B | 2.78 | 127.64 | 124.17 |
| 12 | X3 | 201 | CYC | C2C-C1C-NC | 2.78 | 110.67 | 108.27 |
| 12 | X1 | 201 | CYC | C2C-C1C-NC | 2.78 | 110.67 | 108.27 |
| 12 | EA | 201 | CYC | CBC-CAC-C3C | -2.78 | 107.28 | 113.47 |
| 12 | E9 | 201 | CYC | CBC-CAC-C3C | -2.78 | 107.28 | 113.47 |
| 12 | M4 | 301 | CYC | CHD-C4C-NC | 2.78 | 128.51 | 125.20 |
| 12 | V7 | 201 | CYC | CMB-C2B-C1B | 2.78 | 127.64 | 124.17 |
| 12 | J5 | 201 | CYC | CHD-C4C-NC | 2.78 | 128.51 | 125.20 |
| 12 | VA | 202 | CYC | C1A-C2A-C3A | -2.78 | 103.71 | 106.78 |
| 12 | V9 | 202 | CYC | C1A-C2A-C3A | -2.78 | 103.71 | 106.78 |
| 12 | I2 | 201 | CYC | C1B-C2B-C3B | -2.78 | 104.97 | 107.87 |
| 12 | W3 | 201 | CYC | CBC-CAC-C3C | -2.78 | 107.28 | 113.47 |
| 12 | W1 | 201 | CYC | CBC-CAC-C3C | -2.78 | 107.28 | 113.47 |
| 12 | G6 | 201 | CYC | CBC-CAC-C3C | -2.78 | 107.28 | 113.47 |
| 12 | D7 | 201 | CYC | CHD-C4C-NC | 2.78 | 128.51 | 125.20 |
| 12 | Q9 | 201 | CYC | CBC-CAC-C3C | -2.78 | 107.28 | 113.47 |
| 12 | A2 | 201 | CYC | CBC-CAC-C3C | -2.78 | 107.28 | 113.47 |
| 12 | k5 | 1202 | CYC | CMB-C2B-C1B | 2.78 | 127.63 | 124.17 |
| 12 | K2 | 201 | CYC | CBC-CAC-C3C | -2.78 | 107.29 | 113.47 |
| 12 | E3 | 201 | CYC | CHD-C4C-NC | 2.77 | 128.50 | 125.20 |
| 12 | Z4 | 301 | CYC | CHD-C4C-NC | 2.77 | 128.50 | 125.20 |
| 12 | X4 | 201 | CYC | CBC-CAC-C3C | -2.77 | 107.29 | 113.47 |
| 12 | VA | 201 | CYC | CHD-C4C-NC | 2.77 | 128.50 | 125.20 |
| 12 | V9 | 201 | CYC | CHD-C4C-NC | 2.77 | 128.50 | 125.20 |
| 12 | DA | 201 | CYC | CHD-C4C-NC | 2.77 | 128.50 | 125.20 |
| 12 | R4 | 201 | CYC | CHD-C4C-NC | 2.77 | 128.50 | 125.20 |
| 12 | R8 | 201 | CYC | CHD-C4C-NC | 2.77 | 128.50 | 125.20 |
| 12 | D9 | 201 | CYC | CHD-C4C-NC | 2.77 | 128.50 | 125.20 |
| 12 | R5 | 201 | CYC | CMB-C2B-C1B | 2.77 | 127.63 | 124.17 |
| 12 | G2 | 201 | CYC | CBC-CAC-C3C | -2.77 | 107.30 | 113.47 |
| 12 | D3 | 201 | CYC | C1A-C2A-C3A | -2.77 | 103.72 | 106.78 |
| 12 | D1 | 201 | CYC | C1A-C2A-C3A | -2.77 | 103.72 | 106.78 |
| 12 | D9 | 202 | CYC | C1A-C2A-C3A | -2.77 | 103.72 | 106.78 |
| 12 | L7 | 201 | CYC | CMB-C2B-C1B | 2.77 | 127.62 | 124.17 |
| 12 | f7 | 201 | CYC | CMB-C2B-C1B | 2.77 | 127.62 | 124.17 |
| 12 | J7 | 201 | CYC | CHD-C4C-NC | 2.77 | 128.50 | 125.20 |
| 12 | C3 | 201 | CYC | CBC-CAC-C3C | -2.77 | 107.31 | 113.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | C1 | 201 | CYC | CBC-CAC-C3C | -2.77 | 107.31 | 113.47 |
| 12 | G2 | 201 | CYC | C1B-C2B-C3B | -2.77 | 104.98 | 107.87 |
| 12 | D5 | 201 | CYC | CHD-C4C-NC | 2.77 | 128.50 | 125.20 |
| 12 | AA | 201 | CYC | C1B-C2B-C3B | -2.77 | 104.98 | 107.87 |
| 12 | A9 | 201 | CYC | C1B-C2B-C3B | -2.77 | 104.98 | 107.87 |
| 12 | FA | 301 | CYC | C2C-C1C-NC | 2.77 | 110.66 | 108.27 |
| 12 | F9 | 301 | CYC | C2C-C1C-NC | 2.77 | 110.66 | 108.27 |
| 12 | O1 | 201 | CYC | CBC-CAC-C3C | -2.76 | 107.31 | 113.47 |
| 12 | O3 | 201 | CYC | CBC-CAC-C3C | -2.76 | 107.31 | 113.47 |
| 12 | E3 | 201 | CYC | CBC-CAC-C3C | -2.76 | 107.31 | 113.47 |
| 12 | E1 | 201 | CYC | CBC-CAC-C3C | -2.76 | 107.31 | 113.47 |
| 12 | F7 | 201 | CYC | CMB-C2B-C1B | 2.76 | 127.62 | 124.17 |
| 12 | Z | 201 | CYC | CHD-C4C-NC | 2.76 | 128.49 | 125.20 |
| 12 | H2 | 202 | CYC | C1A-C2A-C3A | -2.76 | 103.72 | 106.78 |
| 12 | H6 | 202 | CYC | C1A-C2A-C3A | -2.76 | 103.72 | 106.78 |
| 12 | RA | 202 | CYC | C1A-C2A-C3A | -2.76 | 103.73 | 106.78 |
| 12 | R9 | 202 | CYC | C1A-C2A-C3A | -2.76 | 103.73 | 106.78 |
| 12 | T7 | 201 | CYC | CMB-C2B-C1B | 2.76 | 127.61 | 124.17 |
| 12 | Z3 | 201 | CYC | CHD-C4C-NC | 2.76 | 128.49 | 125.20 |
| 12 | M8 | 301 | CYC | CHD-C4C-NC | 2.76 | 128.49 | 125.20 |
| 12 | Z1 | 202 | CYC | CHD-C4C-NC | 2.76 | 128.49 | 125.20 |
| 12 | I3 | 201 | CYC | CHD-C4C-NC | 2.76 | 128.49 | 125.20 |
| 12 | Z8 | 301 | CYC | CHD-C4C-NC | 2.76 | 128.49 | 125.20 |
| 12 | I1 | 201 | CYC | CHD-C4C-NC | 2.76 | 128.49 | 125.20 |
| 12 | R7 | 201 | CYC | CMB-C2B-C1B | 2.76 | 127.61 | 124.17 |
| 12 | J4 | 201 | CYC | CHD-C4C-NC | 2.76 | 128.49 | 125.20 |
| 12 | H3 | 201 | CYC | C1A-C2A-C3A | -2.76 | 103.73 | 106.78 |
| 12 | G2 | 201 | CYC | CHD-C4C-NC | 2.76 | 128.49 | 125.20 |
| 12 | S4 | 202 | CYC | CHD-C4C-NC | 2.76 | 128.48 | 125.20 |
| 12 | G4 | 201 | CYC | CBC-CAC-C3C | -2.76 | 107.33 | 113.47 |
| 12 | G8 | 201 | CYC | CBC-CAC-C3C | -2.76 | 107.33 | 113.47 |
| 12 | X5 | 201 | CYC | CMB-C2B-C1B | 2.76 | 127.61 | 124.17 |
| 12 | K4 | 201 | CYC | CHD-C4C-NC | 2.76 | 128.48 | 125.20 |
| 12 | K8 | 201 | CYC | CHD-C4C-NC | 2.76 | 128.48 | 125.20 |
| 12 | h7 | 201 | CYC | CHD-C4C-NC | 2.76 | 128.48 | 125.20 |
| 12 | k5 | 1203 | CYC | C2C-C1C-NC | 2.75 | 110.65 | 108.27 |
| 12 | D2 | 202 | CYC | C1A-C2A-C3A | -2.75 | 103.73 | 106.78 |
| 12 | A4 | 201 | CYC | CHD-C4C-NC | 2.75 | 128.48 | 125.20 |
| 12 | k5 | 1204 | CYC | CHD-C4C-NC | 2.75 | 128.48 | 125.20 |
| 12 | J8 | 201 | CYC | CHD-C4C-NC | 2.75 | 128.48 | 125.20 |
| 12 | A1 | 201 | CYC | CHD-C4C-NC | 2.75 | 128.48 | 125.20 |
| 12 | A3 | 201 | CYC | CHD-C4C-NC | 2.75 | 128.48 | 125.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | Z | 201 | CYC | CMB-C2B-C1B | 2.75 | 127.60 | 124.17 |
| 12 | H9 | 202 | CYC | CHD-C4C-NC | 2.75 | 128.47 | 125.20 |
| 12 | A1 | 201 | CYC | CBC-CAC-C3C | -2.75 | 107.35 | 113.47 |
| 12 | A3 | 201 | CYC | CBC-CAC-C3C | -2.75 | 107.35 | 113.47 |
| 12 | A4 | 201 | CYC | CBC-CAC-C3C | -2.75 | 107.35 | 113.47 |
| 12 | D7 | 201 | CYC | CMB-C2B-C1B | 2.75 | 127.60 | 124.17 |
| 12 | H1 | 202 | CYC | C1A-C2A-C3A | -2.75 | 103.74 | 106.78 |
| 12 | D6 | 201 | CYC | CHD-C4C-NC | 2.75 | 128.47 | 125.20 |
| 12 | G6 | 201 | CYC | CHD-C4C-NC | 2.75 | 128.47 | 125.20 |
| 12 | D2 | 201 | CYC | CHD-C4C-NC | 2.75 | 128.47 | 125.20 |
| 12 | E1 | 201 | CYC | CHD-C4C-NC | 2.75 | 128.47 | 125.20 |
| 12 | J6 | 202 | CYC | CBB-CAB-C3B | -2.74 | 104.86 | 112.43 |
| 12 | U8 | 202 | CYC | C1A-C2A-C3A | -2.74 | 103.75 | 106.78 |
| 12 | A8 | 201 | CYC | CBC-CAC-C3C | -2.74 | 107.36 | 113.47 |
| 12 | L3 | 201 | CYC | C1A-C2A-C3A | -2.74 | 103.75 | 106.78 |
| 12 | U4 | 202 | CYC | C1A-C2A-C3A | -2.74 | 103.75 | 106.78 |
| 12 | L1 | 201 | CYC | C1A-C2A-C3A | -2.74 | 103.75 | 106.78 |
| 12 | F6 | 201 | CYC | CHD-C4C-NC | 2.74 | 128.47 | 125.20 |
| 12 | f7 | 201 | CYC | CAA-C2A-C1A | 2.74 | 129.86 | 125.01 |
| 12 | A | 201 | CYC | CHD-C4C-NC | 2.74 | 128.47 | 125.20 |
| 12 | XA | 201 | CYC | CBB-CAB-C3B | -2.74 | 104.88 | 112.43 |
| 12 | X9 | 201 | CYC | CBB-CAB-C3B | -2.74 | 104.88 | 112.43 |
| 12 | M8 | 302 | CYC | CHD-C4C-NC | 2.74 | 128.46 | 125.20 |
| 12 | OA | 201 | CYC | CBC-CAC-C3C | -2.74 | 107.37 | 113.47 |
| 12 | O9 | 201 | CYC | CBC-CAC-C3C | -2.74 | 107.37 | 113.47 |
| 12 | k5 | 1201 | CYC | C1B-C2B-C3B | -2.74 | 105.01 | 107.87 |
| 12 | GA | 201 | CYC | CHD-C4C-NC | 2.74 | 128.46 | 125.20 |
| 12 | G9 | 201 | CYC | CHD-C4C-NC | 2.74 | 128.46 | 125.20 |
| 12 | U1 | 201 | CYC | CHD-C4C-NC | 2.74 | 128.46 | 125.20 |
| 12 | DA | 202 | CYC | C1A-C2A-C3A | -2.74 | 103.75 | 106.78 |
| 12 | I5 | 201 | CYC | CMB-C2B-C1B | 2.74 | 127.58 | 124.17 |
| 12 | W4 | 201 | CYC | CHD-C4C-NC | 2.74 | 128.46 | 125.20 |
| 12 | W8 | 201 | CYC | CHD-C4C-NC | 2.74 | 128.46 | 125.20 |
| 12 | U3 | 201 | CYC | CHD-C4C-NC | 2.74 | 128.46 | 125.20 |
| 12 | RA | 201 | CYC | CHD-C4C-NC | 2.74 | 128.46 | 125.20 |
| 12 | R9 | 201 | CYC | CHD-C4C-NC | 2.74 | 128.46 | 125.20 |
| 12 | J2 | 202 | CYC | CBB-CAB-C3B | -2.73 | 104.89 | 112.43 |
| 12 | W3 | 201 | CYC | CHD-C4C-NC | 2.73 | 128.46 | 125.20 |
| 12 | W1 | 201 | CYC | CHD-C4C-NC | 2.73 | 128.46 | 125.20 |
| 12 | F3 | 201 | CYC | CHD-C4C-NC | 2.73 | 128.45 | 125.20 |
| 12 | A8 | 201 | CYC | CHD-C4C-NC | 2.73 | 128.45 | 125.20 |
| 12 | F1 | 201 | CYC | CHD-C4C-NC | 2.73 | 128.45 | 125.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | b5 | 201 | CYC | CMB-C2B-C1B | 2.73 | 127.58 | 124.17 |
| 12 | G6 | 201 | CYC | C1B-C2B-C3B | -2.73 | 105.02 | 107.87 |
| 12 | O3 | 201 | CYC | C4A-C3A-C2A | -2.73 | 103.37 | 106.51 |
| 12 | k5 | 1202 | CYC | CAA-C2A-C1A | 2.73 | 129.84 | 125.01 |
| 12 | BA | 202 | CYC | C1A-C2A-C3A | -2.73 | 103.76 | 106.78 |
| 12 | B9 | 202 | CYC | C1A-C2A-C3A | -2.73 | 103.76 | 106.78 |
| 12 | R5 | 201 | CYC | CAA-C2A-C1A | 2.73 | 129.84 | 125.01 |
| 12 | WA | 201 | CYC | CHD-C4C-NC | 2.73 | 128.45 | 125.20 |
| 12 | W9 | 201 | CYC | CHD-C4C-NC | 2.73 | 128.45 | 125.20 |
| 12 | S1 | 201 | CYC | CHD-C4C-NC | 2.73 | 128.45 | 125.20 |
| 12 | S3 | 201 | CYC | CHD-C4C-NC | 2.73 | 128.45 | 125.20 |
| 12 | D6 | 202 | CYC | C1A-C2A-C3A | -2.73 | 103.77 | 106.78 |
| 12 | A | 201 | CYC | CMB-C2B-C1B | 2.72 | 127.57 | 124.17 |
| 12 | X5 | 201 | CYC | CAA-C2A-C1A | 2.72 | 129.83 | 125.01 |
| 12 | HA | 202 | CYC | CHD-C4C-NC | 2.72 | 128.44 | 125.20 |
| 12 | T3 | 301 | CYC | CBB-CAB-C3B | -2.72 | 104.93 | 112.43 |
| 12 | D2 | 201 | CYC | CBB-CAB-C3B | -2.72 | 104.93 | 112.43 |
| 12 | f7 | 201 | CYC | CHD-C4C-NC | 2.72 | 128.44 | 125.20 |
| 12 | N6 | 101 | CYC | CHD-C4C-NC | 2.72 | 128.44 | 125.20 |
| 12 | r7 | 201 | CYC | C2C-C1C-NC | 2.72 | 110.62 | 108.27 |
| 12 | L3 | 202 | CYC | CHD-C4C-NC | 2.72 | 128.44 | 125.20 |
| 12 | aA | 902 | CYC | CHD-C4C-NC | 2.72 | 128.44 | 125.20 |
| 12 | O1 | 201 | CYC | C4A-C3A-C2A | -2.72 | 103.39 | 106.51 |
| 12 | FA | 301 | CYC | CHD-C4C-NC | 2.72 | 128.44 | 125.20 |
| 12 | T7 | 201 | CYC | CHD-C4C-NC | 2.72 | 128.44 | 125.20 |
| 12 | F9 | 301 | CYC | CHD-C4C-NC | 2.72 | 128.44 | 125.20 |
| 12 | B3 | 202 | CYC | CBB-CAB-C3B | -2.72 | 104.94 | 112.43 |
| 12 | N2 | 101 | CYC | CHD-C4C-NC | 2.72 | 128.44 | 125.20 |
| 12 | a9 | 901 | CYC | CHD-C4C-NC | 2.72 | 128.44 | 125.20 |
| 12 | HA | 202 | CYC | CBB-CAB-C3B | -2.72 | 104.94 | 112.43 |
| 12 | N6 | 101 | CYC | CBB-CAB-C3B | -2.72 | 104.94 | 112.43 |
| 12 | H4 | 201 | CYC | CBB-CAB-C3B | -2.72 | 104.94 | 112.43 |
| 12 | H8 | 201 | CYC | CBB-CAB-C3B | -2.72 | 104.94 | 112.43 |
| 12 | KA | 201 | CYC | CHD-C4C-NC | 2.71 | 128.43 | 125.20 |
| 12 | K9 | 201 | CYC | CHD-C4C-NC | 2.71 | 128.43 | 125.20 |
| 12 | T1 | 301 | CYC | CBB-CAB-C3B | -2.71 | 104.95 | 112.43 |
| 12 | T4 | 201 | CYC | C4A-C3A-C2A | -2.71 | 103.39 | 106.51 |
| 12 | T8 | 201 | CYC | C4A-C3A-C2A | -2.71 | 103.39 | 106.51 |
| 12 | L4 | 202 | CYC | CHD-C4C-NC | 2.71 | 128.43 | 125.20 |
| 12 | T5 | 201 | CYC | CHD-C4C-NC | 2.71 | 128.43 | 125.20 |
| 12 | k5 | 1203 | CYC | CMB-C2B-C1B | 2.71 | 127.55 | 124.17 |
| 12 | VA | 201 | CYC | CBB-CAB-C3B | -2.71 | 104.95 | 112.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | K4 | 201 | CYC | C4A-C3A-C2A | -2.71 | 103.39 | 106.51 |
| 12 | J3 | 202 | CYC | CHD-C4C-NC | 2.71 | 128.43 | 125.20 |
| 12 | aA | 901 | CYC | CHD-C4C-NC | 2.71 | 128.43 | 125.20 |
| 12 | F5 | 201 | CYC | CMB-C2B-C1B | 2.71 | 127.55 | 124.17 |
| 12 | K8 | 201 | CYC | C4A-C3A-C2A | -2.71 | 103.40 | 106.51 |
| 12 | G4 | 201 | CYC | CHD-C4C-NC | 2.71 | 128.43 | 125.20 |
| 12 | G8 | 201 | CYC | CHD-C4C-NC | 2.71 | 128.43 | 125.20 |
| 12 | k5 | 1204 | CYC | CMB-C2B-C1B | 2.71 | 127.55 | 124.17 |
| 12 | d5 | 201 | CYC | C2C-C1C-NC | 2.71 | 110.61 | 108.27 |
| 12 | N8 | 201 | CYC | C4A-C3A-C2A | -2.71 | 103.40 | 106.51 |
| 12 | g7 | 201 | CYC | CMB-C2B-C1B | 2.71 | 127.55 | 124.17 |
| 12 | J4 | 201 | CYC | CBB-CAB-C3B | -2.71 | 104.96 | 112.43 |
| 12 | J8 | 201 | CYC | CBB-CAB-C3B | -2.71 | 104.96 | 112.43 |
| 12 | D4 | 202 | CYC | CHD-C4C-NC | 2.71 | 128.43 | 125.20 |
| 12 | H5 | 201 | CYC | C2C-C1C-NC | 2.71 | 110.61 | 108.27 |
| 12 | V3 | 202 | CYC | C1A-C2A-C3A | -2.71 | 103.79 | 106.78 |
| 12 | V1 | 202 | CYC | C1A-C2A-C3A | -2.71 | 103.79 | 106.78 |
| 12 | TA | 301 | CYC | CBB-CAB-C3B | -2.71 | 104.97 | 112.43 |
| 12 | N2 | 101 | CYC | CBB-CAB-C3B | -2.71 | 104.97 | 112.43 |
| 12 | D6 | 201 | CYC | CBB-CAB-C3B | -2.71 | 104.97 | 112.43 |
| 12 | T9 | 301 | CYC | CBB-CAB-C3B | -2.71 | 104.97 | 112.43 |
| 12 | B1 | 202 | CYC | CBB-CAB-C3B | -2.71 | 104.97 | 112.43 |
| 12 | X7 | 201 | CYC | CMB-C2B-C1B | 2.71 | 127.55 | 124.17 |
| 12 | F6 | 201 | CYC | CBB-CAB-C3B | -2.71 | 104.97 | 112.43 |
| 12 | N4 | 201 | CYC | CHD-C4C-NC | 2.70 | 128.42 | 125.20 |
| 12 | N8 | 201 | CYC | CHD-C4C-NC | 2.70 | 128.42 | 125.20 |
| 12 | H9 | 202 | CYC | CBB-CAB-C3B | -2.70 | 104.97 | 112.43 |
| 12 | a7 | 201 | CYC | CMB-C2B-C1B | 2.70 | 127.54 | 124.17 |
| 12 | C5 | 201 | CYC | CMB-C2B-C1B | 2.70 | 127.54 | 124.17 |
| 12 | R1 | 201 | CYC | CHD-C4C-NC | 2.70 | 128.42 | 125.20 |
| 12 | R3 | 201 | CYC | CHD-C4C-NC | 2.70 | 128.42 | 125.20 |
| 12 | P7 | 201 | CYC | CMB-C2B-C1B | 2.70 | 127.54 | 124.17 |
| 12 | Z8 | 301 | CYC | CBB-CAB-C3B | -2.70 | 104.98 | 112.43 |
| 12 | Q1 | 201 | CYC | CHD-C4C-NC | 2.70 | 128.42 | 125.20 |
| 12 | Q3 | 201 | CYC | CHD-C4C-NC | 2.70 | 128.42 | 125.20 |
| 12 | b7 | 201 | CYC | CHD-C4C-NC | 2.70 | 128.42 | 125.20 |
| 12 | L8 | 201 | CYC | C1A-C2A-C3A | -2.70 | 103.79 | 106.78 |
| 12 | P3 | 201 | CYC | CHD-C4C-NC | 2.70 | 128.41 | 125.20 |
| 12 | I4 | 201 | CYC | CHD-C4C-NC | 2.70 | 128.41 | 125.20 |
| 12 | F3 | 201 | CYC | CBB-CAB-C3B | -2.70 | 104.99 | 112.43 |
| 12 | R9 | 201 | CYC | CBB-CAB-C3B | -2.70 | 104.99 | 112.43 |
| 12 | O4 | 201 | CYC | CHD-C4C-NC | 2.70 | 128.41 | 125.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | X7 | 201 | CYC | CAA-C2A-C1A | 2.70 | 129.78 | 125.01 |
| 12 | r7 | 201 | CYC | CMB-C2B-C1B | 2.70 | 127.54 | 124.17 |
| 12 | b7 | 201 | CYC | C2C-C1C-NC | 2.70 | 110.60 | 108.27 |
| 12 | PA | 201 | CYC | CHD-C4C-NC | 2.70 | 128.41 | 125.20 |
| 12 | P9 | 201 | CYC | CHD-C4C-NC | 2.70 | 128.41 | 125.20 |
| 12 | V9 | 201 | CYC | CBB-CAB-C3B | -2.70 | 104.99 | 112.43 |
| 12 | DA | 201 | CYC | CBB-CAB-C3B | -2.70 | 105.00 | 112.43 |
| 12 | D9 | 201 | CYC | CBB-CAB-C3B | -2.70 | 105.00 | 112.43 |
| 12 | B5 | 201 | CYC | CMB-C2B-C1B | 2.70 | 127.53 | 124.17 |
| 12 | V5 | 201 | CYC | CMB-C2B-C1B | 2.70 | 127.53 | 124.17 |
| 12 | F1 | 201 | CYC | CBB-CAB-C3B | -2.70 | 105.00 | 112.43 |
| 12 | U4 | 201 | CYC | CBB-CAB-C3B | -2.70 | 105.00 | 112.43 |
| 12 | O4 | 201 | CYC | CBB-CAB-C3B | -2.70 | 105.00 | 112.43 |
| 12 | U8 | 201 | CYC | CBB-CAB-C3B | -2.70 | 105.00 | 112.43 |
| 12 | O8 | 201 | CYC | CBB-CAB-C3B | -2.70 | 105.00 | 112.43 |
| 12 | N4 | 201 | CYC | C4A-C3A-C2A | -2.69 | 103.41 | 106.51 |
| 12 | IA | 201 | CYC | CHD-C4C-NC | 2.69 | 128.41 | 125.20 |
| 12 | PA | 201 | CYC | CBB-CAB-C3B | -2.69 | 105.01 | 112.43 |
| 12 | RA | 201 | CYC | CBB-CAB-C3B | -2.69 | 105.01 | 112.43 |
| 12 | P9 | 201 | CYC | CBB-CAB-C3B | -2.69 | 105.01 | 112.43 |
| 12 | h7 | 201 | CYC | C2C-C1C-NC | 2.69 | 110.59 | 108.27 |
| 12 | F5 | 201 | CYC | CHD-C4C-NC | 2.69 | 128.41 | 125.20 |
| 12 | Z4 | 301 | CYC | CBB-CAB-C3B | -2.69 | 105.01 | 112.43 |
| 12 | p7 | 201 | CYC | CAA-C2A-C1A | 2.69 | 129.77 | 125.01 |
| 12 | D3 | 202 | CYC | CBB-CAB-C3B | -2.69 | 105.01 | 112.43 |
| 12 | j5 | 1201 | CYC | C1B-C2B-C3B | -2.69 | 105.06 | 107.87 |
| 12 | K1 | 201 | CYC | C4A-C3A-C2A | -2.69 | 103.42 | 106.51 |
| 12 | R1 | 201 | CYC | CBB-CAB-C3B | -2.69 | 105.02 | 112.43 |
| 12 | R3 | 201 | CYC | CBB-CAB-C3B | -2.69 | 105.02 | 112.43 |
| 12 | D8 | 202 | CYC | CHD-C4C-NC | 2.69 | 128.40 | 125.20 |
| 12 | FA | 301 | CYC | CBB-CAB-C3B | -2.69 | 105.02 | 112.43 |
| 12 | F9 | 301 | CYC | CBB-CAB-C3B | -2.69 | 105.02 | 112.43 |
| 12 | U4 | 201 | CYC | CHD-C4C-NC | 2.69 | 128.40 | 125.20 |
| 12 | U8 | 201 | CYC | CHD-C4C-NC | 2.69 | 128.40 | 125.20 |
| 12 | A1 | 201 | CYC | C4A-C3A-C2A | -2.69 | 103.42 | 106.51 |
| 12 | A3 | 201 | CYC | C4A-C3A-C2A | -2.69 | 103.42 | 106.51 |
| 12 | P5 | 201 | CYC | CMB-C2B-C1B | 2.69 | 127.52 | 124.17 |
| 12 | SA | 201 | CYC | CHD-C4C-NC | 2.69 | 128.40 | 125.20 |
| 12 | S9 | 201 | CYC | CHD-C4C-NC | 2.69 | 128.40 | 125.20 |
| 12 | F4 | 202 | CYC | CBB-CAB-C3B | -2.69 | 105.03 | 112.43 |
| 12 | F2 | 201 | CYC | CBB-CAB-C3B | -2.69 | 105.03 | 112.43 |
| 12 | G2 | 201 | CYC | C4A-C3A-C2A | -2.69 | 103.42 | 106.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | C3 | 201 | CYC | CHD-C4C-NC | 2.69 | 128.40 | 125.20 |
| 12 | C1 | 201 | CYC | CHD-C4C-NC | 2.69 | 128.40 | 125.20 |
| 12 | I9 | 201 | CYC | CHD-C4C-NC | 2.69 | 128.40 | 125.20 |
| 12 | J5 | 201 | CYC | CAA-C2A-C1A | 2.69 | 129.76 | 125.01 |
| 12 | j5 | 1202 | CYC | CMB-C2B-C1B | 2.68 | 127.52 | 124.17 |
| 12 | J7 | 201 | CYC | CMB-C2B-C1B | 2.68 | 127.52 | 124.17 |
| 12 | ZA | 201 | CYC | C1A-C2A-C3A | -2.68 | 103.81 | 106.78 |
| 12 | Z9 | 201 | CYC | C1A-C2A-C3A | -2.68 | 103.81 | 106.78 |
| 12 | I3 | 201 | CYC | C4A-C3A-C2A | -2.68 | 103.43 | 106.51 |
| 12 | XA | 201 | CYC | CHD-C4C-NC | 2.68 | 128.39 | 125.20 |
| 12 | K2 | 201 | CYC | CHD-C4C-NC | 2.68 | 128.39 | 125.20 |
| 12 | E6 | 201 | CYC | CHD-C4C-NC | 2.68 | 128.39 | 125.20 |
| 12 | X9 | 201 | CYC | CHD-C4C-NC | 2.68 | 128.39 | 125.20 |
| 12 | k5 | 1202 | CYC | CHD-C4C-NC | 2.68 | 128.39 | 125.20 |
| 12 | d7 | 201 | CYC | CHD-C4C-NC | 2.68 | 128.39 | 125.20 |
| 12 | O8 | 201 | CYC | CHD-C4C-NC | 2.68 | 128.39 | 125.20 |
| 12 | ZA | 202 | CYC | CBB-CAB-C3B | -2.68 | 105.04 | 112.43 |
| 12 | Z9 | 202 | CYC | CBB-CAB-C3B | -2.68 | 105.04 | 112.43 |
| 12 | V4 | 201 | CYC | CHD-C4C-NC | 2.68 | 128.39 | 125.20 |
| 12 | V8 | 201 | CYC | CHD-C4C-NC | 2.68 | 128.39 | 125.20 |
| 12 | CA | 201 | CYC | C4A-C3A-C2A | -2.68 | 103.43 | 106.51 |
| 12 | C9 | 201 | CYC | C4A-C3A-C2A | -2.68 | 103.43 | 106.51 |
| 12 | N7 | 201 | CYC | CHD-C4C-NC | 2.68 | 128.39 | 125.20 |
| 12 | S4 | 202 | CYC | CBB-CAB-C3B | -2.68 | 105.04 | 112.43 |
| 12 | D4 | 202 | CYC | CBB-CAB-C3B | -2.68 | 105.05 | 112.43 |
| 12 | D8 | 202 | CYC | CBB-CAB-C3B | -2.68 | 105.05 | 112.43 |
| 12 | W8 | 201 | CYC | CBB-CAB-C3B | -2.68 | 105.05 | 112.43 |
| 12 | K3 | 201 | CYC | C4A-C3A-C2A | -2.68 | 103.43 | 106.51 |
| 12 | BA | 201 | CYC | CBB-CAB-C3B | -2.68 | 105.05 | 112.43 |
| 12 | B9 | 201 | CYC | CBB-CAB-C3B | -2.68 | 105.05 | 112.43 |
| 12 | T4 | 201 | CYC | CHD-C4C-NC | 2.68 | 128.39 | 125.20 |
| 12 | T8 | 201 | CYC | CHD-C4C-NC | 2.68 | 128.39 | 125.20 |
| 12 | I8 | 201 | CYC | CHD-C4C-NC | 2.68 | 128.39 | 125.20 |
| 12 | X1 | 201 | CYC | CBB-CAB-C3B | -2.67 | 105.06 | 112.43 |
| 12 | F8 | 202 | CYC | CBB-CAB-C3B | -2.67 | 105.06 | 112.43 |
| 12 | d7 | 201 | CYC | CAA-C2A-C1A | 2.67 | 129.74 | 125.01 |
| 12 | D1 | 202 | CYC | CBB-CAB-C3B | -2.67 | 105.06 | 112.43 |
| 12 | D7 | 201 | CYC | C2C-C1C-NC | 2.67 | 110.58 | 108.27 |
| 12 | aA | 901 | CYC | CBB-CAB-C3B | -2.67 | 105.06 | 112.43 |
| 12 | W4 | 201 | CYC | CBB-CAB-C3B | -2.67 | 105.06 | 112.43 |
| 12 | X3 | 201 | CYC | CBB-CAB-C3B | -2.67 | 105.07 | 112.43 |
| 12 | L5 | 201 | CYC | CMB-C2B-C1B | 2.67 | 127.50 | 124.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | M8 | 302 | CYC | CBB-CAB-C3B | -2.67 | 105.07 | 112.43 |
| 12 | J7 | 201 | CYC | C2C-C1C-NC | 2.67 | 110.58 | 108.27 |
| 12 | T7 | 201 | CYC | C2C-C1C-NC | 2.67 | 110.58 | 108.27 |
| 12 | JA | 202 | CYC | CBB-CAB-C3B | -2.67 | 105.07 | 112.43 |
| 12 | J3 | 202 | CYC | CBB-CAB-C3B | -2.67 | 105.07 | 112.43 |
| 12 | J9 | 202 | CYC | CBB-CAB-C3B | -2.67 | 105.07 | 112.43 |
| 12 | L4 | 201 | CYC | C1A-C2A-C3A | -2.67 | 103.83 | 106.78 |
| 12 | L7 | 201 | CYC | CAA-C2A-C1A | 2.67 | 129.73 | 125.01 |
| 12 | L5 | 201 | CYC | C2C-C1C-NC | 2.67 | 110.57 | 108.27 |
| 12 | T5 | 201 | CYC | C2C-C1C-NC | 2.67 | 110.57 | 108.27 |
| 12 | h7 | 201 | CYC | CAA-C2A-C1A | 2.67 | 129.73 | 125.01 |
| 12 | D3 | 202 | CYC | CHD-C4C-NC | 2.67 | 128.38 | 125.20 |
| 12 | L5 | 201 | CYC | CHD-C4C-NC | 2.67 | 128.38 | 125.20 |
| 12 | D1 | 202 | CYC | CHD-C4C-NC | 2.67 | 128.38 | 125.20 |
| 12 | P7 | 201 | CYC | CHD-C4C-NC | 2.67 | 128.38 | 125.20 |
| 12 | G6 | 201 | CYC | C4A-C3A-C2A | -2.67 | 103.44 | 106.51 |
| 12 | F7 | 201 | CYC | CAA-C2A-C1A | 2.67 | 129.73 | 125.01 |
| 12 | b7 | 201 | CYC | CAA-C2A-C1A | 2.67 | 129.73 | 125.01 |
| 12 | P1 | 201 | CYC | CHD-C4C-NC | 2.67 | 128.38 | 125.20 |
| 12 | E4 | 201 | CYC | CHD-C4C-NC | 2.67 | 128.38 | 125.20 |
| 12 | E8 | 201 | CYC | CHD-C4C-NC | 2.67 | 128.38 | 125.20 |
| 12 | R7 | 201 | CYC | CAA-C2A-C1A | 2.67 | 129.72 | 125.01 |
| 12 | H5 | 201 | CYC | CMB-C2B-C1B | 2.66 | 127.49 | 124.17 |
| 12 | O1 | 201 | CYC | CHD-C4C-NC | 2.66 | 128.37 | 125.20 |
| 12 | O3 | 201 | CYC | CHD-C4C-NC | 2.66 | 128.37 | 125.20 |
| 12 | P5 | 201 | CYC | CHD-C4C-NC | 2.66 | 128.37 | 125.20 |
| 12 | B8 | 202 | CYC | CBB-CAB-C3B | -2.66 | 105.09 | 112.43 |
| 12 | H6 | 201 | CYC | CBB-CAB-C3B | -2.66 | 105.09 | 112.43 |
| 12 | I1 | 201 | CYC | C4A-C3A-C2A | -2.66 | 103.45 | 106.51 |
| 12 | B7 | 201 | CYC | CAA-C2A-C1A | 2.66 | 129.72 | 125.01 |
| 12 | L2 | 201 | CYC | CHD-C4C-NC | 2.66 | 128.37 | 125.20 |
| 12 | B8 | 202 | CYC | CHD-C4C-NC | 2.66 | 128.37 | 125.20 |
| 12 | j7 | 201 | CYC | CMB-C2B-C1B | 2.66 | 127.49 | 124.17 |
| 12 | F4 | 202 | CYC | CHD-C4C-NC | 2.66 | 128.37 | 125.20 |
| 12 | F8 | 202 | CYC | CHD-C4C-NC | 2.66 | 128.37 | 125.20 |
| 12 | F5 | 201 | CYC | CAA-C2A-C1A | 2.66 | 129.71 | 125.01 |
| 12 | P5 | 201 | CYC | CAA-C2A-C1A | 2.66 | 129.71 | 125.01 |
| 12 | B5 | 201 | CYC | C2C-C1C-NC | 2.66 | 110.56 | 108.27 |
| 12 | j7 | 201 | CYC | C2C-C1C-NC | 2.66 | 110.56 | 108.27 |
| 12 | D5 | 201 | CYC | CAA-C2A-C1A | 2.66 | 129.71 | 125.01 |
| 12 | T5 | 201 | CYC | CMB-C2B-C1B | 2.66 | 127.49 | 124.17 |
| 12 | J7 | 201 | CYC | CAA-C2A-C1A | 2.66 | 129.71 | 125.01 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | H2 | 201 | CYC | CBB-CAB-C3B | -2.66 | 105.11 | 112.43 |
| 12 | K2 | 201 | CYC | C4A-C3A-C2A | -2.66 | 103.46 | 106.51 |
| 12 | K6 | 201 | CYC | C4A-C3A-C2A | -2.66 | 103.46 | 106.51 |
| 12 | K6 | 201 | CYC | CHD-C4C-NC | 2.66 | 128.36 | 125.20 |
| 12 | j7 | 201 | CYC | CAA-C2A-C1A | 2.66 | 129.71 | 125.01 |
| 12 | F5 | 201 | CYC | C2C-C1C-NC | 2.66 | 110.56 | 108.27 |
| 12 | L6 | 201 | CYC | CHD-C4C-NC | 2.66 | 128.36 | 125.20 |
| 12 | B7 | 201 | CYC | CHD-C4C-NC | 2.66 | 128.36 | 125.20 |
| 12 | j7 | 201 | CYC | CHD-C4C-NC | 2.65 | 128.36 | 125.20 |
| 12 | v7 | 201 | CYC | CAA-C2A-C1A | 2.65 | 129.70 | 125.01 |
| 12 | P1 | 201 | CYC | CBB-CAB-C3B | -2.65 | 105.11 | 112.43 |
| 12 | H3 | 202 | CYC | CBB-CAB-C3B | -2.65 | 105.11 | 112.43 |
| 12 | P3 | 201 | CYC | CBB-CAB-C3B | -2.65 | 105.11 | 112.43 |
| 12 | b5 | 201 | CYC | CAA-C2A-C1A | 2.65 | 129.70 | 125.01 |
| 12 | EA | 201 | CYC | CHD-C4C-NC | 2.65 | 128.36 | 125.20 |
| 12 | B5 | 201 | CYC | CHD-C4C-NC | 2.65 | 128.36 | 125.20 |
| 12 | E9 | 201 | CYC | CHD-C4C-NC | 2.65 | 128.36 | 125.20 |
| 12 | A | 201 | CYC | CAA-C2A-C1A | 2.65 | 129.70 | 125.01 |
| 12 | K5 | 201 | CYC | CMB-C2B-C1B | 2.65 | 127.48 | 124.17 |
| 12 | v7 | 201 | CYC | CHD-C4C-NC | 2.65 | 128.36 | 125.20 |
| 12 | B4 | 202 | CYC | CBB-CAB-C3B | -2.65 | 105.12 | 112.43 |
| 12 | f5 | 201 | CYC | CAA-C2A-C1A | 2.65 | 129.70 | 125.01 |
| 12 | H5 | 201 | CYC | CHD-C4C-NC | 2.65 | 128.36 | 125.20 |
| 12 | H7 | 201 | CYC | CAA-C2A-C1A | 2.65 | 129.70 | 125.01 |
| 12 | E5 | 201 | CYC | CMB-C2B-C1B | 2.65 | 127.48 | 124.17 |
| 12 | JA | 202 | CYC | CHD-C4C-NC | 2.65 | 128.35 | 125.20 |
| 12 | J9 | 202 | CYC | CHD-C4C-NC | 2.65 | 128.35 | 125.20 |
| 12 | H1 | 201 | CYC | CBB-CAB-C3B | -2.65 | 105.13 | 112.43 |
| 12 | M8 | 301 | CYC | CBB-CAB-C3B | -2.65 | 105.13 | 112.43 |
| 12 | R7 | 201 | CYC | C2C-C1C-NC | 2.65 | 110.56 | 108.27 |
| 12 | M4 | 301 | CYC | CBB-CAB-C3B | -2.65 | 105.14 | 112.43 |
| 12 | i7 | 201 | CYC | CMB-C2B-C1B | 2.65 | 127.47 | 124.17 |
| 12 | LA | 202 | CYC | CHD-C4C-NC | 2.65 | 128.35 | 125.20 |
| 12 | K3 | 201 | CYC | CHD-C4C-NC | 2.65 | 128.35 | 125.20 |
| 12 | L9 | 202 | CYC | CHD-C4C-NC | 2.65 | 128.35 | 125.20 |
| 12 | K1 | 201 | CYC | CHD-C4C-NC | 2.65 | 128.35 | 125.20 |
| 12 | X4 | 201 | CYC | CHD-C4C-NC | 2.64 | 128.35 | 125.20 |
| 12 | X8 | 201 | CYC | CHD-C4C-NC | 2.64 | 128.35 | 125.20 |
| 12 | d5 | 201 | CYC | CAA-C2A-C1A | 2.64 | 129.69 | 125.01 |
| 12 | f7 | 201 | CYC | C2C-C1C-NC | 2.64 | 110.55 | 108.27 |
| 12 | L4 | 202 | CYC | CBB-CAB-C3B | -2.64 | 105.15 | 112.43 |
| 12 | L6 | 201 | CYC | CBB-CAB-C3B | -2.64 | 105.15 | 112.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | G4 | 201 | CYC | C4A-C3A-C2A | -2.64 | 103.48 | 106.51 |
| 12 | G8 | 201 | CYC | C4A-C3A-C2A | -2.64 | 103.48 | 106.51 |
| 12 | a9 | 901 | CYC | CBB-CAB-C3B | -2.64 | 105.16 | 112.43 |
| 12 | KA | 201 | CYC | C4A-C3A-C2A | -2.64 | 103.48 | 106.51 |
| 12 | K9 | 201 | CYC | C4A-C3A-C2A | -2.64 | 103.48 | 106.51 |
| 12 | d5 | 201 | CYC | CMB-C2B-C1B | 2.64 | 127.46 | 124.17 |
| 12 | R7 | 201 | CYC | CHD-C4C-NC | 2.64 | 128.34 | 125.20 |
| 12 | Z3 | 201 | CYC | CBB-CAB-C3B | -2.64 | 105.16 | 112.43 |
| 12 | Z1 | 202 | CYC | CBB-CAB-C3B | -2.64 | 105.16 | 112.43 |
| 12 | N5 | 201 | CYC | CMB-C2B-C1B | 2.64 | 127.46 | 124.17 |
| 12 | L7 | 201 | CYC | CHD-C4C-NC | 2.64 | 128.34 | 125.20 |
| 12 | X4 | 201 | CYC | C4A-C3A-C2A | -2.64 | 103.48 | 106.51 |
| 12 | X8 | 201 | CYC | C4A-C3A-C2A | -2.64 | 103.48 | 106.51 |
| 12 | AA | 201 | CYC | CHD-C4C-NC | 2.64 | 128.34 | 125.20 |
| 12 | A9 | 201 | CYC | CHD-C4C-NC | 2.64 | 128.34 | 125.20 |
| 12 | T1 | 301 | CYC | CHD-C4C-NC | 2.64 | 128.34 | 125.20 |
| 12 | N5 | 201 | CYC | C2C-C1C-NC | 2.64 | 110.55 | 108.27 |
| 12 | Y3 | 201 | CYC | C4A-C3A-C2A | -2.64 | 103.48 | 106.51 |
| 12 | Y1 | 201 | CYC | C4A-C3A-C2A | -2.64 | 103.48 | 106.51 |
| 12 | H7 | 201 | CYC | CHD-C4C-NC | 2.63 | 128.34 | 125.20 |
| 12 | H8 | 201 | CYC | CHD-C4C-NC | 2.63 | 128.34 | 125.20 |
| 12 | LA | 202 | CYC | CBB-CAB-C3B | -2.63 | 105.17 | 112.43 |
| 12 | L9 | 202 | CYC | CBB-CAB-C3B | -2.63 | 105.17 | 112.43 |
| 12 | N5 | 201 | CYC | CHD-C4C-NC | 2.63 | 128.33 | 125.20 |
| 12 | E2 | 201 | CYC | CHD-C4C-NC | 2.63 | 128.33 | 125.20 |
| 12 | p7 | 201 | CYC | CHD-C4C-NC | 2.63 | 128.33 | 125.20 |
| 12 | V5 | 201 | CYC | CAA-C2A-C1A | 2.63 | 129.66 | 125.01 |
| 12 | d7 | 201 | CYC | CMB-C2B-C1B | 2.63 | 127.45 | 124.17 |
| 12 | o7 | 201 | CYC | CMB-C2B-C1B | 2.63 | 127.45 | 124.17 |
| 12 | A4 | 201 | CYC | C4A-C3A-C2A | -2.63 | 103.49 | 106.51 |
| 12 | A8 | 201 | CYC | C4A-C3A-C2A | -2.63 | 103.49 | 106.51 |
| 12 | T3 | 301 | CYC | CHD-C4C-NC | 2.63 | 128.33 | 125.20 |
| 12 | P7 | 201 | CYC | CAA-C2A-C1A | 2.63 | 129.66 | 125.01 |
| 12 | H4 | 201 | CYC | CHD-C4C-NC | 2.63 | 128.33 | 125.20 |
| 12 | L5 | 201 | CYC | CAA-C2A-C1A | 2.63 | 129.65 | 125.01 |
| 12 | V3 | 201 | CYC | CBB-CAB-C3B | -2.63 | 105.19 | 112.43 |
| 12 | V1 | 201 | CYC | CBB-CAB-C3B | -2.63 | 105.19 | 112.43 |
| 12 | L7 | 201 | CYC | C2C-C1C-NC | 2.63 | 110.54 | 108.27 |
| 12 | B4 | 202 | CYC | CHD-C4C-NC | 2.62 | 128.33 | 125.20 |
| 12 | V7 | 201 | CYC | CAA-C2A-C1A | 2.62 | 129.65 | 125.01 |
| 12 | D7 | 201 | CYC | CAA-C2A-C1A | 2.62 | 129.65 | 125.01 |
| 12 | O7 | 201 | CYC | CMB-C2B-C1B | 2.62 | 127.44 | 124.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | Z5 | 201 | CYC | CAA-C2A-C1A | 2.62 | 129.65 | 125.01 |
| 12 | m7 | 201 | CYC | CMB-C2B-C1B | 2.62 | 127.44 | 124.17 |
| 12 | L3 | 202 | CYC | CBB-CAB-C3B | -2.62 | 105.20 | 112.43 |
| 12 | aA | 902 | CYC | CBB-CAB-C3B | -2.62 | 105.20 | 112.43 |
| 12 | V5 | 201 | CYC | CHD-C4C-NC | 2.62 | 128.32 | 125.20 |
| 12 | F7 | 201 | CYC | C2C-C1C-NC | 2.62 | 110.53 | 108.27 |
| 12 | L2 | 201 | CYC | CBB-CAB-C3B | -2.62 | 105.20 | 112.43 |
| 12 | Z5 | 201 | CYC | C2C-C1C-NC | 2.62 | 110.53 | 108.27 |
| 12 | V7 | 201 | CYC | C2C-C1C-NC | 2.62 | 110.53 | 108.27 |
| 12 | V7 | 201 | CYC | CHD-C4C-NC | 2.62 | 128.32 | 125.20 |
| 12 | Z | 201 | CYC | CAA-C2A-C1A | 2.62 | 129.64 | 125.01 |
| 12 | H7 | 201 | CYC | C2C-C1C-NC | 2.62 | 110.53 | 108.27 |
| 12 | p7 | 201 | CYC | C2C-C1C-NC | 2.62 | 110.53 | 108.27 |
| 12 | R5 | 201 | CYC | C2C-C1C-NC | 2.62 | 110.53 | 108.27 |
| 12 | T5 | 201 | CYC | CAA-C2A-C1A | 2.62 | 129.64 | 125.01 |
| 12 | P4 | 201 | CYC | CHD-C4C-NC | 2.62 | 128.32 | 125.20 |
| 12 | P8 | 201 | CYC | CHD-C4C-NC | 2.62 | 128.32 | 125.20 |
| 12 | k5 | 1202 | CYC | C2C-C1C-NC | 2.62 | 110.53 | 108.27 |
| 12 | Z5 | 201 | CYC | CMB-C2B-C1B | 2.62 | 127.43 | 124.17 |
| 12 | U7 | 201 | CYC | CMB-C2B-C1B | 2.62 | 127.43 | 124.17 |
| 12 | Z5 | 201 | CYC | CHD-C4C-NC | 2.61 | 128.31 | 125.20 |
| 12 | Y1 | 201 | CYC | CHD-C4C-NC | 2.61 | 128.31 | 125.20 |
| 12 | CA | 201 | CYC | CHB-C4A-NA | -2.61 | 119.47 | 124.93 |
| 12 | W7 | 201 | CYC | CMB-C2B-C1B | 2.61 | 127.43 | 124.17 |
| 12 | Q9 | 201 | CYC | CHB-C4A-NA | -2.61 | 119.47 | 124.93 |
| 12 | f5 | 201 | CYC | CHD-C4C-NC | 2.61 | 128.31 | 125.20 |
| 12 | P4 | 201 | CYC | C4A-C3A-C2A | -2.61 | 103.51 | 106.51 |
| 12 | P8 | 201 | CYC | C4A-C3A-C2A | -2.61 | 103.51 | 106.51 |
| 12 | YA | 201 | CYC | C4A-C3A-C2A | -2.61 | 103.51 | 106.51 |
| 12 | Y9 | 201 | CYC | C4A-C3A-C2A | -2.61 | 103.51 | 106.51 |
| 12 | e5 | 201 | CYC | CMB-C2B-C1B | 2.61 | 127.42 | 124.17 |
| 12 | c7 | 201 | CYC | CMB-C2B-C1B | 2.61 | 127.42 | 124.17 |
| 12 | C6 | 201 | CYC | C4A-C3A-C2A | -2.61 | 103.52 | 106.51 |
| 12 | v7 | 201 | CYC | C2C-C1C-NC | 2.61 | 110.52 | 108.27 |
| 12 | X7 | 201 | CYC | CHD-C4C-NC | 2.61 | 128.30 | 125.20 |
| 12 | B7 | 201 | CYC | C2C-C1C-NC | 2.61 | 110.52 | 108.27 |
| 12 | AA | 201 | CYC | C4A-C3A-C2A | -2.60 | 103.52 | 106.51 |
| 12 | A9 | 201 | CYC | C4A-C3A-C2A | -2.60 | 103.52 | 106.51 |
| 12 | N7 | 201 | CYC | CAA-C2A-C1A | 2.60 | 129.61 | 125.01 |
| 12 | P7 | 201 | CYC | C2C-C1C-NC | 2.60 | 110.52 | 108.27 |
| 12 | r7 | 201 | CYC | CAA-C2A-C1A | 2.60 | 129.61 | 125.01 |
| 12 | H6 | 201 | CYC | CHD-C4C-NC | 2.60 | 128.30 | 125.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | I7 | 201 | CYC | CMB-C2B-C1B | 2.60 | 127.41 | 124.17 |
| 12 | C9 | 201 | CYC | CHB-C4A-NA | -2.60 | 119.49 | 124.93 |
| 12 | N5 | 201 | CYC | CAA-C2A-C1A | 2.60 | 129.61 | 125.01 |
| 12 | K2 | 201 | CYC | CHB-C4A-NA | -2.60 | 119.50 | 124.93 |
| 12 | O1 | 201 | CYC | C2A-C1A-NA | 2.60 | 113.83 | 110.05 |
| 12 | O3 | 201 | CYC | C2A-C1A-NA | 2.60 | 113.83 | 110.05 |
| 12 | I2 | 201 | CYC | CHD-C4C-NC | 2.60 | 128.29 | 125.20 |
| 12 | I6 | 201 | CYC | CHD-C4C-NC | 2.60 | 128.29 | 125.20 |
| 12 | d5 | 201 | CYC | CHD-C4C-NC | 2.60 | 128.29 | 125.20 |
| 12 | s7 | 201 | CYC | CMB-C2B-C1B | 2.60 | 127.41 | 124.17 |
| 12 | d7 | 201 | CYC | C2C-C1C-NC | 2.59 | 110.51 | 108.27 |
| 12 | YA | 201 | CYC | CHD-C4C-NC | 2.59 | 128.29 | 125.20 |
| 12 | C9 | 201 | CYC | CHD-C4C-NC | 2.59 | 128.29 | 125.20 |
| 12 | K6 | 201 | CYC | CHB-C4A-NA | -2.59 | 119.51 | 124.93 |
| 12 | E7 | 201 | CYC | CMB-C2B-C1B | 2.59 | 127.40 | 124.17 |
| 12 | F7 | 201 | CYC | CHD-C4C-NC | 2.59 | 128.28 | 125.20 |
| 12 | QA | 201 | CYC | CHB-C4A-NA | -2.59 | 119.52 | 124.93 |
| 12 | C2 | 201 | CYC | CHB-C4A-NA | -2.59 | 119.52 | 124.93 |
| 12 | Y9 | 201 | CYC | CHD-C4C-NC | 2.59 | 128.28 | 125.20 |
| 12 | a5 | 201 | CYC | CMB-C2B-C1B | 2.59 | 127.39 | 124.17 |
| 12 | u7 | 201 | CYC | CMB-C2B-C1B | 2.59 | 127.39 | 124.17 |
| 12 | Y3 | 201 | CYC | CHD-C4C-NC | 2.59 | 128.28 | 125.20 |
| 12 | M7 | 201 | CYC | CMB-C2B-C1B | 2.58 | 127.39 | 124.17 |
| 12 | O9 | 201 | CYC | C4A-C3A-C2A | -2.58 | 103.54 | 106.51 |
| 12 | T7 | 201 | CYC | CAA-C2A-C1A | 2.58 | 129.57 | 125.01 |
| 12 | k5 | 1203 | CYC | CAA-C2A-C1A | 2.58 | 129.57 | 125.01 |
| 12 | Q9 | 201 | CYC | CHD-C4C-NC | 2.58 | 128.27 | 125.20 |
| 12 | Q9 | 201 | CYC | C4A-C3A-C2A | -2.58 | 103.55 | 106.51 |
| 12 | C3 | 201 | CYC | C2A-C1A-NA | 2.58 | 113.80 | 110.05 |
| 12 | C1 | 201 | CYC | C2A-C1A-NA | 2.58 | 113.80 | 110.05 |
| 12 | QA | 201 | CYC | C4A-C3A-C2A | -2.58 | 103.55 | 106.51 |
| 12 | A2 | 201 | CYC | C4A-C3A-C2A | -2.58 | 103.55 | 106.51 |
| 12 | b5 | 201 | CYC | CHD-C4C-NC | 2.58 | 128.27 | 125.20 |
| 12 | X5 | 201 | CYC | C2C-C1C-NC | 2.58 | 110.50 | 108.27 |
| 12 | X7 | 201 | CYC | C2C-C1C-NC | 2.58 | 110.50 | 108.27 |
| 12 | O5 | 201 | CYC | CMB-C2B-C1B | 2.58 | 127.38 | 124.17 |
| 12 | C1 | 201 | CYC | CHB-C4A-NA | -2.58 | 119.55 | 124.93 |
| 12 | b5 | 201 | CYC | C2C-C1C-NC | 2.57 | 110.49 | 108.27 |
| 12 | G3 | 201 | CYC | C4A-C3A-C2A | -2.57 | 103.55 | 106.51 |
| 12 | I6 | 201 | CYC | C4A-C3A-C2A | -2.57 | 103.55 | 106.51 |
| 12 | YA | 201 | CYC | CHB-C4A-NA | -2.57 | 119.56 | 124.93 |
| 12 | Y9 | 201 | CYC | CHB-C4A-NA | -2.57 | 119.56 | 124.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | k5 | 1204 | CYC | CAA-C2A-C1A | 2.57 | 129.55 | 125.01 |
| 12 | Z | 201 | CYC | C2C-C1C-NC | 2.57 | 110.49 | 108.27 |
| 12 | k5 | 1203 | CYC | C4A-C3A-C2A | -2.57 | 103.56 | 106.51 |
| 12 | CA | 201 | CYC | CHD-C4C-NC | 2.57 | 128.26 | 125.20 |
| 12 | X5 | 201 | CYC | CHD-C4C-NC | 2.57 | 128.25 | 125.20 |
| 12 | j5 | 1202 | CYC | CAA-C2A-C1A | 2.56 | 129.55 | 125.01 |
| 12 | C6 | 201 | CYC | CHB-C4A-NA | -2.56 | 119.57 | 124.93 |
| 12 | L4 | 202 | CYC | C1A-C2A-C3A | -2.56 | 103.94 | 106.78 |
| 12 | C7 | 201 | CYC | CMB-C2B-C1B | 2.56 | 127.37 | 124.17 |
| 12 | OA | 201 | CYC | C4A-C3A-C2A | -2.56 | 103.56 | 106.51 |
| 12 | I2 | 201 | CYC | C4A-C3A-C2A | -2.56 | 103.56 | 106.51 |
| 12 | G1 | 201 | CYC | C4A-C3A-C2A | -2.56 | 103.56 | 106.51 |
| 12 | U5 | 201 | CYC | CMB-C2B-C1B | 2.56 | 127.37 | 124.17 |
| 12 | LA | 202 | CYC | CAA-C2A-C1A | 2.56 | 129.54 | 125.01 |
| 12 | L9 | 202 | CYC | CAA-C2A-C1A | 2.56 | 129.54 | 125.01 |
| 12 | H2 | 201 | CYC | CHD-C4C-NC | 2.56 | 128.25 | 125.20 |
| 12 | H5 | 201 | CYC | CAA-C2A-C1A | 2.56 | 129.54 | 125.01 |
| 12 | K3 | 201 | CYC | CHB-C4A-NA | -2.56 | 119.57 | 124.93 |
| 12 | K1 | 201 | CYC | CHB-C4A-NA | -2.56 | 119.57 | 124.93 |
| 12 | A6 | 201 | CYC | C4A-C3A-C2A | -2.56 | 103.57 | 106.51 |
| 12 | A2 | 201 | CYC | CHB-C4A-NA | -2.56 | 119.58 | 124.93 |
| 12 | CA | 201 | CYC | C2A-C1A-NA | 2.56 | 113.78 | 110.05 |
| 12 | E6 | 201 | CYC | C2A-C1A-NA | 2.56 | 113.78 | 110.05 |
| 12 | C9 | 201 | CYC | C2A-C1A-NA | 2.56 | 113.78 | 110.05 |
| 12 | W5 | 201 | CYC | CMB-C2B-C1B | 2.56 | 127.36 | 124.17 |
| 12 | C3 | 201 | CYC | CHB-C4A-NA | -2.56 | 119.58 | 124.93 |
| 12 | j5 | 1202 | CYC | C2C-C1C-NC | 2.56 | 110.48 | 108.27 |
| 12 | c5 | 201 | CYC | CMB-C2B-C1B | 2.56 | 127.36 | 124.17 |
| 12 | QA | 201 | CYC | CHD-C4C-NC | 2.56 | 128.25 | 125.20 |
| 12 | A7 | 201 | CYC | CMB-C2B-C1B | 2.56 | 127.36 | 124.17 |
| 12 | B3 | 202 | CYC | CHD-C4C-NC | 2.56 | 128.25 | 125.20 |
| 12 | r7 | 201 | CYC | CHD-C4C-NC | 2.56 | 128.25 | 125.20 |
| 12 | A | 201 | CYC | C2C-C1C-NC | 2.56 | 110.48 | 108.27 |
| 12 | C2 | 201 | CYC | C4A-C3A-C2A | -2.56 | 103.57 | 106.51 |
| 12 | UA | 201 | CYC | C4A-C3A-C2A | -2.56 | 103.57 | 106.51 |
| 12 | a9 | 901 | CYC | C1A-C2A-C3A | -2.56 | 103.95 | 106.78 |
| 12 | Q1 | 201 | CYC | C4A-C3A-C2A | -2.55 | 103.58 | 106.51 |
| 12 | Q3 | 201 | CYC | C4A-C3A-C2A | -2.55 | 103.58 | 106.51 |
| 12 | G3 | 201 | CYC | CHB-C4A-NA | -2.55 | 119.59 | 124.93 |
| 12 | G1 | 201 | CYC | CHB-C4A-NA | -2.55 | 119.59 | 124.93 |
| 12 | C6 | 201 | CYC | CHD-C4C-NC | 2.55 | 128.24 | 125.20 |
| 12 | OA | 201 | CYC | CHB-C4A-NA | -2.55 | 119.59 | 124.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | O9 | 201 | CYC | CHB-C4A-NA | -2.55 | 119.59 | 124.93 |
| 12 | C8 | 201 | CYC | CHB-C4A-NA | -2.55 | 119.59 | 124.93 |
| 12 | S1 | 201 | CYC | C4A-C3A-C2A | -2.55 | 103.58 | 106.51 |
| 12 | S3 | 201 | CYC | C4A-C3A-C2A | -2.55 | 103.58 | 106.51 |
| 12 | C3 | 201 | CYC | C4A-C3A-C2A | -2.55 | 103.58 | 106.51 |
| 12 | C1 | 201 | CYC | C4A-C3A-C2A | -2.55 | 103.58 | 106.51 |
| 12 | K4 | 201 | CYC | CHB-C4A-NA | -2.55 | 119.60 | 124.93 |
| 12 | K8 | 201 | CYC | CHB-C4A-NA | -2.55 | 119.60 | 124.93 |
| 12 | B5 | 201 | CYC | CAA-C2A-C1A | 2.55 | 129.52 | 125.01 |
| 12 | I6 | 201 | CYC | C2A-C1A-NA | 2.55 | 113.76 | 110.05 |
| 12 | K7 | 201 | CYC | CMB-C2B-C1B | 2.55 | 127.35 | 124.17 |
| 12 | C4 | 201 | CYC | CHD-C4C-NC | 2.55 | 128.24 | 125.20 |
| 12 | C8 | 201 | CYC | CHD-C4C-NC | 2.55 | 128.24 | 125.20 |
| 12 | E3 | 201 | CYC | C4A-C3A-C2A | -2.55 | 103.58 | 106.51 |
| 12 | E1 | 201 | CYC | C4A-C3A-C2A | -2.55 | 103.58 | 106.51 |
| 12 | Y5 | 201 | CYC | CMB-C2B-C1B | 2.55 | 127.35 | 124.17 |
| 12 | X4 | 201 | CYC | C2A-C1A-NA | 2.55 | 113.75 | 110.05 |
| 12 | X8 | 201 | CYC | C2A-C1A-NA | 2.55 | 113.75 | 110.05 |
| 12 | k5 | 1203 | CYC | CHD-C4C-NC | 2.55 | 128.23 | 125.20 |
| 12 | I6 | 201 | CYC | CHB-C4A-NA | -2.55 | 119.61 | 124.93 |
| 12 | E4 | 201 | CYC | C4A-C3A-C2A | -2.55 | 103.58 | 106.51 |
| 12 | A1 | 201 | CYC | CAC-C3C-C4C | 2.55 | 119.21 | 112.67 |
| 12 | A3 | 201 | CYC | CAC-C3C-C4C | 2.55 | 119.21 | 112.67 |
| 12 | R9 | 201 | CYC | CAA-C2A-C1A | 2.55 | 129.51 | 125.01 |
| 12 | N7 | 201 | CYC | C2C-C1C-NC | 2.55 | 110.47 | 108.27 |
| 12 | C4 | 201 | CYC | CHB-C4A-NA | -2.54 | 119.61 | 124.93 |
| 12 | F2 | 201 | CYC | C1A-C2A-C3A | -2.54 | 103.97 | 106.78 |
| 12 | f5 | 201 | CYC | C2C-C1C-NC | 2.54 | 110.47 | 108.27 |
| 12 | Z3 | 201 | CYC | C1A-C2A-C3A | -2.54 | 103.97 | 106.78 |
| 12 | Z1 | 202 | CYC | C1A-C2A-C3A | -2.54 | 103.97 | 106.78 |
| 12 | C2 | 201 | CYC | CHD-C4C-NC | 2.54 | 128.23 | 125.20 |
| 12 | LA | 202 | CYC | C1A-C2A-C3A | -2.54 | 103.97 | 106.78 |
| 12 | L9 | 202 | CYC | C1A-C2A-C3A | -2.54 | 103.97 | 106.78 |
| 12 | R4 | 201 | CYC | C4A-C3A-C2A | -2.54 | 103.59 | 106.51 |
| 12 | AA | 201 | CYC | CHB-C4A-NA | -2.54 | 119.62 | 124.93 |
| 12 | r7 | 201 | CYC | C4A-C3A-C2A | -2.54 | 103.59 | 106.51 |
| 12 | V5 | 201 | CYC | C4A-C3A-C2A | -2.54 | 103.59 | 106.51 |
| 12 | A1 | 201 | CYC | CHB-C4A-NA | -2.54 | 119.62 | 124.93 |
| 12 | A3 | 201 | CYC | CHB-C4A-NA | -2.54 | 119.62 | 124.93 |
| 12 | A1 | 201 | CYC | C2A-C1A-NA | 2.54 | 113.74 | 110.05 |
| 12 | A3 | 201 | CYC | C2A-C1A-NA | 2.54 | 113.74 | 110.05 |
| 12 | A6 | 201 | CYC | C2A-C1A-NA | 2.54 | 113.74 | 110.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | A2 | 201 | CYC | C2A-C1A-NA | 2.54 | 113.74 | 110.05 |
| 12 | A9 | 201 | CYC | CHB-C4A-NA | -2.54 | 119.63 | 124.93 |
| 12 | R5 | 201 | CYC | CHD-C4C-NC | 2.54 | 128.22 | 125.20 |
| 12 | S5 | 201 | CYC | CMB-C2B-C1B | 2.54 | 127.33 | 124.17 |
| 12 | X4 | 201 | CYC | CHB-C4A-NA | -2.54 | 119.63 | 124.93 |
| 12 | X8 | 201 | CYC | CHB-C4A-NA | -2.54 | 119.63 | 124.93 |
| 12 | E2 | 201 | CYC | C2A-C1A-NA | 2.54 | 113.74 | 110.05 |
| 12 | A4 | 201 | CYC | CHB-C4A-NA | -2.53 | 119.63 | 124.93 |
| 12 | A8 | 201 | CYC | CHB-C4A-NA | -2.53 | 119.63 | 124.93 |
| 12 | U9 | 201 | CYC | C4A-C3A-C2A | -2.53 | 103.60 | 106.51 |
| 12 | Q1 | 201 | CYC | CHB-C4A-NA | -2.53 | 119.63 | 124.93 |
| 12 | Q3 | 201 | CYC | CHB-C4A-NA | -2.53 | 119.63 | 124.93 |
| 12 | BA | 201 | CYC | CAA-C2A-C1A | 2.53 | 129.49 | 125.01 |
| 12 | B9 | 201 | CYC | CAA-C2A-C1A | 2.53 | 129.49 | 125.01 |
| 12 | R8 | 201 | CYC | C4A-C3A-C2A | -2.53 | 103.60 | 106.51 |
| 12 | KA | 201 | CYC | CHB-C4A-NA | -2.53 | 119.64 | 124.93 |
| 12 | K9 | 201 | CYC | CHB-C4A-NA | -2.53 | 119.64 | 124.93 |
| 12 | HA | 202 | CYC | C1A-C2A-C3A | -2.53 | 103.98 | 106.78 |
| 12 | M5 | 201 | CYC | CMB-C2B-C1B | 2.53 | 127.33 | 124.17 |
| 12 | E9 | 201 | CYC | CHB-C4A-NA | -2.53 | 119.64 | 124.93 |
| 12 | V4 | 201 | CYC | C2A-C1A-NA | 2.53 | 113.73 | 110.05 |
| 12 | A6 | 201 | CYC | CHB-C4A-NA | -2.53 | 119.64 | 124.93 |
| 12 | RA | 201 | CYC | CAA-C2A-C1A | 2.53 | 129.48 | 125.01 |
| 12 | H4 | 201 | CYC | CAA-C2A-C1A | 2.53 | 129.48 | 125.01 |
| 12 | H8 | 201 | CYC | CAA-C2A-C1A | 2.53 | 129.48 | 125.01 |
| 12 | U3 | 201 | CYC | C4A-C3A-C2A | -2.53 | 103.61 | 106.51 |
| 12 | U1 | 201 | CYC | C4A-C3A-C2A | -2.53 | 103.61 | 106.51 |
| 12 | Q7 | 201 | CYC | CMB-C2B-C1B | 2.53 | 127.32 | 124.17 |
| 12 | SA | 201 | CYC | C2A-C1A-NA | 2.52 | 113.72 | 110.05 |
| 12 | WA | 201 | CYC | C2A-C1A-NA | 2.52 | 113.72 | 110.05 |
| 12 | S9 | 201 | CYC | C2A-C1A-NA | 2.52 | 113.72 | 110.05 |
| 12 | IA | 201 | CYC | CHB-C4A-NA | -2.52 | 119.65 | 124.93 |
| 12 | I9 | 201 | CYC | CHB-C4A-NA | -2.52 | 119.65 | 124.93 |
| 12 | W9 | 201 | CYC | C2A-C1A-NA | 2.52 | 113.72 | 110.05 |
| 12 | P5 | 201 | CYC | C4A-C3A-C2A | -2.52 | 103.61 | 106.51 |
| 12 | Y3 | 201 | CYC | CHB-C4A-NA | -2.52 | 119.66 | 124.93 |
| 12 | Y1 | 201 | CYC | CHB-C4A-NA | -2.52 | 119.66 | 124.93 |
| 12 | TA | 301 | CYC | CHD-C4C-NC | 2.52 | 128.20 | 125.20 |
| 12 | T9 | 301 | CYC | CHD-C4C-NC | 2.52 | 128.20 | 125.20 |
| 12 | I4 | 201 | CYC | C2A-C1A-NA | 2.52 | 113.72 | 110.05 |
| 12 | I8 | 201 | CYC | C2A-C1A-NA | 2.52 | 113.72 | 110.05 |
| 12 | R8 | 201 | CYC | C2A-C1A-NA | 2.52 | 113.72 | 110.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | EA | 201 | CYC | CHB-C4A-NA | -2.52 | 119.66 | 124.93 |
| 12 | X1 | 201 | CYC | CAA-C2A-C1A | 2.52 | 129.47 | 125.01 |
| 12 | IA | 201 | CYC | C4A-C3A-C2A | -2.52 | 103.61 | 106.51 |
| 12 | I9 | 201 | CYC | C4A-C3A-C2A | -2.52 | 103.61 | 106.51 |
| 12 | K2 | 201 | CYC | CAC-C3C-C4C | 2.52 | 119.14 | 112.67 |
| 12 | J4 | 201 | CYC | CAA-C2A-C1A | 2.52 | 129.46 | 125.01 |
| 12 | J8 | 201 | CYC | CAA-C2A-C1A | 2.52 | 129.46 | 125.01 |
| 12 | A2 | 201 | CYC | CAC-C3C-C4C | 2.52 | 119.14 | 112.67 |
| 12 | E4 | 201 | CYC | C2A-C1A-NA | 2.52 | 113.71 | 110.05 |
| 12 | W1 | 201 | CYC | CAC-C3C-C4C | 2.52 | 119.14 | 112.67 |
| 12 | HA | 202 | CYC | CAA-C2A-C1A | 2.52 | 129.46 | 125.01 |
| 12 | O3 | 201 | CYC | CHB-C4A-NA | -2.52 | 119.67 | 124.93 |
| 12 | SA | 201 | CYC | CHB-C4A-NA | -2.52 | 119.67 | 124.93 |
| 12 | S9 | 201 | CYC | CHB-C4A-NA | -2.52 | 119.67 | 124.93 |
| 12 | G7 | 201 | CYC | CMB-C2B-C1B | 2.51 | 127.31 | 124.17 |
| 12 | T4 | 201 | CYC | C2A-C1A-NA | 2.51 | 113.71 | 110.05 |
| 12 | T8 | 201 | CYC | C2A-C1A-NA | 2.51 | 113.71 | 110.05 |
| 12 | Y5 | 201 | CYC | C2C-C1C-NC | 2.51 | 110.44 | 108.27 |
| 12 | I4 | 201 | CYC | CHB-C4A-NA | -2.51 | 119.67 | 124.93 |
| 12 | I8 | 201 | CYC | CHB-C4A-NA | -2.51 | 119.67 | 124.93 |
| 12 | E8 | 201 | CYC | C4A-C3A-C2A | -2.51 | 103.62 | 106.51 |
| 12 | S4 | 202 | CYC | CAA-C2A-C1A | 2.51 | 129.45 | 125.01 |
| 12 | W1 | 201 | CYC | C4A-C3A-C2A | -2.51 | 103.62 | 106.51 |
| 12 | M4 | 301 | CYC | CAA-C2A-C1A | 2.51 | 129.45 | 125.01 |
| 12 | A6 | 201 | CYC | CAC-C3C-C4C | 2.51 | 119.12 | 112.67 |
| 12 | Q5 | 201 | CYC | CMB-C2B-C1B | 2.51 | 127.30 | 124.17 |
| 12 | I2 | 201 | CYC | CHB-C4A-NA | -2.51 | 119.68 | 124.93 |
| 12 | D6 | 201 | CYC | CAA-C2A-C1A | 2.51 | 129.45 | 125.01 |
| 12 | OA | 201 | CYC | CAC-C3C-C4C | 2.51 | 119.12 | 112.67 |
| 12 | O9 | 201 | CYC | CAC-C3C-C4C | 2.51 | 119.12 | 112.67 |
| 12 | E6 | 201 | CYC | CHB-C4A-NA | -2.51 | 119.68 | 124.93 |
| 12 | R4 | 201 | CYC | C2A-C1A-NA | 2.51 | 113.70 | 110.05 |
| 12 | M8 | 301 | CYC | CAA-C2A-C1A | 2.51 | 129.45 | 125.01 |
| 12 | AA | 201 | CYC | C2A-C1A-NA | 2.51 | 113.70 | 110.05 |
| 12 | A9 | 201 | CYC | C2A-C1A-NA | 2.51 | 113.70 | 110.05 |
| 12 | C4 | 201 | CYC | C4A-C3A-C2A | -2.51 | 103.63 | 106.51 |
| 12 | C8 | 201 | CYC | C4A-C3A-C2A | -2.51 | 103.63 | 106.51 |
| 12 | G5 | 201 | CYC | CMB-C2B-C1B | 2.51 | 127.30 | 124.17 |
| 12 | W3 | 201 | CYC | C4A-C3A-C2A | -2.51 | 103.63 | 106.51 |
| 12 | B1 | 202 | CYC | CHD-C4C-NC | 2.51 | 128.19 | 125.20 |
| 12 | E4 | 201 | CYC | CHB-C4A-NA | -2.51 | 119.69 | 124.93 |
| 12 | E8 | 201 | CYC | CHB-C4A-NA | -2.51 | 119.69 | 124.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | OA | 201 | CYC | C2A-C1A-NA | 2.51 | 113.70 | 110.05 |
| 12 | V8 | 201 | CYC | C2A-C1A-NA | 2.51 | 113.70 | 110.05 |
| 12 | E3 | 201 | CYC | CHB-C4A-NA | -2.51 | 119.69 | 124.93 |
| 12 | E1 | 201 | CYC | CHB-C4A-NA | -2.51 | 119.69 | 124.93 |
| 12 | W3 | 201 | CYC | CAC-C3C-C4C | 2.51 | 119.11 | 112.67 |
| 12 | G4 | 201 | CYC | CAC-C3C-C4C | 2.51 | 119.11 | 112.67 |
| 12 | G8 | 201 | CYC | CAC-C3C-C4C | 2.51 | 119.11 | 112.67 |
| 12 | N4 | 201 | CYC | C2A-C1A-NA | 2.51 | 113.69 | 110.05 |
| 12 | O1 | 201 | CYC | CHB-C4A-NA | -2.51 | 119.69 | 124.93 |
| 12 | I2 | 201 | CYC | C2A-C1A-NA | 2.51 | 113.69 | 110.05 |
| 12 | K6 | 201 | CYC | CAC-C3C-C4C | 2.51 | 119.11 | 112.67 |
| 12 | N4 | 201 | CYC | CHB-C4A-NA | -2.51 | 119.69 | 124.93 |
| 12 | N8 | 201 | CYC | CHB-C4A-NA | -2.51 | 119.69 | 124.93 |
| 12 | VA | 201 | CYC | C1A-C2A-C3A | -2.51 | 104.01 | 106.78 |
| 12 | K8 | 201 | CYC | C2A-C1A-NA | 2.51 | 113.69 | 110.05 |
| 12 | T3 | 301 | CYC | C1A-C2A-C3A | -2.50 | 104.01 | 106.78 |
| 12 | T1 | 301 | CYC | C1A-C2A-C3A | -2.50 | 104.01 | 106.78 |
| 12 | X3 | 201 | CYC | CAA-C2A-C1A | 2.50 | 129.44 | 125.01 |
| 12 | H9 | 202 | CYC | CAA-C2A-C1A | 2.50 | 129.44 | 125.01 |
| 12 | Y7 | 201 | CYC | CMB-C2B-C1B | 2.50 | 127.29 | 124.17 |
| 12 | Q1 | 201 | CYC | CAC-C3C-C4C | 2.50 | 119.10 | 112.67 |
| 12 | Q3 | 201 | CYC | CAC-C3C-C4C | 2.50 | 119.10 | 112.67 |
| 12 | GA | 201 | CYC | C4A-C3A-C2A | -2.50 | 103.64 | 106.51 |
| 12 | G9 | 201 | CYC | C4A-C3A-C2A | -2.50 | 103.64 | 106.51 |
| 12 | M8 | 302 | CYC | CAA-C2A-C1A | 2.50 | 129.43 | 125.01 |
| 12 | K4 | 201 | CYC | CAC-C3C-C4C | 2.50 | 119.09 | 112.67 |
| 12 | K8 | 201 | CYC | CAC-C3C-C4C | 2.50 | 119.09 | 112.67 |
| 12 | GA | 201 | CYC | CHB-C4A-NA | -2.50 | 119.70 | 124.93 |
| 12 | YA | 201 | CYC | CAC-C3C-C4C | 2.50 | 119.09 | 112.67 |
| 12 | Y9 | 201 | CYC | CAC-C3C-C4C | 2.50 | 119.09 | 112.67 |
| 12 | L6 | 201 | CYC | C1A-C2A-C3A | -2.50 | 104.02 | 106.78 |
| 12 | M8 | 301 | CYC | C1A-C2A-C3A | -2.50 | 104.02 | 106.78 |
| 12 | UA | 201 | CYC | CHB-C4A-NA | -2.50 | 119.71 | 124.93 |
| 12 | H6 | 201 | CYC | CAA-C2A-C1A | 2.50 | 129.43 | 125.01 |
| 12 | U1 | 201 | CYC | CHB-C4A-NA | -2.50 | 119.71 | 124.93 |
| 12 | I5 | 201 | CYC | CHB-C1B-C2B | -2.50 | 122.00 | 126.95 |
| 12 | a9 | 901 | CYC | CAA-C2A-C1A | 2.50 | 129.42 | 125.01 |
| 12 | L4 | 202 | CYC | CAA-C2A-C1A | 2.49 | 129.42 | 125.01 |
| 12 | KA | 201 | CYC | CAC-C3C-C4C | 2.49 | 119.08 | 112.67 |
| 12 | SA | 201 | CYC | CAC-C3C-C4C | 2.49 | 119.08 | 112.67 |
| 12 | O1 | 201 | CYC | CAC-C3C-C4C | 2.49 | 119.08 | 112.67 |
| 12 | O3 | 201 | CYC | CAC-C3C-C4C | 2.49 | 119.08 | 112.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | K9 | 201 | CYC | CAC-C3C-C4C | 2.49 | 119.08 | 112.67 |
| 12 | S9 | 201 | CYC | CAC-C3C-C4C | 2.49 | 119.08 | 112.67 |
| 12 | X4 | 201 | CYC | CAC-C3C-C4C | 2.49 | 119.08 | 112.67 |
| 12 | X8 | 201 | CYC | CAC-C3C-C4C | 2.49 | 119.08 | 112.67 |
| 12 | T4 | 201 | CYC | CHB-C4A-NA | -2.49 | 119.72 | 124.93 |
| 12 | T8 | 201 | CYC | CHB-C4A-NA | -2.49 | 119.72 | 124.93 |
| 12 | D2 | 201 | CYC | CAA-C2A-C1A | 2.49 | 129.42 | 125.01 |
| 12 | A5 | 201 | CYC | CMB-C2B-C1B | 2.49 | 127.28 | 124.17 |
| 12 | e7 | 201 | CYC | CMB-C2B-C1B | 2.49 | 127.28 | 124.17 |
| 12 | E2 | 201 | CYC | CHB-C4A-NA | -2.49 | 119.72 | 124.93 |
| 12 | L6 | 201 | CYC | C2A-C1A-NA | 2.49 | 113.68 | 110.05 |
| 12 | L2 | 201 | CYC | C1A-C2A-C3A | -2.49 | 104.02 | 106.78 |
| 12 | G9 | 201 | CYC | CHB-C4A-NA | -2.49 | 119.72 | 124.93 |
| 12 | Q9 | 201 | CYC | CAC-C3C-C4C | 2.49 | 119.07 | 112.67 |
| 12 | Q1 | 201 | CYC | C2A-C1A-NA | 2.49 | 113.67 | 110.05 |
| 12 | Q3 | 201 | CYC | C2A-C1A-NA | 2.49 | 113.67 | 110.05 |
| 12 | E8 | 201 | CYC | C2A-C1A-NA | 2.49 | 113.67 | 110.05 |
| 12 | Z | 201 | CYC | C4A-C3A-C2A | -2.49 | 103.65 | 106.51 |
| 12 | N2 | 101 | CYC | CAA-C2A-C1A | 2.49 | 129.42 | 125.01 |
| 12 | N6 | 101 | CYC | CAA-C2A-C1A | 2.49 | 129.42 | 125.01 |
| 12 | aA | 901 | CYC | CAA-C2A-C1A | 2.49 | 129.42 | 125.01 |
| 12 | TA | 301 | CYC | CAA-C2A-C1A | 2.49 | 129.41 | 125.01 |
| 12 | T9 | 301 | CYC | CAA-C2A-C1A | 2.49 | 129.41 | 125.01 |
| 12 | V4 | 201 | CYC | CAC-C3C-C4C | 2.49 | 119.07 | 112.67 |
| 12 | V8 | 201 | CYC | CAC-C3C-C4C | 2.49 | 119.07 | 112.67 |
| 12 | W3 | 201 | CYC | CHB-C4A-NA | -2.49 | 119.72 | 124.93 |
| 12 | I3 | 201 | CYC | CAC-C3C-C4C | 2.49 | 119.07 | 112.67 |
| 12 | I1 | 201 | CYC | CAC-C3C-C4C | 2.49 | 119.07 | 112.67 |
| 12 | F9 | 301 | CYC | C1A-C2A-C3A | -2.49 | 104.03 | 106.78 |
| 12 | E9 | 201 | CYC | C4A-C3A-C2A | -2.49 | 103.65 | 106.51 |
| 12 | L2 | 201 | CYC | C2A-C1A-NA | 2.49 | 113.67 | 110.05 |
| 12 | C5 | 201 | CYC | CHB-C1B-C2B | -2.49 | 122.02 | 126.95 |
| 12 | H2 | 201 | CYC | CAA-C2A-C1A | 2.49 | 129.41 | 125.01 |
| 12 | U9 | 201 | CYC | CHB-C4A-NA | -2.49 | 119.73 | 124.93 |
| 12 | U3 | 201 | CYC | CHB-C4A-NA | -2.49 | 119.73 | 124.93 |
| 12 | W1 | 201 | CYC | CHB-C4A-NA | -2.49 | 119.73 | 124.93 |
| 12 | QA | 201 | CYC | CAC-C3C-C4C | 2.49 | 119.06 | 112.67 |
| 12 | V4 | 201 | CYC | CHB-C4A-NA | -2.49 | 119.73 | 124.93 |
| 12 | V8 | 201 | CYC | CHB-C4A-NA | -2.49 | 119.73 | 124.93 |
| 12 | WA | 201 | CYC | C4A-C3A-C2A | -2.48 | 103.66 | 106.51 |
| 12 | P4 | 201 | CYC | CAC-C3C-C4C | 2.48 | 119.05 | 112.67 |
| 12 | I3 | 201 | CYC | CHB-C4A-NA | -2.48 | 119.74 | 124.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | I1 | 201 | CYC | CHB-C4A-NA | -2.48 | 119.74 | 124.93 |
| 12 | E6 | 201 | CYC | C4A-C3A-C2A | -2.48 | 103.66 | 106.51 |
| 12 | N8 | 201 | CYC | C2A-C1A-NA | 2.48 | 113.66 | 110.05 |
| 12 | H2 | 201 | CYC | C1A-C2A-C3A | -2.48 | 104.03 | 106.78 |
| 12 | C6 | 201 | CYC | CAC-C3C-C4C | 2.48 | 119.05 | 112.67 |
| 12 | XA | 201 | CYC | CAA-C2A-C1A | 2.48 | 129.40 | 125.01 |
| 12 | E3 | 201 | CYC | C2A-C1A-NA | 2.48 | 113.66 | 110.05 |
| 12 | E1 | 201 | CYC | C2A-C1A-NA | 2.48 | 113.66 | 110.05 |
| 12 | IA | 201 | CYC | CAC-C3C-C4C | 2.48 | 119.05 | 112.67 |
| 12 | I9 | 201 | CYC | CAC-C3C-C4C | 2.48 | 119.05 | 112.67 |
| 12 | J7 | 201 | CYC | C4A-C3A-C2A | -2.48 | 103.66 | 106.51 |
| 12 | FA | 301 | CYC | C1A-C2A-C3A | -2.48 | 104.04 | 106.78 |
| 12 | K4 | 201 | CYC | C2A-C1A-NA | 2.48 | 113.66 | 110.05 |
| 12 | V3 | 201 | CYC | CAA-C2A-C1A | 2.48 | 129.40 | 125.01 |
| 12 | X9 | 201 | CYC | CAA-C2A-C1A | 2.48 | 129.40 | 125.01 |
| 12 | V1 | 201 | CYC | CAA-C2A-C1A | 2.48 | 129.40 | 125.01 |
| 12 | H6 | 201 | CYC | C1A-C2A-C3A | -2.48 | 104.04 | 106.78 |
| 12 | O9 | 201 | CYC | C2A-C1A-NA | 2.48 | 113.66 | 110.05 |
| 12 | K2 | 201 | CYC | C2A-C1A-NA | 2.48 | 113.66 | 110.05 |
| 12 | B4 | 202 | CYC | CAA-C2A-C1A | 2.48 | 129.39 | 125.01 |
| 12 | QA | 201 | CYC | C2A-C1A-NA | 2.48 | 113.66 | 110.05 |
| 12 | N2 | 101 | CYC | C1A-C2A-C3A | -2.48 | 104.04 | 106.78 |
| 12 | N6 | 101 | CYC | C1A-C2A-C3A | -2.48 | 104.04 | 106.78 |
| 12 | W3 | 201 | CYC | C2A-C1A-NA | 2.48 | 113.65 | 110.05 |
| 12 | W1 | 201 | CYC | C2A-C1A-NA | 2.48 | 113.65 | 110.05 |
| 12 | E8 | 201 | CYC | CAC-C3C-C4C | 2.48 | 119.04 | 112.67 |
| 12 | PA | 201 | CYC | CAA-C2A-C1A | 2.48 | 129.39 | 125.01 |
| 12 | P9 | 201 | CYC | CAA-C2A-C1A | 2.48 | 129.39 | 125.01 |
| 12 | q7 | 201 | CYC | CMB-C2B-C1B | 2.48 | 127.26 | 124.17 |
| 12 | N8 | 201 | CYC | CAC-C3C-C4C | 2.48 | 119.03 | 112.67 |
| 12 | K6 | 201 | CYC | C2A-C1A-NA | 2.48 | 113.65 | 110.05 |
| 12 | V4 | 201 | CYC | C4A-C3A-C2A | -2.48 | 103.66 | 106.51 |
| 12 | I4 | 201 | CYC | C4A-C3A-C2A | -2.48 | 103.66 | 106.51 |
| 12 | I8 | 201 | CYC | C4A-C3A-C2A | -2.48 | 103.66 | 106.51 |
| 12 | J3 | 202 | CYC | CAA-C2A-C1A | 2.48 | 129.39 | 125.01 |
| 12 | A | 201 | CYC | C4A-C3A-C2A | -2.48 | 103.67 | 106.51 |
| 12 | W9 | 201 | CYC | C4A-C3A-C2A | -2.48 | 103.67 | 106.51 |
| 12 | C2 | 201 | CYC | CAC-C3C-C4C | 2.47 | 119.03 | 112.67 |
| 12 | A4 | 201 | CYC | CAC-C3C-C4C | 2.47 | 119.02 | 112.67 |
| 12 | A8 | 201 | CYC | CAC-C3C-C4C | 2.47 | 119.02 | 112.67 |
| 12 | P8 | 201 | CYC | CAC-C3C-C4C | 2.47 | 119.02 | 112.67 |
| 12 | X3 | 201 | CYC | C1A-C2A-C3A | -2.47 | 104.05 | 106.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | V9 | 201 | CYC | C1A-C2A-C3A | -2.47 | 104.05 | 106.78 |
| 12 | C3 | 201 | CYC | CAC-C3C-C4C | 2.47 | 119.02 | 112.67 |
| 12 | E4 | 201 | CYC | CAC-C3C-C4C | 2.47 | 119.02 | 112.67 |
| 12 | C1 | 201 | CYC | CAC-C3C-C4C | 2.47 | 119.02 | 112.67 |
| 12 | Q9 | 201 | CYC | C2A-C1A-NA | 2.47 | 113.64 | 110.05 |
| 12 | WA | 201 | CYC | CAC-C3C-C4C | 2.47 | 119.02 | 112.67 |
| 12 | W9 | 201 | CYC | CAC-C3C-C4C | 2.47 | 119.02 | 112.67 |
| 12 | G2 | 201 | CYC | CHB-C4A-NA | -2.47 | 119.77 | 124.93 |
| 12 | L4 | 202 | CYC | C2A-C1A-NA | 2.47 | 113.64 | 110.05 |
| 12 | F9 | 301 | CYC | CAA-C2A-C1A | 2.47 | 129.37 | 125.01 |
| 12 | B8 | 202 | CYC | CAA-C2A-C1A | 2.47 | 129.37 | 125.01 |
| 12 | J3 | 202 | CYC | C1A-C2A-C3A | -2.47 | 104.05 | 106.78 |
| 12 | X1 | 201 | CYC | C1A-C2A-C3A | -2.47 | 104.05 | 106.78 |
| 12 | B9 | 201 | CYC | C1A-C2A-C3A | -2.46 | 104.06 | 106.78 |
| 12 | k5 | 1202 | CYC | C4A-C3A-C2A | -2.46 | 103.68 | 106.51 |
| 12 | E2 | 201 | CYC | C4A-C3A-C2A | -2.46 | 103.68 | 106.51 |
| 12 | N4 | 201 | CYC | CAC-C3C-C4C | 2.46 | 119.00 | 112.67 |
| 12 | BA | 201 | CYC | C1A-C2A-C3A | -2.46 | 104.06 | 106.78 |
| 12 | VA | 201 | CYC | CAA-C2A-C1A | 2.46 | 129.37 | 125.01 |
| 12 | Z3 | 201 | CYC | CAA-C2A-C1A | 2.46 | 129.37 | 125.01 |
| 12 | Z1 | 202 | CYC | CAA-C2A-C1A | 2.46 | 129.37 | 125.01 |
| 12 | H9 | 202 | CYC | C1A-C2A-C3A | -2.46 | 104.06 | 106.78 |
| 12 | v7 | 201 | CYC | C4A-C3A-C2A | -2.46 | 103.68 | 106.51 |
| 12 | G8 | 201 | CYC | CHB-C4A-NA | -2.46 | 119.78 | 124.93 |
| 12 | FA | 301 | CYC | CAA-C2A-C1A | 2.46 | 129.36 | 125.01 |
| 12 | V5 | 201 | CYC | C2C-C1C-NC | 2.46 | 110.39 | 108.27 |
| 12 | EA | 201 | CYC | C4A-C3A-C2A | -2.46 | 103.68 | 106.51 |
| 12 | F3 | 201 | CYC | C1A-C2A-C3A | -2.46 | 104.06 | 106.78 |
| 12 | F1 | 201 | CYC | C1A-C2A-C3A | -2.46 | 104.06 | 106.78 |
| 12 | G6 | 201 | CYC | CHB-C4A-NA | -2.46 | 119.78 | 124.93 |
| 12 | U5 | 201 | CYC | CHB-C1B-C2B | -2.46 | 122.07 | 126.95 |
| 12 | c5 | 201 | CYC | C2C-C1C-NC | 2.46 | 110.39 | 108.27 |
| 12 | D7 | 201 | CYC | C4A-C3A-C2A | -2.46 | 103.68 | 106.51 |
| 12 | F6 | 201 | CYC | CAA-C2A-C1A | 2.46 | 129.36 | 125.01 |
| 12 | e7 | 201 | CYC | CHB-C1B-C2B | -2.46 | 122.08 | 126.95 |
| 12 | WA | 201 | CYC | CHB-C4A-NA | -2.46 | 119.79 | 124.93 |
| 12 | W9 | 201 | CYC | CHB-C4A-NA | -2.46 | 119.79 | 124.93 |
| 12 | L3 | 202 | CYC | CAA-C2A-C1A | 2.46 | 129.35 | 125.01 |
| 12 | aA | 902 | CYC | CAA-C2A-C1A | 2.46 | 129.35 | 125.01 |
| 12 | Y3 | 201 | CYC | C2A-C1A-NA | 2.46 | 113.62 | 110.05 |
| 12 | Y1 | 201 | CYC | C2A-C1A-NA | 2.46 | 113.62 | 110.05 |
| 12 | G2 | 201 | CYC | C2A-C1A-NA | 2.46 | 113.62 | 110.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | G6 | 201 | CYC | C2A-C1A-NA | 2.46 | 113.62 | 110.05 |
| 12 | G4 | 201 | CYC | CHB-C4A-NA | -2.46 | 119.80 | 124.93 |
| 12 | T4 | 201 | CYC | CAC-C3C-C4C | 2.46 | 118.98 | 112.67 |
| 12 | T8 | 201 | CYC | CAC-C3C-C4C | 2.46 | 118.98 | 112.67 |
| 12 | R4 | 201 | CYC | CAC-C3C-C4C | 2.46 | 118.98 | 112.67 |
| 12 | R8 | 201 | CYC | CAC-C3C-C4C | 2.46 | 118.98 | 112.67 |
| 12 | S7 | 201 | CYC | CMB-C2B-C1B | 2.46 | 127.23 | 124.17 |
| 12 | UA | 201 | CYC | C2A-C1A-NA | 2.45 | 113.62 | 110.05 |
| 12 | U9 | 201 | CYC | C2A-C1A-NA | 2.45 | 113.62 | 110.05 |
| 12 | P4 | 201 | CYC | CHB-C4A-NA | -2.45 | 119.80 | 124.93 |
| 12 | P8 | 201 | CYC | CHB-C4A-NA | -2.45 | 119.80 | 124.93 |
| 12 | I2 | 201 | CYC | CAC-C3C-C4C | 2.45 | 118.97 | 112.67 |
| 12 | I6 | 201 | CYC | CAC-C3C-C4C | 2.45 | 118.97 | 112.67 |
| 12 | U3 | 201 | CYC | CAC-C3C-C4C | 2.45 | 118.97 | 112.67 |
| 12 | XA | 201 | CYC | C1A-C2A-C3A | -2.45 | 104.07 | 106.78 |
| 12 | X9 | 201 | CYC | C1A-C2A-C3A | -2.45 | 104.07 | 106.78 |
| 12 | YA | 201 | CYC | C2A-C1A-NA | 2.45 | 113.62 | 110.05 |
| 12 | Y9 | 201 | CYC | C2A-C1A-NA | 2.45 | 113.62 | 110.05 |
| 12 | L7 | 201 | CYC | C4A-C3A-C2A | -2.45 | 103.69 | 106.51 |
| 12 | ZA | 202 | CYC | C1A-C2A-C3A | -2.45 | 104.07 | 106.78 |
| 12 | Z9 | 202 | CYC | C1A-C2A-C3A | -2.45 | 104.07 | 106.78 |
| 12 | K1 | 201 | CYC | CAC-C3C-C4C | 2.45 | 118.97 | 112.67 |
| 12 | Y7 | 201 | CYC | CHB-C1B-C2B | -2.45 | 122.09 | 126.95 |
| 12 | R7 | 201 | CYC | C4A-C3A-C2A | -2.45 | 103.69 | 106.51 |
| 12 | Z4 | 301 | CYC | CAA-C2A-C1A | 2.45 | 129.34 | 125.01 |
| 12 | F2 | 201 | CYC | CAA-C2A-C1A | 2.45 | 129.34 | 125.01 |
| 12 | k5 | 1204 | CYC | C2C-C1C-NC | 2.45 | 110.39 | 108.27 |
| 12 | W4 | 201 | CYC | CAA-C2A-C1A | 2.45 | 129.34 | 125.01 |
| 12 | W8 | 201 | CYC | CAA-C2A-C1A | 2.45 | 129.34 | 125.01 |
| 12 | PA | 201 | CYC | C1A-C2A-C3A | -2.45 | 104.07 | 106.78 |
| 12 | S1 | 201 | CYC | CHB-C4A-NA | -2.45 | 119.81 | 124.93 |
| 12 | S3 | 201 | CYC | CHB-C4A-NA | -2.45 | 119.81 | 124.93 |
| 12 | U3 | 201 | CYC | C2A-C1A-NA | 2.45 | 113.61 | 110.05 |
| 12 | U1 | 201 | CYC | C2A-C1A-NA | 2.45 | 113.61 | 110.05 |
| 12 | a9 | 901 | CYC | C2A-C1A-NA | 2.45 | 113.61 | 110.05 |
| 12 | D4 | 202 | CYC | C1A-C2A-C3A | -2.45 | 104.07 | 106.78 |
| 12 | D8 | 202 | CYC | C1A-C2A-C3A | -2.45 | 104.07 | 106.78 |
| 12 | p7 | 201 | CYC | C4A-C3A-C2A | -2.45 | 103.70 | 106.51 |
| 12 | k7 | 201 | CYC | CMB-C2B-C1B | 2.45 | 127.22 | 124.17 |
| 12 | CA | 201 | CYC | CAC-C3C-C4C | 2.45 | 118.96 | 112.67 |
| 12 | C9 | 201 | CYC | CAC-C3C-C4C | 2.45 | 118.96 | 112.67 |
| 12 | L3 | 202 | CYC | C1A-C2A-C3A | -2.45 | 104.07 | 106.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | f5 | 201 | CYC | C4A-C3A-C2A | -2.45 | 103.70 | 106.51 |
| 12 | C4 | 201 | CYC | CAC-C3C-C4C | 2.45 | 118.95 | 112.67 |
| 12 | C8 | 201 | CYC | CAC-C3C-C4C | 2.45 | 118.95 | 112.67 |
| 12 | G2 | 201 | CYC | CAC-C3C-C4C | 2.45 | 118.95 | 112.67 |
| 12 | M4 | 301 | CYC | C1A-C2A-C3A | -2.45 | 104.08 | 106.78 |
| 12 | UA | 201 | CYC | CAC-C3C-C4C | 2.45 | 118.95 | 112.67 |
| 12 | V8 | 201 | CYC | C4A-C3A-C2A | -2.44 | 103.70 | 106.51 |
| 12 | U1 | 201 | CYC | CAC-C3C-C4C | 2.44 | 118.95 | 112.67 |
| 12 | R4 | 201 | CYC | CHB-C4A-NA | -2.44 | 119.82 | 124.93 |
| 12 | O5 | 201 | CYC | CHB-C1B-C2B | -2.44 | 122.11 | 126.95 |
| 12 | q7 | 201 | CYC | C2C-C1C-NC | 2.44 | 110.38 | 108.27 |
| 12 | T3 | 301 | CYC | CAA-C2A-C1A | 2.44 | 129.33 | 125.01 |
| 12 | T1 | 301 | CYC | CAA-C2A-C1A | 2.44 | 129.33 | 125.01 |
| 12 | F6 | 201 | CYC | C1A-C2A-C3A | -2.44 | 104.08 | 106.78 |
| 12 | G3 | 201 | CYC | CAC-C3C-C4C | 2.44 | 118.95 | 112.67 |
| 12 | G1 | 201 | CYC | CAC-C3C-C4C | 2.44 | 118.95 | 112.67 |
| 12 | V3 | 201 | CYC | C1A-C2A-C3A | -2.44 | 104.08 | 106.78 |
| 12 | V1 | 201 | CYC | C1A-C2A-C3A | -2.44 | 104.08 | 106.78 |
| 12 | a7 | 201 | CYC | CHB-C1B-C2B | -2.44 | 122.11 | 126.95 |
| 12 | K3 | 201 | CYC | CAC-C3C-C4C | 2.44 | 118.94 | 112.67 |
| 12 | V9 | 201 | CYC | CAA-C2A-C1A | 2.44 | 129.33 | 125.01 |
| 12 | M8 | 302 | CYC | C1A-C2A-C3A | -2.44 | 104.08 | 106.78 |
| 12 | R1 | 201 | CYC | CAA-C2A-C1A | 2.44 | 129.33 | 125.01 |
| 12 | R3 | 201 | CYC | CAA-C2A-C1A | 2.44 | 129.33 | 125.01 |
| 12 | V3 | 201 | CYC | C2A-C1A-NA | 2.44 | 113.60 | 110.05 |
| 12 | V1 | 201 | CYC | C2A-C1A-NA | 2.44 | 113.60 | 110.05 |
| 12 | E7 | 201 | CYC | CHB-C1B-C2B | -2.44 | 122.11 | 126.95 |
| 12 | D4 | 202 | CYC | CAA-C2A-C1A | 2.44 | 129.33 | 125.01 |
| 12 | L6 | 201 | CYC | CAA-C2A-C1A | 2.44 | 129.33 | 125.01 |
| 12 | D8 | 202 | CYC | CAA-C2A-C1A | 2.44 | 129.33 | 125.01 |
| 12 | R8 | 201 | CYC | CHB-C4A-NA | -2.44 | 119.83 | 124.93 |
| 12 | J4 | 201 | CYC | C1A-C2A-C3A | -2.44 | 104.08 | 106.78 |
| 12 | EA | 201 | CYC | CAC-C3C-C4C | 2.44 | 118.94 | 112.67 |
| 12 | E9 | 201 | CYC | CAC-C3C-C4C | 2.44 | 118.94 | 112.67 |
| 12 | P1 | 201 | CYC | CAA-C2A-C1A | 2.44 | 129.32 | 125.01 |
| 12 | P3 | 201 | CYC | CAA-C2A-C1A | 2.44 | 129.32 | 125.01 |
| 12 | Y3 | 201 | CYC | CAC-C3C-C4C | 2.44 | 118.94 | 112.67 |
| 12 | Y1 | 201 | CYC | CAC-C3C-C4C | 2.44 | 118.94 | 112.67 |
| 12 | C4 | 201 | CYC | C2A-C1A-NA | 2.44 | 113.60 | 110.05 |
| 12 | C8 | 201 | CYC | C2A-C1A-NA | 2.44 | 113.60 | 110.05 |
| 12 | S1 | 201 | CYC | CAC-C3C-C4C | 2.44 | 118.94 | 112.67 |
| 12 | S3 | 201 | CYC | CAC-C3C-C4C | 2.44 | 118.94 | 112.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | H5 | 201 | CYC | C4A-C3A-C2A | -2.44 | 103.71 | 106.51 |
| 12 | k5 | 1204 | CYC | C4A-C3A-C2A | -2.44 | 103.71 | 106.51 |
| 12 | i7 | 201 | CYC | CHB-C1B-C2B | -2.44 | 122.12 | 126.95 |
| 12 | aA | 901 | CYC | C1A-C2A-C3A | -2.44 | 104.08 | 106.78 |
| 12 | DA | 201 | CYC | CAA-C2A-C1A | 2.44 | 129.32 | 125.01 |
| 12 | D9 | 201 | CYC | CAA-C2A-C1A | 2.44 | 129.32 | 125.01 |
| 12 | A4 | 201 | CYC | C2A-C1A-NA | 2.44 | 113.59 | 110.05 |
| 12 | A8 | 201 | CYC | C2A-C1A-NA | 2.44 | 113.59 | 110.05 |
| 12 | F4 | 202 | CYC | C2C-C3C-C4C | 2.44 | 104.99 | 101.34 |
| 12 | F8 | 202 | CYC | C2C-C3C-C4C | 2.44 | 104.99 | 101.34 |
| 12 | P9 | 201 | CYC | C1A-C2A-C3A | -2.44 | 104.09 | 106.78 |
| 12 | U9 | 201 | CYC | CAC-C3C-C4C | 2.44 | 118.93 | 112.67 |
| 12 | g7 | 201 | CYC | CHB-C1B-C2B | -2.44 | 122.12 | 126.95 |
| 12 | F3 | 201 | CYC | CAA-C2A-C1A | 2.43 | 129.32 | 125.01 |
| 12 | F1 | 201 | CYC | CAA-C2A-C1A | 2.43 | 129.32 | 125.01 |
| 12 | F4 | 202 | CYC | CAA-C2A-C1A | 2.43 | 129.31 | 125.01 |
| 12 | M8 | 301 | CYC | C2A-C1A-NA | 2.43 | 113.59 | 110.05 |
| 12 | f7 | 201 | CYC | C4A-C3A-C2A | -2.43 | 103.71 | 106.51 |
| 12 | aA | 902 | CYC | C1A-C2A-C3A | -2.43 | 104.09 | 106.78 |
| 12 | G6 | 201 | CYC | CAC-C3C-C4C | 2.43 | 118.92 | 112.67 |
| 12 | IA | 201 | CYC | C2A-C1A-NA | 2.43 | 113.59 | 110.05 |
| 12 | LA | 202 | CYC | C2A-C1A-NA | 2.43 | 113.59 | 110.05 |
| 12 | P4 | 201 | CYC | C2A-C1A-NA | 2.43 | 113.59 | 110.05 |
| 12 | P8 | 201 | CYC | C2A-C1A-NA | 2.43 | 113.59 | 110.05 |
| 12 | L9 | 202 | CYC | C2A-C1A-NA | 2.43 | 113.59 | 110.05 |
| 12 | I9 | 201 | CYC | C2A-C1A-NA | 2.43 | 113.59 | 110.05 |
| 12 | I1 | 201 | CYC | C2A-C1A-NA | 2.43 | 113.59 | 110.05 |
| 12 | EA | 201 | CYC | C2A-C1A-NA | 2.43 | 113.59 | 110.05 |
| 12 | S1 | 201 | CYC | C2A-C1A-NA | 2.43 | 113.59 | 110.05 |
| 12 | e5 | 201 | CYC | CHB-C1B-C2B | -2.43 | 122.13 | 126.95 |
| 12 | S4 | 202 | CYC | C2C-C3C-C4C | 2.43 | 104.98 | 101.34 |
| 12 | KA | 201 | CYC | C2A-C1A-NA | 2.43 | 113.58 | 110.05 |
| 12 | K9 | 201 | CYC | C2A-C1A-NA | 2.43 | 113.58 | 110.05 |
| 12 | m7 | 201 | CYC | CHB-C1B-C2B | -2.43 | 122.13 | 126.95 |
| 12 | o7 | 201 | CYC | CHB-C1B-C2B | -2.43 | 122.13 | 126.95 |
| 12 | HA | 202 | CYC | C2C-C3C-C4C | 2.43 | 104.98 | 101.34 |
| 12 | E3 | 201 | CYC | CAC-C3C-C4C | 2.43 | 118.91 | 112.67 |
| 12 | E1 | 201 | CYC | CAC-C3C-C4C | 2.43 | 118.91 | 112.67 |
| 12 | AA | 201 | CYC | CAC-C3C-C4C | 2.43 | 118.91 | 112.67 |
| 12 | J8 | 201 | CYC | C1A-C2A-C3A | -2.43 | 104.09 | 106.78 |
| 12 | W4 | 202 | CYC | O2D-CGD-CBD | 2.43 | 121.83 | 114.03 |
| 12 | S3 | 201 | CYC | C2A-C1A-NA | 2.43 | 113.58 | 110.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | a5 | 201 | CYC | CHB-C1B-C2B | -2.43 | 122.14 | 126.95 |
| 12 | F4 | 202 | CYC | C1A-C2A-C3A | -2.43 | 104.09 | 106.78 |
| 12 | F8 | 202 | CYC | C1A-C2A-C3A | -2.43 | 104.09 | 106.78 |
| 12 | D3 | 202 | CYC | CAA-C2A-C1A | 2.43 | 129.30 | 125.01 |
| 12 | d7 | 201 | CYC | C4A-C3A-C2A | -2.43 | 103.72 | 106.51 |
| 12 | H4 | 201 | CYC | C2A-C1A-NA | 2.43 | 113.58 | 110.05 |
| 12 | H8 | 201 | CYC | C2A-C1A-NA | 2.43 | 113.58 | 110.05 |
| 12 | D5 | 201 | CYC | C4A-C3A-C2A | -2.43 | 103.72 | 106.51 |
| 12 | I3 | 201 | CYC | C2A-C1A-NA | 2.43 | 113.58 | 110.05 |
| 12 | D1 | 202 | CYC | CAA-C2A-C1A | 2.43 | 129.30 | 125.01 |
| 12 | Z8 | 301 | CYC | CAA-C2A-C1A | 2.43 | 129.30 | 125.01 |
| 12 | L2 | 201 | CYC | CAA-C2A-C1A | 2.43 | 129.30 | 125.01 |
| 12 | s7 | 201 | CYC | CHB-C1B-C2B | -2.43 | 122.14 | 126.95 |
| 12 | h7 | 201 | CYC | C4A-C3A-C2A | -2.42 | 103.72 | 106.51 |
| 12 | W5 | 201 | CYC | CHB-C1B-C2B | -2.42 | 122.15 | 126.95 |
| 12 | BA | 201 | CYC | C2A-C1A-NA | 2.42 | 113.57 | 110.05 |
| 12 | B9 | 201 | CYC | C2A-C1A-NA | 2.42 | 113.57 | 110.05 |
| 12 | W8 | 202 | CYC | O2D-CGD-CBD | 2.42 | 121.81 | 114.03 |
| 12 | E5 | 201 | CYC | CHB-C1B-C2B | -2.42 | 122.15 | 126.95 |
| 12 | C7 | 201 | CYC | CHB-C1B-C2B | -2.42 | 122.15 | 126.95 |
| 12 | u7 | 201 | CYC | CHB-C1B-C2B | -2.42 | 122.15 | 126.95 |
| 12 | K7 | 201 | CYC | CHB-C1B-C2B | -2.42 | 122.15 | 126.95 |
| 12 | b7 | 201 | CYC | C4A-C3A-C2A | -2.42 | 103.73 | 106.51 |
| 12 | S5 | 201 | CYC | CHB-C1B-C2B | -2.42 | 122.15 | 126.95 |
| 12 | M7 | 201 | CYC | C2C-C1C-NC | 2.42 | 110.36 | 108.27 |
| 12 | M5 | 201 | CYC | CHB-C1B-C2B | -2.42 | 122.15 | 126.95 |
| 12 | P5 | 201 | CYC | C2C-C1C-NC | 2.42 | 110.36 | 108.27 |
| 12 | B1 | 202 | CYC | CAA-C2A-C1A | 2.42 | 129.29 | 125.01 |
| 12 | J5 | 201 | CYC | C4A-C3A-C2A | -2.42 | 103.73 | 106.51 |
| 12 | W4 | 201 | CYC | C1A-C2A-C3A | -2.42 | 104.11 | 106.78 |
| 12 | W8 | 201 | CYC | C1A-C2A-C3A | -2.42 | 104.11 | 106.78 |
| 12 | A9 | 201 | CYC | CAC-C3C-C4C | 2.42 | 118.88 | 112.67 |
| 12 | D1 | 201 | CYC | O2D-CGD-CBD | 2.42 | 121.79 | 114.03 |
| 12 | Z9 | 201 | CYC | O2D-CGD-CBD | 2.42 | 121.79 | 114.03 |
| 12 | D3 | 201 | CYC | O2D-CGD-CBD | 2.42 | 121.79 | 114.03 |
| 12 | Y5 | 201 | CYC | CHB-C1B-C2B | -2.42 | 122.16 | 126.95 |
| 12 | Z8 | 301 | CYC | C1A-C2A-C3A | -2.42 | 104.11 | 106.78 |
| 12 | B3 | 202 | CYC | CAA-C2A-C1A | 2.42 | 129.28 | 125.01 |
| 12 | a7 | 201 | CYC | C2C-C1C-NC | 2.42 | 110.36 | 108.27 |
| 12 | K5 | 201 | CYC | CHB-C1B-C2B | -2.42 | 122.16 | 126.95 |
| 12 | A7 | 201 | CYC | CHB-C1B-C2B | -2.42 | 122.16 | 126.95 |
| 12 | k7 | 201 | CYC | CHB-C1B-C2B | -2.42 | 122.16 | 126.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | X5 | 201 | CYC | C4A-C3A-C2A | -2.42 | 103.73 | 106.51 |
| 12 | F2 | 201 | CYC | C2C-C3C-C4C | 2.41 | 104.96 | 101.34 |
| 12 | I7 | 201 | CYC | CHB-C1B-C2B | -2.41 | 122.16 | 126.95 |
| 12 | M4 | 301 | CYC | C2A-C1A-NA | 2.41 | 113.56 | 110.05 |
| 12 | Z4 | 301 | CYC | C1A-C2A-C3A | -2.41 | 104.11 | 106.78 |
| 12 | F8 | 202 | CYC | CAA-C2A-C1A | 2.41 | 129.28 | 125.01 |
| 12 | S4 | 202 | CYC | C1A-C2A-C3A | -2.41 | 104.11 | 106.78 |
| 12 | XA | 202 | CYC | O2D-CGD-CBD | 2.41 | 121.78 | 114.03 |
| 12 | X9 | 202 | CYC | O2D-CGD-CBD | 2.41 | 121.78 | 114.03 |
| 12 | H3 | 201 | CYC | O2D-CGD-CBD | 2.41 | 121.78 | 114.03 |
| 12 | H1 | 202 | CYC | O2D-CGD-CBD | 2.41 | 121.78 | 114.03 |
| 12 | O8 | 201 | CYC | CAA-C2A-C1A | 2.41 | 129.28 | 125.01 |
| 12 | M7 | 201 | CYC | CHB-C1B-C2B | -2.41 | 122.17 | 126.95 |
| 12 | O4 | 201 | CYC | CAA-C2A-C1A | 2.41 | 129.28 | 125.01 |
| 12 | G3 | 201 | CYC | C2A-C1A-NA | 2.41 | 113.56 | 110.05 |
| 12 | F9 | 301 | CYC | C2A-C1A-NA | 2.41 | 113.56 | 110.05 |
| 12 | G1 | 201 | CYC | C2A-C1A-NA | 2.41 | 113.56 | 110.05 |
| 12 | I4 | 201 | CYC | CAC-C3C-C4C | 2.41 | 118.86 | 112.67 |
| 12 | I8 | 201 | CYC | CAC-C3C-C4C | 2.41 | 118.86 | 112.67 |
| 12 | E2 | 201 | CYC | CAC-C3C-C4C | 2.41 | 118.86 | 112.67 |
| 12 | J2 | 202 | CYC | CAA-C2A-C1A | 2.41 | 129.27 | 125.01 |
| 12 | SA | 201 | CYC | C4A-C3A-C2A | -2.41 | 103.74 | 106.51 |
| 12 | X7 | 201 | CYC | C4A-C3A-C2A | -2.41 | 103.74 | 106.51 |
| 12 | S9 | 201 | CYC | C4A-C3A-C2A | -2.41 | 103.74 | 106.51 |
| 12 | R9 | 201 | CYC | C1A-C2A-C3A | -2.41 | 104.12 | 106.78 |
| 12 | k7 | 201 | CYC | C2C-C1C-NC | 2.41 | 110.35 | 108.27 |
| 12 | TA | 301 | CYC | C1A-C2A-C3A | -2.41 | 104.12 | 106.78 |
| 12 | T9 | 301 | CYC | C1A-C2A-C3A | -2.41 | 104.12 | 106.78 |
| 12 | c7 | 201 | CYC | CHB-C1B-C2B | -2.41 | 122.18 | 126.95 |
| 12 | O4 | 201 | CYC | C1A-C2A-C3A | -2.41 | 104.12 | 106.78 |
| 12 | c5 | 201 | CYC | CHB-C1B-C2B | -2.41 | 122.18 | 126.95 |
| 12 | O7 | 201 | CYC | CHB-C1B-C2B | -2.41 | 122.18 | 126.95 |
| 12 | q7 | 201 | CYC | CHB-C1B-C2B | -2.41 | 122.18 | 126.95 |
| 12 | Q7 | 201 | CYC | CHB-C1B-C2B | -2.41 | 122.18 | 126.95 |
| 12 | RA | 201 | CYC | C1A-C2A-C3A | -2.41 | 104.12 | 106.78 |
| 12 | O8 | 201 | CYC | C1A-C2A-C3A | -2.41 | 104.12 | 106.78 |
| 12 | E9 | 201 | CYC | C2A-C1A-NA | 2.41 | 113.55 | 110.05 |
| 12 | L4 | 201 | CYC | O2D-CGD-CBD | 2.41 | 121.76 | 114.03 |
| 12 | L8 | 201 | CYC | O2D-CGD-CBD | 2.41 | 121.76 | 114.03 |
| 12 | A5 | 201 | CYC | CHB-C1B-C2B | -2.41 | 122.18 | 126.95 |
| 12 | Z3 | 202 | CYC | O2D-CGD-CBD | 2.41 | 121.76 | 114.03 |
| 12 | Z1 | 201 | CYC | O2D-CGD-CBD | 2.41 | 121.76 | 114.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | ZA | 201 | CYC | O2D-CGD-CBD | 2.41 | 121.76 | 114.03 |
| 12 | H9 | 202 | CYC | C2C-C3C-C4C | 2.40 | 104.94 | 101.34 |
| 12 | g7 | 201 | CYC | C2C-C1C-NC | 2.40 | 110.35 | 108.27 |
| 12 | H3 | 202 | CYC | C1A-C2A-C3A | -2.40 | 104.12 | 106.78 |
| 12 | GA | 201 | CYC | CAC-C3C-C4C | 2.40 | 118.84 | 112.67 |
| 12 | E6 | 201 | CYC | CAC-C3C-C4C | 2.40 | 118.84 | 112.67 |
| 12 | H1 | 201 | CYC | C1A-C2A-C3A | -2.40 | 104.12 | 106.78 |
| 12 | D5 | 201 | CYC | C2C-C1C-NC | 2.40 | 110.34 | 108.27 |
| 12 | G7 | 201 | CYC | CHB-C1B-C2B | -2.40 | 122.19 | 126.95 |
| 12 | F6 | 201 | CYC | C2C-C3C-C4C | 2.40 | 104.93 | 101.34 |
| 12 | H3 | 202 | CYC | CAA-C2A-C1A | 2.40 | 129.25 | 125.01 |
| 12 | H4 | 201 | CYC | C1A-C2A-C3A | -2.40 | 104.13 | 106.78 |
| 12 | H8 | 201 | CYC | C1A-C2A-C3A | -2.40 | 104.13 | 106.78 |
| 12 | Z3 | 201 | CYC | C2A-C1A-NA | 2.40 | 113.54 | 110.05 |
| 12 | Z1 | 202 | CYC | C2A-C1A-NA | 2.40 | 113.54 | 110.05 |
| 12 | B8 | 202 | CYC | C2A-C1A-NA | 2.40 | 113.54 | 110.05 |
| 12 | J5 | 201 | CYC | C2C-C1C-NC | 2.40 | 110.34 | 108.27 |
| 12 | F7 | 201 | CYC | C4A-C3A-C2A | -2.40 | 103.76 | 106.51 |
| 12 | U4 | 202 | CYC | O2D-CGD-CBD | 2.40 | 121.72 | 114.03 |
| 12 | D6 | 202 | CYC | O2D-CGD-CBD | 2.40 | 121.72 | 114.03 |
| 12 | U8 | 202 | CYC | O2D-CGD-CBD | 2.40 | 121.72 | 114.03 |
| 12 | J3 | 201 | CYC | O2D-CGD-CBD | 2.39 | 121.72 | 114.03 |
| 12 | J1 | 201 | CYC | O2D-CGD-CBD | 2.39 | 121.72 | 114.03 |
| 12 | B4 | 202 | CYC | C2A-C1A-NA | 2.39 | 113.53 | 110.05 |
| 12 | LA | 201 | CYC | O2D-CGD-CBD | 2.39 | 121.72 | 114.03 |
| 12 | L9 | 201 | CYC | O2D-CGD-CBD | 2.39 | 121.72 | 114.03 |
| 12 | P1 | 201 | CYC | C1A-C2A-C3A | -2.39 | 104.14 | 106.78 |
| 12 | P3 | 201 | CYC | C1A-C2A-C3A | -2.39 | 104.14 | 106.78 |
| 12 | H7 | 201 | CYC | C4A-C3A-C2A | -2.39 | 103.76 | 106.51 |
| 12 | GA | 201 | CYC | C2A-C1A-NA | 2.39 | 113.53 | 110.05 |
| 12 | G9 | 201 | CYC | C2A-C1A-NA | 2.39 | 113.53 | 110.05 |
| 12 | R1 | 202 | CYC | O2D-CGD-CBD | 2.39 | 121.72 | 114.03 |
| 12 | R3 | 202 | CYC | O2D-CGD-CBD | 2.39 | 121.72 | 114.03 |
| 12 | G5 | 201 | CYC | CHB-C1B-C2B | -2.39 | 122.21 | 126.95 |
| 12 | V7 | 201 | CYC | C4A-C3A-C2A | -2.39 | 103.76 | 106.51 |
| 12 | U7 | 201 | CYC | CHB-C1B-C2B | -2.39 | 122.21 | 126.95 |
| 12 | B5 | 201 | CYC | C4A-C3A-C2A | -2.39 | 103.76 | 106.51 |
| 12 | G9 | 201 | CYC | CAC-C3C-C4C | 2.39 | 118.81 | 112.67 |
| 12 | D6 | 201 | CYC | C1A-C2A-C3A | -2.39 | 104.14 | 106.78 |
| 12 | FA | 301 | CYC | C2A-C1A-NA | 2.39 | 113.52 | 110.05 |
| 12 | H2 | 202 | CYC | O2D-CGD-CBD | 2.39 | 121.70 | 114.03 |
| 12 | Q5 | 201 | CYC | CHB-C1B-C2B | -2.39 | 122.22 | 126.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | L3 | 201 | CYC | O2D-CGD-CBD | 2.39 | 121.70 | 114.03 |
| 12 | L1 | 201 | CYC | O2D-CGD-CBD | 2.39 | 121.70 | 114.03 |
| 12 | H1 | 201 | CYC | CAA-C2A-C1A | 2.39 | 129.23 | 125.01 |
| 12 | H6 | 202 | CYC | O2D-CGD-CBD | 2.39 | 121.70 | 114.03 |
| 12 | H4 | 202 | CYC | O2D-CGD-CBD | 2.39 | 121.70 | 114.03 |
| 12 | H8 | 202 | CYC | O2D-CGD-CBD | 2.39 | 121.70 | 114.03 |
| 12 | j5 | 1202 | CYC | C4A-C3A-C2A | -2.39 | 103.77 | 106.51 |
| 12 | S4 | 201 | CYC | O2D-CGD-CBD | 2.39 | 121.69 | 114.03 |
| 12 | S8 | 201 | CYC | O2D-CGD-CBD | 2.39 | 121.69 | 114.03 |
| 12 | JA | 202 | CYC | CAA-C2A-C1A | 2.39 | 129.23 | 125.01 |
| 12 | J9 | 202 | CYC | CAA-C2A-C1A | 2.39 | 129.23 | 125.01 |
| 12 | G4 | 201 | CYC | C2A-C1A-NA | 2.38 | 113.52 | 110.05 |
| 12 | G8 | 201 | CYC | C2A-C1A-NA | 2.38 | 113.52 | 110.05 |
| 12 | H9 | 201 | CYC | O2D-CGD-CBD | 2.38 | 121.69 | 114.03 |
| 12 | F2 | 201 | CYC | C2A-C1A-NA | 2.38 | 113.52 | 110.05 |
| 12 | P3 | 202 | CYC | O2D-CGD-CBD | 2.38 | 121.68 | 114.03 |
| 12 | j7 | 201 | CYC | C4A-C3A-C2A | -2.38 | 103.77 | 106.51 |
| 12 | F4 | 201 | CYC | O2D-CGD-CBD | 2.38 | 121.68 | 114.03 |
| 12 | F8 | 201 | CYC | O2D-CGD-CBD | 2.38 | 121.68 | 114.03 |
| 12 | VA | 201 | CYC | C2C-C3C-C4C | 2.38 | 104.91 | 101.34 |
| 12 | V9 | 201 | CYC | C2C-C3C-C4C | 2.38 | 104.91 | 101.34 |
| 12 | B7 | 201 | CYC | C4A-C3A-C2A | -2.38 | 103.78 | 106.51 |
| 12 | PA | 202 | CYC | O2D-CGD-CBD | 2.38 | 121.68 | 114.03 |
| 12 | T3 | 302 | CYC | O2D-CGD-CBD | 2.38 | 121.67 | 114.03 |
| 12 | T1 | 302 | CYC | O2D-CGD-CBD | 2.38 | 121.67 | 114.03 |
| 12 | DA | 202 | CYC | O2D-CGD-CBD | 2.38 | 121.67 | 114.03 |
| 12 | D9 | 202 | CYC | O2D-CGD-CBD | 2.38 | 121.67 | 114.03 |
| 12 | ZA | 202 | CYC | CAA-C2A-C1A | 2.38 | 129.22 | 125.01 |
| 12 | Z9 | 202 | CYC | CAA-C2A-C1A | 2.38 | 129.22 | 125.01 |
| 12 | P9 | 202 | CYC | O2D-CGD-CBD | 2.38 | 121.67 | 114.03 |
| 12 | T3 | 301 | CYC | C2C-C3C-C4C | 2.38 | 104.90 | 101.34 |
| 12 | T1 | 301 | CYC | C2C-C3C-C4C | 2.38 | 104.90 | 101.34 |
| 12 | BA | 202 | CYC | O2D-CGD-CBD | 2.38 | 121.67 | 114.03 |
| 12 | B4 | 201 | CYC | O2D-CGD-CBD | 2.38 | 121.67 | 114.03 |
| 12 | B9 | 202 | CYC | O2D-CGD-CBD | 2.38 | 121.67 | 114.03 |
| 12 | JA | 201 | CYC | O2D-CGD-CBD | 2.38 | 121.67 | 114.03 |
| 12 | J9 | 201 | CYC | O2D-CGD-CBD | 2.38 | 121.67 | 114.03 |
| 12 | D2 | 202 | CYC | O2D-CGD-CBD | 2.38 | 121.67 | 114.03 |
| 12 | J4 | 202 | CYC | O2D-CGD-CBD | 2.38 | 121.66 | 114.03 |
| 12 | L6 | 202 | CYC | O2D-CGD-CBD | 2.38 | 121.66 | 114.03 |
| 12 | J8 | 202 | CYC | O2D-CGD-CBD | 2.38 | 121.66 | 114.03 |
| 12 | P7 | 201 | CYC | C4A-C3A-C2A | -2.38 | 103.78 | 106.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | PA | 201 | CYC | C2A-C1A-NA | 2.38 | 113.50 | 110.05 |
| 12 | F3 | 202 | CYC | O2D-CGD-CBD | 2.38 | 121.66 | 114.03 |
| 12 | F1 | 202 | CYC | O2D-CGD-CBD | 2.38 | 121.66 | 114.03 |
| 12 | j5 | 1201 | CYC | C1B-NB-C4B | -2.37 | 107.64 | 110.67 |
| 12 | V3 | 202 | CYC | O2D-CGD-CBD | 2.37 | 121.66 | 114.03 |
| 12 | V1 | 202 | CYC | O2D-CGD-CBD | 2.37 | 121.66 | 114.03 |
| 12 | P1 | 201 | CYC | C2A-C1A-NA | 2.37 | 113.50 | 110.05 |
| 12 | P3 | 201 | CYC | C2A-C1A-NA | 2.37 | 113.50 | 110.05 |
| 12 | J6 | 202 | CYC | CAA-C2A-C1A | 2.37 | 129.21 | 125.01 |
| 12 | C2 | 201 | CYC | C2A-C1A-NA | 2.37 | 113.50 | 110.05 |
| 12 | C6 | 201 | CYC | C2A-C1A-NA | 2.37 | 113.50 | 110.05 |
| 12 | X3 | 202 | CYC | O2D-CGD-CBD | 2.37 | 121.65 | 114.03 |
| 12 | X1 | 202 | CYC | O2D-CGD-CBD | 2.37 | 121.65 | 114.03 |
| 12 | P9 | 201 | CYC | C2A-C1A-NA | 2.37 | 113.50 | 110.05 |
| 12 | P1 | 202 | CYC | O2D-CGD-CBD | 2.37 | 121.65 | 114.03 |
| 12 | X9 | 201 | CYC | C2C-C3C-C4C | 2.37 | 104.89 | 101.34 |
| 12 | HA | 201 | CYC | O2D-CGD-CBD | 2.37 | 121.65 | 114.03 |
| 12 | B8 | 201 | CYC | O2D-CGD-CBD | 2.37 | 121.65 | 114.03 |
| 12 | B3 | 201 | CYC | O2D-CGD-CBD | 2.37 | 121.65 | 114.03 |
| 12 | B1 | 201 | CYC | O2D-CGD-CBD | 2.37 | 121.65 | 114.03 |
| 12 | B2 | 201 | CYC | O2D-CGD-CBD | 2.37 | 121.65 | 114.03 |
| 12 | H3 | 202 | CYC | C2C-C3C-C4C | 2.37 | 104.89 | 101.34 |
| 12 | L2 | 202 | CYC | O2D-CGD-CBD | 2.37 | 121.64 | 114.03 |
| 12 | B6 | 201 | CYC | O2D-CGD-CBD | 2.37 | 121.64 | 114.03 |
| 12 | W7 | 201 | CYC | CHB-C1B-C2B | -2.37 | 122.26 | 126.95 |
| 12 | B4 | 202 | CYC | C1A-C2A-C3A | -2.37 | 104.16 | 106.78 |
| 12 | Z8 | 301 | CYC | C2A-C1A-NA | 2.37 | 113.49 | 110.05 |
| 12 | S7 | 201 | CYC | C2C-C1C-NC | 2.37 | 110.31 | 108.27 |
| 12 | M8 | 302 | CYC | C2A-C1A-NA | 2.36 | 113.49 | 110.05 |
| 12 | F9 | 302 | CYC | O2D-CGD-CBD | 2.36 | 121.62 | 114.03 |
| 12 | VA | 202 | CYC | O2D-CGD-CBD | 2.36 | 121.62 | 114.03 |
| 12 | Y8 | 201 | CYC | O2D-CGD-CBD | 2.36 | 121.62 | 114.03 |
| 12 | V9 | 202 | CYC | O2D-CGD-CBD | 2.36 | 121.62 | 114.03 |
| 12 | VA | 201 | CYC | C2A-C1A-NA | 2.36 | 113.48 | 110.05 |
| 12 | M8 | 302 | CYC | C2C-C3C-C4C | 2.36 | 104.88 | 101.34 |
| 12 | S4 | 202 | CYC | C2A-C1A-NA | 2.36 | 113.48 | 110.05 |
| 12 | Y4 | 201 | CYC | O2D-CGD-CBD | 2.36 | 121.62 | 114.03 |
| 12 | R1 | 201 | CYC | C1A-C2A-C3A | -2.36 | 104.17 | 106.78 |
| 12 | R3 | 201 | CYC | C1A-C2A-C3A | -2.36 | 104.17 | 106.78 |
| 12 | H6 | 201 | CYC | C2A-C1A-NA | 2.36 | 113.48 | 110.05 |
| 12 | RA | 201 | CYC | C2A-C1A-NA | 2.36 | 113.48 | 110.05 |
| 12 | R9 | 201 | CYC | C2A-C1A-NA | 2.36 | 113.48 | 110.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | D3 | 202 | CYC | C1A-C2A-C3A | -2.36 | 104.17 | 106.78 |
| 12 | JA | 202 | CYC | C1A-C2A-C3A | -2.36 | 104.17 | 106.78 |
| 12 | J9 | 202 | CYC | C1A-C2A-C3A | -2.36 | 104.17 | 106.78 |
| 12 | FA | 301 | CYC | C2C-C3C-C4C | 2.36 | 104.87 | 101.34 |
| 12 | F9 | 301 | CYC | C2C-C3C-C4C | 2.36 | 104.87 | 101.34 |
| 12 | R5 | 201 | CYC | C4A-C3A-C2A | -2.36 | 103.80 | 106.51 |
| 12 | DA | 201 | CYC | C1A-C2A-C3A | -2.36 | 104.17 | 106.78 |
| 12 | D9 | 201 | CYC | C1A-C2A-C3A | -2.36 | 104.17 | 106.78 |
| 12 | F9 | 303 | CYC | O2D-CGD-CBD | 2.36 | 121.60 | 114.03 |
| 12 | L5 | 201 | CYC | C4A-C3A-C2A | -2.35 | 103.80 | 106.51 |
| 12 | U4 | 201 | CYC | CAA-C2A-C1A | 2.35 | 129.17 | 125.01 |
| 12 | V3 | 201 | CYC | C2C-C3C-C4C | 2.35 | 104.86 | 101.34 |
| 12 | V1 | 201 | CYC | C2C-C3C-C4C | 2.35 | 104.86 | 101.34 |
| 12 | K3 | 201 | CYC | C2A-C1A-NA | 2.35 | 113.47 | 110.05 |
| 12 | J2 | 201 | CYC | O2D-CGD-CBD | 2.35 | 121.59 | 114.03 |
| 12 | XA | 201 | CYC | C2C-C3C-C4C | 2.35 | 104.86 | 101.34 |
| 12 | XA | 201 | CYC | C2A-C1A-NA | 2.35 | 113.47 | 110.05 |
| 12 | X9 | 201 | CYC | C2A-C1A-NA | 2.35 | 113.47 | 110.05 |
| 12 | H2 | 201 | CYC | C2A-C1A-NA | 2.35 | 113.47 | 110.05 |
| 12 | K1 | 201 | CYC | C2A-C1A-NA | 2.35 | 113.47 | 110.05 |
| 12 | H6 | 201 | CYC | C2C-C3C-C4C | 2.35 | 104.86 | 101.34 |
| 12 | O4 | 202 | CYC | O2D-CGD-CBD | 2.35 | 121.58 | 114.03 |
| 12 | O8 | 202 | CYC | O2D-CGD-CBD | 2.35 | 121.58 | 114.03 |
| 12 | U8 | 201 | CYC | CAA-C2A-C1A | 2.35 | 129.17 | 125.01 |
| 12 | D1 | 202 | CYC | C1A-C2A-C3A | -2.35 | 104.18 | 106.78 |
| 12 | TA | 301 | CYC | C2A-C1A-NA | 2.35 | 113.47 | 110.05 |
| 12 | F6 | 201 | CYC | C2A-C1A-NA | 2.35 | 113.47 | 110.05 |
| 12 | T9 | 301 | CYC | C2A-C1A-NA | 2.35 | 113.47 | 110.05 |
| 12 | T7 | 201 | CYC | C4A-C3A-C2A | -2.35 | 103.81 | 106.51 |
| 12 | B8 | 202 | CYC | C1A-C2A-C3A | -2.35 | 104.18 | 106.78 |
| 12 | J6 | 201 | CYC | O2D-CGD-CBD | 2.35 | 121.57 | 114.03 |
| 12 | TA | 301 | CYC | C2C-C3C-C4C | 2.35 | 104.85 | 101.34 |
| 12 | T9 | 301 | CYC | C2C-C3C-C4C | 2.35 | 104.85 | 101.34 |
| 12 | H1 | 201 | CYC | C2C-C3C-C4C | 2.35 | 104.85 | 101.34 |
| 12 | JA | 202 | CYC | C2C-C3C-C4C | 2.35 | 104.85 | 101.34 |
| 12 | J2 | 202 | CYC | C2C-C3C-C4C | 2.35 | 104.85 | 101.34 |
| 12 | J9 | 202 | CYC | C2C-C3C-C4C | 2.35 | 104.85 | 101.34 |
| 12 | R9 | 202 | CYC | O2D-CGD-CBD | 2.35 | 121.57 | 114.03 |
| 12 | F2 | 202 | CYC | O2D-CGD-CBD | 2.35 | 121.57 | 114.03 |
| 12 | TA | 302 | CYC | O2D-CGD-CBD | 2.34 | 121.56 | 114.03 |
| 12 | T9 | 302 | CYC | O2D-CGD-CBD | 2.34 | 121.56 | 114.03 |
| 12 | D4 | 201 | CYC | O2D-CGD-CBD | 2.34 | 121.56 | 114.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | D8 | 201 | CYC | O2D-CGD-CBD | 2.34 | 121.56 | 114.03 |
| 12 | D4 | 202 | CYC | C2A-C1A-NA | 2.34 | 113.45 | 110.05 |
| 12 | D8 | 202 | CYC | C2A-C1A-NA | 2.34 | 113.45 | 110.05 |
| 12 | b5 | 201 | CYC | C4A-C3A-C2A | -2.34 | 103.82 | 106.51 |
| 12 | HA | 202 | CYC | C2A-C1A-NA | 2.34 | 113.45 | 110.05 |
| 12 | N2 | 101 | CYC | C2A-C1A-NA | 2.34 | 113.45 | 110.05 |
| 12 | J4 | 201 | CYC | C2A-C1A-NA | 2.34 | 113.45 | 110.05 |
| 12 | N6 | 101 | CYC | C2A-C1A-NA | 2.34 | 113.45 | 110.05 |
| 12 | B1 | 202 | CYC | C2C-C3C-C4C | 2.34 | 104.84 | 101.34 |
| 12 | Z5 | 201 | CYC | C4A-C3A-C2A | -2.34 | 103.83 | 106.51 |
| 12 | F6 | 202 | CYC | O2D-CGD-CBD | 2.34 | 121.54 | 114.03 |
| 12 | V9 | 201 | CYC | C2A-C1A-NA | 2.34 | 113.45 | 110.05 |
| 12 | F5 | 201 | CYC | C4A-C3A-C2A | -2.34 | 103.83 | 106.51 |
| 12 | S7 | 201 | CYC | CHB-C1B-C2B | -2.33 | 122.32 | 126.95 |
| 12 | RA | 202 | CYC | O2D-CGD-CBD | 2.33 | 121.52 | 114.03 |
| 12 | R1 | 201 | CYC | C2A-C1A-NA | 2.33 | 113.44 | 110.05 |
| 12 | R3 | 201 | CYC | C2A-C1A-NA | 2.33 | 113.44 | 110.05 |
| 12 | H2 | 201 | CYC | C2C-C3C-C4C | 2.33 | 104.83 | 101.34 |
| 12 | J8 | 201 | CYC | C2A-C1A-NA | 2.33 | 113.44 | 110.05 |
| 12 | H4 | 201 | CYC | C2C-C3C-C4C | 2.33 | 104.83 | 101.34 |
| 12 | J4 | 201 | CYC | C2C-C3C-C4C | 2.33 | 104.83 | 101.34 |
| 12 | F4 | 202 | CYC | C2A-C1A-NA | 2.33 | 113.44 | 110.05 |
| 12 | F8 | 202 | CYC | C2A-C1A-NA | 2.33 | 113.44 | 110.05 |
| 12 | L3 | 202 | CYC | C2C-C3C-C4C | 2.33 | 104.83 | 101.34 |
| 12 | aA | 902 | CYC | C2C-C3C-C4C | 2.33 | 104.83 | 101.34 |
| 12 | U4 | 201 | CYC | C2C-C3C-C4C | 2.33 | 104.82 | 101.34 |
| 12 | U8 | 201 | CYC | C2C-C3C-C4C | 2.33 | 104.82 | 101.34 |
| 12 | X1 | 201 | CYC | C2A-C1A-NA | 2.33 | 113.43 | 110.05 |
| 12 | X3 | 201 | CYC | C2C-C3C-C4C | 2.33 | 104.82 | 101.34 |
| 12 | J6 | 202 | CYC | C2C-C3C-C4C | 2.33 | 104.82 | 101.34 |
| 12 | H8 | 201 | CYC | C2C-C3C-C4C | 2.33 | 104.82 | 101.34 |
| 12 | X1 | 201 | CYC | C2C-C3C-C4C | 2.33 | 104.82 | 101.34 |
| 12 | B3 | 202 | CYC | C1A-C2A-C3A | -2.32 | 104.21 | 106.78 |
| 12 | F3 | 201 | CYC | C2A-C1A-NA | 2.32 | 113.43 | 110.05 |
| 12 | F1 | 201 | CYC | C2A-C1A-NA | 2.32 | 113.43 | 110.05 |
| 12 | F3 | 201 | CYC | C2C-C3C-C4C | 2.32 | 104.81 | 101.34 |
| 12 | D1 | 202 | CYC | C2C-C3C-C4C | 2.32 | 104.81 | 101.34 |
| 12 | F1 | 201 | CYC | C2C-C3C-C4C | 2.32 | 104.81 | 101.34 |
| 12 | D6 | 201 | CYC | C2A-C1A-NA | 2.32 | 113.42 | 110.05 |
| 12 | N5 | 201 | CYC | C4A-C3A-C2A | -2.32 | 103.84 | 106.51 |
| 12 | Z4 | 301 | CYC | C2A-C1A-NA | 2.32 | 113.42 | 110.05 |
| 12 | J8 | 201 | CYC | C2C-C3C-C4C | 2.32 | 104.81 | 101.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | aA | 901 | CYC | C2A-C1A-NA | 2.32 | 113.42 | 110.05 |
| 12 | Q8 | 201 | CYC | O2D-CGD-CBD | 2.32 | 121.47 | 114.03 |
| 12 | a9 | 901 | CYC | C2C-C3C-C4C | 2.31 | 104.81 | 101.34 |
| 12 | J3 | 202 | CYC | C2A-C1A-NA | 2.31 | 113.42 | 110.05 |
| 12 | d5 | 201 | CYC | C4A-C3A-C2A | -2.31 | 103.85 | 106.51 |
| 12 | D2 | 201 | CYC | C1A-C2A-C3A | -2.31 | 104.22 | 106.78 |
| 12 | R3 | 201 | CYC | C2C-C3C-C4C | 2.31 | 104.80 | 101.34 |
| 12 | L4 | 202 | CYC | C2C-C3C-C4C | 2.31 | 104.80 | 101.34 |
| 12 | H9 | 202 | CYC | C2A-C1A-NA | 2.31 | 113.41 | 110.05 |
| 12 | G5 | 201 | CYC | C2C-C1C-NC | 2.31 | 110.26 | 108.27 |
| 12 | B3 | 202 | CYC | C2C-C3C-C4C | 2.31 | 104.80 | 101.34 |
| 12 | D3 | 202 | CYC | C2A-C1A-NA | 2.31 | 113.41 | 110.05 |
| 12 | B1 | 202 | CYC | C2A-C1A-NA | 2.31 | 113.41 | 110.05 |
| 12 | B1 | 202 | CYC | C1A-C2A-C3A | -2.31 | 104.23 | 106.78 |
| 12 | X3 | 201 | CYC | C2A-C1A-NA | 2.31 | 113.41 | 110.05 |
| 12 | Q4 | 201 | CYC | O2D-CGD-CBD | 2.31 | 121.44 | 114.03 |
| 12 | H3 | 202 | CYC | C2A-C1A-NA | 2.30 | 113.40 | 110.05 |
| 12 | L6 | 201 | CYC | C2C-C3C-C4C | 2.30 | 104.79 | 101.34 |
| 12 | N7 | 201 | CYC | C4A-C3A-C2A | -2.30 | 103.86 | 106.51 |
| 12 | T3 | 301 | CYC | C2A-C1A-NA | 2.30 | 113.40 | 110.05 |
| 12 | D1 | 202 | CYC | C2A-C1A-NA | 2.30 | 113.40 | 110.05 |
| 12 | T1 | 301 | CYC | C2A-C1A-NA | 2.30 | 113.40 | 110.05 |
| 12 | ZA | 202 | CYC | C2C-C3C-C4C | 2.30 | 104.79 | 101.34 |
| 12 | Z9 | 202 | CYC | C2C-C3C-C4C | 2.30 | 104.79 | 101.34 |
| 12 | D2 | 201 | CYC | C2A-C1A-NA | 2.30 | 113.39 | 110.05 |
| 12 | R1 | 201 | CYC | C2C-C3C-C4C | 2.30 | 104.78 | 101.34 |
| 12 | D3 | 202 | CYC | C2C-C3C-C4C | 2.30 | 104.78 | 101.34 |
| 12 | LA | 202 | CYC | C2C-C3C-C4C | 2.30 | 104.78 | 101.34 |
| 12 | L9 | 202 | CYC | C2C-C3C-C4C | 2.30 | 104.78 | 101.34 |
| 12 | H1 | 201 | CYC | C2A-C1A-NA | 2.30 | 113.39 | 110.05 |
| 12 | J2 | 202 | CYC | C1A-C2A-C3A | -2.29 | 104.24 | 106.78 |
| 12 | B3 | 202 | CYC | C2A-C1A-NA | 2.29 | 113.39 | 110.05 |
| 12 | k5 | 1201 | CYC | C1B-NB-C4B | -2.29 | 107.75 | 110.67 |
| 12 | W4 | 201 | CYC | C2C-C3C-C4C | 2.29 | 104.77 | 101.34 |
| 12 | W8 | 201 | CYC | C2C-C3C-C4C | 2.29 | 104.77 | 101.34 |
| 12 | Z3 | 201 | CYC | C2C-C3C-C4C | 2.29 | 104.77 | 101.34 |
| 12 | Z1 | 202 | CYC | C2C-C3C-C4C | 2.29 | 104.77 | 101.34 |
| 12 | T5 | 201 | CYC | C4A-C3A-C2A | -2.29 | 103.88 | 106.51 |
| 12 | L3 | 202 | CYC | C2A-C1A-NA | 2.29 | 113.38 | 110.05 |
| 12 | N2 | 101 | CYC | C2C-C3C-C4C | 2.29 | 104.76 | 101.34 |
| 12 | L2 | 201 | CYC | C2C-C3C-C4C | 2.28 | 104.76 | 101.34 |
| 12 | C5 | 201 | CYC | C2C-C1C-NC | 2.28 | 110.24 | 108.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | O4 | 201 | CYC | C2A-C1A-NA | 2.28 | 113.37 | 110.05 |
| 12 | O8 | 201 | CYC | C2A-C1A-NA | 2.28 | 113.37 | 110.05 |
| 12 | c7 | 201 | CYC | C2C-C1C-NC | 2.28 | 110.24 | 108.27 |
| 12 | aA | 902 | CYC | C2A-C1A-NA | 2.28 | 113.36 | 110.05 |
| 12 | W5 | 201 | CYC | C2C-C1C-NC | 2.28 | 110.24 | 108.27 |
| 12 | Q5 | 201 | CYC | C2C-C1C-NC | 2.28 | 110.23 | 108.27 |
| 12 | J3 | 202 | CYC | C2C-C3C-C4C | 2.27 | 104.75 | 101.34 |
| 12 | aA | 901 | CYC | C2C-C3C-C4C | 2.27 | 104.75 | 101.34 |
| 12 | M5 | 201 | CYC | C2C-C1C-NC | 2.27 | 110.23 | 108.27 |
| 12 | A5 | 201 | CYC | C2C-C1C-NC | 2.27 | 110.23 | 108.27 |
| 12 | RA | 201 | CYC | C2C-C3C-C4C | 2.27 | 104.74 | 101.34 |
| 12 | R9 | 201 | CYC | C2C-C3C-C4C | 2.27 | 104.74 | 101.34 |
| 12 | S5 | 201 | CYC | C2C-C1C-NC | 2.27 | 110.23 | 108.27 |
| 12 | J6 | 202 | CYC | C1A-C2A-C3A | -2.26 | 104.28 | 106.78 |
| 12 | JA | 202 | CYC | C2A-C1A-NA | 2.26 | 113.34 | 110.05 |
| 12 | J9 | 202 | CYC | C2A-C1A-NA | 2.26 | 113.34 | 110.05 |
| 12 | O4 | 201 | CYC | C4D-CHA-C1A | 2.26 | 131.51 | 128.81 |
| 12 | O8 | 201 | CYC | C4D-CHA-C1A | 2.26 | 131.51 | 128.81 |
| 12 | M7 | 201 | CYC | CAA-CBA-CGA | -2.26 | 108.74 | 113.60 |
| 12 | P9 | 201 | CYC | C2C-C3C-C4C | 2.26 | 104.72 | 101.34 |
| 12 | DA | 201 | CYC | C2A-C1A-NA | 2.26 | 113.33 | 110.05 |
| 12 | D9 | 201 | CYC | C2A-C1A-NA | 2.26 | 113.33 | 110.05 |
| 12 | O4 | 202 | CYC | CAA-C2A-C1A | 2.26 | 129.00 | 125.01 |
| 12 | O8 | 202 | CYC | CAA-C2A-C1A | 2.26 | 129.00 | 125.01 |
| 12 | U4 | 201 | CYC | C2A-C1A-NA | 2.25 | 113.33 | 110.05 |
| 12 | U8 | 201 | CYC | C2A-C1A-NA | 2.25 | 113.33 | 110.05 |
| 12 | M4 | 301 | CYC | C2C-C3C-C4C | 2.25 | 104.71 | 101.34 |
| 12 | ZA | 202 | CYC | C2A-C1A-NA | 2.25 | 113.33 | 110.05 |
| 12 | Z9 | 202 | CYC | C2A-C1A-NA | 2.25 | 113.33 | 110.05 |
| 12 | O4 | 201 | CYC | C2C-C3C-C4C | 2.25 | 104.71 | 101.34 |
| 12 | O8 | 201 | CYC | C2C-C3C-C4C | 2.25 | 104.71 | 101.34 |
| 12 | N6 | 101 | CYC | C2C-C3C-C4C | 2.25 | 104.71 | 101.34 |
| 12 | P1 | 202 | CYC | CAA-C2A-C1A | 2.25 | 128.99 | 125.01 |
| 12 | P3 | 202 | CYC | CAA-C2A-C1A | 2.25 | 128.99 | 125.01 |
| 12 | Z8 | 301 | CYC | C2C-C3C-C4C | 2.25 | 104.70 | 101.34 |
| 12 | k5 | 1201 | CYC | O2A-CGA-CBA | 2.24 | 121.24 | 114.03 |
| 12 | DA | 201 | CYC | C2C-C3C-C4C | 2.24 | 104.70 | 101.34 |
| 12 | j5 | 1201 | CYC | C2B-C1B-NB | 2.24 | 110.27 | 106.99 |
| 12 | U4 | 201 | CYC | C1A-C2A-C3A | -2.24 | 104.30 | 106.78 |
| 12 | U8 | 201 | CYC | C1A-C2A-C3A | -2.24 | 104.30 | 106.78 |
| 12 | F9 | 302 | CYC | CAA-C2A-C1A | 2.24 | 128.97 | 125.01 |
| 12 | T9 | 302 | CYC | CAA-C2A-C1A | 2.24 | 128.97 | 125.01 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | PA | 201 | CYC | C2C-C3C-C4C | 2.24 | 104.69 | 101.34 |
| 12 | I5 | 201 | CYC | C2C-C1C-NC | 2.24 | 110.20 | 108.27 |
| 12 | G7 | 201 | CYC | CAA-CBA-CGA | -2.24 | 108.79 | 113.60 |
| 12 | F9 | 303 | CYC | CAA-C2A-C1A | 2.23 | 128.96 | 125.01 |
| 12 | S7 | 201 | CYC | CAA-CBA-CGA | -2.23 | 108.79 | 113.60 |
| 12 | B2 | 201 | CYC | CAA-C2A-C1A | 2.23 | 128.96 | 125.01 |
| 12 | u7 | 201 | CYC | C2C-C1C-NC | 2.23 | 110.20 | 108.27 |
| 12 | K7 | 201 | CYC | C2C-C1C-NC | 2.23 | 110.20 | 108.27 |
| 12 | D6 | 201 | CYC | C2C-C3C-C4C | 2.23 | 104.68 | 101.34 |
| 12 | D2 | 201 | CYC | C2C-C3C-C4C | 2.23 | 104.68 | 101.34 |
| 12 | o7 | 201 | CYC | C2C-C1C-NC | 2.23 | 110.19 | 108.27 |
| 12 | G5 | 201 | CYC | CAA-CBA-CGA | -2.23 | 108.81 | 113.60 |
| 12 | B6 | 201 | CYC | CAA-C2A-C1A | 2.23 | 128.95 | 125.01 |
| 12 | J2 | 202 | CYC | C2A-C1A-NA | 2.23 | 113.29 | 110.05 |
| 12 | E7 | 201 | CYC | C2C-C1C-NC | 2.23 | 110.19 | 108.27 |
| 12 | k5 | 1201 | CYC | C2B-C1B-NB | 2.23 | 110.25 | 106.99 |
| 12 | j5 | 1201 | CYC | O2A-CGA-CBA | 2.22 | 121.18 | 114.03 |
| 12 | A7 | 201 | CYC | CAA-CBA-CGA | -2.22 | 108.82 | 113.60 |
| 12 | Z4 | 301 | CYC | C2C-C3C-C4C | 2.22 | 104.66 | 101.34 |
| 12 | TA | 302 | CYC | CAA-C2A-C1A | 2.22 | 128.93 | 125.01 |
| 12 | D9 | 201 | CYC | C2C-C3C-C4C | 2.22 | 104.66 | 101.34 |
| 12 | A5 | 201 | CYC | CAA-CBA-CGA | -2.22 | 108.83 | 113.60 |
| 12 | D4 | 202 | CYC | C2C-C3C-C4C | 2.22 | 104.66 | 101.34 |
| 12 | T3 | 302 | CYC | CAA-C2A-C1A | 2.21 | 128.92 | 125.01 |
| 12 | T1 | 302 | CYC | CAA-C2A-C1A | 2.21 | 128.92 | 125.01 |
| 12 | a5 | 201 | CYC | CBD-CAD-C3D | -2.21 | 108.84 | 112.62 |
| 12 | D8 | 202 | CYC | C2C-C3C-C4C | 2.21 | 104.65 | 101.34 |
| 12 | U5 | 201 | CYC | C2C-C1C-NC | 2.21 | 110.18 | 108.27 |
| 12 | P9 | 202 | CYC | CAA-C2A-C1A | 2.21 | 128.92 | 125.01 |
| 12 | C7 | 201 | CYC | CBD-CAD-C3D | -2.21 | 108.85 | 112.62 |
| 12 | U5 | 201 | CYC | CAA-CBA-CGA | -2.20 | 108.86 | 113.60 |
| 12 | O5 | 201 | CYC | CAA-CBA-CGA | -2.20 | 108.86 | 113.60 |
| 12 | c5 | 201 | CYC | CAA-CBA-CGA | -2.20 | 108.86 | 113.60 |
| 12 | S5 | 201 | CYC | CBD-CAD-C3D | -2.20 | 108.86 | 112.62 |
| 12 | J2 | 201 | CYC | CAA-C2A-C1A | 2.20 | 128.90 | 125.01 |
| 12 | e7 | 201 | CYC | CBD-CAD-C3D | -2.20 | 108.87 | 112.62 |
| 12 | B4 | 201 | CYC | CAA-C2A-C1A | 2.20 | 128.90 | 125.01 |
| 12 | I7 | 201 | CYC | CBD-CAD-C3D | -2.20 | 108.87 | 112.62 |
| 12 | BA | 201 | CYC | C2C-C3C-C4C | 2.20 | 104.63 | 101.34 |
| 12 | B9 | 201 | CYC | C2C-C3C-C4C | 2.20 | 104.63 | 101.34 |
| 12 | X5 | 201 | CYC | CHB-C1B-C2B | -2.20 | 122.59 | 126.95 |
| 12 | B4 | 202 | CYC | C4D-CHA-C1A | 2.20 | 131.43 | 128.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | I7 | 201 | CYC | CAA-CBA-CGA | -2.20 | 108.88 | 113.60 |
| 12 | U4 | 202 | CYC | CBC-CAC-C3C | 2.20 | 118.36 | 113.47 |
| 12 | U8 | 202 | CYC | CBC-CAC-C3C | 2.20 | 118.36 | 113.47 |
| 12 | L4 | 201 | CYC | CBC-CAC-C3C | 2.20 | 118.36 | 113.47 |
| 12 | L8 | 201 | CYC | CBC-CAC-C3C | 2.20 | 118.36 | 113.47 |
| 12 | D2 | 201 | CYC | C4D-CHA-C1A | 2.20 | 131.43 | 128.81 |
| 12 | e5 | 201 | CYC | CBD-CAD-C3D | -2.19 | 108.88 | 112.62 |
| 12 | S4 | 201 | CYC | CAA-C2A-C1A | 2.19 | 128.89 | 125.01 |
| 12 | S8 | 201 | CYC | CAA-C2A-C1A | 2.19 | 128.89 | 125.01 |
| 12 | O7 | 201 | CYC | CBD-CAD-C3D | -2.19 | 108.88 | 112.62 |
| 12 | K7 | 201 | CYC | CBD-CAD-C3D | -2.19 | 108.88 | 112.62 |
| 12 | q7 | 201 | CYC | CAA-CBA-CGA | -2.19 | 108.89 | 113.60 |
| 12 | k7 | 201 | CYC | CAA-CBA-CGA | -2.19 | 108.89 | 113.60 |
| 12 | PA | 202 | CYC | CAA-C2A-C1A | 2.19 | 128.88 | 125.01 |
| 12 | F4 | 201 | CYC | CAA-C2A-C1A | 2.19 | 128.88 | 125.01 |
| 12 | F8 | 201 | CYC | CAA-C2A-C1A | 2.19 | 128.88 | 125.01 |
| 12 | Q7 | 201 | CYC | C2C-C1C-NC | 2.19 | 110.16 | 108.27 |
| 12 | G7 | 201 | CYC | C2C-C1C-NC | 2.19 | 110.16 | 108.27 |
| 12 | V3 | 202 | CYC | CBC-CAC-C3C | 2.19 | 118.34 | 113.47 |
| 12 | V1 | 202 | CYC | CBC-CAC-C3C | 2.19 | 118.34 | 113.47 |
| 12 | A7 | 201 | CYC | CBD-CAD-C3D | -2.19 | 108.88 | 112.62 |
| 12 | B8 | 201 | CYC | CAA-C2A-C1A | 2.19 | 128.88 | 125.01 |
| 12 | J6 | 201 | CYC | CAA-C2A-C1A | 2.19 | 128.88 | 125.01 |
| 12 | A7 | 201 | CYC | C2C-C1C-NC | 2.19 | 110.16 | 108.27 |
| 12 | W4 | 201 | CYC | C2A-C1A-NA | 2.19 | 113.23 | 110.05 |
| 12 | W8 | 201 | CYC | C2A-C1A-NA | 2.19 | 113.23 | 110.05 |
| 12 | i7 | 201 | CYC | C2C-C1C-NC | 2.19 | 110.16 | 108.27 |
| 12 | a7 | 201 | CYC | CAA-CBA-CGA | -2.18 | 108.90 | 113.60 |
| 12 | Z4 | 301 | CYC | C4D-CHA-C1A | 2.18 | 131.42 | 128.81 |
| 12 | s7 | 201 | CYC | CAA-CBA-CGA | -2.18 | 108.91 | 113.60 |
| 12 | PA | 201 | CYC | C4D-CHA-C1A | 2.18 | 131.41 | 128.81 |
| 12 | L3 | 202 | CYC | C4D-CHA-C1A | 2.18 | 131.41 | 128.81 |
| 12 | P9 | 201 | CYC | C4D-CHA-C1A | 2.18 | 131.41 | 128.81 |
| 12 | aA | 902 | CYC | C4D-CHA-C1A | 2.18 | 131.41 | 128.81 |
| 12 | FA | 301 | CYC | C4D-CHA-C1A | 2.18 | 131.41 | 128.81 |
| 12 | R5 | 201 | CYC | CHB-C1B-C2B | -2.18 | 122.63 | 126.95 |
| 12 | s7 | 201 | CYC | CBD-CAD-C3D | -2.18 | 108.90 | 112.62 |
| 12 | k5 | 1201 | CYC | CBB-CAB-C3B | -2.18 | 106.42 | 112.43 |
| 12 | M8 | 301 | CYC | C2C-C3C-C4C | 2.18 | 104.60 | 101.34 |
| 12 | M5 | 201 | CYC | CBD-CAD-C3D | -2.18 | 108.90 | 112.62 |
| 12 | k7 | 201 | CYC | CBD-CAD-C3D | -2.18 | 108.90 | 112.62 |
| 12 | M7 | 201 | CYC | CBD-CAD-C3D | -2.18 | 108.91 | 112.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | WA | 201 | CYC | CAA-C2A-C1A | 2.18 | 128.86 | 125.01 |
| 12 | W9 | 201 | CYC | CAA-C2A-C1A | 2.18 | 128.86 | 125.01 |
| 12 | Y7 | 201 | CYC | CBD-CAD-C3D | -2.18 | 108.91 | 112.62 |
| 12 | L6 | 202 | CYC | CAA-C2A-C1A | 2.18 | 128.86 | 125.01 |
| 12 | H2 | 202 | CYC | CAA-C2A-C1A | 2.18 | 128.86 | 125.01 |
| 12 | H6 | 202 | CYC | CAA-C2A-C1A | 2.18 | 128.86 | 125.01 |
| 12 | BA | 201 | CYC | C4D-CHA-C1A | 2.17 | 131.41 | 128.81 |
| 12 | B9 | 201 | CYC | C4D-CHA-C1A | 2.17 | 131.41 | 128.81 |
| 12 | Q5 | 201 | CYC | C2C-C3C-C4C | 2.17 | 104.60 | 101.34 |
| 12 | m7 | 201 | CYC | CBD-CAD-C3D | -2.17 | 108.91 | 112.62 |
| 12 | H1 | 201 | CYC | C4D-CHA-C1A | 2.17 | 131.41 | 128.81 |
| 12 | Y5 | 201 | CYC | CAA-CBA-CGA | -2.17 | 108.93 | 113.60 |
| 12 | m7 | 201 | CYC | CAA-CBA-CGA | -2.17 | 108.93 | 113.60 |
| 12 | q7 | 201 | CYC | CBD-CAD-C3D | -2.17 | 108.91 | 112.62 |
| 12 | H3 | 202 | CYC | C4D-CHA-C1A | 2.17 | 131.40 | 128.81 |
| 12 | Y7 | 201 | CYC | C2C-C1C-NC | 2.17 | 110.14 | 108.27 |
| 12 | N7 | 201 | CYC | CHB-C1B-C2B | -2.17 | 122.65 | 126.95 |
| 12 | C7 | 201 | CYC | CAA-CBA-CGA | -2.17 | 108.93 | 113.60 |
| 12 | X3 | 202 | CYC | CBC-CAC-C3C | 2.17 | 118.30 | 113.47 |
| 12 | X1 | 202 | CYC | CBC-CAC-C3C | 2.17 | 118.30 | 113.47 |
| 12 | H8 | 202 | CYC | CAA-C2A-C1A | 2.17 | 128.85 | 125.01 |
| 12 | i7 | 201 | CYC | CBD-CAD-C3D | -2.17 | 108.92 | 112.62 |
| 12 | O5 | 201 | CYC | C2C-C1C-NC | 2.17 | 110.14 | 108.27 |
| 12 | B3 | 201 | CYC | CAA-C2A-C1A | 2.17 | 128.84 | 125.01 |
| 12 | B1 | 201 | CYC | CAA-C2A-C1A | 2.17 | 128.84 | 125.01 |
| 12 | W8 | 202 | CYC | CAA-C2A-C1A | 2.17 | 128.84 | 125.01 |
| 12 | Z3 | 202 | CYC | CAA-C2A-C1A | 2.17 | 128.84 | 125.01 |
| 12 | Z1 | 201 | CYC | CAA-C2A-C1A | 2.17 | 128.84 | 125.01 |
| 12 | M7 | 201 | CYC | C2C-C3C-C4C | 2.17 | 104.58 | 101.34 |
| 12 | e7 | 201 | CYC | C2C-C1C-NC | 2.17 | 110.14 | 108.27 |
| 12 | J6 | 202 | CYC | C2A-C1A-NA | 2.17 | 113.20 | 110.05 |
| 12 | LA | 201 | CYC | CAA-C2A-C1A | 2.17 | 128.84 | 125.01 |
| 12 | L9 | 201 | CYC | CAA-C2A-C1A | 2.17 | 128.84 | 125.01 |
| 12 | g7 | 201 | CYC | CAA-CBA-CGA | -2.17 | 108.94 | 113.60 |
| 12 | W4 | 202 | CYC | CAA-C2A-C1A | 2.17 | 128.84 | 125.01 |
| 12 | Z3 | 201 | CYC | C4D-CHA-C1A | 2.17 | 131.40 | 128.81 |
| 12 | Z1 | 202 | CYC | C4D-CHA-C1A | 2.17 | 131.40 | 128.81 |
| 12 | H7 | 201 | CYC | CHB-C1B-C2B | -2.16 | 122.66 | 126.95 |
| 12 | CA | 201 | CYC | CAA-C2A-C1A | 2.16 | 128.84 | 125.01 |
| 12 | C9 | 201 | CYC | CAA-C2A-C1A | 2.16 | 128.84 | 125.01 |
| 12 | D6 | 201 | CYC | C4D-CHA-C1A | 2.16 | 131.39 | 128.81 |
| 12 | v7 | 201 | CYC | CHB-C1B-C2B | -2.16 | 122.66 | 126.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | B4 | 202 | CYC | C2C-C3C-C4C | 2.16 | 104.58 | 101.34 |
| 12 | Q5 | 201 | CYC | CBD-CAD-C3D | -2.16 | 108.93 | 112.62 |
| 12 | U5 | 201 | CYC | CBD-CAD-C3D | -2.16 | 108.93 | 112.62 |
| 12 | B8 | 202 | CYC | C2C-C3C-C4C | 2.16 | 104.58 | 101.34 |
| 12 | E7 | 201 | CYC | CBD-CAD-C3D | -2.16 | 108.93 | 112.62 |
| 12 | J8 | 202 | CYC | CBC-CAC-C3C | 2.16 | 118.28 | 113.47 |
| 12 | a5 | 201 | CYC | CAA-CBA-CGA | -2.16 | 108.95 | 113.60 |
| 12 | W5 | 201 | CYC | CBD-CAD-C3D | -2.16 | 108.93 | 112.62 |
| 12 | J4 | 202 | CYC | CAA-C2A-C1A | 2.16 | 128.83 | 125.01 |
| 12 | J8 | 202 | CYC | CAA-C2A-C1A | 2.16 | 128.83 | 125.01 |
| 12 | u7 | 201 | CYC | C2C-C3C-C4C | 2.16 | 104.57 | 101.34 |
| 12 | Y7 | 201 | CYC | CAA-CBA-CGA | -2.16 | 108.96 | 113.60 |
| 12 | J9 | 201 | CYC | CBC-CAC-C3C | 2.16 | 118.27 | 113.47 |
| 12 | L2 | 202 | CYC | CAA-C2A-C1A | 2.16 | 128.83 | 125.01 |
| 12 | L7 | 201 | CYC | CHB-C1B-C2B | -2.16 | 122.67 | 126.95 |
| 12 | A5 | 201 | CYC | CBD-CAD-C3D | -2.16 | 108.94 | 112.62 |
| 12 | K5 | 201 | CYC | C2C-C1C-NC | 2.16 | 110.13 | 108.27 |
| 12 | B8 | 202 | CYC | C4D-CHA-C1A | 2.16 | 131.39 | 128.81 |
| 12 | F9 | 301 | CYC | C4D-CHA-C1A | 2.16 | 131.39 | 128.81 |
| 12 | H4 | 202 | CYC | CAA-C2A-C1A | 2.16 | 128.82 | 125.01 |
| 12 | P1 | 201 | CYC | C2C-C3C-C4C | 2.16 | 104.57 | 101.34 |
| 12 | P3 | 201 | CYC | C2C-C3C-C4C | 2.16 | 104.57 | 101.34 |
| 12 | F7 | 201 | CYC | CHB-C1B-C2B | -2.16 | 122.68 | 126.95 |
| 12 | F2 | 202 | CYC | CBC-CAC-C3C | 2.15 | 118.27 | 113.47 |
| 12 | ZA | 202 | CYC | C4D-CHA-C1A | 2.15 | 131.38 | 128.81 |
| 12 | Z9 | 202 | CYC | C4D-CHA-C1A | 2.15 | 131.38 | 128.81 |
| 12 | D5 | 201 | CYC | CHB-C1B-C2B | -2.15 | 122.68 | 126.95 |
| 12 | HA | 201 | CYC | CAA-C2A-C1A | 2.15 | 128.82 | 125.01 |
| 12 | H9 | 201 | CYC | CAA-C2A-C1A | 2.15 | 128.82 | 125.01 |
| 12 | o7 | 201 | CYC | C2C-C3C-C4C | 2.15 | 104.56 | 101.34 |
| 12 | O5 | 201 | CYC | CBD-CAD-C3D | -2.15 | 108.95 | 112.62 |
| 12 | W7 | 201 | CYC | CBD-CAD-C3D | -2.15 | 108.95 | 112.62 |
| 12 | K2 | 201 | CYC | CAA-C2A-C1A | 2.15 | 128.81 | 125.01 |
| 12 | e5 | 201 | CYC | C2C-C1C-NC | 2.15 | 110.13 | 108.27 |
| 12 | S7 | 201 | CYC | CBD-CAD-C3D | -2.15 | 108.95 | 112.62 |
| 12 | P1 | 201 | CYC | C4D-CHA-C1A | 2.15 | 131.38 | 128.81 |
| 12 | P3 | 201 | CYC | C4D-CHA-C1A | 2.15 | 131.38 | 128.81 |
| 12 | K6 | 201 | CYC | CAA-C2A-C1A | 2.15 | 128.81 | 125.01 |
| 12 | LA | 201 | CYC | CBC-CAC-C3C | 2.15 | 118.26 | 113.47 |
| 12 | H3 | 201 | CYC | CBC-CAC-C3C | 2.15 | 118.26 | 113.47 |
| 12 | L9 | 201 | CYC | CBC-CAC-C3C | 2.15 | 118.26 | 113.47 |
| 12 | H1 | 202 | CYC | CBC-CAC-C3C | 2.15 | 118.26 | 113.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | L2 | 201 | CYC | C4D-CHA-C1A | 2.15 | 131.38 | 128.81 |
| 12 | L6 | 201 | CYC | C4D-CHA-C1A | 2.15 | 131.38 | 128.81 |
| 12 | HA | 201 | CYC | CBC-CAC-C3C | 2.15 | 118.25 | 113.47 |
| 12 | H9 | 201 | CYC | CBC-CAC-C3C | 2.15 | 118.25 | 113.47 |
| 12 | W5 | 201 | CYC | C2C-C3C-C4C | 2.15 | 104.56 | 101.34 |
| 12 | H2 | 202 | CYC | CBC-CAC-C3C | 2.15 | 118.25 | 113.47 |
| 12 | L3 | 201 | CYC | CAA-C2A-C1A | 2.15 | 128.81 | 125.01 |
| 12 | L1 | 201 | CYC | CAA-C2A-C1A | 2.15 | 128.81 | 125.01 |
| 12 | DA | 202 | CYC | CBC-CAC-C3C | 2.15 | 118.25 | 113.47 |
| 12 | D9 | 202 | CYC | CBC-CAC-C3C | 2.15 | 118.25 | 113.47 |
| 12 | C3 | 201 | CYC | CAA-C2A-C1A | 2.15 | 128.81 | 125.01 |
| 12 | C1 | 201 | CYC | CAA-C2A-C1A | 2.15 | 128.81 | 125.01 |
| 12 | I5 | 201 | CYC | CAA-CBA-CGA | -2.15 | 108.98 | 113.60 |
| 12 | JA | 201 | CYC | CAA-C2A-C1A | 2.15 | 128.81 | 125.01 |
| 12 | J9 | 201 | CYC | CAA-C2A-C1A | 2.15 | 128.81 | 125.01 |
| 12 | O1 | 201 | CYC | CAA-C2A-C1A | 2.15 | 128.81 | 125.01 |
| 12 | O3 | 201 | CYC | CAA-C2A-C1A | 2.15 | 128.81 | 125.01 |
| 12 | JA | 201 | CYC | CBC-CAC-C3C | 2.15 | 118.25 | 113.47 |
| 12 | J2 | 201 | CYC | CBC-CAC-C3C | 2.15 | 118.24 | 113.47 |
| 12 | X1 | 202 | CYC | CAA-C2A-C1A | 2.15 | 128.80 | 125.01 |
| 12 | J4 | 202 | CYC | CBC-CAC-C3C | 2.15 | 118.24 | 113.47 |
| 12 | U7 | 201 | CYC | C2C-C1C-NC | 2.14 | 110.12 | 108.27 |
| 12 | XA | 202 | CYC | CBC-CAC-C3C | 2.14 | 118.24 | 113.47 |
| 12 | L3 | 201 | CYC | CBC-CAC-C3C | 2.14 | 118.24 | 113.47 |
| 12 | H6 | 202 | CYC | CBC-CAC-C3C | 2.14 | 118.24 | 113.47 |
| 12 | X9 | 202 | CYC | CBC-CAC-C3C | 2.14 | 118.24 | 113.47 |
| 12 | L1 | 201 | CYC | CBC-CAC-C3C | 2.14 | 118.24 | 113.47 |
| 12 | B7 | 201 | CYC | CHB-C1B-C2B | -2.14 | 122.70 | 126.95 |
| 12 | F6 | 202 | CYC | CBC-CAC-C3C | 2.14 | 118.24 | 113.47 |
| 12 | O7 | 201 | CYC | C2C-C1C-NC | 2.14 | 110.12 | 108.27 |
| 12 | L4 | 202 | CYC | C4D-CHA-C1A | 2.14 | 131.37 | 128.81 |
| 12 | j5 | 1201 | CYC | CBB-CAB-C3B | -2.14 | 106.52 | 112.43 |
| 12 | e5 | 201 | CYC | CAA-CBA-CGA | -2.14 | 108.99 | 113.60 |
| 12 | f5 | 201 | CYC | CHB-C1B-C2B | -2.14 | 122.70 | 126.95 |
| 12 | S4 | 201 | CYC | CBC-CAC-C3C | 2.14 | 118.24 | 113.47 |
| 12 | S8 | 201 | CYC | CBC-CAC-C3C | 2.14 | 118.24 | 113.47 |
| 12 | Q5 | 201 | CYC | CAA-CBA-CGA | -2.14 | 108.99 | 113.60 |
| 12 | T8 | 201 | CYC | CAA-C2A-C1A | 2.14 | 128.80 | 125.01 |
| 12 | Y4 | 201 | CYC | CHB-C4A-C3A | 2.14 | 130.41 | 124.90 |
| 12 | Y8 | 201 | CYC | CHB-C4A-C3A | 2.14 | 130.41 | 124.90 |
| 12 | E5 | 201 | CYC | CBD-CAD-C3D | -2.14 | 108.97 | 112.62 |
| 12 | G5 | 201 | CYC | CBD-CAD-C3D | -2.14 | 108.97 | 112.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | G7 | 201 | CYC | CBD-CAD-C3D | -2.14 | 108.97 | 112.62 |
| 12 | b5 | 201 | CYC | CHB-C1B-C2B | -2.14 | 122.71 | 126.95 |
| 12 | R7 | 201 | CYC | CHB-C1B-C2B | -2.14 | 122.71 | 126.95 |
| 12 | p7 | 201 | CYC | CHB-C1B-C2B | -2.14 | 122.71 | 126.95 |
| 12 | W5 | 201 | CYC | CAA-CBA-CGA | -2.14 | 109.00 | 113.60 |
| 12 | J3 | 201 | CYC | CBC-CAC-C3C | 2.14 | 118.23 | 113.47 |
| 12 | J1 | 201 | CYC | CBC-CAC-C3C | 2.14 | 118.23 | 113.47 |
| 12 | T4 | 201 | CYC | CAA-C2A-C1A | 2.14 | 128.79 | 125.01 |
| 12 | o7 | 201 | CYC | CBD-CAD-C3D | -2.14 | 108.97 | 112.62 |
| 12 | M8 | 302 | CYC | C4D-CHA-C1A | 2.14 | 131.37 | 128.81 |
| 12 | g7 | 201 | CYC | CBD-CAD-C3D | -2.14 | 108.97 | 112.62 |
| 12 | D4 | 201 | CYC | CBC-CAC-C3C | 2.14 | 118.23 | 113.47 |
| 12 | W7 | 201 | CYC | C2C-C1C-NC | 2.14 | 110.12 | 108.27 |
| 12 | O7 | 201 | CYC | CAA-CBA-CGA | -2.14 | 109.00 | 113.60 |
| 12 | K7 | 201 | CYC | CAA-CBA-CGA | -2.14 | 109.00 | 113.60 |
| 12 | v7 | 201 | CYC | C2C-C3C-C4C | 2.14 | 104.54 | 101.34 |
| 12 | I6 | 201 | CYC | CAA-C2A-C1A | 2.14 | 128.79 | 125.01 |
| 12 | X3 | 202 | CYC | CAA-C2A-C1A | 2.14 | 128.79 | 125.01 |
| 12 | D3 | 201 | CYC | CBC-CAC-C3C | 2.14 | 118.22 | 113.47 |
| 12 | D1 | 201 | CYC | CBC-CAC-C3C | 2.14 | 118.22 | 113.47 |
| 12 | J5 | 201 | CYC | CHB-C1B-C2B | -2.14 | 122.71 | 126.95 |
| 12 | K5 | 201 | CYC | CBD-CAD-C3D | -2.14 | 108.97 | 112.62 |
| 12 | B5 | 201 | CYC | CHB-C1B-C2B | -2.14 | 122.72 | 126.95 |
| 12 | C5 | 201 | CYC | CAA-CBA-CGA | -2.14 | 109.01 | 113.60 |
| 12 | Y4 | 201 | CYC | CBC-CAC-C3C | 2.14 | 118.22 | 113.47 |
| 12 | Y8 | 201 | CYC | CBC-CAC-C3C | 2.14 | 118.22 | 113.47 |
| 12 | R5 | 201 | CYC | C2C-C3C-C4C | 2.14 | 104.54 | 101.34 |
| 12 | AA | 201 | CYC | CAA-C2A-C1A | 2.14 | 128.79 | 125.01 |
| 12 | D4 | 201 | CYC | CAA-C2A-C1A | 2.14 | 128.79 | 125.01 |
| 12 | D8 | 201 | CYC | CAA-C2A-C1A | 2.14 | 128.79 | 125.01 |
| 12 | A9 | 201 | CYC | CAA-C2A-C1A | 2.14 | 128.79 | 125.01 |
| 12 | a7 | 201 | CYC | CBD-CAD-C3D | -2.14 | 108.98 | 112.62 |
| 12 | O4 | 202 | CYC | CBC-CAC-C3C | 2.14 | 118.22 | 113.47 |
| 12 | O8 | 202 | CYC | CBC-CAC-C3C | 2.14 | 118.22 | 113.47 |
| 12 | V9 | 202 | CYC | CBC-CAC-C3C | 2.14 | 118.22 | 113.47 |
| 12 | a5 | 201 | CYC | C2C-C1C-NC | 2.13 | 110.11 | 108.27 |
| 12 | Q8 | 201 | CYC | CAA-C2A-C1A | 2.13 | 128.78 | 125.01 |
| 12 | F3 | 202 | CYC | CAA-C2A-C1A | 2.13 | 128.78 | 125.01 |
| 12 | F1 | 202 | CYC | CAA-C2A-C1A | 2.13 | 128.78 | 125.01 |
| 12 | W4 | 201 | CYC | C4D-CHA-C1A | 2.13 | 131.36 | 128.81 |
| 12 | W8 | 201 | CYC | C4D-CHA-C1A | 2.13 | 131.36 | 128.81 |
| 12 | Z3 | 202 | CYC | CBC-CAC-C3C | 2.13 | 118.22 | 113.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | Z1 | 201 | CYC | CBC-CAC-C3C | 2.13 | 118.22 | 113.47 |
| 12 | R8 | 201 | CYC | CAA-C2A-C1A | 2.13 | 128.78 | 125.01 |
| 12 | e7 | 201 | CYC | CAA-CBA-CGA | -2.13 | 109.01 | 113.60 |
| 12 | X7 | 201 | CYC | CHB-C1B-C2B | -2.13 | 122.72 | 126.95 |
| 12 | B3 | 201 | CYC | CBC-CAC-C3C | 2.13 | 118.21 | 113.47 |
| 12 | B4 | 201 | CYC | CBC-CAC-C3C | 2.13 | 118.21 | 113.47 |
| 12 | B1 | 201 | CYC | CBC-CAC-C3C | 2.13 | 118.21 | 113.47 |
| 12 | J6 | 201 | CYC | CBC-CAC-C3C | 2.13 | 118.21 | 113.47 |
| 12 | B8 | 201 | CYC | CBC-CAC-C3C | 2.13 | 118.21 | 113.47 |
| 12 | X5 | 201 | CYC | C2C-C3C-C4C | 2.13 | 104.53 | 101.34 |
| 12 | L2 | 202 | CYC | CBC-CAC-C3C | 2.13 | 118.21 | 113.47 |
| 12 | V4 | 201 | CYC | CAA-C2A-C1A | 2.13 | 128.78 | 125.01 |
| 12 | V8 | 201 | CYC | CAA-C2A-C1A | 2.13 | 128.78 | 125.01 |
| 12 | Y5 | 201 | CYC | CBD-CAD-C3D | -2.13 | 108.98 | 112.62 |
| 12 | D8 | 201 | CYC | CBC-CAC-C3C | 2.13 | 118.21 | 113.47 |
| 12 | G6 | 201 | CYC | CAA-C2A-C1A | 2.13 | 128.78 | 125.01 |
| 12 | T3 | 302 | CYC | CBC-CAC-C3C | 2.13 | 118.21 | 113.47 |
| 12 | T1 | 302 | CYC | CBC-CAC-C3C | 2.13 | 118.21 | 113.47 |
| 12 | BA | 202 | CYC | CAA-C2A-C1A | 2.13 | 128.78 | 125.01 |
| 12 | B9 | 202 | CYC | CAA-C2A-C1A | 2.13 | 128.78 | 125.01 |
| 12 | VA | 202 | CYC | CBC-CAC-C3C | 2.13 | 118.21 | 113.47 |
| 12 | F4 | 202 | CYC | C4D-CHA-C1A | 2.13 | 131.35 | 128.81 |
| 12 | H4 | 201 | CYC | C4D-CHA-C1A | 2.13 | 131.35 | 128.81 |
| 12 | F8 | 202 | CYC | C4D-CHA-C1A | 2.13 | 131.35 | 128.81 |
| 12 | H8 | 201 | CYC | C4D-CHA-C1A | 2.13 | 131.35 | 128.81 |
| 12 | R1 | 202 | CYC | CBC-CAC-C3C | 2.13 | 118.21 | 113.47 |
| 12 | R3 | 202 | CYC | CBC-CAC-C3C | 2.13 | 118.21 | 113.47 |
| 12 | U4 | 201 | CYC | C4D-CHA-C1A | 2.13 | 131.35 | 128.81 |
| 12 | U8 | 201 | CYC | C4D-CHA-C1A | 2.13 | 131.35 | 128.81 |
| 12 | Z3 | 202 | CYC | CMB-C2B-C1B | 2.13 | 126.82 | 124.17 |
| 12 | Z1 | 201 | CYC | CMB-C2B-C1B | 2.13 | 126.82 | 124.17 |
| 12 | u7 | 201 | CYC | CBD-CAD-C3D | -2.13 | 108.99 | 112.62 |
| 12 | K5 | 201 | CYC | CAA-CBA-CGA | -2.13 | 109.03 | 113.60 |
| 12 | c5 | 201 | CYC | CBD-CAD-C3D | -2.13 | 108.99 | 112.62 |
| 12 | D2 | 202 | CYC | CHB-C4A-C3A | 2.13 | 130.37 | 124.90 |
| 12 | F2 | 202 | CYC | CAA-C2A-C1A | 2.13 | 128.77 | 125.01 |
| 12 | J3 | 201 | CYC | CAA-C2A-C1A | 2.13 | 128.77 | 125.01 |
| 12 | I2 | 201 | CYC | CAA-C2A-C1A | 2.13 | 128.77 | 125.01 |
| 12 | g7 | 201 | CYC | C2C-C3C-C4C | 2.13 | 104.52 | 101.34 |
| 12 | R4 | 201 | CYC | CAA-C2A-C1A | 2.12 | 128.77 | 125.01 |
| 12 | F6 | 202 | CYC | CAA-C2A-C1A | 2.12 | 128.77 | 125.01 |
| 12 | a9 | 901 | CYC | C4D-CHA-C1A | 2.12 | 131.35 | 128.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | G2 | 201 | CYC | CAA-C2A-C1A | 2.12 | 128.76 | 125.01 |
| 12 | h7 | 201 | CYC | CHB-C1B-C2B | -2.12 | 122.74 | 126.95 |
| 12 | E7 | 201 | CYC | CAA-CBA-CGA | -2.12 | 109.03 | 113.60 |
| 12 | W3 | 201 | CYC | CAA-C2A-C1A | 2.12 | 128.76 | 125.01 |
| 12 | b7 | 201 | CYC | CHB-C1B-C2B | -2.12 | 122.74 | 126.95 |
| 12 | TA | 302 | CYC | CBC-CAC-C3C | 2.12 | 118.19 | 113.47 |
| 12 | T9 | 302 | CYC | CBC-CAC-C3C | 2.12 | 118.19 | 113.47 |
| 12 | F3 | 202 | CYC | CMB-C2B-C1B | 2.12 | 126.81 | 124.17 |
| 12 | F1 | 202 | CYC | CMB-C2B-C1B | 2.12 | 126.81 | 124.17 |
| 12 | V3 | 202 | CYC | CAA-C2A-C1A | 2.12 | 128.76 | 125.01 |
| 12 | V1 | 202 | CYC | CAA-C2A-C1A | 2.12 | 128.76 | 125.01 |
| 12 | c7 | 201 | CYC | CBD-CAD-C3D | -2.12 | 109.00 | 112.62 |
| 12 | U7 | 201 | CYC | CAA-CBA-CGA | -2.12 | 109.04 | 113.60 |
| 12 | f7 | 201 | CYC | CHB-C1B-C2B | -2.12 | 122.75 | 126.95 |
| 12 | u7 | 201 | CYC | CAA-CBA-CGA | -2.12 | 109.04 | 113.60 |
| 12 | k5 | 1202 | CYC | CHB-C1B-C2B | -2.12 | 122.75 | 126.95 |
| 12 | XA | 202 | CYC | CAA-C2A-C1A | 2.12 | 128.76 | 125.01 |
| 12 | W7 | 201 | CYC | C2C-C3C-C4C | 2.12 | 104.51 | 101.34 |
| 12 | X7 | 201 | CYC | C2C-C3C-C4C | 2.12 | 104.51 | 101.34 |
| 12 | D7 | 201 | CYC | CHB-C1B-C2B | -2.12 | 122.75 | 126.95 |
| 12 | F3 | 202 | CYC | CBC-CAC-C3C | 2.12 | 118.18 | 113.47 |
| 12 | L6 | 202 | CYC | CBC-CAC-C3C | 2.12 | 118.18 | 113.47 |
| 12 | F1 | 202 | CYC | CBC-CAC-C3C | 2.12 | 118.18 | 113.47 |
| 12 | V3 | 202 | CYC | CMB-C2B-C1B | 2.12 | 126.81 | 124.17 |
| 12 | V1 | 202 | CYC | CMB-C2B-C1B | 2.12 | 126.81 | 124.17 |
| 12 | L8 | 201 | CYC | CAA-C2A-C1A | 2.12 | 128.75 | 125.01 |
| 12 | X4 | 201 | CYC | CAA-C2A-C1A | 2.12 | 128.75 | 125.01 |
| 12 | X8 | 201 | CYC | CAA-C2A-C1A | 2.12 | 128.75 | 125.01 |
| 12 | T7 | 201 | CYC | CHB-C1B-C2B | -2.12 | 122.75 | 126.95 |
| 12 | T5 | 201 | CYC | CHB-C1B-C2B | -2.12 | 122.75 | 126.95 |
| 12 | Q7 | 201 | CYC | CAA-CBA-CGA | -2.12 | 109.05 | 113.60 |
| 12 | Q7 | 201 | CYC | CBD-CAD-C3D | -2.12 | 109.01 | 112.62 |
| 12 | q7 | 201 | CYC | C2C-C3C-C4C | 2.12 | 104.51 | 101.34 |
| 12 | E5 | 201 | CYC | CAA-CBA-CGA | -2.12 | 109.05 | 113.60 |
| 12 | p7 | 201 | CYC | C2C-C3C-C4C | 2.12 | 104.51 | 101.34 |
| 12 | PA | 202 | CYC | CBC-CAC-C3C | 2.12 | 118.18 | 113.47 |
| 12 | P9 | 202 | CYC | CBC-CAC-C3C | 2.12 | 118.18 | 113.47 |
| 12 | JA | 201 | CYC | CHB-C4A-C3A | 2.12 | 130.34 | 124.90 |
| 12 | J9 | 201 | CYC | CHB-C4A-C3A | 2.12 | 130.34 | 124.90 |
| 12 | E5 | 201 | CYC | C2C-C1C-NC | 2.11 | 110.10 | 108.27 |
| 12 | Y4 | 201 | CYC | CAA-C2A-C1A | 2.11 | 128.75 | 125.01 |
| 12 | Y8 | 201 | CYC | CAA-C2A-C1A | 2.11 | 128.75 | 125.01 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | J1 | 201 | CYC | CAA-C2A-C1A | 2.11 | 128.75 | 125.01 |
| 12 | A2 | 201 | CYC | CAA-C2A-C1A | 2.11 | 128.75 | 125.01 |
| 12 | F9 | 303 | CYC | CBC-CAC-C3C | 2.11 | 118.17 | 113.47 |
| 12 | D6 | 202 | CYC | CHB-C4A-C3A | 2.11 | 130.34 | 124.90 |
| 12 | P4 | 201 | CYC | CAA-C2A-C1A | 2.11 | 128.75 | 125.01 |
| 12 | K8 | 201 | CYC | CAA-C2A-C1A | 2.11 | 128.75 | 125.01 |
| 12 | P8 | 201 | CYC | CAA-C2A-C1A | 2.11 | 128.75 | 125.01 |
| 12 | Q4 | 201 | CYC | CAA-C2A-C1A | 2.11 | 128.74 | 125.01 |
| 12 | F5 | 201 | CYC | CHB-C1B-C2B | -2.11 | 122.77 | 126.95 |
| 12 | F7 | 201 | CYC | C2C-C3C-C4C | 2.11 | 104.50 | 101.34 |
| 12 | Z8 | 301 | CYC | C4D-CHA-C1A | 2.11 | 131.33 | 128.81 |
| 12 | M5 | 201 | CYC | CAA-CBA-CGA | -2.11 | 109.06 | 113.60 |
| 12 | BA | 202 | CYC | CBC-CAC-C3C | 2.11 | 118.17 | 113.47 |
| 12 | B9 | 202 | CYC | CBC-CAC-C3C | 2.11 | 118.17 | 113.47 |
| 12 | c7 | 201 | CYC | C2C-C3C-C4C | 2.11 | 104.50 | 101.34 |
| 12 | OA | 201 | CYC | CAA-C2A-C1A | 2.11 | 128.74 | 125.01 |
| 12 | O9 | 201 | CYC | CAA-C2A-C1A | 2.11 | 128.74 | 125.01 |
| 12 | Q7 | 201 | CYC | C2C-C3C-C4C | 2.11 | 104.50 | 101.34 |
| 12 | W4 | 202 | CYC | CBC-CAC-C3C | 2.11 | 118.16 | 113.47 |
| 12 | W8 | 202 | CYC | CBC-CAC-C3C | 2.11 | 118.16 | 113.47 |
| 12 | N5 | 201 | CYC | CHB-C1B-C2B | -2.11 | 122.77 | 126.95 |
| 12 | U4 | 202 | CYC | CMB-C2B-C1B | 2.11 | 126.80 | 124.17 |
| 12 | U8 | 202 | CYC | CMB-C2B-C1B | 2.11 | 126.80 | 124.17 |
| 12 | Q4 | 201 | CYC | CBC-CAC-C3C | 2.11 | 118.16 | 113.47 |
| 12 | YA | 201 | CYC | CAA-C2A-C1A | 2.11 | 128.74 | 125.01 |
| 12 | Y9 | 201 | CYC | CAA-C2A-C1A | 2.11 | 128.74 | 125.01 |
| 12 | RA | 202 | CYC | CBC-CAC-C3C | 2.11 | 118.16 | 113.47 |
| 12 | R9 | 202 | CYC | CBC-CAC-C3C | 2.11 | 118.16 | 113.47 |
| 12 | W7 | 201 | CYC | CAA-CBA-CGA | -2.11 | 109.07 | 113.60 |
| 12 | k7 | 201 | CYC | C2C-C3C-C4C | 2.11 | 104.49 | 101.34 |
| 12 | k5 | 1201 | CYC | CAA-C2A-C1A | 2.11 | 128.73 | 125.01 |
| 12 | s7 | 201 | CYC | C2C-C1C-NC | 2.11 | 110.09 | 108.27 |
| 12 | e7 | 201 | CYC | C2C-C3C-C4C | 2.11 | 104.49 | 101.34 |
| 12 | DA | 202 | CYC | CAA-C2A-C1A | 2.10 | 128.73 | 125.01 |
| 12 | D9 | 202 | CYC | CAA-C2A-C1A | 2.10 | 128.73 | 125.01 |
| 12 | V7 | 201 | CYC | CHB-C1B-C2B | -2.10 | 122.78 | 126.95 |
| 12 | X9 | 202 | CYC | CAA-C2A-C1A | 2.10 | 128.73 | 125.01 |
| 12 | E5 | 201 | CYC | C2C-C3C-C4C | 2.10 | 104.49 | 101.34 |
| 12 | o7 | 201 | CYC | CAA-CBA-CGA | -2.10 | 109.08 | 113.60 |
| 12 | IA | 201 | CYC | CAA-C2A-C1A | 2.10 | 128.73 | 125.01 |
| 12 | UA | 201 | CYC | CAA-C2A-C1A | 2.10 | 128.73 | 125.01 |
| 12 | I9 | 201 | CYC | CAA-C2A-C1A | 2.10 | 128.73 | 125.01 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | U9 | 201 | CYC | CAA-C2A-C1A | 2.10 | 128.73 | 125.01 |
| 12 | Y1 | 201 | CYC | CAA-C2A-C1A | 2.10 | 128.73 | 125.01 |
| 12 | A6 | 201 | CYC | CAA-C2A-C1A | 2.10 | 128.73 | 125.01 |
| 12 | W1 | 201 | CYC | CAA-C2A-C1A | 2.10 | 128.73 | 125.01 |
| 12 | L5 | 201 | CYC | CHB-C1B-C2B | -2.10 | 122.78 | 126.95 |
| 12 | j5 | 1201 | CYC | CAA-C2A-C1A | 2.10 | 128.73 | 125.01 |
| 12 | A5 | 201 | CYC | C2C-C3C-C4C | 2.10 | 104.49 | 101.34 |
| 12 | F4 | 201 | CYC | CBC-CAC-C3C | 2.10 | 118.15 | 113.47 |
| 12 | F8 | 201 | CYC | CBC-CAC-C3C | 2.10 | 118.15 | 113.47 |
| 12 | Q8 | 201 | CYC | CBC-CAC-C3C | 2.10 | 118.14 | 113.47 |
| 12 | Y3 | 201 | CYC | CAA-C2A-C1A | 2.10 | 128.72 | 125.01 |
| 12 | J7 | 201 | CYC | CHB-C1B-C2B | -2.10 | 122.79 | 126.95 |
| 12 | k5 | 1204 | CYC | CHB-C1B-C2B | -2.10 | 122.79 | 126.95 |
| 12 | PA | 202 | CYC | CHB-C4A-C3A | 2.10 | 130.30 | 124.90 |
| 12 | P9 | 202 | CYC | CHB-C4A-C3A | 2.10 | 130.30 | 124.90 |
| 12 | K5 | 201 | CYC | C2C-C3C-C4C | 2.10 | 104.48 | 101.34 |
| 12 | L4 | 201 | CYC | CAA-C2A-C1A | 2.10 | 128.72 | 125.01 |
| 12 | R1 | 202 | CYC | CAA-C2A-C1A | 2.10 | 128.72 | 125.01 |
| 12 | S4 | 202 | CYC | C4D-CHA-C1A | 2.10 | 131.31 | 128.81 |
| 12 | ZA | 201 | CYC | CBC-CAC-C3C | 2.10 | 118.14 | 113.47 |
| 12 | P3 | 202 | CYC | CBC-CAC-C3C | 2.10 | 118.14 | 113.47 |
| 12 | TA | 301 | CYC | C4D-CHA-C1A | 2.10 | 131.31 | 128.81 |
| 12 | T9 | 301 | CYC | C4D-CHA-C1A | 2.10 | 131.31 | 128.81 |
| 12 | c7 | 201 | CYC | CAA-CBA-CGA | -2.10 | 109.09 | 113.60 |
| 12 | D9 | 202 | CYC | CHB-C4A-C3A | 2.10 | 130.29 | 124.90 |
| 12 | D3 | 201 | CYC | CHB-C4A-C3A | 2.10 | 130.29 | 124.90 |
| 12 | D1 | 201 | CYC | CHB-C4A-C3A | 2.10 | 130.29 | 124.90 |
| 12 | G5 | 201 | CYC | C2C-C3C-C4C | 2.10 | 104.48 | 101.34 |
| 12 | K2 | 201 | CYC | C1B-CHB-C4A | -2.10 | 122.96 | 128.08 |
| 12 | SA | 201 | CYC | CAA-C2A-C1A | 2.10 | 128.72 | 125.01 |
| 12 | P1 | 202 | CYC | CBC-CAC-C3C | 2.09 | 118.13 | 113.47 |
| 12 | H4 | 202 | CYC | CBC-CAC-C3C | 2.09 | 118.13 | 113.47 |
| 12 | H8 | 202 | CYC | CBC-CAC-C3C | 2.09 | 118.13 | 113.47 |
| 12 | S9 | 201 | CYC | CAA-C2A-C1A | 2.09 | 128.71 | 125.01 |
| 12 | H1 | 202 | CYC | CAA-C2A-C1A | 2.09 | 128.71 | 125.01 |
| 12 | K4 | 201 | CYC | CAA-C2A-C1A | 2.09 | 128.71 | 125.01 |
| 12 | I7 | 201 | CYC | C2C-C3C-C4C | 2.09 | 104.47 | 101.34 |
| 12 | j5 | 1202 | CYC | CHB-C1B-C2B | -2.09 | 122.80 | 126.95 |
| 12 | K4 | 201 | CYC | C1B-CHB-C4A | -2.09 | 122.97 | 128.08 |
| 12 | K8 | 201 | CYC | C1B-CHB-C4A | -2.09 | 122.97 | 128.08 |
| 12 | Y7 | 201 | CYC | C2C-C3C-C4C | 2.09 | 104.47 | 101.34 |
| 12 | k5 | 1203 | CYC | CHB-C1B-C2B | -2.09 | 122.80 | 126.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | S5 | 201 | CYC | CAA-CBA-CGA | -2.09 | 109.10 | 113.60 |
| 12 | N6 | 101 | CYC | C4D-CHA-C1A | 2.09 | 131.31 | 128.81 |
| 12 | JA | 201 | CYC | CMB-C2B-C1B | 2.09 | 126.78 | 124.17 |
| 12 | J9 | 201 | CYC | CMB-C2B-C1B | 2.09 | 126.78 | 124.17 |
| 12 | C7 | 201 | CYC | C2C-C3C-C4C | 2.09 | 104.47 | 101.34 |
| 12 | R7 | 201 | CYC | C2C-C3C-C4C | 2.09 | 104.47 | 101.34 |
| 12 | d7 | 201 | CYC | CHB-C1B-C2B | -2.09 | 122.80 | 126.95 |
| 12 | E4 | 201 | CYC | CAA-C2A-C1A | 2.09 | 128.71 | 125.01 |
| 12 | E8 | 201 | CYC | CAA-C2A-C1A | 2.09 | 128.71 | 125.01 |
| 12 | XA | 202 | CYC | CMB-C2B-C1B | 2.09 | 126.78 | 124.17 |
| 12 | X9 | 202 | CYC | CMB-C2B-C1B | 2.09 | 126.78 | 124.17 |
| 12 | P1 | 202 | CYC | CHB-C4A-C3A | 2.09 | 130.28 | 124.90 |
| 12 | P3 | 202 | CYC | CHB-C4A-C3A | 2.09 | 130.28 | 124.90 |
| 12 | K7 | 201 | CYC | C2C-C3C-C4C | 2.09 | 104.47 | 101.34 |
| 12 | F2 | 201 | CYC | C1B-CHB-C4A | -2.09 | 122.97 | 128.08 |
| 12 | D8 | 201 | CYC | CMB-C2B-C1B | 2.09 | 126.78 | 124.17 |
| 12 | P5 | 201 | CYC | CHB-C1B-C2B | -2.09 | 122.81 | 126.95 |
| 12 | j7 | 201 | CYC | CHB-C1B-C2B | -2.09 | 122.81 | 126.95 |
| 12 | QA | 201 | CYC | CAA-C2A-C1A | 2.09 | 128.70 | 125.01 |
| 12 | H3 | 201 | CYC | CAA-C2A-C1A | 2.09 | 128.70 | 125.01 |
| 12 | Z9 | 201 | CYC | CBC-CAC-C3C | 2.09 | 118.12 | 113.47 |
| 12 | O5 | 201 | CYC | C2C-C3C-C4C | 2.09 | 104.47 | 101.34 |
| 12 | k5 | 1201 | CYC | C1A-C2A-C3A | -2.09 | 104.47 | 106.78 |
| 12 | B6 | 201 | CYC | CBC-CAC-C3C | 2.09 | 118.12 | 113.47 |
| 12 | A8 | 201 | CYC | CAA-C2A-C1A | 2.09 | 128.70 | 125.01 |
| 12 | VA | 201 | CYC | C4D-CHA-C1A | 2.09 | 131.30 | 128.81 |
| 12 | V9 | 201 | CYC | C4D-CHA-C1A | 2.09 | 131.30 | 128.81 |
| 12 | E7 | 201 | CYC | C2C-C3C-C4C | 2.09 | 104.47 | 101.34 |
| 12 | R3 | 202 | CYC | CAA-C2A-C1A | 2.09 | 128.70 | 125.01 |
| 12 | U4 | 202 | CYC | CAA-C2A-C1A | 2.09 | 128.70 | 125.01 |
| 12 | U5 | 201 | CYC | C2C-C3C-C4C | 2.09 | 104.46 | 101.34 |
| 12 | DA | 202 | CYC | CHB-C4A-C3A | 2.09 | 130.26 | 124.90 |
| 12 | T4 | 201 | CYC | C1B-CHB-C4A | -2.09 | 122.98 | 128.08 |
| 12 | K6 | 201 | CYC | C1B-CHB-C4A | -2.09 | 122.98 | 128.08 |
| 12 | T8 | 201 | CYC | C1B-CHB-C4A | -2.09 | 122.98 | 128.08 |
| 12 | J4 | 202 | CYC | CMB-C2B-C1B | 2.09 | 126.77 | 124.17 |
| 12 | P7 | 201 | CYC | C2C-C3C-C4C | 2.09 | 104.46 | 101.34 |
| 12 | C7 | 201 | CYC | C2C-C1C-NC | 2.08 | 110.07 | 108.27 |
| 12 | D4 | 202 | CYC | C4D-CHA-C1A | 2.08 | 131.30 | 128.81 |
| 12 | F6 | 201 | CYC | C4D-CHA-C1A | 2.08 | 131.30 | 128.81 |
| 12 | D8 | 202 | CYC | C4D-CHA-C1A | 2.08 | 131.30 | 128.81 |
| 12 | Q1 | 201 | CYC | CAA-C2A-C1A | 2.08 | 128.69 | 125.01 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | Q3 | 201 | CYC | CAA-C2A-C1A | 2.08 | 128.69 | 125.01 |
| 12 | M5 | 201 | CYC | C2C-C3C-C4C | 2.08 | 104.46 | 101.34 |
| 12 | A4 | 201 | CYC | CAA-C2A-C1A | 2.08 | 128.69 | 125.01 |
| 12 | I1 | 201 | CYC | CAA-C2A-C1A | 2.08 | 128.69 | 125.01 |
| 12 | Z | 201 | CYC | CHB-C1B-C2B | -2.08 | 122.82 | 126.95 |
| 12 | h7 | 201 | CYC | C2C-C3C-C4C | 2.08 | 104.46 | 101.34 |
| 12 | H3 | 201 | CYC | CMB-C2B-C1B | 2.08 | 126.77 | 124.17 |
| 12 | H1 | 202 | CYC | CMB-C2B-C1B | 2.08 | 126.77 | 124.17 |
| 12 | H5 | 201 | CYC | CHB-C1B-C2B | -2.08 | 122.82 | 126.95 |
| 12 | L5 | 201 | CYC | C2C-C3C-C4C | 2.08 | 104.46 | 101.34 |
| 12 | U7 | 201 | CYC | CBD-CAD-C3D | -2.08 | 109.07 | 112.62 |
| 12 | X3 | 202 | CYC | CHB-C4A-C3A | 2.08 | 130.25 | 124.90 |
| 12 | X1 | 202 | CYC | CHB-C4A-C3A | 2.08 | 130.25 | 124.90 |
| 12 | V1 | 201 | CYC | C4D-CHA-C1A | 2.08 | 131.30 | 128.81 |
| 12 | i7 | 201 | CYC | C2C-C3C-C4C | 2.08 | 104.46 | 101.34 |
| 12 | L2 | 201 | CYC | CAB-C3B-C2B | 2.08 | 131.09 | 127.53 |
| 12 | U7 | 201 | CYC | C2C-C3C-C4C | 2.08 | 104.46 | 101.34 |
| 12 | a7 | 201 | CYC | C2C-C3C-C4C | 2.08 | 104.46 | 101.34 |
| 12 | YA | 201 | CYC | C1B-CHB-C4A | -2.08 | 123.00 | 128.08 |
| 12 | Y9 | 201 | CYC | C1B-CHB-C4A | -2.08 | 123.00 | 128.08 |
| 12 | i7 | 201 | CYC | CAA-CBA-CGA | -2.08 | 109.12 | 113.60 |
| 12 | L3 | 201 | CYC | CHB-C4A-C3A | 2.08 | 130.25 | 124.90 |
| 12 | L1 | 201 | CYC | CHB-C4A-C3A | 2.08 | 130.25 | 124.90 |
| 12 | XA | 201 | CYC | C4D-CHA-C1A | 2.08 | 131.29 | 128.81 |
| 12 | X9 | 201 | CYC | C4D-CHA-C1A | 2.08 | 131.29 | 128.81 |
| 12 | RA | 202 | CYC | CMB-C2B-C1B | 2.08 | 126.76 | 124.17 |
| 12 | R9 | 202 | CYC | CMB-C2B-C1B | 2.08 | 126.76 | 124.17 |
| 12 | O7 | 201 | CYC | C2C-C3C-C4C | 2.08 | 104.45 | 101.34 |
| 12 | OA | 201 | CYC | C1B-CHB-C4A | -2.08 | 123.00 | 128.08 |
| 12 | O9 | 201 | CYC | C1B-CHB-C4A | -2.08 | 123.00 | 128.08 |
| 12 | E9 | 201 | CYC | C1B-CHB-C4A | -2.08 | 123.00 | 128.08 |
| 12 | I3 | 201 | CYC | CAA-C2A-C1A | 2.08 | 128.69 | 125.01 |
| 12 | f7 | 201 | CYC | C2C-C3C-C4C | 2.08 | 104.45 | 101.34 |
| 12 | I7 | 201 | CYC | C2C-C1C-NC | 2.08 | 110.06 | 108.27 |
| 12 | F9 | 302 | CYC | CBC-CAC-C3C | 2.08 | 118.09 | 113.47 |
| 12 | B2 | 201 | CYC | CBC-CAC-C3C | 2.08 | 118.09 | 113.47 |
| 12 | VA | 202 | CYC | CAA-C2A-C1A | 2.08 | 128.68 | 125.01 |
| 12 | V9 | 202 | CYC | CAA-C2A-C1A | 2.08 | 128.68 | 125.01 |
| 12 | G3 | 201 | CYC | C1B-CHB-C4A | -2.08 | 123.01 | 128.08 |
| 12 | G1 | 201 | CYC | C1B-CHB-C4A | -2.08 | 123.01 | 128.08 |
| 12 | F8 | 202 | CYC | CHB-C1B-C2B | -2.08 | 122.83 | 126.95 |
| 12 | L7 | 201 | CYC | C2C-C3C-C4C | 2.08 | 104.45 | 101.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | b7 | 201 | CYC | C2C-C3C-C4C | 2.08 | 104.45 | 101.34 |
| 12 | I5 | 201 | CYC | CBD-CAD-C3D | -2.08 | 109.08 | 112.62 |
| 12 | A7 | 201 | CYC | C2C-C3C-C4C | 2.08 | 104.45 | 101.34 |
| 12 | U8 | 202 | CYC | CAA-C2A-C1A | 2.08 | 128.68 | 125.01 |
| 12 | F4 | 201 | CYC | CHB-C4A-C3A | 2.08 | 130.24 | 124.90 |
| 12 | F8 | 201 | CYC | CHB-C4A-C3A | 2.08 | 130.24 | 124.90 |
| 12 | D4 | 201 | CYC | CMB-C2B-C1B | 2.07 | 126.76 | 124.17 |
| 12 | T3 | 301 | CYC | C4D-CHA-C1A | 2.07 | 131.29 | 128.81 |
| 12 | T1 | 301 | CYC | C4D-CHA-C1A | 2.07 | 131.29 | 128.81 |
| 12 | ZA | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.68 | 125.01 |
| 12 | Z9 | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.68 | 125.01 |
| 12 | Q8 | 201 | CYC | CHB-C4A-C3A | 2.07 | 130.23 | 124.90 |
| 12 | D3 | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.68 | 125.01 |
| 12 | D1 | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.68 | 125.01 |
| 12 | D6 | 202 | CYC | CBC-CAC-C3C | 2.07 | 118.08 | 113.47 |
| 12 | Q9 | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.68 | 125.01 |
| 12 | BA | 202 | CYC | CHB-C4A-C3A | 2.07 | 130.23 | 124.90 |
| 12 | L6 | 202 | CYC | CHB-C4A-C3A | 2.07 | 130.23 | 124.90 |
| 12 | B9 | 202 | CYC | CHB-C4A-C3A | 2.07 | 130.23 | 124.90 |
| 12 | M8 | 301 | CYC | CAB-C3B-C2B | 2.07 | 131.07 | 127.53 |
| 12 | Z1 | 201 | CYC | CHB-C4A-C3A | 2.07 | 130.23 | 124.90 |
| 12 | L2 | 202 | CYC | CHB-C4A-C3A | 2.07 | 130.23 | 124.90 |
| 12 | J9 | 202 | CYC | C4D-CHA-C1A | 2.07 | 131.28 | 128.81 |
| 12 | EA | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.67 | 125.01 |
| 12 | RA | 202 | CYC | CAA-C2A-C1A | 2.07 | 128.67 | 125.01 |
| 12 | I4 | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.67 | 125.01 |
| 12 | I8 | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.67 | 125.01 |
| 12 | R9 | 202 | CYC | CAA-C2A-C1A | 2.07 | 128.67 | 125.01 |
| 12 | WA | 201 | CYC | C1B-CHB-C4A | -2.07 | 123.02 | 128.08 |
| 12 | W9 | 201 | CYC | C1B-CHB-C4A | -2.07 | 123.02 | 128.08 |
| 12 | E2 | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.67 | 125.01 |
| 12 | F5 | 201 | CYC | C2C-C3C-C4C | 2.07 | 104.44 | 101.34 |
| 12 | D3 | 201 | CYC | CMB-C2B-C1B | 2.07 | 126.75 | 124.17 |
| 12 | D1 | 201 | CYC | CMB-C2B-C1B | 2.07 | 126.75 | 124.17 |
| 12 | J8 | 202 | CYC | CMB-C2B-C1B | 2.07 | 126.75 | 124.17 |
| 12 | N4 | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.67 | 125.01 |
| 12 | N8 | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.67 | 125.01 |
| 12 | K3 | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.67 | 125.01 |
| 12 | K1 | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.67 | 125.01 |
| 12 | L9 | 201 | CYC | CHB-C4A-C3A | 2.07 | 130.22 | 124.90 |
| 12 | D2 | 202 | CYC | CBC-CAC-C3C | 2.07 | 118.07 | 113.47 |
| 12 | X3 | 201 | CYC | C4D-CHA-C1A | 2.07 | 131.28 | 128.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | X1 | 201 | CYC | C4D-CHA-C1A | 2.07 | 131.28 | 128.81 |
| 12 | V5 | 201 | CYC | CHB-C1B-C2B | -2.07 | 122.85 | 126.95 |
| 12 | A1 | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.67 | 125.01 |
| 12 | A3 | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.67 | 125.01 |
| 12 | E6 | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.67 | 125.01 |
| 12 | GA | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.66 | 125.01 |
| 12 | G9 | 201 | CYC | CAA-C2A-C1A | 2.07 | 128.66 | 125.01 |
| 12 | K3 | 201 | CYC | C1B-CHB-C4A | -2.07 | 123.03 | 128.08 |
| 12 | X4 | 201 | CYC | C1B-CHB-C4A | -2.07 | 123.03 | 128.08 |
| 12 | K1 | 201 | CYC | C1B-CHB-C4A | -2.07 | 123.03 | 128.08 |
| 12 | S5 | 201 | CYC | C2C-C3C-C4C | 2.07 | 104.44 | 101.34 |
| 12 | V5 | 201 | CYC | C2C-C3C-C4C | 2.07 | 104.44 | 101.34 |
| 12 | M8 | 301 | CYC | C4D-CHA-C1A | 2.07 | 131.28 | 128.81 |
| 12 | j5 | 1201 | CYC | CHB-C1B-C2B | -2.07 | 122.85 | 126.95 |
| 12 | P7 | 201 | CYC | CHB-C1B-C2B | -2.07 | 122.85 | 126.95 |
| 12 | O1 | 201 | CYC | C1B-CHB-C4A | -2.07 | 123.03 | 128.08 |
| 12 | O3 | 201 | CYC | C1B-CHB-C4A | -2.07 | 123.03 | 128.08 |
| 12 | ZA | 202 | CYC | CHB-C1B-C2B | -2.06 | 122.86 | 126.95 |
| 12 | J6 | 201 | CYC | CMB-C2B-C1B | 2.06 | 126.74 | 124.17 |
| 12 | ZA | 201 | CYC | CHB-C4A-C3A | 2.06 | 130.21 | 124.90 |
| 12 | Z9 | 201 | CYC | CHB-C4A-C3A | 2.06 | 130.21 | 124.90 |
| 12 | U3 | 201 | CYC | CAA-C2A-C1A | 2.06 | 128.66 | 125.01 |
| 12 | U1 | 201 | CYC | CAA-C2A-C1A | 2.06 | 128.66 | 125.01 |
| 12 | C5 | 201 | CYC | C2C-C3C-C4C | 2.06 | 104.43 | 101.34 |
| 12 | EA | 201 | CYC | C1B-CHB-C4A | -2.06 | 123.04 | 128.08 |
| 12 | Z3 | 202 | CYC | CHB-C4A-C3A | 2.06 | 130.21 | 124.90 |
| 12 | D4 | 201 | CYC | CHB-C4A-C3A | 2.06 | 130.21 | 124.90 |
| 12 | D8 | 201 | CYC | CHB-C4A-C3A | 2.06 | 130.21 | 124.90 |
| 12 | E9 | 201 | CYC | CAA-C2A-C1A | 2.06 | 128.66 | 125.01 |
| 12 | A | 201 | CYC | CHB-C1B-C2B | -2.06 | 122.86 | 126.95 |
| 12 | T7 | 201 | CYC | C2C-C3C-C4C | 2.06 | 104.43 | 101.34 |
| 12 | V3 | 201 | CYC | C4D-CHA-C1A | 2.06 | 131.27 | 128.81 |
| 12 | Q4 | 201 | CYC | CHB-C4A-C3A | 2.06 | 130.21 | 124.90 |
| 12 | F4 | 202 | CYC | CHB-C1B-C2B | -2.06 | 122.86 | 126.95 |
| 12 | U4 | 202 | CYC | CHB-C4A-C3A | 2.06 | 130.20 | 124.90 |
| 12 | U8 | 202 | CYC | CHB-C4A-C3A | 2.06 | 130.20 | 124.90 |
| 12 | P1 | 202 | CYC | CHD-C4C-NC | 2.06 | 127.66 | 125.20 |
| 12 | P3 | 202 | CYC | CHD-C4C-NC | 2.06 | 127.66 | 125.20 |
| 12 | k5 | 1201 | CYC | CHB-C1B-C2B | -2.06 | 122.86 | 126.95 |
| 12 | Z9 | 202 | CYC | CHB-C1B-C2B | -2.06 | 122.86 | 126.95 |
| 12 | H6 | 201 | CYC | C4D-CHA-C1A | 2.06 | 131.27 | 128.81 |
| 12 | B1 | 202 | CYC | CHB-C1B-C2B | -2.06 | 122.86 | 126.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | F6 | 201 | CYC | C1B-CHB-C4A | -2.06 | 123.04 | 128.08 |
| 12 | N2 | 101 | CYC | C4D-CHA-C1A | 2.06 | 131.27 | 128.81 |
| 12 | C4 | 201 | CYC | CAA-C2A-C1A | 2.06 | 128.65 | 125.01 |
| 12 | C8 | 201 | CYC | CAA-C2A-C1A | 2.06 | 128.65 | 125.01 |
| 12 | W4 | 202 | CYC | CMB-C2B-C1B | 2.06 | 126.74 | 124.17 |
| 12 | W8 | 202 | CYC | CMB-C2B-C1B | 2.06 | 126.74 | 124.17 |
| 12 | T9 | 302 | CYC | CHB-C4A-C3A | 2.06 | 130.20 | 124.90 |
| 12 | R1 | 201 | CYC | C4D-CHA-C1A | 2.06 | 131.27 | 128.81 |
| 12 | R3 | 201 | CYC | C4D-CHA-C1A | 2.06 | 131.27 | 128.81 |
| 12 | LA | 201 | CYC | CHB-C4A-C3A | 2.06 | 130.20 | 124.90 |
| 12 | G4 | 201 | CYC | CAA-C2A-C1A | 2.06 | 128.65 | 125.01 |
| 12 | G8 | 201 | CYC | CAA-C2A-C1A | 2.06 | 128.65 | 125.01 |
| 12 | B3 | 202 | CYC | CHB-C1B-C2B | -2.06 | 122.87 | 126.95 |
| 12 | J3 | 202 | CYC | C4D-CHA-C1A | 2.06 | 131.27 | 128.81 |
| 12 | aA | 901 | CYC | C4D-CHA-C1A | 2.06 | 131.27 | 128.81 |
| 12 | s7 | 201 | CYC | C2C-C3C-C4C | 2.06 | 104.42 | 101.34 |
| 12 | TA | 302 | CYC | CHB-C4A-C3A | 2.06 | 130.19 | 124.90 |
| 12 | C5 | 201 | CYC | CBD-CAD-C3D | -2.06 | 109.11 | 112.62 |
| 12 | V3 | 202 | CYC | CHB-C4A-C3A | 2.06 | 130.19 | 124.90 |
| 12 | V1 | 202 | CYC | CHB-C4A-C3A | 2.06 | 130.19 | 124.90 |
| 12 | S7 | 201 | CYC | C2C-C3C-C4C | 2.06 | 104.42 | 101.34 |
| 12 | G3 | 201 | CYC | CAA-C2A-C1A | 2.06 | 128.65 | 125.01 |
| 12 | G1 | 201 | CYC | CAA-C2A-C1A | 2.06 | 128.65 | 125.01 |
| 12 | aA | 901 | CYC | CAB-C3B-C2B | 2.06 | 131.05 | 127.53 |
| 12 | m7 | 201 | CYC | C2C-C3C-C4C | 2.06 | 104.42 | 101.34 |
| 12 | i7 | 201 | CYC | OC-C1C-NC | 2.06 | 127.43 | 124.94 |
| 12 | Y3 | 201 | CYC | C1B-CHB-C4A | -2.06 | 123.06 | 128.08 |
| 12 | Y1 | 201 | CYC | C1B-CHB-C4A | -2.06 | 123.06 | 128.08 |
| 12 | Y5 | 201 | CYC | C2C-C3C-C4C | 2.05 | 104.42 | 101.34 |
| 12 | IA | 201 | CYC | C1B-CHB-C4A | -2.05 | 123.06 | 128.08 |
| 12 | X8 | 201 | CYC | C1B-CHB-C4A | -2.05 | 123.06 | 128.08 |
| 12 | I9 | 201 | CYC | C1B-CHB-C4A | -2.05 | 123.06 | 128.08 |
| 12 | D6 | 202 | CYC | CAA-C2A-C1A | 2.05 | 128.64 | 125.01 |
| 12 | DA | 201 | CYC | C4D-CHA-C1A | 2.05 | 131.26 | 128.81 |
| 12 | D9 | 201 | CYC | C4D-CHA-C1A | 2.05 | 131.26 | 128.81 |
| 12 | D4 | 202 | CYC | CHB-C1B-C2B | -2.05 | 122.88 | 126.95 |
| 12 | D8 | 202 | CYC | CHB-C1B-C2B | -2.05 | 122.88 | 126.95 |
| 12 | J3 | 201 | CYC | CHB-C4A-C3A | 2.05 | 130.18 | 124.90 |
| 12 | J1 | 201 | CYC | CHB-C4A-C3A | 2.05 | 130.18 | 124.90 |
| 12 | AA | 201 | CYC | C1B-CHB-C4A | -2.05 | 123.06 | 128.08 |
| 12 | B6 | 201 | CYC | CHB-C4A-C3A | 2.05 | 130.18 | 124.90 |
| 12 | Z5 | 201 | CYC | CHB-C1B-C2B | -2.05 | 122.88 | 126.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | b5 | 201 | CYC | C2C-C3C-C4C | 2.05 | 104.41 | 101.34 |
| 12 | d5 | 201 | CYC | CHB-C1B-C2B | -2.05 | 122.88 | 126.95 |
| 12 | RA | 202 | CYC | CHB-C4A-C3A | 2.05 | 130.18 | 124.90 |
| 12 | R9 | 202 | CYC | CHB-C4A-C3A | 2.05 | 130.18 | 124.90 |
| 12 | r7 | 201 | CYC | CHB-C1B-C2B | -2.05 | 122.88 | 126.95 |
| 12 | D1 | 202 | CYC | CAB-C3B-C2B | 2.05 | 131.04 | 127.53 |
| 12 | B1 | 202 | CYC | C3A-C4A-NA | 2.05 | 114.91 | 110.53 |
| 12 | f5 | 201 | CYC | C2C-C3C-C4C | 2.05 | 104.41 | 101.34 |
| 12 | j7 | 201 | CYC | C2C-C3C-C4C | 2.05 | 104.41 | 101.34 |
| 12 | Q4 | 201 | CYC | CMB-C2B-C1B | 2.05 | 126.73 | 124.17 |
| 12 | F9 | 302 | CYC | CHB-C4A-C3A | 2.05 | 130.17 | 124.90 |
| 12 | B1 | 202 | CYC | C1B-CHB-C4A | -2.05 | 123.07 | 128.08 |
| 12 | A6 | 201 | CYC | C1B-CHB-C4A | -2.05 | 123.07 | 128.08 |
| 12 | F3 | 201 | CYC | CHB-C1B-C2B | -2.05 | 122.89 | 126.95 |
| 12 | F1 | 201 | CYC | CHB-C1B-C2B | -2.05 | 122.89 | 126.95 |
| 12 | L6 | 201 | CYC | CAB-C3B-C2B | 2.05 | 131.04 | 127.53 |
| 12 | J3 | 202 | CYC | CAB-C3B-C2B | 2.05 | 131.03 | 127.53 |
| 12 | KA | 201 | CYC | CAA-C2A-C1A | 2.05 | 128.63 | 125.01 |
| 12 | K9 | 201 | CYC | CAA-C2A-C1A | 2.05 | 128.63 | 125.01 |
| 12 | I5 | 201 | CYC | C2C-C3C-C4C | 2.05 | 104.41 | 101.34 |
| 12 | A1 | 201 | CYC | C1B-CHB-C4A | -2.05 | 123.07 | 128.08 |
| 12 | A3 | 201 | CYC | C1B-CHB-C4A | -2.05 | 123.07 | 128.08 |
| 12 | B3 | 202 | CYC | C1B-CHB-C4A | -2.05 | 123.07 | 128.08 |
| 12 | I4 | 201 | CYC | C1B-CHB-C4A | -2.05 | 123.07 | 128.08 |
| 12 | O4 | 201 | CYC | C1B-CHB-C4A | -2.05 | 123.07 | 128.08 |
| 12 | I8 | 201 | CYC | C1B-CHB-C4A | -2.05 | 123.07 | 128.08 |
| 12 | O8 | 201 | CYC | C1B-CHB-C4A | -2.05 | 123.07 | 128.08 |
| 12 | VA | 202 | CYC | CHB-C4A-C3A | 2.05 | 130.17 | 124.90 |
| 12 | V9 | 202 | CYC | CHB-C4A-C3A | 2.05 | 130.17 | 124.90 |
| 12 | O4 | 201 | CYC | CHB-C1B-C2B | -2.05 | 122.89 | 126.95 |
| 12 | O8 | 201 | CYC | CHB-C1B-C2B | -2.05 | 122.89 | 126.95 |
| 12 | T3 | 302 | CYC | CMB-C2B-C1B | 2.05 | 126.72 | 124.17 |
| 12 | T1 | 302 | CYC | CMB-C2B-C1B | 2.05 | 126.72 | 124.17 |
| 12 | L4 | 201 | CYC | CHB-C4A-C3A | 2.05 | 130.17 | 124.90 |
| 12 | L8 | 201 | CYC | CHB-C4A-C3A | 2.05 | 130.17 | 124.90 |
| 12 | R1 | 201 | CYC | CHB-C1B-C2B | -2.05 | 122.89 | 126.95 |
| 12 | R3 | 201 | CYC | CHB-C1B-C2B | -2.05 | 122.89 | 126.95 |
| 12 | I6 | 201 | CYC | C1B-CHB-C4A | -2.05 | 123.08 | 128.08 |
| 12 | X3 | 201 | CYC | C3A-C4A-NA | 2.05 | 114.90 | 110.53 |
| 12 | Z8 | 301 | CYC | CAB-C3B-C2B | 2.05 | 131.03 | 127.53 |
| 12 | L2 | 202 | CYC | CHD-C4C-NC | 2.05 | 127.64 | 125.20 |
| 12 | D2 | 202 | CYC | CAA-C2A-C1A | 2.05 | 128.63 | 125.01 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | F6 | 202 | CYC | CHB-C4A-C3A | 2.05 | 130.16 | 124.90 |
| 12 | F2 | 202 | CYC | CHB-C4A-C3A | 2.05 | 130.16 | 124.90 |
| 12 | B2 | 201 | CYC | CHB-C4A-C3A | 2.05 | 130.16 | 124.90 |
| 12 | C3 | 201 | CYC | C1B-CHB-C4A | -2.04 | 123.08 | 128.08 |
| 12 | C1 | 201 | CYC | C1B-CHB-C4A | -2.04 | 123.08 | 128.08 |
| 12 | C9 | 201 | CYC | C1B-CHB-C4A | -2.04 | 123.08 | 128.08 |
| 12 | Y4 | 201 | CYC | CMB-C2B-C1B | 2.04 | 126.72 | 124.17 |
| 12 | J1 | 201 | CYC | CMB-C2B-C1B | 2.04 | 126.72 | 124.17 |
| 12 | R3 | 202 | CYC | CHB-C4A-C3A | 2.04 | 130.16 | 124.90 |
| 12 | A4 | 201 | CYC | C1B-CHB-C4A | -2.04 | 123.09 | 128.08 |
| 12 | A8 | 201 | CYC | C1B-CHB-C4A | -2.04 | 123.09 | 128.08 |
| 12 | A9 | 201 | CYC | C1B-CHB-C4A | -2.04 | 123.09 | 128.08 |
| 12 | F9 | 303 | CYC | CHB-C4A-C3A | 2.04 | 130.16 | 124.90 |
| 12 | G2 | 201 | CYC | C1B-CHB-C4A | -2.04 | 123.09 | 128.08 |
| 12 | PA | 201 | CYC | C3A-C4A-NA | 2.04 | 114.89 | 110.53 |
| 12 | P9 | 201 | CYC | C3A-C4A-NA | 2.04 | 114.89 | 110.53 |
| 12 | j5 | 1201 | CYC | C1A-C2A-C3A | -2.04 | 104.52 | 106.78 |
| 12 | B3 | 201 | CYC | CHD-C4C-NC | 2.04 | 127.63 | 125.20 |
| 12 | JA | 202 | CYC | C4D-CHA-C1A | 2.04 | 131.25 | 128.81 |
| 12 | R1 | 201 | CYC | C1B-CHB-C4A | -2.04 | 123.09 | 128.08 |
| 12 | R3 | 201 | CYC | C1B-CHB-C4A | -2.04 | 123.09 | 128.08 |
| 12 | S1 | 201 | CYC | C1B-CHB-C4A | -2.04 | 123.09 | 128.08 |
| 12 | S3 | 201 | CYC | C1B-CHB-C4A | -2.04 | 123.09 | 128.08 |
| 12 | Q7 | 201 | CYC | OC-C1C-NC | 2.04 | 127.42 | 124.94 |
| 12 | C9 | 201 | CYC | C2C-C1C-NC | -2.04 | 106.51 | 108.27 |
| 12 | R1 | 202 | CYC | CMB-C2B-C1B | 2.04 | 126.72 | 124.17 |
| 12 | R3 | 202 | CYC | CMB-C2B-C1B | 2.04 | 126.72 | 124.17 |
| 12 | F4 | 202 | CYC | CAB-C3B-C2B | 2.04 | 131.02 | 127.53 |
| 12 | CA | 201 | CYC | C1B-CHB-C4A | -2.04 | 123.09 | 128.08 |
| 12 | B4 | 202 | CYC | CHB-C1B-C2B | -2.04 | 122.91 | 126.95 |
| 12 | M4 | 301 | CYC | C4D-CHA-C1A | 2.04 | 131.25 | 128.81 |
| 12 | Y8 | 201 | CYC | CMB-C2B-C1B | 2.04 | 126.71 | 124.17 |
| 12 | H2 | 202 | CYC | CHB-C4A-C3A | 2.04 | 130.15 | 124.90 |
| 12 | H6 | 202 | CYC | CHB-C4A-C3A | 2.04 | 130.15 | 124.90 |
| 12 | U4 | 201 | CYC | CHB-C1B-C2B | -2.04 | 122.91 | 126.95 |
| 12 | U8 | 201 | CYC | CHB-C1B-C2B | -2.04 | 122.91 | 126.95 |
| 12 | FA | 301 | CYC | C1B-CHB-C4A | -2.04 | 123.10 | 128.08 |
| 12 | F9 | 301 | CYC | C1B-CHB-C4A | -2.04 | 123.10 | 128.08 |
| 12 | X3 | 201 | CYC | CHB-C1B-C2B | -2.04 | 122.91 | 126.95 |
| 12 | X1 | 201 | CYC | CHB-C1B-C2B | -2.04 | 122.91 | 126.95 |
| 12 | U4 | 201 | CYC | C1B-CHB-C4A | -2.04 | 123.10 | 128.08 |
| 12 | U8 | 201 | CYC | C1B-CHB-C4A | -2.04 | 123.10 | 128.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | H6 | 202 | CYC | CMB-C2B-C1B | 2.04 | 126.71 | 124.17 |
| 12 | D3 | 202 | CYC | CAB-C3B-C2B | 2.04 | 131.01 | 127.53 |
| 12 | F3 | 201 | CYC | CAB-C3B-C2B | 2.04 | 131.01 | 127.53 |
| 12 | B3 | 201 | CYC | CHB-C4A-C3A | 2.04 | 130.14 | 124.90 |
| 12 | B1 | 201 | CYC | CHB-C4A-C3A | 2.04 | 130.14 | 124.90 |
| 12 | J4 | 202 | CYC | CHB-C4A-C3A | 2.04 | 130.14 | 124.90 |
| 12 | J8 | 202 | CYC | CHB-C4A-C3A | 2.04 | 130.14 | 124.90 |
| 12 | R4 | 201 | CYC | C1B-CHB-C4A | -2.04 | 123.11 | 128.08 |
| 12 | F9 | 303 | CYC | CMB-C2B-C1B | 2.04 | 126.71 | 124.17 |
| 12 | Z4 | 301 | CYC | CHB-C1B-C2B | -2.04 | 122.91 | 126.95 |
| 12 | aA | 901 | CYC | CHB-C1B-C2B | -2.04 | 122.91 | 126.95 |
| 12 | E5 | 201 | CYC | OC-C1C-NC | 2.04 | 127.41 | 124.94 |
| 12 | W7 | 201 | CYC | OC-C1C-NC | 2.04 | 127.41 | 124.94 |
| 12 | XA | 202 | CYC | CHB-C4A-C3A | 2.04 | 130.14 | 124.90 |
| 12 | J6 | 201 | CYC | CHB-C4A-C3A | 2.04 | 130.14 | 124.90 |
| 12 | F1 | 202 | CYC | CHB-C4A-C3A | 2.04 | 130.14 | 124.90 |
| 12 | LA | 202 | CYC | C4D-CHA-C1A | 2.04 | 131.24 | 128.81 |
| 12 | L9 | 202 | CYC | C4D-CHA-C1A | 2.04 | 131.24 | 128.81 |
| 12 | D8 | 202 | CYC | CAB-C3B-C2B | 2.04 | 131.01 | 127.53 |
| 12 | T3 | 302 | CYC | CHB-C4A-C3A | 2.04 | 130.13 | 124.90 |
| 12 | S4 | 201 | CYC | CHB-C4A-C3A | 2.04 | 130.13 | 124.90 |
| 12 | S8 | 201 | CYC | CHB-C4A-C3A | 2.04 | 130.13 | 124.90 |
| 12 | T1 | 302 | CYC | CHB-C4A-C3A | 2.04 | 130.13 | 124.90 |
| 12 | E3 | 201 | CYC | CAA-C2A-C1A | 2.04 | 128.61 | 125.01 |
| 12 | E1 | 201 | CYC | CAA-C2A-C1A | 2.04 | 128.61 | 125.01 |
| 12 | A2 | 201 | CYC | C1B-CHB-C4A | -2.04 | 123.11 | 128.08 |
| 12 | KA | 201 | CYC | C1B-CHB-C4A | -2.03 | 123.11 | 128.08 |
| 12 | G8 | 201 | CYC | C1B-CHB-C4A | -2.03 | 123.11 | 128.08 |
| 12 | K9 | 201 | CYC | C1B-CHB-C4A | -2.03 | 123.11 | 128.08 |
| 12 | W3 | 201 | CYC | C2C-C1C-NC | -2.03 | 106.52 | 108.27 |
| 12 | D3 | 202 | CYC | CHB-C1B-C2B | -2.03 | 122.92 | 126.95 |
| 12 | D1 | 202 | CYC | CHB-C1B-C2B | -2.03 | 122.92 | 126.95 |
| 12 | H4 | 202 | CYC | CHB-C4A-C3A | 2.03 | 130.13 | 124.90 |
| 12 | H8 | 202 | CYC | CHB-C4A-C3A | 2.03 | 130.13 | 124.90 |
| 12 | M4 | 301 | CYC | CAB-C3B-C2B | 2.03 | 131.01 | 127.53 |
| 12 | D1 | 202 | CYC | C3A-C4A-NA | 2.03 | 114.87 | 110.53 |
| 12 | VA | 201 | CYC | C3A-C4A-NA | 2.03 | 114.87 | 110.53 |
| 12 | SA | 201 | CYC | C1B-CHB-C4A | -2.03 | 123.12 | 128.08 |
| 12 | S9 | 201 | CYC | C1B-CHB-C4A | -2.03 | 123.12 | 128.08 |
| 12 | A | 201 | CYC | C2C-C3C-C4C | 2.03 | 104.38 | 101.34 |
| 12 | Z | 201 | CYC | C2C-C3C-C4C | 2.03 | 104.38 | 101.34 |
| 12 | Z8 | 301 | CYC | CHB-C1B-C2B | -2.03 | 122.92 | 126.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | DA | 201 | CYC | C1B-CHB-C4A | -2.03 | 123.12 | 128.08 |
| 12 | D9 | 201 | CYC | C1B-CHB-C4A | -2.03 | 123.12 | 128.08 |
| 12 | D3 | 202 | CYC | C3A-C4A-NA | 2.03 | 114.86 | 110.53 |
| 12 | J4 | 201 | CYC | C4D-CHA-C1A | 2.03 | 131.24 | 128.81 |
| 12 | J8 | 201 | CYC | C4D-CHA-C1A | 2.03 | 131.24 | 128.81 |
| 12 | R1 | 202 | CYC | CHB-C4A-C3A | 2.03 | 130.12 | 124.90 |
| 12 | J2 | 201 | CYC | CHB-C4A-C3A | 2.03 | 130.12 | 124.90 |
| 12 | d7 | 201 | CYC | C2C-C3C-C4C | 2.03 | 104.38 | 101.34 |
| 12 | M4 | 301 | CYC | C1B-CHB-C4A | -2.03 | 123.12 | 128.08 |
| 12 | VA | 201 | CYC | CHB-C1B-C2B | -2.03 | 122.93 | 126.95 |
| 12 | c5 | 201 | CYC | C2C-C3C-C4C | 2.03 | 104.38 | 101.34 |
| 12 | e5 | 201 | CYC | C2C-C3C-C4C | 2.03 | 104.38 | 101.34 |
| 12 | c7 | 201 | CYC | OC-C1C-NC | 2.03 | 127.40 | 124.94 |
| 12 | X1 | 201 | CYC | C3A-C4A-NA | 2.03 | 114.86 | 110.53 |
| 12 | H9 | 201 | CYC | CMB-C2B-C1B | 2.03 | 126.70 | 124.17 |
| 12 | O4 | 202 | CYC | CHB-C4A-C3A | 2.03 | 130.12 | 124.90 |
| 12 | O8 | 202 | CYC | CHB-C4A-C3A | 2.03 | 130.12 | 124.90 |
| 12 | W1 | 201 | CYC | C2C-C1C-NC | -2.03 | 106.52 | 108.27 |
| 12 | HA | 201 | CYC | CHB-C4A-C3A | 2.03 | 130.12 | 124.90 |
| 12 | H9 | 201 | CYC | CHB-C4A-C3A | 2.03 | 130.12 | 124.90 |
| 12 | P5 | 201 | CYC | C2C-C3C-C4C | 2.03 | 104.38 | 101.34 |
| 12 | K5 | 201 | CYC | OC-C1C-NC | 2.03 | 127.40 | 124.94 |
| 12 | P1 | 201 | CYC | CHB-C1B-C2B | -2.03 | 122.93 | 126.95 |
| 12 | P3 | 201 | CYC | CHB-C1B-C2B | -2.03 | 122.93 | 126.95 |
| 12 | D3 | 202 | CYC | C1B-CHB-C4A | -2.03 | 123.13 | 128.08 |
| 12 | D1 | 202 | CYC | C1B-CHB-C4A | -2.03 | 123.13 | 128.08 |
| 12 | H2 | 201 | CYC | CAB-C3B-C2B | 2.03 | 131.00 | 127.53 |
| 12 | e5 | 201 | CYC | OC-C1C-NC | 2.03 | 127.40 | 124.94 |
| 12 | J2 | 201 | CYC | CMB-C2B-C1B | 2.03 | 126.70 | 124.17 |
| 12 | F9 | 302 | CYC | CMB-C2B-C1B | 2.03 | 126.70 | 124.17 |
| 12 | GA | 201 | CYC | C1B-CHB-C4A | -2.03 | 123.13 | 128.08 |
| 12 | Z1 | 202 | CYC | CHB-C1B-C2B | -2.03 | 122.93 | 126.95 |
| 12 | TA | 301 | CYC | CAB-C3B-C2B | 2.03 | 131.00 | 127.53 |
| 12 | T9 | 301 | CYC | CAB-C3B-C2B | 2.03 | 131.00 | 127.53 |
| 12 | TA | 301 | CYC | C3A-C4A-NA | 2.03 | 114.85 | 110.53 |
| 12 | T9 | 301 | CYC | C3A-C4A-NA | 2.03 | 114.85 | 110.53 |
| 12 | FA | 301 | CYC | CHB-C1B-C2B | -2.03 | 122.93 | 126.95 |
| 12 | J3 | 202 | CYC | CHB-C1B-C2B | -2.03 | 122.93 | 126.95 |
| 12 | F9 | 301 | CYC | CHB-C1B-C2B | -2.03 | 122.93 | 126.95 |
| 12 | H7 | 201 | CYC | C2C-C3C-C4C | 2.03 | 104.37 | 101.34 |
| 12 | R8 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.13 | 128.08 |
| 12 | F3 | 202 | CYC | CHB-C4A-C3A | 2.02 | 130.11 | 124.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | I2 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.14 | 128.08 |
| 12 | D4 | 202 | CYC | C1B-CHB-C4A | -2.02 | 123.14 | 128.08 |
| 12 | D8 | 202 | CYC | C1B-CHB-C4A | -2.02 | 123.14 | 128.08 |
| 12 | W4 | 202 | CYC | CHB-C4A-C3A | 2.02 | 130.10 | 124.90 |
| 12 | W8 | 202 | CYC | CHB-C4A-C3A | 2.02 | 130.10 | 124.90 |
| 12 | F8 | 202 | CYC | CAB-C3B-C2B | 2.02 | 130.99 | 127.53 |
| 12 | B3 | 202 | CYC | C3A-C4A-NA | 2.02 | 114.85 | 110.53 |
| 12 | X9 | 202 | CYC | CHB-C4A-C3A | 2.02 | 130.10 | 124.90 |
| 12 | W3 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.14 | 128.08 |
| 12 | E2 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.14 | 128.08 |
| 12 | k5 | 1202 | CYC | C2C-C3C-C4C | 2.02 | 104.37 | 101.34 |
| 12 | H2 | 202 | CYC | CMB-C2B-C1B | 2.02 | 126.69 | 124.17 |
| 12 | H2 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.14 | 128.08 |
| 12 | B4 | 202 | CYC | C1B-CHB-C4A | -2.02 | 123.14 | 128.08 |
| 12 | L3 | 202 | CYC | CHB-C1B-C2B | -2.02 | 122.94 | 126.95 |
| 12 | V9 | 201 | CYC | CHB-C1B-C2B | -2.02 | 122.94 | 126.95 |
| 12 | R1 | 201 | CYC | CAB-C3B-C2B | 2.02 | 130.99 | 127.53 |
| 12 | H1 | 201 | CYC | C3A-C4A-NA | 2.02 | 114.84 | 110.53 |
| 12 | E4 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.14 | 128.08 |
| 12 | E6 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.14 | 128.08 |
| 12 | E8 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.14 | 128.08 |
| 12 | M8 | 301 | CYC | C1B-CHB-C4A | -2.02 | 123.14 | 128.08 |
| 12 | U1 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.14 | 128.08 |
| 12 | L6 | 202 | CYC | CHD-C4C-NC | 2.02 | 127.61 | 125.20 |
| 12 | H3 | 201 | CYC | CHB-C4A-C3A | 2.02 | 130.10 | 124.90 |
| 12 | H1 | 202 | CYC | CHB-C4A-C3A | 2.02 | 130.10 | 124.90 |
| 12 | G4 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.14 | 128.08 |
| 12 | B8 | 202 | CYC | CHB-C1B-C2B | -2.02 | 122.94 | 126.95 |
| 12 | B1 | 201 | CYC | CHD-C4C-NC | 2.02 | 127.61 | 125.20 |
| 12 | UA | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.14 | 128.08 |
| 12 | U9 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.14 | 128.08 |
| 12 | aA | 901 | CYC | C1B-CHB-C4A | -2.02 | 123.14 | 128.08 |
| 12 | H3 | 202 | CYC | C3A-C4A-NA | 2.02 | 114.84 | 110.53 |
| 12 | F1 | 201 | CYC | CAB-C3B-C2B | 2.02 | 130.99 | 127.53 |
| 12 | a5 | 201 | CYC | C2C-C3C-C4C | 2.02 | 104.36 | 101.34 |
| 12 | B4 | 201 | CYC | CHB-C4A-C3A | 2.02 | 130.09 | 124.90 |
| 12 | B8 | 201 | CYC | CHB-C4A-C3A | 2.02 | 130.09 | 124.90 |
| 12 | F3 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.15 | 128.08 |
| 12 | F1 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.15 | 128.08 |
| 12 | Z8 | 301 | CYC | C1B-CHB-C4A | -2.02 | 123.15 | 128.08 |
| 12 | J3 | 201 | CYC | CMB-C2B-C1B | 2.02 | 126.69 | 124.17 |
| 12 | B1 | 202 | CYC | C4D-CHA-C1A | 2.02 | 131.22 | 128.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | m7 | 201 | CYC | C2C-C1C-NC | 2.02 | 110.01 | 108.27 |
| 12 | P1 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.15 | 128.08 |
| 12 | P3 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.15 | 128.08 |
| 12 | B8 | 202 | CYC | C1B-CHB-C4A | -2.02 | 123.15 | 128.08 |
| 12 | a9 | 901 | CYC | CAB-C3B-C2B | 2.02 | 130.98 | 127.53 |
| 12 | X3 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.15 | 128.08 |
| 12 | X1 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.15 | 128.08 |
| 12 | S4 | 201 | CYC | CMB-C2B-C1B | 2.02 | 126.69 | 124.17 |
| 12 | S8 | 201 | CYC | CMB-C2B-C1B | 2.02 | 126.69 | 124.17 |
| 12 | BA | 201 | CYC | CAB-C3B-C2B | 2.02 | 130.98 | 127.53 |
| 12 | B9 | 201 | CYC | CAB-C3B-C2B | 2.02 | 130.98 | 127.53 |
| 12 | X1 | 201 | CYC | CAB-C3B-C2B | 2.02 | 130.98 | 127.53 |
| 12 | U4 | 201 | CYC | C3A-C4A-NA | 2.02 | 114.83 | 110.53 |
| 12 | J6 | 202 | CYC | C3A-C4A-NA | 2.02 | 114.83 | 110.53 |
| 12 | U8 | 201 | CYC | C3A-C4A-NA | 2.02 | 114.83 | 110.53 |
| 12 | G7 | 201 | CYC | C2C-C3C-C4C | 2.02 | 104.36 | 101.34 |
| 12 | Z3 | 202 | CYC | CHD-C4C-NC | 2.02 | 127.60 | 125.20 |
| 12 | Z1 | 201 | CYC | CHD-C4C-NC | 2.02 | 127.60 | 125.20 |
| 12 | V9 | 201 | CYC | C3A-C4A-NA | 2.02 | 114.83 | 110.53 |
| 12 | Q9 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.16 | 128.08 |
| 12 | BA | 201 | CYC | CHB-C1B-C2B | -2.02 | 122.95 | 126.95 |
| 12 | B9 | 201 | CYC | CHB-C1B-C2B | -2.02 | 122.95 | 126.95 |
| 12 | aA | 902 | CYC | CHB-C1B-C2B | -2.02 | 122.95 | 126.95 |
| 12 | Q8 | 201 | CYC | CMB-C2B-C1B | 2.02 | 126.68 | 124.17 |
| 12 | I7 | 201 | CYC | OC-C1C-NC | 2.02 | 127.38 | 124.94 |
| 12 | BA | 201 | CYC | C3A-C4A-NA | 2.02 | 114.83 | 110.53 |
| 12 | G9 | 201 | CYC | C1B-CHB-C4A | -2.02 | 123.16 | 128.08 |
| 12 | Z4 | 301 | CYC | CAB-C3B-C2B | 2.02 | 130.98 | 127.53 |
| 12 | H8 | 201 | CYC | CAB-C3B-C2B | 2.02 | 130.98 | 127.53 |
| 12 | W4 | 202 | CYC | CHD-C4C-NC | 2.02 | 127.60 | 125.20 |
| 12 | W8 | 202 | CYC | CHD-C4C-NC | 2.02 | 127.60 | 125.20 |
| 12 | W4 | 201 | CYC | CHB-C1B-C2B | -2.01 | 122.96 | 126.95 |
| 12 | W8 | 201 | CYC | CHB-C1B-C2B | -2.01 | 122.96 | 126.95 |
| 12 | Z3 | 201 | CYC | CAB-C3B-C2B | 2.01 | 130.97 | 127.53 |
| 12 | Z1 | 202 | CYC | CAB-C3B-C2B | 2.01 | 130.97 | 127.53 |
| 12 | G6 | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.16 | 128.08 |
| 12 | B9 | 201 | CYC | C3A-C4A-NA | 2.01 | 114.83 | 110.53 |
| 12 | Z3 | 201 | CYC | CHB-C1B-C2B | -2.01 | 122.96 | 126.95 |
| 12 | J3 | 202 | CYC | C1B-CHB-C4A | -2.01 | 123.16 | 128.08 |
| 12 | C7 | 201 | CYC | OC-C1C-NC | 2.01 | 127.38 | 124.94 |
| 12 | H4 | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.16 | 128.08 |
| 12 | H8 | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.16 | 128.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12 | LA | 202 | CYC | CHB-C1B-C2B | -2.01 | 122.96 | 126.95 |
| 12 | D4 | 202 | CYC | CAB-C3B-C2B | 2.01 | 130.97 | 127.53 |
| 12 | H6 | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.17 | 128.08 |
| 12 | W1 | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.17 | 128.08 |
| 12 | H4 | 201 | CYC | CAB-C3B-C2B | 2.01 | 130.97 | 127.53 |
| 12 | H4 | 202 | CYC | CMB-C2B-C1B | 2.01 | 126.68 | 124.17 |
| 12 | H8 | 202 | CYC | CMB-C2B-C1B | 2.01 | 126.68 | 124.17 |
| 12 | J7 | 201 | CYC | C2C-C3C-C4C | 2.01 | 104.35 | 101.34 |
| 12 | N6 | 101 | CYC | CAB-C3B-C2B | 2.01 | 130.97 | 127.53 |
| 12 | HA | 201 | CYC | CMB-C2B-C1B | 2.01 | 126.67 | 124.17 |
| 12 | X3 | 202 | CYC | CMB-C2B-C1B | 2.01 | 126.67 | 124.17 |
| 12 | X1 | 202 | CYC | CMB-C2B-C1B | 2.01 | 126.67 | 124.17 |
| 12 | PA | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.17 | 128.08 |
| 12 | P9 | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.17 | 128.08 |
| 12 | DA | 201 | CYC | CHB-C1B-C2B | -2.01 | 122.97 | 126.95 |
| 12 | C2 | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.17 | 128.08 |
| 12 | H4 | 201 | CYC | CHB-C1B-C2B | -2.01 | 122.97 | 126.95 |
| 12 | H8 | 201 | CYC | CHB-C1B-C2B | -2.01 | 122.97 | 126.95 |
| 12 | E3 | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.17 | 128.08 |
| 12 | E1 | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.17 | 128.08 |
| 12 | PA | 201 | CYC | CHB-C1B-C2B | -2.01 | 122.97 | 126.95 |
| 12 | P9 | 201 | CYC | CHB-C1B-C2B | -2.01 | 122.97 | 126.95 |
| 12 | C6 | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.17 | 128.08 |
| 12 | B4 | 201 | CYC | CMB-C2B-C1B | 2.01 | 126.67 | 124.17 |
| 12 | B3 | 202 | CYC | CAB-C3B-C2B | 2.01 | 130.96 | 127.53 |
| 12 | T3 | 301 | CYC | C1B-CHB-C4A | -2.01 | 123.18 | 128.08 |
| 12 | U3 | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.18 | 128.08 |
| 12 | T1 | 301 | CYC | C1B-CHB-C4A | -2.01 | 123.18 | 128.08 |
| 12 | J4 | 202 | CYC | CHD-C4C-NC | 2.01 | 127.59 | 125.20 |
| 12 | J8 | 202 | CYC | CHD-C4C-NC | 2.01 | 127.59 | 125.20 |
| 12 | L1 | 201 | CYC | CHD-C4C-NC | 2.01 | 127.59 | 125.20 |
| 12 | k5 | 1203 | CYC | C2C-C3C-C4C | 2.01 | 104.35 | 101.34 |
| 12 | B4 | 202 | CYC | C3A-C4A-NA | 2.01 | 114.81 | 110.53 |
| 12 | S1 | 201 | CYC | CAA-C2A-C1A | 2.01 | 128.56 | 125.01 |
| 12 | N4 | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.18 | 128.08 |
| 12 | N8 | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.18 | 128.08 |
| 12 | J2 | 202 | CYC | C4D-CHA-C1A | 2.01 | 131.21 | 128.81 |
| 12 | J4 | 201 | CYC | CAB-C3B-C2B | 2.01 | 130.96 | 127.53 |
| 12 | J8 | 201 | CYC | CAB-C3B-C2B | 2.01 | 130.96 | 127.53 |
| 12 | BA | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.18 | 128.08 |
| 12 | Z3 | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.18 | 128.08 |
| 12 | B9 | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.18 | 128.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12 | Z1 | 202 | CYC | C1B-CHB-C4A | -2.01 | 123.18 | 128.08 |
| 12 | W4 | 201 | CYC | C3A-C4A-NA | 2.01 | 114.81 | 110.53 |
| 12 | W8 | 201 | CYC | C3A-C4A-NA | 2.01 | 114.81 | 110.53 |
| 12 | B3 | 202 | CYC | C4D-CHA-C1A | 2.01 | 131.21 | 128.81 |
| 12 | F6 | 201 | CYC | CHB-C1B-C2B | -2.01 | 122.97 | 126.95 |
| 12 | R3 | 201 | CYC | CAB-C3B-C2B | 2.01 | 130.96 | 127.53 |
| 12 | H1 | 201 | CYC | CHB-C1B-C2B | -2.01 | 122.97 | 126.95 |
| 12 | H2 | 201 | CYC | C4D-CHA-C1A | 2.00 | 131.20 | 128.81 |
| 12 | V4 | 201 | CYC | C1B-CHB-C4A | -2.00 | 123.18 | 128.08 |
| 12 | V8 | 201 | CYC | C1B-CHB-C4A | -2.00 | 123.18 | 128.08 |
| 12 | DA | 201 | CYC | CAB-C3B-C2B | 2.00 | 130.96 | 127.53 |
| 12 | D9 | 201 | CYC | CAB-C3B-C2B | 2.00 | 130.96 | 127.53 |
| 12 | J2 | 202 | CYC | C3A-C4A-NA | 2.00 | 114.81 | 110.53 |
| 12 | JA | 202 | CYC | C1B-CHB-C4A | -2.00 | 123.19 | 128.08 |
| 12 | J9 | 202 | CYC | C1B-CHB-C4A | -2.00 | 123.19 | 128.08 |
| 12 | V1 | 201 | CYC | CHB-C1B-C2B | -2.00 | 122.98 | 126.95 |
| 12 | L4 | 202 | CYC | CAB-C3B-C2B | 2.00 | 130.96 | 127.53 |
| 12 | TA | 301 | CYC | C1B-CHB-C4A | -2.00 | 123.19 | 128.08 |
| 12 | T9 | 301 | CYC | C1B-CHB-C4A | -2.00 | 123.19 | 128.08 |
| 12 | X3 | 201 | CYC | CAB-C3B-C2B | 2.00 | 130.95 | 127.53 |
| 12 | BA | 202 | CYC | CHD-C4C-NC | 2.00 | 127.58 | 125.20 |
| 12 | B9 | 202 | CYC | CHD-C4C-NC | 2.00 | 127.58 | 125.20 |
| 12 | S4 | 202 | CYC | CHB-C1B-C2B | -2.00 | 122.98 | 126.95 |
| 12 | D4 | 202 | CYC | C3A-C4A-NA | 2.00 | 114.80 | 110.53 |
| 12 | D8 | 202 | CYC | C3A-C4A-NA | 2.00 | 114.80 | 110.53 |
| 12 | H3 | 202 | CYC | CHB-C1B-C2B | -2.00 | 122.98 | 126.95 |
| 12 | LA | 202 | CYC | C3A-C4A-NA | 2.00 | 114.80 | 110.53 |
| 12 | L9 | 202 | CYC | C3A-C4A-NA | 2.00 | 114.80 | 110.53 |

