



Full wwPDB NMR Structure Validation Report ⓘ

Sep 28, 2025 – 02:34 PM EDT

PDB ID : 9ONB / pdb_00009onb
BMRB ID : 31248
Title : Immature HIV-1 CACTD-SP1 lattice with Maturation inhibitor PF-46396 (S) and Inositol hexakisphosphate (IP6)
Authors : Zadorozhnyi, R.; Quinn, C.M.; Zadrozny, K.K.; Ablan, S.D.; Kennedy, B.J.; Yap, G.P.A.; Sanner, D.; Kraml, C.; Freed, E.O.; Ganser-Pornillos, B.K.; Pornillos, O.; Gronenborn, A.M.; Polenova, T.
Deposited on : 2025-05-14

This is a Full wwPDB NMR Structure 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/NMRValidationReportHelp>

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](#) ①) were used in the production of this report:

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| wwPDB-RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| wwPDB-ShiftChecker | : | v1.2 |
| BMRB Restraints Analysis | : | v1.2 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.46 |

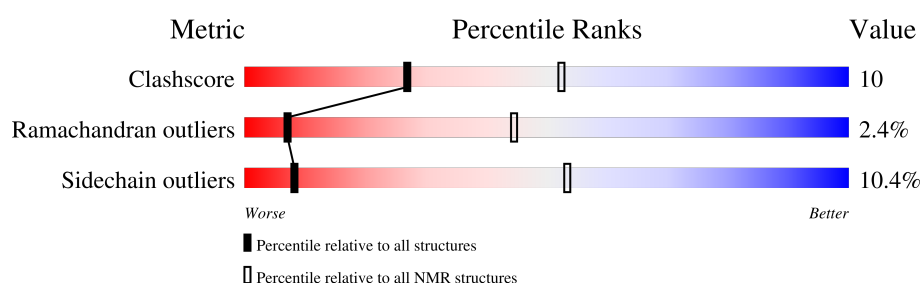
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 6%.

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) | NMR archive (#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore | 210492 | 14027 |
| Ramachandran outliers | 207382 | 12486 |
| Sidechain outliers | 206894 | 12463 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | G | 102 | 73% 23% .. |
| 1 | H | 102 | 66% 26% . . . |
| 1 | I | 102 | 57% 26% 5% 12% |
| 1 | J | 102 | 69% 22% . . 7% |
| 1 | K | 102 | 69% 21% 5% 6% |
| 1 | L | 102 | 68% 25% 5% . |

2 Ensemble composition and analysis

This entry contains 10 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues | | | |
|--------------------------------------|---|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | G:146-G:244, H:147-H:245, I:147-I:148, I:153-I:205, I:210-I:244, J:147-J:205, J:210-J:245, K:144-K:147, K:154-K:245, L:147-L:245 (578) | 0.62 | 2 |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 2 single-model clusters were found.

| Cluster number | Models |
|-----------------------|-------------|
| 1 | 1, 3, 4, 8 |
| 2 | 2, 6, 9, 10 |
| Single-model clusters | 5; 7 |

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9410 atoms, of which 4703 are hydrogens and 0 are deuteriums.

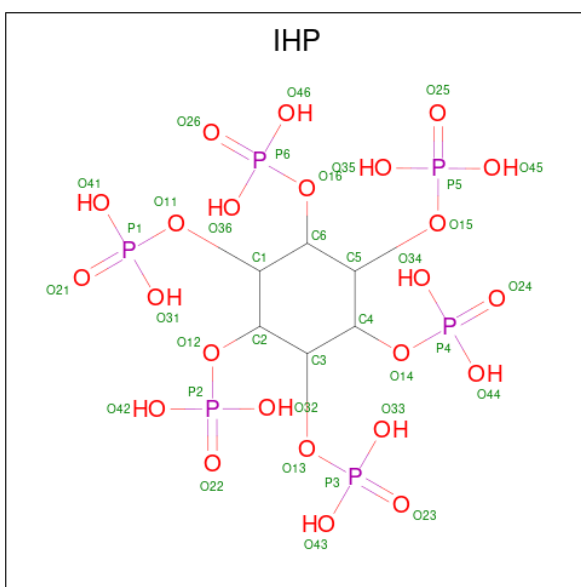
- Molecule 1 is a protein called Capsid protein p24.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1 | G | 102 | Total | C | H | N | O | S | 0 |
| | | | 1551 | 479 | 778 | 136 | 151 | 7 | |
| 1 | H | 102 | Total | C | H | N | O | S | 0 |
| | | | 1551 | 479 | 778 | 136 | 151 | 7 | |
| 1 | I | 102 | Total | C | H | N | O | S | 0 |
| | | | 1551 | 479 | 778 | 136 | 151 | 7 | |
| 1 | J | 102 | Total | C | H | N | O | S | 0 |
| | | | 1551 | 479 | 778 | 136 | 151 | 7 | |
| 1 | K | 102 | Total | C | H | N | O | S | 0 |
| | | | 1551 | 479 | 778 | 136 | 151 | 7 | |
| 1 | L | 102 | Total | C | H | N | O | S | 0 |
| | | | 1551 | 479 | 778 | 136 | 151 | 7 | |

There are 18 discrepancies between the modelled and reference sequences:

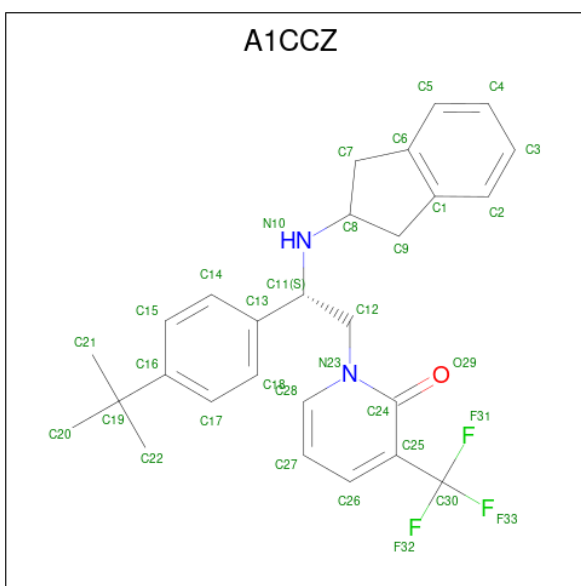
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| G | 144 | GLY | - | expression tag | UNP P12497 |
| G | 145 | GLY | - | expression tag | UNP P12497 |
| G | 241 | THR | PRO | conflict | UNP P12497 |
| H | 144 | GLY | - | expression tag | UNP P12497 |
| H | 145 | GLY | - | expression tag | UNP P12497 |
| H | 241 | THR | PRO | conflict | UNP P12497 |
| I | 144 | GLY | - | expression tag | UNP P12497 |
| I | 145 | GLY | - | expression tag | UNP P12497 |
| I | 241 | THR | PRO | conflict | UNP P12497 |
| J | 144 | GLY | - | expression tag | UNP P12497 |
| J | 145 | GLY | - | expression tag | UNP P12497 |
| J | 241 | THR | PRO | conflict | UNP P12497 |
| K | 144 | GLY | - | expression tag | UNP P12497 |
| K | 145 | GLY | - | expression tag | UNP P12497 |
| K | 241 | THR | PRO | conflict | UNP P12497 |
| L | 144 | GLY | - | expression tag | UNP P12497 |
| L | 145 | GLY | - | expression tag | UNP P12497 |
| L | 241 | THR | PRO | conflict | UNP P12497 |

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | |
|-----|-------|----------|-------|---|---|----|---|
| 2 | H | 1 | Total | C | H | O | P |
| | | | 42 | 6 | 6 | 24 | 6 |

- Molecule 3 is 1-{(2S)-2-(4-tert-butylphenyl)-2-[(2,3-dihydro-1H-inden-2-yl)amino]ethyl}-3-(trifluoromethyl)pyridin-2(1H)-one (CCD ID: A1CCZ) (formula: $C_{27}H_{29}F_3N_2O$) (labeled as "Ligand of Interest" by depositor).



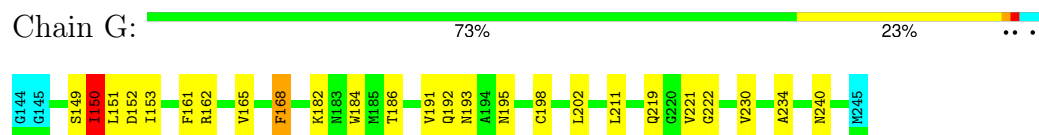
| Mol | Chain | Residues | Atoms | | | | | |
|-----|-------|----------|-------|----|---|----|---|---|
| 3 | H | 1 | Total | C | F | H | N | O |
| | | | 62 | 27 | 3 | 29 | 2 | 1 |

4 Residue-property plots [i](#)

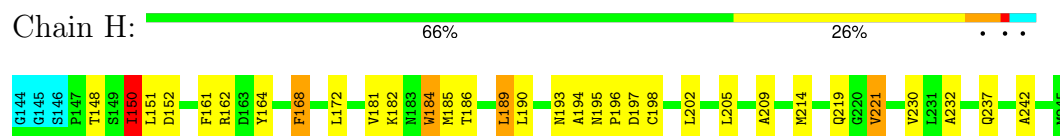
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

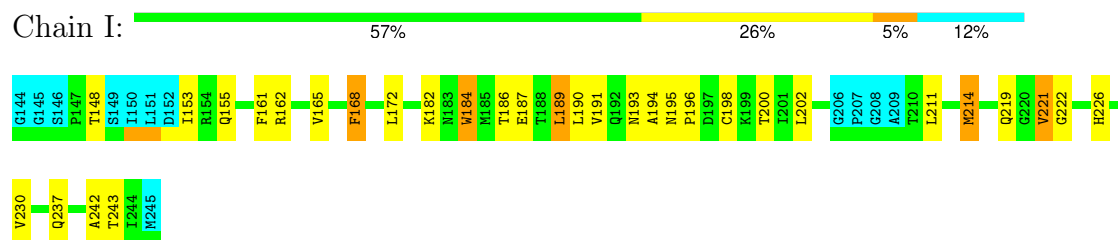
- Molecule 1: Capsid protein p24



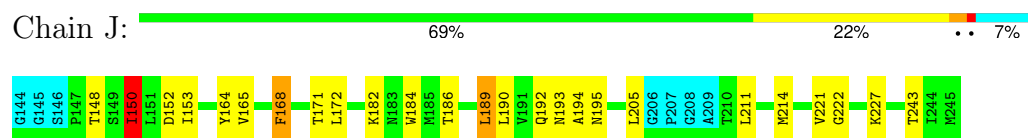
- Molecule 1: Capsid protein p24



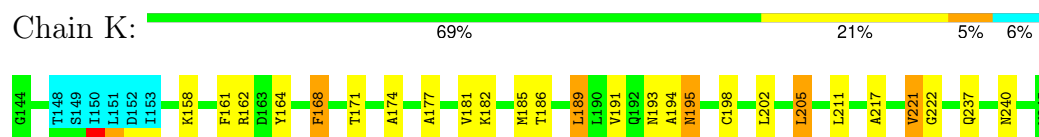
- Molecule 1: Capsid protein p24



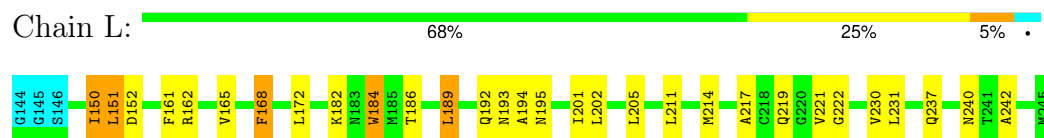
- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24

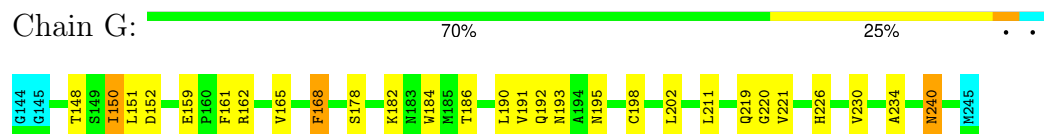


4.2 Scores per residue for each member of the ensemble

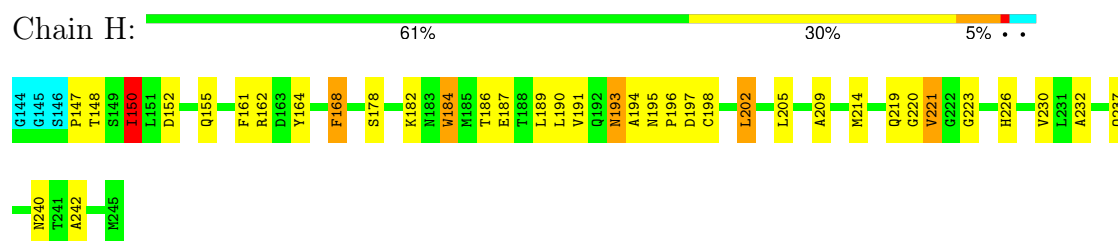
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

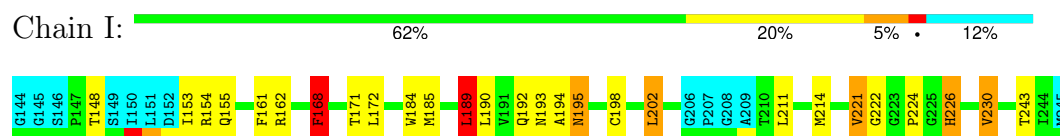
- Molecule 1: Capsid protein p24



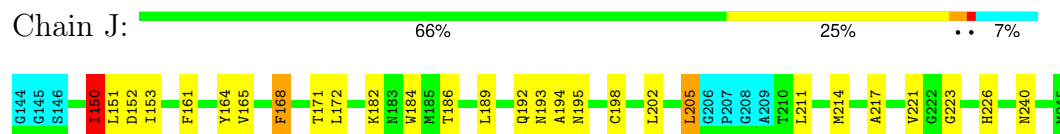
- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24

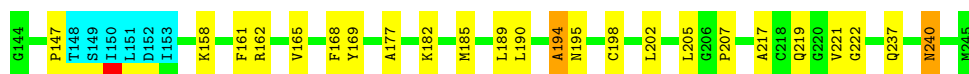


- Molecule 1: Capsid protein p24



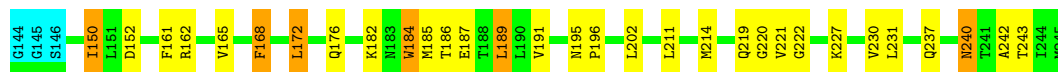
- Molecule 1: Capsid protein p24





- Molecule 1: Capsid protein p24

Chain L: 67% 25% 6% •



4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Capsid protein p24

Chain G: 66% 29% • •



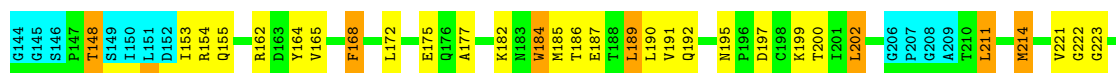
- Molecule 1: Capsid protein p24

Chain H: 60% 27% 9% • •



- Molecule 1: Capsid protein p24

Chain I: 52% 29% 7% 12%



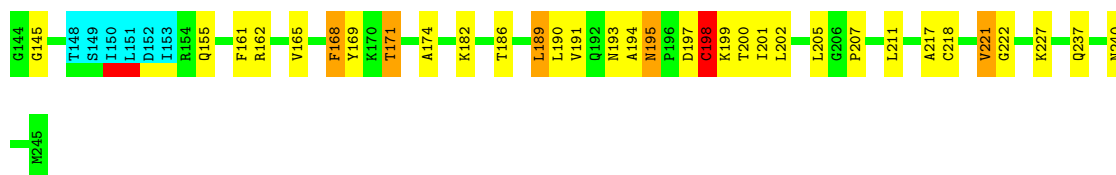
- Molecule 1: Capsid protein p24

Chain J: 64% 20% 9% 7%



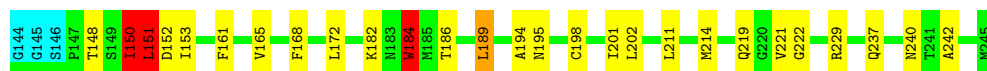
- Molecule 1: Capsid protein p24

Chain K: 62% 26% 5% 6%



- Molecule 1: Capsid protein p24

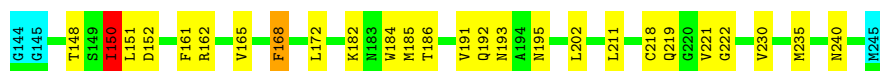
Chain L: 71% 23% ..



4.2.3 Score per residue for model 3

- Molecule 1: Capsid protein p24

Chain G: 72% 24% ..



- Molecule 1: Capsid protein p24

Chain H: 65% 25% 8% .