There are no chirality outliers.

All (2898) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | A | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | A | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | A | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | Z | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Z | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Z | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | AA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | AA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | AA | 201 | CYC | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | AA | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | AA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | AA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | BA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | BA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | BA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | BA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | BA | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | BA | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | BA | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | BA | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | CA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | CA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | CA | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | CA | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | CA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | CA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | DA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | DA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | DA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | DA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | DA | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | DA | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | DA | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | DA | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | EA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | EA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | EA | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | EA | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | EA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | EA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | FA | 301 | CYC | NA-C4A-CHB-C1B |
| 12 | FA | 301 | CYC | C3A-C4A-CHB-C1B |
| 12 | FA | 301 | CYC | ND-C1D-CHD-C4C |
| 12 | FA | 301 | CYC | C2D-C1D-CHD-C4C |
| 12 | GA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | GA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | GA | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | GA | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | GA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | GA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | HA | 201 | CYC | NA-C4A-CHB-C1B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | HA | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | HA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | HA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | HA | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | HA | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | HA | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | HA | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | IA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | IA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | IA | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | IA | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | IA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | IA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | JA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | JA | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | JA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | JA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | JA | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | JA | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | JA | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | JA | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | KA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | KA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | KA | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | KA | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | KA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | KA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | LA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | LA | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | LA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | LA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | LA | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | LA | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | LA | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | LA | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | OA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | OA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | OA | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | OA | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | OA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | OA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | PA | 201 | CYC | NA-C4A-CHB-C1B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | PA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | PA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | PA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | PA | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | PA | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | PA | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | PA | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | QA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | QA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | QA | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | QA | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | QA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | QA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | RA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | RA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | RA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | RA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | RA | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | RA | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | RA | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | RA | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | SA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | SA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | SA | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | SA | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | SA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | SA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | TA | 301 | CYC | NA-C4A-CHB-C1B |
| 12 | TA | 301 | CYC | C3A-C4A-CHB-C1B |
| 12 | TA | 301 | CYC | ND-C1D-CHD-C4C |
| 12 | TA | 301 | CYC | C2D-C1D-CHD-C4C |
| 12 | TA | 302 | CYC | NA-C4A-CHB-C1B |
| 12 | TA | 302 | CYC | C4C-C3C-CAC-CBC |
| 12 | TA | 302 | CYC | ND-C1D-CHD-C4C |
| 12 | TA | 302 | CYC | C2D-C1D-CHD-C4C |
| 12 | UA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | UA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | UA | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | UA | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | UA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | UA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | VA | 201 | CYC | NA-C4A-CHB-C1B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | VA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | VA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | VA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | VA | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | VA | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | VA | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | VA | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | WA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | WA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | WA | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | WA | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | WA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | WA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | XA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | XA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | XA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | XA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | XA | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | XA | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | XA | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | XA | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | YA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | YA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | YA | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | YA | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | YA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | YA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | ZA | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | ZA | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | ZA | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | ZA | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | ZA | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | ZA | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | ZA | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | ZA | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | O1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | O1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | O1 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | O1 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | O1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | O1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | P1 | 201 | CYC | NA-C4A-CHB-C1B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | P1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | P1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | P1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | P1 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | P1 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | P1 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | P1 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | Q1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Q1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | Q1 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | Q1 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | Q1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Q1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | R1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | R1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | R1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | R1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | R1 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | R1 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | R1 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | R1 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | S1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | S1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | S1 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | S1 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | S1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | S1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | A1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | A1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | A1 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | A1 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | A1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | A1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | G3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | G3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | G3 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | G3 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | G3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | G3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | H3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | H3 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | H3 | 201 | CYC | ND-C1D-CHD-C4C |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | H3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | H3 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | H3 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | H3 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | H3 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | I3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | I3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | I3 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | I3 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | I3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | I3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | J3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | J3 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | J3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | J3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | J3 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | J3 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | J3 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | J3 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | K3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | K3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | K3 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | K3 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | K3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | K3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | G2 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | G2 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | G2 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | G2 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | G2 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | G2 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | H2 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | H2 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | H2 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | H2 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | H2 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | H2 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | H2 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | H2 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | I2 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | I2 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | I2 | 201 | CYC | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | I2 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | I2 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | I2 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | J2 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | J2 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | J2 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | J2 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | J2 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | J2 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | J2 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | J2 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | K2 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | K2 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | K2 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | K2 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | K2 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | K2 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | L2 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | L2 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | L2 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | L2 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | L2 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | L2 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | L2 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | L2 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | N2 | 101 | CYC | NA-C4A-CHB-C1B |
| 12 | N2 | 101 | CYC | C3A-C4A-CHB-C1B |
| 12 | N2 | 101 | CYC | ND-C1D-CHD-C4C |
| 12 | N2 | 101 | CYC | C2D-C1D-CHD-C4C |
| 12 | A3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | A3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | A3 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | A3 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | A3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | A3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | B3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | B3 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | B3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | B3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | B3 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | B3 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | B3 | 202 | CYC | ND-C1D-CHD-C4C |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | B3 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | C3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | C3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | C3 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | C3 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | C3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | C3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | D3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | D3 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | D3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | D3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | D3 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | D3 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | D3 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | D3 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | E3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | E3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | E3 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | E3 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | E3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | E3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | F3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | F3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | F3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | F3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | F3 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | F3 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | F3 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | F3 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | Z3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Z3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | Z3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Z3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | Z3 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | Z3 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | Z3 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | Z3 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | A4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | A4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | A4 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | A4 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | A4 | 201 | CYC | ND-C1D-CHD-C4C |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | A4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | B4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | B4 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | B4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | B4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | B4 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | B4 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | B4 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | B4 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | C4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | C4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | C4 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | C4 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | C4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | C4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | D4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | D4 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | D4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | D4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | D4 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | D4 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | D4 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | D4 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | L3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | L3 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | L3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | L3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | L3 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | L3 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | L3 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | L3 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | O3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | O3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | O3 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | O3 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | O3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | O3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | P3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | P3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | P3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | P3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | P3 | 202 | CYC | NA-C4A-CHB-C1B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | P3 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | P3 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | P3 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | Q3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Q3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | Q3 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | Q3 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | Q3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Q3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | R3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | R3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | R3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | R3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | R3 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | R3 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | R3 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | R3 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | S3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | S3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | S3 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | S3 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | S3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | S3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | T3 | 301 | CYC | NA-C4A-CHB-C1B |
| 12 | T3 | 301 | CYC | C3A-C4A-CHB-C1B |
| 12 | T3 | 301 | CYC | ND-C1D-CHD-C4C |
| 12 | T3 | 301 | CYC | C2D-C1D-CHD-C4C |
| 12 | T3 | 302 | CYC | NA-C4A-CHB-C1B |
| 12 | T3 | 302 | CYC | C4C-C3C-CAC-CBC |
| 12 | T3 | 302 | CYC | ND-C1D-CHD-C4C |
| 12 | T3 | 302 | CYC | C2D-C1D-CHD-C4C |
| 12 | U3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | U3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | U3 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | U3 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | U3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | U3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | V3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | V3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | V3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | V3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | V3 | 202 | CYC | NA-C4A-CHB-C1B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | V3 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | V3 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | V3 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | W3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | W3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | W3 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | W3 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | W3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | W3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | X3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | X3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | X3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | X3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | X3 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | X3 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | X3 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | X3 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | Y3 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Y3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | Y3 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | Y3 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | Y3 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Y3 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | B1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | B1 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | B1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | B1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | B1 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | B1 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | B1 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | B1 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | S4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | S4 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | S4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | S4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | S4 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | S4 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | S4 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | S4 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | T4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | T4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | T4 | 201 | CYC | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | T4 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | T4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | T4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | U4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | U4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | U4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | U4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | U4 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | U4 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | U4 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | U4 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | V4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | V4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | V4 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | V4 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | V4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | V4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | W4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | W4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | W4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | W4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | W4 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | W4 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | W4 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | W4 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | E4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | E4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | E4 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | E4 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | E4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | E4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | F4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | F4 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | F4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | F4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | F4 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | F4 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | F4 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | F4 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | G4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | G4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | G4 | 201 | CYC | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | G4 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | G4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | G4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | H4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | H4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | H4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | H4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | H4 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | H4 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | H4 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | H4 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | I4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | I4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | I4 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | I4 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | I4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | I4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | J4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | J4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | J4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | J4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | J4 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | J4 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | J4 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | J4 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | K4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | K4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | K4 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | K4 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | K4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | K4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | L4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | L4 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | L4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | L4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | L4 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | L4 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | L4 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | L4 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | M4 | 301 | CYC | NA-C4A-CHB-C1B |
| 12 | M4 | 301 | CYC | C3A-C4A-CHB-C1B |
| 12 | M4 | 301 | CYC | ND-C1D-CHD-C4C |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | M4 | 301 | CYC | C2D-C1D-CHD-C4C |
| 12 | N4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | N4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | N4 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | N4 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | N4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | N4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | O4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | O4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | O4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | O4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | O4 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | O4 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | O4 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | O4 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | P4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | P4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | P4 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | P4 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | P4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | P4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | Q4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Q4 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | Q4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Q4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | R4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | R4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | R4 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | R4 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | R4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | R4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | K5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | K5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | L5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | L5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | L5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | M5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | M5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | N5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | N5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | N5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | O5 | 201 | CYC | ND-C1D-CHD-C4C |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | O5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | X4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | X4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | X4 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | X4 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | X4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | X4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | Y4 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Y4 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | Y4 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Y4 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | Z4 | 301 | CYC | NA-C4A-CHB-C1B |
| 12 | Z4 | 301 | CYC | C3A-C4A-CHB-C1B |
| 12 | Z4 | 301 | CYC | ND-C1D-CHD-C4C |
| 12 | Z4 | 301 | CYC | C2D-C1D-CHD-C4C |
| 12 | A5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | A5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | B5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | B5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | B5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | C5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | C5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | D5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | D5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | D5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | E5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | E5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | F5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | F5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | F5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | G5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | G5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | H5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | H5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | H5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | I5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | I5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | J5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | J5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | J5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | C1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | C1 | 201 | CYC | C3A-C4A-CHB-C1B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | C1 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | C1 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | C1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | C1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | c5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | c5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | d5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | d5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | d5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | e5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | e5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | f5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | f5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | f5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | P5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | P5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | P5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | Q5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Q5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | R5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | R5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | R5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | S5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | S5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | T5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | T5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | T5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | U5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | U5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | V5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | V5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | V5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | W5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | W5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | X5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | X5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | X5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | Y5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Y5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | Z5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Z5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Z5 | 201 | CYC | C2D-C1D-CHD-C4C |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 12 | a5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | a5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | b5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | b5 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | b5 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | J6 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | J6 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | J6 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | J6 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | J6 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | J6 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | J6 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | J6 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | K6 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | K6 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | K6 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | K6 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | K6 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | K6 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | L6 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | L6 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | L6 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | L6 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | L6 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | L6 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | L6 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | L6 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | N6 | 101 | CYC | NA-C4A-CHB-C1B |
| 12 | N6 | 101 | CYC | C3A-C4A-CHB-C1B |
| 12 | N6 | 101 | CYC | ND-C1D-CHD-C4C |
| 12 | N6 | 101 | CYC | C2D-C1D-CHD-C4C |
| 12 | A7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | A7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | j5 | 1201 | CYC | NA-C4A-CHB-C1B |
| 12 | j5 | 1201 | CYC | C3A-C4A-CHB-C1B |
| 12 | j5 | 1201 | CYC | C3D-CAD-CBD-CGD |
| 12 | j5 | 1202 | CYC | NA-C4A-CHB-C1B |
| 12 | j5 | 1202 | CYC | ND-C1D-CHD-C4C |
| 12 | j5 | 1202 | CYC | C2D-C1D-CHD-C4C |
| 12 | k5 | 1201 | CYC | NA-C4A-CHB-C1B |
| 12 | k5 | 1201 | CYC | C3A-C4A-CHB-C1B |
| 12 | k5 | 1201 | CYC | C3D-CAD-CBD-CGD |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 12 | k5 | 1202 | CYC | NA-C4A-CHB-C1B |
| 12 | k5 | 1202 | CYC | ND-C1D-CHD-C4C |
| 12 | k5 | 1202 | CYC | C2D-C1D-CHD-C4C |
| 12 | k5 | 1203 | CYC | NA-C4A-CHB-C1B |
| 12 | k5 | 1203 | CYC | ND-C1D-CHD-C4C |
| 12 | k5 | 1203 | CYC | C2D-C1D-CHD-C4C |
| 12 | k5 | 1204 | CYC | NA-C4A-CHB-C1B |
| 12 | k5 | 1204 | CYC | ND-C1D-CHD-C4C |
| 12 | k5 | 1204 | CYC | C2D-C1D-CHD-C4C |
| 12 | A6 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | A6 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | A6 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | A6 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | A6 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | A6 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | B6 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | B6 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | B6 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | B6 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | C6 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | C6 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | C6 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | C6 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | C6 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | C6 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | D6 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | D6 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | D6 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | D6 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | D6 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | D6 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | D6 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | D6 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | E6 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | E6 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | E6 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | E6 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | E6 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | E6 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | F6 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | F6 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | F6 | 201 | CYC | ND-C1D-CHD-C4C |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | F6 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | F6 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | F6 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | F6 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | F6 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | G6 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | G6 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | G6 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | G6 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | G6 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | G6 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | H6 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | H6 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | H6 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | H6 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | H6 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | H6 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | H6 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | H6 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | I6 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | I6 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | I6 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | I6 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | I6 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | I6 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | D1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | D1 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | D1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | D1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | D1 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | D1 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | D1 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | D1 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | O7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | O7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | P7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | P7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | P7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | Q7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Q7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | R7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | R7 | 201 | CYC | ND-C1D-CHD-C4C |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | R7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | S7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | S7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | B7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | B7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | B7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | C7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | C7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | D7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | D7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | D7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | E7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | E7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | F7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | F7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | F7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | G7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | G7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | H7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | H7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | H7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | I7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | I7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | J7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | J7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | J7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | K7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | K7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | L7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | L7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | L7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | M7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | M7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | N7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | N7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | N7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | g7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | g7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | h7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | h7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | h7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | i7 | 201 | CYC | ND-C1D-CHD-C4C |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | i7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | j7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | j7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | j7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | k7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | k7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | T7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | T7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | T7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | U7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | U7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | V7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | V7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | V7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | W7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | W7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | X7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | X7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | X7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | Y7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Y7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | a7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | a7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | b7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | b7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | b7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | c7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | c7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | d7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | d7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | d7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | e7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | e7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | f7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | f7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | f7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | E1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | E1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | E1 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | E1 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | E1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | E1 | 201 | CYC | C2D-C1D-CHD-C4C |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | A8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | A8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | A8 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | A8 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | A8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | A8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | B8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | B8 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | B8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | B8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | B8 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | B8 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | B8 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | B8 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | C8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | C8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | C8 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | C8 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | C8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | C8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | D8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | D8 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | D8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | D8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | D8 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | D8 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | D8 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | D8 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | E8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | E8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | E8 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | E8 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | E8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | E8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | m7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | m7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | o7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | o7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | p7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | p7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | p7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | q7 | 201 | CYC | ND-C1D-CHD-C4C |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | q7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | r7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | r7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | r7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | s7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | s7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | u7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | u7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | v7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | v7 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | v7 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | T8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | T8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | T8 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | T8 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | T8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | T8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | U8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | U8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | U8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | U8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | U8 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | U8 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | U8 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | U8 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | V8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | V8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | V8 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | V8 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | V8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | V8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | W8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | W8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | W8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | W8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | W8 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | W8 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | W8 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | W8 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | X8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | X8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | X8 | 201 | CYC | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | X8 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | X8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | X8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | F8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | F8 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | F8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | F8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | F8 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | F8 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | F8 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | F8 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | G8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | G8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | G8 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | G8 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | G8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | G8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | H8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | H8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | H8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | H8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | H8 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | H8 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | H8 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | H8 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | I8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | I8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | I8 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | I8 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | I8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | I8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | J8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | J8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | J8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | J8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | J8 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | J8 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | J8 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | J8 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | K8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | K8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | K8 | 201 | CYC | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | K8 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | K8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | K8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | L8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | L8 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | L8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | L8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | M8 | 301 | CYC | NA-C4A-CHB-C1B |
| 12 | M8 | 301 | CYC | C3A-C4A-CHB-C1B |
| 12 | M8 | 301 | CYC | ND-C1D-CHD-C4C |
| 12 | M8 | 301 | CYC | C2D-C1D-CHD-C4C |
| 12 | M8 | 302 | CYC | NA-C4A-CHB-C1B |
| 12 | M8 | 302 | CYC | C3A-C4A-CHB-C1B |
| 12 | M8 | 302 | CYC | ND-C1D-CHD-C4C |
| 12 | M8 | 302 | CYC | C2D-C1D-CHD-C4C |
| 12 | N8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | N8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | N8 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | N8 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | N8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | N8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | O8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | O8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | O8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | O8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | O8 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | O8 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | O8 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | O8 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | P8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | P8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | P8 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | P8 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | P8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | P8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | Q8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Q8 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | Q8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Q8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | R8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | R8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | R8 | 201 | CYC | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | R8 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | R8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | R8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | S8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | S8 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | S8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | S8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | F1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | F1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | F1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | F1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | F1 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | F1 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | F1 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | F1 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | L9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | L9 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | L9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | L9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | L9 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | L9 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | L9 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | L9 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | O9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | O9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | O9 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | O9 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | O9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | O9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | P9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | P9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | P9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | P9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | P9 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | P9 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | P9 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | P9 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | Q9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Q9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | Q9 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | Q9 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | Q9 | 201 | CYC | ND-C1D-CHD-C4C |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | Q9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | Y8 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Y8 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | Y8 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Y8 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | Z8 | 301 | CYC | NA-C4A-CHB-C1B |
| 12 | Z8 | 301 | CYC | C3A-C4A-CHB-C1B |
| 12 | Z8 | 301 | CYC | ND-C1D-CHD-C4C |
| 12 | Z8 | 301 | CYC | C2D-C1D-CHD-C4C |
| 12 | A9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | A9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | A9 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | A9 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | A9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | A9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | B9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | B9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | B9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | B9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | B9 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | B9 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | B9 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | B9 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | C9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | C9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | C9 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | C9 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | C9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | C9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | D9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | D9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | D9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | D9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | D9 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | D9 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | D9 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | D9 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | E9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | E9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | E9 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | E9 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | E9 | 201 | CYC | ND-C1D-CHD-C4C |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | E9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | F9 | 301 | CYC | NA-C4A-CHB-C1B |
| 12 | F9 | 301 | CYC | C3A-C4A-CHB-C1B |
| 12 | F9 | 301 | CYC | ND-C1D-CHD-C4C |
| 12 | F9 | 301 | CYC | C2D-C1D-CHD-C4C |
| 12 | F9 | 302 | CYC | NA-C4A-CHB-C1B |
| 12 | F9 | 302 | CYC | C4C-C3C-CAC-CBC |
| 12 | F9 | 302 | CYC | ND-C1D-CHD-C4C |
| 12 | F9 | 302 | CYC | C2D-C1D-CHD-C4C |
| 12 | F9 | 303 | CYC | NA-C4A-CHB-C1B |
| 12 | F9 | 303 | CYC | C4C-C3C-CAC-CBC |
| 12 | F9 | 303 | CYC | ND-C1D-CHD-C4C |
| 12 | F9 | 303 | CYC | C2D-C1D-CHD-C4C |
| 12 | G9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | G9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | G9 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | G9 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | G9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | G9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | H9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | H9 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | H9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | H9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | H9 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | H9 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | H9 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | H9 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | I9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | I9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | I9 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | I9 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | I9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | I9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | J9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | J9 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | J9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | J9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | J9 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | J9 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | J9 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | J9 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | K9 | 201 | CYC | NA-C4A-CHB-C1B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | K9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | K9 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | K9 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | K9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | K9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | R9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | R9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | R9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | R9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | R9 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | R9 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | R9 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | R9 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | S9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | S9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | S9 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | S9 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | S9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | S9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | T9 | 301 | CYC | NA-C4A-CHB-C1B |
| 12 | T9 | 301 | CYC | C3A-C4A-CHB-C1B |
| 12 | T9 | 301 | CYC | ND-C1D-CHD-C4C |
| 12 | T9 | 301 | CYC | C2D-C1D-CHD-C4C |
| 12 | T9 | 302 | CYC | NA-C4A-CHB-C1B |
| 12 | T9 | 302 | CYC | C4C-C3C-CAC-CBC |
| 12 | T9 | 302 | CYC | ND-C1D-CHD-C4C |
| 12 | T9 | 302 | CYC | C2D-C1D-CHD-C4C |
| 12 | U9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | U9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | U9 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | U9 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | U9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | U9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | V9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | V9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | V9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | V9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | V9 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | V9 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | V9 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | V9 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | W9 | 201 | CYC | NA-C4A-CHB-C1B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | W9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | W9 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | W9 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | W9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | W9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | X9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | X9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | X9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | X9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | X9 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | X9 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | X9 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | X9 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | Y9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Y9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | Y9 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | Y9 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | Y9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Y9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | Z9 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Z9 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | Z9 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Z9 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | Z9 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | Z9 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | Z9 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | Z9 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | G1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | G1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | G1 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | G1 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | G1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | G1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | a9 | 901 | CYC | NA-C4A-CHB-C1B |
| 12 | a9 | 901 | CYC | C3A-C4A-CHB-C1B |
| 12 | a9 | 901 | CYC | ND-C1D-CHD-C4C |
| 12 | a9 | 901 | CYC | C2D-C1D-CHD-C4C |
| 12 | aA | 901 | CYC | NA-C4A-CHB-C1B |
| 12 | aA | 901 | CYC | C3A-C4A-CHB-C1B |
| 12 | aA | 901 | CYC | ND-C1D-CHD-C4C |
| 12 | aA | 901 | CYC | C2D-C1D-CHD-C4C |
| 12 | aA | 902 | CYC | NA-C4A-CHB-C1B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | aA | 902 | CYC | C3A-C4A-CHB-C1B |
| 12 | aA | 902 | CYC | ND-C1D-CHD-C4C |
| 12 | aA | 902 | CYC | C2D-C1D-CHD-C4C |
| 12 | H1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | H1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | H1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | H1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | H1 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | H1 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | H1 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | H1 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | I1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | I1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | I1 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | I1 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | I1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | I1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | J1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | J1 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | J1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | J1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | K1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | K1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | K1 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | K1 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | K1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | K1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | L1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | L1 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | L1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | L1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | T1 | 301 | CYC | NA-C4A-CHB-C1B |
| 12 | T1 | 301 | CYC | C3A-C4A-CHB-C1B |
| 12 | T1 | 301 | CYC | ND-C1D-CHD-C4C |
| 12 | T1 | 301 | CYC | C2D-C1D-CHD-C4C |
| 12 | T1 | 302 | CYC | NA-C4A-CHB-C1B |
| 12 | T1 | 302 | CYC | C4C-C3C-CAC-CBC |
| 12 | T1 | 302 | CYC | ND-C1D-CHD-C4C |
| 12 | T1 | 302 | CYC | C2D-C1D-CHD-C4C |
| 12 | U1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | U1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | U1 | 201 | CYC | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | U1 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | U1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | U1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | V1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | V1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | V1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | V1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | V1 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | V1 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | V1 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | V1 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | W1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | W1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | W1 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | W1 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | W1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | W1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | X1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | X1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | X1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | X1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | X1 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | X1 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | X1 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | X1 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | Y1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Y1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | Y1 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | Y1 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | Y1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Y1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | Z1 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Z1 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | Z1 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | Z1 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | Z1 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | Z1 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | Z1 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | Z1 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | A2 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | A2 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | A2 | 201 | CYC | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | A2 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | A2 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | A2 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | B2 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | B2 | 201 | CYC | C4C-C3C-CAC-CBC |
| 12 | B2 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | B2 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | C2 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | C2 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | C2 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | C2 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | C2 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | C2 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | D2 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | D2 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | D2 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | D2 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | D2 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | D2 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | D2 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | D2 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | E2 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | E2 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | E2 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | E2 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | E2 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | E2 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | F2 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | F2 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | F2 | 201 | CYC | ND-C1D-CHD-C4C |
| 12 | F2 | 201 | CYC | C2D-C1D-CHD-C4C |
| 12 | F2 | 202 | CYC | NA-C4A-CHB-C1B |
| 12 | F2 | 202 | CYC | C4C-C3C-CAC-CBC |
| 12 | F2 | 202 | CYC | ND-C1D-CHD-C4C |
| 12 | F2 | 202 | CYC | C2D-C1D-CHD-C4C |
| 12 | L5 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | N5 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | B5 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | D5 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | F5 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | H5 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | J5 | 201 | CYC | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 12 | d5 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | f5 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | P5 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | R5 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | T5 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | V5 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | Z5 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | b5 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | j5 | 1202 | CYC | C2B-C3B-CAB-CBB |
| 12 | k5 | 1204 | CYC | C2B-C3B-CAB-CBB |
| 12 | P7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | D7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | F7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | J7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | L7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | N7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | h7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | j7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | V7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | X7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | b7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | f7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | A | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | Z | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | X5 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | k5 | 1202 | CYC | C2B-C3B-CAB-CBB |
| 12 | k5 | 1203 | CYC | C2B-C3B-CAB-CBB |
| 12 | R7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | B7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | H7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | T7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | d7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | p7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | r7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | v7 | 201 | CYC | C2B-C3B-CAB-CBB |
| 12 | A | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | Z | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | L5 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | N5 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | B5 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | D5 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | F5 | 201 | CYC | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 12 | H5 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | J5 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | d5 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | f5 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | P5 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | R5 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | T5 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | V5 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | X5 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | Z5 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | b5 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | j5 | 1202 | CYC | C4B-C3B-CAB-CBB |
| 12 | k5 | 1202 | CYC | C4B-C3B-CAB-CBB |
| 12 | k5 | 1203 | CYC | C4B-C3B-CAB-CBB |
| 12 | k5 | 1204 | CYC | C4B-C3B-CAB-CBB |
| 12 | P7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | R7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | B7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | D7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | F7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | H7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | J7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | L7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | N7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | h7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | j7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | T7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | V7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | X7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | b7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | d7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | f7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | p7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | r7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | v7 | 201 | CYC | C4B-C3B-CAB-CBB |
| 12 | K5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | M5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | O5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | A5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | C5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | E5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | G5 | 201 | CYC | C3A-C4A-CHB-C1B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | I5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | c5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | e5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | Q5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | S5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | U5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | W5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | Y5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | a5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | A7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | O7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | Q7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | S7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | C7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | E7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | G7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | I7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | K7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | M7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | g7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | i7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | k7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | U7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | W7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | Y7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | a7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | c7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | e7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | m7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | o7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | q7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | s7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | u7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | K5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | M5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | O5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | A5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | C5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | E5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | G5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | I5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | c5 | 201 | CYC | NA-C4A-CHB-C1B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | e5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Q5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | S5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | U5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | W5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Y5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | a5 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | A7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | O7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Q7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | S7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | C7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | E7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | G7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | I7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | K7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | M7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | g7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | i7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | k7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | U7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | W7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | Y7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | a7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | c7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | e7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | m7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | o7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | q7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | s7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | u7 | 201 | CYC | NA-C4A-CHB-C1B |
| 12 | A | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | Z | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | BA | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | DA | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | HA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | JA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | LA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | PA | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | RA | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | TA | 302 | CYC | C3A-C4A-CHB-C1B |
| 12 | VA | 202 | CYC | C3A-C4A-CHB-C1B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | XA | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | ZA | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | P1 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | R1 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | H3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | J3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | H2 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | J2 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | L2 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | B3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | D3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | F3 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | Z3 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | B4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | D4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | L3 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | P3 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | R3 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | T3 | 302 | CYC | C3A-C4A-CHB-C1B |
| 12 | V3 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | X3 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | B1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | S4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | U4 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | W4 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | F4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | H4 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | J4 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | L4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | O4 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | Q4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | L5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | N5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | Y4 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | B5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | D5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | F5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | H5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | J5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | d5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | f5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | P5 | 201 | CYC | C3A-C4A-CHB-C1B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 12 | R5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | T5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | V5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | X5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | Z5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | b5 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | J6 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | L6 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | j5 | 1202 | CYC | C3A-C4A-CHB-C1B |
| 12 | k5 | 1202 | CYC | C3A-C4A-CHB-C1B |
| 12 | k5 | 1203 | CYC | C3A-C4A-CHB-C1B |
| 12 | k5 | 1204 | CYC | C3A-C4A-CHB-C1B |
| 12 | B6 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | D6 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | F6 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | H6 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | D1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | P7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | R7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | B7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | D7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | F7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | H7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | J7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | L7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | N7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | h7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | j7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | T7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | V7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | X7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | b7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | d7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | f7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | B8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | D8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | p7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | r7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | v7 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | U8 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | W8 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | F8 | 201 | CYC | C3A-C4A-CHB-C1B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | H8 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | J8 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | L8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | O8 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | Q8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | S8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | F1 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | L9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | P9 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | Y8 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | B9 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | D9 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | F9 | 302 | CYC | C3A-C4A-CHB-C1B |
| 12 | F9 | 303 | CYC | C3A-C4A-CHB-C1B |
| 12 | H9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | J9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | R9 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | T9 | 302 | CYC | C3A-C4A-CHB-C1B |
| 12 | V9 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | X9 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | Z9 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | H1 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | J1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | L1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | T1 | 302 | CYC | C3A-C4A-CHB-C1B |
| 12 | V1 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | X1 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | Z1 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | B2 | 201 | CYC | C3A-C4A-CHB-C1B |
| 12 | D2 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | F2 | 202 | CYC | C3A-C4A-CHB-C1B |
| 12 | BA | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | DA | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | HA | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | JA | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | LA | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | PA | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | RA | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | TA | 302 | CYC | C2C-C3C-CAC-CBC |
| 12 | VA | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | XA | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | ZA | 201 | CYC | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | P1 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | R1 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | H3 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | J3 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | H2 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | J2 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | L2 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | B3 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | D3 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | F3 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | Z3 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | B4 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | D4 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | L3 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | P3 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | R3 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | T3 | 302 | CYC | C2C-C3C-CAC-CBC |
| 12 | V3 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | X3 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | B1 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | S4 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | U4 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | W4 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | F4 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | H4 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | J4 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | L4 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | O4 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | Q4 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | Y4 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | J6 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | L6 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | B6 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | D6 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | F6 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | H6 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | D1 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | B8 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | D8 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | U8 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | W8 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | F8 | 201 | CYC | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | H8 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | J8 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | L8 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | O8 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | Q8 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | S8 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | F1 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | L9 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | P9 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | Y8 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | B9 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | D9 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | F9 | 302 | CYC | C2C-C3C-CAC-CBC |
| 12 | F9 | 303 | CYC | C2C-C3C-CAC-CBC |
| 12 | H9 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | J9 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | R9 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | T9 | 302 | CYC | C2C-C3C-CAC-CBC |
| 12 | V9 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | X9 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | Z9 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | H1 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | J1 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | L1 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | T1 | 302 | CYC | C2C-C3C-CAC-CBC |
| 12 | V1 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | X1 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | Z1 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | B2 | 201 | CYC | C2C-C3C-CAC-CBC |
| 12 | D2 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | F2 | 202 | CYC | C2C-C3C-CAC-CBC |
| 12 | K5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | M5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | O5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | A5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | C5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | E5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | G5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | I5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | c5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | e5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | Q5 | 201 | CYC | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | S5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | U5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | W5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | Y5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | a5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | A7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | O7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | Q7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | S7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | C7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | E7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | G7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | I7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | K7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | M7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | g7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | i7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | k7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | U7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | W7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | Y7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | a7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | c7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | e7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | o7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | q7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | u7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | s7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | m7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | DA | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | JA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | PA | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | RA | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | TA | 302 | CYC | CAD-CBD-CGD-O1D |
| 12 | VA | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | P1 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | J3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | H2 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | J2 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | B3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | Z3 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | L3 | 201 | CYC | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | P3 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | T3 | 302 | CYC | CAD-CBD-CGD-O1D |
| 12 | V3 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | X3 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | B1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | S4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | U4 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | W4 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | F4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | H4 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | J4 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | L4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | O4 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | J6 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | D6 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | F6 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | H6 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | B8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | U8 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | W8 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | F8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | H8 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | J8 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | L8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | O8 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | Q8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | S8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | P9 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | D9 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | F9 | 303 | CYC | CAD-CBD-CGD-O1D |
| 12 | J9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | R9 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | T9 | 302 | CYC | CAD-CBD-CGD-O1D |
| 12 | V9 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | Z9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | J1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | L1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | T1 | 302 | CYC | CAD-CBD-CGD-O1D |
| 12 | V1 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | X1 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | Z1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | B2 | 201 | CYC | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | D2 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | BA | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | HA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | LA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | XA | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | ZA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | R1 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | H3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | L2 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | D3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | F3 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | B4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | D4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | R3 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | Q4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | Y4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | L6 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | B6 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | D1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | D8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | F1 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | L9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | Y8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | B9 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | F9 | 302 | CYC | CAD-CBD-CGD-O1D |
| 12 | H9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | X9 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | H1 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | F2 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | Z9 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | TA | 302 | CYC | CAA-CBA-CGA-O2A |
| 12 | ZA | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | D3 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | J4 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | Y4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | D1 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | J8 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | Y8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | T9 | 302 | CYC | CAA-CBA-CGA-O2A |
| 12 | BA | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | DA | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | HA | 201 | CYC | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | JA | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | LA | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | PA | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | RA | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | VA | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | R1 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | H3 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | J3 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | H2 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | J2 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | L2 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | F3 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | Z3 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | L3 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | R3 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | T3 | 302 | CYC | CAA-CBA-CGA-O2A |
| 12 | V3 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | S4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | U4 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | W4 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | F4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | H4 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | L4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | Q4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | J6 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | L6 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | D6 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | F6 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | H6 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | U8 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | W8 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | F8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | H8 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | L8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | Q8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | S8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | F1 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | L9 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | P9 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | B9 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | D9 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | F9 | 302 | CYC | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | F9 | 303 | CYC | CAA-CBA-CGA-O2A |
| 12 | H9 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | J9 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | R9 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | V9 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | X9 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | H1 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | J1 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | L1 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | T1 | 302 | CYC | CAA-CBA-CGA-O2A |
| 12 | V1 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | Z1 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | D2 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | F2 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | AA | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | IA | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | OA | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | QA | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | UA | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | WA | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | XA | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | Q1 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | G3 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | I2 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | K2 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | B3 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | C3 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | A4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | C4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | Q3 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | S3 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | U3 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | B1 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | E4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | G4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | I4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | N4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | C1 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | K6 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | E6 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | I6 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | A8 | 201 | CYC | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | C8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | E8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | G8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | I8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | N8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | O9 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | Q9 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | A9 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | I9 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | S9 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | U9 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | W9 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | G1 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | U1 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | A2 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | E2 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | CA | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | EA | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | GA | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | HA | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | KA | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | PA | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | SA | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | YA | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | ZA | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | O1 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | S1 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | A1 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | I3 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | K3 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | G2 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | A3 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | B3 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | D3 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | E3 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | Z3 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | B4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | D4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | O3 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | W3 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | X3 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | Y3 | 201 | CYC | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | B1 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | T4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | V4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | K4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | O4 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | O4 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | P4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | Q4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | R4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | X4 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | Y4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | L6 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | A6 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | C6 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | G6 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | D1 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | E1 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | B8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | D8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | T8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | V8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | X8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | K8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | O8 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | O8 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | P8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | R8 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | P9 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | Y8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | C9 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | E9 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | F9 | 302 | CYC | CAA-CBA-CGA-O1A |
| 12 | F9 | 303 | CYC | CAA-CBA-CGA-O1A |
| 12 | G9 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | H9 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | K9 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | Y9 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | H1 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | I1 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | K1 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | W1 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | X1 | 202 | CYC | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | Y1 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | Z1 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | B2 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | C2 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | BA | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | DA | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | JA | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | LA | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | RA | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | TA | 302 | CYC | CAA-CBA-CGA-O1A |
| 12 | VA | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | XA | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | P1 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | P1 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | R1 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | H3 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | J3 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | H2 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | J2 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | L2 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | F3 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | B4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | D4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | L3 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | P3 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | P3 | 202 | CYC | CAA-CBA-CGA-O2A |
| 12 | R3 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | T3 | 302 | CYC | CAA-CBA-CGA-O1A |
| 12 | V3 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | X3 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | S4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | U4 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | W4 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | F4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | H4 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | J4 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | L4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | J6 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | B6 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | B6 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | D6 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | F6 | 202 | CYC | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | H6 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | B8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | D8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | U8 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | W8 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | F8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | H8 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | J8 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | L8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | Q8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | S8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | F1 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | L9 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | B9 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | D9 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | J9 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | R9 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | T9 | 302 | CYC | CAA-CBA-CGA-O1A |
| 12 | V9 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | X9 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | Z9 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | J1 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | L1 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | T1 | 302 | CYC | CAA-CBA-CGA-O1A |
| 12 | V1 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | X1 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | B2 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | D2 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | F2 | 202 | CYC | CAA-CBA-CGA-O1A |
| 12 | K8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | CA | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | CA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | OA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | QA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | WA | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | WA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | H3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | I2 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | I2 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | B3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | D3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | A4 | 201 | CYC | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 12 | W3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | B1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | U4 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | K4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | N4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | j5 | 1201 | CYC | CAA-CBA-CGA-O2A |
| 12 | k5 | 1201 | CYC | CAA-CBA-CGA-O2A |
| 12 | A6 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | A6 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | E6 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | I6 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | A8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | U8 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | N8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | O9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | P9 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | C9 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | F9 | 303 | CYC | CAD-CBD-CGD-O2D |
| 12 | R9 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | W9 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | W9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | H1 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | W1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | A2 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | A2 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | C2 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | E2 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | AA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | BA | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | EA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | GA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | HA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | IA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | KA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | KA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | PA | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | RA | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | YA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | P1 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | R1 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | G3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | I3 | 201 | CYC | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 12 | G2 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | C3 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | P3 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | R3 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | V3 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | Y3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | V4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | F4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | L4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | O4 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | M5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | X4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | E5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | C1 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | c5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | Q5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | W5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | j5 | 1201 | CYC | CAA-CBA-CGA-O1A |
| 12 | k5 | 1201 | CYC | CAA-CBA-CGA-O1A |
| 12 | C6 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | E6 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | F6 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | I6 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | O7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | i7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | k7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | W7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | Y7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | c7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | e7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | B8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | o7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | u7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | V8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | X8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | F8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | L8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | O8 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | A9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | B9 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | C9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | E9 | 201 | CYC | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | F9 | 302 | CYC | CAD-CBD-CGD-O2D |
| 12 | G9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | H9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | I9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | K9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | K9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | Y9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | G1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | I1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | V1 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | Y1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | E2 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | IA | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | OA | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | OA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | SA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | SA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | UA | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | VA | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | YA | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | O1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | S1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | A1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | A1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | I3 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | G2 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | J2 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | L2 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | A3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | A3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | C3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | E3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | E3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | F3 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | B4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | C4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | C4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | O3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | S3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | U3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | W3 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | Y3 | 201 | CYC | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | S4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | V4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | E4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | I4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | K4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | N4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | P4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | P4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | Q4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | R4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | K5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | O5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | X4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | A5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | C5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | G5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | C1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | e5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | S5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | U5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | Y5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | a5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | J6 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | A7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | G6 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | D1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | Q7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | S7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | C7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | G7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | I7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | M7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | g7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | U7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | a7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | E1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | E1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | C8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | C8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | E8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | m7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | q7 | 201 | CYC | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | s7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | X8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | I8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | K8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | N8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | P8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | P8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | Q8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | R8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | S8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | F1 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | O9 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | O9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | Q9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | I9 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | S9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | U9 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | V9 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | Y9 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | I1 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | U1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | W1 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | C2 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | F2 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | CA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | EA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | IA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | QA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | O1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | S1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | G3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | J3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | K3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | H2 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | I2 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | K2 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | C3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | A4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | C4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | D4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | O3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | S3 | 201 | CYC | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | T4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | V4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | E4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | G4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | I4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | P4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | R4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | I5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | C1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | K6 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | C6 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | I6 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | E7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | K7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | A8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | C8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | E8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | T8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | V8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | G8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | I8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | P8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | R8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | Q9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | C9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | E9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | I9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | S9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | G1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | J1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | K1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | C2 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | AA | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | AA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | EA | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | GA | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | GA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | KA | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | QA | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | SA | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | UA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | UA | 201 | CYC | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | WA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | YA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | O1 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | Q1 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | Q1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | Q1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | S1 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | A1 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | G3 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | I3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | K3 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | K3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | G2 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | K2 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | K2 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | A3 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | E3 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | A4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | O3 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | Q3 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | Q3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | Q3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | S3 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | U3 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | U3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | W3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | Y3 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | T4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | G4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | H4 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | I4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | N4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | X4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | K6 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | A6 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | C6 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | E6 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | G6 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | G6 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | E1 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | A8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | T8 | 201 | CYC | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | V8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | X8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | G8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | H8 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | I8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | K8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | N8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | Q9 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | A9 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | A9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | E9 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | G9 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | G9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | K9 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | S9 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | U9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | U9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | W9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | Y9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | G1 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | I1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | K1 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | K1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | U1 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | U1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | W1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | Y1 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | Y1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | A2 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | D2 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | E2 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | DA | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | ZA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | X3 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | T4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | E4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | G4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | K4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | R4 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | K6 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | L6 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | D6 | 202 | CYC | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | H6 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | D8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | E8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | T8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | G8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | R8 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | D9 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | X1 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | A5 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | G5 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | Q5 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | K7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | TA | 302 | CYC | CAD-CBD-CGD-O2D |
| 12 | XA | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | Z3 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | L3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | T3 | 302 | CYC | CAD-CBD-CGD-O2D |
| 12 | J4 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | W8 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | J8 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | T9 | 302 | CYC | CAD-CBD-CGD-O2D |
| 12 | X9 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | Z9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | L1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | T1 | 302 | CYC | CAD-CBD-CGD-O2D |
| 12 | Z1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | L5 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | H5 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | B6 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | b7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | A | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | Z | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | N5 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | D5 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | F5 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | J5 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | f5 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | P5 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | R5 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | T5 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | V5 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | X5 | 201 | CYC | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 12 | b5 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | j5 | 1202 | CYC | CAD-CBD-CGD-O2D |
| 12 | k5 | 1202 | CYC | CAD-CBD-CGD-O2D |
| 12 | k5 | 1203 | CYC | CAD-CBD-CGD-O2D |
| 12 | k5 | 1204 | CYC | CAD-CBD-CGD-O2D |
| 12 | P7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | R7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | B7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | D7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | F7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | H7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | J7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | L7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | N7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | h7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | j7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | T7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | X7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | d7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | f7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | r7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | W4 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | Y4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | B5 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | d5 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | Z5 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | V7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | p7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | v7 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | B2 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | JA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | LA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | L9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | Y8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | J9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | L5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | D5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | F5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | P5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | V5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | j5 | 1202 | CYC | CAA-CBA-CGA-O2A |
| 12 | k5 | 1204 | CYC | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 12 | P7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | D7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | V7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | f7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | A | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | Z | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | DA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | JA | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | RA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | R1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | D3 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | F3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | R3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | N5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | Z4 | 301 | CYC | CAD-CBD-CGD-O2D |
| 12 | B5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | H5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | J5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | d5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | f5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | R5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | T5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | X5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | b5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | k5 | 1202 | CYC | CAA-CBA-CGA-O2A |
| 12 | k5 | 1203 | CYC | CAA-CBA-CGA-O2A |
| 12 | D6 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | D1 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | R7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | B7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | F7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | H7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | J7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | L7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | N7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | h7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | j7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | T7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | X7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | b7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | d7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | r7 | 201 | CYC | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 12 | v7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | F1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | Z8 | 301 | CYC | CAD-CBD-CGD-O2D |
| 12 | B9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | D9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | F9 | 301 | CYC | CAD-CBD-CGD-O2D |
| 12 | J9 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | O5 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | U5 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | W5 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | E7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | I7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | M7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | BA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | FA | 301 | CYC | CAD-CBD-CGD-O2D |
| 12 | H2 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | B4 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | D4 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | L3 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | Z5 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | D8 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | p7 | 201 | CYC | CAA-CBA-CGA-O2A |
| 12 | M8 | 301 | CYC | CAD-CBD-CGD-O2D |
| 12 | R9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | D2 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | T3 | 301 | CYC | CAD-CBD-CGD-O2D |
| 12 | L5 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | B5 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | H5 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | J5 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | T5 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | V5 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | Z5 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | j5 | 1202 | CYC | CAD-CBD-CGD-O1D |
| 12 | k5 | 1202 | CYC | CAD-CBD-CGD-O1D |
| 12 | k5 | 1204 | CYC | CAD-CBD-CGD-O1D |
| 12 | H6 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | P7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | B7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | H7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | h7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | T7 | 201 | CYC | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 12 | X7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | b7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | f7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | p7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | r7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | v7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | aA | 902 | CYC | CAD-CBD-CGD-O2D |
| 12 | LA | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | PA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | VA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | XA | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | ZA | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | P1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | H3 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | J3 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | J2 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | N2 | 101 | CYC | CAD-CBD-CGD-O2D |
| 12 | B3 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | Z3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | P3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | B1 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | S4 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | W4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | F4 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | J4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | L4 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | M4 | 301 | CYC | CAD-CBD-CGD-O2D |
| 12 | O4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | N5 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | D5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | F5 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | d5 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | P5 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | J6 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | N6 | 101 | CYC | CAD-CBD-CGD-O2D |
| 12 | j5 | 1202 | CYC | CAA-CBA-CGA-O1A |
| 12 | k5 | 1202 | CYC | CAA-CBA-CGA-O1A |
| 12 | k5 | 1203 | CYC | CAA-CBA-CGA-O1A |
| 12 | k5 | 1204 | CYC | CAA-CBA-CGA-O1A |
| 12 | F6 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | P7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | R7 | 201 | CYC | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | B7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | F7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | H7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | J7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | L7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | N7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | N7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | h7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | j7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | T7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | X7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | b7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | d7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | f7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | B8 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | W8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | F8 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | J8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | M8 | 302 | CYC | CAD-CBD-CGD-O2D |
| 12 | O8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | L9 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | P9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | V9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | X9 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | Z9 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | a9 | 901 | CYC | CAD-CBD-CGD-O2D |
| 12 | aA | 901 | CYC | CAD-CBD-CGD-O2D |
| 12 | H1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | T1 | 301 | CYC | CAD-CBD-CGD-O2D |
| 12 | Z1 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | TA | 301 | CYC | CAD-CBD-CGD-O2D |
| 12 | L2 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | V3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | X3 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | H4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | D5 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | d5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | b5 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | L6 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | H8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | T9 | 301 | CYC | CAD-CBD-CGD-O2D |
| 12 | V1 | 201 | CYC | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 12 | X1 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | F2 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | A | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | A | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | Z | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | HA | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | U4 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | N5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | B5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | J5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | f5 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | P5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | R5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | R5 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | T5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | V5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | X5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | X5 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | Z5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | k5 | 1203 | CYC | CAD-CBD-CGD-O1D |
| 12 | R7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | D7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | D7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | J7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | j7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | V7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | V7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | d7 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | p7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | r7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | v7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | U8 | 201 | CYC | CAD-CBD-CGD-O2D |
| 12 | H9 | 202 | CYC | CAD-CBD-CGD-O2D |
| 12 | Z | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | L5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | F5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | H5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | f5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | b5 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | F7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | L7 | 201 | CYC | CAA-CBA-CGA-O1A |
| 12 | DA | 201 | CYC | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 12 | FA | 301 | CYC | CAD-CBD-CGD-O1D |
| 12 | JA | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | LA | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | PA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | TA | 301 | CYC | CAD-CBD-CGD-O1D |
| 12 | VA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | XA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | H3 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | J3 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | H2 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | N2 | 101 | CYC | CAD-CBD-CGD-O1D |
| 12 | B3 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | D3 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | F3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | Z3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | V3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | X3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | B1 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | S4 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | F4 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | O4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | N6 | 101 | CYC | CAD-CBD-CGD-O1D |
| 12 | j5 | 1201 | CYC | CAD-CBD-CGD-O1D |
| 12 | j5 | 1201 | CYC | CAD-CBD-CGD-O2D |
| 12 | k5 | 1201 | CYC | CAD-CBD-CGD-O1D |
| 12 | k5 | 1201 | CYC | CAD-CBD-CGD-O2D |
| 12 | F6 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | H6 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | D1 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | F8 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | M8 | 302 | CYC | CAD-CBD-CGD-O1D |
| 12 | O8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | F1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | L9 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | P9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | Z8 | 301 | CYC | CAD-CBD-CGD-O1D |
| 12 | D9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | F9 | 301 | CYC | CAD-CBD-CGD-O1D |
| 12 | J9 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | T9 | 301 | CYC | CAD-CBD-CGD-O1D |
| 12 | V9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | X9 | 201 | CYC | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | aA | 901 | CYC | CAD-CBD-CGD-O1D |
| 12 | H1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | V1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | X1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | Z1 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | F2 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | K5 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | C5 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | E5 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | I5 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | c5 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | e5 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | Y5 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | Q7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | C7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | g7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | i7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | k7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | W7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | Y7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | a7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | e7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | q7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | u7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | L2 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | B4 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | W4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | J4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | M4 | 301 | CYC | CAD-CBD-CGD-O1D |
| 12 | L6 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | W8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | J8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | a9 | 901 | CYC | CAD-CBD-CGD-O1D |
| 12 | RA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | ZA | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | P1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | J2 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | D4 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | L3 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | P3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | T3 | 301 | CYC | CAD-CBD-CGD-O1D |
| 12 | Z4 | 301 | CYC | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 12 | J6 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | D8 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | M8 | 301 | CYC | CAD-CBD-CGD-O1D |
| 12 | B9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | R9 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | Z9 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | T1 | 301 | CYC | CAD-CBD-CGD-O1D |
| 12 | BA | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | HA | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | R1 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | R3 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | U4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | H4 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | L4 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | D6 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | B8 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | U8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | H8 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | H9 | 202 | CYC | CAD-CBD-CGD-O1D |
| 12 | aA | 902 | CYC | CAD-CBD-CGD-O1D |
| 12 | D2 | 201 | CYC | CAD-CBD-CGD-O1D |
| 12 | M5 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | S5 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | a5 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | A7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | O7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | S7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | G7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | U7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | c7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | m7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | o7 | 201 | CYC | C2A-CAA-CBA-CGA |
| 12 | s7 | 201 | CYC | C2A-CAA-CBA-CGA |

There are no ring outliers.

336 monomers are involved in 5213 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12 | I8 | 201 | CYC | 8 | 0 |
| 12 | P8 | 201 | CYC | 8 | 0 |
| 12 | PA | 202 | CYC | 7 | 0 |
| 12 | J6 | 201 | CYC | 7 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12 | D4 | 201 | CYC | 6 | 0 |
| 12 | j7 | 201 | CYC | 15 | 0 |
| 12 | X7 | 201 | CYC | 8 | 0 |
| 12 | P1 | 202 | CYC | 7 | 0 |
| 12 | a9 | 901 | CYC | 106 | 0 |
| 12 | E1 | 201 | CYC | 8 | 0 |
| 12 | E3 | 201 | CYC | 8 | 0 |
| 12 | E8 | 201 | CYC | 8 | 0 |
| 12 | EA | 201 | CYC | 7 | 0 |
| 12 | c5 | 201 | CYC | 3 | 0 |
| 12 | HA | 201 | CYC | 6 | 0 |
| 12 | T8 | 201 | CYC | 8 | 0 |
| 12 | P9 | 201 | CYC | 11 | 0 |
| 12 | D5 | 201 | CYC | 11 | 0 |
| 12 | A2 | 201 | CYC | 8 | 0 |
| 12 | T4 | 201 | CYC | 8 | 0 |
| 12 | G6 | 201 | CYC | 8 | 0 |
| 12 | TA | 302 | CYC | 8 | 0 |
| 12 | Y3 | 201 | CYC | 8 | 0 |
| 12 | S4 | 201 | CYC | 6 | 0 |
| 12 | C3 | 201 | CYC | 8 | 0 |
| 12 | B9 | 202 | CYC | 7 | 0 |
| 12 | BA | 202 | CYC | 8 | 0 |
| 12 | V1 | 202 | CYC | 6 | 0 |
| 12 | U4 | 201 | CYC | 13 | 0 |
| 12 | LA | 202 | CYC | 21 | 0 |
| 12 | SA | 201 | CYC | 8 | 0 |
| 12 | M4 | 301 | CYC | 76 | 0 |
| 12 | v7 | 201 | CYC | 22 | 0 |
| 12 | C6 | 201 | CYC | 8 | 0 |
| 12 | L6 | 202 | CYC | 10 | 0 |
| 12 | B1 | 202 | CYC | 68 | 0 |
| 12 | P1 | 201 | CYC | 18 | 0 |
| 12 | X8 | 201 | CYC | 8 | 0 |
| 12 | G4 | 201 | CYC | 8 | 0 |
| 12 | B5 | 201 | CYC | 26 | 0 |
| 12 | K4 | 201 | CYC | 8 | 0 |
| 12 | Z5 | 201 | CYC | 15 | 0 |
| 12 | Z1 | 202 | CYC | 28 | 0 |
| 12 | L3 | 202 | CYC | 21 | 0 |
| 12 | E5 | 201 | CYC | 27 | 0 |
| 12 | D6 | 201 | CYC | 8 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 12 | V1 | 201 | CYC | 7 | 0 |
| 12 | F3 | 201 | CYC | 24 | 0 |
| 12 | k5 | 1204 | CYC | 40 | 0 |
| 12 | A1 | 201 | CYC | 8 | 0 |
| 12 | JA | 201 | CYC | 8 | 0 |
| 12 | I5 | 201 | CYC | 8 | 0 |
| 12 | Q5 | 201 | CYC | 15 | 0 |
| 12 | R8 | 201 | CYC | 8 | 0 |
| 12 | V9 | 201 | CYC | 42 | 0 |
| 12 | V7 | 201 | CYC | 10 | 0 |
| 12 | g7 | 201 | CYC | 3 | 0 |
| 12 | R9 | 202 | CYC | 6 | 0 |
| 12 | OA | 201 | CYC | 8 | 0 |
| 12 | M8 | 302 | CYC | 80 | 0 |
| 12 | D8 | 202 | CYC | 21 | 0 |
| 12 | T3 | 301 | CYC | 23 | 0 |
| 12 | F6 | 201 | CYC | 63 | 0 |
| 12 | G3 | 201 | CYC | 8 | 0 |
| 12 | o7 | 201 | CYC | 18 | 0 |
| 12 | XA | 202 | CYC | 6 | 0 |
| 12 | H9 | 201 | CYC | 6 | 0 |
| 12 | J7 | 201 | CYC | 23 | 0 |
| 12 | I9 | 201 | CYC | 8 | 0 |
| 12 | K9 | 201 | CYC | 8 | 0 |
| 12 | ZA | 202 | CYC | 12 | 0 |
| 12 | J9 | 201 | CYC | 9 | 0 |
| 12 | BA | 201 | CYC | 18 | 0 |
| 12 | N4 | 201 | CYC | 8 | 0 |
| 12 | S3 | 201 | CYC | 9 | 0 |
| 12 | H8 | 202 | CYC | 6 | 0 |
| 12 | M8 | 301 | CYC | 101 | 0 |
| 12 | F8 | 201 | CYC | 6 | 0 |
| 12 | R3 | 201 | CYC | 25 | 0 |
| 12 | N2 | 101 | CYC | 13 | 0 |
| 12 | K1 | 201 | CYC | 8 | 0 |
| 12 | F3 | 202 | CYC | 7 | 0 |
| 12 | k5 | 1202 | CYC | 15 | 0 |
| 12 | JA | 202 | CYC | 39 | 0 |
| 12 | ZA | 201 | CYC | 9 | 0 |
| 12 | IA | 201 | CYC | 8 | 0 |
| 12 | A3 | 201 | CYC | 8 | 0 |
| 12 | a7 | 201 | CYC | 3 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 12 | D2 | 202 | CYC | 7 | 0 |
| 12 | L2 | 202 | CYC | 10 | 0 |
| 12 | V3 | 202 | CYC | 6 | 0 |
| 12 | S9 | 201 | CYC | 8 | 0 |
| 12 | K5 | 201 | CYC | 28 | 0 |
| 12 | N8 | 201 | CYC | 12 | 0 |
| 12 | U1 | 201 | CYC | 8 | 0 |
| 12 | U9 | 201 | CYC | 8 | 0 |
| 12 | P3 | 202 | CYC | 8 | 0 |
| 12 | Y8 | 201 | CYC | 10 | 0 |
| 12 | XA | 201 | CYC | 7 | 0 |
| 12 | R4 | 201 | CYC | 8 | 0 |
| 12 | D7 | 201 | CYC | 32 | 0 |
| 12 | LA | 201 | CYC | 12 | 0 |
| 12 | HA | 202 | CYC | 82 | 0 |
| 12 | QA | 201 | CYC | 49 | 0 |
| 12 | k5 | 1201 | CYC | 30 | 0 |
| 12 | B9 | 201 | CYC | 20 | 0 |
| 12 | J1 | 201 | CYC | 7 | 0 |
| 12 | DA | 202 | CYC | 6 | 0 |
| 12 | F2 | 202 | CYC | 5 | 0 |
| 12 | E9 | 201 | CYC | 7 | 0 |
| 12 | X1 | 201 | CYC | 18 | 0 |
| 12 | e7 | 201 | CYC | 3 | 0 |
| 12 | J9 | 202 | CYC | 39 | 0 |
| 12 | H1 | 202 | CYC | 6 | 0 |
| 12 | Z8 | 301 | CYC | 163 | 0 |
| 12 | J3 | 201 | CYC | 6 | 0 |
| 12 | Q9 | 201 | CYC | 8 | 0 |
| 12 | s7 | 201 | CYC | 3 | 0 |
| 12 | O7 | 201 | CYC | 3 | 0 |
| 12 | j5 | 1202 | CYC | 31 | 0 |
| 12 | Y9 | 201 | CYC | 8 | 0 |
| 12 | W3 | 201 | CYC | 8 | 0 |
| 12 | E7 | 201 | CYC | 13 | 0 |
| 12 | C4 | 201 | CYC | 8 | 0 |
| 12 | W5 | 201 | CYC | 14 | 0 |
| 12 | Z1 | 201 | CYC | 9 | 0 |
| 12 | Z4 | 301 | CYC | 104 | 0 |
| 12 | A7 | 201 | CYC | 3 | 0 |
| 12 | I2 | 201 | CYC | 8 | 0 |
| 12 | d5 | 201 | CYC | 16 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12 | W7 | 201 | CYC | 14 | 0 |
| 12 | J2 | 202 | CYC | 10 | 0 |
| 12 | h7 | 201 | CYC | 15 | 0 |
| 12 | H1 | 201 | CYC | 56 | 0 |
| 12 | O1 | 201 | CYC | 11 | 0 |
| 12 | L5 | 201 | CYC | 14 | 0 |
| 12 | N5 | 201 | CYC | 14 | 0 |
| 12 | J4 | 202 | CYC | 6 | 0 |
| 12 | S5 | 201 | CYC | 3 | 0 |
| 12 | i7 | 201 | CYC | 13 | 0 |
| 12 | Z9 | 202 | CYC | 11 | 0 |
| 12 | FA | 301 | CYC | 19 | 0 |
| 12 | WA | 201 | CYC | 8 | 0 |
| 12 | J2 | 201 | CYC | 8 | 0 |
| 12 | B8 | 201 | CYC | 8 | 0 |
| 12 | DA | 201 | CYC | 14 | 0 |
| 12 | P5 | 201 | CYC | 18 | 0 |
| 12 | V4 | 201 | CYC | 8 | 0 |
| 12 | I4 | 201 | CYC | 8 | 0 |
| 12 | O8 | 202 | CYC | 9 | 0 |
| 12 | B2 | 201 | CYC | 7 | 0 |
| 12 | L2 | 201 | CYC | 8 | 0 |
| 12 | k7 | 201 | CYC | 3 | 0 |
| 12 | D9 | 201 | CYC | 14 | 0 |
| 12 | c7 | 201 | CYC | 10 | 0 |
| 12 | E6 | 201 | CYC | 8 | 0 |
| 12 | F1 | 202 | CYC | 6 | 0 |
| 12 | L8 | 201 | CYC | 10 | 0 |
| 12 | L4 | 201 | CYC | 9 | 0 |
| 12 | R1 | 202 | CYC | 7 | 0 |
| 12 | A5 | 201 | CYC | 69 | 0 |
| 12 | N6 | 101 | CYC | 13 | 0 |
| 12 | W8 | 202 | CYC | 8 | 0 |
| 12 | T9 | 302 | CYC | 6 | 0 |
| 12 | C1 | 201 | CYC | 8 | 0 |
| 12 | F1 | 201 | CYC | 25 | 0 |
| 12 | f7 | 201 | CYC | 16 | 0 |
| 12 | L1 | 201 | CYC | 9 | 0 |
| 12 | aA | 901 | CYC | 52 | 0 |
| 12 | Y4 | 201 | CYC | 8 | 0 |
| 12 | L9 | 202 | CYC | 21 | 0 |
| 12 | H5 | 201 | CYC | 21 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12 | I1 | 201 | CYC | 8 | 0 |
| 12 | S7 | 201 | CYC | 4 | 0 |
| 12 | G8 | 201 | CYC | 8 | 0 |
| 12 | M7 | 201 | CYC | 3 | 0 |
| 12 | R7 | 201 | CYC | 9 | 0 |
| 12 | p7 | 201 | CYC | 16 | 0 |
| 12 | Q1 | 201 | CYC | 8 | 0 |
| 12 | B8 | 202 | CYC | 84 | 0 |
| 12 | m7 | 201 | CYC | 4 | 0 |
| 12 | A6 | 201 | CYC | 8 | 0 |
| 12 | J4 | 201 | CYC | 12 | 0 |
| 12 | J8 | 202 | CYC | 8 | 0 |
| 12 | R9 | 201 | CYC | 19 | 0 |
| 12 | P7 | 201 | CYC | 13 | 0 |
| 12 | L3 | 201 | CYC | 9 | 0 |
| 12 | D8 | 201 | CYC | 6 | 0 |
| 12 | B1 | 201 | CYC | 7 | 0 |
| 12 | N7 | 201 | CYC | 10 | 0 |
| 12 | L4 | 202 | CYC | 21 | 0 |
| 12 | U8 | 202 | CYC | 8 | 0 |
| 12 | H3 | 202 | CYC | 14 | 0 |
| 12 | Z3 | 202 | CYC | 12 | 0 |
| 12 | L6 | 201 | CYC | 8 | 0 |
| 12 | B3 | 202 | CYC | 67 | 0 |
| 12 | S1 | 201 | CYC | 8 | 0 |
| 12 | W4 | 202 | CYC | 7 | 0 |
| 12 | f5 | 201 | CYC | 6 | 0 |
| 12 | E4 | 201 | CYC | 8 | 0 |
| 12 | b7 | 201 | CYC | 18 | 0 |
| 12 | K8 | 201 | CYC | 8 | 0 |
| 12 | W4 | 201 | CYC | 7 | 0 |
| 12 | Y7 | 201 | CYC | 3 | 0 |
| 12 | J8 | 201 | CYC | 12 | 0 |
| 12 | F9 | 301 | CYC | 20 | 0 |
| 12 | P4 | 201 | CYC | 8 | 0 |
| 12 | G5 | 201 | CYC | 70 | 0 |
| 12 | Z3 | 201 | CYC | 26 | 0 |
| 12 | M5 | 201 | CYC | 4 | 0 |
| 12 | O9 | 201 | CYC | 8 | 0 |
| 12 | u7 | 201 | CYC | 19 | 0 |
| 12 | F4 | 202 | CYC | 9 | 0 |
| 12 | B7 | 201 | CYC | 12 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12 | e5 | 201 | CYC | 8 | 0 |
| 12 | r7 | 201 | CYC | 17 | 0 |
| 12 | A4 | 201 | CYC | 8 | 0 |
| 12 | I3 | 201 | CYC | 8 | 0 |
| 12 | D1 | 202 | CYC | 9 | 0 |
| 12 | X5 | 201 | CYC | 16 | 0 |
| 12 | Y5 | 201 | CYC | 3 | 0 |
| 12 | F5 | 201 | CYC | 17 | 0 |
| 12 | KA | 201 | CYC | 8 | 0 |
| 12 | P3 | 201 | CYC | 17 | 0 |
| 12 | D4 | 202 | CYC | 9 | 0 |
| 12 | K2 | 201 | CYC | 8 | 0 |
| 12 | X3 | 202 | CYC | 8 | 0 |
| 12 | R1 | 201 | CYC | 26 | 0 |
| 12 | C8 | 201 | CYC | 8 | 0 |
| 12 | q7 | 201 | CYC | 3 | 0 |
| 12 | D2 | 201 | CYC | 8 | 0 |
| 12 | H3 | 201 | CYC | 6 | 0 |
| 12 | W8 | 201 | CYC | 7 | 0 |
| 12 | H4 | 202 | CYC | 6 | 0 |
| 12 | Q4 | 201 | CYC | 6 | 0 |
| 12 | H8 | 201 | CYC | 28 | 0 |
| 12 | F2 | 201 | CYC | 54 | 0 |
| 12 | D1 | 201 | CYC | 6 | 0 |
| 12 | P9 | 202 | CYC | 9 | 0 |
| 12 | V3 | 201 | CYC | 7 | 0 |
| 12 | a5 | 201 | CYC | 8 | 0 |
| 12 | U7 | 201 | CYC | 3 | 0 |
| 12 | B4 | 201 | CYC | 8 | 0 |
| 12 | F9 | 302 | CYC | 35 | 0 |
| 12 | I6 | 201 | CYC | 8 | 0 |
| 12 | R5 | 201 | CYC | 15 | 0 |
| 12 | X3 | 201 | CYC | 18 | 0 |
| 12 | G2 | 201 | CYC | 11 | 0 |
| 12 | L9 | 201 | CYC | 14 | 0 |
| 12 | F7 | 201 | CYC | 17 | 0 |
| 12 | G9 | 201 | CYC | 8 | 0 |
| 12 | O3 | 201 | CYC | 8 | 0 |
| 12 | C9 | 201 | CYC | 8 | 0 |
| 12 | Q7 | 201 | CYC | 14 | 0 |
| 12 | H4 | 201 | CYC | 29 | 0 |
| 12 | K3 | 201 | CYC | 8 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 12 | X9 | 201 | CYC | 7 | 0 |
| 12 | E2 | 201 | CYC | 7 | 0 |
| 12 | T5 | 201 | CYC | 19 | 0 |
| 12 | G1 | 201 | CYC | 8 | 0 |
| 12 | k5 | 1203 | CYC | 34 | 0 |
| 12 | W1 | 201 | CYC | 8 | 0 |
| 12 | C5 | 201 | CYC | 7 | 0 |
| 12 | K6 | 201 | CYC | 8 | 0 |
| 12 | F9 | 303 | CYC | 18 | 0 |
| 12 | B6 | 201 | CYC | 7 | 0 |
| 12 | YA | 201 | CYC | 8 | 0 |
| 12 | H6 | 202 | CYC | 6 | 0 |
| 12 | A9 | 201 | CYC | 8 | 0 |
| 12 | D9 | 202 | CYC | 7 | 0 |
| 12 | A8 | 201 | CYC | 8 | 0 |
| 12 | T7 | 201 | CYC | 16 | 0 |
| 12 | T3 | 302 | CYC | 5 | 0 |
| 12 | B3 | 201 | CYC | 8 | 0 |
| 12 | RA | 201 | CYC | 19 | 0 |
| 12 | H9 | 202 | CYC | 82 | 0 |
| 12 | D6 | 202 | CYC | 6 | 0 |
| 12 | U3 | 201 | CYC | 8 | 0 |
| 12 | T1 | 301 | CYC | 23 | 0 |
| 12 | b5 | 201 | CYC | 7 | 0 |
| 12 | J5 | 201 | CYC | 12 | 0 |
| 12 | Y1 | 201 | CYC | 8 | 0 |
| 12 | J6 | 202 | CYC | 10 | 0 |
| 12 | U5 | 201 | CYC | 3 | 0 |
| 12 | V9 | 202 | CYC | 6 | 0 |
| 12 | V5 | 201 | CYC | 18 | 0 |
| 12 | j5 | 1201 | CYC | 26 | 0 |
| 12 | X4 | 201 | CYC | 8 | 0 |
| 12 | C7 | 201 | CYC | 4 | 0 |
| 12 | F6 | 202 | CYC | 6 | 0 |
| 12 | F4 | 201 | CYC | 8 | 0 |
| 12 | V8 | 201 | CYC | 8 | 0 |
| 12 | T1 | 302 | CYC | 5 | 0 |
| 12 | A | 201 | CYC | 9 | 0 |
| 12 | S8 | 201 | CYC | 6 | 0 |
| 12 | J3 | 202 | CYC | 45 | 0 |
| 12 | Z9 | 201 | CYC | 9 | 0 |
| 12 | O8 | 201 | CYC | 18 | 0 |

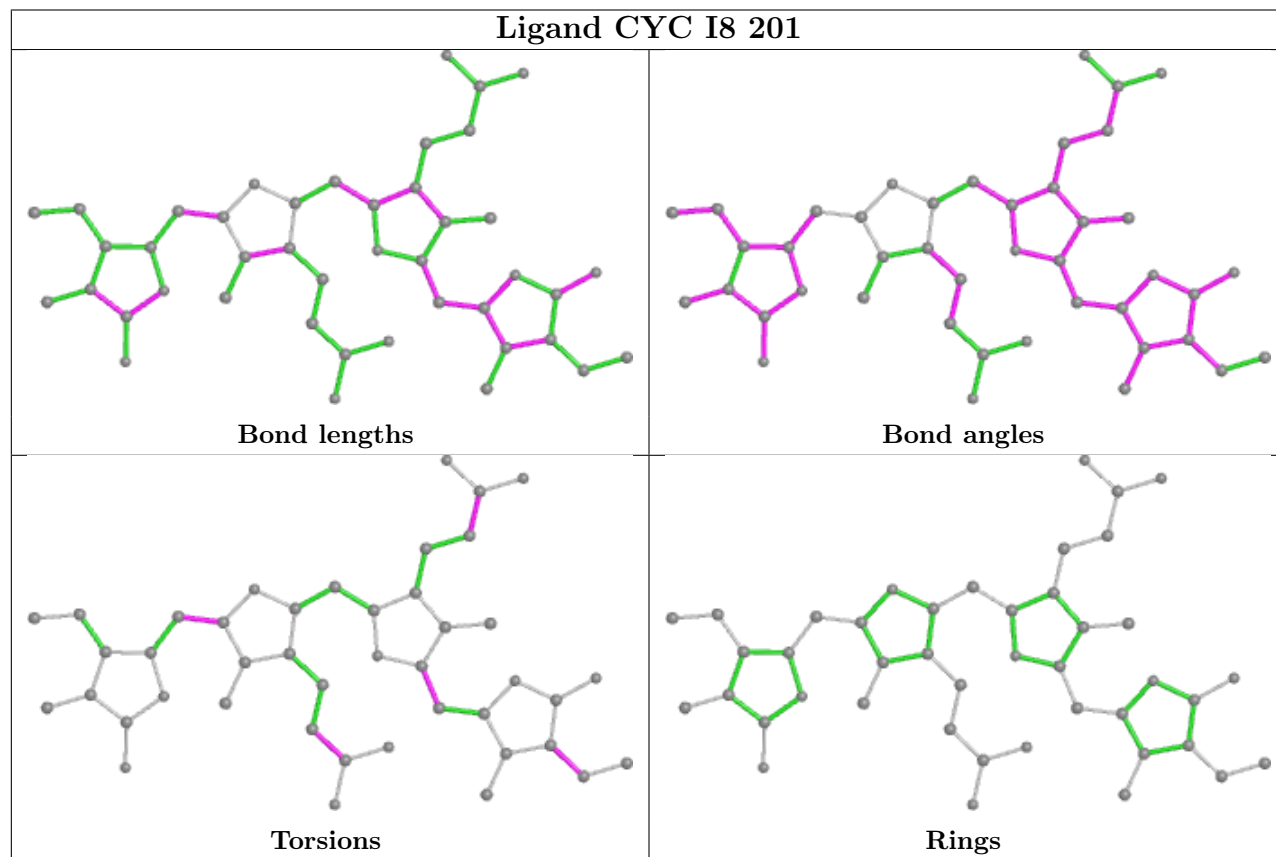
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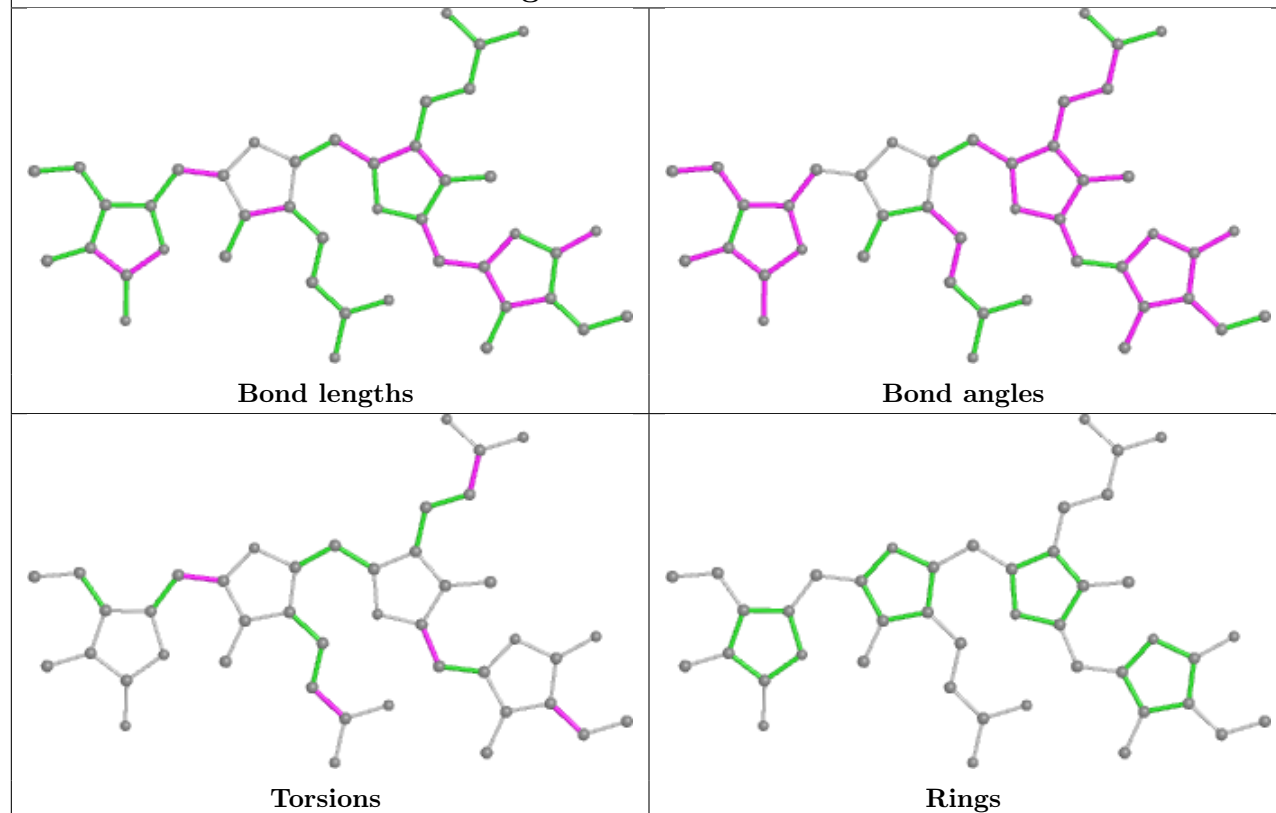
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12 | Q3 | 201 | CYC | 8 | 0 |
| 12 | GA | 201 | CYC | 8 | 0 |
| 12 | VA | 202 | CYC | 19 | 0 |
| 12 | RA | 202 | CYC | 8 | 0 |
| 12 | Q8 | 201 | CYC | 6 | 0 |
| 12 | F8 | 202 | CYC | 8 | 0 |
| 12 | R3 | 202 | CYC | 7 | 0 |
| 12 | D3 | 202 | CYC | 9 | 0 |
| 12 | O5 | 201 | CYC | 4 | 0 |
| 12 | O4 | 202 | CYC | 10 | 0 |
| 12 | H6 | 201 | CYC | 19 | 0 |
| 12 | aA | 902 | CYC | 20 | 0 |
| 12 | TA | 301 | CYC | 45 | 0 |
| 12 | U8 | 201 | CYC | 13 | 0 |
| 12 | L7 | 201 | CYC | 13 | 0 |
| 12 | I7 | 201 | CYC | 3 | 0 |
| 12 | VA | 201 | CYC | 41 | 0 |
| 12 | AA | 201 | CYC | 8 | 0 |
| 12 | D3 | 201 | CYC | 6 | 0 |
| 12 | H7 | 201 | CYC | 11 | 0 |
| 12 | X9 | 202 | CYC | 8 | 0 |
| 12 | G7 | 201 | CYC | 3 | 0 |
| 12 | O4 | 201 | CYC | 22 | 0 |
| 12 | U4 | 202 | CYC | 6 | 0 |
| 12 | d7 | 201 | CYC | 19 | 0 |
| 12 | CA | 201 | CYC | 8 | 0 |
| 12 | PA | 201 | CYC | 12 | 0 |
| 12 | UA | 201 | CYC | 9 | 0 |
| 12 | H2 | 202 | CYC | 8 | 0 |
| 12 | C2 | 201 | CYC | 8 | 0 |
| 12 | K7 | 201 | CYC | 14 | 0 |
| 12 | X1 | 202 | CYC | 5 | 0 |
| 12 | W9 | 201 | CYC | 8 | 0 |
| 12 | S4 | 202 | CYC | 33 | 0 |
| 12 | T9 | 301 | CYC | 46 | 0 |
| 12 | H2 | 201 | CYC | 19 | 0 |
| 12 | B4 | 202 | CYC | 116 | 0 |
| 12 | Z | 201 | CYC | 8 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

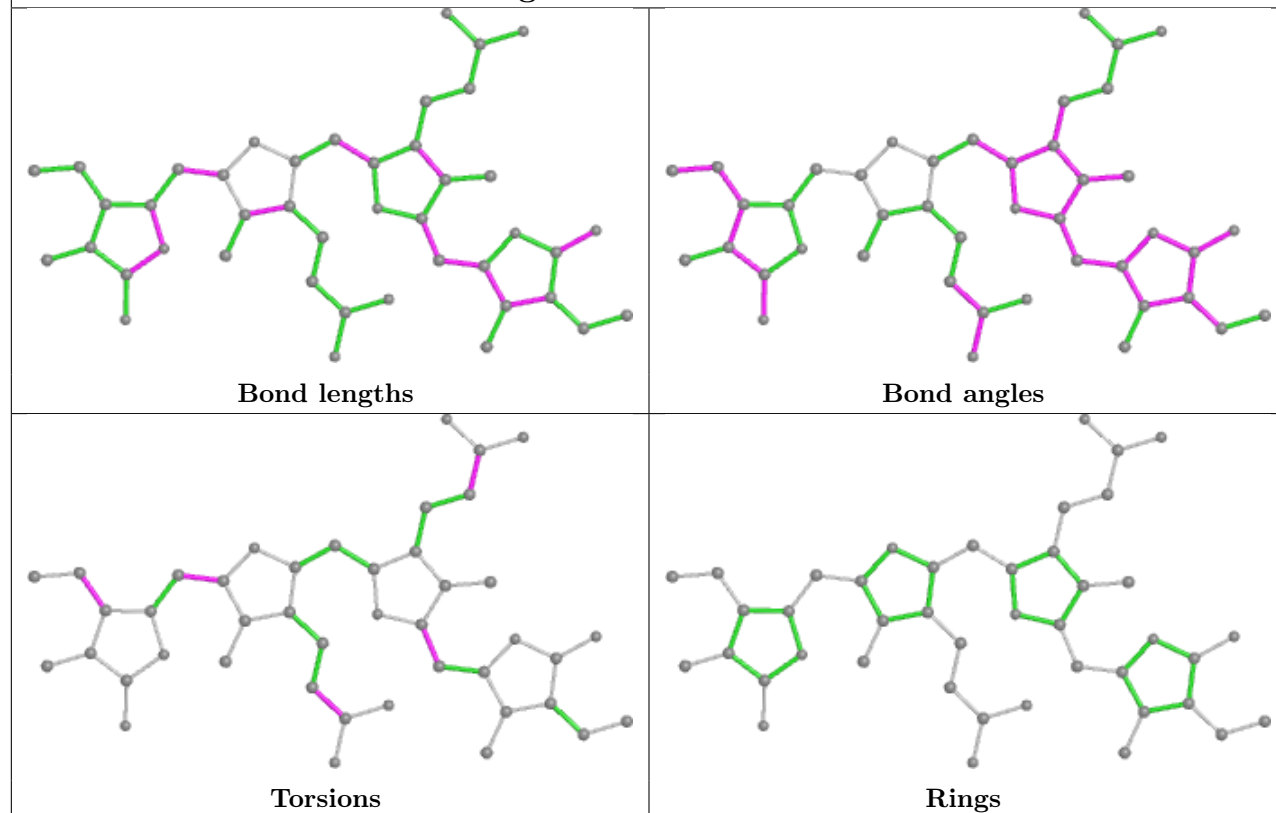
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

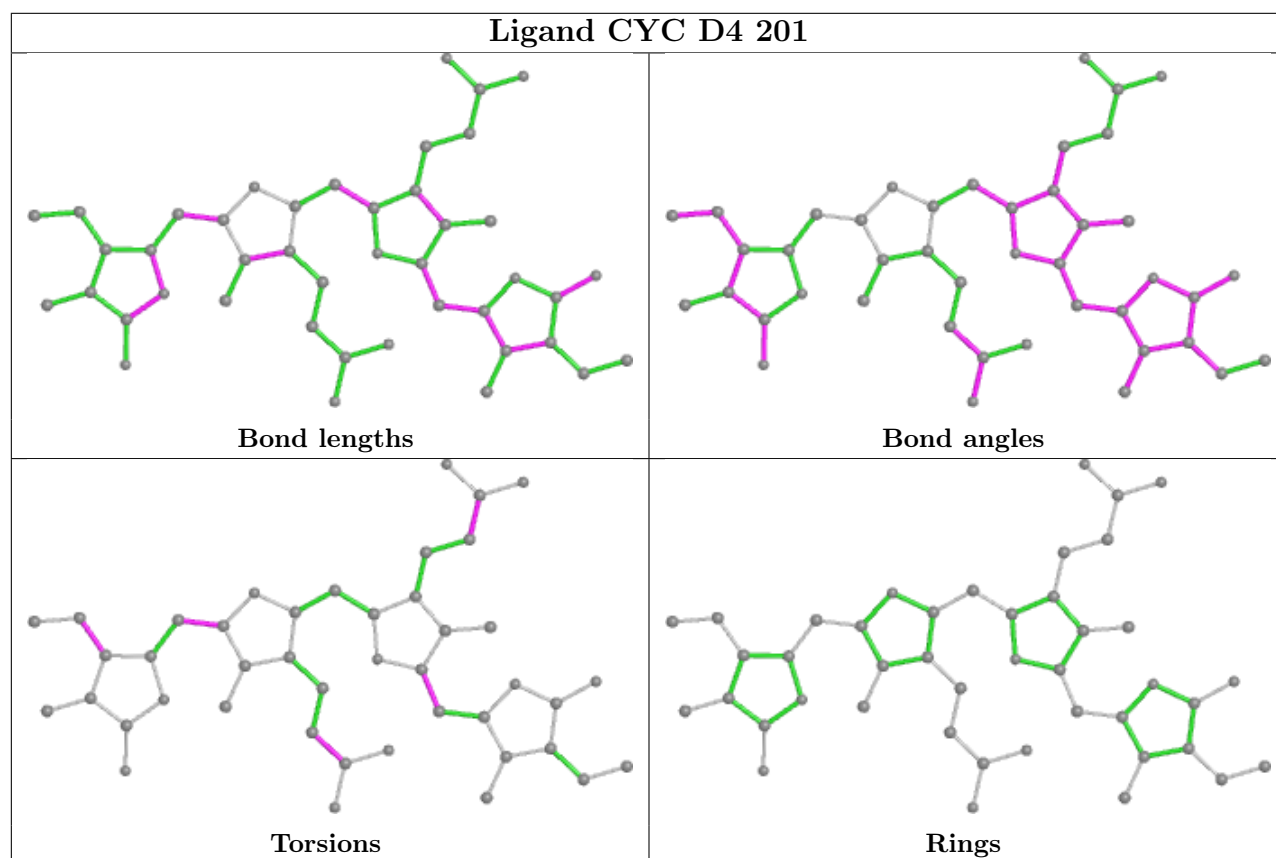
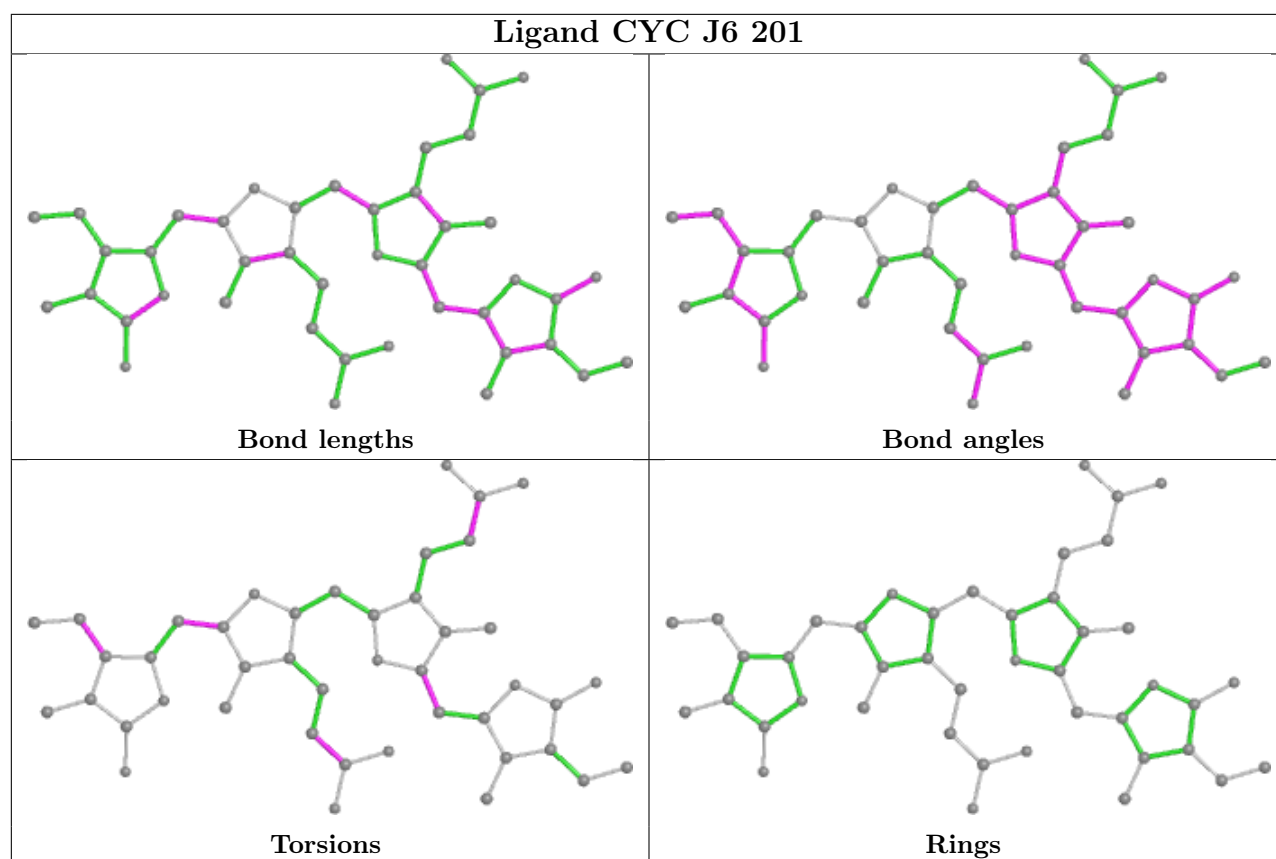


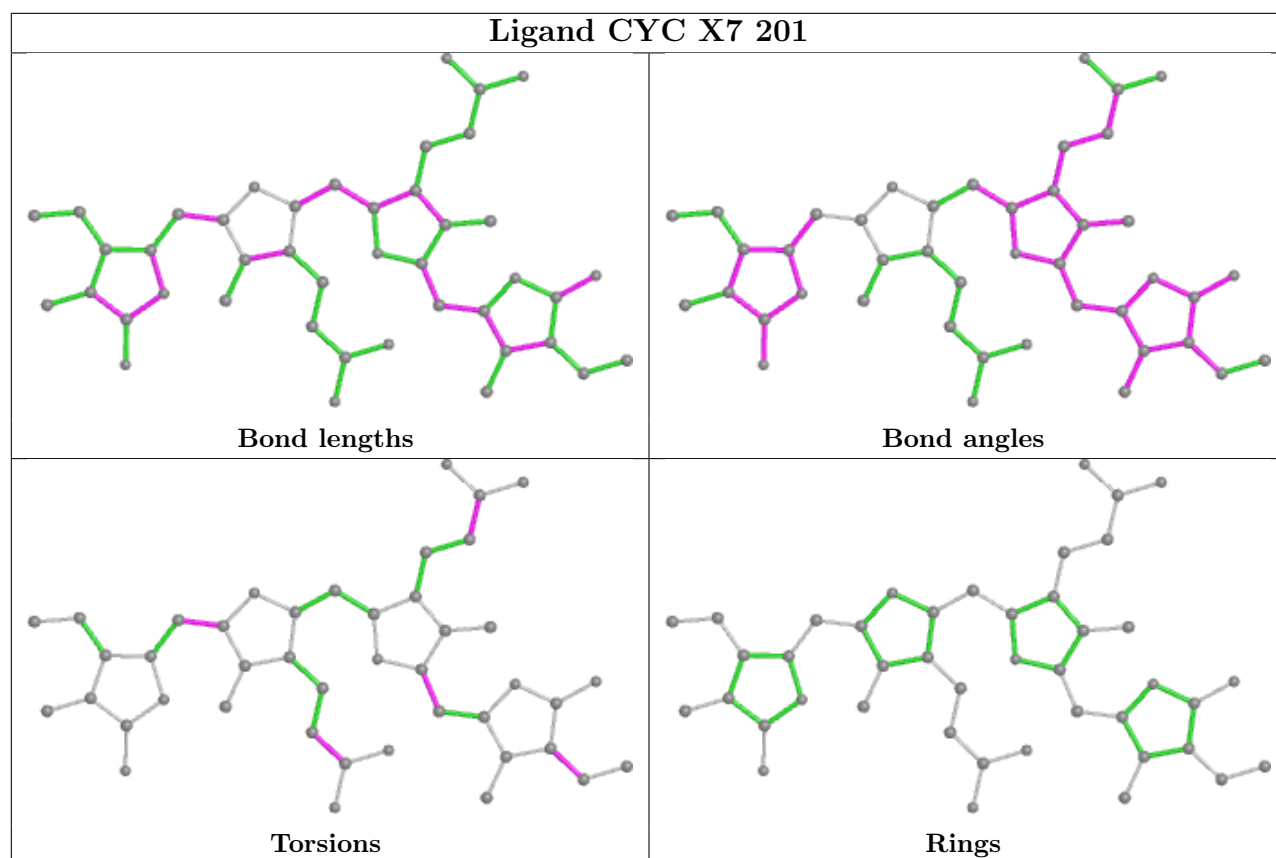
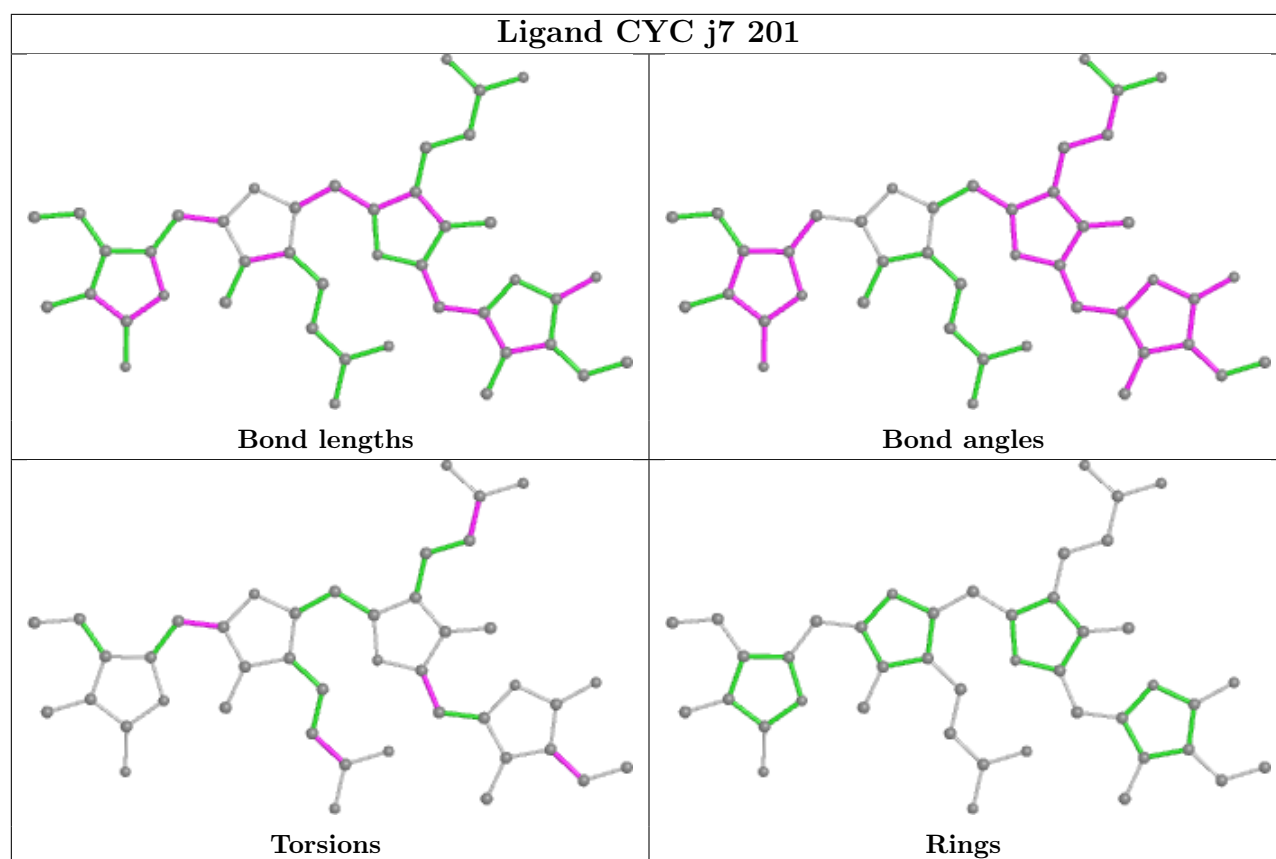
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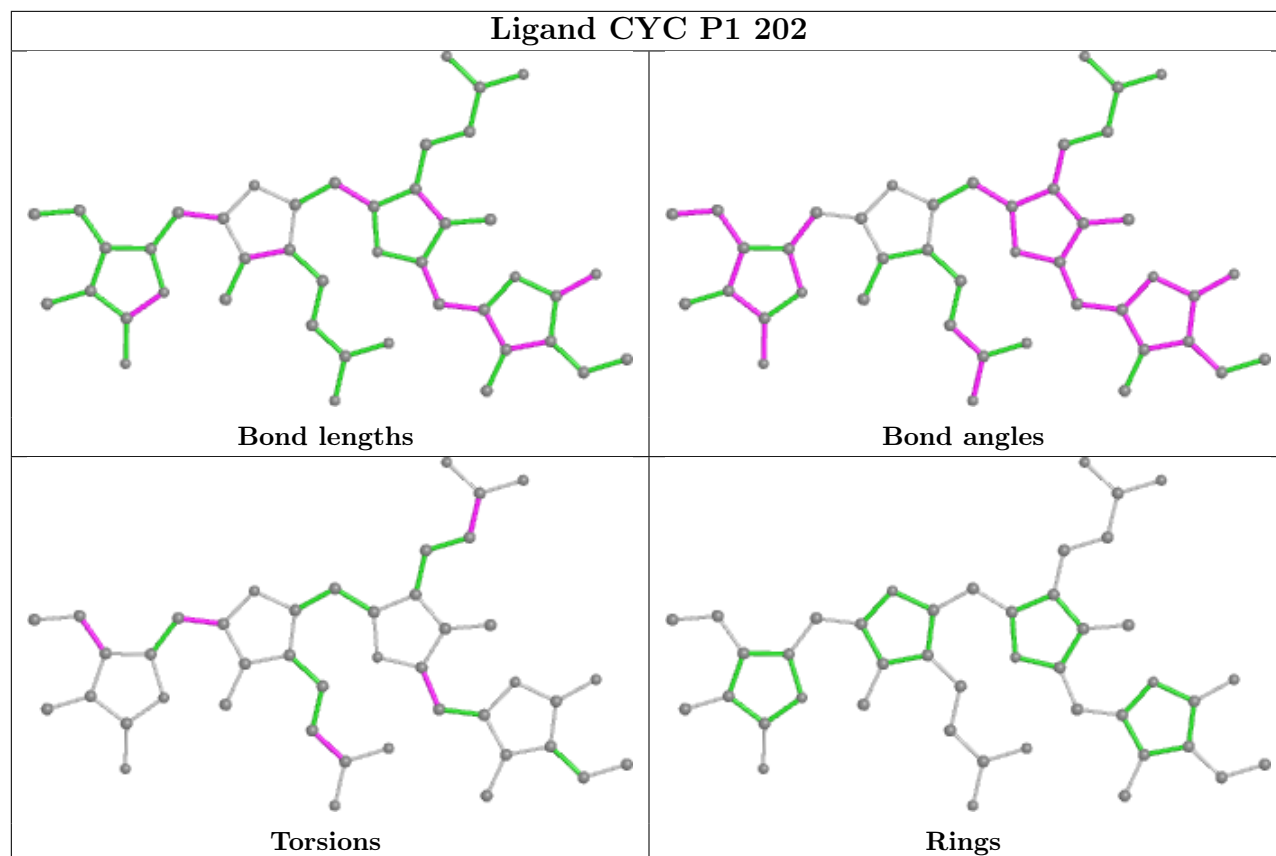
Ligand CYC PA 202



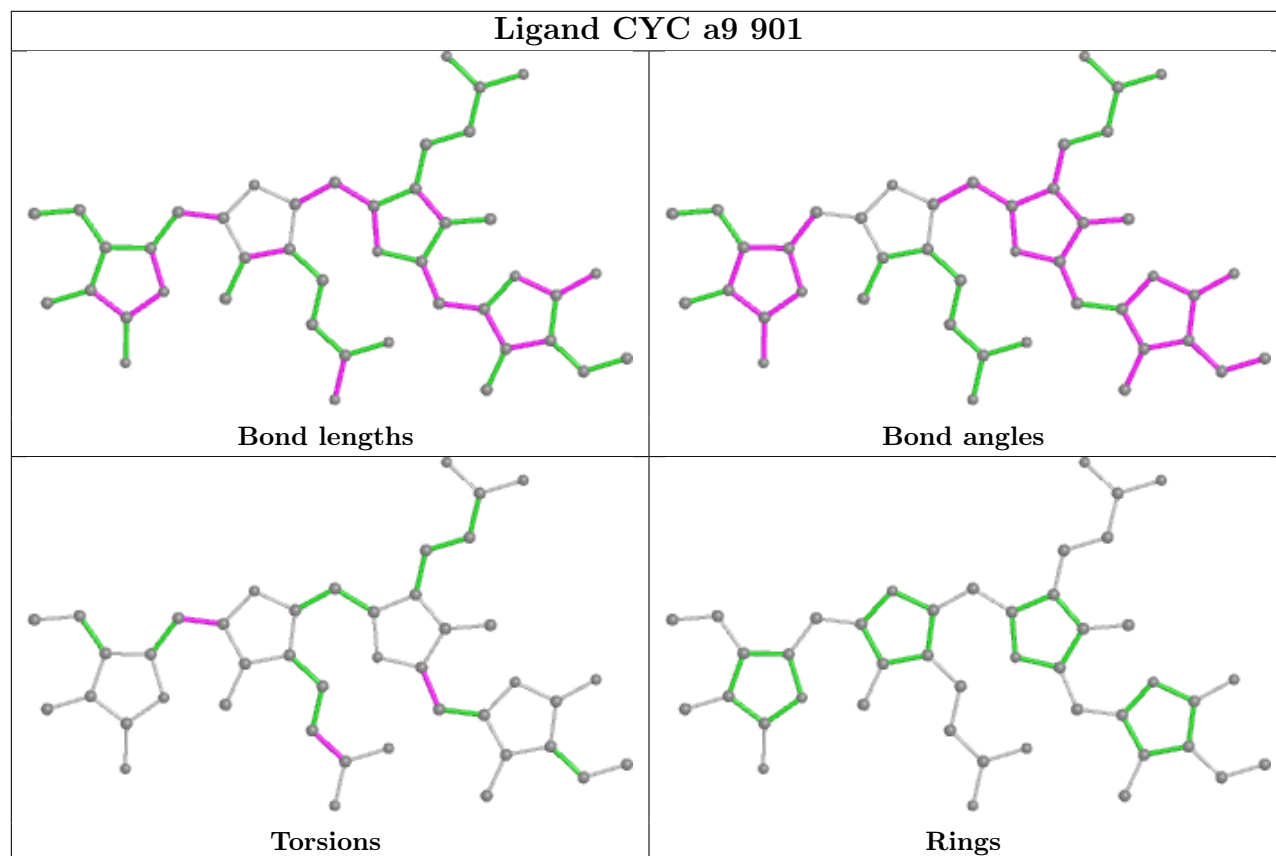




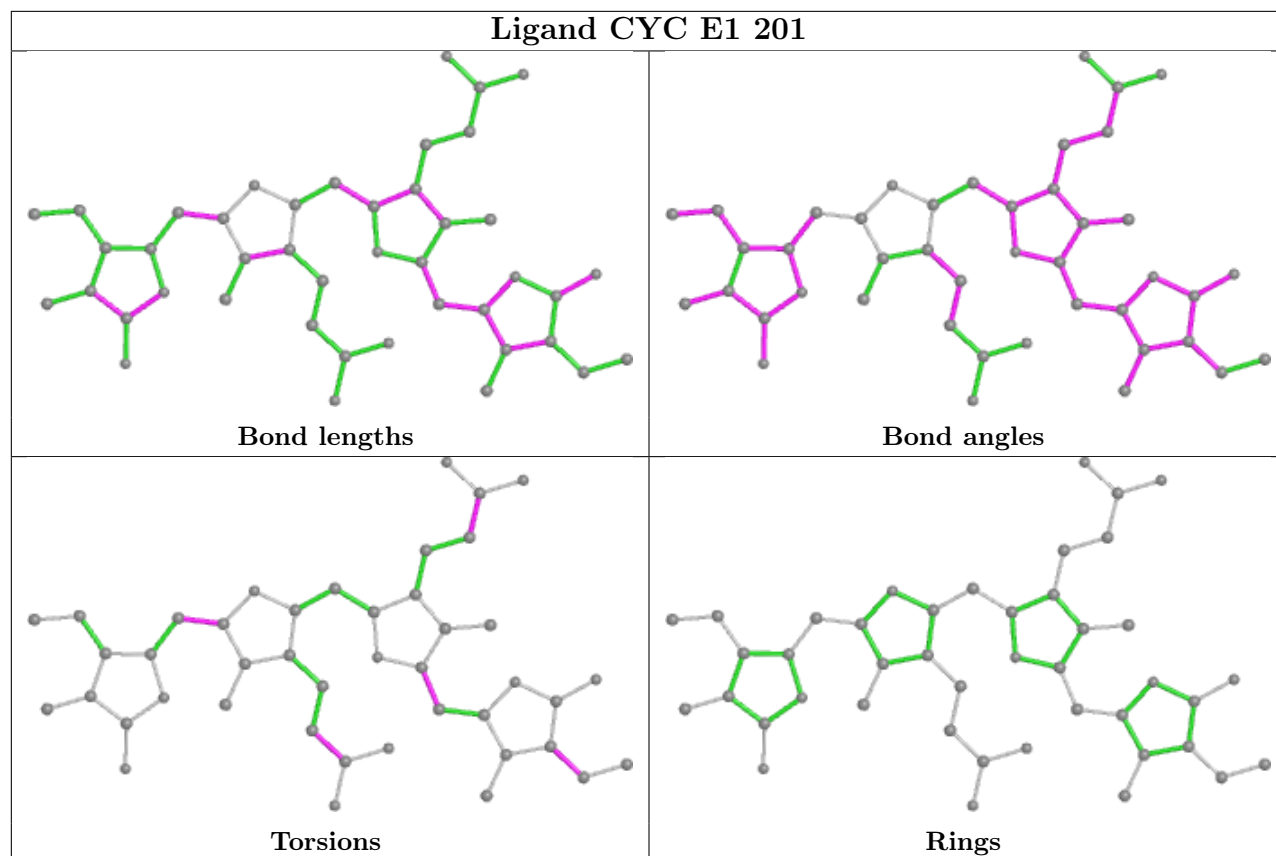
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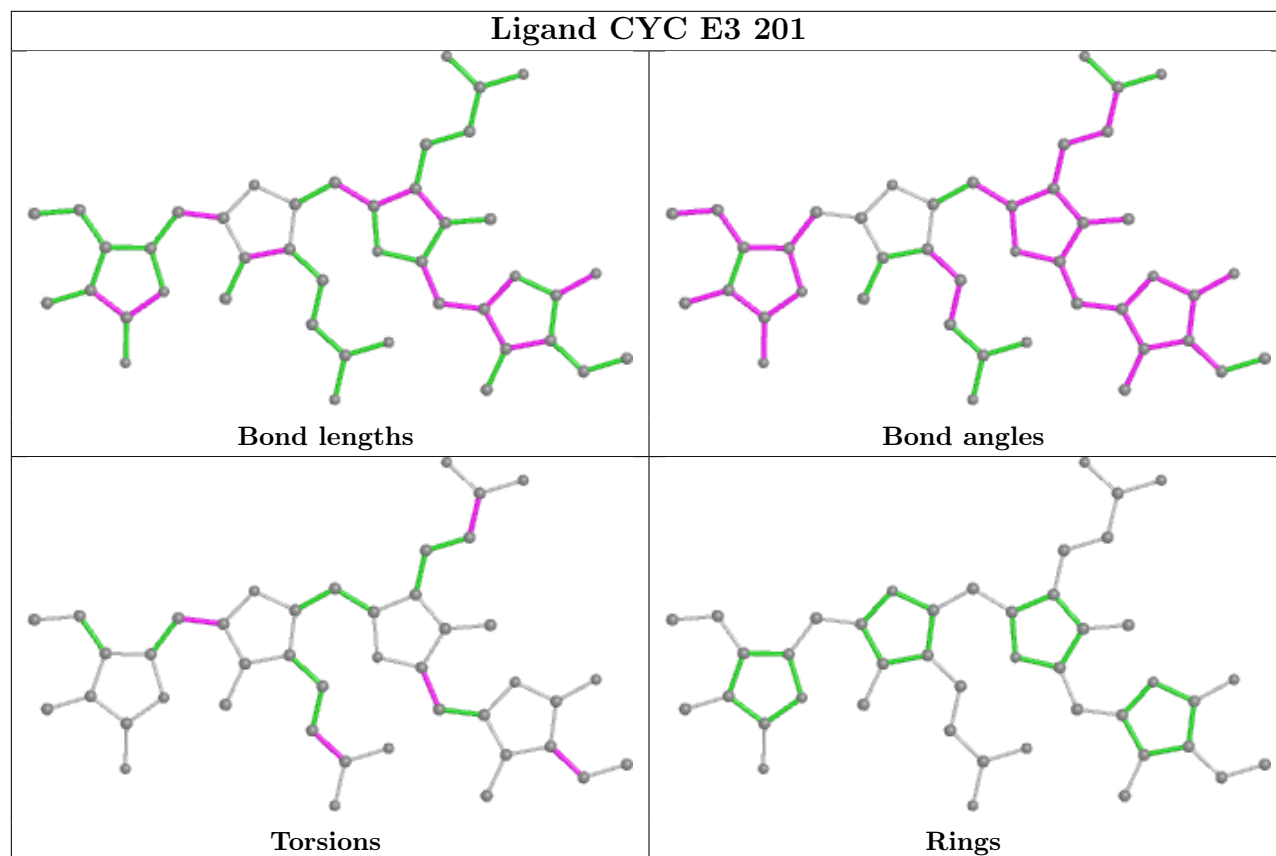
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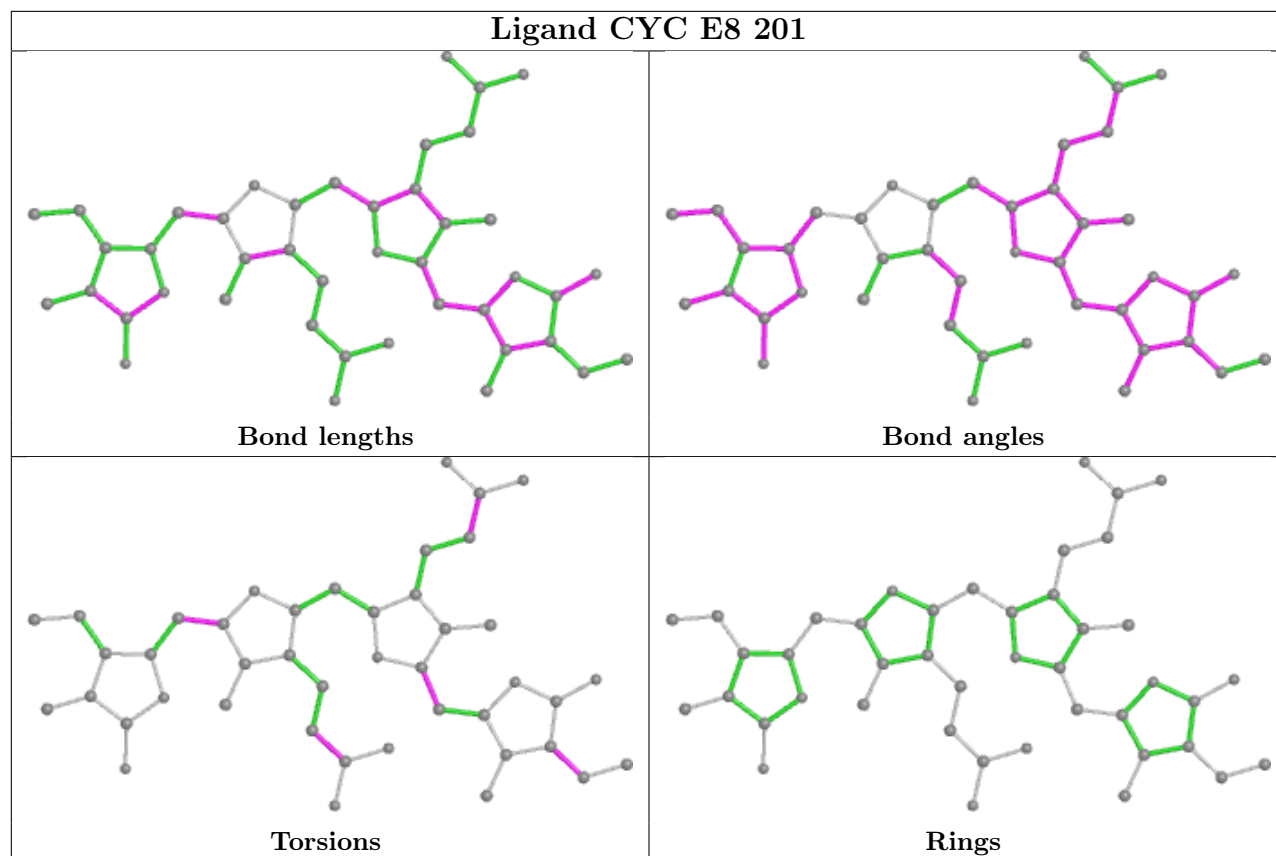
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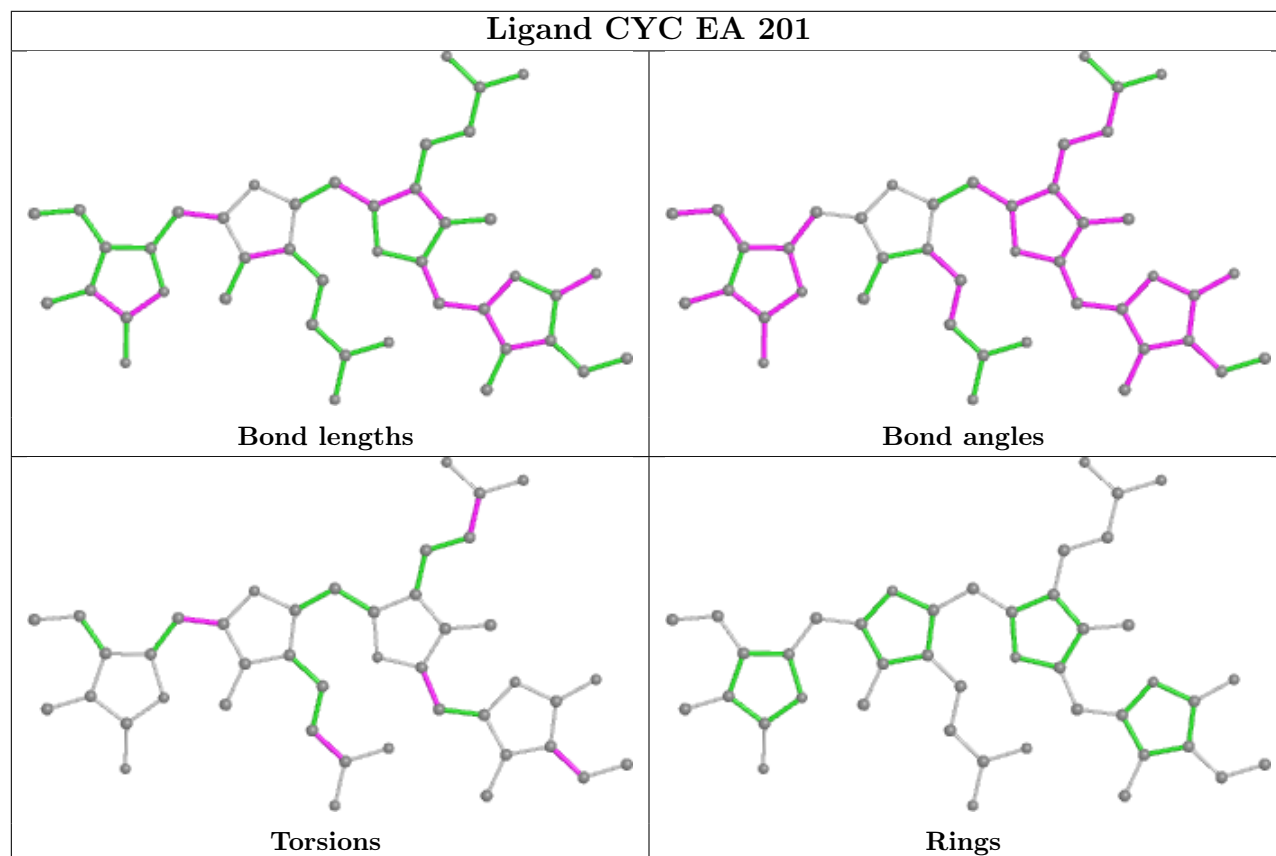
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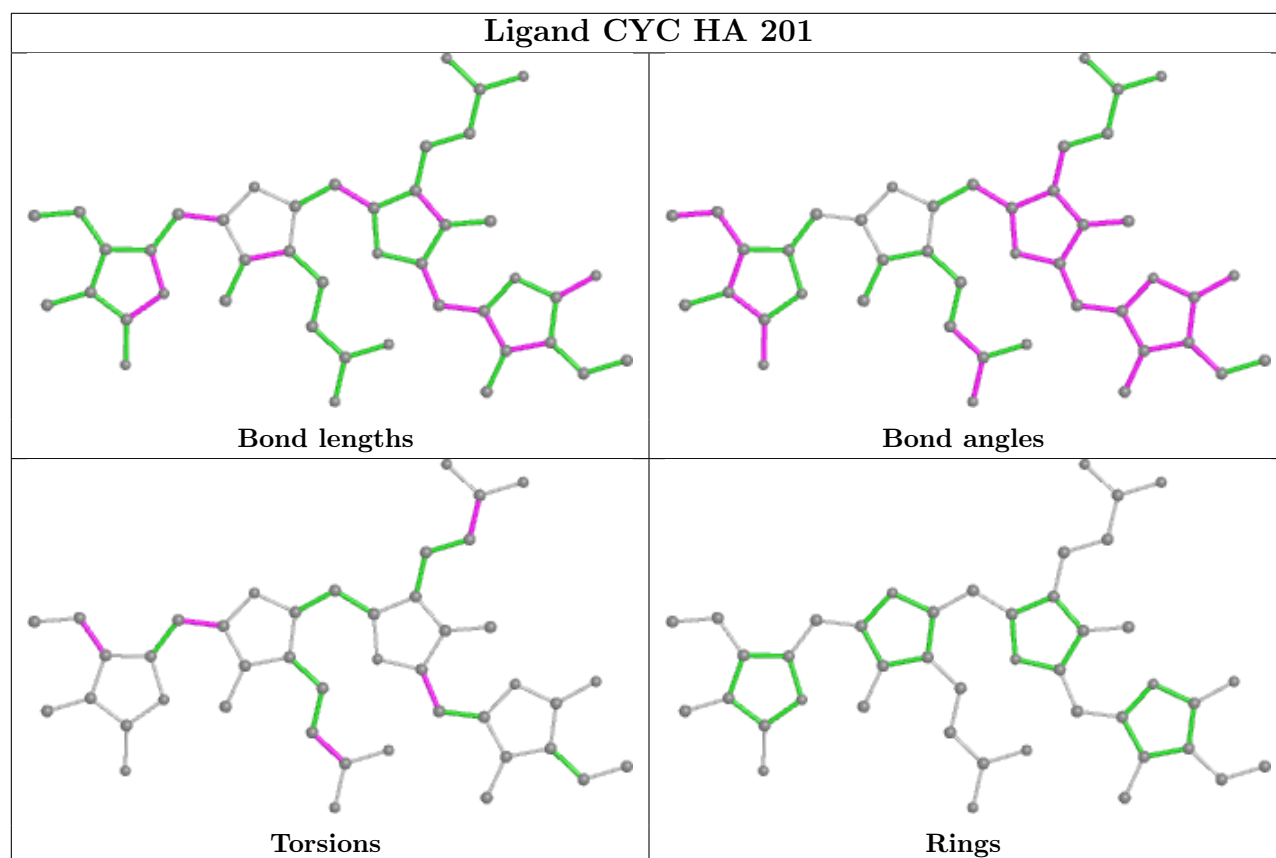
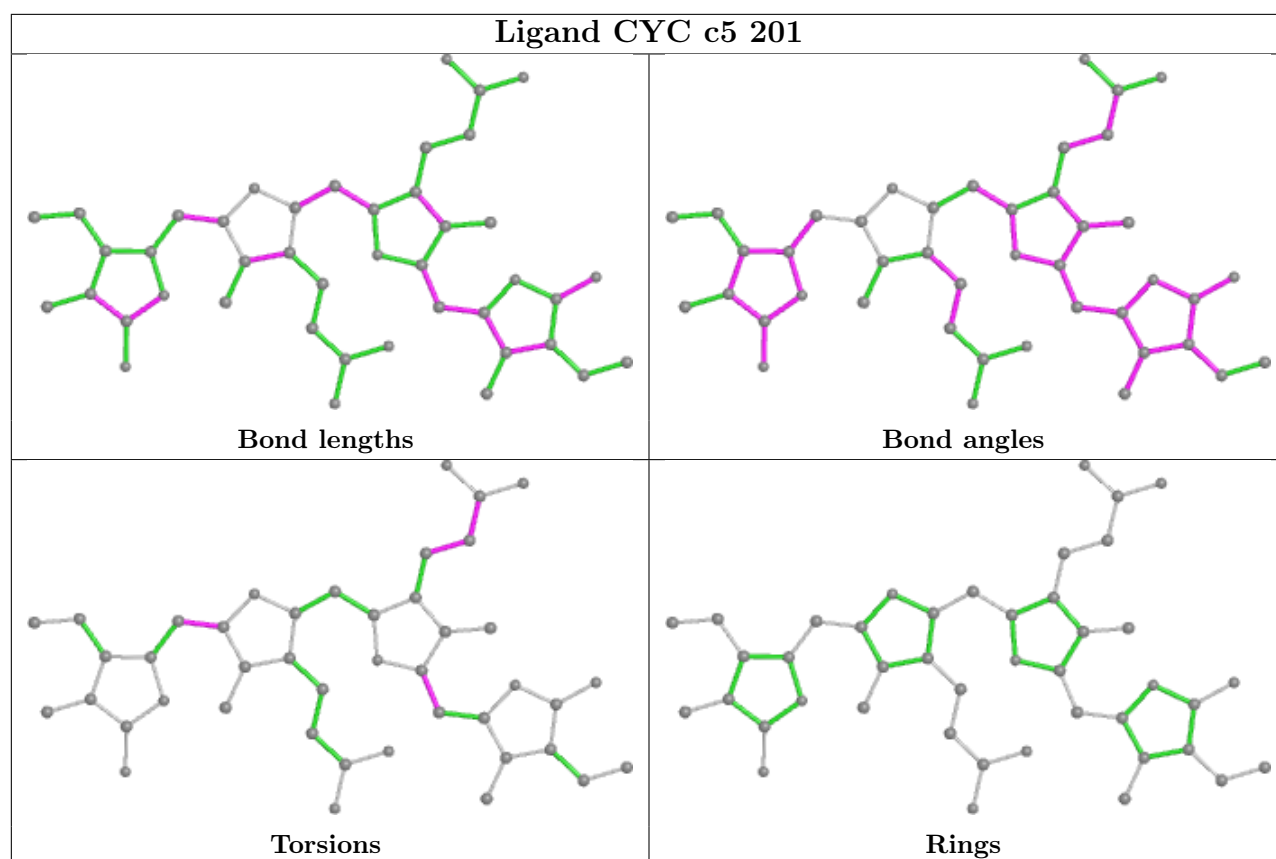


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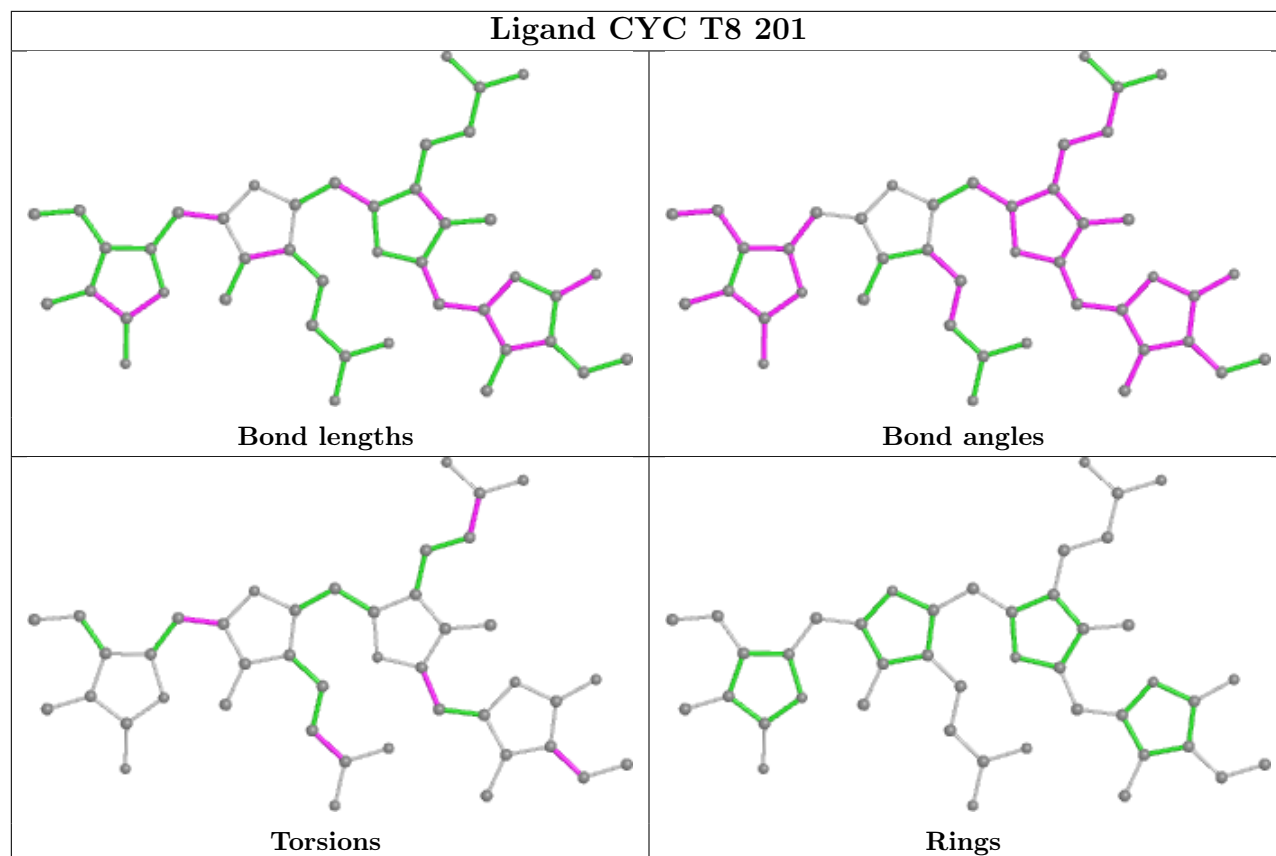


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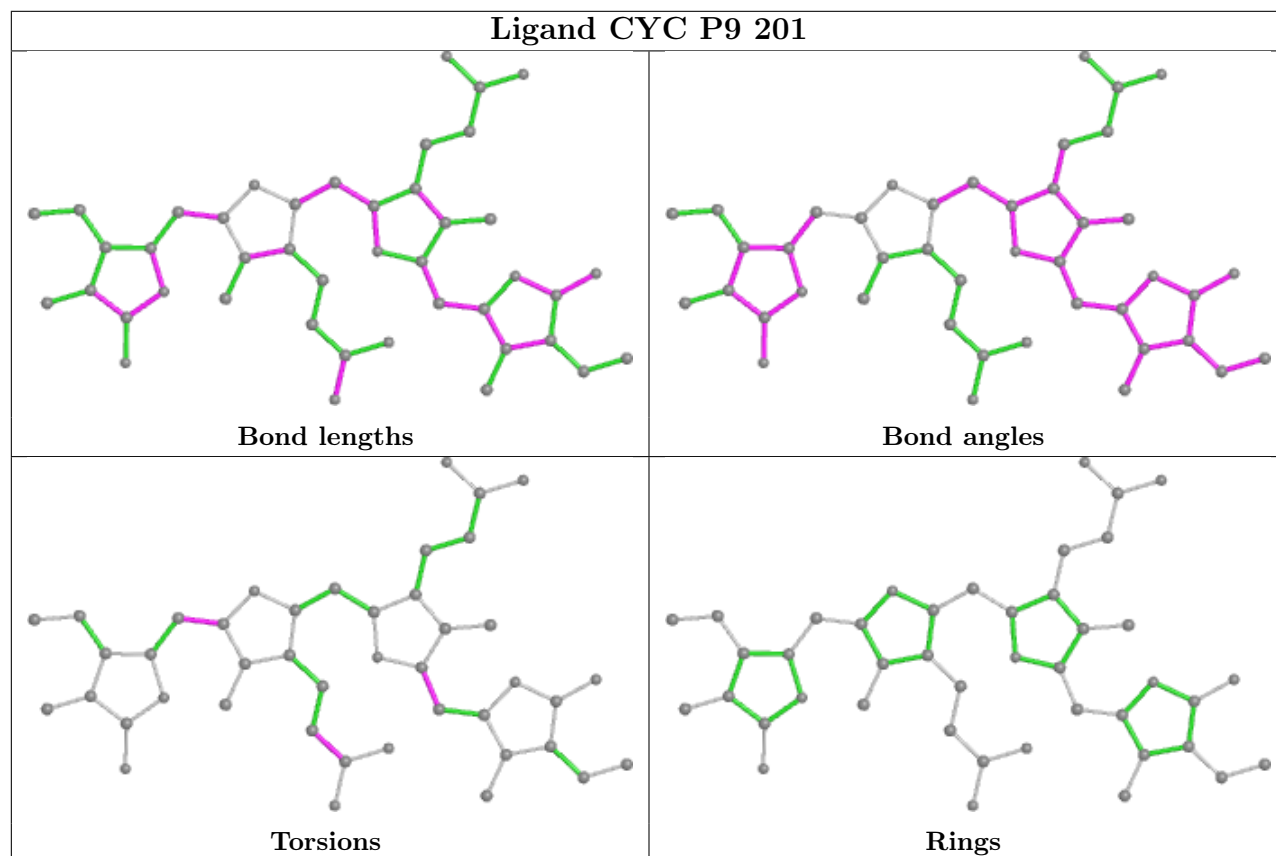




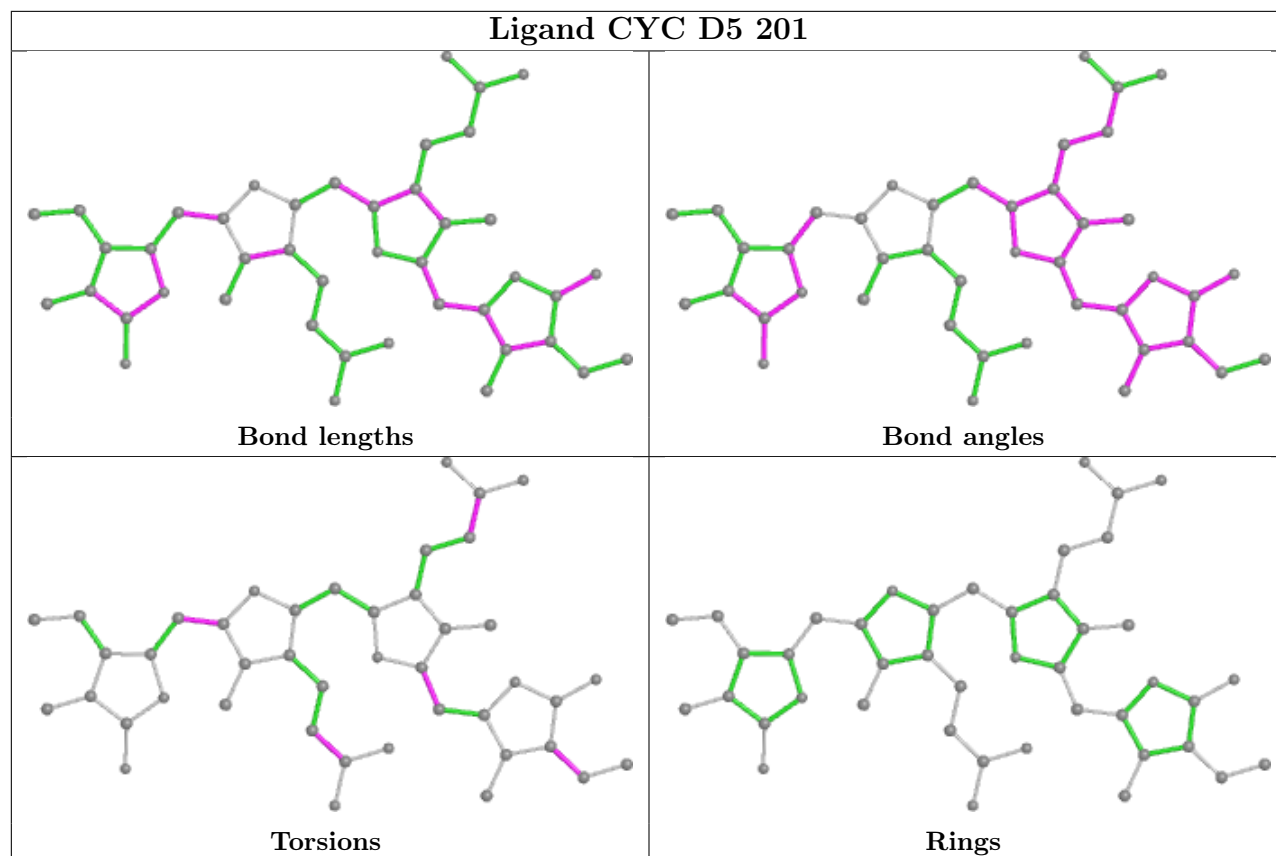
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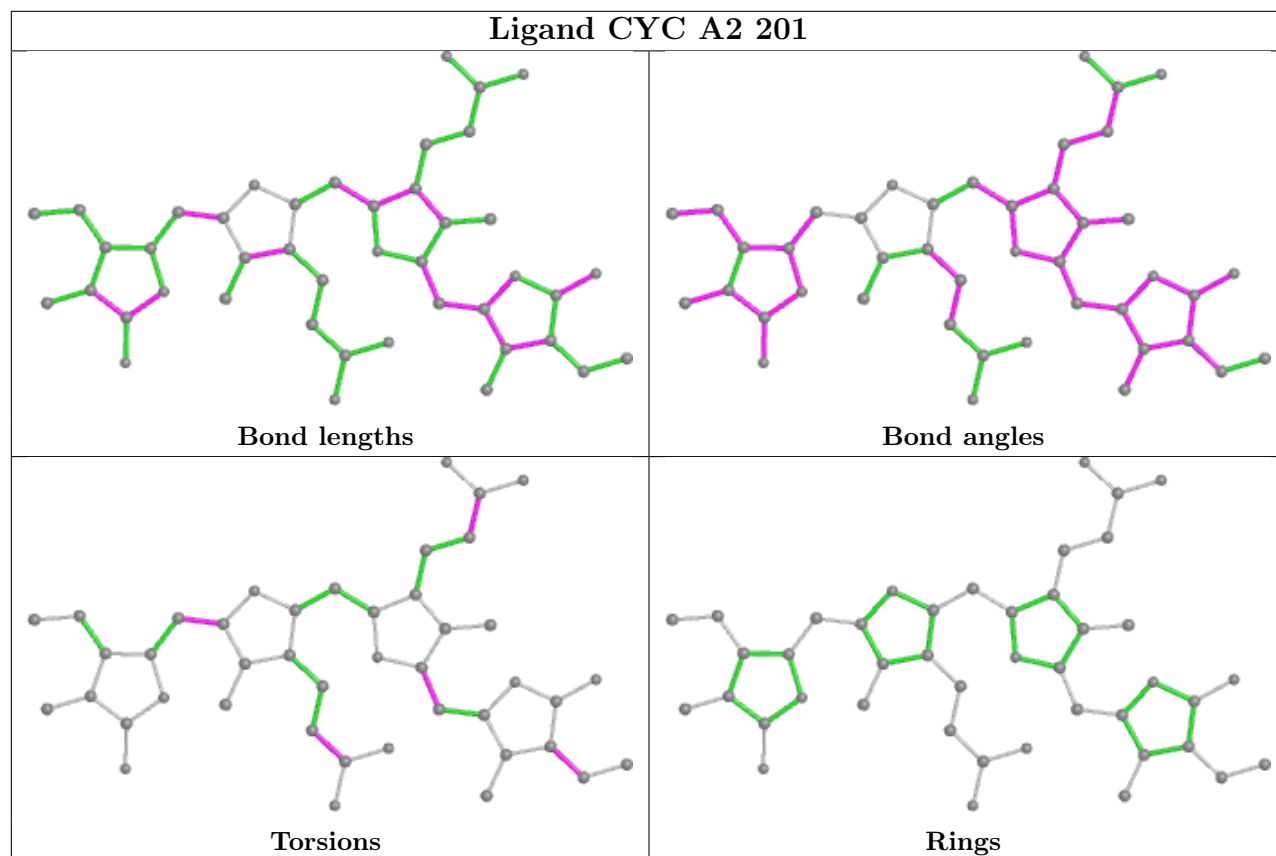
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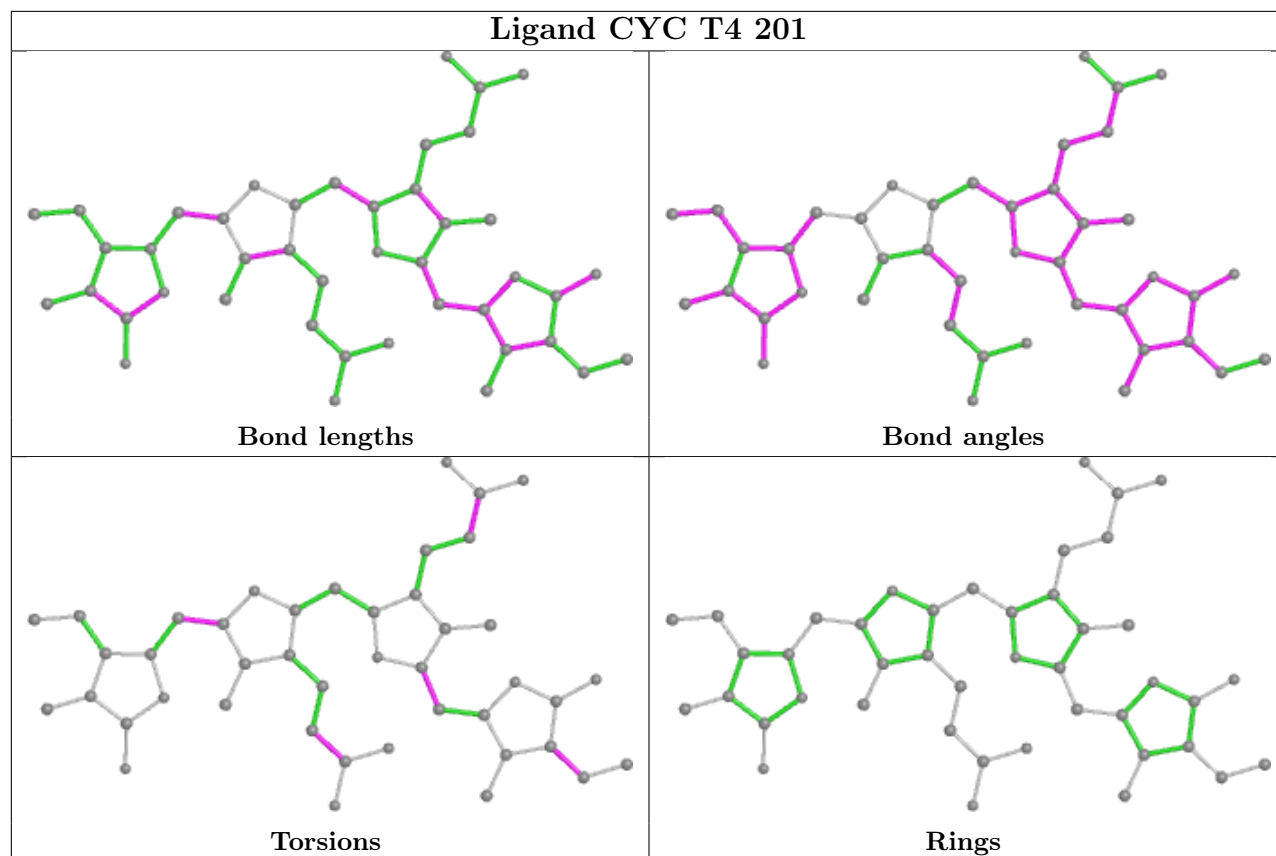
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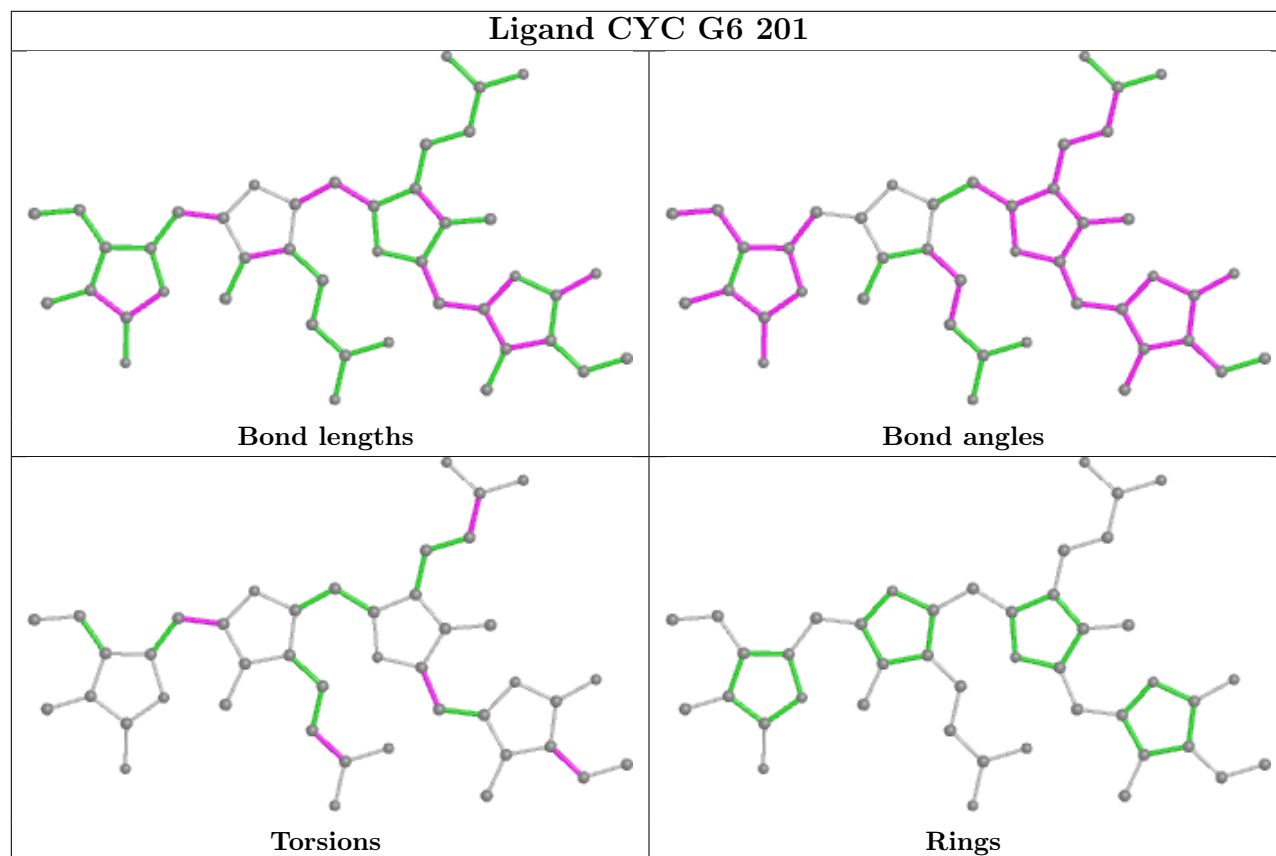
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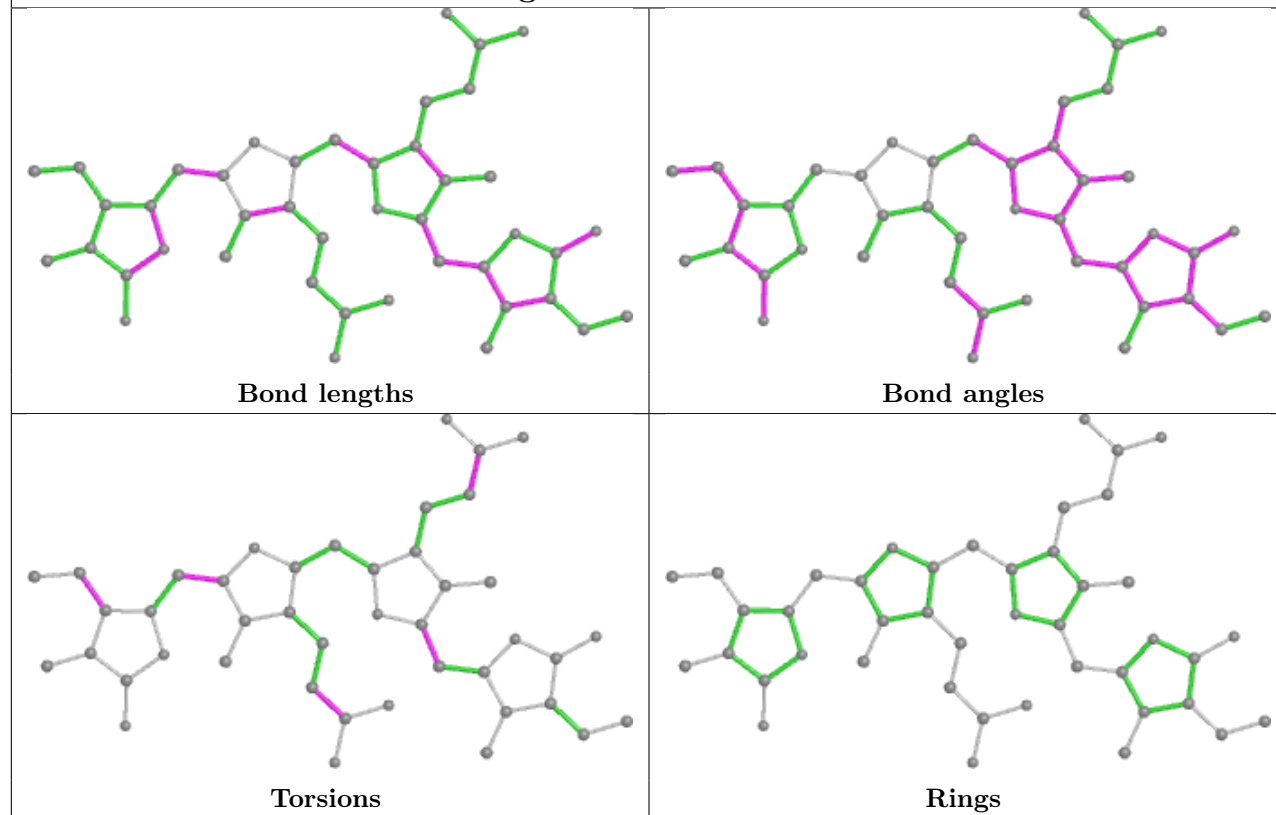
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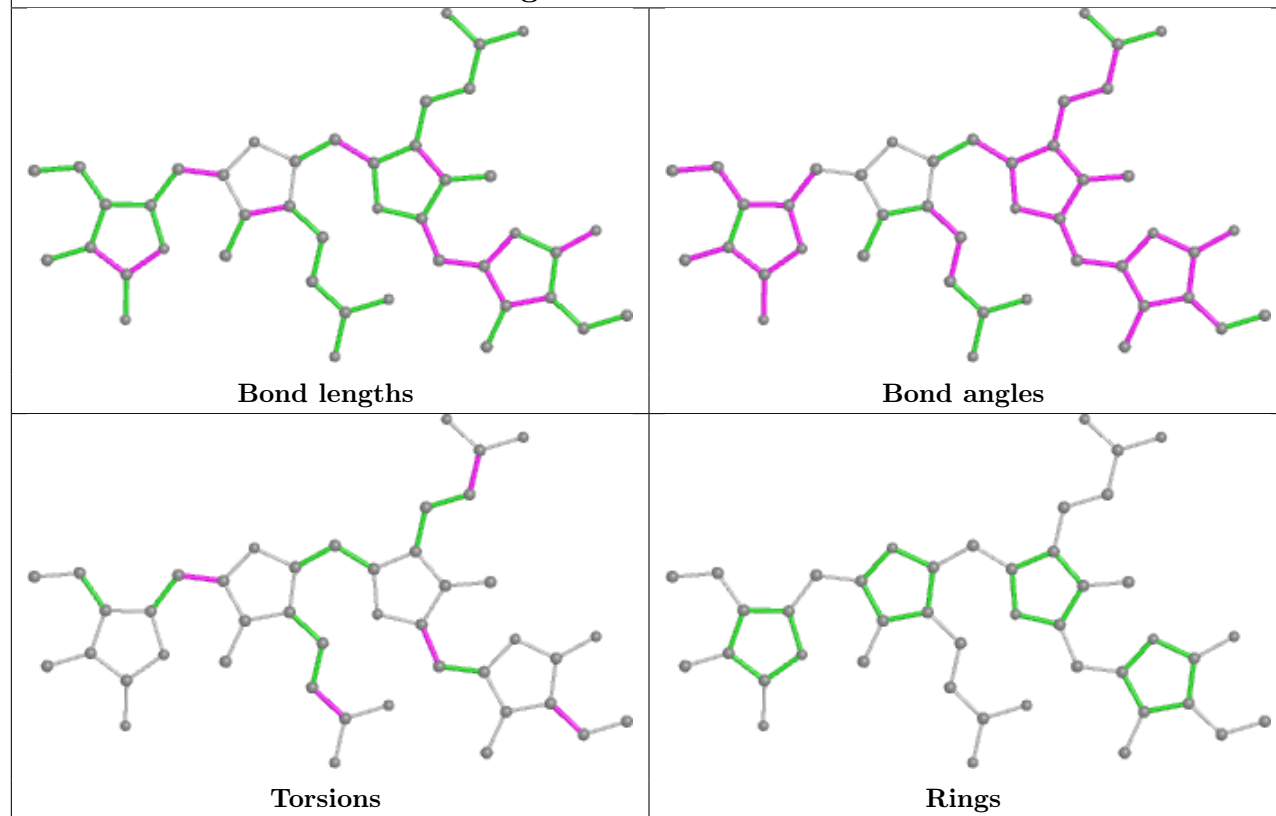
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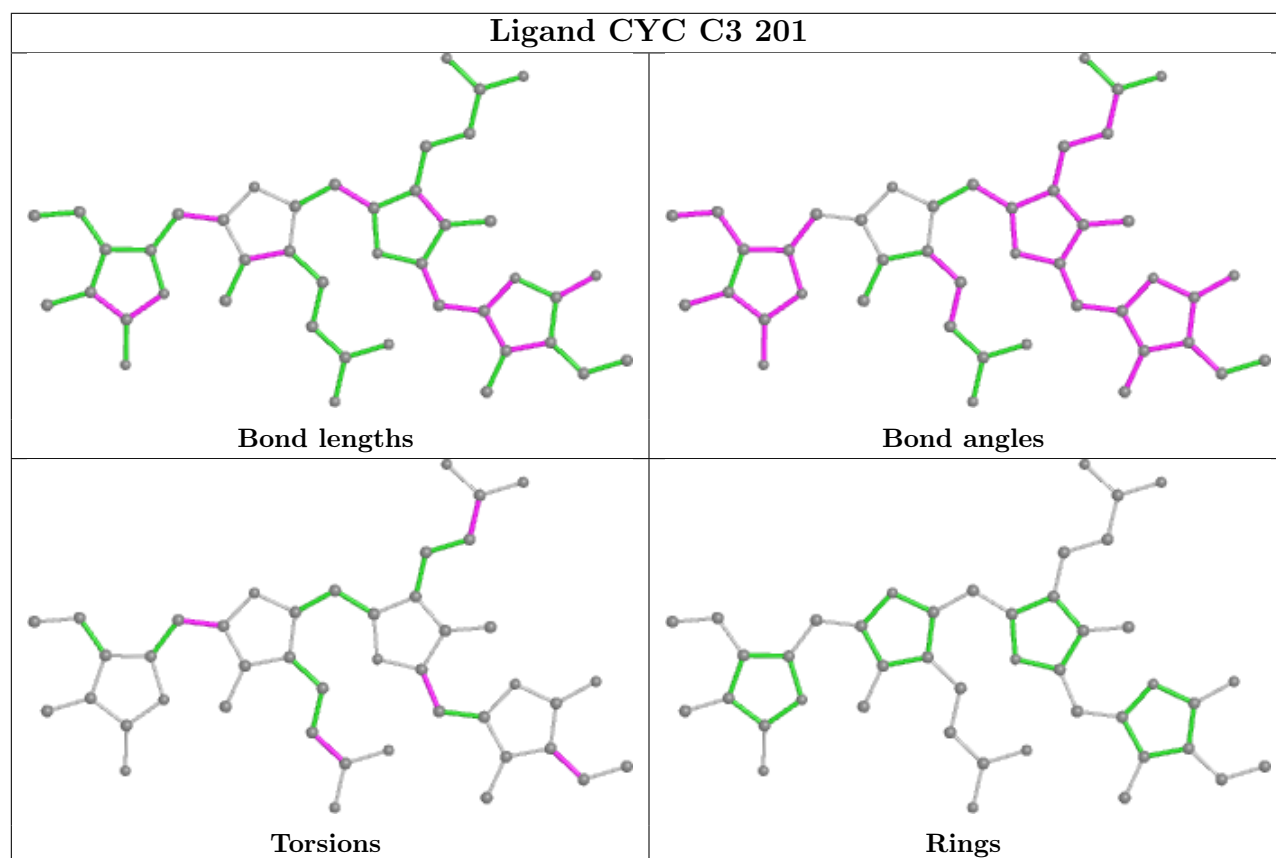
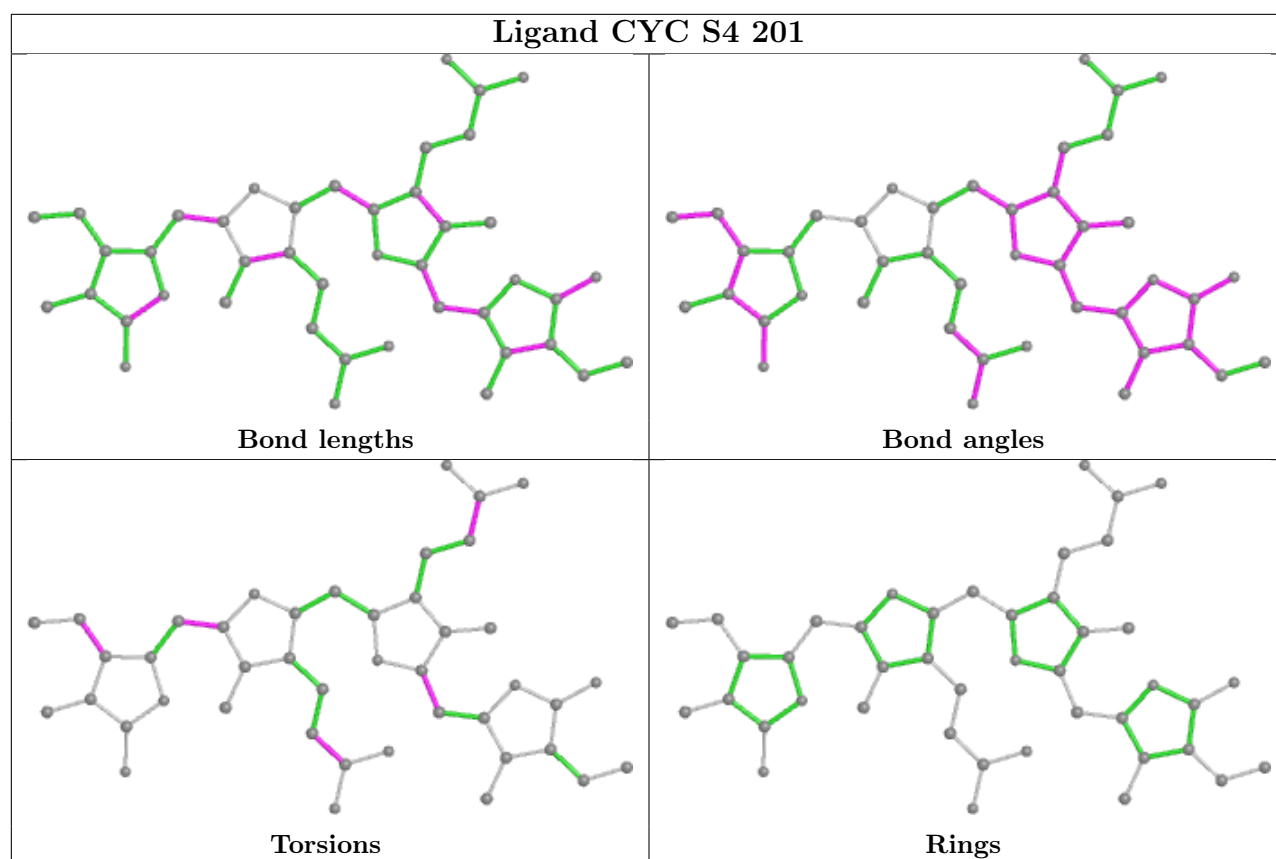


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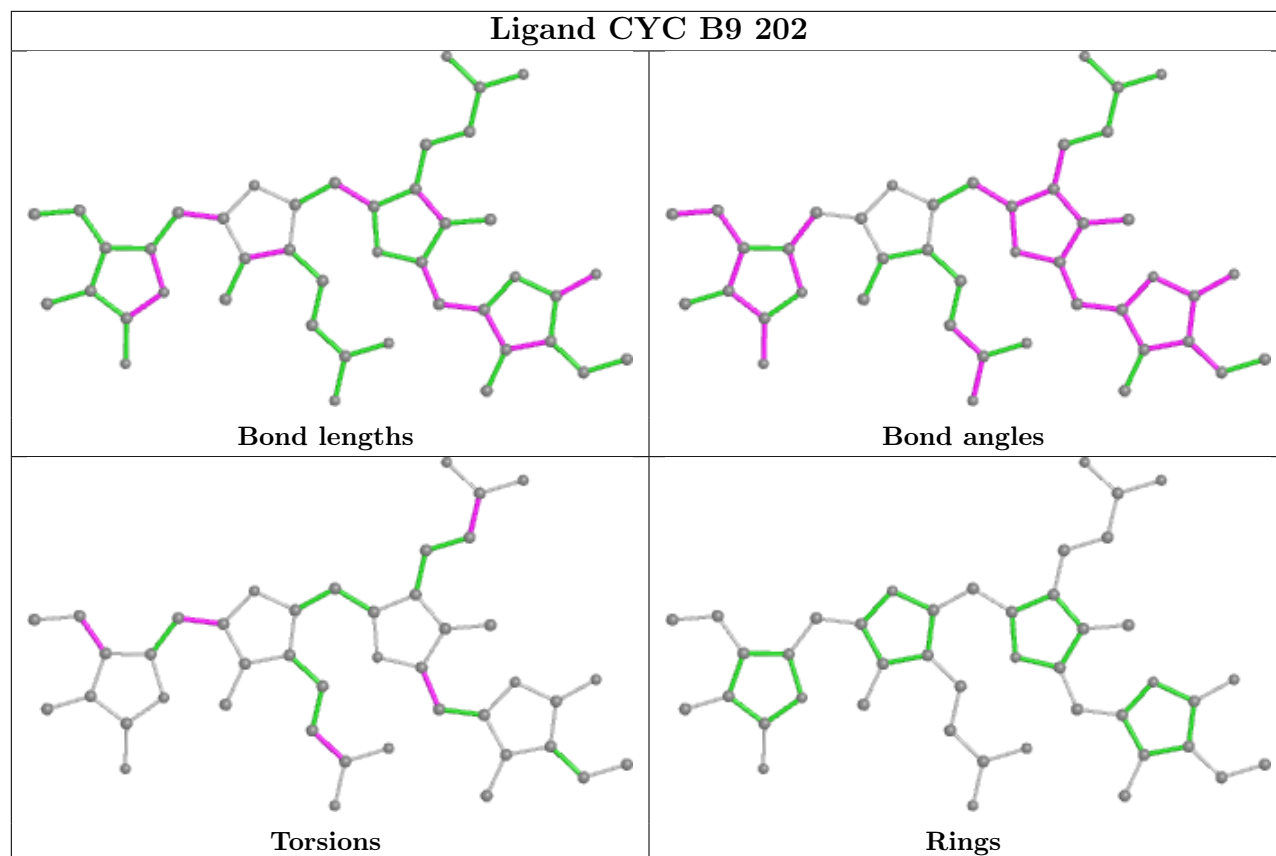


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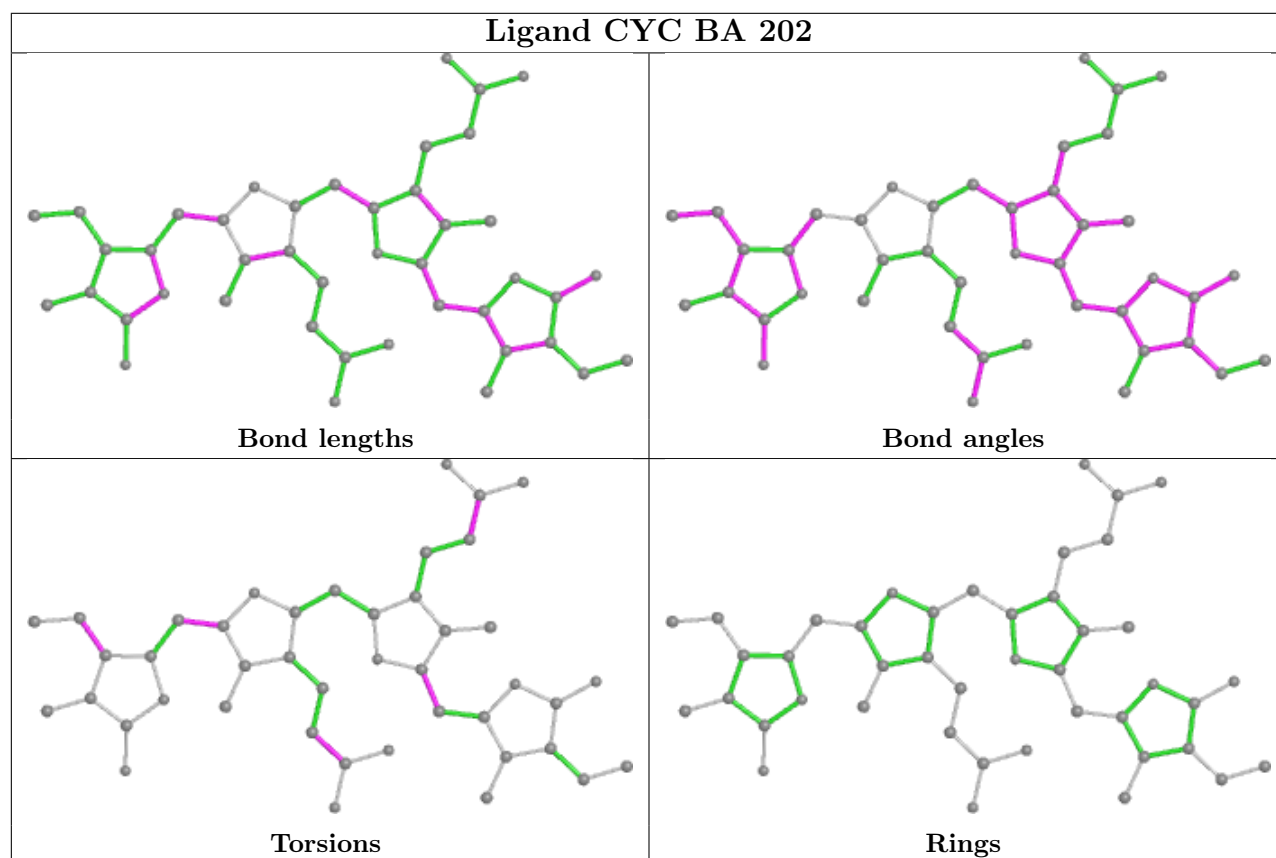




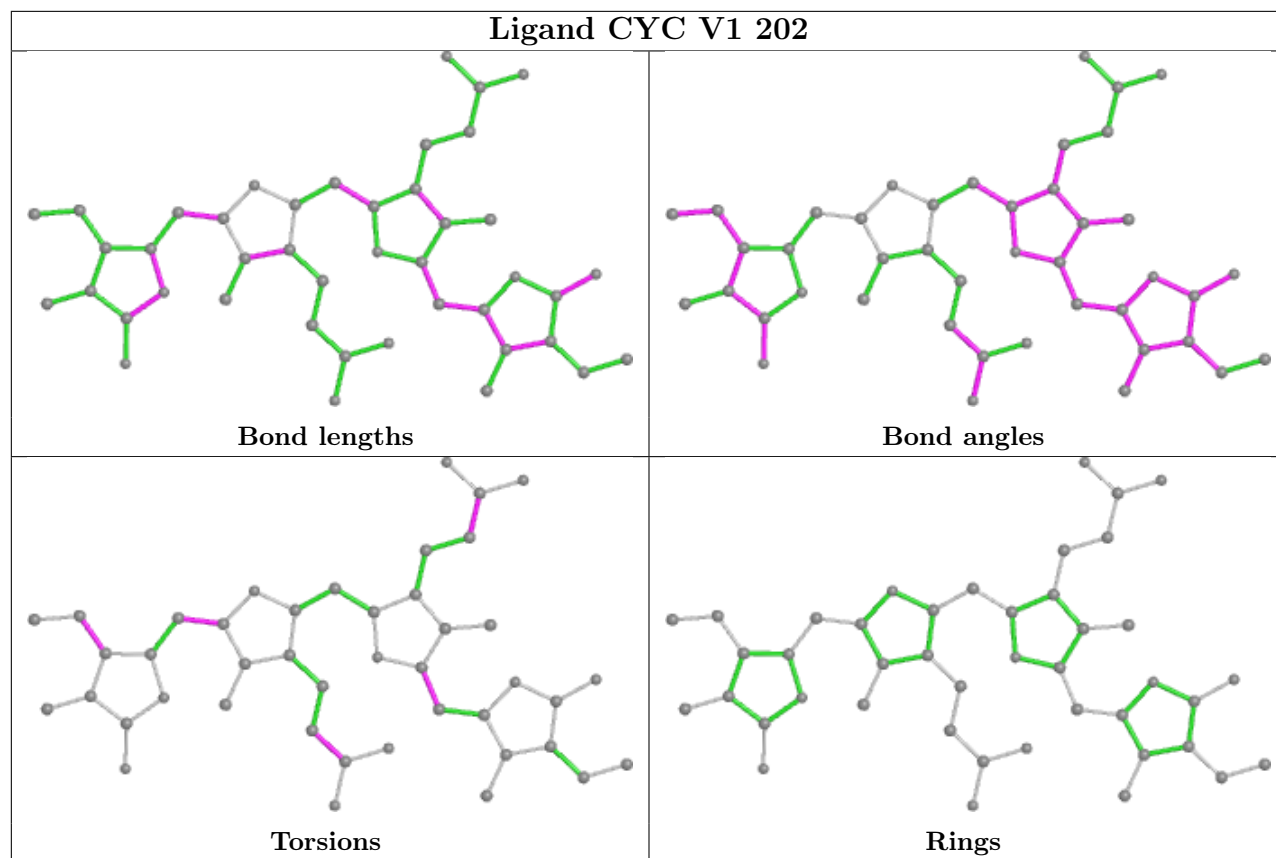
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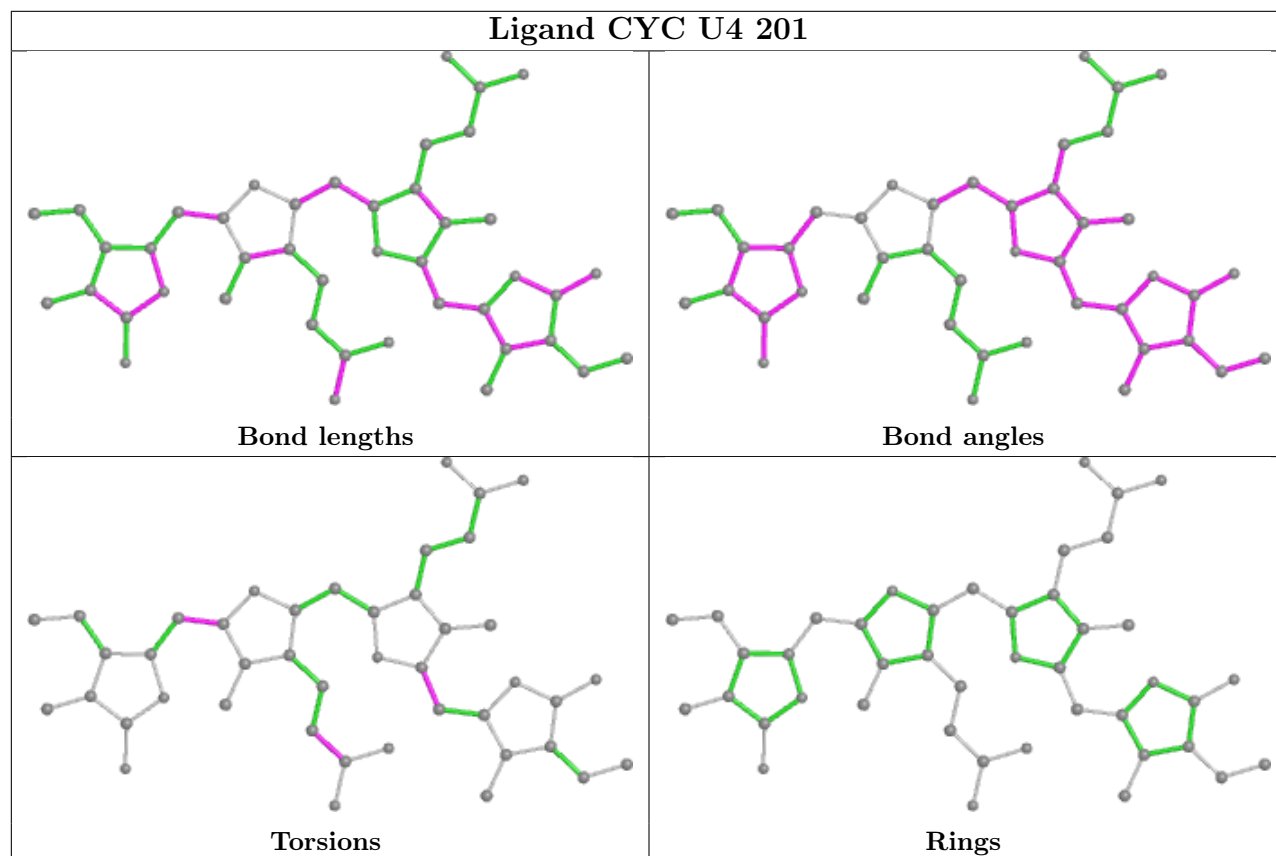
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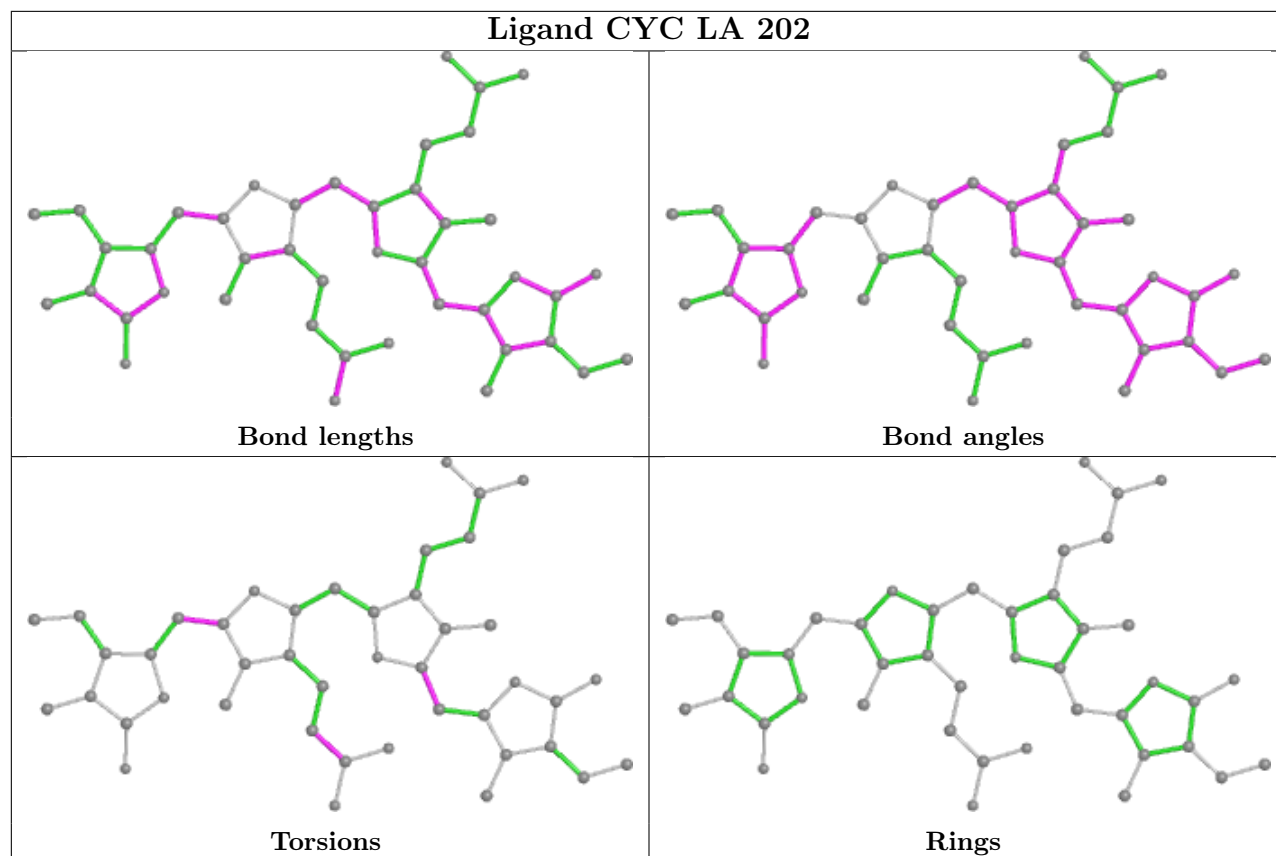
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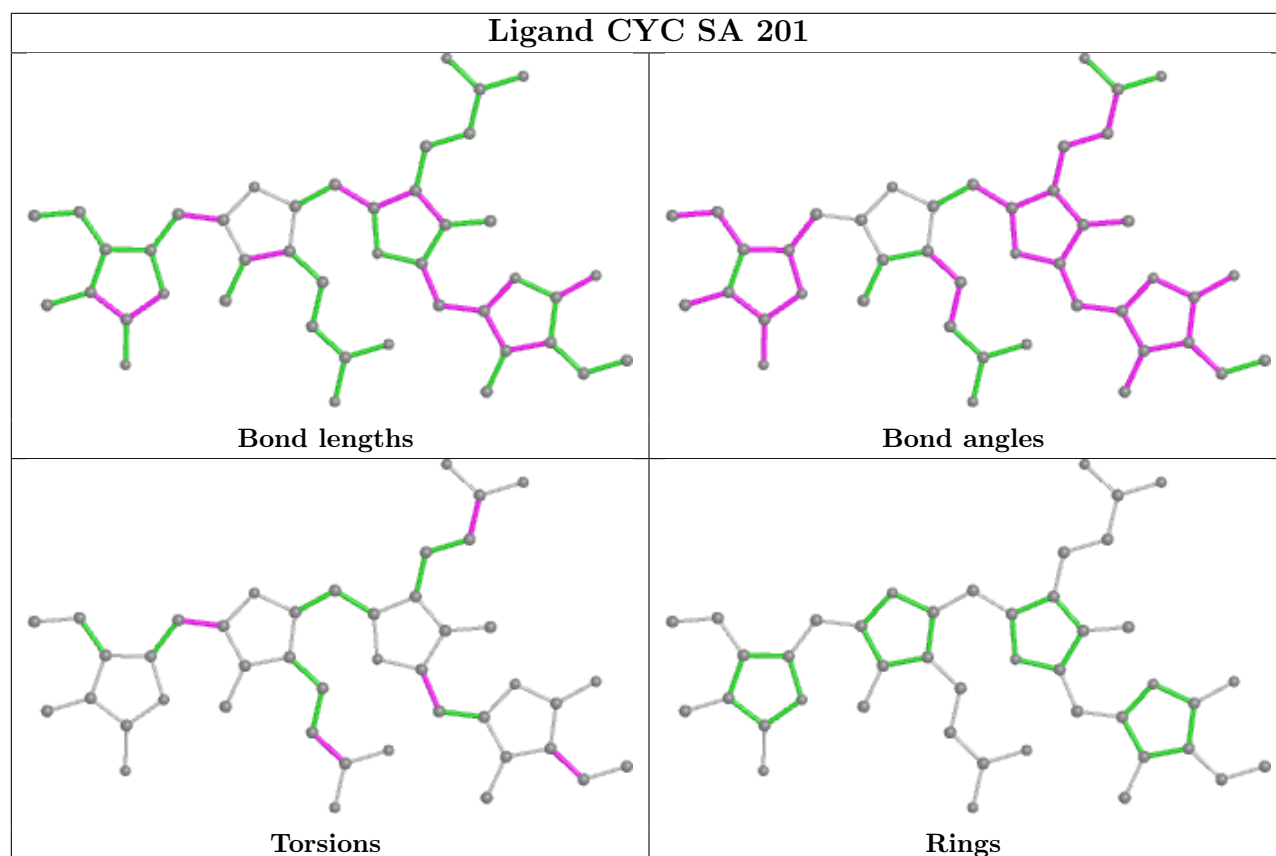
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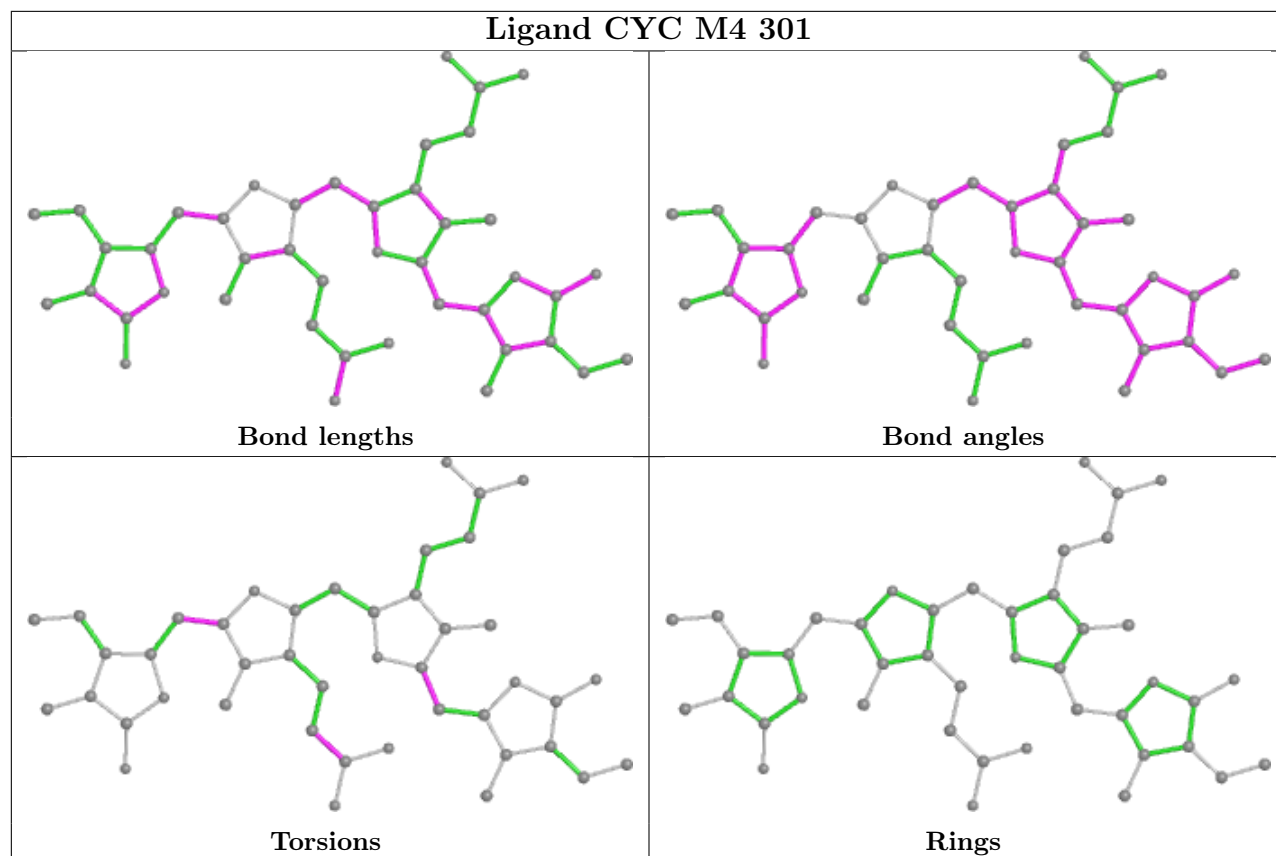
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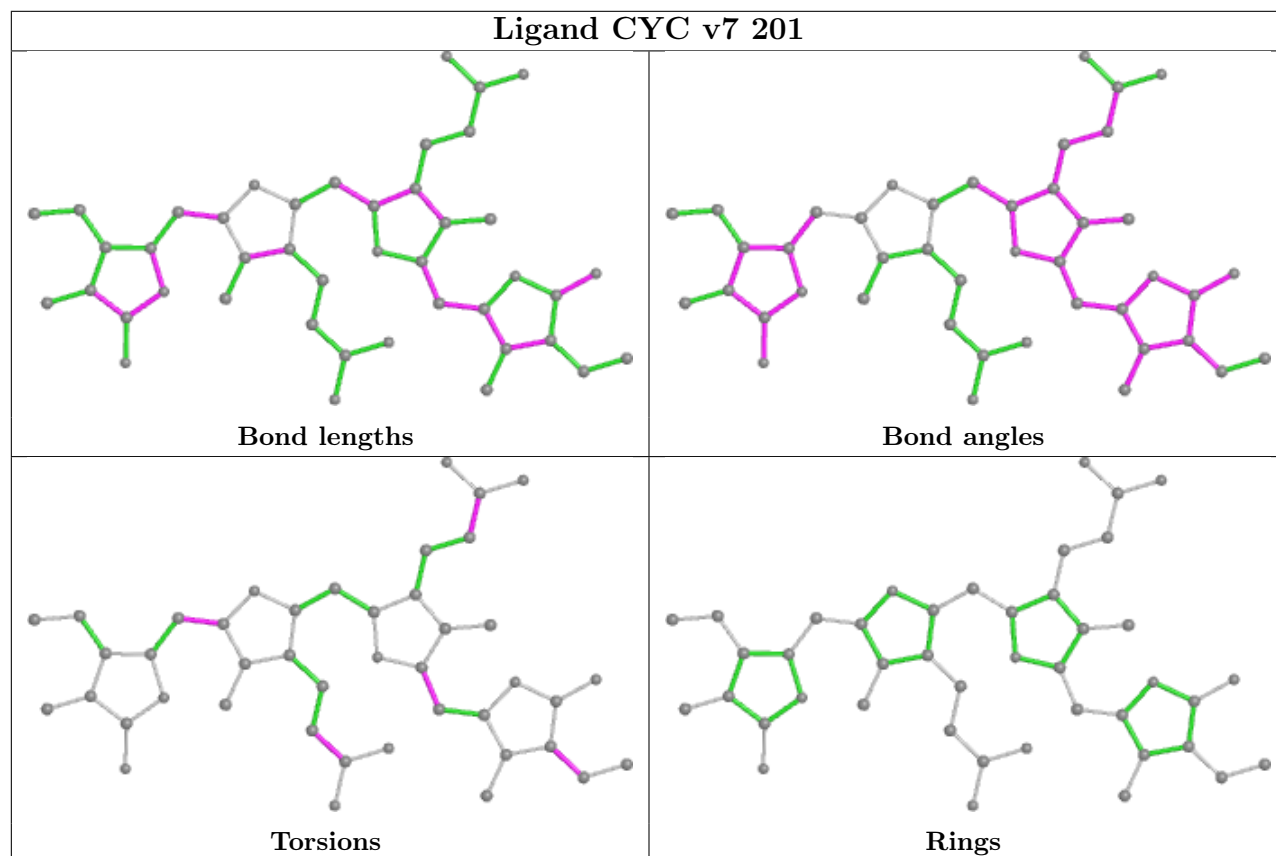
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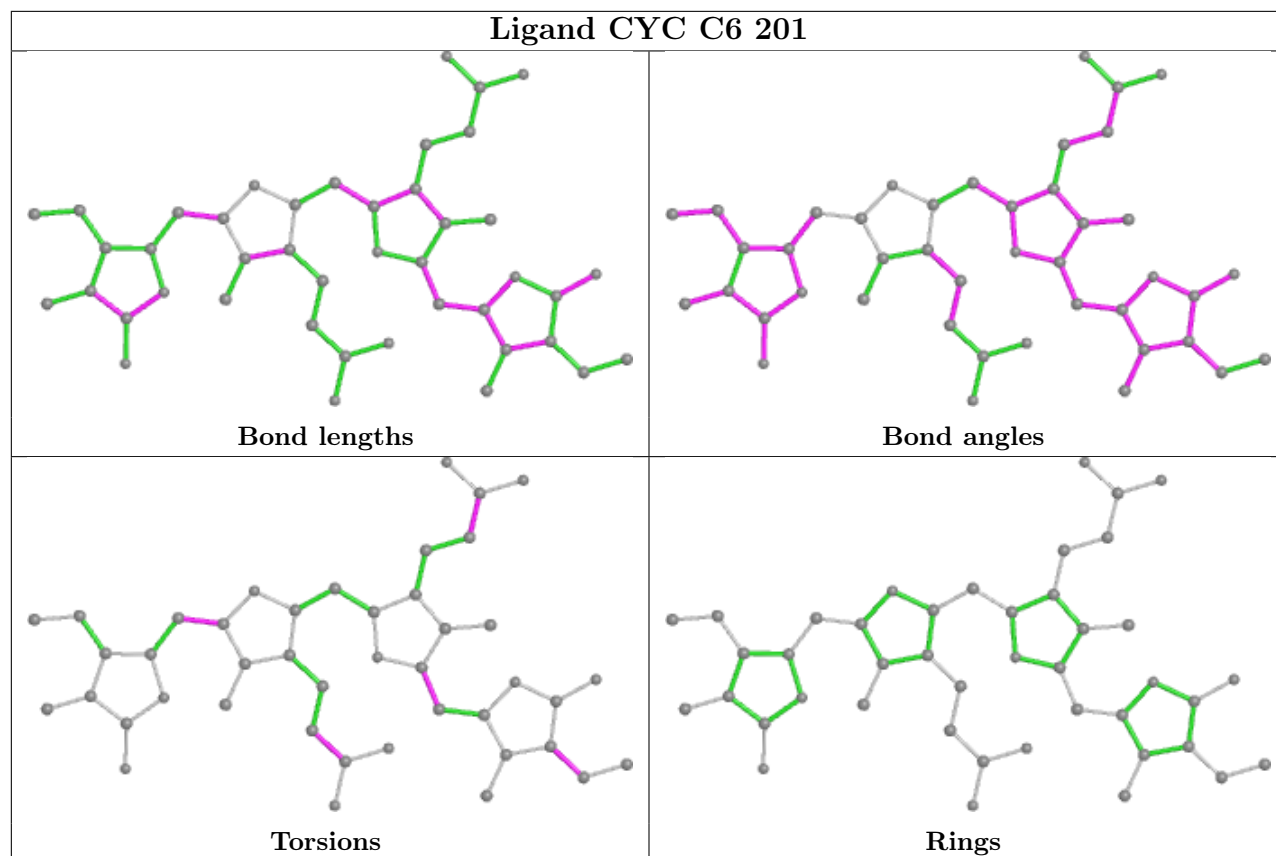
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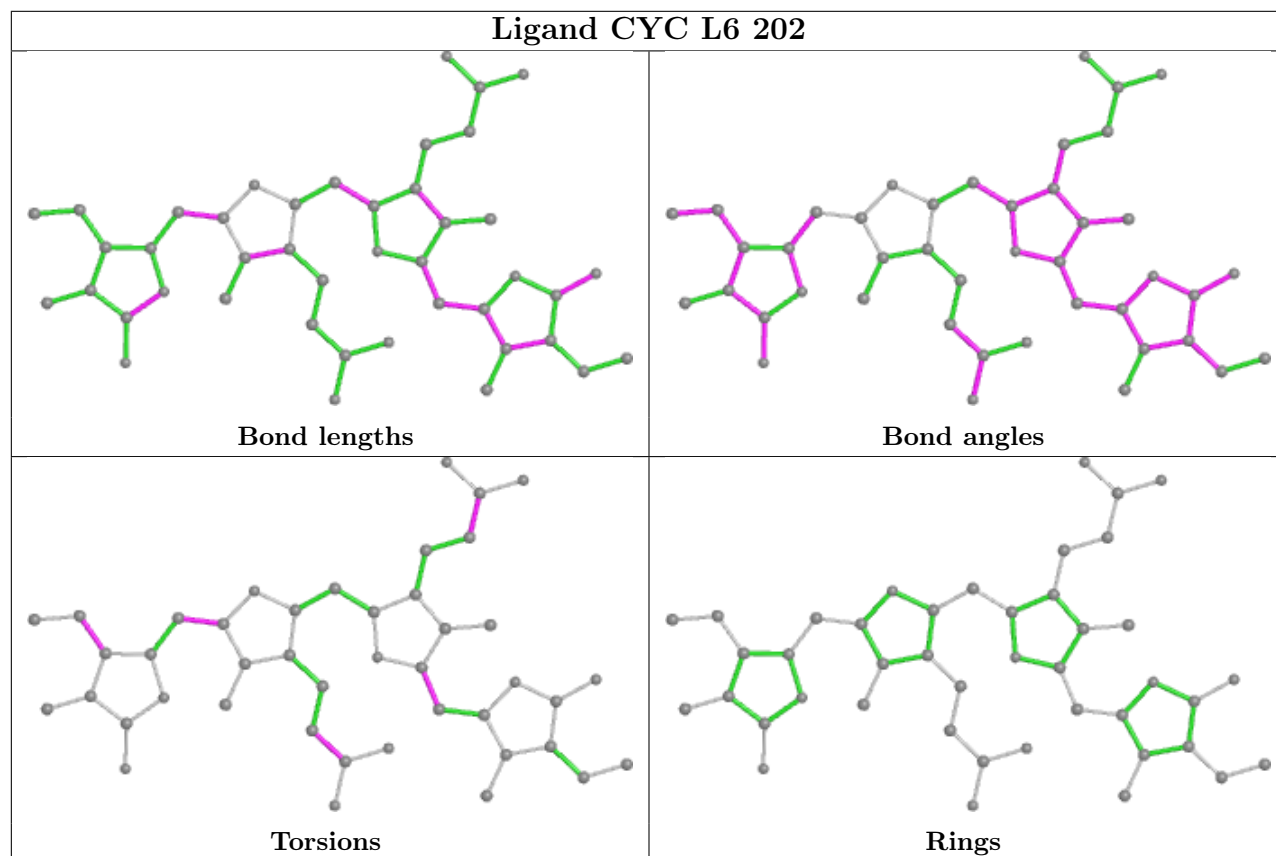
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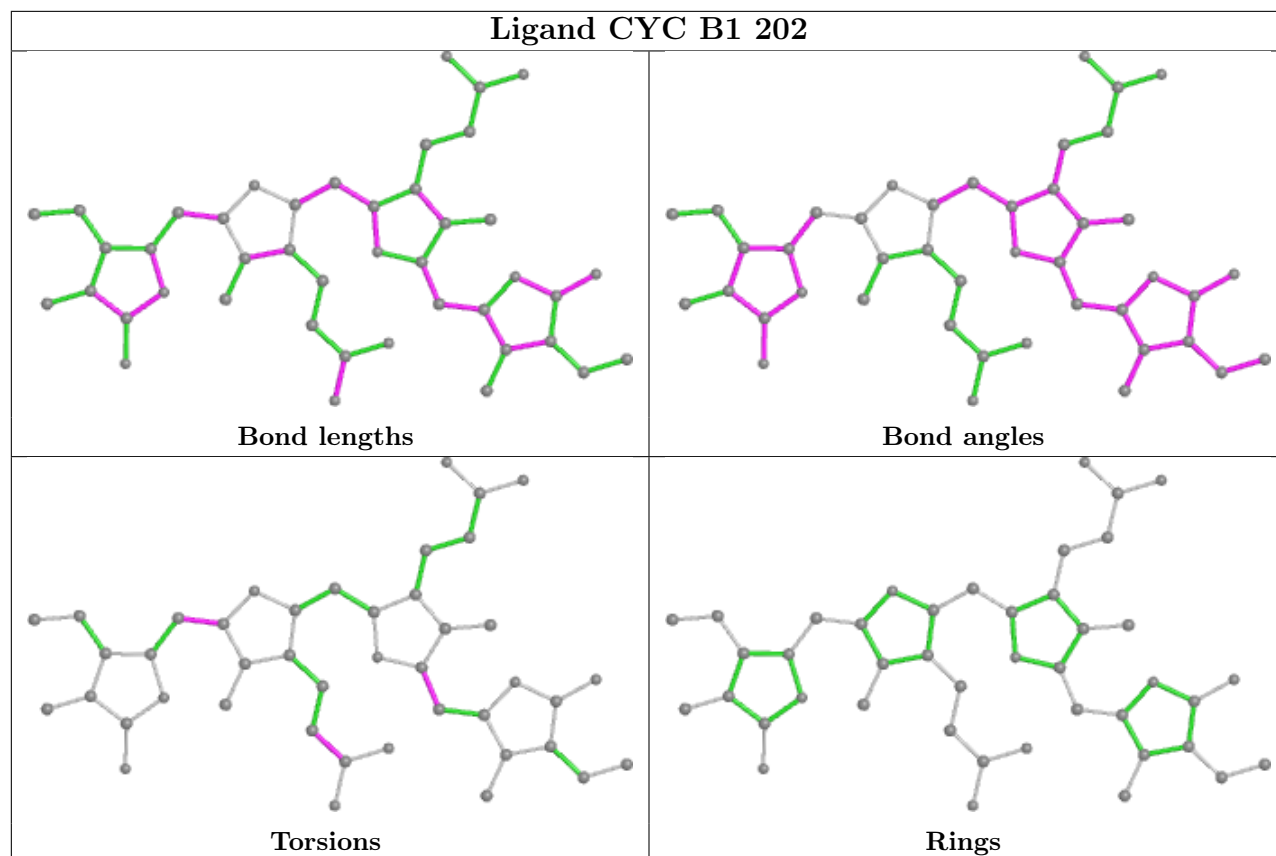
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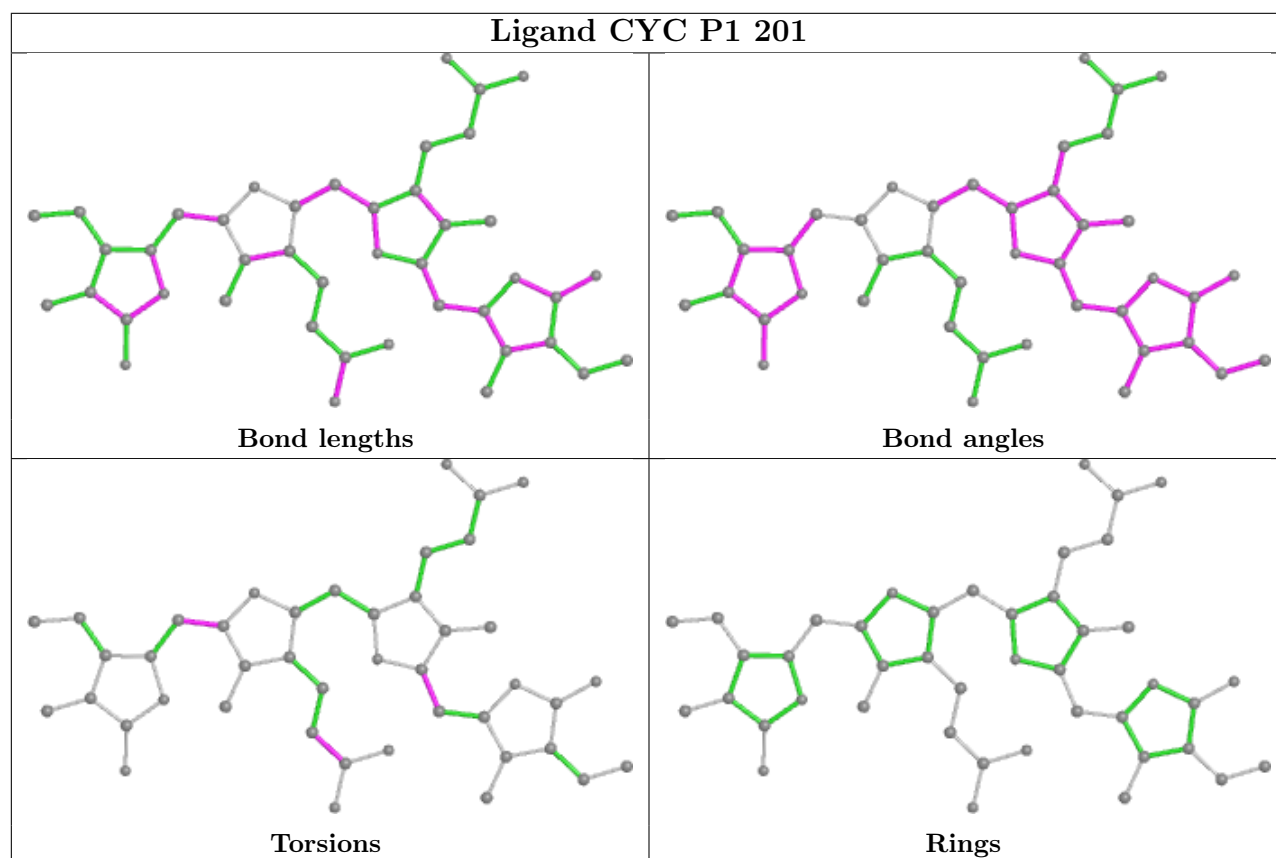
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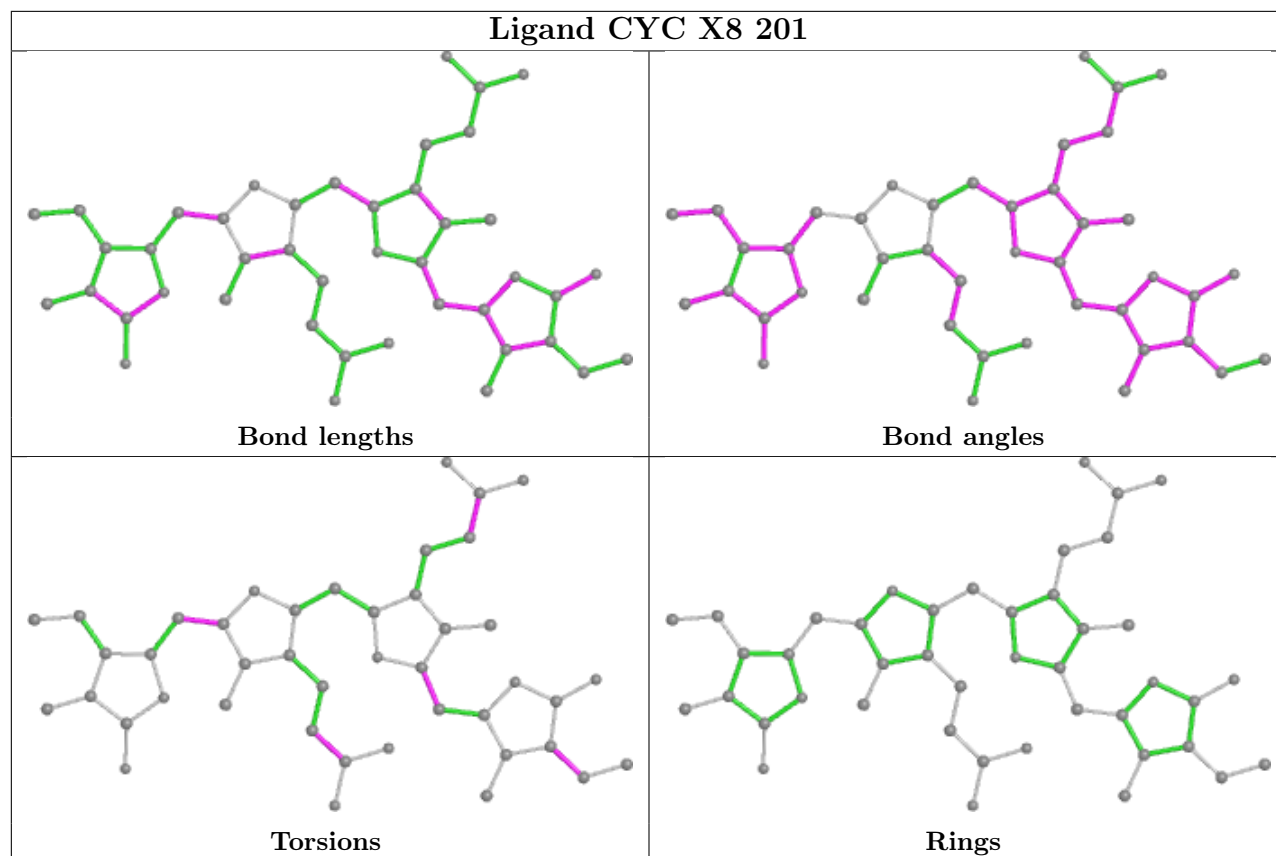
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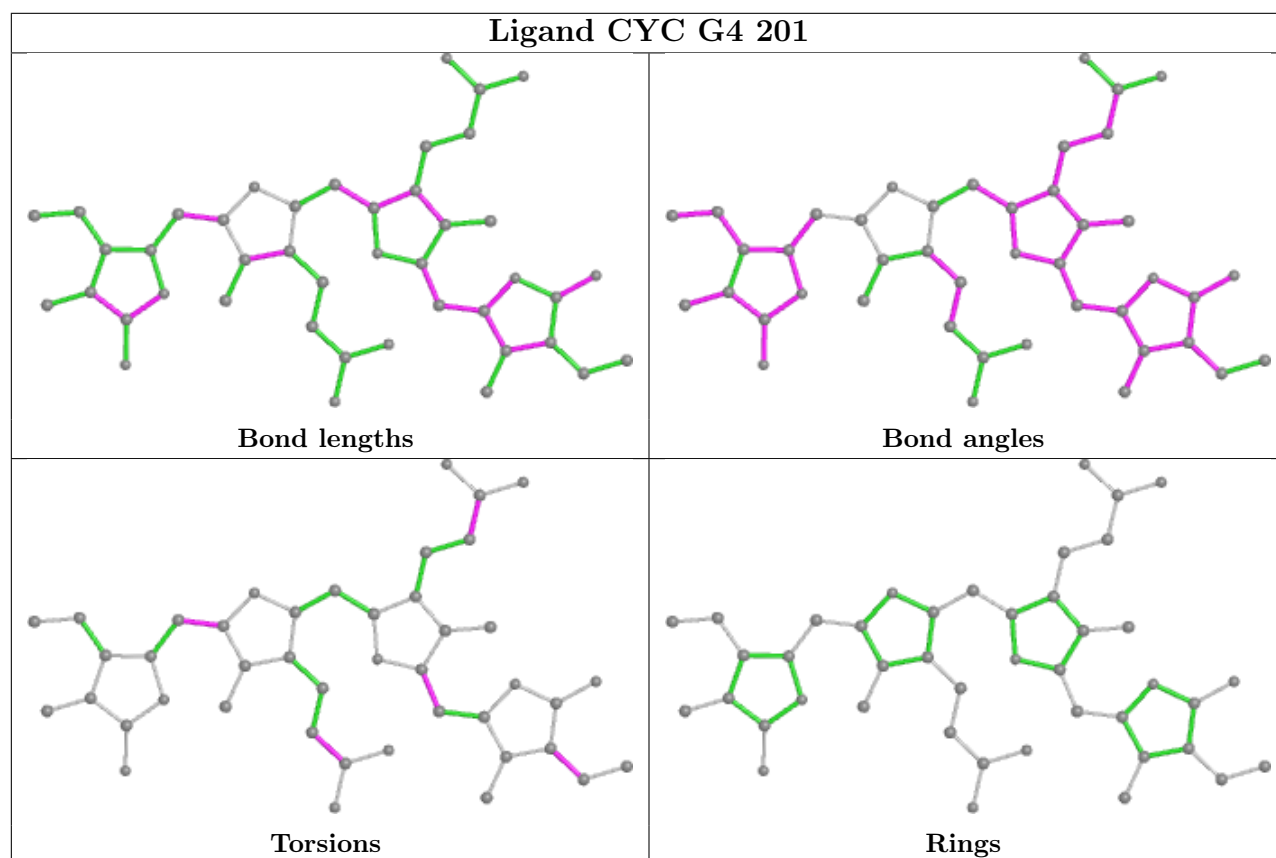
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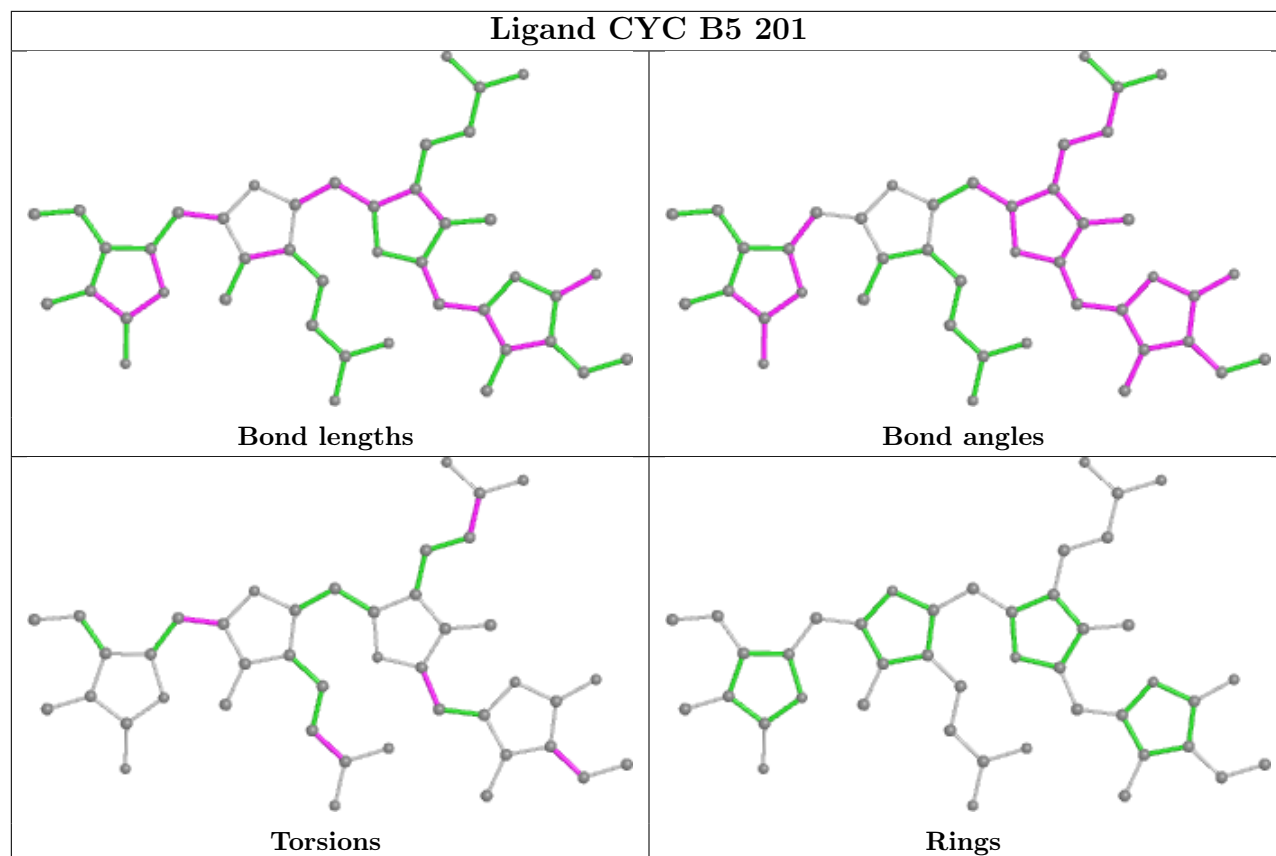
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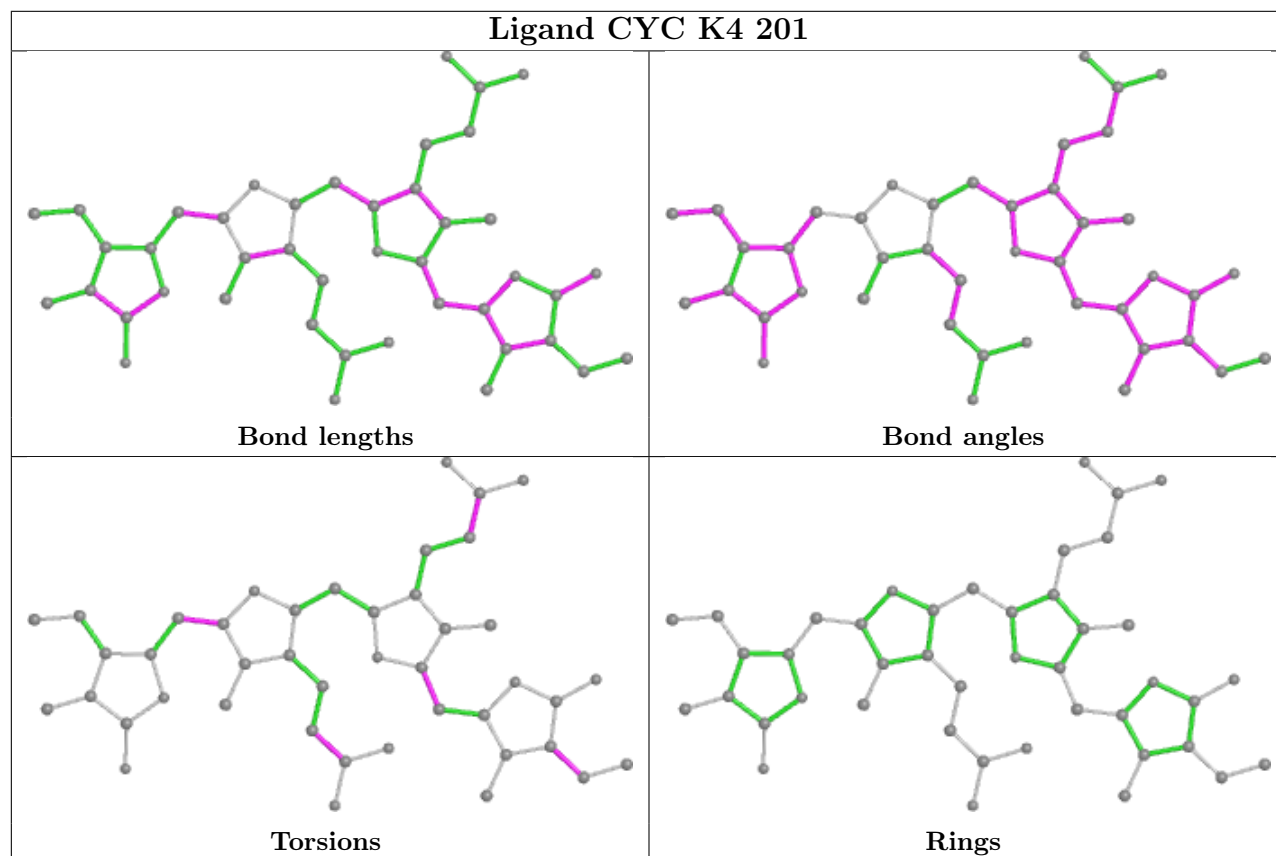
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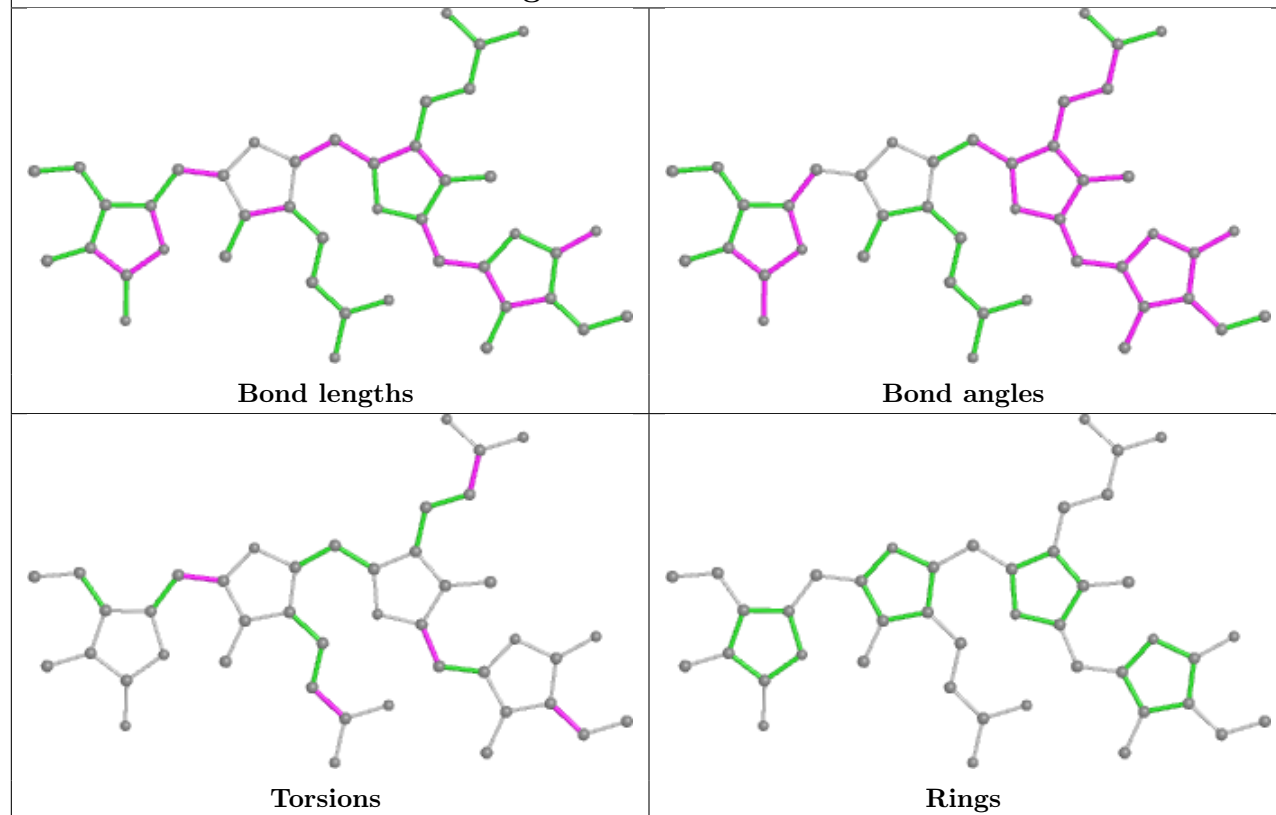
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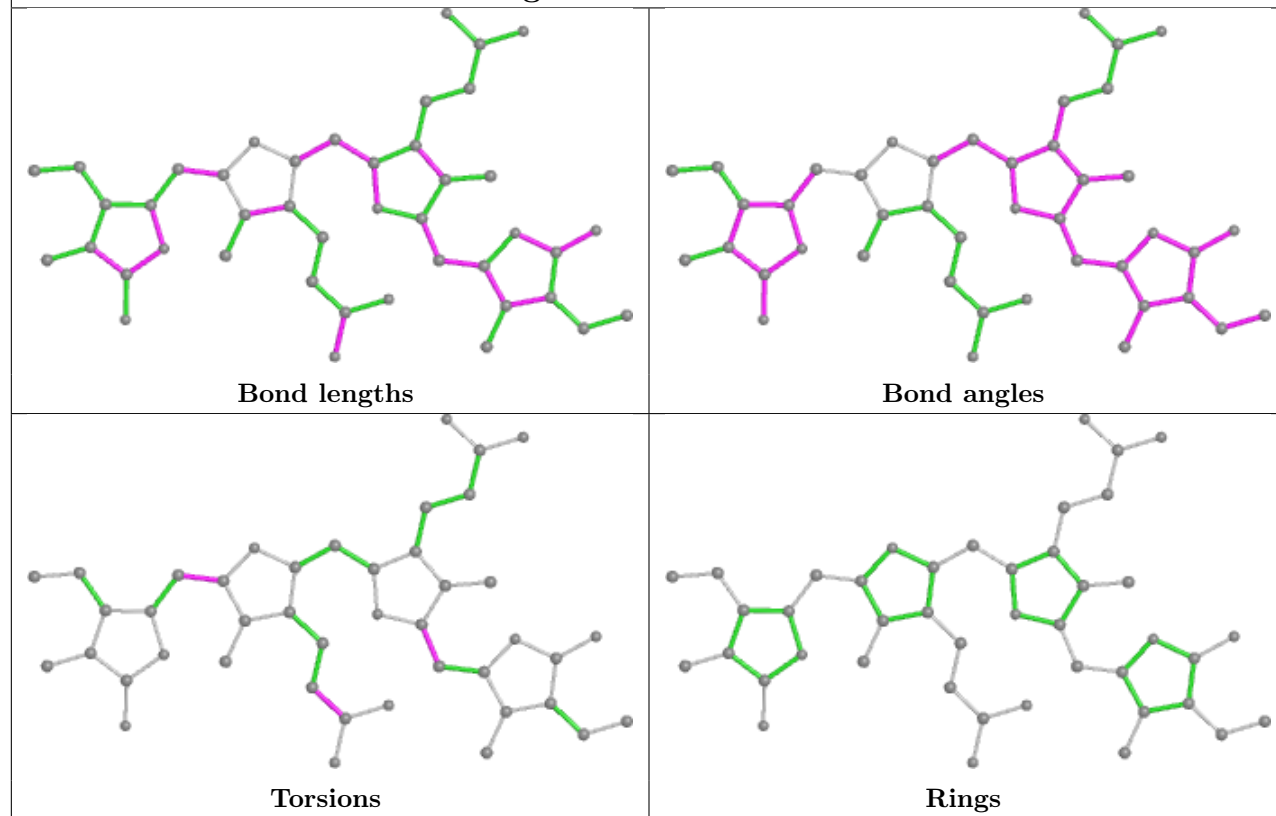
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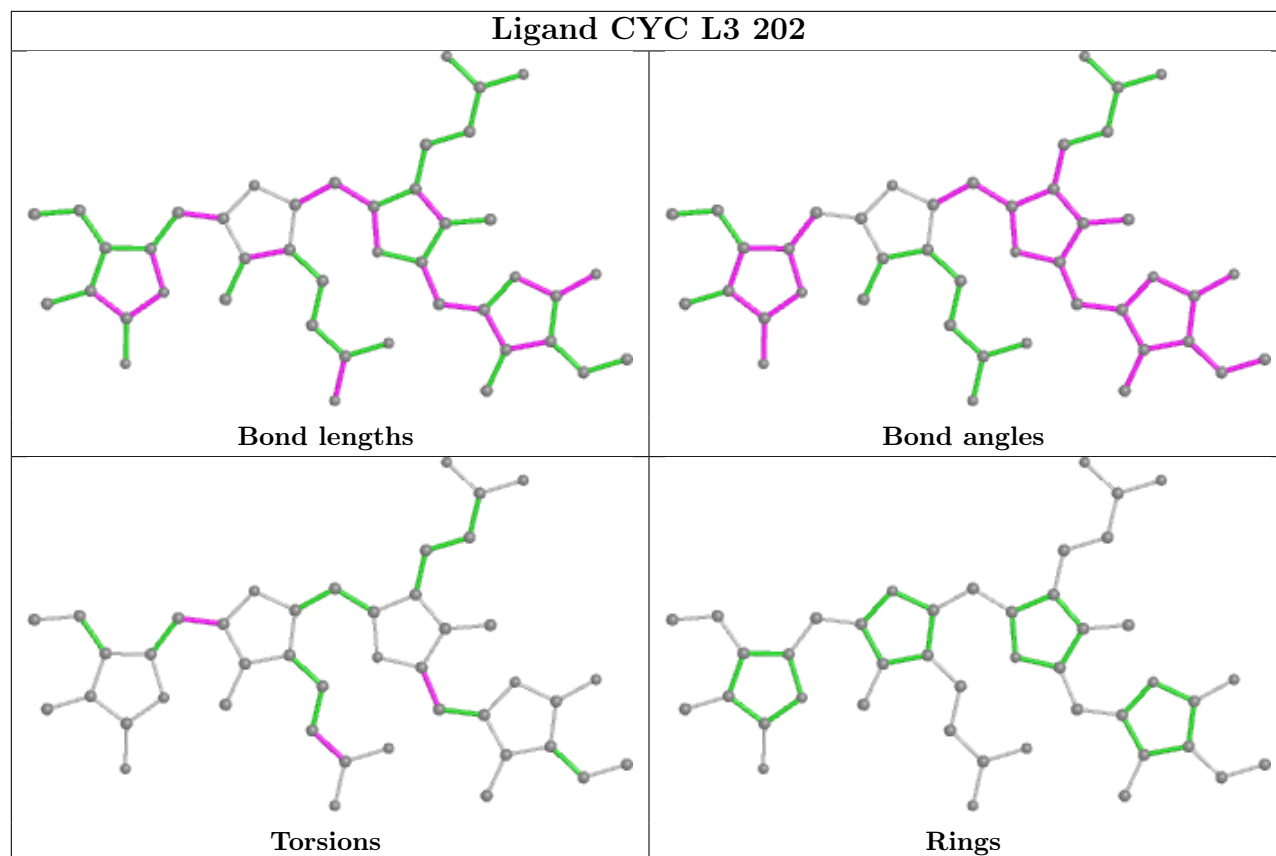
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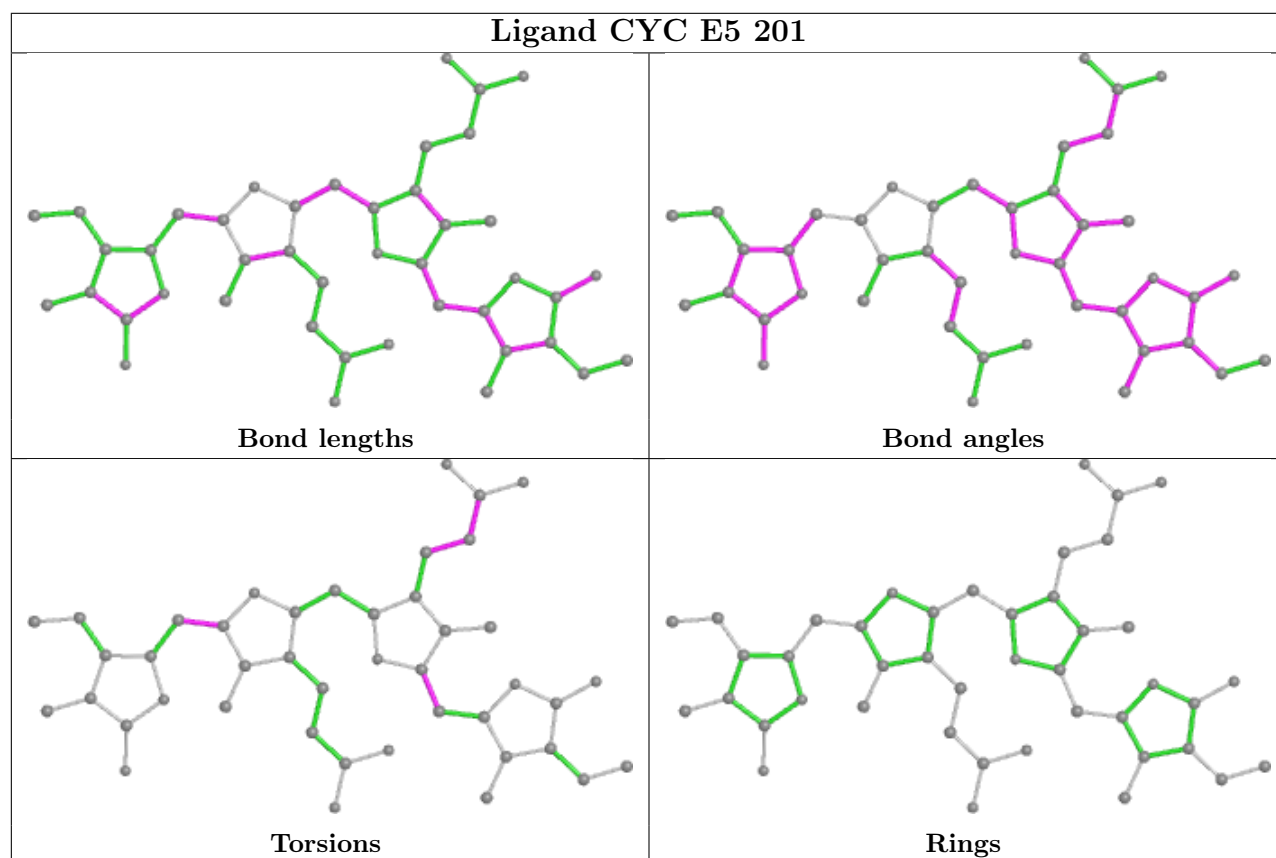
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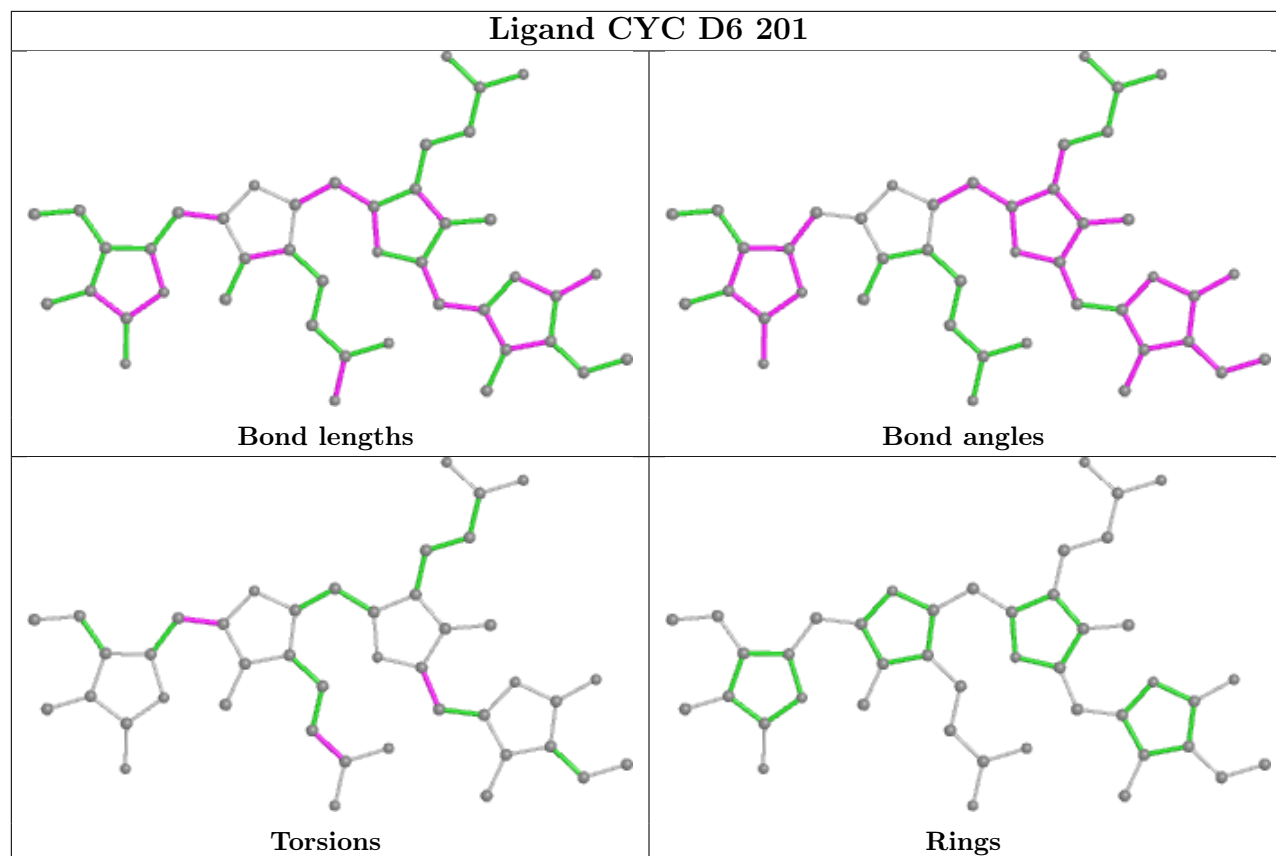
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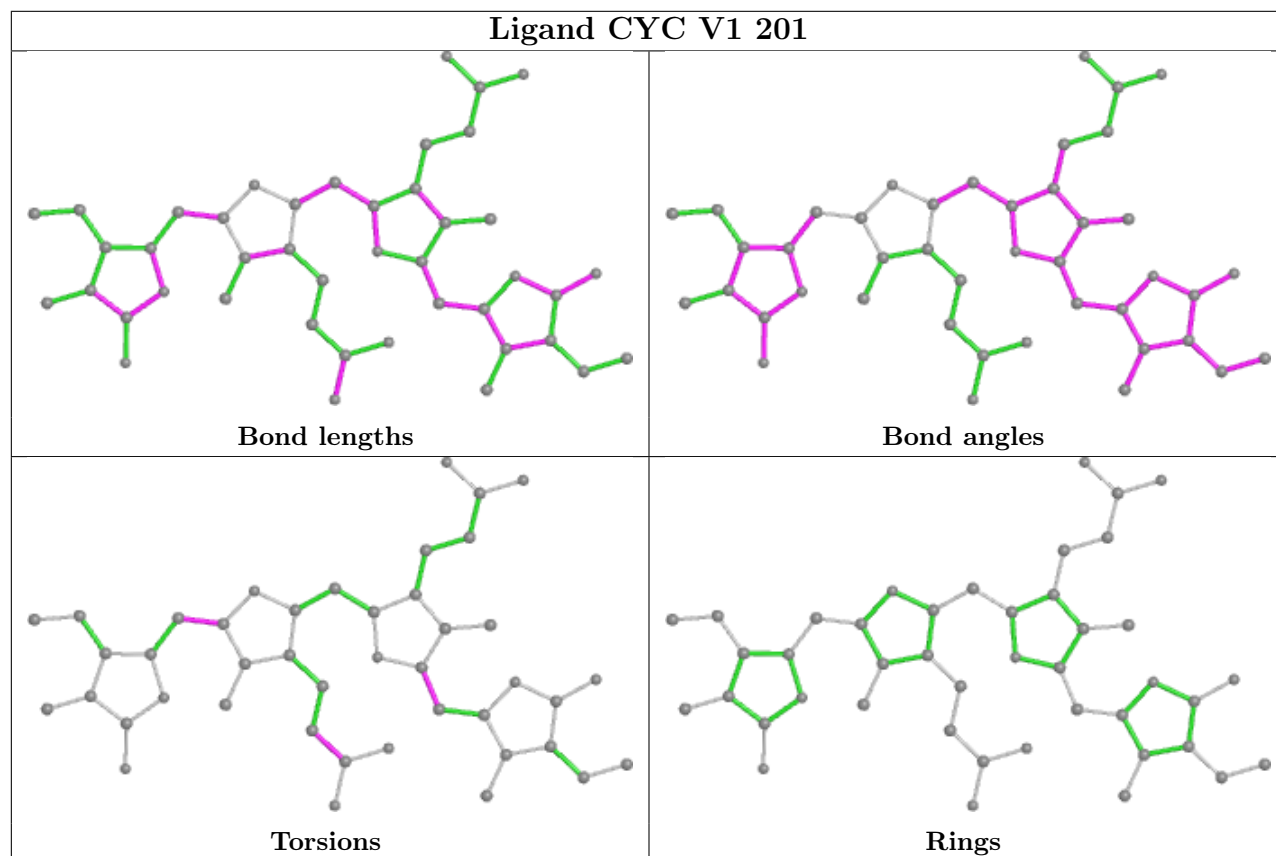
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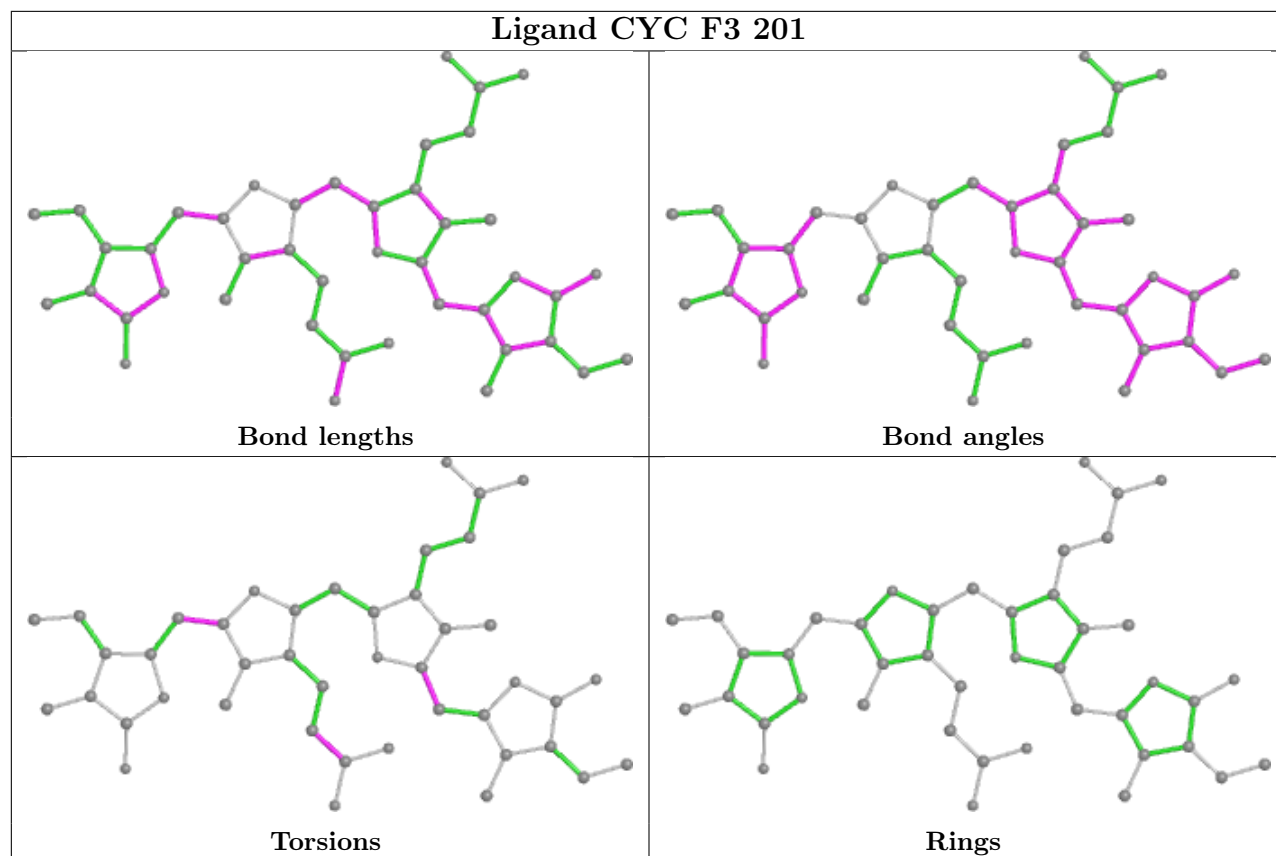
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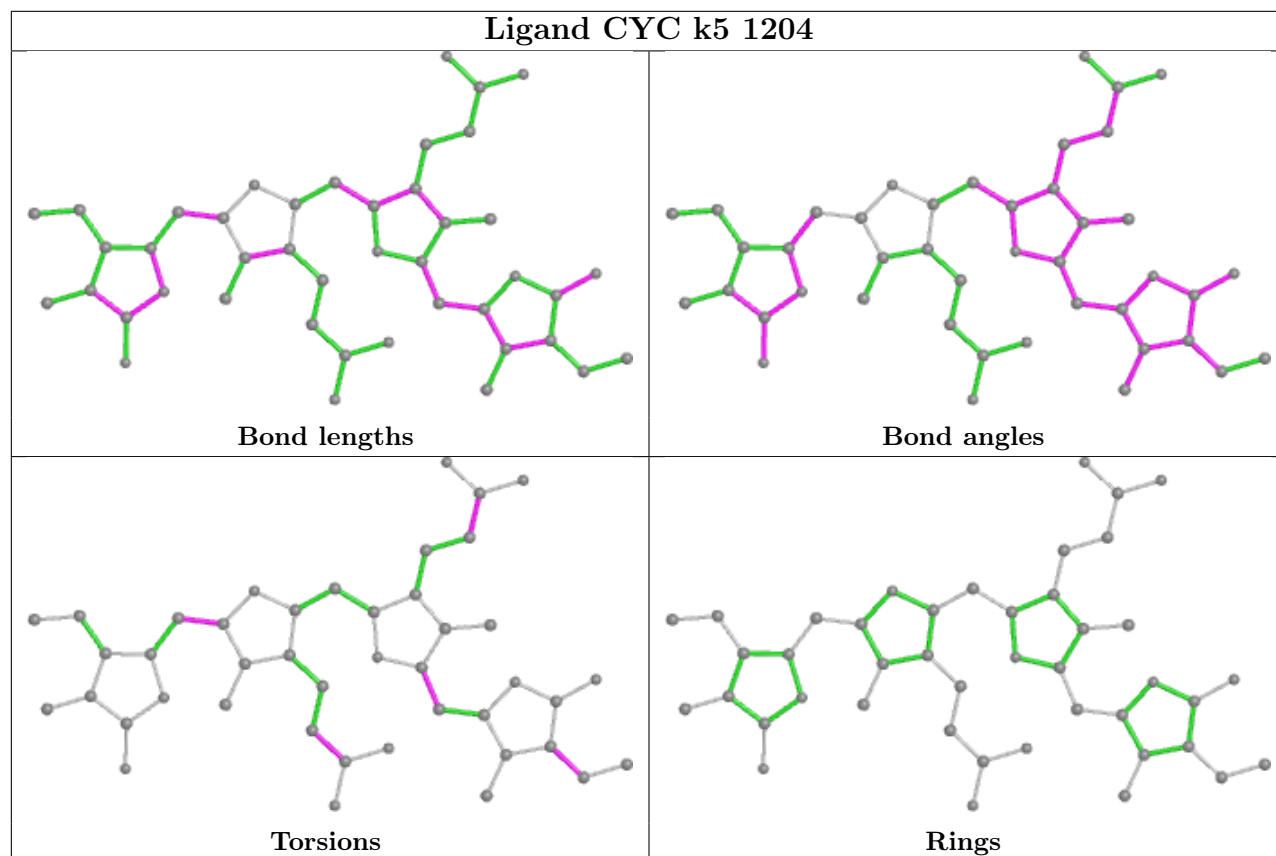
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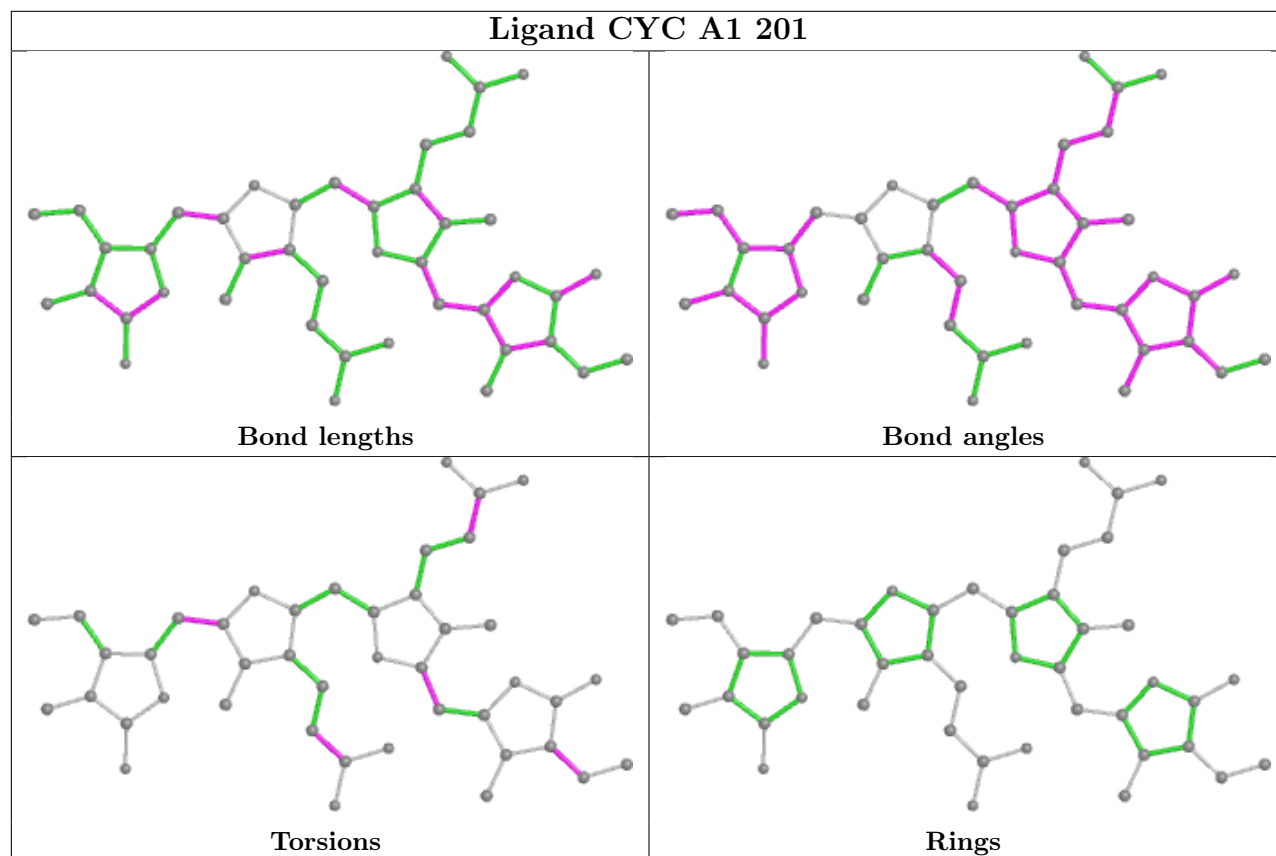
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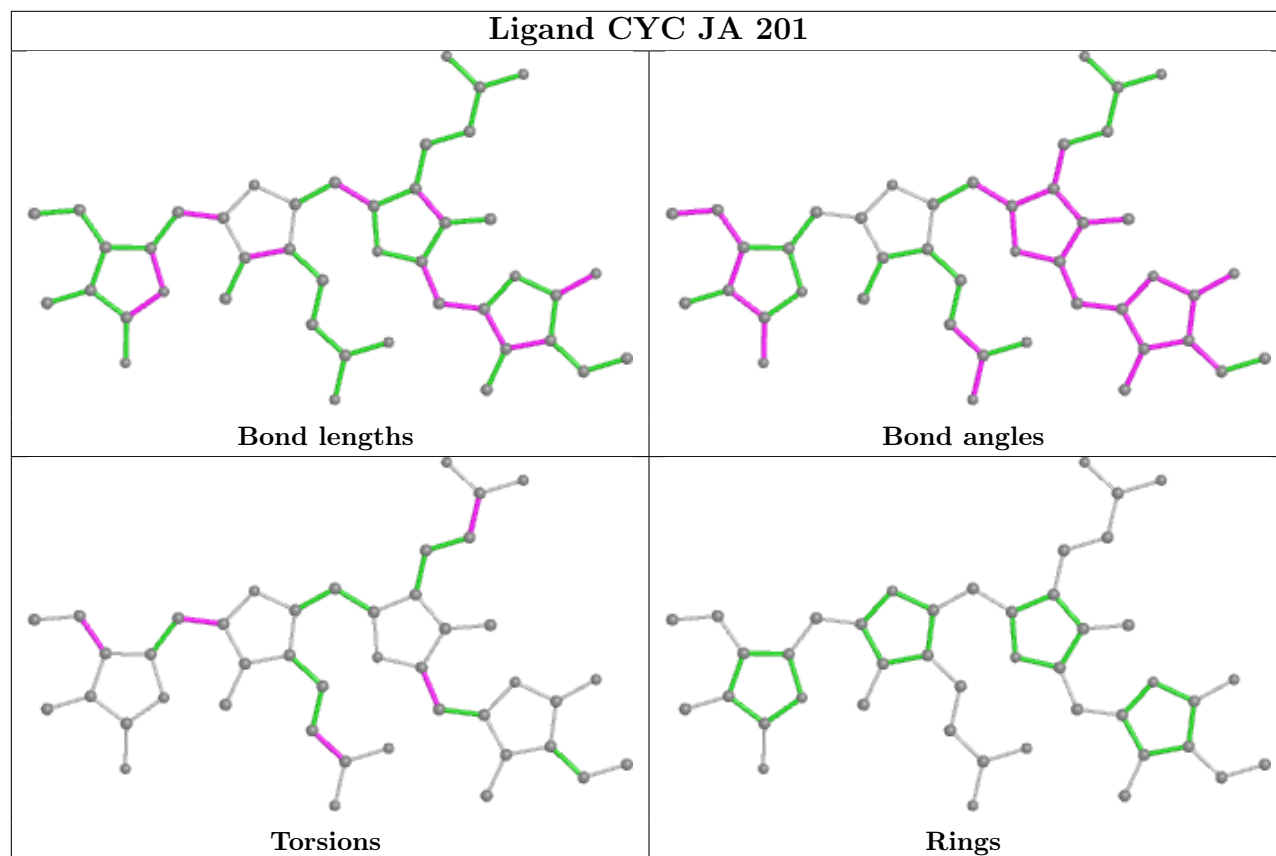
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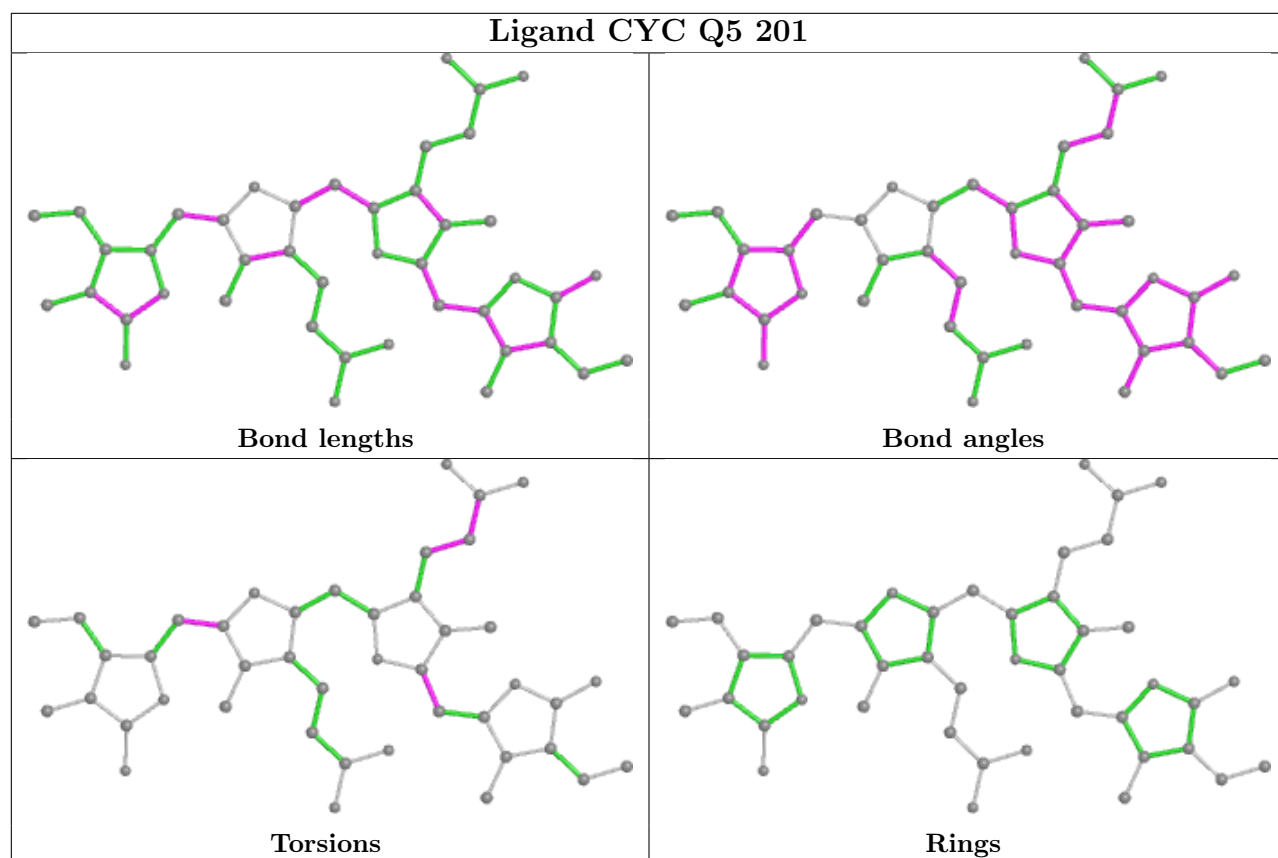
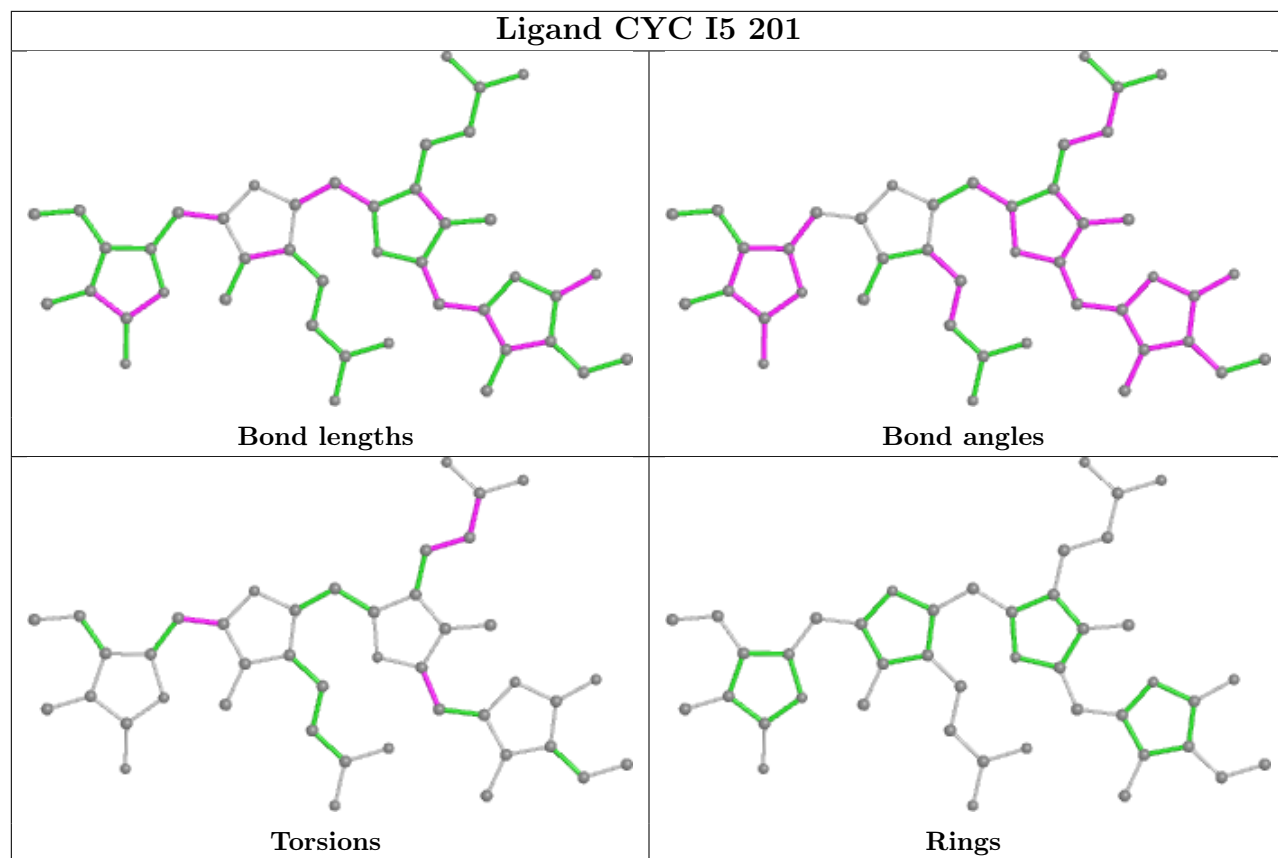


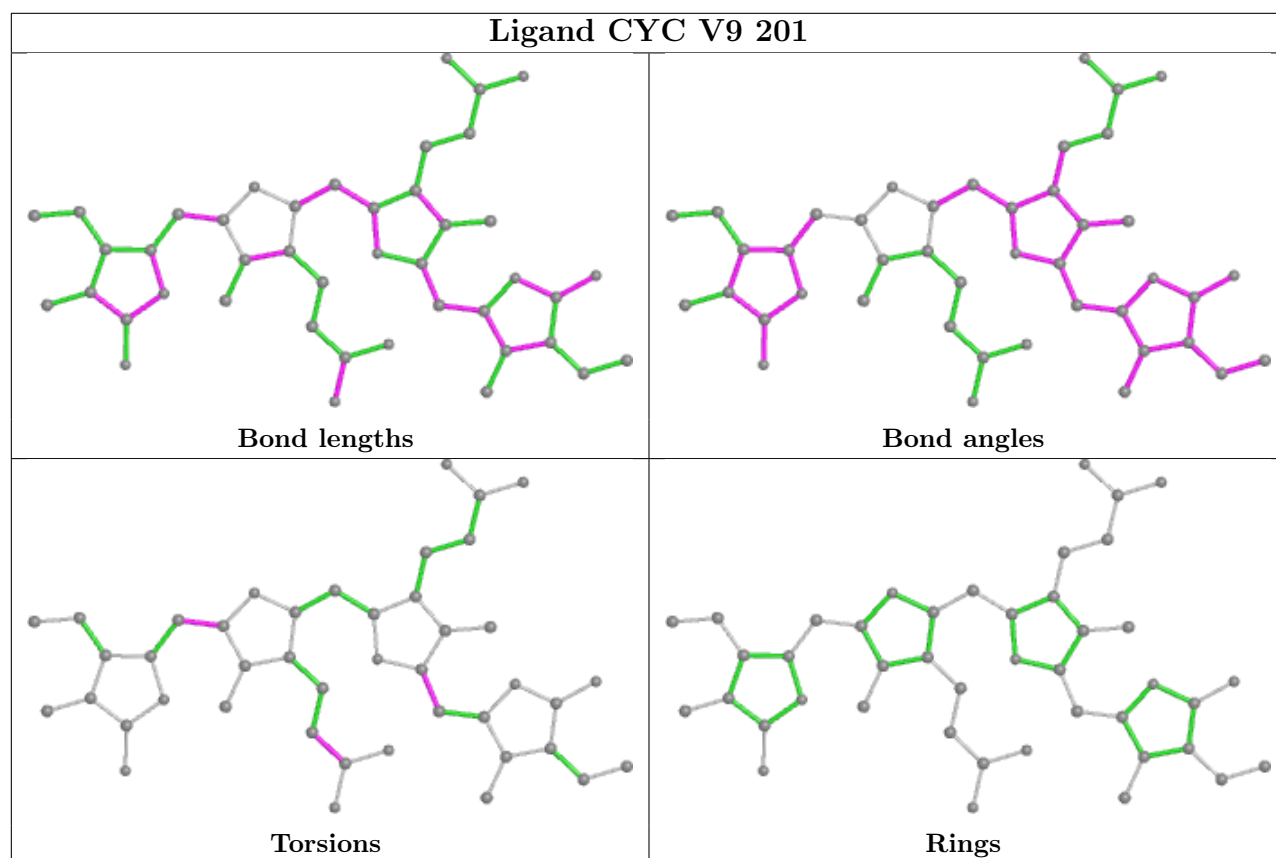
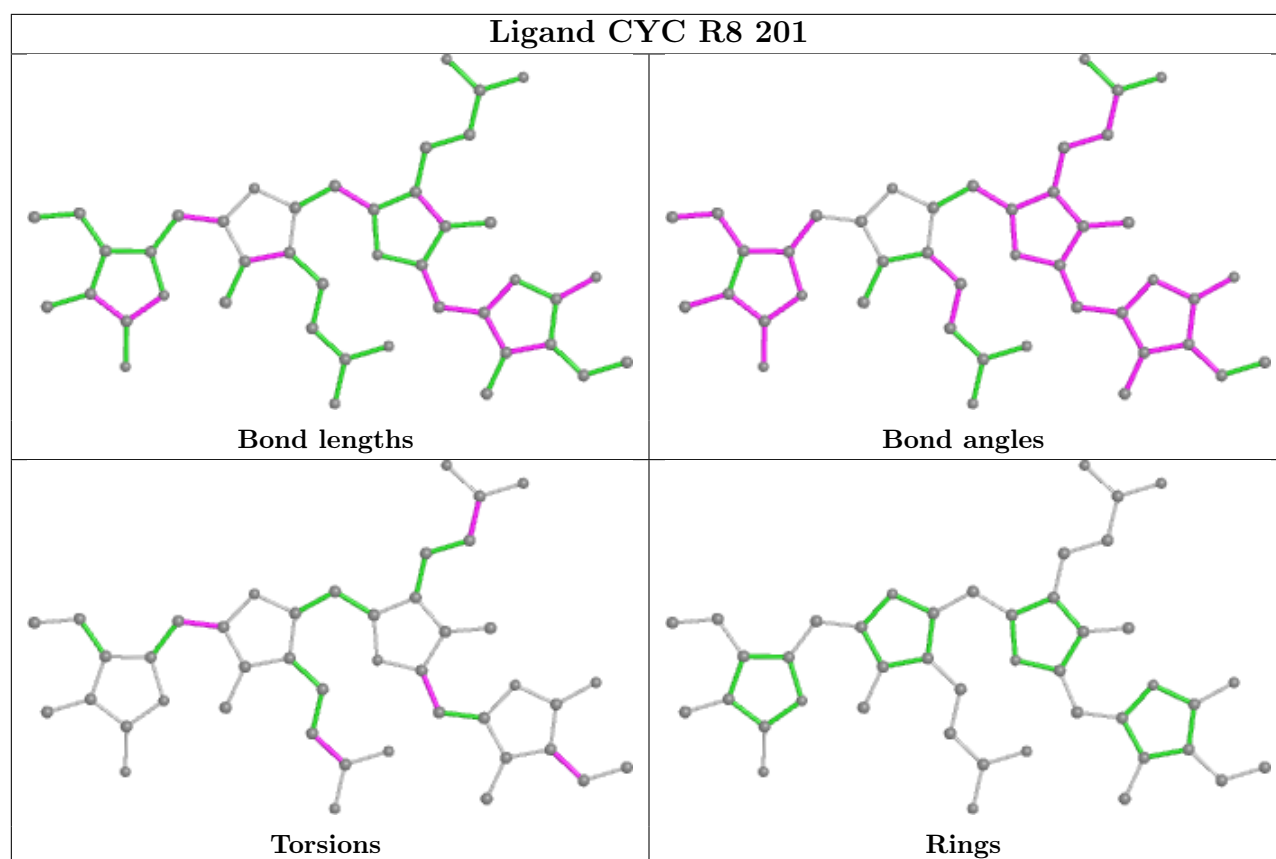
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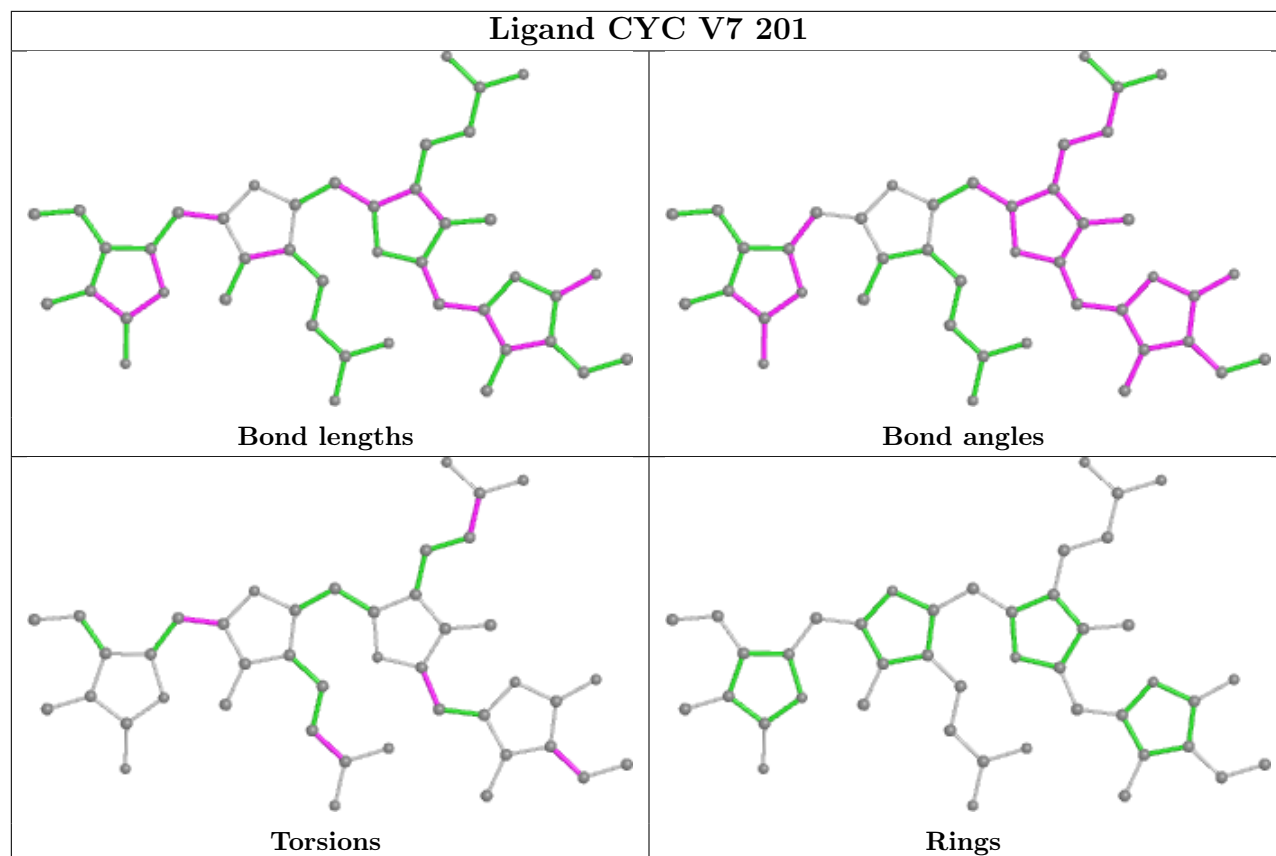
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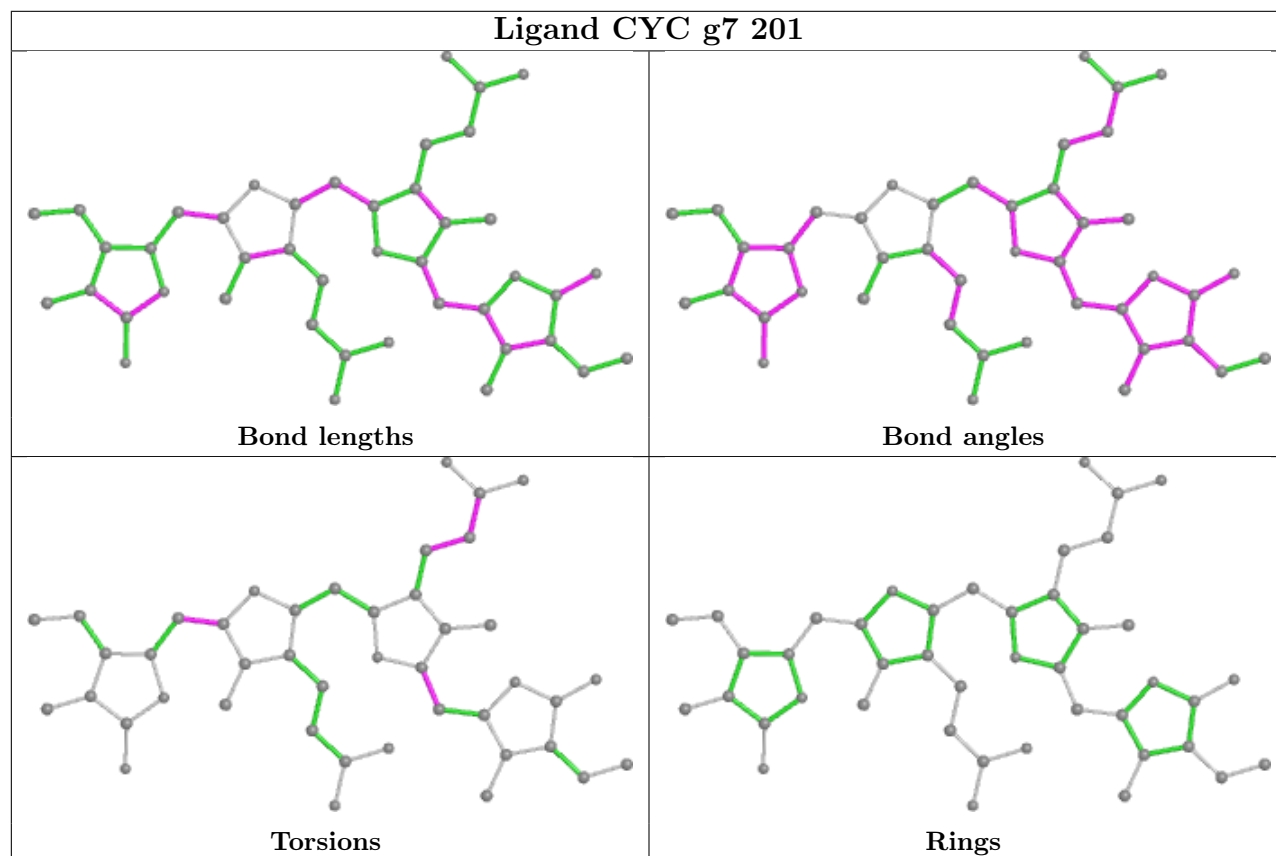




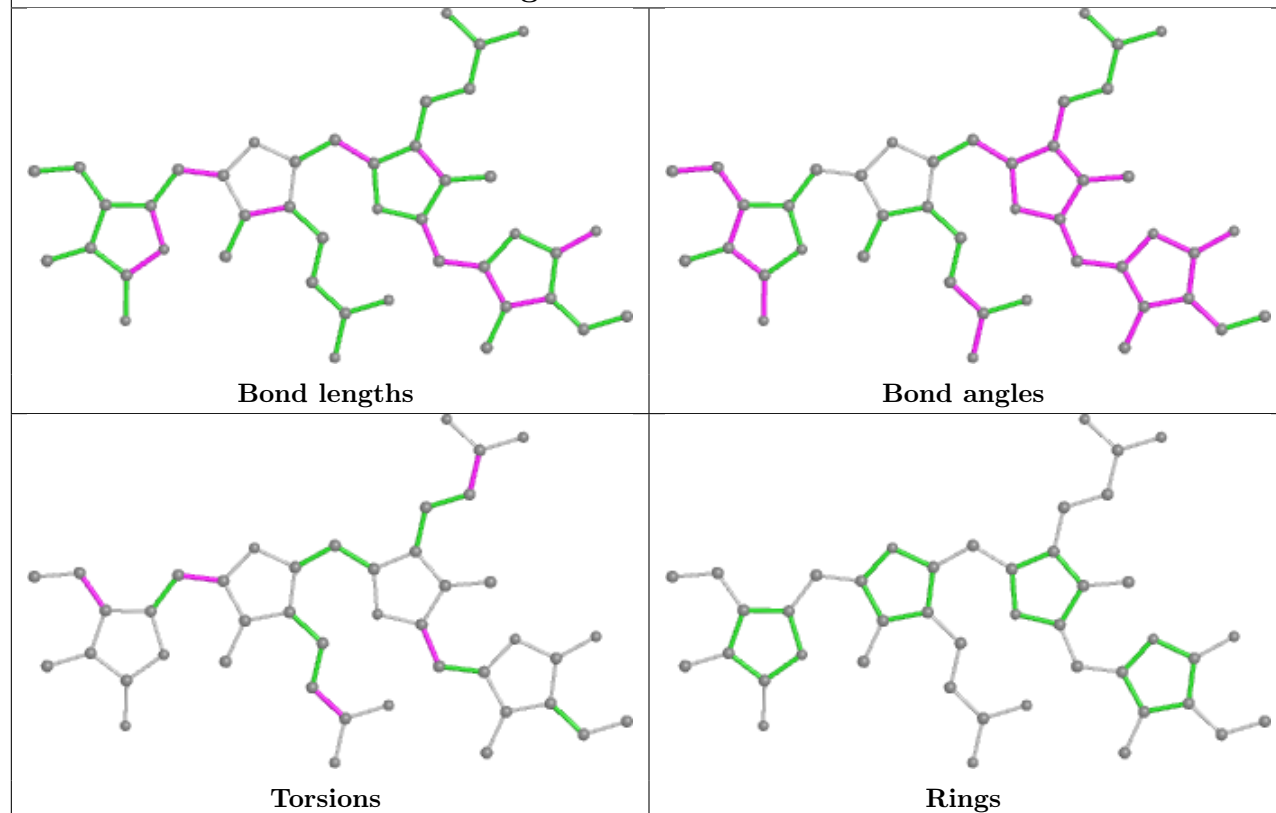
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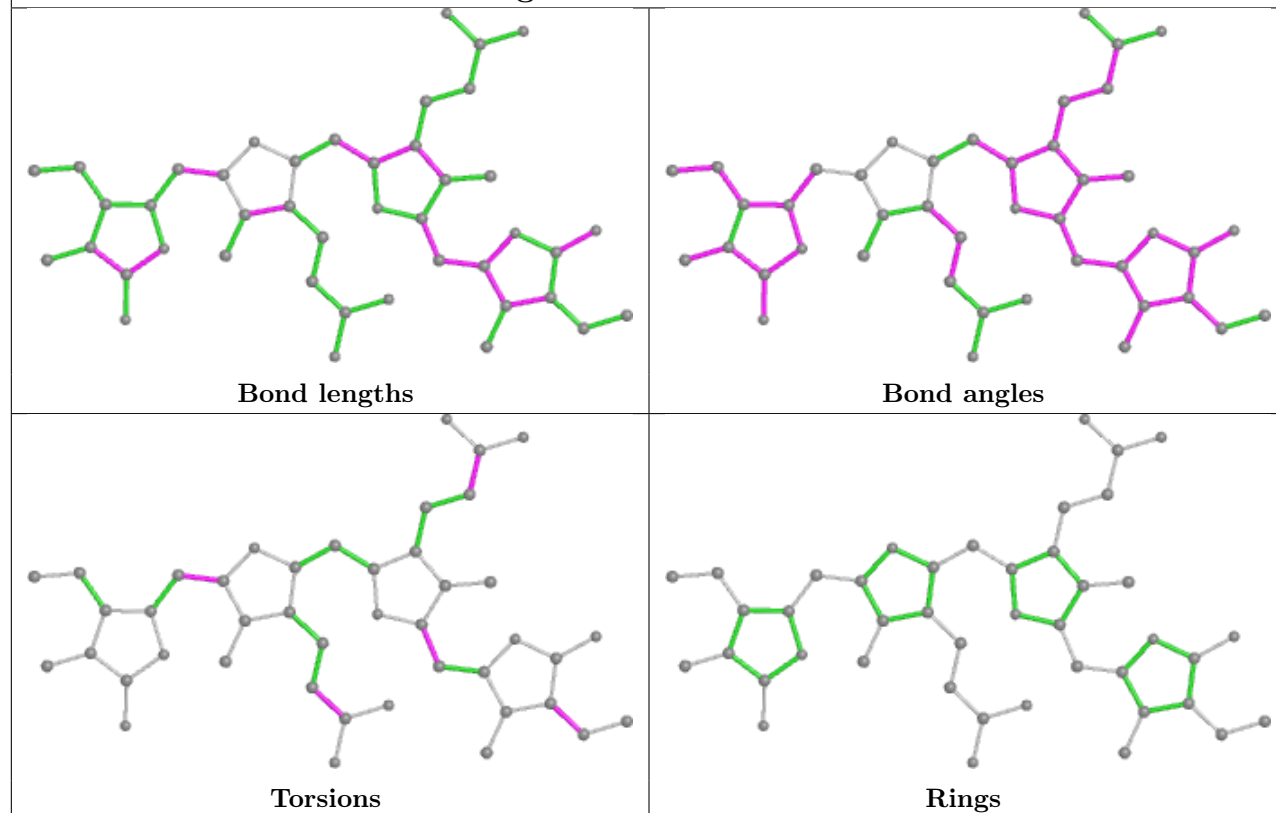
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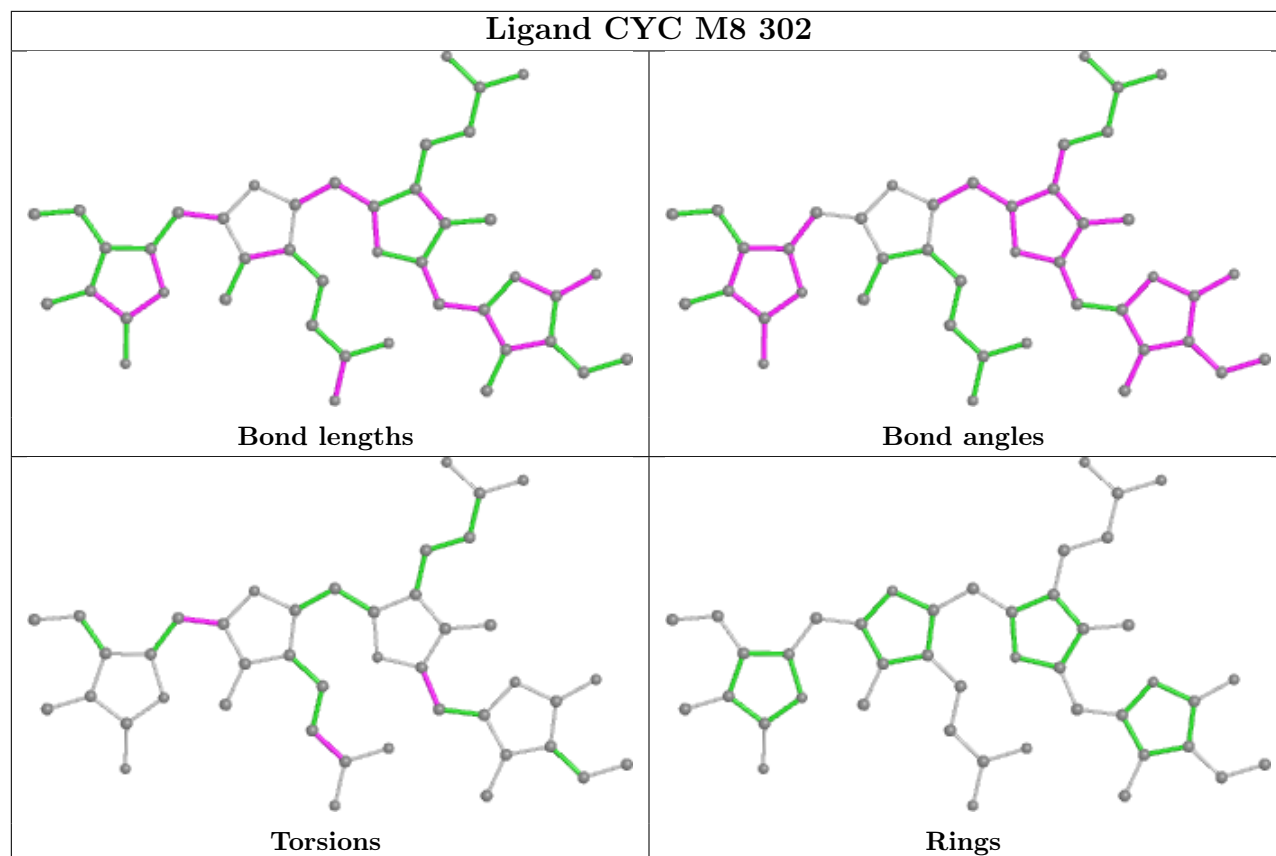
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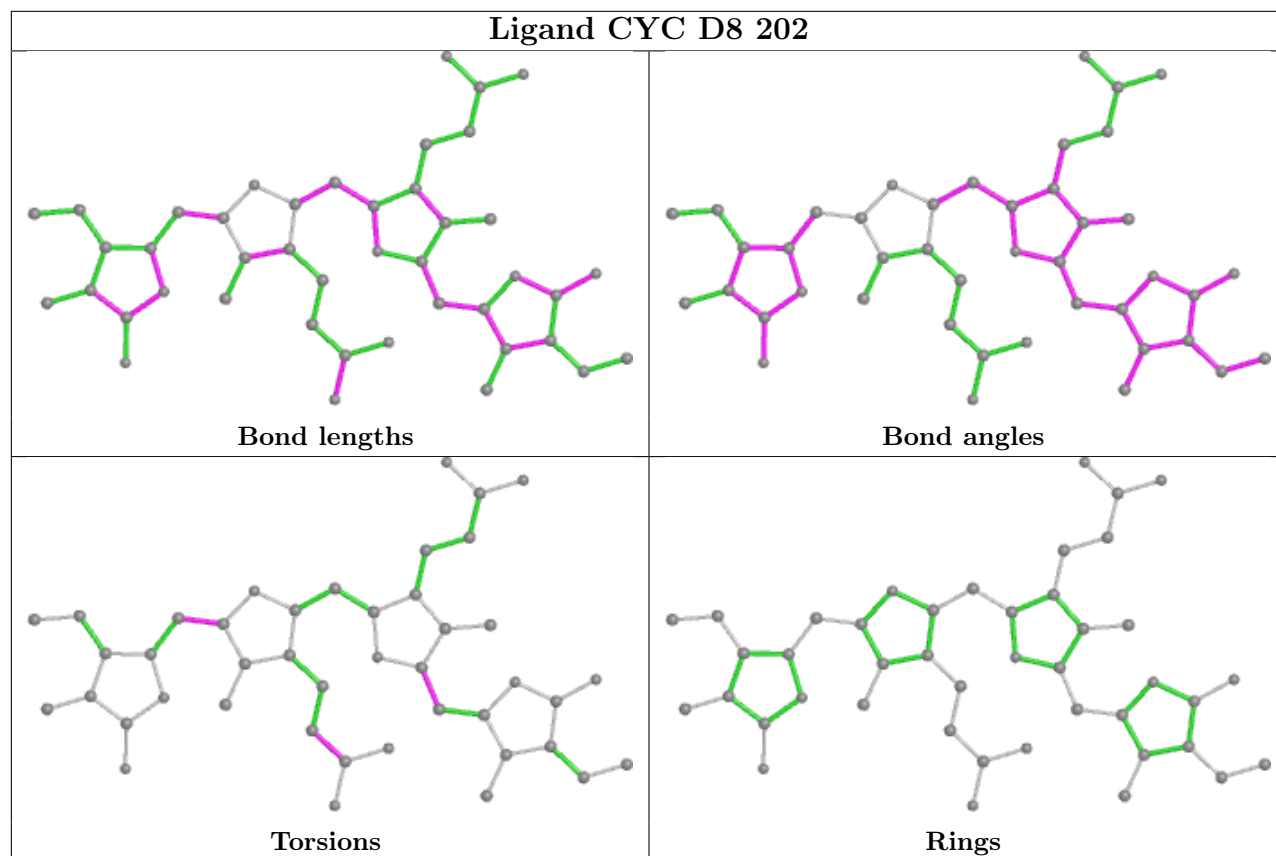
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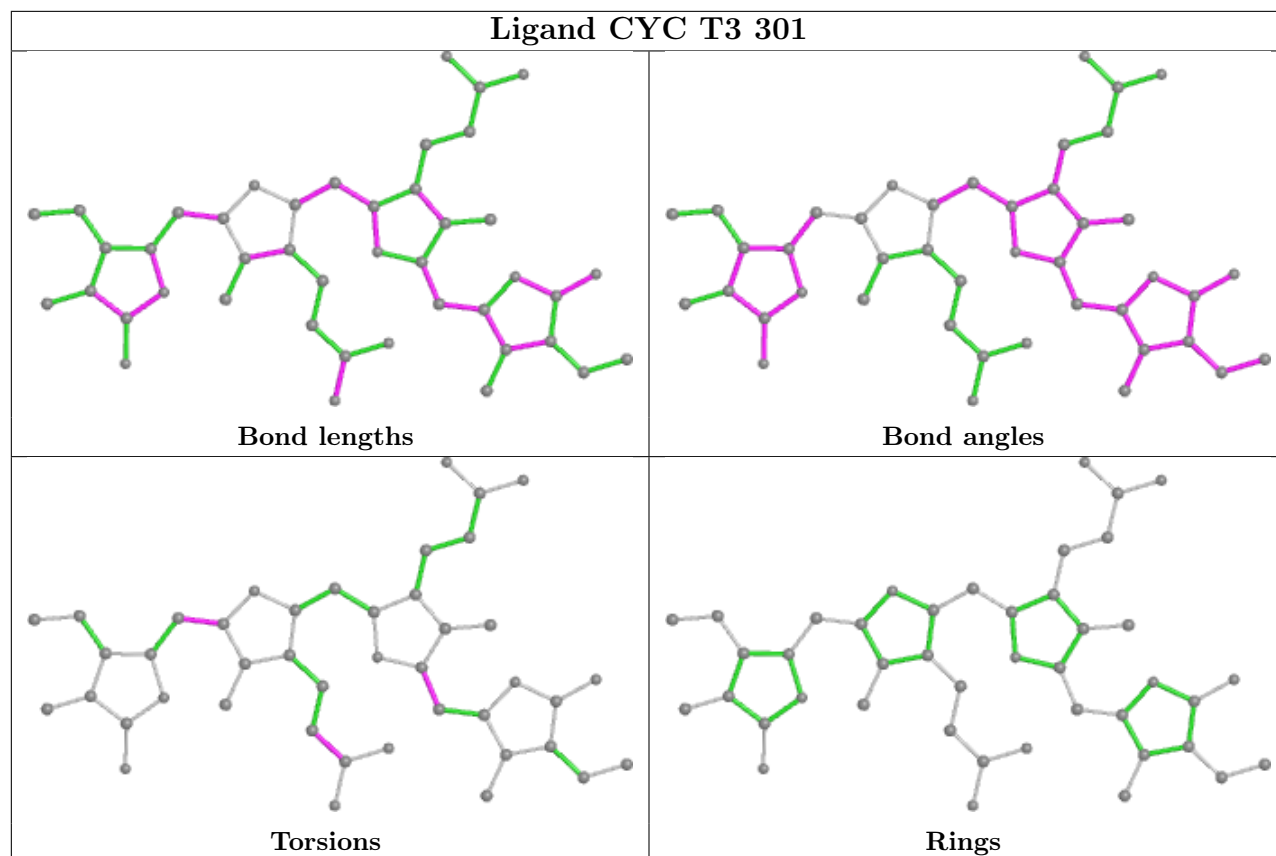
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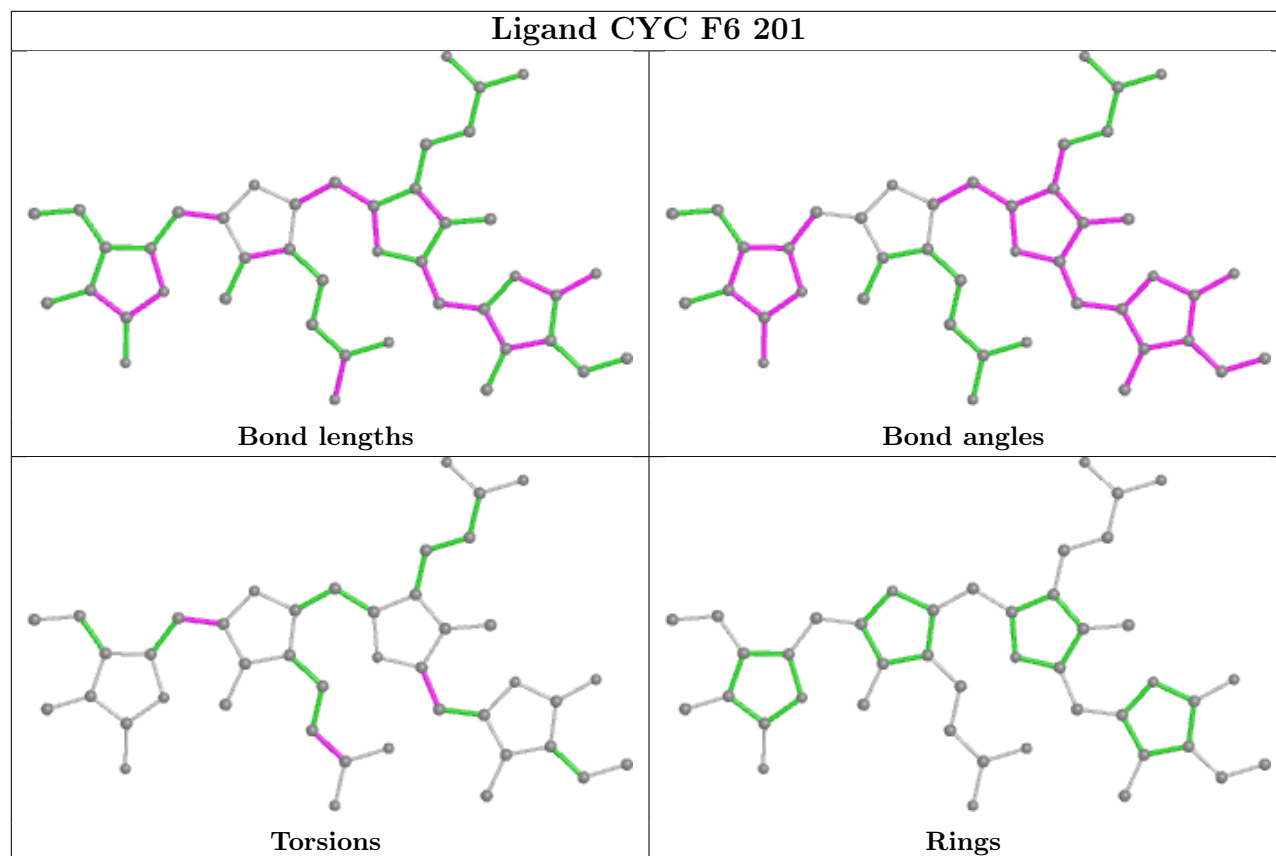
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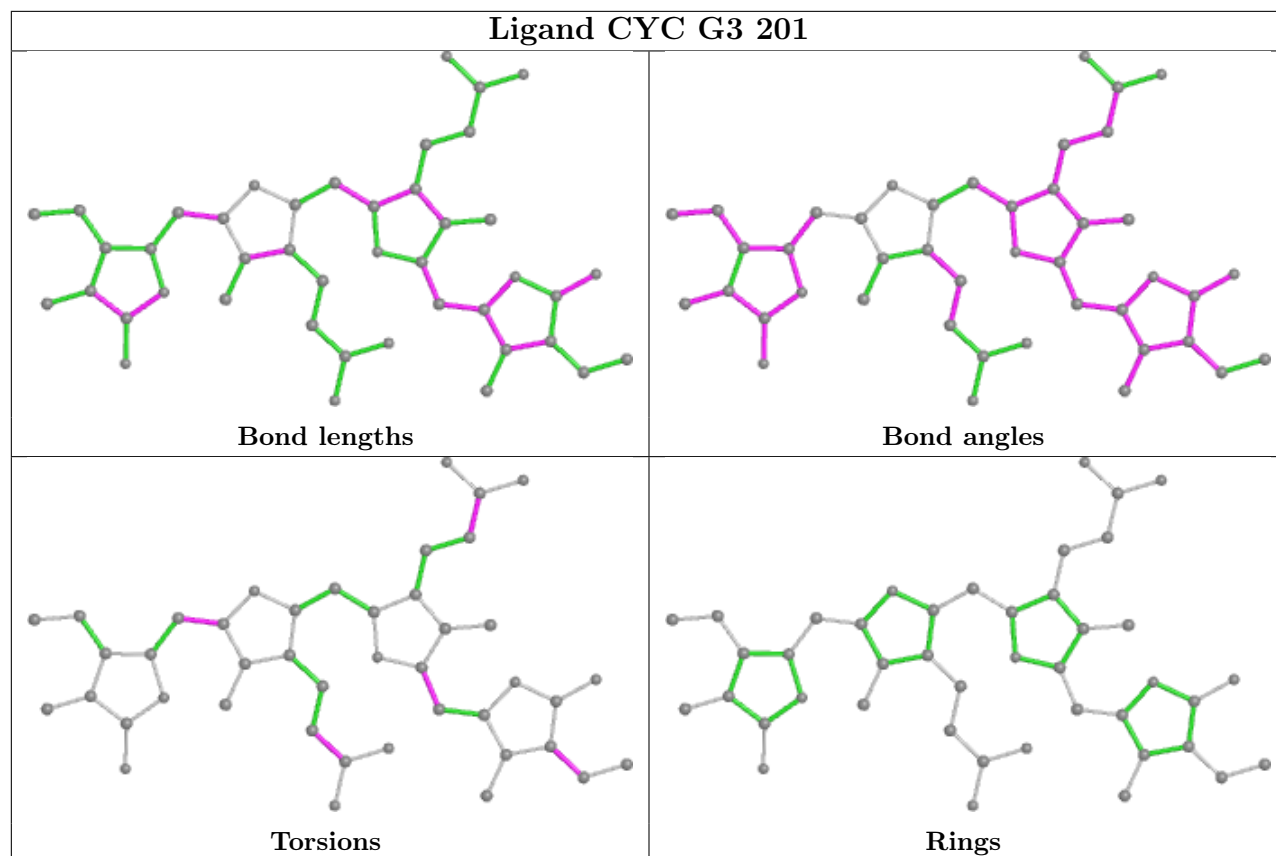
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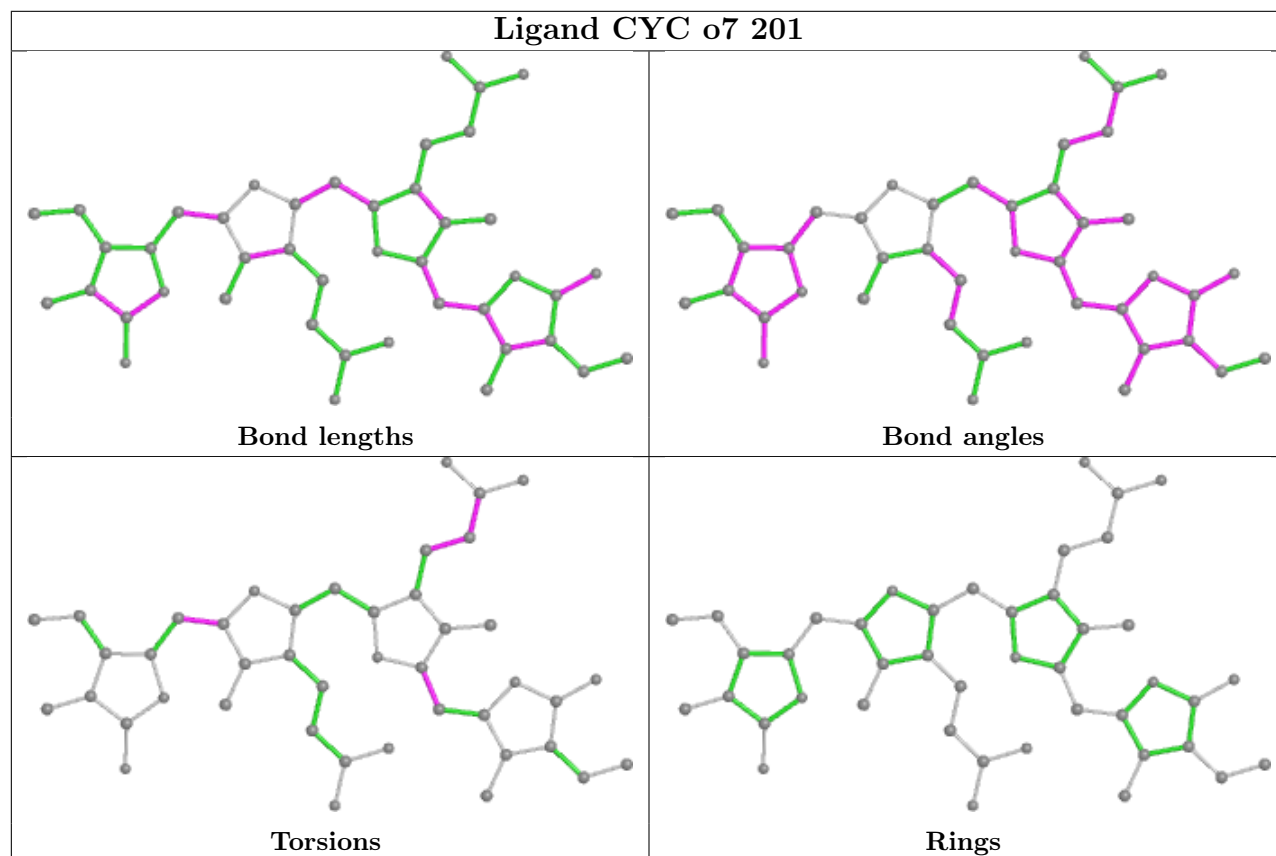
Ligand CYC F6 201



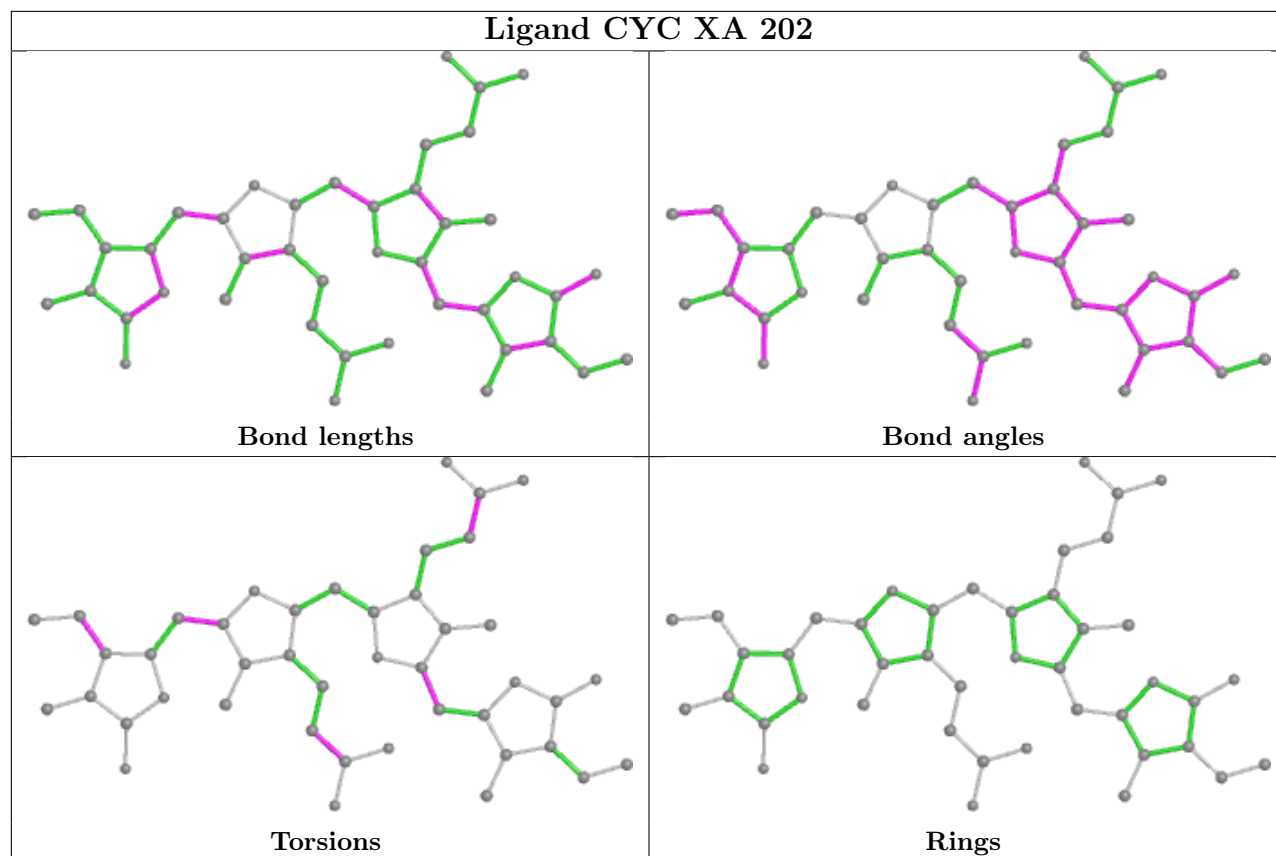
Ligand CYC G3 201



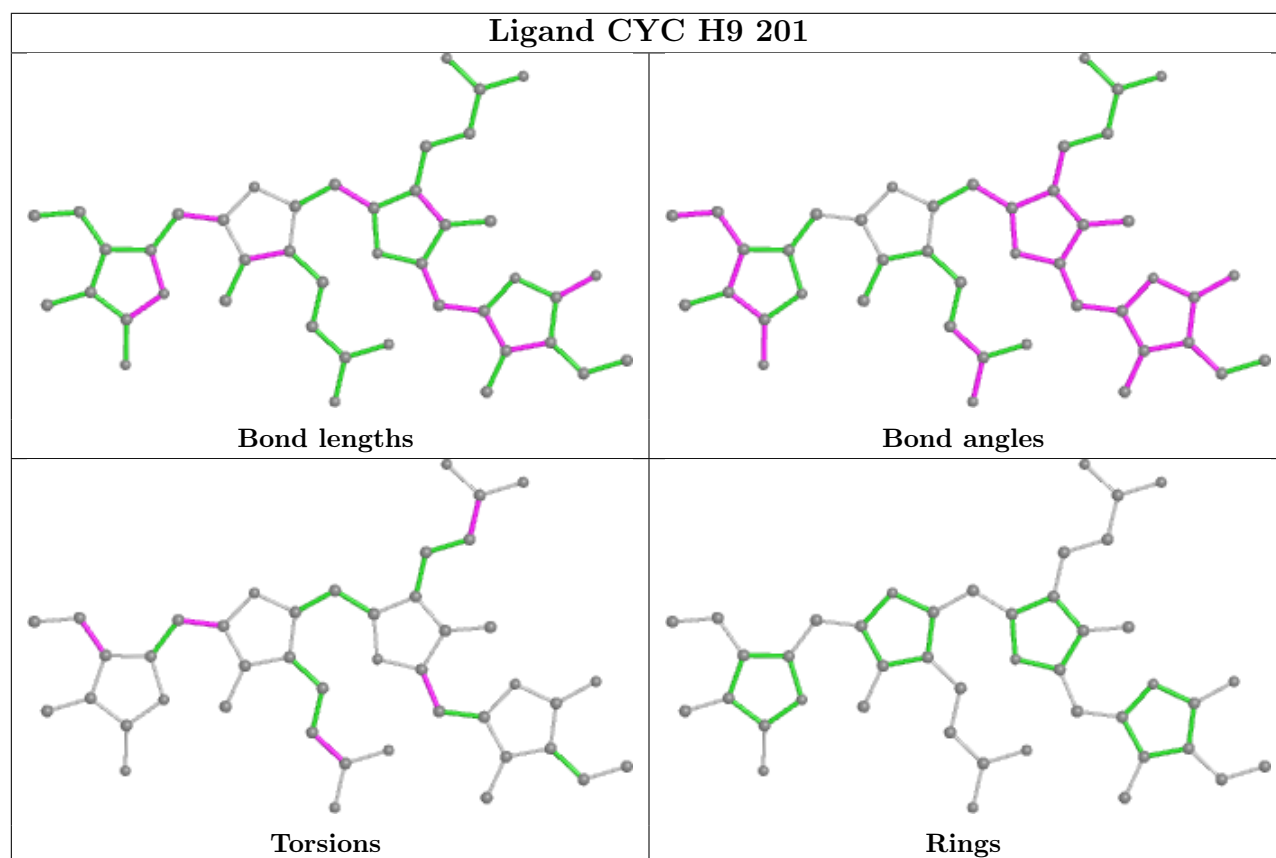
Ligand CYC o7 201



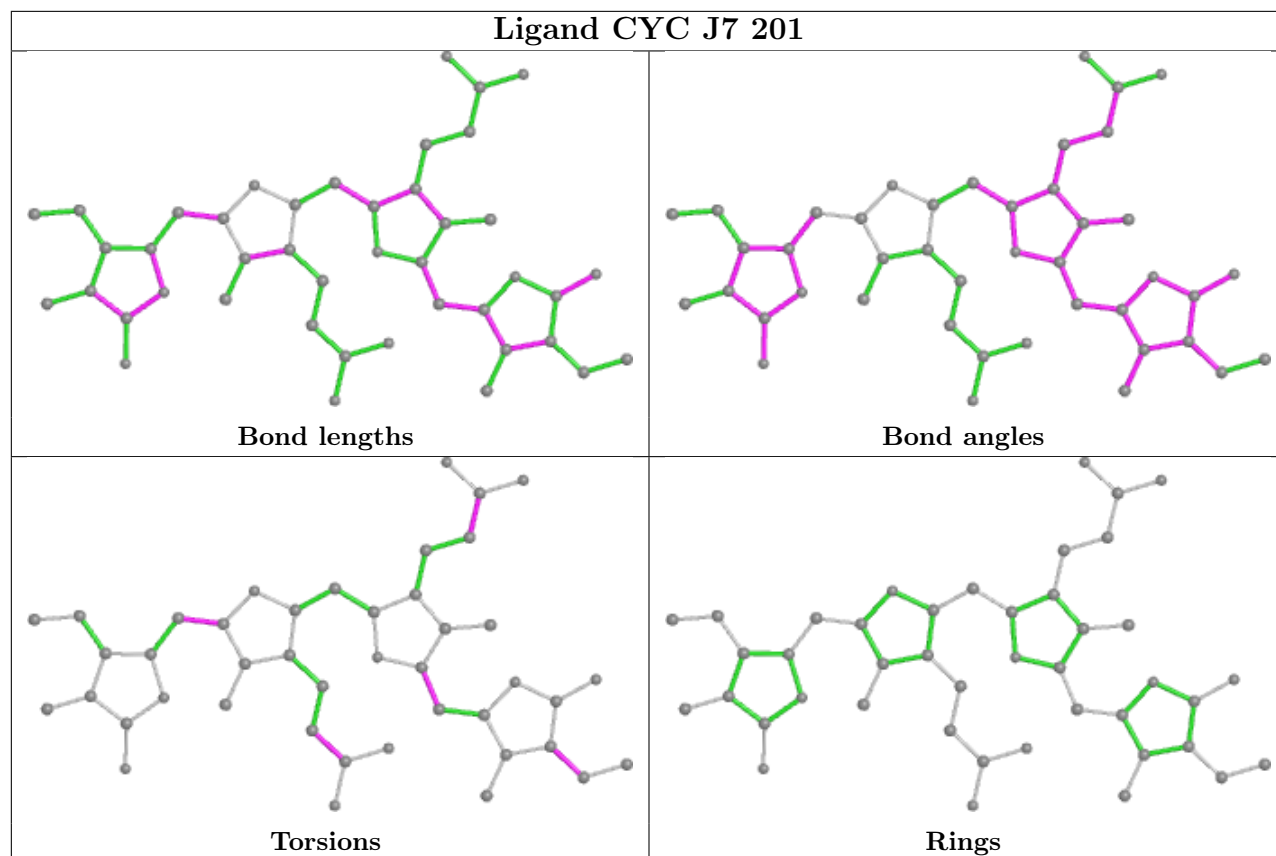
Ligand CYC XA 202



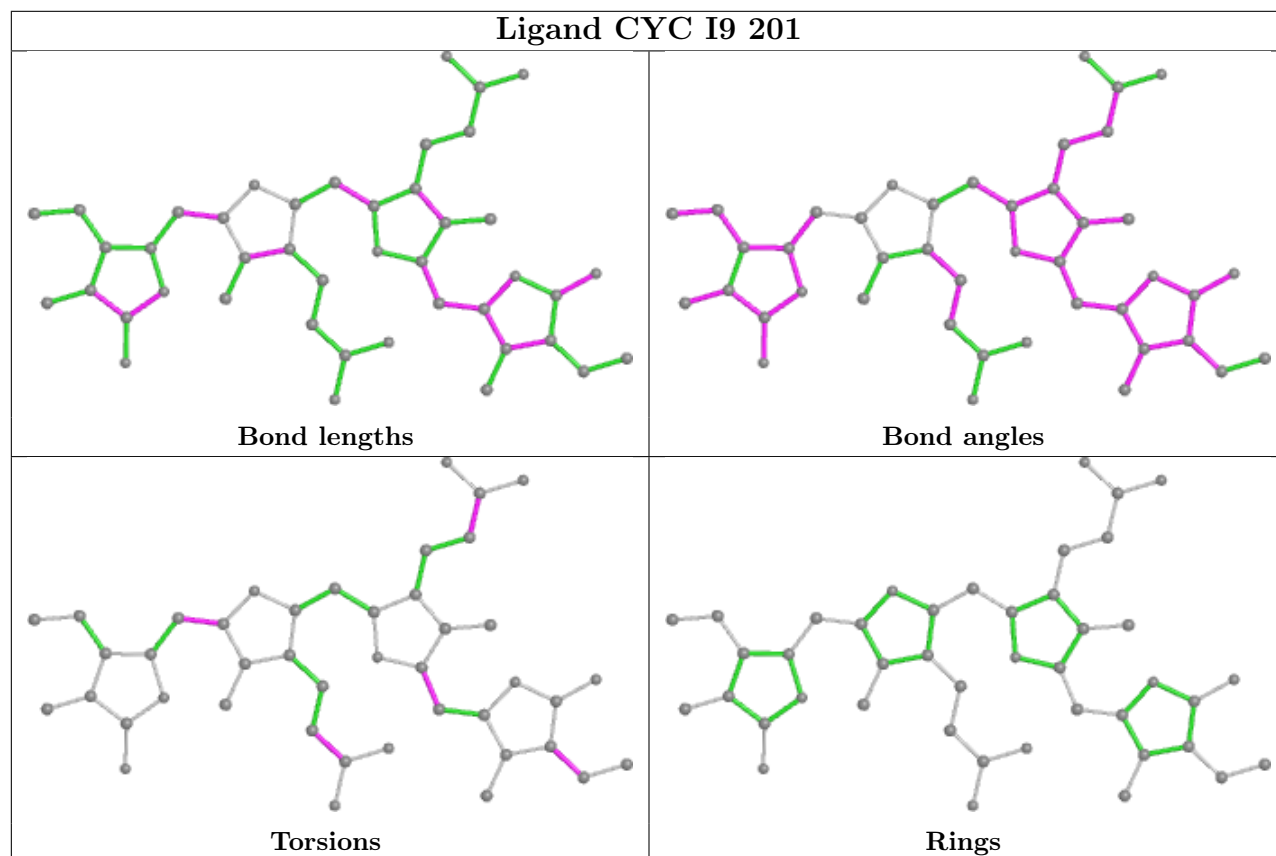
Ligand CYC H9 201



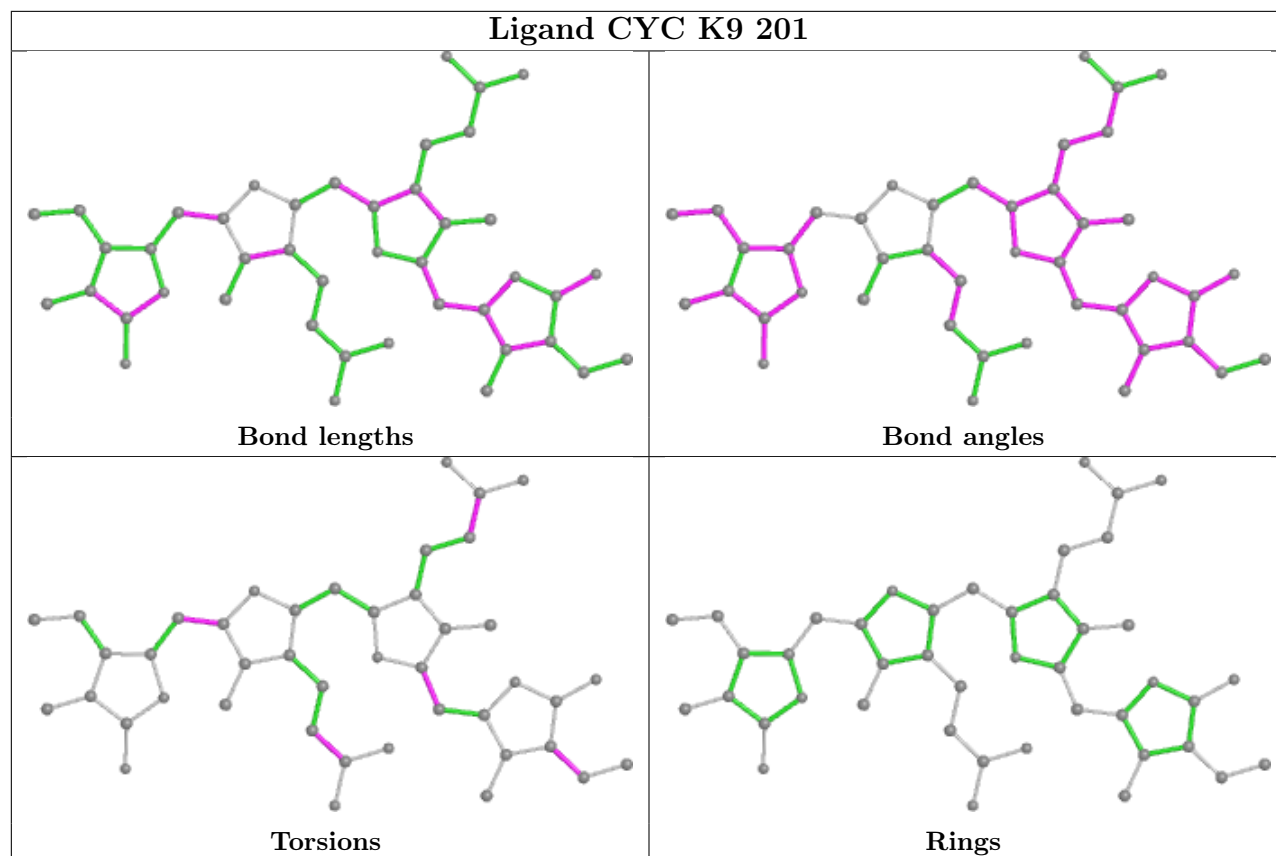
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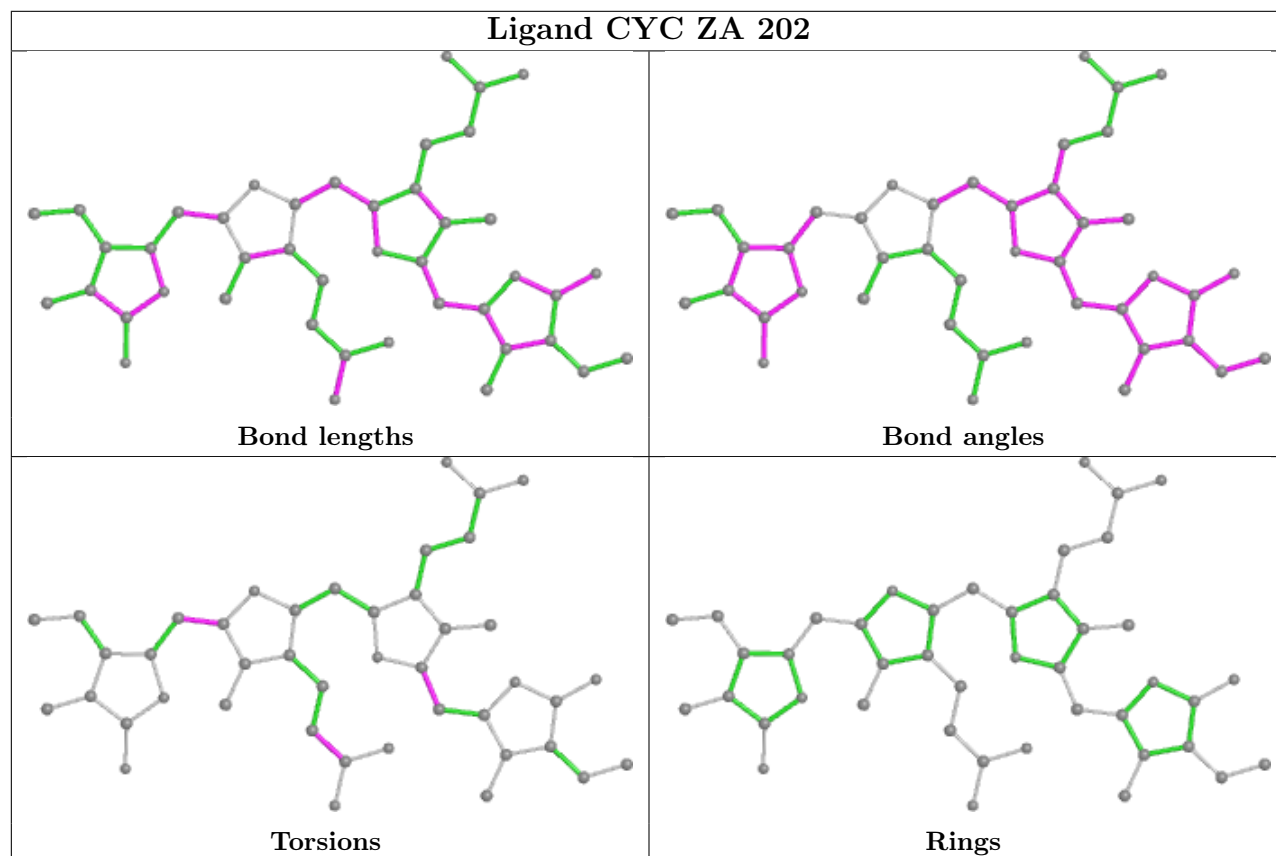
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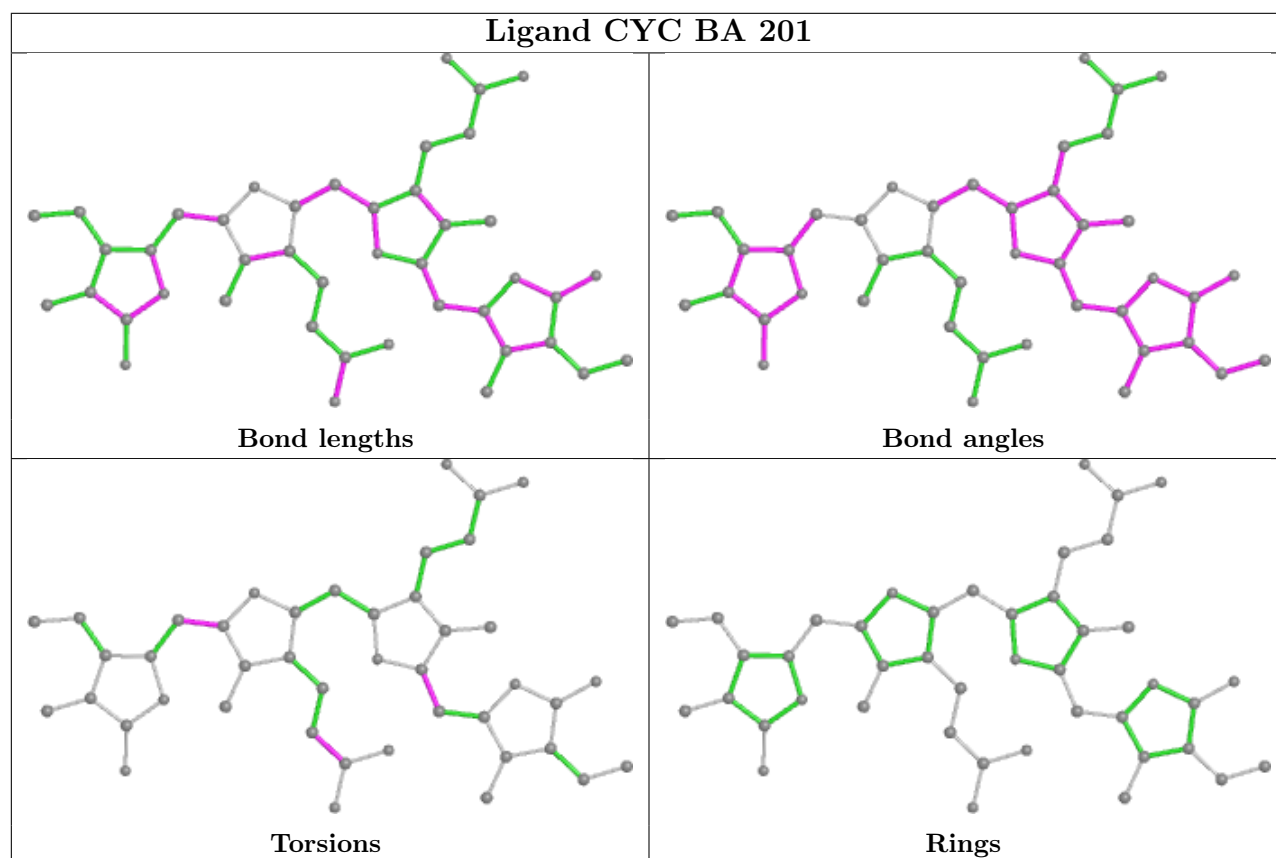
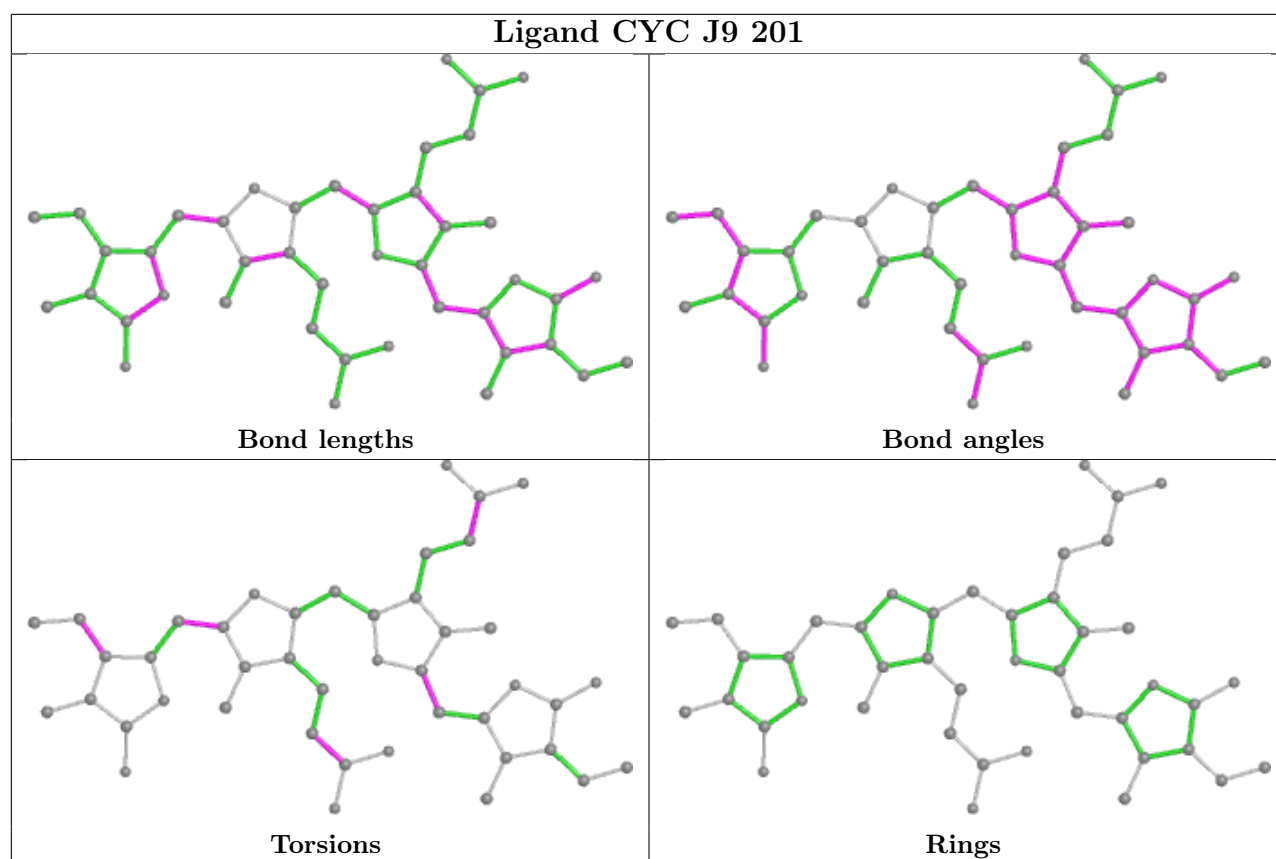