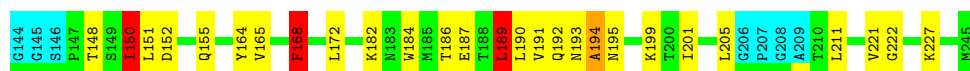
- Molecule 1: Capsid protein p24

Chain I: 51% 30% 6% 12%

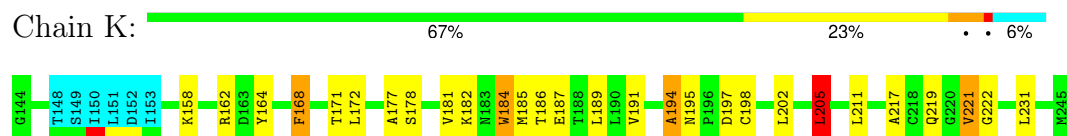


- Molecule 1: Capsid protein p24

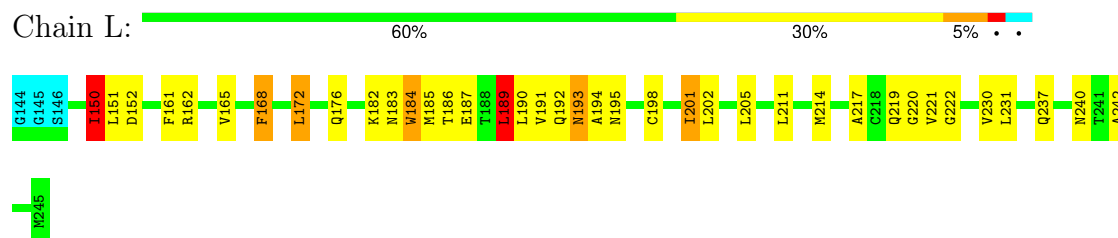
Chain J: 67% 23% 7%



- Molecule 1: Capsid protein p24

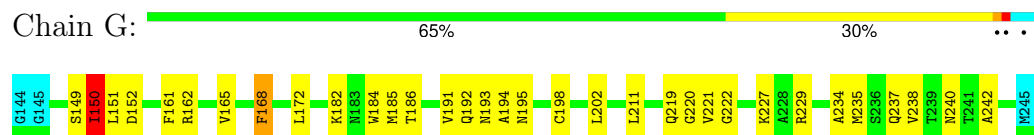


- Molecule 1: Capsid protein p24

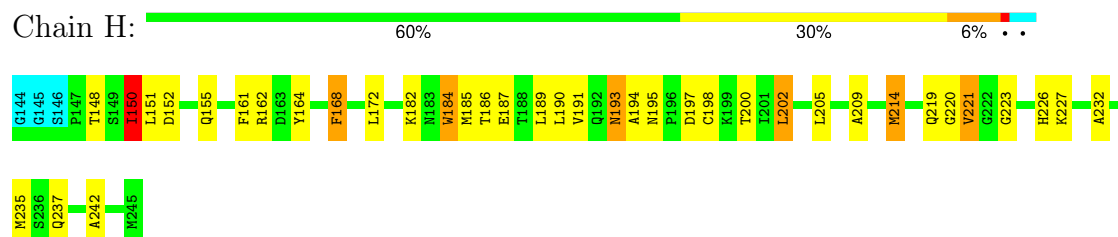


4.2.4 Score per residue for model 4

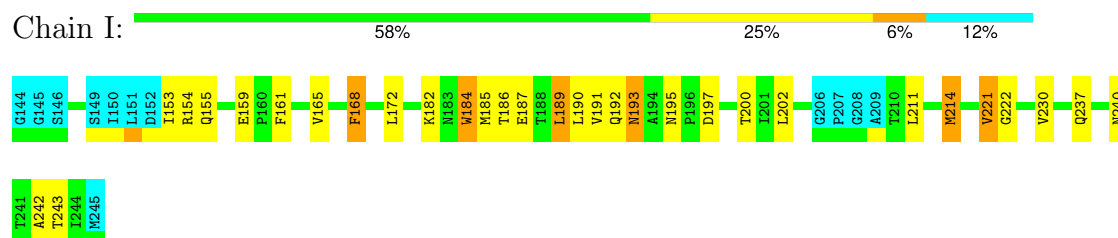
- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24

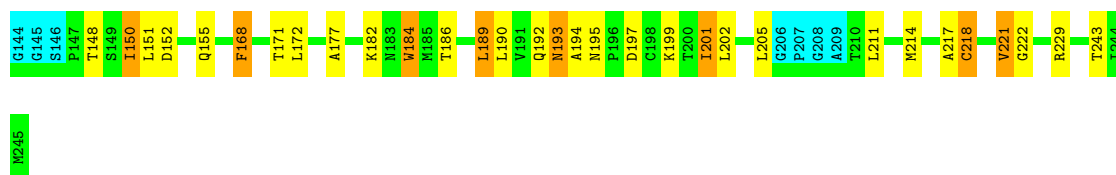


- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24





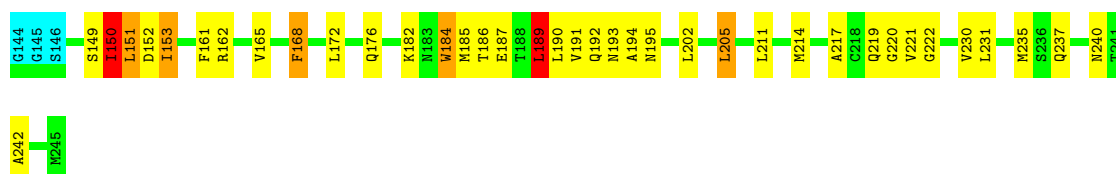
- Molecule 1: Capsid protein p24

Chain K: 65% 25% 5% 6%



- Molecule 1: Capsid protein p24

Chain L: 60% 30% 5% • •



4.2.5 Score per residue for model 5

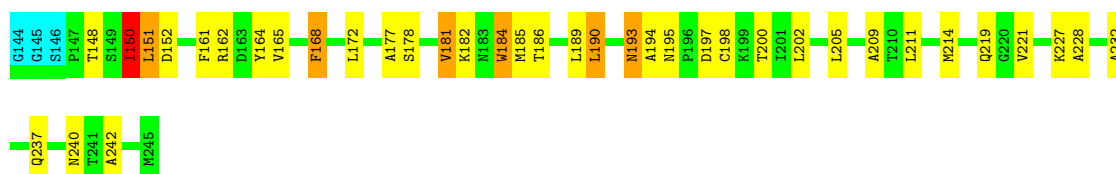
- Molecule 1: Capsid protein p24

Chain G: 61% 33% • • •



- Molecule 1: Capsid protein p24

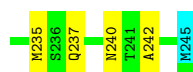
Chain H: 60% 30% 6% • •



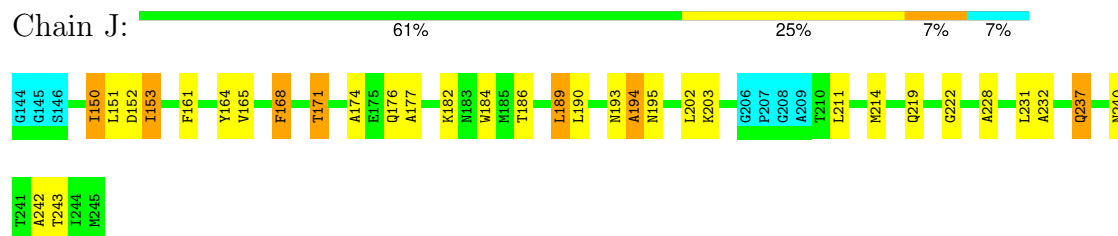
- Molecule 1: Capsid protein p24

Chain I: 55% 26% 6% • 12%

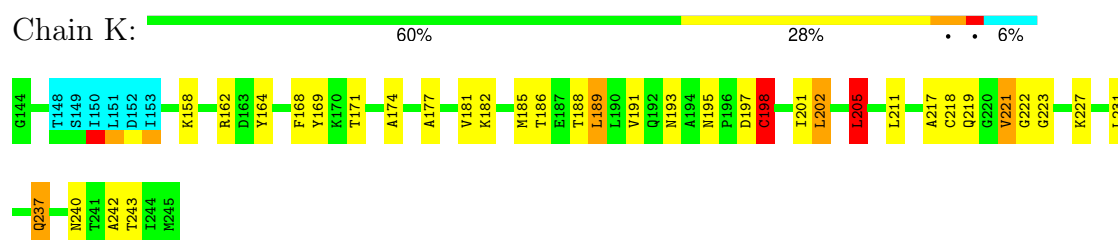




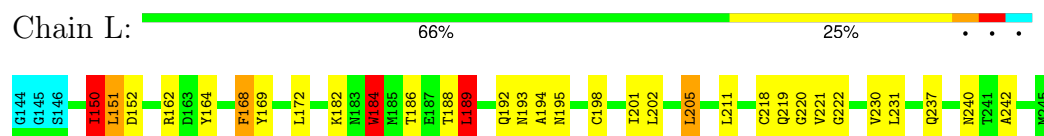
- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24

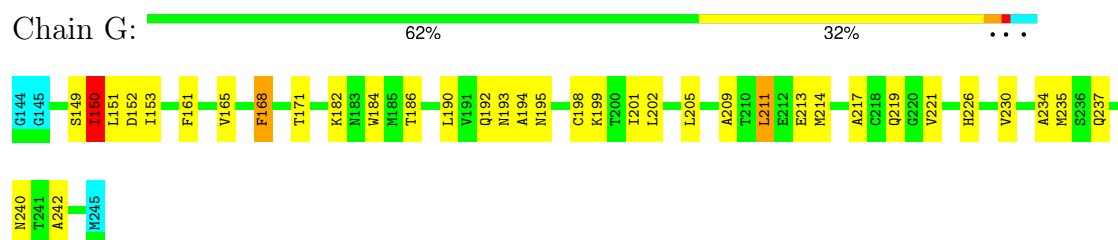


- Molecule 1: Capsid protein p24

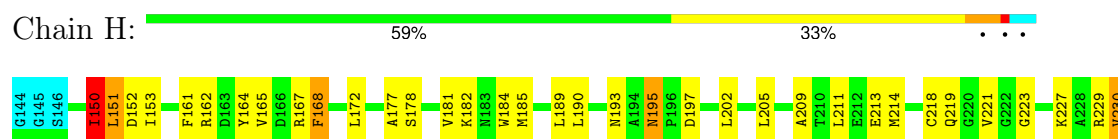


4.2.6 Score per residue for model 6

- Molecule 1: Capsid protein p24

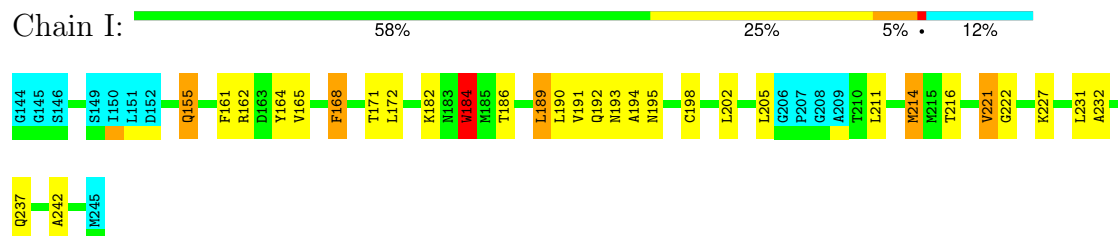


- Molecule 1: Capsid protein p24

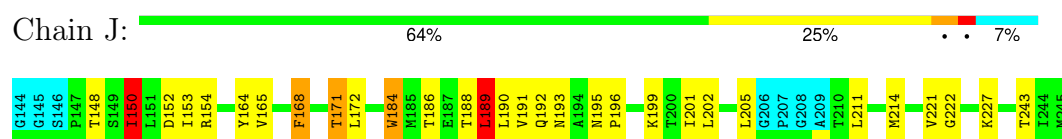




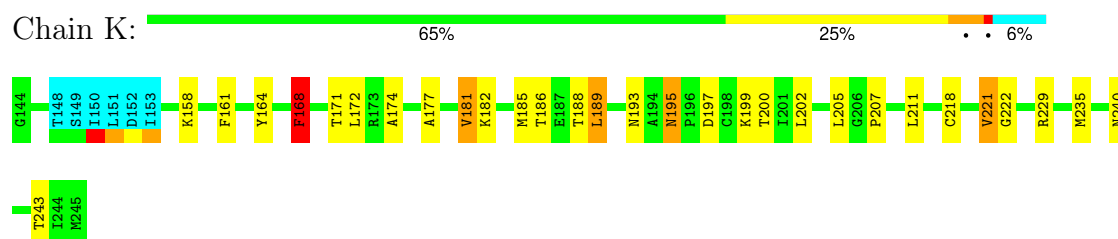
- Molecule 1: Capsid protein p24



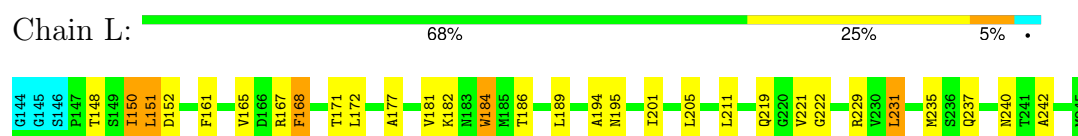
- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24

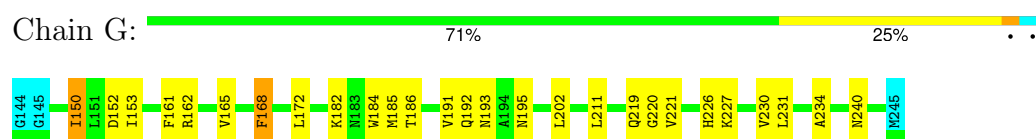


- Molecule 1: Capsid protein p24



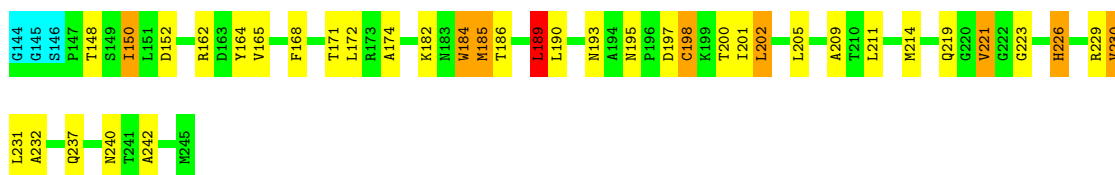
4.2.7 Score per residue for model 7

- Molecule 1: Capsid protein p24

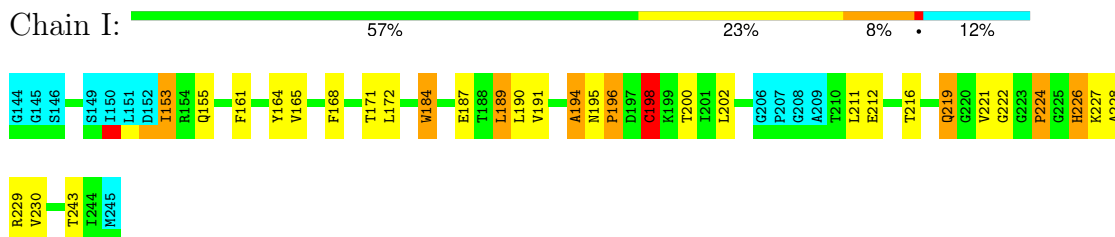


- Molecule 1: Capsid protein p24

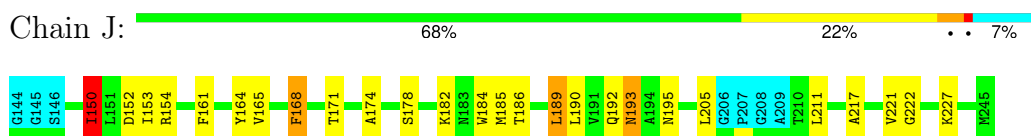




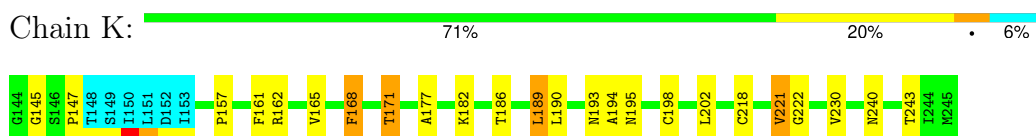
- Molecule 1: Capsid protein p24



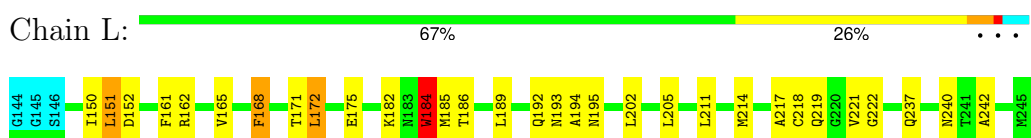
- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24



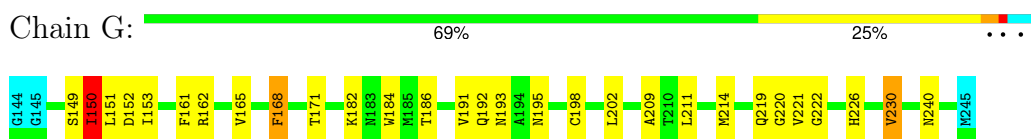
- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24

4.2.8 Score per residue for model 8

- Molecule 1: Capsid protein p24



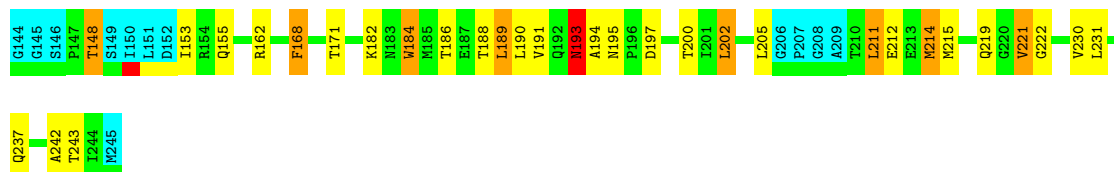
- Molecule 1: Capsid protein p24





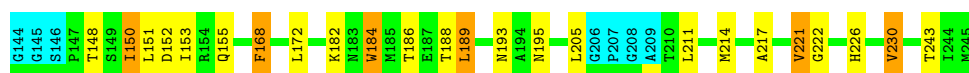
- Molecule 1: Capsid protein p24

Chain I: 57% 23% 8% 12%



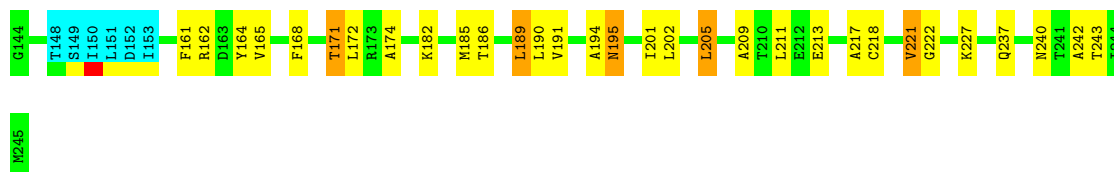
- Molecule 1: Capsid protein p24

Chain J: 70% 18% 6% 7%



- Molecule 1: Capsid protein p24

Chain K: 64% 25% 5% 6%



- Molecule 1: Capsid protein p24

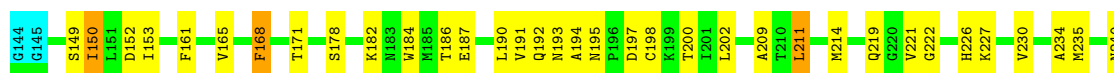
Chain L: 64% 27% 6% 3%



4.2.9 Score per residue for model 9

- Molecule 1: Capsid protein p24

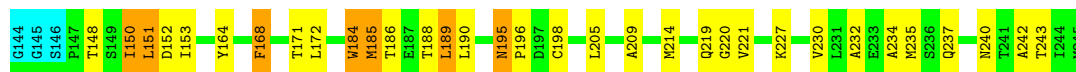
Chain G: 63% 31% 6% 0%





- Molecule 1: Capsid protein p24

Chain H: 65% 25% 7%



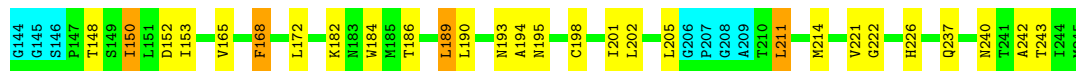
- Molecule 1: Capsid protein p24

Chain I: 58% 25% 6% 12%



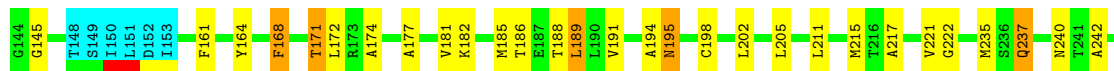
- Molecule 1: Capsid protein p24

Chain J: 66% 24% 7%



- Molecule 1: Capsid protein p24

Chain K: 66% 24% 5% 6%



- Molecule 1: Capsid protein p24

Chain L: 64% 29%



4.2.10 Score per residue for model 10

- Molecule 1: Capsid protein p24

Chain G:  71% 25% • •



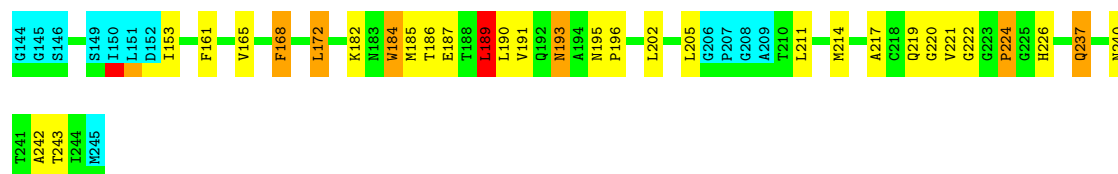
- Molecule 1: Capsid protein p24

Chain H:  65% 25% 7% • •



- Molecule 1: Capsid protein p24

Chain I:  58% 24% 6% • 12%



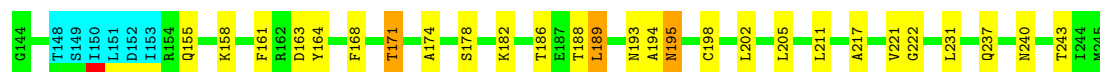
- Molecule 1: Capsid protein p24

Chain J:  72% 19% • 7%



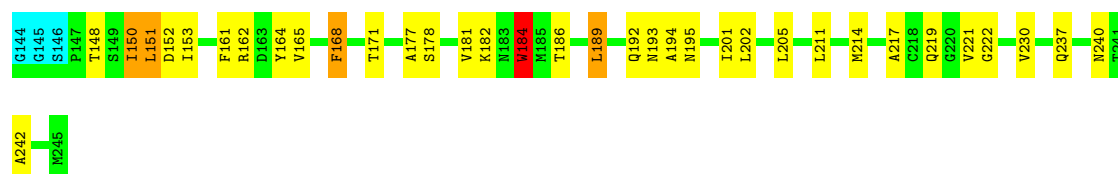
- Molecule 1: Capsid protein p24

Chain K:  68% 24% • 6%



- Molecule 1: Capsid protein p24

Chain L:  63% 29% • • •



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification | Version |
|---------------|-----------------------|---------|
| X-PLOR NIH | structure calculation | |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| | |
|--|----------------|
| Chemical shift file(s) | working_cs.cif |
| Number of chemical shift lists | 1 |
| Total number of shifts | 514 |
| Number of shifts mapped to atoms | 514 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 6% |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, A1CCZ