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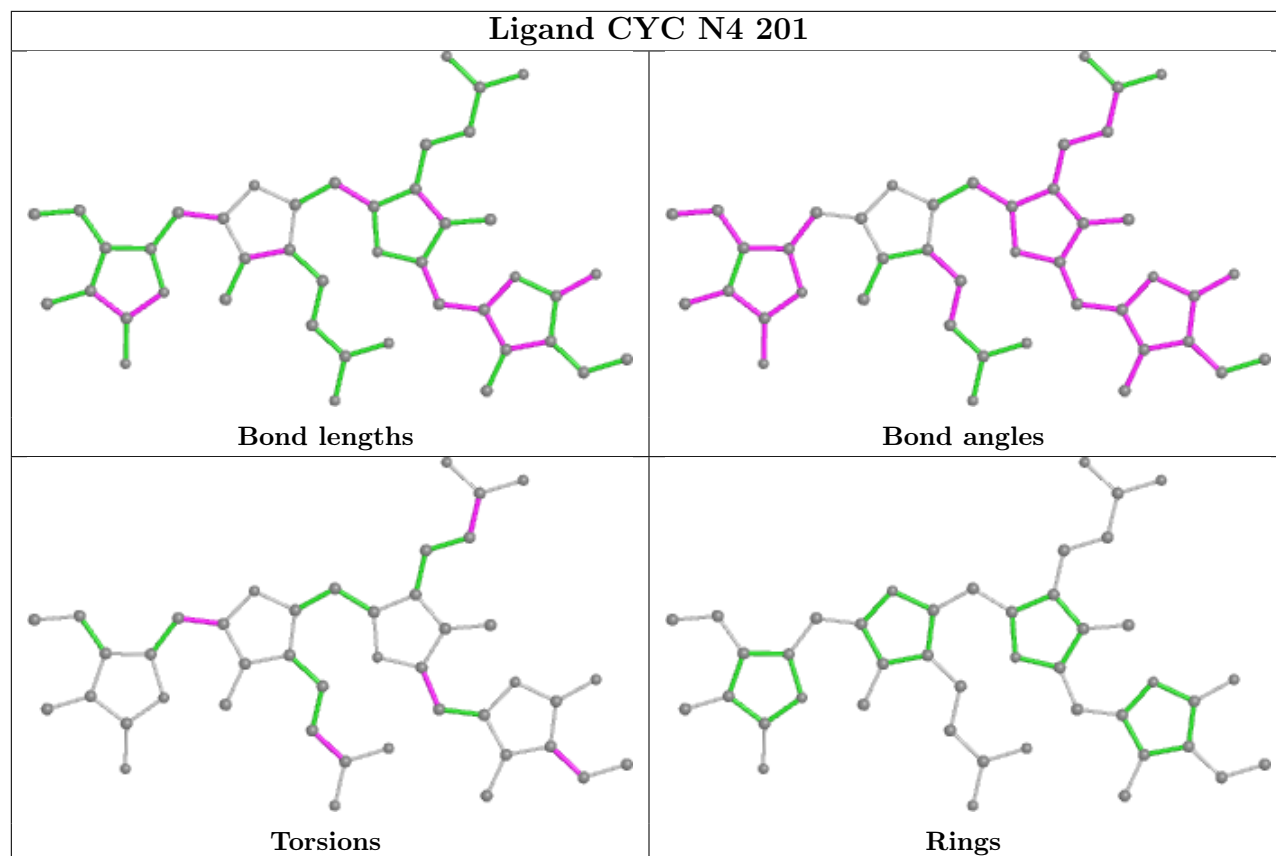


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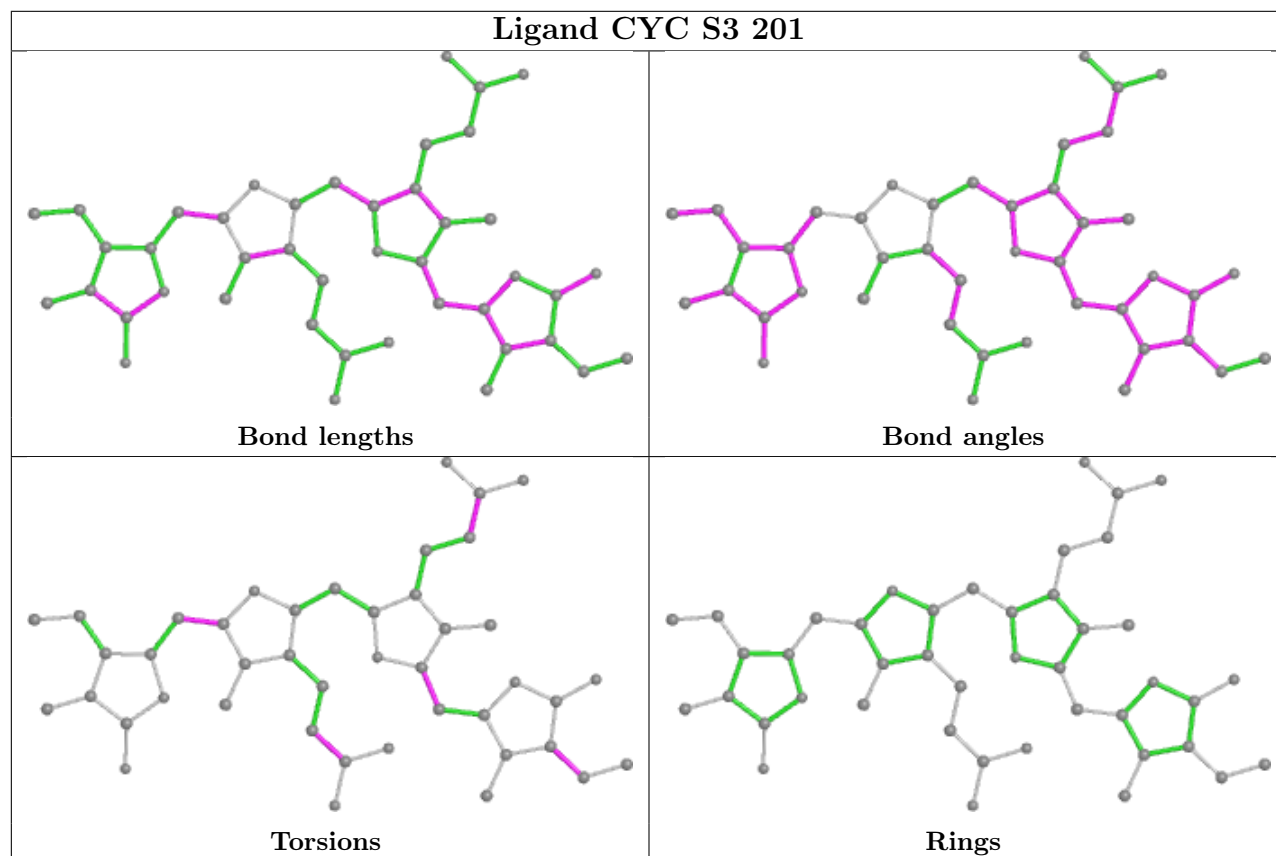




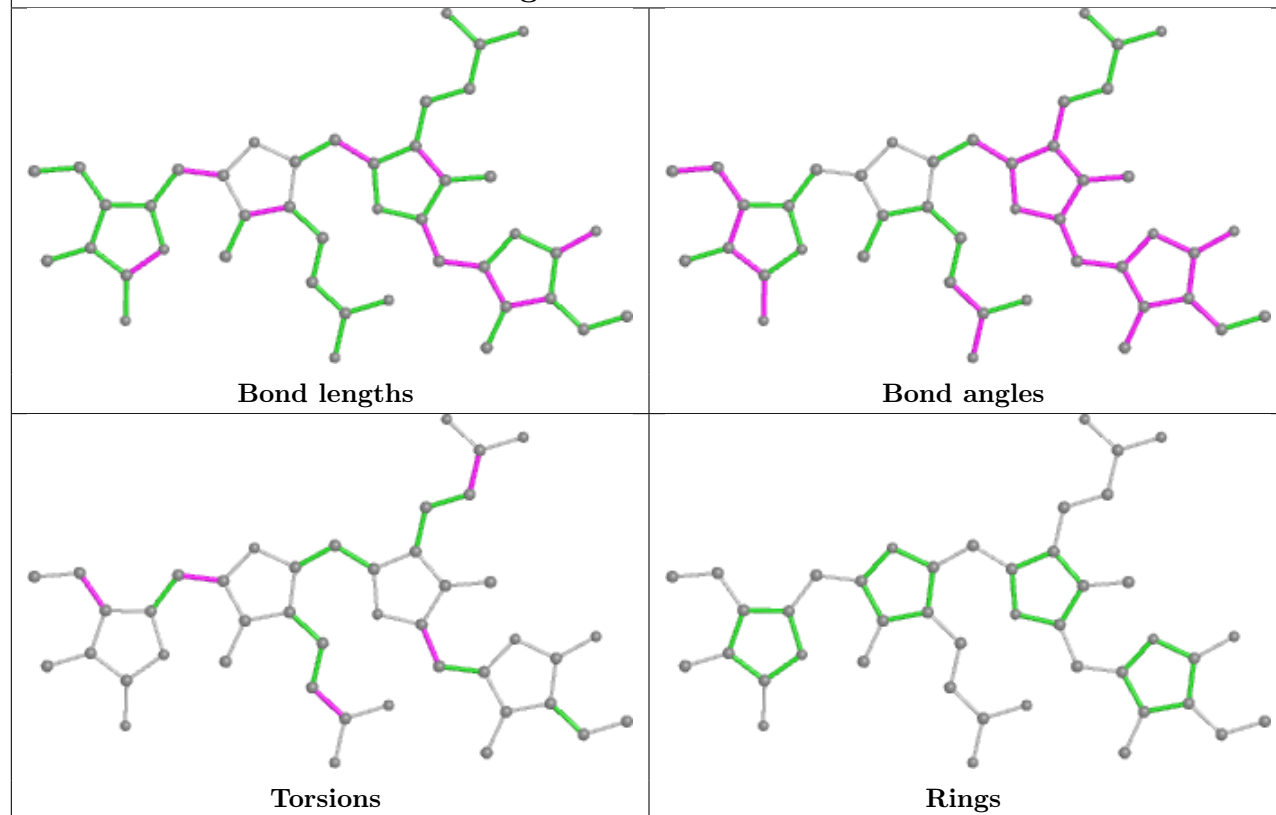
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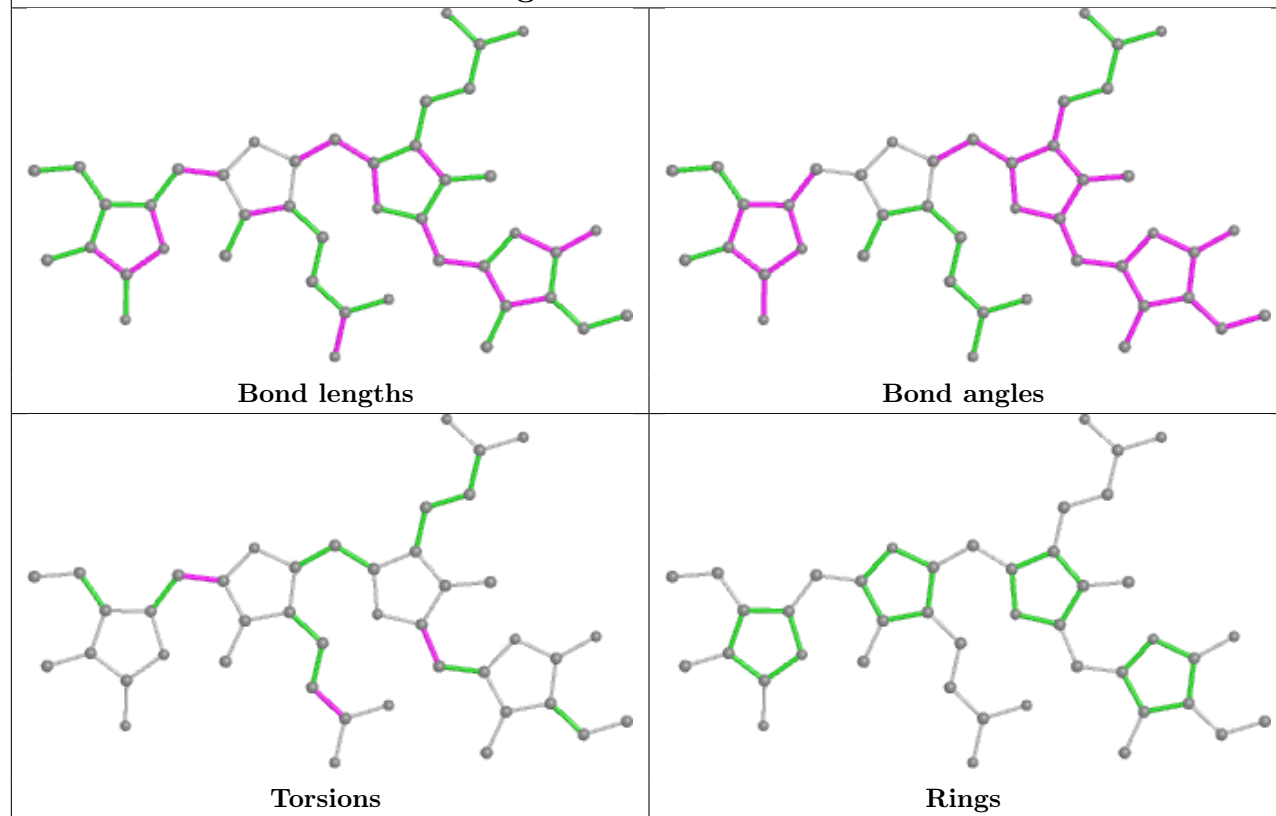
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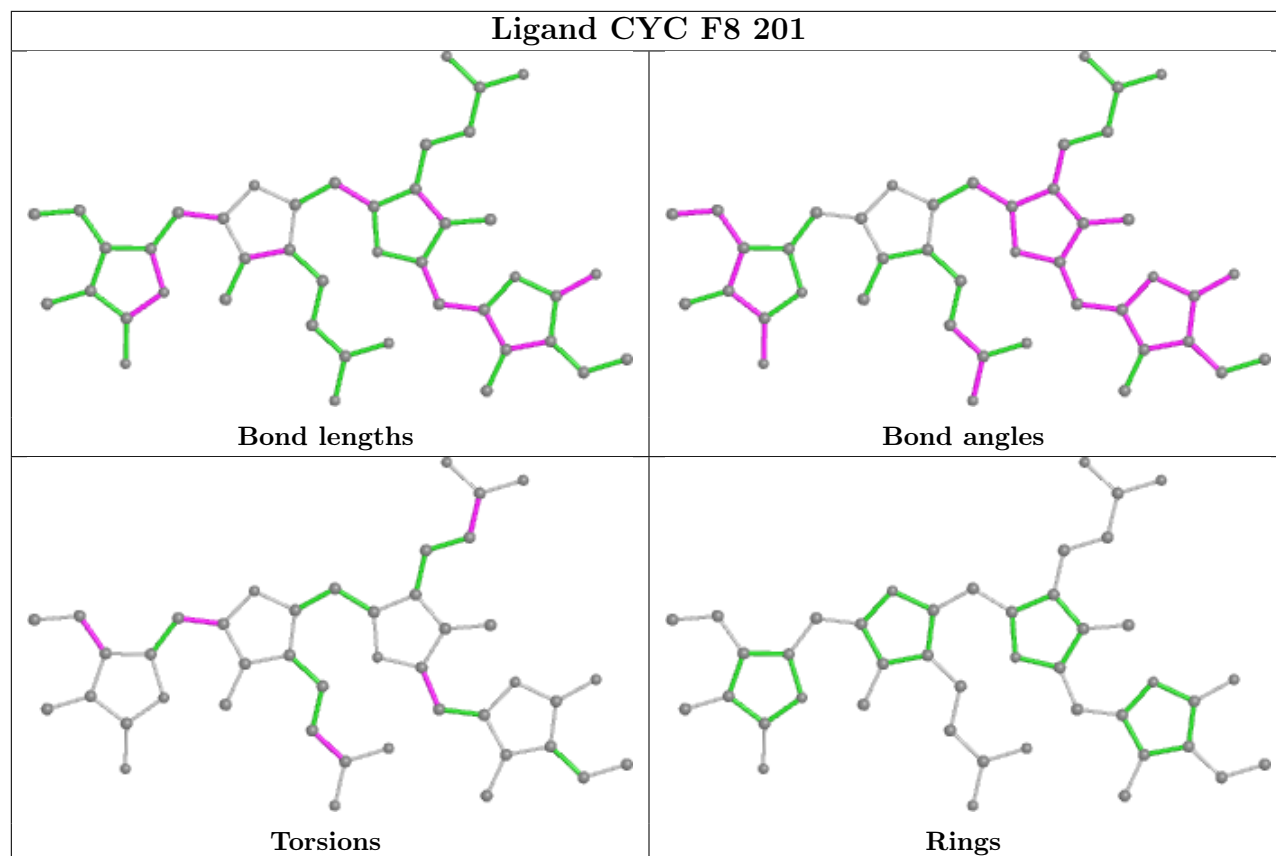
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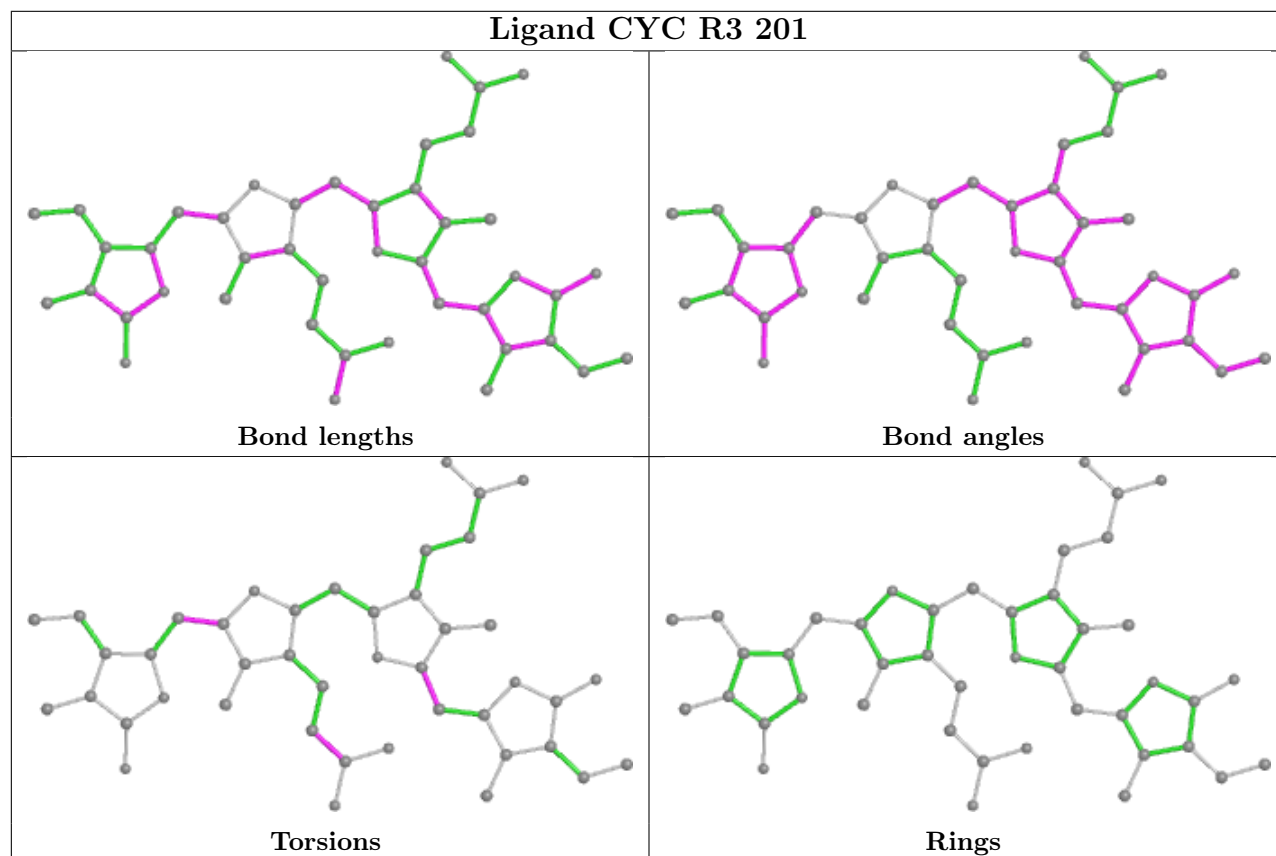
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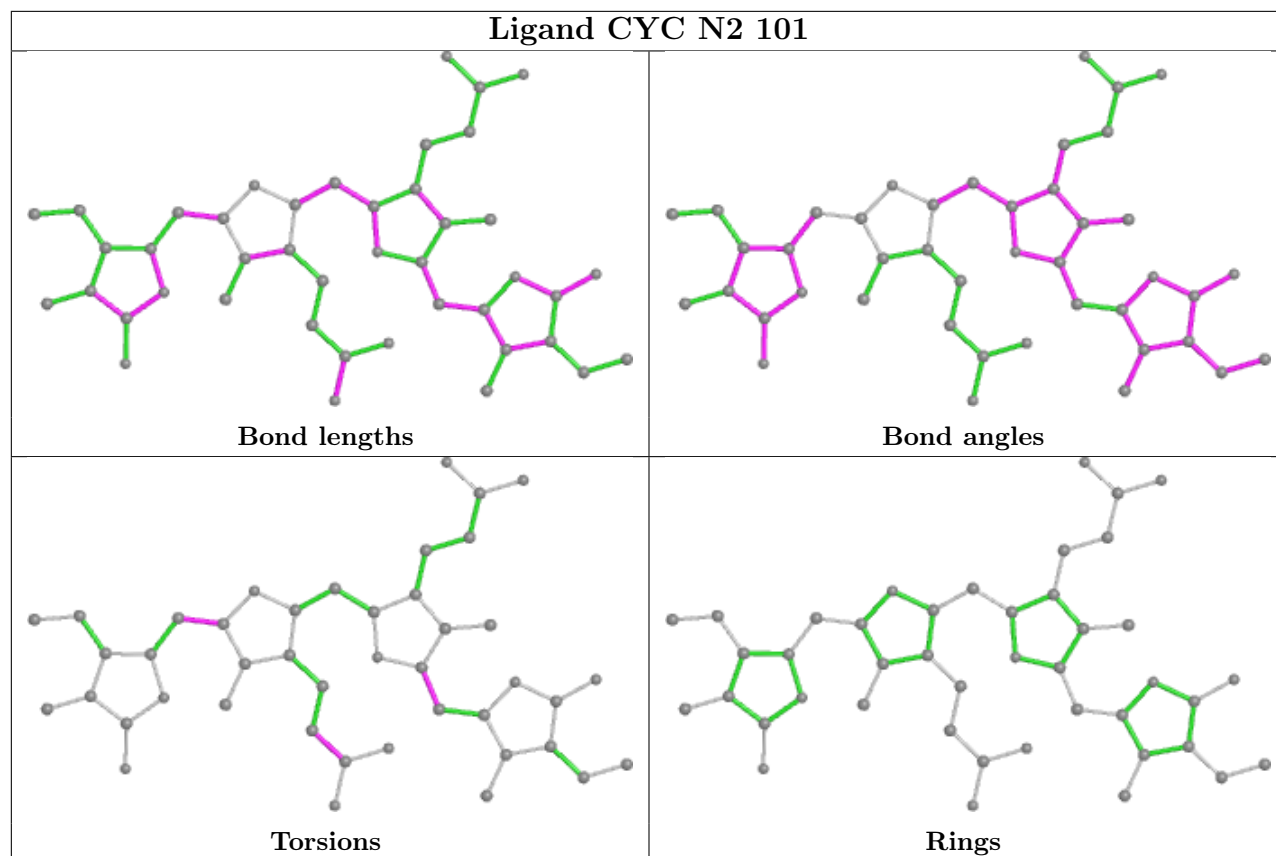
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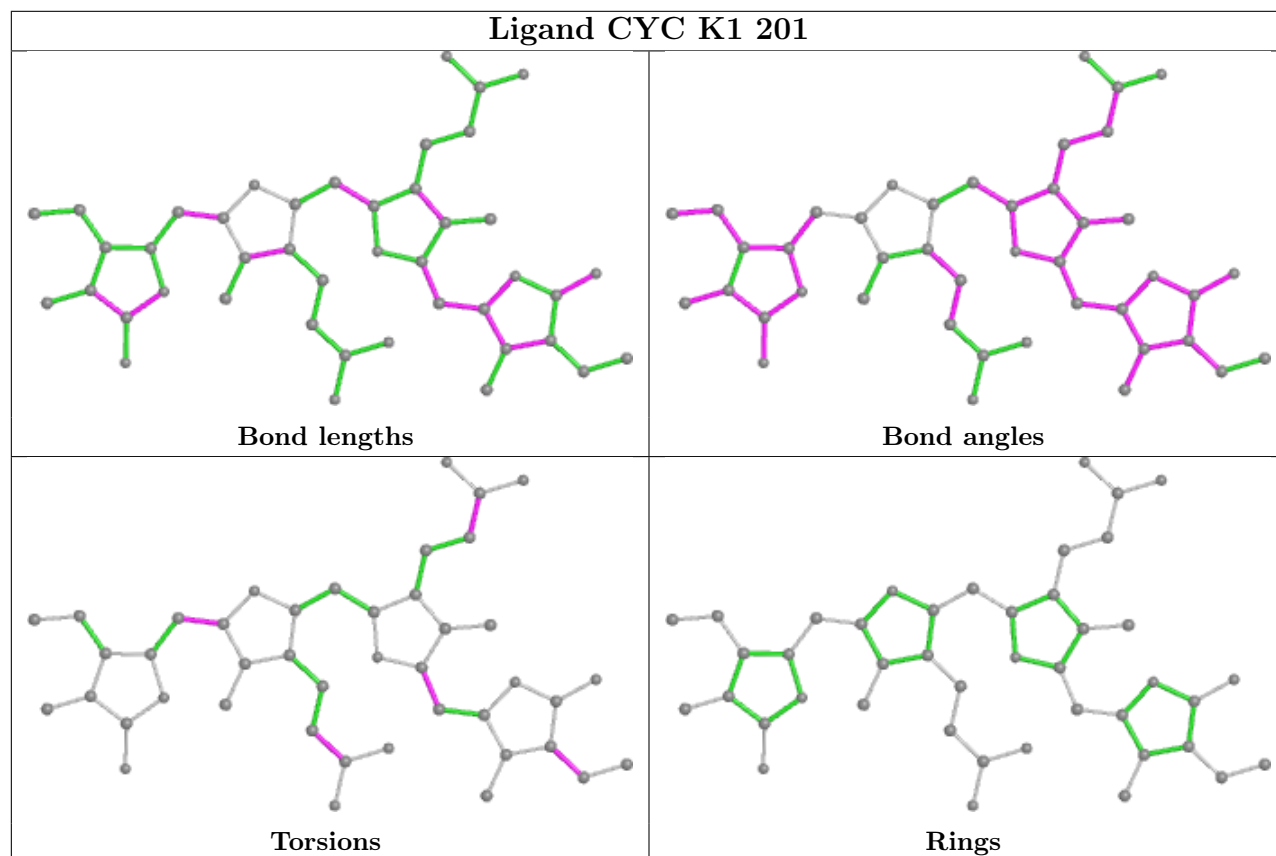
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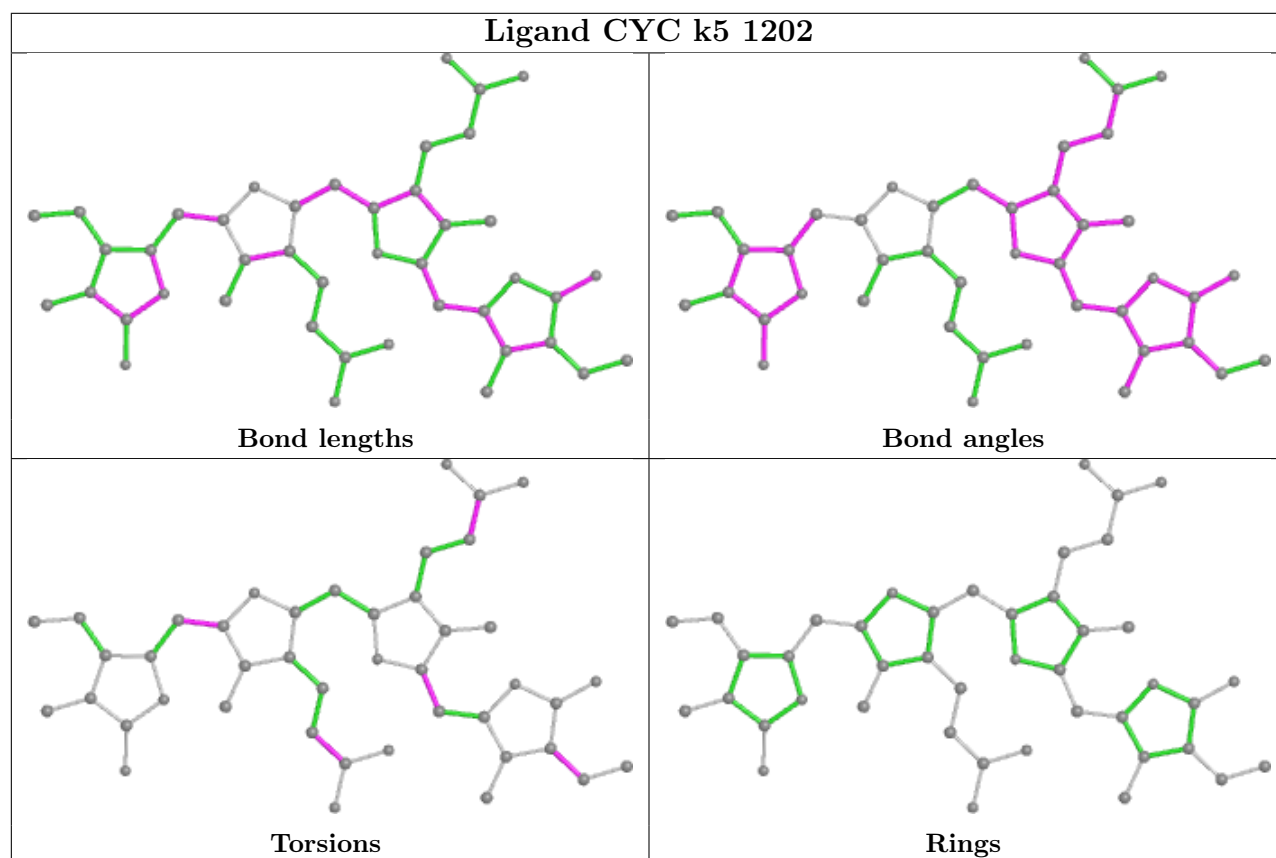
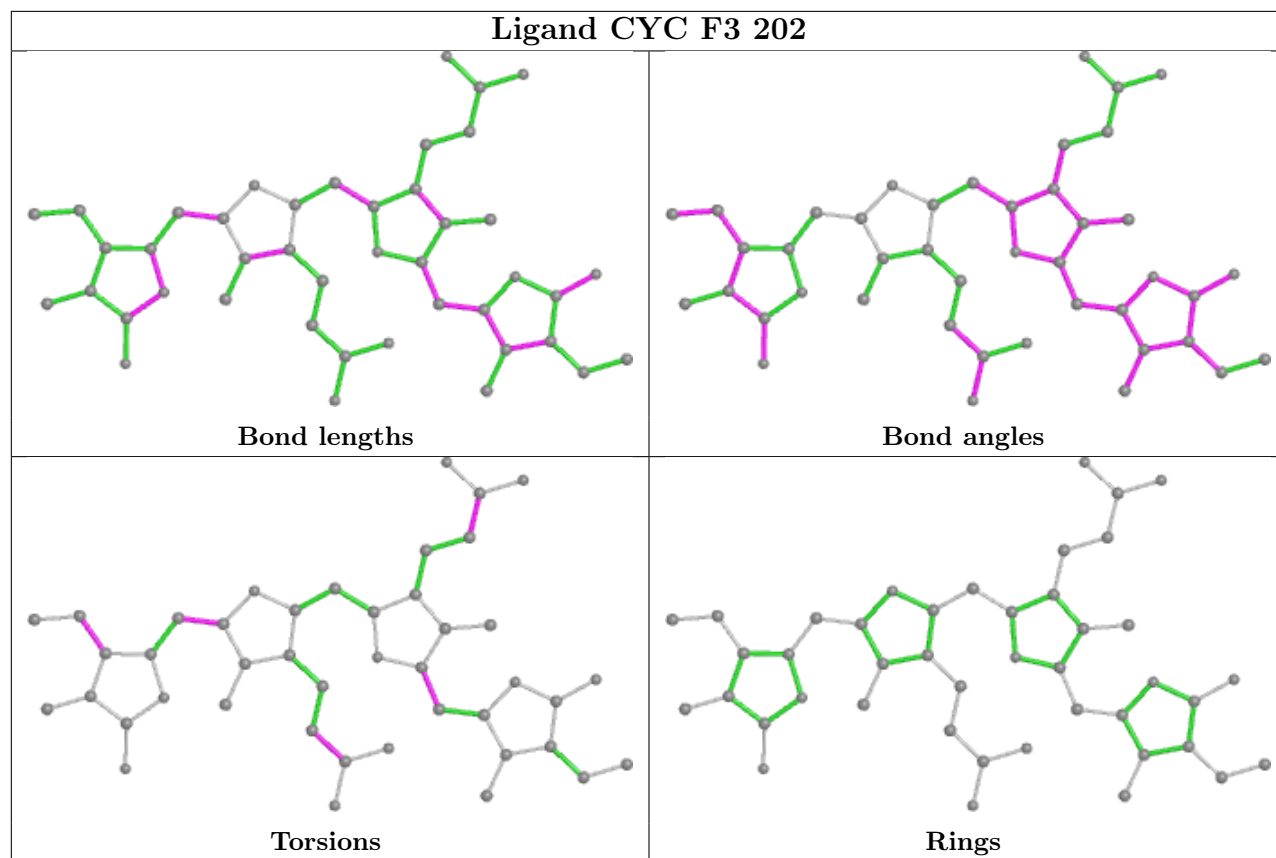


Ligand CYC N2 101

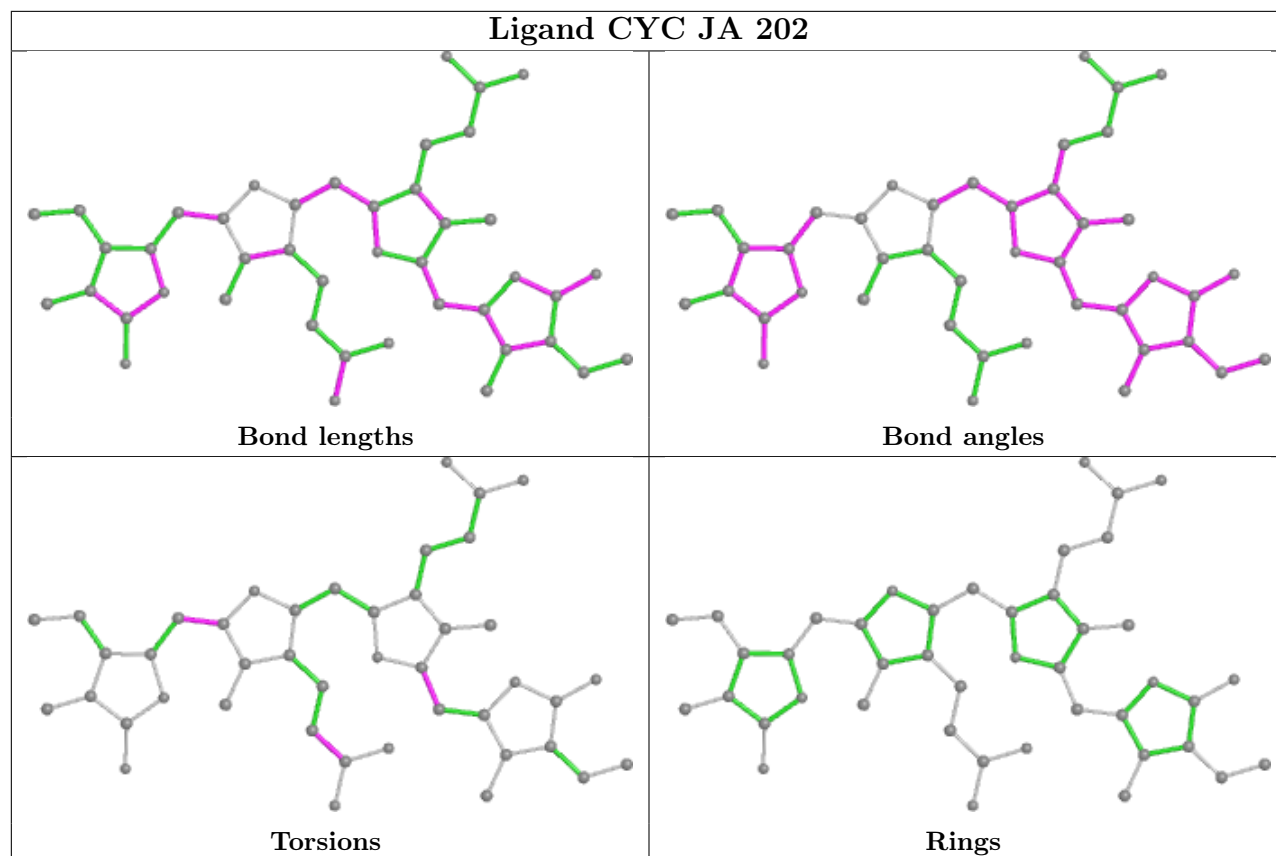


Ligand CYC K1 201

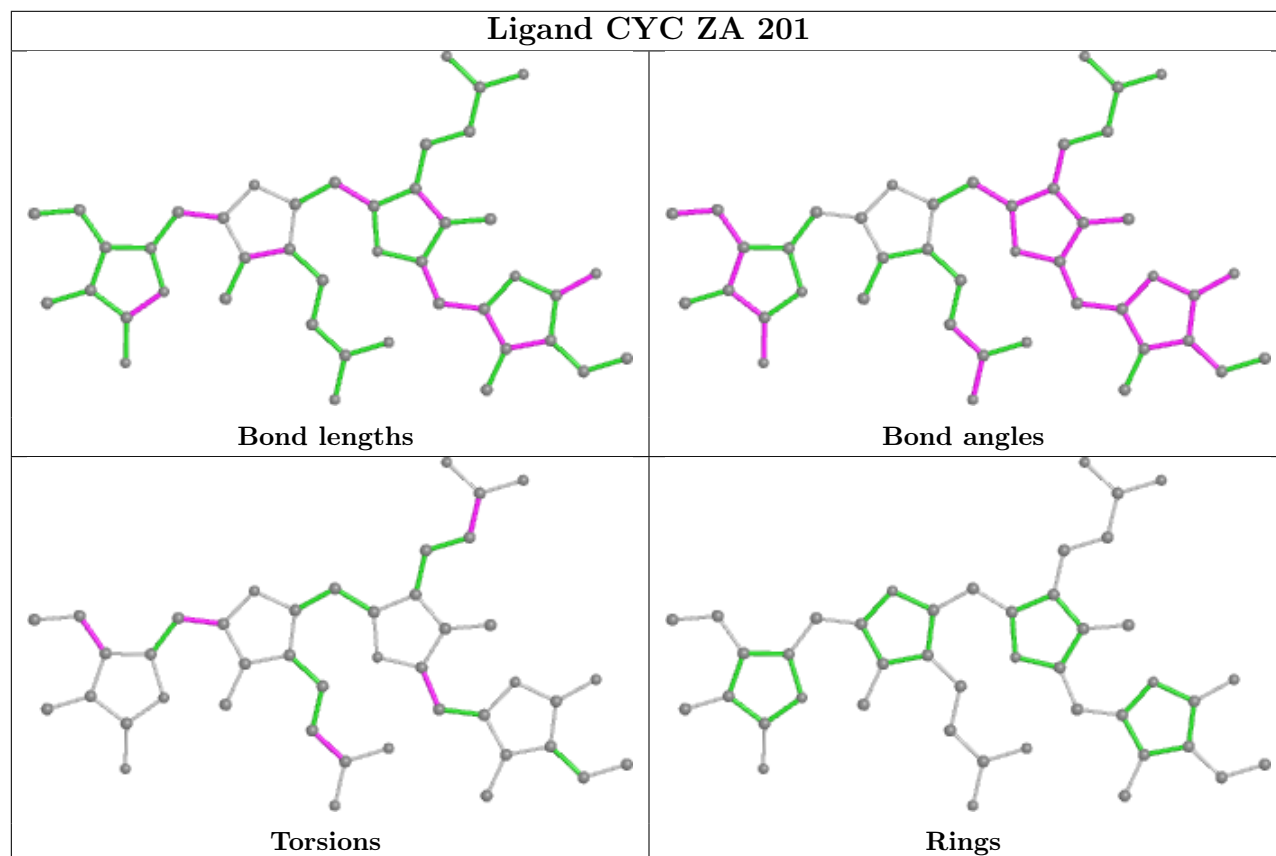




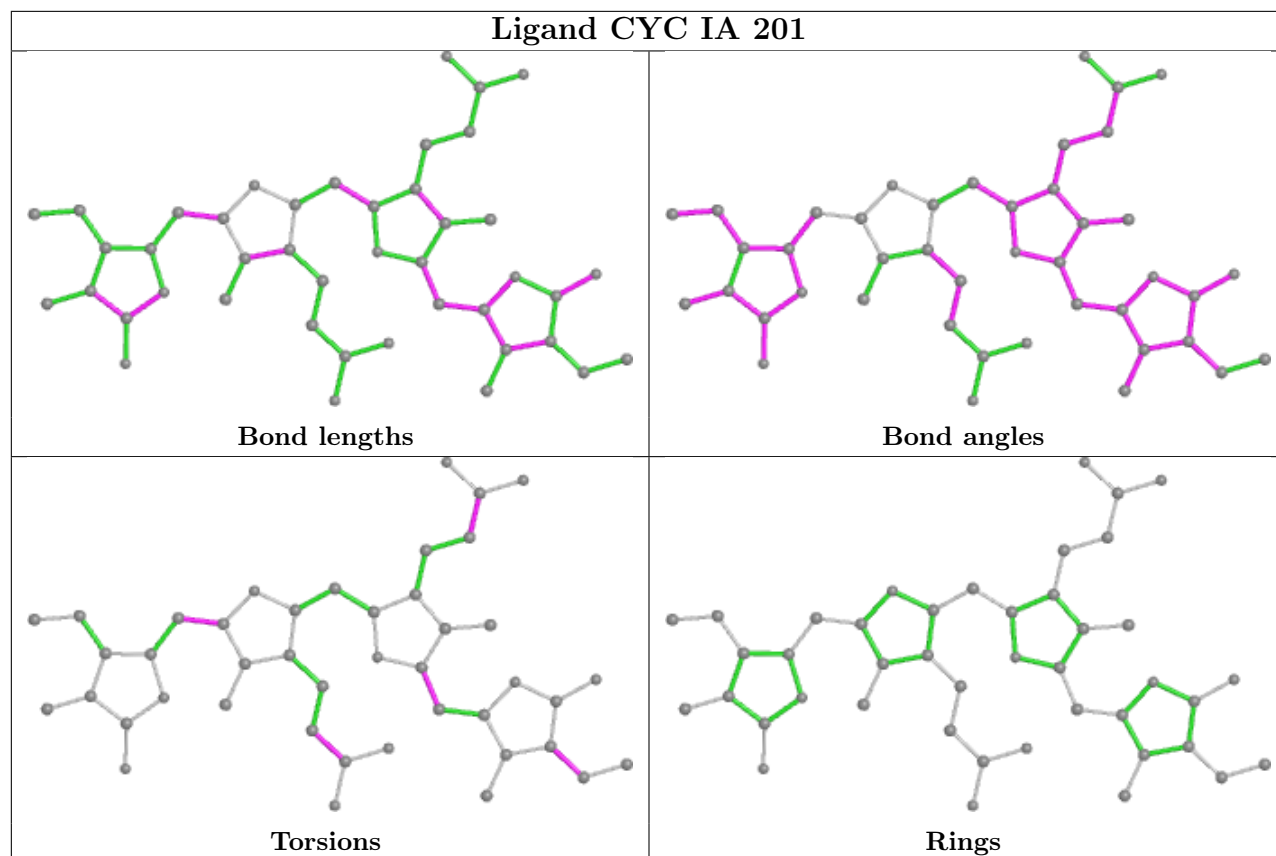
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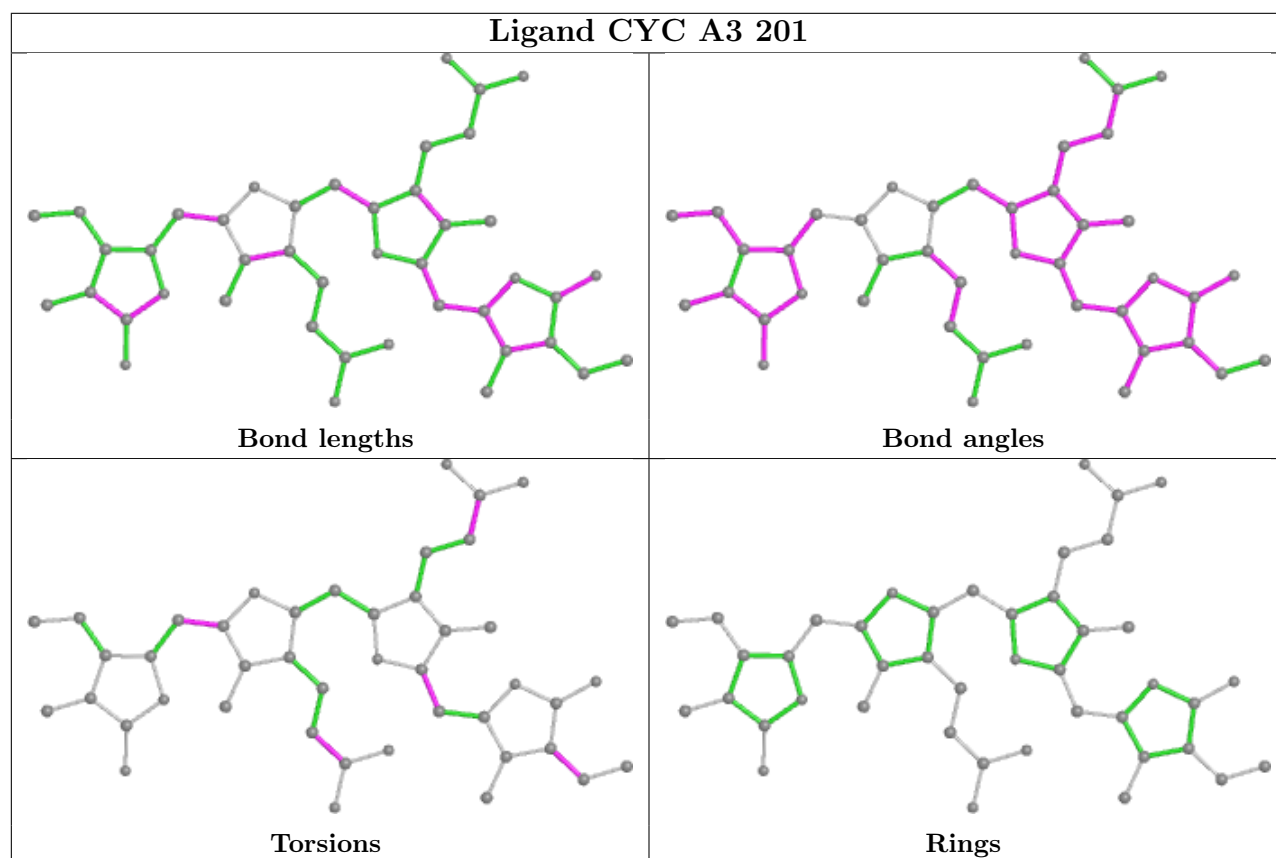
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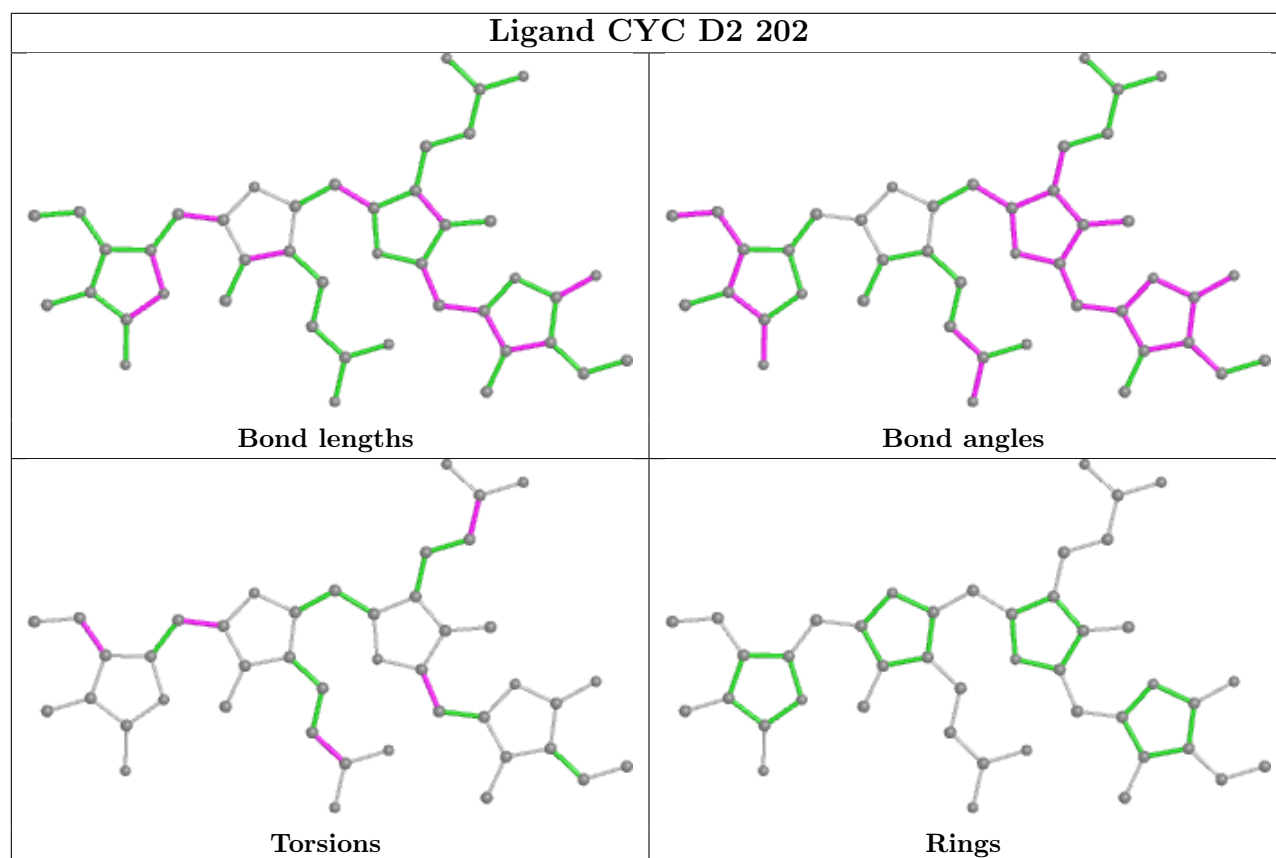
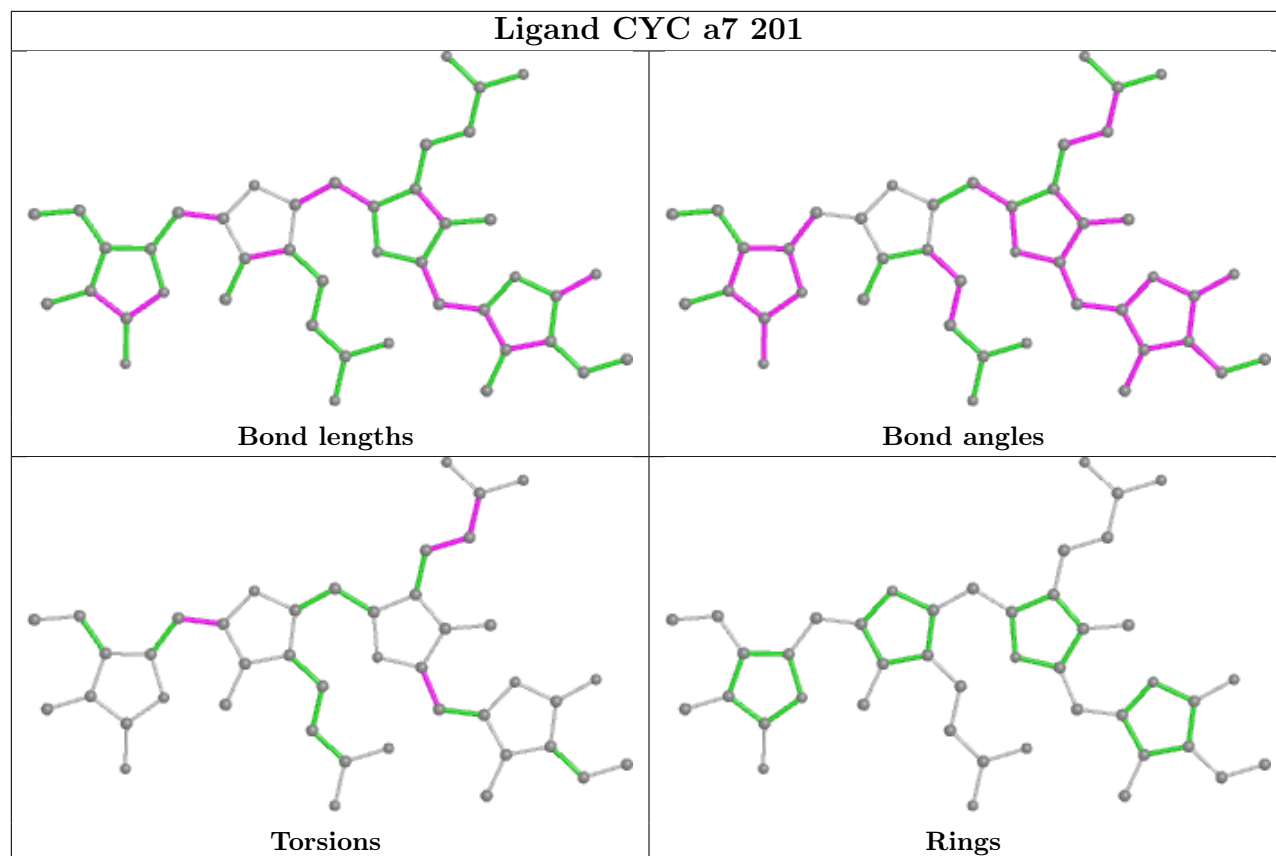


Ligand CYC IA 201

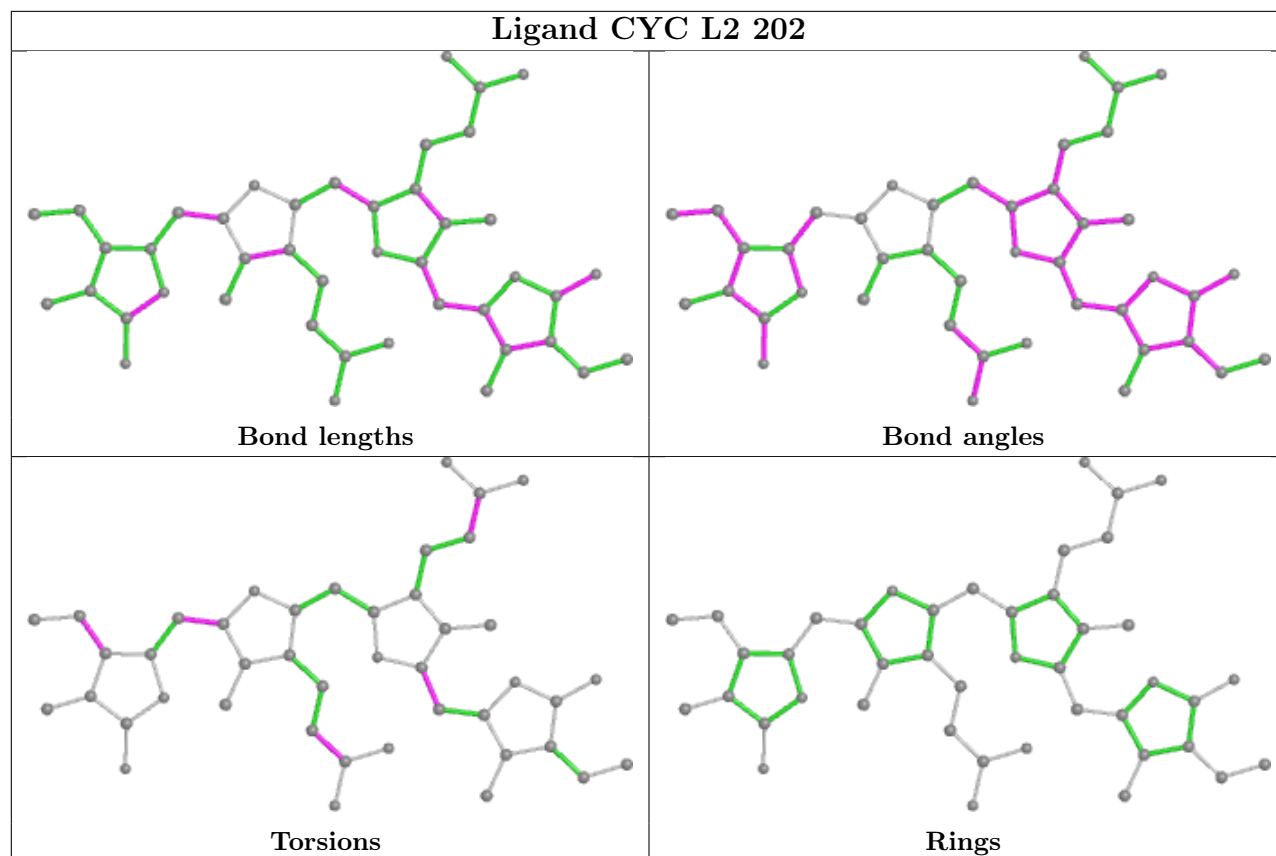


Ligand CYC A3 201

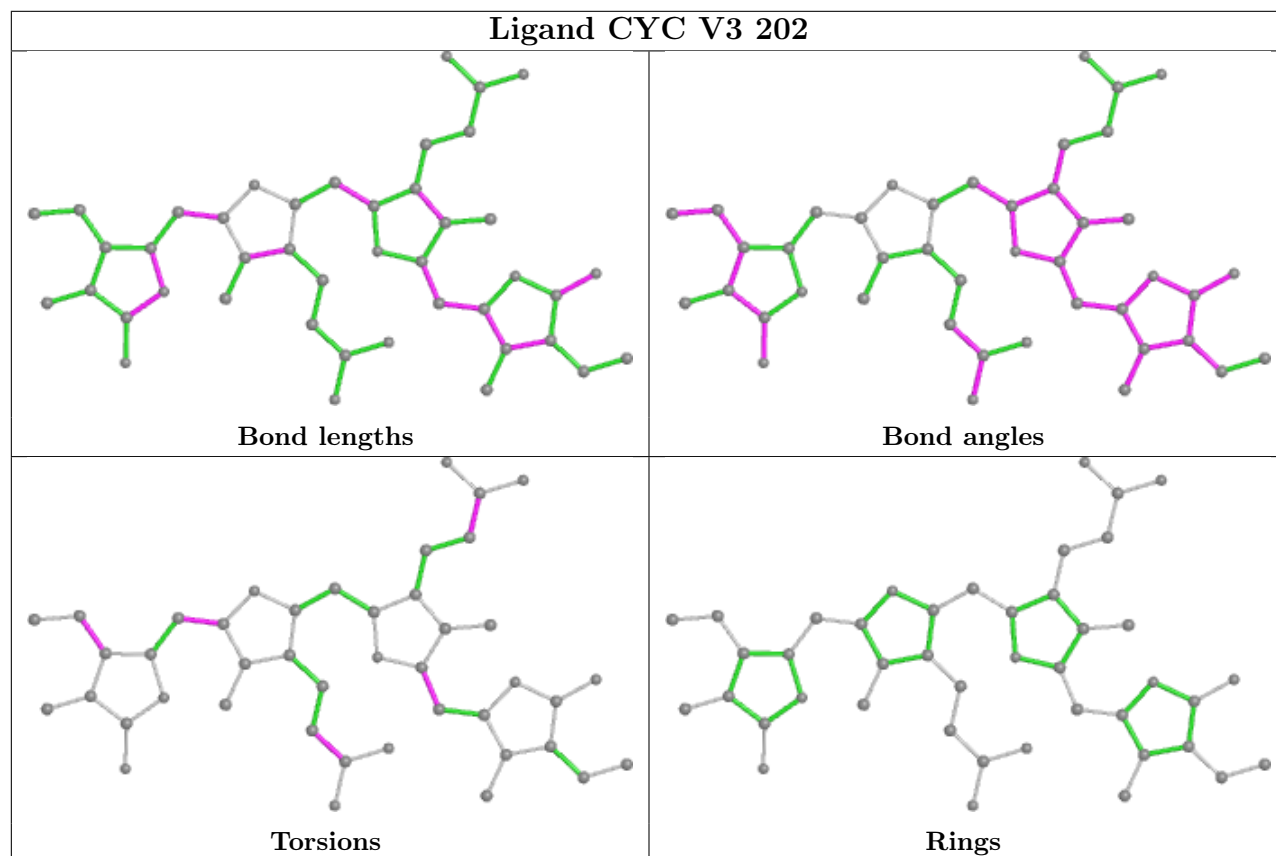


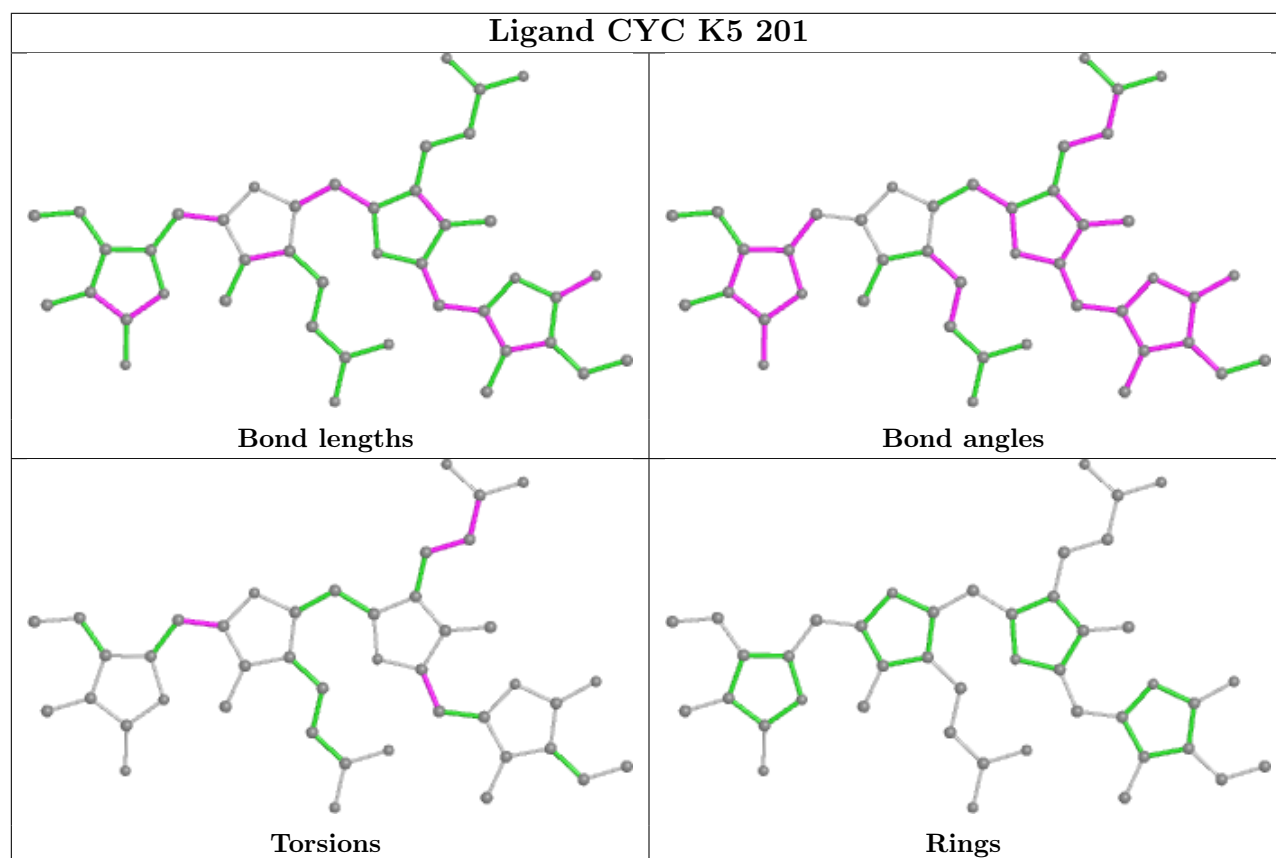
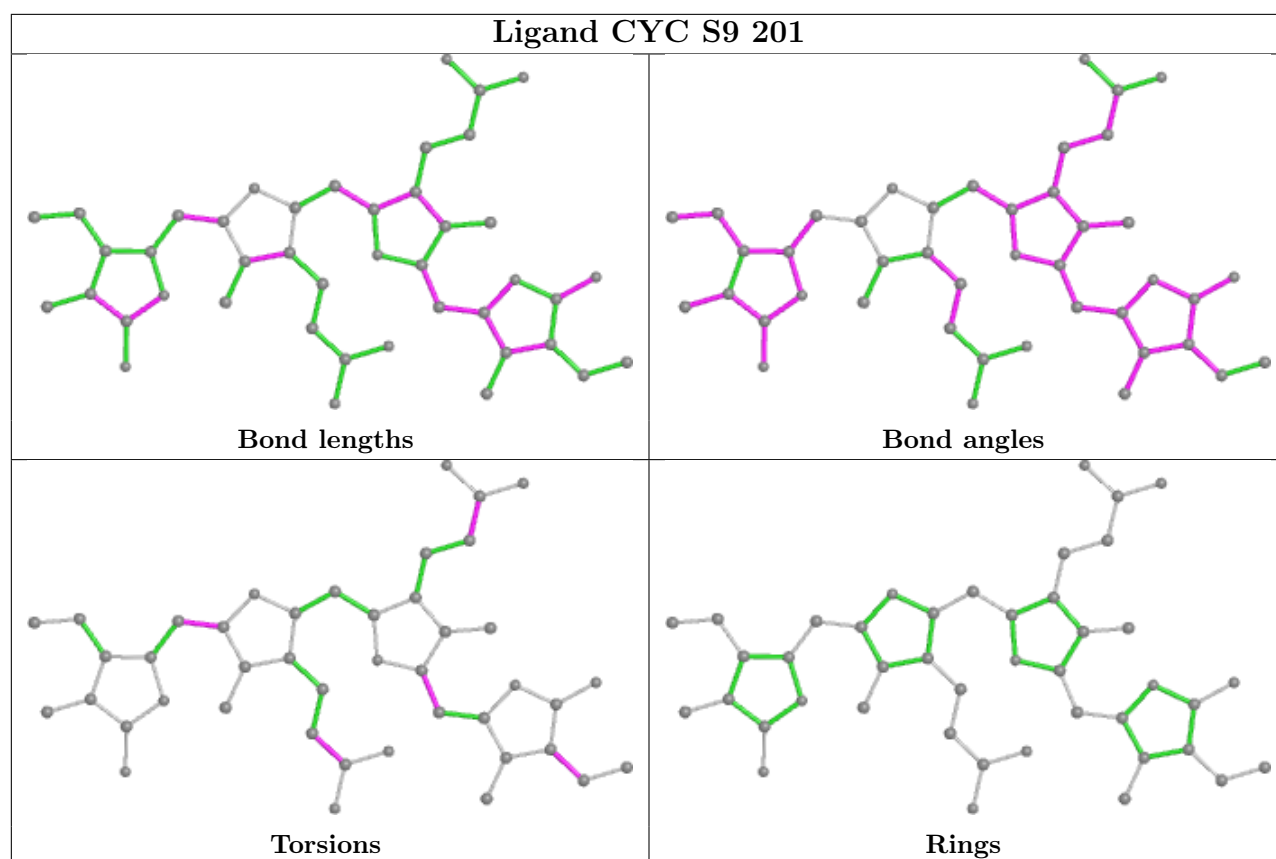


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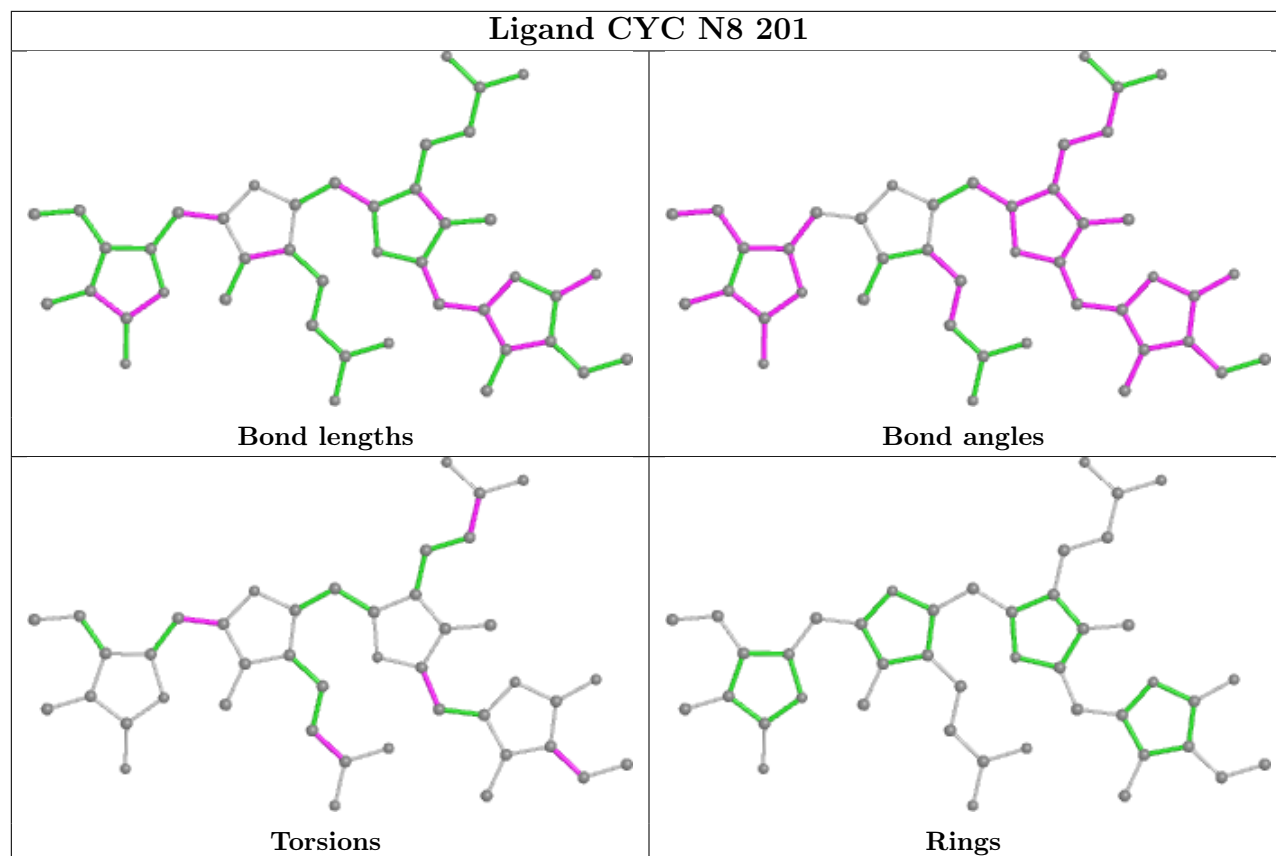


Ligand CYC V3 202

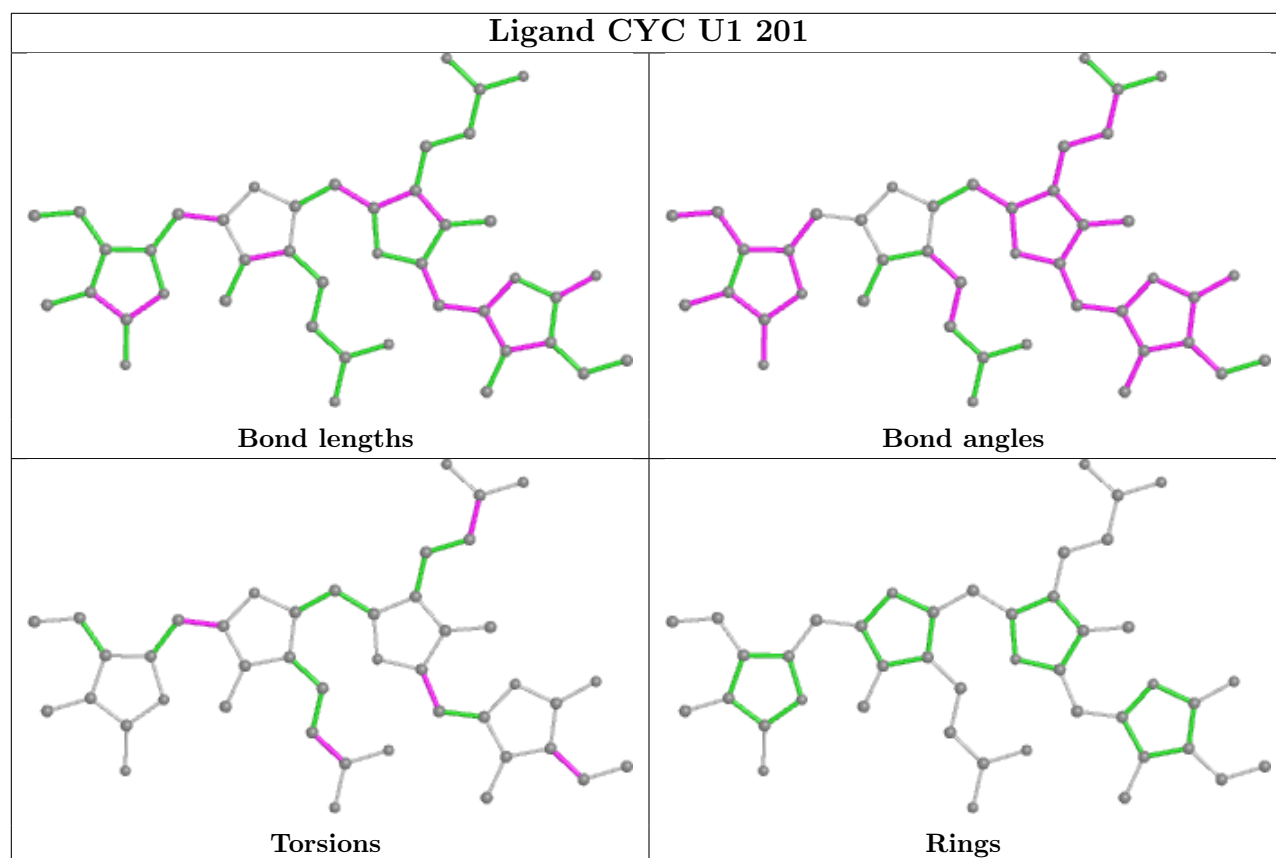




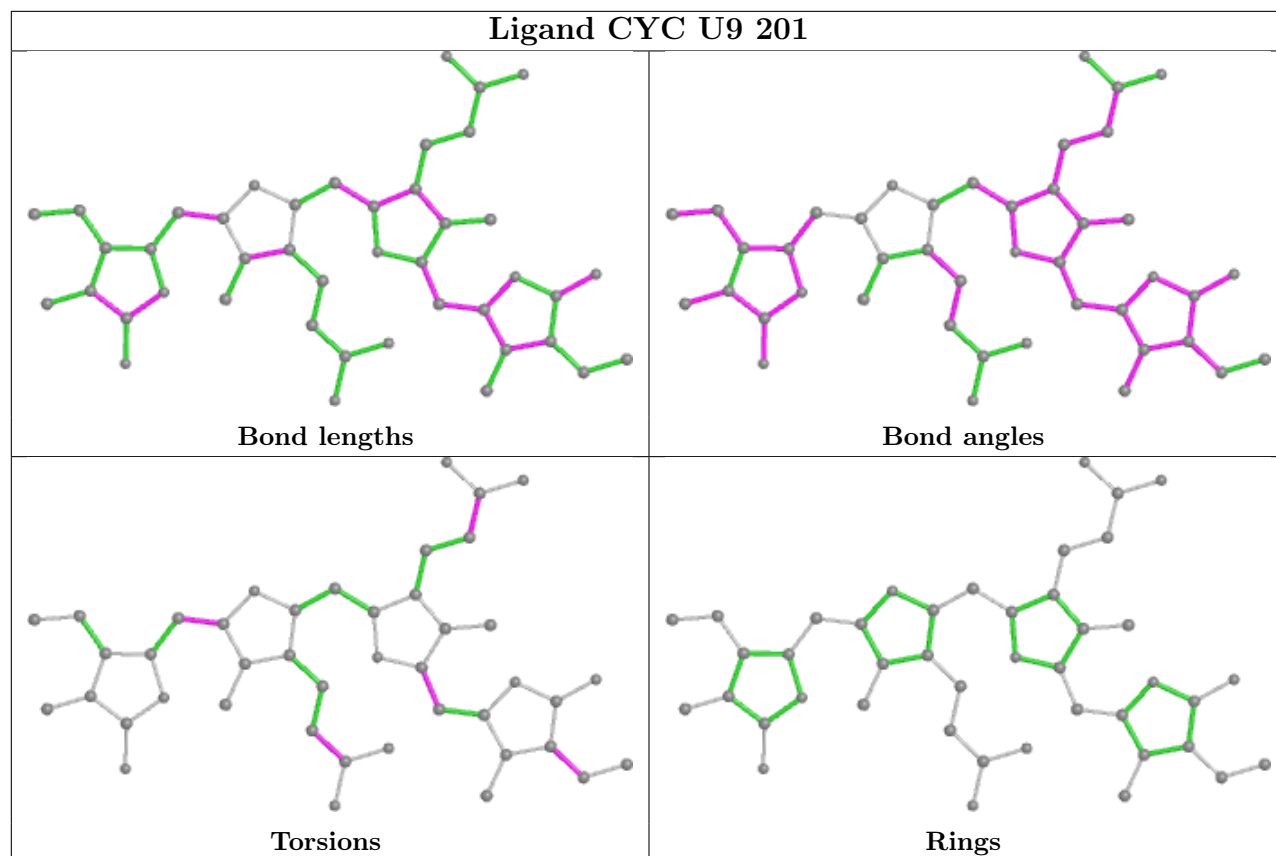
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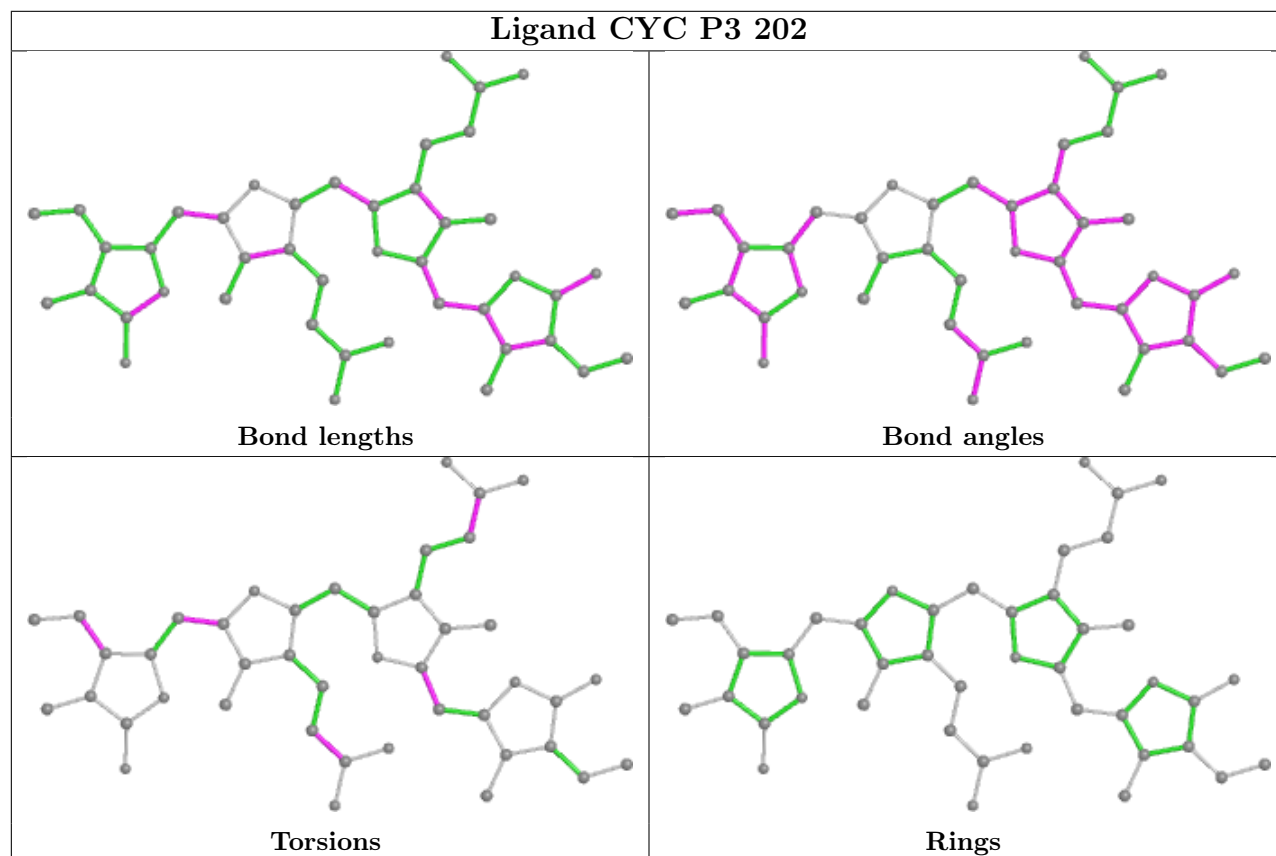
Ligand CYC U1 201



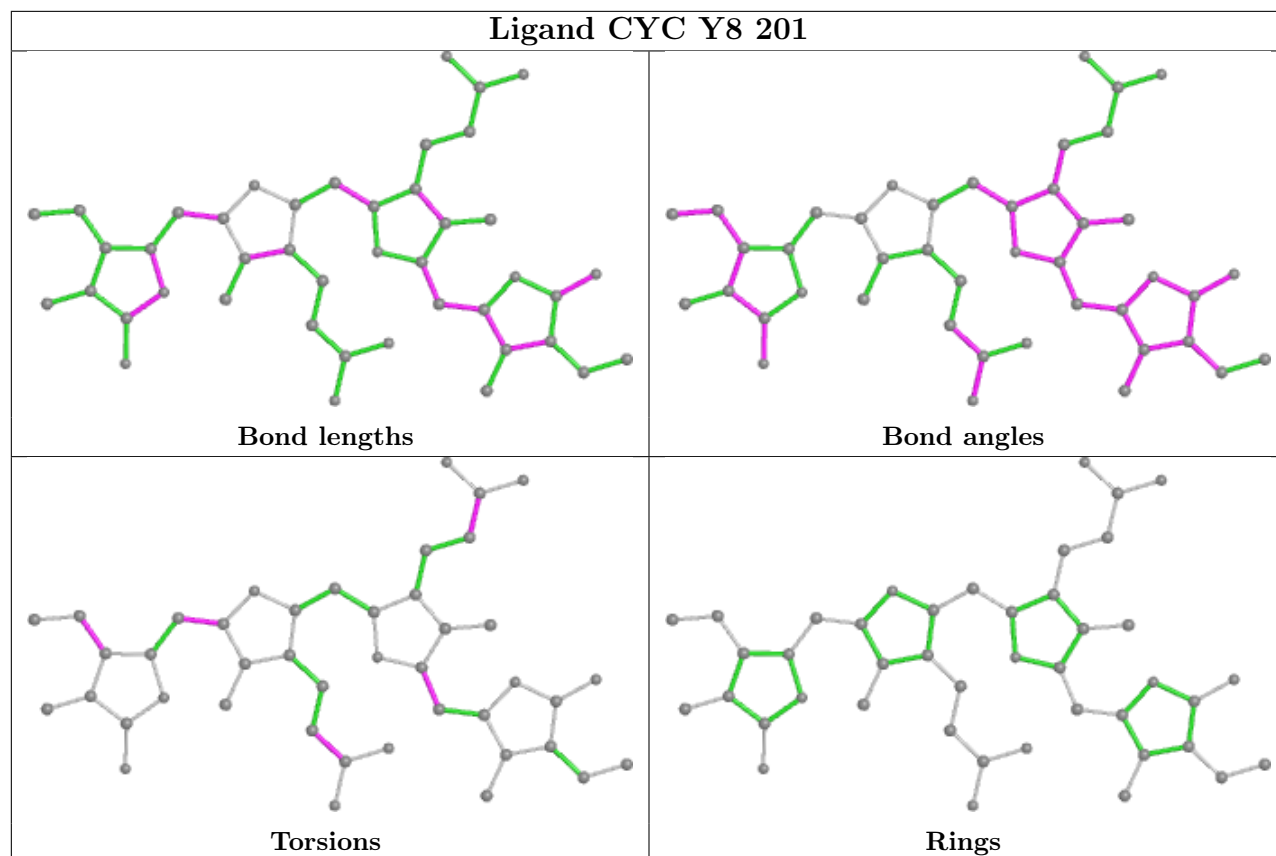
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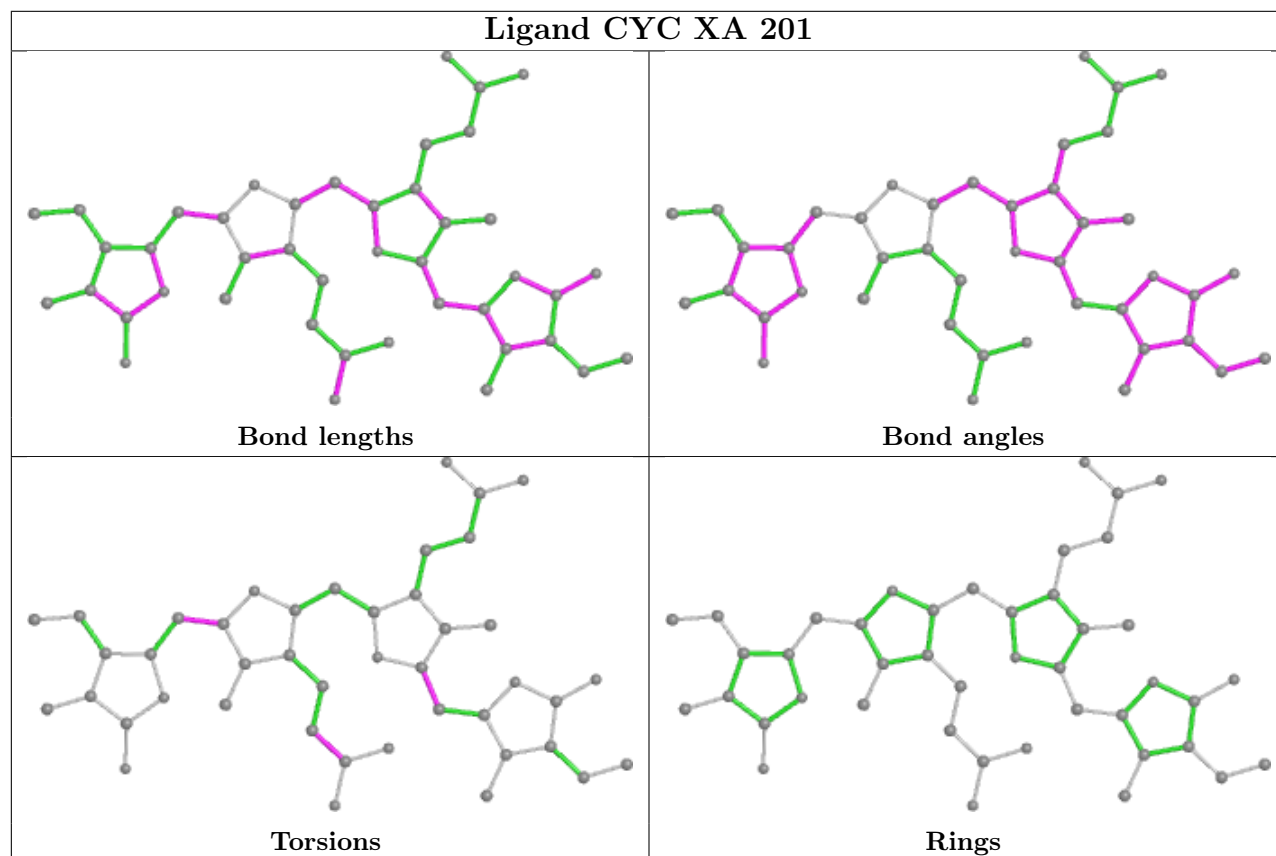
Ligand CYC P3 202



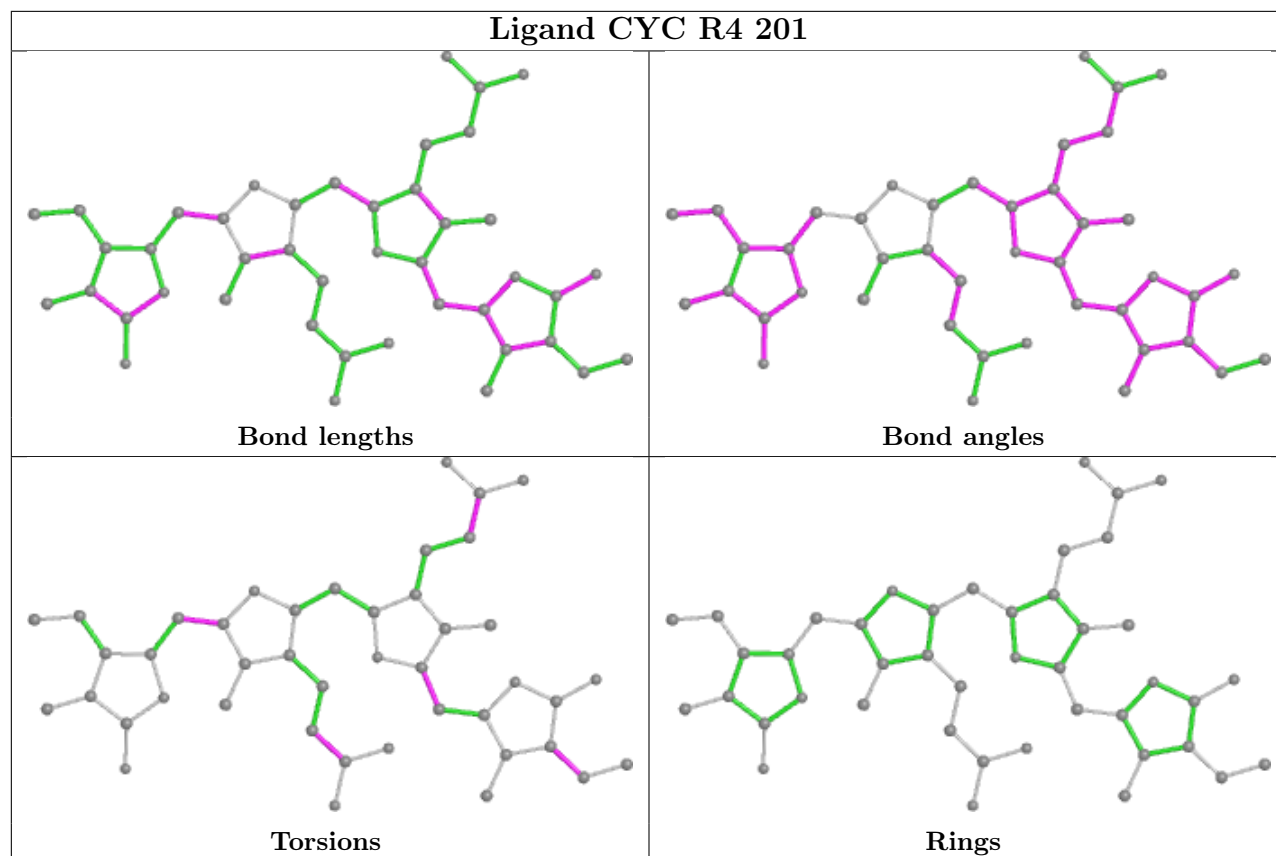
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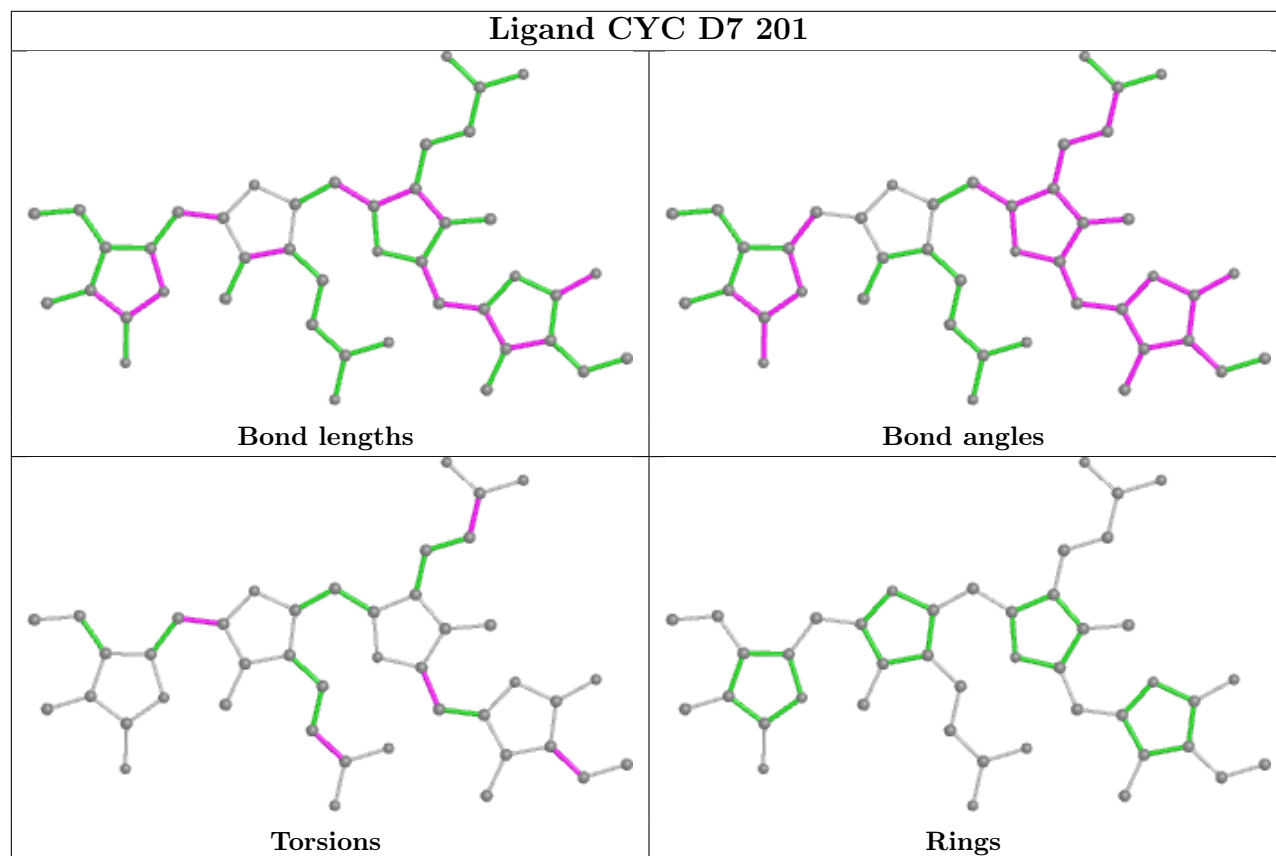
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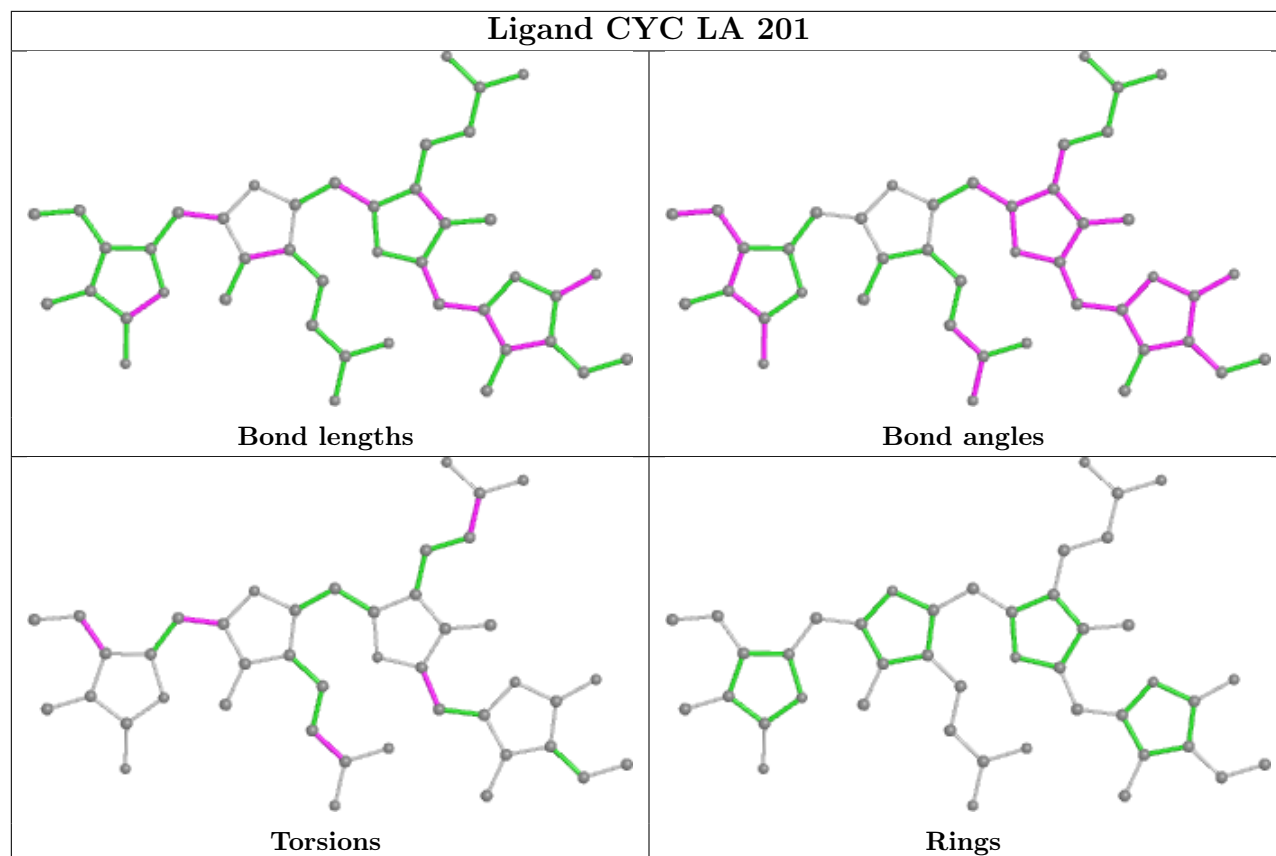
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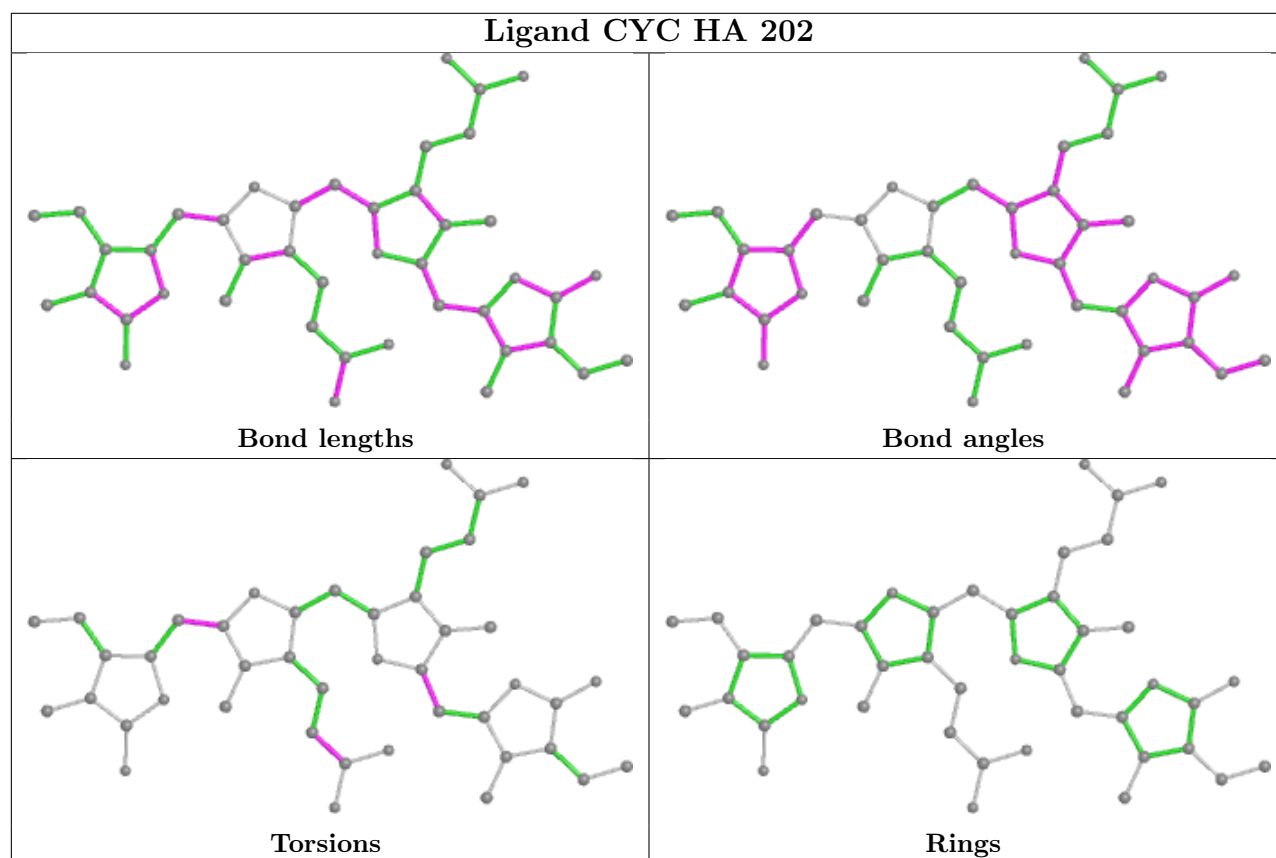
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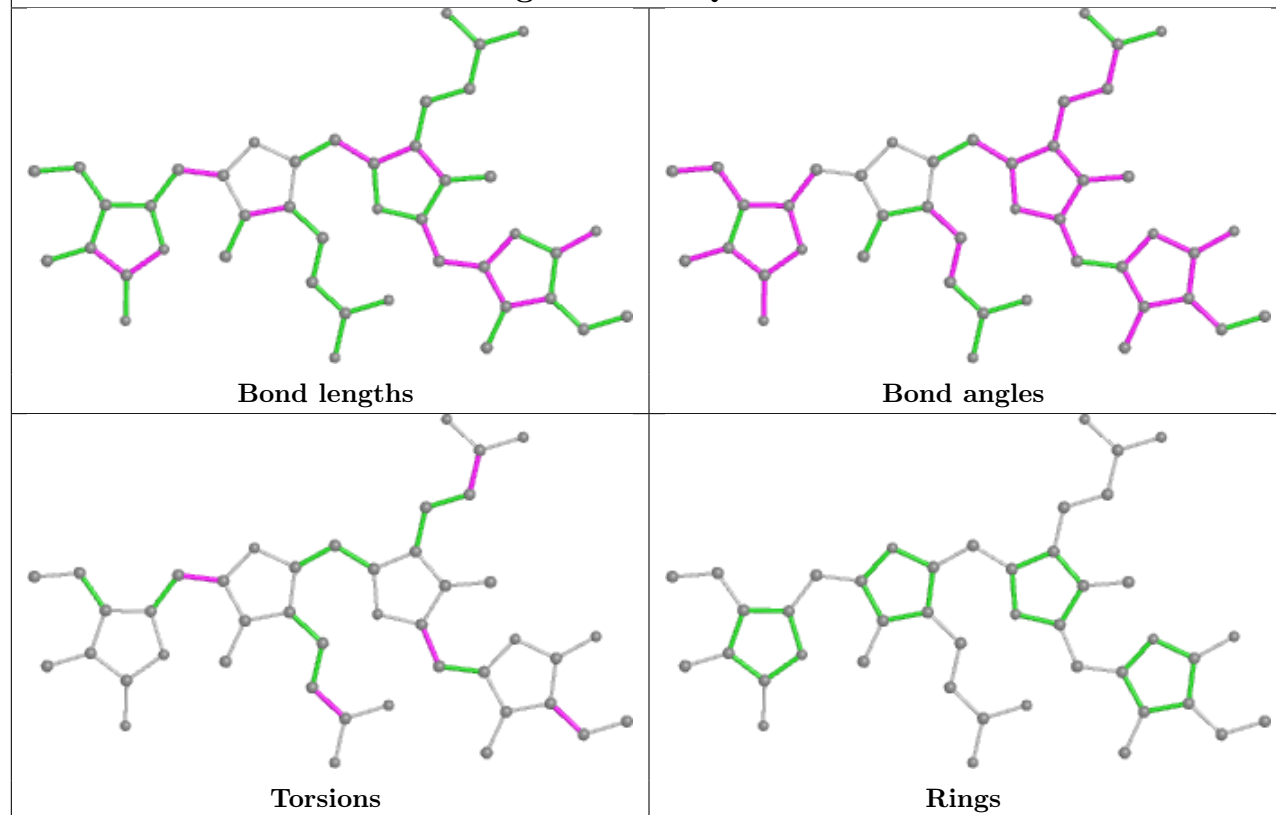
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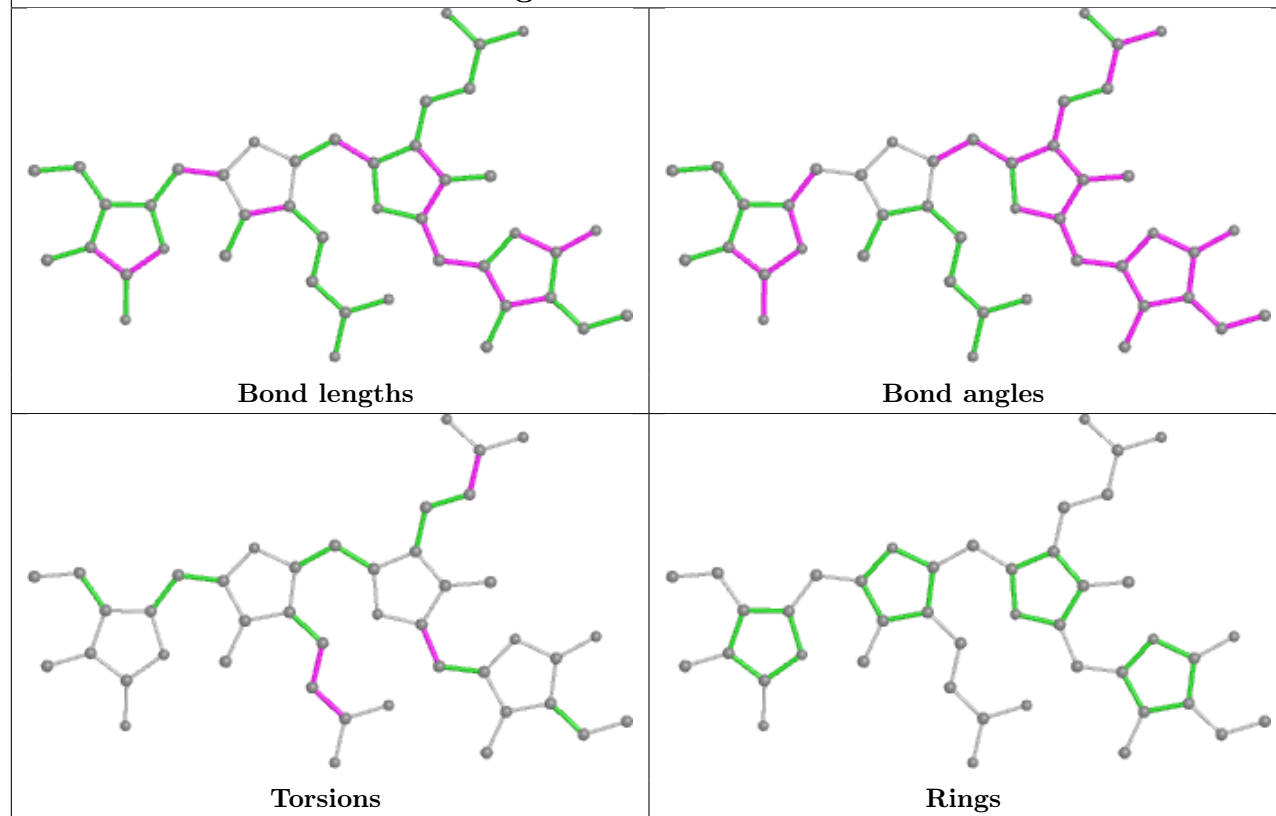
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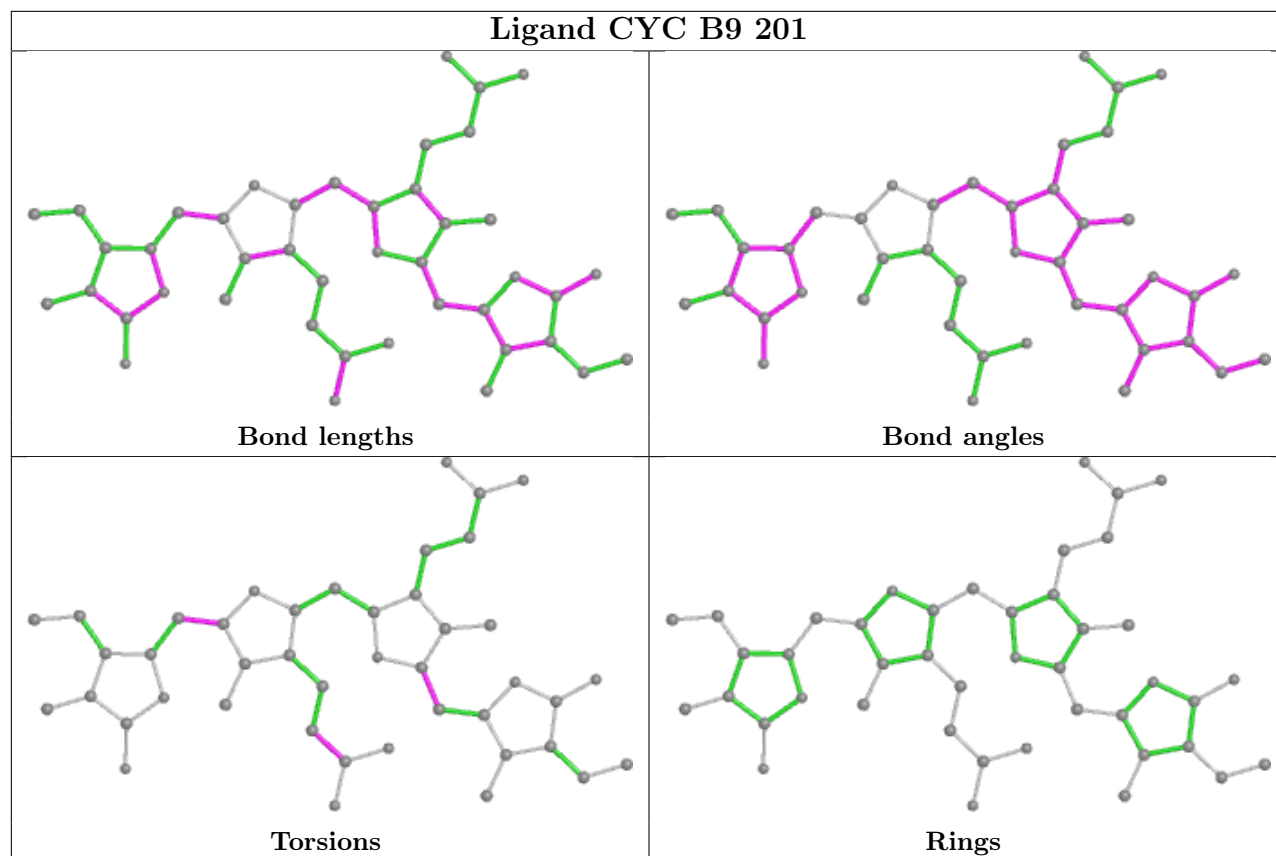
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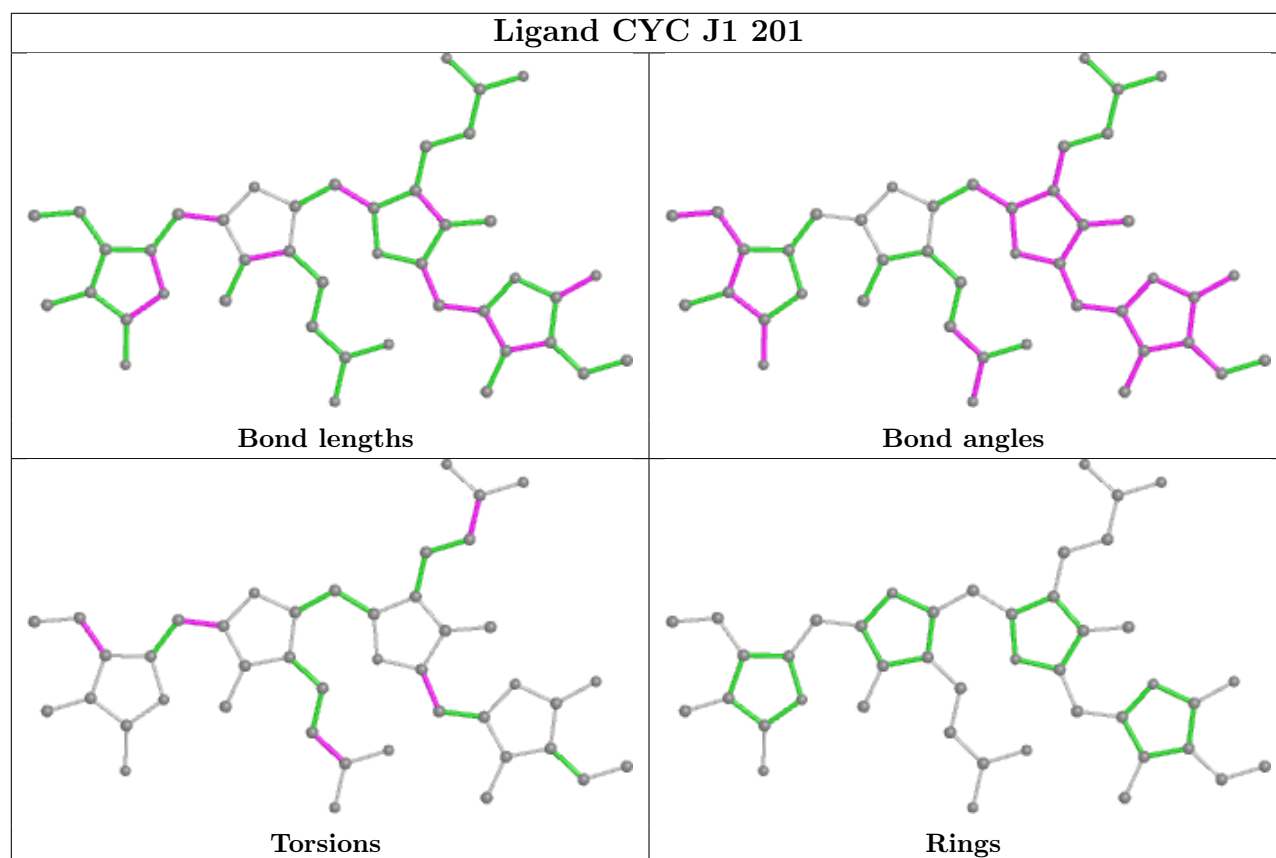
Ligand CYC k5 1201



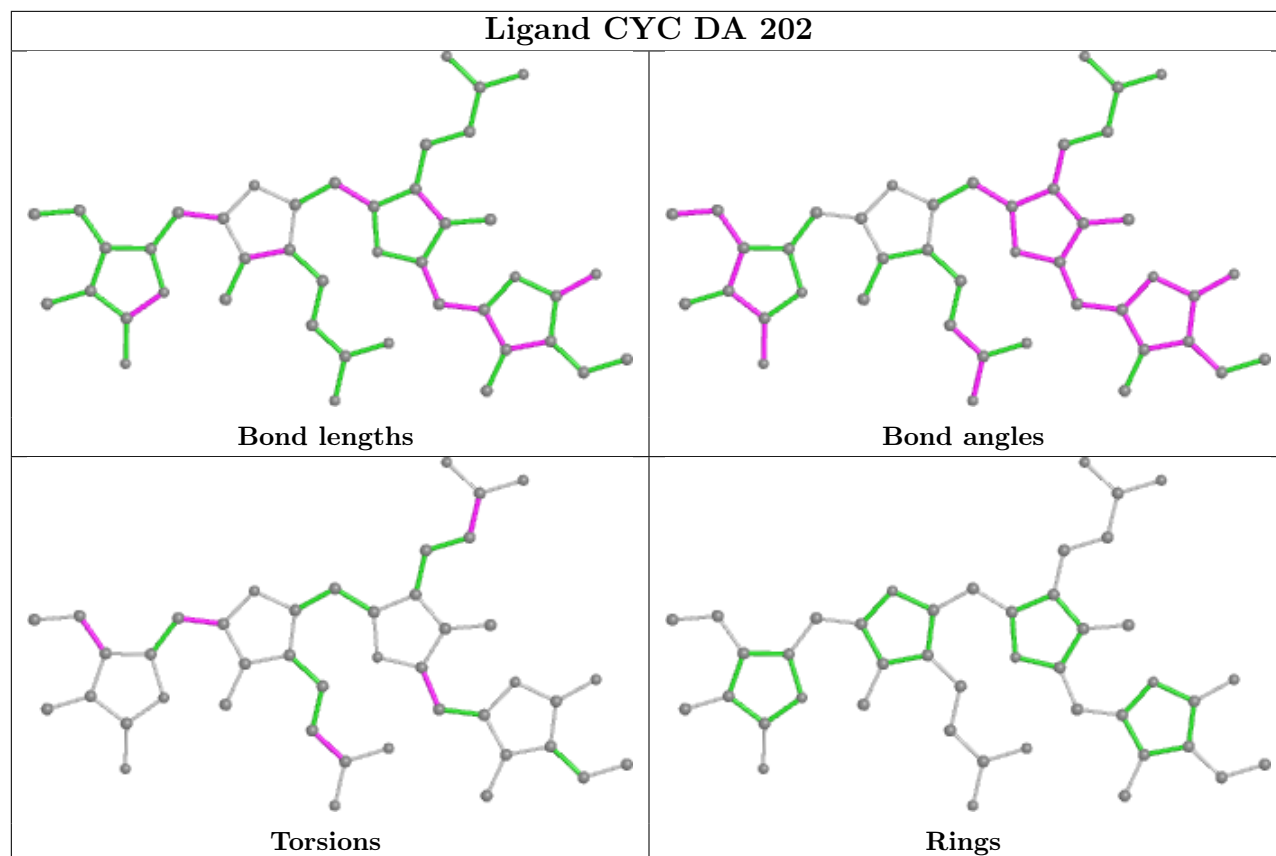
Ligand CYC B9 201



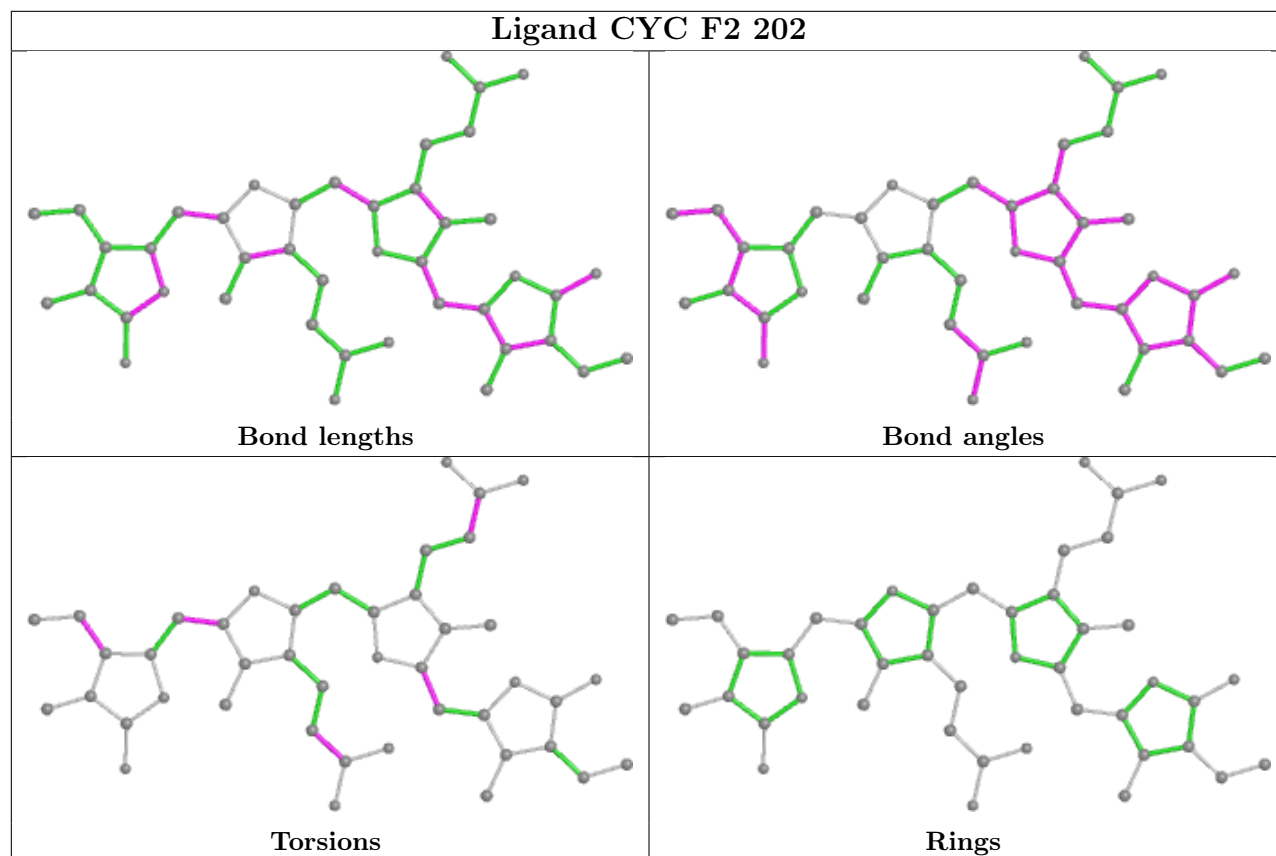
Ligand CYC J1 201



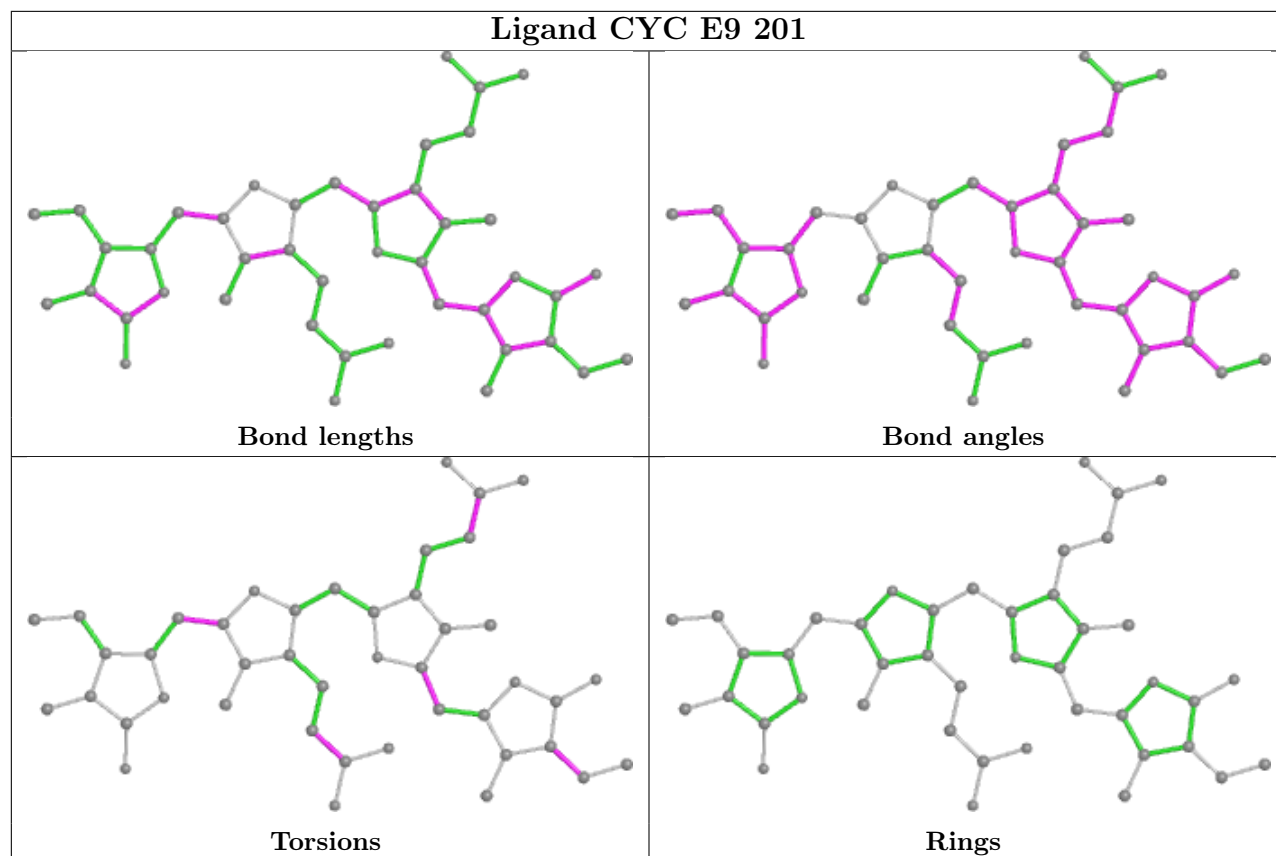
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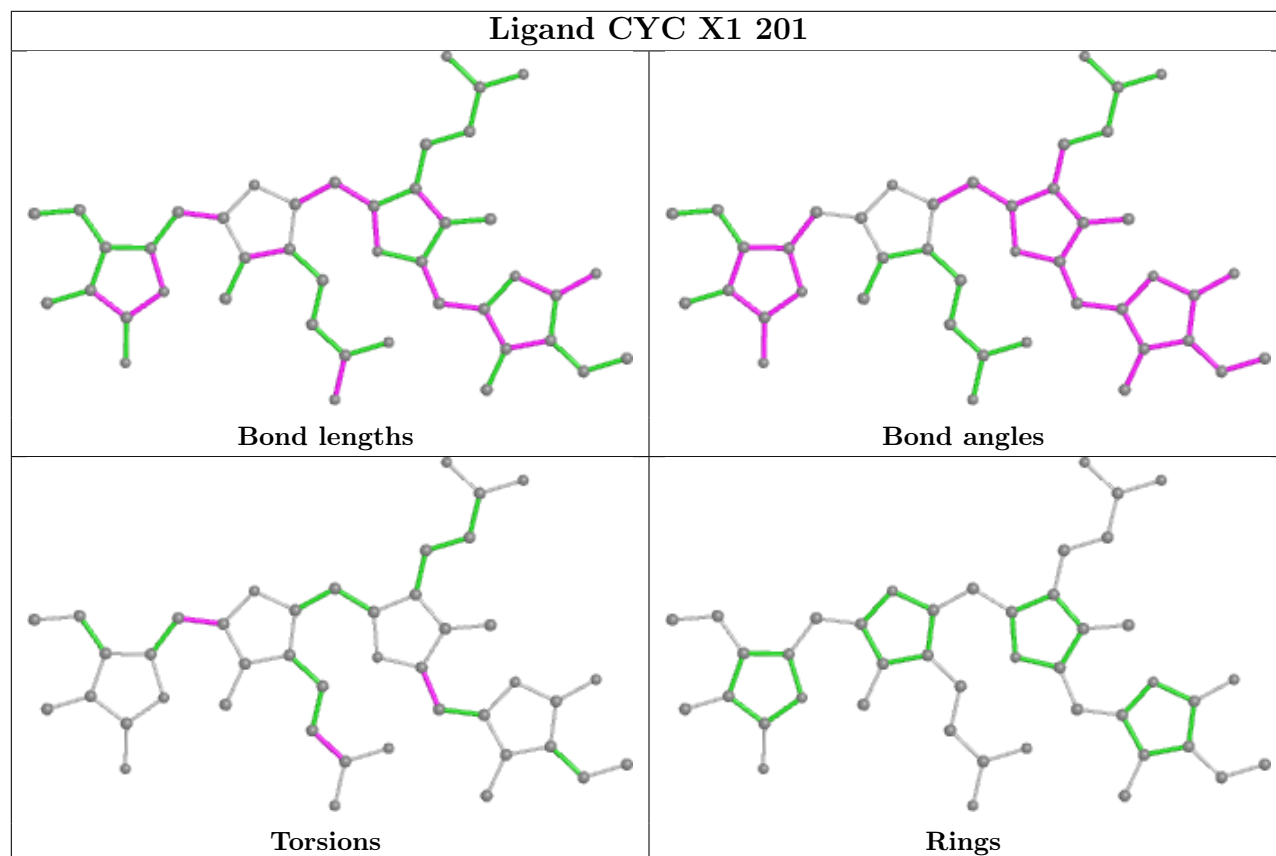
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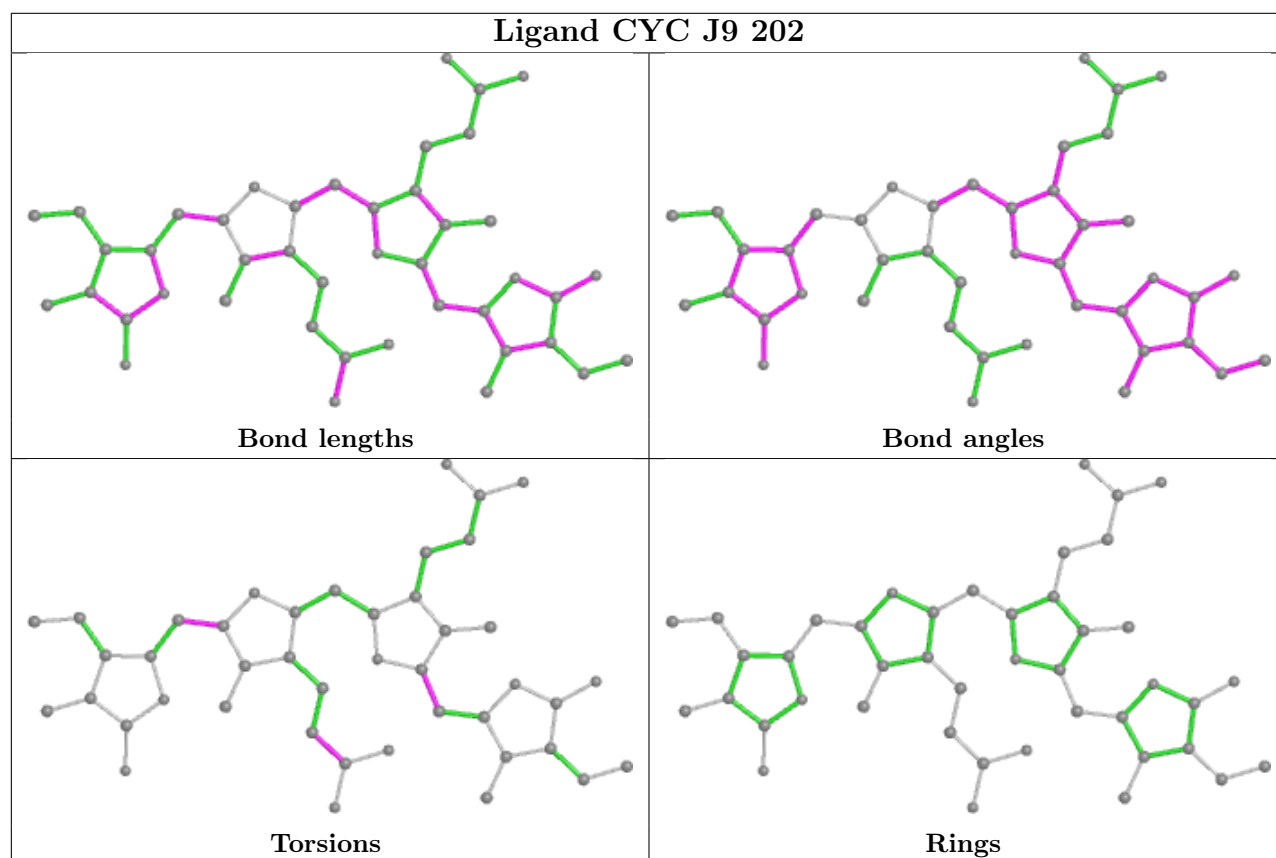
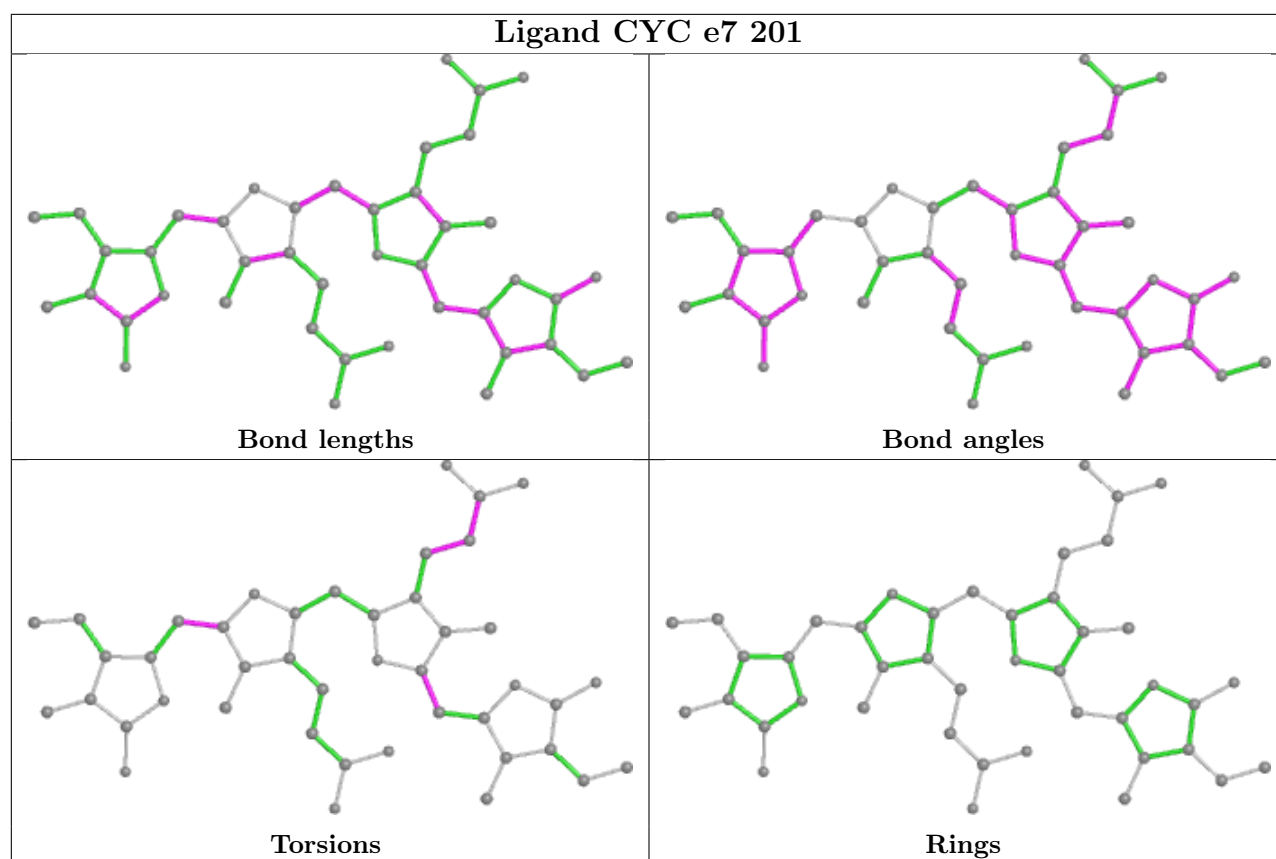


Ligand CYC E9 201

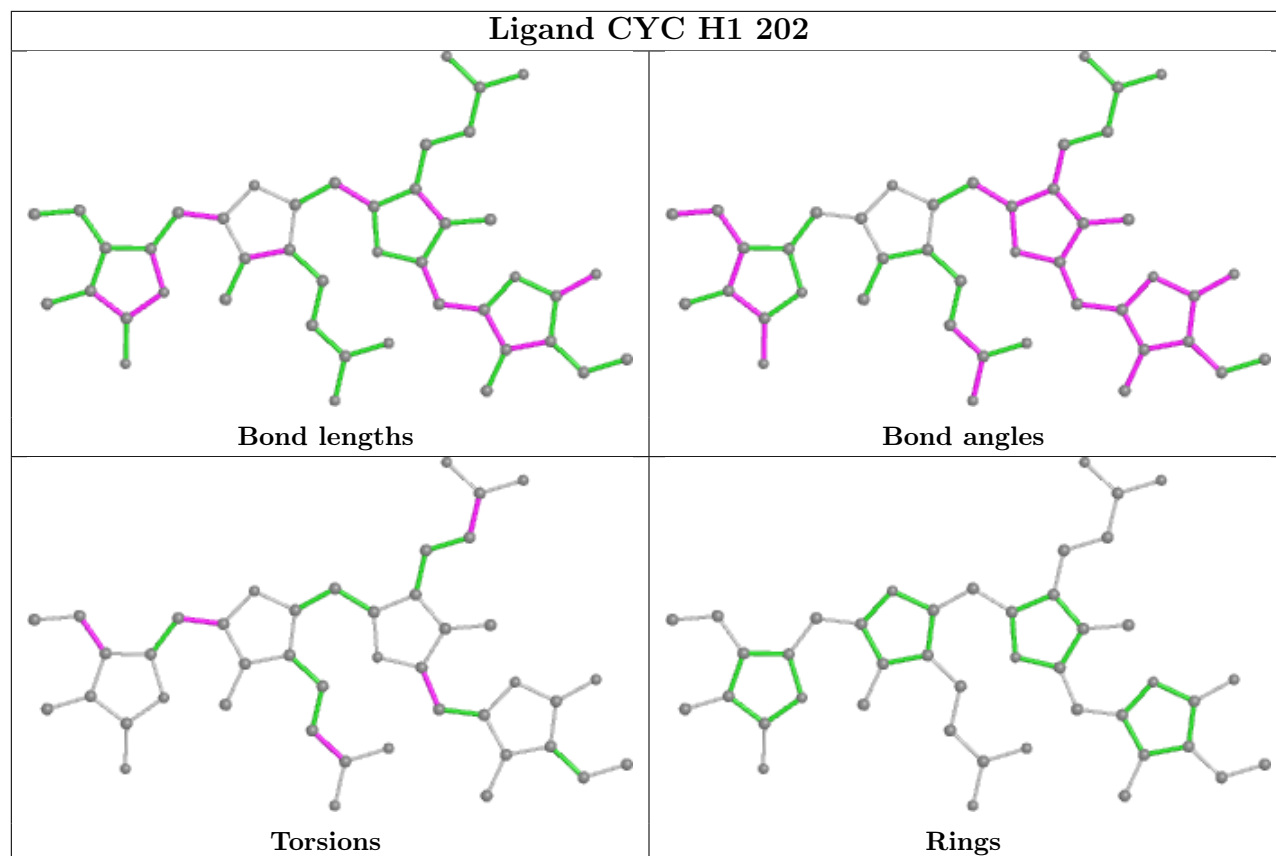


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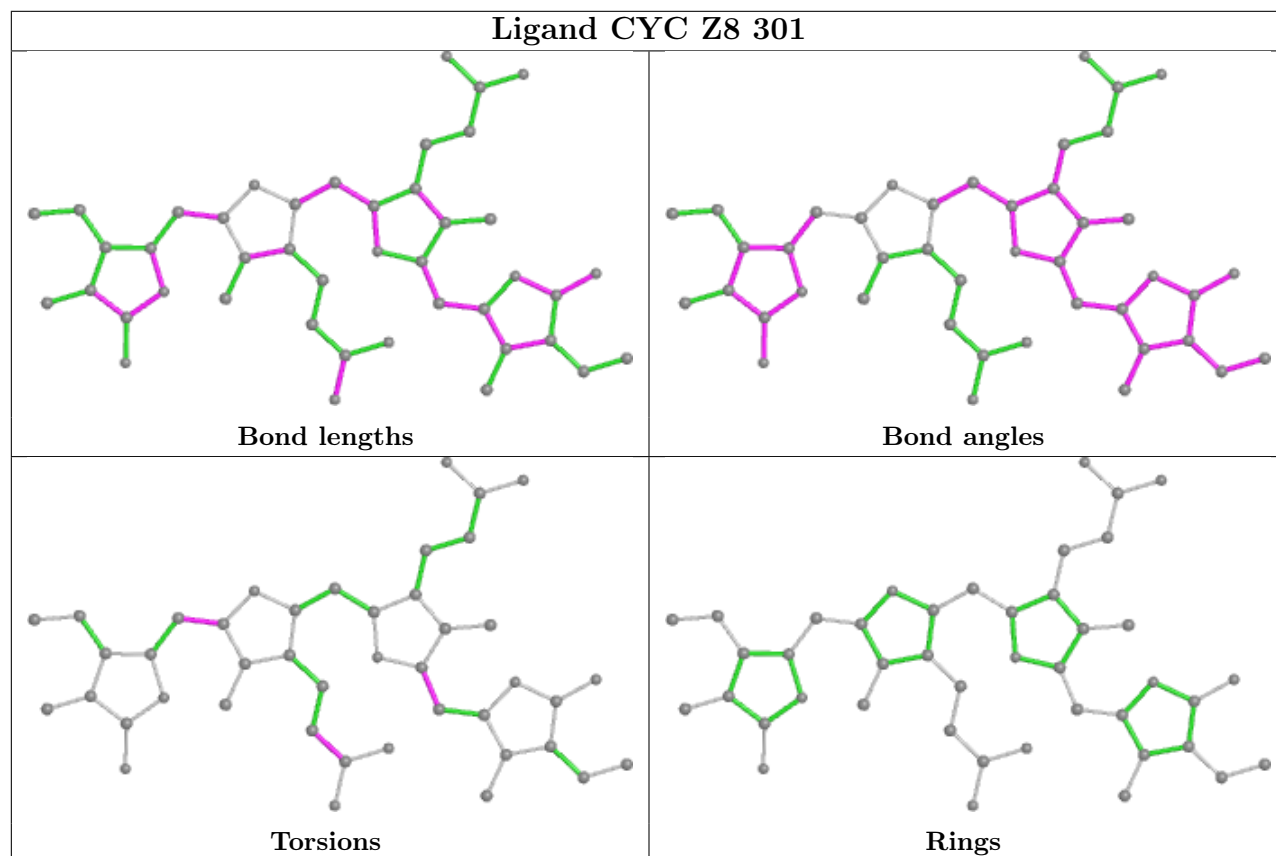


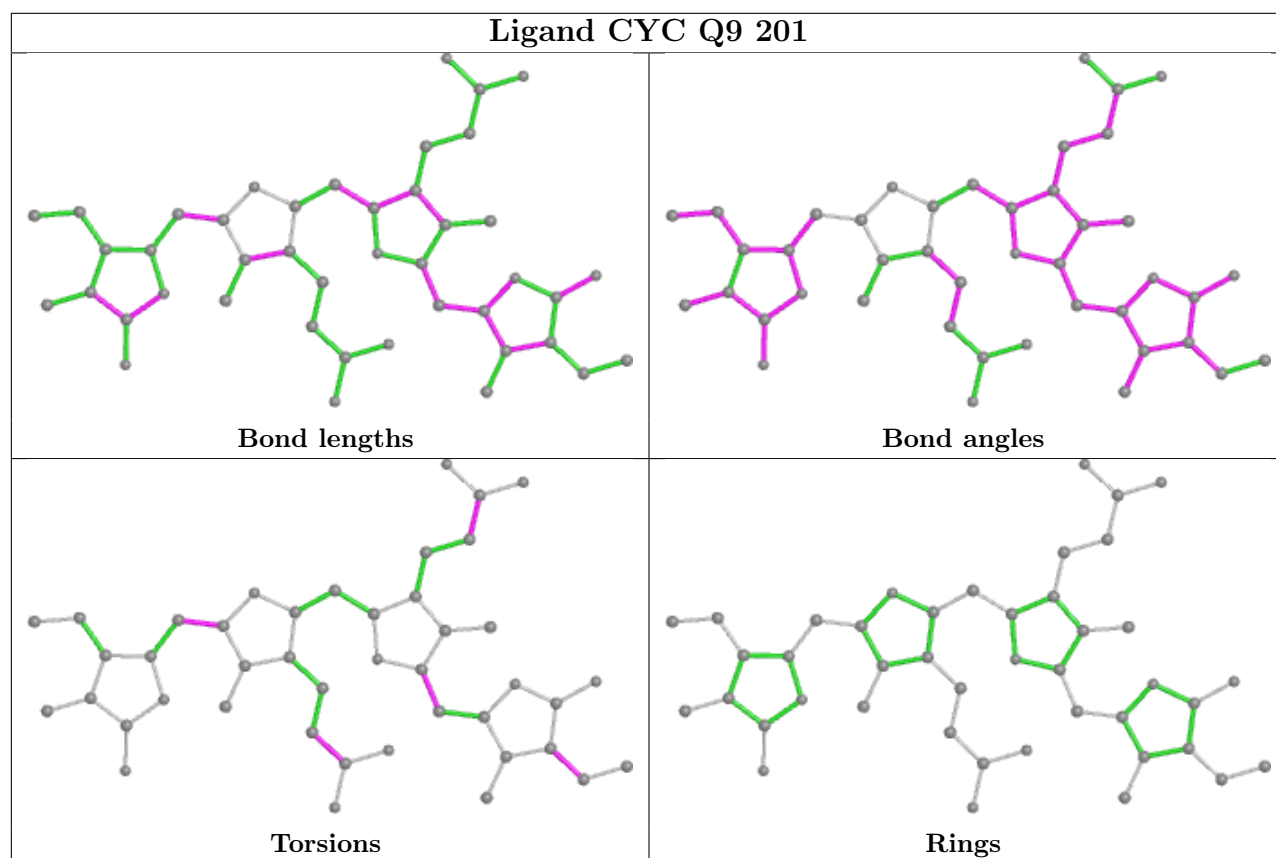
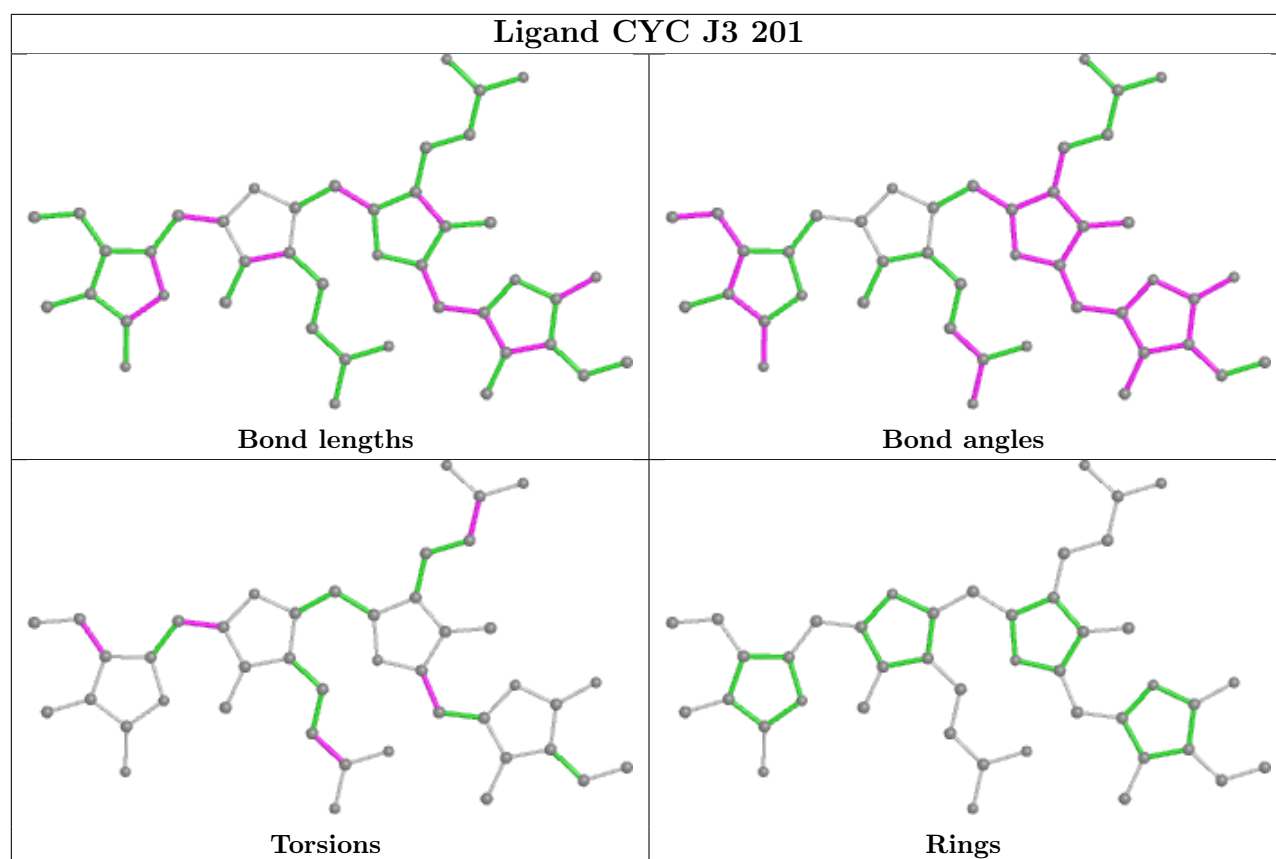


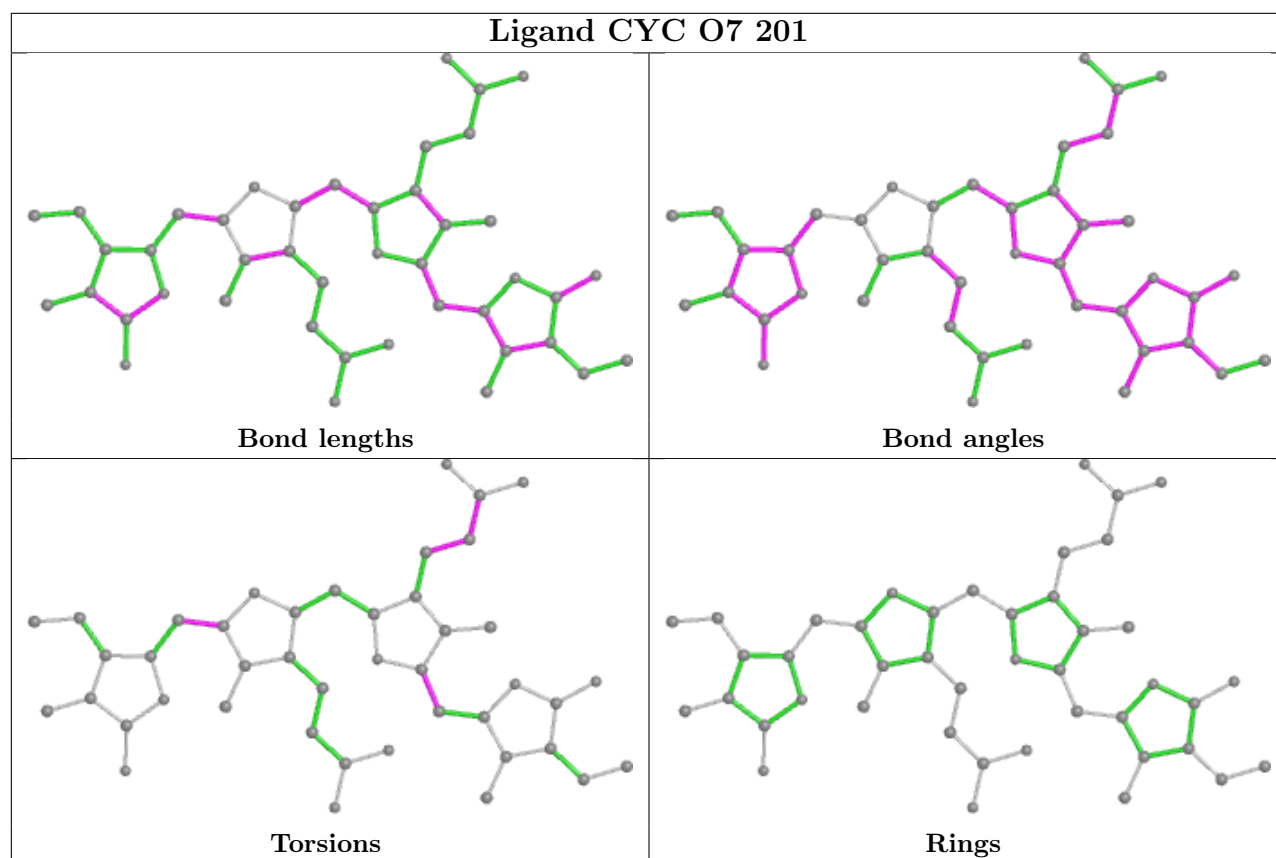
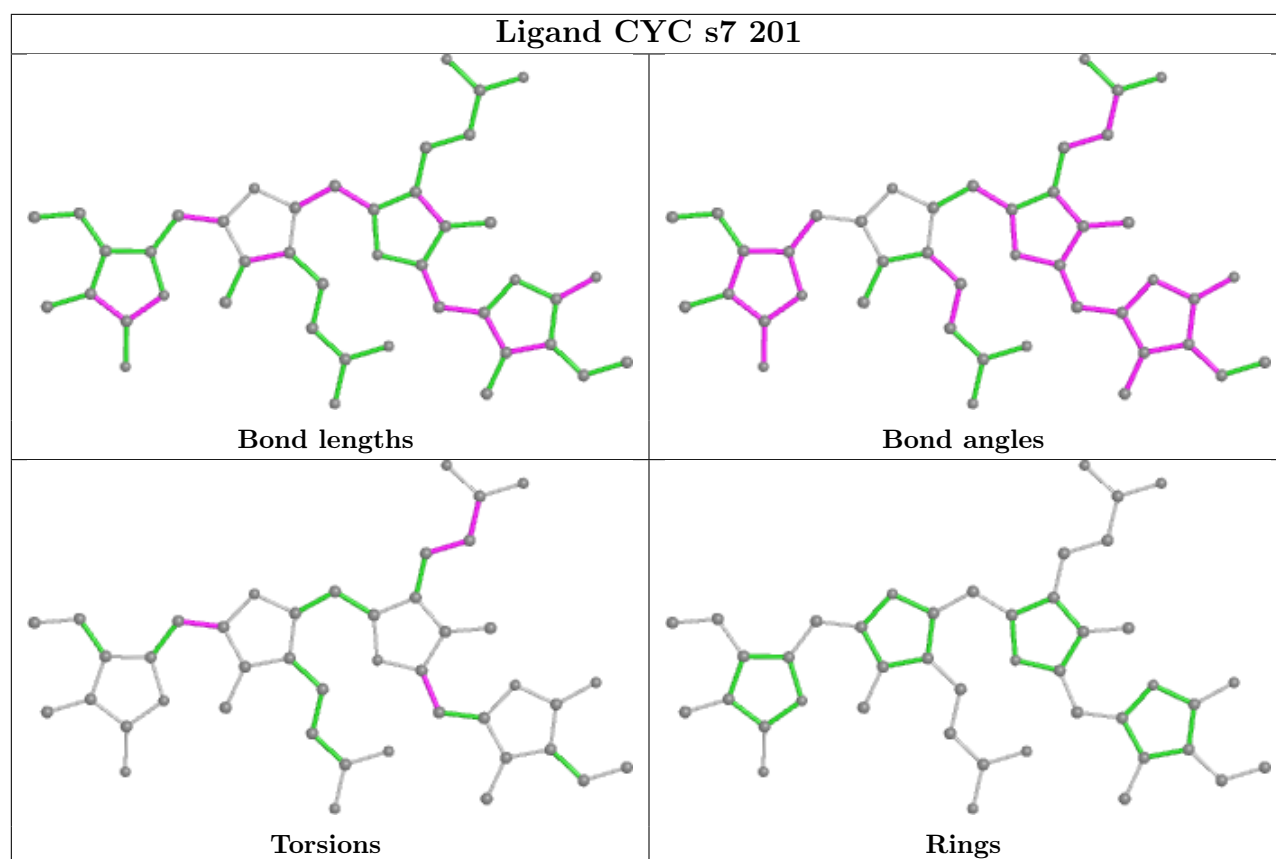
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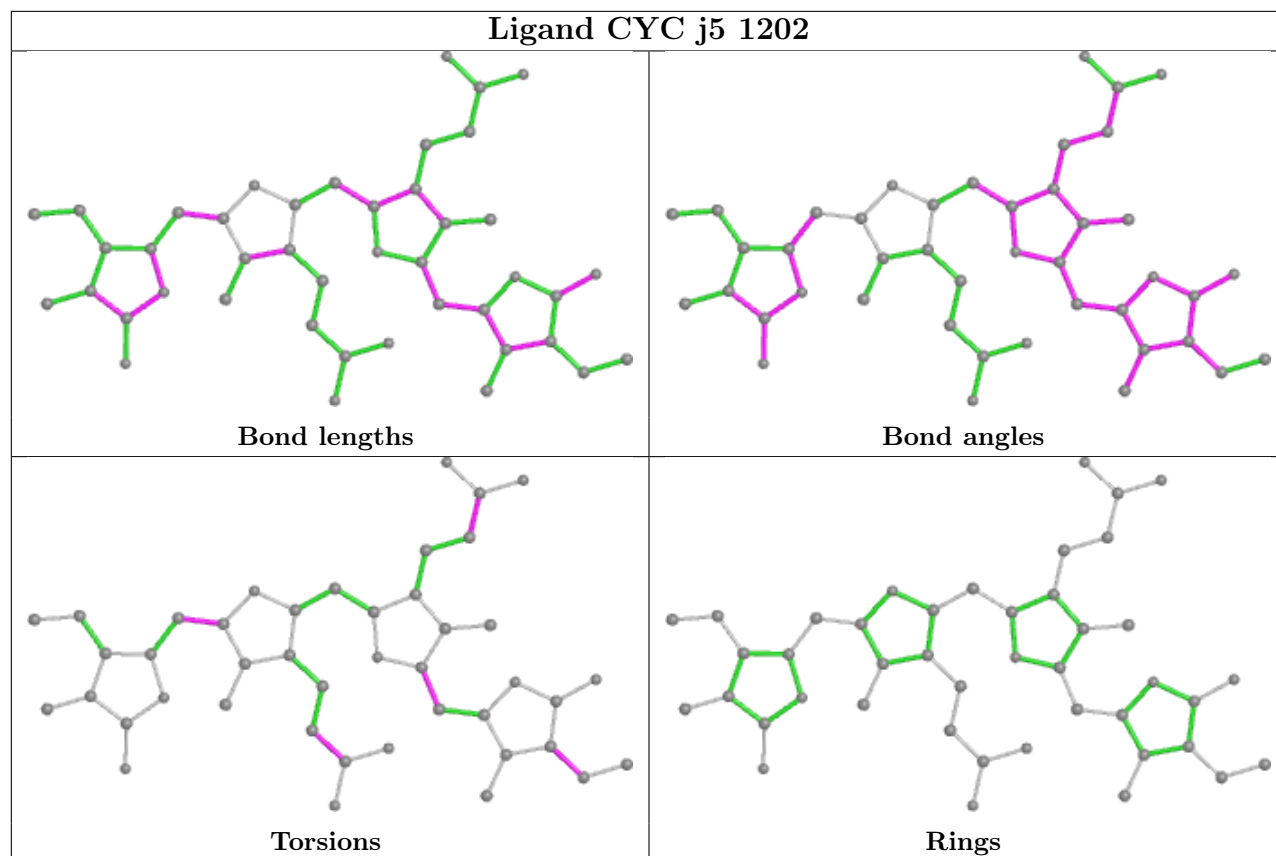
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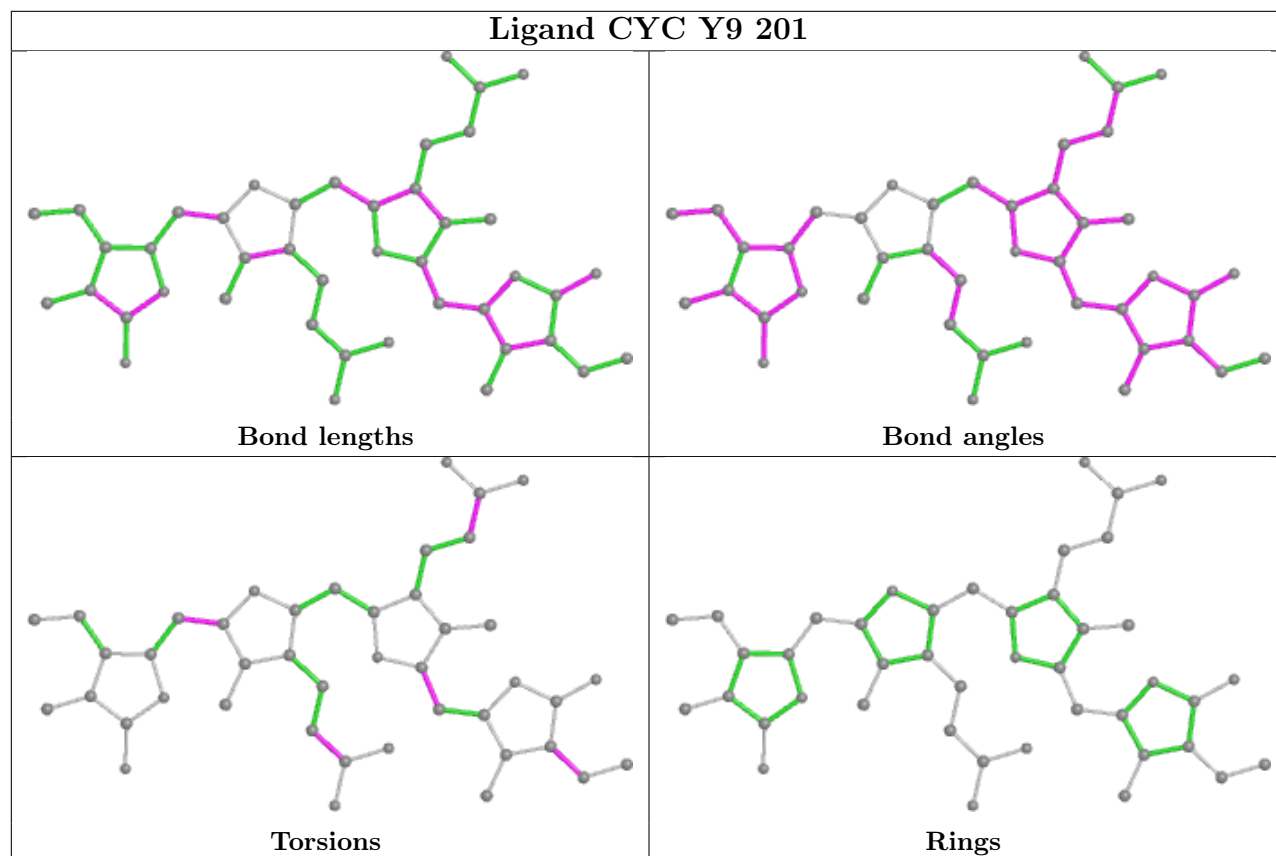




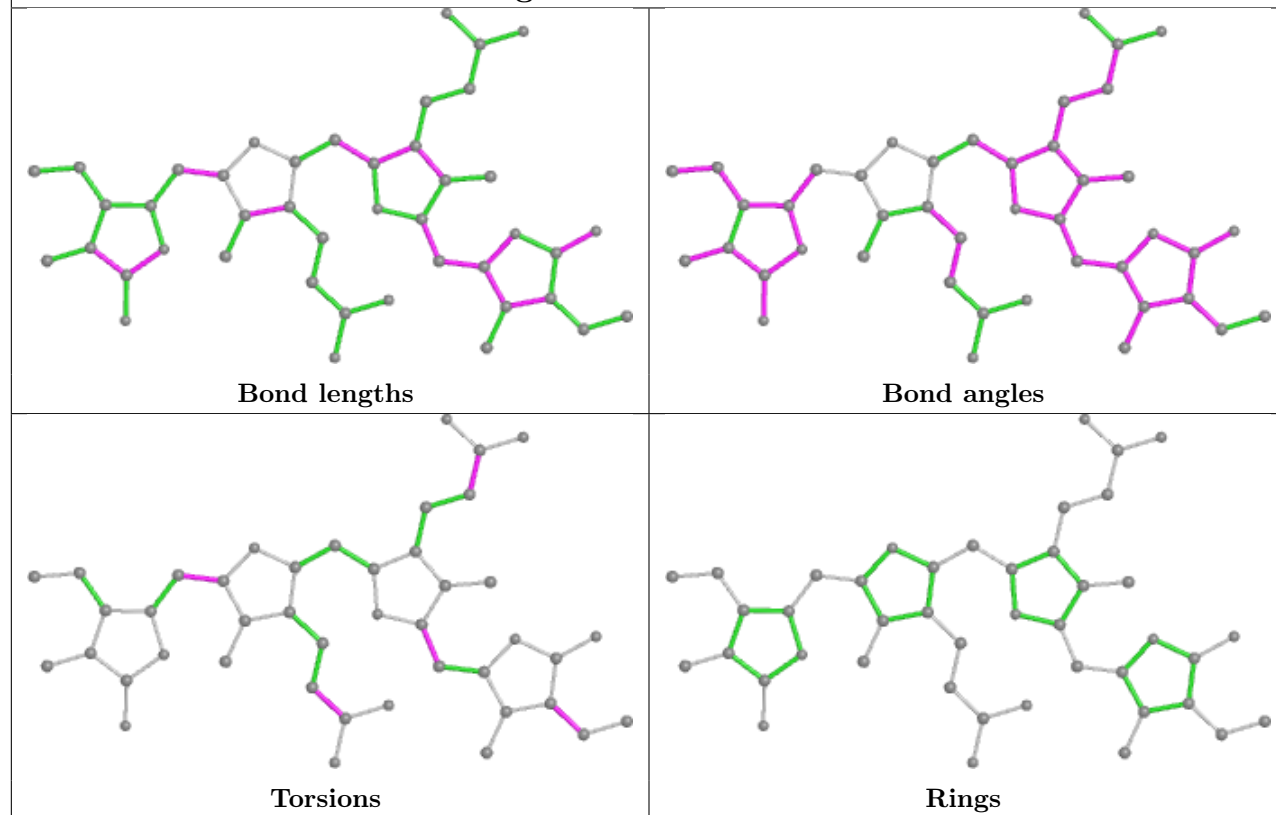
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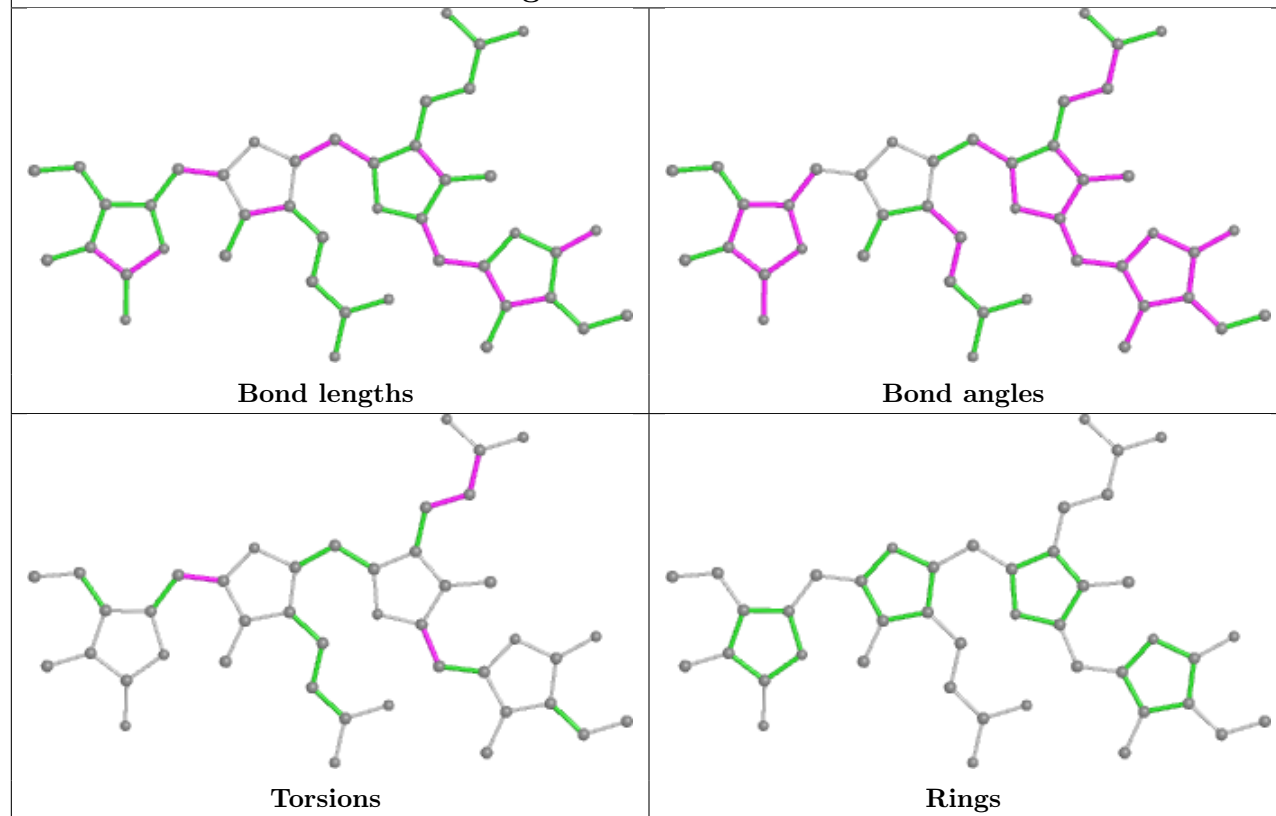
Ligand CYC Y9 201



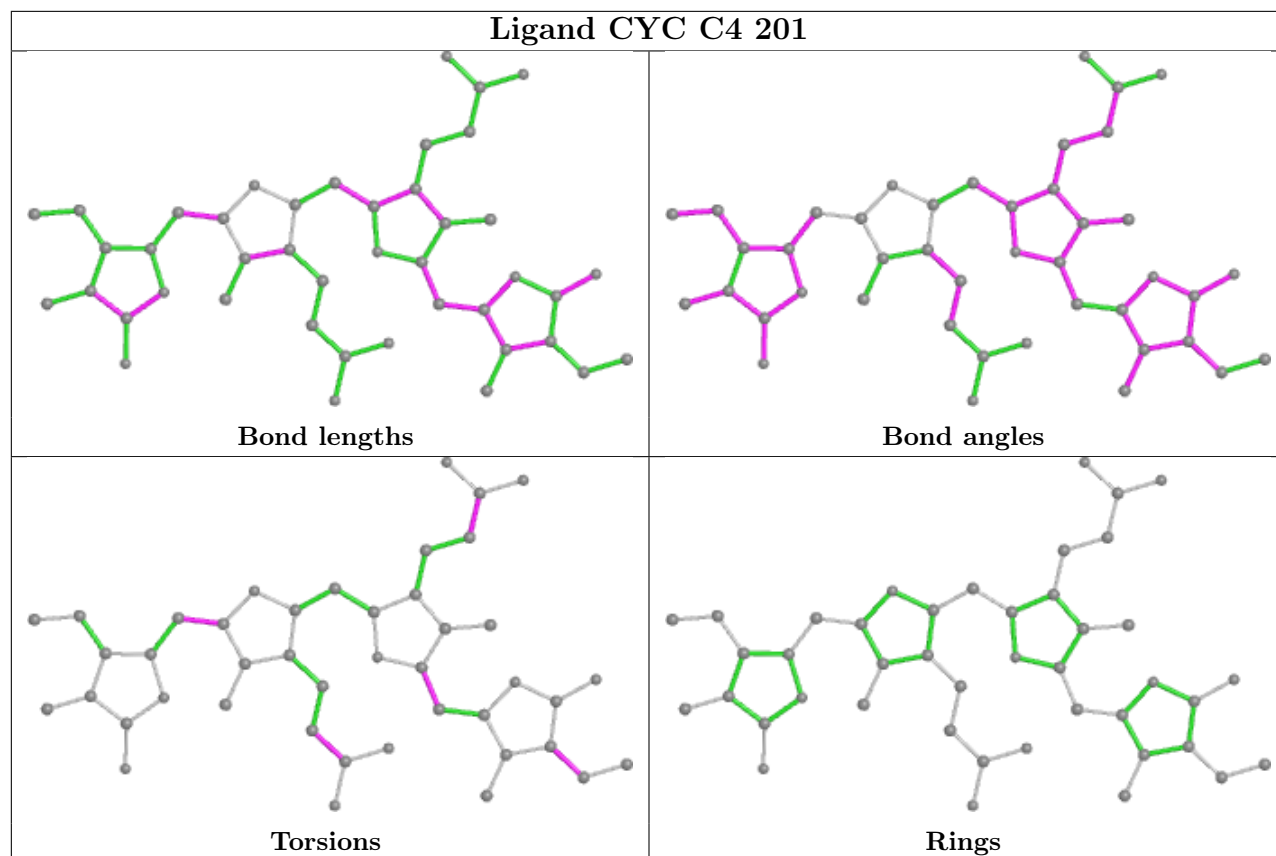
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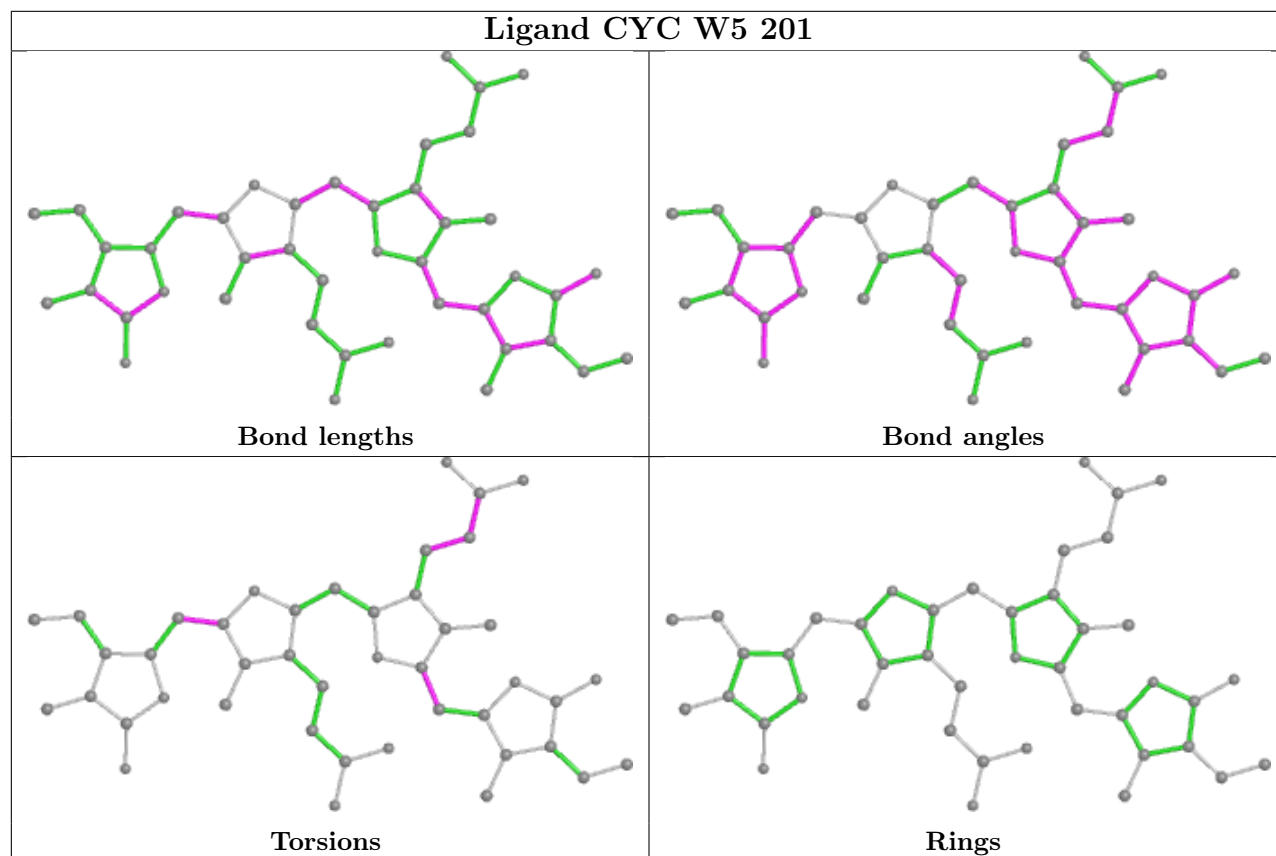
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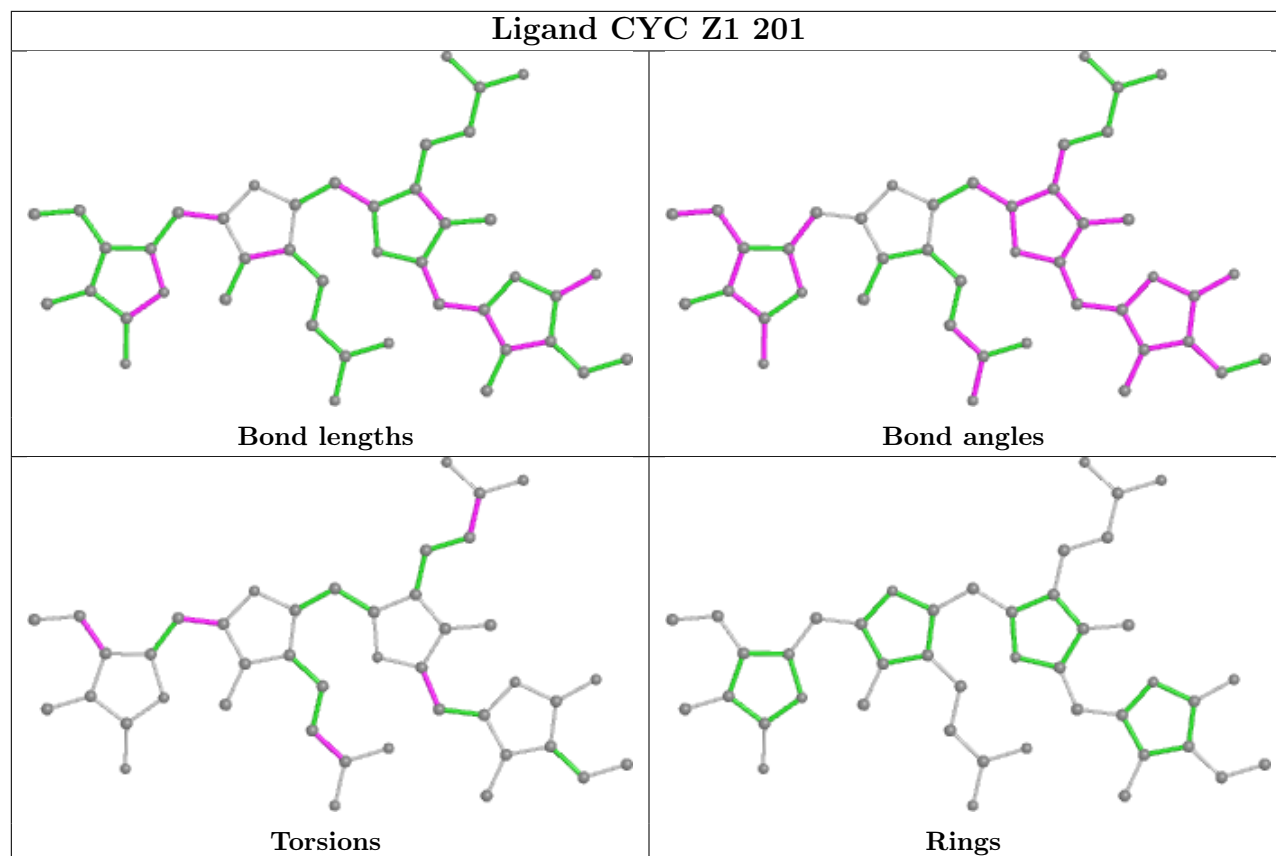
Ligand CYC C4 201



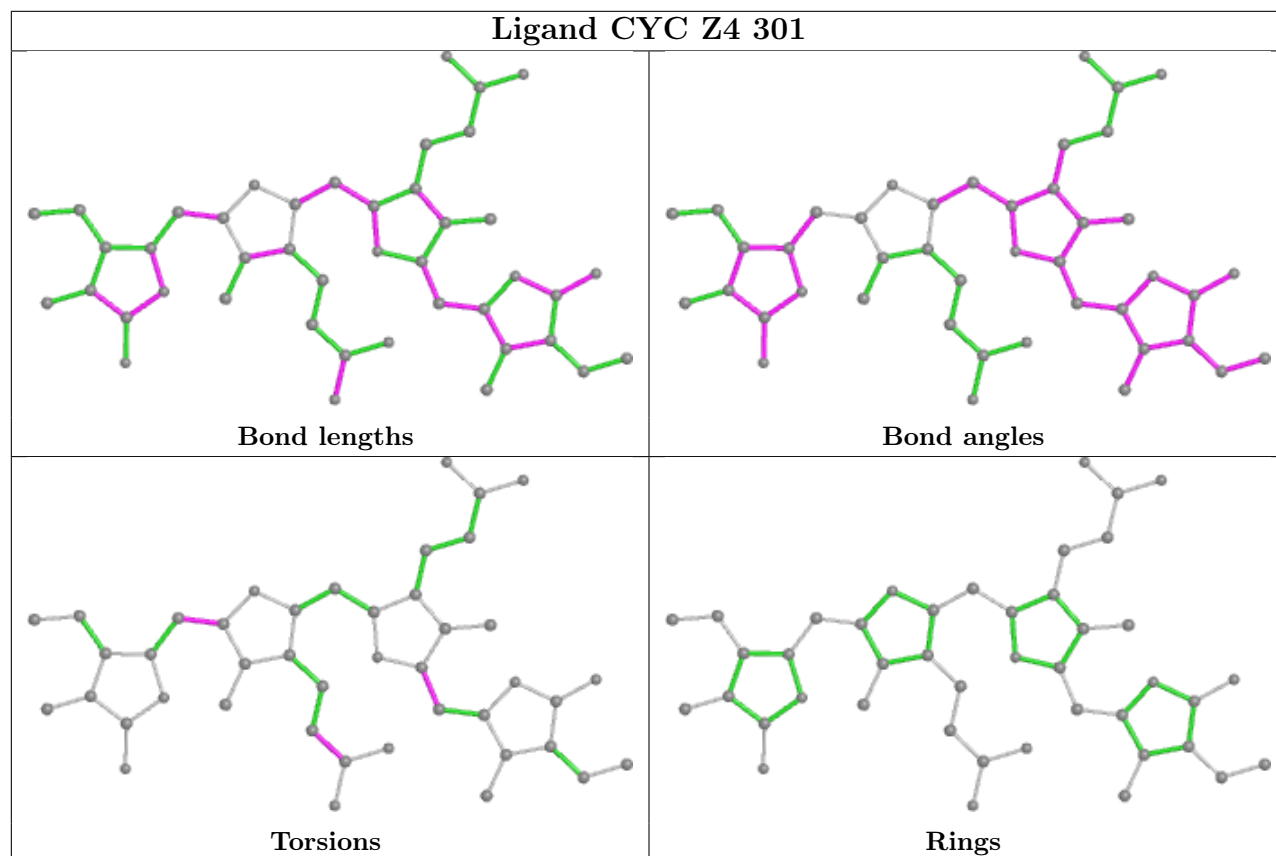
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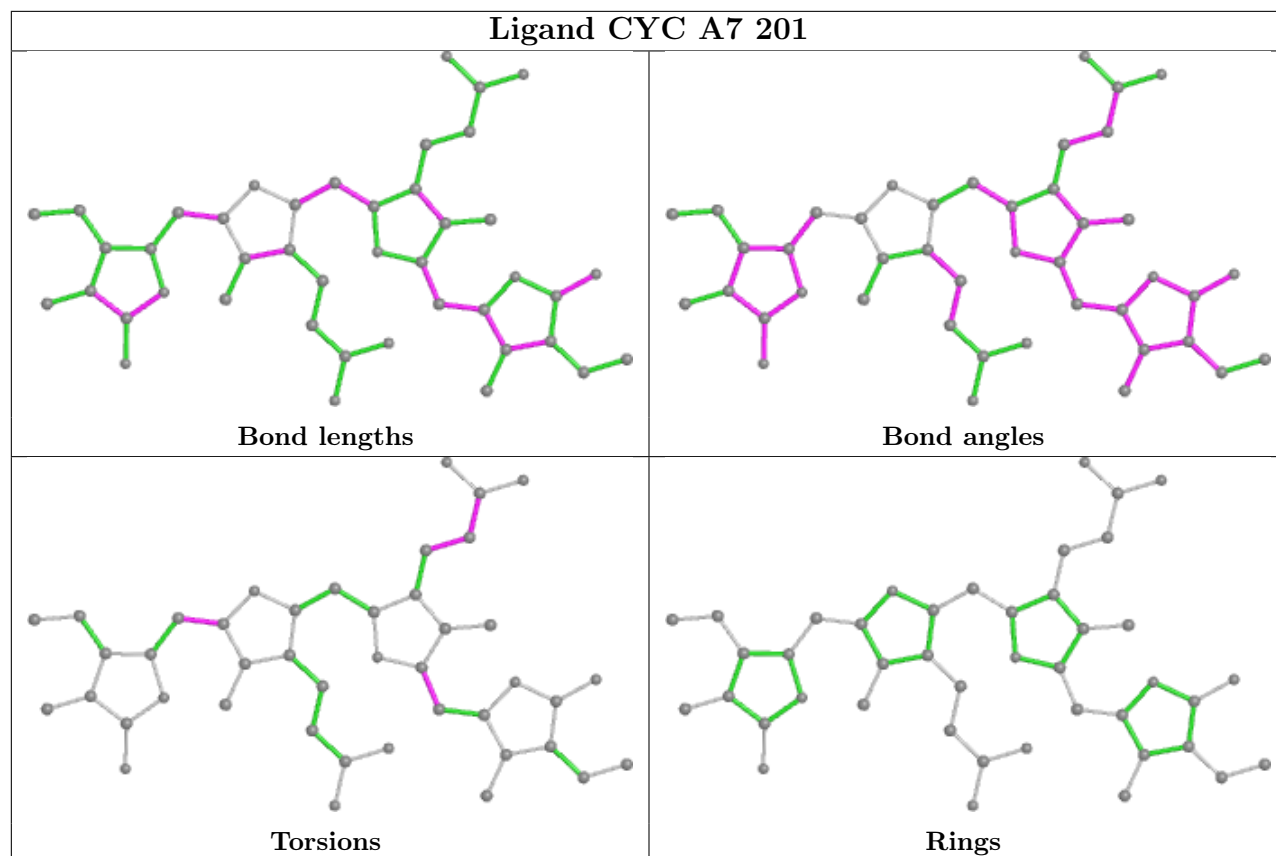
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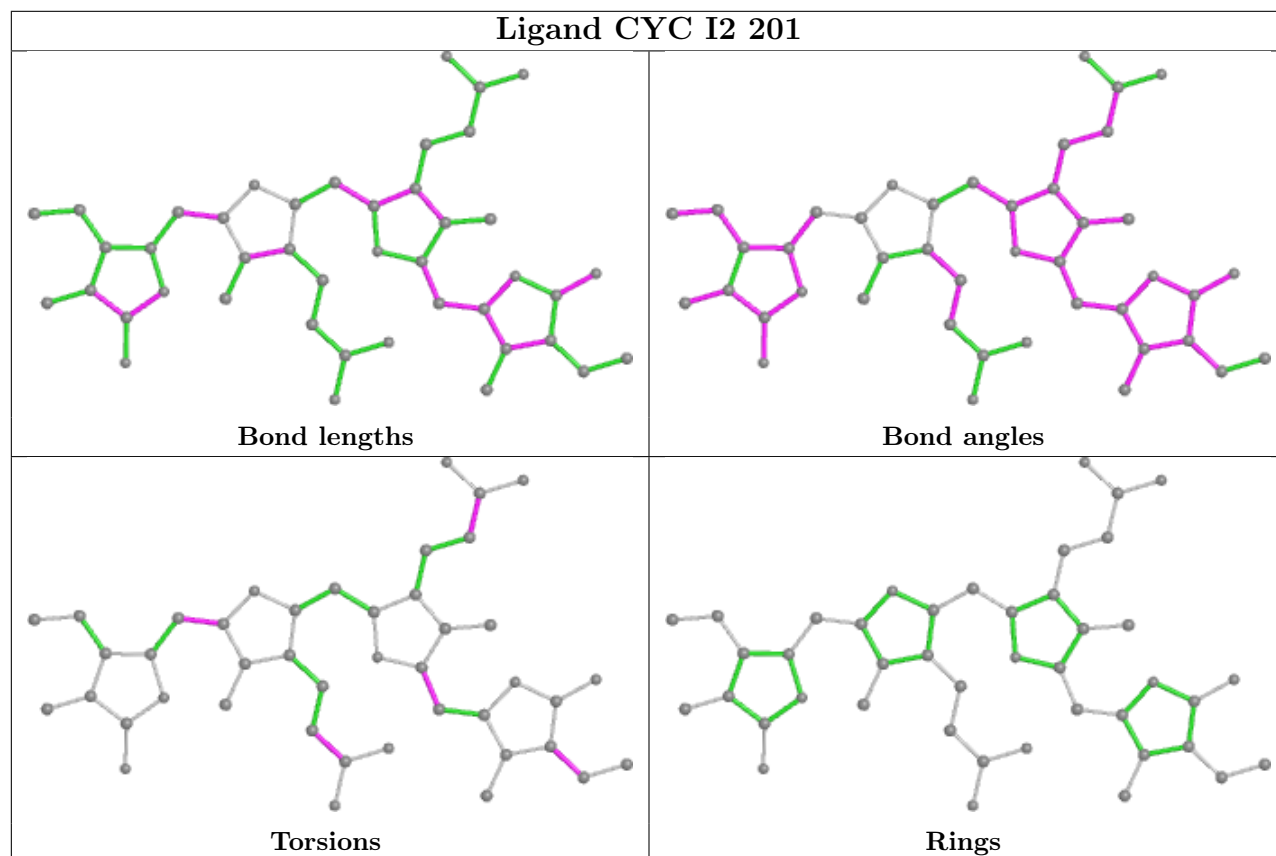
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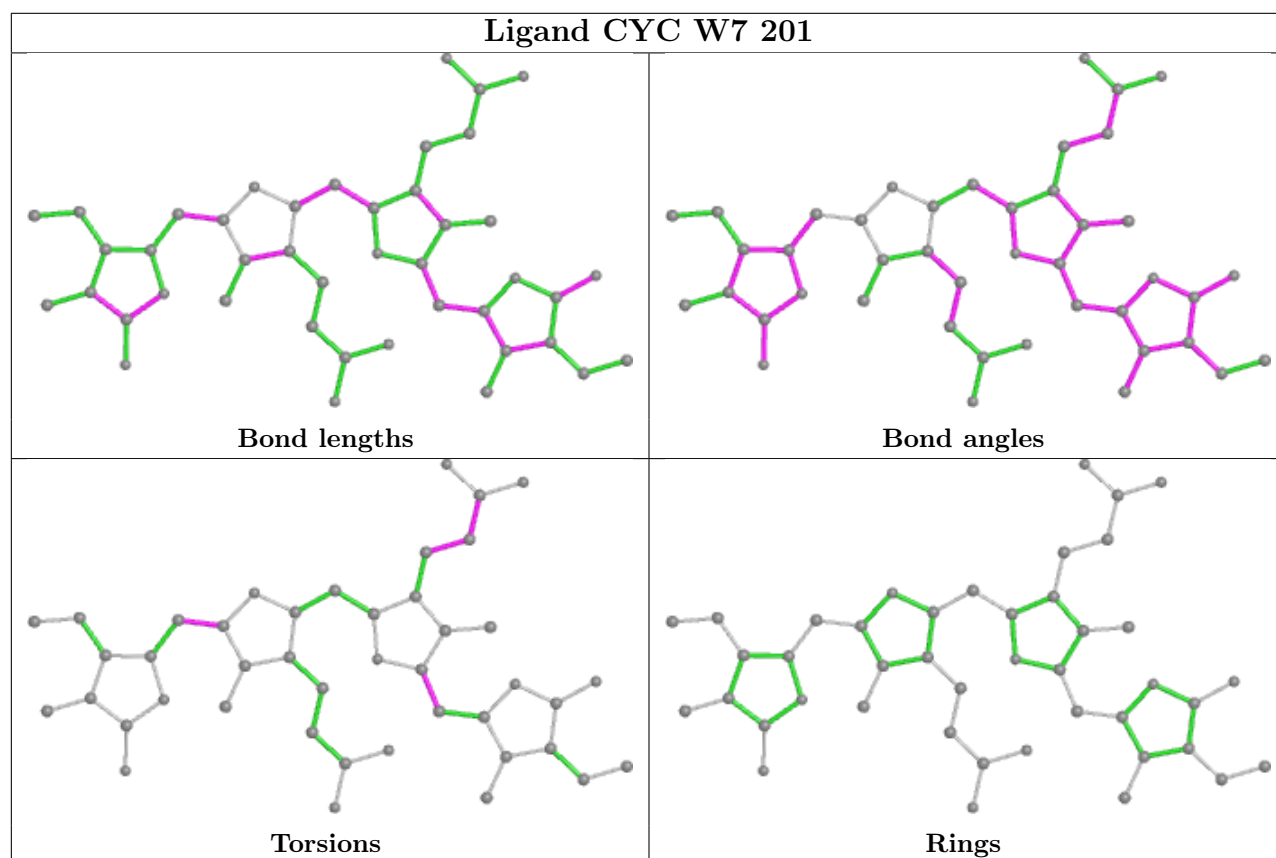
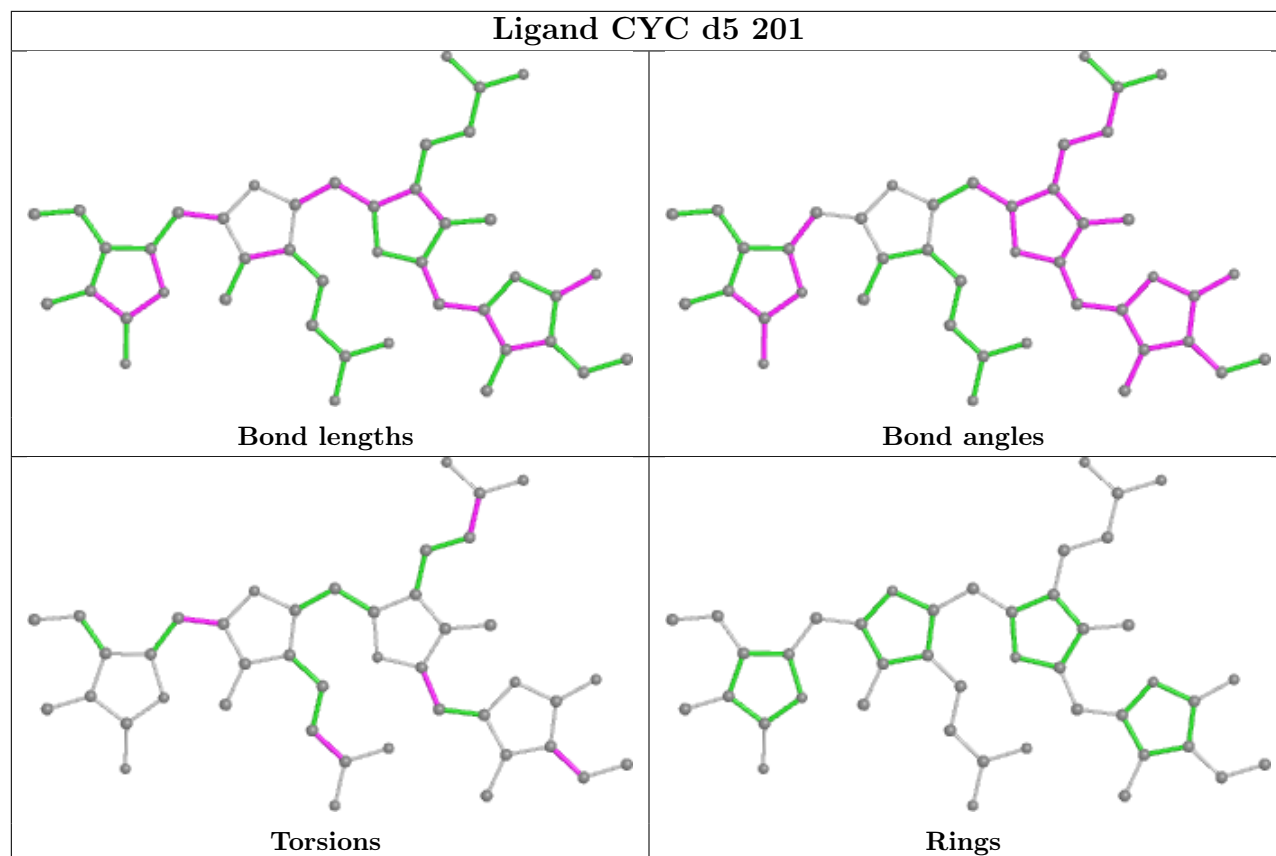


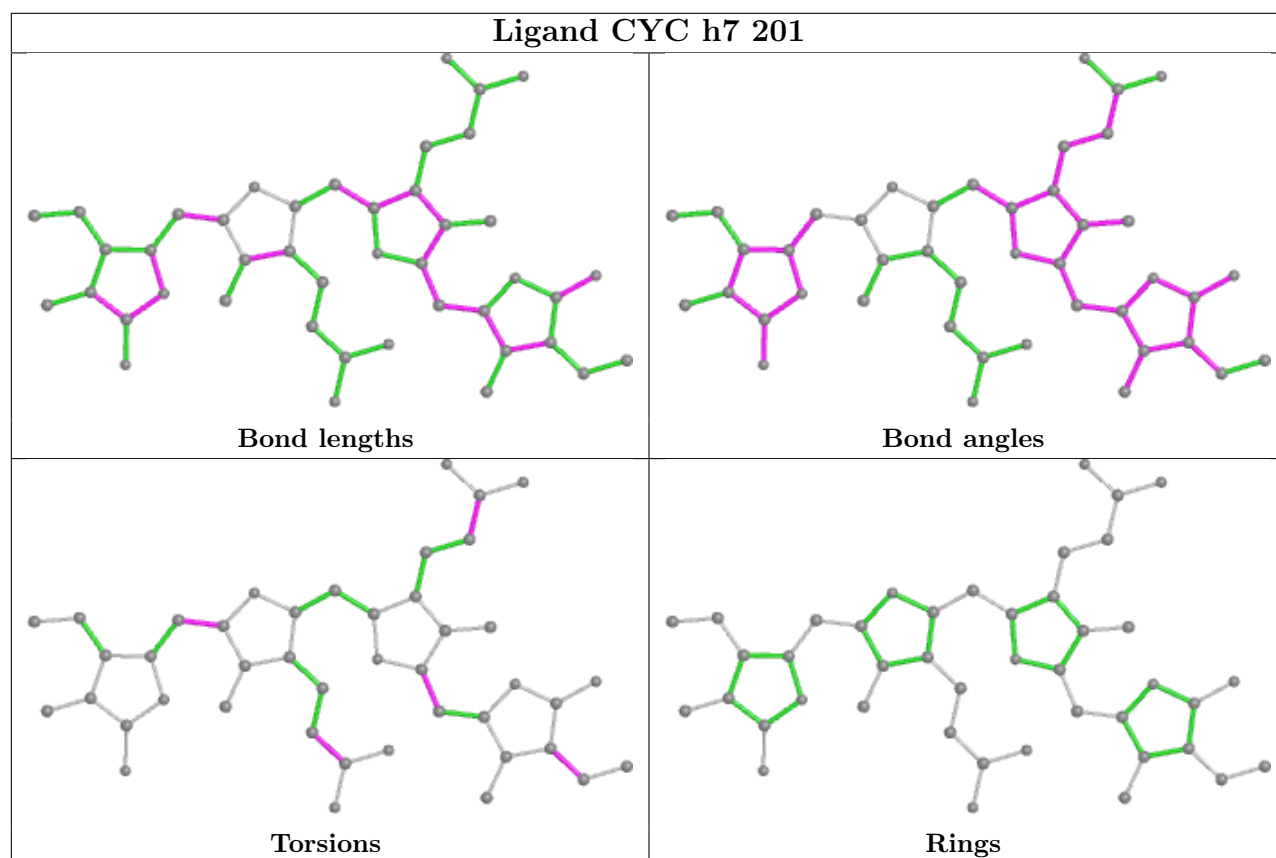
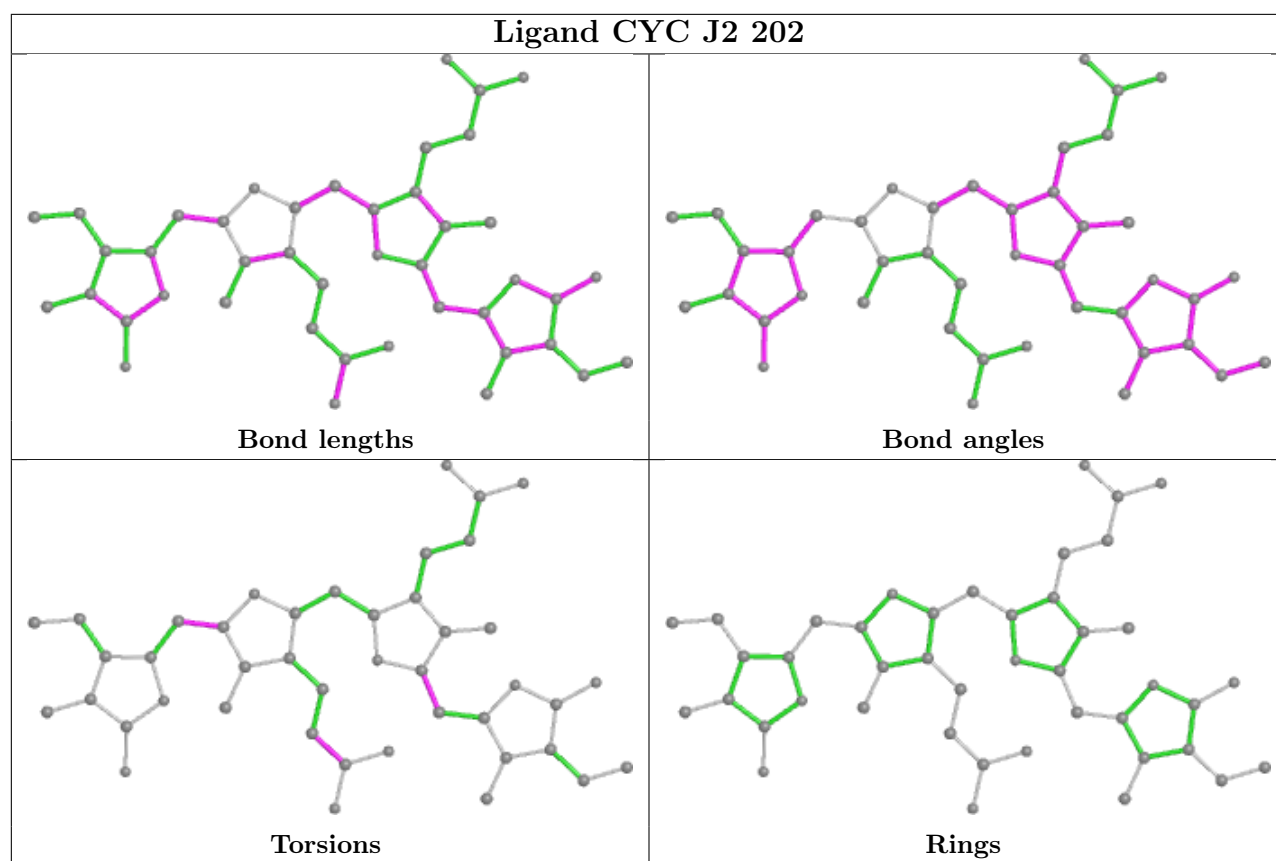
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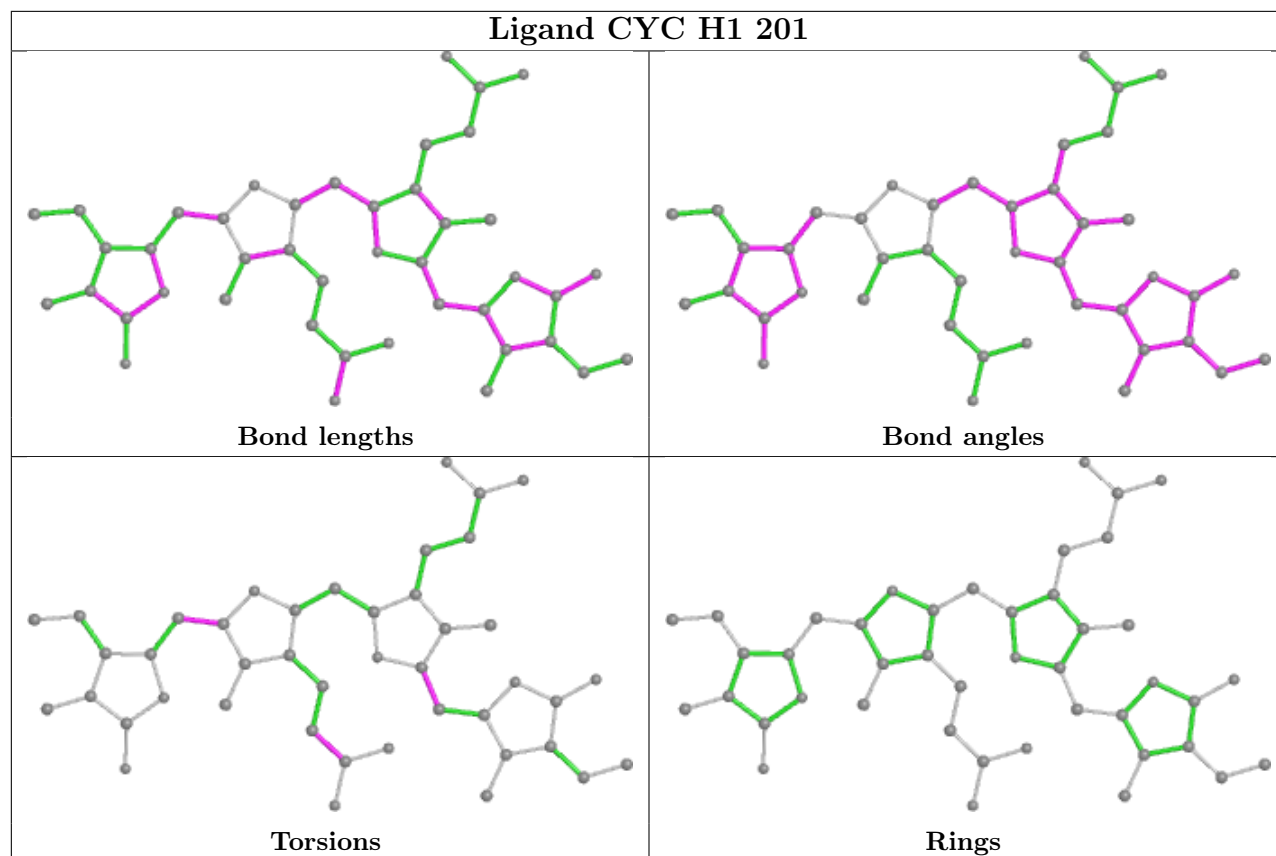
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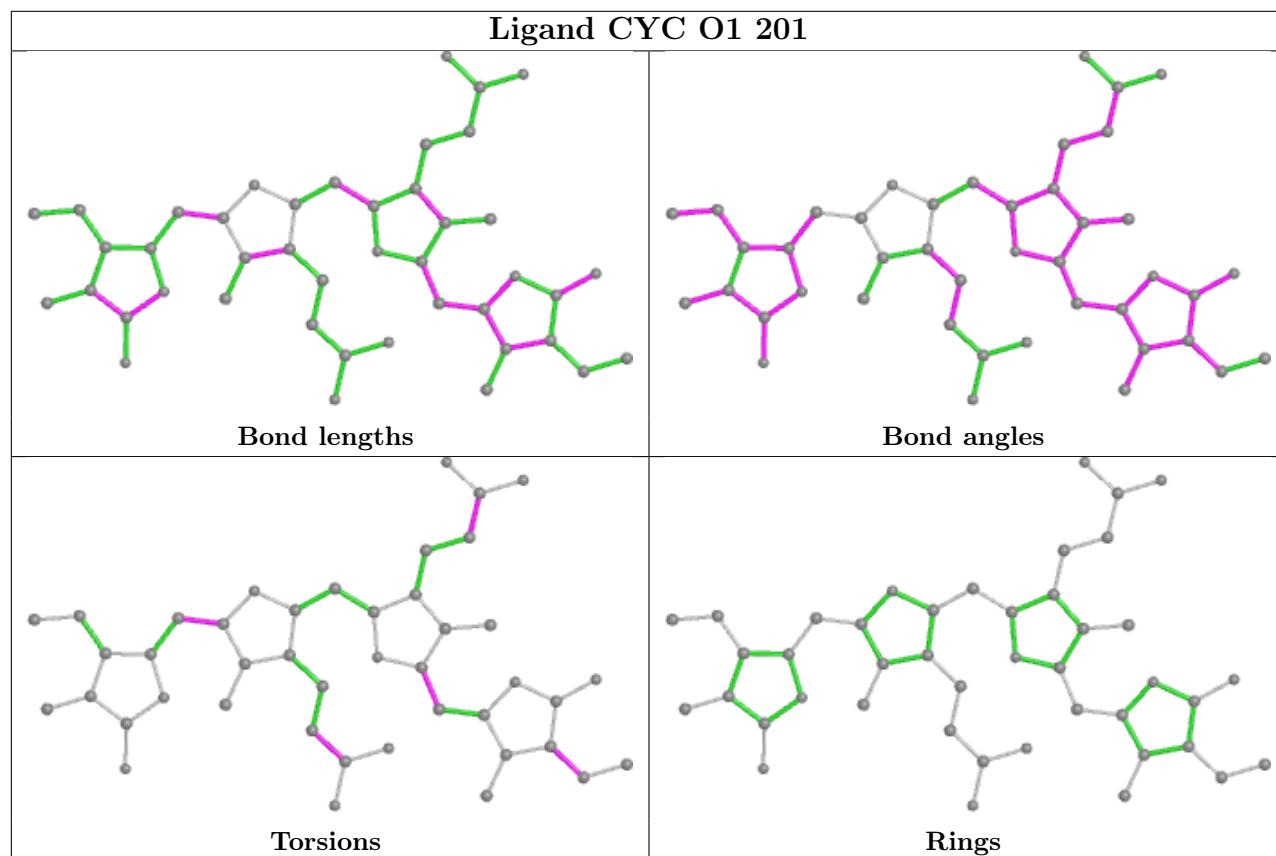




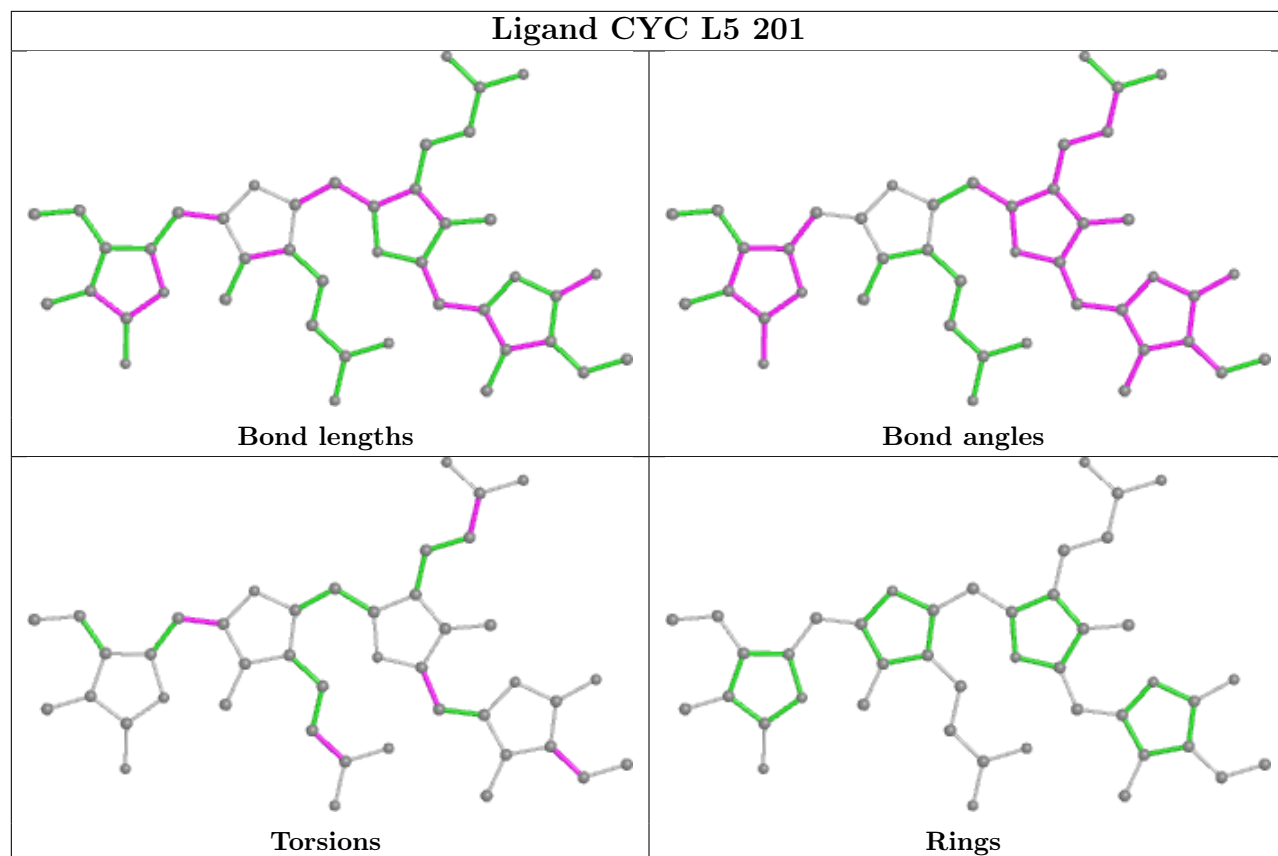
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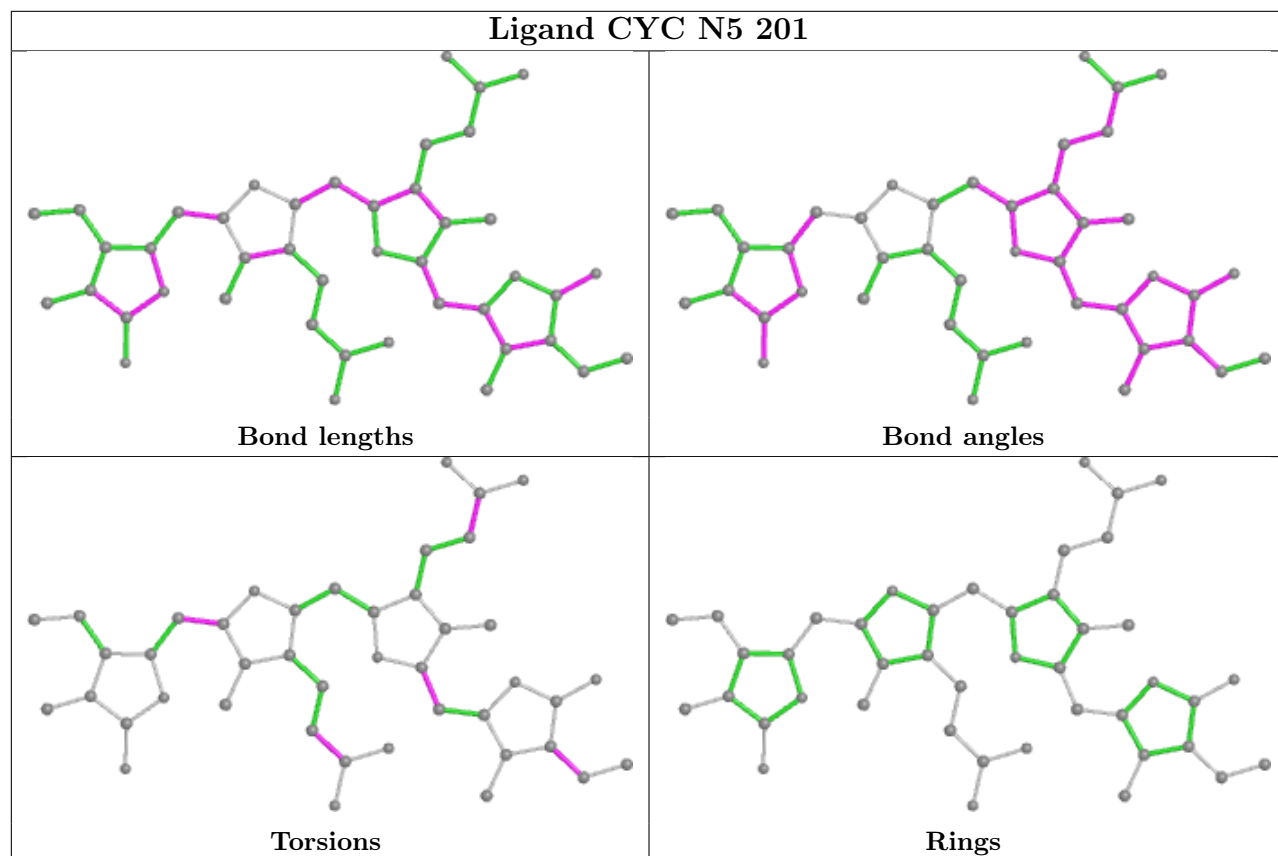
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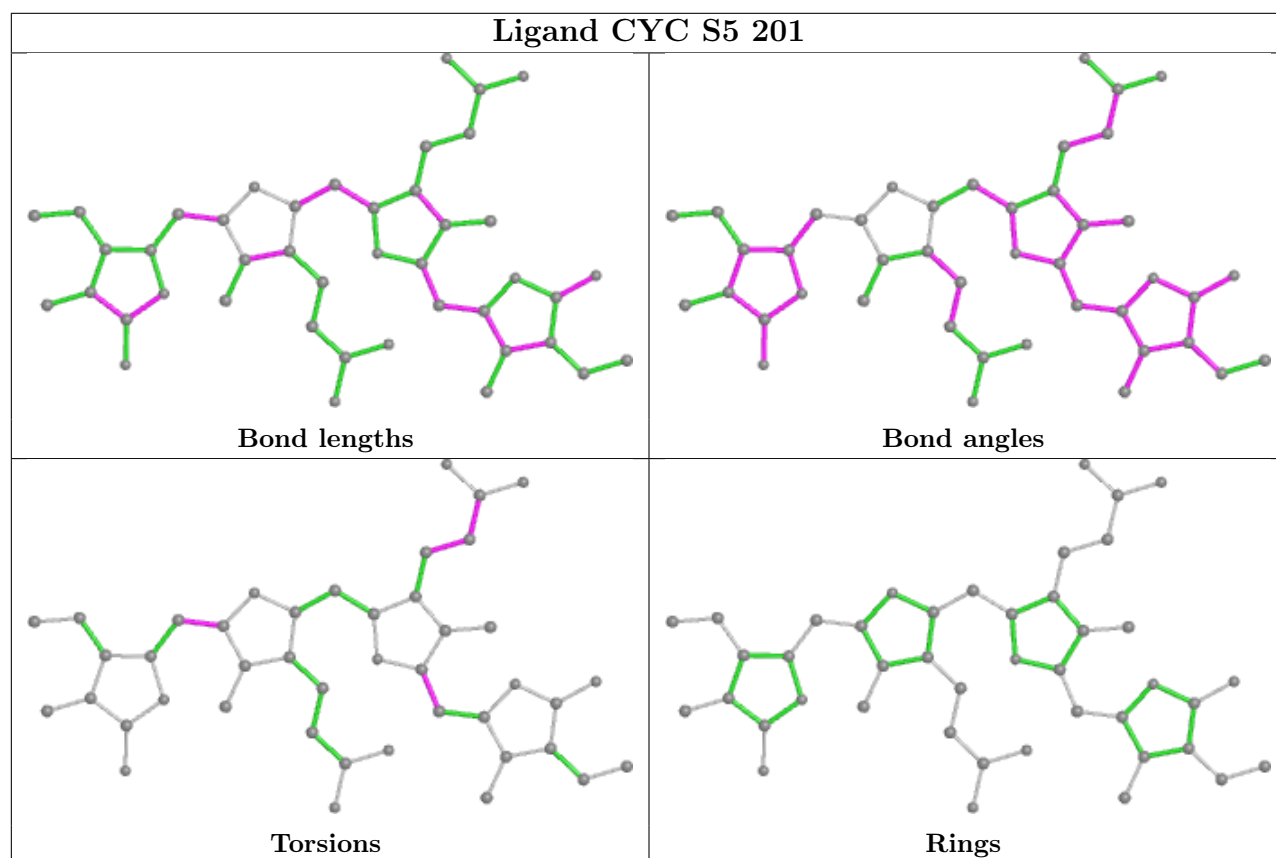
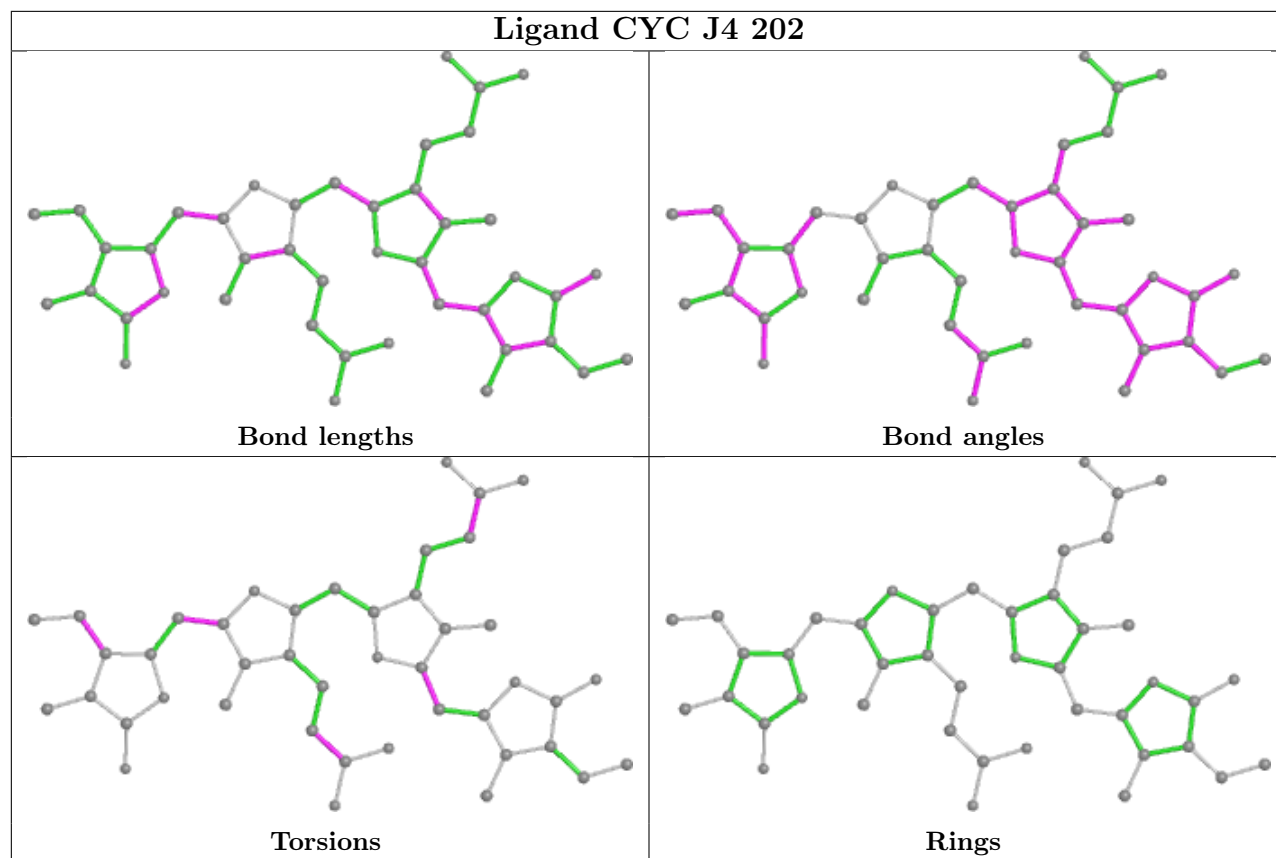


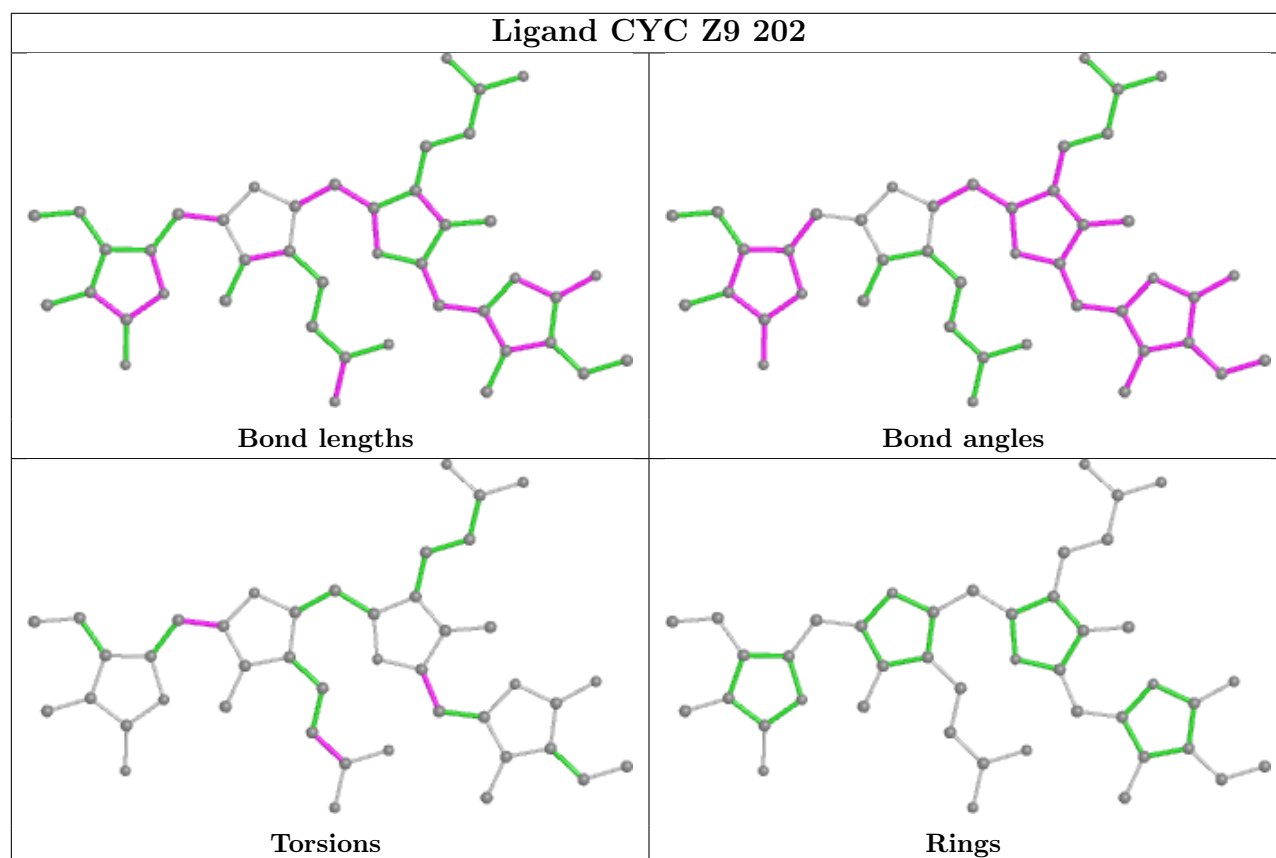
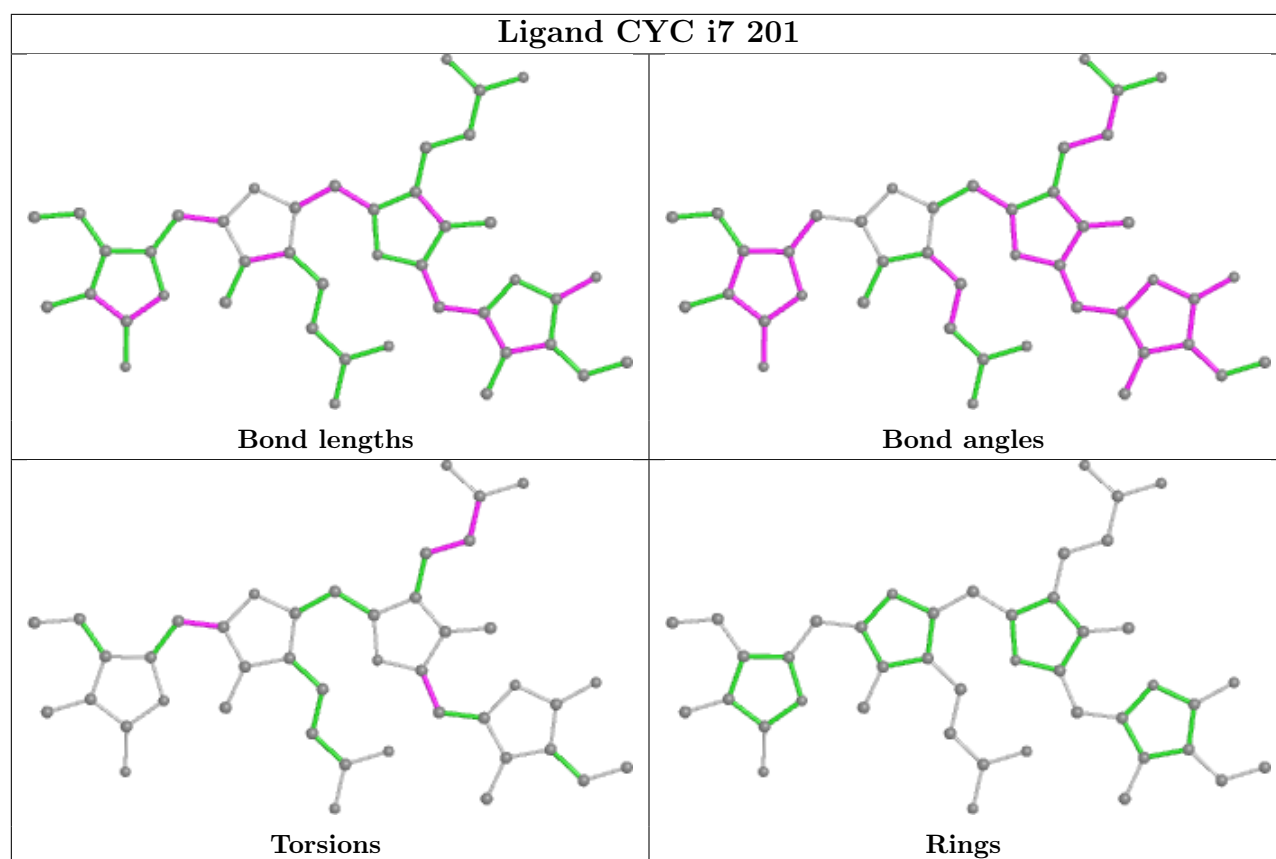
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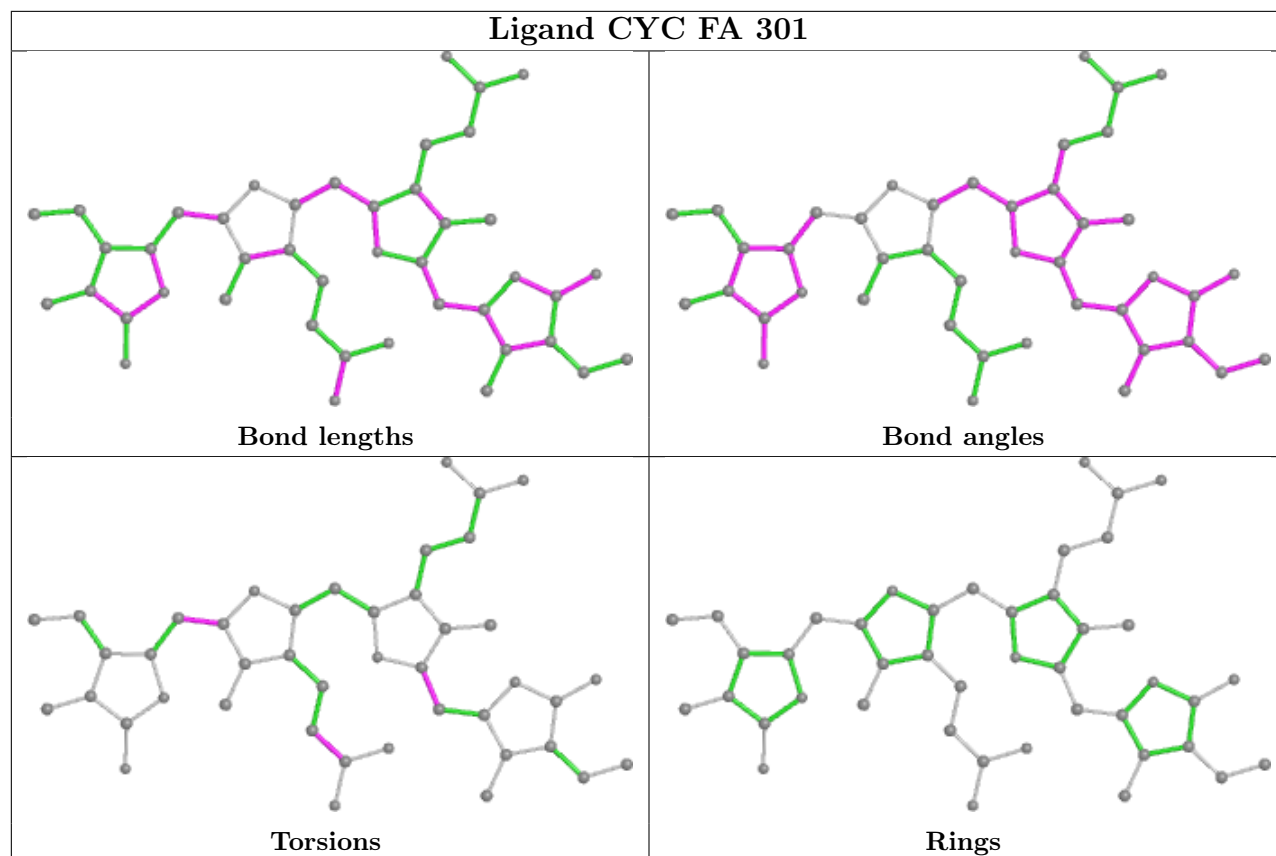
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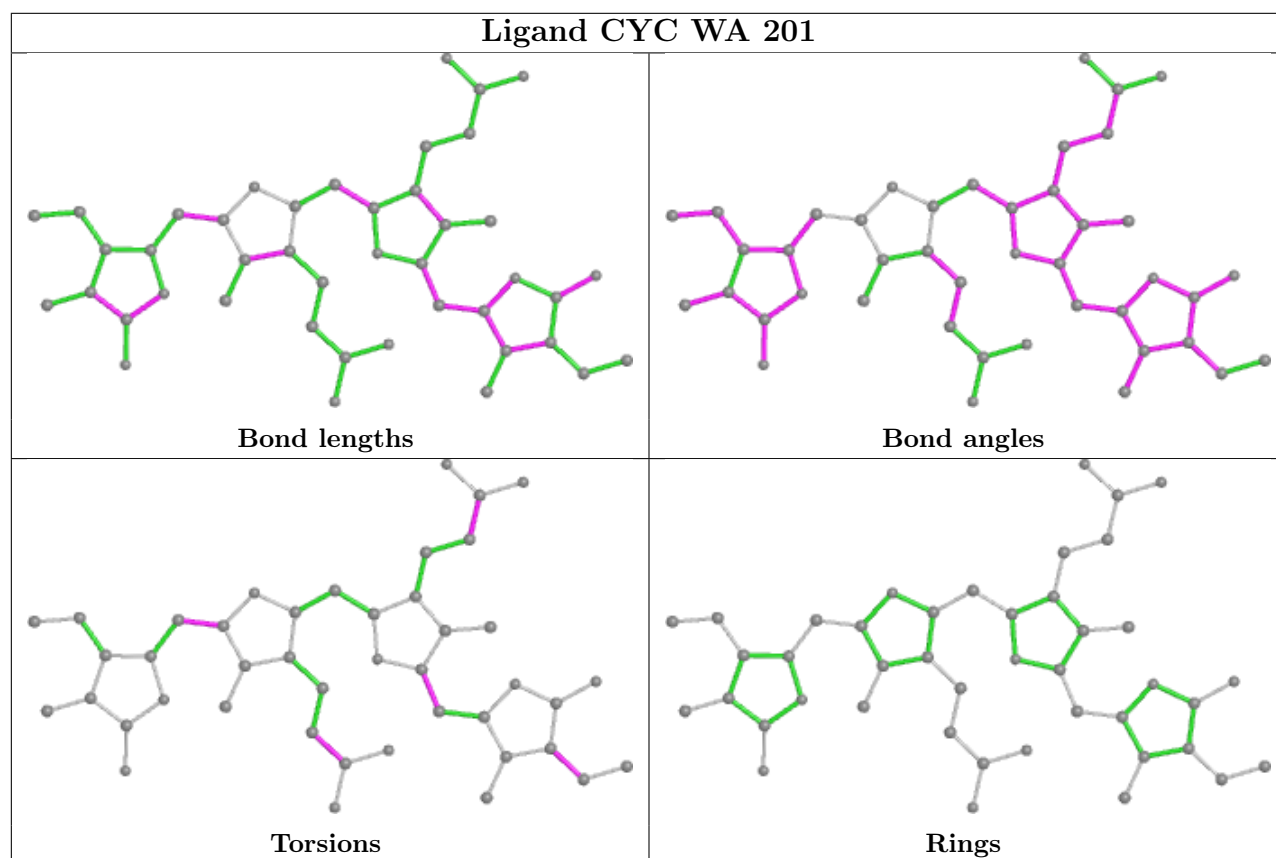


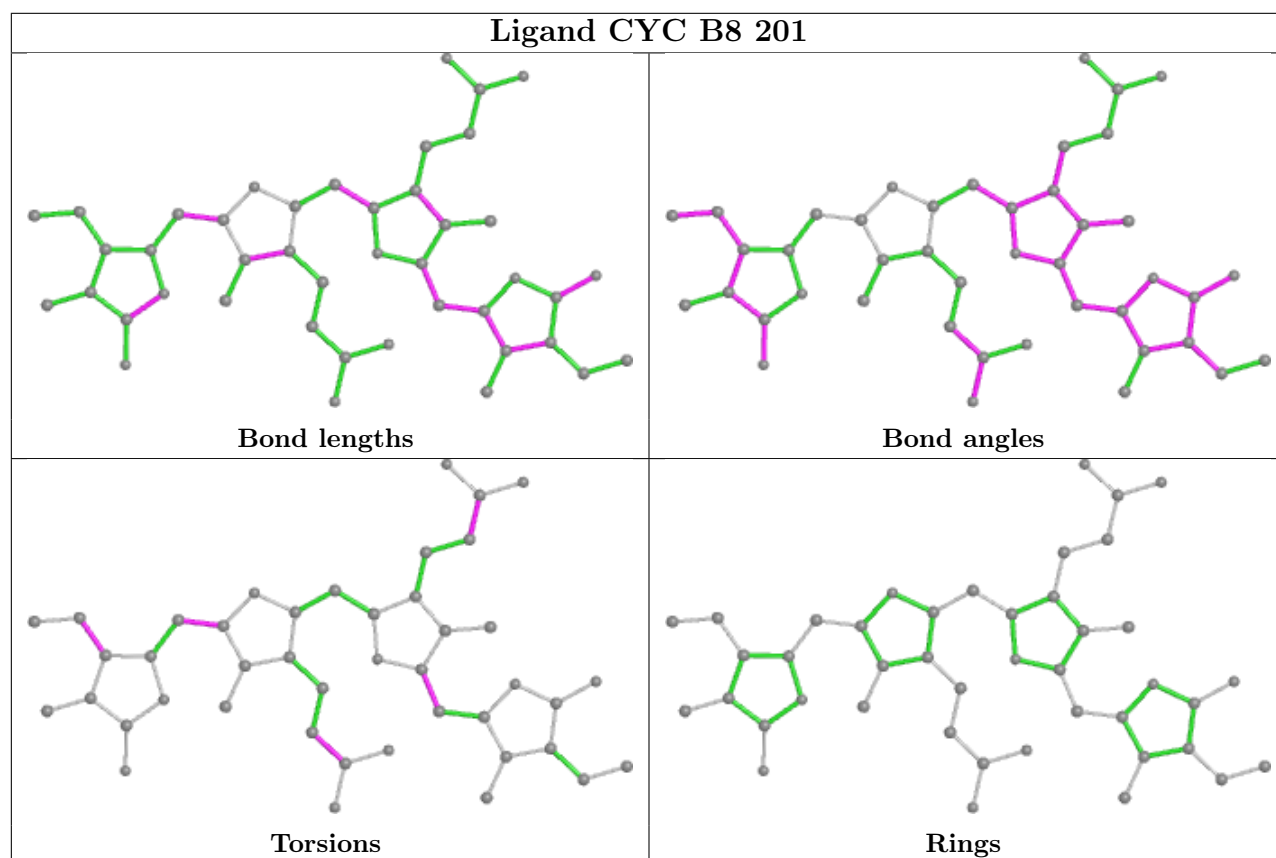
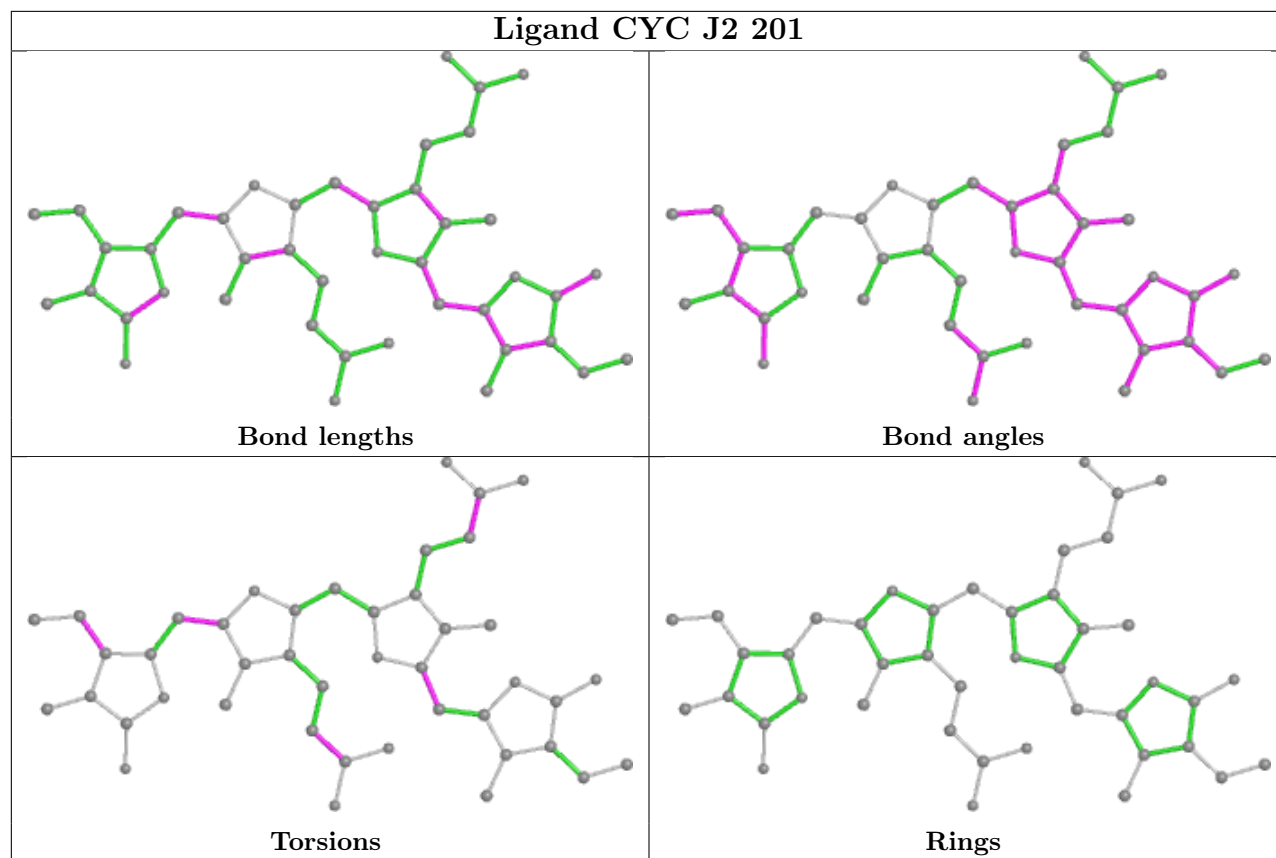


Ligand CYC FA 301

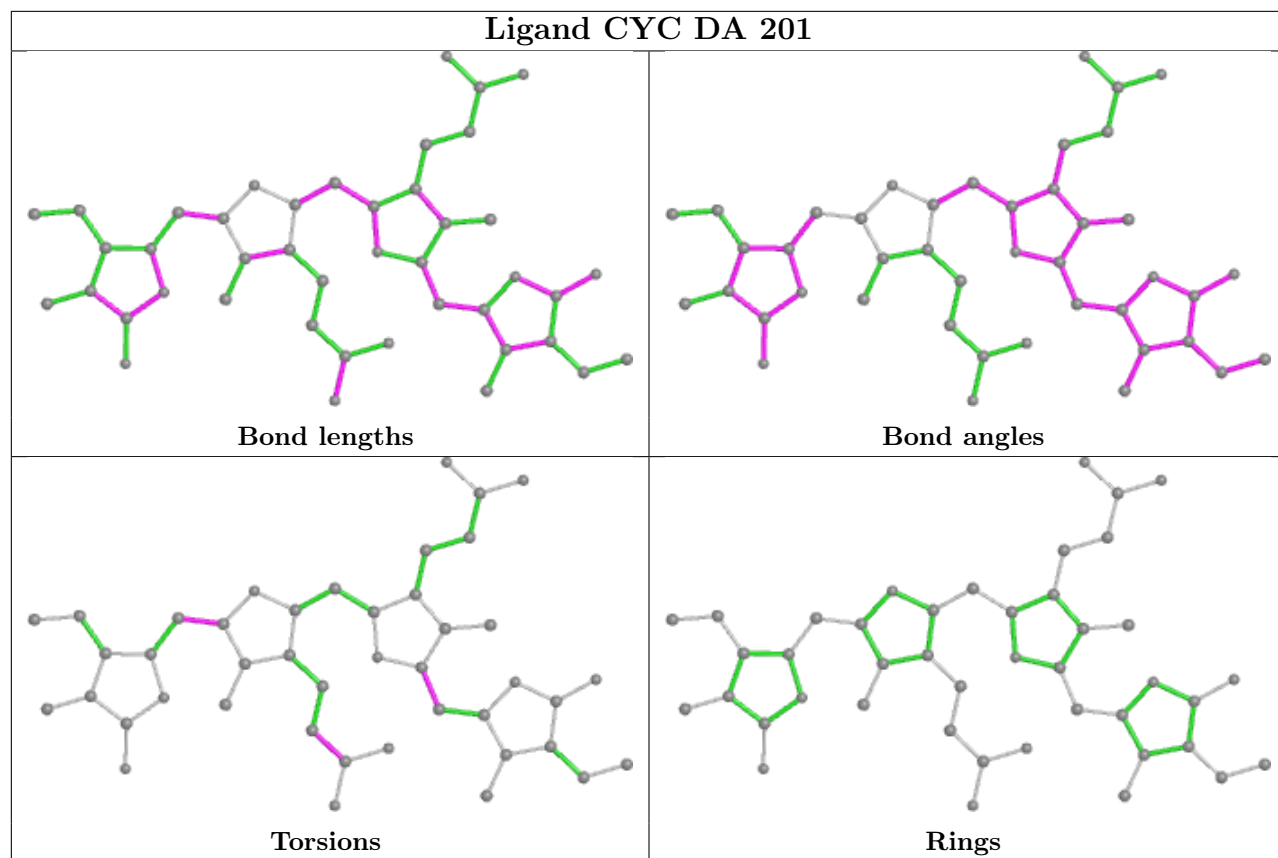


Ligand CYC WA 201

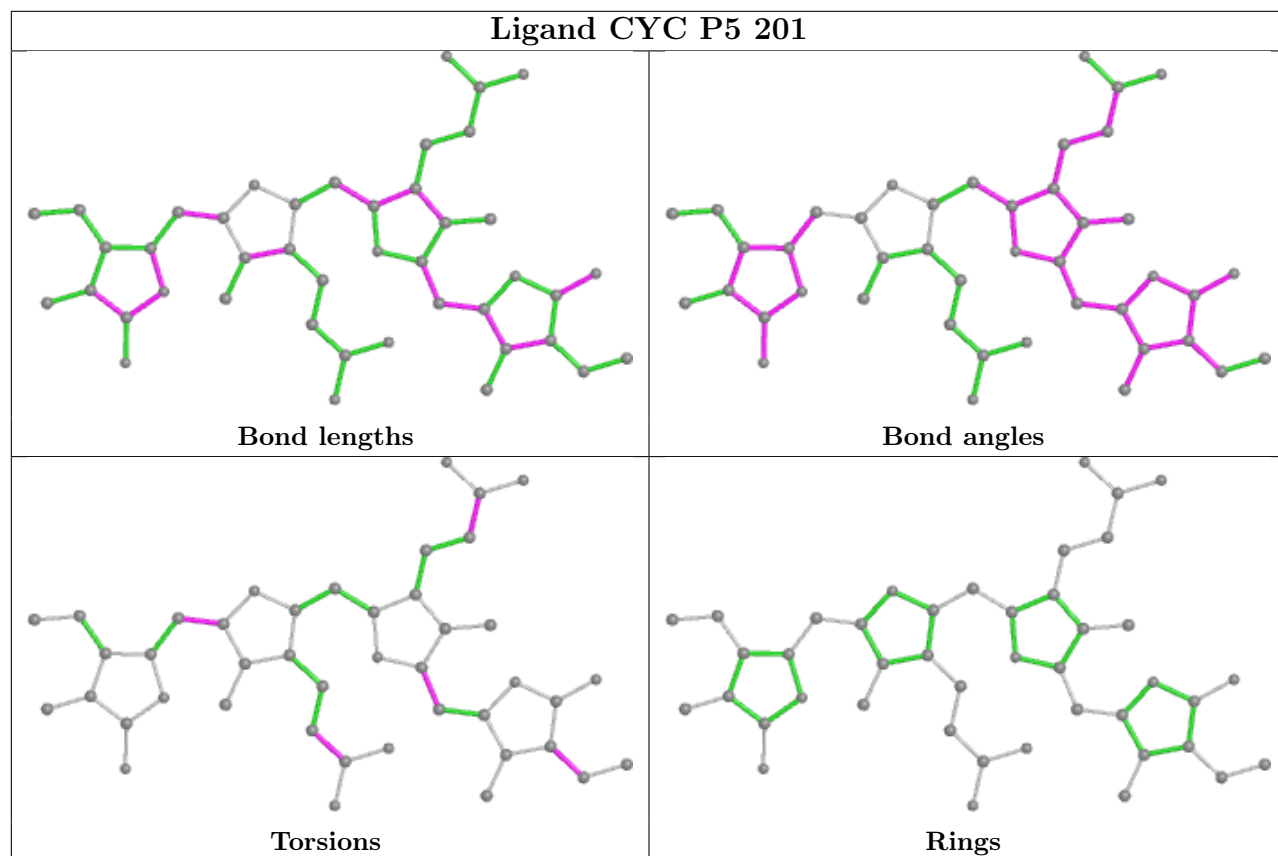




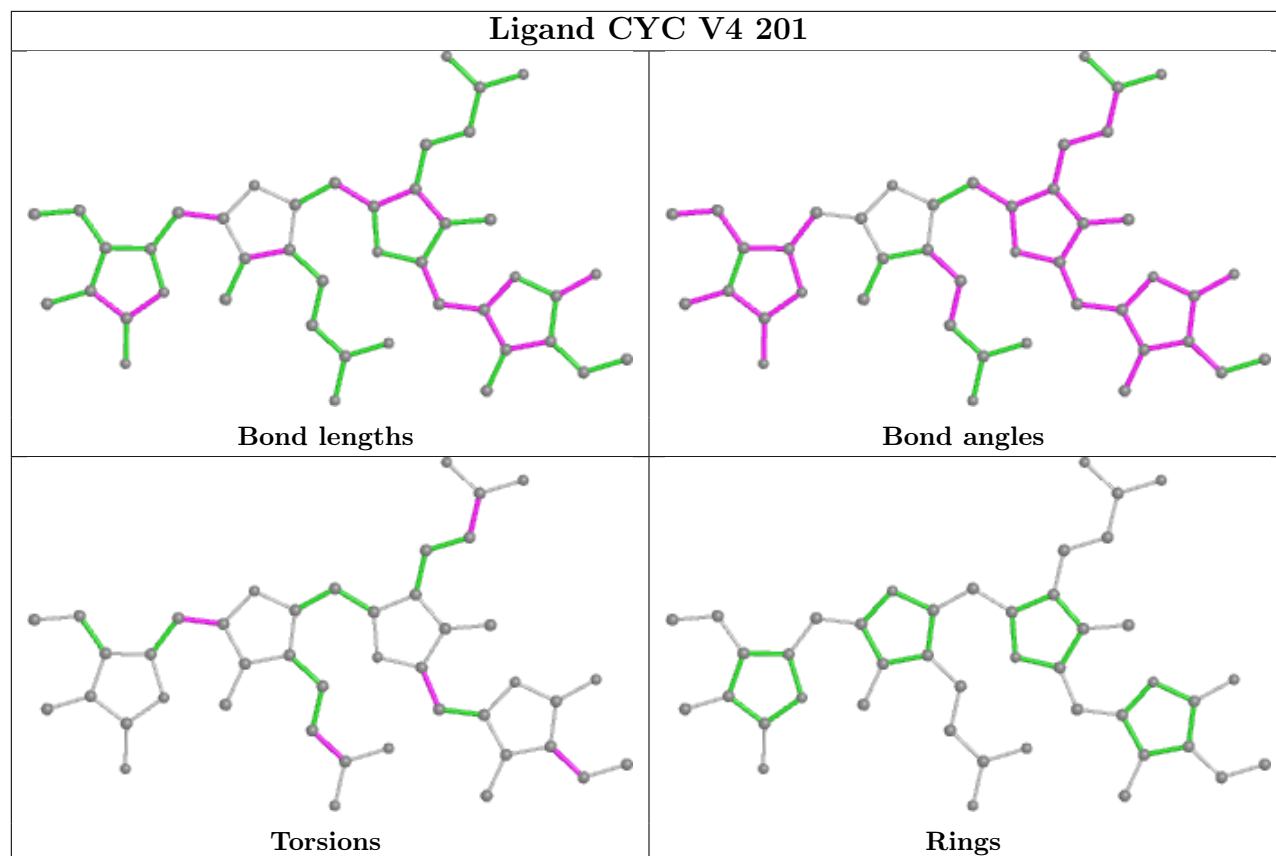
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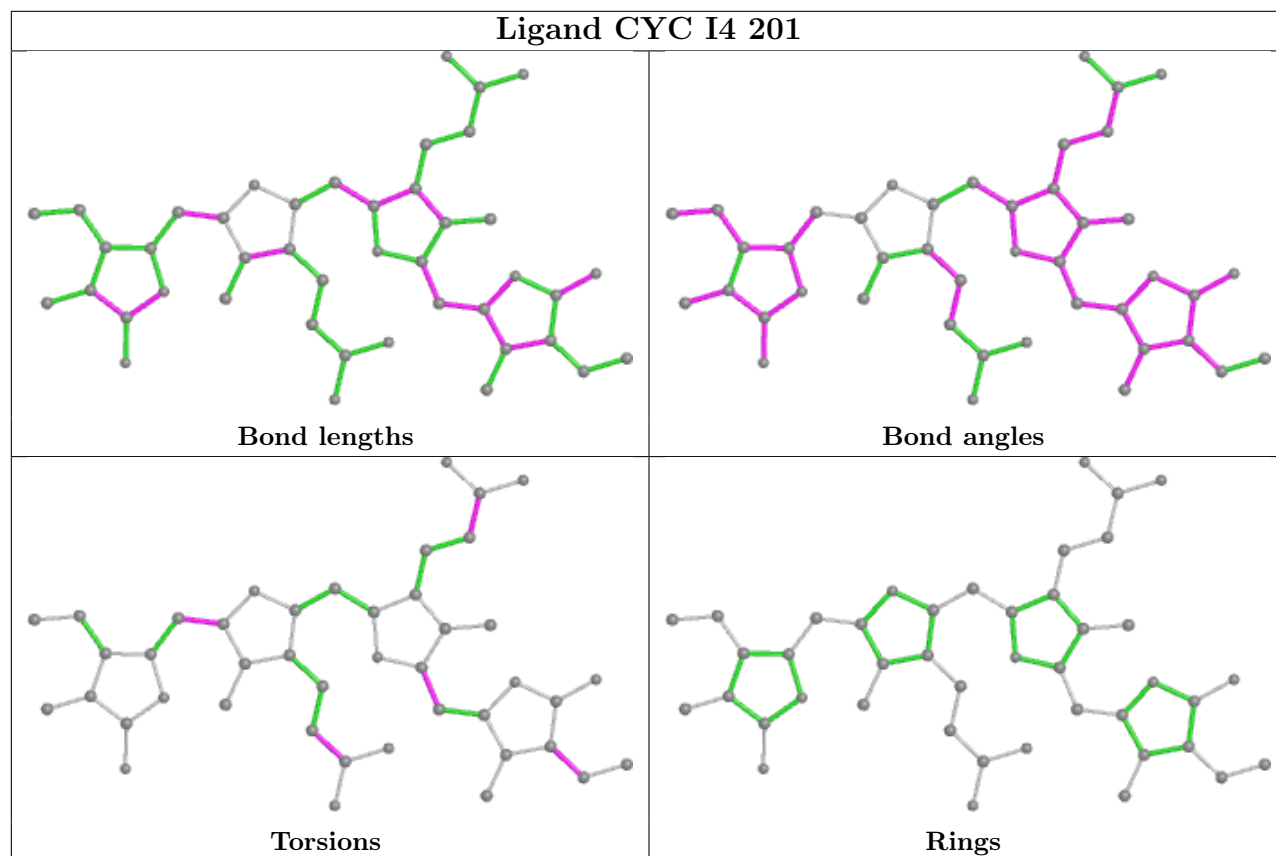
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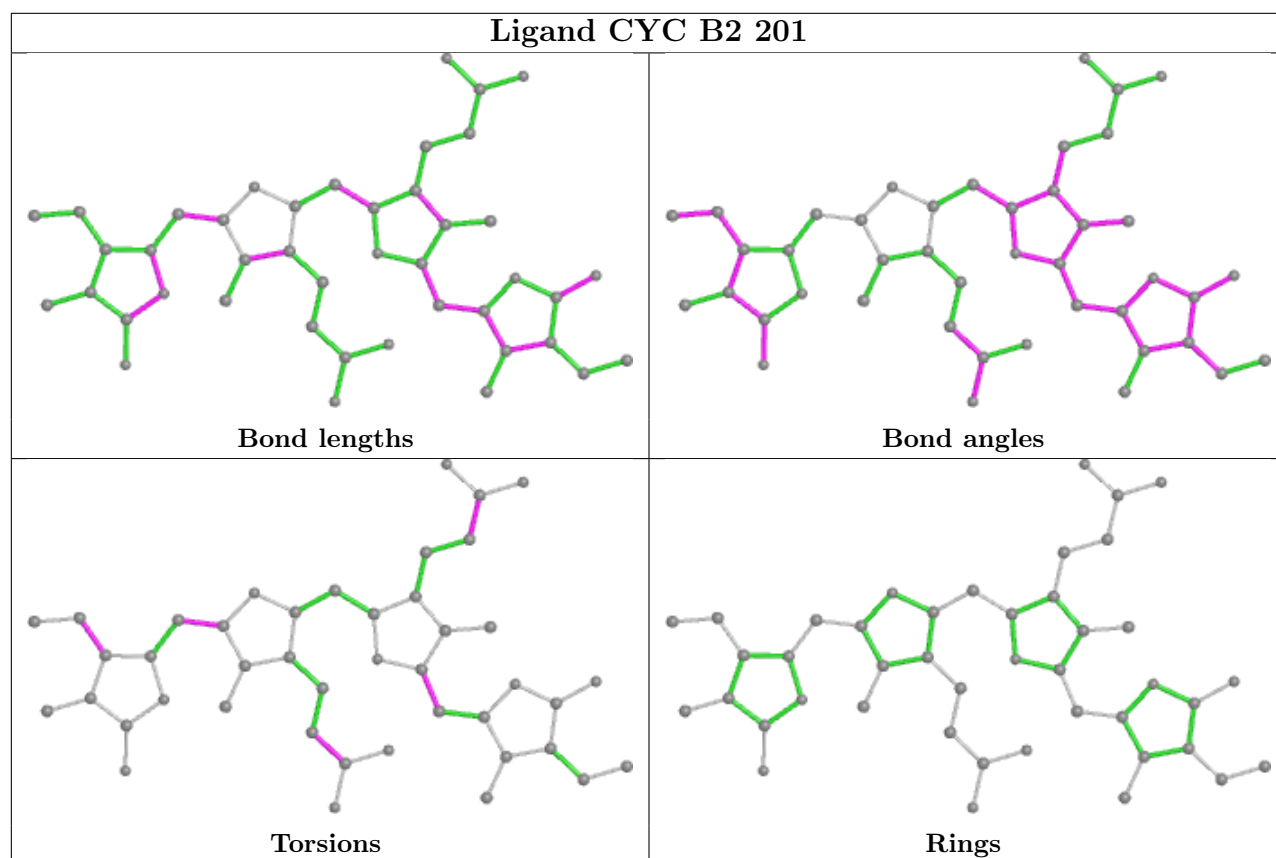
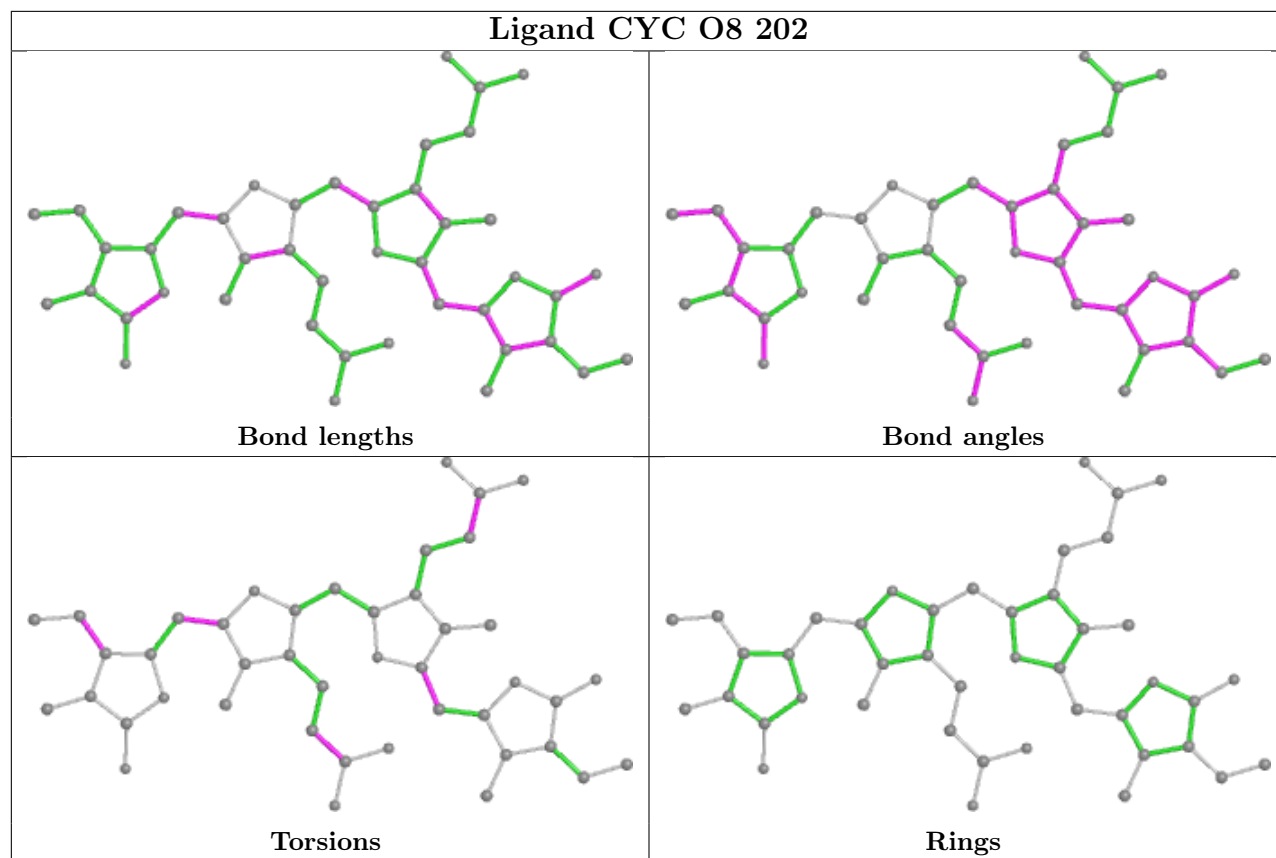


Ligand CYC V4 201

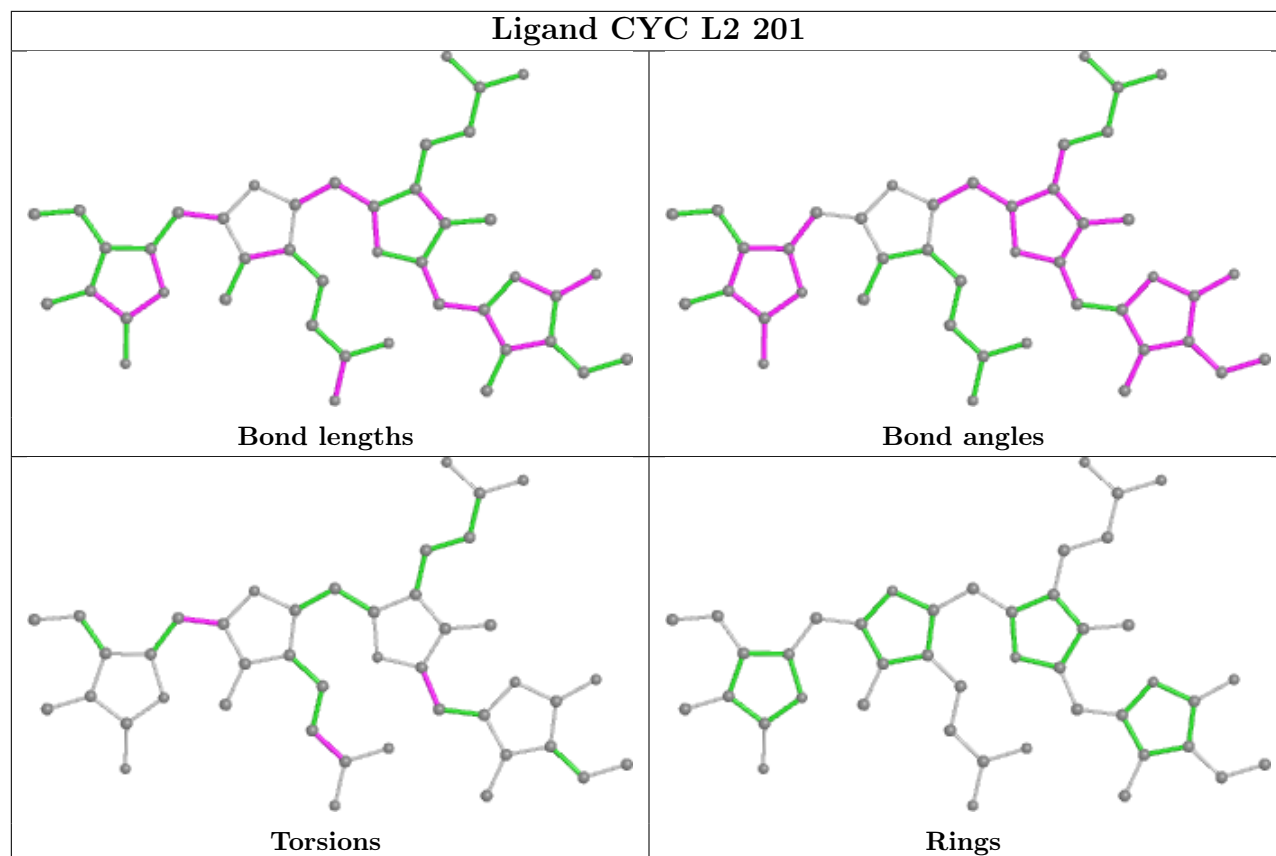


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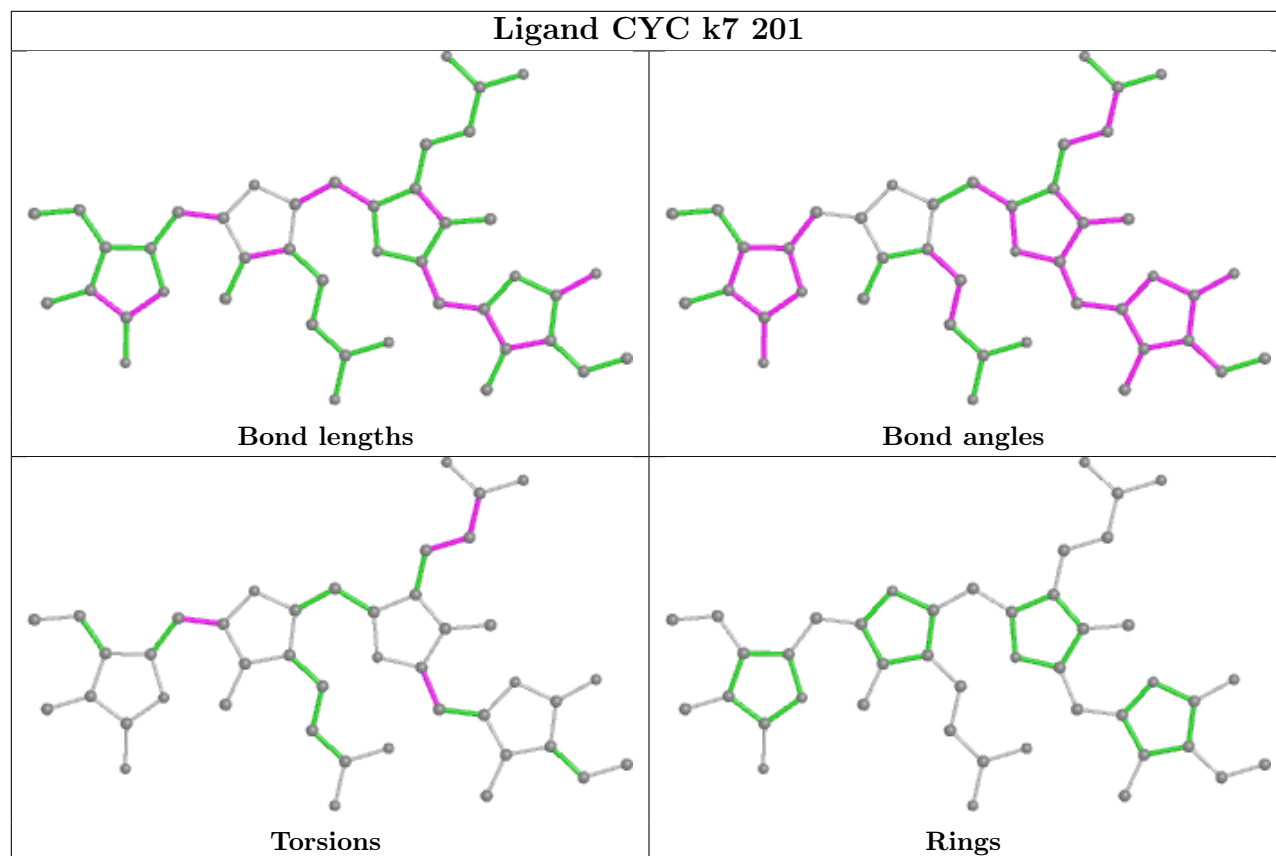




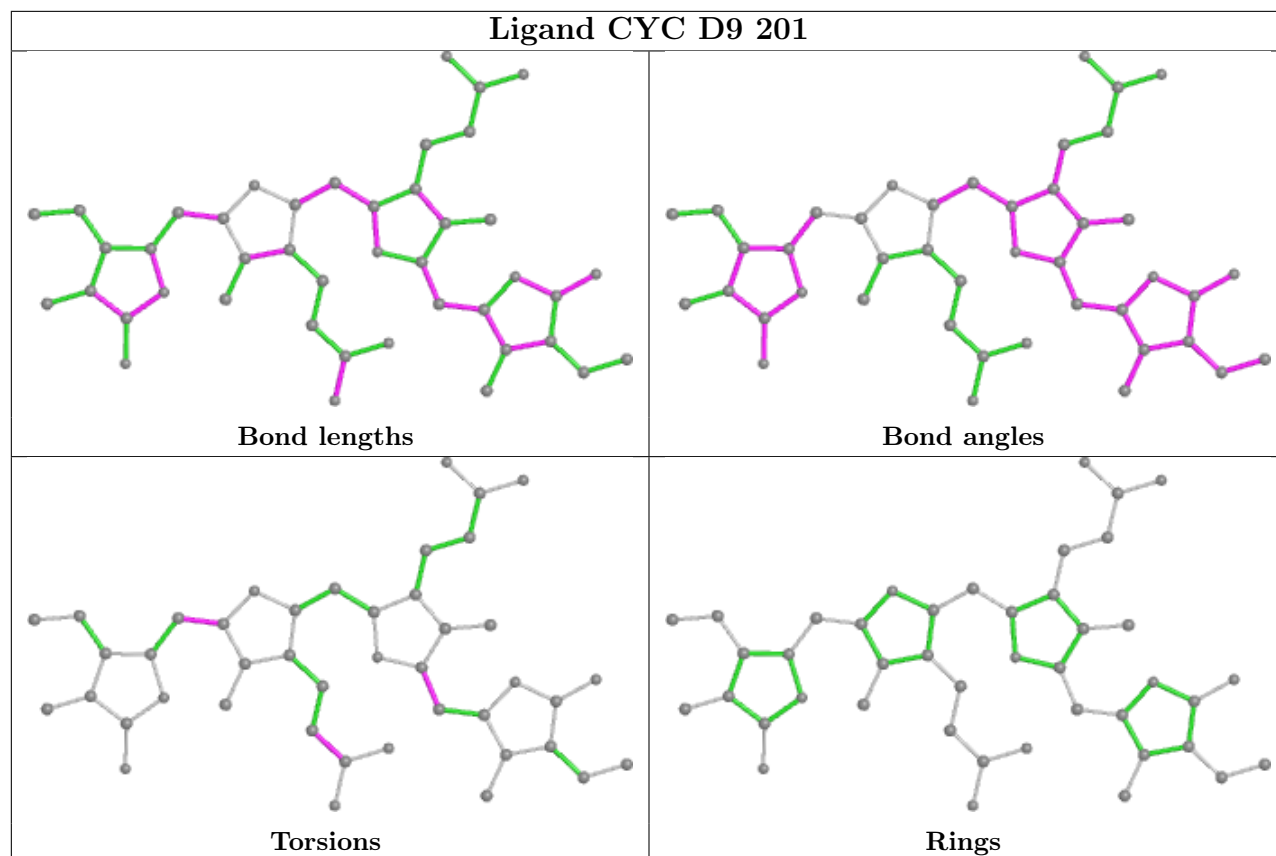
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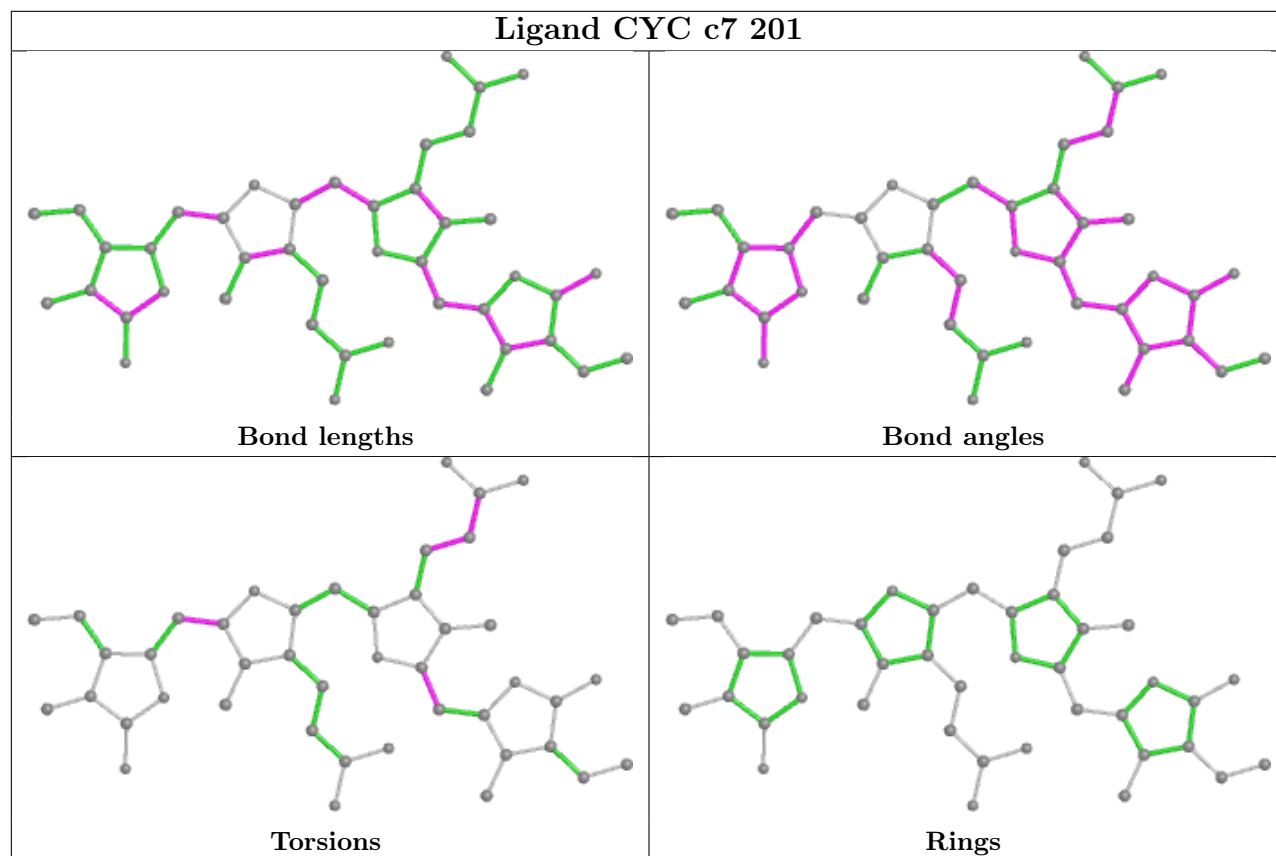
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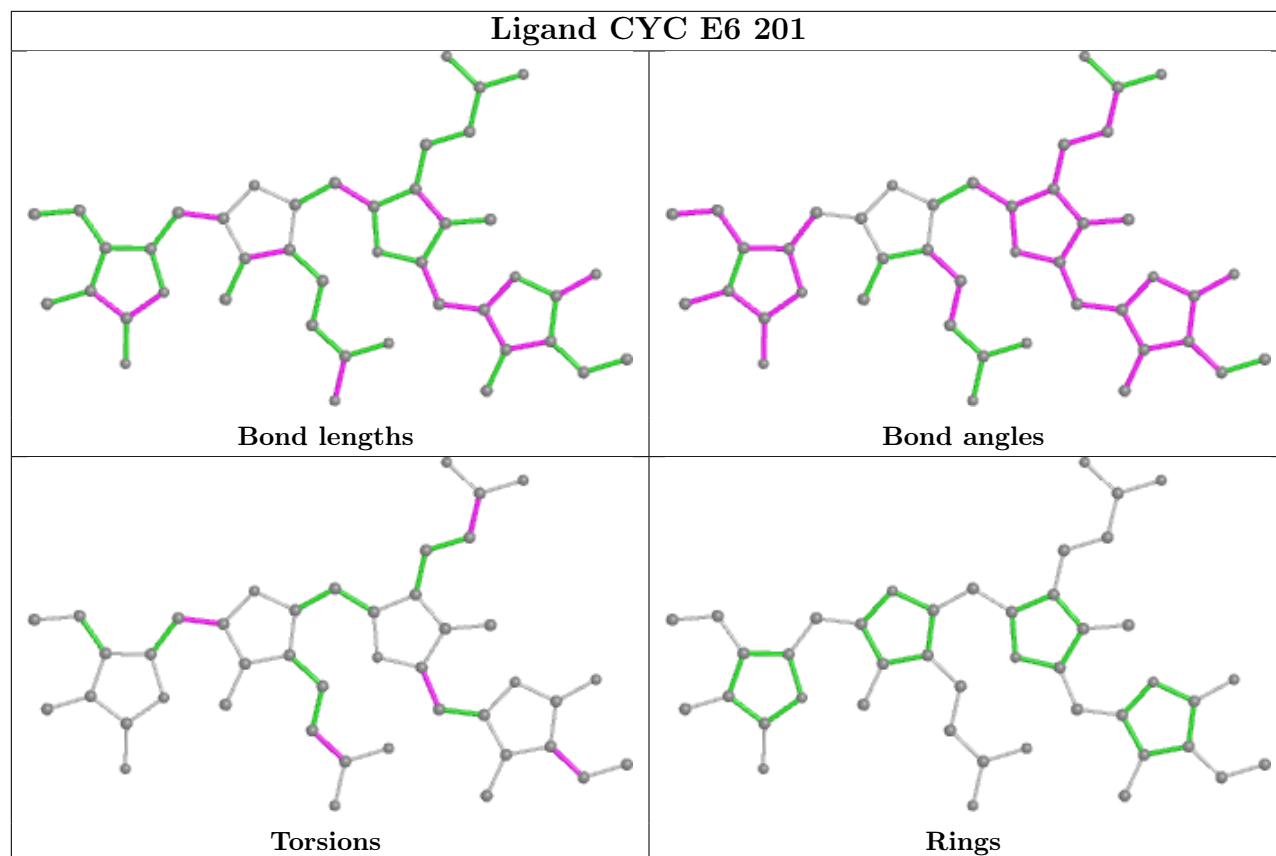
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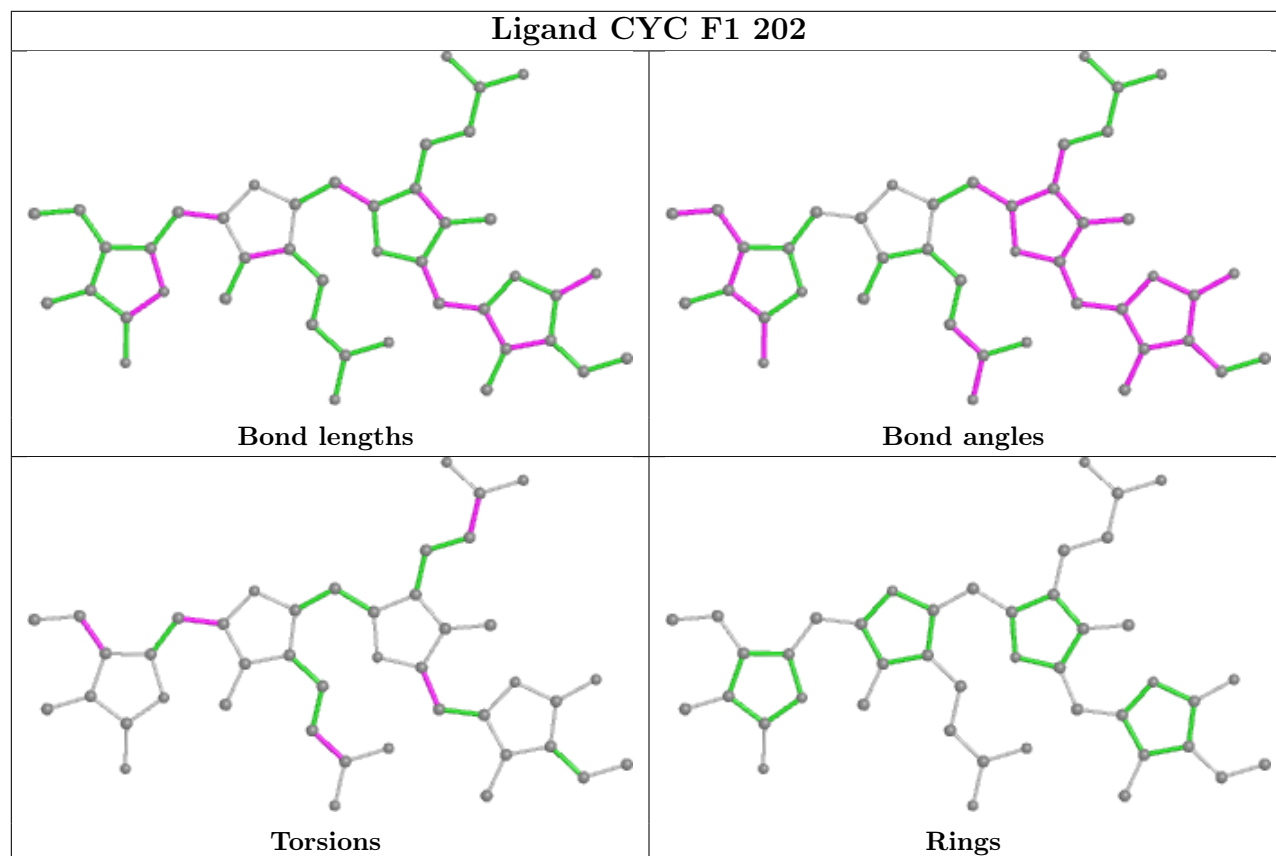
Ligand CYC c7 201



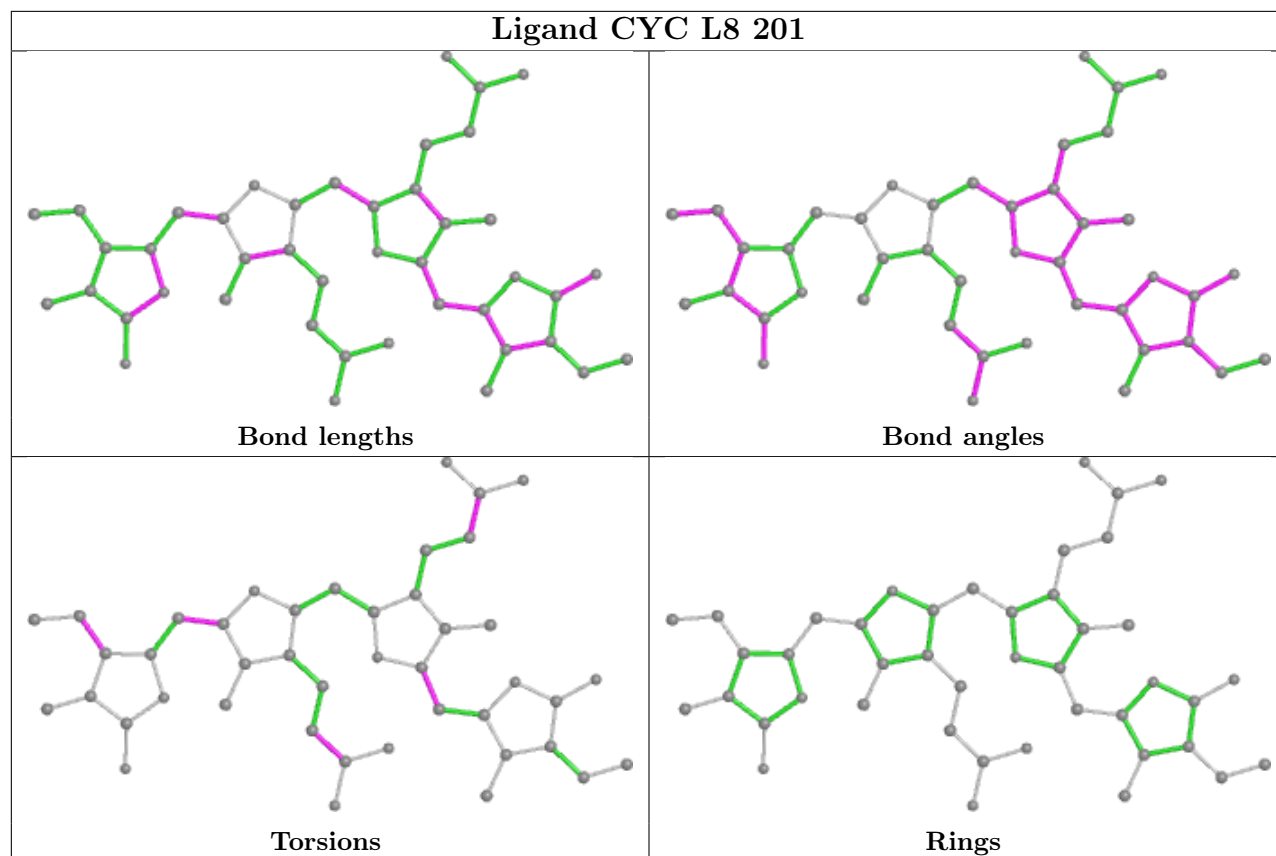
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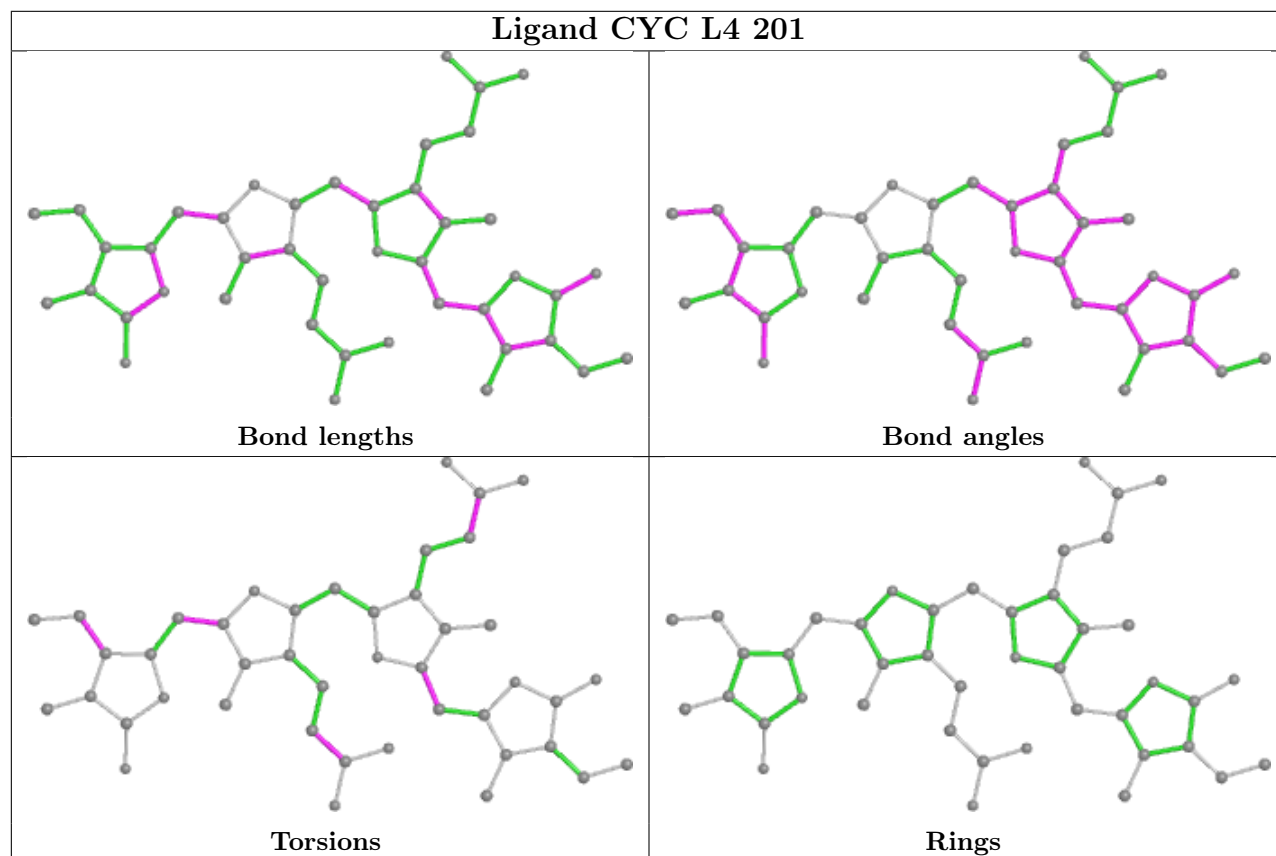
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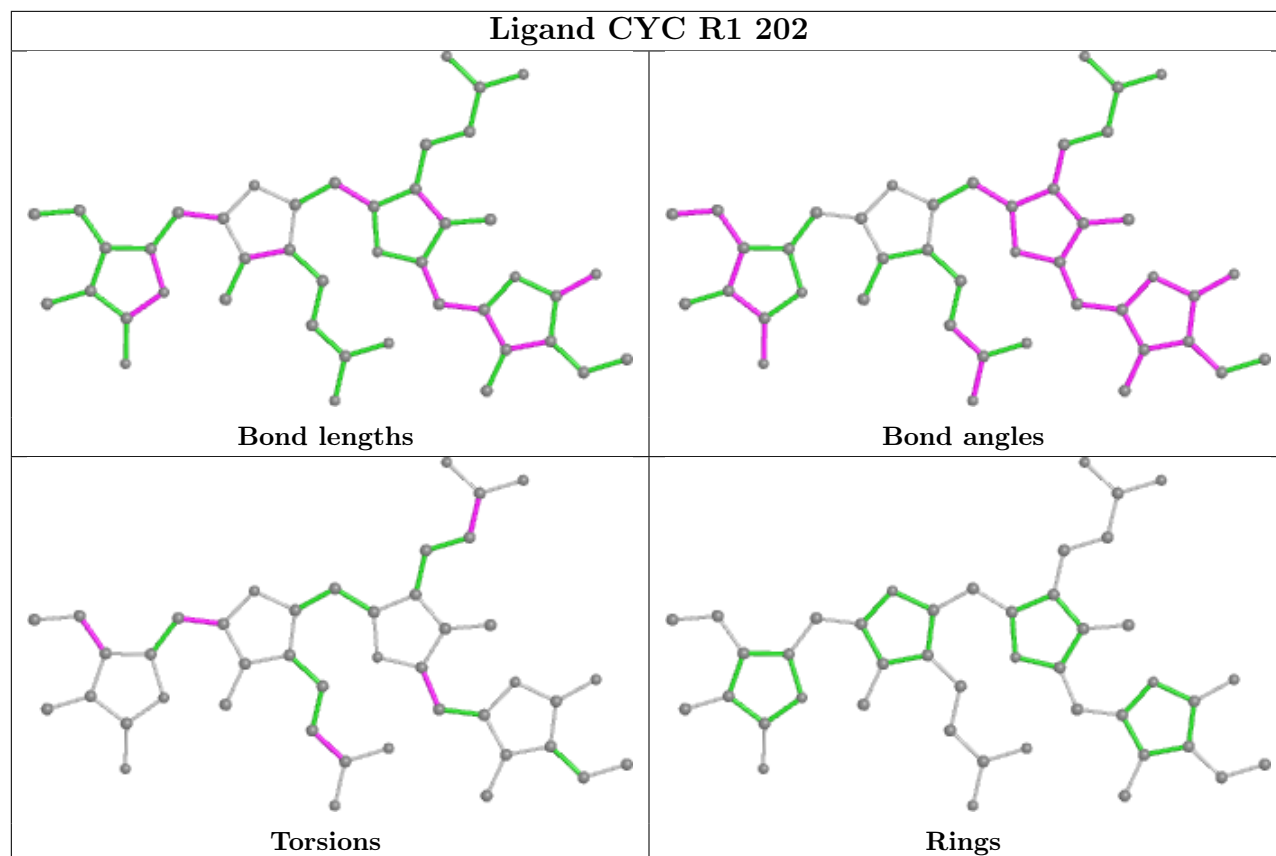
Ligand CYC L8 201



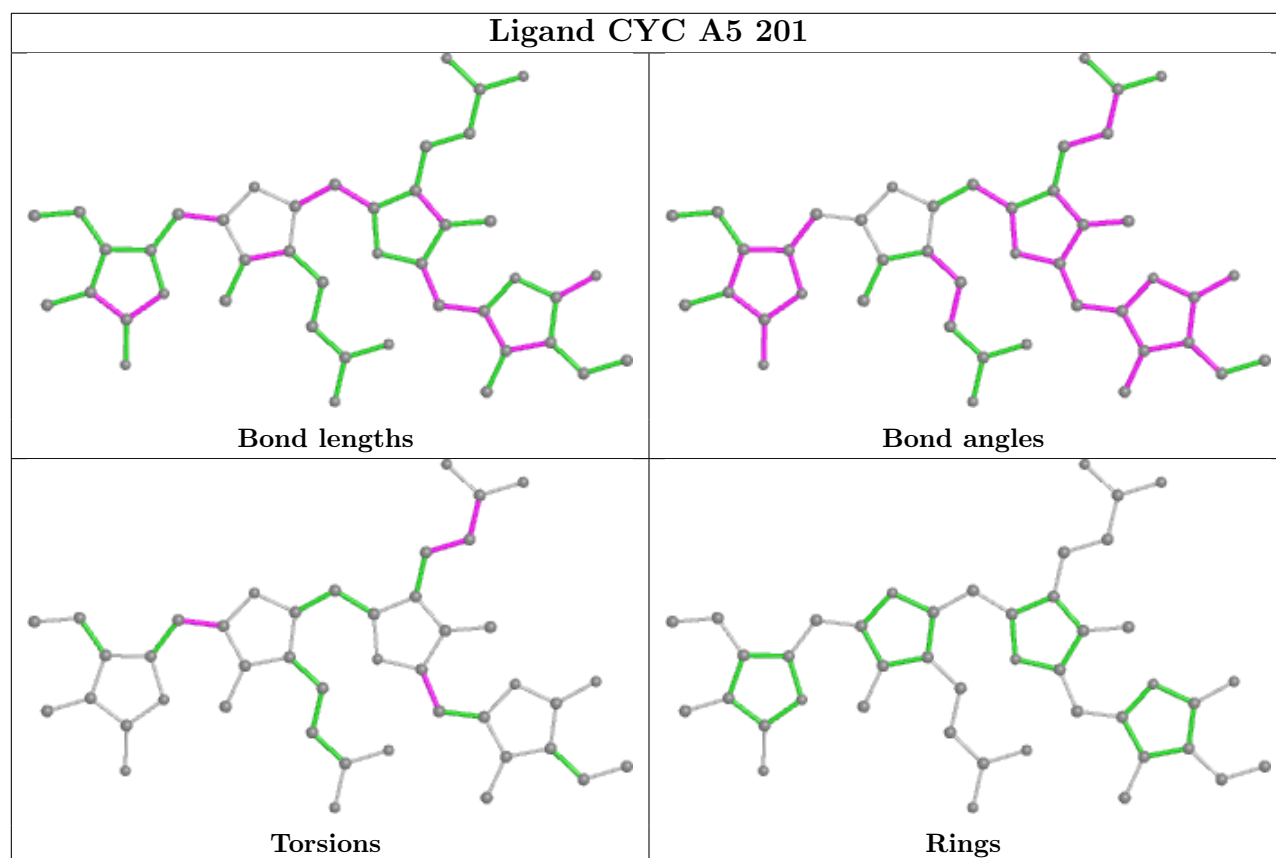
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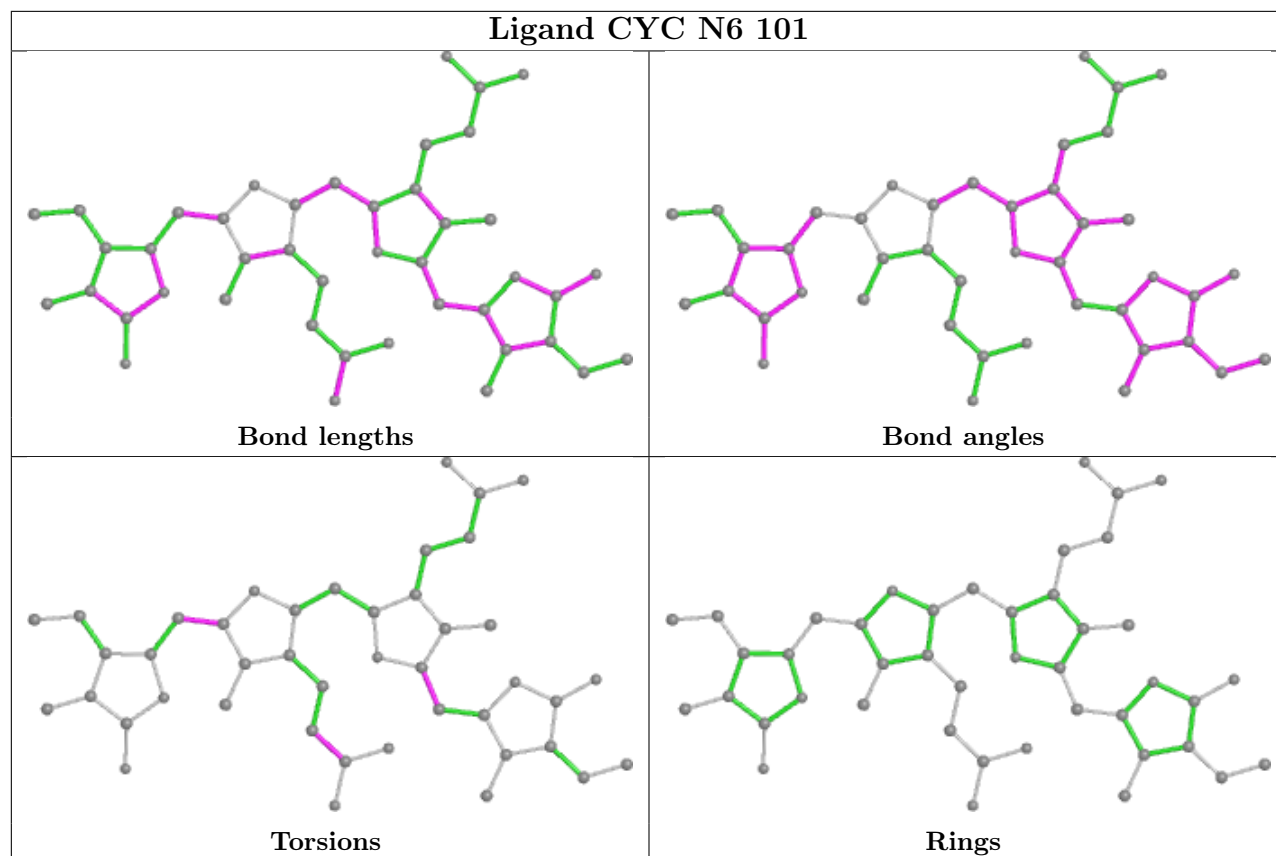
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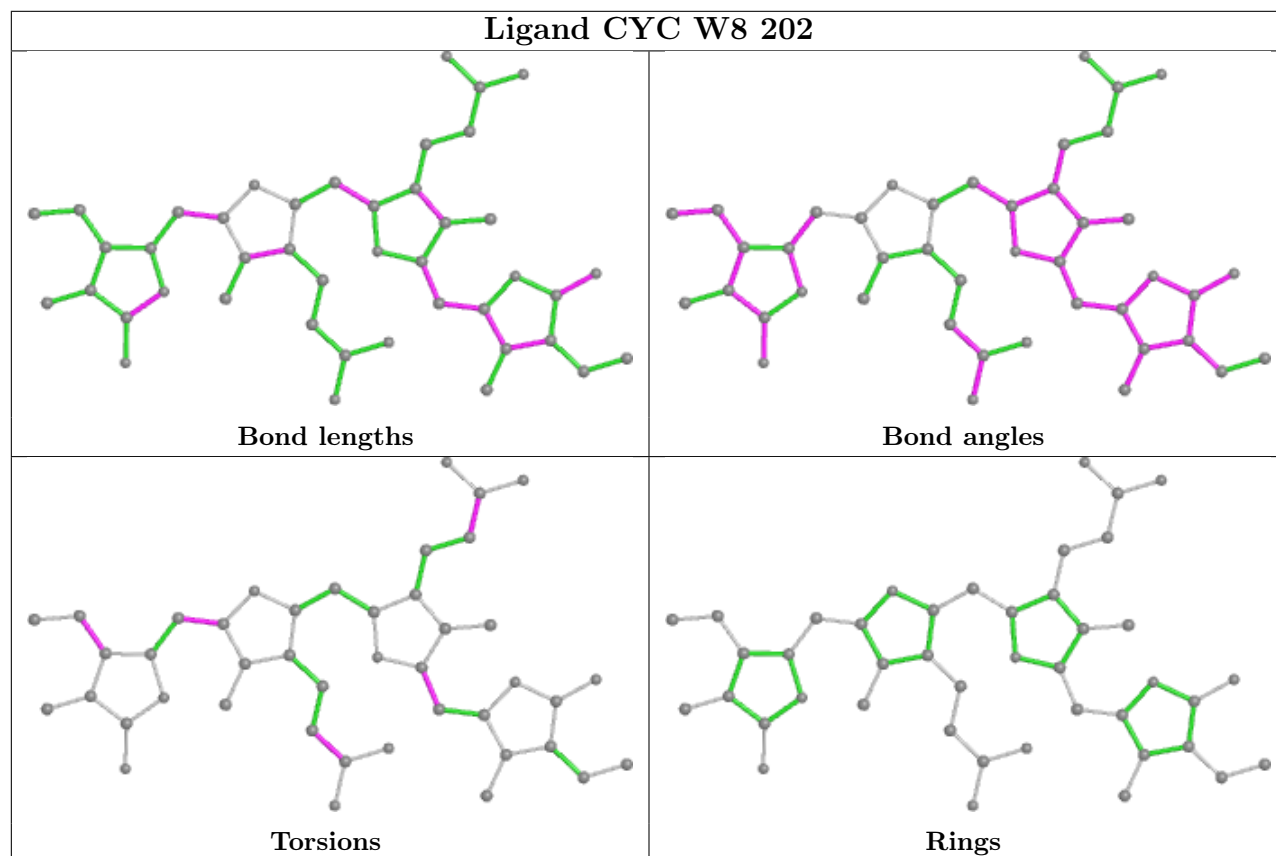
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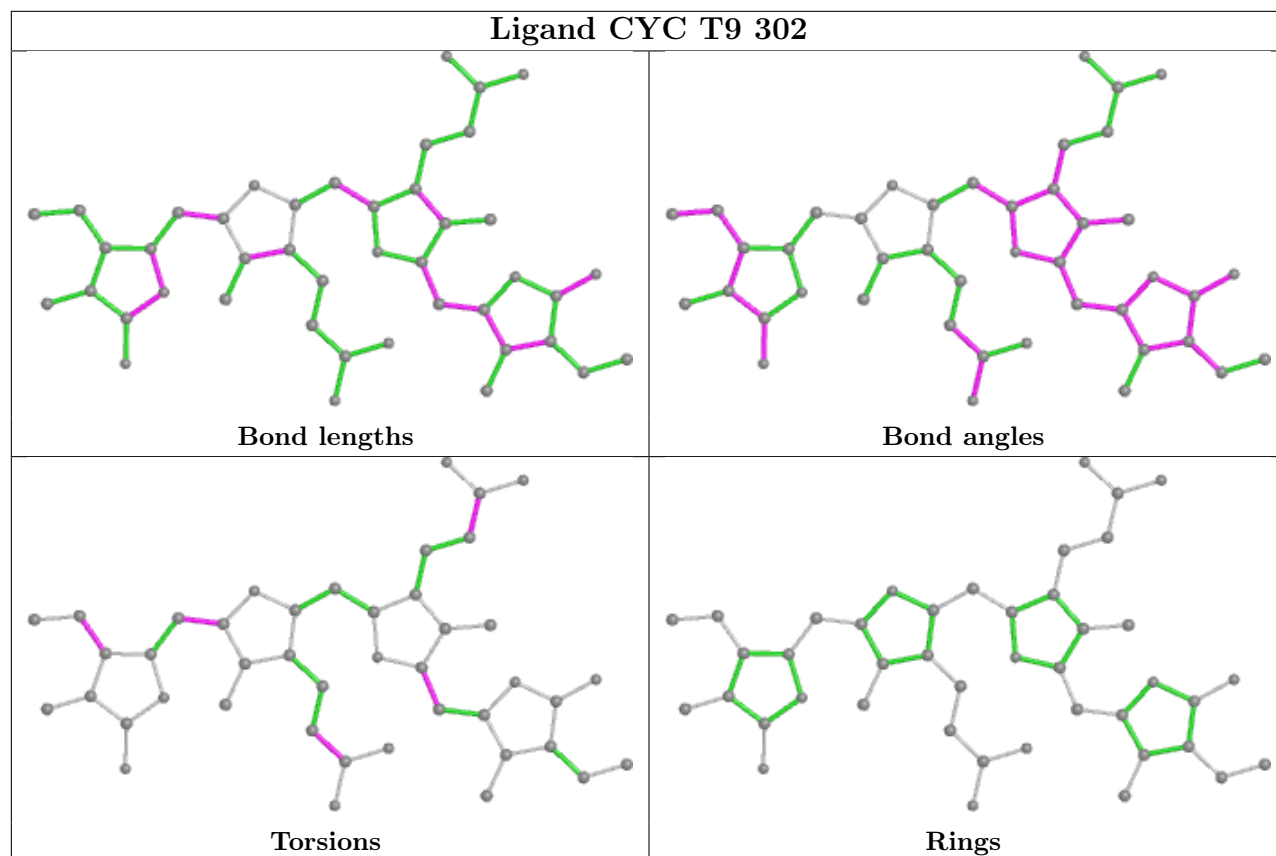
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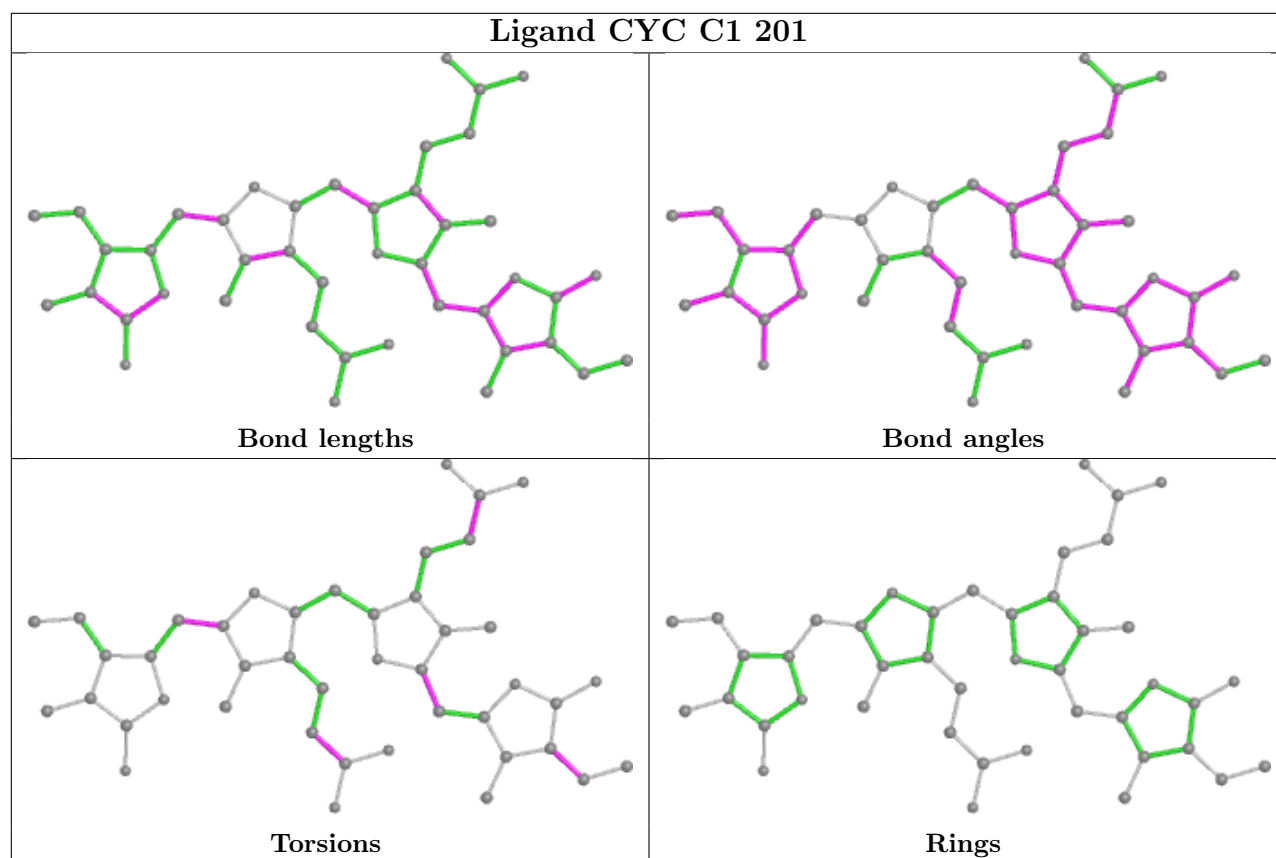
Ligand CYC W8 202



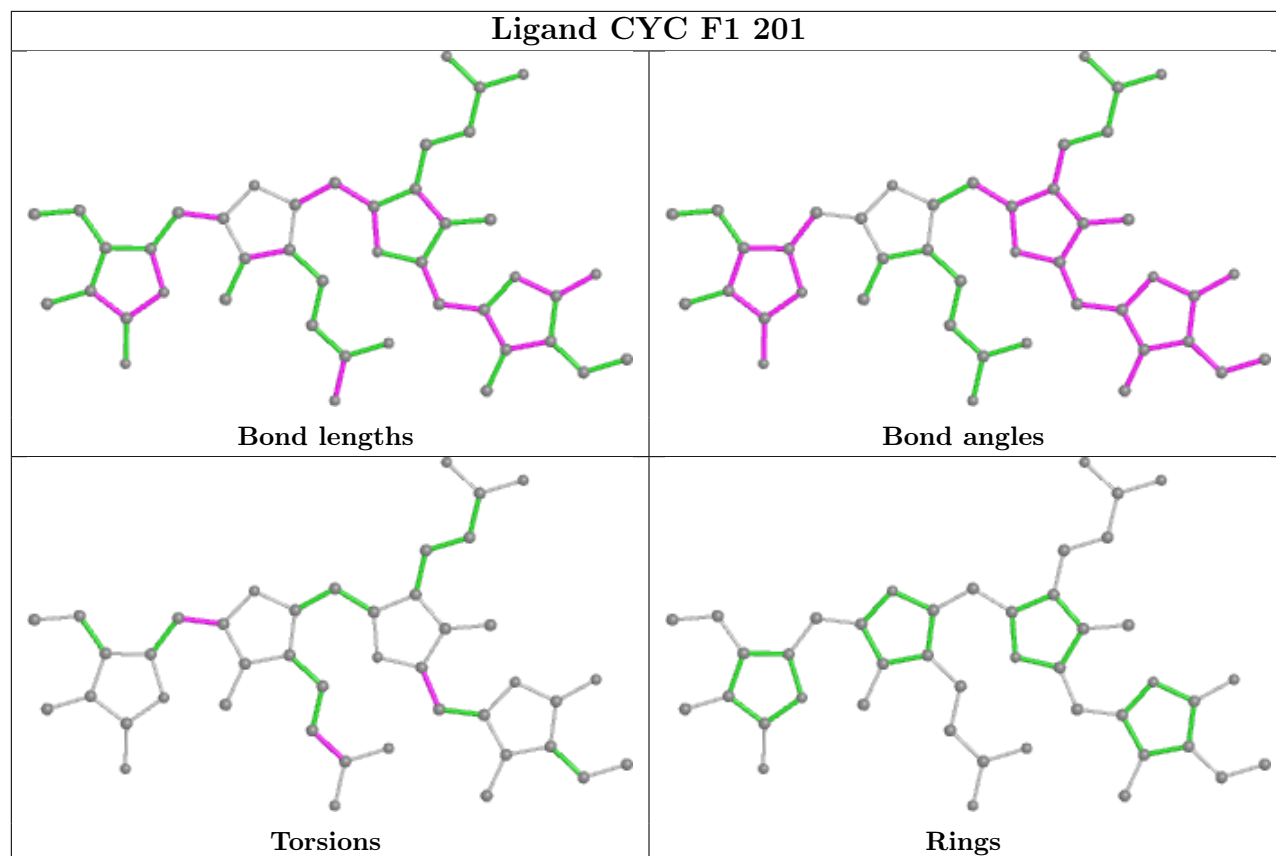
Ligand CYC T9 302



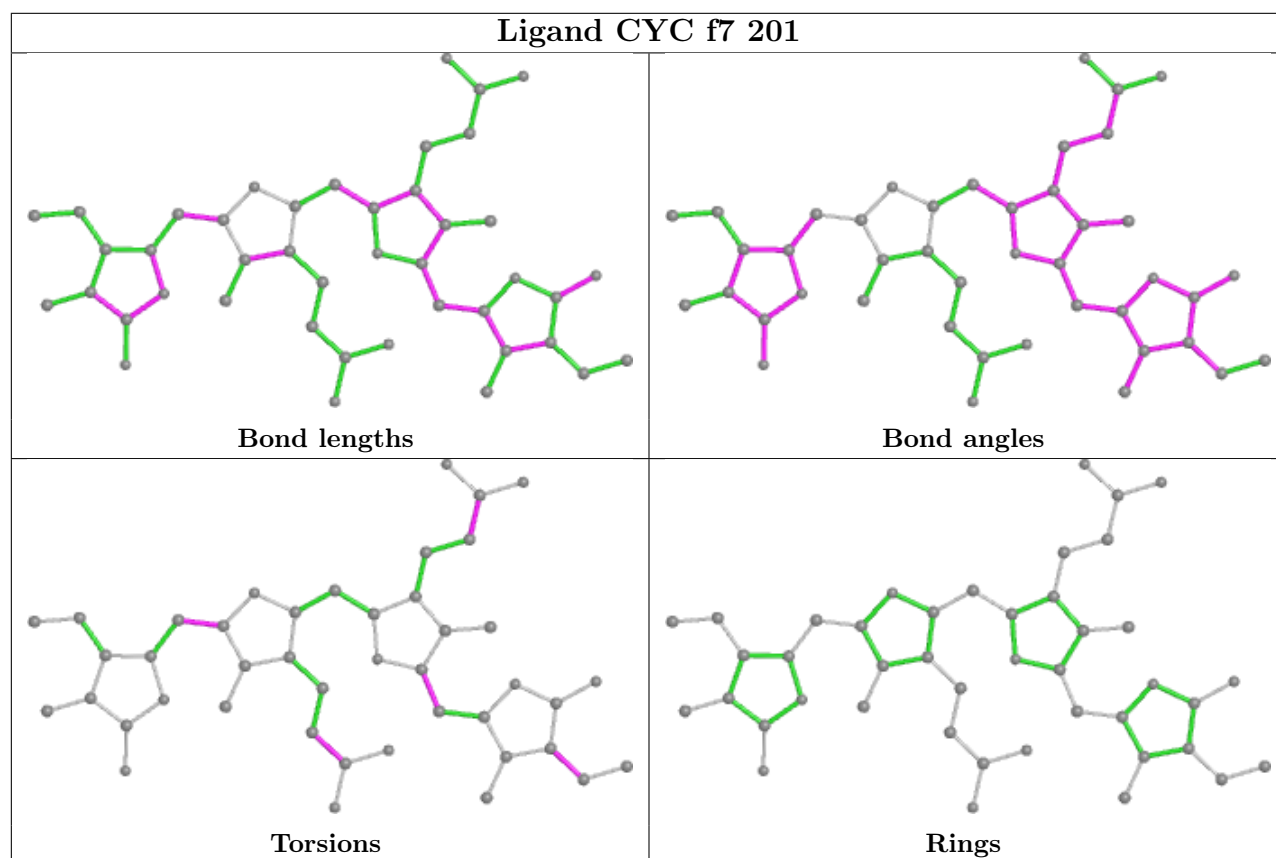
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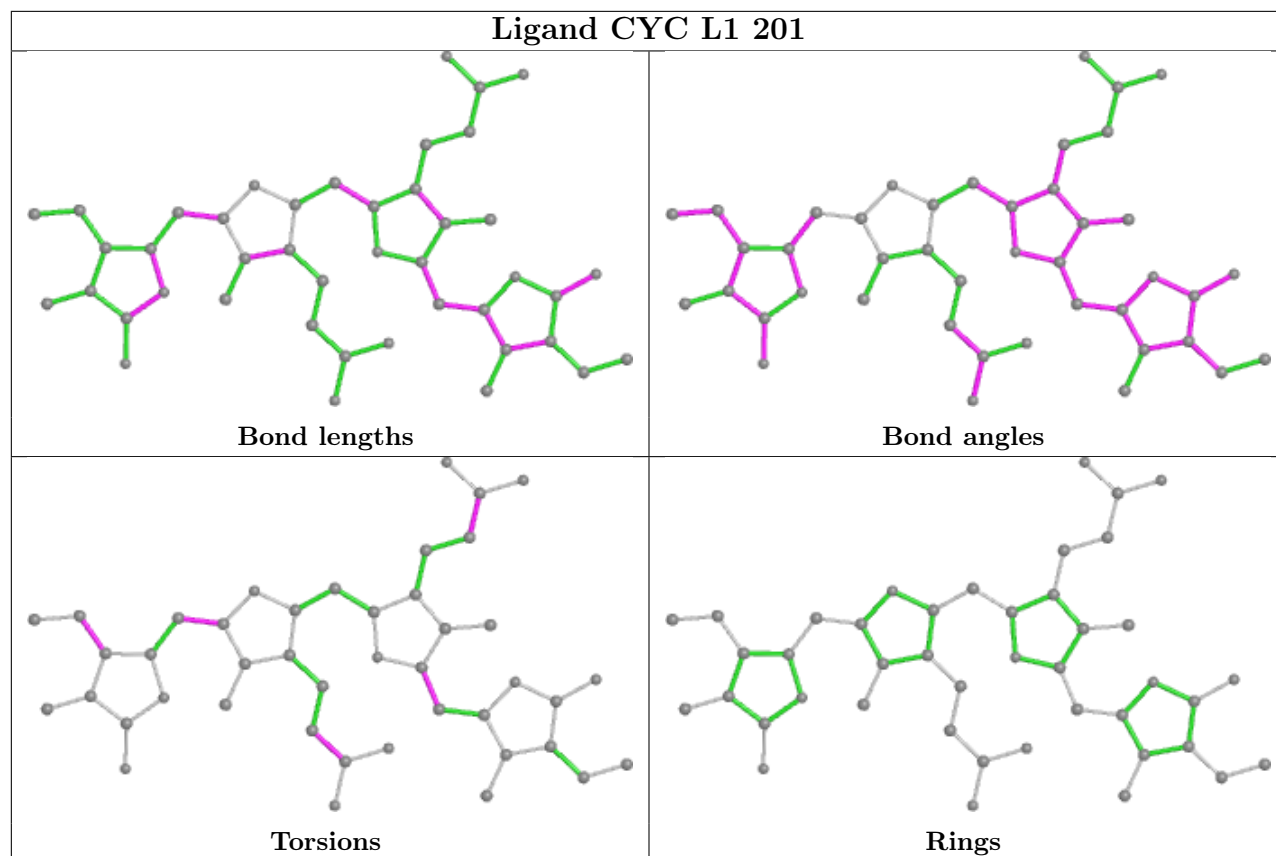
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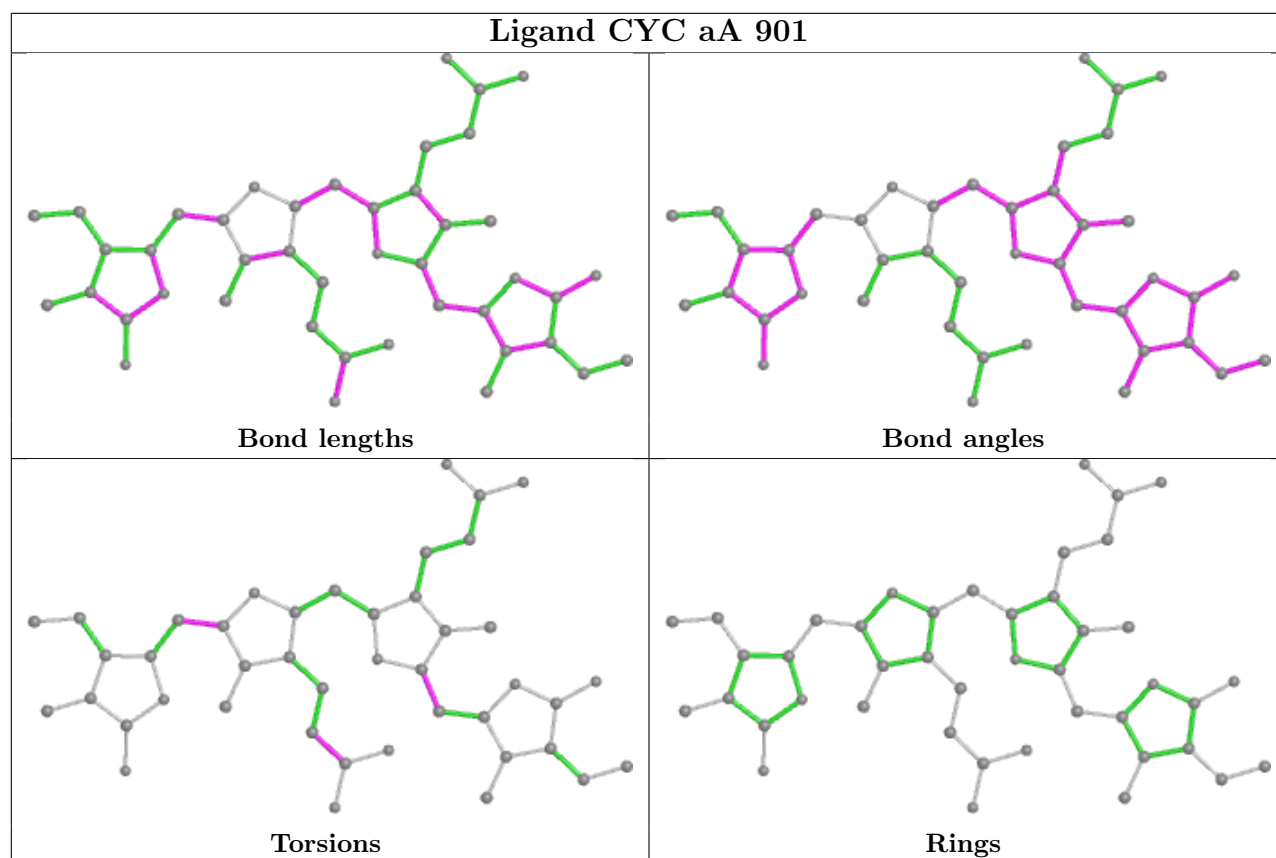
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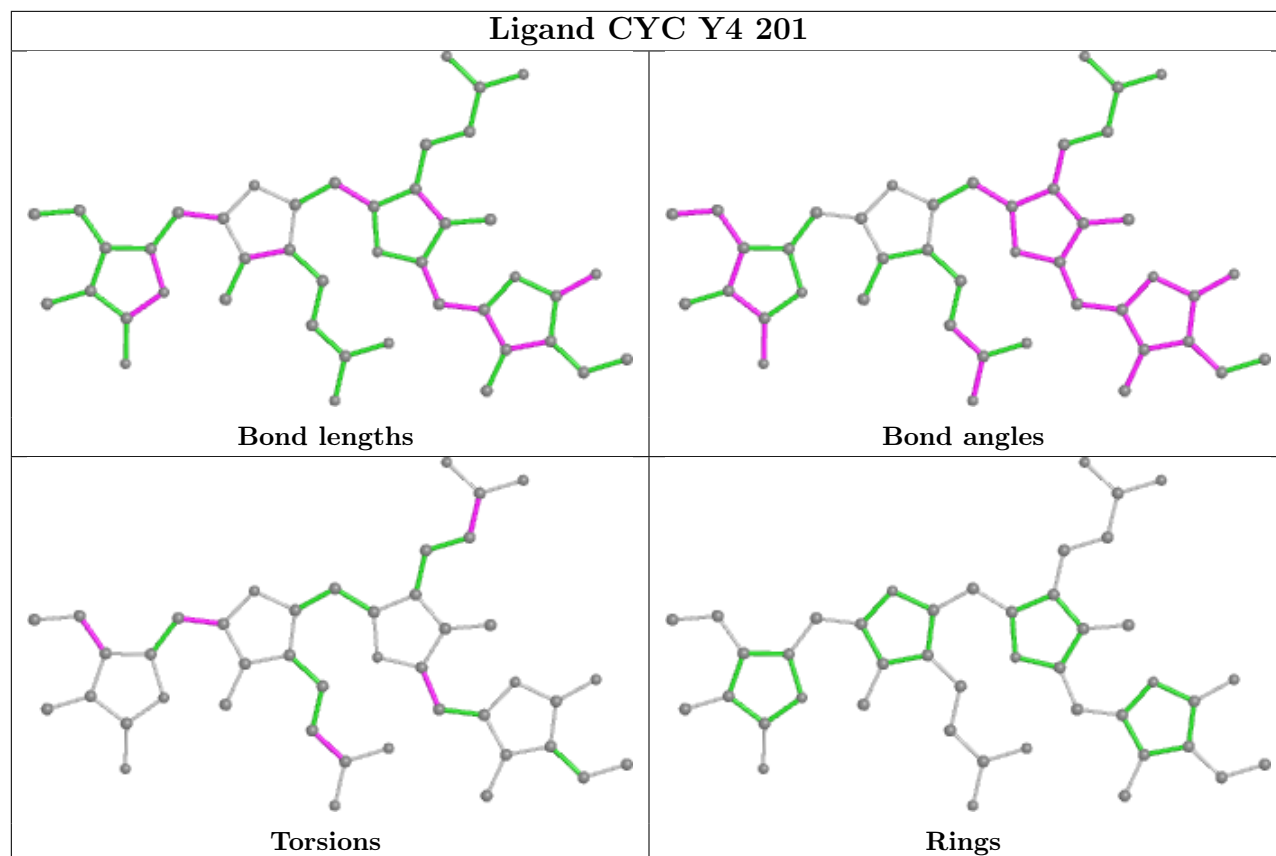
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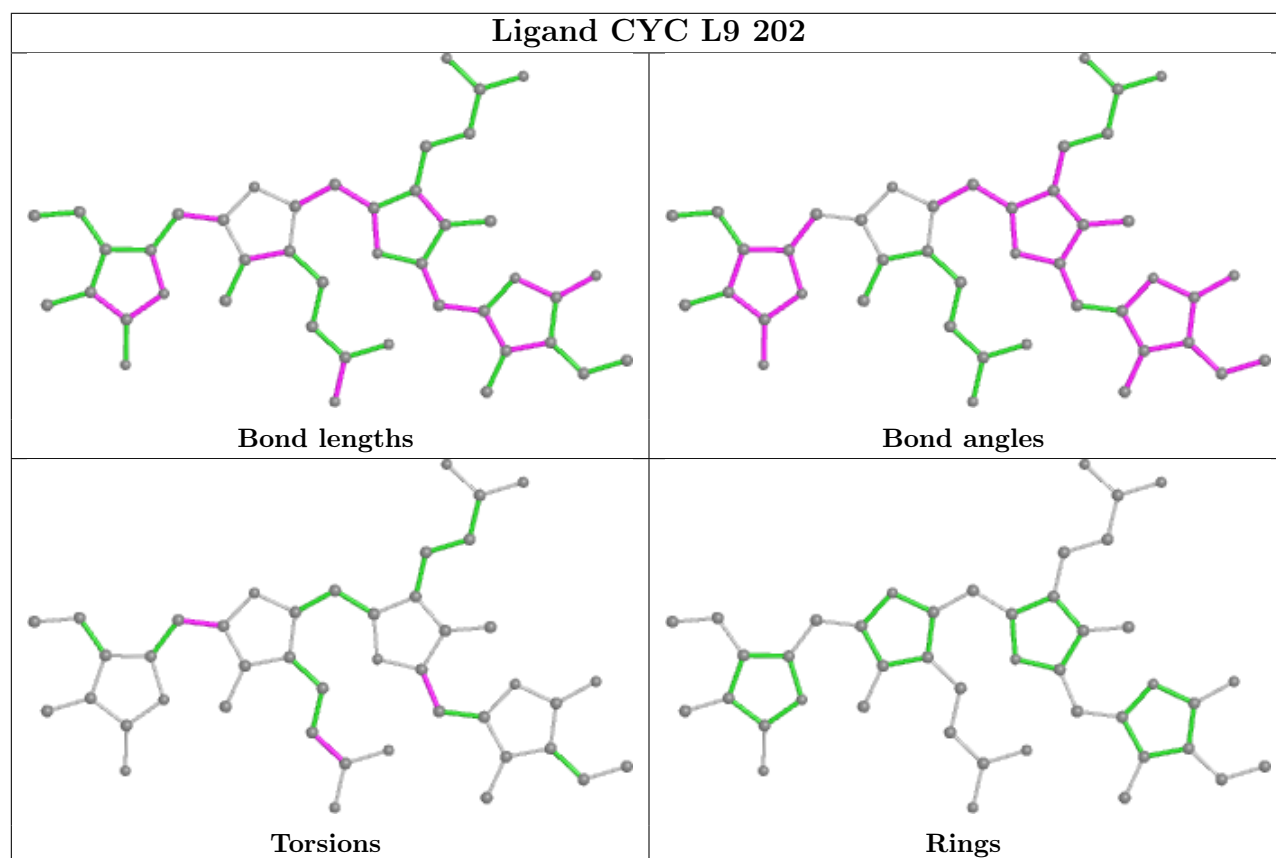
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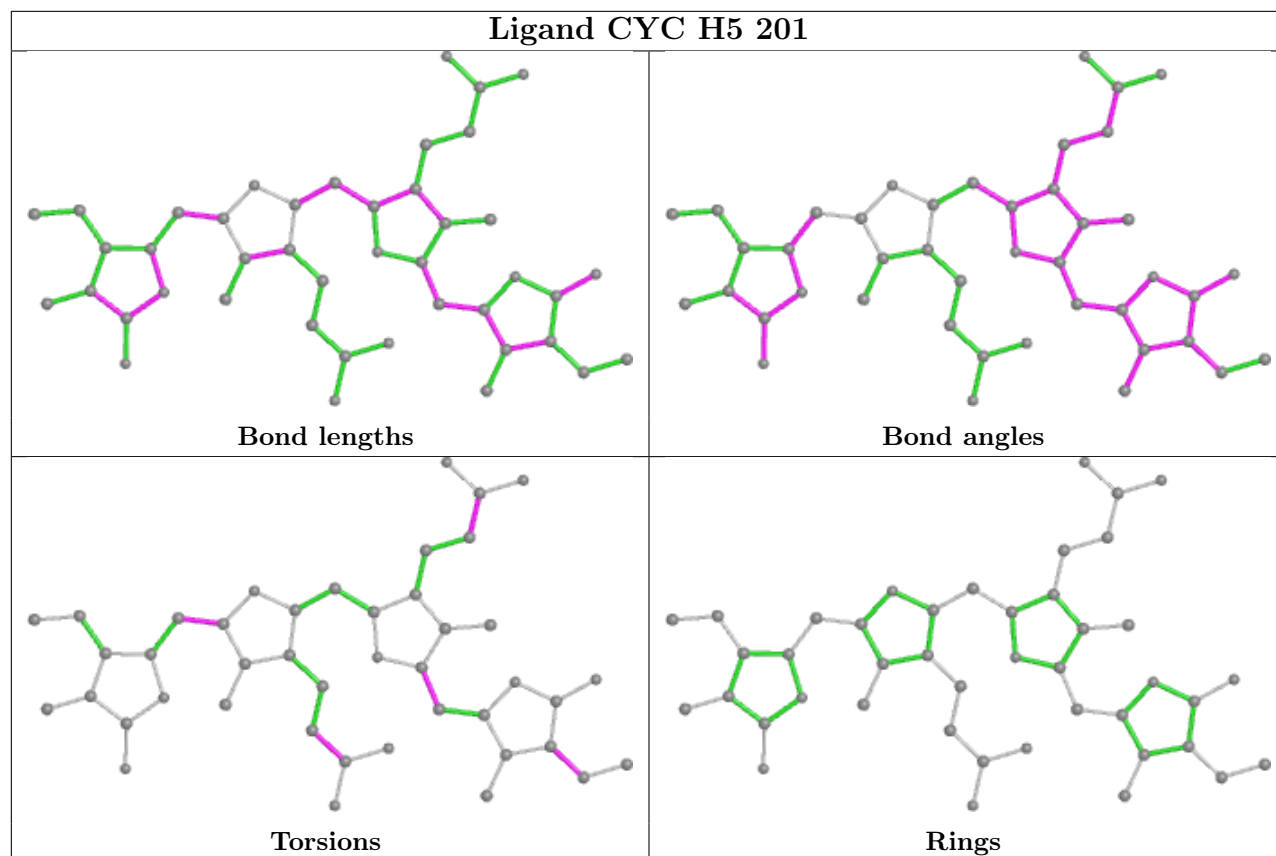
Ligand CYC Y4 201



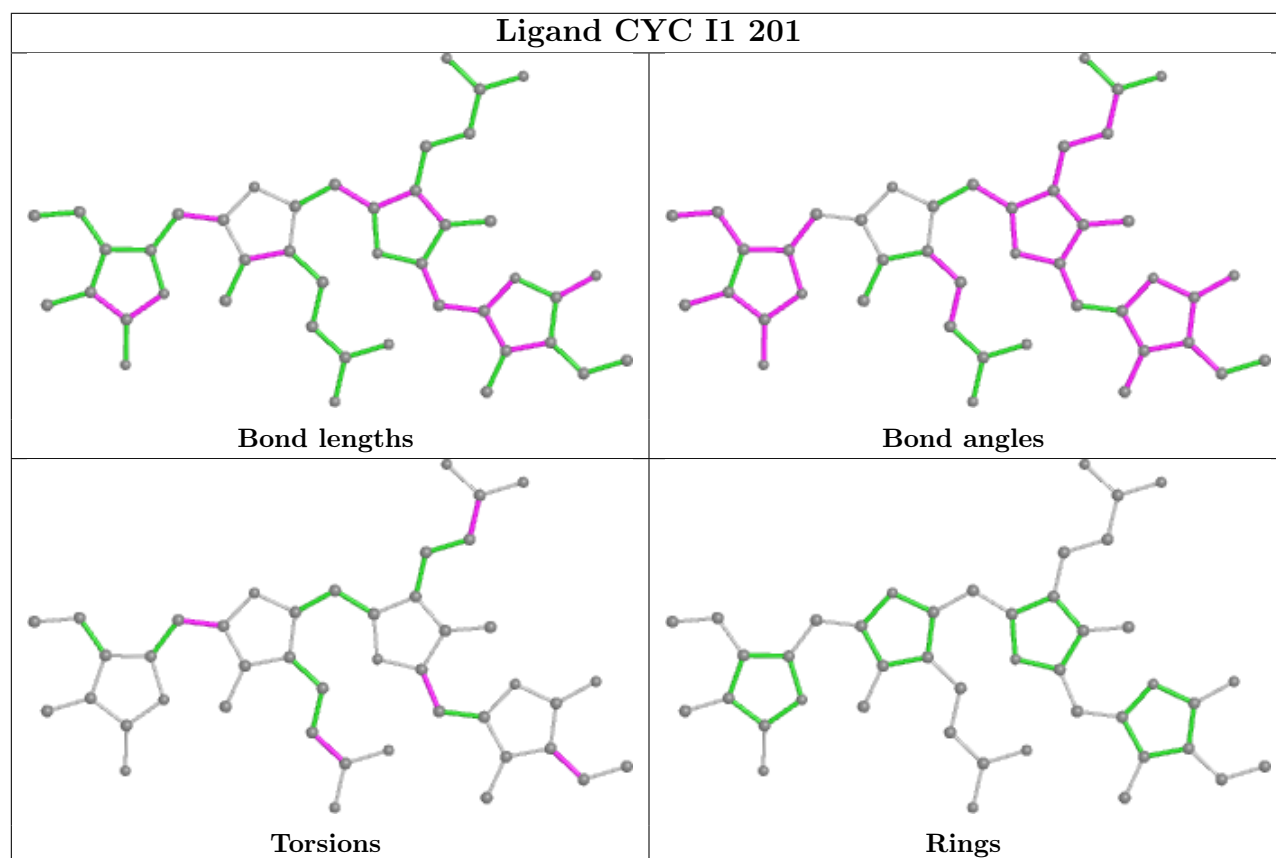
Ligand CYC L9 202

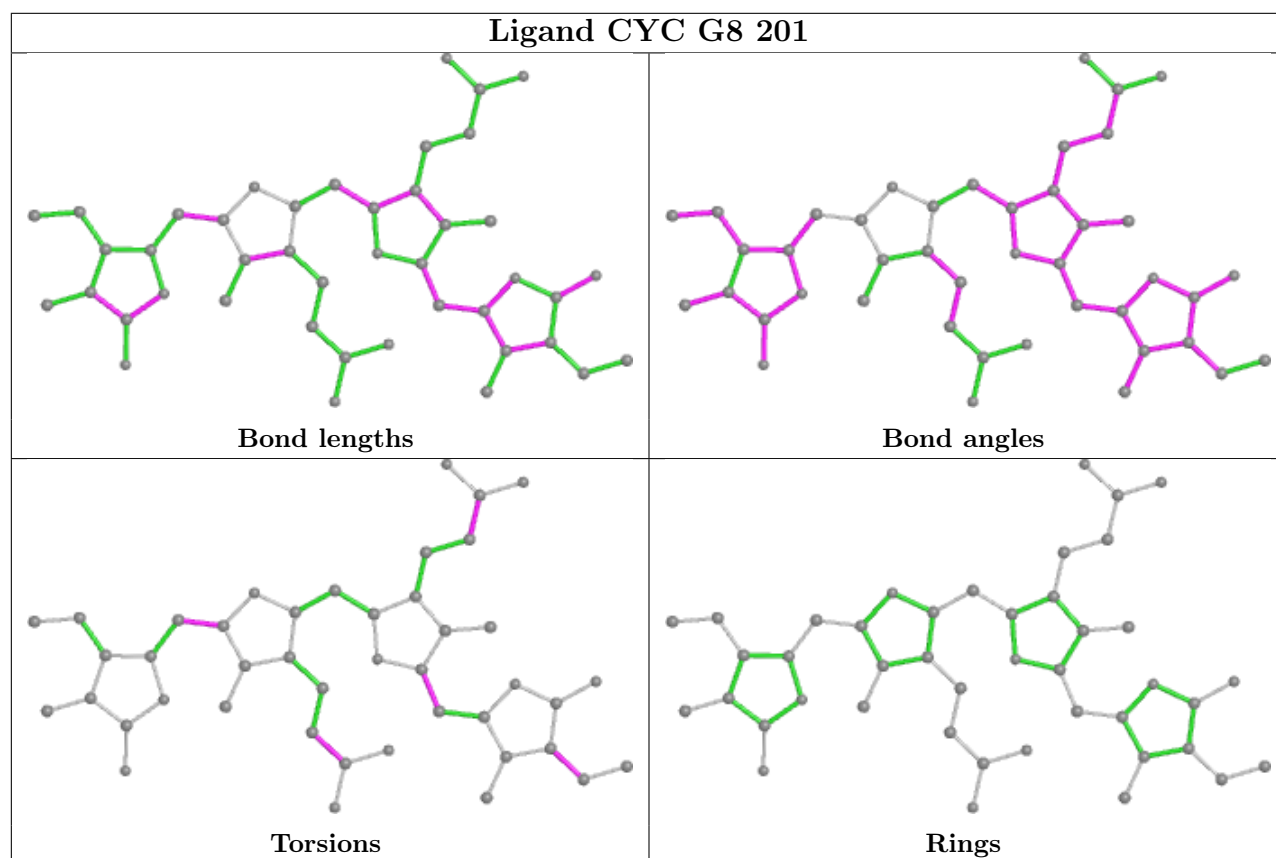
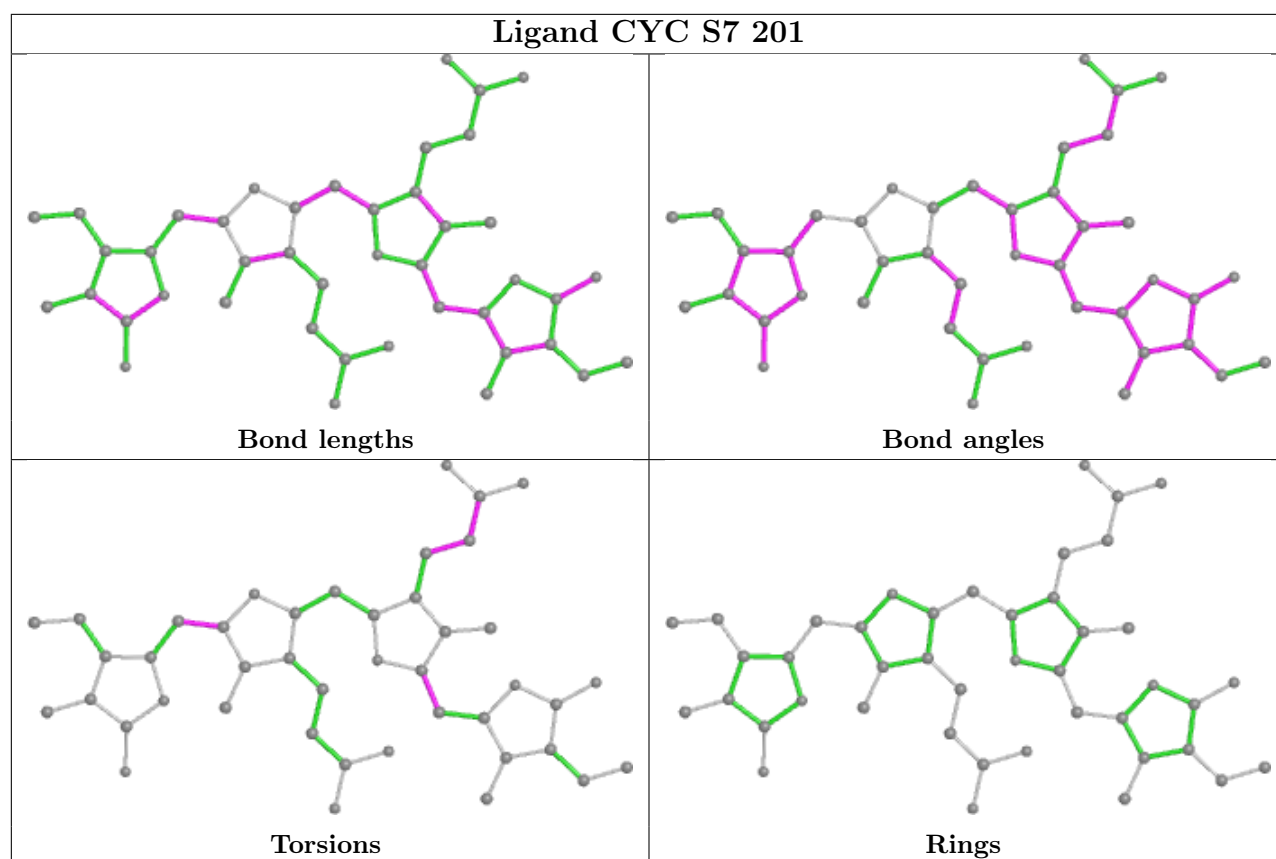


Ligand CYC H5 201

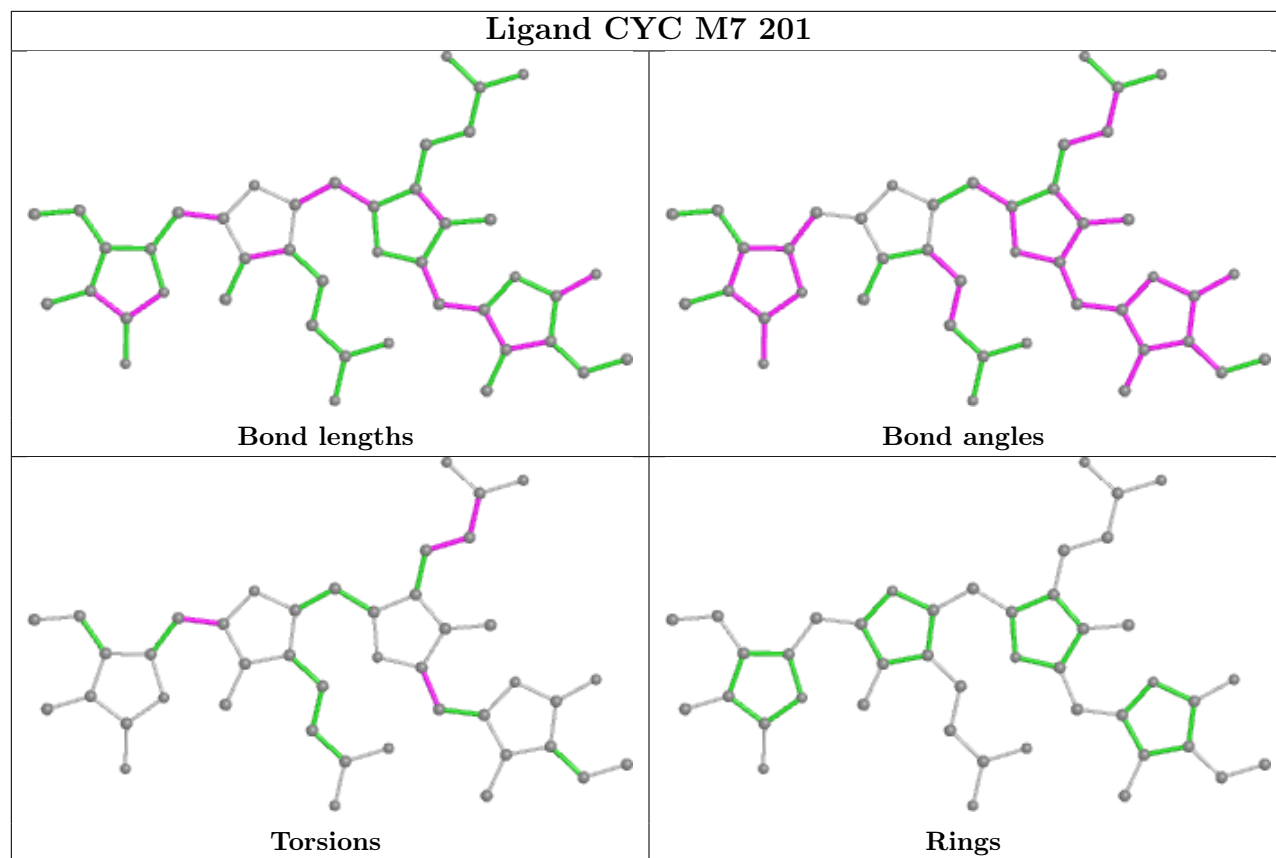


Ligand CYC I1 201

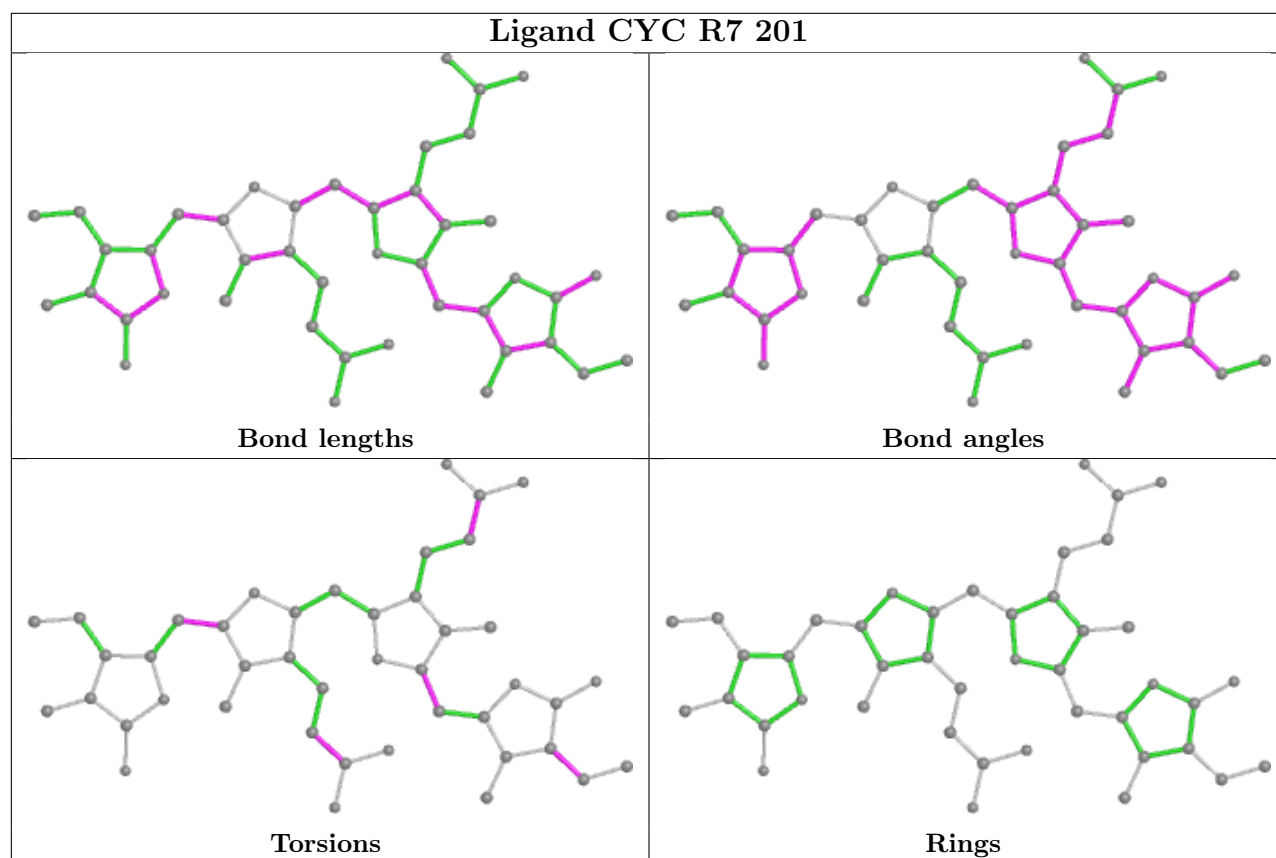


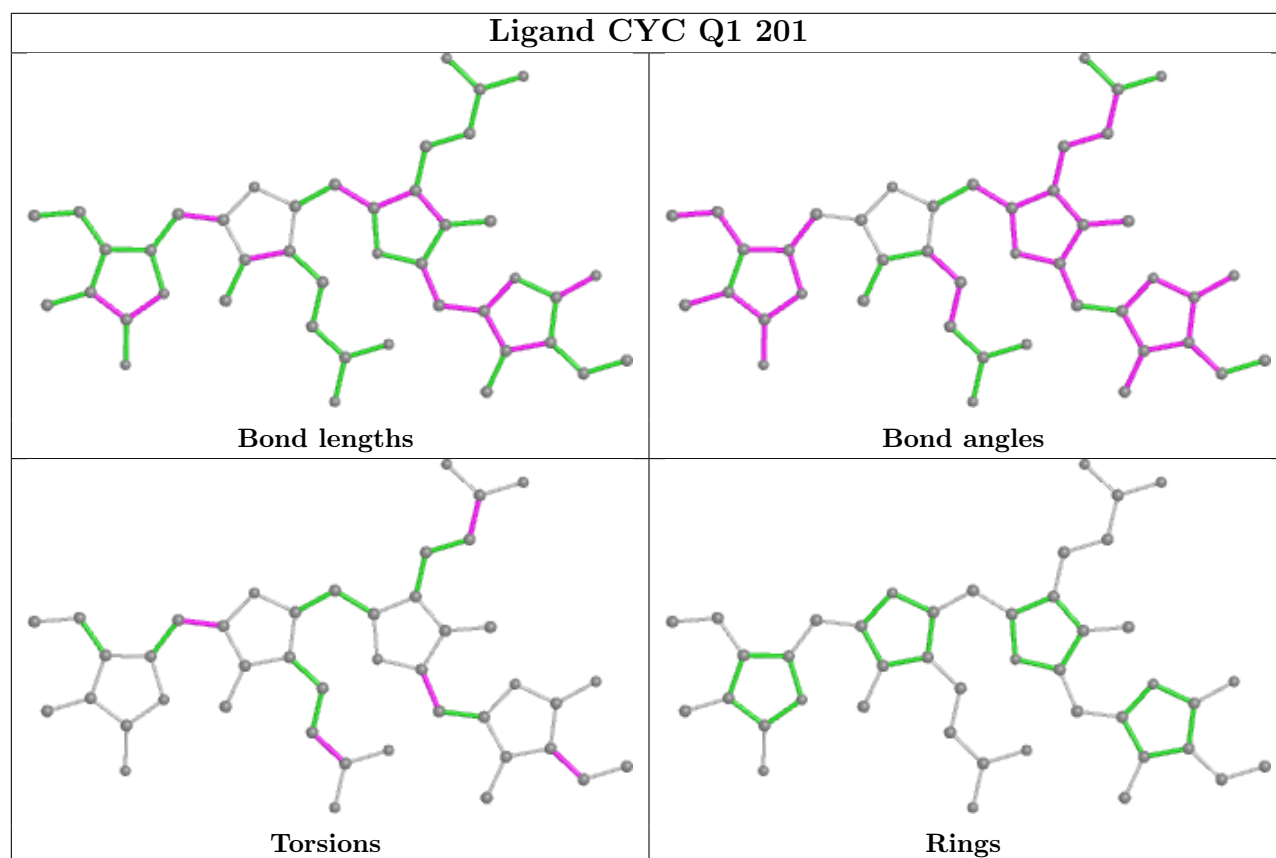
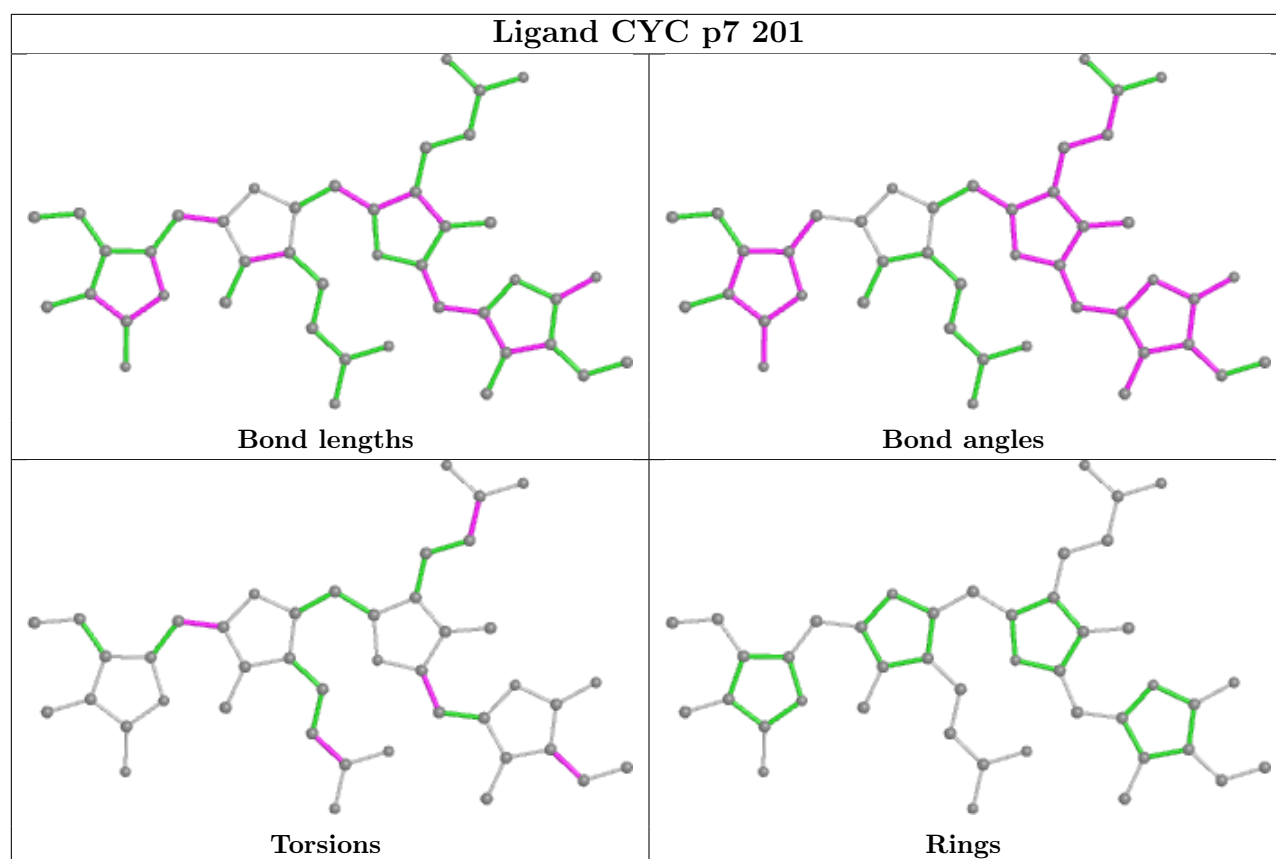


Ligand CYC M7 201

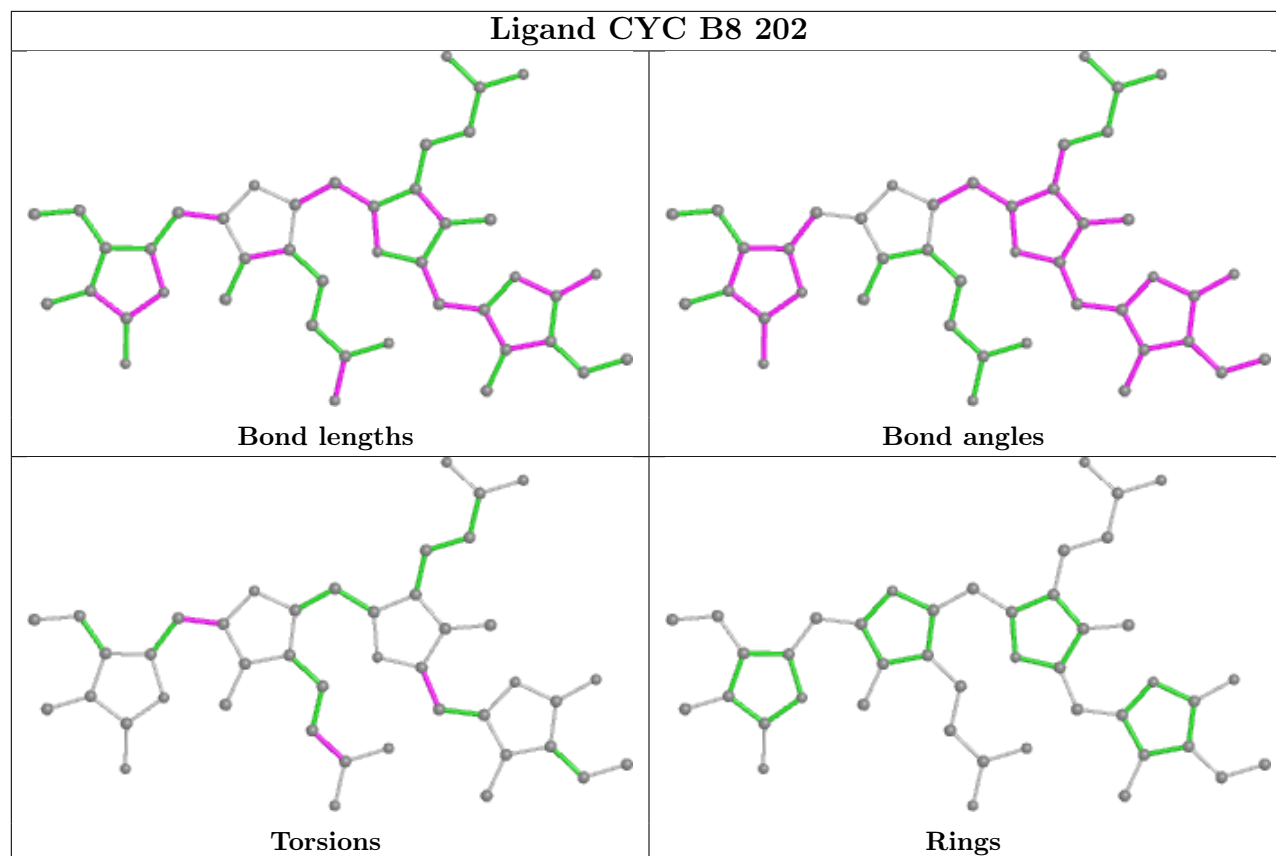


Ligand CYC R7 201

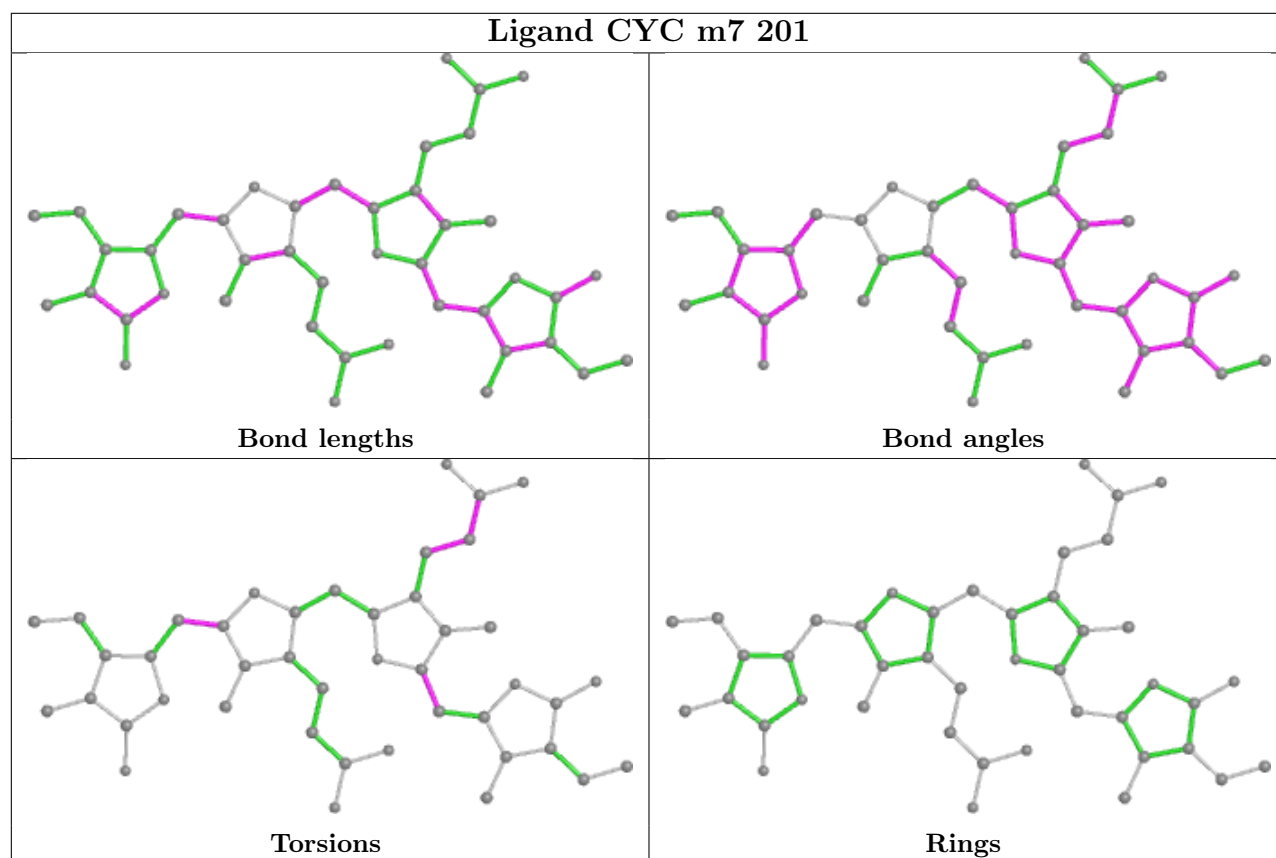




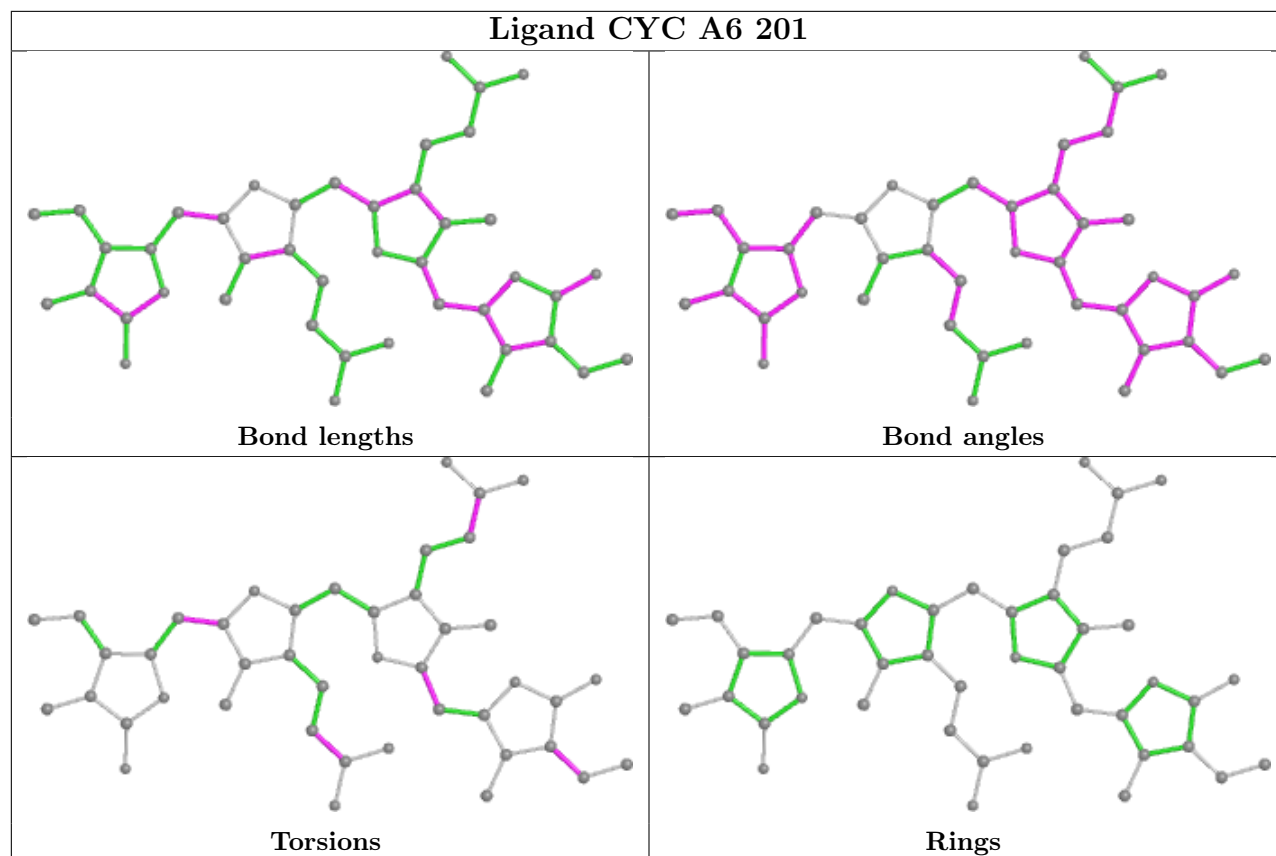
Ligand CYC B8 202



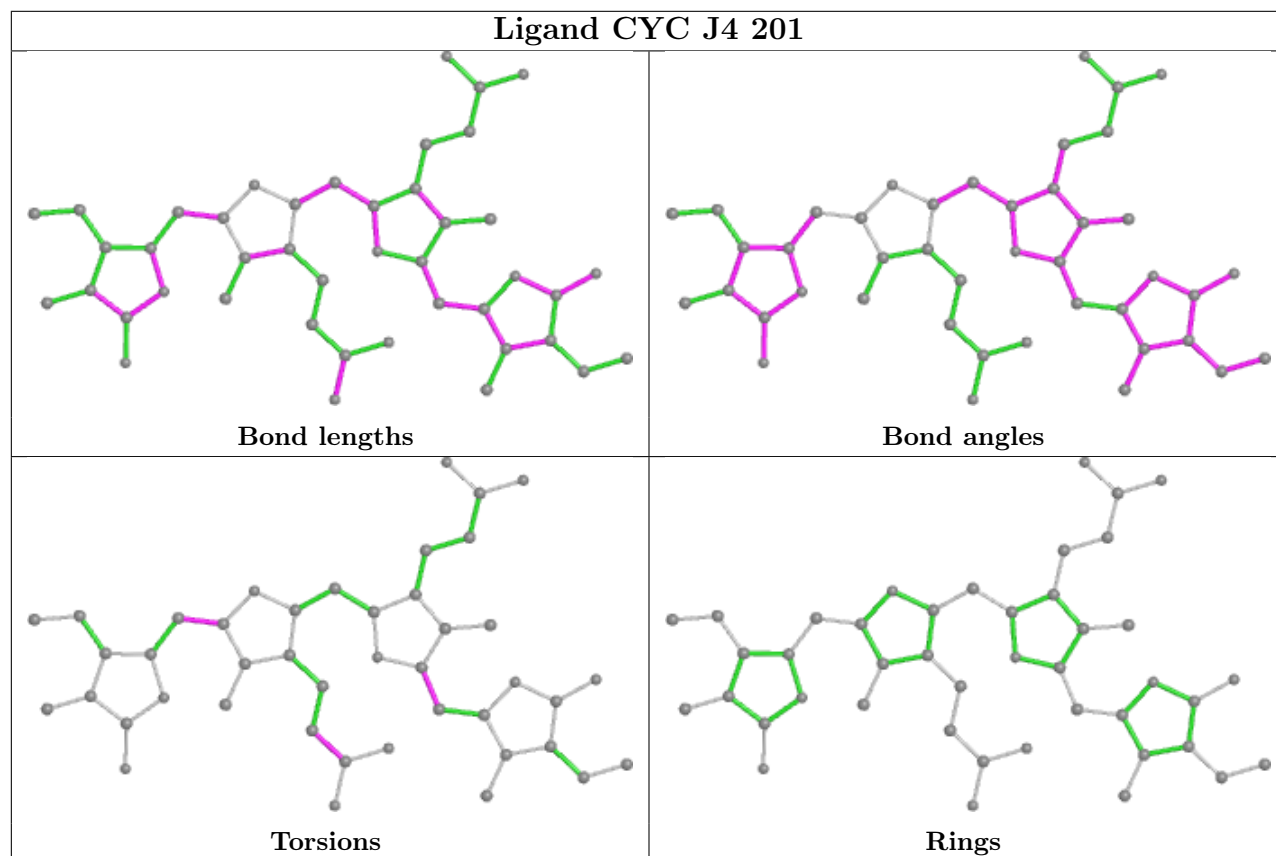
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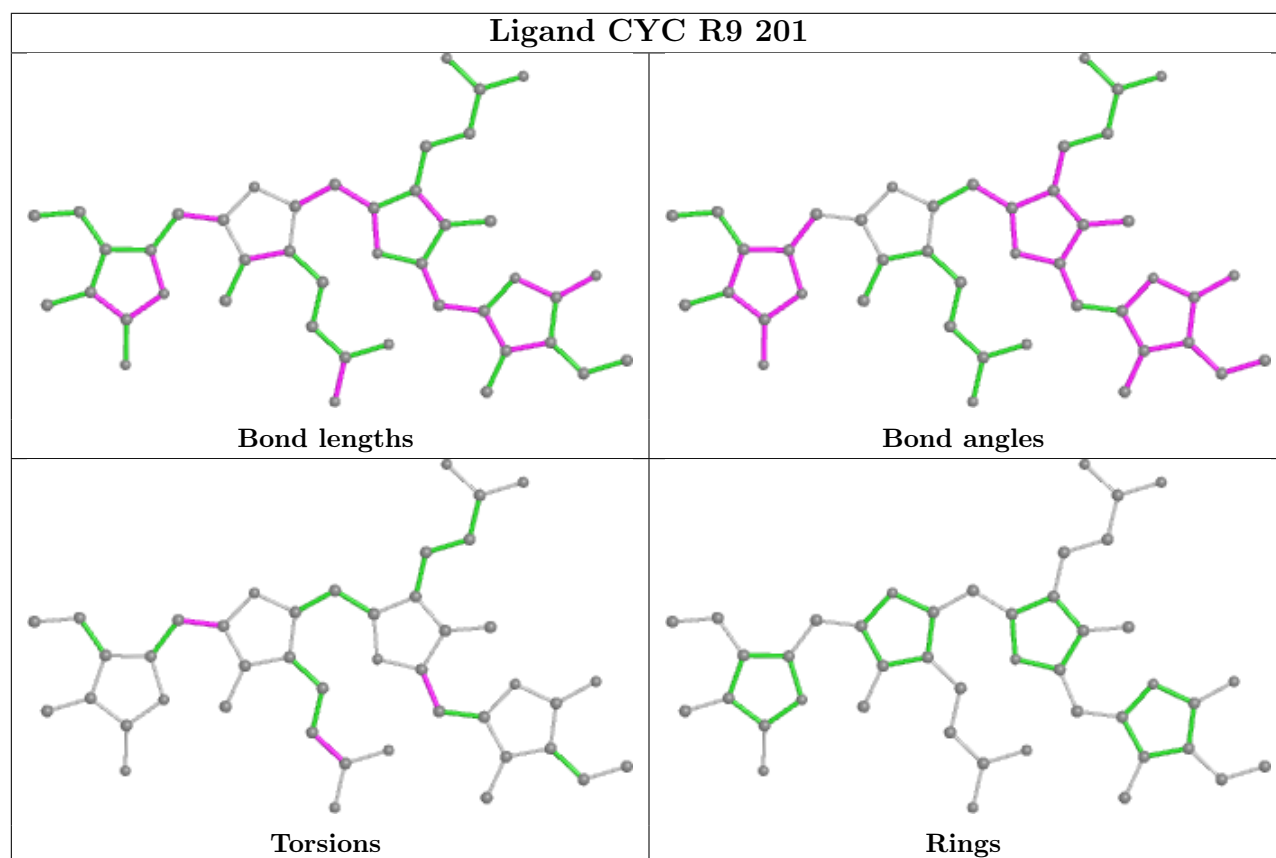
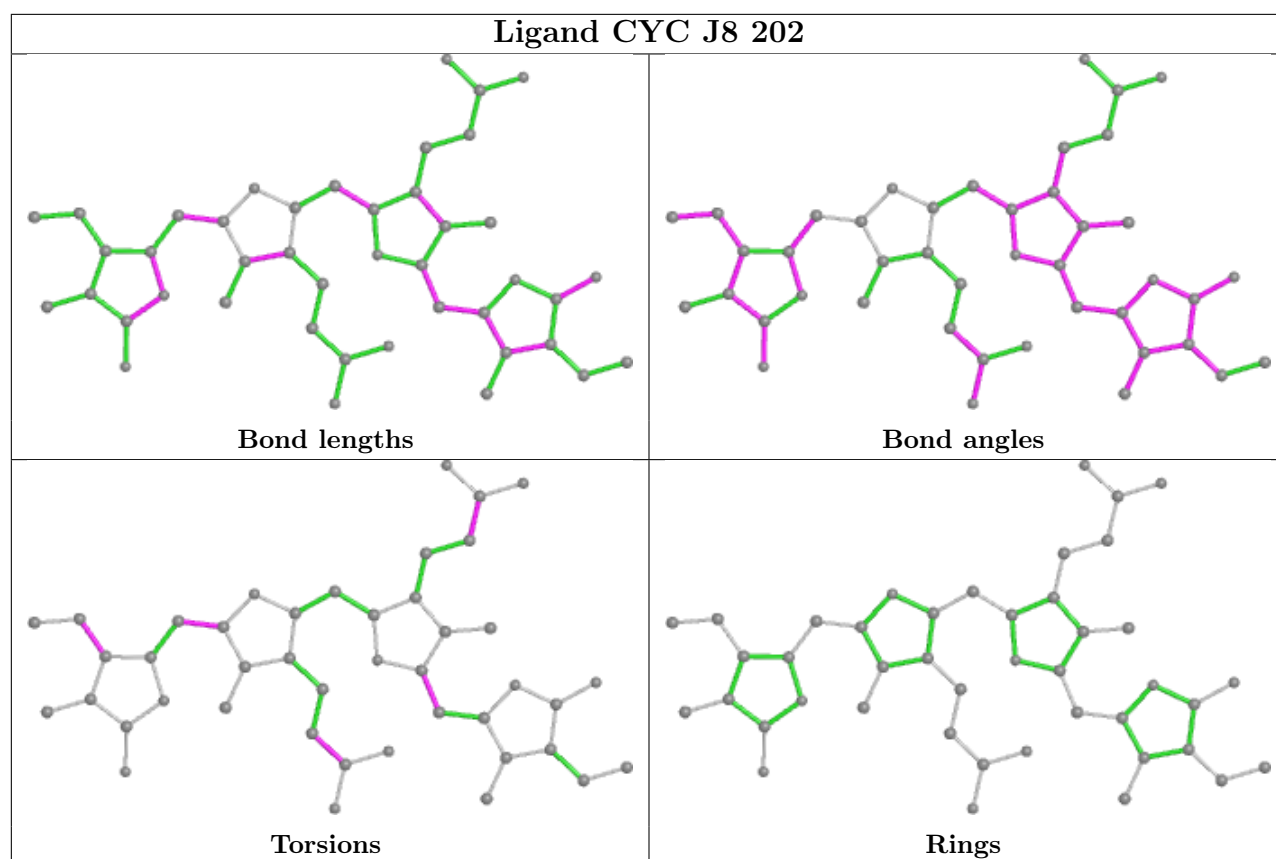