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 (average) 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 | G | 1.39±0.02 | 6±1/769 (0.7± 0.2%) | 1.50±0.02 | 10±2/1043 (1.0± 0.1%) |
| 1 | H | 1.33±0.03 | 4±2/771 (0.6± 0.3%) | 1.54±0.03 | 10±2/1041 (1.0± 0.2%) |
| 1 | I | 1.27±0.05 | 2±2/712 (0.3± 0.2%) | 1.56±0.03 | 11±2/964 (1.1± 0.2%) |
| 1 | J | 1.17±0.02 | 1±1/750 (0.2± 0.1%) | 1.48±0.04 | 11±2/1012 (1.0± 0.2%) |
| 1 | K | 1.12±0.04 | 1±1/740 (0.2± 0.1%) | 1.42±0.04 | 7±1/998 (0.7± 0.1%) |
| 1 | L | 1.25±0.04 | 4±2/771 (0.5± 0.2%) | 1.56±0.05 | 15±4/1041 (1.4± 0.4%) |
| All | All | 1.26 | 185/45130 (0.4%) | 1.51 | 635/60990 (1.0%) |

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 | Planarity |
|-----|-------|-----------|-----------|
| 1 | I | 0.0±0.0 | 0.1±0.3 |
| All | All | 0 | 1 |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | L | 221 | VAL | C-N | 13.95 | 1.44 | 1.33 | 7 | 10 |
| 1 | I | 221 | VAL | C-N | 9.88 | 1.42 | 1.32 | 10 | 4 |
| 1 | L | 152 | ASP | C-N | 9.85 | 1.43 | 1.33 | 9 | 6 |
| 1 | J | 221 | VAL | C-N | 9.01 | 1.41 | 1.32 | 9 | 5 |
| 1 | H | 152 | ASP | C-N | 8.13 | 1.41 | 1.33 | 9 | 2 |
| 1 | J | 152 | ASP | C-N | 8.02 | 1.44 | 1.33 | 8 | 3 |
| 1 | H | 198 | CYS | C-O | -7.37 | 1.14 | 1.24 | 3 | 5 |
| 1 | K | 221 | VAL | C-N | 7.14 | 1.42 | 1.33 | 3 | 8 |
| 1 | G | 221 | VAL | C-N | 7.12 | 1.41 | 1.32 | 2 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | I | 219 | GLN | C-N | 6.91 | 1.41 | 1.33 | 10 | 1 |
| 1 | H | 185 | MET | N-CA | -6.72 | 1.39 | 1.46 | 7 | 5 |
| 1 | G | 219 | GLN | C-N | 6.70 | 1.42 | 1.33 | 2 | 8 |
| 1 | H | 152 | ASP | N-CA | -6.58 | 1.38 | 1.46 | 2 | 2 |
| 1 | G | 221 | VAL | N-CA | 6.49 | 1.54 | 1.46 | 1 | 10 |
| 1 | H | 151 | LEU | CA-C | -6.48 | 1.45 | 1.52 | 2 | 2 |
| 1 | G | 150 | ILE | C-N | -6.35 | 1.25 | 1.33 | 6 | 5 |
| 1 | G | 149 | SER | C-N | 6.27 | 1.42 | 1.33 | 2 | 6 |
| 1 | G | 198 | CYS | C-O | -6.15 | 1.16 | 1.24 | 4 | 6 |
| 1 | H | 151 | LEU | C-N | 6.14 | 1.41 | 1.33 | 5 | 1 |
| 1 | H | 219 | GLN | C-N | 6.14 | 1.40 | 1.33 | 4 | 2 |
| 1 | H | 221 | VAL | C-N | 6.11 | 1.42 | 1.33 | 10 | 6 |
| 1 | I | 221 | VAL | N-CA | 6.04 | 1.54 | 1.46 | 1 | 3 |
| 1 | L | 152 | ASP | N-CA | -6.00 | 1.39 | 1.46 | 8 | 2 |
| 1 | I | 196 | PRO | N-CA | 5.99 | 1.54 | 1.47 | 7 | 4 |
| 1 | G | 150 | ILE | C-O | -5.99 | 1.17 | 1.24 | 6 | 5 |
| 1 | H | 184 | TRP | N-CA | 5.93 | 1.53 | 1.46 | 2 | 7 |
| 1 | I | 198 | CYS | C-O | -5.92 | 1.16 | 1.24 | 7 | 2 |
| 1 | I | 202 | LEU | N-CA | -5.91 | 1.38 | 1.46 | 9 | 1 |
| 1 | H | 150 | ILE | C-N | -5.79 | 1.26 | 1.33 | 2 | 1 |
| 1 | H | 194 | ALA | CA-C | -5.77 | 1.47 | 1.53 | 5 | 1 |
| 1 | L | 150 | ILE | CA-C | -5.76 | 1.45 | 1.52 | 2 | 2 |
| 1 | I | 155 | GLN | CA-C | -5.74 | 1.45 | 1.52 | 6 | 1 |
| 1 | I | 189 | LEU | CA-C | -5.73 | 1.45 | 1.52 | 9 | 3 |
| 1 | H | 189 | LEU | N-CA | 5.70 | 1.53 | 1.46 | 9 | 2 |
| 1 | G | 220 | GLY | C-O | -5.62 | 1.18 | 1.24 | 7 | 5 |
| 1 | H | 194 | ALA | N-CA | -5.56 | 1.39 | 1.46 | 2 | 2 |
| 1 | H | 229 | ARG | CA-C | 5.54 | 1.60 | 1.52 | 7 | 2 |
| 1 | L | 221 | VAL | N-CA | 5.50 | 1.53 | 1.46 | 5 | 2 |
| 1 | I | 224 | PRO | C-N | -5.43 | 1.26 | 1.33 | 10 | 1 |
| 1 | K | 184 | TRP | CA-C | 5.43 | 1.60 | 1.52 | 3 | 1 |
| 1 | L | 198 | CYS | C-O | -5.42 | 1.17 | 1.24 | 2 | 2 |
| 1 | L | 151 | LEU | N-CA | -5.42 | 1.40 | 1.46 | 4 | 1 |
| 1 | L | 194 | ALA | CA-C | -5.42 | 1.47 | 1.53 | 7 | 1 |
| 1 | H | 150 | ILE | N-CA | 5.41 | 1.53 | 1.46 | 1 | 2 |
| 1 | I | 153 | ILE | C-O | -5.39 | 1.17 | 1.24 | 8 | 1 |
| 1 | L | 220 | GLY | C-O | -5.36 | 1.17 | 1.23 | 1 | 4 |
| 1 | I | 220 | GLY | C-O | -5.34 | 1.18 | 1.24 | 10 | 1 |
| 1 | H | 196 | PRO | N-CA | 5.34 | 1.54 | 1.47 | 8 | 1 |
| 1 | I | 191 | VAL | N-CA | 5.32 | 1.53 | 1.46 | 5 | 1 |
| 1 | L | 189 | LEU | CA-C | -5.30 | 1.46 | 1.52 | 4 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | J | 151 | LEU | N-CA | -5.26 | 1.40 | 1.46 | 1 | 1 |
| 1 | G | 150 | ILE | N-CA | 5.25 | 1.52 | 1.46 | 5 | 1 |
| 1 | H | 198 | CYS | N-CA | -5.25 | 1.39 | 1.46 | 5 | 1 |
| 1 | K | 201 | ILE | C-O | -5.22 | 1.19 | 1.24 | 2 | 1 |
| 1 | J | 152 | ASP | CA-C | 5.21 | 1.59 | 1.53 | 9 | 1 |
| 1 | K | 223 | GLY | C-N | -5.15 | 1.27 | 1.34 | 5 | 1 |
| 1 | J | 153 | ILE | CA-CB | 5.11 | 1.60 | 1.54 | 5 | 1 |
| 1 | I | 222 | GLY | CA-C | -5.10 | 1.46 | 1.52 | 1 | 1 |
| 1 | H | 184 | TRP | CG-CD2 | 5.08 | 1.52 | 1.43 | 3 | 1 |
| 1 | L | 169 | TYR | CA-C | 5.06 | 1.59 | 1.52 | 5 | 1 |
| 1 | G | 152 | ASP | N-CA | -5.06 | 1.40 | 1.46 | 9 | 1 |
| 1 | J | 194 | ALA | N-CA | -5.06 | 1.40 | 1.46 | 3 | 1 |
| 1 | L | 183 | ASN | CA-C | 5.02 | 1.59 | 1.52 | 3 | 1 |
| 1 | K | 219 | GLN | C-N | 5.00 | 1.40 | 1.33 | 3 | 1 |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|--------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | L | 184 | TRP | N-CA-C | -10.72 | 99.56 | 111.14 | 5 | 10 |
| 1 | L | 151 | LEU | N-CA-C | -10.49 | 98.72 | 112.68 | 7 | 6 |
| 1 | I | 222 | GLY | CA-C-O | -10.25 | 115.07 | 122.45 | 1 | 5 |
| 1 | H | 151 | LEU | N-CA-C | -9.94 | 99.46 | 112.68 | 2 | 3 |
| 1 | H | 152 | ASP | N-CA-CB | -8.69 | 96.22 | 111.42 | 2 | 1 |
| 1 | I | 192 | GLN | N-CA-C | 8.63 | 120.30 | 111.07 | 2 | 4 |
| 1 | I | 189 | LEU | N-CA-C | -8.46 | 102.00 | 111.14 | 1 | 8 |
| 1 | G | 192 | GLN | N-CA-C | 8.33 | 119.99 | 111.07 | 4 | 10 |
| 1 | H | 219 | GLN | N-CA-C | -8.23 | 102.50 | 112.54 | 4 | 10 |
| 1 | J | 222 | GLY | CA-C-O | -8.10 | 116.62 | 122.45 | 4 | 4 |
| 1 | G | 219 | GLN | N-CA-C | -8.02 | 102.75 | 112.54 | 5 | 10 |
| 1 | I | 193 | ASN | CA-CB-CG | -7.98 | 104.62 | 112.60 | 1 | 3 |
| 1 | L | 189 | LEU | N-CA-CB | 7.97 | 122.07 | 110.20 | 9 | 8 |
| 1 | L | 193 | ASN | OD1-CG-ND2 | -7.94 | 114.66 | 122.60 | 5 | 3 |
| 1 | H | 197 | ASP | N-CA-C | -7.85 | 102.41 | 110.97 | 8 | 2 |
| 1 | I | 184 | TRP | N-CA-C | -7.78 | 102.88 | 111.36 | 10 | 4 |
| 1 | H | 152 | ASP | CA-C-O | -7.77 | 112.67 | 119.97 | 2 | 1 |
| 1 | I | 222 | GLY | N-CA-C | -7.67 | 104.22 | 112.04 | 1 | 2 |
| 1 | K | 194 | ALA | N-CA-C | 7.65 | 120.92 | 107.61 | 3 | 7 |
| 1 | G | 152 | ASP | CA-C-N | -7.55 | 110.42 | 120.91 | 8 | 10 |
| 1 | G | 152 | ASP | C-N-CA | -7.55 | 110.42 | 120.91 | 8 | 10 |
| 1 | K | 221 | VAL | CA-C-O | -7.51 | 114.61 | 121.97 | 1 | 9 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | J | 192 | GLN | N-CA-C | 7.42 | 119.00 | 111.07 | 4 | 7 |
| 1 | J | 152 | ASP | CA-C-N | -7.38 | 110.64 | 120.91 | 9 | 10 |
| 1 | J | 152 | ASP | C-N-CA | -7.38 | 110.64 | 120.91 | 9 | 10 |
| 1 | I | 221 | VAL | CA-C-O | -7.29 | 114.83 | 121.97 | 8 | 4 |
| 1 | H | 221 | VAL | CA-C-O | -7.28 | 114.30 | 121.58 | 6 | 10 |
| 1 | I | 202 | LEU | N-CA-C | -7.19 | 103.44 | 111.28 | 1 | 5 |
| 1 | H | 192 | GLN | N-CA-C | 7.17 | 118.89 | 111.14 | 2 | 1 |
| 1 | I | 214 | MET | N-CA-C | -7.12 | 103.45 | 111.07 | 4 | 6 |
| 1 | J | 201 | ILE | CB-CA-C | -7.05 | 102.78 | 112.02 | 3 | 4 |
| 1 | G | 221 | VAL | CA-C-O | -6.91 | 114.48 | 121.59 | 7 | 10 |
| 1 | L | 152 | ASP | CA-C-N | -6.82 | 110.11 | 121.63 | 9 | 10 |
| 1 | L | 152 | ASP | C-N-CA | -6.82 | 110.11 | 121.63 | 9 | 10 |
| 1 | I | 193 | ASN | CB-CG-ND2 | 6.81 | 126.61 | 116.40 | 5 | 2 |
| 1 | H | 161 | PHE | CA-CB-CG | -6.80 | 107.00 | 113.80 | 1 | 4 |
| 1 | I | 219 | GLN | N-CA-C | -6.77 | 104.88 | 113.01 | 7 | 4 |
| 1 | I | 155 | GLN | N-CA-CB | 6.74 | 121.16 | 110.23 | 6 | 1 |
| 1 | L | 152 | ASP | N-CA-CB | -6.72 | 101.79 | 111.54 | 2 | 4 |
| 1 | J | 194 | ALA | N-CA-C | 6.71 | 120.24 | 107.75 | 5 | 5 |
| 1 | L | 221 | VAL | CA-C-N | -6.67 | 113.53 | 122.54 | 5 | 5 |
| 1 | L | 221 | VAL | C-N-CA | -6.67 | 113.53 | 122.54 | 5 | 5 |
| 1 | H | 152 | ASP | CA-C-N | -6.66 | 112.55 | 122.01 | 9 | 9 |
| 1 | H | 152 | ASP | C-N-CA | -6.66 | 112.55 | 122.01 | 9 | 9 |
| 1 | I | 168 | PHE | N-CA-C | -6.65 | 104.11 | 111.36 | 1 | 2 |
| 1 | H | 221 | VAL | CA-C-N | -6.63 | 113.59 | 122.54 | 4 | 5 |
| 1 | H | 221 | VAL | C-N-CA | -6.63 | 113.59 | 122.54 | 4 | 5 |
| 1 | J | 152 | ASP | N-CA-CB | -6.62 | 101.06 | 111.39 | 10 | 1 |