Ligand CYC A6 201

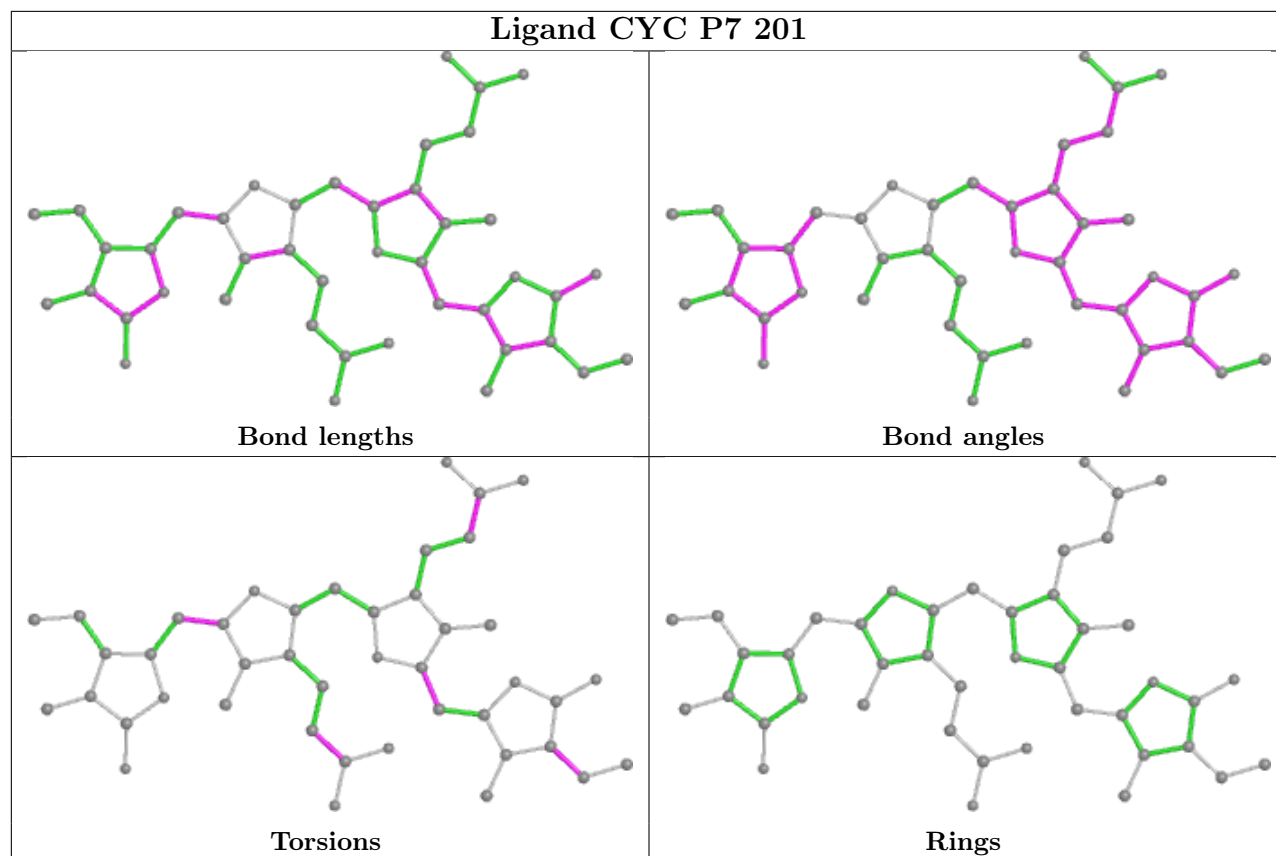


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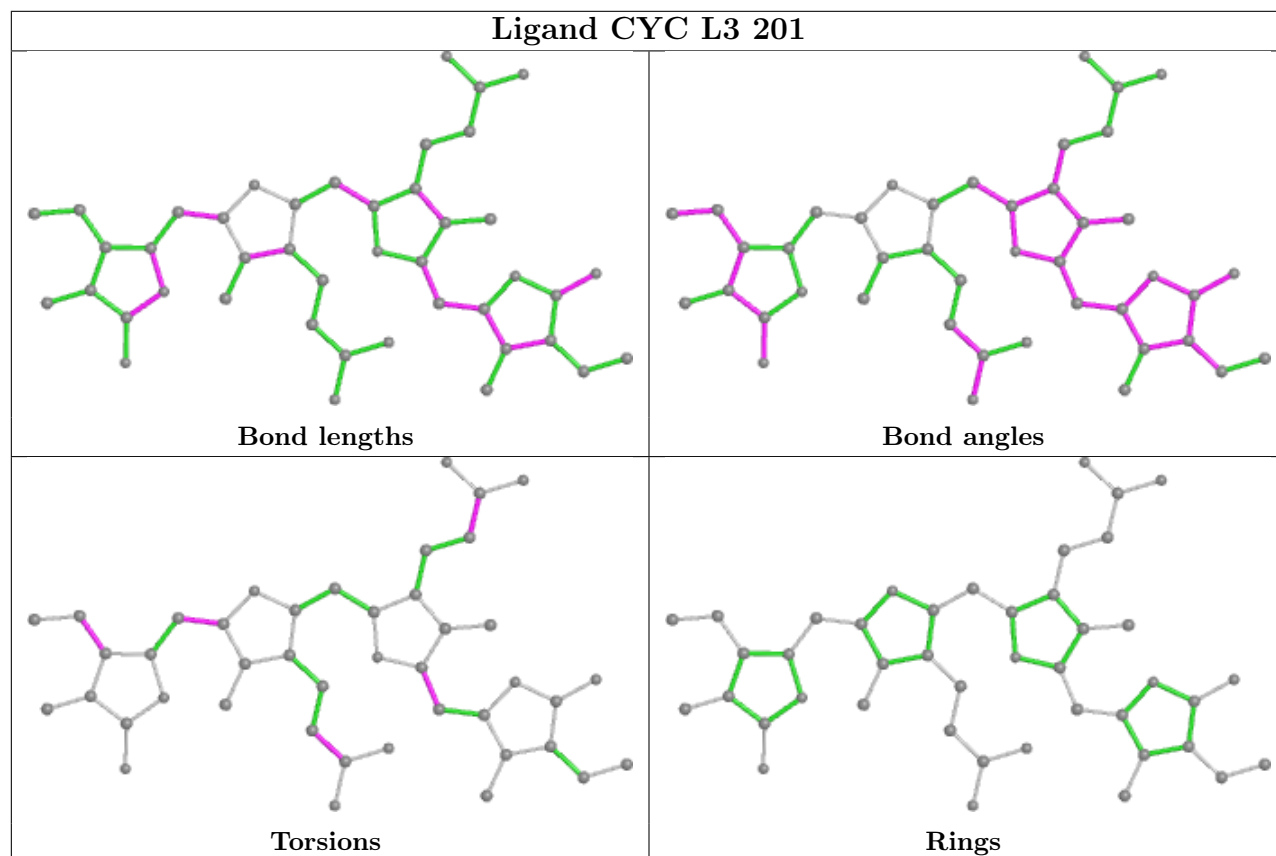




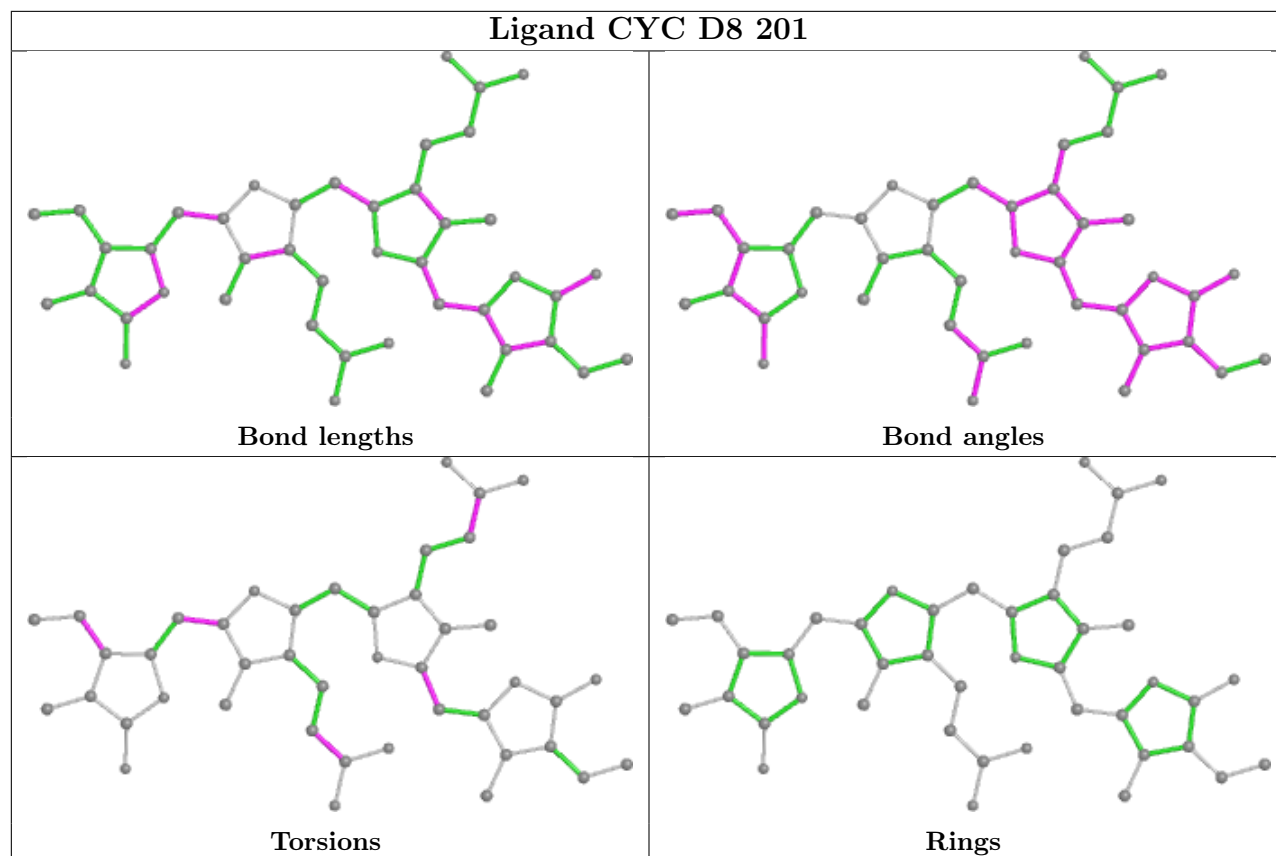
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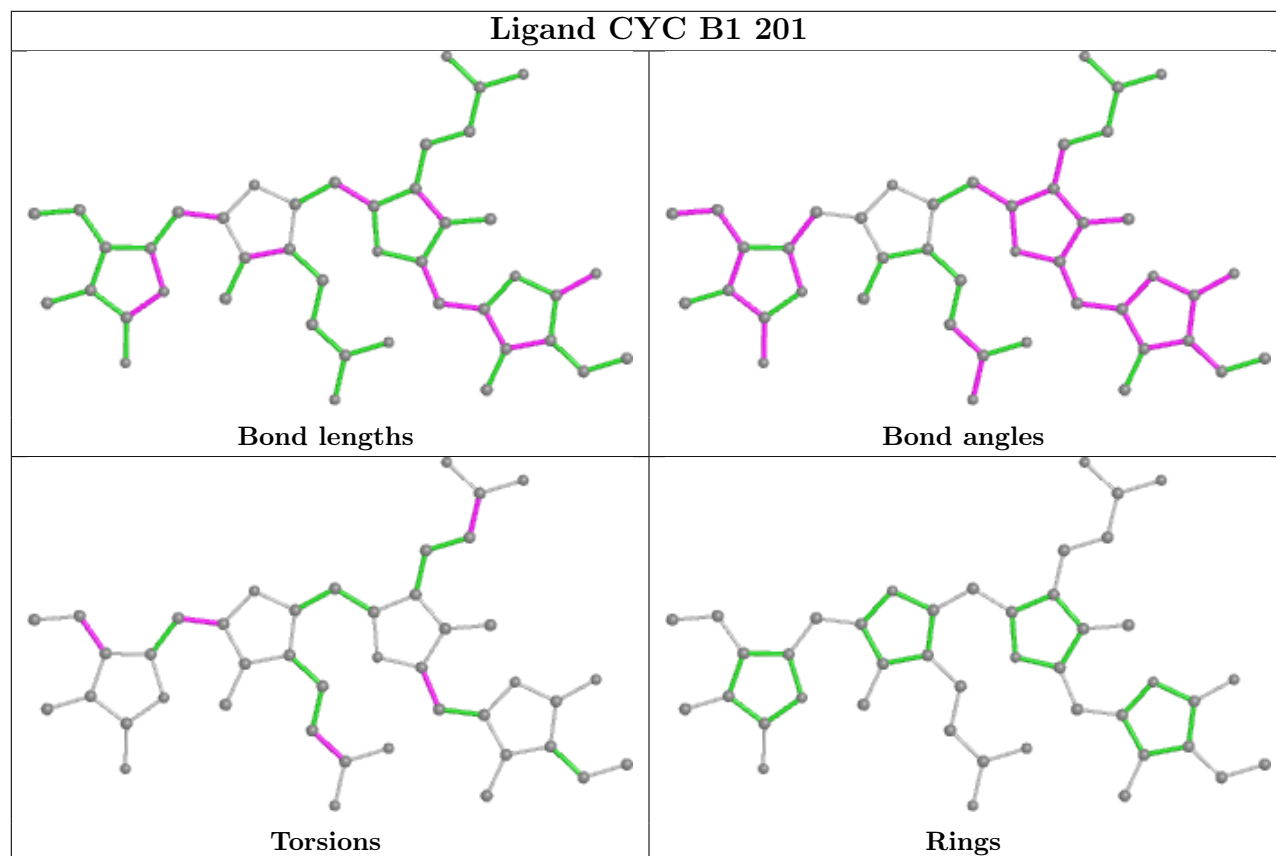
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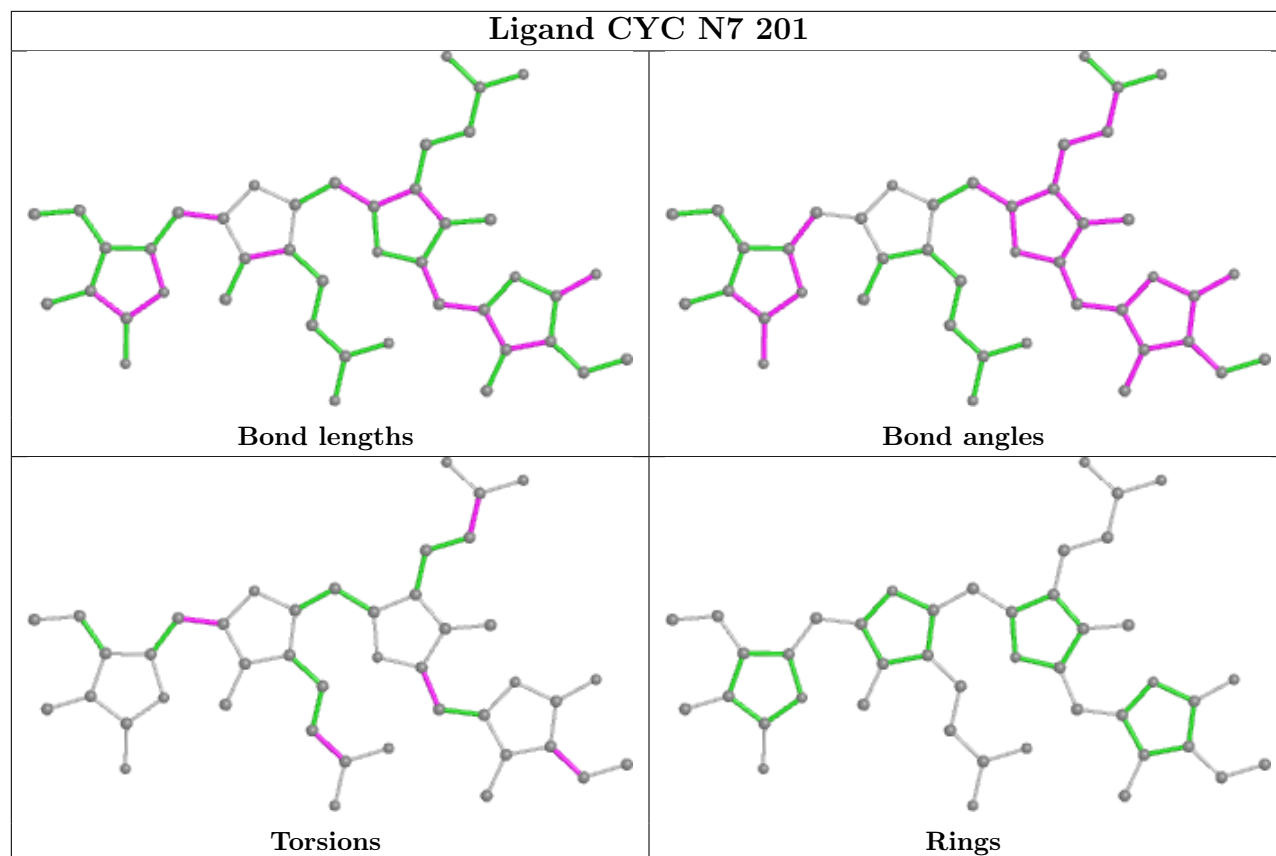
Ligand CYC D8 201



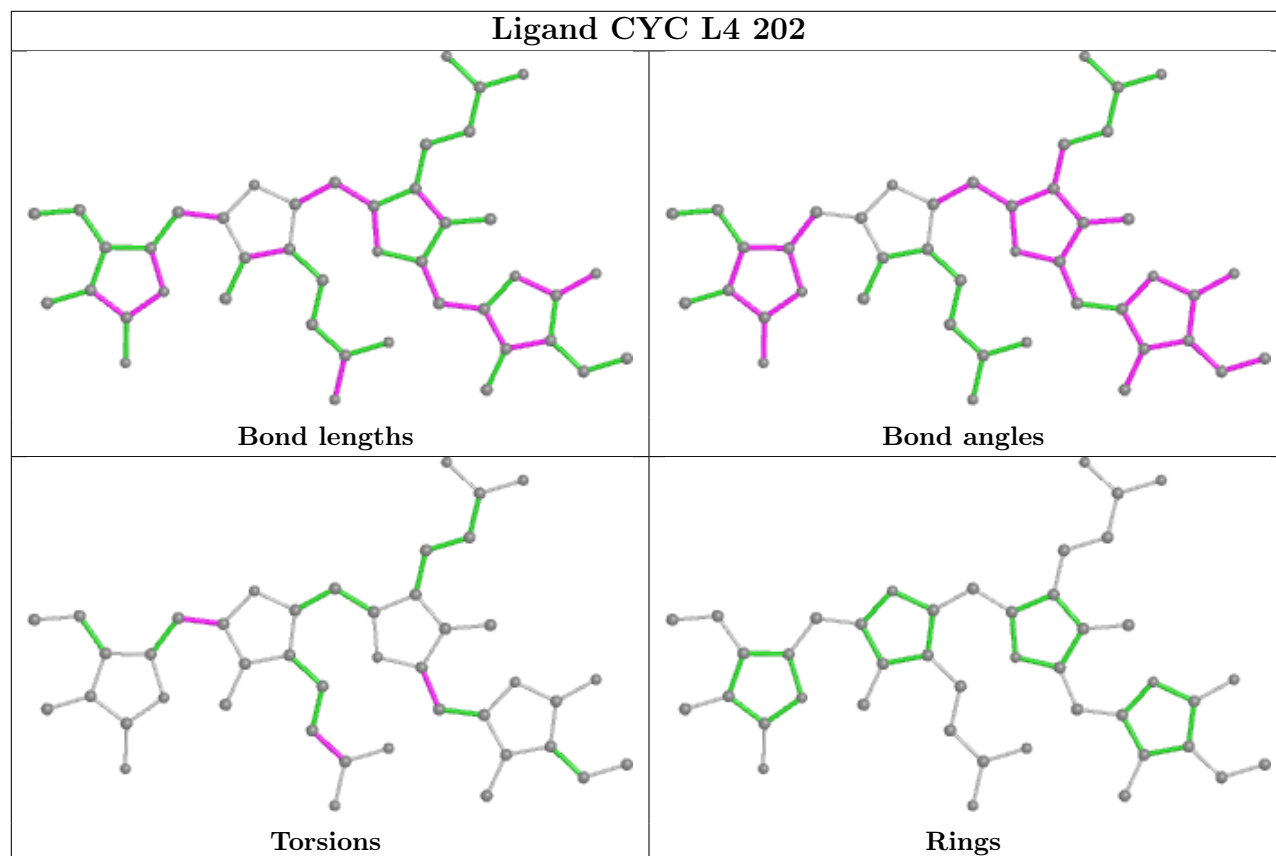
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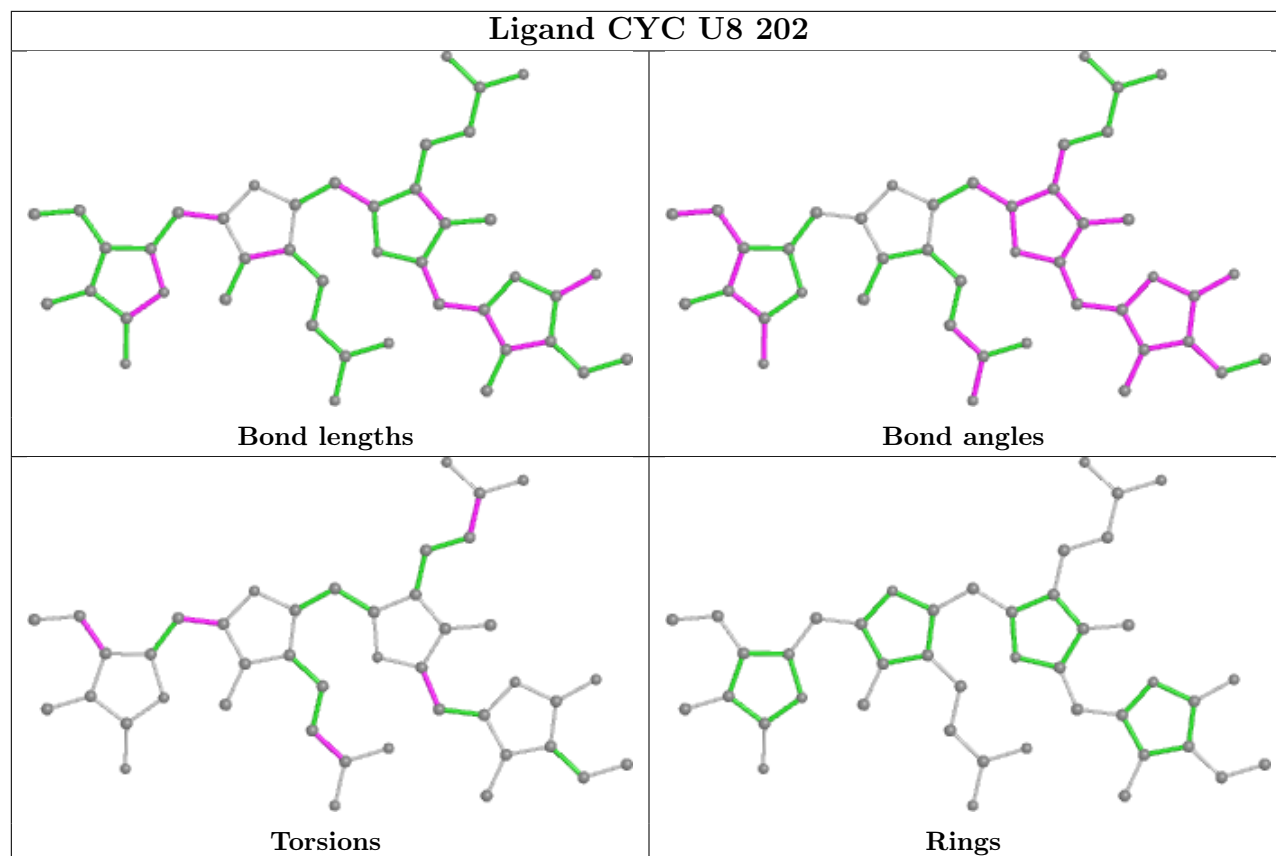
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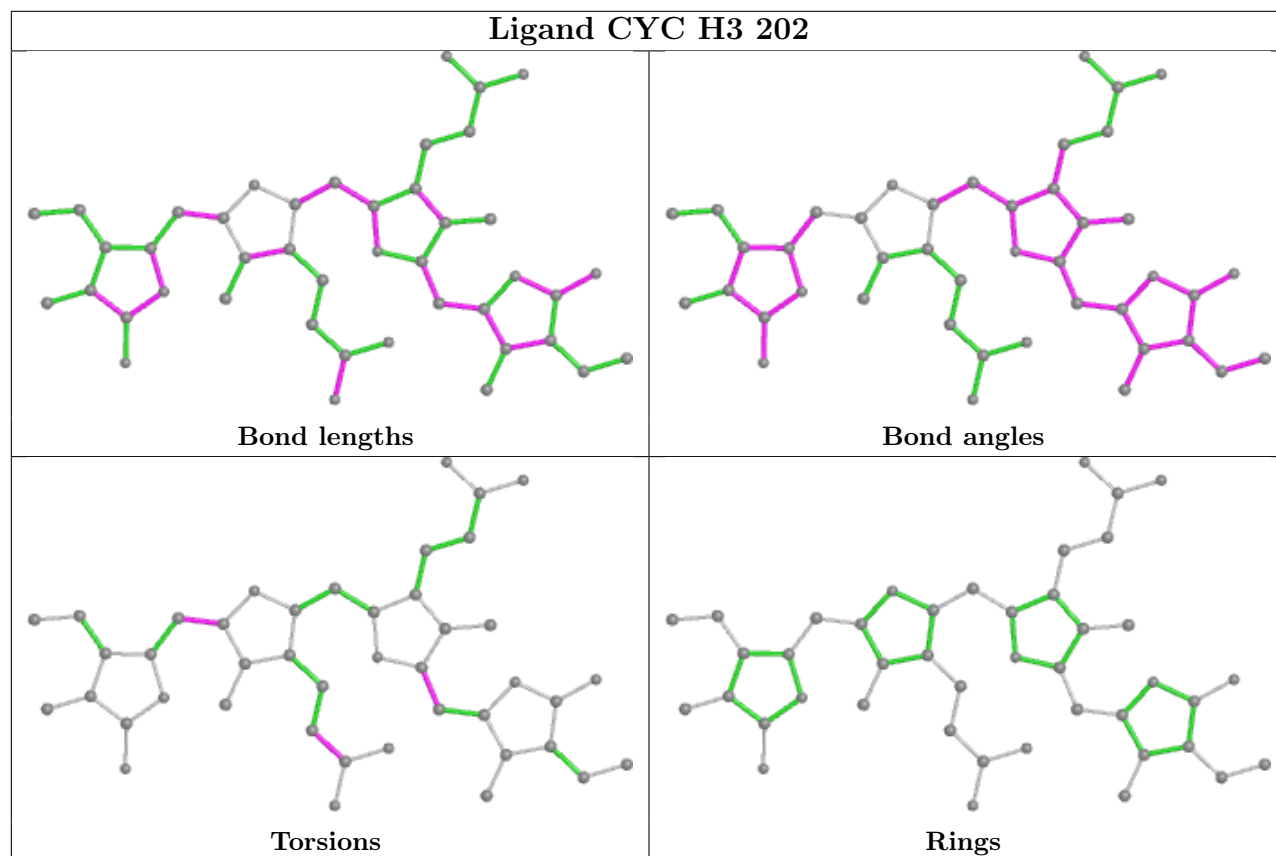
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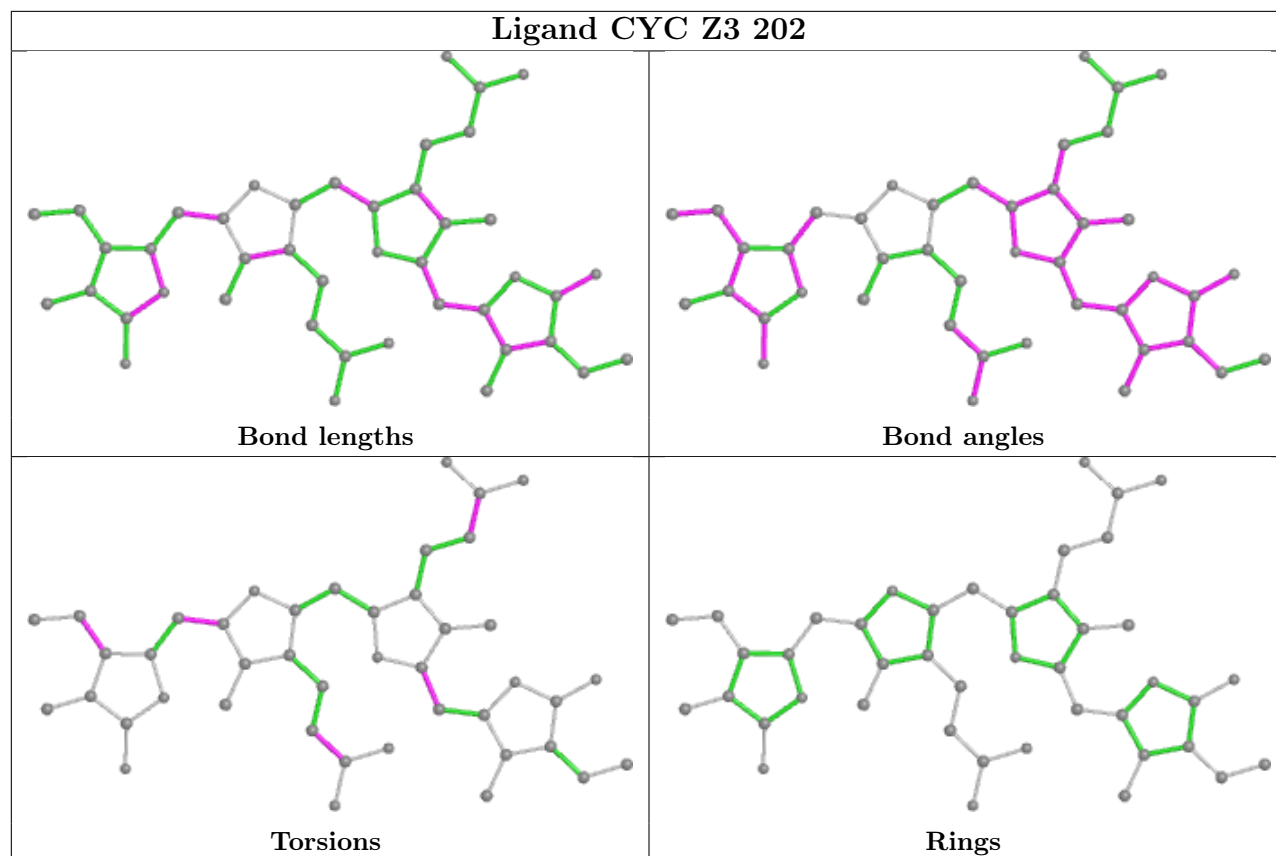
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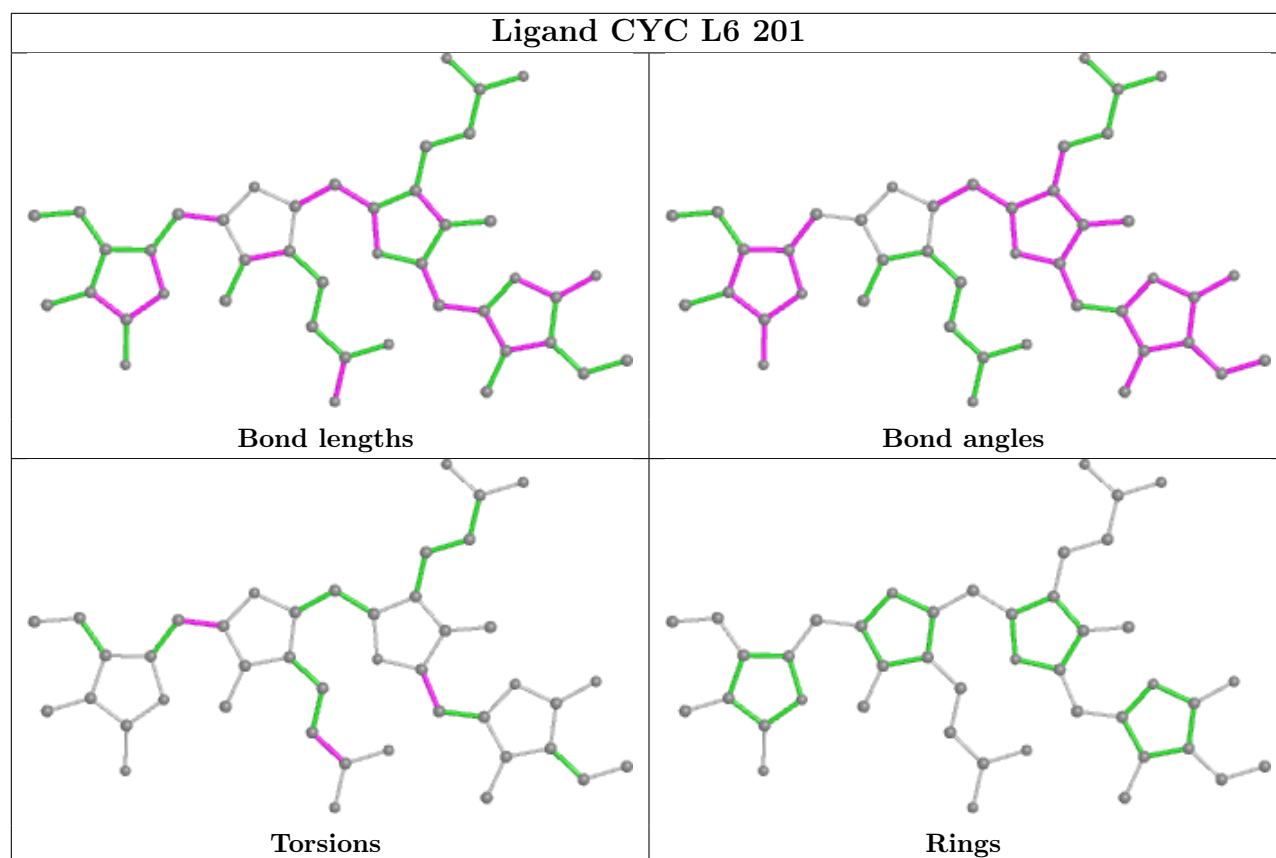
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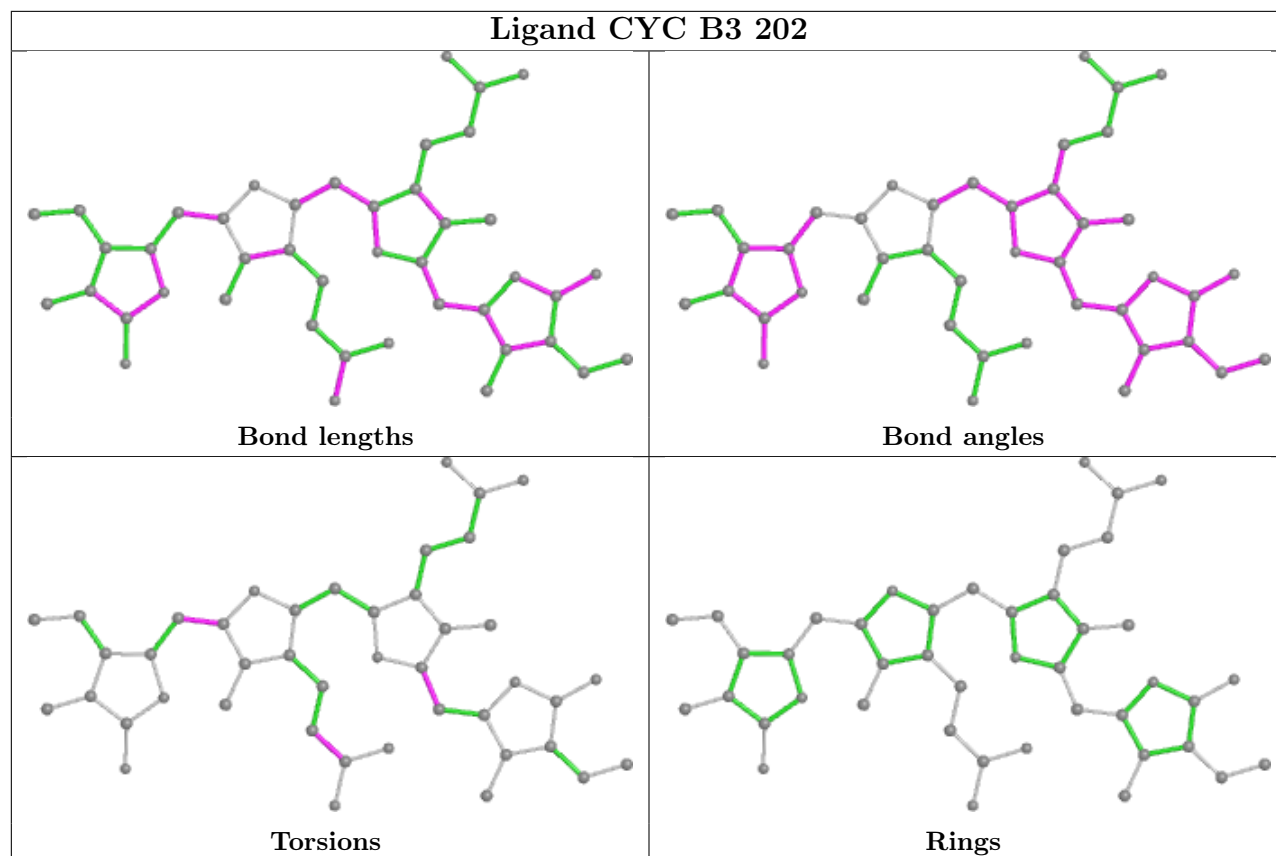
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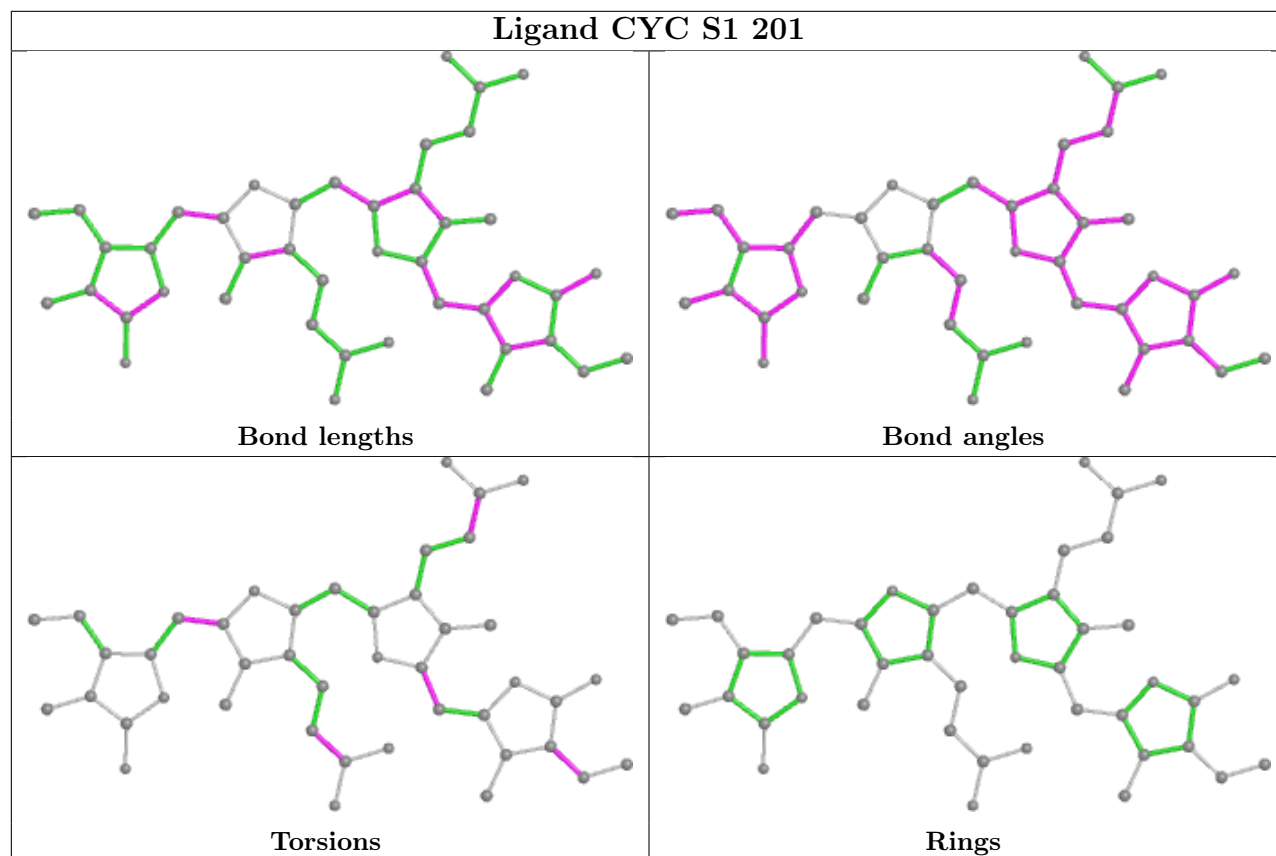
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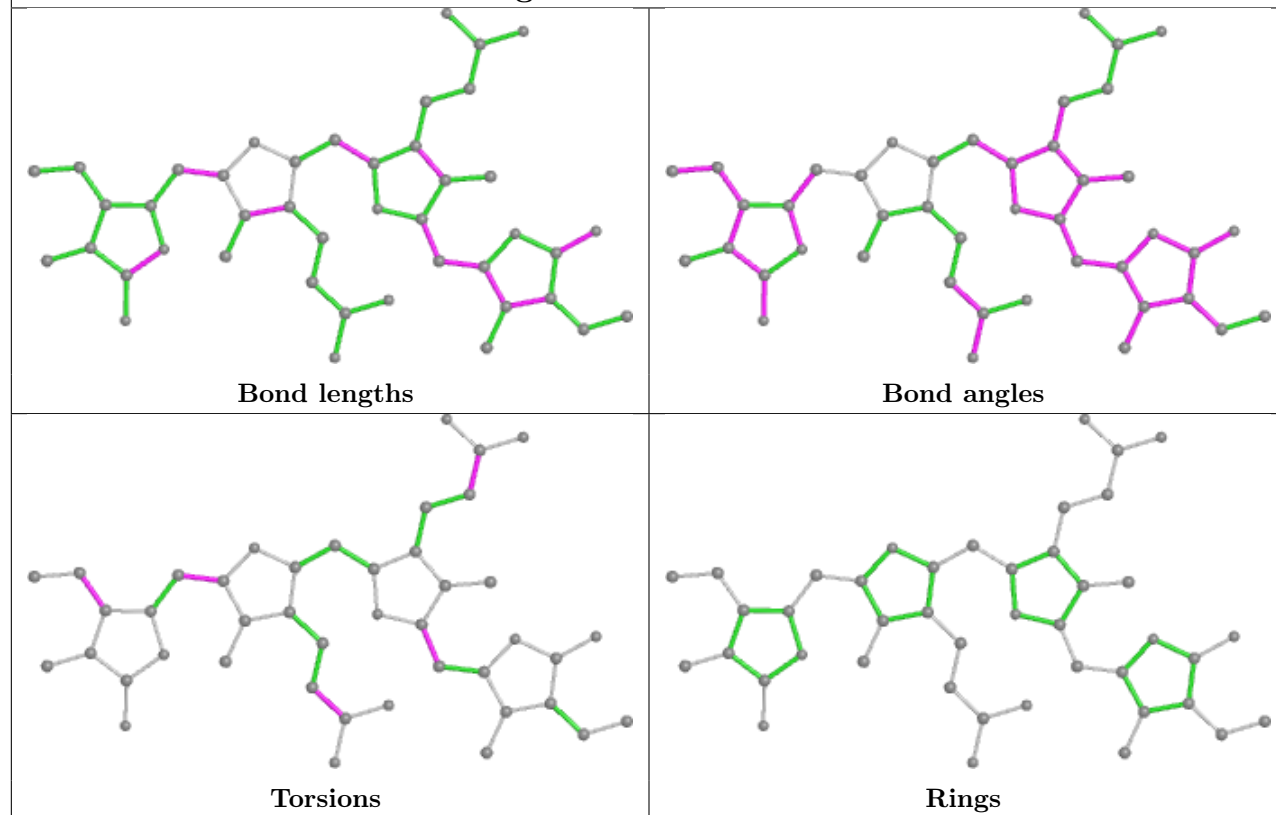
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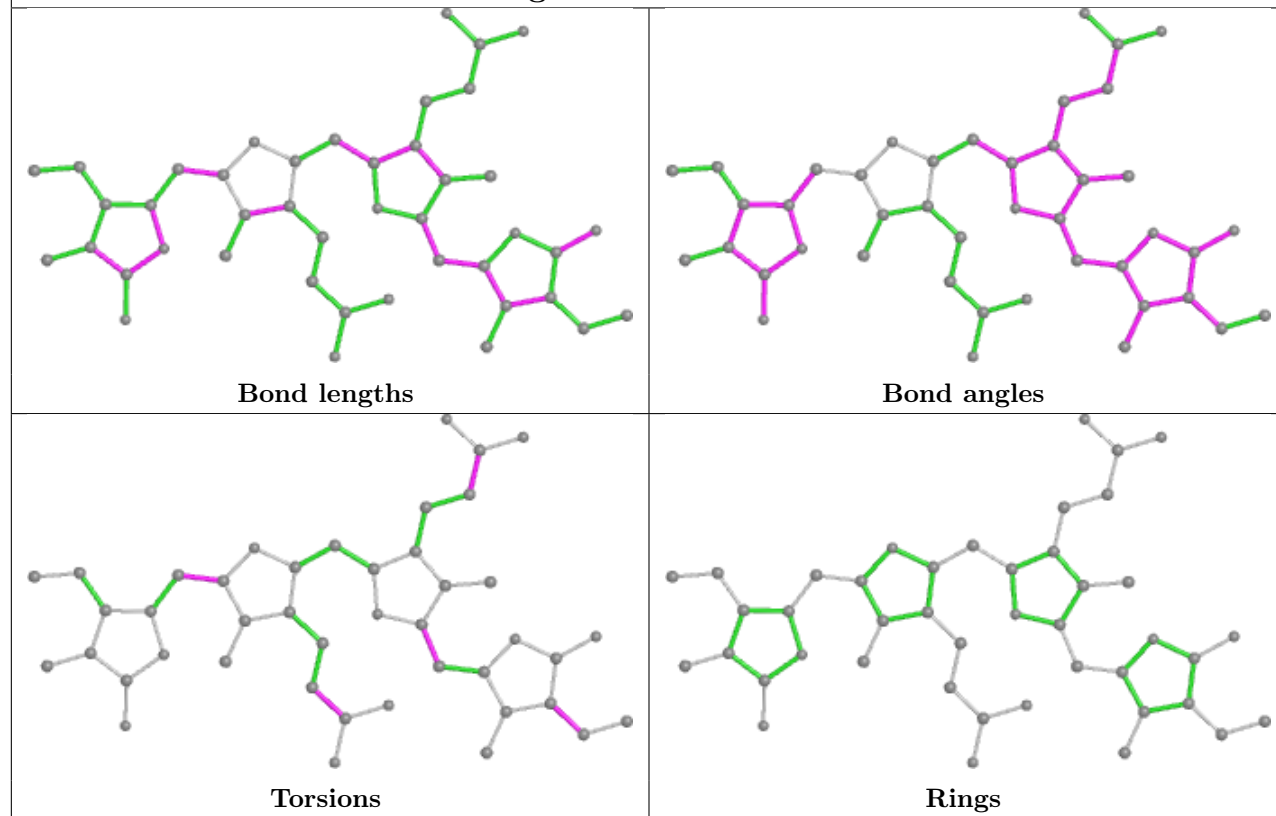
Ligand CYC S1 201



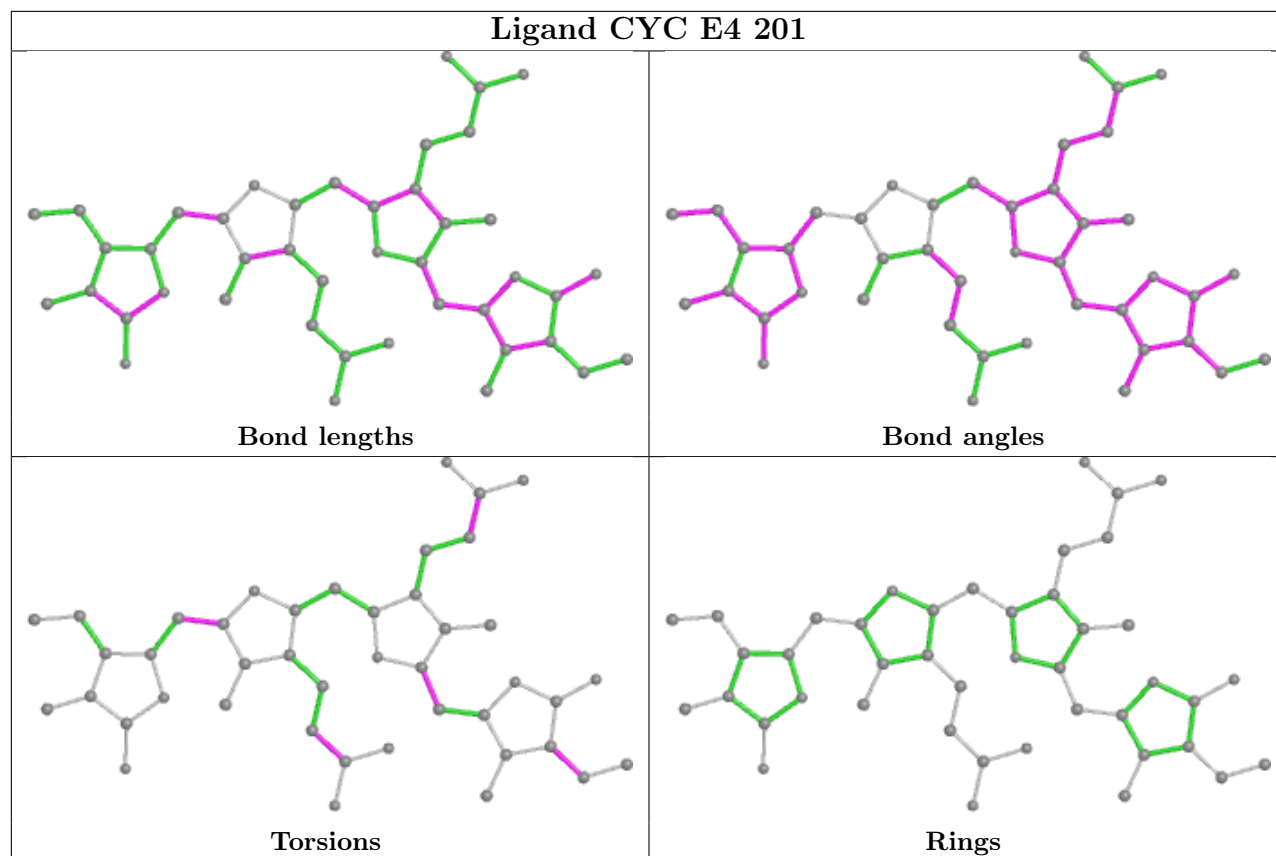
Ligand CYC W4 202



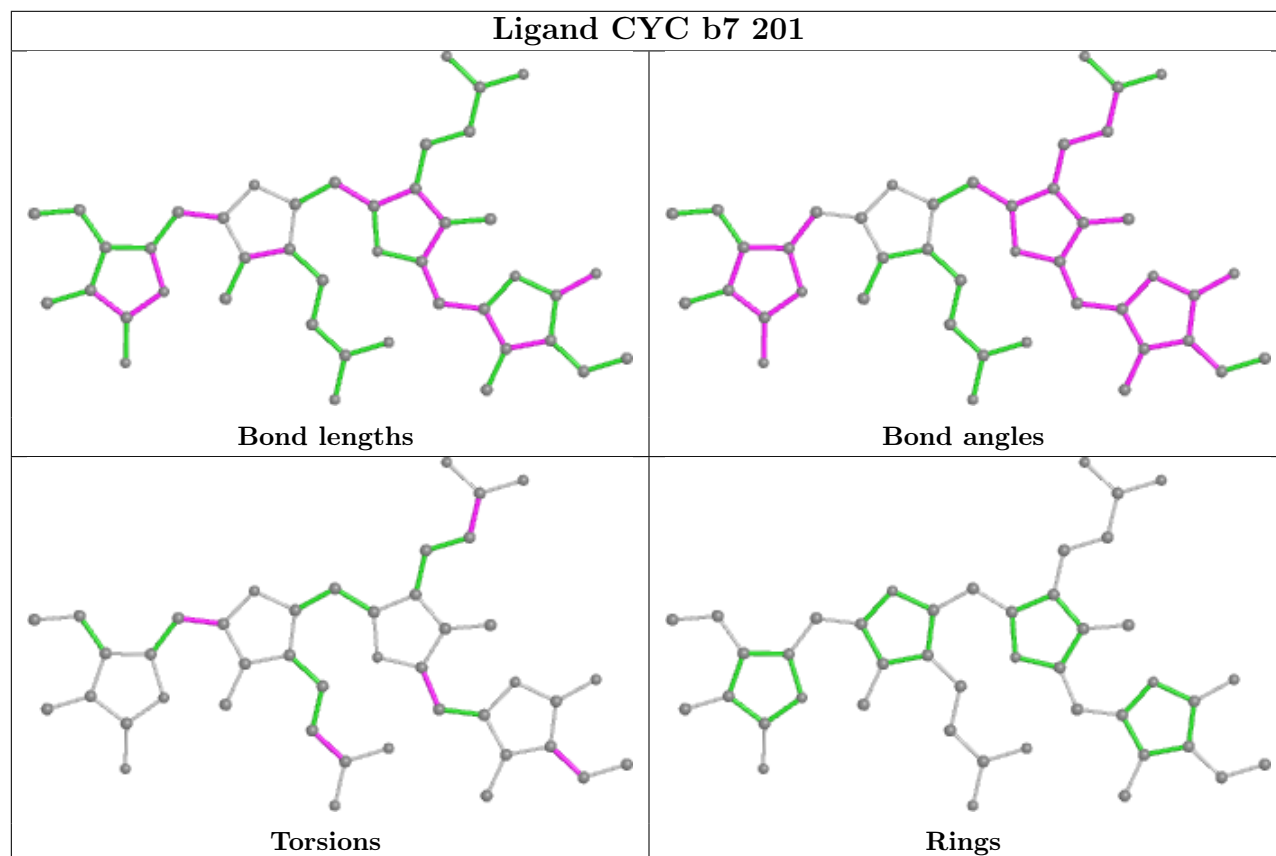
Ligand CYC f5 201

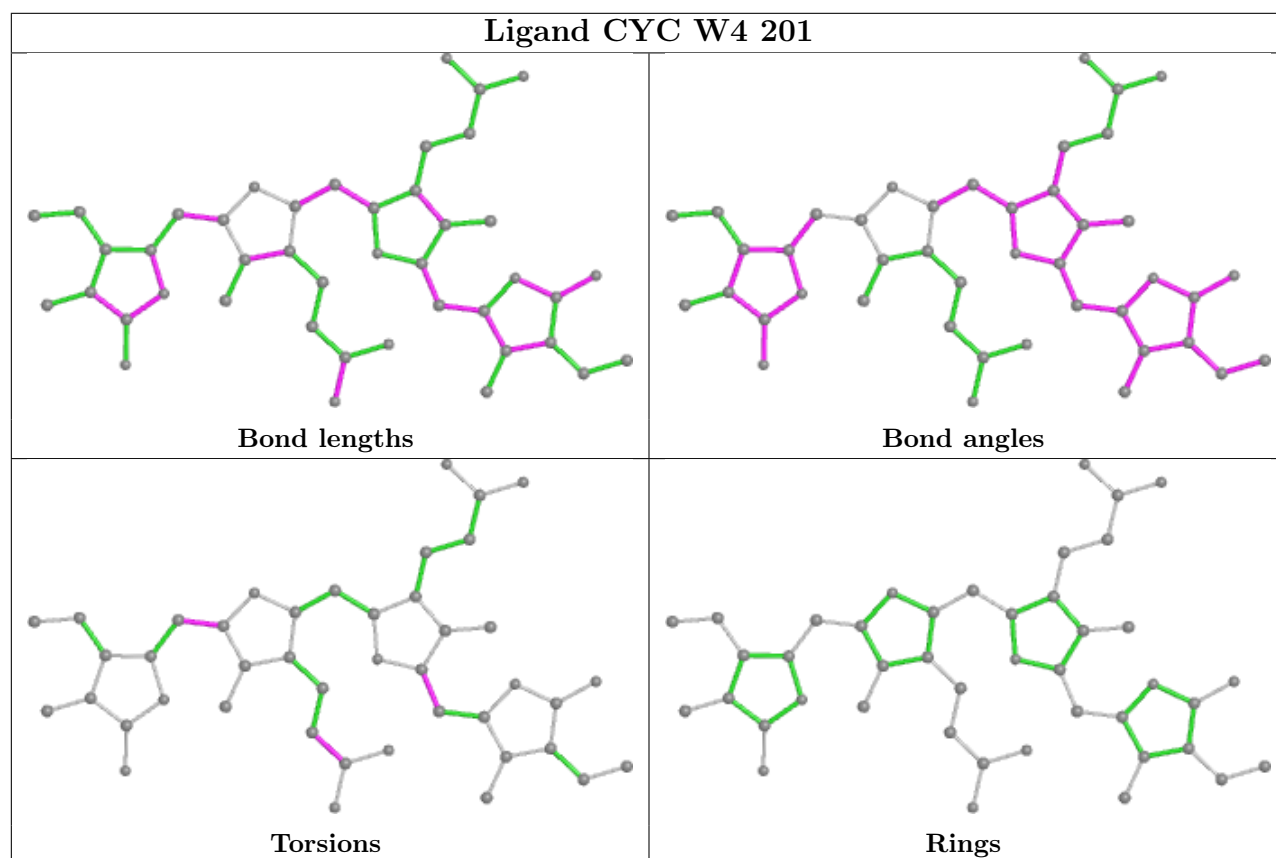
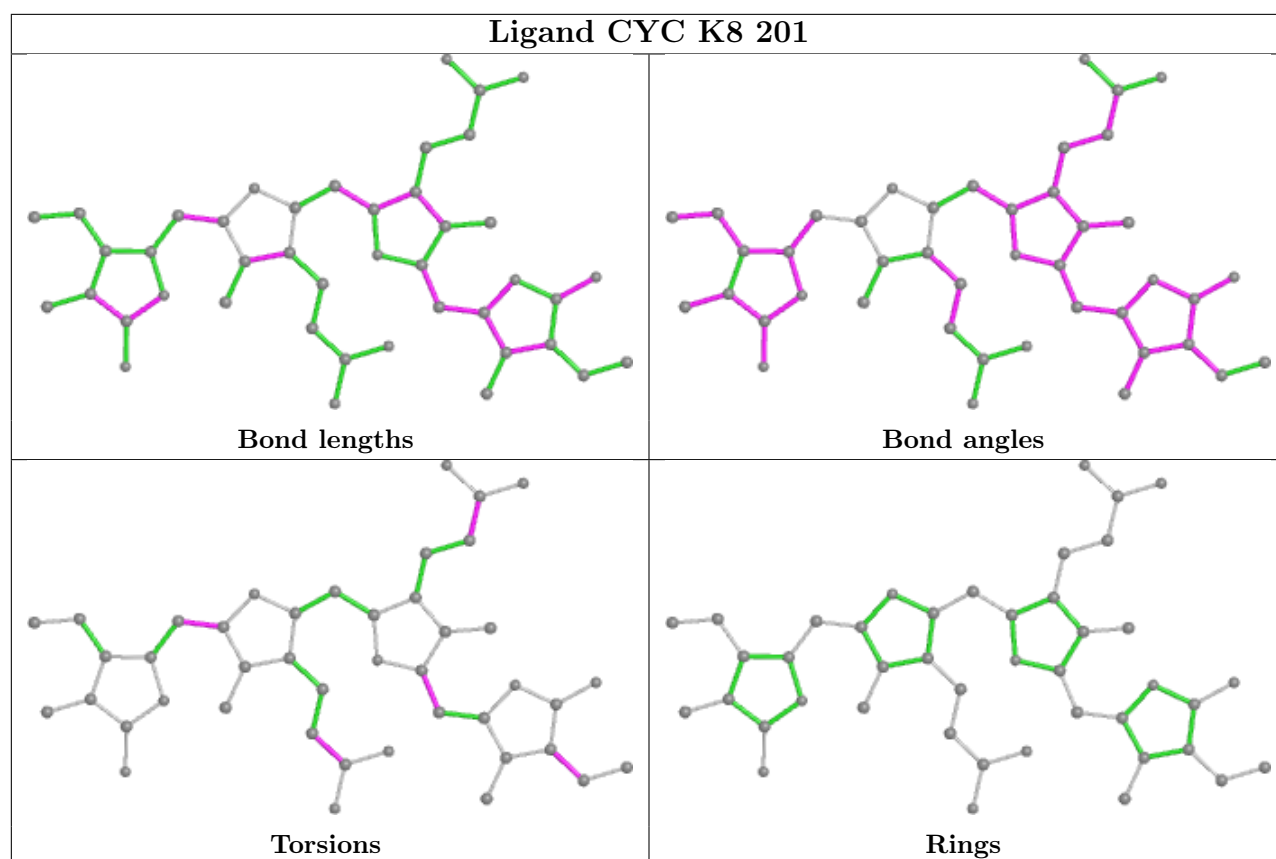


Ligand CYC E4 201

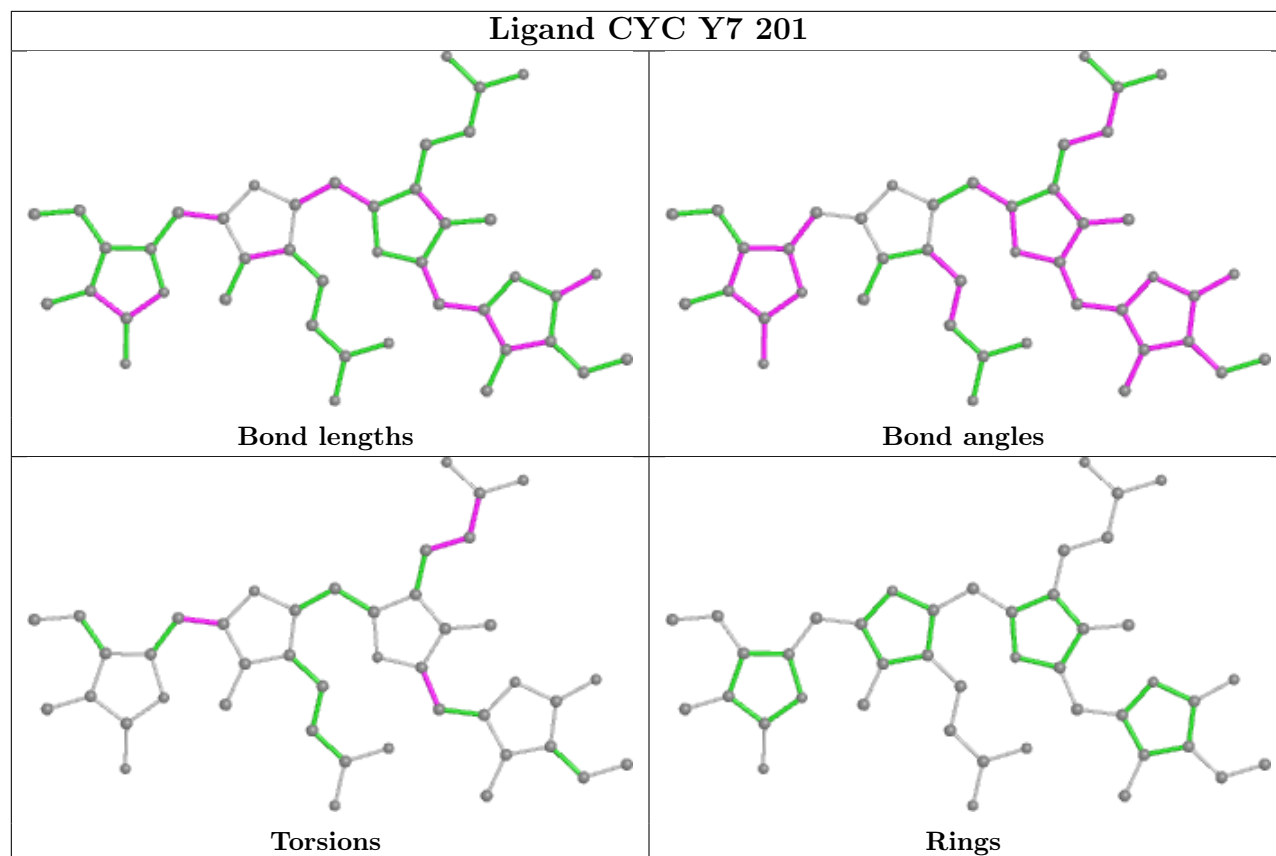


Ligand CYC b7 201

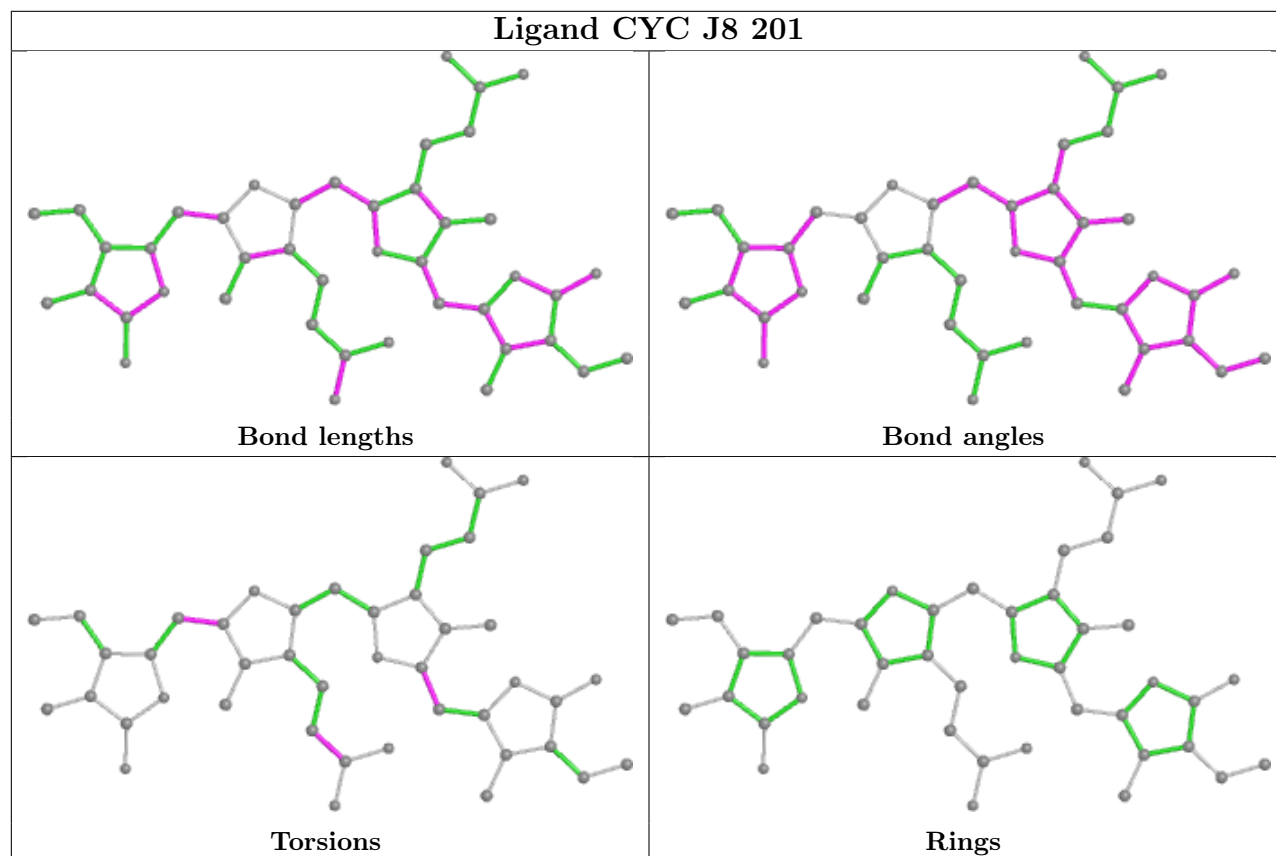




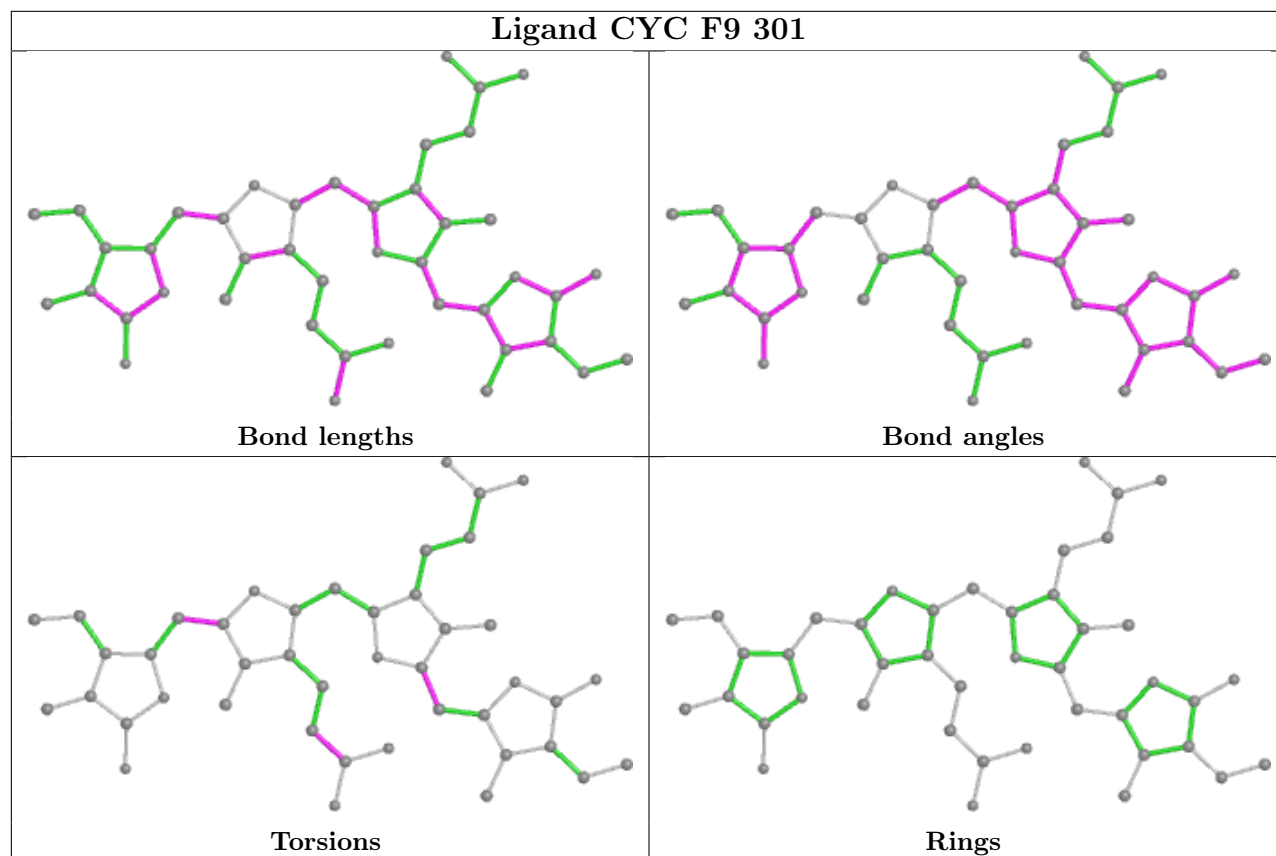
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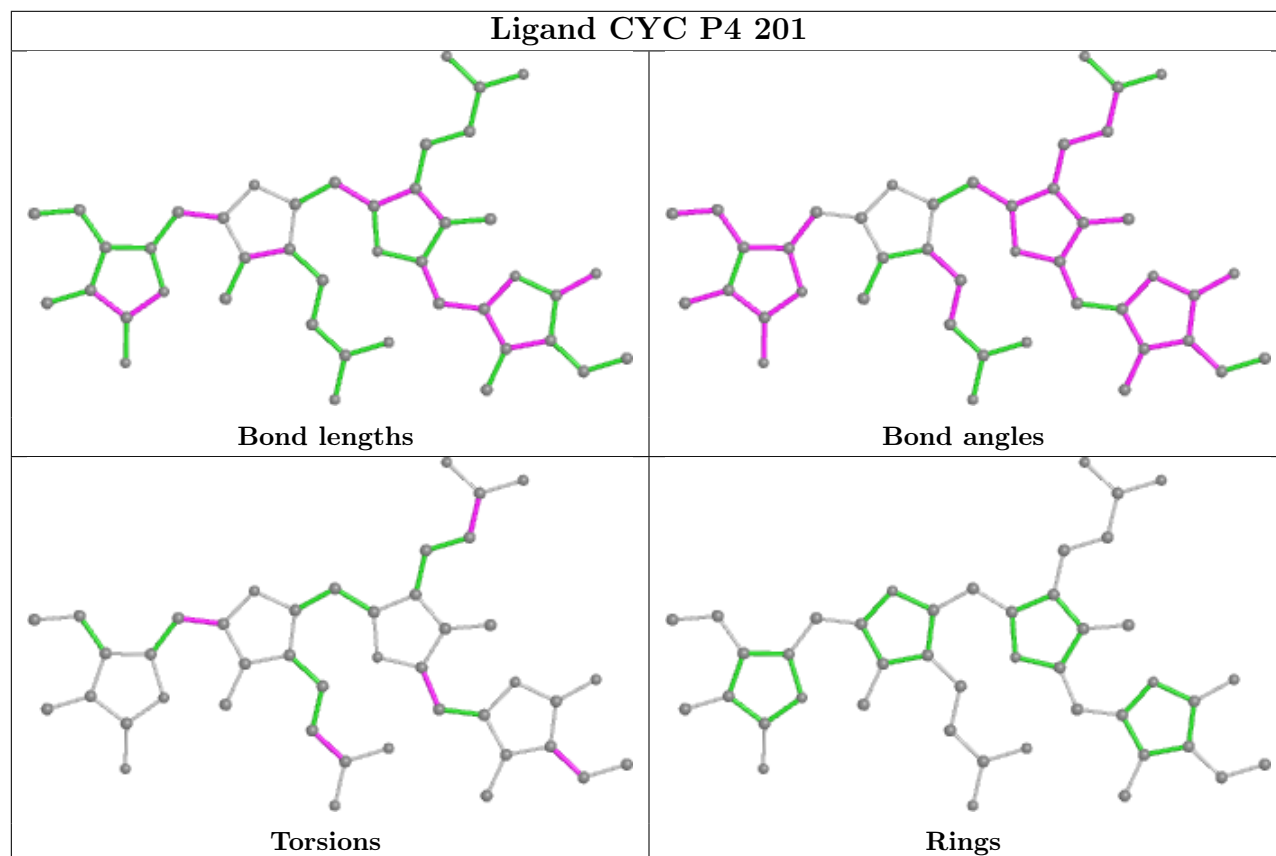
Ligand CYC J8 201



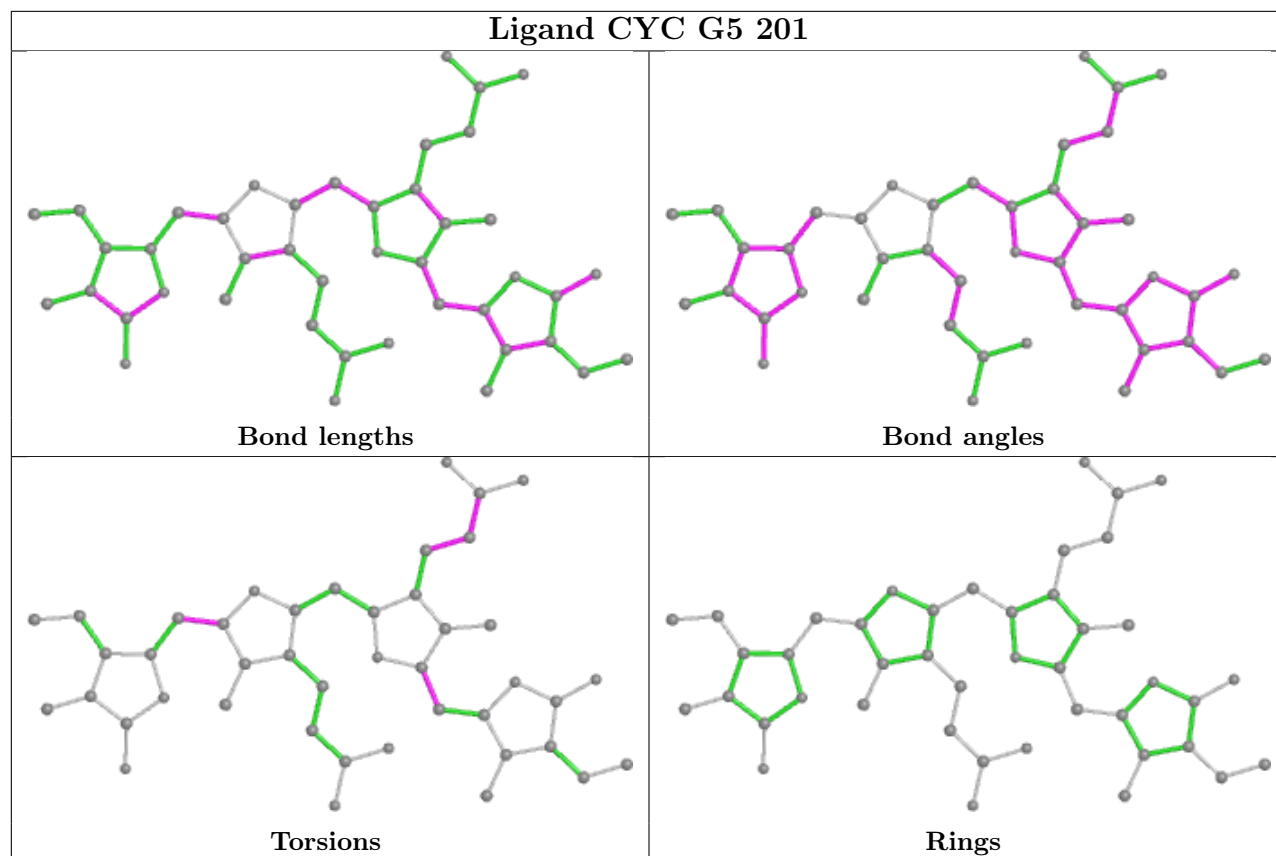
Ligand CYC F9 301



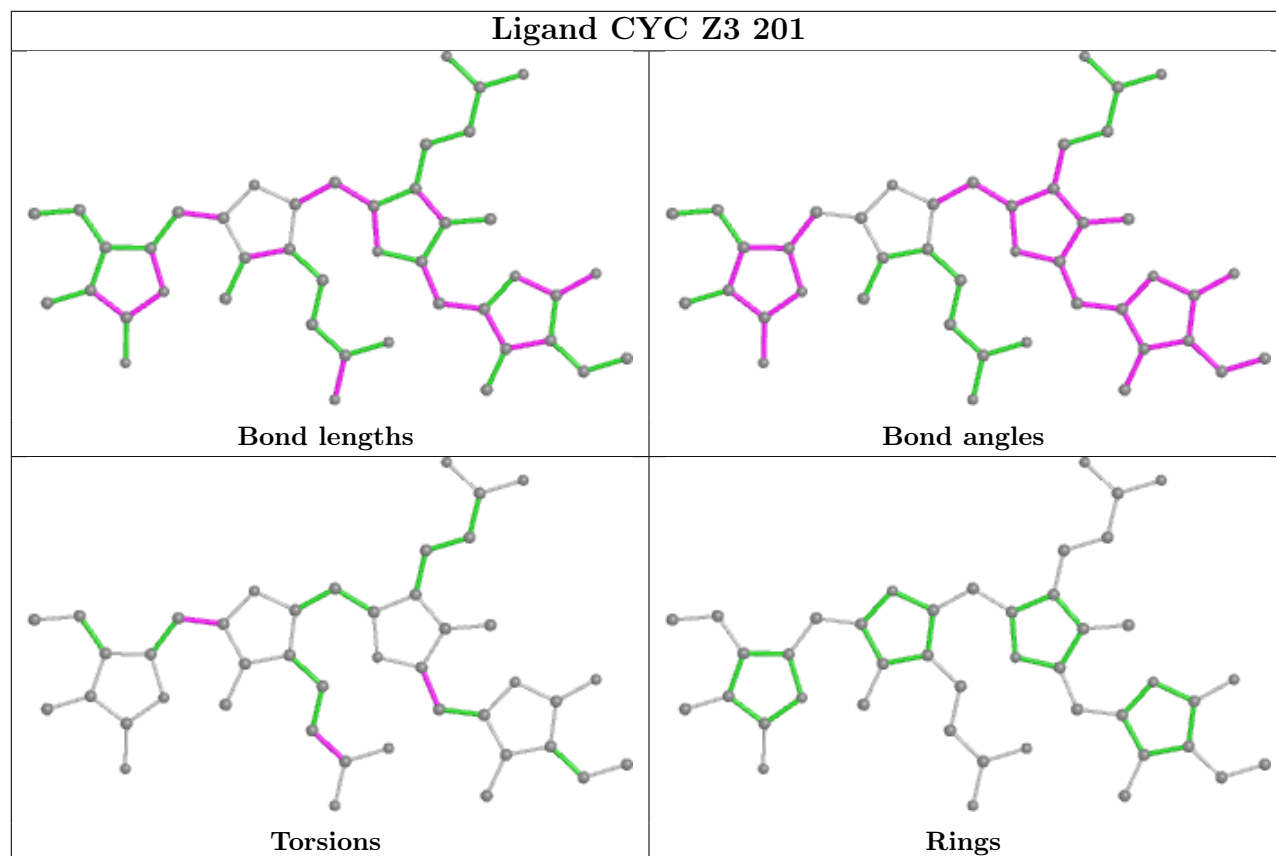
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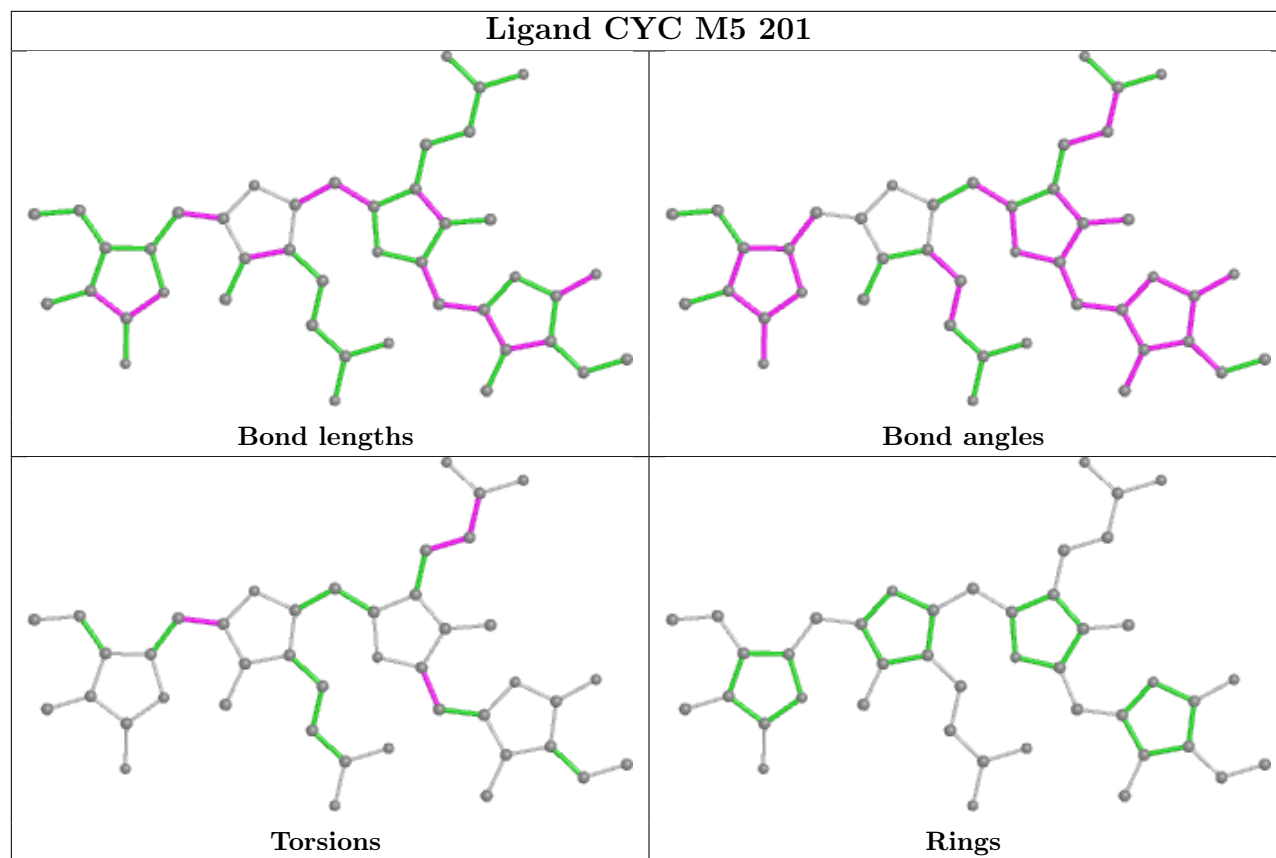
Ligand CYC G5 201



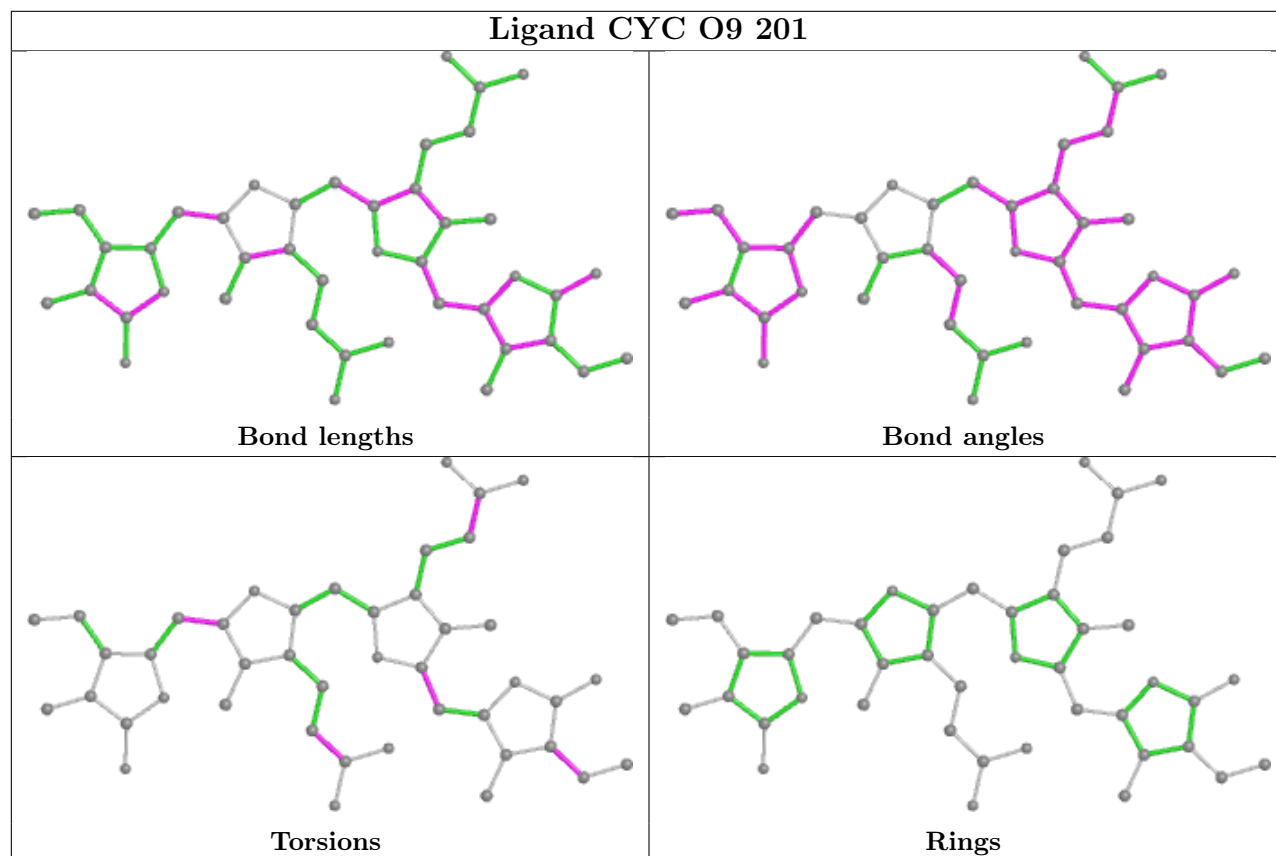
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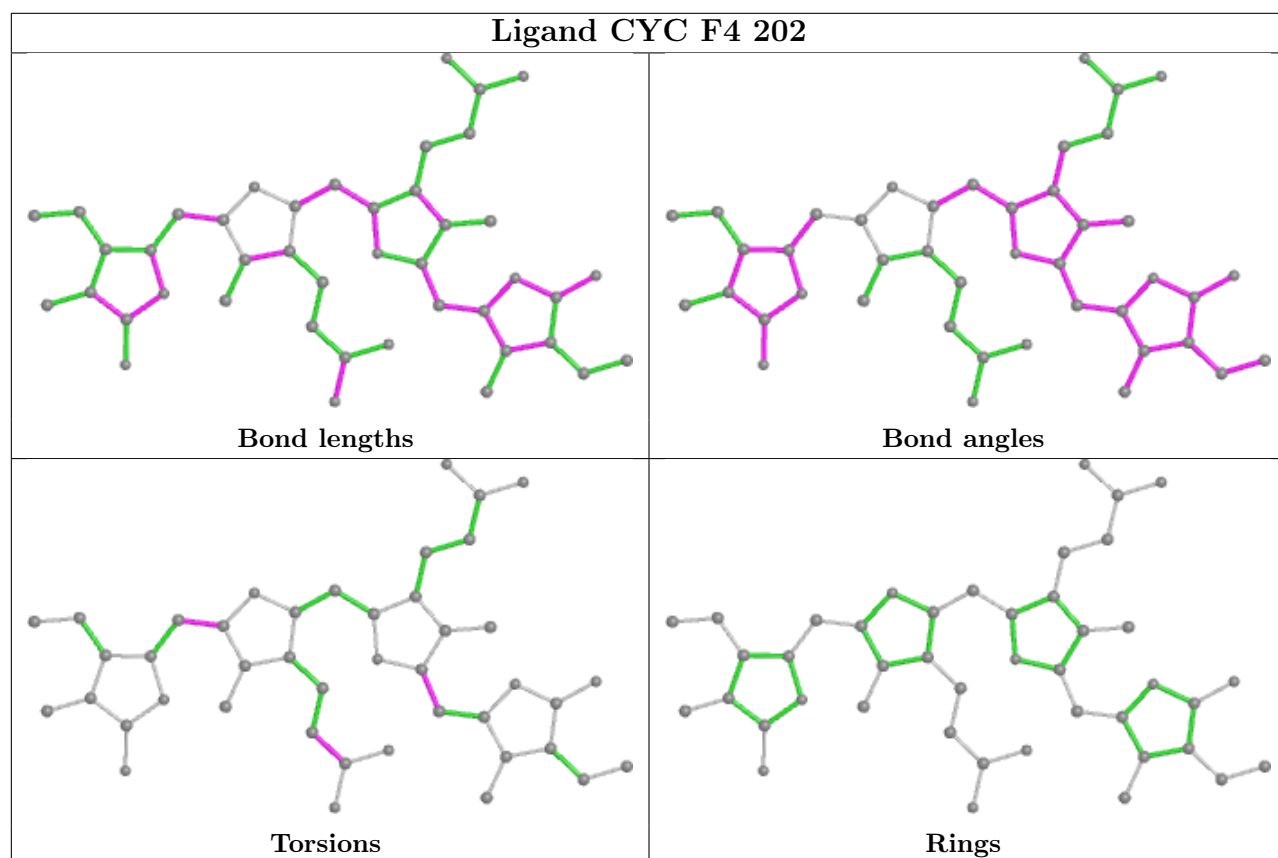
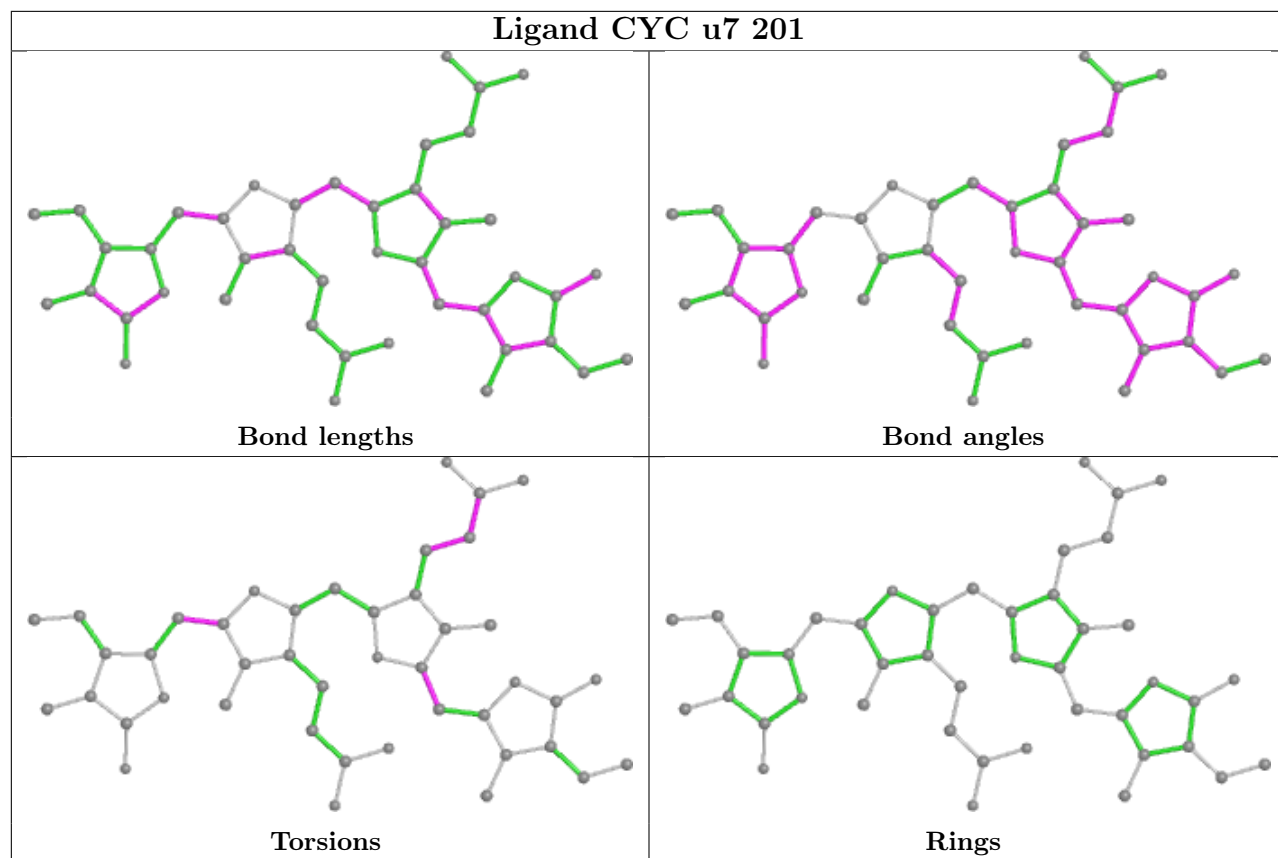


Ligand CYC M5 201

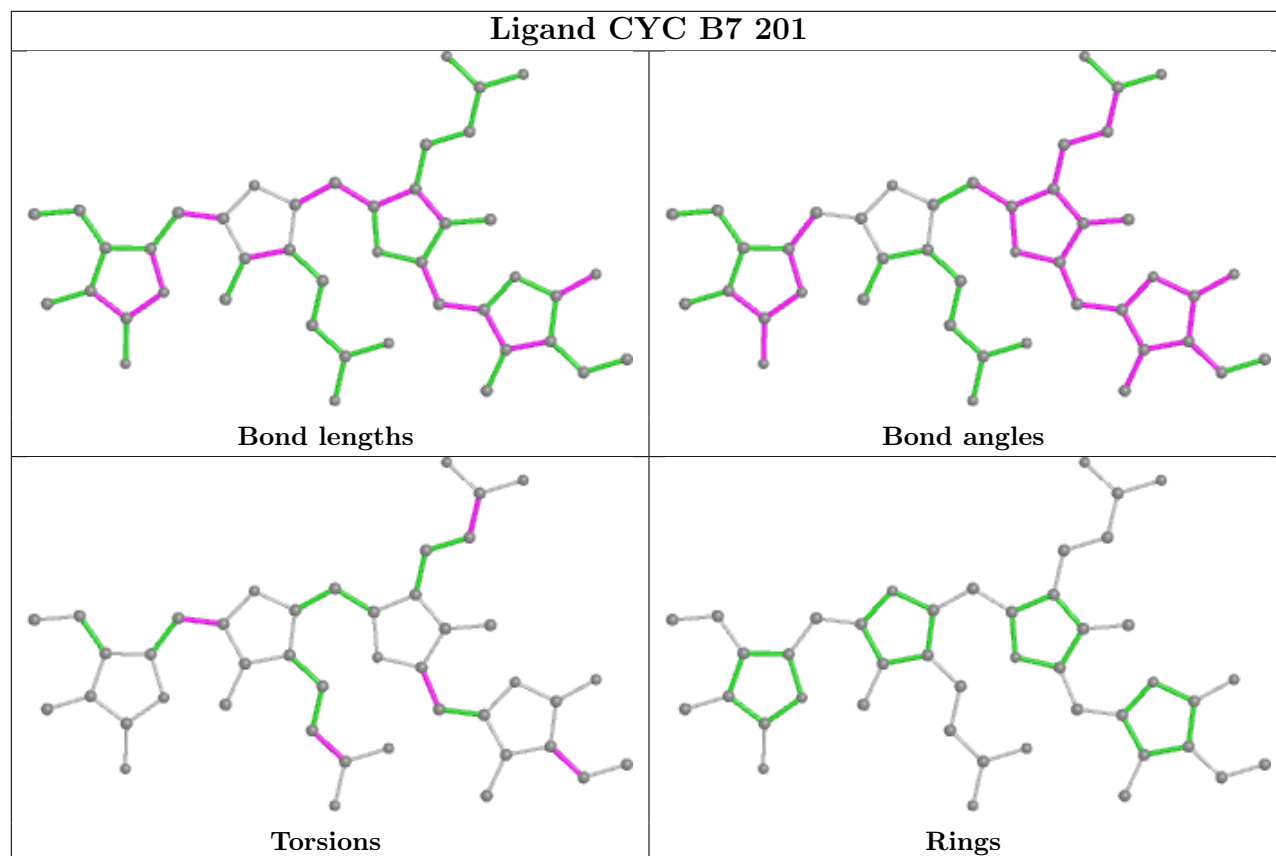


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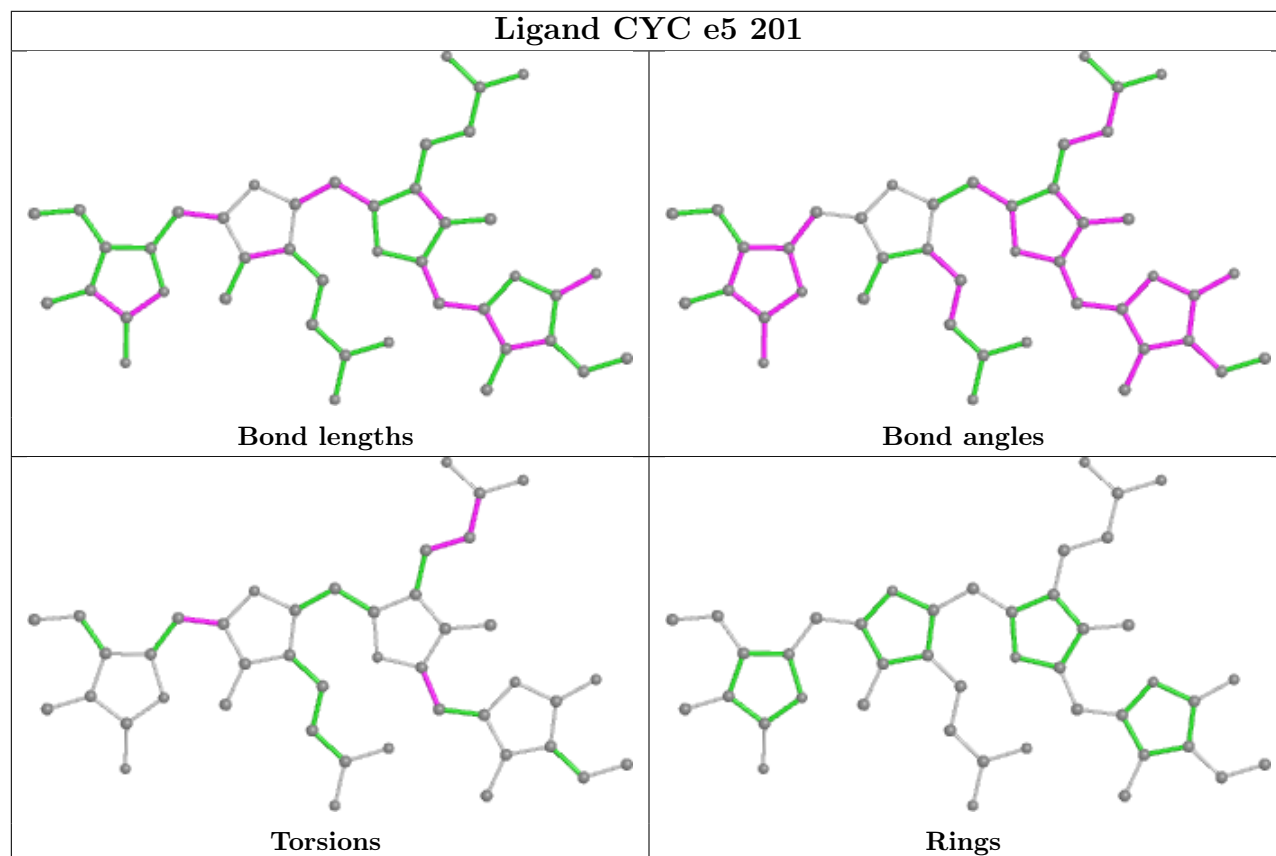


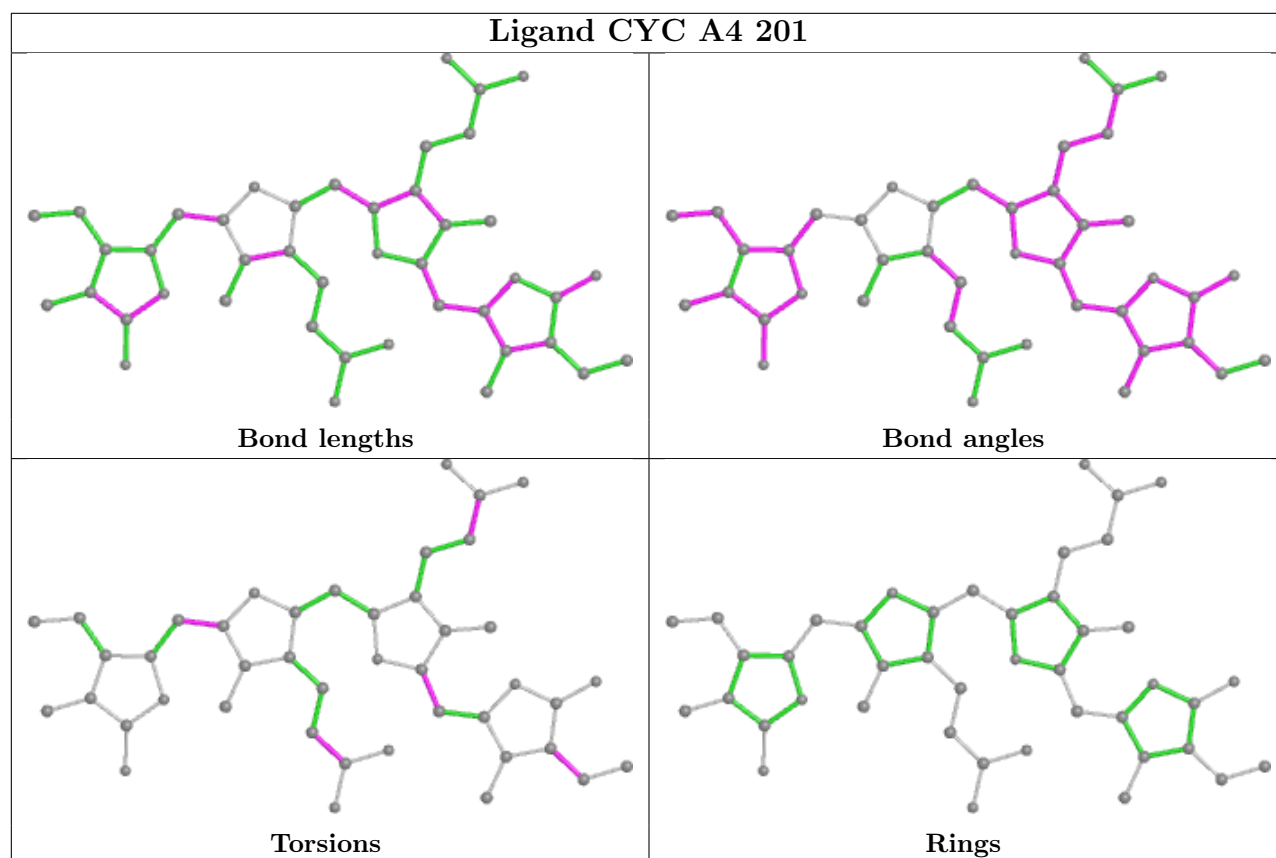
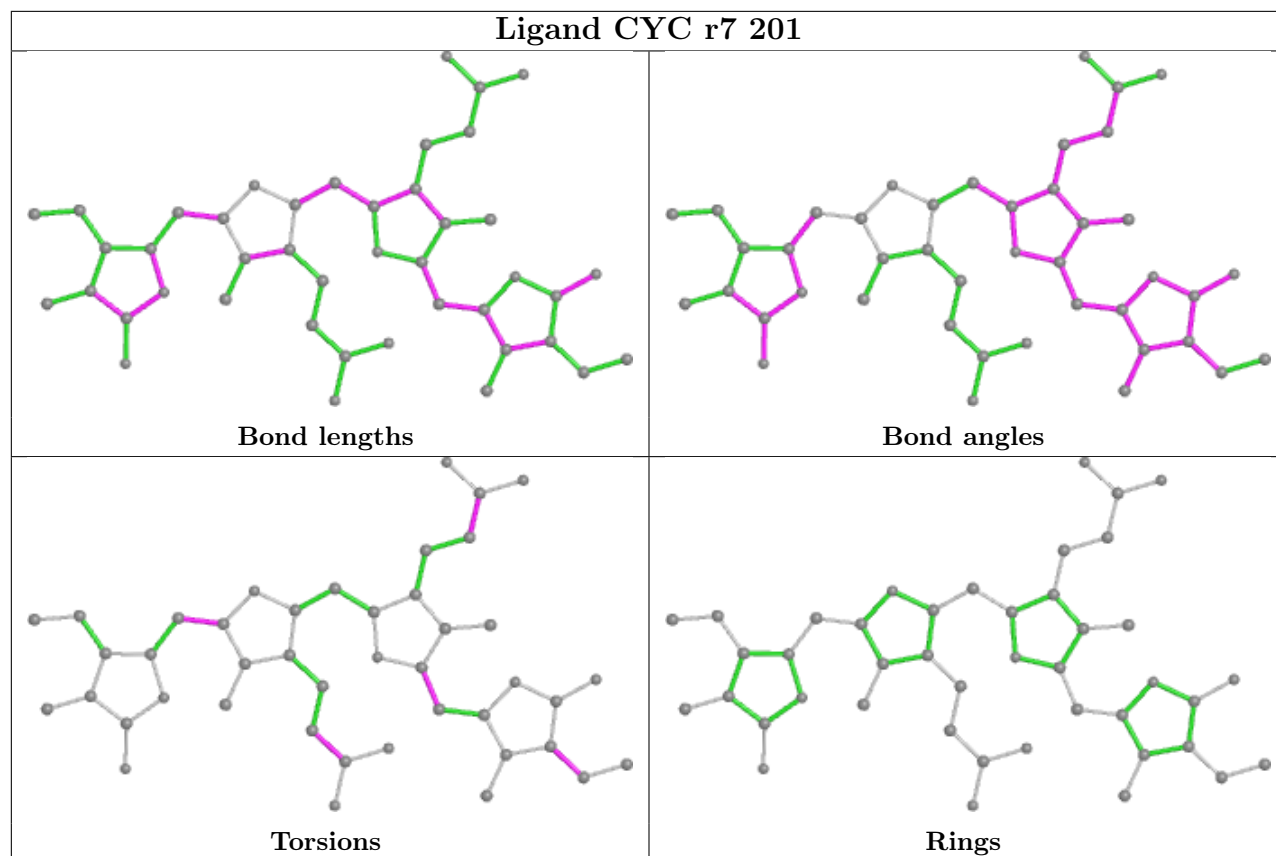


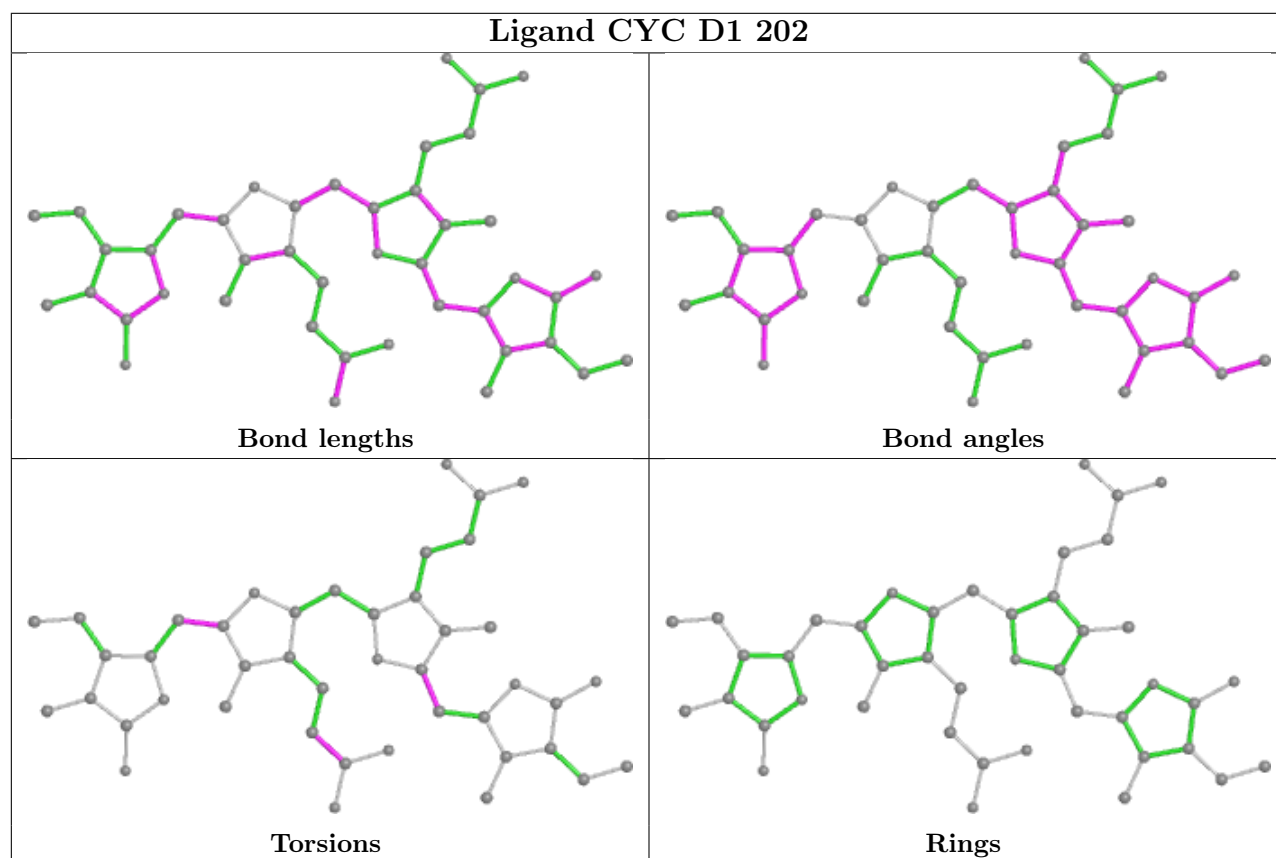
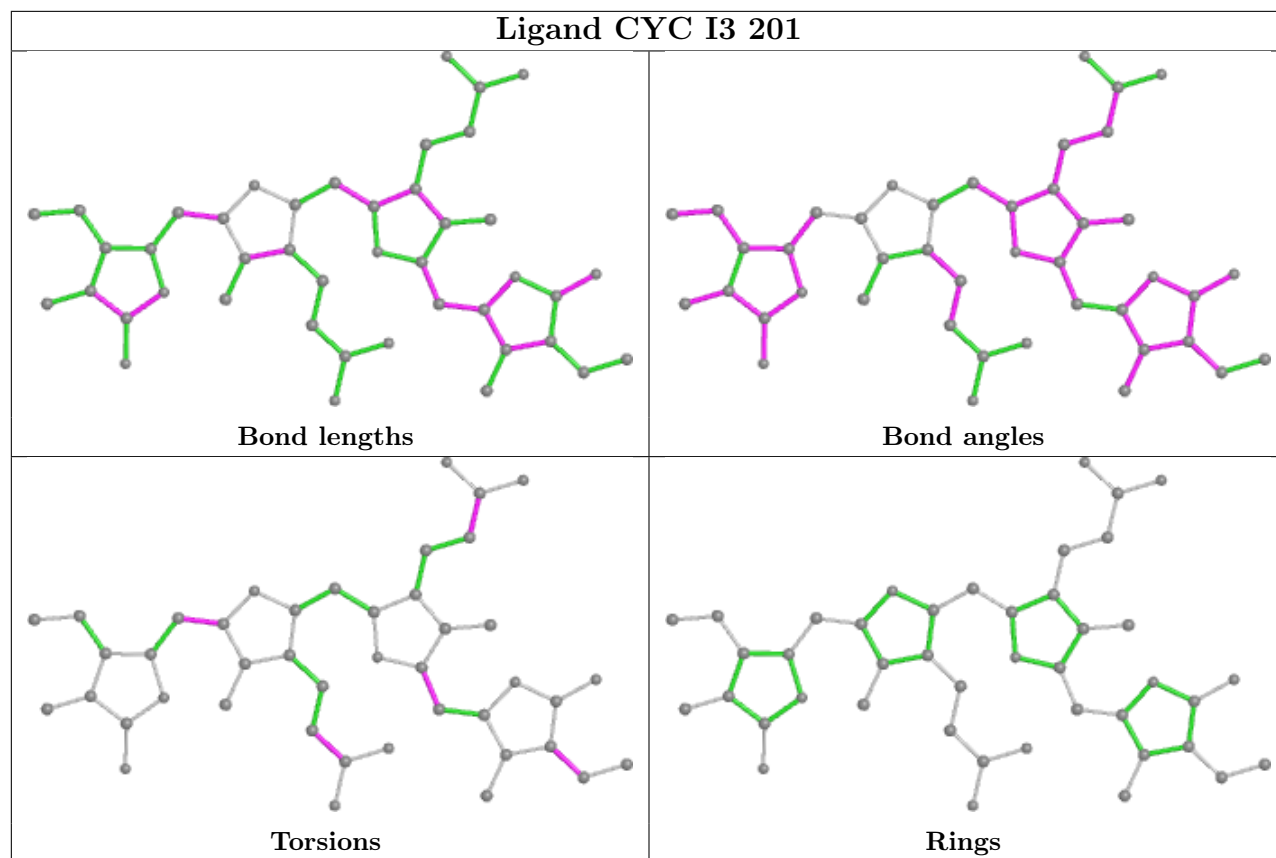
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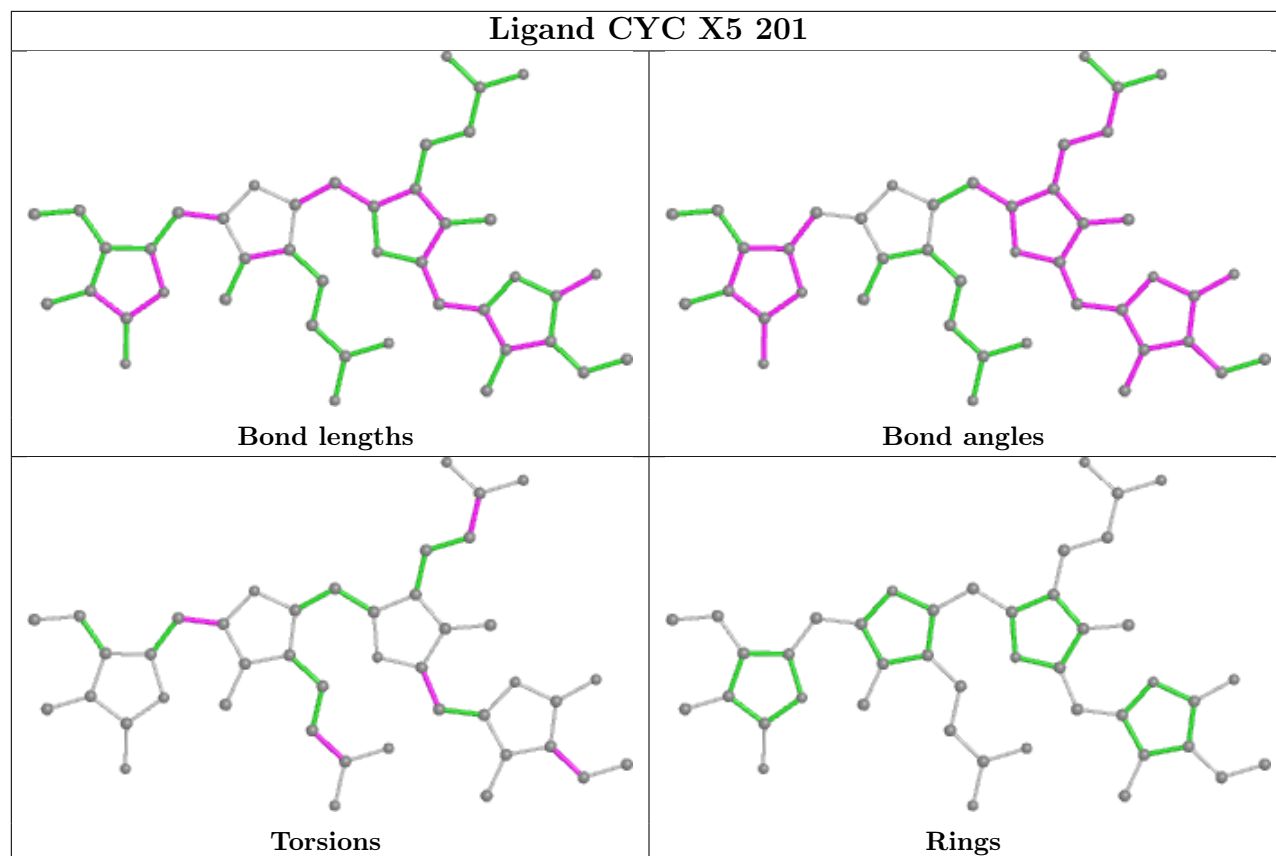
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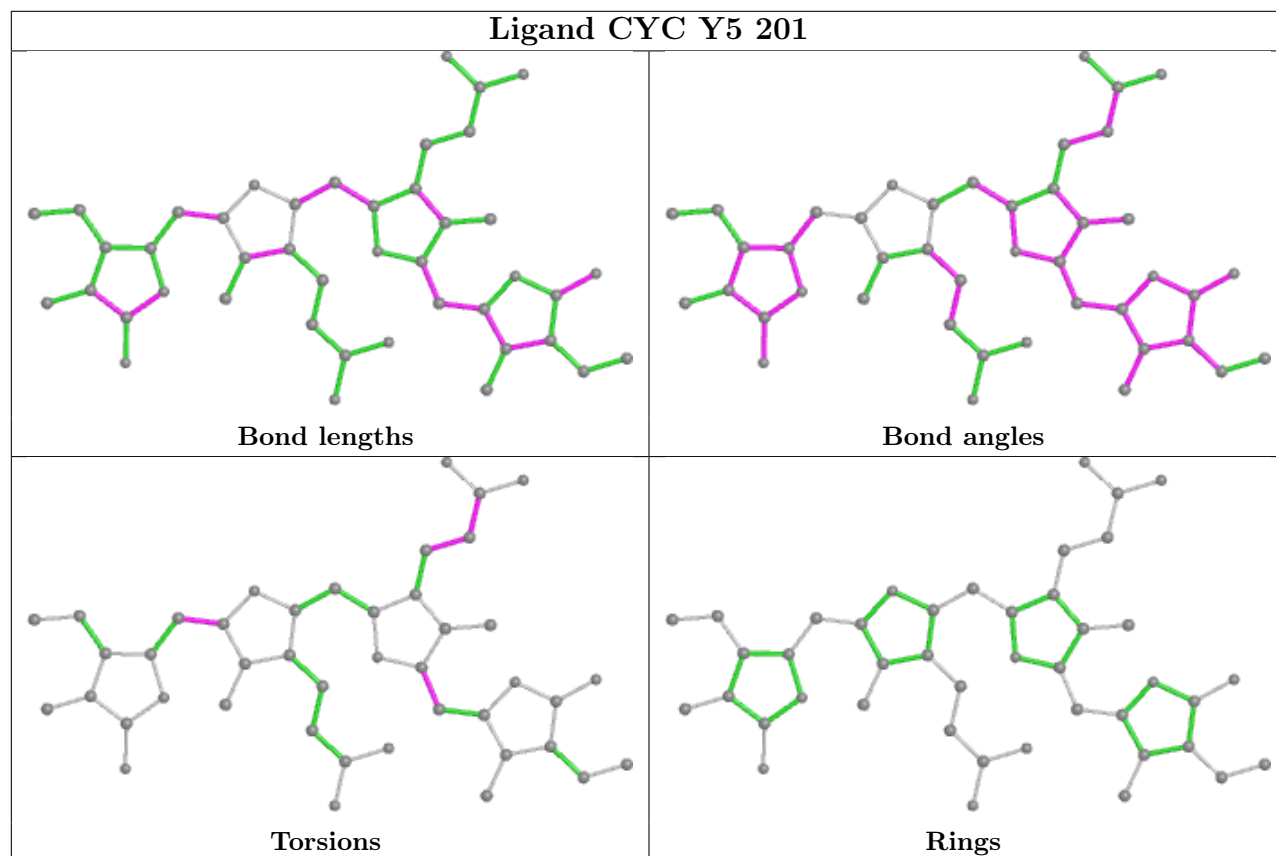




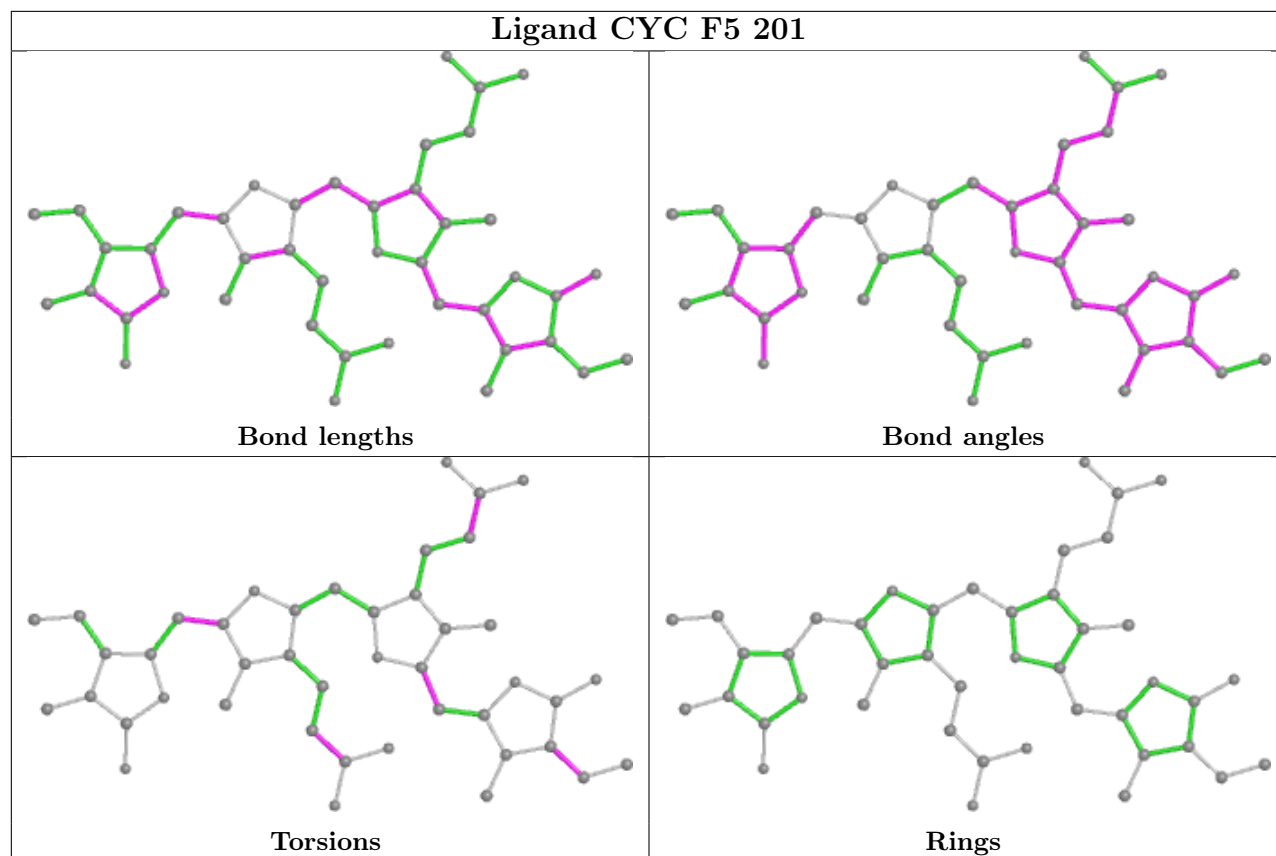
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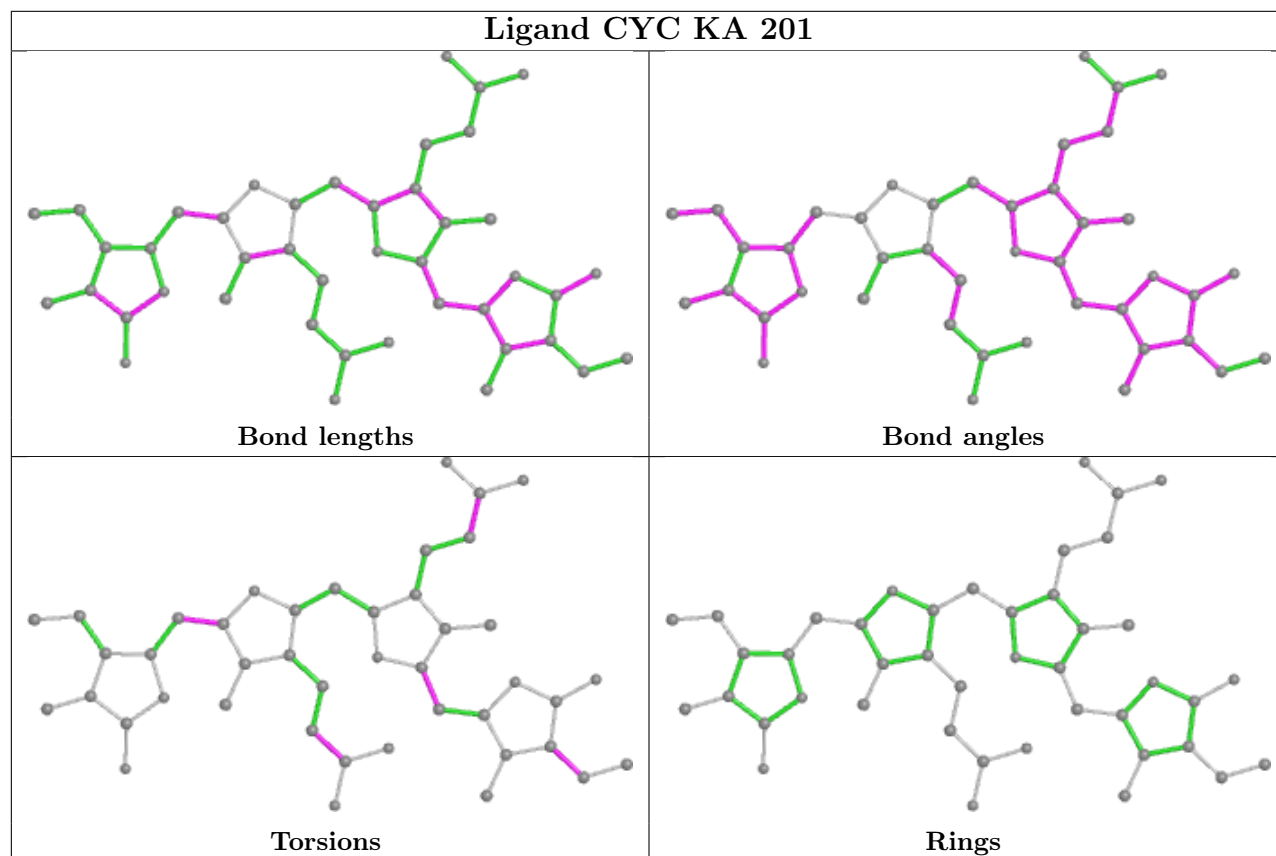
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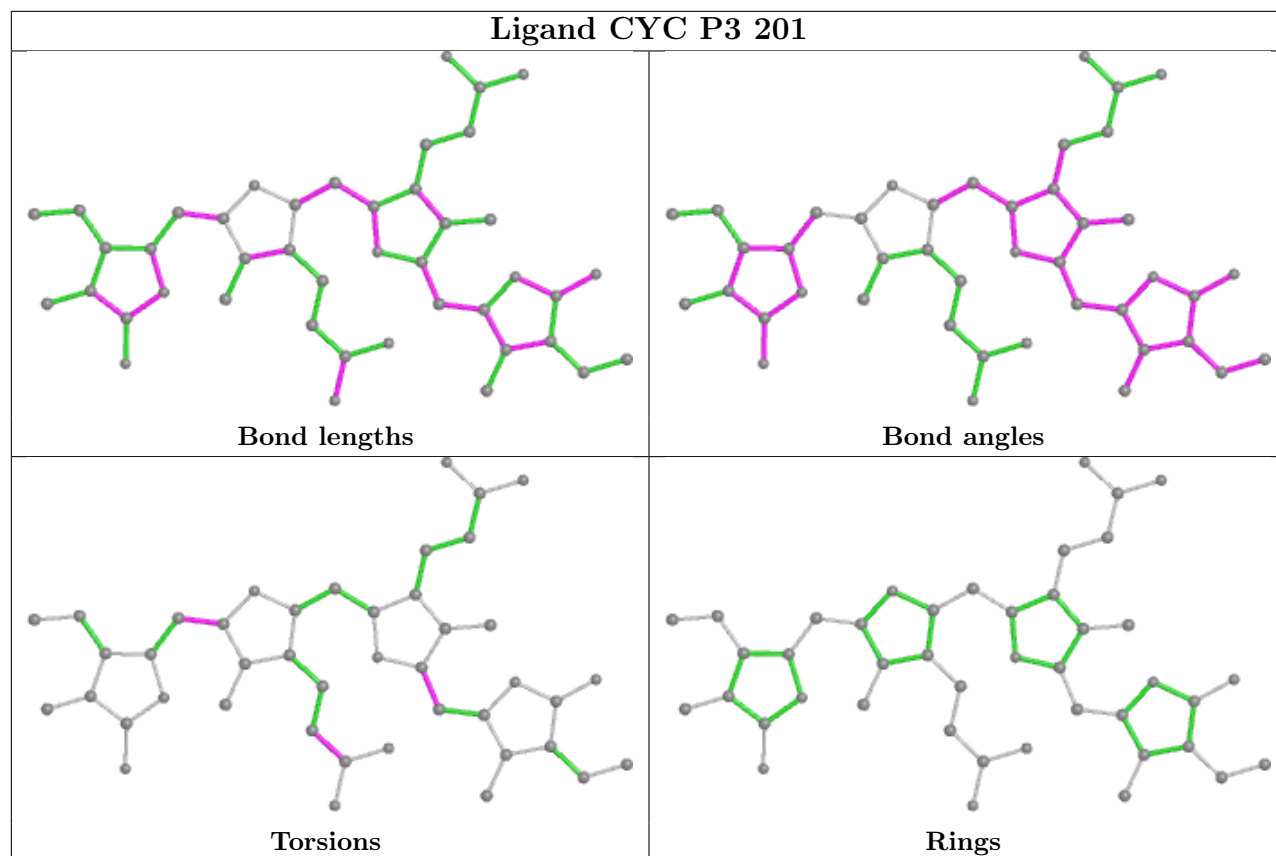
Ligand CYC F5 201



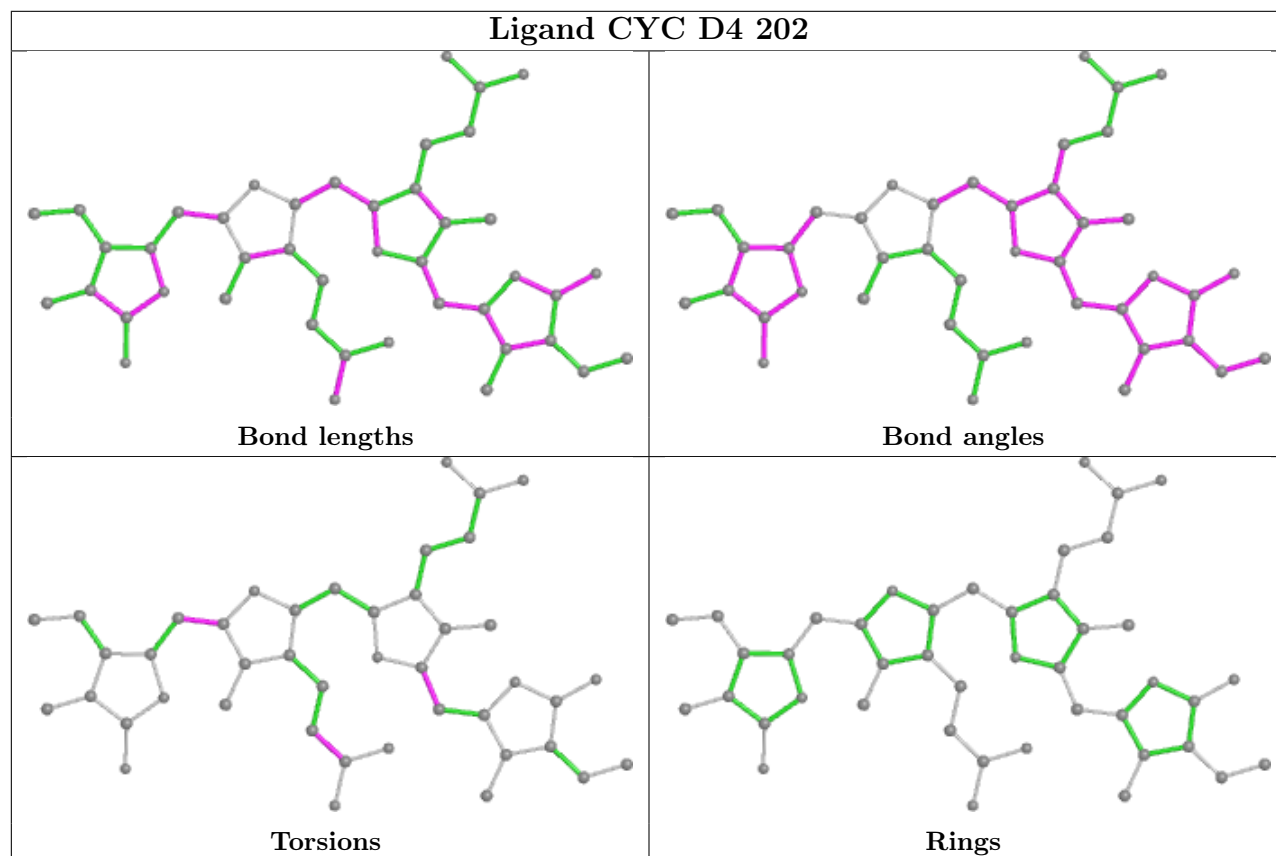
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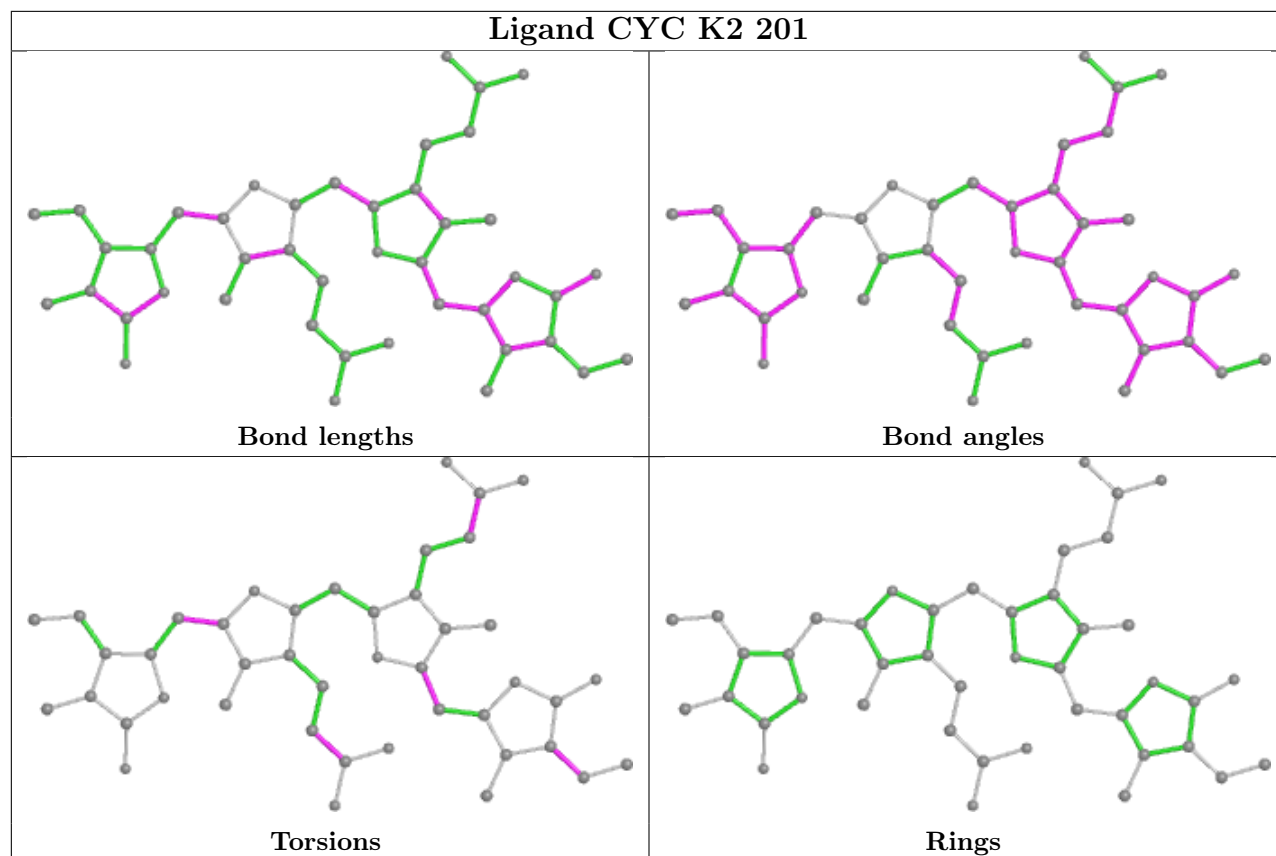
Ligand CYC P3 201



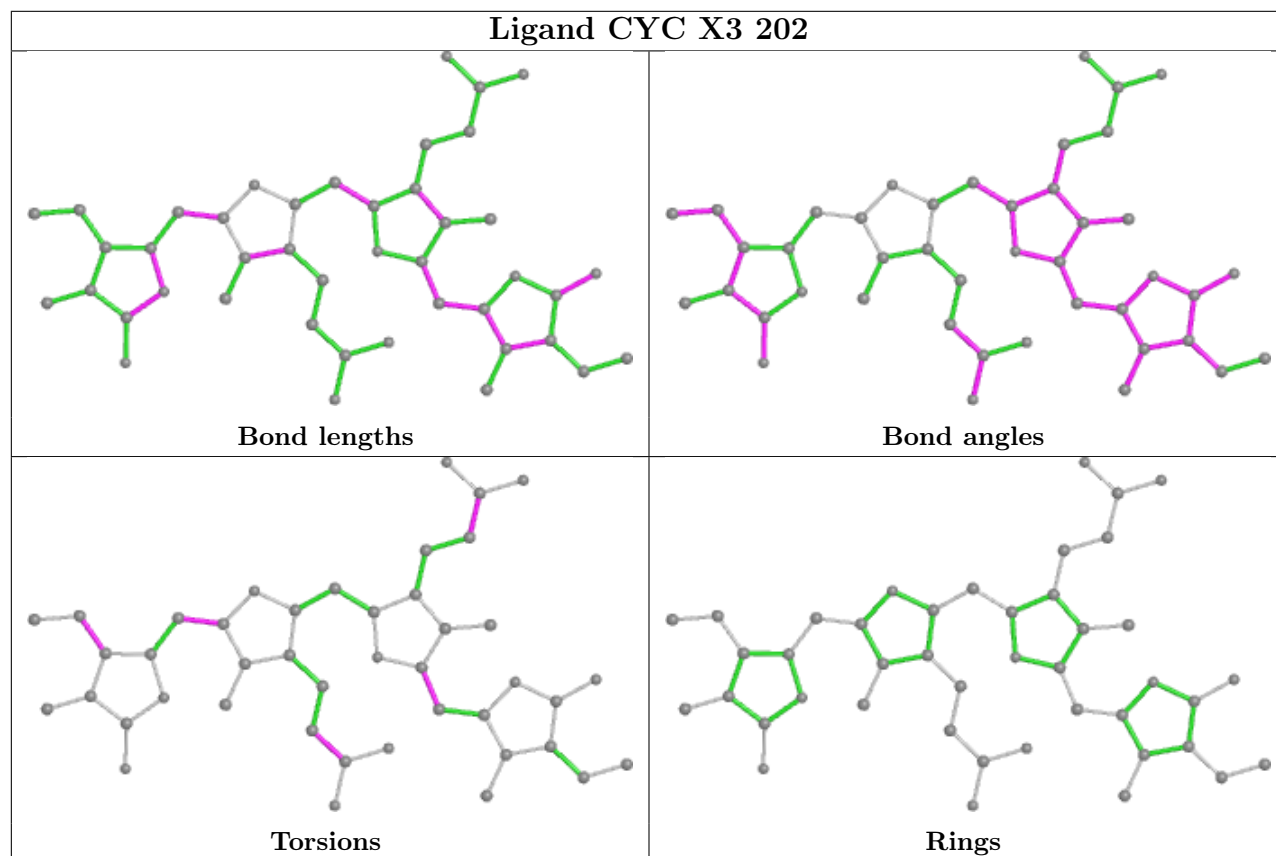
Ligand CYC D4 202



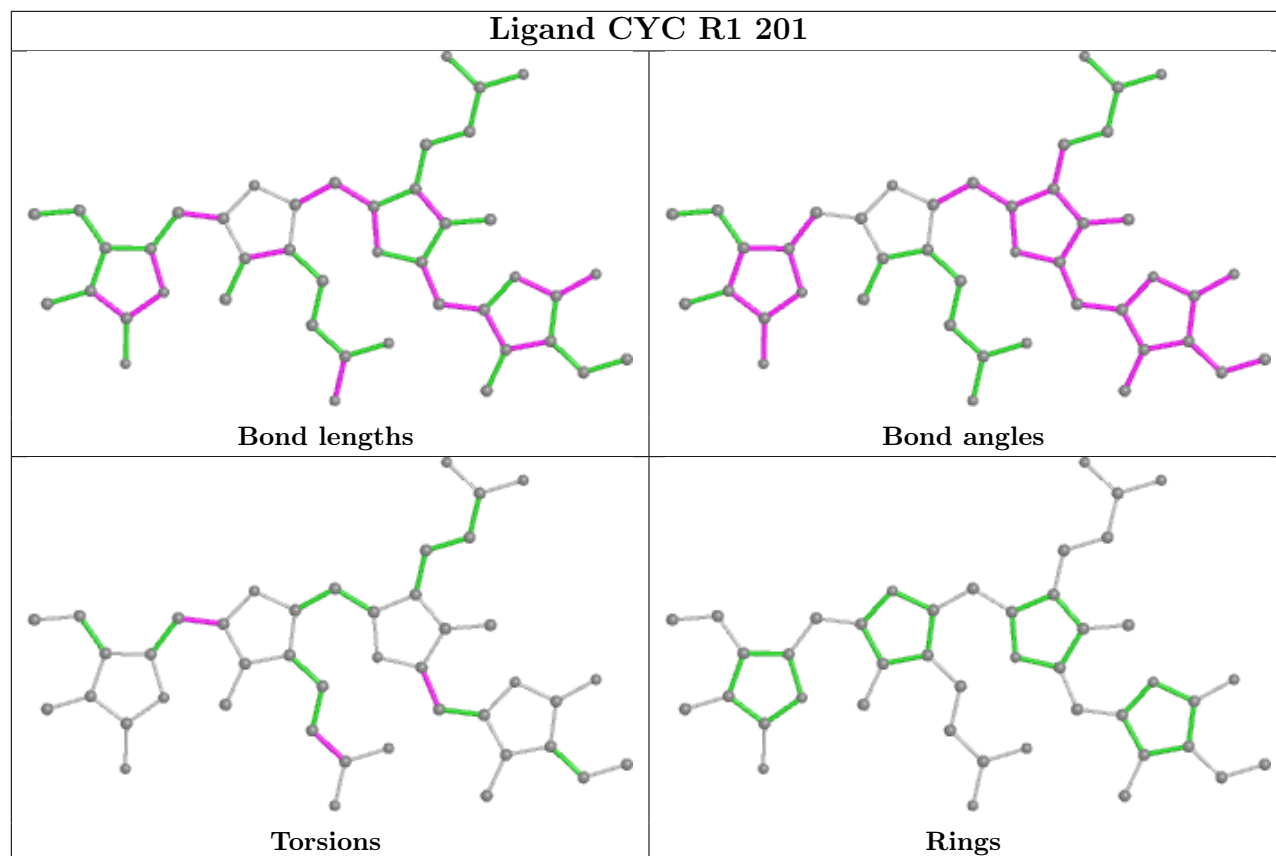
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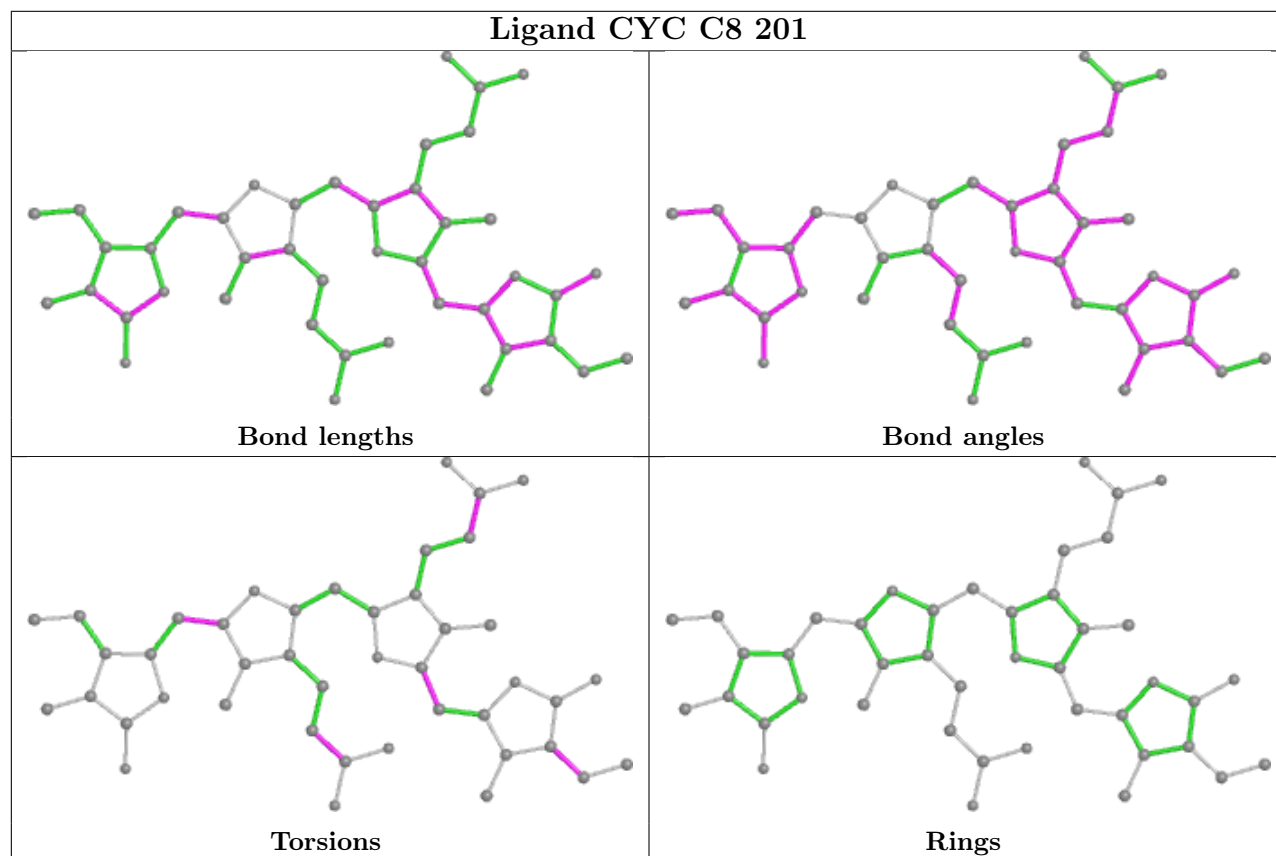
Ligand CYC X3 202

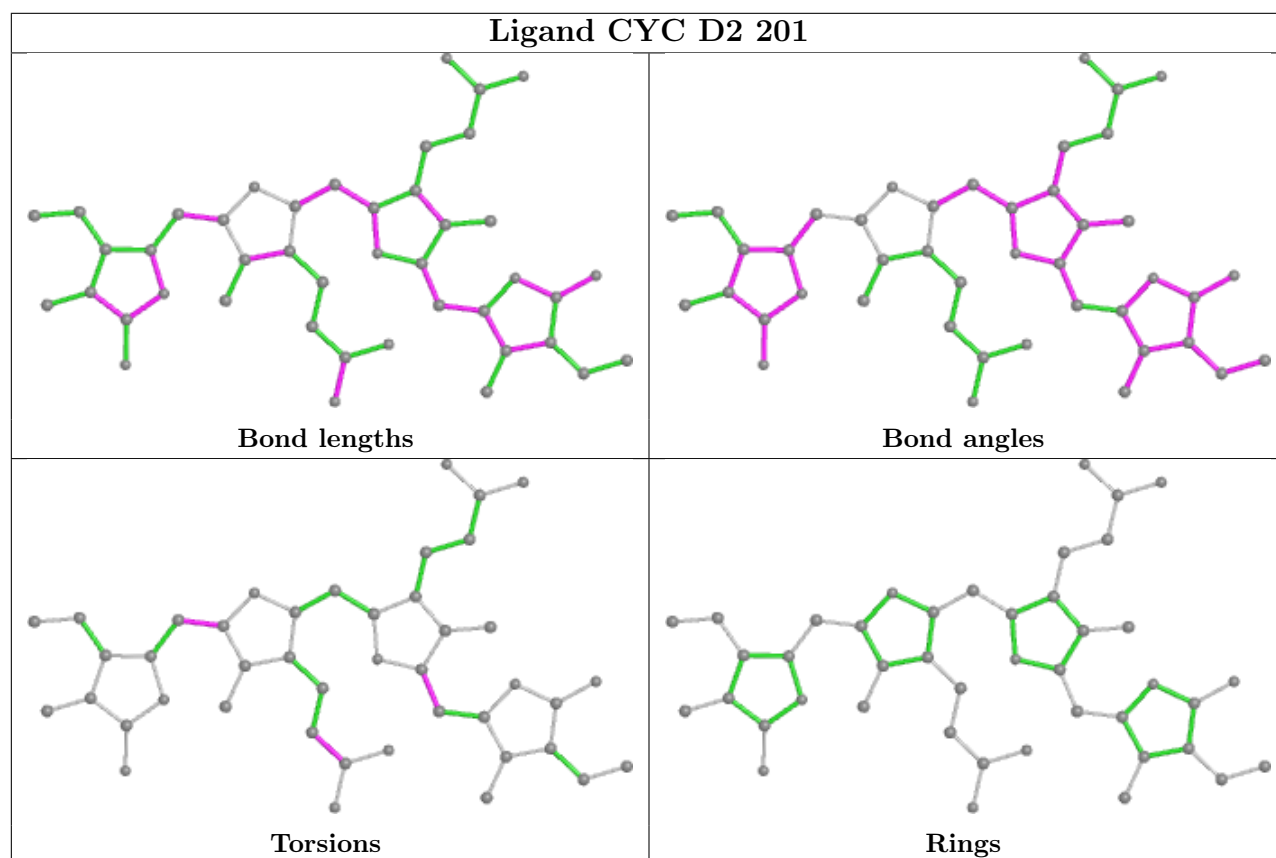
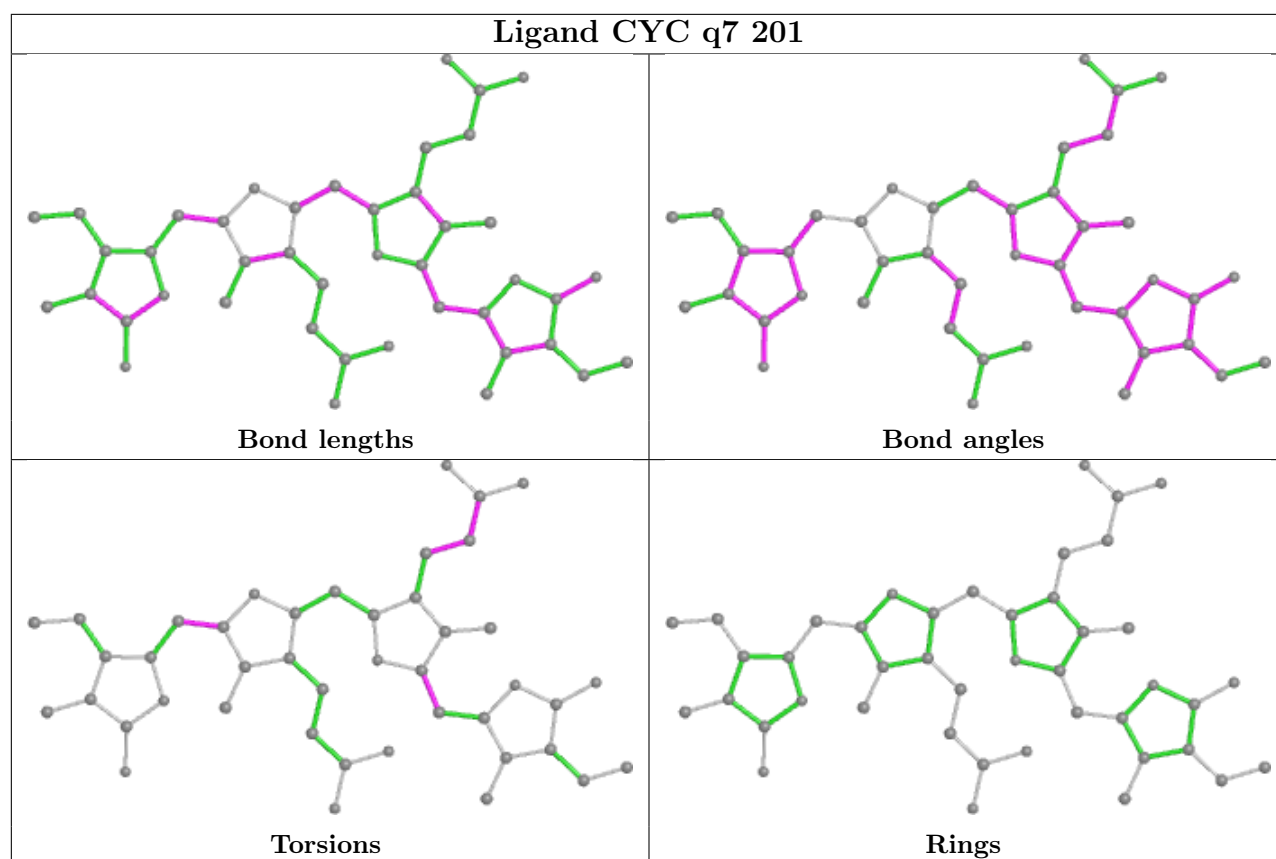


Ligand CYC R1 201

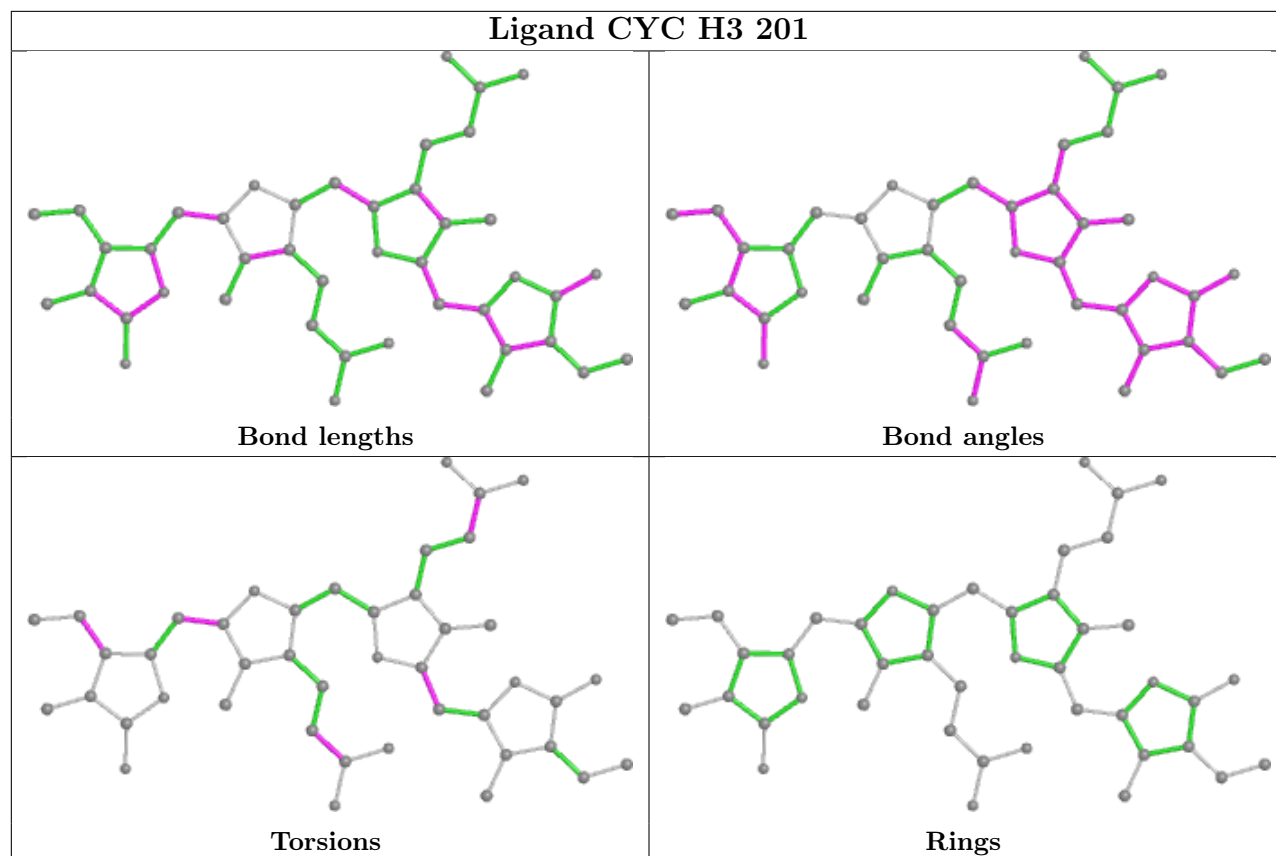


Ligand CYC C8 201

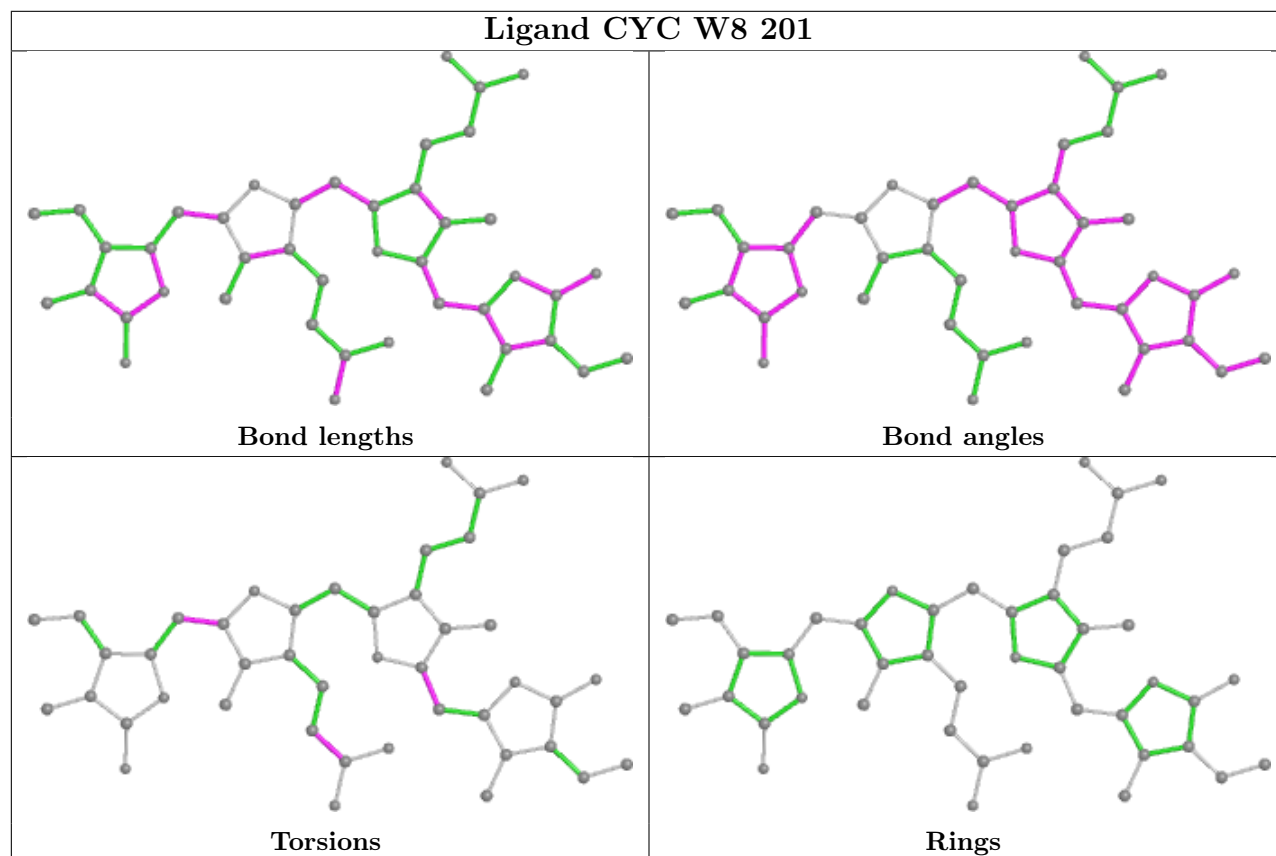




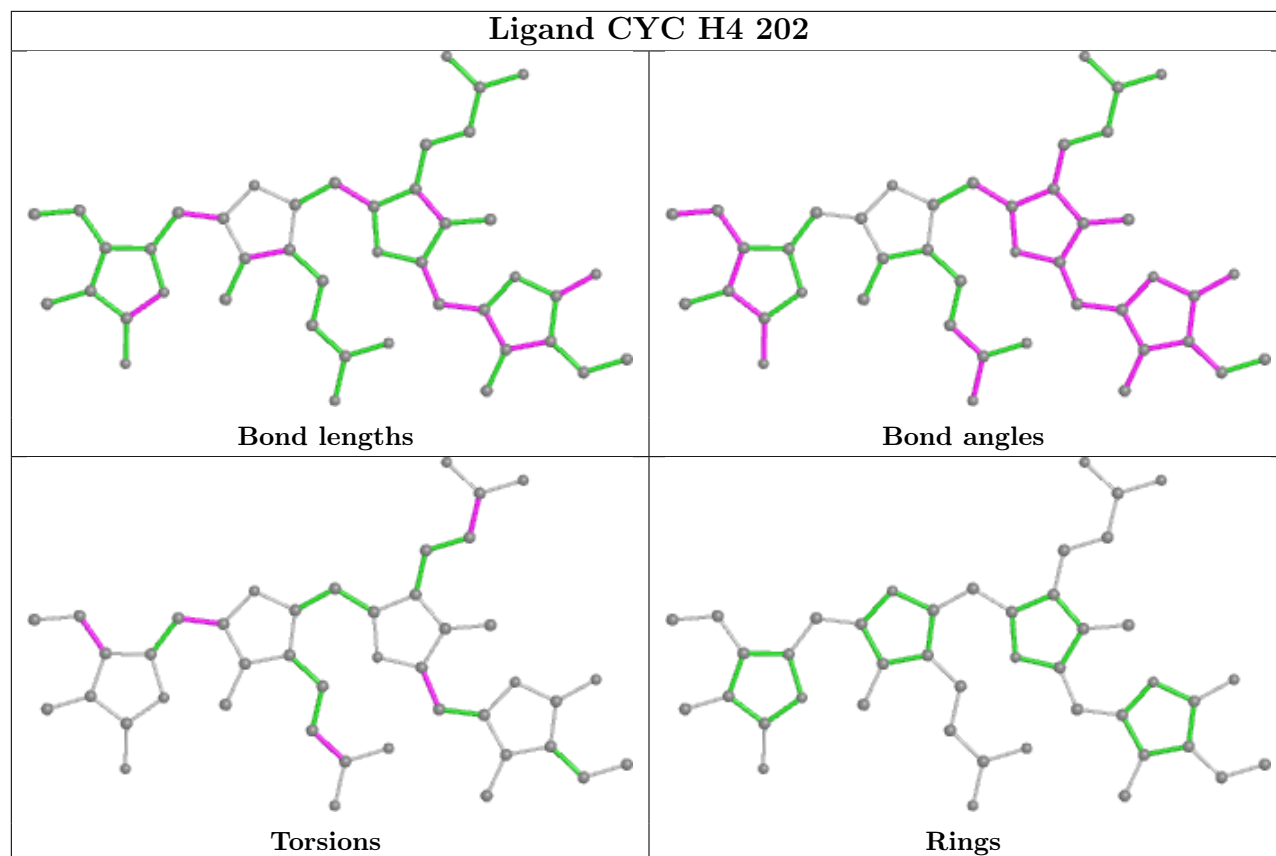
Ligand CYC H3 201



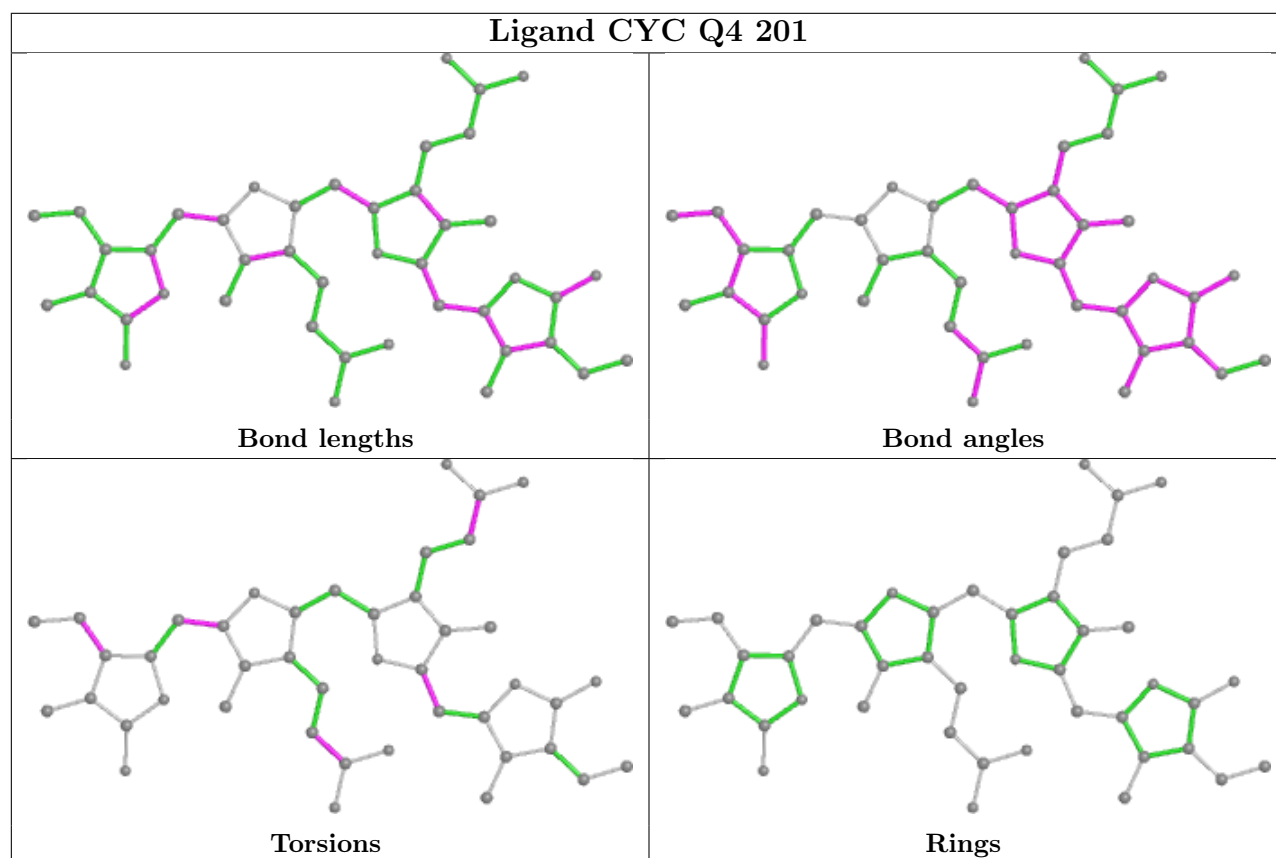
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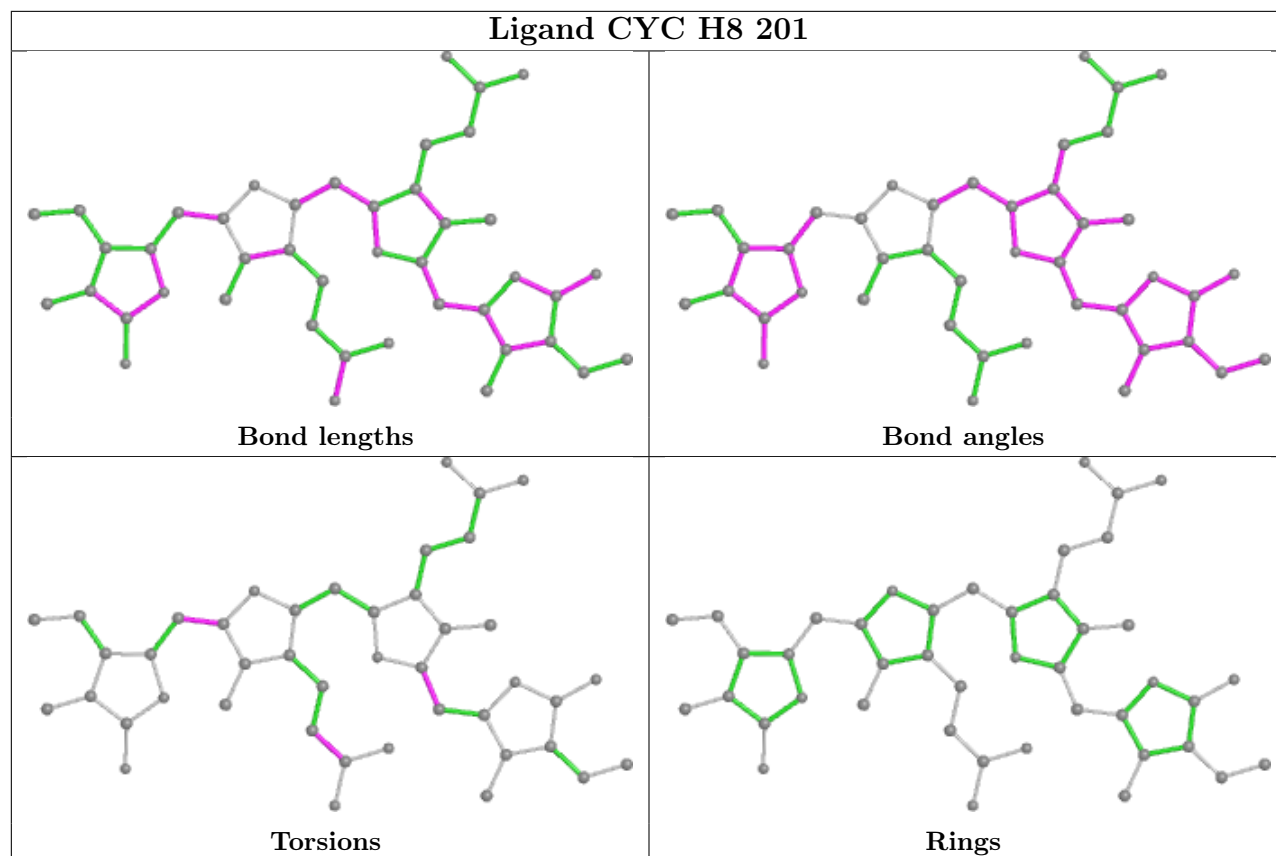
Ligand CYC H4 202



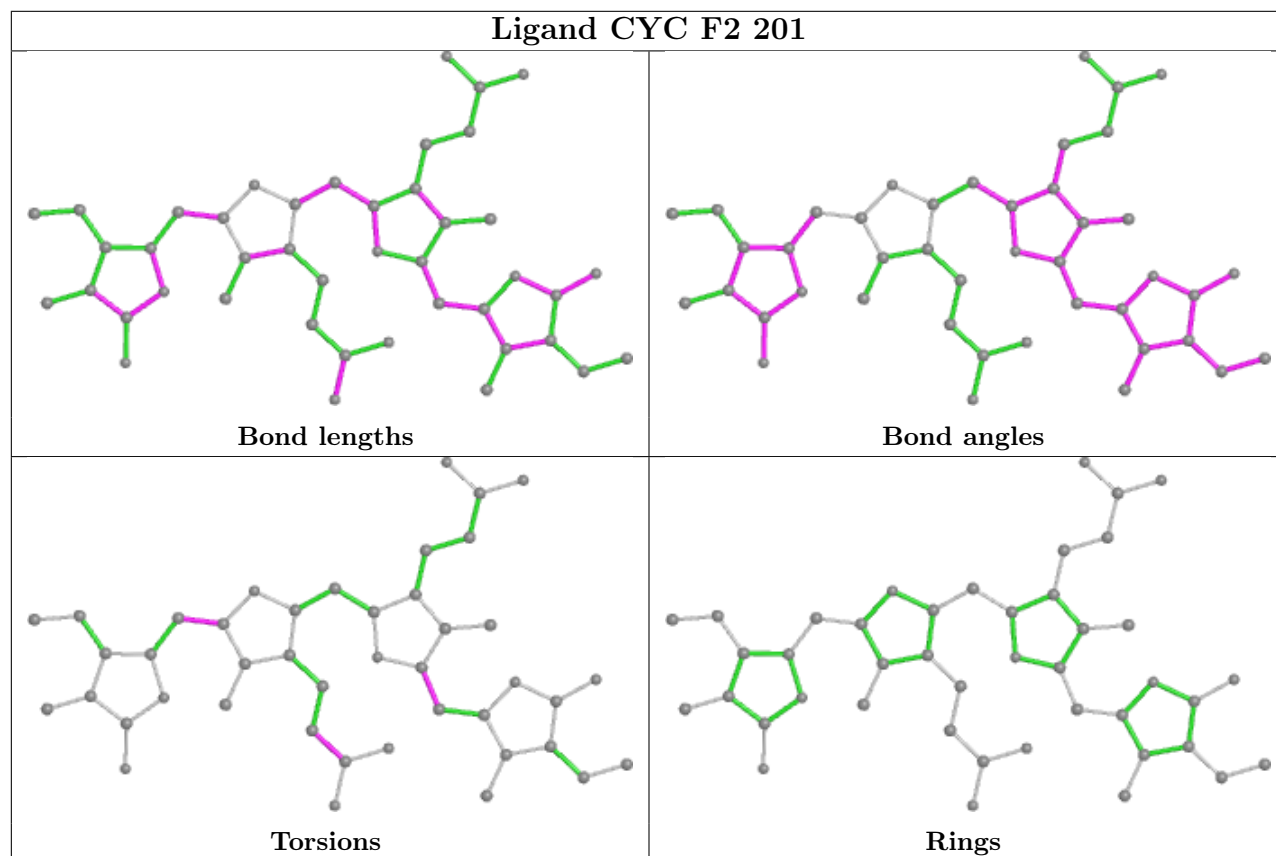
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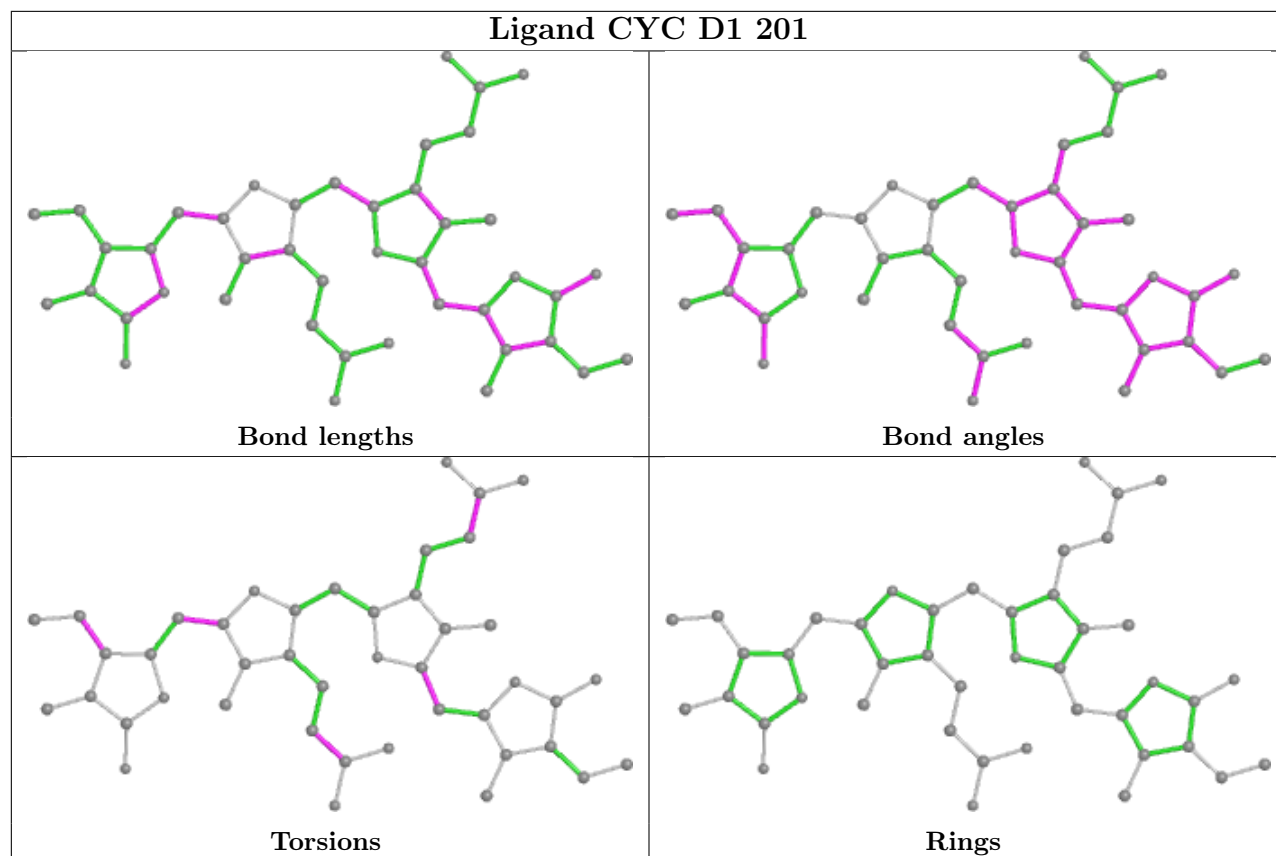
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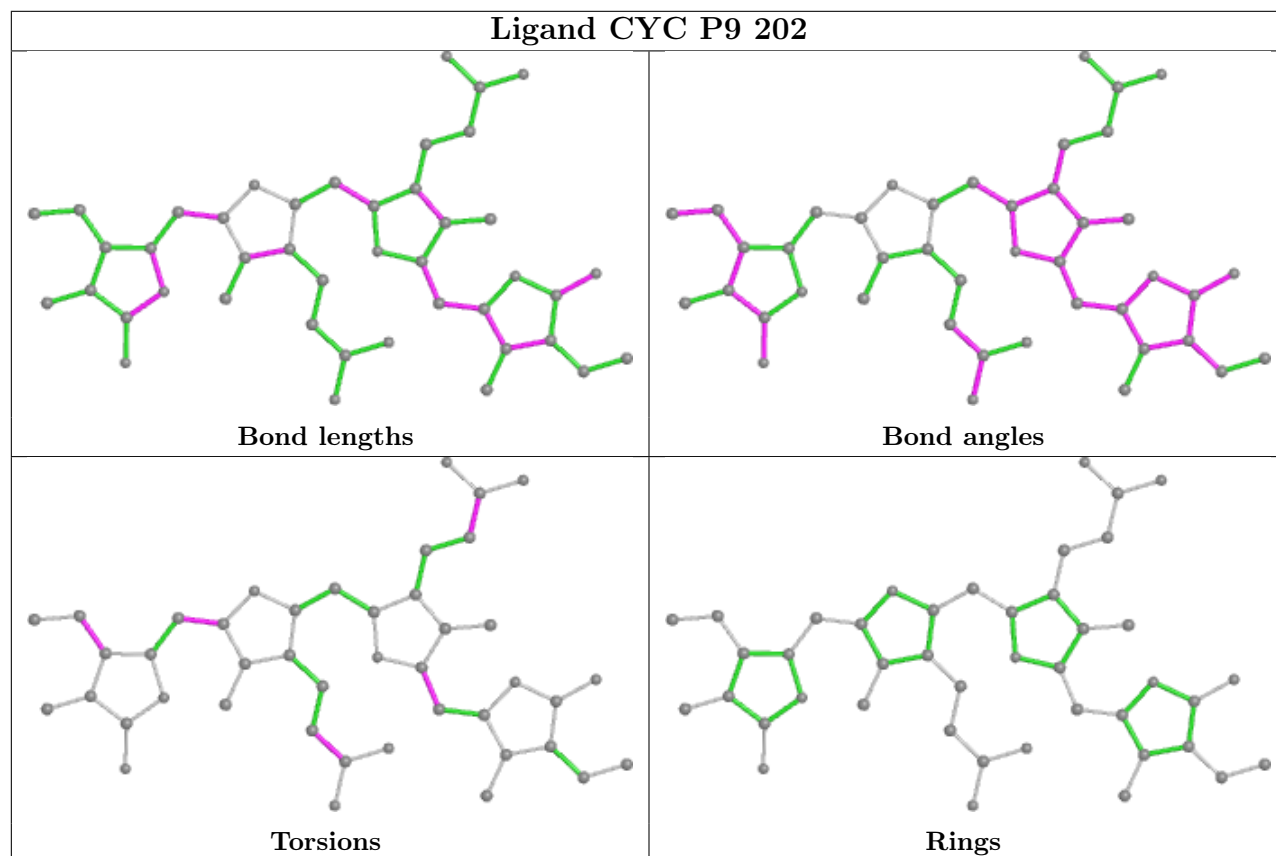
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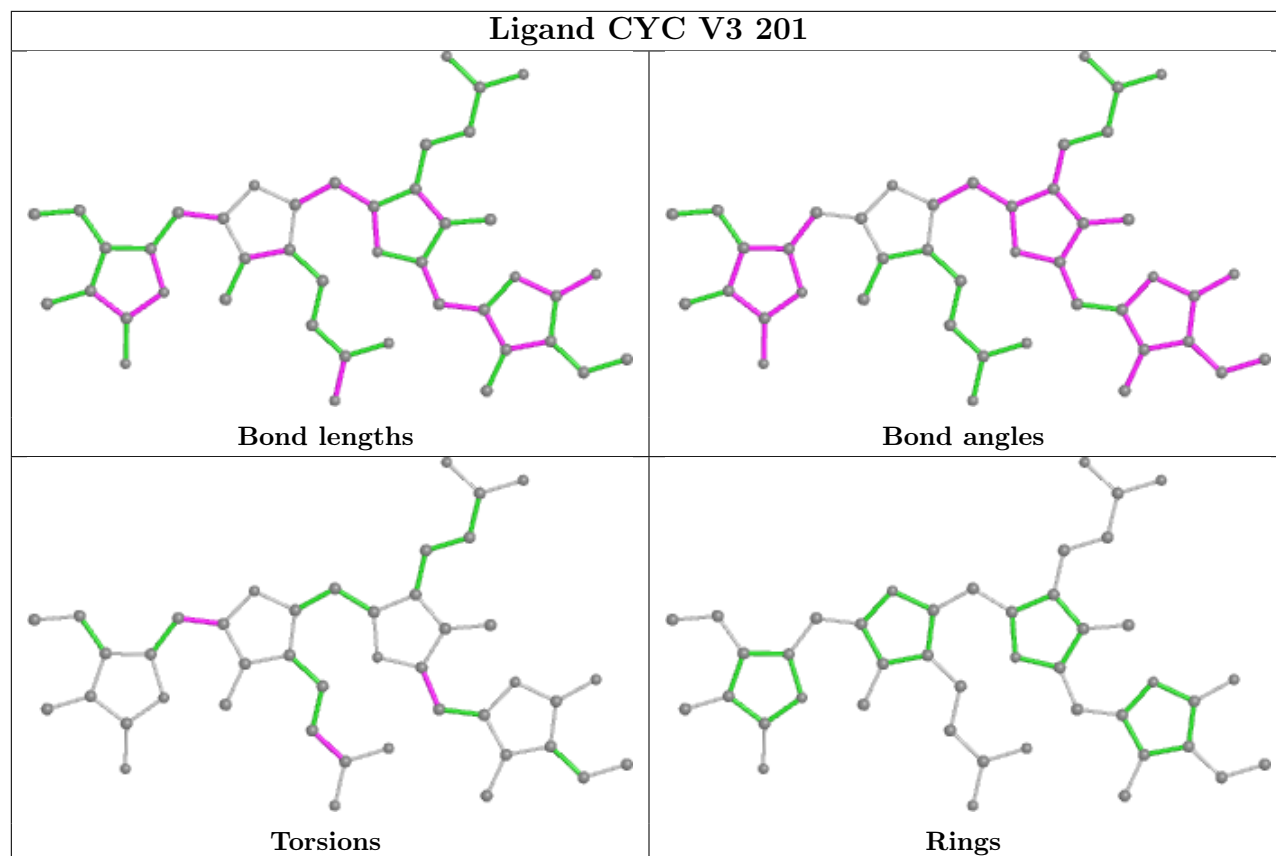
Ligand CYC D1 201



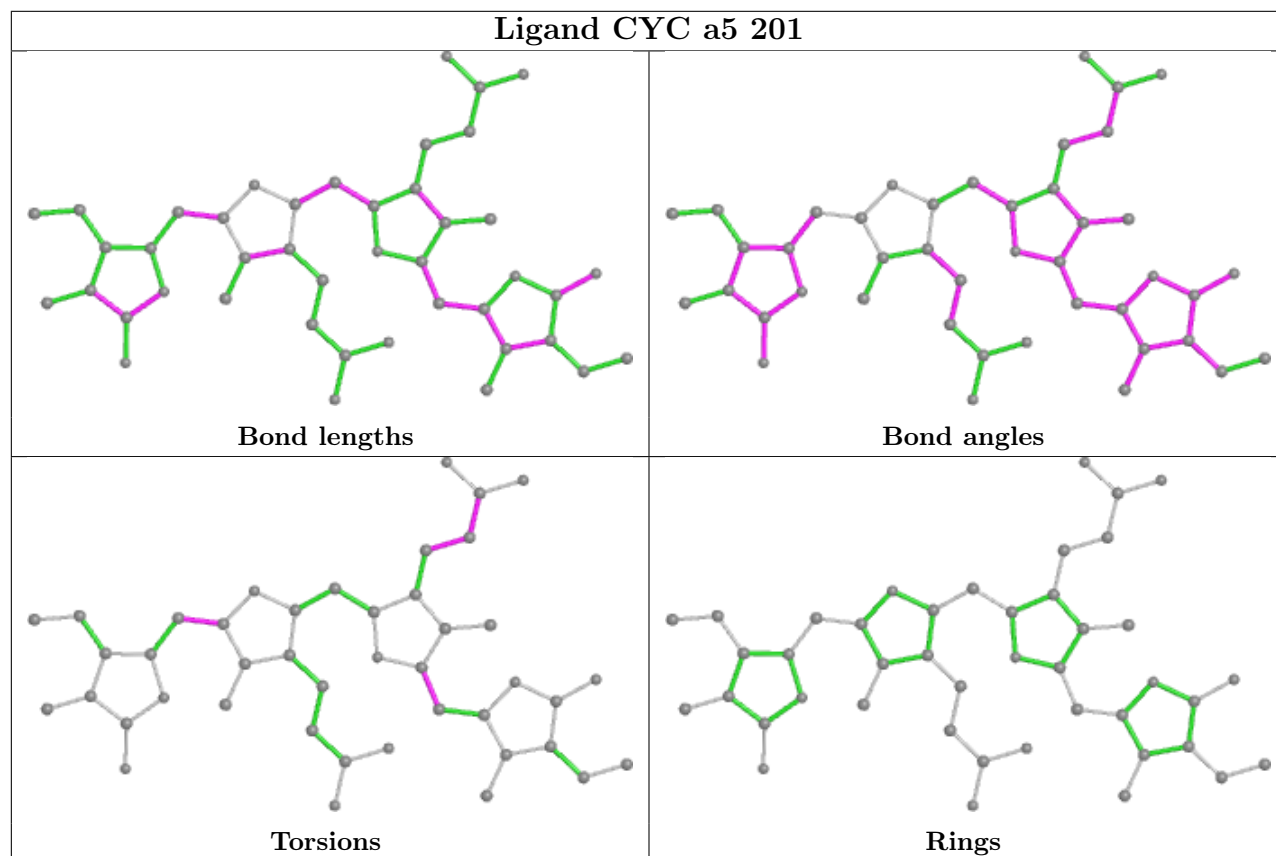
Ligand CYC P9 202



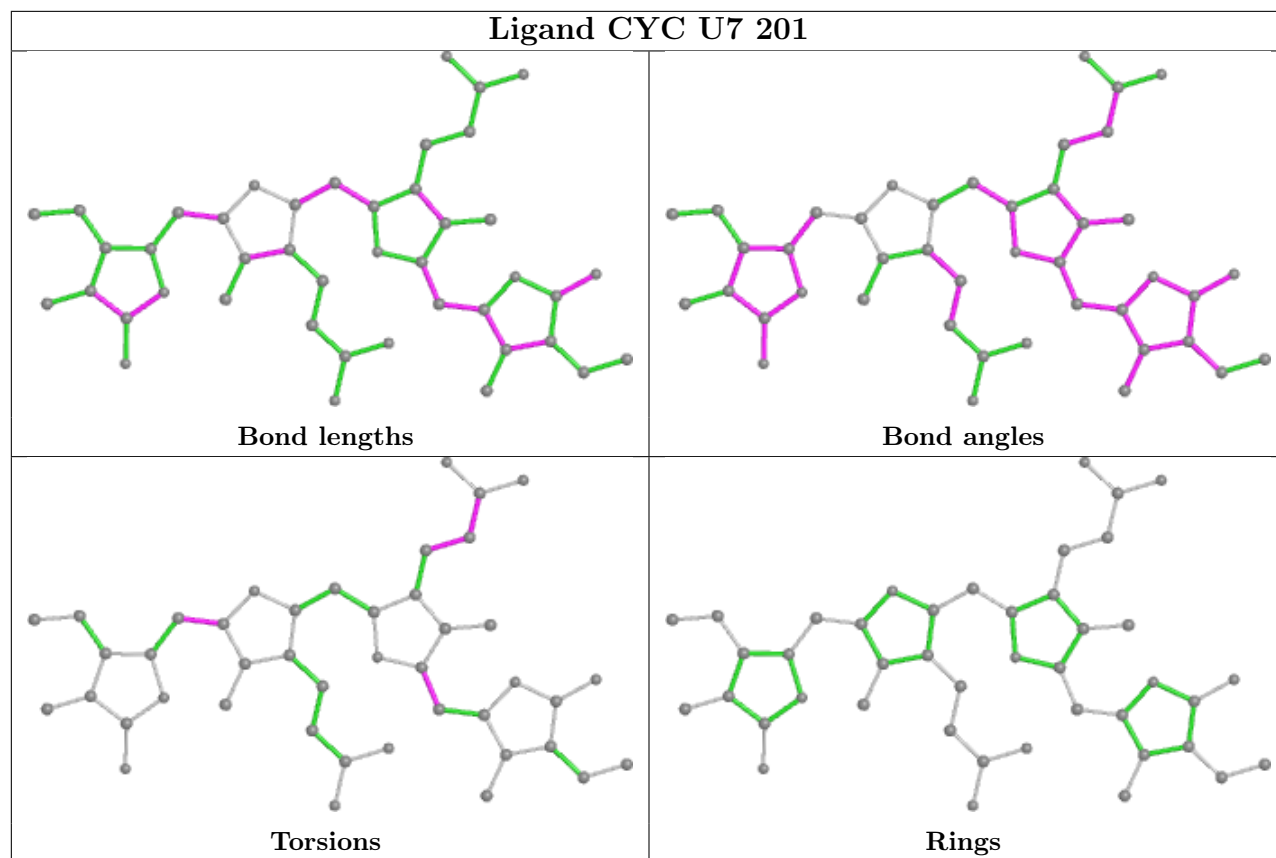
Ligand CYC V3 201



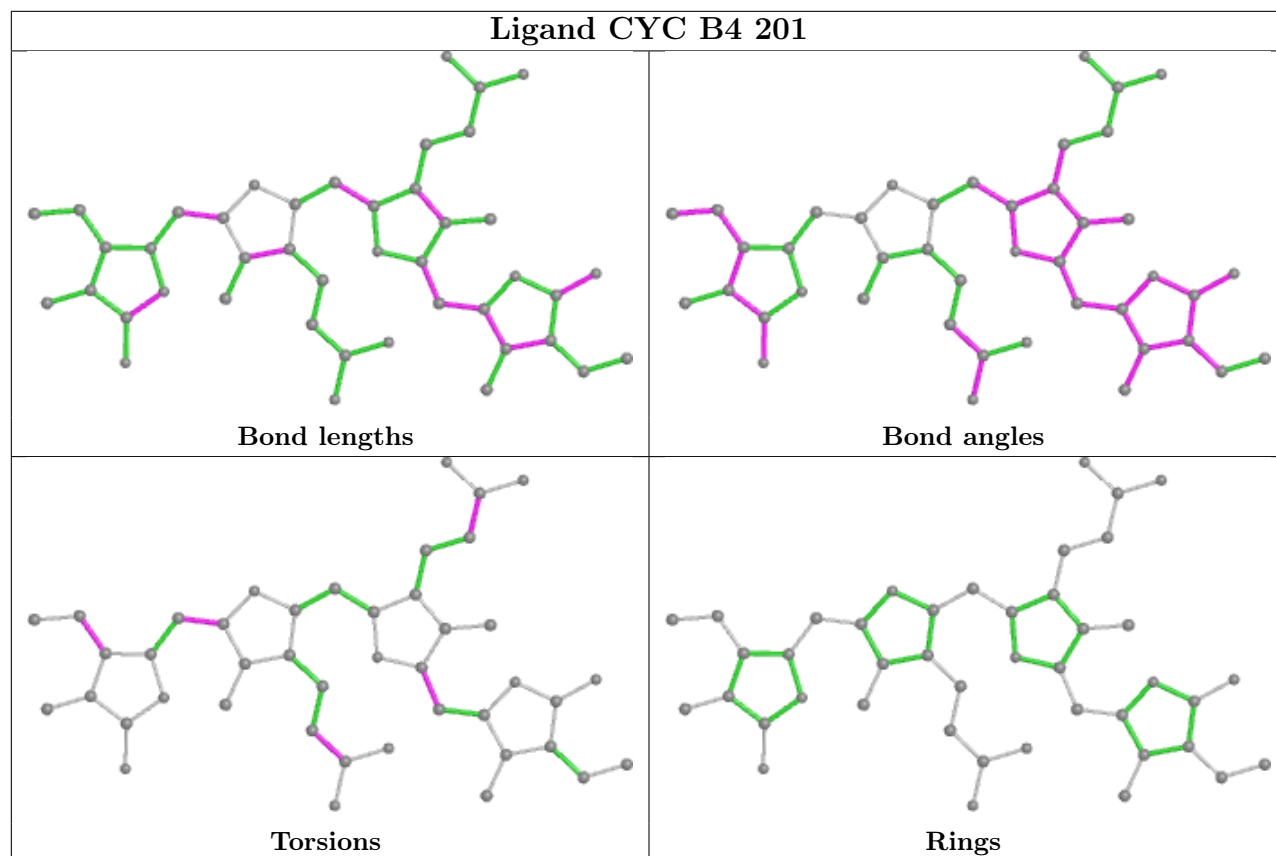
Ligand CYC a5 201



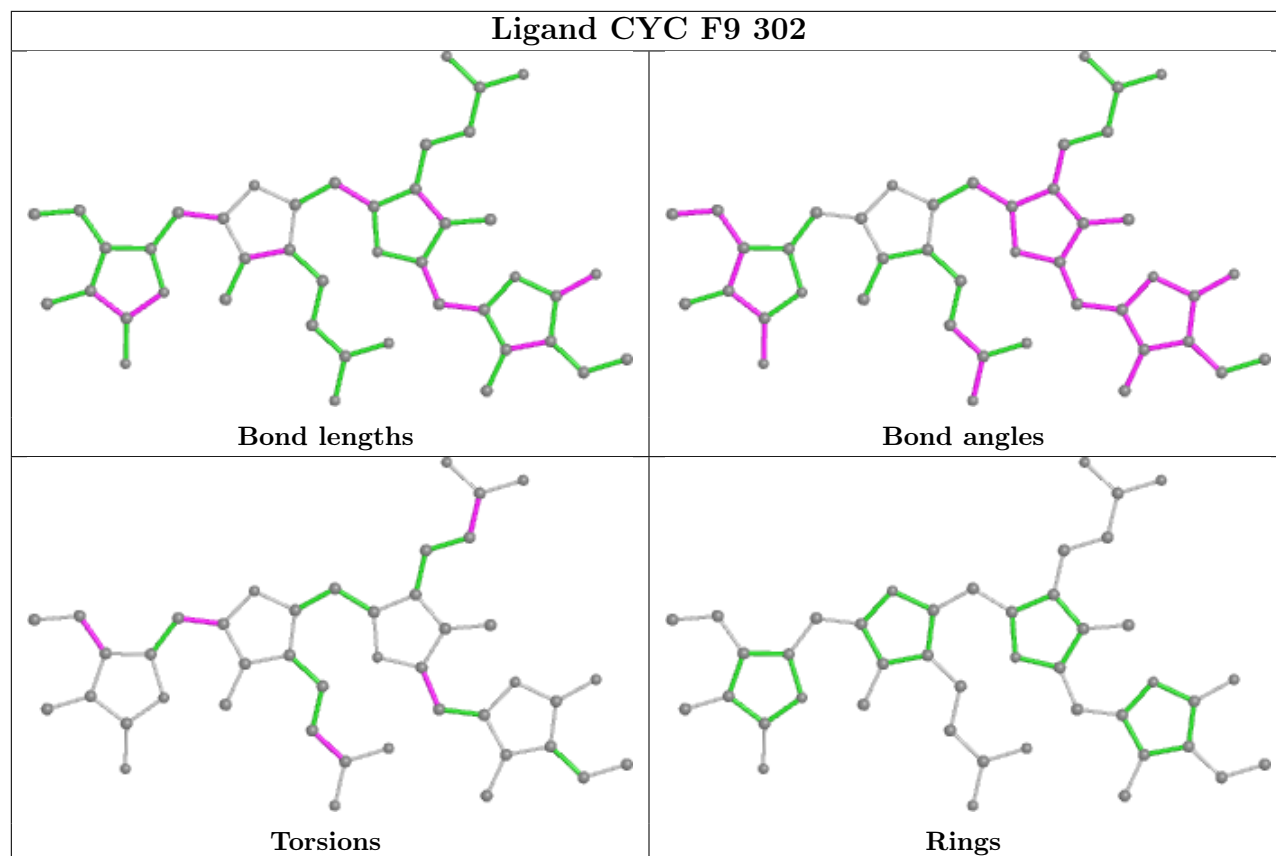
Ligand CYC U7 201



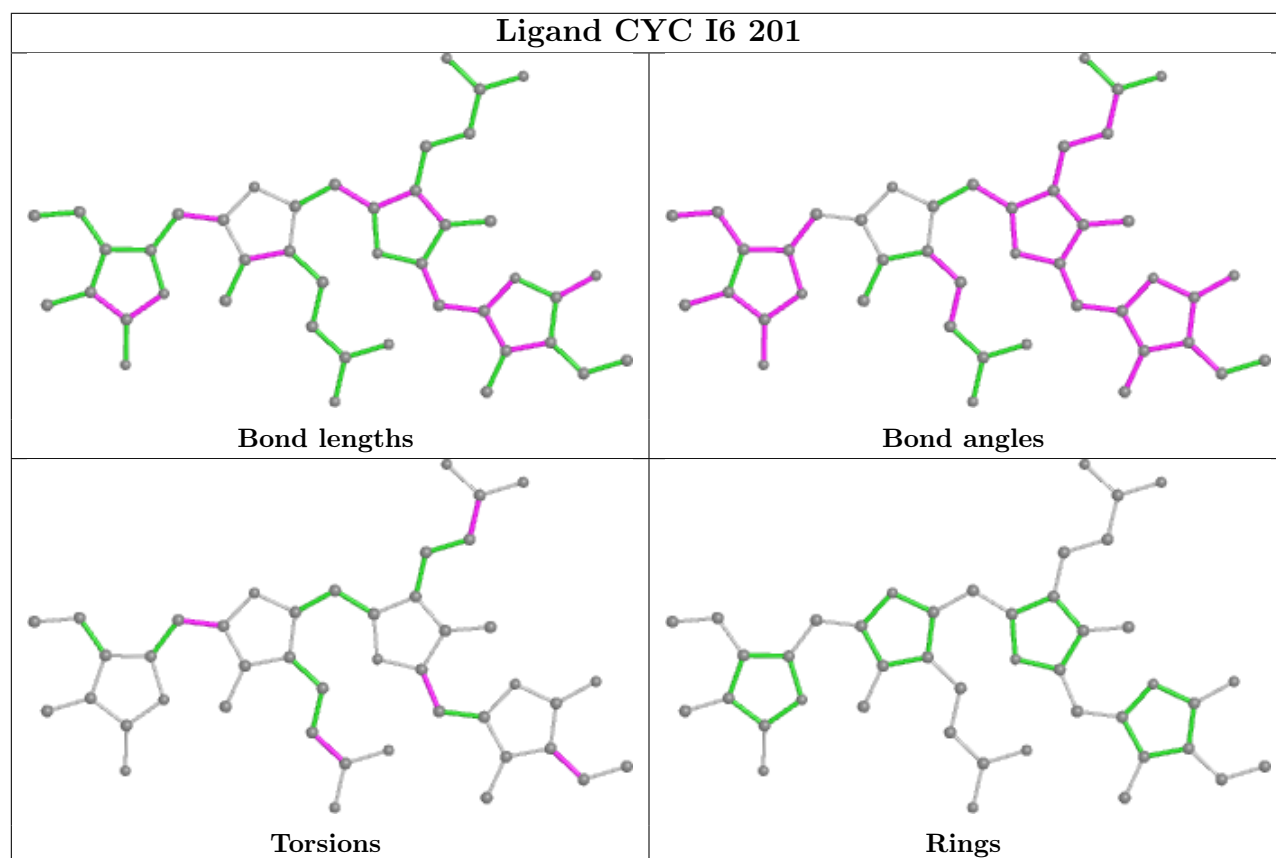
Ligand CYC B4 201



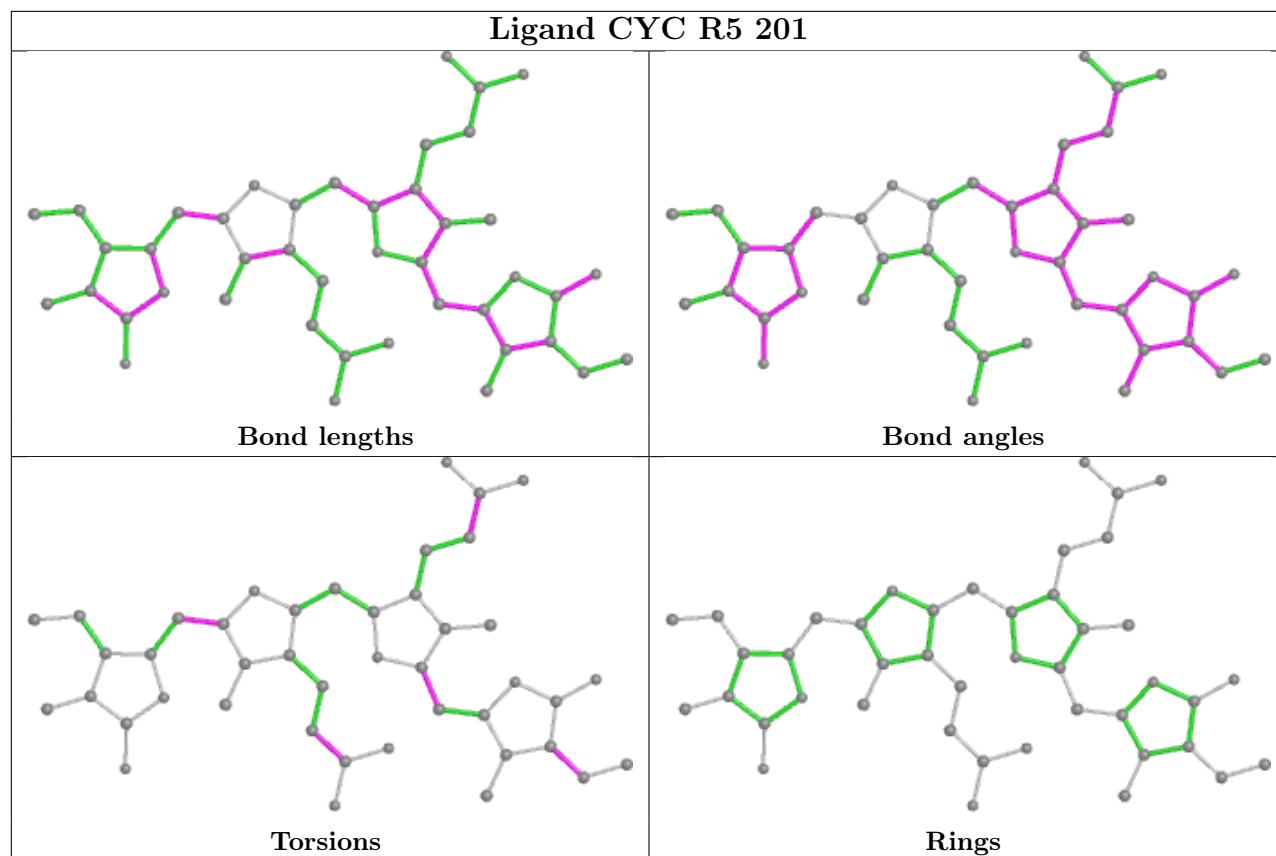
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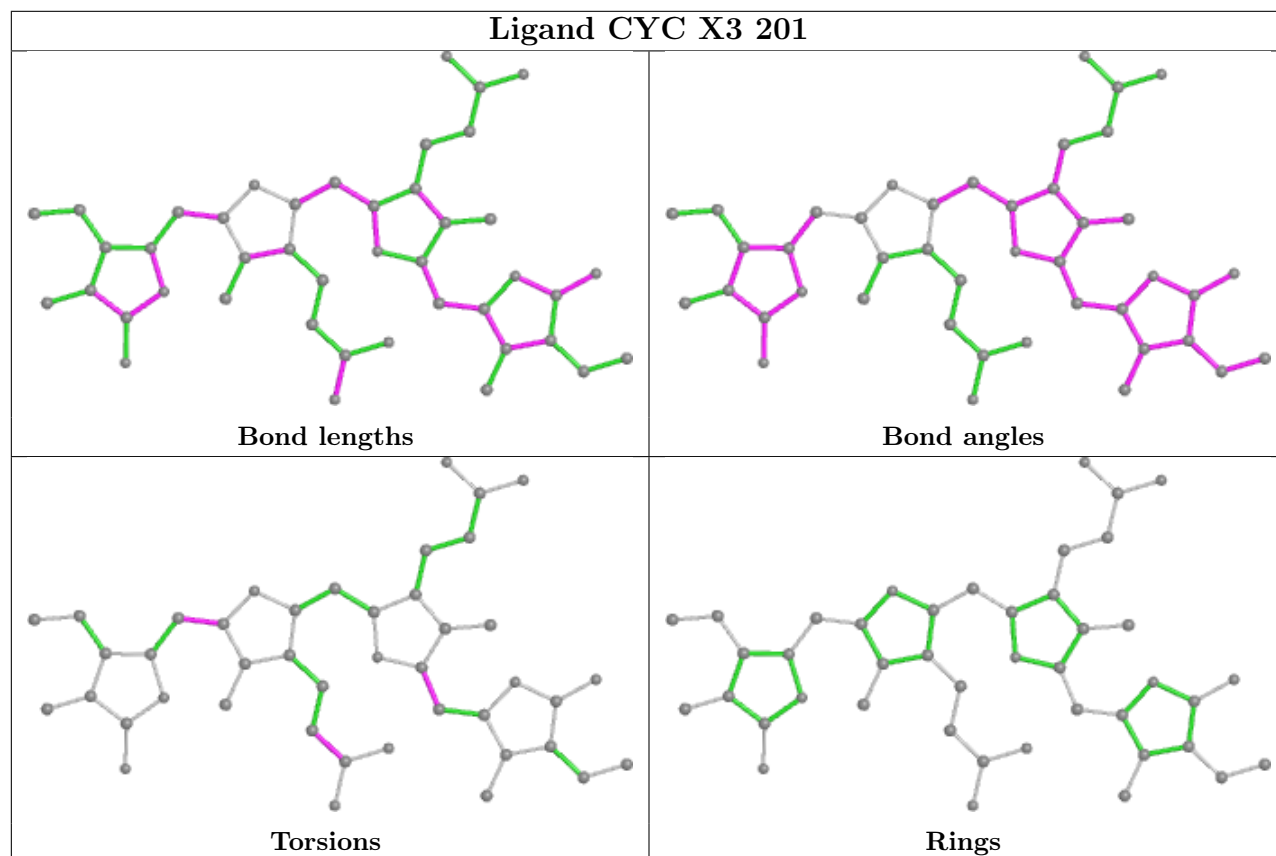
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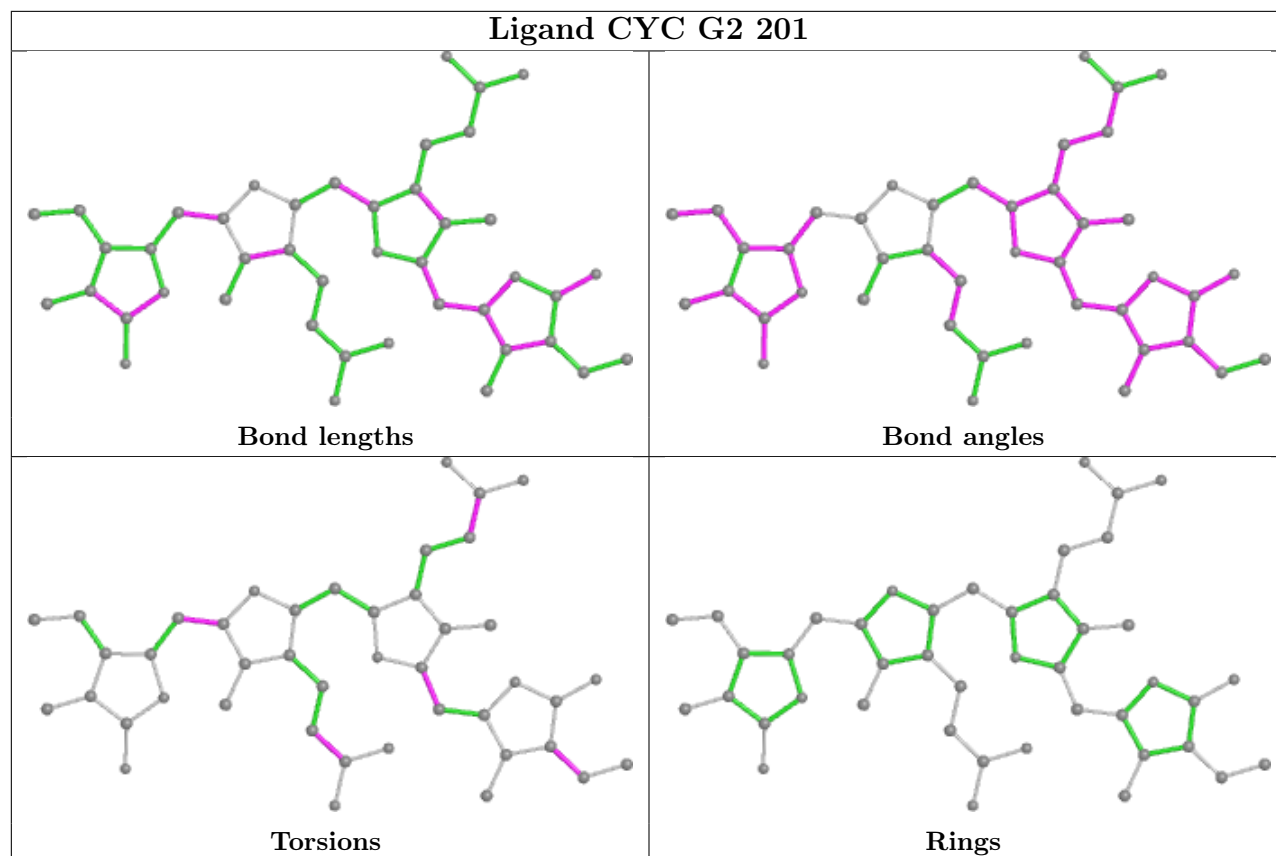
Ligand CYC R5 201



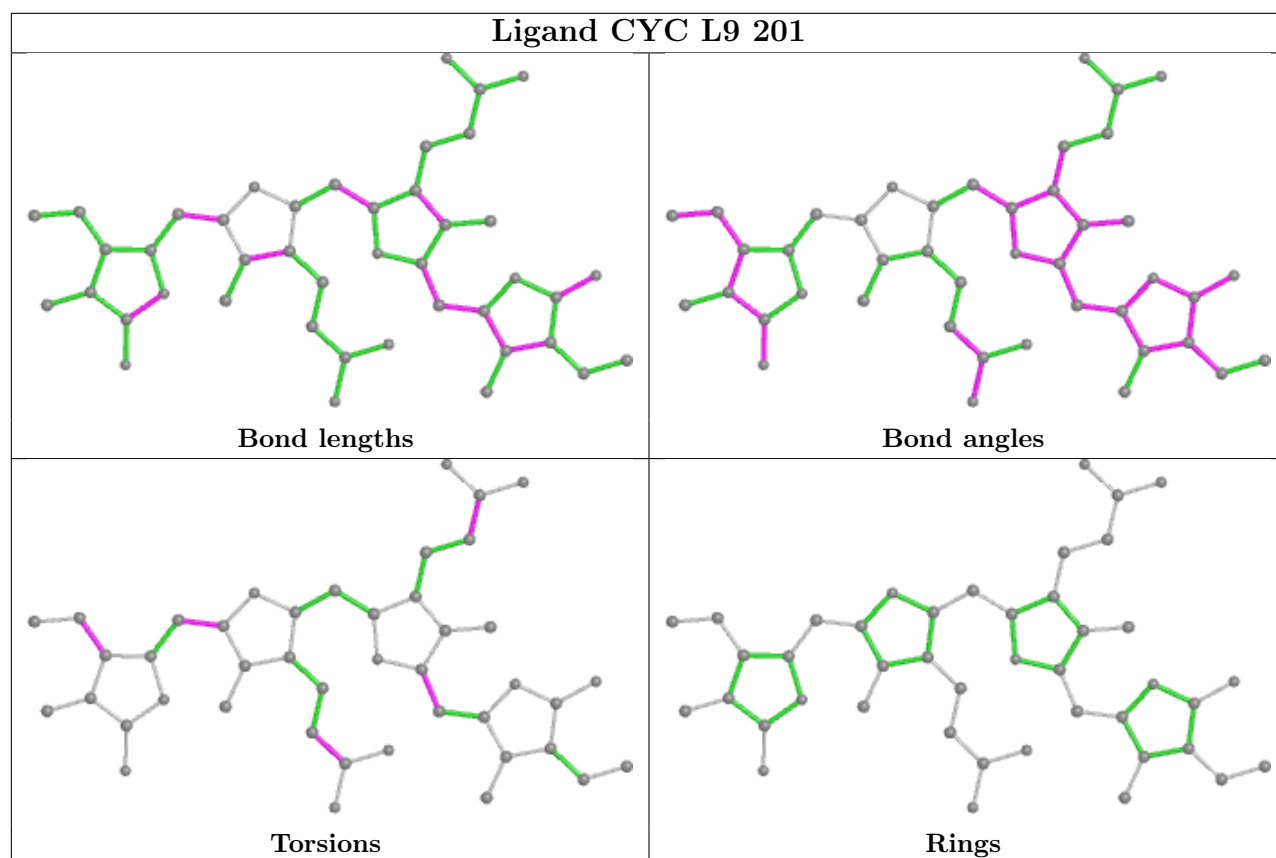
Ligand CYC X3 201



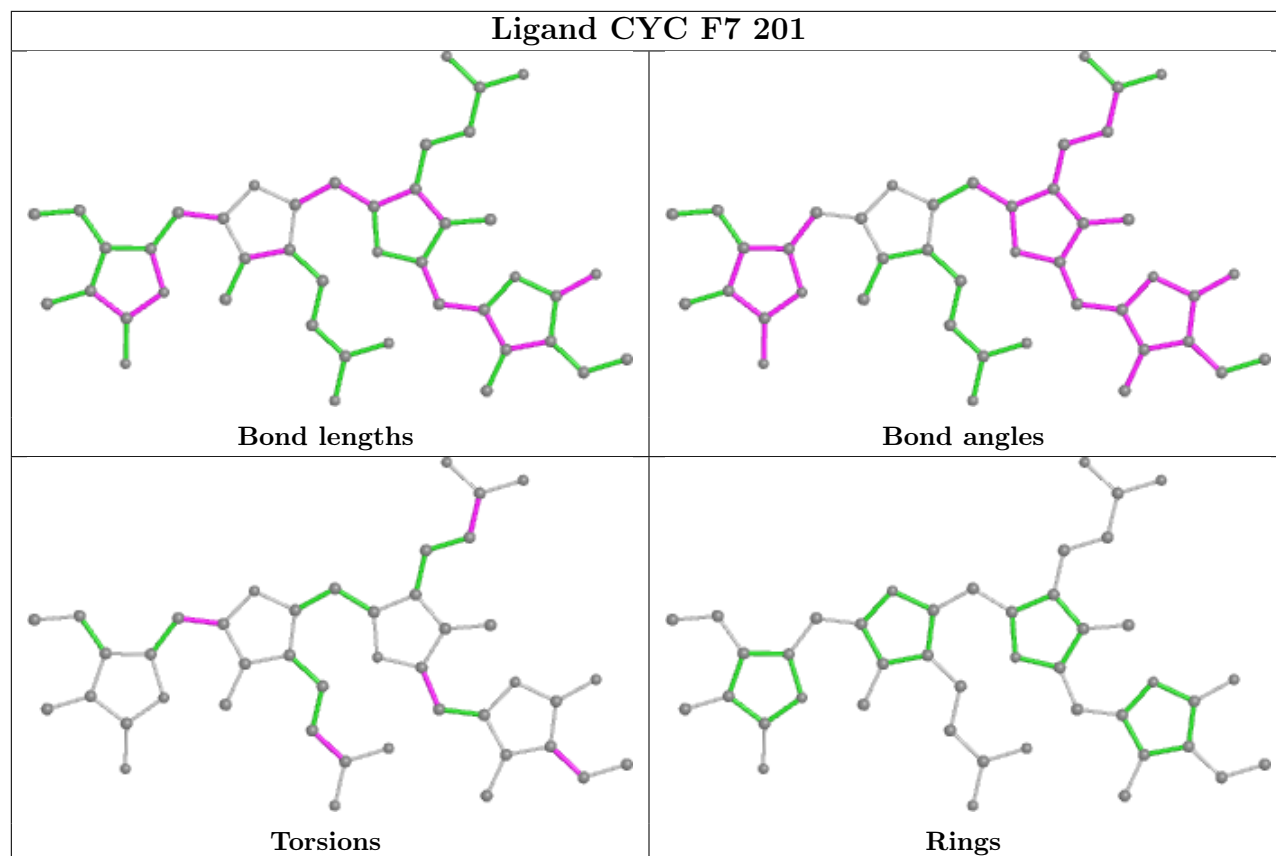
Ligand CYC G2 201



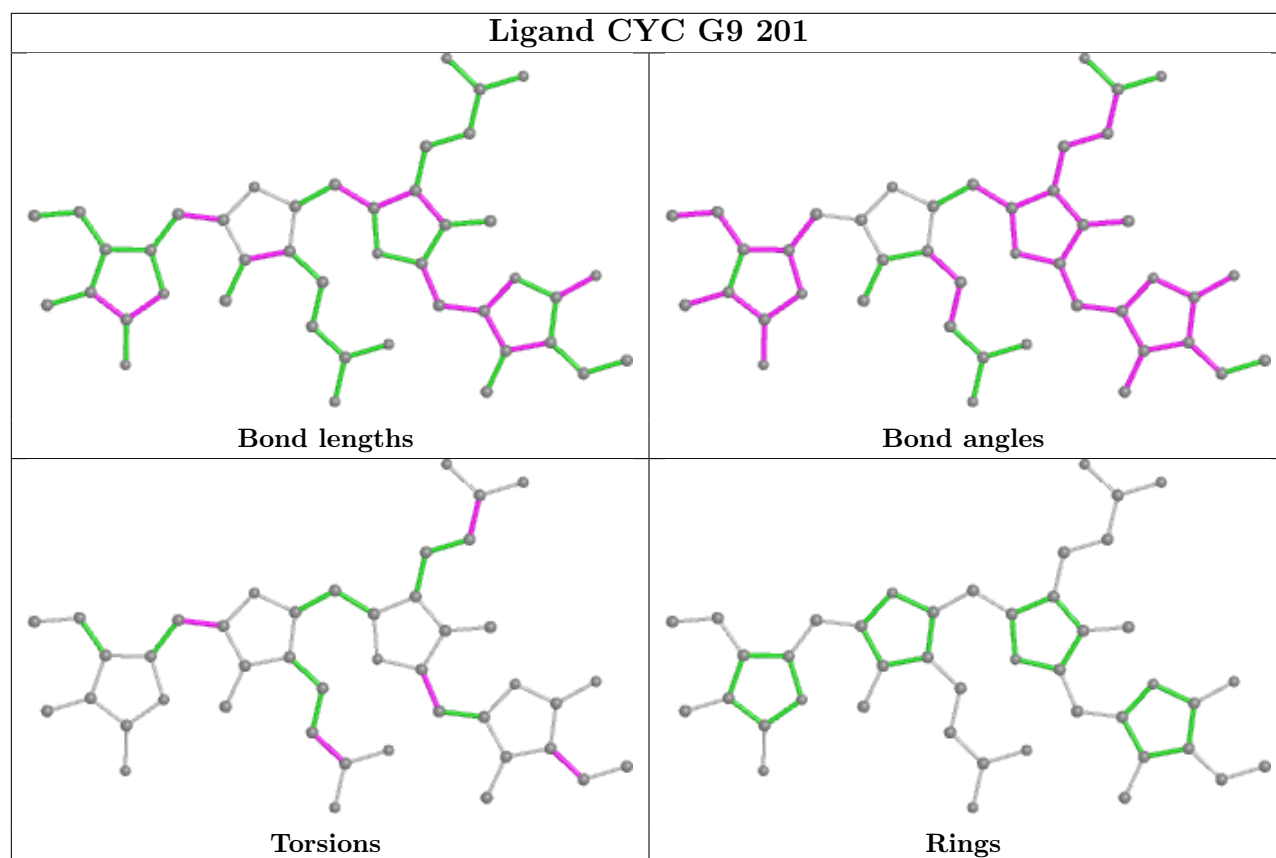
Ligand CYC L9 201



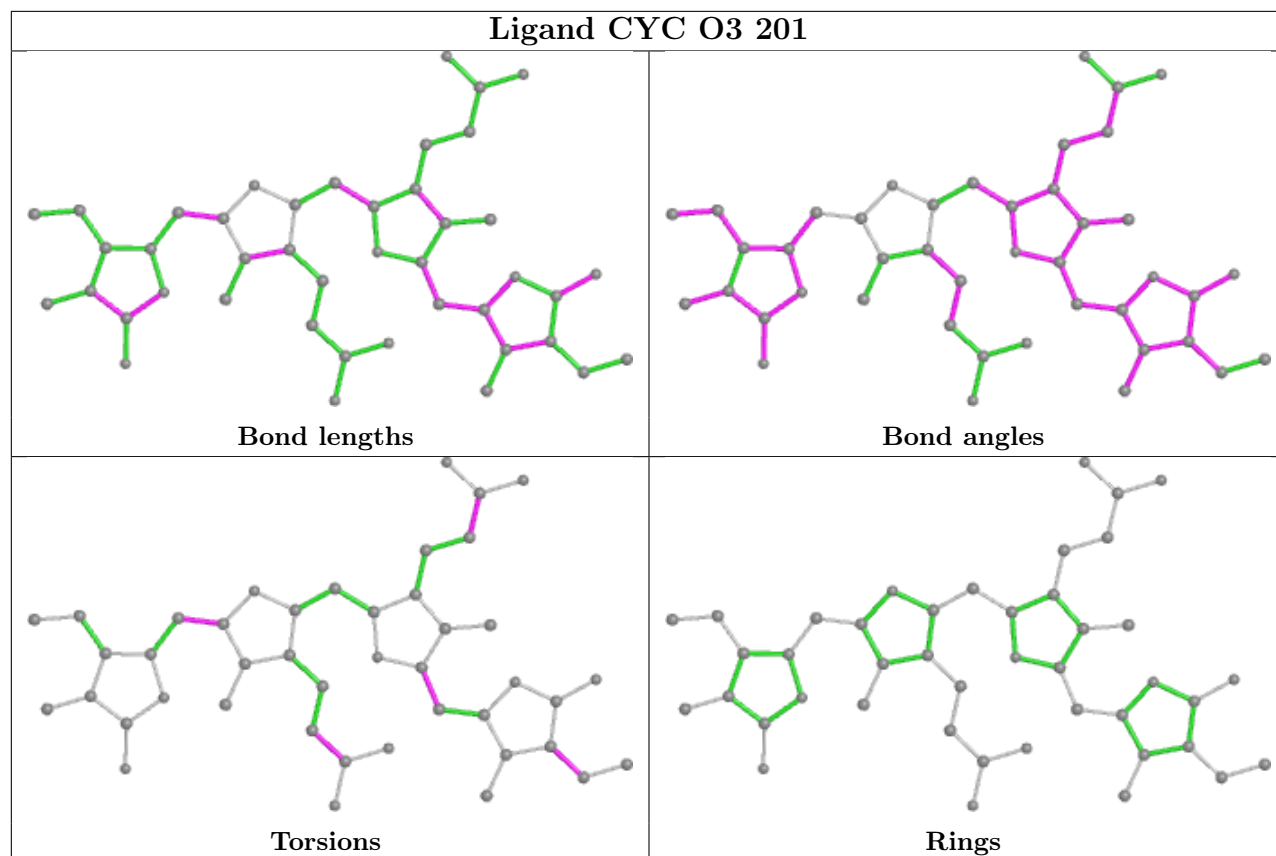
Ligand CYC F7 201



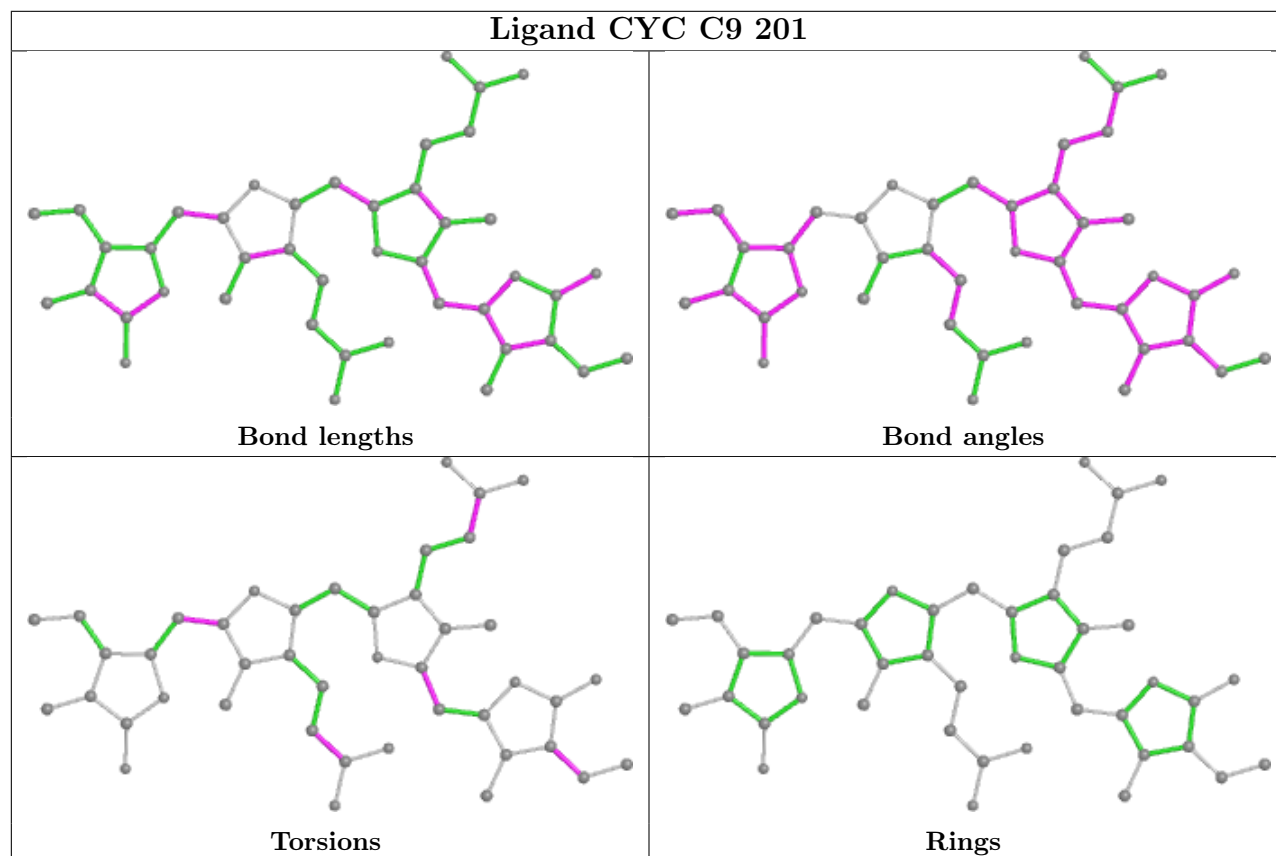
Ligand CYC G9 201



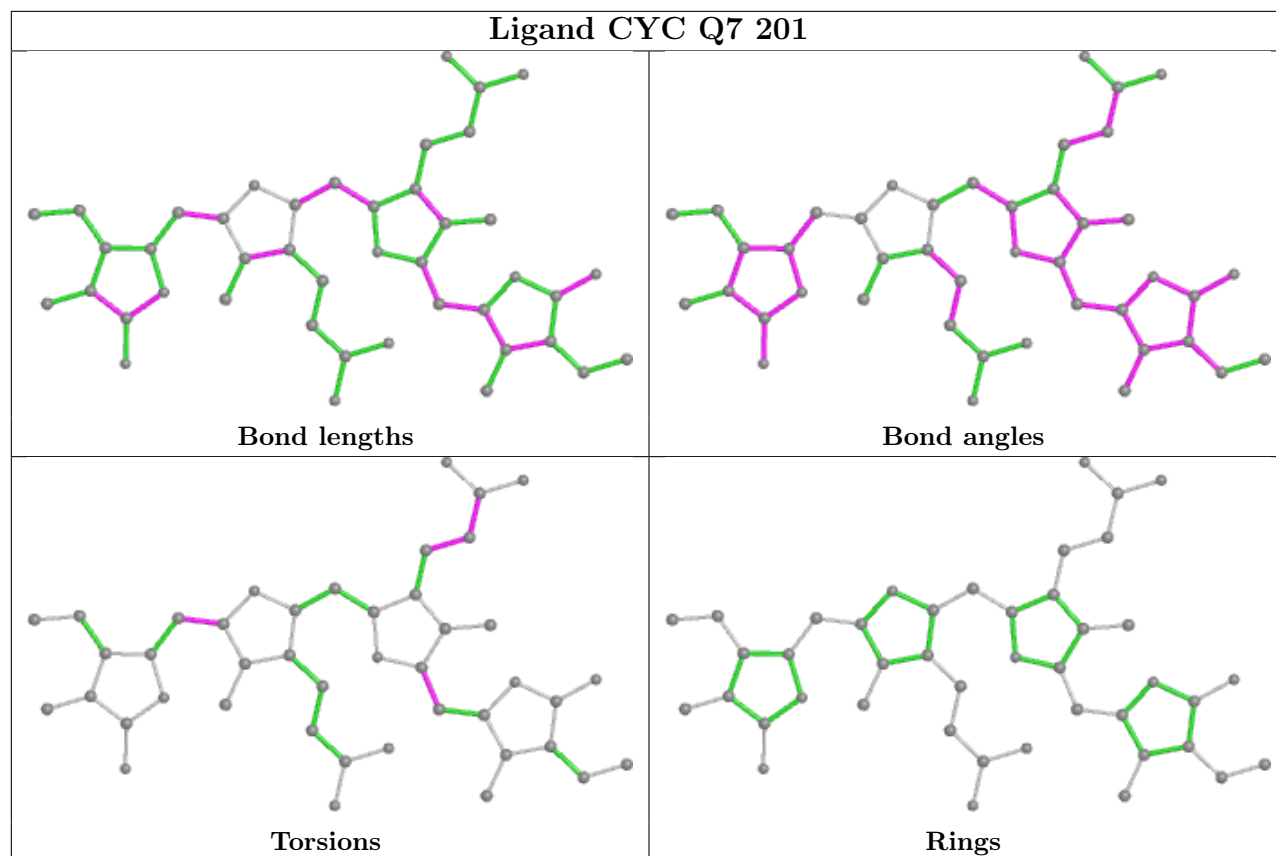
Ligand CYC O3 201



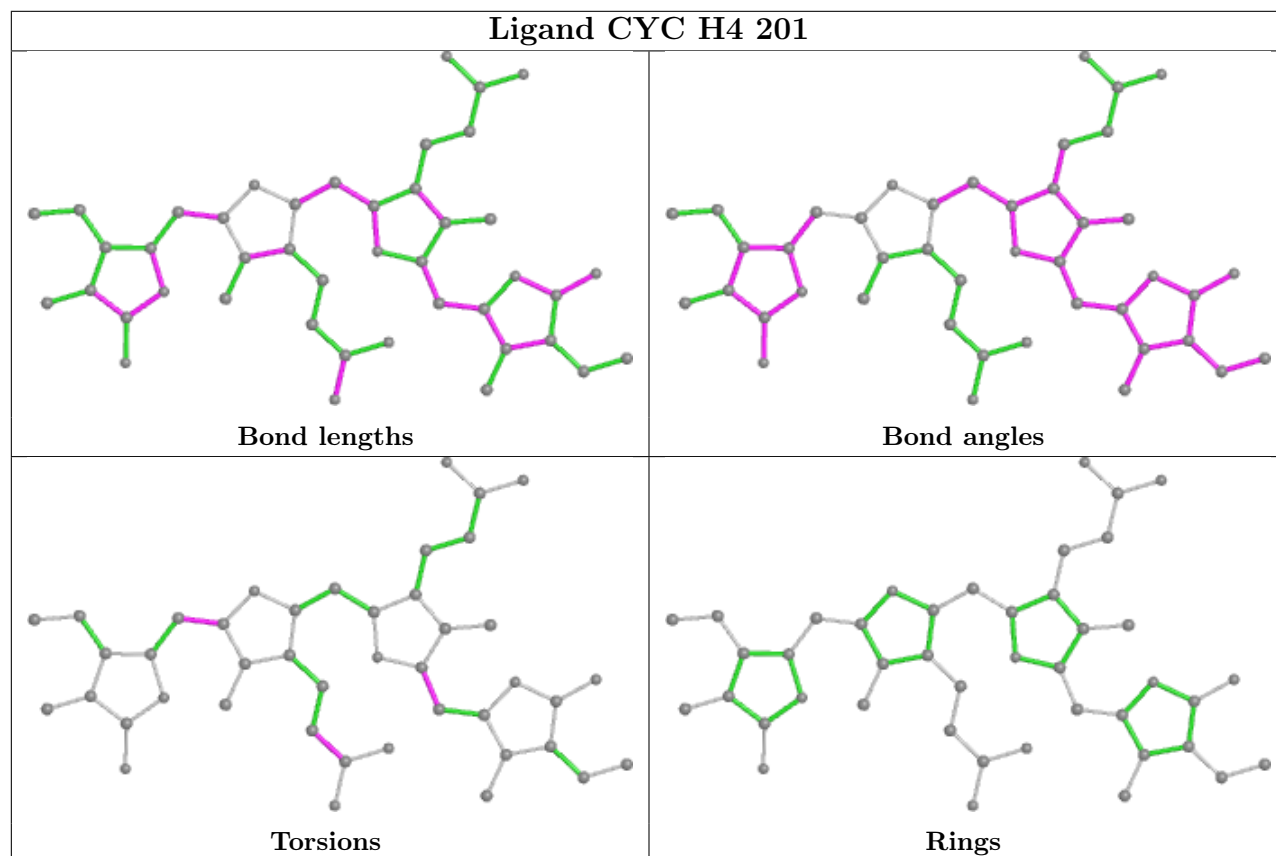
Ligand CYC C9 201



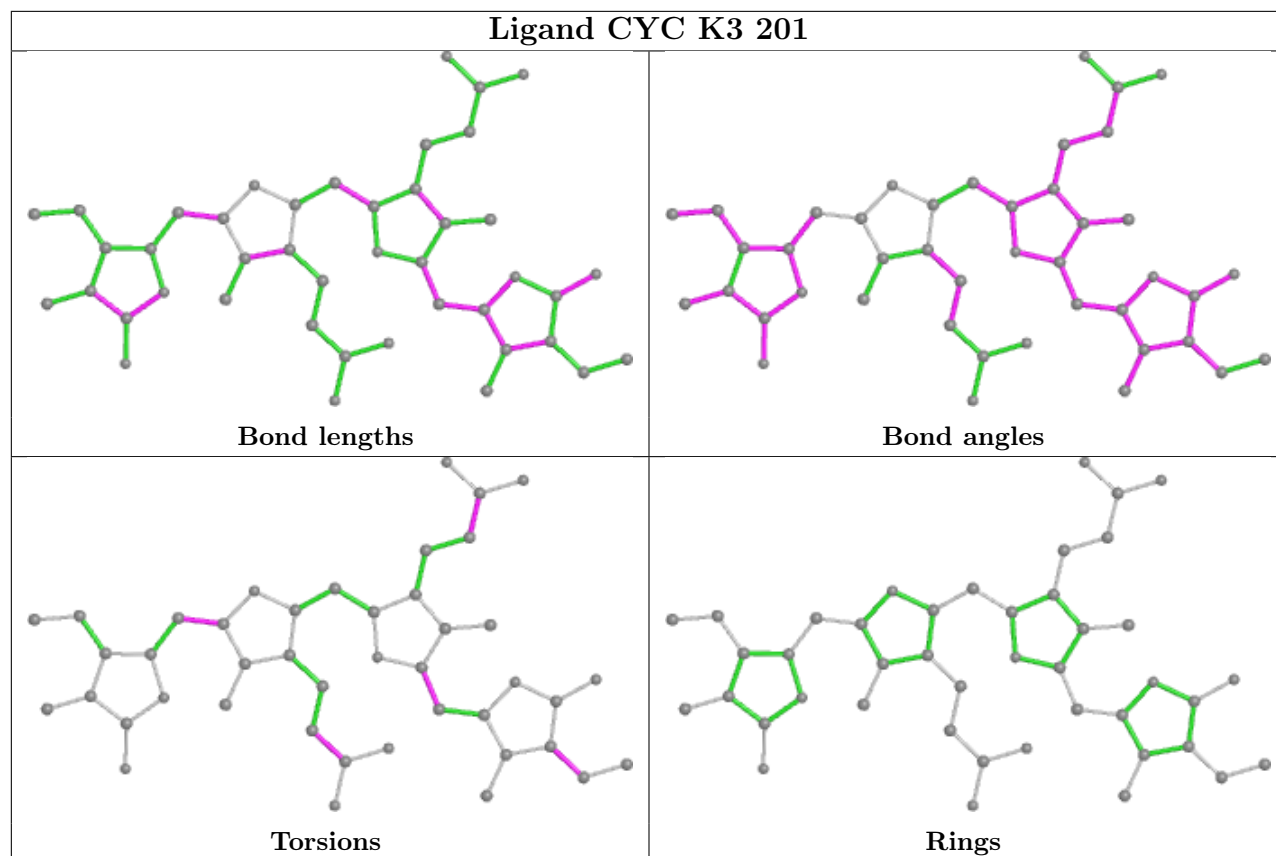
Ligand CYC Q7 201



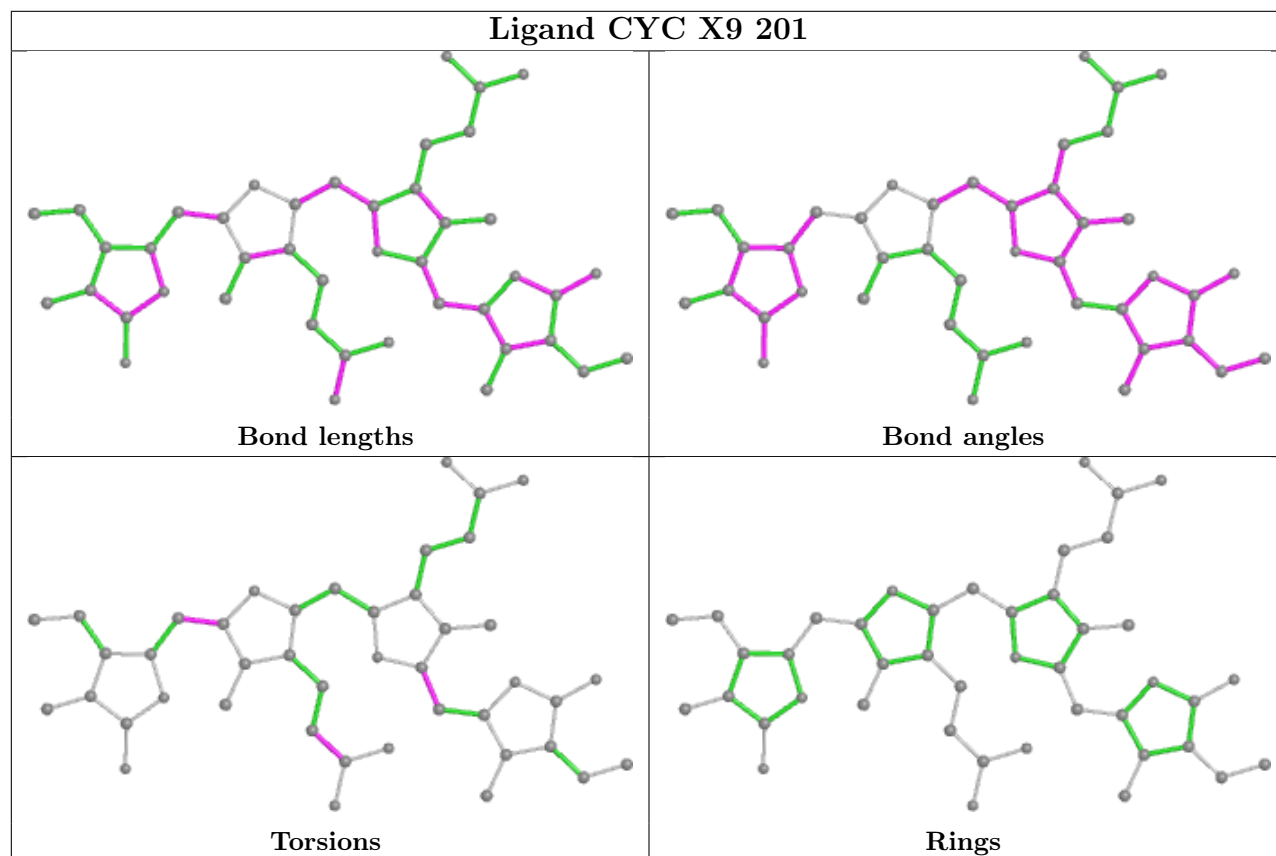
Ligand CYC H4 201

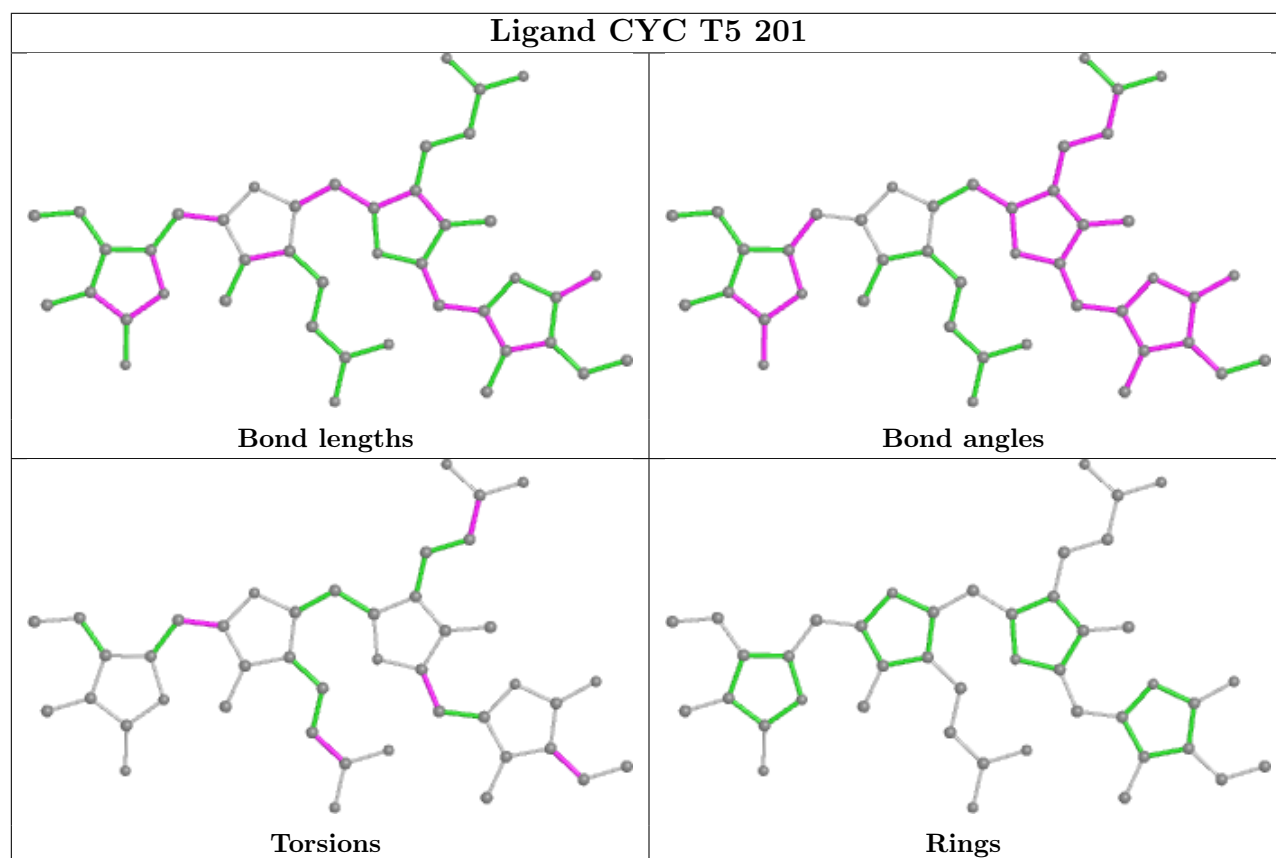
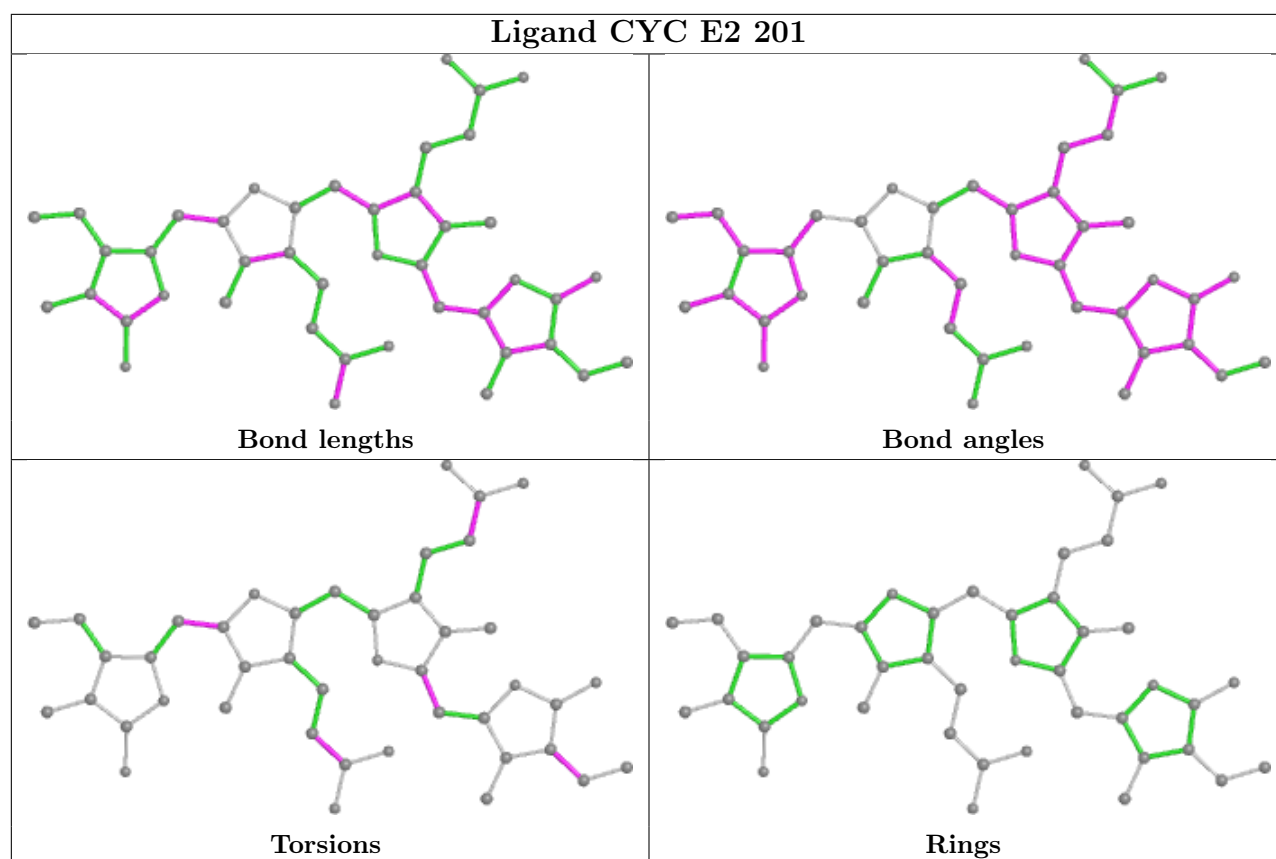


Ligand CYC K3 201

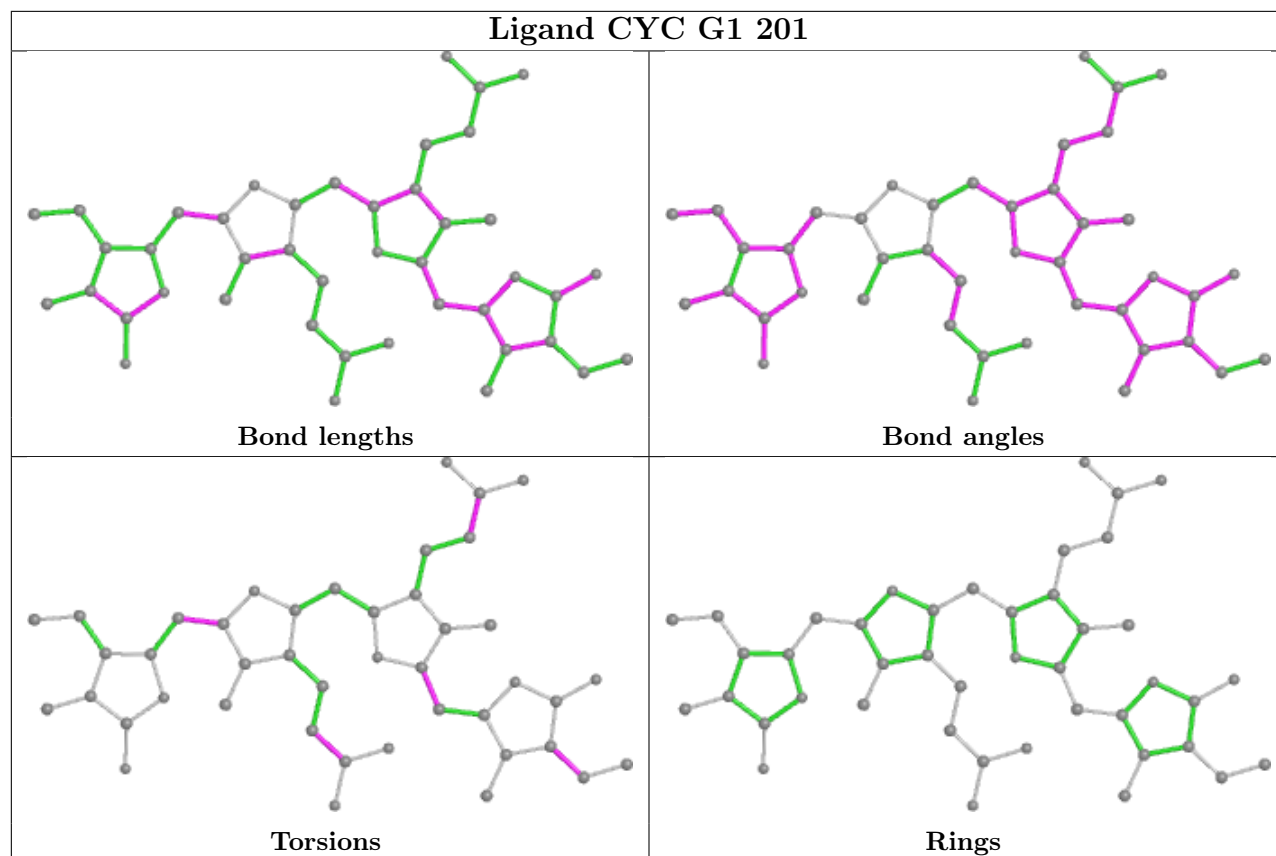


Ligand CYC X9 201

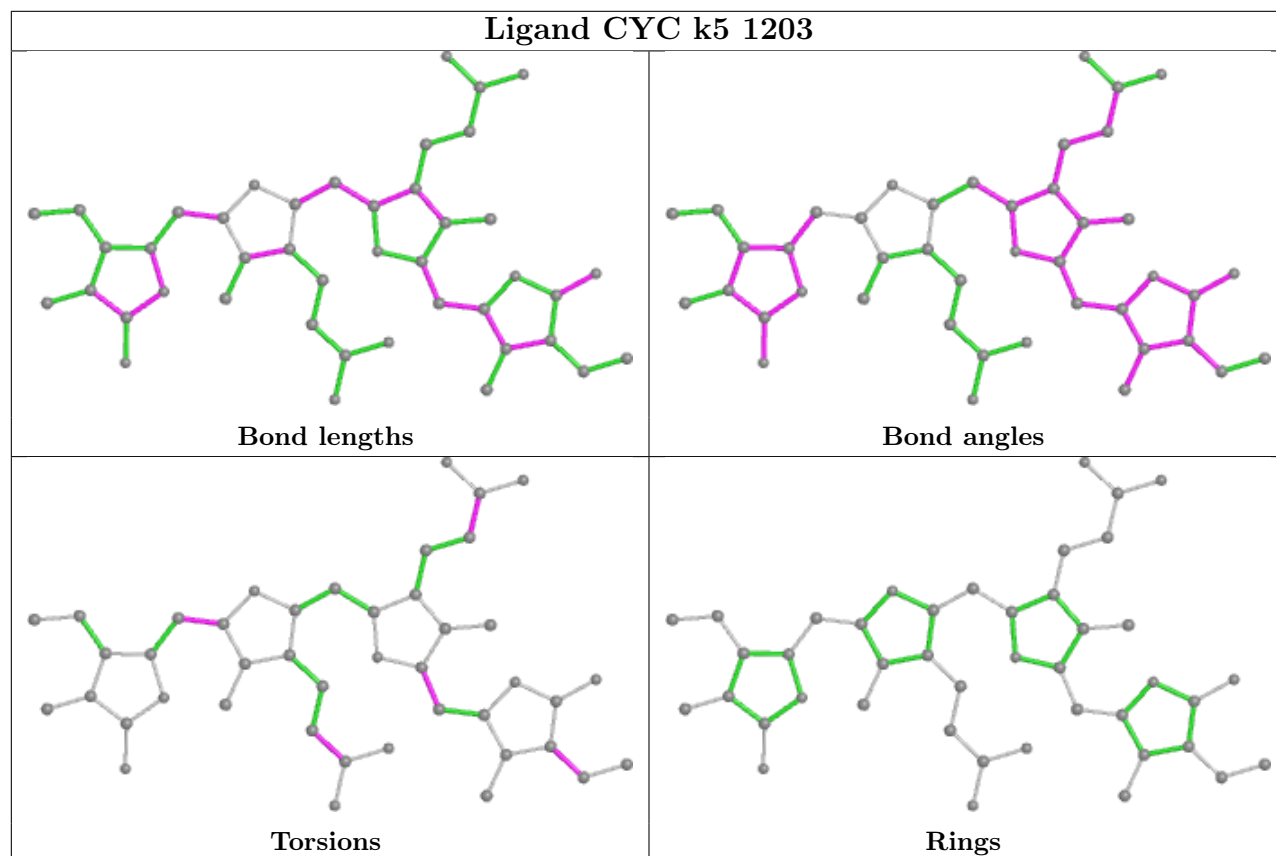




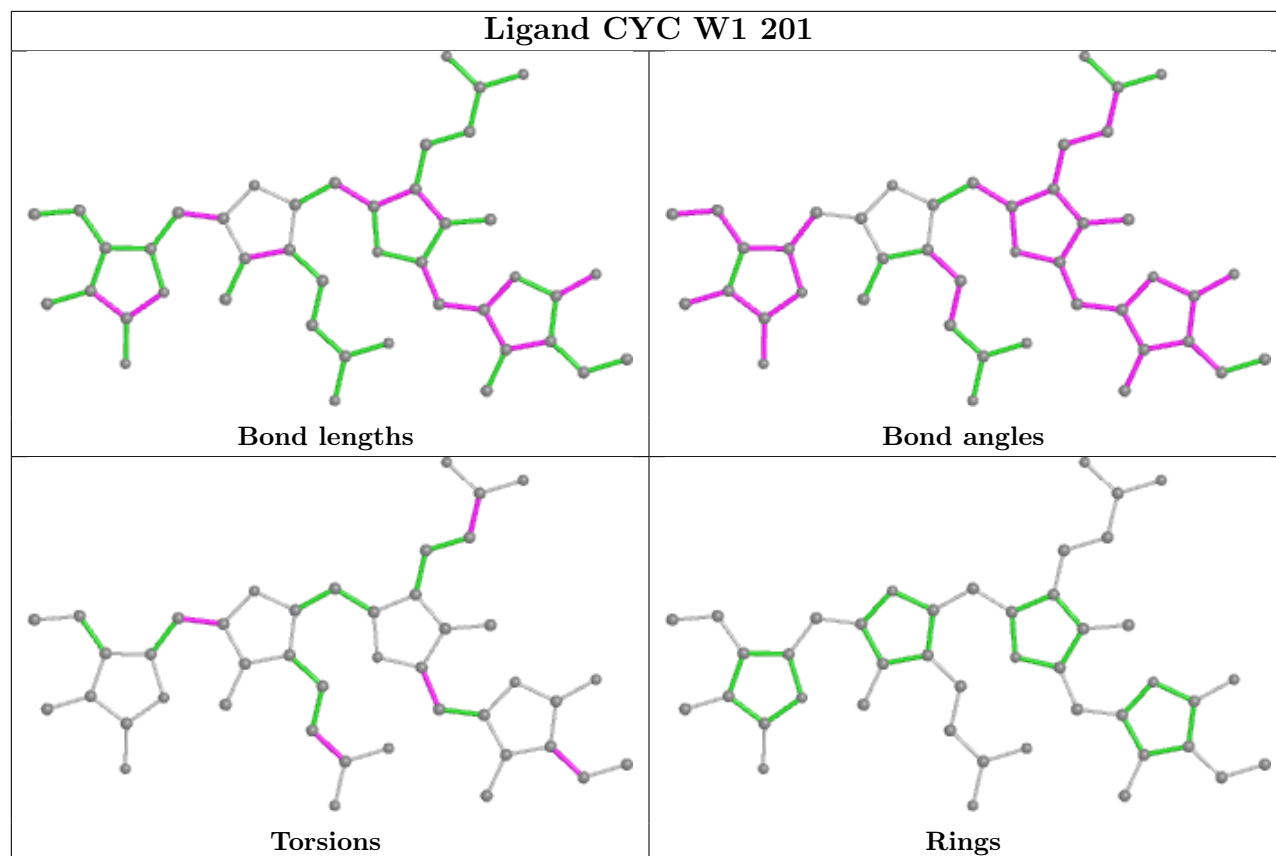
Ligand CYC G1 201



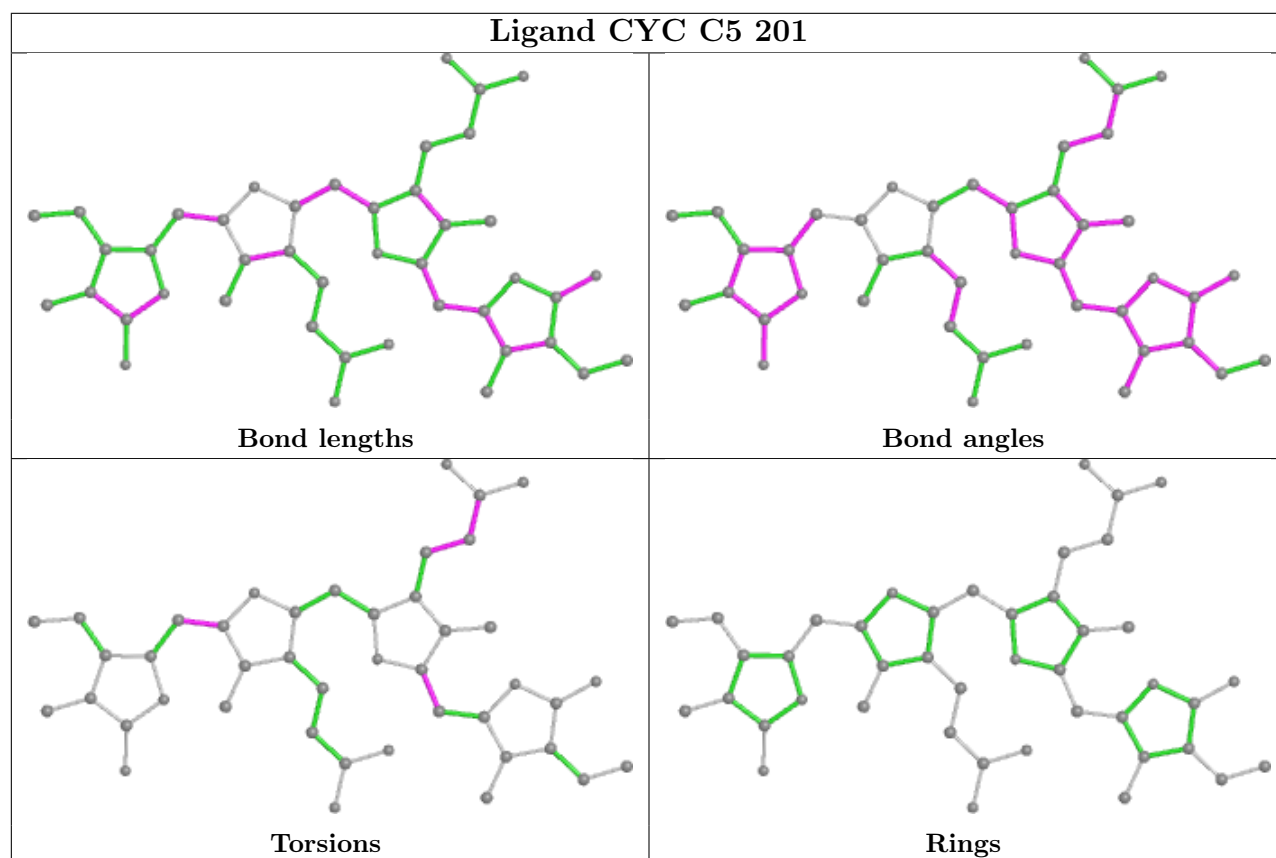
Ligand CYC k5 1203



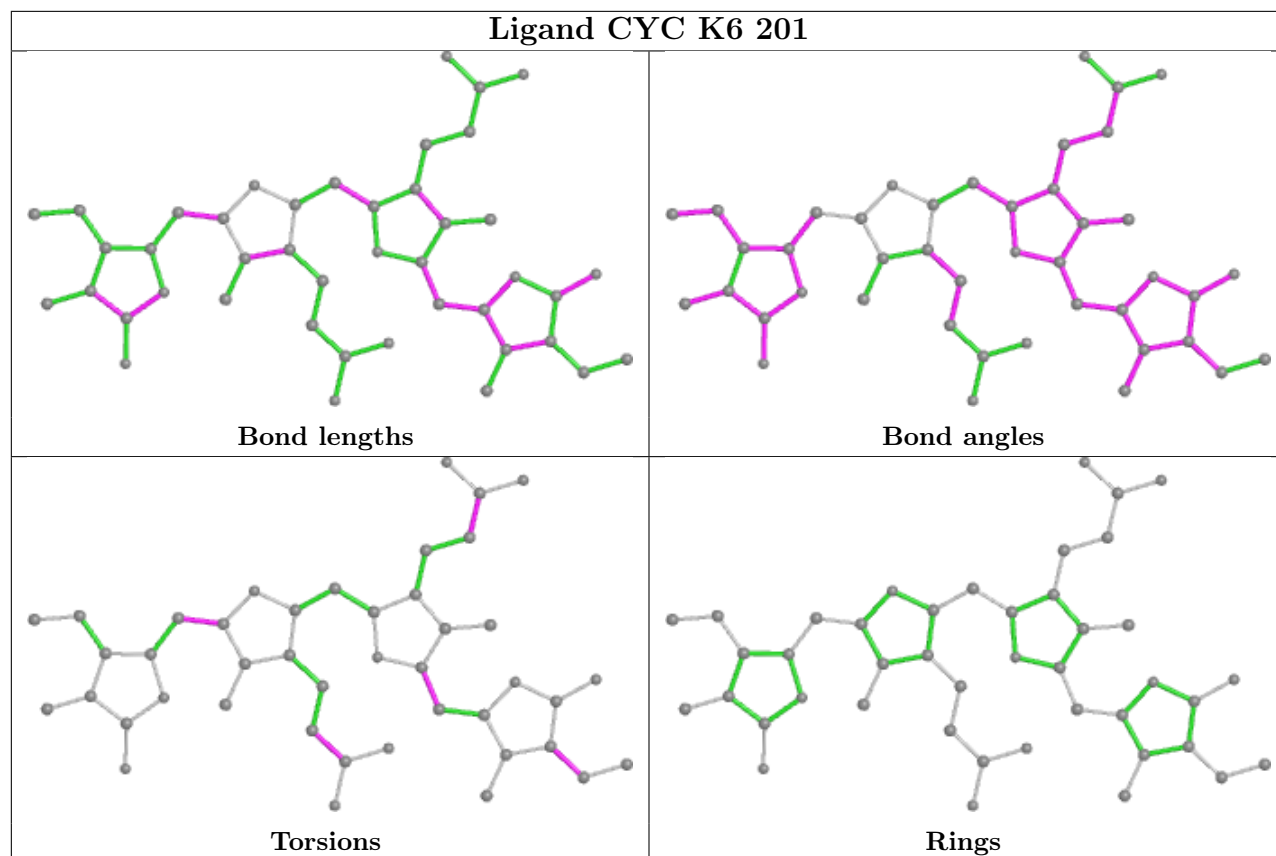
Ligand CYC W1 201



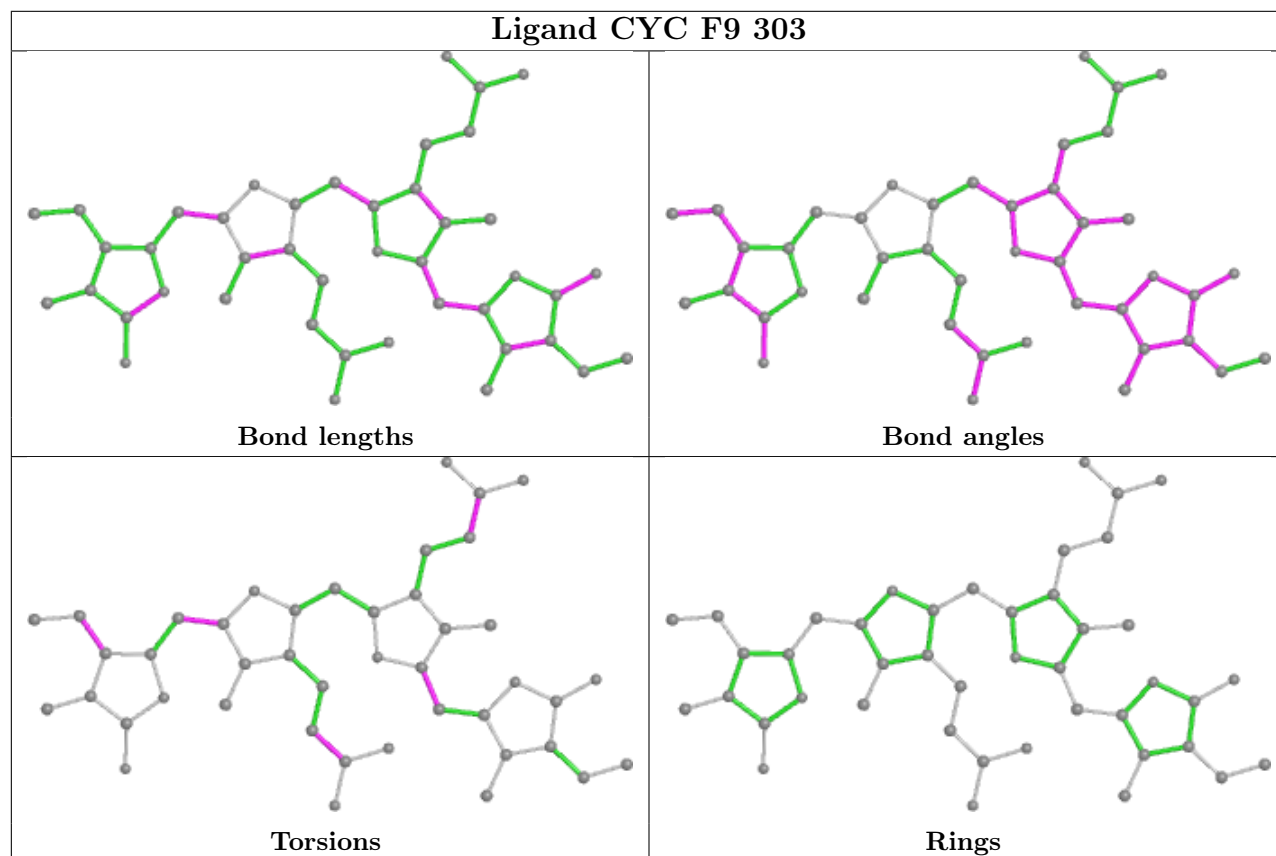
Ligand CYC C5 201



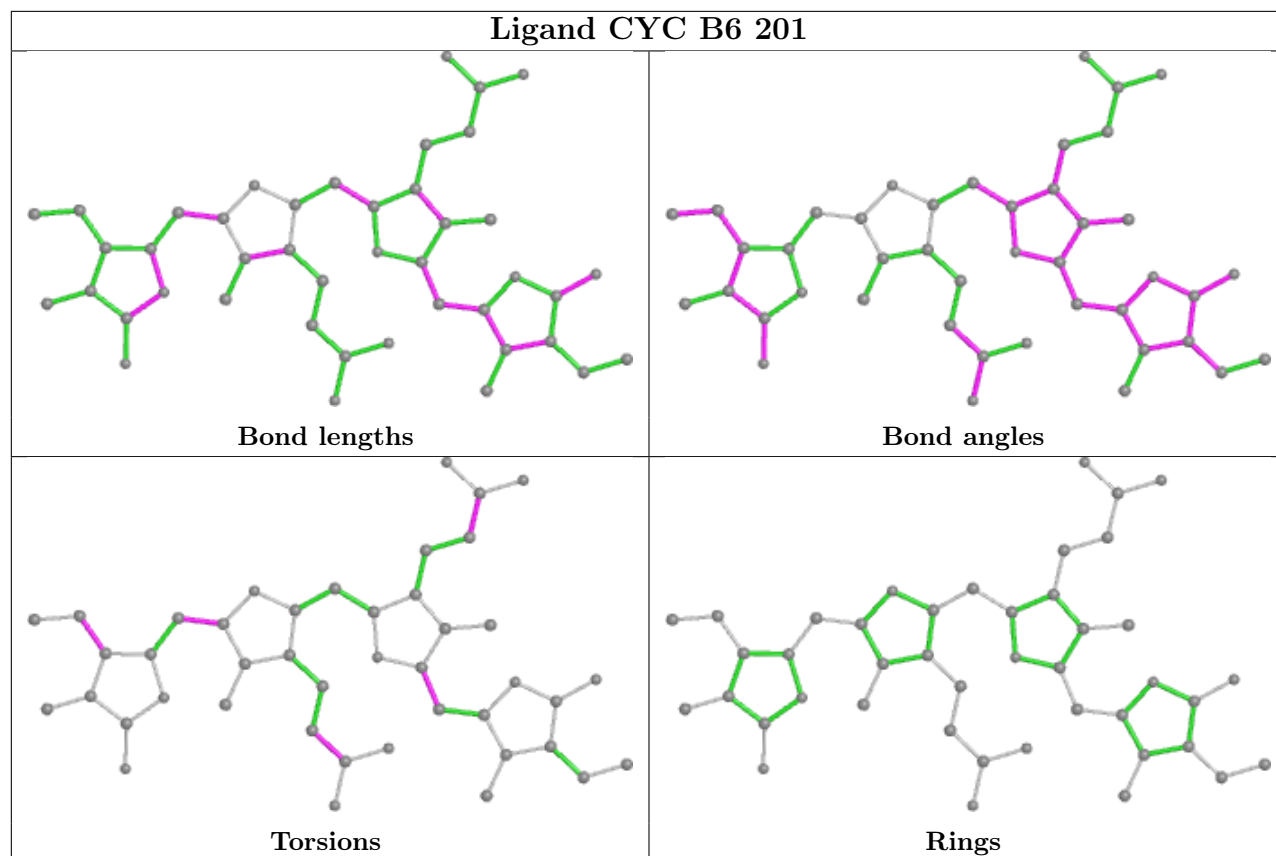
Ligand CYC K6 201



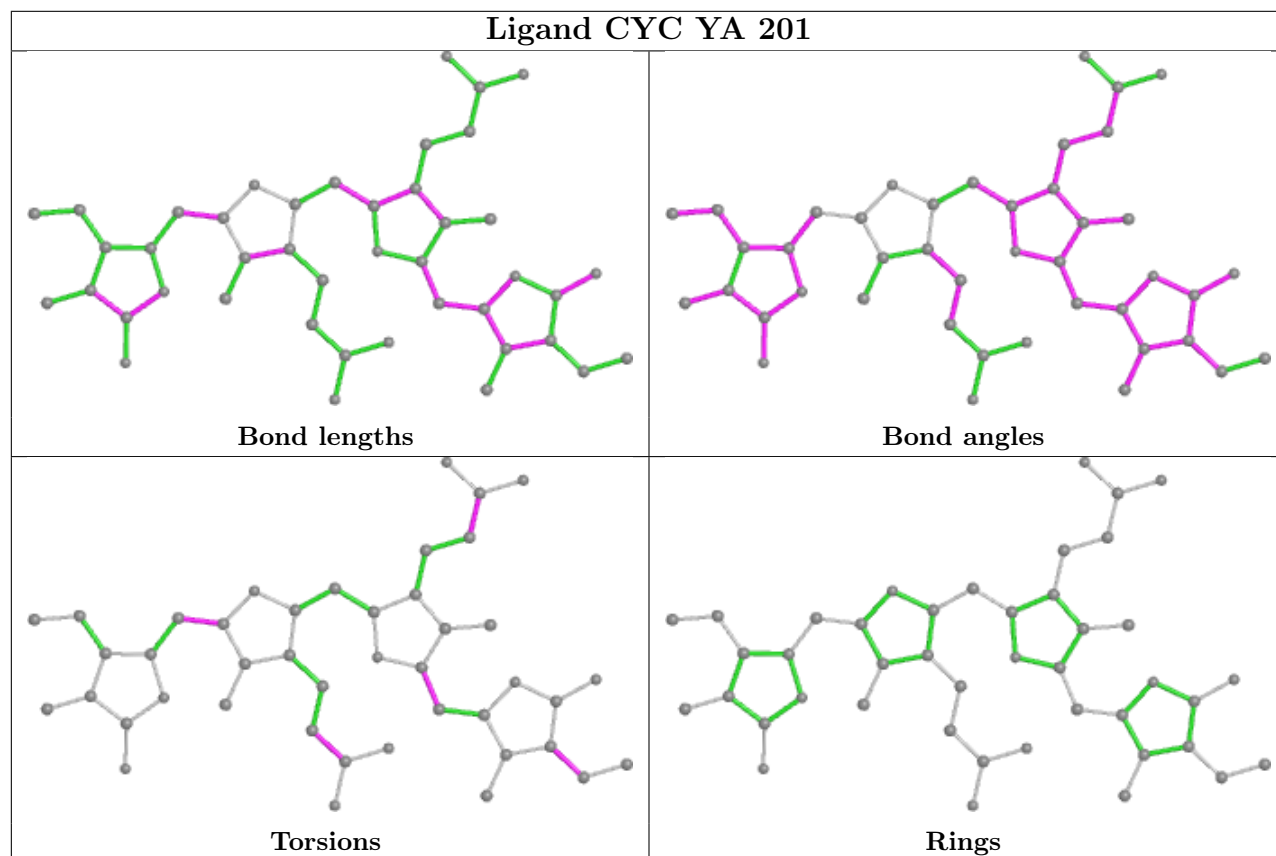
Ligand CYC F9 303



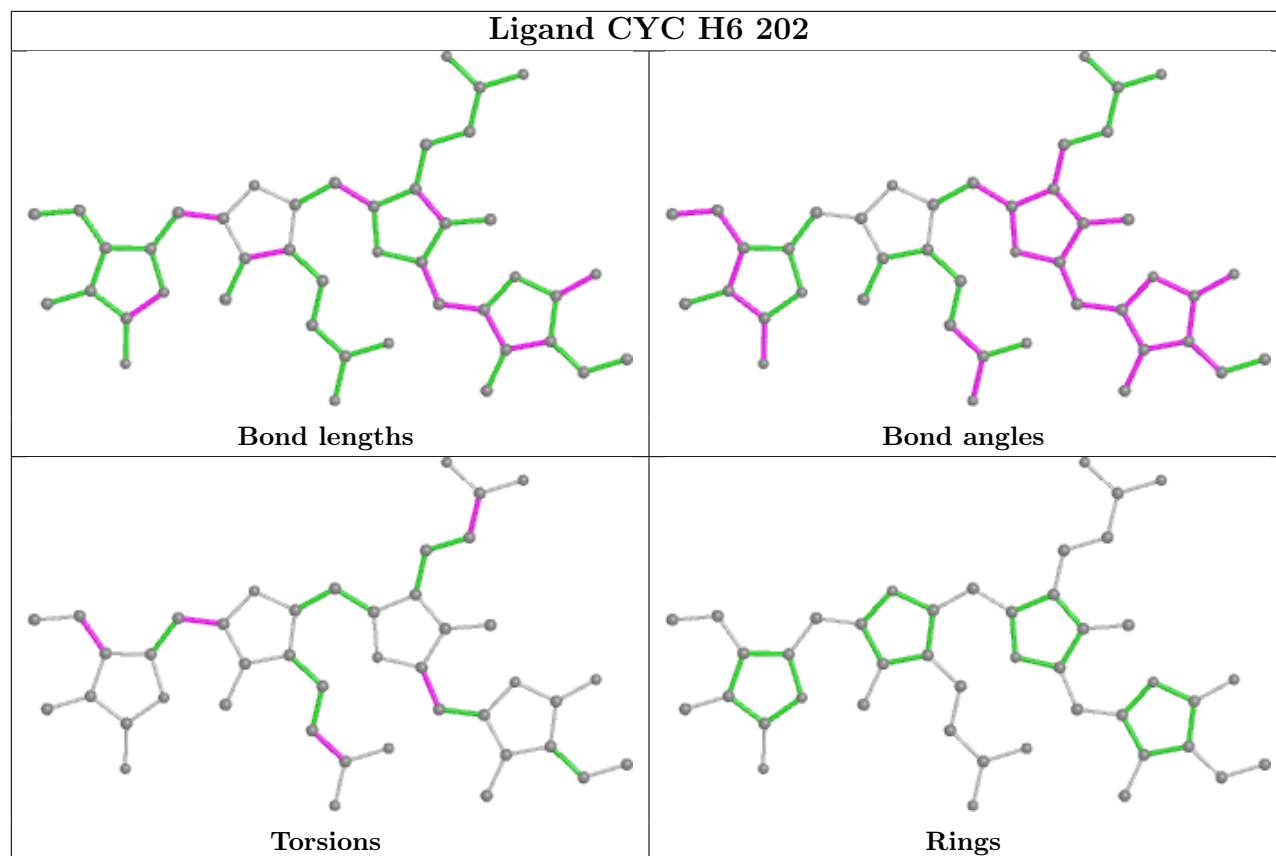
Ligand CYC B6 201



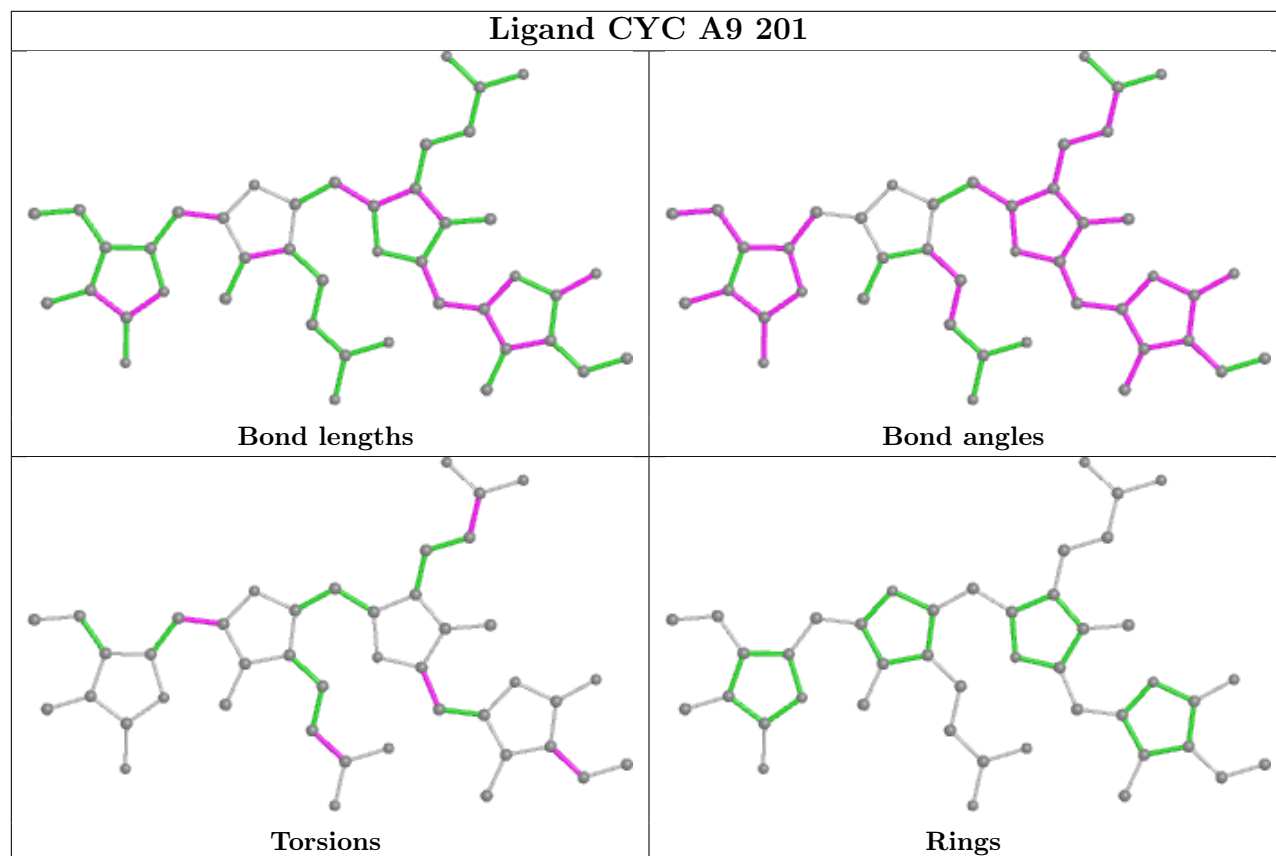
Ligand CYC YA 201



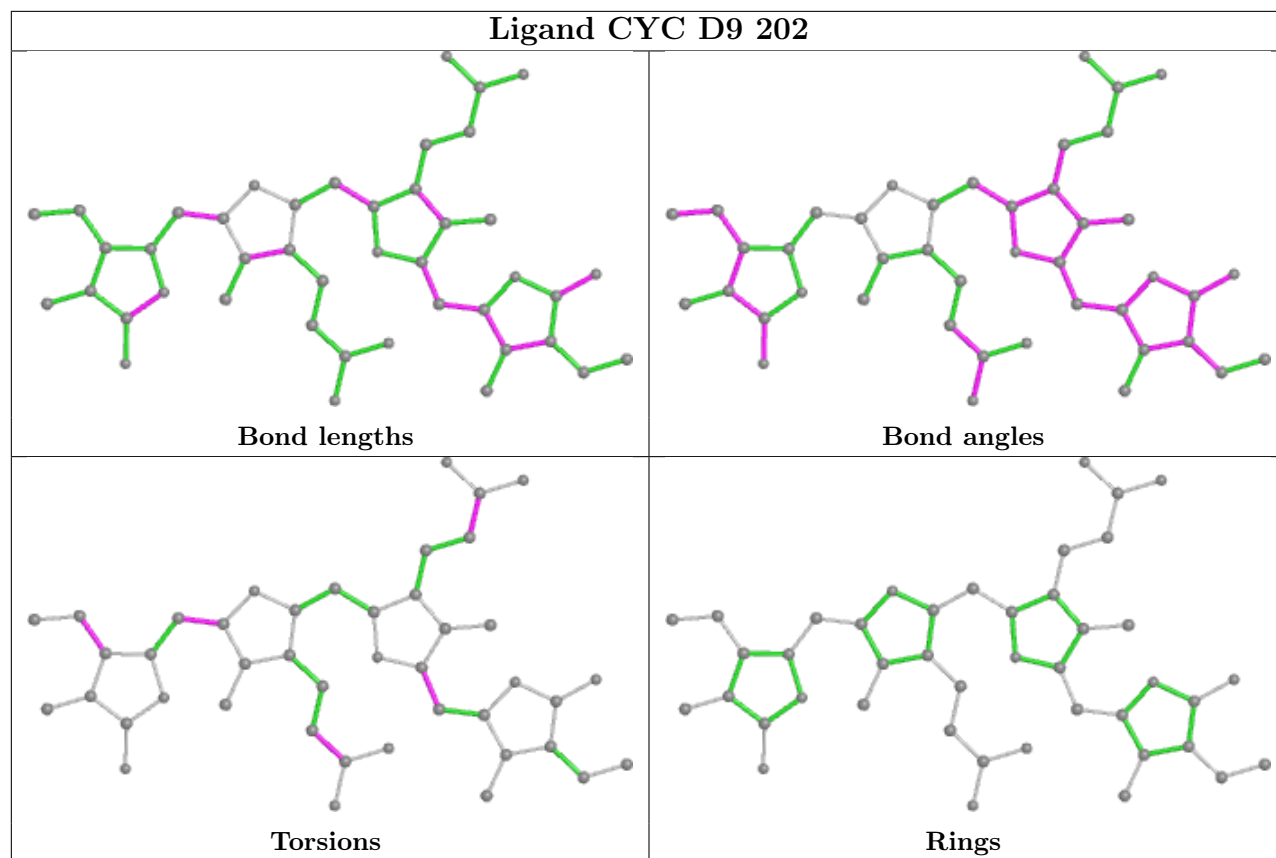
Ligand CYC H6 202



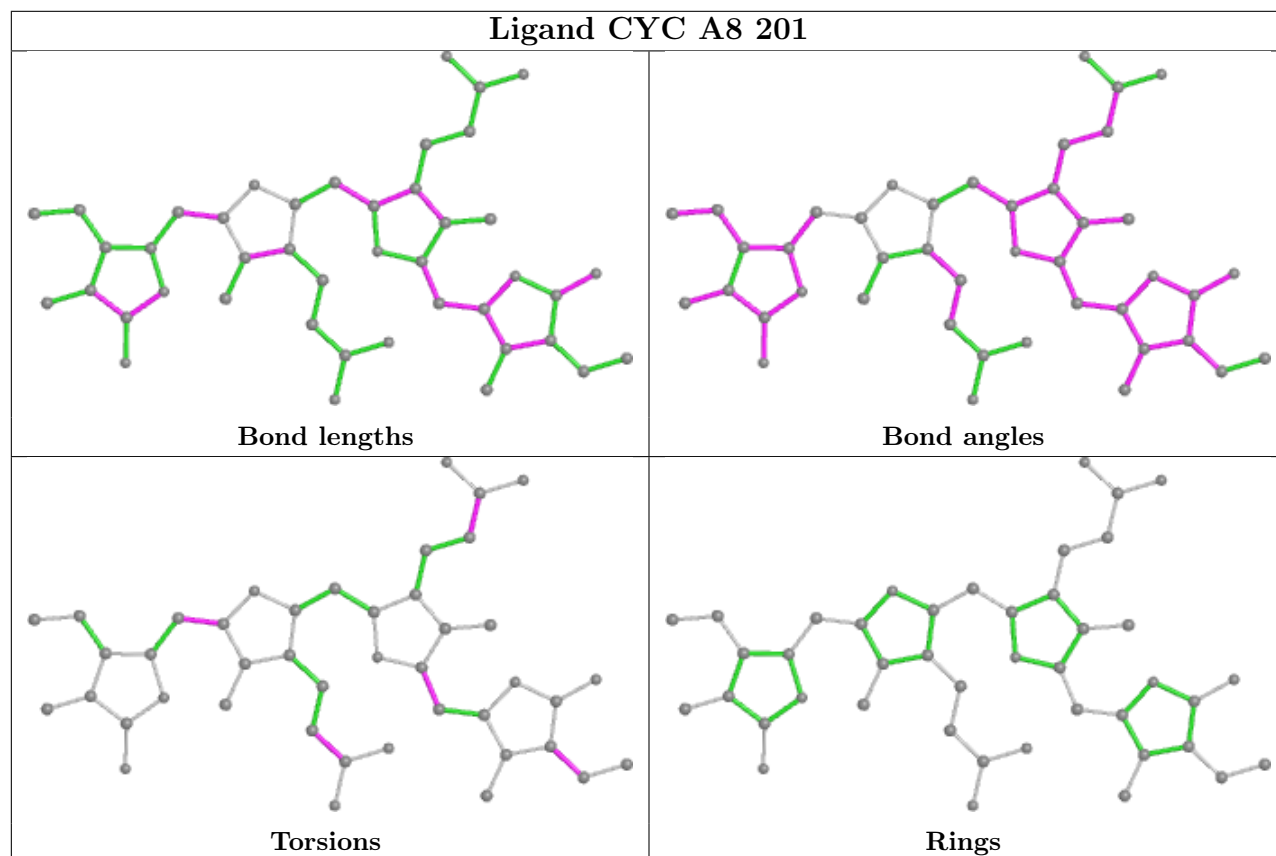
Ligand CYC A9 201



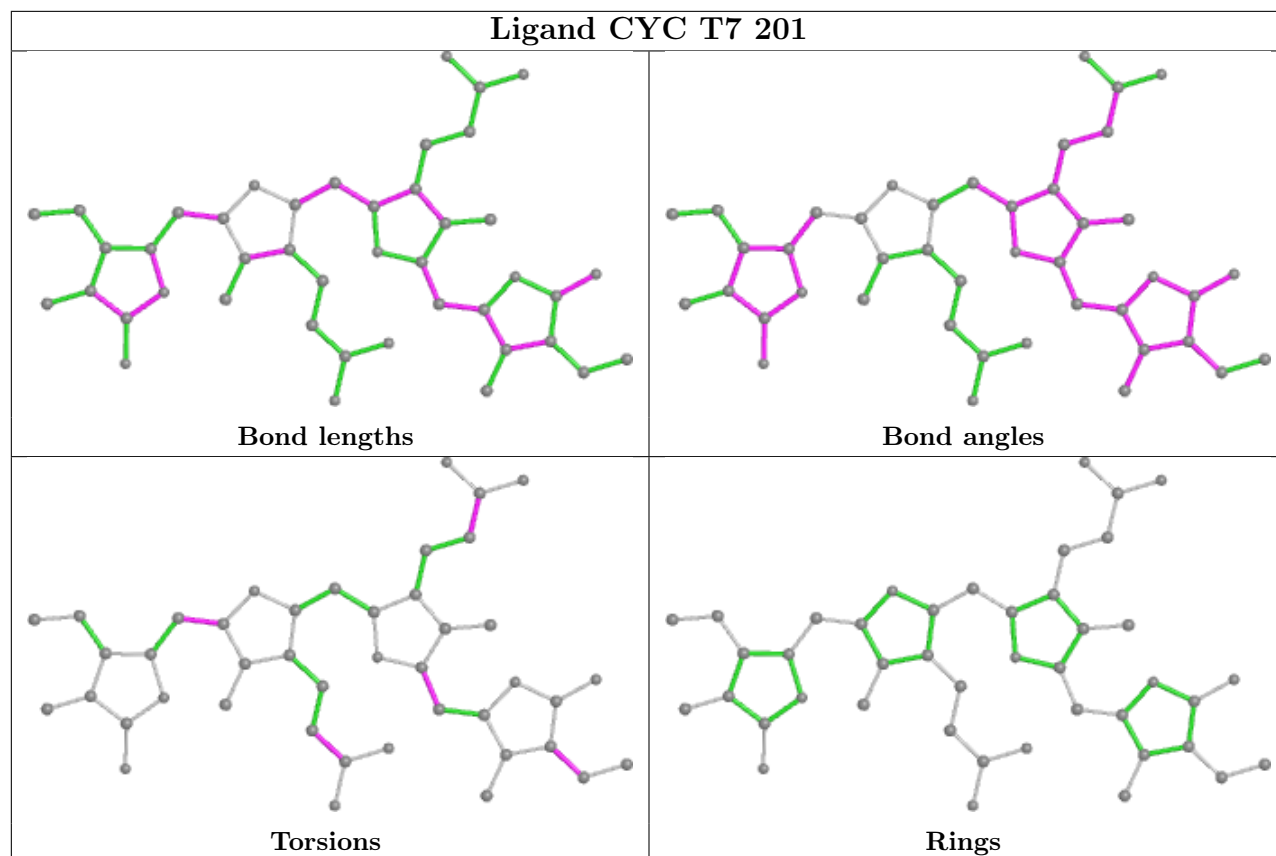
Ligand CYC D9 202



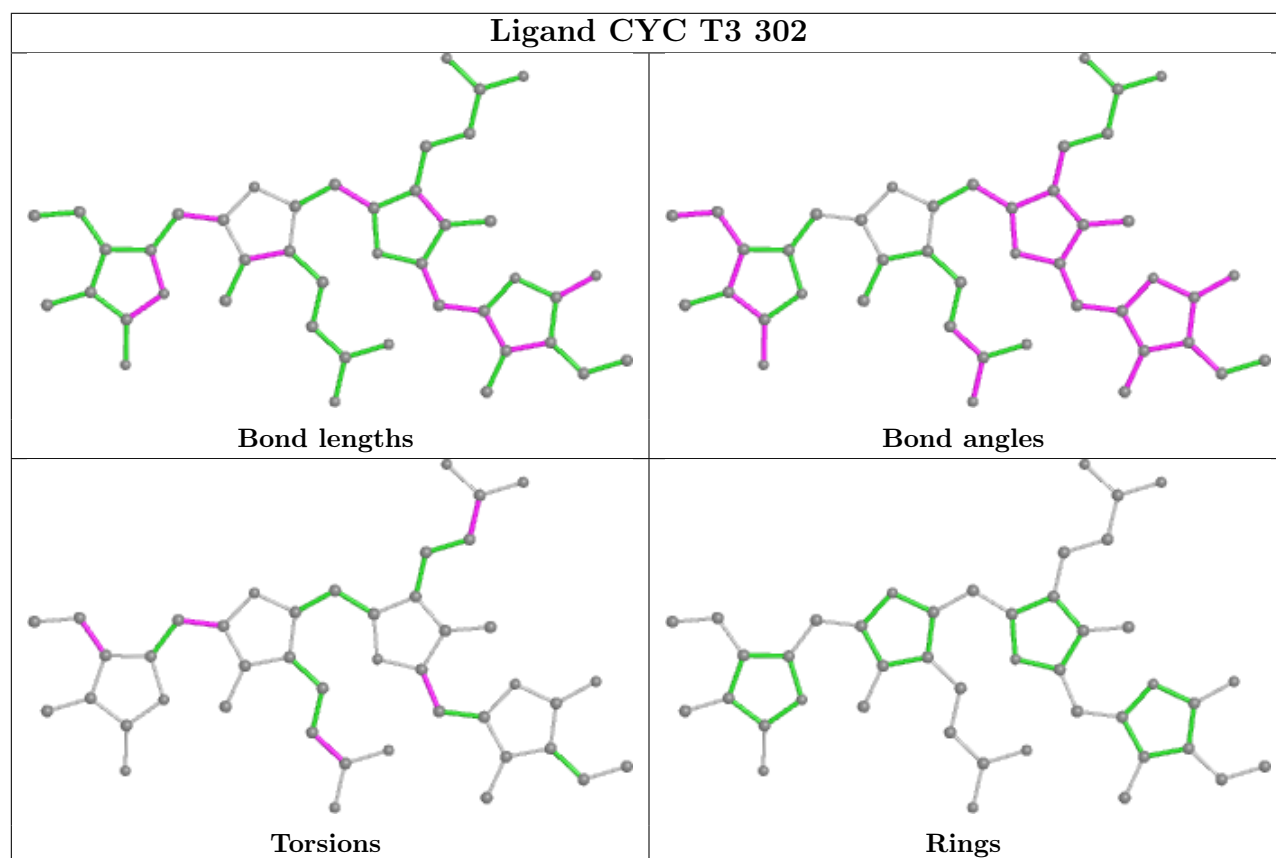
Ligand CYC A8 201



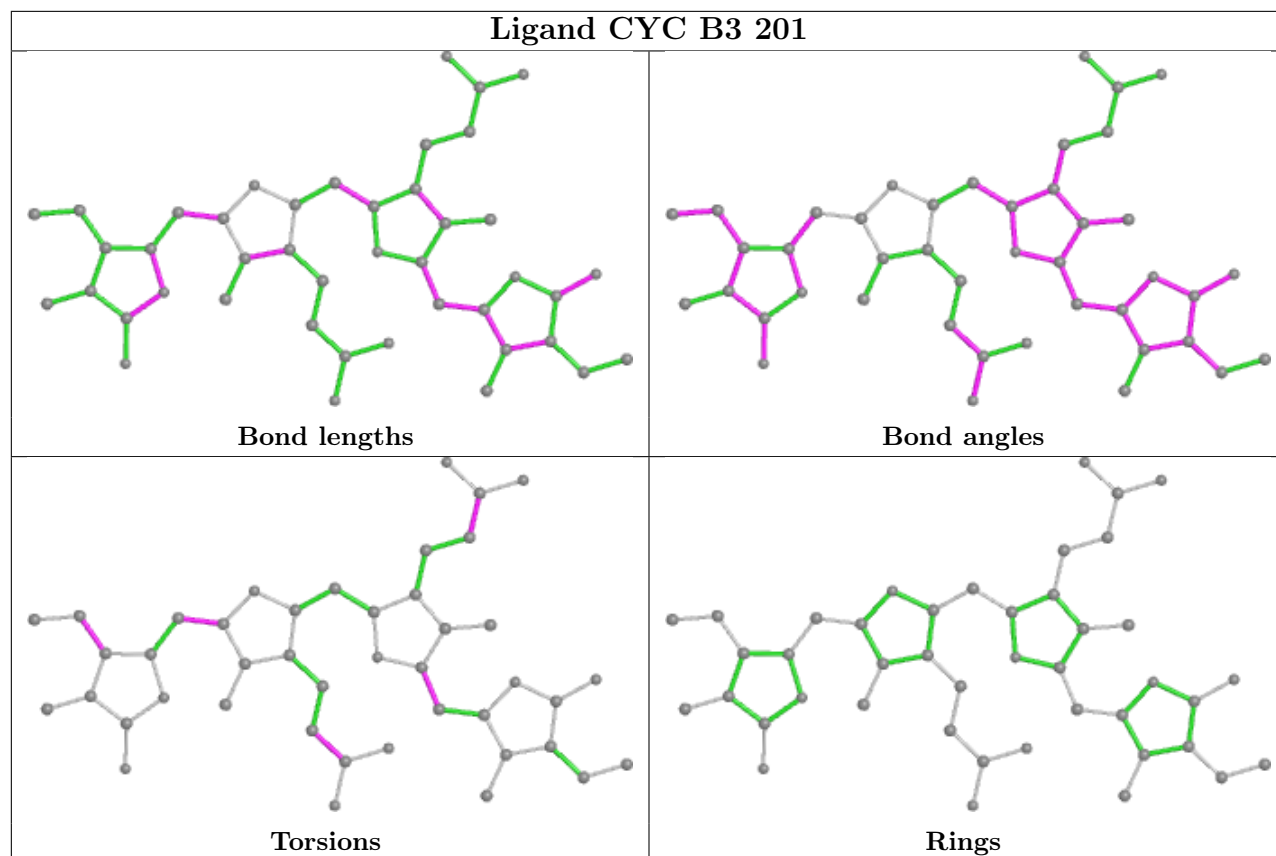
Ligand CYC T7 201



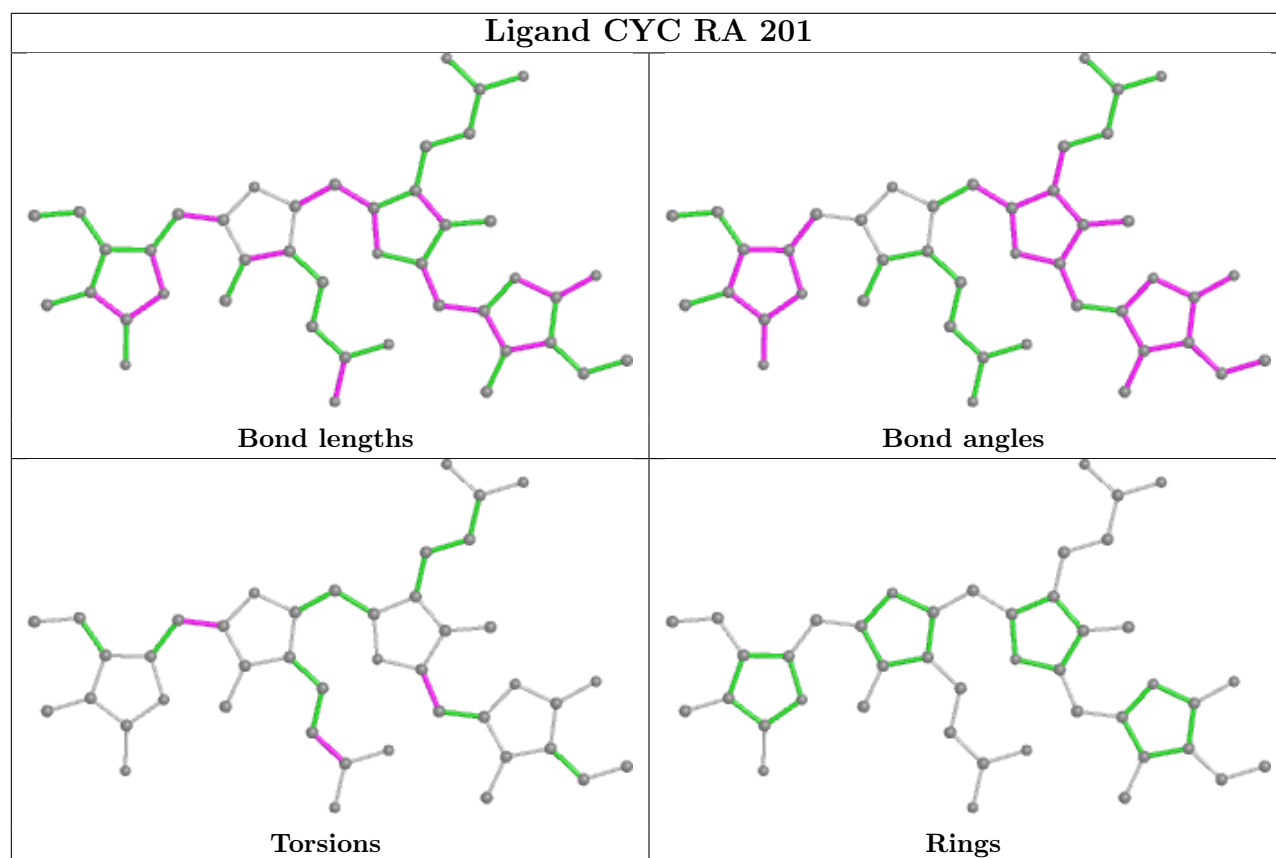
Ligand CYC T3 302



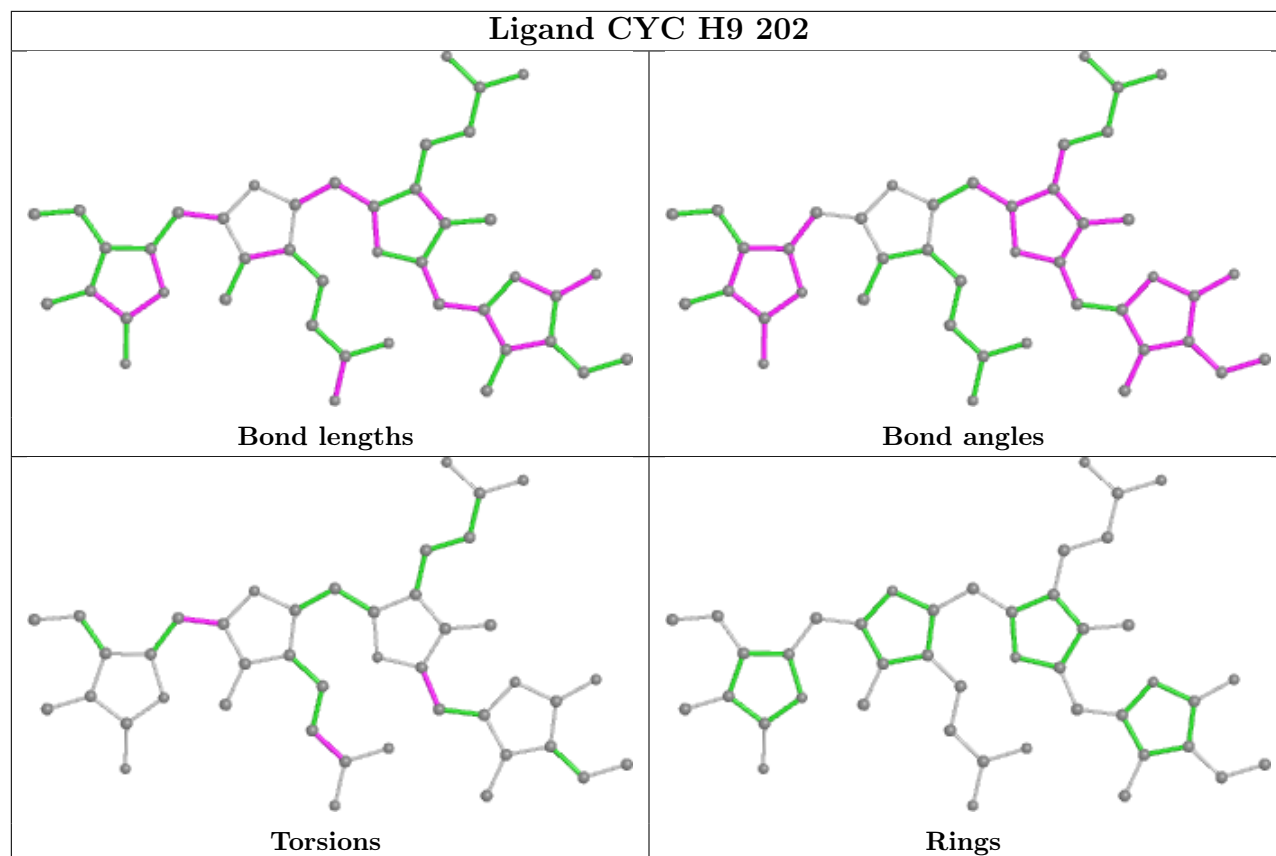
Ligand CYC B3 201



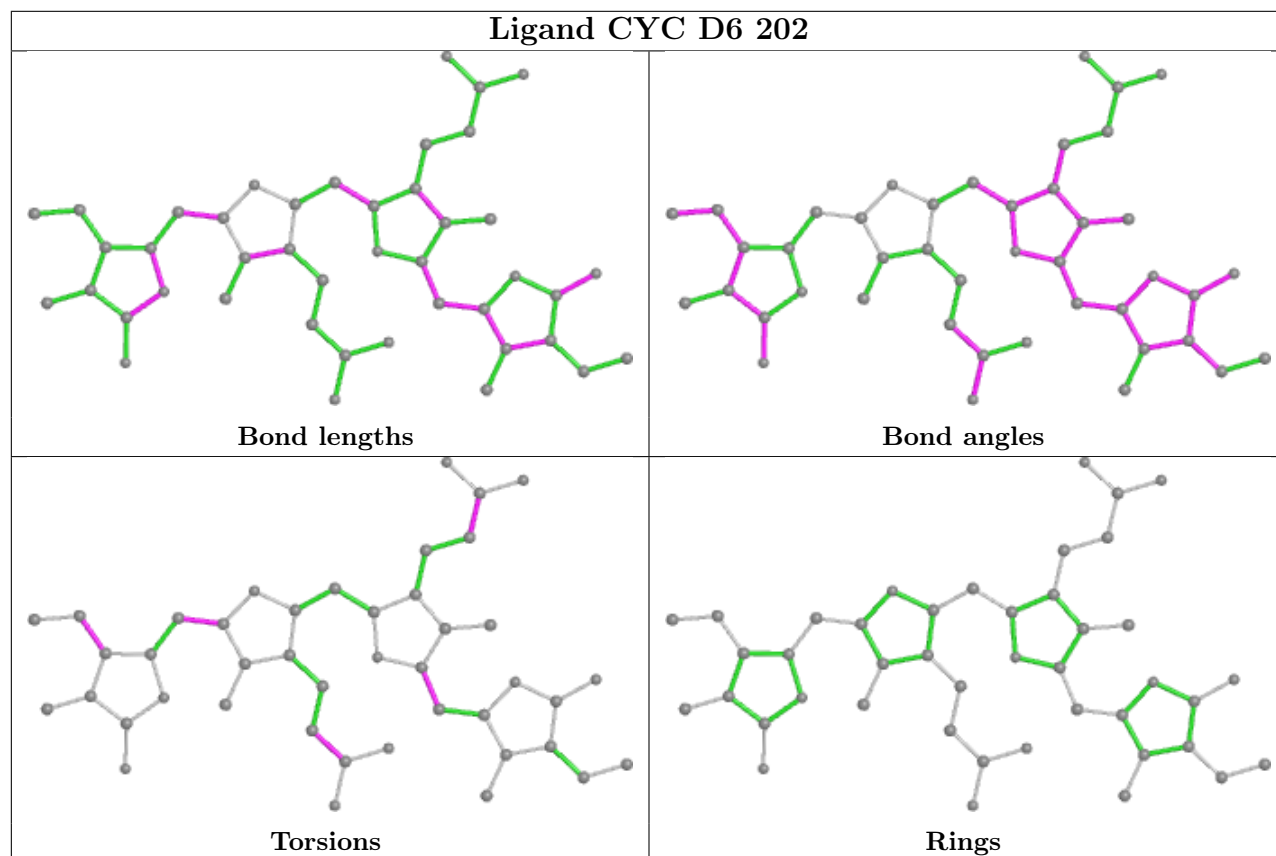
Ligand CYC RA 201



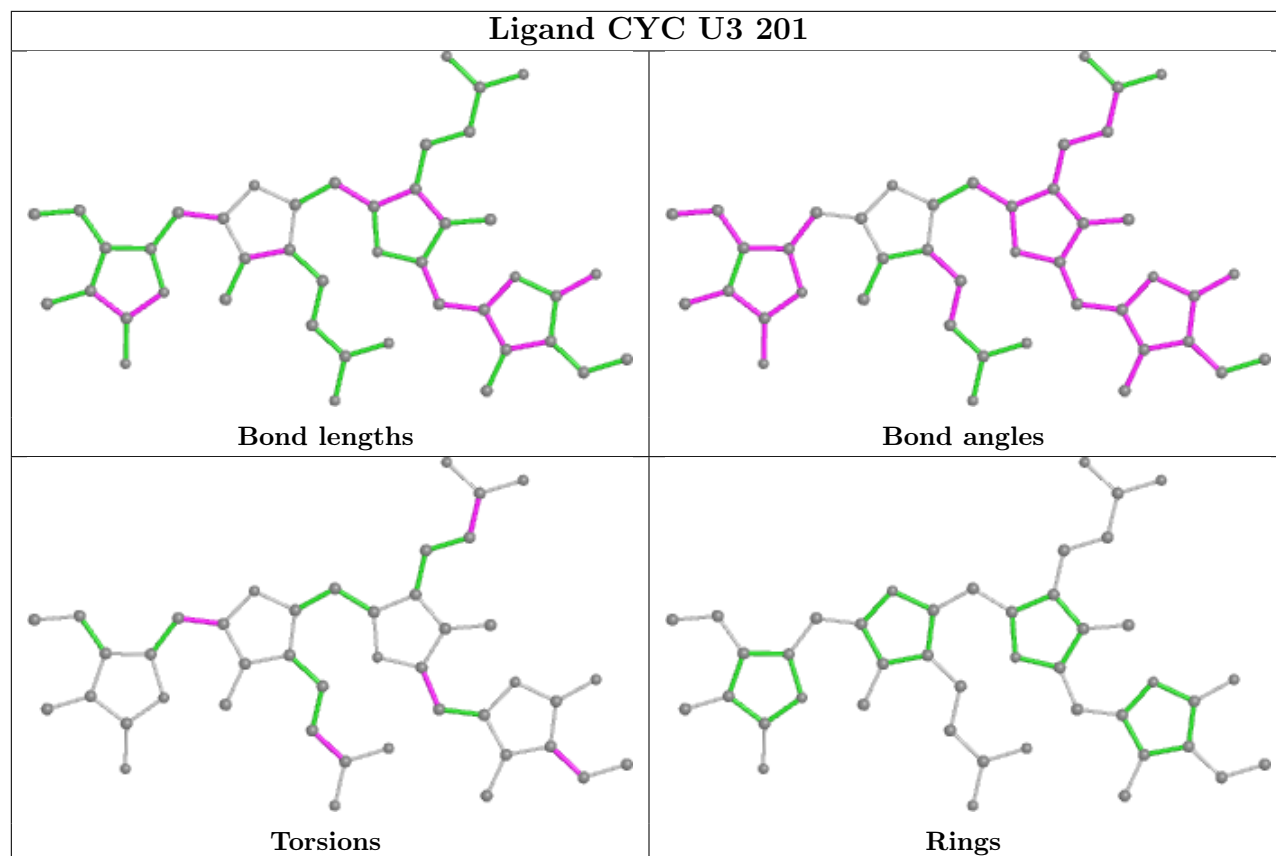
Ligand CYC H9 202



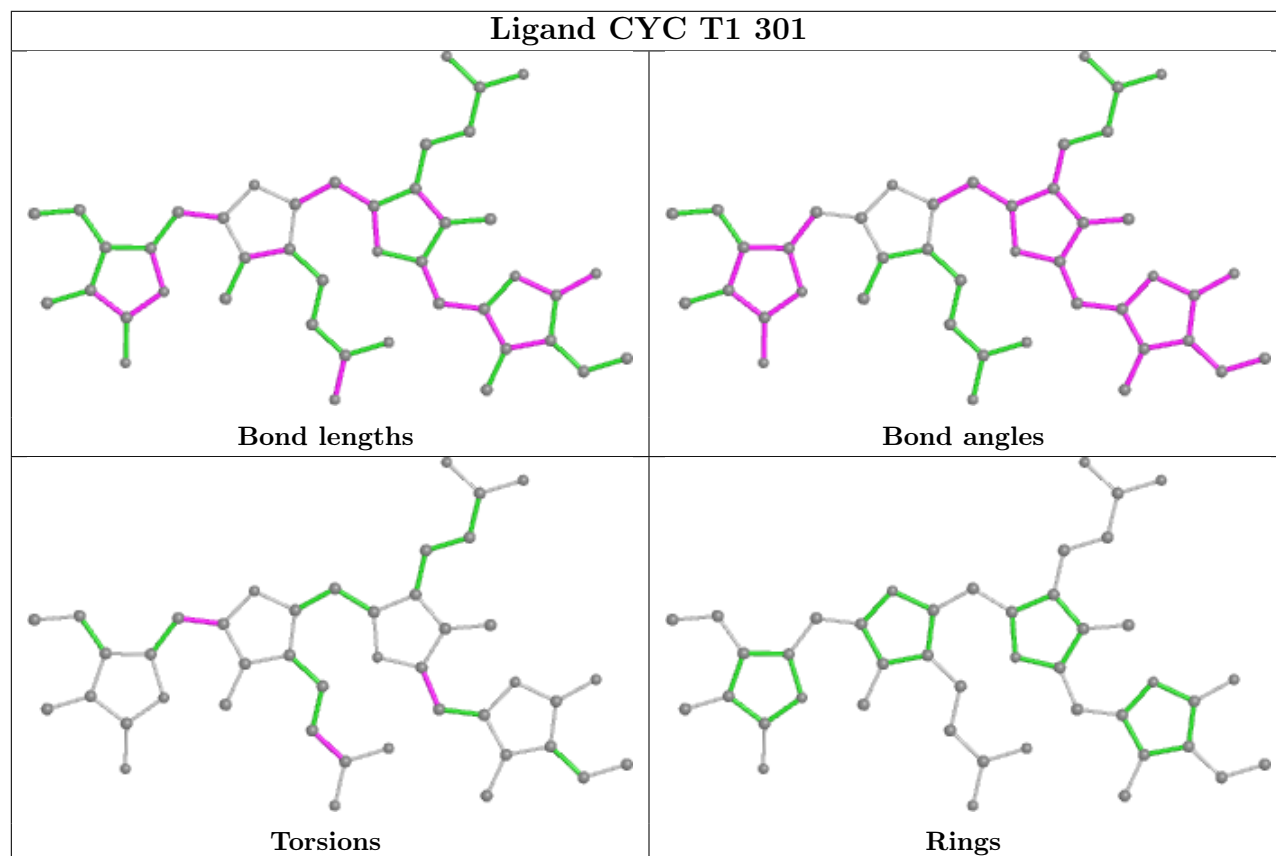
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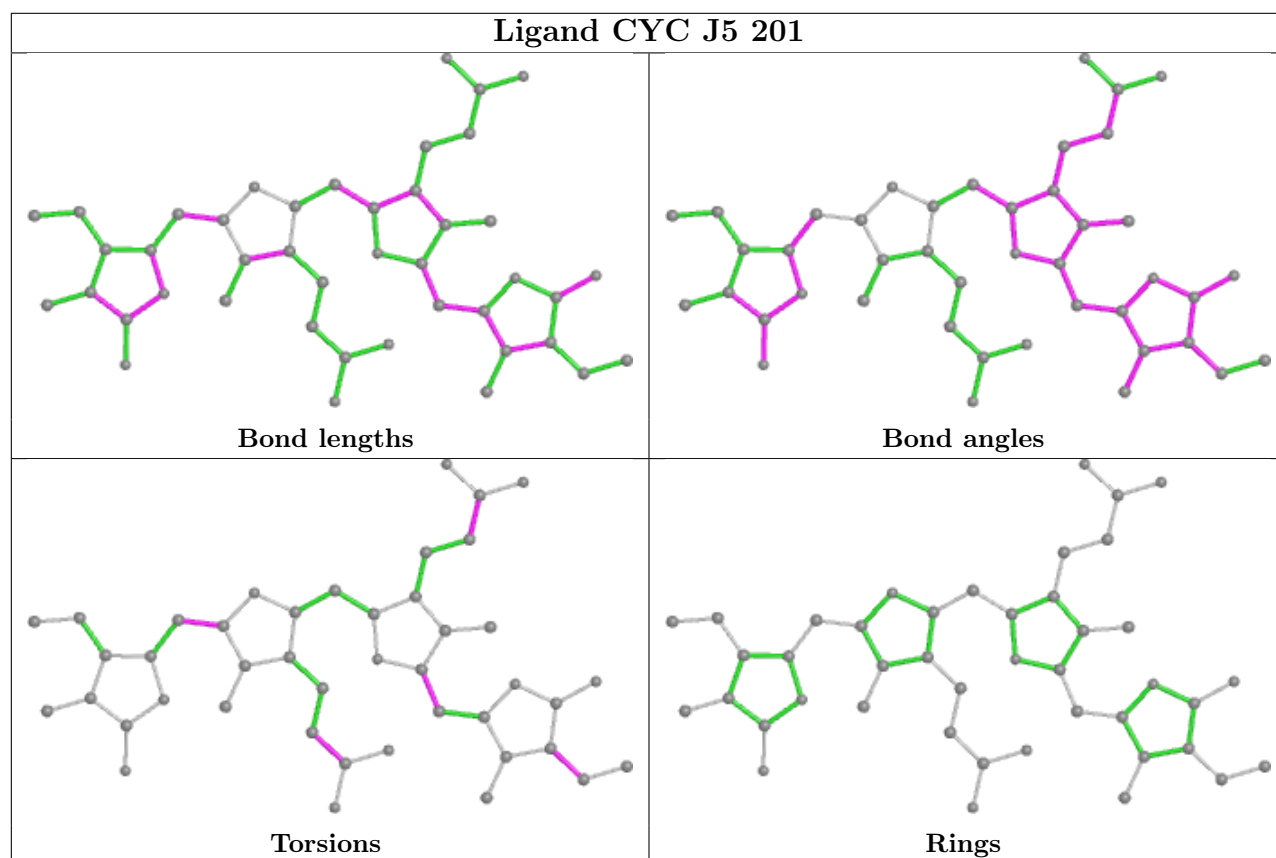
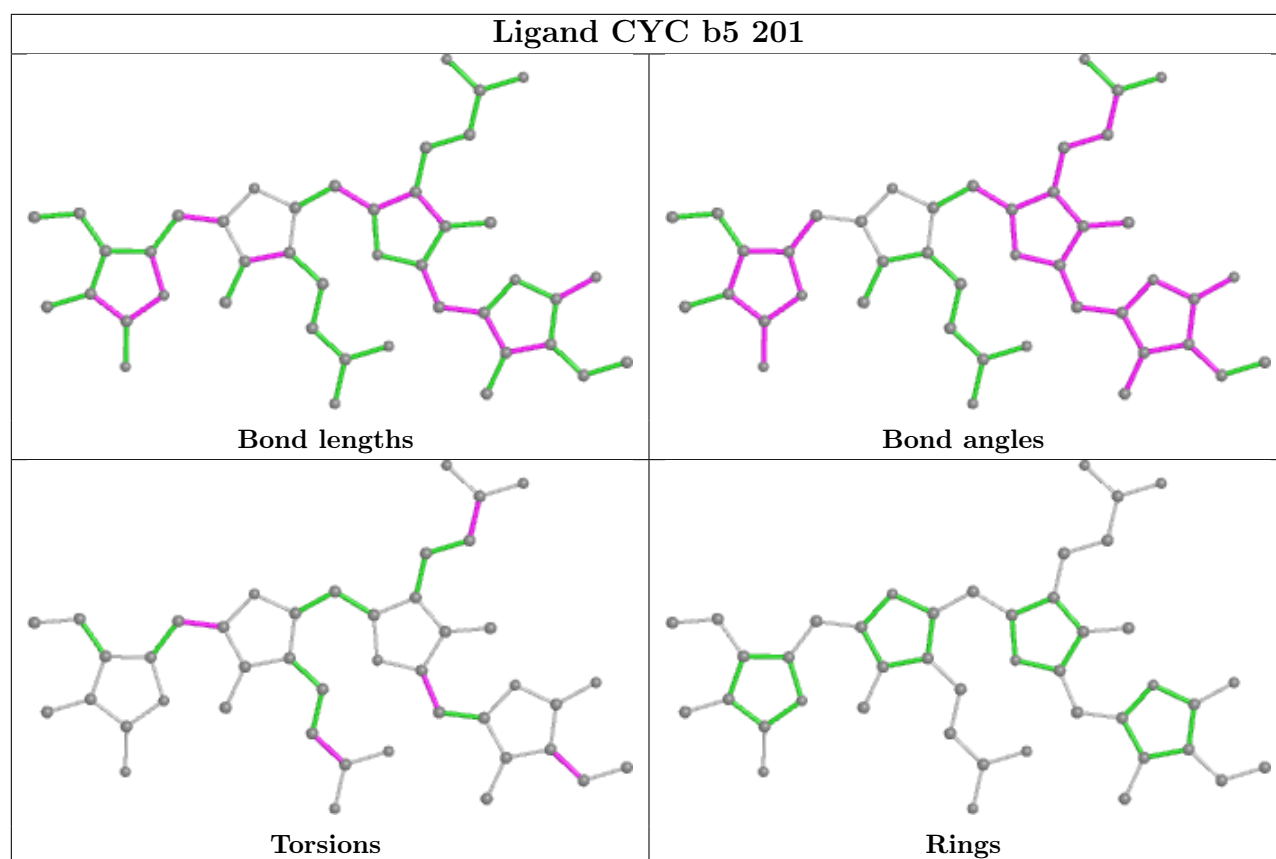


Ligand CYC U3 201

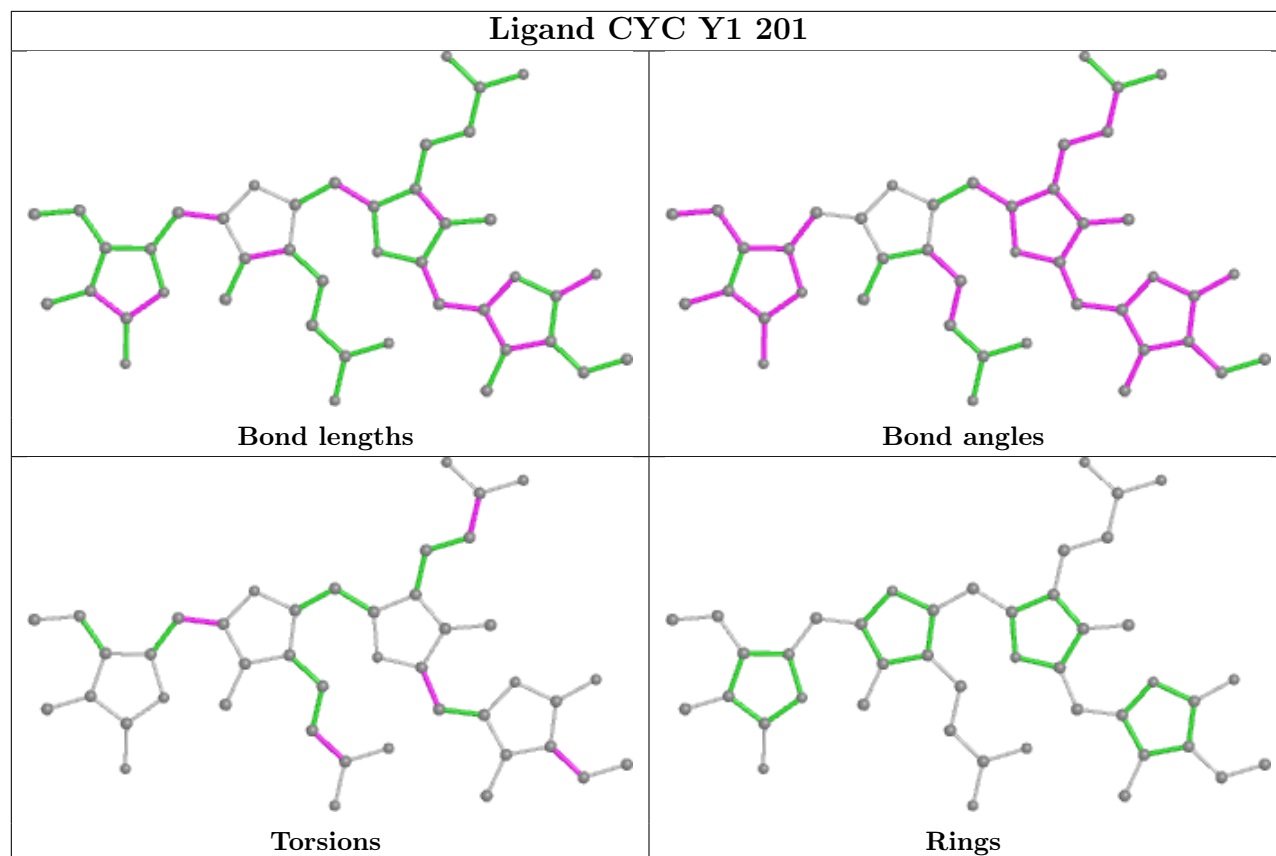


Ligand CYC T1 301

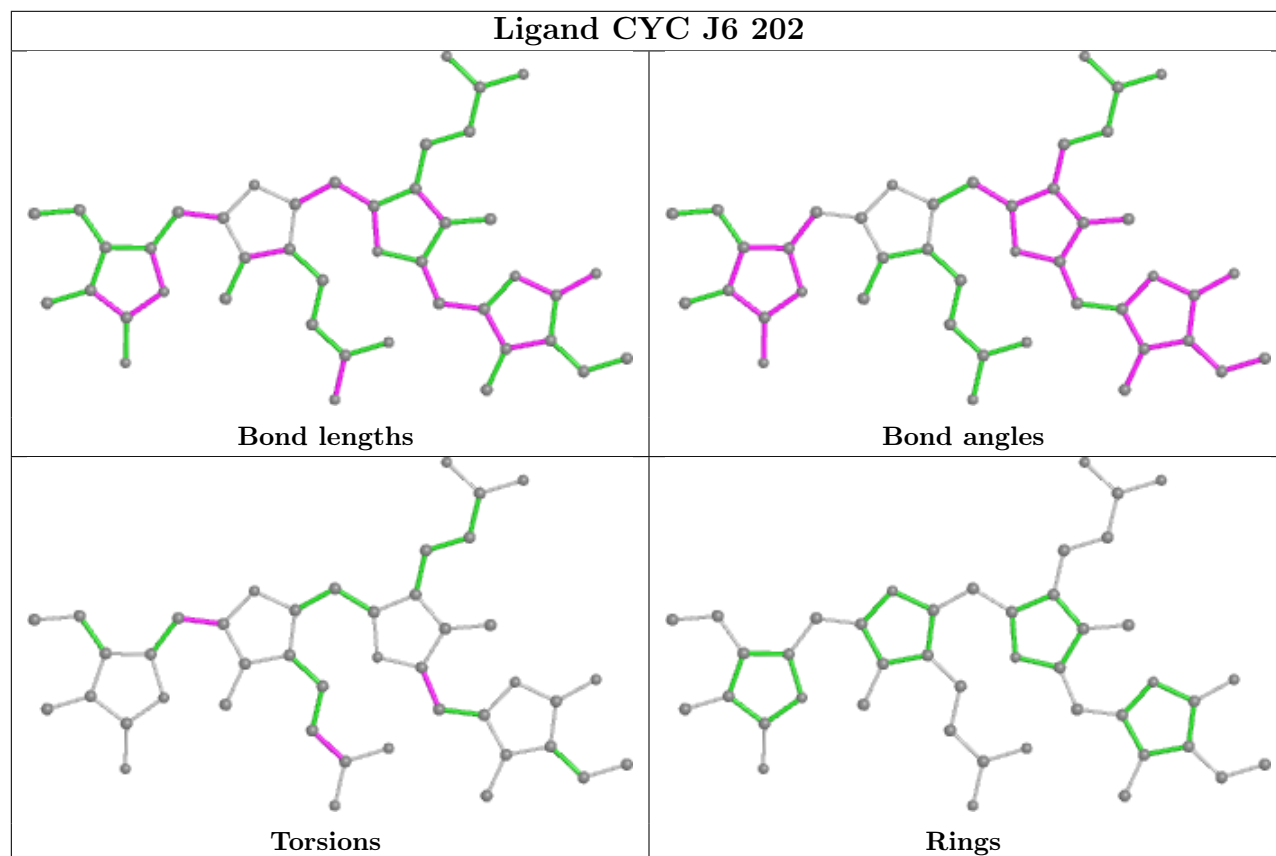




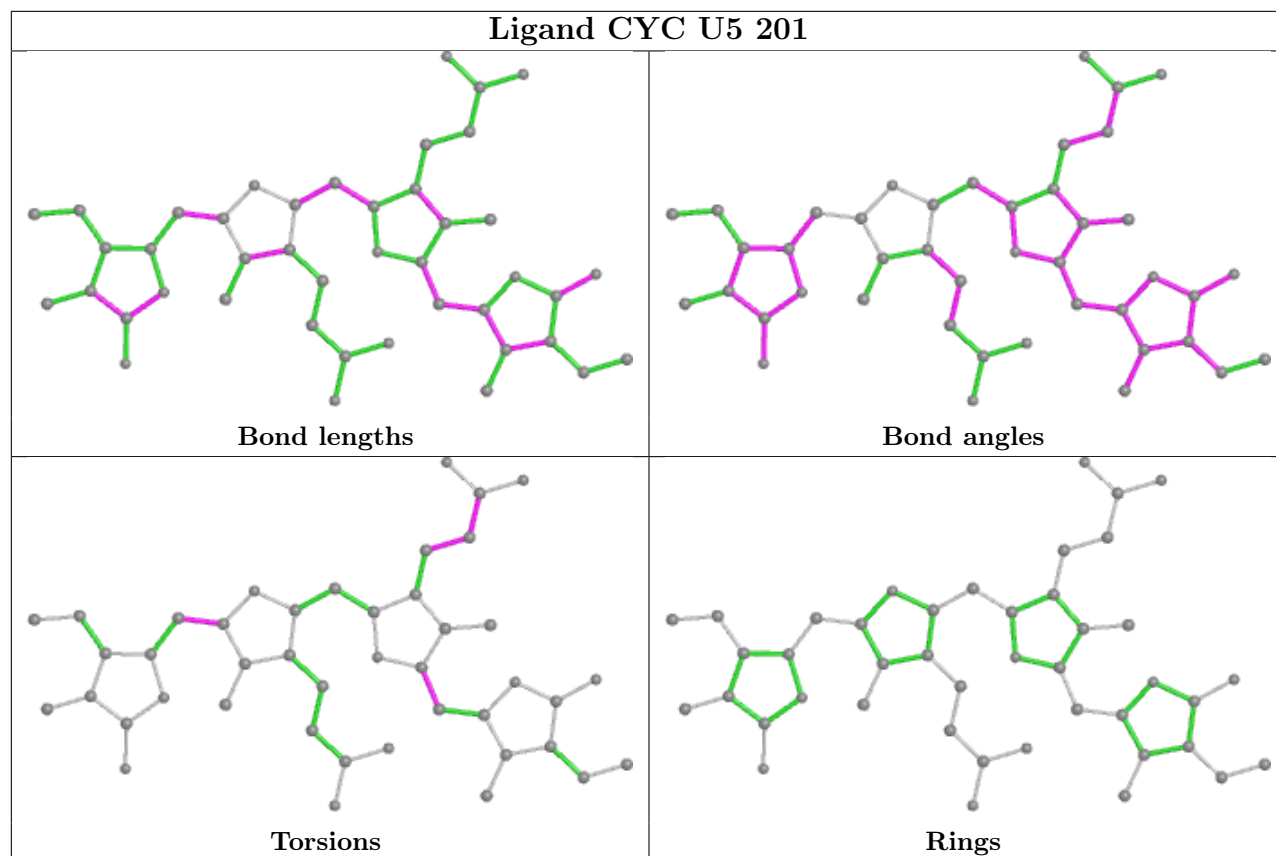
Ligand CYC Y1 201



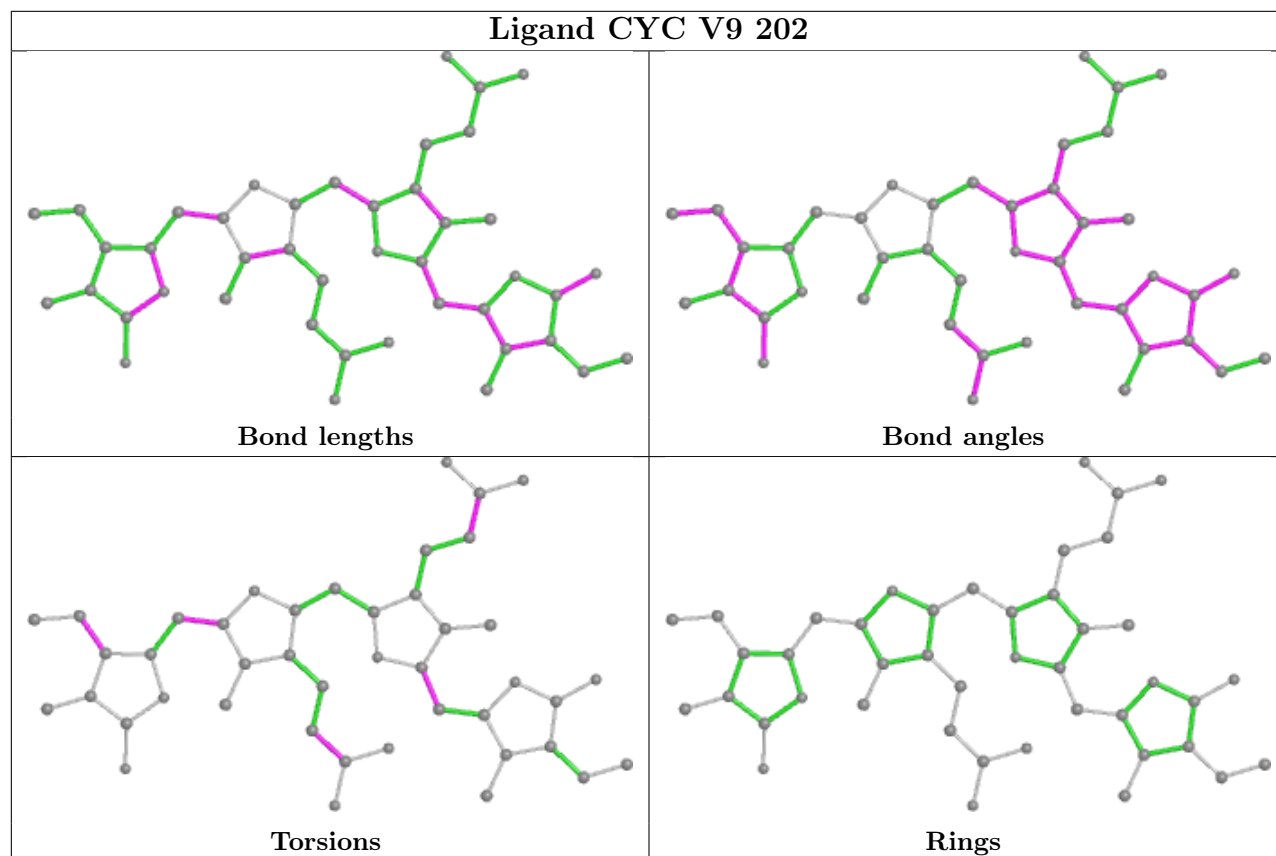
Ligand CYC J6 202

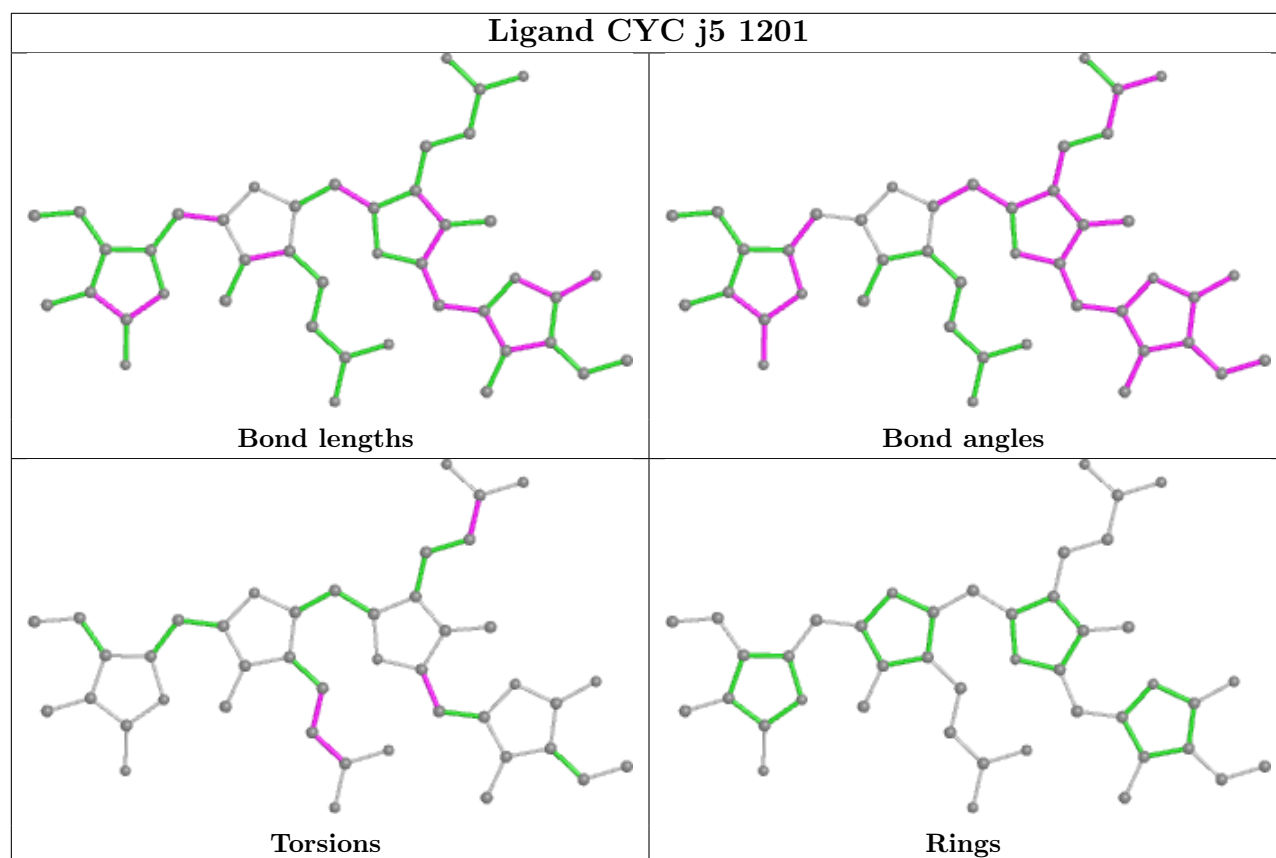
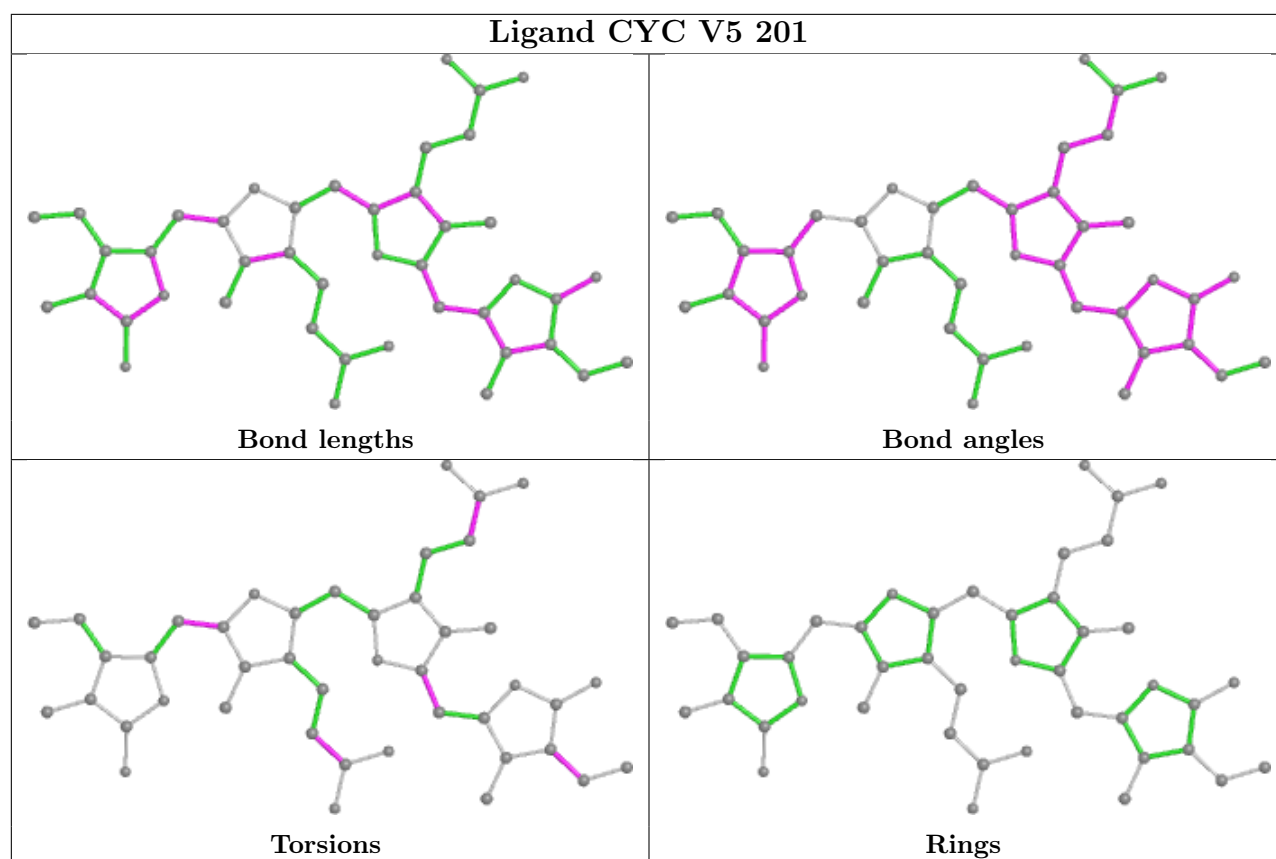


Ligand CYC U5 201

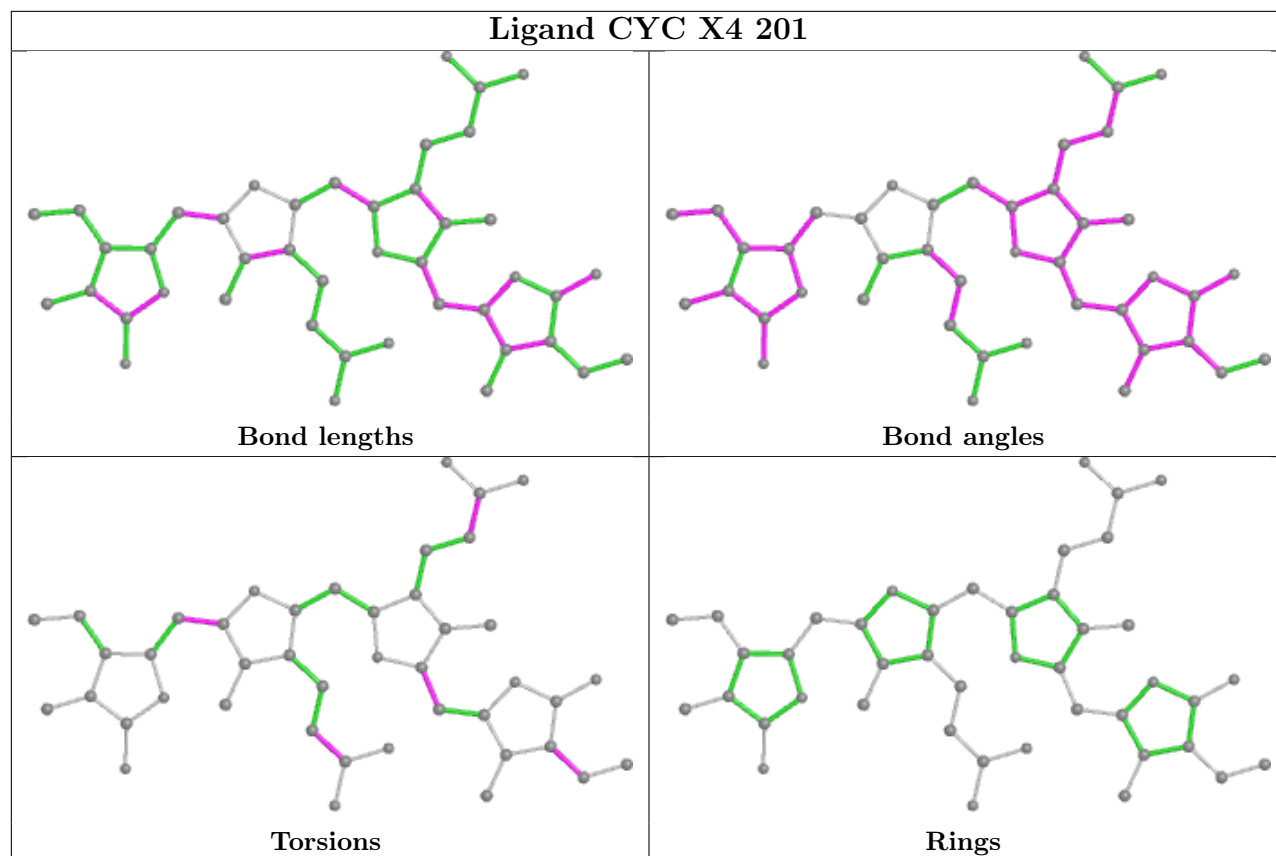


Ligand CYC V9 202

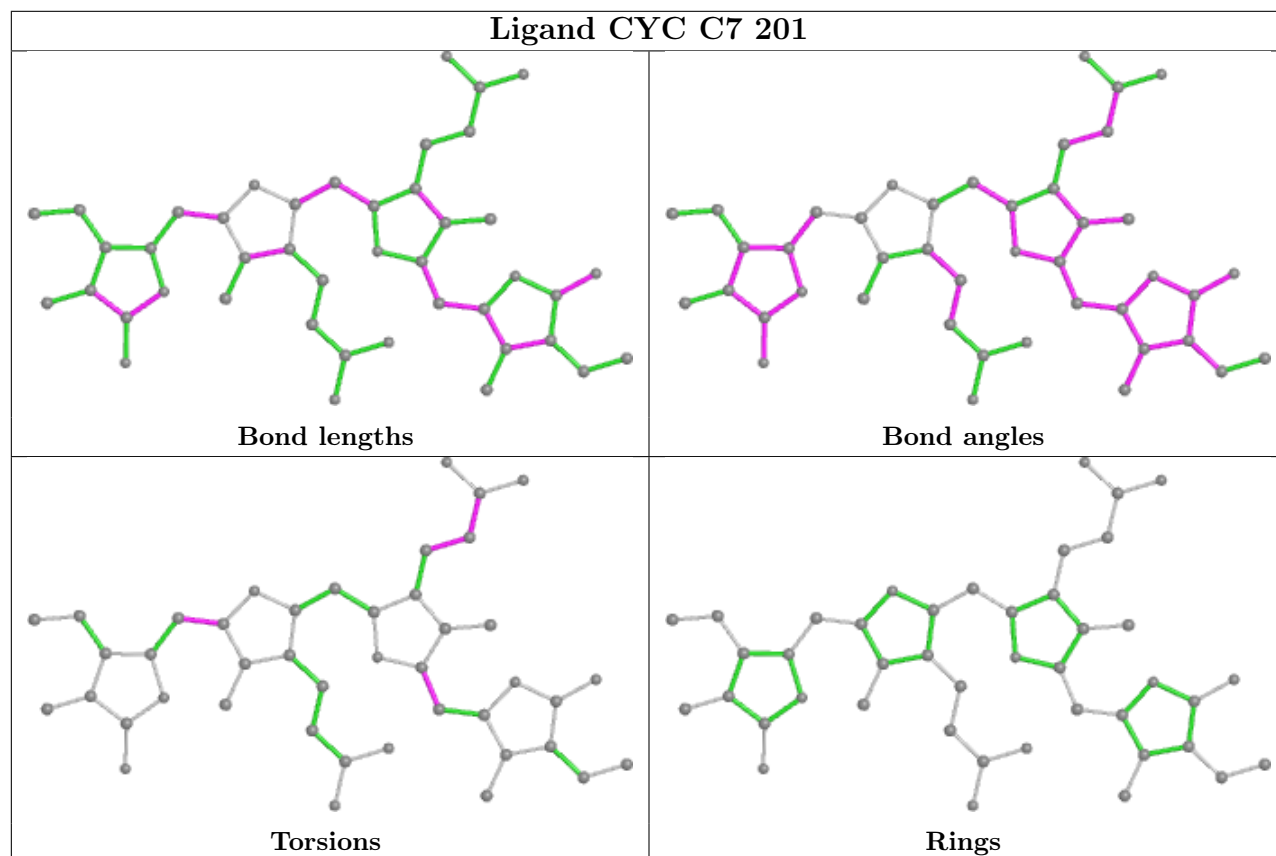




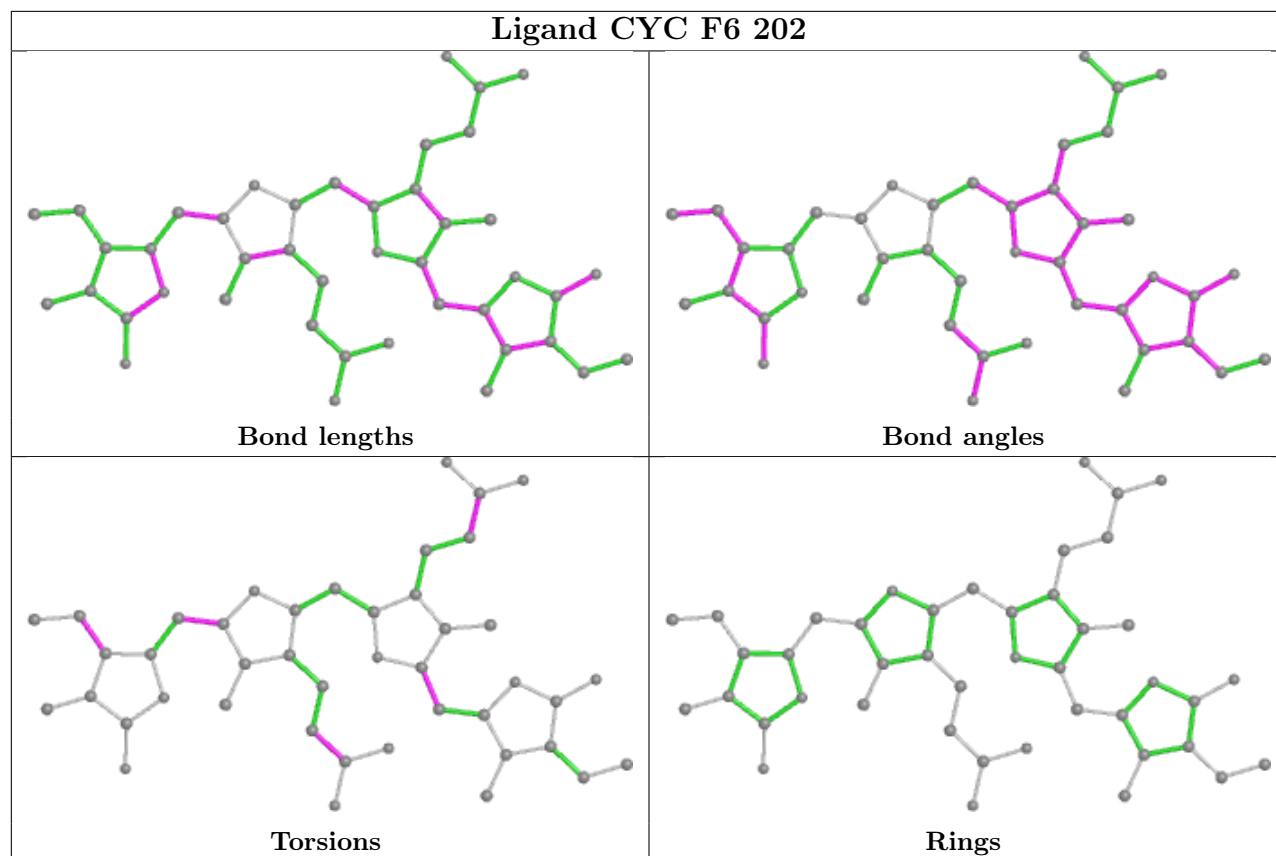
Ligand CYC X4 201



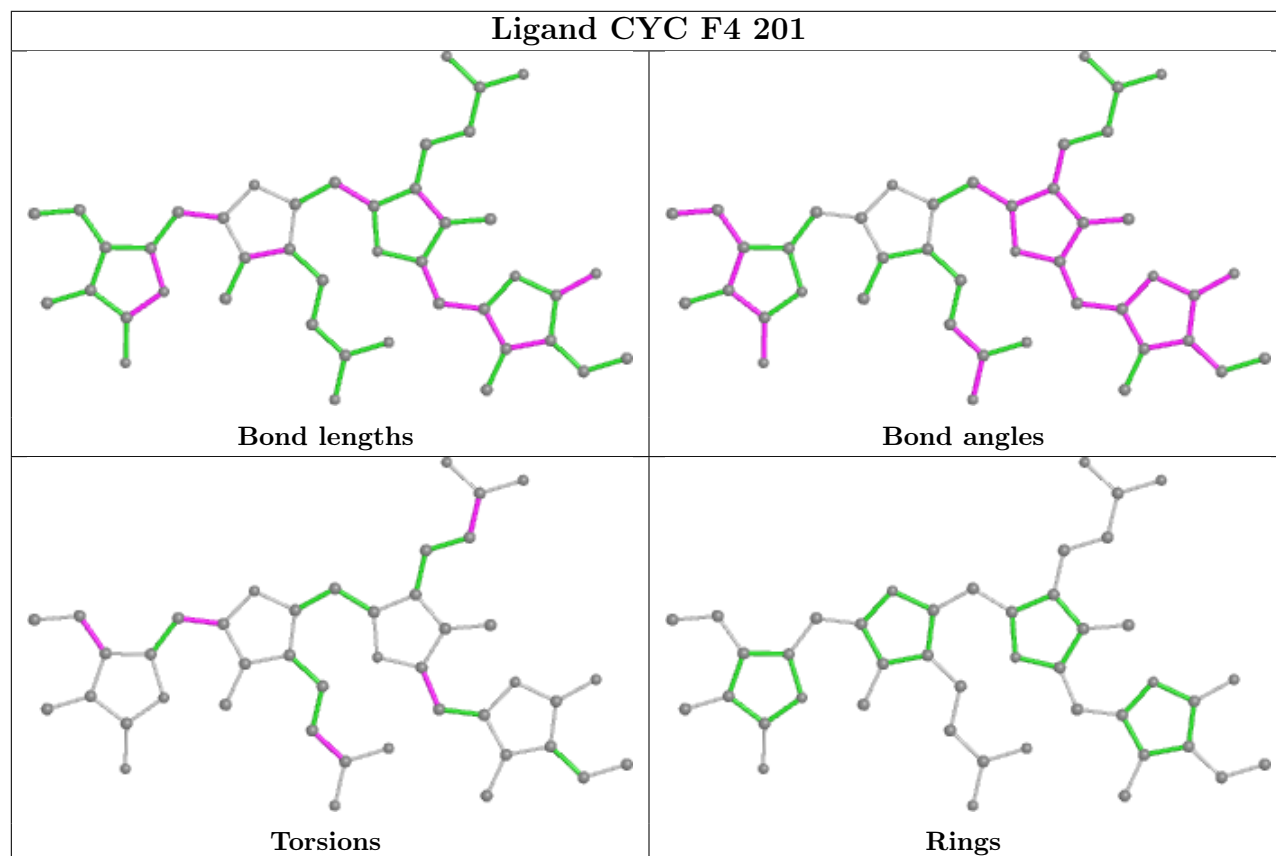
Ligand CYC C7 201



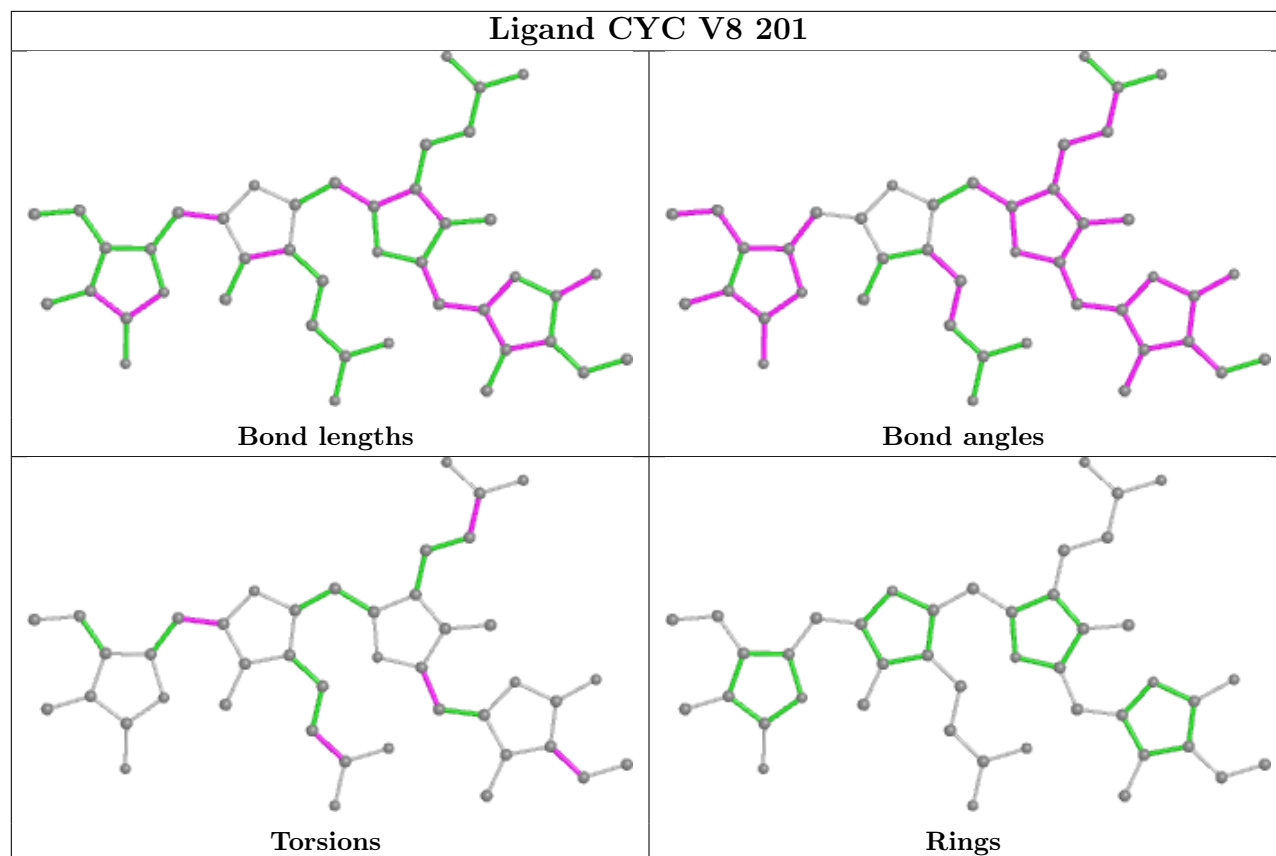
Ligand CYC F6 202



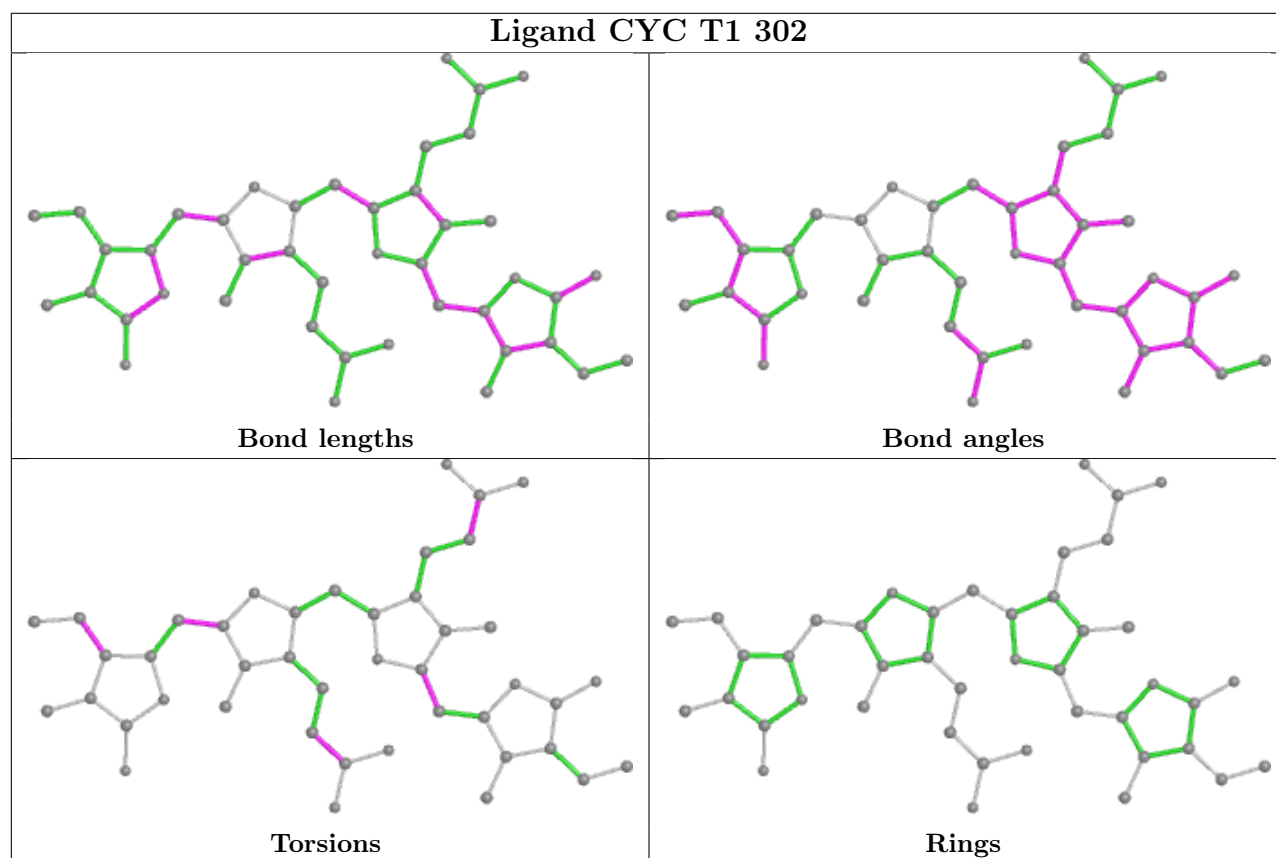
Ligand CYC F4 201

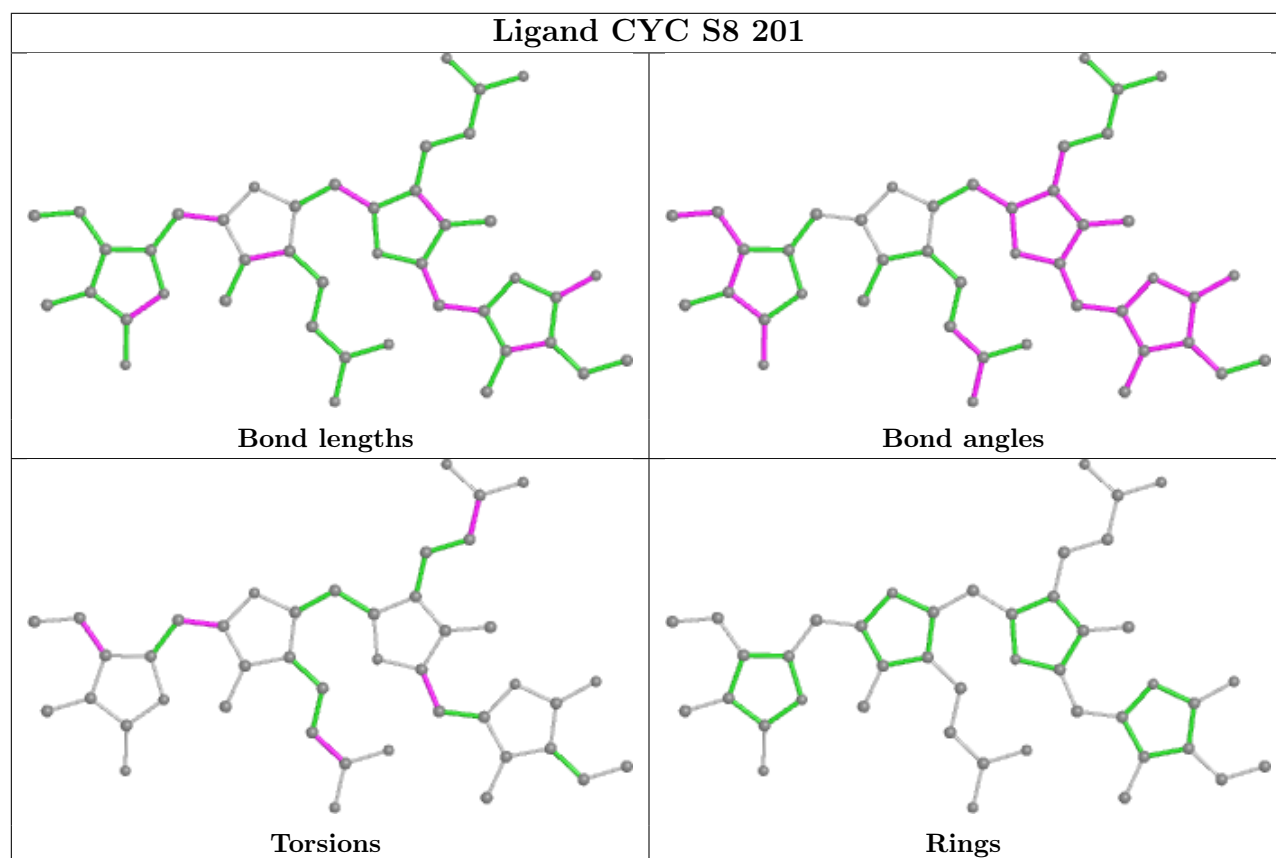
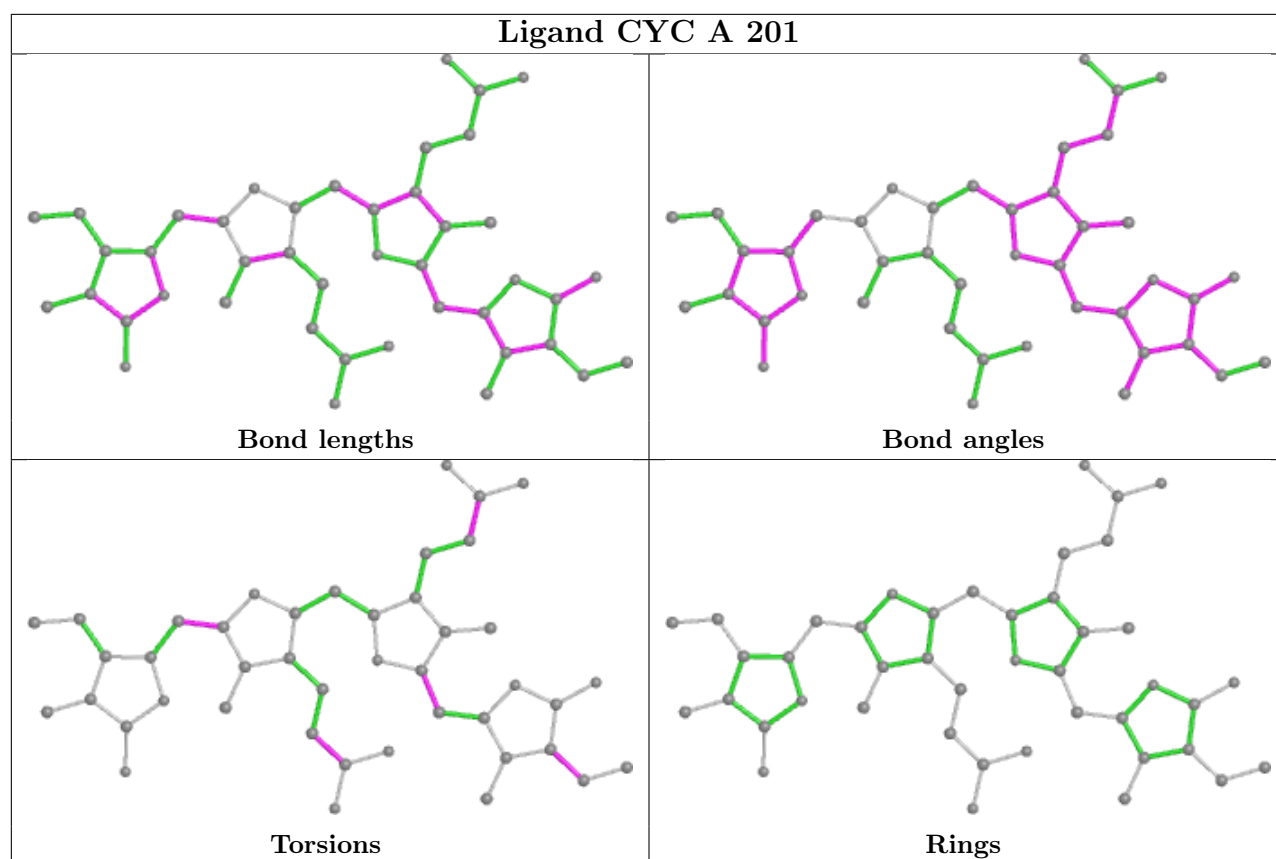