| 1 | I | 222 | GLY | CA-C-N | -6.58 | 111.54 | 121.87 | 1 | 9 |
| 1 | I | 222 | GLY | C-N-CA | -6.58 | 111.54 | 121.87 | 1 | 9 |
| 1 | J | 221 | VAL | CA-C-O | -6.49 | 113.82 | 121.80 | 4 | 6 |
| 1 | H | 150 | ILE | CA-C-O | 6.49 | 128.89 | 120.78 | 2 | 1 |
| 1 | L | 151 | LEU | CA-C-O | -6.46 | 114.03 | 120.82 | 5 | 1 |
| 1 | L | 150 | ILE | N-CA-CB | 6.43 | 121.84 | 111.23 | 8 | 3 |
| 1 | I | 165 | VAL | N-CA-C | -6.38 | 104.11 | 110.62 | 3 | 2 |
| 1 | L | 201 | ILE | CB-CA-C | -6.36 | 103.82 | 111.97 | 2 | 6 |
| 1 | L | 193 | ASN | CA-CB-CG | -6.32 | 106.28 | 112.60 | 5 | 2 |
| 1 | I | 228 | ALA | N-CA-C | -6.26 | 104.46 | 111.28 | 2 | 3 |
| 1 | J | 222 | GLY | CA-C-N | -6.25 | 112.05 | 121.87 | 6 | 8 |
| 1 | J | 222 | GLY | C-N-CA | -6.25 | 112.05 | 121.87 | 6 | 8 |
| 1 | H | 205 | LEU | CB-CA-C | -6.25 | 101.02 | 110.90 | 8 | 2 |
| 1 | L | 222 | GLY | CA-C-O | -6.24 | 117.27 | 122.33 | 7 | 3 |
| 1 | H | 230 | VAL | N-CA-C | 6.23 | 117.72 | 110.62 | 1 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | L | 219 | GLN | N-CA-C | -6.22 | 104.55 | 111.71 | 2 | 10 |
| 1 | H | 151 | LEU | CA-C-O | -6.22 | 113.96 | 120.55 | 6 | 3 |
| 1 | L | 184 | TRP | N-CA-CB | 6.22 | 119.09 | 110.07 | 5 | 1 |
| 1 | J | 221 | VAL | CA-C-N | -6.19 | 114.18 | 122.54 | 10 | 5 |
| 1 | J | 221 | VAL | C-N-CA | -6.19 | 114.18 | 122.54 | 10 | 5 |
| 1 | H | 200 | THR | N-CA-C | -6.19 | 104.61 | 111.36 | 3 | 1 |
| 1 | K | 222 | GLY | CA-C-N | -6.18 | 112.16 | 121.87 | 6 | 9 |
| 1 | K | 222 | GLY | C-N-CA | -6.18 | 112.16 | 121.87 | 6 | 9 |
| 1 | K | 221 | VAL | CA-C-N | -6.18 | 114.20 | 122.54 | 6 | 2 |
| 1 | K | 221 | VAL | C-N-CA | -6.18 | 114.20 | 122.54 | 6 | 2 |
| 1 | I | 189 | LEU | N-CA-CB | 6.17 | 119.28 | 110.16 | 2 | 2 |
| 1 | J | 154 | ARG | N-CA-C | 6.15 | 118.96 | 109.07 | 7 | 4 |
| 1 | H | 228 | ALA | N-CA-C | -6.14 | 104.59 | 111.28 | 5 | 1 |
| 1 | L | 192 | GLN | N-CA-C | 6.12 | 117.95 | 111.28 | 8 | 5 |
| 1 | H | 194 | ALA | CA-C-O | -6.07 | 114.30 | 122.44 | 5 | 1 |
| 1 | L | 194 | ALA | N-CA-C | 6.07 | 119.67 | 107.41 | 6 | 6 |
| 1 | G | 221 | VAL | CA-C-N | -6.06 | 114.36 | 122.54 | 5 | 8 |
| 1 | G | 221 | VAL | C-N-CA | -6.06 | 114.36 | 122.54 | 5 | 8 |
| 1 | J | 153 | ILE | N-CA-C | -5.99 | 101.84 | 109.80 | 5 | 1 |
| 1 | I | 153 | ILE | N-CA-C | -5.97 | 101.86 | 109.80 | 8 | 3 |
| 1 | I | 153 | ILE | CA-C-O | -5.96 | 115.45 | 121.59 | 8 | 1 |
| 1 | L | 231 | LEU | N-CA-C | -5.93 | 104.72 | 111.07 | 8 | 4 |
| 1 | H | 226 | HIS | CA-CB-CG | -5.92 | 107.88 | 113.80 | 7 | 1 |
| 1 | H | 190 | LEU | N-CA-C | -5.91 | 105.33 | 112.54 | 3 | 3 |
| 1 | J | 150 | ILE | N-CA-CB | 5.88 | 120.94 | 111.23 | 6 | 3 |
| 1 | K | 172 | LEU | N-CA-C | -5.87 | 105.01 | 111.82 | 8 | 3 |
| 1 | I | 223 | GLY | CA-C-N | 5.86 | 126.00 | 119.32 | 9 | 2 |
| 1 | I | 223 | GLY | C-N-CA | 5.86 | 126.00 | 119.32 | 9 | 2 |
| 1 | L | 240 | ASN | N-CA-C | 5.85 | 120.22 | 111.96 | 4 | 10 |
| 1 | L | 193 | ASN | CB-CG-ND2 | 5.85 | 125.17 | 116.40 | 5 | 1 |
| 1 | J | 184 | TRP | N-CA-C | -5.78 | 104.98 | 111.28 | 4 | 1 |
| 1 | I | 198 | CYS | N-CA-C | -5.74 | 104.63 | 111.69 | 5 | 1 |
| 1 | I | 221 | VAL | CA-C-N | -5.74 | 114.94 | 122.63 | 10 | 2 |
| 1 | I | 221 | VAL | C-N-CA | -5.74 | 114.94 | 122.63 | 10 | 2 |
| 1 | L | 151 | LEU | CA-C-N | -5.74 | 113.49 | 122.73 | 4 | 3 |
| 1 | L | 151 | LEU | C-N-CA | -5.74 | 113.49 | 122.73 | 4 | 3 |
| 1 | K | 201 | ILE | CB-CA-C | -5.74 | 104.37 | 111.94 | 2 | 1 |
| 1 | J | 151 | LEU | CA-C-N | -5.73 | 114.01 | 122.83 | 1 | 4 |
| 1 | J | 151 | LEU | C-N-CA | -5.73 | 114.01 | 122.83 | 1 | 4 |
| 1 | I | 224 | PRO | N-CA-C | 5.70 | 124.22 | 112.47 | 7 | 1 |
| 1 | G | 222 | GLY | CA-C-N | -5.69 | 112.94 | 121.87 | 3 | 7 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | G | 222 | GLY | C-N-CA | -5.69 | 112.94 | 121.87 | 3 | 7 |
| 1 | I | 226 | HIS | CA-CB-CG | -5.67 | 108.12 | 113.80 | 7 | 1 |
| 1 | J | 205 | LEU | N-CA-C | -5.66 | 104.49 | 111.33 | 1 | 1 |
| 1 | L | 222 | GLY | CA-C-N | -5.64 | 113.02 | 121.87 | 5 | 7 |
| 1 | L | 222 | GLY | C-N-CA | -5.64 | 113.02 | 121.87 | 5 | 7 |
| 1 | J | 189 | LEU | N-CA-CB | 5.64 | 118.36 | 110.07 | 5 | 3 |
| 1 | H | 154 | ARG | N-CA-C | 5.63 | 118.62 | 108.48 | 8 | 2 |
| 1 | K | 237 | GLN | N-CA-C | -5.62 | 105.24 | 111.36 | 10 | 6 |
| 1 | K | 219 | GLN | N-CA-C | -5.61 | 105.70 | 112.54 | 3 | 3 |
| 1 | J | 189 | LEU | CB-CA-C | -5.60 | 101.84 | 110.81 | 2 | 2 |
| 1 | I | 193 | ASN | OD1-CG-ND2 | -5.57 | 117.03 | 122.60 | 5 | 1 |
| 1 | H | 150 | ILE | N-CA-CB | 5.56 | 120.41 | 111.23 | 2 | 1 |
| 1 | K | 240 | ASN | N-CA-C | 5.55 | 120.05 | 111.56 | 5 | 9 |
| 1 | H | 151 | LEU | CA-C-N | -5.53 | 113.83 | 122.73 | 5 | 1 |
| 1 | H | 151 | LEU | C-N-CA | -5.53 | 113.83 | 122.73 | 5 | 1 |
| 1 | I | 154 | ARG | N-CA-C | 5.52 | 118.81 | 109.76 | 4 | 4 |
| 1 | J | 151 | LEU | CA-C-O | -5.52 | 115.00 | 120.90 | 5 | 2 |
| 1 | J | 151 | LEU | N-CA-C | -5.51 | 104.91 | 111.69 | 4 | 1 |
| 1 | L | 222 | GLY | N-CA-C | 5.51 | 117.69 | 111.85 | 2 | 2 |
| 1 | J | 240 | ASN | N-CA-C | 5.50 | 119.97 | 111.56 | 9 | 2 |
| 1 | K | 169 | TYR | N-CA-C | -5.47 | 105.39 | 111.36 | 5 | 2 |
| 1 | K | 222 | GLY | CA-C-O | -5.47 | 116.84 | 121.66 | 2 | 2 |
| 1 | I | 240 | ASN | N-CA-C | 5.46 | 119.92 | 111.56 | 4 | 5 |
| 1 | I | 194 | ALA | N-CA-C | 5.45 | 118.10 | 108.24 | 7 | 2 |
| 1 | H | 201 | ILE | CB-CA-C | -5.45 | 104.85 | 111.87 | 7 | 1 |
| 1 | L | 189 | LEU | N-CA-C | -5.43 | 105.01 | 111.69 | 1 | 1 |
| 1 | J | 219 | GLN | N-CA-C | -5.42 | 105.93 | 112.54 | 5 | 1 |
| 1 | L | 221 | VAL | CA-C-O | -5.41 | 114.02 | 120.78 | 5 | 4 |
| 1 | G | 240 | ASN | N-CA-C | 5.39 | 119.81 | 111.56 | 1 | 10 |
| 1 | K | 205 | LEU | N-CA-C | -5.38 | 105.42 | 111.28 | 5 | 3 |
| 1 | L | 193 | ASN | CB-CA-C | -5.38 | 99.20 | 110.17 | 5 | 1 |
| 1 | G | 152 | ASP | CA-C-O | -5.35 | 114.08 | 120.55 | 5 | 4 |
| 1 | L | 205 | LEU | N-CA-C | -5.34 | 105.35 | 111.07 | 8 | 4 |
| 1 | J | 231 | LEU | N-CA-C | -5.32 | 105.56 | 111.36 | 5 | 1 |
| 1 | K | 172 | LEU | N-CA-CB | 5.32 | 118.55 | 110.14 | 3 | 1 |
| 1 | G | 194 | ALA | N-CA-C | 5.32 | 116.66 | 109.11 | 5 | 4 |
| 1 | G | 201 | ILE | CB-CA-C | -5.31 | 105.06 | 112.02 | 6 | 1 |
| 1 | H | 151 | LEU | CB-CA-C | 5.31 | 117.57 | 109.34 | 9 | 1 |
| 1 | H | 201 | ILE | N-CA-CB | 5.30 | 116.64 | 110.65 | 7 | 1 |
| 1 | L | 218 | CYS | CA-CB-SG | -5.30 | 102.22 | 114.40 | 7 | 1 |
| 1 | K | 168 | PHE | CA-CB-CG | -5.29 | 108.51 | 113.80 | 6 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | G | 218 | CYS | CA-CB-SG | -5.28 | 102.25 | 114.40 | 5 | 2 |
| 1 | G | 155 | GLN | OE1-CD-NE2 | -5.28 | 117.32 | 122.60 | 2 | 1 |
| 1 | I | 155 | GLN | CB-CA-C | -5.28 | 100.82 | 109.53 | 6 | 1 |
| 1 | H | 195 | ASN | CA-CB-CG | -5.26 | 107.34 | 112.60 | 6 | 1 |
| 1 | H | 157 | PRO | N-CA-C | -5.24 | 106.57 | 113.65 | 2 | 1 |
| 1 | H | 240 | ASN | N-CA-C | 5.23 | 119.56 | 111.56 | 5 | 4 |
| 1 | H | 193 | ASN | OD1-CG-ND2 | -5.23 | 117.37 | 122.60 | 8 | 1 |
| 1 | H | 188 | THR | N-CA-C | 5.21 | 119.61 | 112.68 | 9 | 1 |
| 1 | I | 184 | TRP | O-C-N | 5.21 | 127.72 | 122.09 | 6 | 1 |
| 1 | L | 153 | ILE | N-CA-C | -5.20 | 102.38 | 109.55 | 4 | 1 |
| 1 | H | 220 | GLY | N-CA-C | -5.19 | 106.44 | 113.24 | 8 | 4 |
| 1 | J | 237 | GLN | N-CA-C | -5.18 | 105.72 | 111.36 | 5 | 1 |
| 1 | H | 198 | CYS | N-CA-CB | 5.18 | 117.58 | 110.07 | 8 | 1 |
| 1 | J | 226 | HIS | CA-CB-CG | -5.14 | 108.66 | 113.80 | 1 | 1 |
| 1 | G | 220 | GLY | N-CA-C | -5.09 | 109.07 | 114.67 | 7 | 1 |
| 1 | I | 205 | LEU | N-CA-C | -5.08 | 105.74 | 111.28 | 8 | 1 |
| 1 | H | 148 | THR | N-CA-C | 5.08 | 118.21 | 111.30 | 7 | 1 |
| 1 | I | 237 | GLN | N-CA-C | -5.08 | 105.82 | 111.36 | 10 | 1 |
| 1 | H | 195 | ASN | CA-C-N | 5.07 | 126.18 | 119.84 | 9 | 1 |
| 1 | H | 195 | ASN | C-N-CA | 5.07 | 126.18 | 119.84 | 9 | 1 |
| 1 | L | 154 | ARG | N-CA-C | 5.04 | 118.34 | 110.32 | 8 | 1 |
| 1 | J | 168 | PHE | CA-CB-CG | -5.02 | 108.78 | 113.80 | 3 | 1 |
| 1 | K | 198 | CYS | N-CA-C | -5.01 | 106.00 | 111.82 | 2 | 2 |
| 1 | L | 189 | LEU | O-C-N | 5.01 | 127.50 | 122.09 | 4 | 1 |

There are no chirality outliers.

All unique planar outliers are listed below.

| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1 | I | 162 | ARG | Sidechain | 1 |

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | G | 756 | 761 | 761 | 12±3 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | H | 759 | 765 | 765 | 21±4 |
| 1 | I | 700 | 707 | 707 | 18±6 |
| 1 | J | 739 | 747 | 747 | 13±4 |
| 1 | K | 728 | 729 | 726 | 13±3 |
| 1 | L | 759 | 765 | 765 | 14±2 |
| 3 | H | 33 | 29 | 0 | 0±1 |
| All | All | 45100 | 45090 | 44770 | 868 |

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 10.

All unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:L:150:ILE:HD11 | 1:L:171:THR:HG23 | 0.87 | 1.44 | 6 | 4 |
| 1:G:234:ALA:HB1 | 1:H:232:ALA:HB2 | 0.85 | 1.47 | 1 | 7 |
| 1:H:234:ALA:HB1 | 1:I:232:ALA:HB2 | 0.80 | 1.53 | 9 | 2 |
| 1:I:153:ILE:HG22 | 1:I:189:LEU:HD21 | 0.79 | 1.53 | 9 | 3 |
| 1:H:152:ASP:HA | 1:H:189:LEU:HD11 | 0.79 | 1.54 | 2 | 1 |
| 1:H:234:ALA:HB3 | 1:I:231:LEU:HD23 | 0.77 | 1.57 | 8 | 1 |
| 1:I:165:VAL:HG22 | 1:I:190:LEU:HD11 | 0.76 | 1.55 | 6 | 3 |
| 1:L:165:VAL:HG22 | 1:L:190:LEU:HD11 | 0.75 | 1.58 | 8 | 3 |
| 1:K:165:VAL:HG22 | 1:K:190:LEU:HD11 | 0.75 | 1.59 | 1 | 4 |
| 1:K:235:MET:SD | 1:L:235:MET:HE2 | 0.74 | 2.23 | 4 | 2 |
| 1:H:164:TYR:CE2 | 1:H:190:LEU:HD12 | 0.73 | 2.19 | 8 | 10 |
| 1:J:165:VAL:HG22 | 1:J:190:LEU:HD11 | 0.73 | 1.59 | 5 | 4 |
| 1:J:153:ILE:HG22 | 1:J:189:LEU:HD21 | 0.73 | 1.59 | 10 | 3 |
| 1:L:150:ILE:HG23 | 1:L:189:LEU:HD22 | 0.72 | 1.61 | 4 | 2 |
| 1:K:205:LEU:HD11 | 1:K:217:ALA:HB2 | 0.72 | 1.59 | 8 | 4 |
| 1:J:153:ILE:HG23 | 1:J:164:TYR:CE1 | 0.72 | 2.20 | 7 | 3 |
| 1:K:191:VAL:HG22 | 1:K:202:LEU:HD23 | 0.71 | 1.62 | 2 | 3 |
| 1:K:182:LYS:O | 1:K:186:THR:HG23 | 0.70 | 1.86 | 10 | 9 |
| 1:G:182:LYS:O | 1:G:186:THR:HG23 | 0.70 | 1.87 | 3 | 10 |
| 1:H:153:ILE:HG23 | 1:H:164:TYR:CE1 | 0.70 | 2.21 | 2 | 2 |
| 1:J:182:LYS:O | 1:J:186:THR:HG23 | 0.70 | 1.87 | 1 | 6 |
| 1:L:182:LYS:O | 1:L:186:THR:HG23 | 0.70 | 1.87 | 1 | 10 |
| 1:H:168:PHE:CD2 | 1:H:190:LEU:HD13 | 0.69 | 2.21 | 8 | 4 |
| 1:H:165:VAL:HG22 | 1:H:190:LEU:HD11 | 0.69 | 1.64 | 6 | 2 |
| 1:H:191:VAL:HG22 | 1:H:202:LEU:HD23 | 0.69 | 1.64 | 2 | 2 |
| 1:L:184:TRP:CH2 | 1:L:189:LEU:HD23 | 0.69 | 2.23 | 7 | 1 |
| 1:H:182:LYS:O | 1:H:186:THR:HG23 | 0.69 | 1.87 | 2 | 6 |
| 1:I:153:ILE:CG2 | 1:I:189:LEU:HD21 | 0.69 | 2.18 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:I:161:PHE:O | 1:I:165:VAL:HG23 | 0.68 | 1.88 | 9 | 6 |
| 1:G:209:ALA:O | 1:G:214:MET:HE2 | 0.68 | 1.88 | 8 | 4 |
| 1:L:150:ILE:HG22 | 1:L:189:LEU:HD23 | 0.68 | 1.66 | 8 | 2 |
| 1:J:150:ILE:HD11 | 1:J:168:PHE:O | 0.68 | 1.89 | 3 | 1 |
| 1:H:172:LEU:HD21 | 1:H:185:MET:SD | 0.68 | 2.29 | 8 | 8 |
| 1:L:184:TRP:CZ2 | 1:L:189:LEU:HD22 | 0.67 | 2.24 | 2 | 2 |
| 1:L:153:ILE:HG21 | 1:L:168:PHE:HB2 | 0.67 | 1.65 | 4 | 2 |
| 1:K:161:PHE:CE1 | 1:K:202:LEU:HD11 | 0.67 | 2.24 | 9 | 5 |
| 1:J:168:PHE:CE1 | 1:J:186:THR:HG22 | 0.67 | 2.24 | 5 | 4 |
| 1:J:153:ILE:HD13 | 1:J:171:THR:HG21 | 0.67 | 1.64 | 6 | 2 |
| 1:H:234:ALA:CB | 1:I:232:ALA:HB2 | 0.66 | 2.20 | 9 | 2 |
| 1:G:238:VAL:HG21 | 1:H:235:MET:CB | 0.66 | 2.20 | 2 | 2 |
| 1:H:197:ASP:HB2 | 1:H:221:VAL:HG13 | 0.66 | 1.68 | 1 | 5 |
| 1:I:189:LEU:HD11 | 1:I:193:ASN:ND2 | 0.65 | 2.07 | 6 | 3 |
| 1:K:198:CYS:SG | 1:K:202:LEU:HD22 | 0.65 | 2.32 | 5 | 1 |
| 1:G:235:MET:SD | 1:H:235:MET:HE2 | 0.65 | 2.32 | 3 | 4 |
| 1:K:201:ILE:CG2 | 1:K:217:ALA:HB1 | 0.64 | 2.22 | 8 | 3 |
| 1:I:202:LEU:HD23 | 1:I:214:MET:SD | 0.64 | 2.32 | 8 | 2 |
| 1:I:190:LEU:O | 1:I:194:ALA:HB3 | 0.64 | 1.93 | 8 | 4 |
| 1:L:161:PHE:O | 1:L:165:VAL:HG23 | 0.64 | 1.93 | 4 | 9 |
| 1:K:161:PHE:O | 1:K:165:VAL:HG23 | 0.63 | 1.93 | 8 | 4 |
| 1:L:168:PHE:CE1 | 1:L:172:LEU:HD11 | 0.63 | 2.27 | 8 | 3 |
| 1:H:153:ILE:HG22 | 1:H:189:LEU:CD2 | 0.63 | 2.22 | 2 | 1 |
| 1:I:153:ILE:HG22 | 1:I:189:LEU:CD2 | 0.62 | 2.24 | 4 | 1 |
| 1:G:238:VAL:HG21 | 1:H:235:MET:HB2 | 0.62 | 1.72 | 4 | 2 |
| 1:I:187:GLU:O | 1:I:191:VAL:HG23 | 0.62 | 1.93 | 7 | 6 |
| 1:I:189:LEU:HD11 | 1:I:193:ASN:HD21 | 0.62 | 1.54 | 3 | 1 |
| 1:H:161:PHE:O | 1:H:165:VAL:HG23 | 0.62 | 1.94 | 6 | 3 |
| 1:K:197:ASP:O | 1:K:200:THR:HG22 | 0.62 | 1.95 | 2 | 2 |
| 1:I:189:LEU:HD21 | 1:I:193:ASN:OD1 | 0.62 | 1.95 | 8 | 1 |
| 1:L:151:LEU:O | 1:L:189:LEU:HD21 | 0.62 | 1.95 | 2 | 1 |
| 1:I:184:TRP:CZ3 | 1:I:188:THR:HG22 | 0.62 | 2.29 | 9 | 3 |
| 1:J:187:GLU:O | 1:J:191:VAL:HG23 | 0.62 | 1.95 | 3 | 1 |
| 1:L:150:ILE:O | 1:L:189:LEU:HD23 | 0.61 | 1.94 | 8 | 2 |
| 1:I:175:GLU:OE1 | 1:I:177:ALA:HB2 | 0.61 | 1.95 | 2 | 1 |
| 1:J:153:ILE:HG21 | 1:J:168:PHE:HB2 | 0.61 | 1.70 | 6 | 6 |
| 1:H:209:ALA:O | 1:H:214:MET:HE2 | 0.61 | 1.95 | 9 | 3 |
| 1:K:168:PHE:CE1 | 1:K:186:THR:HG22 | 0.60 | 2.31 | 4 | 9 |
| 1:H:205:LEU:HD11 | 1:H:217:ALA:CB | 0.60 | 2.27 | 8 | 2 |
| 1:J:189:LEU:HD21 | 1:J:193:ASN:CG | 0.60 | 2.21 | 7 | 2 |
| 1:L:165:VAL:HG13 | 1:L:168:PHE:CE2 | 0.60 | 2.32 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:G:234:ALA:CB | 1:H:232:ALA:HB2 | 0.60 | 2.25 | 1 | 1 |
| 1:I:184:TRP:CZ2 | 1:I:189:LEU:HD12 | 0.60 | 2.32 | 4 | 4 |
| 1:I:189:LEU:HD11 | 1:I:193:ASN:OD1 | 0.60 | 1.96 | 5 | 3 |
| 1:J:168:PHE:CE1 | 1:J:172:LEU:HD11 | 0.60 | 2.32 | 1 | 7 |
| 1:H:197:ASP:O | 1:H:200:THR:HG22 | 0.59 | 1.97 | 7 | 3 |
| 1:G:205:LEU:HD11 | 1:G:217:ALA:CB | 0.59 | 2.27 | 6 | 1 |
| 1:H:150:ILE:HG23 | 1:H:189:LEU:HD22 | 0.59 | 1.74 | 2 | 5 |
| 1:H:153:ILE:N | 1:H:189:LEU:HD21 | 0.59 | 2.13 | 2 | 1 |
| 1:L:167:ARG:O | 1:L:171:THR:HG22 | 0.59 | 1.97 | 6 | 1 |
| 1:I:155:GLN:HE21 | 1:I:194:ALA:HB1 | 0.59 | 1.57 | 8 | 1 |
| 1:J:150:ILE:HG23 | 1:J:189:LEU:HG | 0.59 | 1.74 | 7 | 1 |
| 1:K:205:LEU:CD1 | 1:K:217:ALA:HB2 | 0.59 | 2.28 | 8 | 3 |
| 1:L:184:TRP:HZ2 | 1:L:189:LEU:HD22 | 0.59 | 1.58 | 8 | 2 |
| 1:L:168:PHE:CZ | 1:L:186:THR:HG22 | 0.58 | 2.33 | 5 | 6 |
| 1:K:184:TRP:CZ2 | 1:K:185:MET:HE3 | 0.58 | 2.33 | 3 | 1 |
| 1:L:189:LEU:HD13 | 1:L:189:LEU:O | 0.58 | 1.97 | 7 | 2 |
| 1:J:205:LEU:HD11 | 1:J:217:ALA:HB3 | 0.58 | 1.74 | 7 | 3 |
| 1:K:205:LEU:HD11 | 1:K:217:ALA:CB | 0.58 | 2.29 | 1 | 5 |
| 1:H:153:ILE:HG23 | 1:H:164:TYR:HE1 | 0.57 | 1.59 | 2 | 1 |
| 1:L:150:ILE:HD13 | 1:L:172:LEU:HG | 0.57 | 1.76 | 7 | 1 |
| 1:L:168:PHE:CE1 | 1:L:186:THR:HG22 | 0.57 | 2.35 | 10 | 2 |
| 1:L:205:LEU:HD11 | 1:L:217:ALA:HB3 | 0.56 | 1.75 | 3 | 5 |
| 1:H:177:ALA:HB3 | 1:H:182:LYS:HE3 | 0.56 | 1.77 | 5 | 2 |
| 1:I:164:TYR:CZ | 1:I:194:ALA:HB2 | 0.56 | 2.34 | 6 | 1 |
| 1:I:165:VAL:HG13 | 1:I:168:PHE:CD2 | 0.56 | 2.36 | 2 | 3 |
| 1:H:150:ILE:C | 1:H:151:LEU:HD12 | 0.56 | 2.25 | 9 | 1 |
| 1:G:191:VAL:HG22 | 1:G:202:LEU:HD23 | 0.56 | 1.77 | 3 | 6 |
| 1:K:205:LEU:HD11 | 1:K:217:ALA:HB3 | 0.56 | 1.77 | 1 | 2 |
| 1:K:161:PHE:CZ | 1:K:202:LEU:HD11 | 0.56 | 2.36 | 10 | 1 |
| 1:L:153:ILE:HG21 | 1:L:168:PHE:CB | 0.56 | 2.31 | 10 | 1 |
| 1:L:165:VAL:HG13 | 1:L:168:PHE:CD2 | 0.55 | 2.36 | 9 | 1 |
| 1:H:209:ALA:N | 1:H:214:MET:HE3 | 0.55 | 2.16 | 7 | 3 |
| 1:G:211:LEU:HD22 | 1:G:214:MET:HE3 | 0.55 | 1.78 | 6 | 2 |
| 1:H:209:ALA:HB3 | 1:H:214:MET:HG3 | 0.55 | 1.79 | 4 | 10 |
| 3:H:302:A1CCZ:C14 | 1:I:231:LEU:HD22 | 0.55 | 2.31 | 9 | 2 |
| 1:I:189:LEU:HD11 | 1:I:193:ASN:CG | 0.55 | 2.26 | 10 | 2 |
| 1:K:171:THR:O | 1:K:174:ALA:HB3 | 0.55 | 2.02 | 10 | 7 |
| 1:H:150:ILE:HG21 | 1:H:185:MET:CG | 0.55 | 2.32 | 9 | 1 |
| 1:I:226:HIS:CE1 | 1:I:230:VAL:HG21 | 0.55 | 2.35 | 7 | 2 |
| 1:K:177:ALA:HB3 | 1:K:182:LYS:CG | 0.55 | 2.32 | 1 | 3 |
| 1:H:168:PHE:CZ | 1:H:186:THR:HG22 | 0.55 | 2.36 | 2 | 7 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:J:161:PHE:CZ | 1:J:165:VAL:HG21 | 0.55 | 2.36 | 5 | 1 |
| 1:I:191:VAL:CG2 | 1:I:202:LEU:HD22 | 0.55 | 2.31 | 8 | 1 |
| 1:J:155:GLN:NE2 | 1:J:221:VAL:HG11 | 0.54 | 2.17 | 4 | 3 |
| 1:H:164:TYR:HE2 | 1:H:190:LEU:HD12 | 0.54 | 1.59 | 9 | 4 |
| 1:H:189:LEU:HD21 | 1:H:193:ASN:OD1 | 0.54 | 2.02 | 6 | 6 |
| 1:G:161:PHE:O | 1:G:165:VAL:HG23 | 0.54 | 2.03 | 5 | 10 |
| 1:I:155:GLN:NE2 | 1:I:221:VAL:HG11 | 0.54 | 2.18 | 4 | 3 |
| 1:H:177:ALA:HB3 | 1:H:182:LYS:CE | 0.54 | 2.33 | 5 | 2 |
| 1:K:187:GLU:O | 1:K:191:VAL:HG23 | 0.54 | 2.03 | 3 | 1 |
| 1:J:153:ILE:HG23 | 1:J:164:TYR:HE1 | 0.54 | 1.62 | 7 | 2 |
| 1:H:187:GLU:O | 1:H:191:VAL:HG23 | 0.53 | 2.02 | 2 | 3 |
| 1:K:198:CYS:HB2 | 1:K:202:LEU:HD13 | 0.53 | 1.80 | 2 | 1 |
| 1:I:229:ARG:O | 1:I:232:ALA:HB3 | 0.53 | 2.03 | 5 | 1 |
| 1:L:150:ILE:CD1 | 1:L:171:THR:HG23 | 0.53 | 2.27 | 6 | 2 |
| 1:I:164:TYR:CE2 | 1:I:190:LEU:HD12 | 0.53 | 2.39 | 6 | 2 |
| 1:H:234:ALA:CB | 1:I:231:LEU:HD23 | 0.53 | 2.33 | 8 | 1 |
| 1:I:168:PHE:CE1 | 1:I:186:THR:HG22 | 0.53 | 2.39 | 8 | 4 |
| 1:H:237:GLN:O | 1:H:242:ALA:HB3 | 0.53 | 2.04 | 4 | 8 |
| 1:G:165:VAL:HG22 | 1:G:190:LEU:HD11 | 0.53 | 1.80 | 9 | 5 |
| 1:G:172:LEU:HD21 | 1:G:185:MET:SD | 0.52 | 2.44 | 7 | 3 |
| 1:I:153:ILE:HG21 | 1:I:168:PHE:HB2 | 0.52 | 1.81 | 10 | 3 |
| 1:I:196:PRO:O | 1:I:200:THR:HG22 | 0.52 | 2.04 | 3 | 3 |
| 1:I:168:PHE:CD1 | 1:I:172:LEU:HD11 | 0.52 | 2.40 | 6 | 1 |
| 1:H:168:PHE:O | 1:H:172:LEU:HD12 | 0.52 | 2.05 | 10 | 7 |
| 1:H:202:LEU:HD21 | 1:H:214:MET:SD | 0.52 | 2.45 | 2 | 1 |
| 1:I:227:LYS:NZ | 1:J:228:ALA:HB2 | 0.52 | 2.20 | 5 | 1 |
| 1:G:231:LEU:HD12 | 1:H:231:LEU:HD22 | 0.52 | 1.81 | 7 | 1 |
| 1:G:168:PHE:CZ | 1:G:186:THR:HG22 | 0.52 | 2.40 | 2 | 10 |
| 1:J:168:PHE:CZ | 1:J:186:THR:HG22 | 0.52 | 2.40 | 4 | 7 |
| 1:J:171:THR:O | 1:J:174:ALA:HB3 | 0.51 | 2.06 | 5 | 2 |
| 1:I:198:CYS:SG | 1:I:202:LEU:HD22 | 0.51 | 2.45 | 3 | 1 |
| 1:J:205:LEU:HD11 | 1:J:217:ALA:CB | 0.51 | 2.35 | 7 | 2 |
| 1:J:202:LEU:HG | 1:J:214:MET:HE3 | 0.51 | 1.81 | 5 | 2 |
| 1:I:202:LEU:HD21 | 1:I:214:MET:HB3 | 0.51 | 1.81 | 6 | 1 |
| 1:I:182:LYS:O | 1:I:186:THR:HG23 | 0.51 | 2.05 | 5 | 5 |
| 1:K:177:ALA:HB1 | 1:K:181:VAL:CG1 | 0.51 | 2.36 | 6 | 5 |
| 1:I:164:TYR:OH | 1:I:189:LEU:HD23 | 0.51 | 2.05 | 2 | 1 |
| 1:H:226:HIS:O | 1:H:230:VAL:HG22 | 0.51 | 2.06 | 7 | 1 |
| 1:I:155:GLN:OE1 | 1:I:221:VAL:HG11 | 0.51 | 2.05 | 8 | 3 |
| 1:K:218:CYS:O | 1:K:221:VAL:HG23 | 0.51 | 2.06 | 8 | 3 |
| 1:K:197:ASP:HB2 | 1:K:221:VAL:HG13 | 0.51 | 1.83 | 3 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:H:191:VAL:CG2 | 1:H:202:LEU:HD23 | 0.51 | 2.36 | 2 | 1 |
| 1:L:184:TRP:CZ3 | 1:L:188:THR:HG22 | 0.51 | 2.41 | 5 | 1 |
| 1:J:153:ILE:HG22 | 1:J:189:LEU:CD2 | 0.50 | 2.36 | 6 | 3 |
| 1:I:202:LEU:HG | 1:I:214:MET:HE2 | 0.50 | 1.82 | 10 | 2 |
| 1:K:155:GLN:CB | 1:K:194:ALA:HB1 | 0.50 | 2.36 | 10 | 1 |
| 1:H:184:TRP:CZ2 | 1:H:189:LEU:HD22 | 0.50 | 2.41 | 8 | 2 |
| 1:L:153:ILE:HG23 | 1:L:164:TYR:OH | 0.50 | 2.05 | 10 | 1 |
| 1:I:165:VAL:HG13 | 1:I:168:PHE:CE2 | 0.50 | 2.41 | 2 | 3 |
| 1:K:235:MET:SD | 1:L:235:MET:HE3 | 0.50 | 2.46 | 6 | 1 |
| 1:I:237:GLN:O | 1:I:242:ALA:HB3 | 0.50 | 2.07 | 2 | 5 |
| 1:H:189:LEU:HD11 | 1:H:193:ASN:OD1 | 0.50 | 2.07 | 1 | 4 |
| 1:H:198:CYS:O | 1:H:202:LEU:HD13 | 0.50 | 2.06 | 2 | 1 |
| 1:K:168:PHE:HE1 | 1:K:186:THR:HG22 | 0.50 | 1.67 | 7 | 9 |
| 1:K:191:VAL:HG22 | 1:K:202:LEU:HD13 | 0.50 | 1.84 | 4 | 2 |
| 1:G:198:CYS:SG | 1:G:202:LEU:HD12 | 0.50 | 2.47 | 6 | 1 |
| 1:J:161:PHE:O | 1:J:165:VAL:HG23 | 0.50 | 2.06 | 7 | 3 |
| 1:H:153:ILE:HG22 | 1:H:189:LEU:HD23 | 0.50 | 1.84 | 2 | 2 |
| 1:G:232:ALA:HB2 | 1:L:237:GLN:OE1 | 0.49 | 2.07 | 2 | 1 |
| 1:L:150:ILE:HG21 | 1:L:185:MET:CG | 0.49 | 2.37 | 4 | 1 |
| 1:H:191:VAL:HG22 | 1:H:202:LEU:HD22 | 0.49 | 1.83 | 1 | 1 |
| 1:I:177:ALA:HB3 | 1:I:182:LYS:CE | 0.49 | 2.37 | 2 | 2 |
| 1:J:177:ALA:HB3 | 1:J:182:LYS:CG | 0.49 | 2.37 | 5 | 2 |
| 1:J:168:PHE:HE1 | 1:J:186:THR:HG22 | 0.49 | 1.63 | 5 | 1 |
| 1:L:202:LEU:HD23 | 1:L:214:MET:SD | 0.49 | 2.47 | 9 | 8 |
| 1:L:237:GLN:HA | 1:L:242:ALA:HB3 | 0.49 | 1.83 | 9 | 8 |
| 1:L:164:TYR:CE2 | 1:L:194:ALA:HB2 | 0.49 | 2.42 | 8 | 2 |