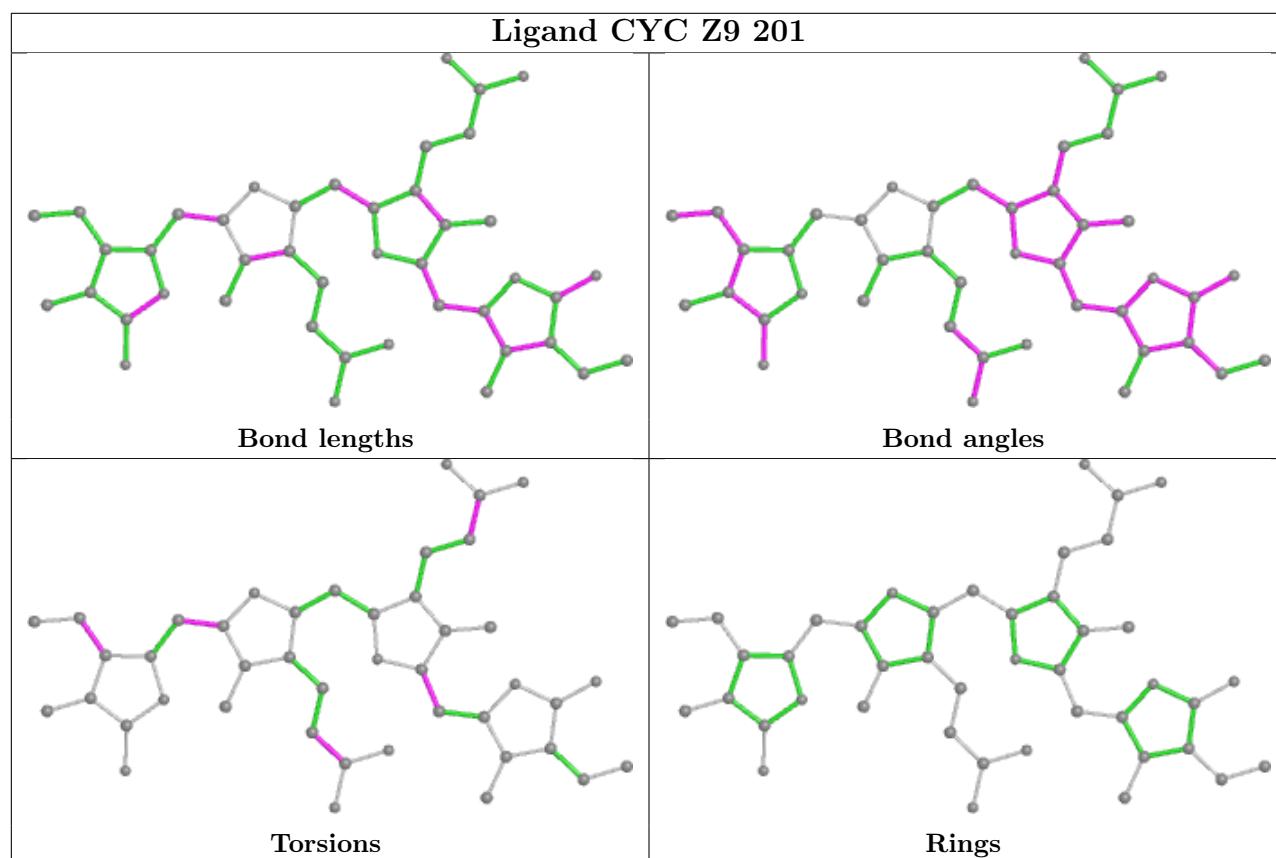
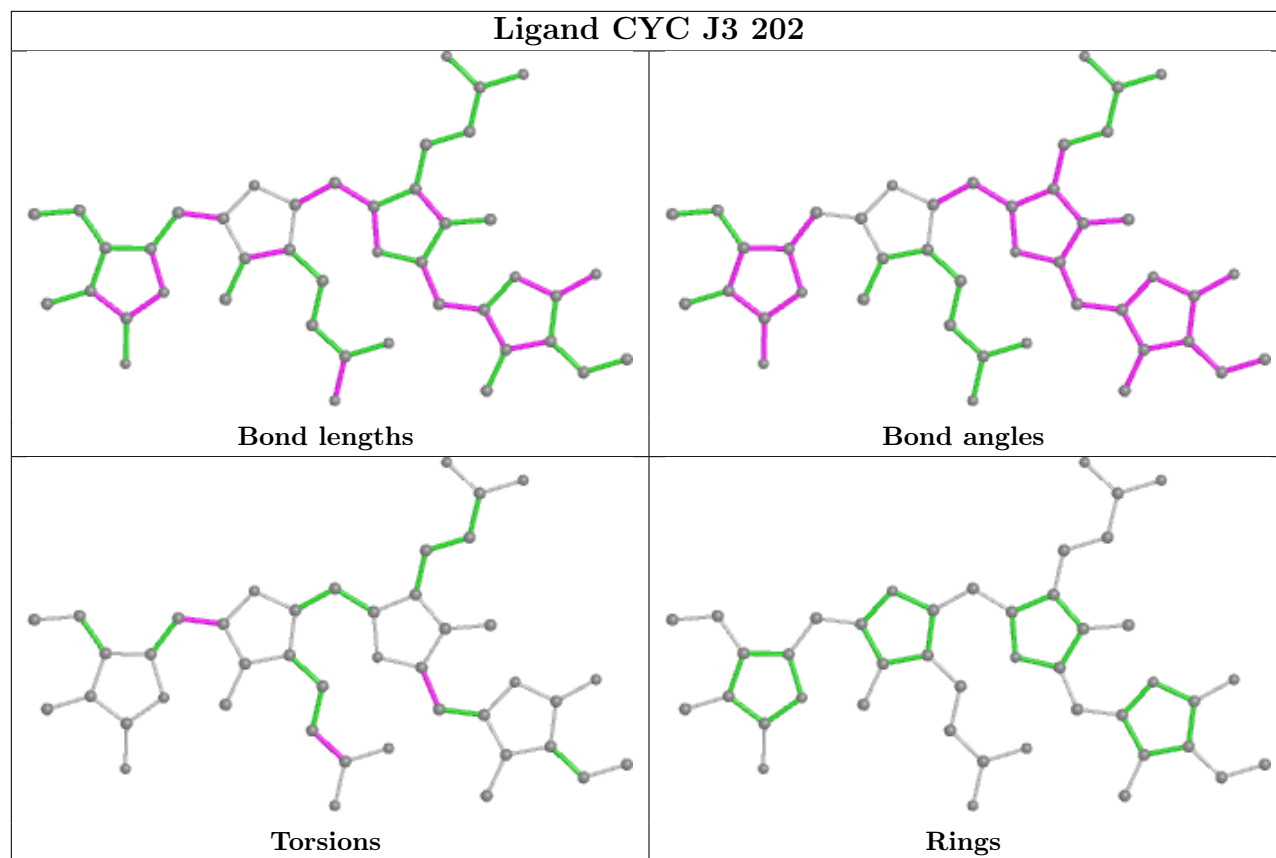
Ligand CYC V8 201



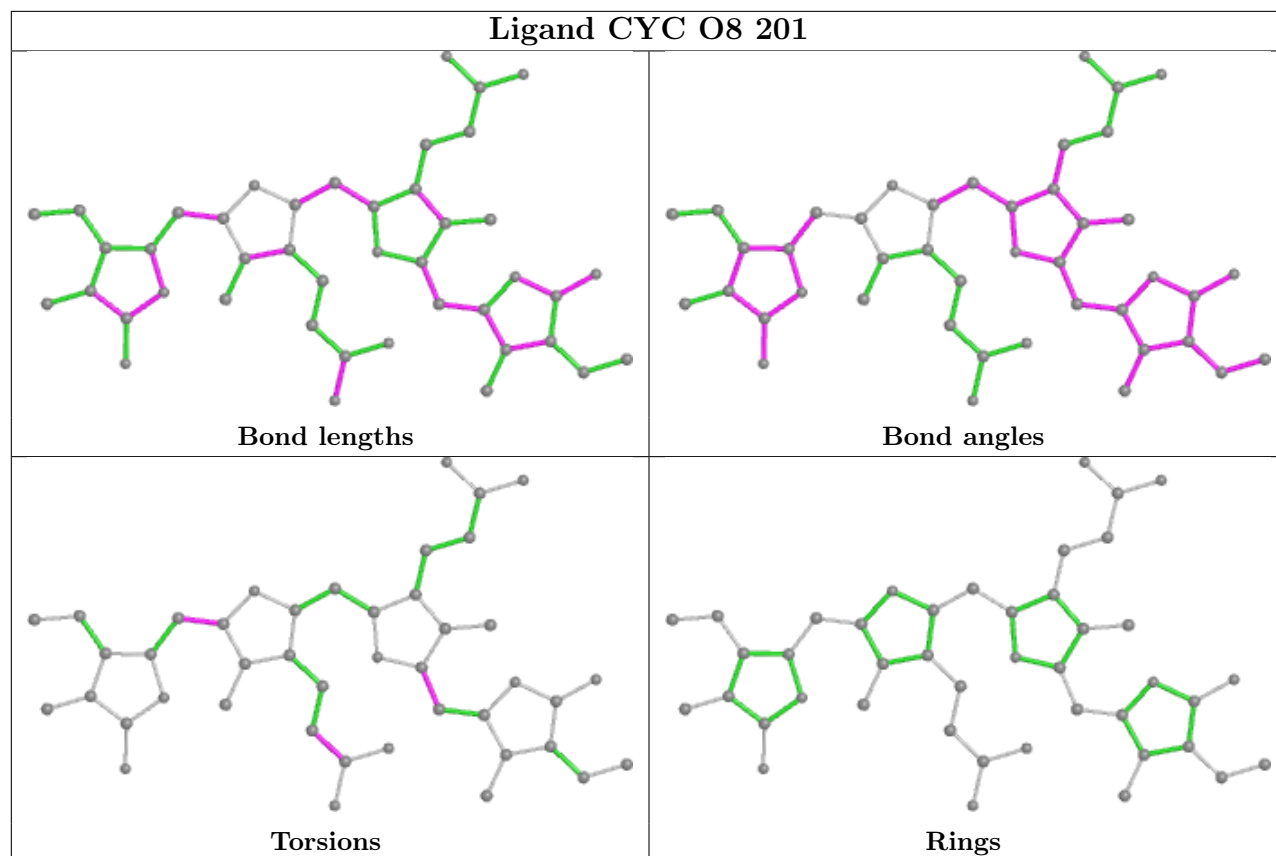
Ligand CYC T1 302



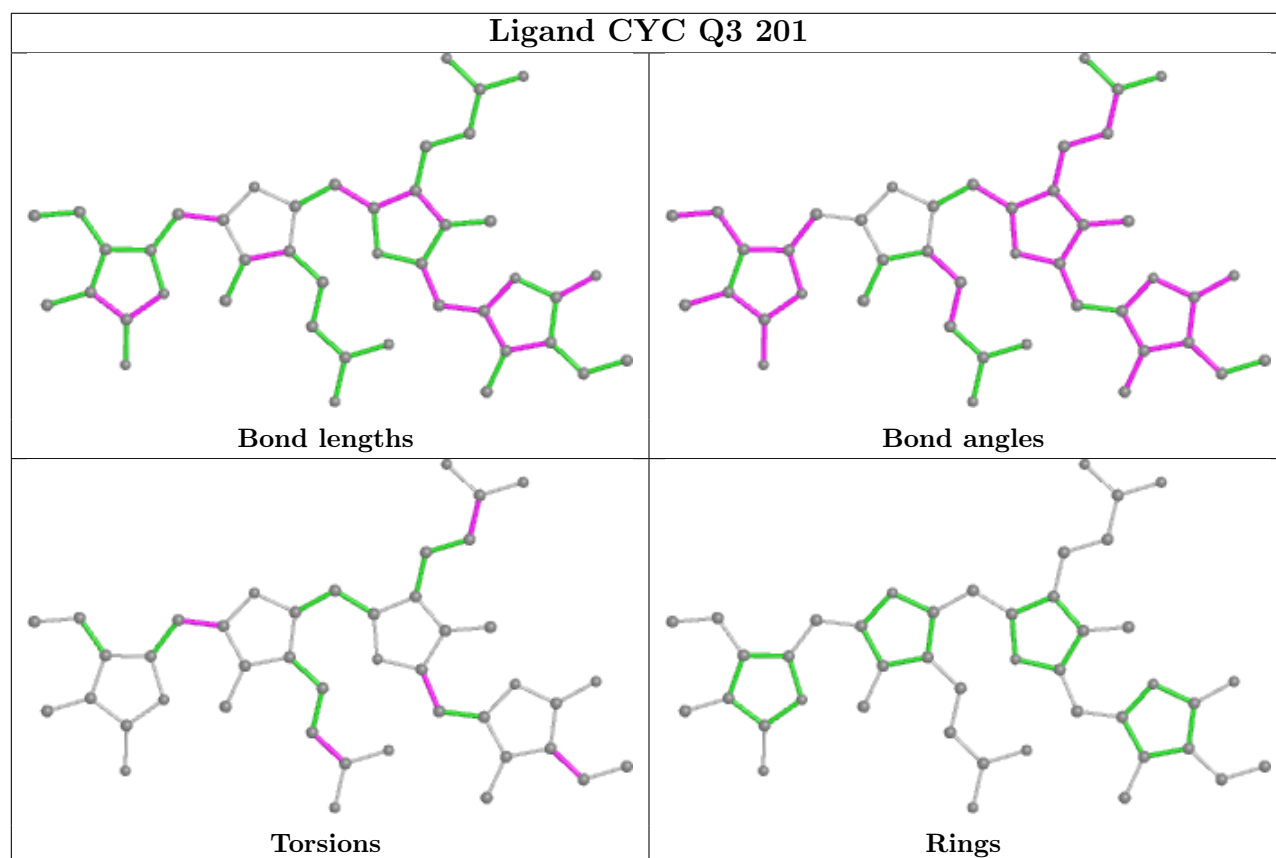




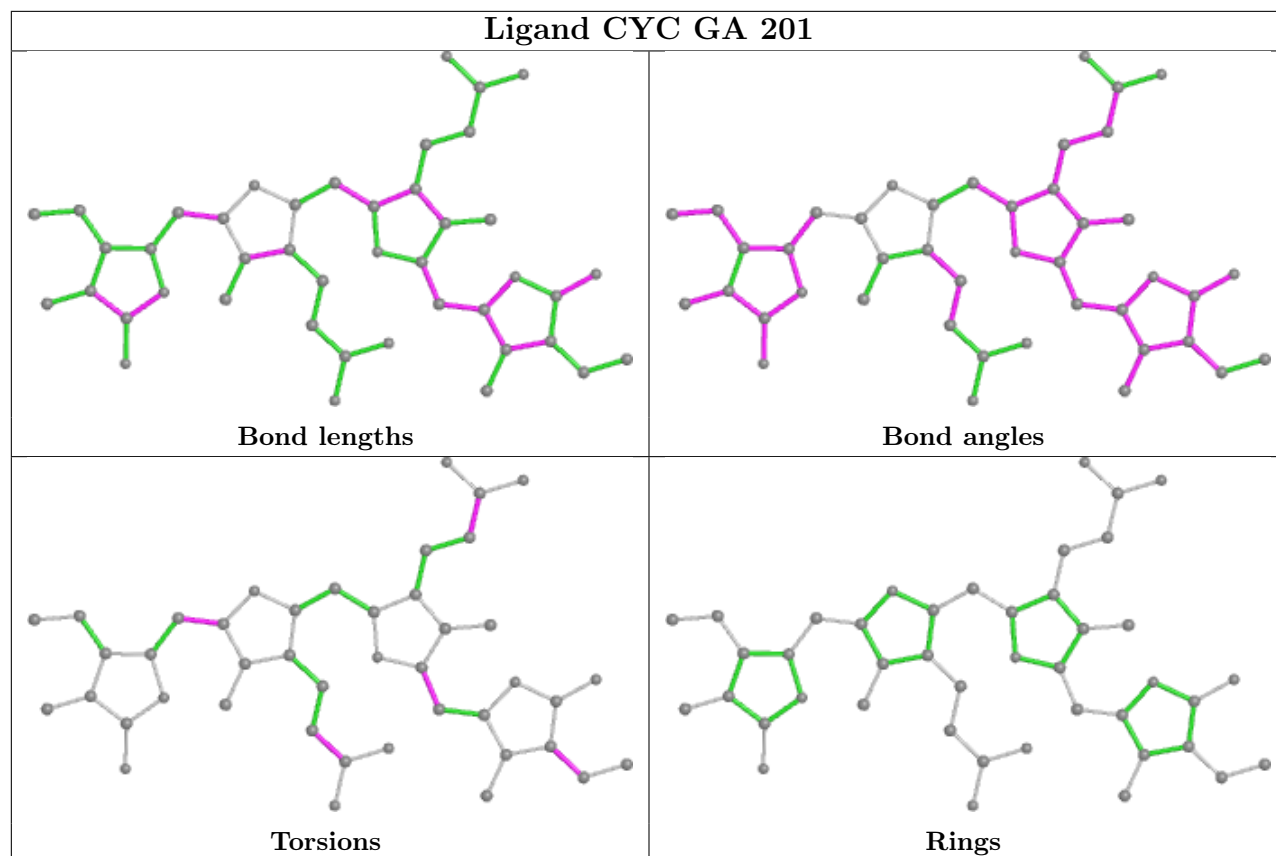
Ligand CYC O8 201



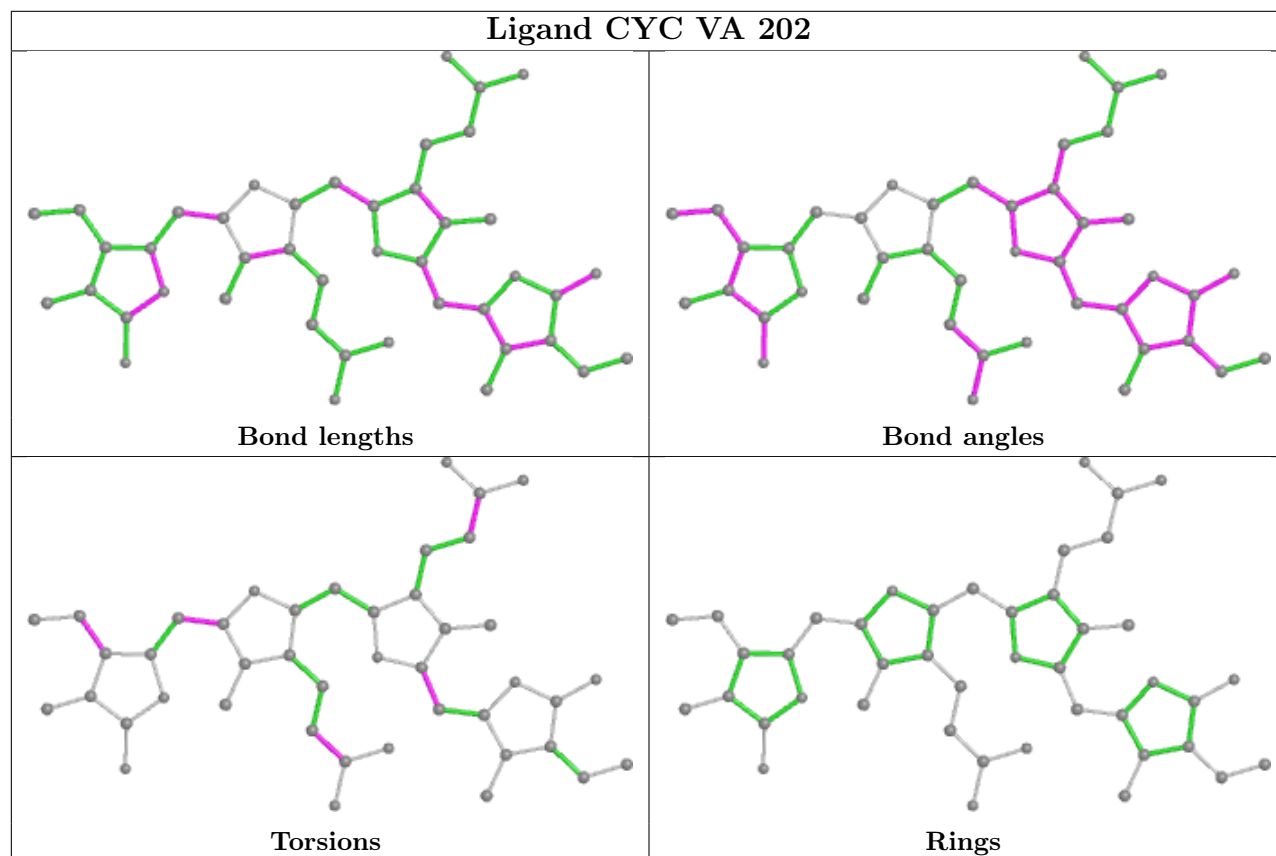
Ligand CYC Q3 201



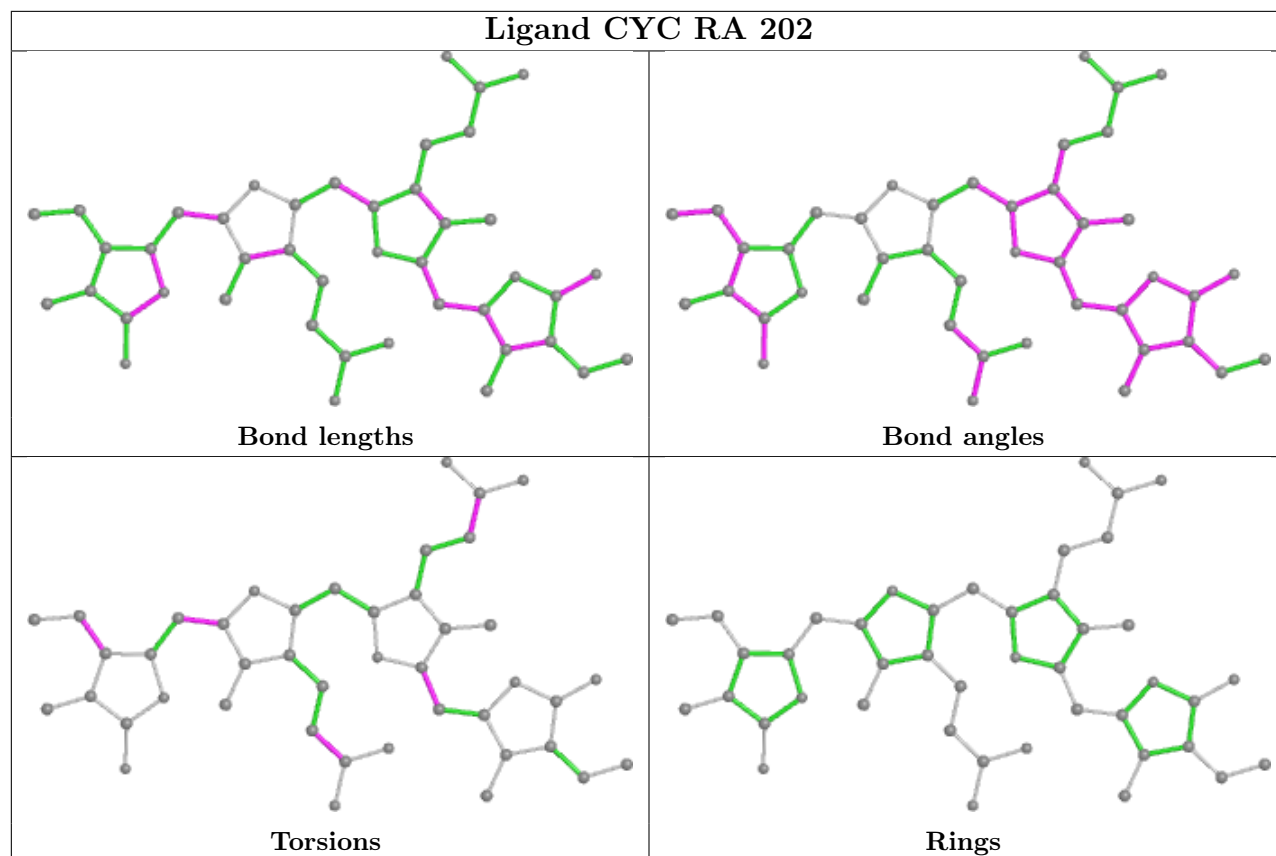
Ligand CYC GA 201



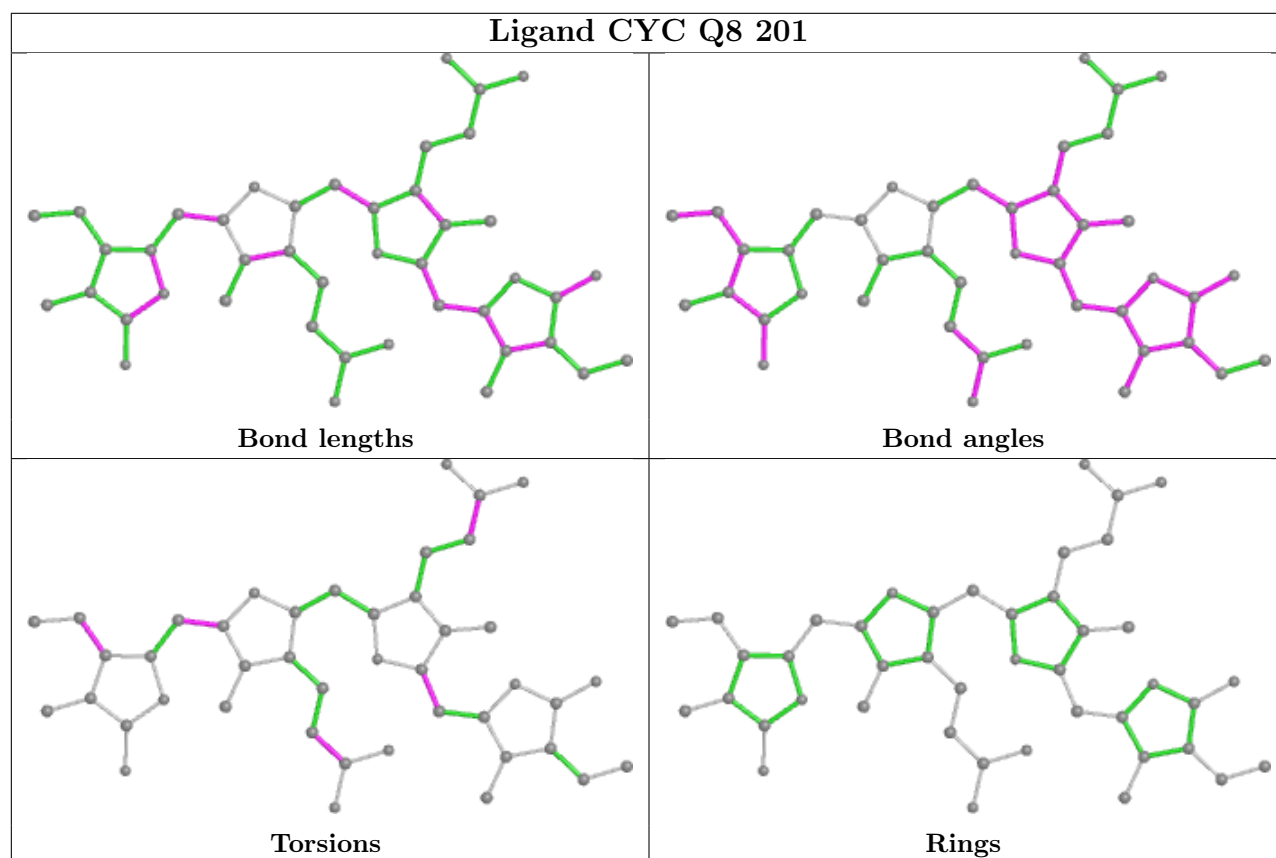
Ligand CYC VA 202



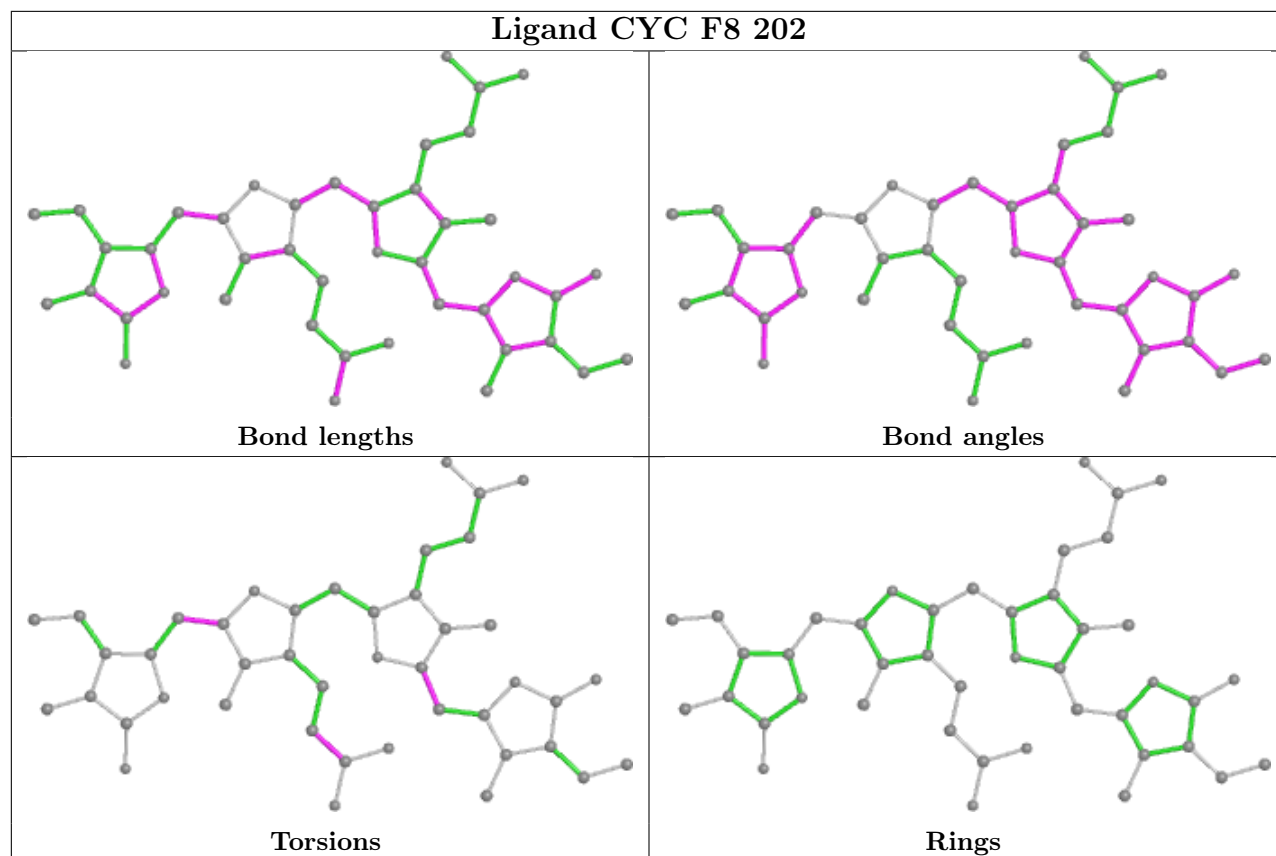
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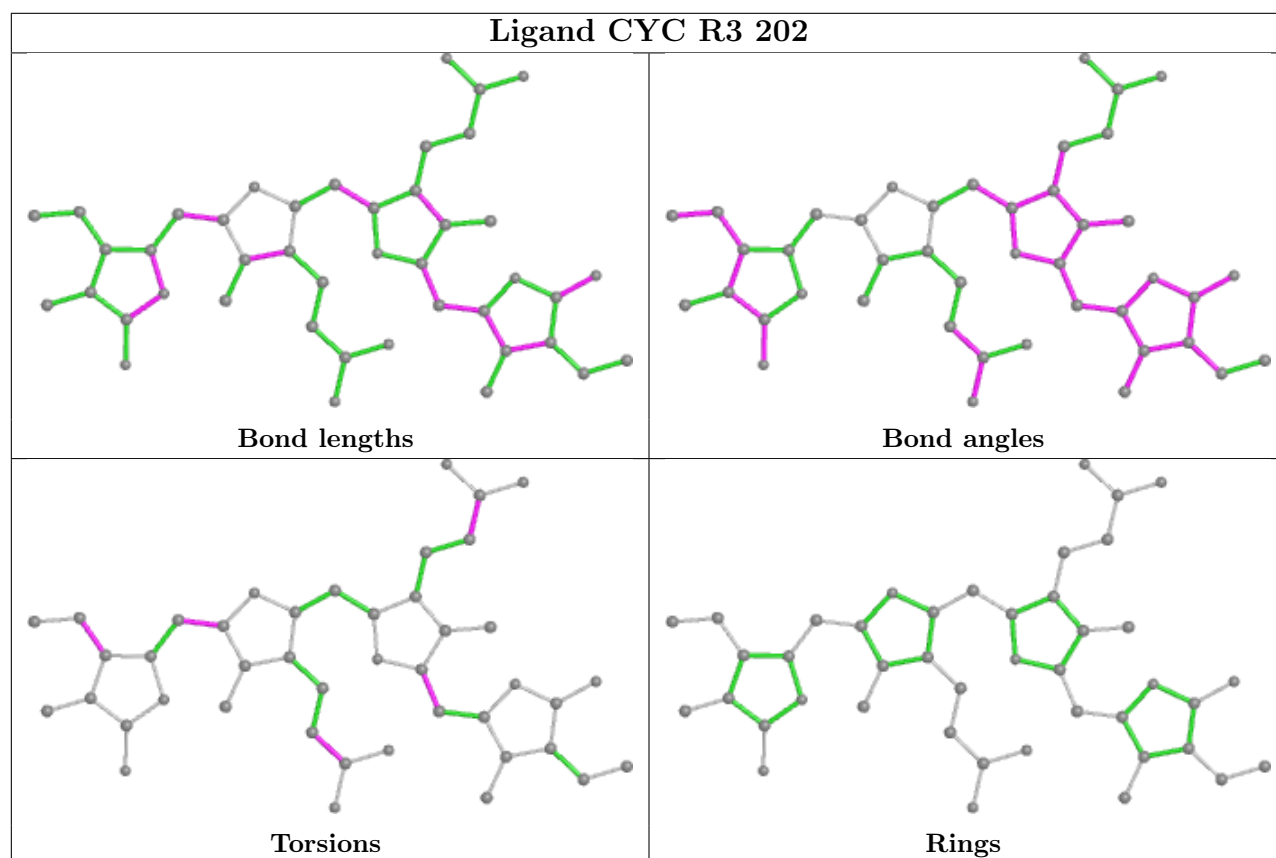
Ligand CYC Q8 201



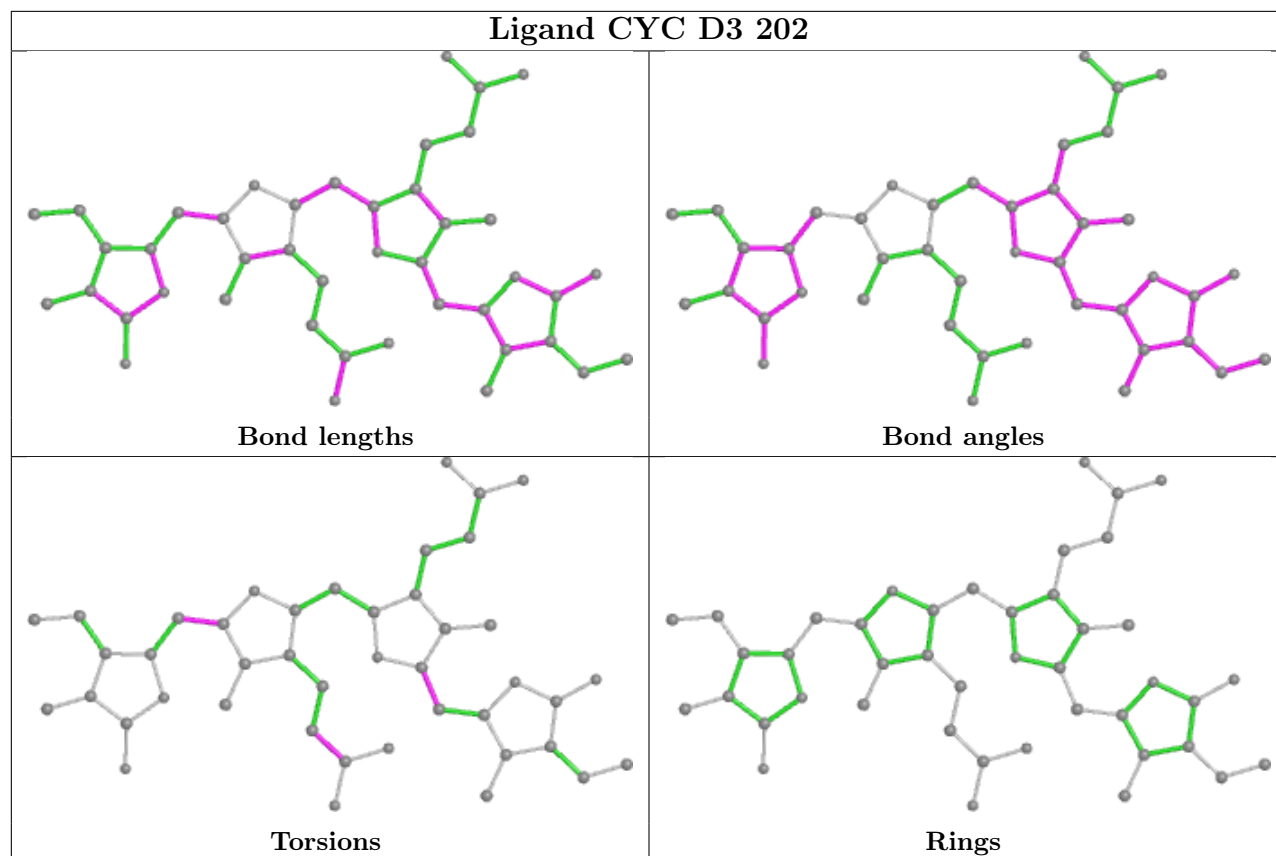
Ligand CYC F8 202



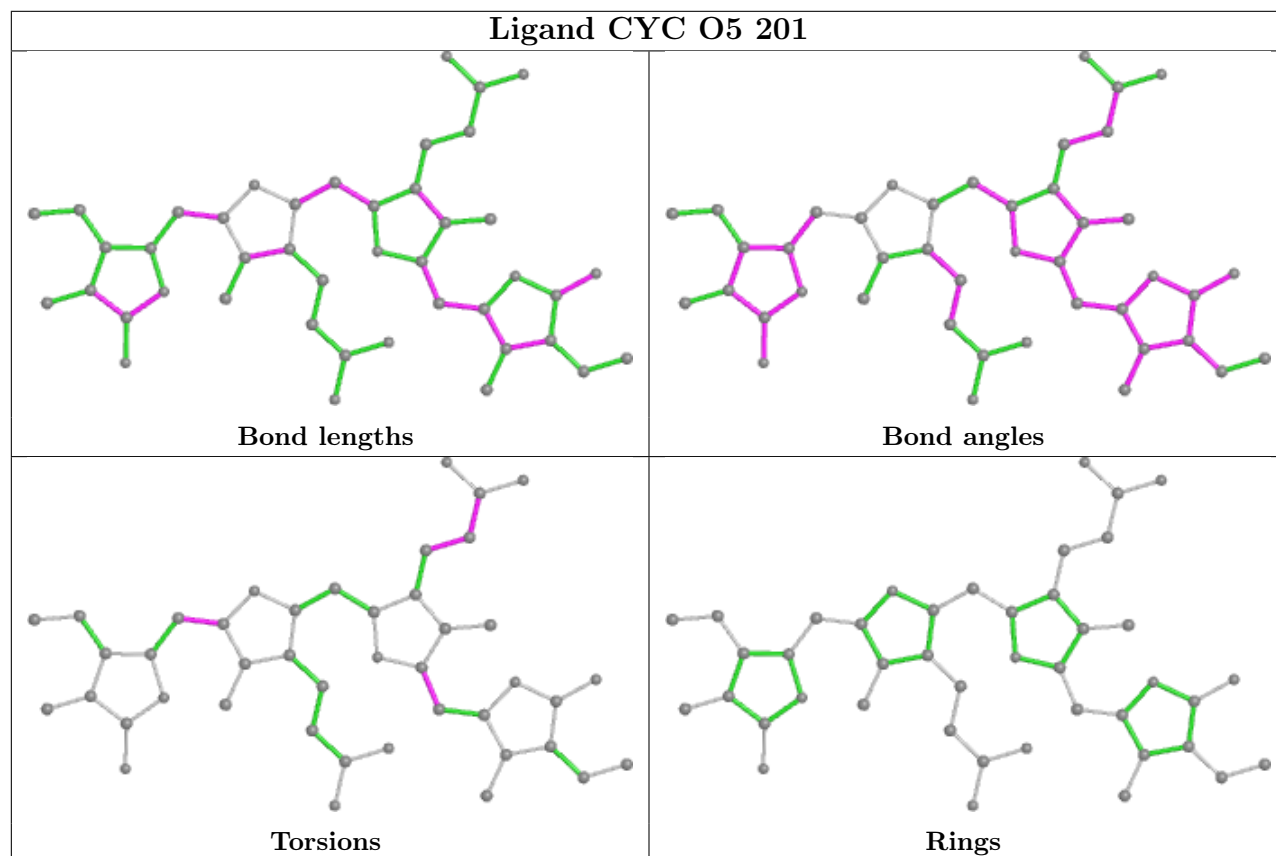
Ligand CYC R3 202



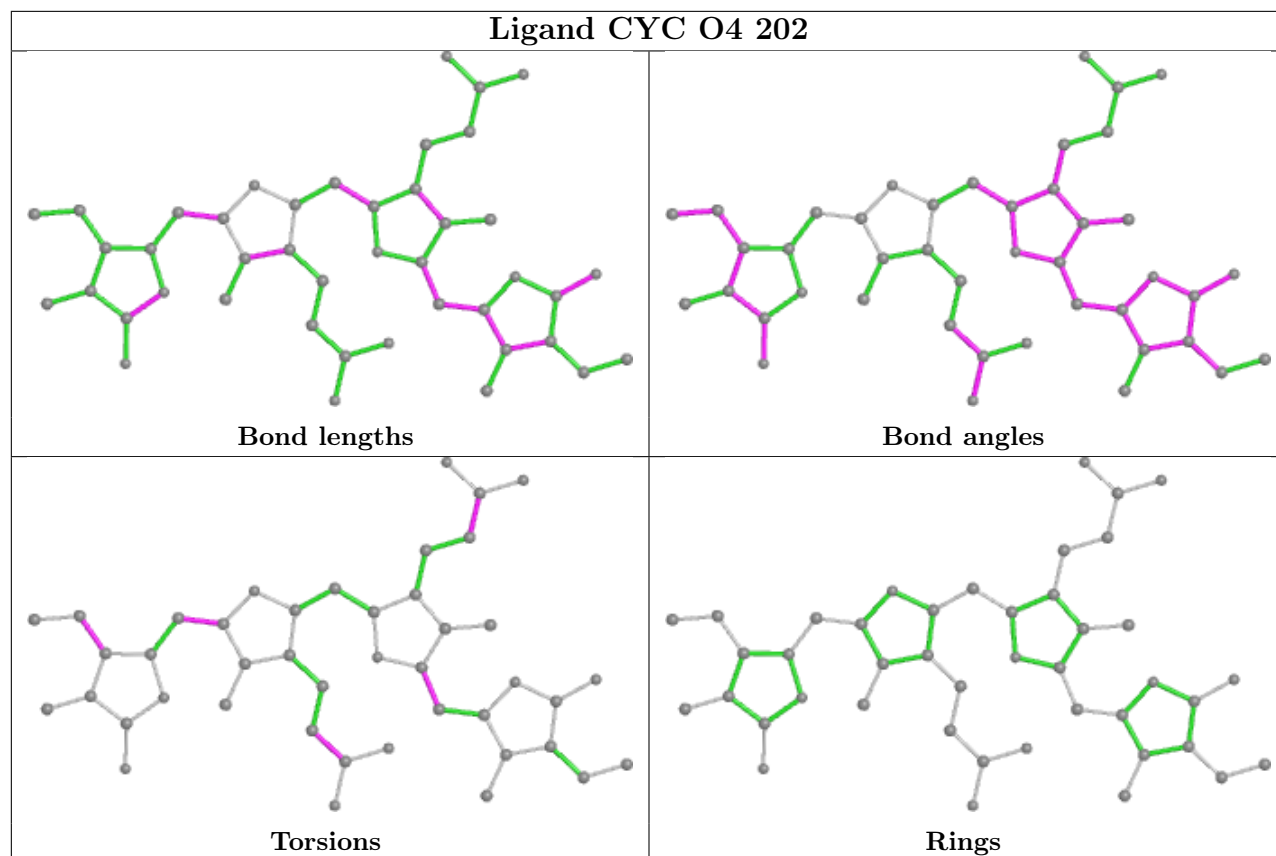
Ligand CYC D3 202



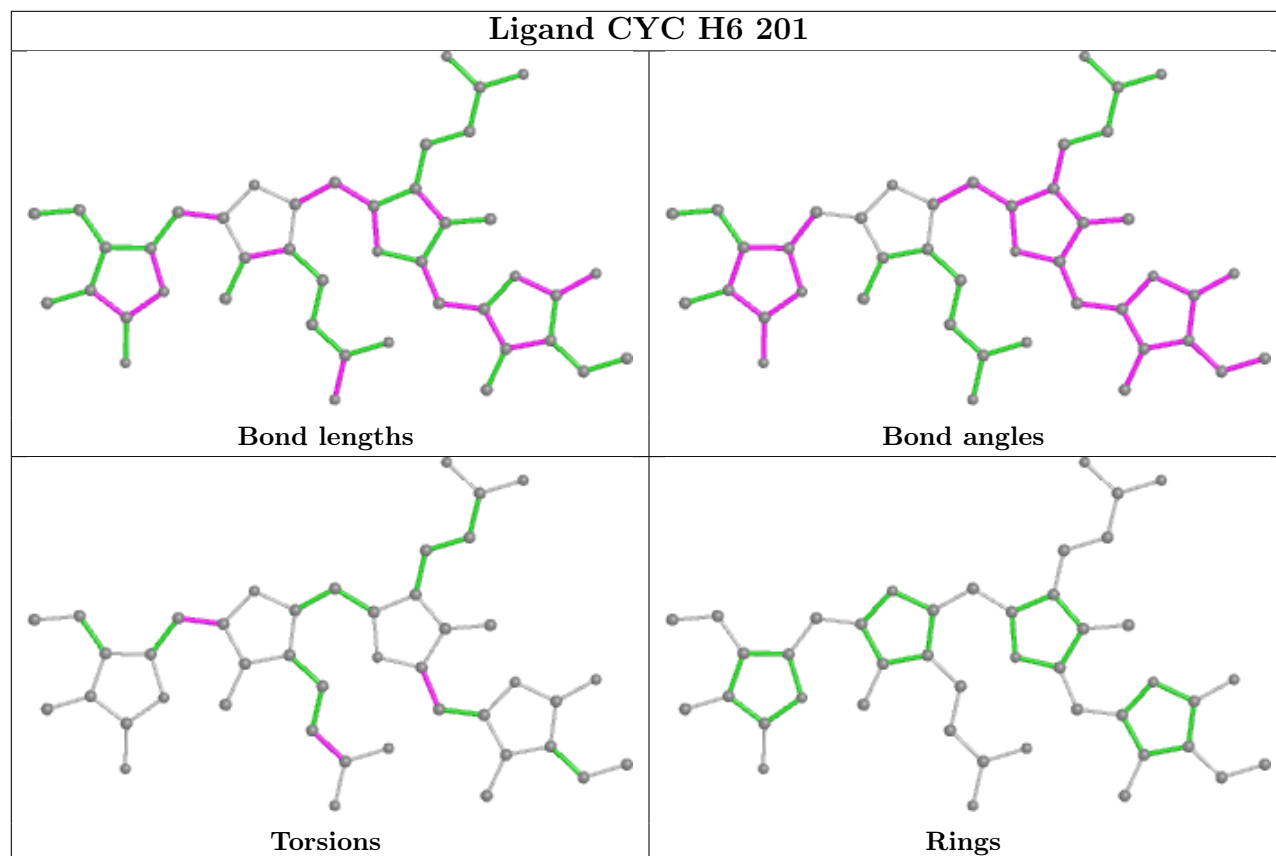
Ligand CYC O5 201



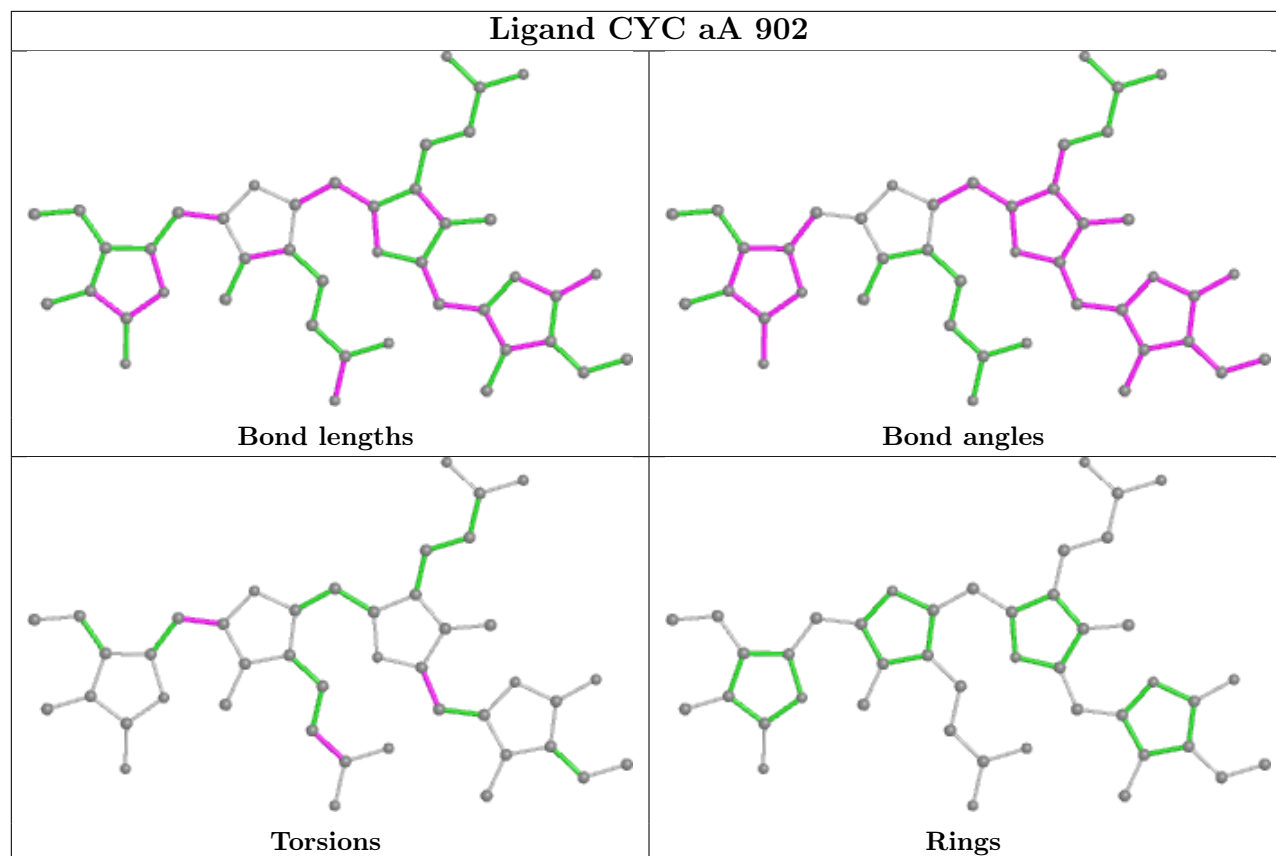
Ligand CYC O4 202



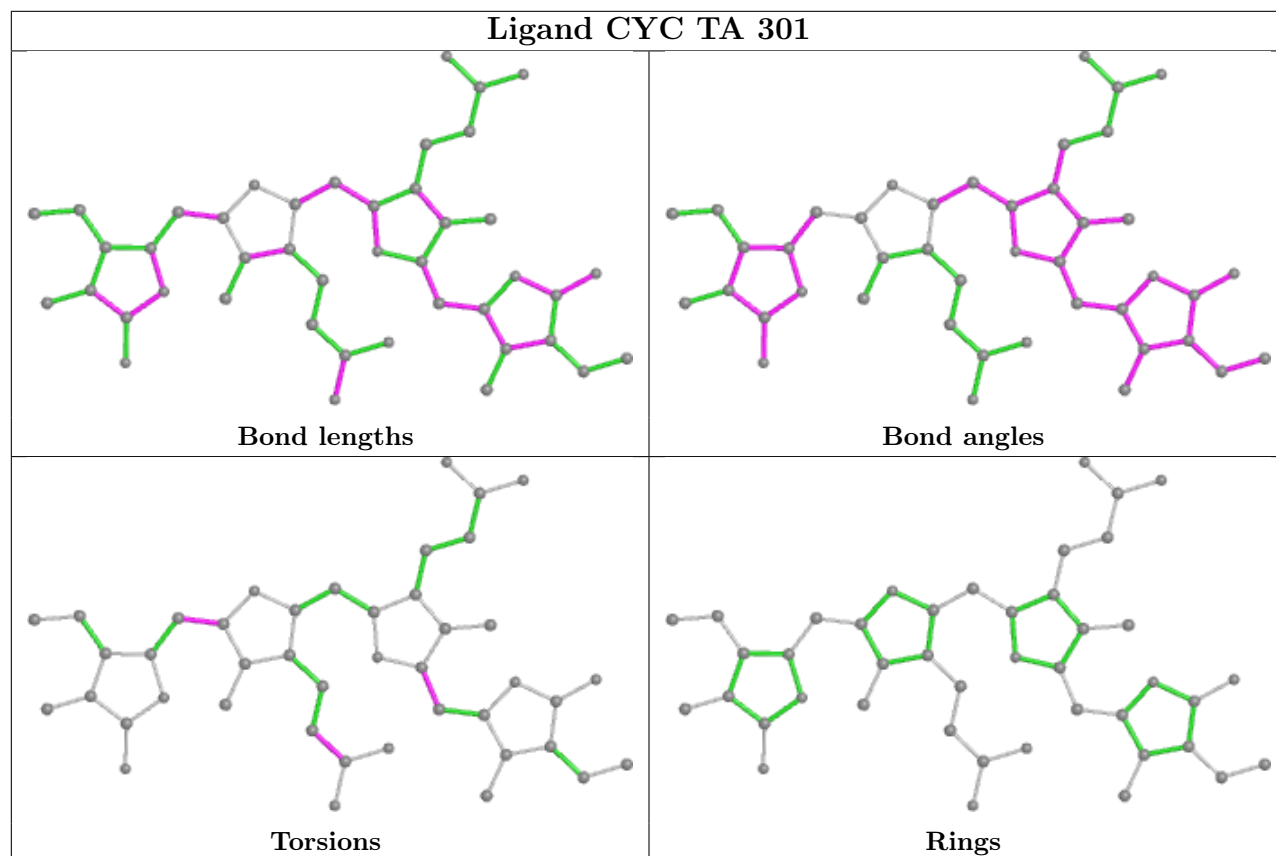
Ligand CYC H6 201



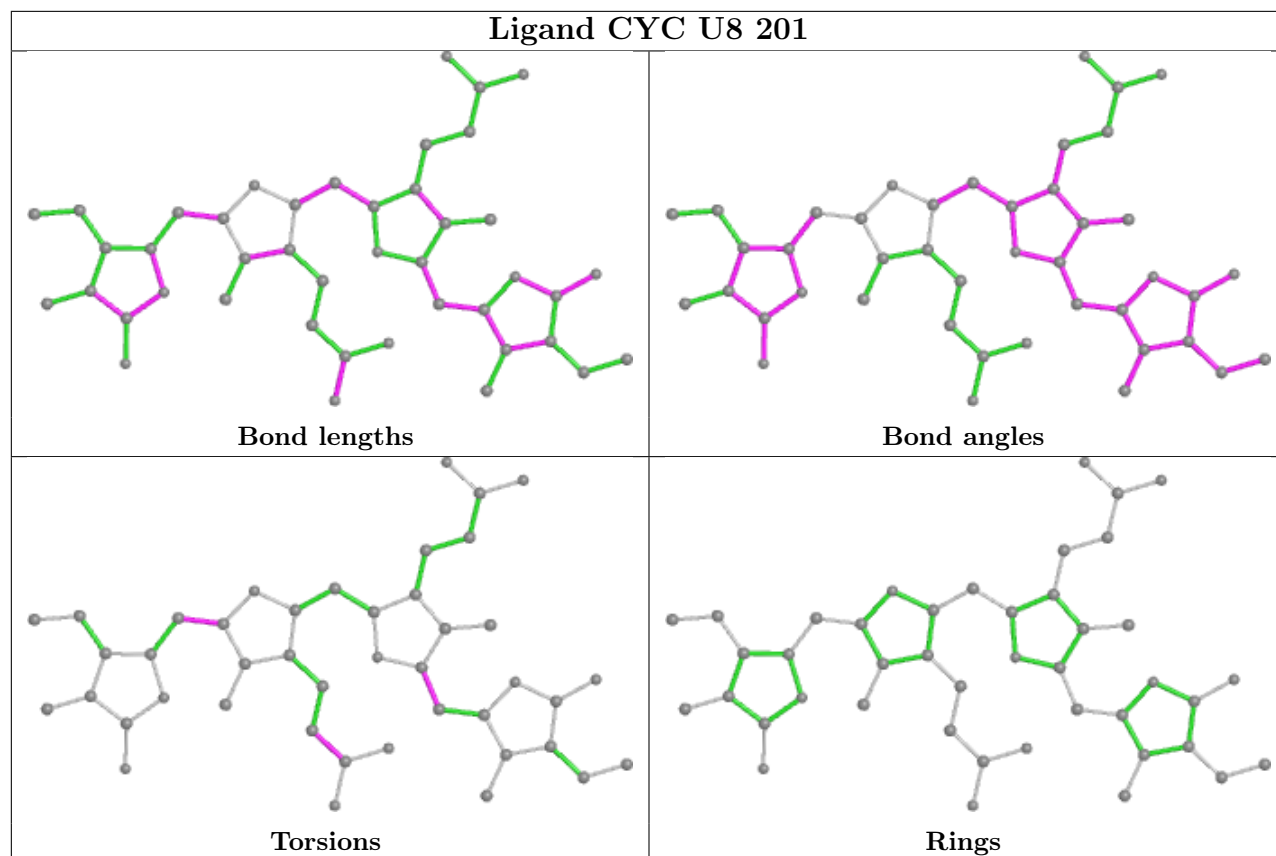
Ligand CYC aA 902



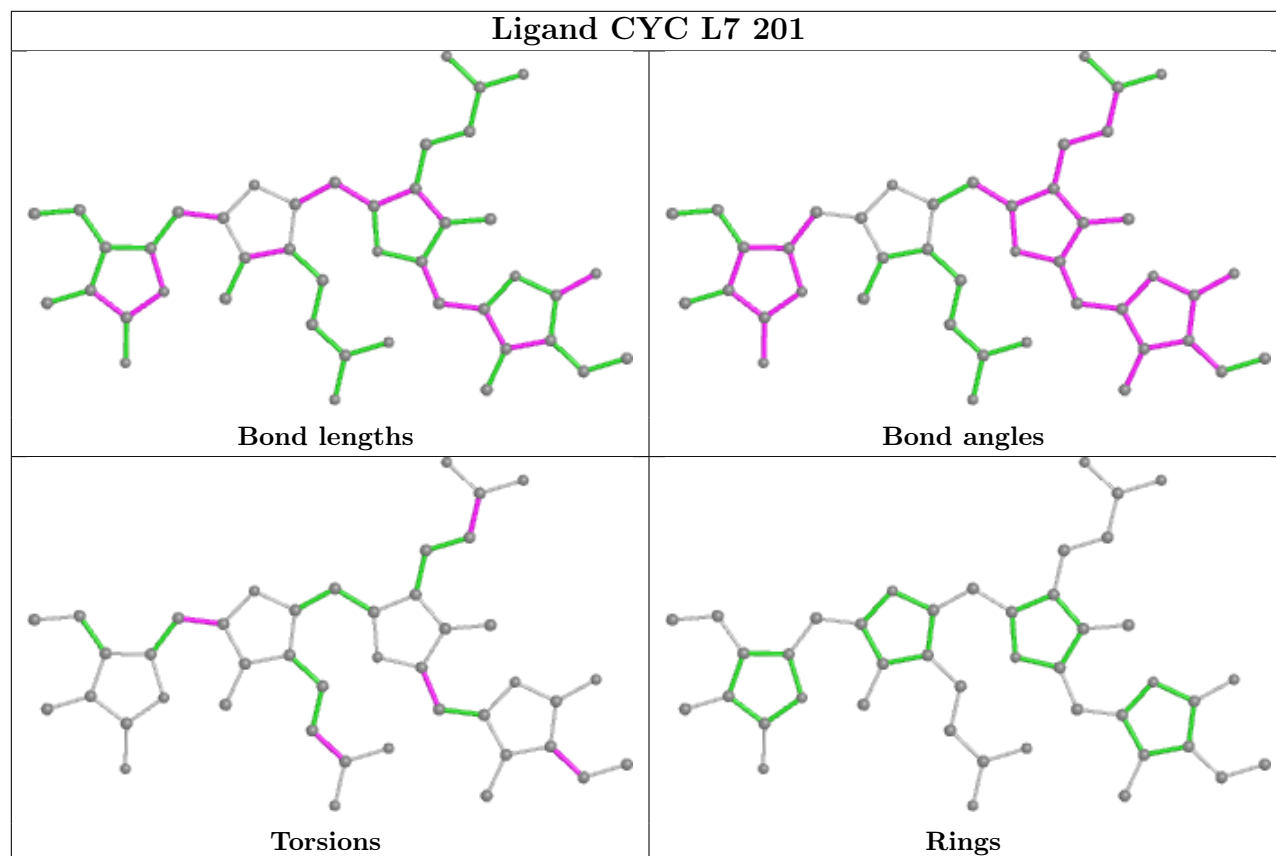
Ligand CYC TA 301

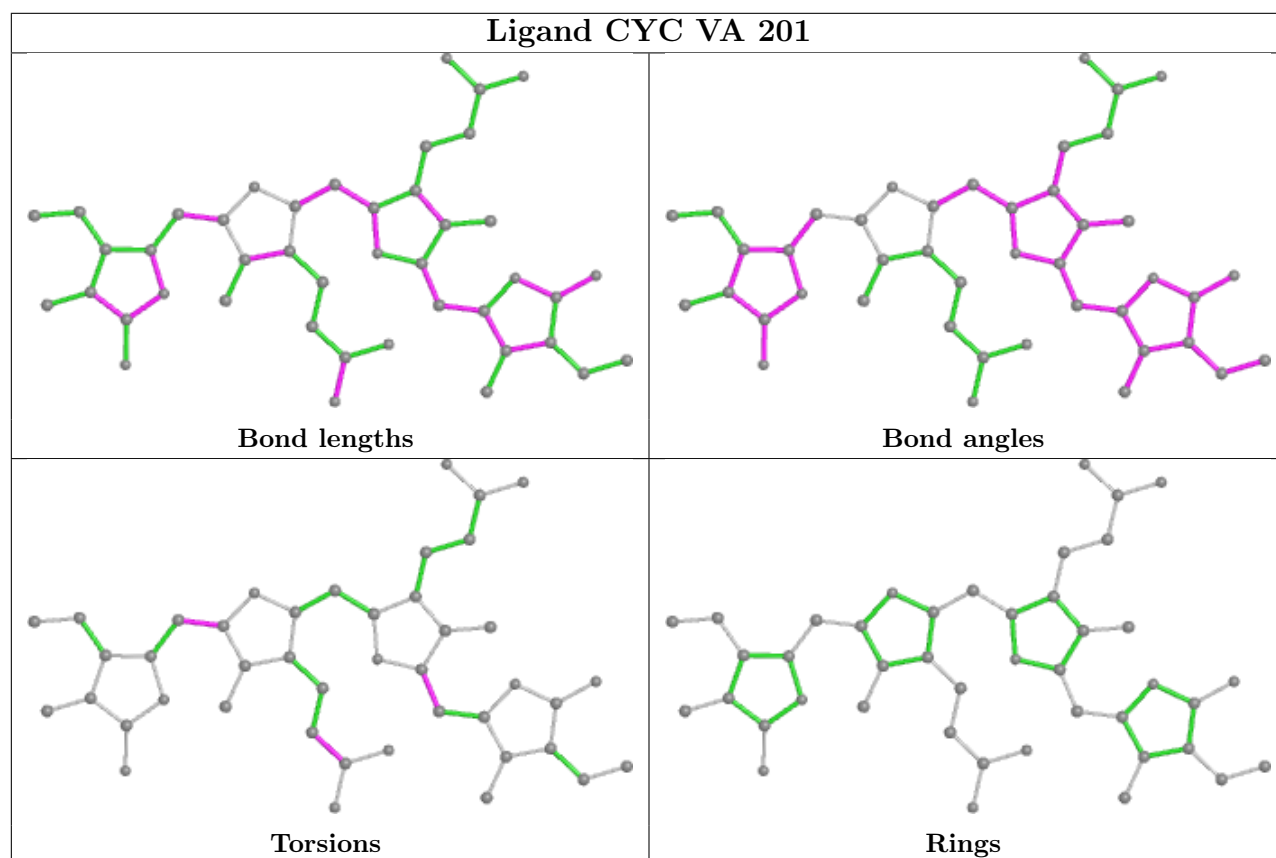
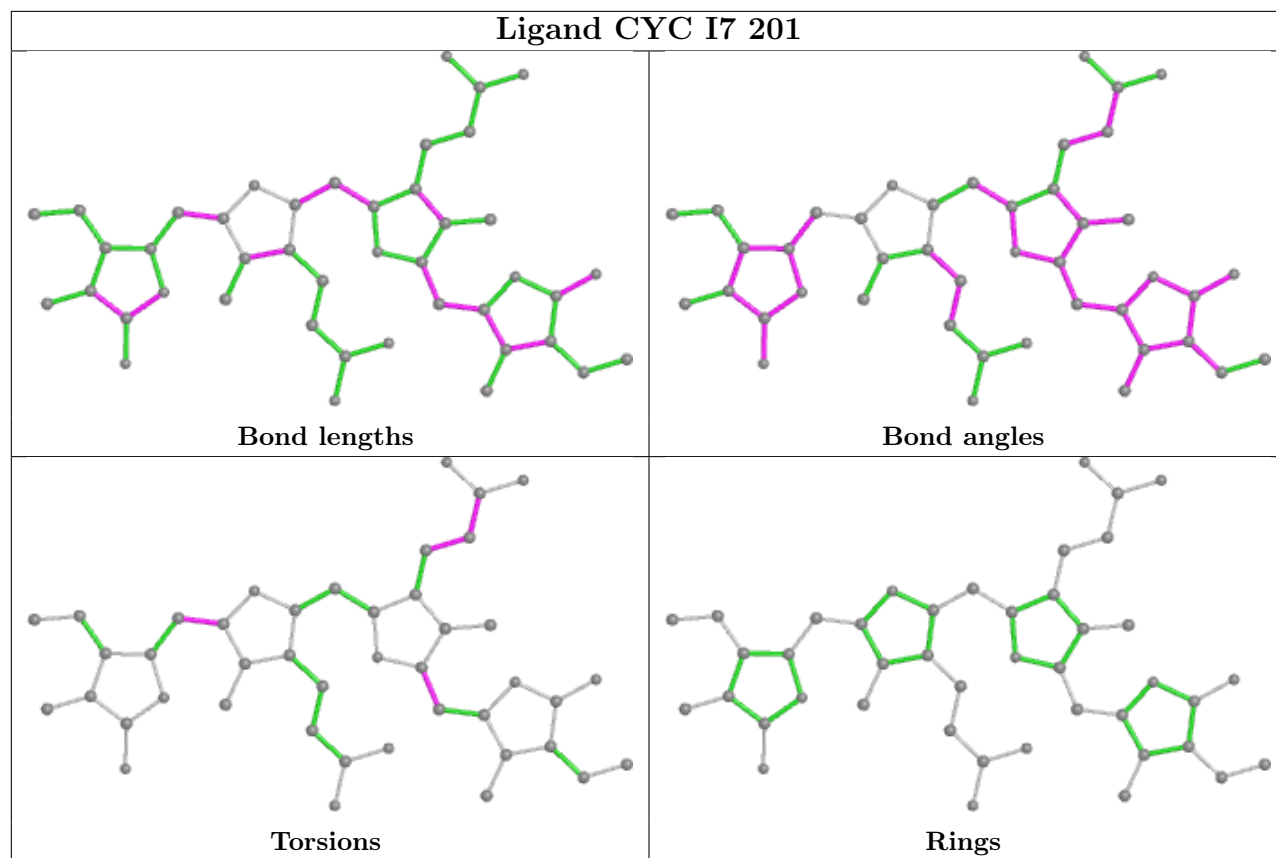


Ligand CYC U8 201

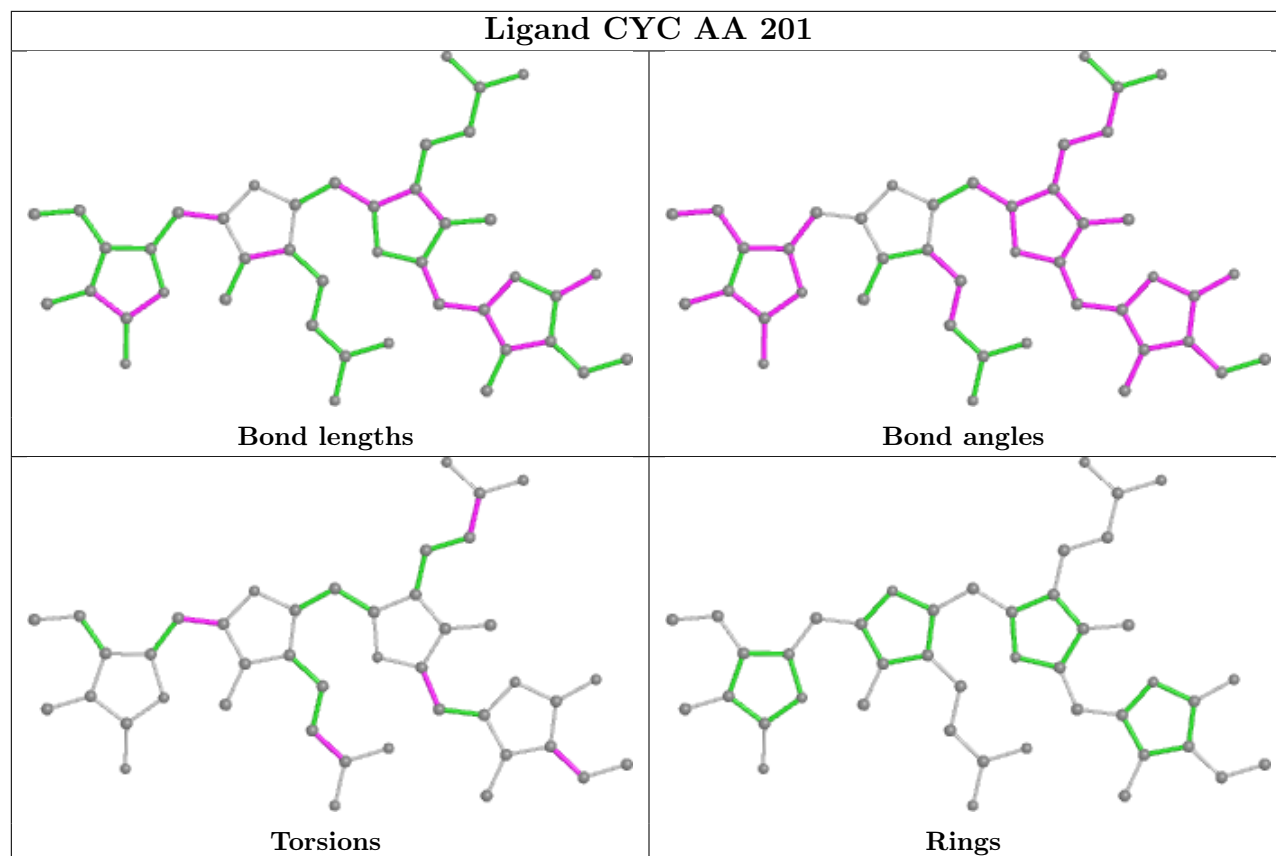


Ligand CYC L7 201

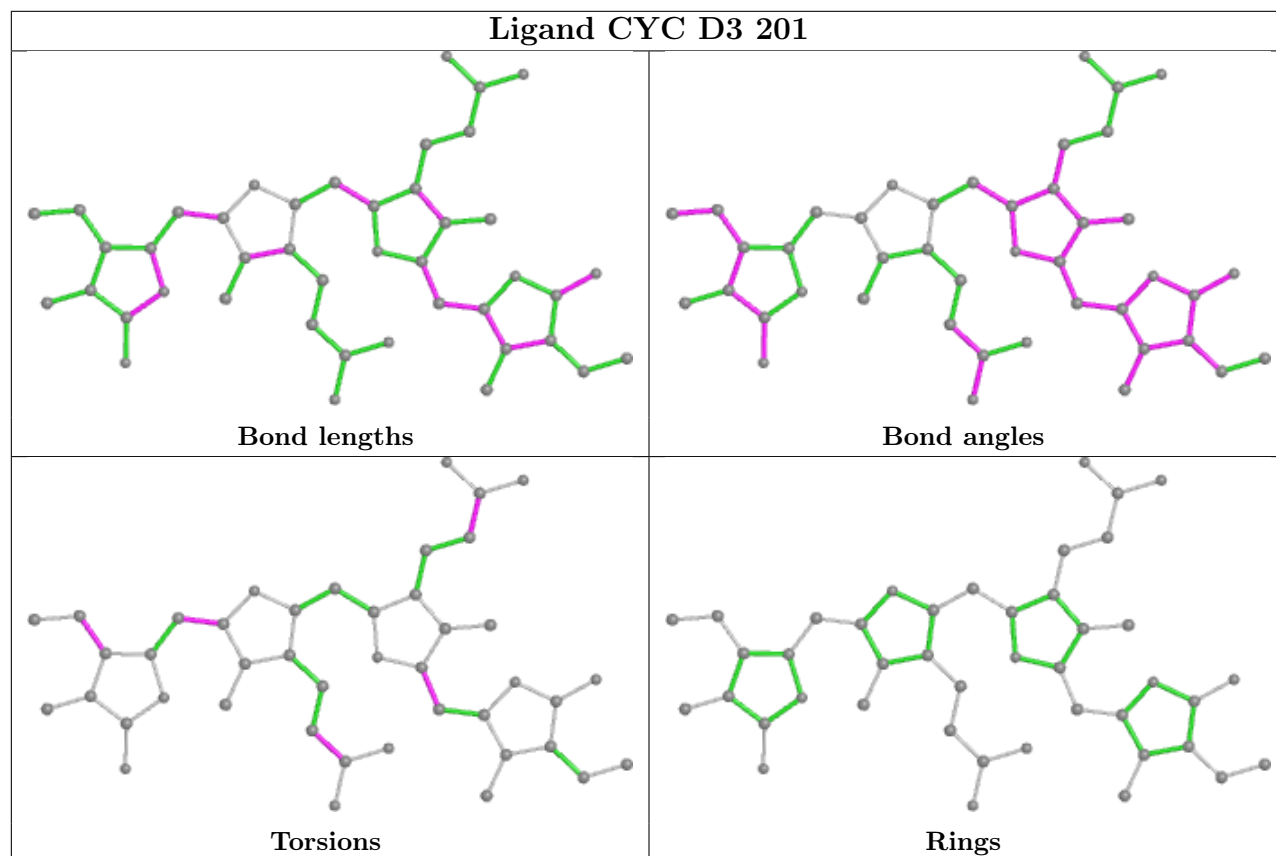




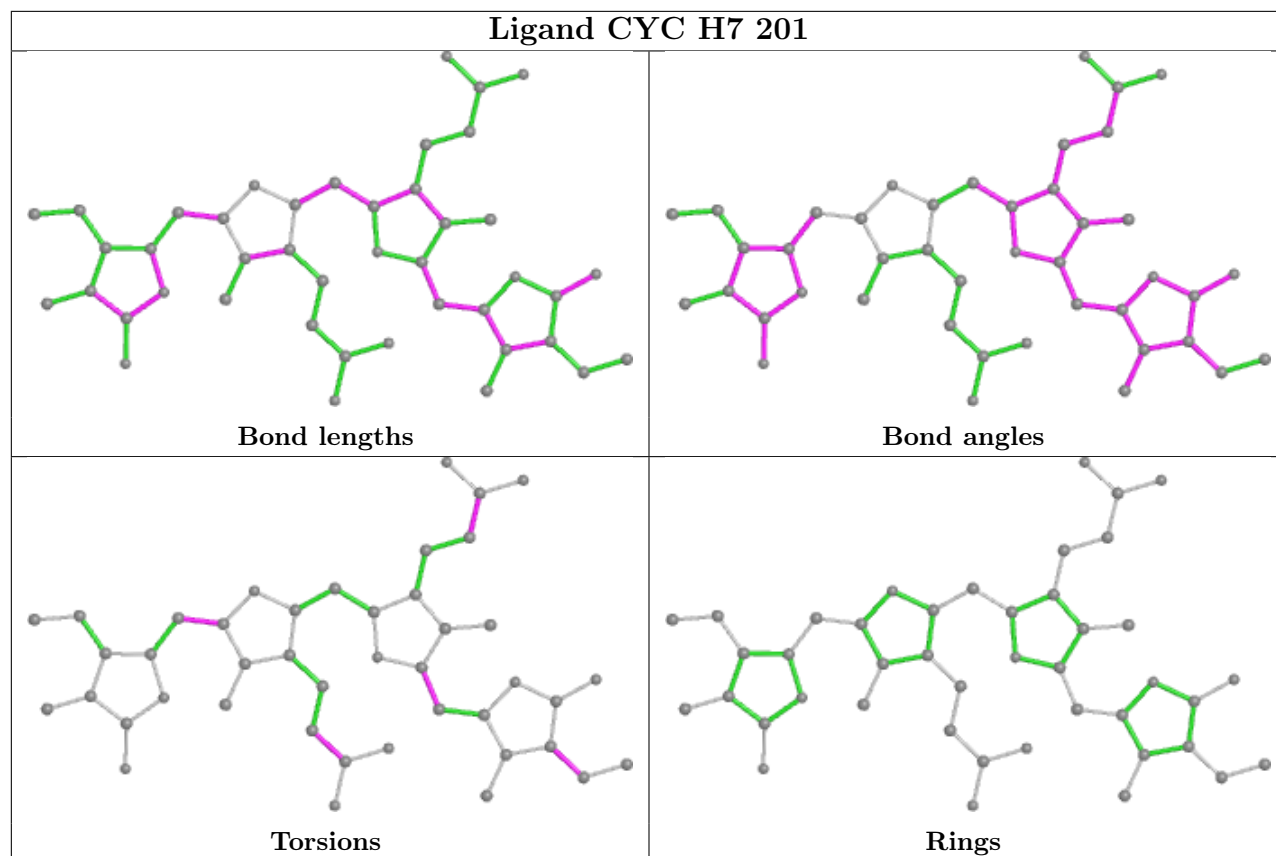
Ligand CYC AA 201



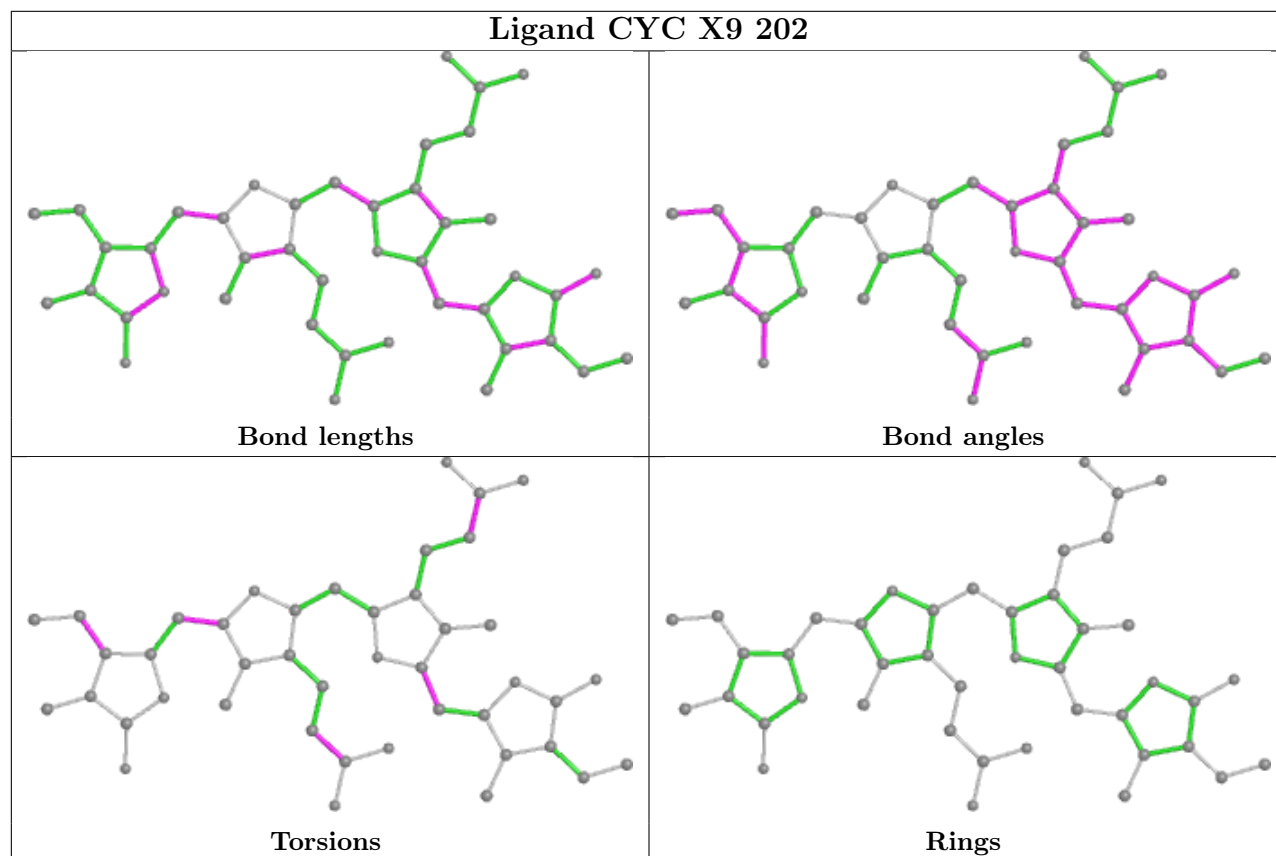
Ligand CYC D3 201



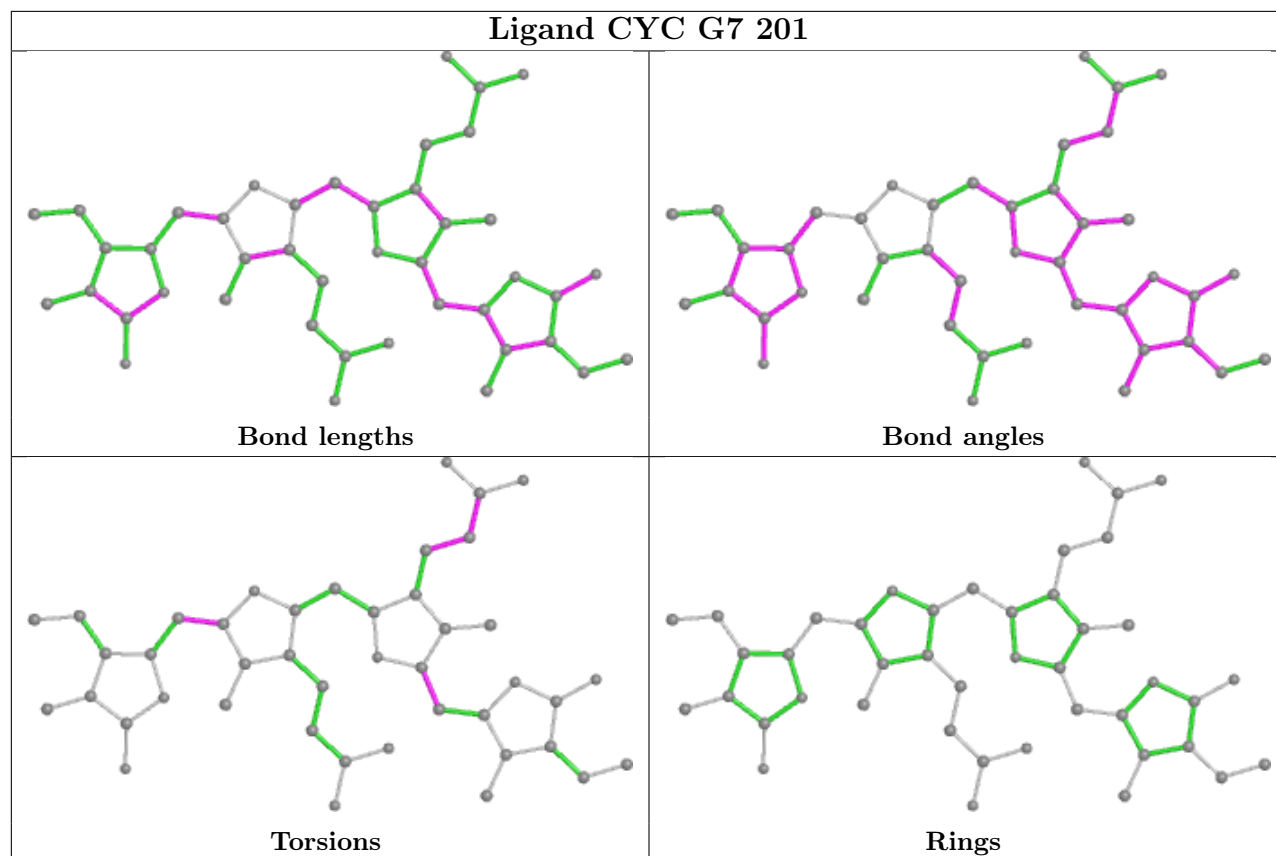
Ligand CYC H7 201



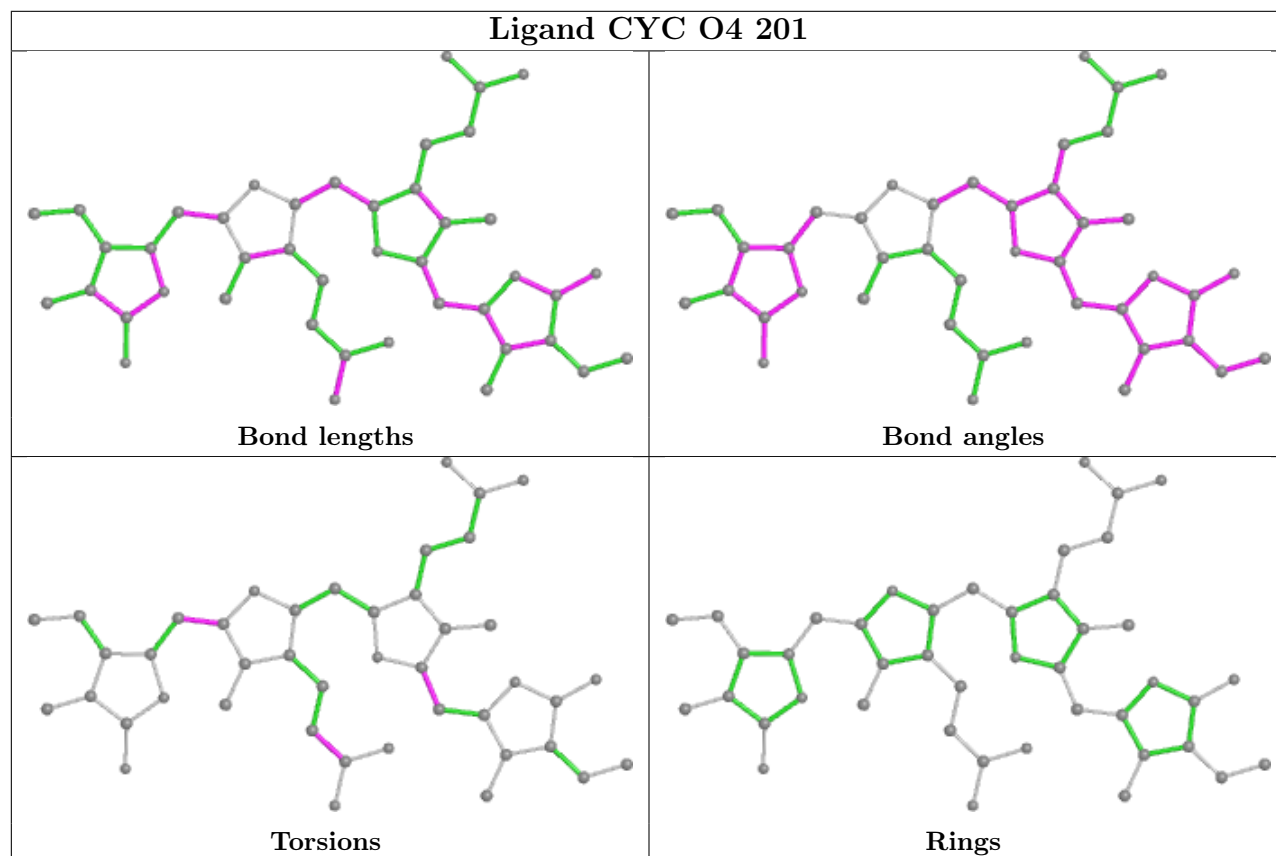
Ligand CYC X9 202



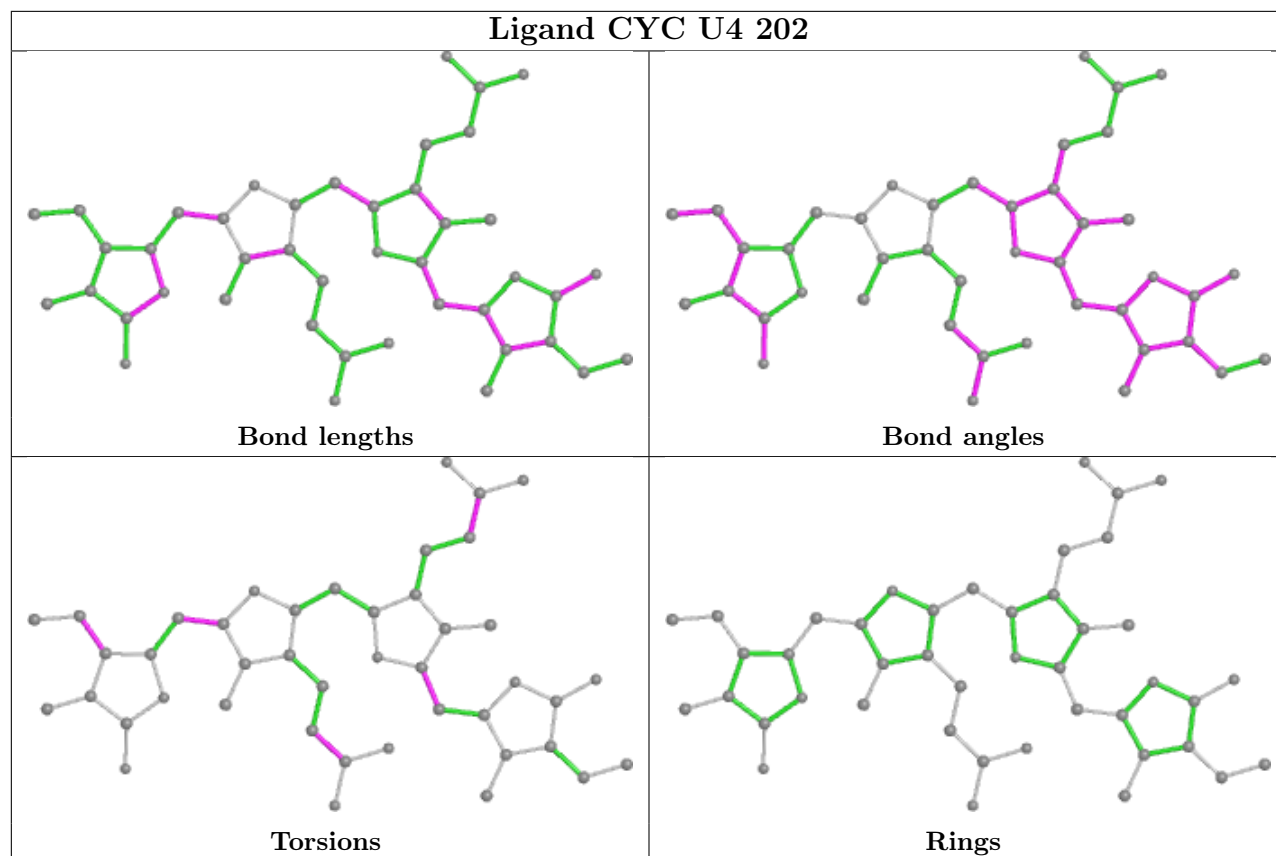
Ligand CYC G7 201



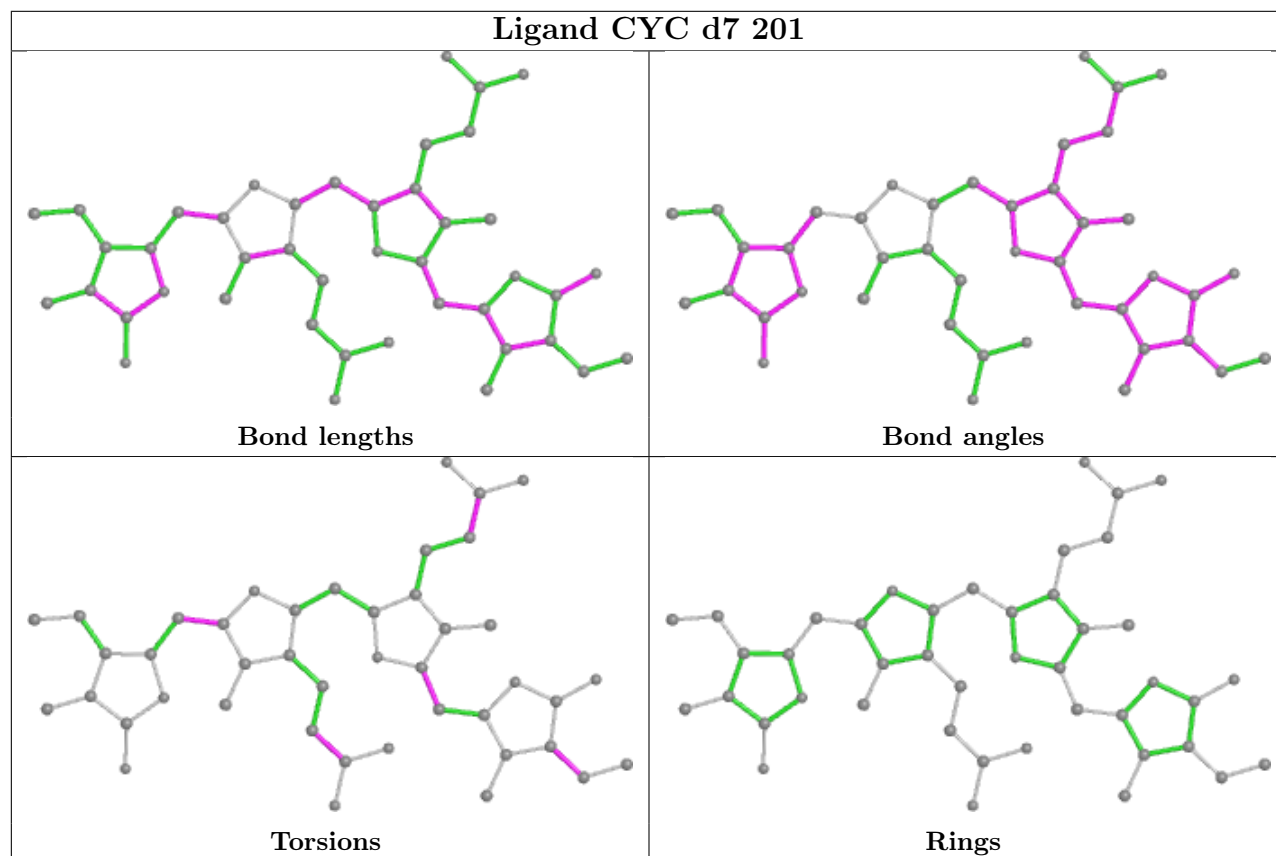
Ligand CYC O4 201



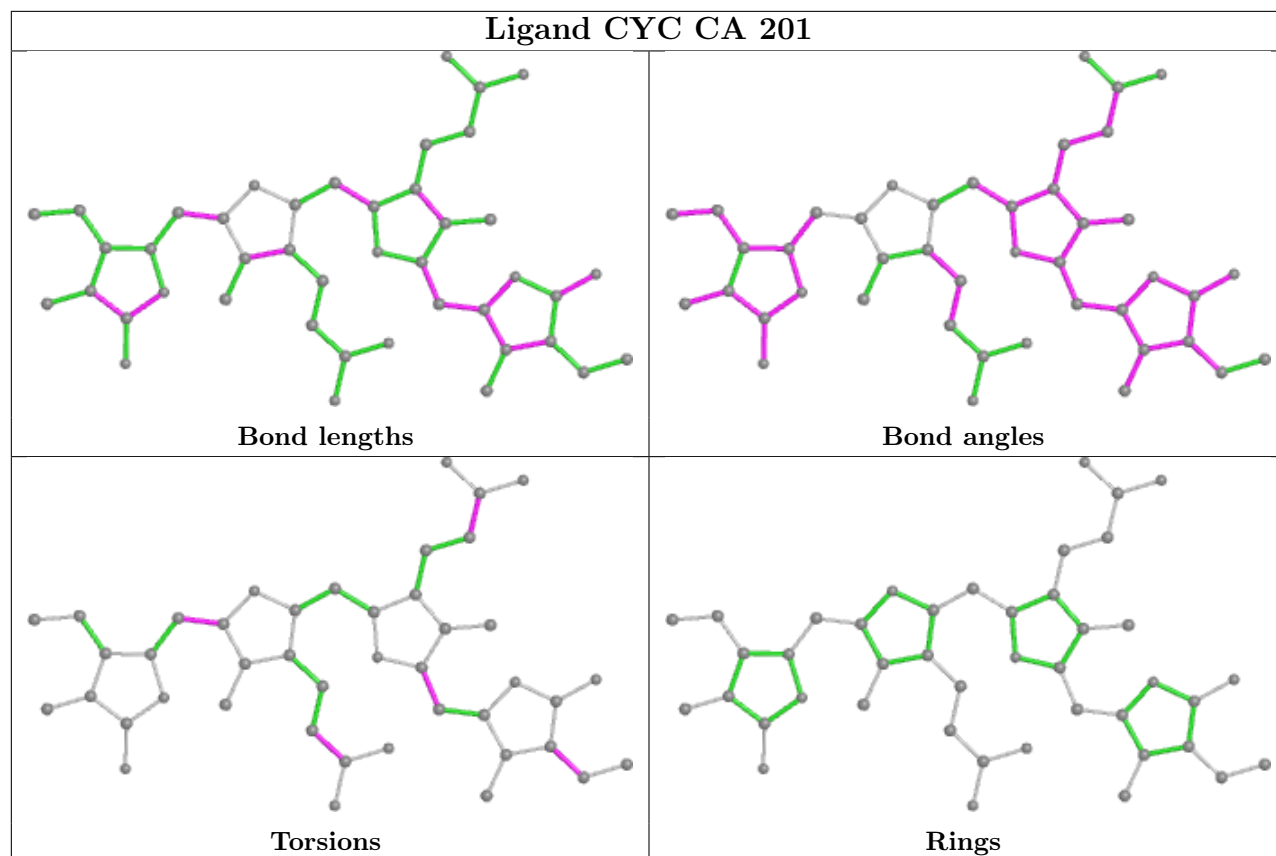
Ligand CYC U4 202



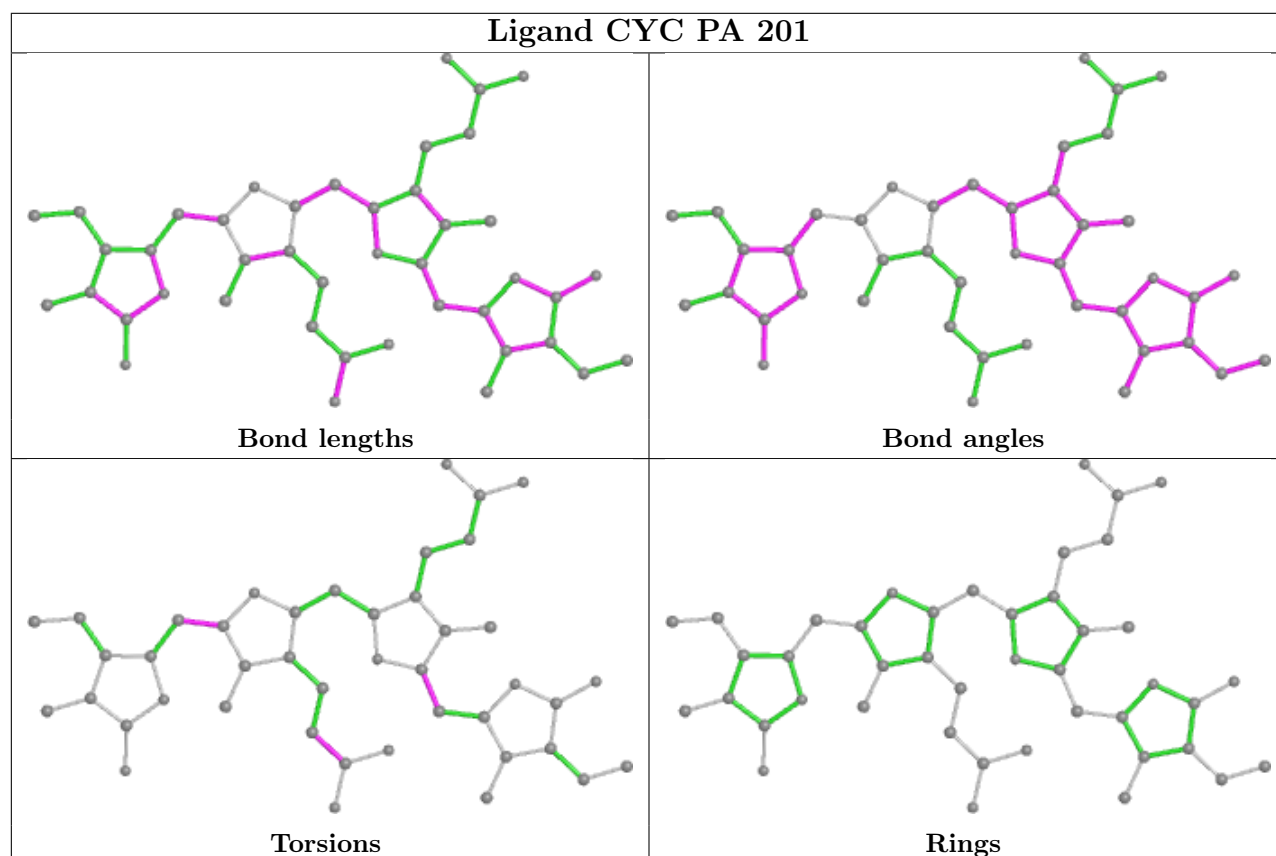
Ligand CYC d7 201



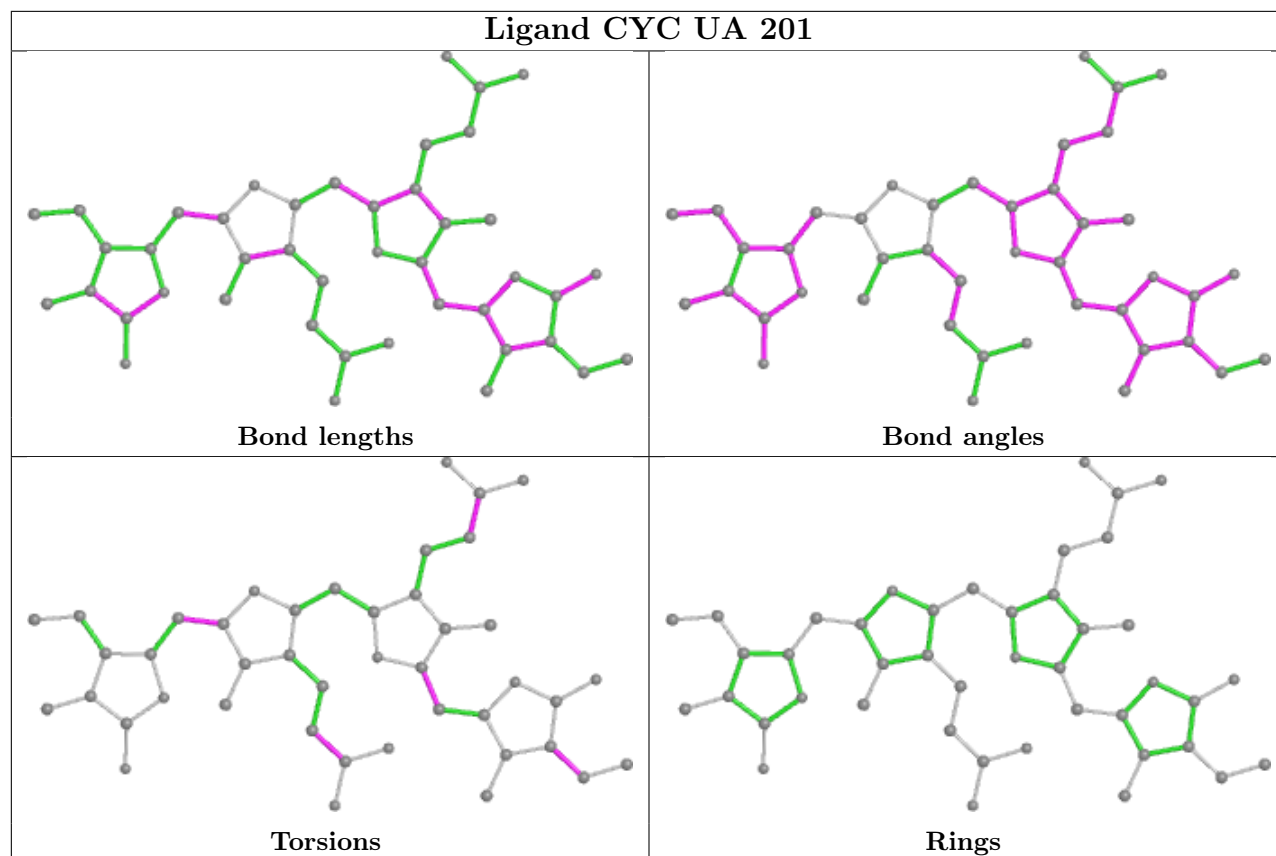
Ligand CYC CA 201



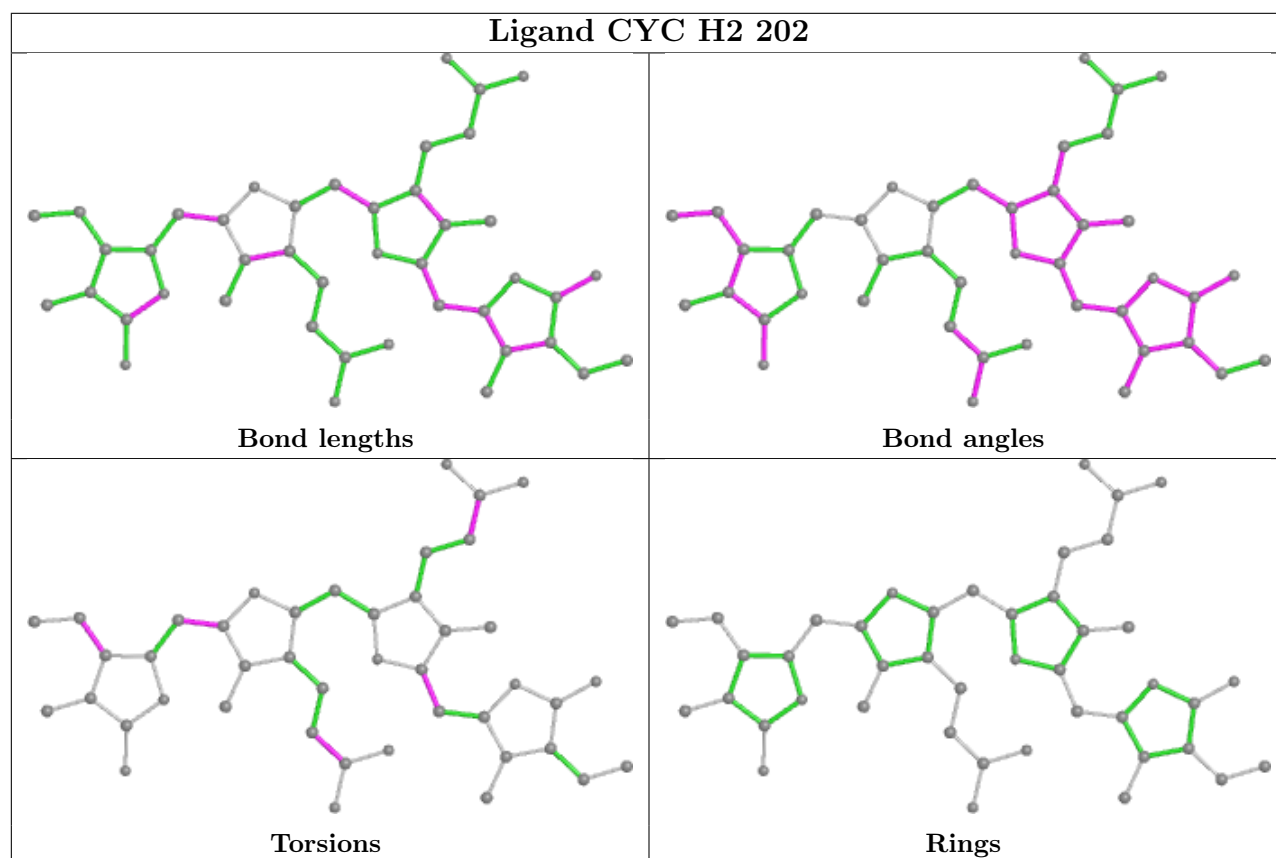
Ligand CYC PA 201



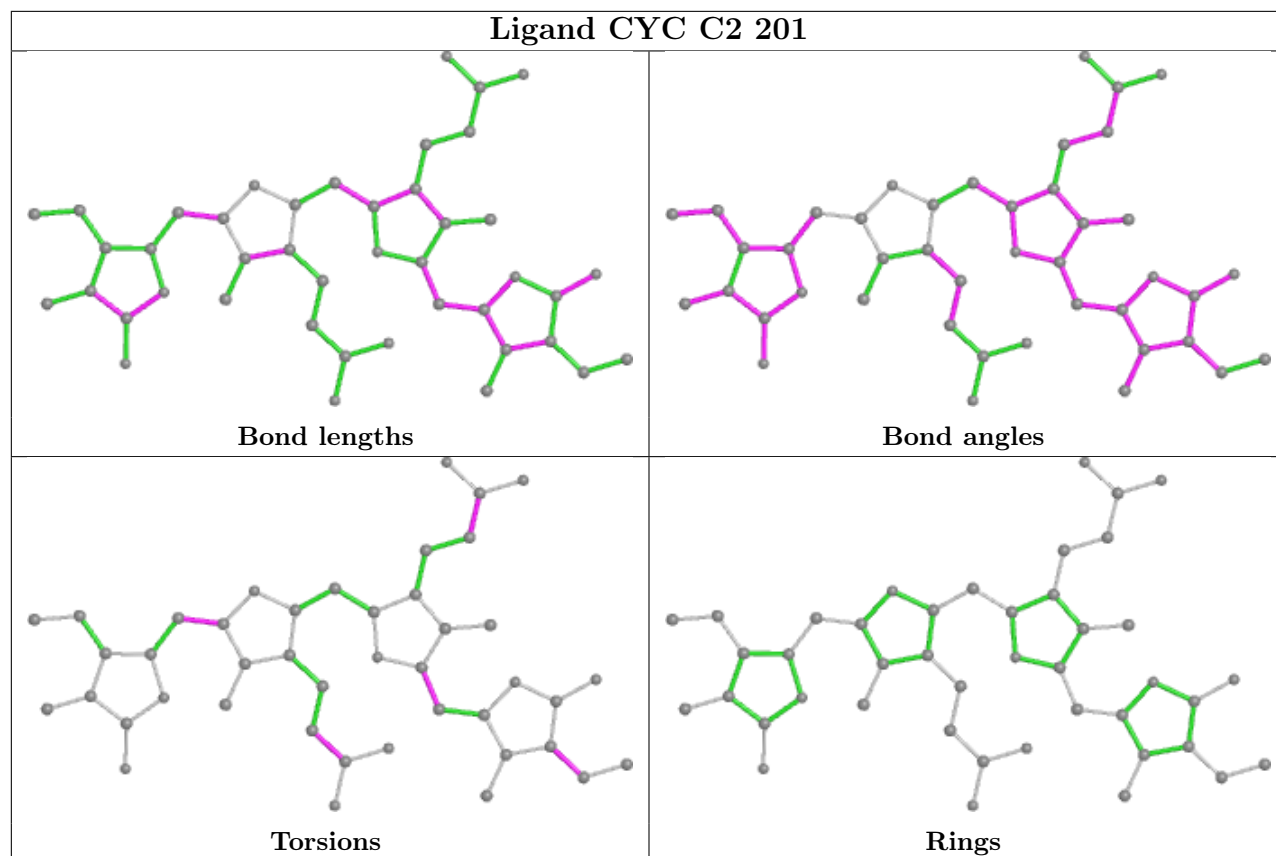
Ligand CYC UA 201



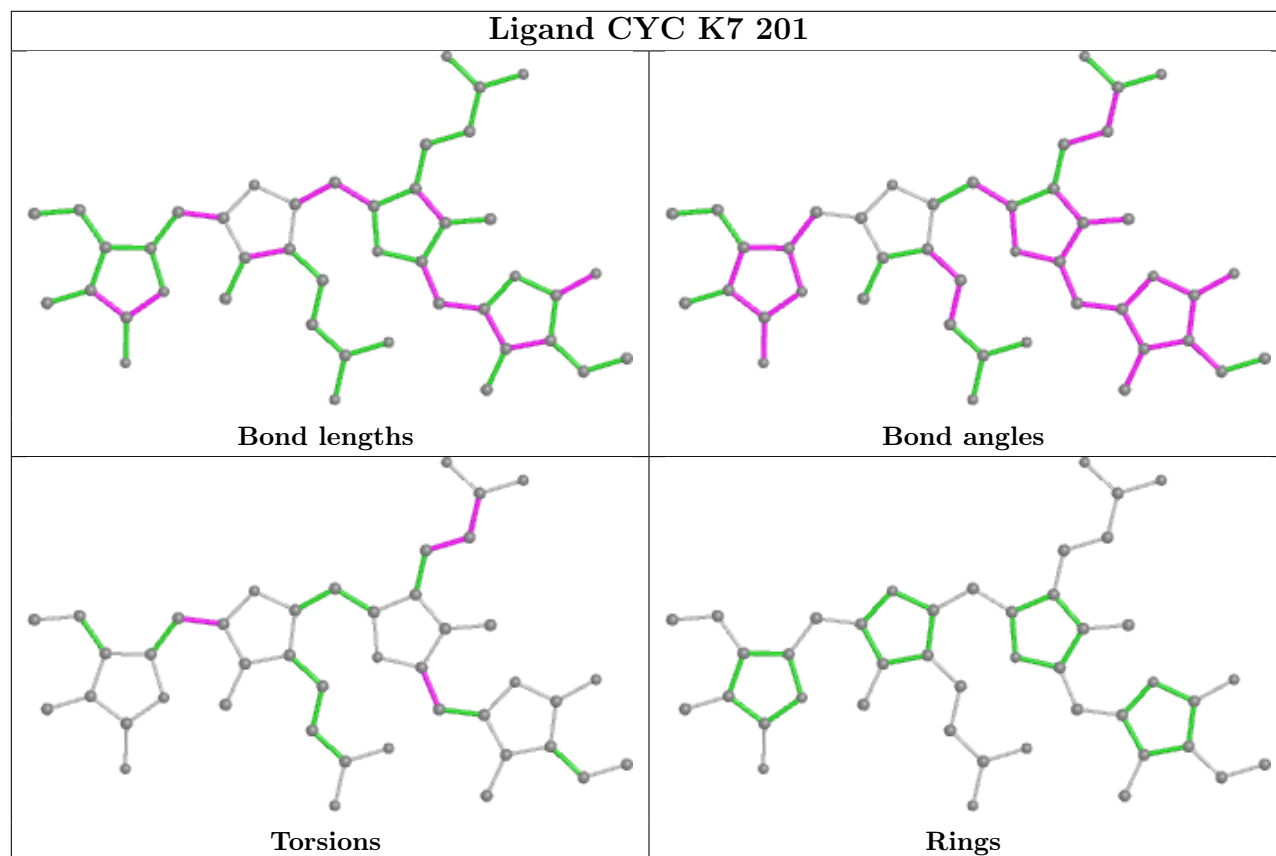
Ligand CYC H2 202



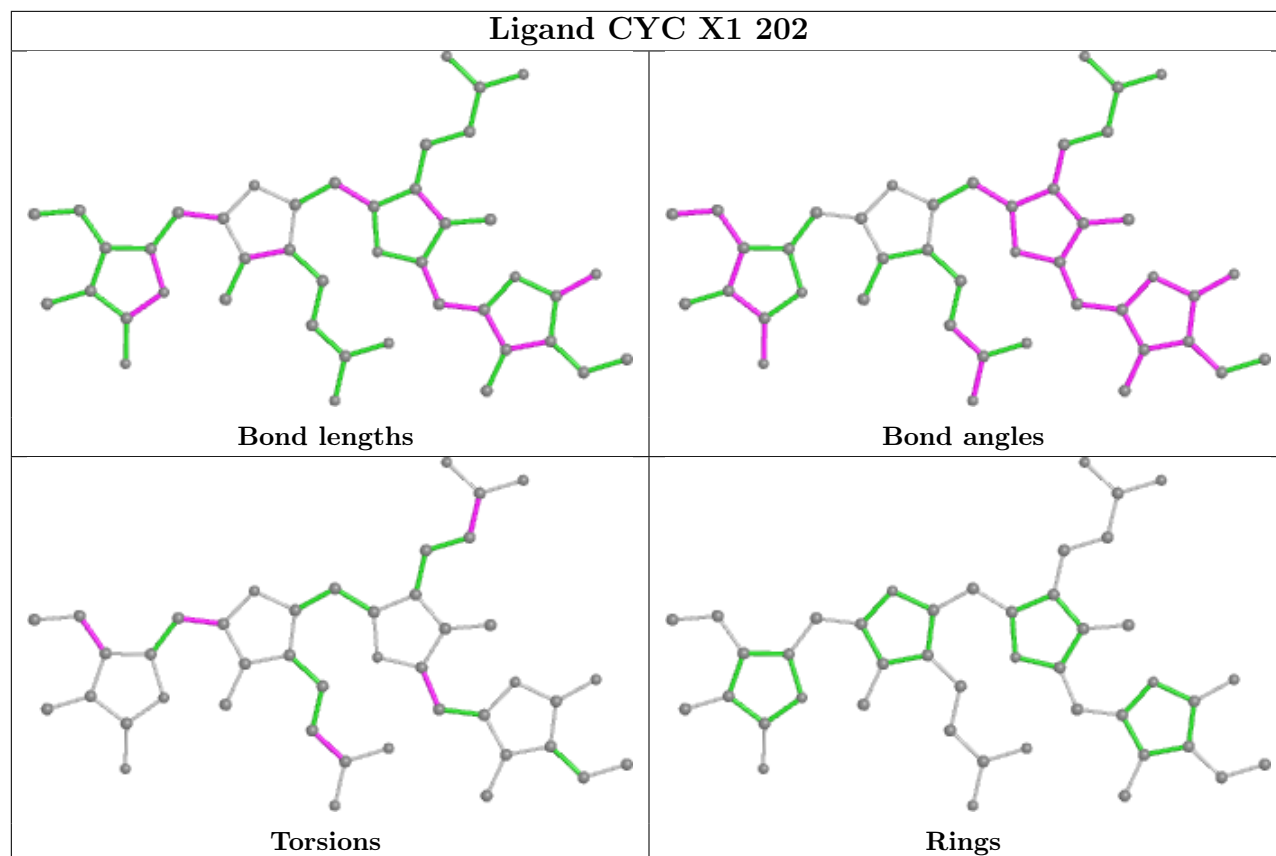
Ligand CYC C2 201



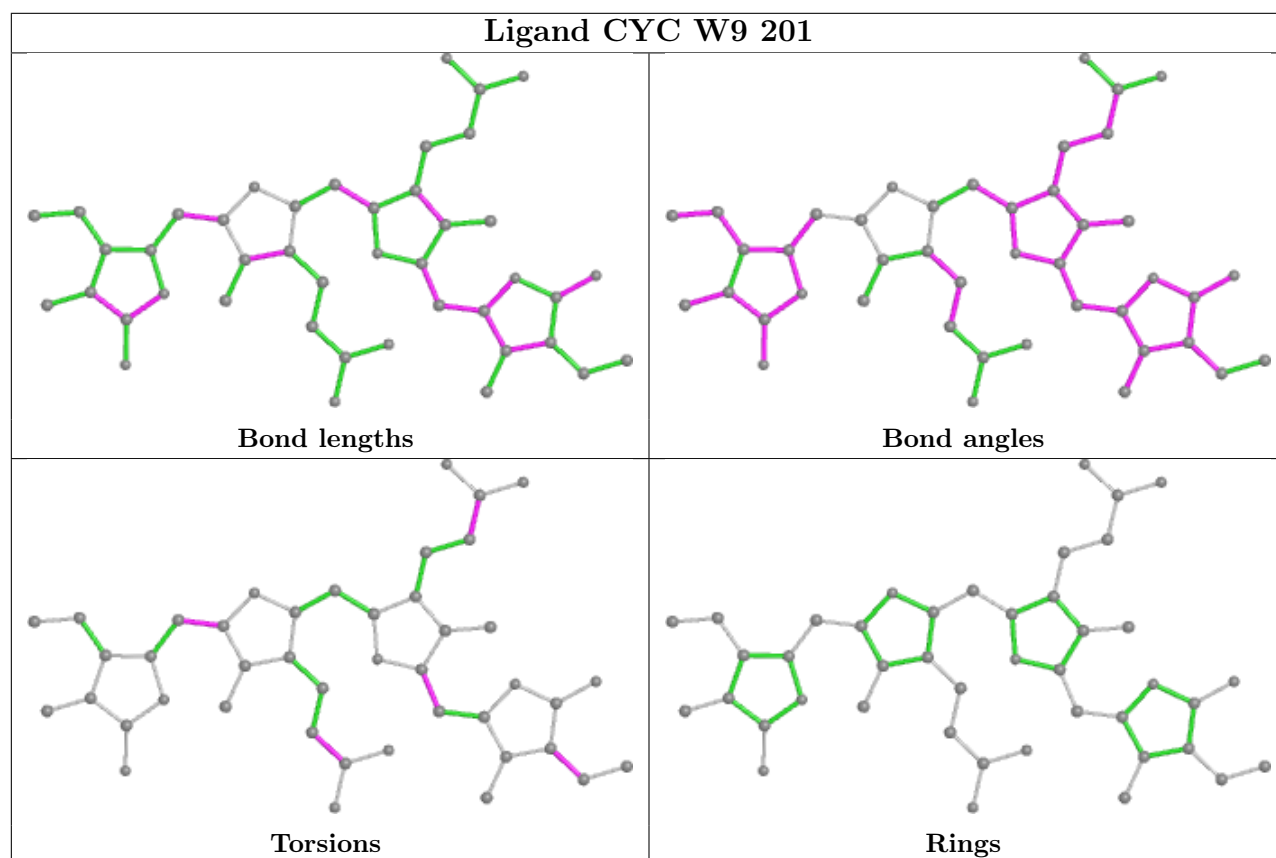
Ligand CYC K7 201



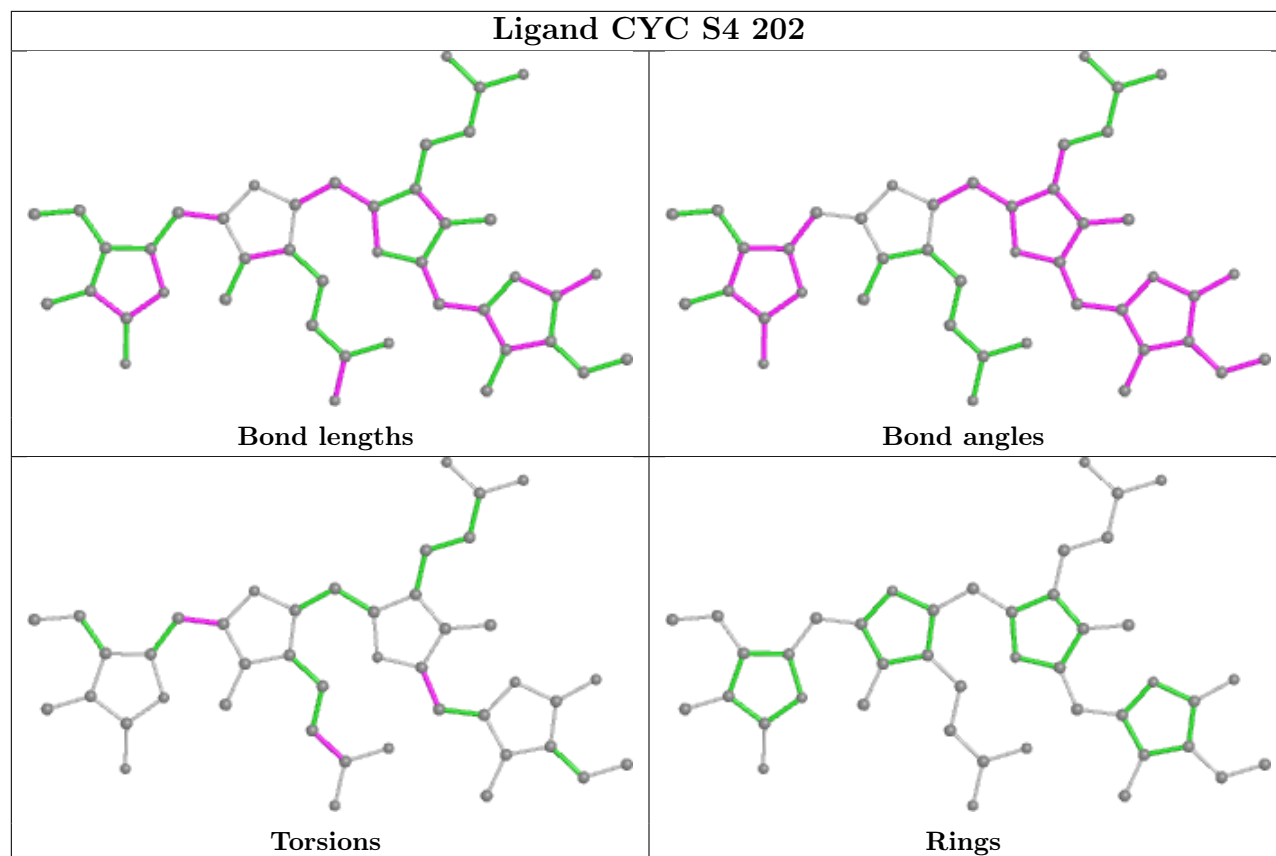
Ligand CYC X1 202



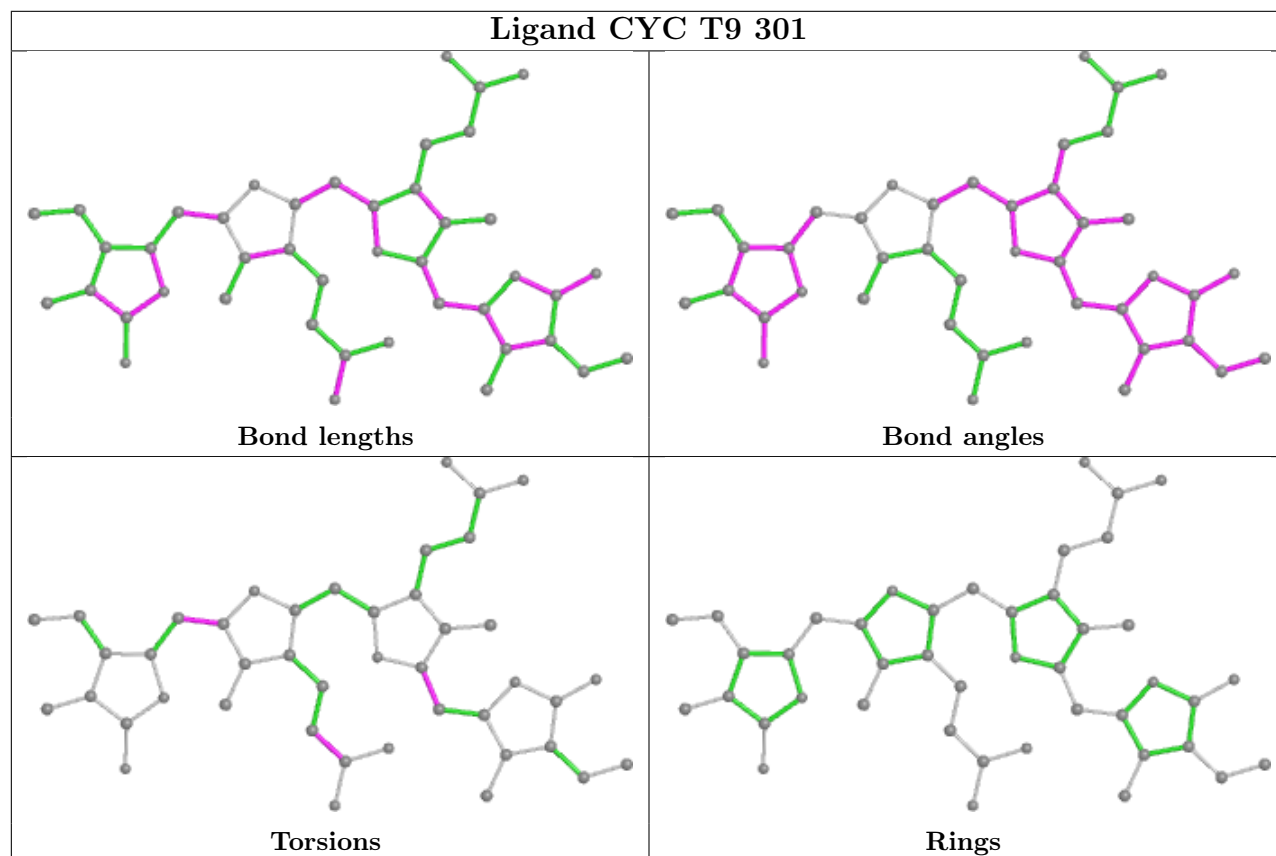
Ligand CYC W9 201



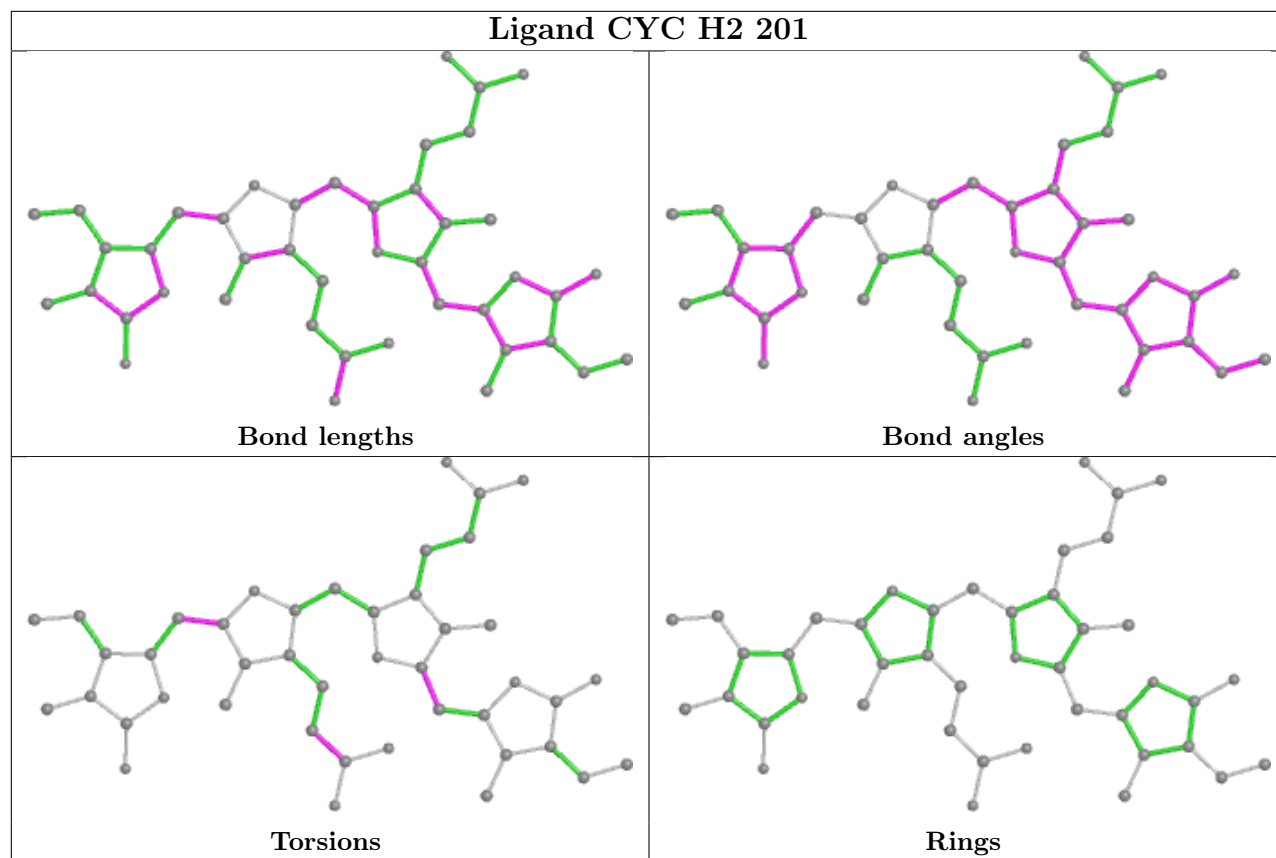
Ligand CYC S4 202



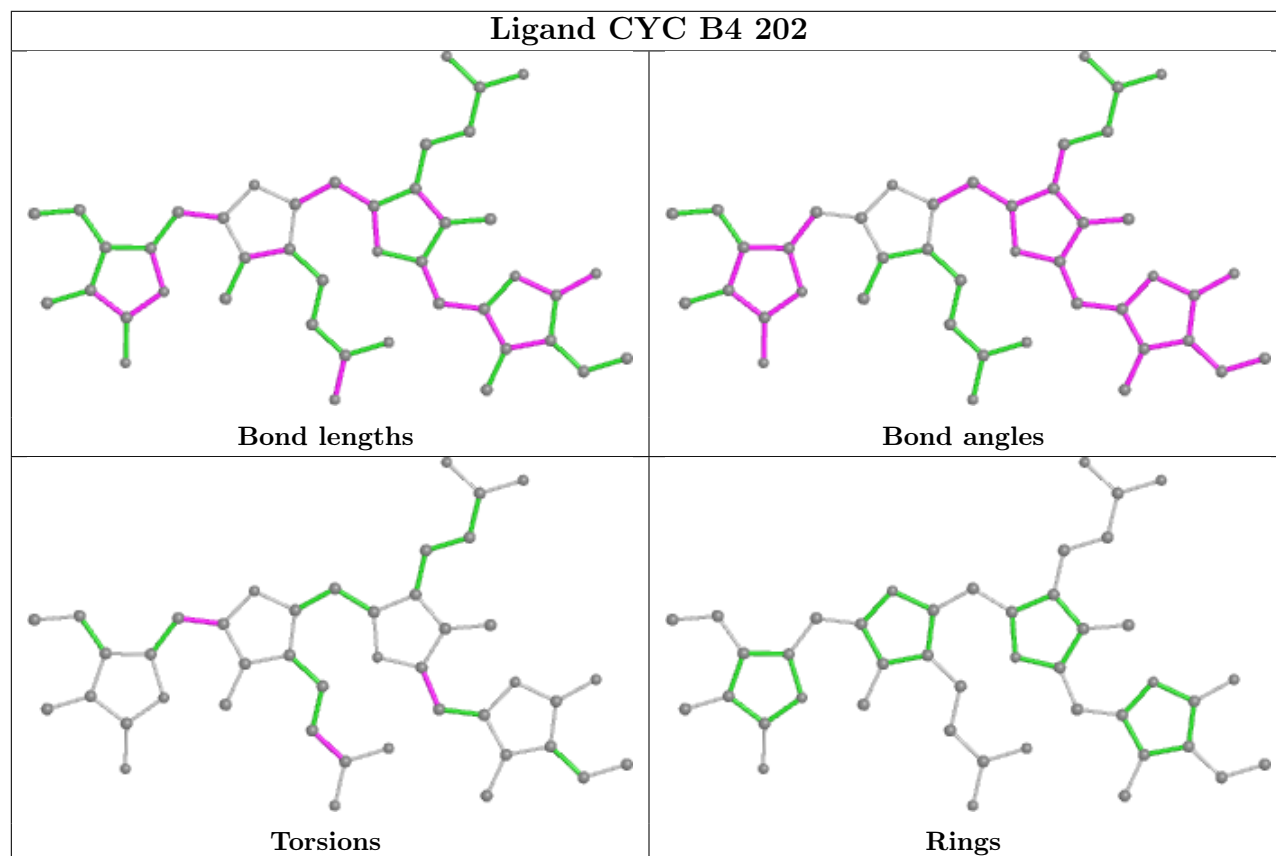
Ligand CYC T9 301

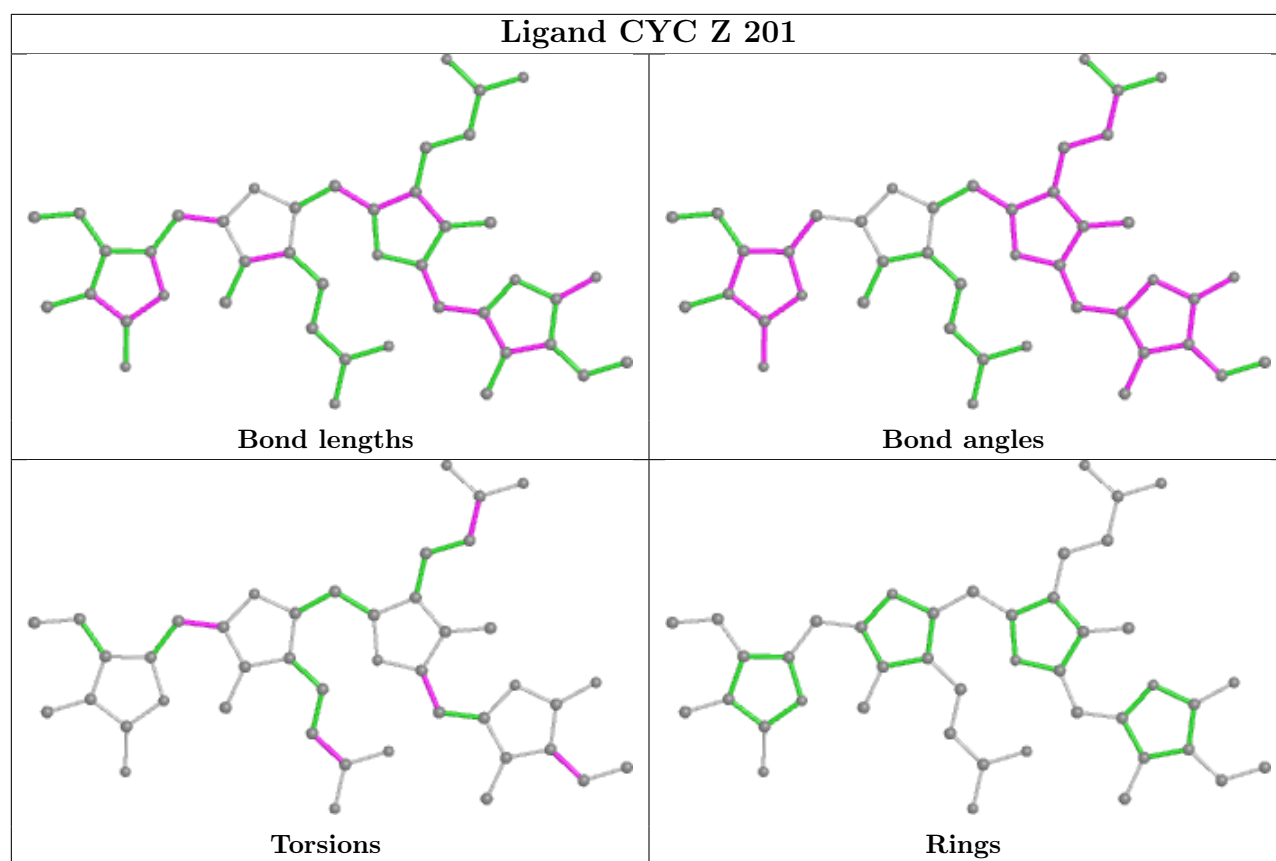


Ligand CYC H2 201



Ligand CYC B4 202





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

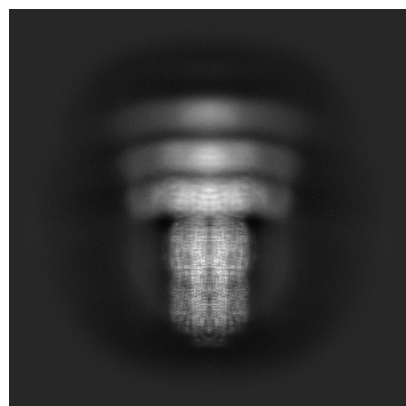
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62201. These allow visual inspection of the internal detail of the map and identification of artifacts.

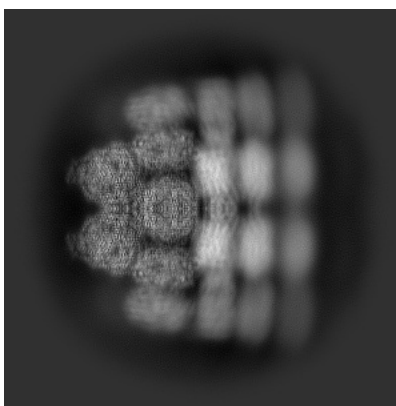
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

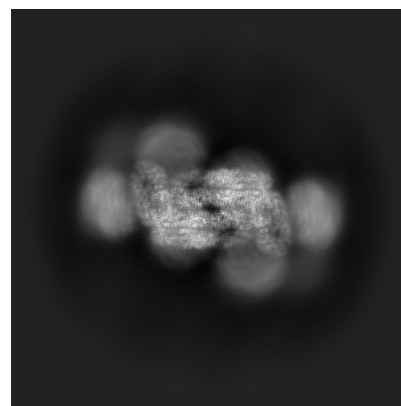
6.1.1 Primary map



X

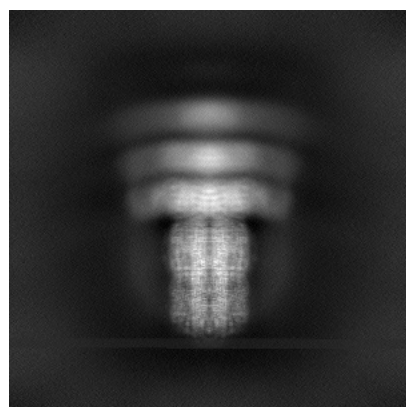


Y

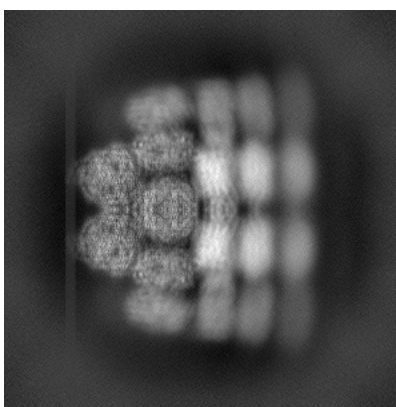


Z

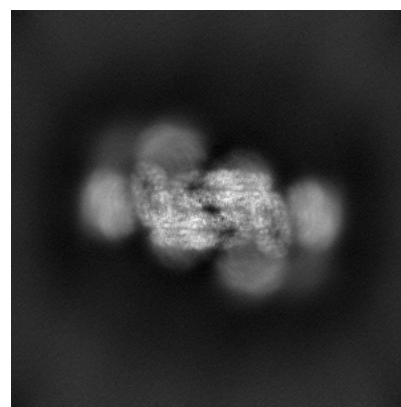
6.1.2 Raw map



X



Y

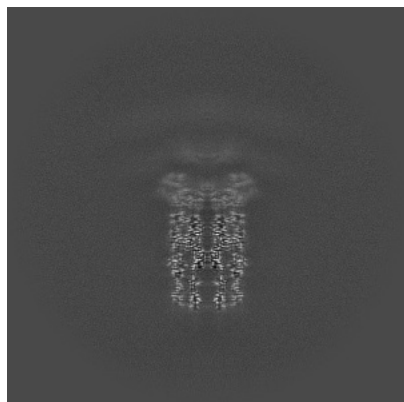


Z

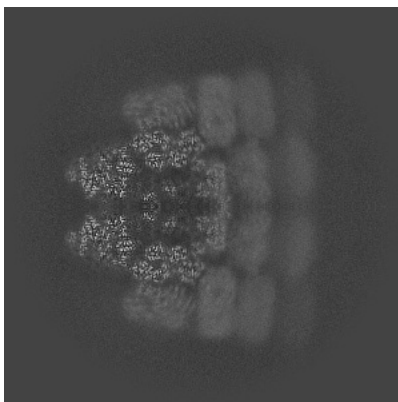
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

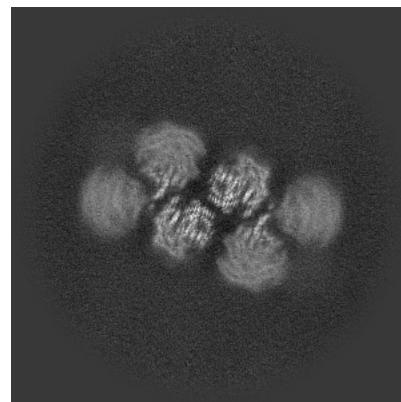
6.2.1 Primary map



X Index: 280

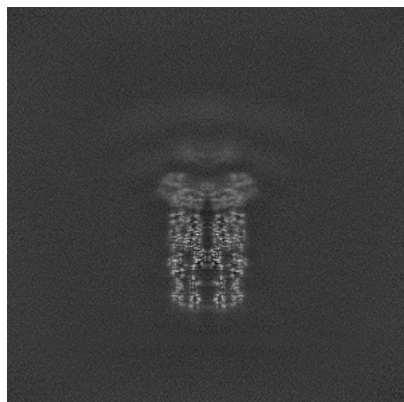


Y Index: 280

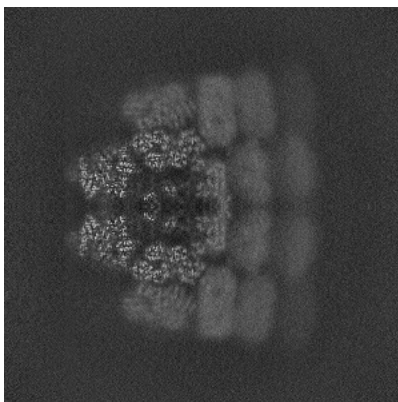


Z Index: 280

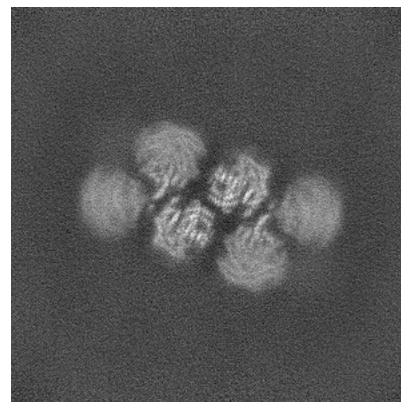
6.2.2 Raw map



X Index: 280



Y Index: 280



Z Index: 280

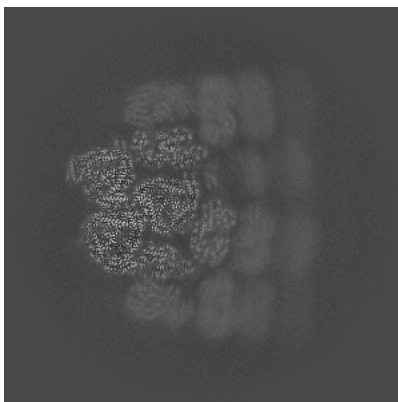
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

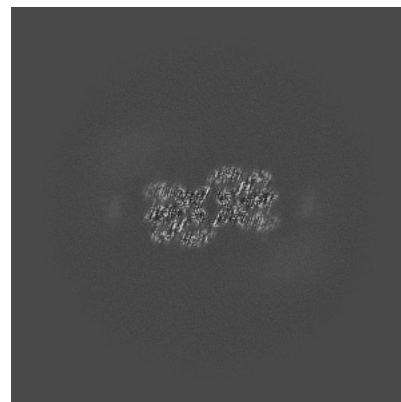
6.3.1 Primary map



X Index: 259



Y Index: 265

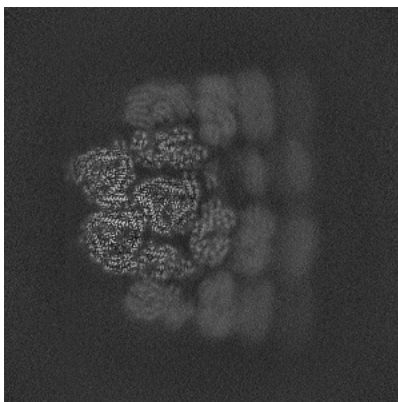


Z Index: 166

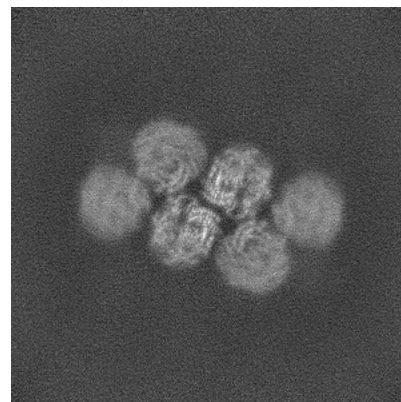
6.3.2 Raw map



X Index: 258



Y Index: 265

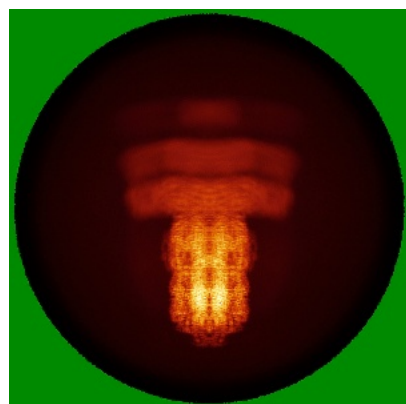


Z Index: 290

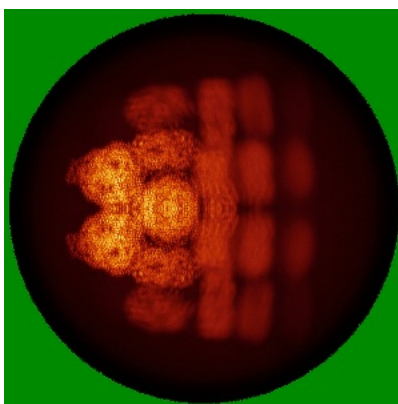
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

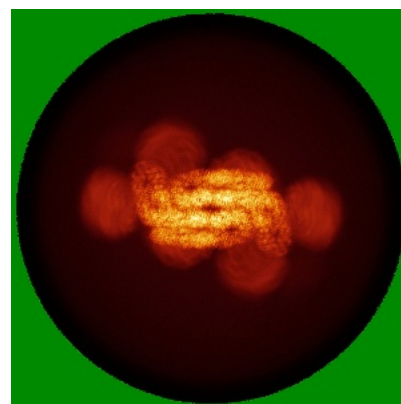
6.4.1 Primary map



X

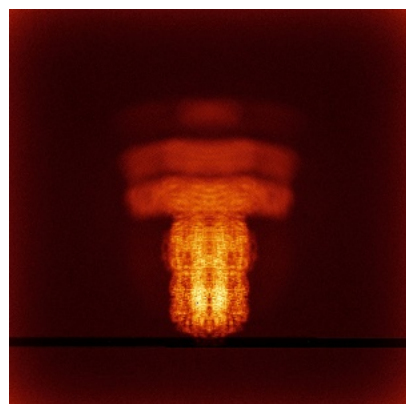


Y

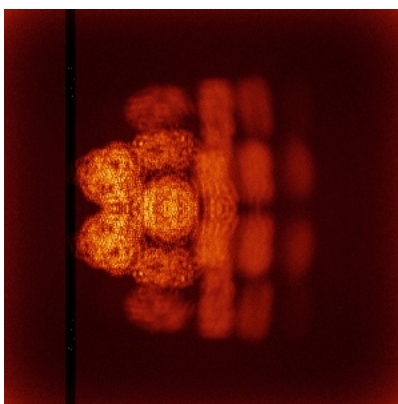


Z

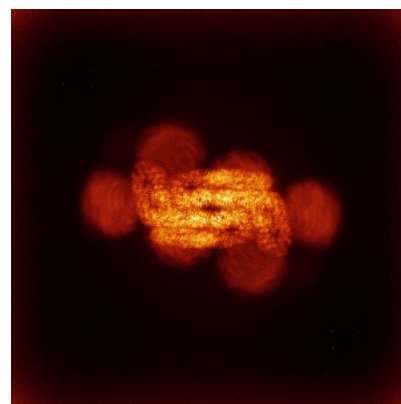
6.4.2 Raw map



X



Y

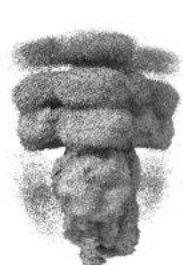


Z

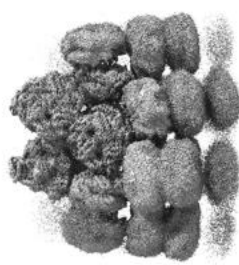
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

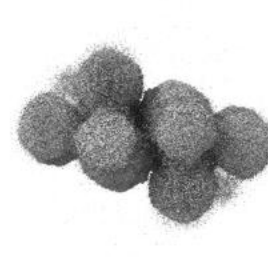
6.5.1 Primary map



X



Y



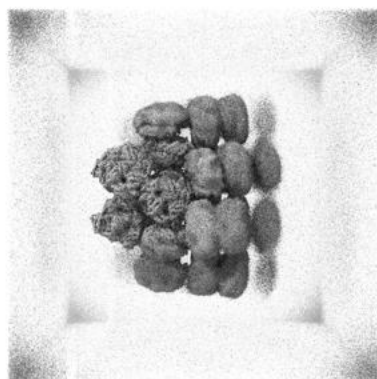
Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

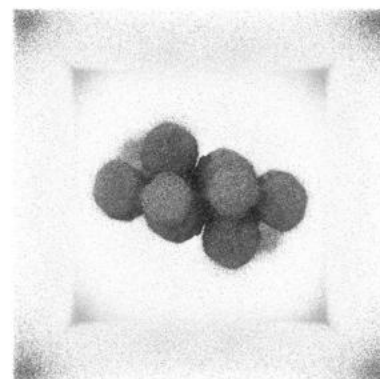
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

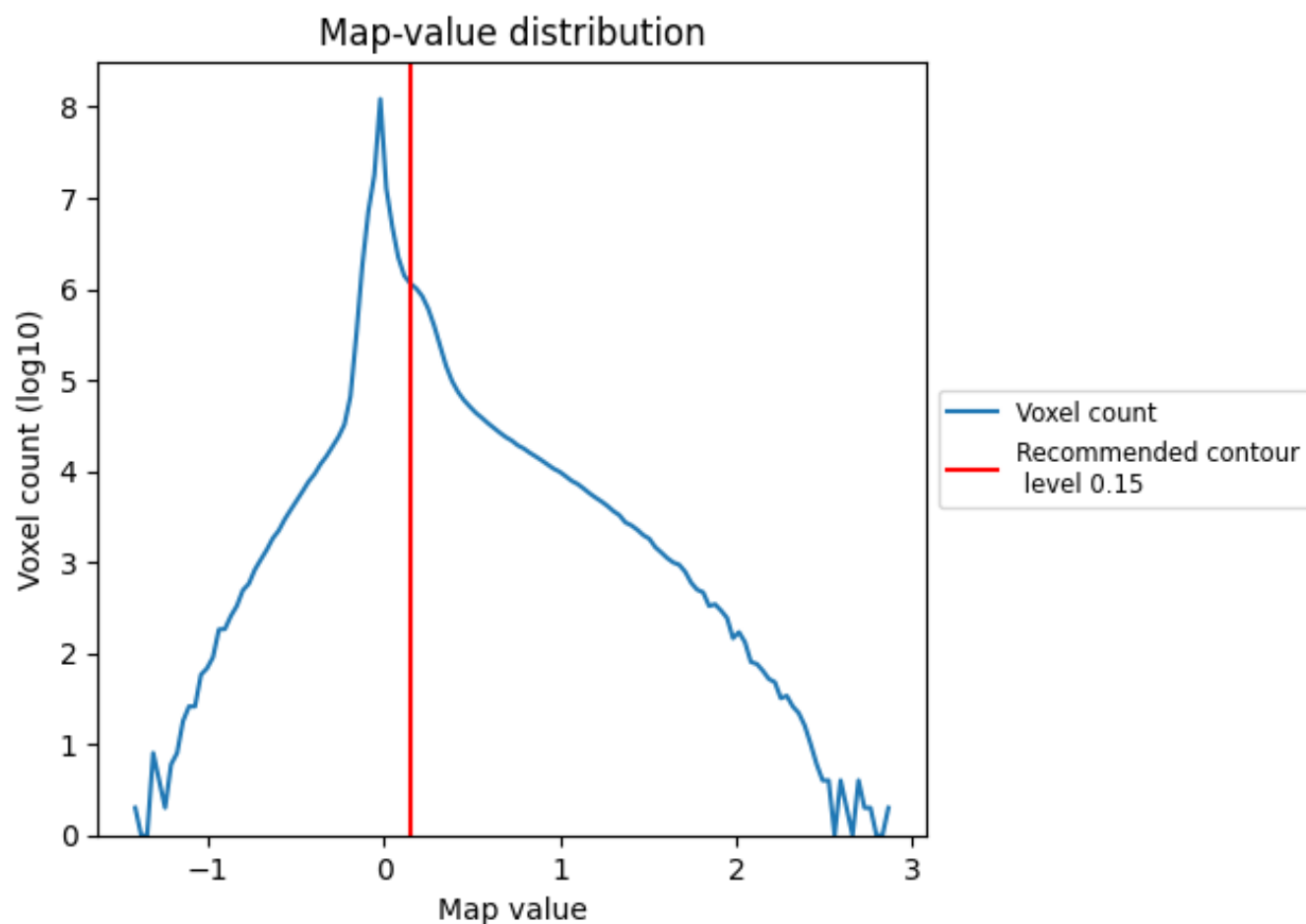
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

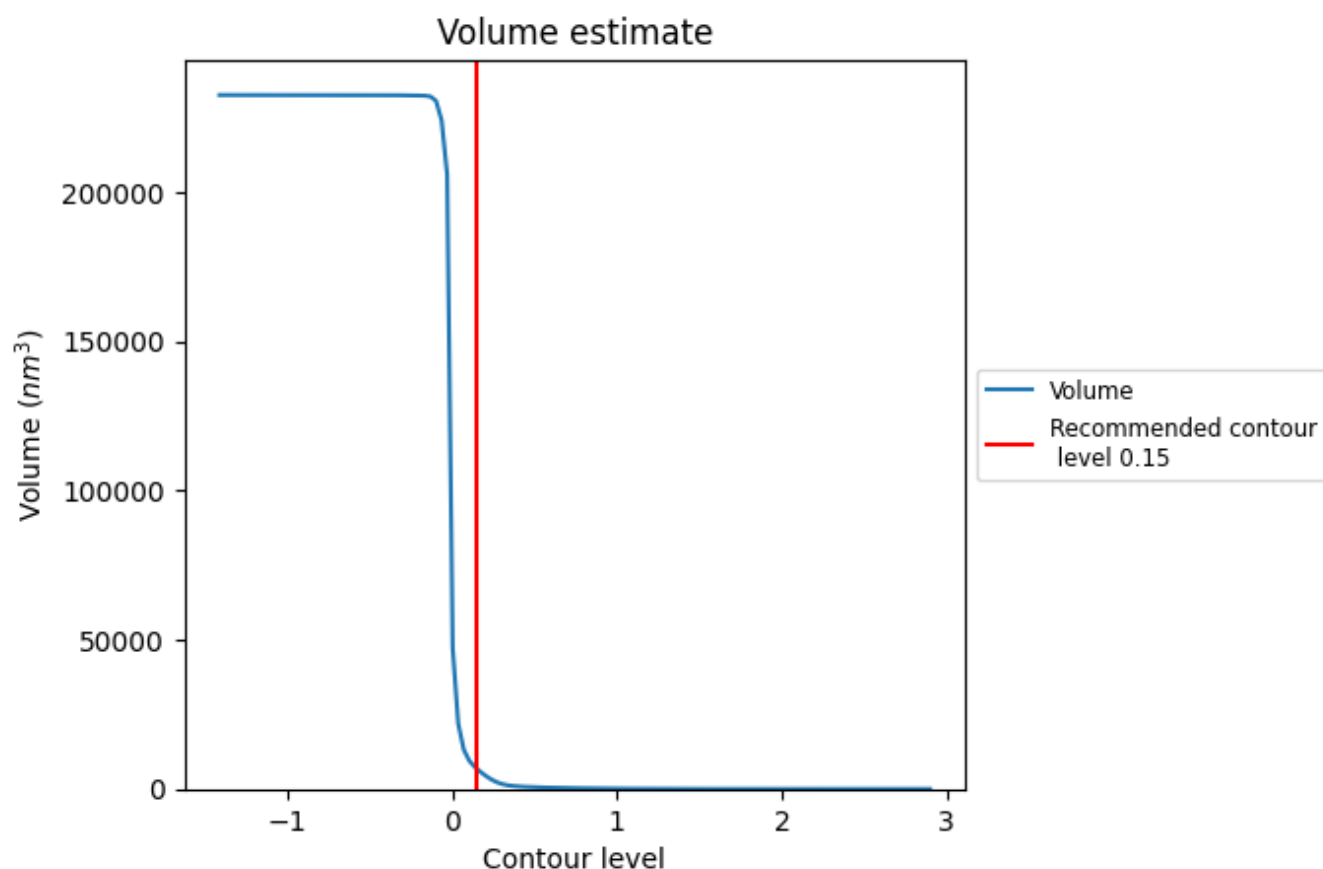
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

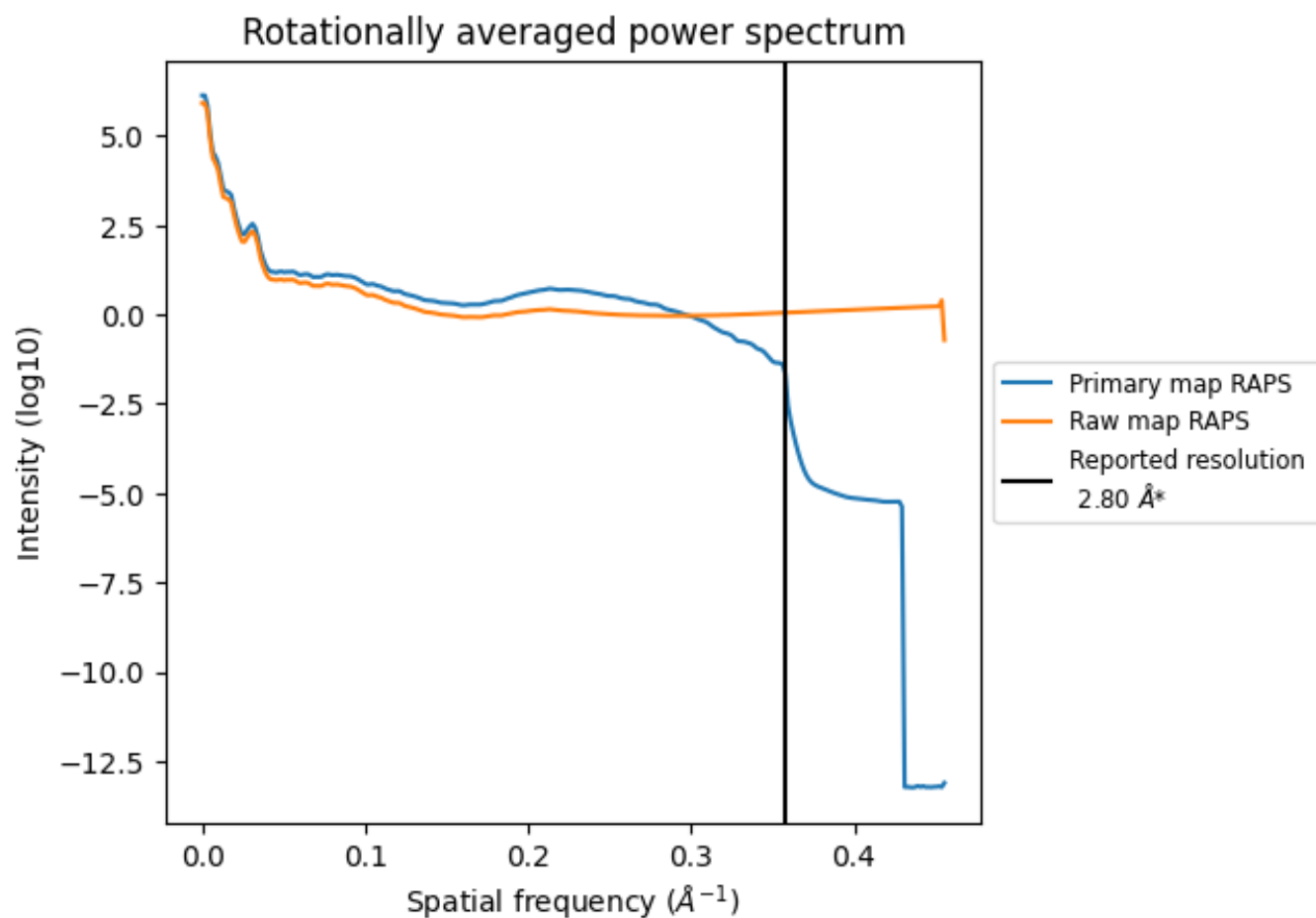
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6773 nm³; this corresponds to an approximate mass of 6118 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

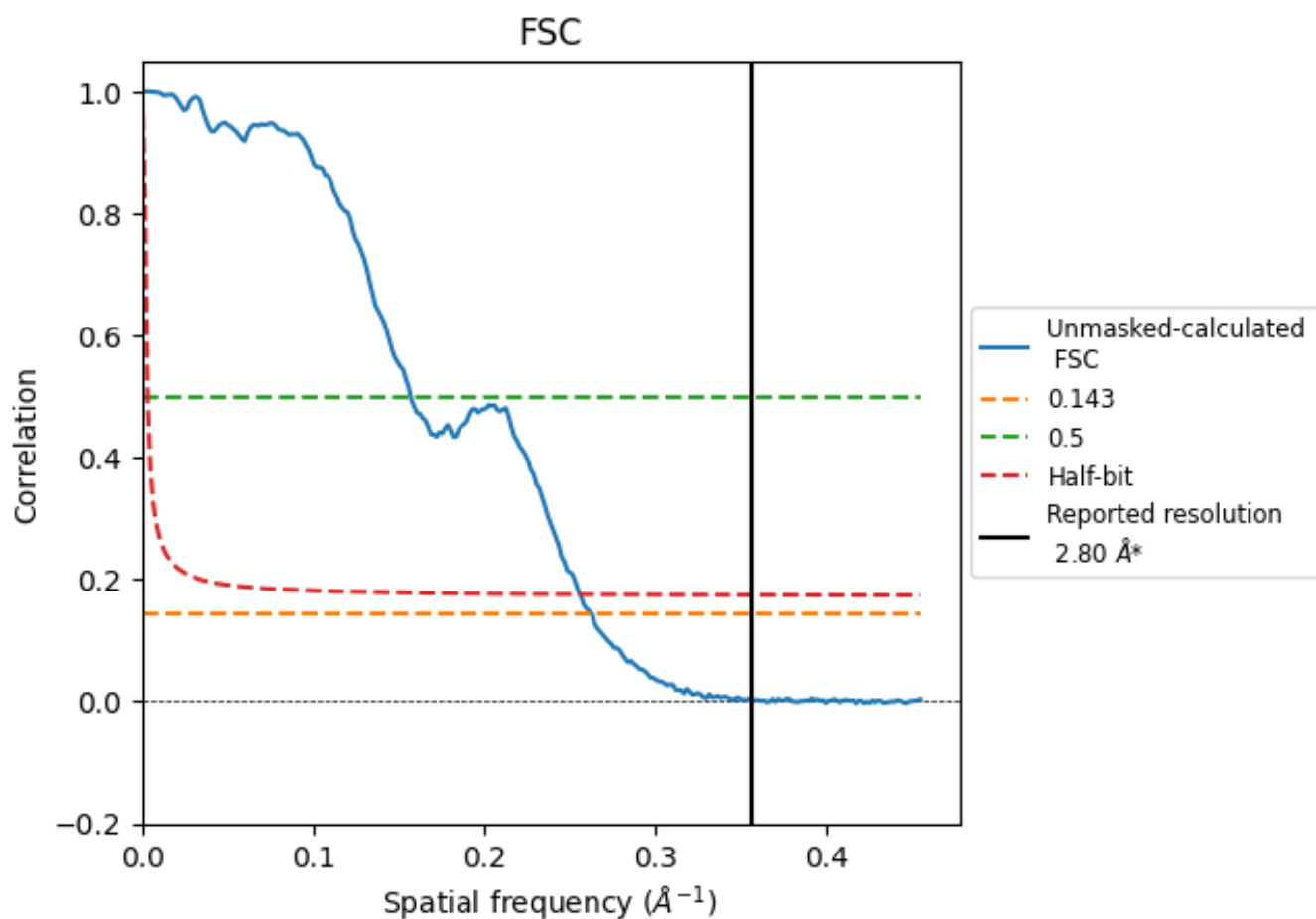


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

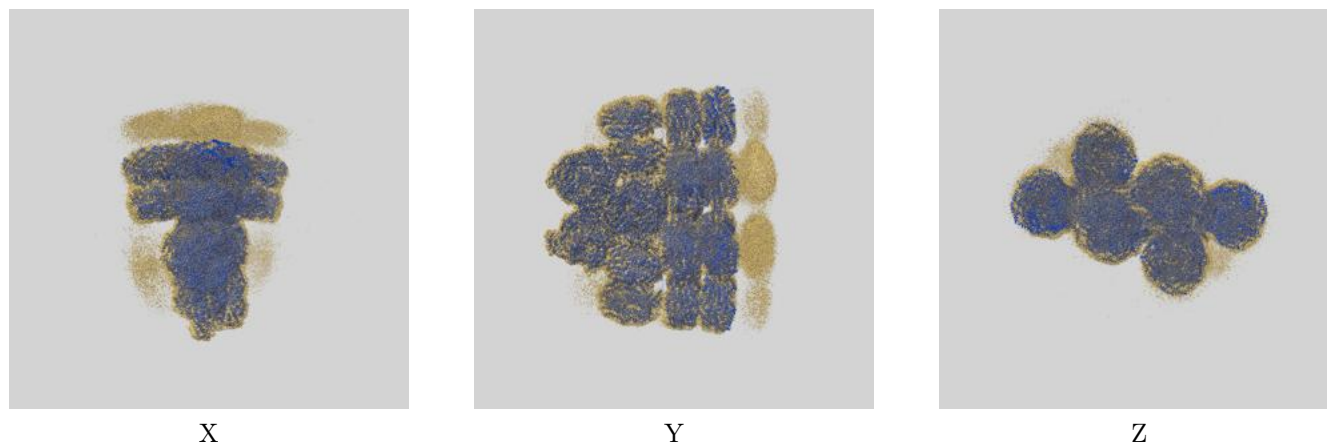
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.80 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 3.80 | 6.36 | 3.90 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

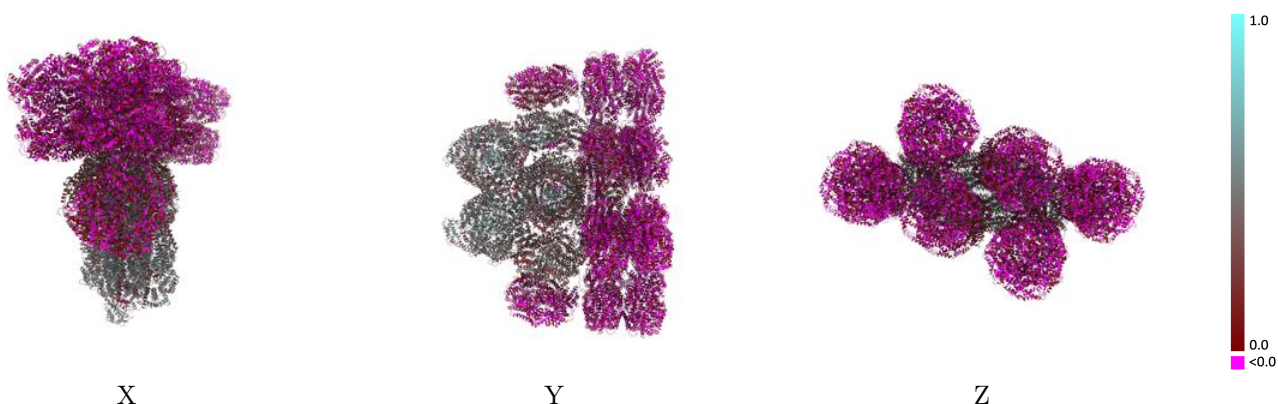
This section contains information regarding the fit between EMDB map EMD-62201 and PDB model 9K9W. Per-residue inclusion information can be found in [section 3](#) on [page 64](#).

9.1 Map-model overlay [i](#)



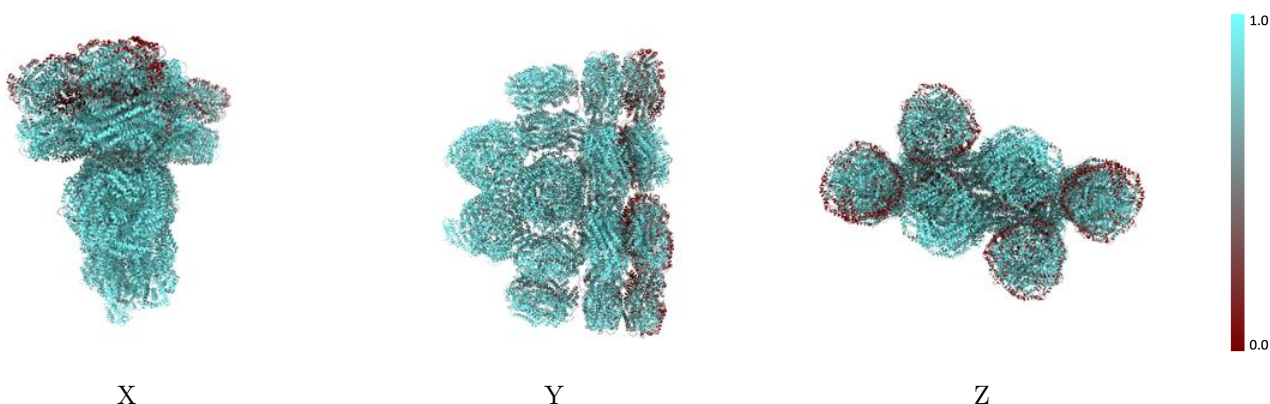
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



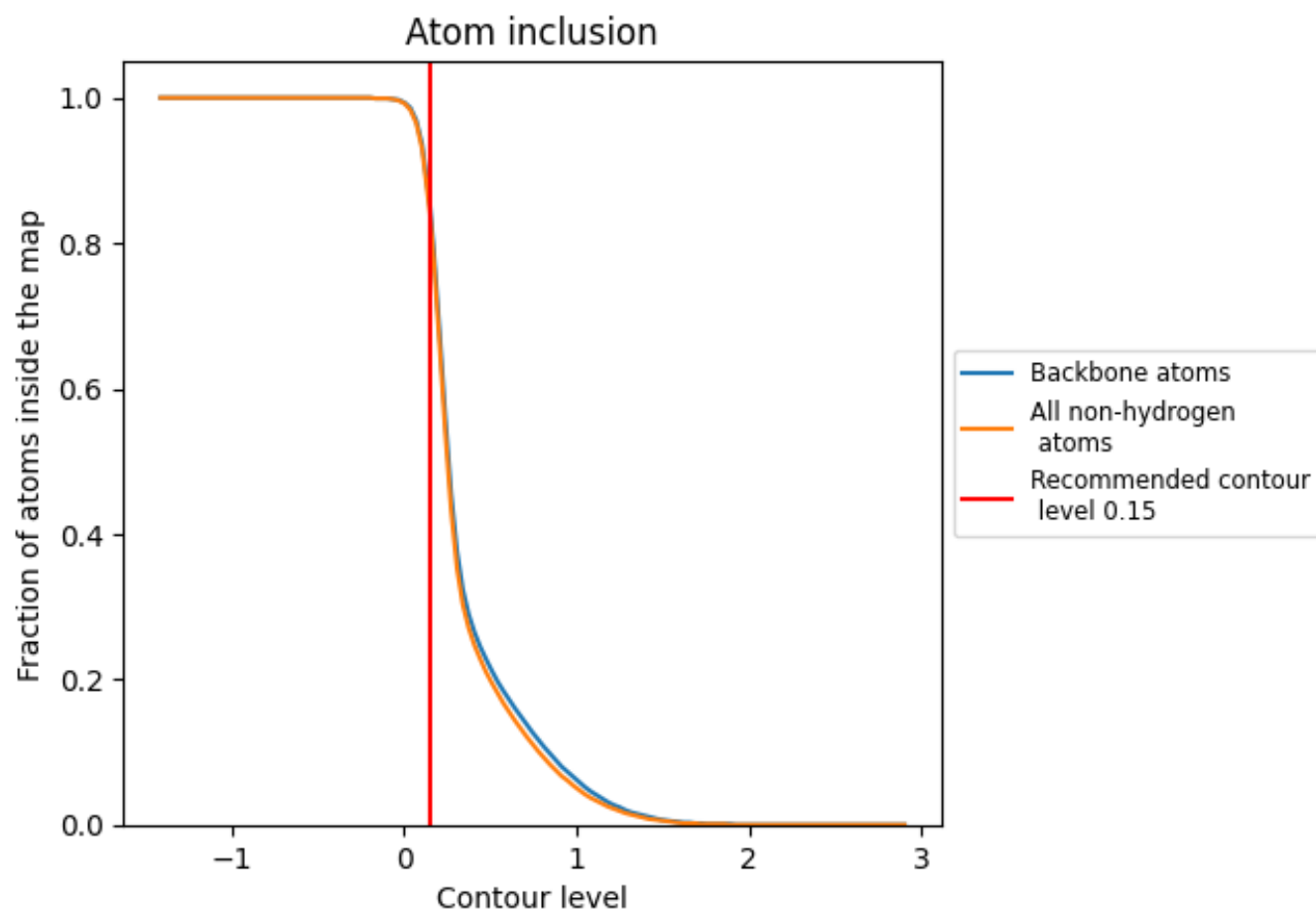
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.8410 |  0.1660 |
| A |  0.9470 |  0.4470 |
| A1 |  0.9680 |  0.0200 |
| A2 |  0.9530 |  0.0760 |
| A3 |  0.9680 |  0.0180 |
| A4 |  0.9620 |  0.0050 |
| A5 |  0.8880 |  0.4010 |
| A6 |  0.9360 |  0.0450 |
| A7 |  0.9070 |  0.4410 |
| A8 |  0.9590 |  0.0050 |
| A9 |  0.9710 |  0.1020 |
| AA |  0.9710 |  0.1010 |
| B1 |  0.9110 |  0.0460 |
| B2 |  0.9180 |  0.0420 |
| B3 |  0.9100 |  0.0450 |
| B4 |  0.8740 |  0.0160 |
| B5 |  0.9300 |  0.4250 |
| B6 |  0.9170 |  0.0210 |
| B7 |  0.9140 |  0.4480 |
| B8 |  0.8760 |  0.0190 |
| B9 |  0.9190 |  0.0640 |
| BA |  0.9200 |  0.0650 |
| C1 |  0.9070 |  0.0260 |
| C2 |  0.9200 |  0.0530 |
| C3 |  0.9060 |  0.0270 |
| C4 |  0.8570 |  0.0230 |
| C5 |  0.9150 |  0.3900 |
| C6 |  0.9070 |  0.0180 |
| C7 |  0.9290 |  0.4230 |
| C8 |  0.8590 |  0.0230 |
| C9 |  0.9440 |  0.1850 |
| CA |  0.9430 |  0.1800 |
| D1 |  0.8770 |  0.0390 |
| D2 |  0.9520 |  0.0480 |
| D3 |  0.8740 |  0.0390 |























































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| D4 |  0.8880 |  0.0350 |
| D5 |  0.9400 |  0.4380 |
| D6 |  0.9460 |  0.0220 |
| D7 |  0.9270 |  0.4710 |
| D8 |  0.8880 |  0.0350 |
| D9 |  0.8880 |  0.0870 |
| DA |  0.8880 |  0.0850 |
| E1 |  0.8780 |  0.0440 |
| E2 |  0.8970 |  0.0370 |
| E3 |  0.8770 |  0.0470 |
| E4 |  0.8810 |  0.0090 |
| E5 |  0.9490 |  0.4440 |
| E6 |  0.8970 |  -0.0060 |
| E7 |  0.9140 |  0.4560 |
| E8 |  0.8810 |  0.0120 |
| E9 |  0.8690 |  0.0360 |
| EA |  0.8690 |  0.0270 |
| F1 |  0.8240 |  0.0690 |
| F2 |  0.9320 |  0.0730 |
| F3 |  0.8230 |  0.0690 |
| F4 |  0.8870 |  0.0200 |
| F5 |  0.9560 |  0.4680 |
| F6 |  0.9450 |  0.0640 |
| F7 |  0.9210 |  0.4680 |
| F8 |  0.8850 |  0.0200 |
| F9 |  0.9370 |  0.1660 |
| FA |  0.9350 |  0.1630 |
| G1 |  0.9550 |  0.0100 |
| G2 |  0.9540 |  0.1620 |
| G3 |  0.9540 |  0.0090 |
| G4 |  0.9650 |  0.0600 |
| G5 |  0.8900 |  0.3950 |
| G6 |  0.9410 |  0.1340 |
| G7 |  0.9180 |  0.4560 |
| G8 |  0.9650 |  0.0560 |
| G9 |  0.9660 |  0.0900 |
| GA |  0.9670 |  0.0890 |
| H1 |  0.9190 |  0.0510 |
| H2 |  0.8170 |  0.1580 |
| H3 |  0.9190 |  0.0480 |
| H4 |  0.8680 |  0.0340 |
| H5 |  0.9390 |  0.4420 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--|---|
| H6 |  0.7890 |  0.1510 |
| H7 |  0.9210 |  0.4490 |
| H8 |  0.8710 |  0.0340 |
| H9 |  0.9440 |  0.1020 |
| HA |  0.9440 |  0.0970 |
| I1 |  0.8110 |  0.0770 |
| I2 |  0.8180 |  0.0700 |
| I3 |  0.8110 |  0.0810 |
| I4 |  0.9300 |  0.0210 |
| I5 |  0.9240 |  0.4120 |
| I6 |  0.8090 |  0.0620 |
| I7 |  0.9310 |  0.4410 |
| I8 |  0.9310 |  0.0240 |
| I9 |  0.9030 |  0.1620 |
| IA |  0.9000 |  0.1510 |
| J1 |  0.8200 |  0.0600 |
| J2 |  0.7860 |  0.0510 |
| J3 |  0.8240 |  0.0640 |
| J4 |  0.9200 |  0.0180 |
| J5 |  0.9480 |  0.4520 |
| J6 |  0.7540 |  0.0390 |
| J7 |  0.9230 |  0.4760 |
| J8 |  0.9220 |  0.0190 |
| J9 |  0.7570 |  0.0370 |
| JA |  0.7580 |  0.0260 |
| K1 |  0.9570 |  0.0210 |
| K2 |  0.9160 |  0.0640 |
| K3 |  0.9570 |  0.0210 |
| K4 |  0.7970 |  -0.0040 |
| K5 |  0.9510 |  0.4480 |
| K6 |  0.8890 |  0.0350 |
| K7 |  0.9200 |  0.4690 |
| K8 |  0.7980 |  -0.0030 |
| K9 |  0.8880 |  0.0330 |
| KA |  0.8860 |  0.0320 |
| L1 |  0.9210 |  0.0140 |
| L2 |  0.8740 |  0.1670 |
| L3 |  0.9230 |  0.0150 |
| L4 |  0.8280 |  0.0190 |
| L5 |  0.9620 |  0.4790 |
| L6 |  0.8280 |  0.0950 |
| L7 |  0.9360 |  0.4950 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--|---|
| L8 |  0.8210 |  0.0170 |
| L9 |  0.9710 |  0.0630 |
| LA |  0.9710 |  0.0640 |
| M1 |  0.8250 |  0.0150 |
| M2 |  0.9060 |  0.1810 |
| M3 |  0.8250 |  0.0150 |
| M4 |  0.9250 |  0.0060 |
| M5 |  0.8880 |  0.3860 |
| M6 |  0.8900 |  0.1380 |
| M7 |  0.9160 |  0.4090 |
| M8 |  0.9220 |  0.0070 |
| M9 |  0.8990 |  0.0260 |
| MA |  0.8970 |  0.0250 |
| N1 |  0.8500 |  0.0180 |
| N2 |  0.9640 |  0.0580 |
| N3 |  0.8520 |  0.0200 |
| N4 |  0.6060 |  0.0320 |
| N5 |  0.9160 |  0.4630 |
| N6 |  0.9390 |  0.0140 |
| N7 |  0.9090 |  0.4070 |
| N8 |  0.6050 |  0.0360 |
| N9 |  0.9770 |  -0.0350 |
| NA |  0.9790 |  -0.0330 |
| O1 |  0.7780 |  -0.0010 |
| O3 |  0.7770 |  -0.0040 |
| O4 |  0.6630 |  0.0210 |
| O5 |  0.9230 |  0.4090 |
| O7 |  0.8320 |  0.3020 |
| O8 |  0.6660 |  0.0190 |
| O9 |  0.9720 |  0.0070 |
| OA |  0.9730 |  0.0100 |
| P1 |  0.6150 |  0.0000 |
| P3 |  0.6130 |  0.0020 |
| P4 |  0.6130 |  0.0150 |
| P5 |  0.9370 |  0.4400 |
| P7 |  0.9210 |  0.3850 |
| P8 |  0.6150 |  0.0170 |
| P9 |  0.9420 |  0.0270 |
| PA |  0.9380 |  0.0260 |
| Q1 |  0.5190 |  0.0250 |
| Q3 |  0.5230 |  0.0260 |
| Q4 |  0.5520 |  0.0070 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--|---|
| Q5 |  0.9170 |  0.3890 |
| Q7 |  0.8470 |  0.2750 |
| Q8 |  0.5340 |  0.0200 |
| Q9 |  0.7250 |  0.0060 |
| QA |  0.7680 |  0.0190 |
| R1 |  0.6870 |  0.0350 |
| R3 |  0.6900 |  0.0360 |
| R4 |  0.4480 |  -0.0020 |
| R5 |  0.9230 |  0.4280 |
| R7 |  0.8980 |  0.3190 |
| R8 |  0.4500 |  -0.0030 |
| R9 |  0.8570 |  0.0320 |
| RA |  0.8570 |  0.0330 |
| S1 |  0.6770 |  0.0090 |
| S3 |  0.6790 |  0.0090 |
| S4 |  0.4190 |  0.0200 |
| S5 |  0.8940 |  0.4090 |
| S7 |  0.8710 |  0.3170 |
| S8 |  0.4070 |  0.0150 |
| S9 |  0.8810 |  0.0320 |
| SA |  0.8810 |  0.0310 |
| T1 |  0.6030 |  -0.0180 |
| T3 |  0.6070 |  -0.0230 |
| T4 |  0.7530 |  0.0090 |
| T5 |  0.9350 |  0.5020 |
| T7 |  0.8800 |  0.3090 |
| T8 |  0.7560 |  0.0060 |
| T9 |  0.8300 |  0.0220 |
| TA |  0.8310 |  0.0190 |
| U1 |  0.4790 |  0.0270 |
| U3 |  0.4730 |  0.0210 |
| U4 |  0.7550 |  0.0020 |
| U5 |  0.9420 |  0.4640 |
| U7 |  0.8160 |  0.2730 |
| U8 |  0.7520 |  0.0020 |
| U9 |  0.8550 |  0.0250 |
| UA |  0.8560 |  0.0280 |
| V1 |  0.3550 |  0.0020 |
| V3 |  0.3550 |  0.0030 |
| V4 |  0.4840 |  0.0010 |
| V5 |  0.9540 |  0.4770 |
| V7 |  0.9130 |  0.3600 |

































































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| Chain | Atom inclusion | Q-score |
|-------|--|---|
| V8 |  0.4810 |  0.0030 |
| V9 |  0.2500 |  0.0030 |
| VA |  0.2510 |  0.0040 |
| W1 |  0.5900 |  0.0200 |
| W3 |  0.5980 |  0.0210 |
| W4 |  0.4270 |  -0.0000 |
| W5 |  0.9240 |  0.4160 |
| W7 |  0.8470 |  0.2670 |
| W8 |  0.4280 |  -0.0020 |
| W9 |  0.3970 |  0.0280 |
| WA |  0.3950 |  0.0270 |
| X1 |  0.7710 |  0.0070 |
| X3 |  0.7700 |  0.0050 |
| X4 |  0.5080 |  0.0090 |
| X5 |  0.9310 |  0.4440 |
| X7 |  0.8850 |  0.2980 |
| X8 |  0.5080 |  0.0050 |
| X9 |  0.5140 |  0.0210 |
| XA |  0.5110 |  0.0180 |
| Y1 |  0.7920 |  0.0060 |
| Y3 |  0.7910 |  0.0010 |
| Y4 |  0.4670 |  -0.0060 |
| Y5 |  0.9370 |  0.4230 |
| Y7 |  0.9380 |  0.3320 |
| Y8 |  0.4750 |  -0.0060 |
| Y9 |  0.9060 |  0.0350 |
| YA |  0.9050 |  0.0340 |
| Z |  0.9530 |  0.4620 |
| Z1 |  0.5710 |  -0.0020 |
| Z3 |  0.5700 |  -0.0040 |
| Z4 |  0.9320 |  0.0790 |
| Z5 |  0.9320 |  0.4750 |
| Z7 |  0.9270 |  0.3800 |
| Z8 |  0.9220 |  0.0570 |
| Z9 |  0.8430 |  0.0200 |
| ZA |  0.8450 |  0.0200 |
| a5 |  0.9420 |  0.4730 |
| a7 |  0.9200 |  0.3710 |
| a9 |  0.9110 |  0.1690 |
| aA |  0.9100 |  0.1710 |
| b5 |  0.8930 |  0.3450 |
| b7 |  0.9550 |  0.4480 |

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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| c5 |  0.9370 |  0.4260 |
| c7 |  0.9330 |  0.3650 |
| d5 |  0.9340 |  0.4700 |
| d7 |  0.9640 |  0.3620 |
| e5 |  0.9400 |  0.4680 |
| e7 |  0.9310 |  0.3250 |
| f5 |  0.9080 |  0.3800 |
| f7 |  0.9320 |  0.3790 |
| g7 |  0.9180 |  0.3670 |
| h7 |  0.9580 |  0.4450 |
| i5 |  0.9710 |  0.5210 |
| i7 |  0.8840 |  0.2520 |
| j5 |  0.9730 |  0.5350 |
| j7 |  0.9600 |  0.3550 |
| k5 |  0.9720 |  0.5330 |
| k7 |  0.8890 |  0.3350 |
| l7 |  0.9090 |  0.3360 |
| m7 |  0.9450 |  0.2980 |
| n7 |  0.8880 |  0.3070 |
| o7 |  0.9420 |  0.4350 |
| p7 |  0.8300 |  0.2650 |
| q7 |  0.8360 |  0.2340 |
| r7 |  0.9070 |  0.3460 |
| s7 |  0.9450 |  0.2960 |
| t7 |  0.8720 |  0.2670 |
| u7 |  0.9530 |  0.4790 |
| v7 |  0.7890 |  0.1970 |
| w7 |  0.9830 |  0.5160 |
| x7 |  0.9810 |  0.5000 |
| y7 |  0.9810 |  0.5050 |
| z5 |  0.9680 |  0.5260 |
| z7 |  0.9870 |  0.5470 |