| 1:G:191:VAL:HG22 | 1:G:202:LEU:CD2 | 0.49 | 2.38 | 9 | 8 |
| 1:J:184:TRP:CZ3 | 1:J:188:THR:HG22 | 0.49 | 2.42 | 6 | 3 |
| 1:I:231:LEU:HD11 | 1:I:235:MET:HE2 | 0.49 | 1.83 | 5 | 1 |
| 1:I:184:TRP:HZ2 | 1:I:189:LEU:HD12 | 0.49 | 1.66 | 4 | 3 |
| 1:L:168:PHE:O | 1:L:172:LEU:HD12 | 0.49 | 2.08 | 7 | 1 |
| 1:I:148:THR:HB | 1:I:153:ILE:HD13 | 0.49 | 1.85 | 2 | 1 |
| 1:K:237:GLN:O | 1:K:242:ALA:HB3 | 0.49 | 2.08 | 9 | 4 |
| 1:I:153:ILE:HD13 | 1:I:171:THR:HG21 | 0.49 | 1.85 | 1 | 1 |
| 1:I:194:ALA:HB3 | 1:I:198:CYS:SG | 0.49 | 2.47 | 1 | 1 |
| 1:J:164:TYR:CE2 | 1:J:194:ALA:HB2 | 0.49 | 2.42 | 3 | 2 |
| 1:L:150:ILE:HG21 | 1:L:185:MET:HG2 | 0.49 | 1.84 | 4 | 1 |
| 1:J:165:VAL:HG13 | 1:J:168:PHE:CE2 | 0.49 | 2.42 | 7 | 2 |
| 1:J:237:GLN:O | 1:J:242:ALA:HB3 | 0.48 | 2.08 | 5 | 1 |
| 1:H:164:TYR:CE2 | 1:H:194:ALA:HB2 | 0.48 | 2.41 | 3 | 5 |
| 1:H:177:ALA:HB1 | 1:H:181:VAL:CG1 | 0.48 | 2.37 | 2 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:L:237:GLN:CA | 1:L:242:ALA:HB3 | 0.48 | 2.38 | 5 | 9 |
| 1:G:205:LEU:HD11 | 1:G:217:ALA:HB3 | 0.48 | 1.85 | 6 | 2 |
| 1:G:150:ILE:HG21 | 1:G:185:MET:HB3 | 0.48 | 1.83 | 5 | 1 |
| 1:J:165:VAL:HG13 | 1:J:168:PHE:CD2 | 0.48 | 2.44 | 7 | 1 |
| 1:G:151:LEU:H | 1:G:151:LEU:HD12 | 0.48 | 1.69 | 3 | 7 |
| 1:L:205:LEU:HD11 | 1:L:217:ALA:HB2 | 0.48 | 1.84 | 9 | 1 |
| 1:G:153:ILE:HD13 | 1:G:171:THR:HG21 | 0.48 | 1.85 | 9 | 5 |
| 1:I:227:LYS:HZ1 | 1:J:228:ALA:HB2 | 0.48 | 1.69 | 5 | 1 |
| 1:K:198:CYS:O | 1:K:202:LEU:HD13 | 0.48 | 2.08 | 7 | 2 |
| 1:G:226:HIS:CE1 | 1:G:230:VAL:HG11 | 0.48 | 2.42 | 7 | 3 |
| 1:J:153:ILE:HD13 | 1:J:171:THR:CG2 | 0.48 | 2.37 | 6 | 1 |
| 1:I:197:ASP:O | 1:I:200:THR:HG22 | 0.48 | 2.09 | 8 | 3 |
| 1:L:205:LEU:HD11 | 1:L:217:ALA:CB | 0.48 | 2.39 | 3 | 1 |
| 1:I:198:CYS:SG | 1:I:202:LEU:HD12 | 0.48 | 2.49 | 6 | 2 |
| 1:H:150:ILE:HG22 | 1:H:150:ILE:O | 0.47 | 2.09 | 2 | 1 |
| 1:I:184:TRP:HZ3 | 1:I:188:THR:HG22 | 0.47 | 1.68 | 3 | 3 |
| 1:J:153:ILE:HG23 | 1:J:164:TYR:OH | 0.47 | 2.09 | 6 | 1 |
| 1:L:172:LEU:HD21 | 1:L:185:MET:SD | 0.47 | 2.50 | 3 | 2 |
| 1:I:237:GLN:OE1 | 1:J:232:ALA:HB1 | 0.47 | 2.09 | 5 | 1 |
| 1:H:209:ALA:HB1 | 1:H:213:GLU:CG | 0.47 | 2.39 | 3 | 4 |
| 1:I:211:LEU:O | 1:I:211:LEU:HD13 | 0.47 | 2.10 | 8 | 2 |
| 1:L:189:LEU:HD21 | 1:L:193:ASN:ND2 | 0.47 | 2.25 | 3 | 1 |
| 1:K:177:ALA:HB1 | 1:K:181:VAL:HG11 | 0.47 | 1.86 | 5 | 4 |
| 1:G:205:LEU:HD13 | 1:G:213:GLU:HG3 | 0.47 | 1.85 | 6 | 1 |
| 1:J:150:ILE:HG21 | 1:J:185:MET:HB3 | 0.47 | 1.86 | 7 | 1 |
| 1:J:150:ILE:HG21 | 1:J:185:MET:CB | 0.47 | 2.40 | 7 | 1 |
| 1:J:189:LEU:HD13 | 1:J:190:LEU:N | 0.47 | 2.25 | 4 | 2 |
| 1:H:168:PHE:HZ | 1:H:186:THR:HG22 | 0.47 | 1.67 | 9 | 7 |
| 1:I:168:PHE:O | 1:I:172:LEU:HD12 | 0.47 | 2.10 | 4 | 3 |
| 1:H:168:PHE:CD1 | 1:H:172:LEU:HD12 | 0.47 | 2.44 | 9 | 1 |
| 1:H:153:ILE:HD11 | 1:H:167:ARG:HB3 | 0.46 | 1.86 | 6 | 1 |
| 1:I:197:ASP:HB2 | 1:I:221:VAL:HG13 | 0.46 | 1.87 | 2 | 2 |
| 1:I:198:CYS:HB3 | 1:I:221:VAL:HG21 | 0.46 | 1.87 | 9 | 2 |
| 1:K:190:LEU:O | 1:K:194:ALA:HB3 | 0.46 | 2.10 | 1 | 1 |
| 1:H:191:VAL:HG22 | 1:H:202:LEU:CD2 | 0.46 | 2.37 | 2 | 2 |
| 1:K:191:VAL:HG22 | 1:K:202:LEU:HD22 | 0.46 | 1.87 | 9 | 1 |
| 1:L:150:ILE:N | 1:L:150:ILE:HD12 | 0.46 | 2.25 | 6 | 3 |
| 1:G:226:HIS:O | 1:G:230:VAL:HG22 | 0.46 | 2.11 | 9 | 1 |
| 1:H:197:ASP:CB | 1:H:221:VAL:HG13 | 0.46 | 2.39 | 8 | 2 |
| 1:G:226:HIS:CE1 | 1:G:230:VAL:HG21 | 0.46 | 2.46 | 1 | 2 |
| 1:J:161:PHE:CZ | 1:J:190:LEU:HD21 | 0.46 | 2.44 | 2 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:L:201:ILE:HG21 | 1:L:218:CYS:SG | 0.46 | 2.50 | 5 | 1 |
| 1:I:198:CYS:O | 1:I:202:LEU:HD12 | 0.46 | 2.11 | 9 | 2 |
| 1:L:184:TRP:CZ2 | 1:L:189:LEU:HD13 | 0.46 | 2.46 | 10 | 1 |
| 1:I:161:PHE:CZ | 1:I:190:LEU:HD21 | 0.46 | 2.46 | 4 | 7 |
| 1:K:218:CYS:SG | 1:K:221:VAL:HG21 | 0.46 | 2.50 | 2 | 1 |
| 1:H:190:LEU:CD2 | 1:H:214:MET:HE1 | 0.46 | 2.41 | 6 | 1 |
| 1:H:237:GLN:HA | 1:H:242:ALA:HB3 | 0.46 | 1.88 | 1 | 1 |
| 1:I:172:LEU:HD21 | 1:I:185:MET:SD | 0.46 | 2.51 | 1 | 5 |
| 1:K:164:TYR:CE2 | 1:K:194:ALA:HB2 | 0.46 | 2.46 | 3 | 1 |
| 1:H:198:CYS:O | 1:H:202:LEU:HD22 | 0.46 | 2.11 | 10 | 1 |
| 1:K:205:LEU:HD21 | 1:K:217:ALA:HB2 | 0.45 | 1.87 | 2 | 1 |
| 1:I:237:GLN:C | 1:I:242:ALA:HB3 | 0.45 | 2.36 | 8 | 1 |
| 1:H:205:LEU:HD11 | 1:H:217:ALA:HB3 | 0.45 | 1.88 | 3 | 1 |
| 1:J:201:ILE:HD13 | 1:J:217:ALA:O | 0.45 | 2.11 | 4 | 1 |
| 1:K:209:ALA:HB1 | 1:K:213:GLU:HB3 | 0.45 | 1.88 | 8 | 1 |
| 1:I:164:TYR:CE2 | 1:I:194:ALA:HB2 | 0.45 | 2.47 | 7 | 1 |
| 1:H:150:ILE:HG21 | 1:H:185:MET:HG2 | 0.45 | 1.89 | 9 | 1 |
| 1:J:198:CYS:HB2 | 1:J:202:LEU:HD13 | 0.45 | 1.88 | 9 | 1 |
| 1:L:148:THR:HB | 1:L:171:THR:HG21 | 0.45 | 1.87 | 10 | 1 |
| 1:K:191:VAL:HA | 1:K:202:LEU:HD23 | 0.45 | 1.88 | 5 | 1 |
| 1:H:198:CYS:HB3 | 1:H:221:VAL:HG21 | 0.45 | 1.87 | 7 | 1 |
| 1:L:189:LEU:HD22 | 1:L:192:GLN:HB2 | 0.45 | 1.87 | 7 | 1 |
| 1:I:168:PHE:HE1 | 1:I:186:THR:HG22 | 0.45 | 1.71 | 3 | 3 |
| 1:J:150:ILE:CD1 | 1:J:171:THR:HG23 | 0.45 | 2.42 | 4 | 1 |
| 1:L:190:LEU:O | 1:L:194:ALA:HB3 | 0.45 | 2.12 | 8 | 1 |
| 1:J:202:LEU:HD23 | 1:J:214:MET:SD | 0.45 | 2.52 | 1 | 1 |
| 1:J:189:LEU:HD22 | 1:J:189:LEU:O | 0.44 | 2.12 | 7 | 1 |
| 1:K:201:ILE:HG22 | 1:K:217:ALA:HB1 | 0.44 | 1.89 | 8 | 1 |
| 1:G:153:ILE:HG21 | 1:G:168:PHE:HB2 | 0.44 | 1.88 | 6 | 4 |
| 1:I:211:LEU:HD22 | 1:I:214:MET:HE3 | 0.44 | 1.89 | 8 | 2 |
| 1:I:168:PHE:CZ | 1:I:186:THR:HG22 | 0.44 | 2.47 | 6 | 3 |
| 1:I:177:ALA:HB3 | 1:I:182:LYS:HE3 | 0.44 | 1.89 | 9 | 3 |
| 1:H:177:ALA:HB1 | 1:H:181:VAL:HG11 | 0.44 | 1.89 | 5 | 2 |
| 1:J:226:HIS:CE1 | 1:J:230:VAL:HG23 | 0.44 | 2.47 | 8 | 1 |
| 1:K:177:ALA:HB1 | 1:K:181:VAL:HG12 | 0.44 | 1.89 | 3 | 1 |
| 1:J:150:ILE:HD11 | 1:J:171:THR:HG23 | 0.44 | 1.88 | 4 | 1 |
| 1:H:209:ALA:HB3 | 1:H:214:MET:CG | 0.44 | 2.42 | 6 | 2 |
| 1:J:189:LEU:HD11 | 1:J:193:ASN:HD21 | 0.44 | 1.73 | 7 | 1 |
| 1:L:150:ILE:HD11 | 1:L:171:THR:CG2 | 0.44 | 2.43 | 7 | 1 |
| 1:G:237:GLN:O | 1:G:242:ALA:HB3 | 0.44 | 2.13 | 4 | 2 |
| 1:J:177:ALA:HB3 | 1:J:182:LYS:HG2 | 0.44 | 1.89 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:I:191:VAL:HG22 | 1:I:202:LEU:HD22 | 0.44 | 1.89 | 8 | 1 |
| 1:K:197:ASP:CB | 1:K:221:VAL:HG13 | 0.44 | 2.43 | 3 | 2 |
| 1:L:177:ALA:HB1 | 1:L:181:VAL:CG1 | 0.44 | 2.42 | 9 | 3 |
| 1:J:190:LEU:O | 1:J:194:ALA:HB3 | 0.43 | 2.13 | 3 | 1 |
| 1:H:235:MET:SD | 1:I:235:MET:HE2 | 0.43 | 2.54 | 3 | 1 |
| 1:K:191:VAL:CG2 | 1:K:202:LEU:HD23 | 0.43 | 2.40 | 3 | 1 |
| 1:G:150:ILE:HG23 | 1:G:189:LEU:HD13 | 0.43 | 1.89 | 5 | 1 |
| 1:J:191:VAL:HG22 | 1:J:202:LEU:HD13 | 0.43 | 1.90 | 6 | 1 |
| 1:K:161:PHE:CZ | 1:K:165:VAL:HG21 | 0.43 | 2.48 | 7 | 2 |
| 1:K:198:CYS:O | 1:K:202:LEU:HD12 | 0.43 | 2.13 | 9 | 2 |
| 1:H:186:THR:O | 1:H:190:LEU:HD23 | 0.43 | 2.13 | 9 | 1 |
| 1:L:187:GLU:O | 1:L:191:VAL:HG23 | 0.43 | 2.13 | 4 | 4 |
| 1:I:226:HIS:C | 1:I:230:VAL:HG12 | 0.43 | 2.39 | 3 | 1 |
| 1:J:189:LEU:HD13 | 1:J:189:LEU:C | 0.43 | 2.38 | 4 | 1 |
| 1:K:177:ALA:HB3 | 1:K:182:LYS:HG3 | 0.43 | 1.89 | 3 | 1 |
| 1:G:238:VAL:HG21 | 1:H:235:MET:HB3 | 0.43 | 1.86 | 2 | 1 |
| 1:L:151:LEU:C | 1:L:189:LEU:HD21 | 0.43 | 2.38 | 2 | 1 |
| 1:K:155:GLN:HB2 | 1:K:194:ALA:HB1 | 0.43 | 1.89 | 10 | 1 |
| 1:J:227:LYS:HA | 1:J:230:VAL:HG22 | 0.43 | 1.91 | 2 | 1 |
| 1:J:237:GLN:HA | 1:J:242:ALA:HB3 | 0.43 | 1.90 | 9 | 1 |
| 1:J:218:CYS:SG | 1:J:221:VAL:HG21 | 0.43 | 2.54 | 4 | 2 |
| 1:L:231:LEU:C | 1:L:231:LEU:HD13 | 0.43 | 2.38 | 6 | 1 |
| 1:K:202:LEU:HD13 | 1:K:218:CYS:SG | 0.43 | 2.54 | 5 | 1 |
| 1:J:165:VAL:HG13 | 1:J:168:PHE:HE2 | 0.42 | 1.74 | 5 | 1 |
| 1:I:161:PHE:CE2 | 1:I:165:VAL:HG21 | 0.42 | 2.49 | 6 | 1 |
| 1:H:147:PRO:C | 1:H:148:THR:HG23 | 0.42 | 2.39 | 1 | 1 |
| 1:L:150:ILE:O | 1:L:189:LEU:HD13 | 0.42 | 2.14 | 5 | 1 |
| 1:H:189:LEU:HD11 | 1:H:193:ASN:ND2 | 0.42 | 2.29 | 6 | 1 |
| 1:H:155:GLN:OE1 | 1:H:221:VAL:HG11 | 0.42 | 2.13 | 4 | 2 |
| 1:I:153:ILE:HG22 | 1:I:189:LEU:HD22 | 0.42 | 1.91 | 4 | 1 |
| 1:I:189:LEU:CD2 | 1:I:193:ASN:HD21 | 0.42 | 2.28 | 4 | 1 |
| 3:H:302:A1CCZ:C15 | 1:I:231:LEU:HD13 | 0.42 | 2.43 | 9 | 1 |
| 1:J:202:LEU:HD22 | 1:J:214:MET:SD | 0.42 | 2.54 | 6 | 1 |
| 1:I:198:CYS:CB | 1:I:221:VAL:HG21 | 0.42 | 2.43 | 7 | 3 |
| 1:J:161:PHE:CE1 | 1:J:190:LEU:HD21 | 0.42 | 2.49 | 5 | 1 |
| 1:K:177:ALA:HB3 | 1:K:182:LYS:HG2 | 0.42 | 1.92 | 1 | 1 |
| 1:G:197:ASP:O | 1:G:200:THR:HG22 | 0.42 | 2.14 | 5 | 3 |
| 1:L:149:SER:O | 1:L:151:LEU:HD12 | 0.42 | 2.15 | 4 | 1 |
| 1:G:231:LEU:HD12 | 1:H:231:LEU:CD2 | 0.42 | 2.44 | 7 | 1 |
| 1:I:189:LEU:C | 1:I:189:LEU:HD13 | 0.42 | 2.40 | 8 | 1 |
| 1:J:164:TYR:CZ | 1:J:194:ALA:HB2 | 0.42 | 2.49 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:J:168:PHE:HZ | 1:J:186:THR:HG22 | 0.42 | 1.75 | 3 | 1 |
| 1:J:191:VAL:HG13 | 1:J:202:LEU:HB2 | 0.42 | 1.91 | 6 | 1 |
| 1:J:211:LEU:HD22 | 1:J:214:MET:HE3 | 0.42 | 1.90 | 9 | 1 |
| 1:H:151:LEU:HD12 | 1:H:151:LEU:N | 0.41 | 2.30 | 4 | 1 |
| 1:L:198:CYS:O | 1:L:202:LEU:HD12 | 0.41 | 2.15 | 5 | 1 |
| 1:I:243:THR:O | 1:I:243:THR:HG23 | 0.41 | 2.16 | 3 | 6 |
| 1:H:202:LEU:HD21 | 1:H:218:CYS:SG | 0.41 | 2.55 | 6 | 1 |
| 1:I:162:ARG:NH2 | 1:I:165:VAL:HG12 | 0.41 | 2.30 | 9 | 1 |
| 1:J:150:ILE:HG23 | 1:J:189:LEU:HD13 | 0.41 | 1.93 | 1 | 2 |
| 1:L:168:PHE:HZ | 1:L:186:THR:HG22 | 0.41 | 1.75 | 1 | 2 |
| 1:L:150:ILE:HG23 | 1:L:153:ILE:HG22 | 0.41 | 1.93 | 2 | 1 |
| 1:G:187:GLU:O | 1:G:191:VAL:HG23 | 0.41 | 2.15 | 2 | 2 |
| 1:J:243:THR:O | 1:J:243:THR:HG23 | 0.41 | 2.16 | 9 | 7 |
| 1:L:168:PHE:CZ | 1:L:172:LEU:HD11 | 0.41 | 2.51 | 2 | 1 |
| 1:J:197:ASP:HB2 | 1:J:221:VAL:HG13 | 0.41 | 1.92 | 4 | 1 |
| 1:G:201:ILE:HG21 | 1:G:218:CYS:SG | 0.41 | 2.56 | 5 | 1 |
| 1:L:243:THR:HG23 | 1:L:243:THR:O | 0.41 | 2.16 | 1 | 2 |
| 1:K:191:VAL:HG22 | 1:K:202:LEU:CD2 | 0.41 | 2.41 | 3 | 1 |
| 1:H:189:LEU:HD21 | 1:H:193:ASN:CG | 0.41 | 2.41 | 6 | 1 |
| 1:H:202:LEU:CD2 | 1:H:214:MET:HE2 | 0.41 | 2.46 | 1 | 1 |
| 1:L:198:CYS:HA | 1:L:201:ILE:HD12 | 0.41 | 1.92 | 3 | 1 |
| 1:K:243:THR:HG23 | 1:K:243:THR:O | 0.41 | 2.16 | 10 | 4 |
| 1:L:151:LEU:HD12 | 1:L:151:LEU:N | 0.41 | 2.31 | 5 | 1 |
| 1:H:237:GLN:OE1 | 1:I:232:ALA:HB2 | 0.41 | 2.15 | 6 | 1 |
| 1:H:198:CYS:CB | 1:H:221:VAL:HG21 | 0.41 | 2.46 | 7 | 1 |
| 1:H:243:THR:HG23 | 1:H:243:THR:O | 0.41 | 2.16 | 9 | 2 |
| 1:H:151:LEU:N | 1:H:151:LEU:HD12 | 0.41 | 2.30 | 10 | 1 |
| 1:I:153:ILE:HG21 | 1:I:168:PHE:HA | 0.41 | 1.93 | 2 | 2 |
| 1:K:165:VAL:HG12 | 1:K:169:TYR:CD1 | 0.41 | 2.51 | 1 | 1 |
| 1:J:151:LEU:HD12 | 1:J:151:LEU:N | 0.41 | 2.31 | 3 | 1 |
| 1:I:205:LEU:HD11 | 1:I:217:ALA:HB3 | 0.41 | 1.92 | 10 | 1 |
| 1:I:201:ILE:HG21 | 1:I:218:CYS:SG | 0.41 | 2.55 | 3 | 1 |
| 1:J:168:PHE:CD2 | 1:J:190:LEU:HD13 | 0.41 | 2.50 | 4 | 1 |
| 1:L:175:GLU:HG2 | 1:L:185:MET:HE1 | 0.41 | 1.92 | 7 | 1 |
| 1:H:181:VAL:HG12 | 1:H:182:LYS:N | 0.41 | 2.31 | 5 | 1 |
| 1:H:198:CYS:O | 1:H:202:LEU:HD12 | 0.41 | 2.16 | 7 | 1 |
| 1:I:237:GLN:CA | 1:I:242:ALA:HB3 | 0.41 | 2.46 | 8 | 1 |
| 1:K:201:ILE:HG21 | 1:K:217:ALA:HB1 | 0.41 | 1.92 | 5 | 1 |
| 1:I:212:GLU:OE1 | 1:I:215:MET:HE1 | 0.41 | 2.15 | 8 | 1 |
| 1:I:237:GLN:CG | 1:I:242:ALA:HB3 | 0.40 | 2.46 | 4 | 1 |
| 1:G:243:THR:O | 1:G:243:THR:HG23 | 0.40 | 2.16 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:I:243:THR:HG23 | 1:I:243:THR:O | 0.40 | 2.16 | 7 | 1 |
| 1:K:172:LEU:HD22 | 1:K:185:MET:SD | 0.40 | 2.57 | 9 | 1 |
| 1:H:202:LEU:CD1 | 1:H:214:MET:HE2 | 0.40 | 2.46 | 5 | 1 |
| 1:H:171:THR:O | 1:H:174:ALA:HB3 | 0.40 | 2.16 | 7 | 1 |
| 1:J:189:LEU:HD11 | 1:J:193:ASN:ND2 | 0.40 | 2.31 | 7 | 1 |
| 1:H:151:LEU:HD12 | 1:H:151:LEU:H | 0.40 | 1.76 | 6 | 1 |
| 1:I:191:VAL:HG22 | 1:I:202:LEU:HD13 | 0.40 | 1.93 | 6 | 1 |
| 1:I:155:GLN:NE2 | 1:I:194:ALA:HB1 | 0.40 | 2.28 | 8 | 1 |
| 1:I:172:LEU:HD22 | 1:I:182:LYS:CD | 0.40 | 2.46 | 4 | 1 |
| 1:K:243:THR:O | 1:K:243:THR:HG23 | 0.40 | 2.16 | 6 | 1 |

6.3 Torsion angles

6.3.1 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 NMR 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 | G | 99/102 (97%) | 91±1 (92±1%) | 6±1 (6±1%) | 2±0 (2±0%) | 8 | 50 |
| 1 | H | 98/102 (96%) | 87±1 (89±1%) | 8±1 (8±1%) | 3±1 (3±1%) | 5 | 34 |
| 1 | I | 90/102 (88%) | 80±2 (89±2%) | 8±2 (9±3%) | 2±0 (2±1%) | 9 | 52 |
| 1 | J | 94/102 (92%) | 82±2 (88±2%) | 9±2 (9±3%) | 3±1 (3±1%) | 6 | 39 |
| 1 | K | 94/102 (92%) | 85±2 (90±2%) | 8±2 (8±2%) | 2±0 (2±1%) | 10 | 55 |
| 1 | L | 98/102 (96%) | 86±1 (88±1%) | 9±1 (9±1%) | 2±1 (3±1%) | 6 | 42 |
| All | All | 5730/6120 (94%) | 5117 (89%) | 477 (8%) | 136 (2%) | 7 | 44 |

All 24 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | G | 150 | ILE | 10 |
| 1 | G | 195 | ASN | 10 |
| 1 | H | 150 | ILE | 10 |
| 1 | H | 195 | ASN | 10 |
| 1 | I | 195 | ASN | 10 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | J | 150 | ILE | 10 |
| 1 | J | 195 | ASN | 10 |
| 1 | K | 195 | ASN | 10 |
| 1 | L | 195 | ASN | 10 |
| 1 | L | 150 | ILE | 8 |
| 1 | H | 196 | PRO | 5 |
| 1 | H | 223 | GLY | 5 |
| 1 | I | 148 | THR | 5 |
| 1 | K | 207 | PRO | 4 |
| 1 | J | 148 | THR | 4 |
| 1 | L | 176 | GLN | 3 |
| 1 | H | 148 | THR | 3 |
| 1 | L | 148 | THR | 3 |
| 1 | J | 223 | GLY | 1 |
| 1 | L | 196 | PRO | 1 |
| 1 | J | 176 | GLN | 1 |
| 1 | J | 196 | PRO | 1 |
| 1 | I | 224 | PRO | 1 |
| 1 | K | 157 | PRO | 1 |

6.3.2 Protein sidechains [i](#)

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 NMR 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 | G | 82/83 (99%) | 74±1 (91±1%) | 8±1 (9±1%) | 10 | 57 |
| 1 | H | 82/83 (99%) | 72±2 (88±2%) | 10±2 (12±2%) | 7 | 50 |
| 1 | I | 76/83 (92%) | 68±1 (90±2%) | 8±1 (10±2%) | 9 | 54 |
| 1 | J | 81/83 (98%) | 72±2 (89±2%) | 9±2 (11±2%) | 7 | 51 |
| 1 | K | 77/83 (93%) | 68±2 (89±3%) | 8±2 (11±3%) | 7 | 52 |
| 1 | L | 82/83 (99%) | 74±2 (91±2%) | 8±2 (9±2%) | 10 | 57 |
| All | All | 4800/4980 (96%) | 4299 (90%) | 501 (10%) | 8 | 53 |

All 129 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | G | 150 | ILE | 10 |
| 1 | G | 168 | PHE | 10 |
| 1 | G | 184 | TRP | 10 |
| 1 | G | 193 | ASN | 10 |
| 1 | G | 211 | LEU | 10 |
| 1 | H | 168 | PHE | 10 |
| 1 | H | 184 | TRP | 10 |
| 1 | I | 184 | TRP | 10 |
| 1 | I | 211 | LEU | 10 |
| 1 | J | 168 | PHE | 10 |
| 1 | J | 184 | TRP | 10 |
| 1 | J | 193 | ASN | 10 |
| 1 | J | 211 | LEU | 10 |
| 1 | L | 184 | TRP | 10 |
| 1 | L | 211 | LEU | 10 |
| 1 | H | 150 | ILE | 9 |
| 1 | I | 168 | PHE | 9 |
| 1 | J | 150 | ILE | 9 |
| 1 | L | 168 | PHE | 9 |
| 1 | J | 189 | LEU | 9 |
| 1 | H | 162 | ARG | 8 |
| 1 | H | 193 | ASN | 8 |
| 1 | H | 205 | LEU | 8 |
| 1 | L | 162 | ARG | 8 |
| 1 | K | 189 | LEU | 8 |
| 1 | K | 211 | LEU | 8 |
| 1 | G | 162 | ARG | 7 |
| 1 | K | 168 | PHE | 7 |
| 1 | K | 171 | THR | 7 |
| 1 | I | 162 | ARG | 6 |
| 1 | K | 158 | LYS | 6 |
| 1 | K | 162 | ARG | 6 |
| 1 | L | 230 | VAL | 6 |
| 1 | J | 205 | LEU | 6 |
| 1 | K | 193 | ASN | 6 |
| 1 | L | 151 | LEU | 6 |
| 1 | H | 202 | LEU | 5 |
| 1 | L | 172 | LEU | 5 |
| 1 | G | 227 | LYS | 5 |
| 1 | H | 181 | VAL | 5 |
| 1 | H | 227 | LYS | 5 |
| 1 | J | 227 | LYS | 5 |
| 1 | K | 195 | ASN | 5 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | L | 189 | LEU | 5 |
| 1 | I | 193 | ASN | 5 |
| 1 | K | 188 | THR | 5 |
| 1 | J | 171 | THR | 4 |
| 1 | L | 150 | ILE | 4 |
| 1 | K | 205 | LEU | 4 |
| 1 | G | 148 | THR | 3 |
| 1 | H | 178 | SER | 3 |
| 1 | H | 226 | HIS | 3 |
| 1 | I | 189 | LEU | 3 |
| 1 | I | 230 | VAL | 3 |
| 1 | H | 189 | LEU | 3 |
| 1 | I | 199 | LYS | 3 |
| 1 | K | 198 | CYS | 3 |
| 1 | K | 227 | LYS | 3 |
| 1 | G | 230 | VAL | 3 |
| 1 | H | 148 | THR | 3 |
| 1 | I | 205 | LEU | 3 |
| 1 | I | 227 | LYS | 3 |
| 1 | J | 199 | LYS | 3 |
| 1 | K | 231 | LEU | 3 |
| 1 | H | 211 | LEU | 3 |
| 1 | I | 172 | LEU | 3 |
| 1 | G | 159 | GLU | 2 |
| 1 | G | 178 | SER | 2 |
| 1 | I | 224 | PRO | 2 |
| 1 | I | 226 | HIS | 2 |
| 1 | L | 227 | LYS | 2 |
| 1 | L | 231 | LEU | 2 |
| 1 | J | 218 | CYS | 2 |
| 1 | J | 229 | ARG | 2 |
| 1 | J | 230 | VAL | 2 |
| 1 | K | 199 | LYS | 2 |
| 1 | L | 229 | ARG | 2 |
| 1 | J | 148 | THR | 2 |
| 1 | K | 178 | SER | 2 |
| 1 | L | 193 | ASN | 2 |
| 1 | L | 205 | LEU | 2 |
| 1 | H | 230 | VAL | 2 |
| 1 | I | 155 | GLN | 2 |
| 1 | I | 216 | THR | 2 |
| 1 | I | 219 | GLN | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | G | 240 | ASN | 1 |
| 1 | I | 195 | ASN | 1 |
| 1 | I | 202 | LEU | 1 |
| 1 | J | 198 | CYS | 1 |
| 1 | J | 240 | ASN | 1 |
| 1 | K | 240 | ASN | 1 |
| 1 | L | 240 | ASN | 1 |
| 1 | H | 219 | GLN | 1 |
| 1 | J | 176 | GLN | 1 |
| 1 | J | 231 | LEU | 1 |
| 1 | K | 155 | GLN | 1 |
| 1 | K | 190 | LEU | 1 |
| 1 | H | 229 | ARG | 1 |
| 1 | I | 203 | LYS | 1 |
| 1 | G | 229 | ARG | 1 |
| 1 | H | 214 | MET | 1 |
| 1 | I | 159 | GLU | 1 |
| 1 | K | 236 | SER | 1 |
| 1 | G | 231 | LEU | 1 |
| 1 | H | 151 | LEU | 1 |
| 1 | J | 203 | LYS | 1 |
| 1 | K | 202 | LEU | 1 |
| 1 | L | 164 | TYR | 1 |
| 1 | G | 199 | LYS | 1 |
| 1 | I | 231 | LEU | 1 |
| 1 | K | 181 | VAL | 1 |
| 1 | K | 229 | ARG | 1 |
| 1 | H | 198 | CYS | 1 |
| 1 | I | 198 | CYS | 1 |
| 1 | I | 212 | GLU | 1 |
| 1 | I | 229 | ARG | 1 |
| 1 | J | 178 | SER | 1 |
| 1 | K | 230 | VAL | 1 |
| 1 | H | 152 | ASP | 1 |
| 1 | H | 192 | GLN | 1 |
| 1 | I | 148 | THR | 1 |
| 1 | H | 171 | THR | 1 |
| 1 | J | 226 | HIS | 1 |
| 1 | K | 215 | MET | 1 |
| 1 | H | 159 | GLU | 1 |
| 1 | H | 201 | ILE | 1 |
| 1 | J | 212 | GLU | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | K | 163 | ASP | 1 |
| 1 | L | 178 | SER | 1 |

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|-------|-------|-----|------|--------------|-----------|--------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | IHP | H | 301 | - | 36,36,36 | 1.67±0.00 | 6±1 (15±1%) |
| 3 | A1CCZ | H | 302 | - | 36,36,36 | 2.03±0.00 | 13±0 (36±0%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|-------|-------|-----|------|-------------|-----------|--------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | IHP | H | 301 | - | 60,60,60 | 1.30±0.00 | 7±0 (11±0%) |
| 3 | A1CCZ | H | 302 | - | 44,54,54 | 2.20±0.00 | 12±0 (27±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 |
|-----|-------|-------|-----|------|---------|--------------|-----------|
| 2 | IHP | H | 301 | - | - | 0±0,30,54,54 | 0±0,1,1,1 |
| 3 | A1CCZ | H | 302 | - | - | 0±0,24,32,32 | 0±0,4,4,4 |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|-------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | H | 301 | IHP | C6-C5 | 5.43 | 1.63 | 1.52 | 3 | 10 |
| 3 | H | 302 | A1CCZ | C12-N23 | 5.05 | 1.53 | 1.47 | 9 | 10 |
| 3 | H | 302 | A1CCZ | C8-N10 | 3.82 | 1.54 | 1.48 | 3 | 10 |
| 3 | H | 302 | A1CCZ | C7-C8 | 3.73 | 1.47 | 1.53 | 1 | 10 |
| 3 | H | 302 | A1CCZ | C18-C17 | 3.53 | 1.33 | 1.38 | 9 | 10 |
| 3 | H | 302 | A1CCZ | O29-C24 | 3.52 | 1.30 | 1.23 | 4 | 10 |
| 2 | H | 301 | IHP | P6-O16 | 3.38 | 1.53 | 1.59 | 5 | 10 |
| 2 | H | 301 | IHP | C5-C4 | 2.99 | 1.58 | 1.52 | 1 | 10 |
| 3 | H | 302 | A1CCZ | C4-C5 | 2.96 | 1.44 | 1.38 | 1 | 10 |
| 3 | H | 302 | A1CCZ | C18-C13 | 2.95 | 1.43 | 1.39 | 7 | 10 |
| 2 | H | 301 | IHP | C2-C1 | 2.88 | 1.58 | 1.52 | 1 | 10 |
| 3 | H | 302 | A1CCZ | C7-C6 | 2.79 | 1.55 | 1.50 | 6 | 10 |
| 3 | H | 302 | A1CCZ | C15-C16 | 2.55 | 1.43 | 1.39 | 4 | 10 |
| 3 | H | 302 | A1CCZ | C19-C16 | 2.47 | 1.48 | 1.53 | 2 | 10 |
| 3 | H | 302 | A1CCZ | C11-N10 | 2.45 | 1.50 | 1.47 | 1 | 10 |
| 3 | H | 302 | A1CCZ | C9-C8 | 2.45 | 1.49 | 1.53 | 8 | 10 |
| 3 | H | 302 | A1CCZ | C12-C11 | 2.32 | 1.56 | 1.53 | 6 | 10 |
| 2 | H | 301 | IHP | P2-O42 | 2.24 | 1.46 | 1.54 | 7 | 10 |
| 2 | H | 301 | IHP | P1-O11 | 2.02 | 1.63 | 1.59 | 8 | 1 |
| 2 | H | 301 | IHP | O13-C3 | 2.01 | 1.37 | 1.44 | 1 | 4 |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|-------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | H | 302 | A1CCZ | C11-C12-N23 | 6.40 | 121.30 | 111.78 | 3 | 10 |
| 3 | H | 302 | A1CCZ | C7-C6-C1 | 6.16 | 106.36 | 110.50 | 10 | 10 |
| 3 | H | 302 | A1CCZ | C1-C9-C8 | 4.94 | 98.02 | 102.89 | 2 | 10 |
| 3 | H | 302 | A1CCZ | C7-C6-C5 | 4.06 | 136.77 | 129.17 | 4 | 10 |
| 2 | H | 301 | IHP | C5-C4-C3 | 3.82 | 102.05 | 110.43 | 9 | 10 |
| 3 | H | 302 | A1CCZ | C5-C6-C1 | 3.35 | 116.32 | 120.12 | 4 | 10 |
| 2 | H | 301 | IHP | O15-C5-C6 | 3.25 | 115.68 | 108.76 | 3 | 10 |
| 2 | H | 301 | IHP | C5-C6-C1 | 3.08 | 103.67 | 110.43 | 7 | 10 |
| 3 | H | 302 | A1CCZ | C2-C1-C6 | 2.80 | 123.31 | 120.12 | 3 | 10 |
| 3 | H | 302 | A1CCZ | C6-C7-C8 | 2.77 | 100.16 | 102.89 | 6 | 10 |
| 3 | H | 302 | A1CCZ | C15-C14-C13 | 2.74 | 118.45 | 121.18 | 6 | 10 |
| 2 | H | 301 | IHP | O34-P4-O14 | 2.69 | 116.32 | 105.85 | 1 | 10 |
| 3 | H | 302 | A1CCZ | C22-C19-C20 | 2.64 | 116.19 | 108.36 | 2 | 10 |
| 2 | H | 301 | IHP | C6-C5-C4 | 2.52 | 104.90 | 110.43 | 3 | 10 |
| 3 | H | 302 | A1CCZ | O29-C24-N23 | 2.44 | 117.28 | 120.53 | 1 | 10 |
| 2 | H | 301 | IHP | O15-P5-O25 | 2.44 | 100.64 | 109.33 | 4 | 10 |
| 3 | H | 302 | A1CCZ | C21-C19-C20 | 2.43 | 101.13 | 108.36 | 10 | 10 |
| 3 | H | 302 | A1CCZ | C17-C16-C15 | 2.07 | 114.94 | 118.03 | 9 | 10 |
| 2 | H | 301 | IHP | O46-P6-O36 | 2.05 | 115.50 | 107.80 | 8 | 10 |

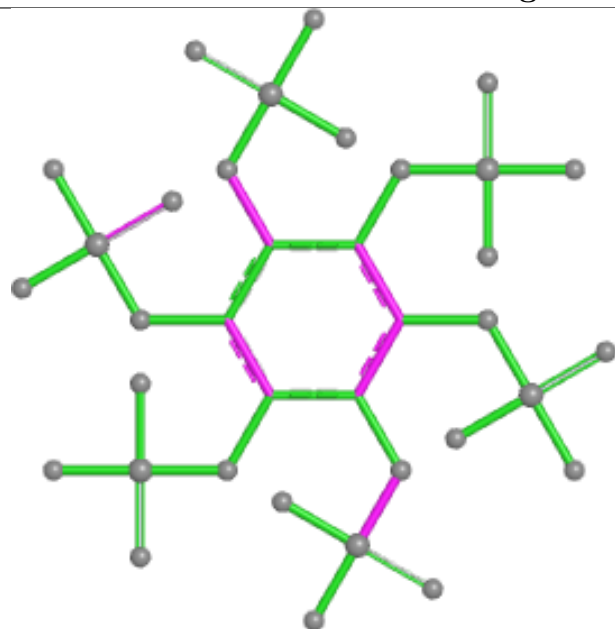
There are no chirality outliers.

There are no torsion outliers.

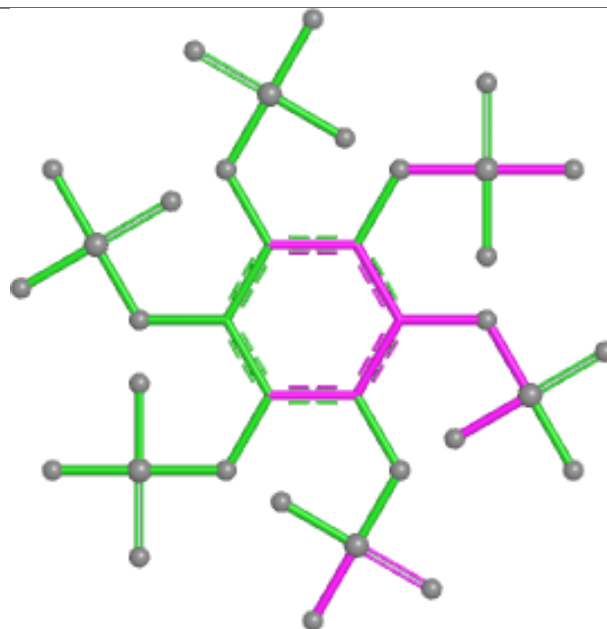
There are no ring outliers.

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.

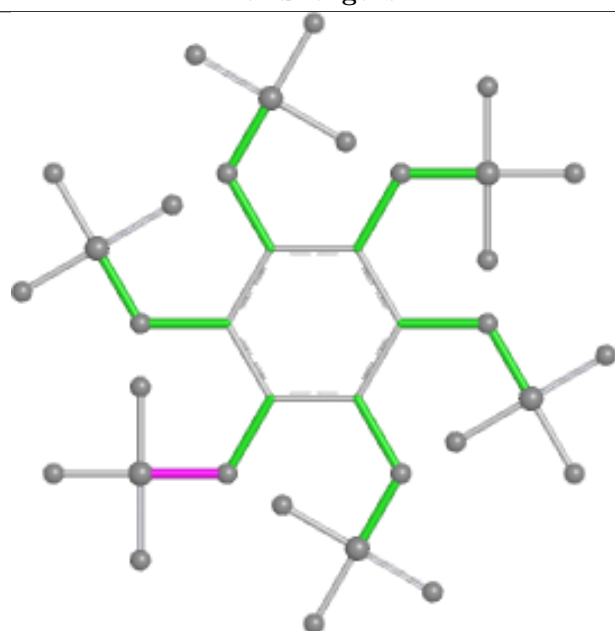
Ligand IHP H 301



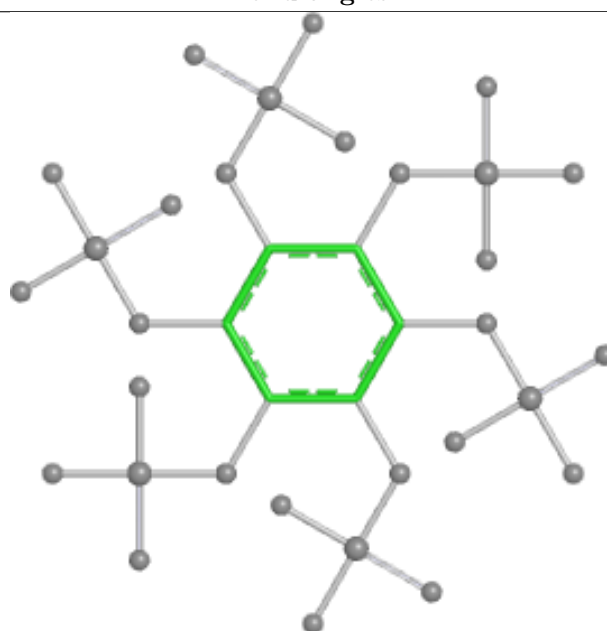
Bond lengths



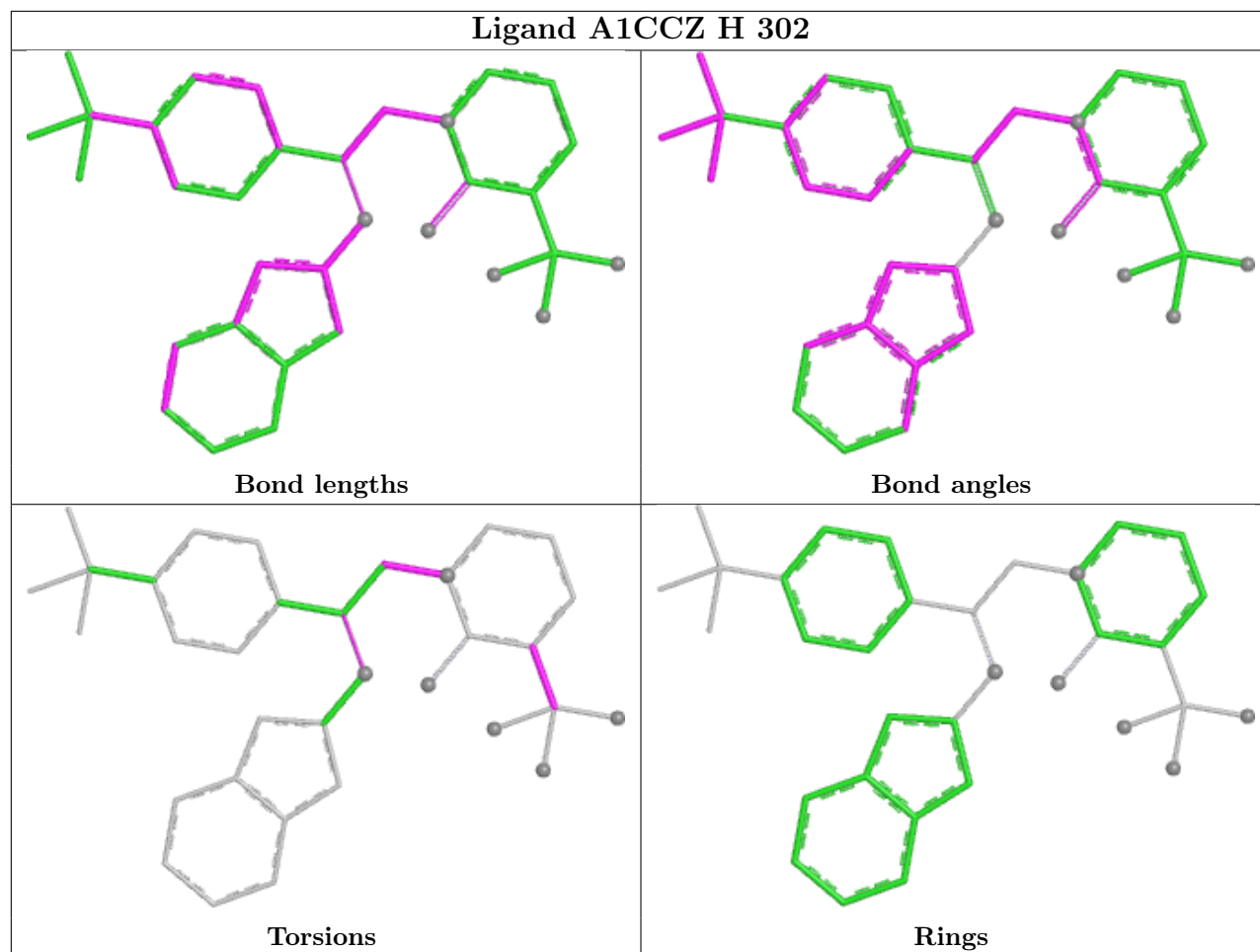
Bond angles



Torsions



Rings



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 6% for the well-defined parts and 6% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *D_1000295827_cs_P1.str.V1*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

| | |
|---|-----|
| Total number of shifts | 514 |
| Number of shifts mapped to atoms | 514 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 2 |

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 96 | -0.78 ± 0.21 | Should be checked |
| $^{13}\text{C}_\beta$ | 87 | 0.07 ± 0.17 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 92 | -0.75 ± 0.16 | Should be applied |
| ^{15}N | 93 | -0.46 ± 0.78 | None needed (< 0.5 ppm) |

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 6%, i.e. 494 atoms were assigned a chemical shift out of a possible 7723. 0 out of 82 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|----------------|--------------|-----------------|-----------------|
| Backbone | 272/2862 (10%) | 2/1162 (0%) | 184/1156 (16%) | 86/544 (16%) |
| Sidechain | 203/4519 (4%) | 6/2939 (0%) | 196/1394 (14%) | 1/186 (1%) |

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| | Total | ¹H | ¹³C | ¹⁵N |
|----------|---------------|----------------------|-----------------------|-----------------------|
| Aromatic | 19/342 (6%) | 1/168 (1%) | 18/162 (11%) | 0/12 (0%) |
| Overall | 494/7723 (6%) | 9/4269 (0%) | 398/2712 (15%) | 87/742 (12%) |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 6%, i.e. 500 atoms were assigned a chemical shift out of a possible 8046. 0 out of 84 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹H | ¹³C | ¹⁵N |
|-----------|---------------|----------------------|-----------------------|-----------------------|
| Backbone | 278/3042 (9%) | 2/1242 (0%) | 188/1224 (15%) | 88/576 (15%) |
| Sidechain | 203/4662 (4%) | 6/3036 (0%) | 196/1440 (14%) | 1/186 (1%) |
| Aromatic | 19/342 (6%) | 1/168 (1%) | 18/162 (11%) | 0/12 (0%) |
| Overall | 500/8046 (6%) | 9/4446 (0%) | 402/2826 (14%) | 89/774 (11%) |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts ⓘ

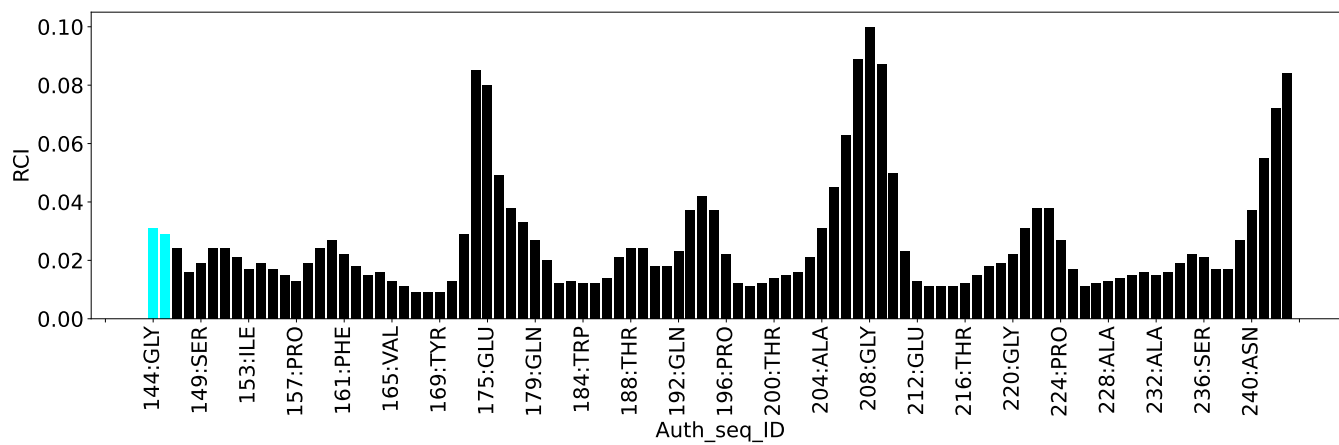
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1 | G | 229 | ARG | NE | 141.70 | 76.53 – 92.65 | 35.4 |
| 1 | G | 158 | LYS | H | 4.70 | 5.24 – 11.12 | -5.9 |

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain G:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

| Description | Value |
|--|-------|
| Total distance restraints | 2427 |
| Intra-residue ($ i-j =0$) | 834 |
| Sequential ($ i-j =1$) | 284 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 488 |
| Long range ($ i-j \geq 5$) | 414 |
| Inter-chain | 407 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 1116 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 5.8 |
| Number of long range restraints per residue ¹ | 0.7 |

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

| Bins (Å) | Average number of violations per model | Max (Å) |
|------------------|--|---------|
| 0.1-0.2 (Small) | 22.2 | 0.2 |
| 0.2-0.5 (Medium) | 42.0 | 0.5 |
| >0.5 (Large) | 20.4 | 1.49 |

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation.

| Bins (°) | Average number of violations per model | Max (°) |
|--------------------|--|---------|
| 1.0-10.0 (Small) | 188.3 | 10.0 |
| 10.0-20.0 (Medium) | 19.8 | 19.86 |
| >20.0 (Large) | 2.2 | 28.71 |

9 Distance violation analysis ⓘ

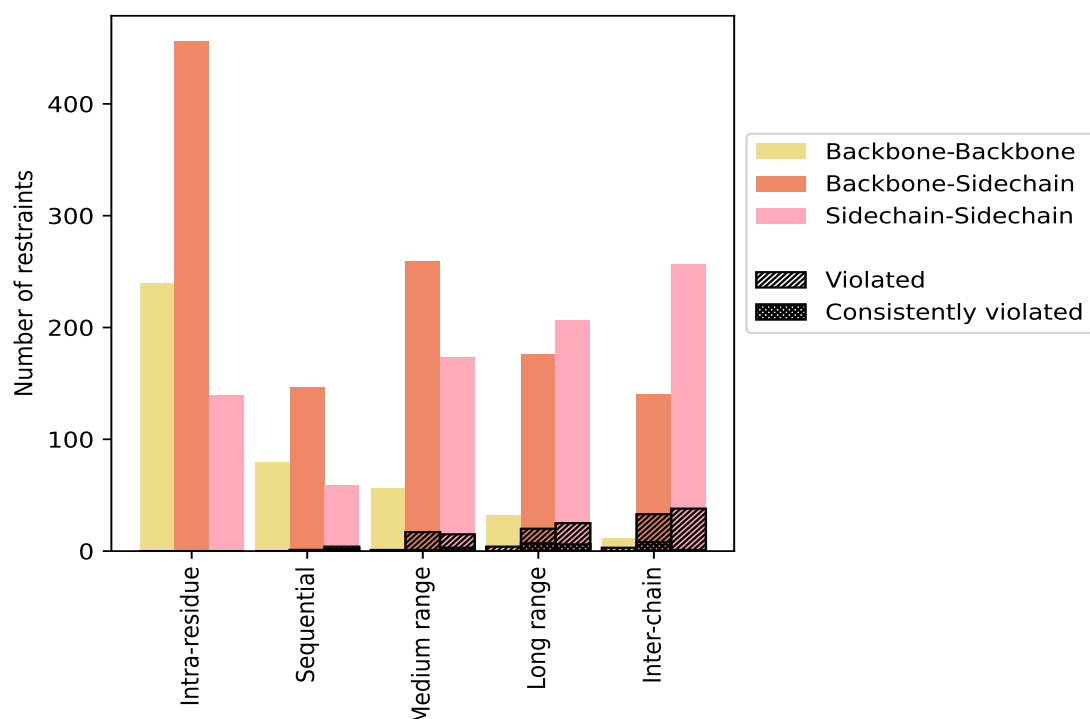
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

| Restrains type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue ($i-j =0$) | 834 | 34.4 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 239 | 9.8 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 456 | 18.8 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 139 | 5.7 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sequential ($i-j =1$) | 284 | 11.7 | 5 | 1.8 | 0.2 | 3 | 1.1 | 0.1 |
| Backbone-Backbone | 79 | 3.3 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 146 | 6.0 | 1 | 0.7 | 0.0 | 1 | 0.7 | 0.0 |
| Sidechain-Sidechain | 59 | 2.4 | 4 | 6.8 | 0.2 | 2 | 3.4 | 0.1 |
| Medium range ($i-j >1$ & $i-j <5$) | 488 | 20.1 | 33 | 6.8 | 1.4 | 4 | 0.8 | 0.2 |
| Backbone-Backbone | 56 | 2.3 | 1 | 1.8 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 259 | 10.7 | 17 | 6.6 | 0.7 | 1 | 0.4 | 0.0 |
| Sidechain-Sidechain | 173 | 7.1 | 15 | 8.7 | 0.6 | 3 | 1.7 | 0.1 |
| Long range ($i-j \geq 5$) | 414 | 17.1 | 49 | 11.8 | 2.0 | 13 | 3.1 | 0.5 |
| Backbone-Backbone | 32 | 1.3 | 4 | 12.5 | 0.2 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 176 | 7.3 | 20 | 11.4 | 0.8 | 7 | 4.0 | 0.3 |
| Sidechain-Sidechain | 206 | 8.5 | 25 | 12.1 | 1.0 | 6 | 2.9 | 0.2 |
| Inter-chain | 407 | 16.8 | 74 | 18.2 | 3.0 | 9 | 2.2 | 0.4 |
| Backbone-Backbone | 11 | 0.5 | 3 | 27.3 | 0.1 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 140 | 5.8 | 33 | 23.6 | 1.4 | 8 | 5.7 | 0.3 |
| Sidechain-Sidechain | 256 | 10.5 | 38 | 14.8 | 1.6 | 1 | 0.4 | 0.0 |
| Hydrogen bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 2427 | 100.0 | 161 | 6.6 | 6.6 | 29 | 1.2 | 1.2 |
| Backbone-Backbone | 417 | 17.2 | 8 | 1.9 | 0.3 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 1177 | 48.5 | 71 | 6.0 | 2.9 | 17 | 1.4 | 0.7 |
| Sidechain-Sidechain | 833 | 34.3 | 82 | 9.8 | 3.4 | 12 | 1.4 | 0.5 |

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfide bonds are counted in their appropriate category on the x-axis

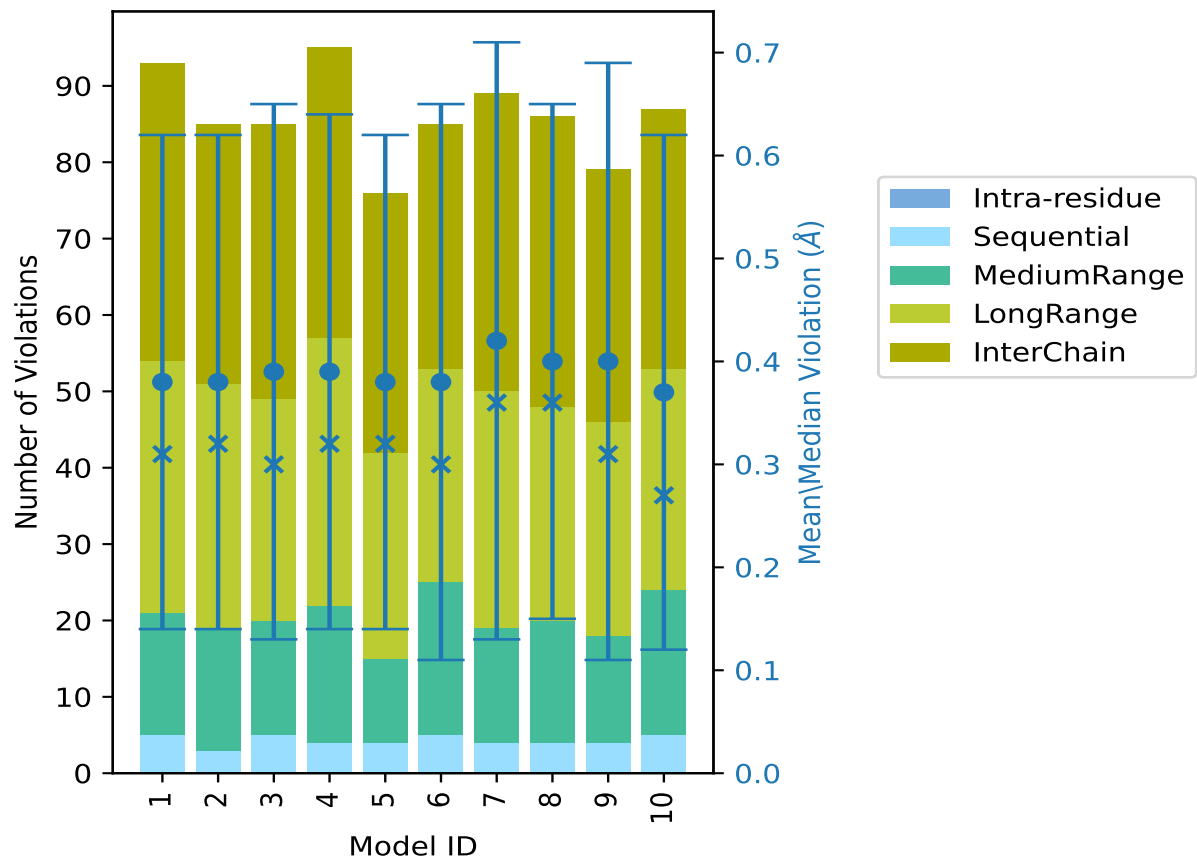
9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 1 | 0 | 5 | 16 | 33 | 39 | 93 | 0.38 | 1.19 | 0.24 | 0.31 |
| 2 | 0 | 3 | 16 | 32 | 34 | 85 | 0.38 | 1.25 | 0.24 | 0.32 |
| 3 | 0 | 5 | 15 | 29 | 36 | 85 | 0.39 | 1.24 | 0.26 | 0.3 |
| 4 | 0 | 4 | 18 | 35 | 38 | 95 | 0.39 | 1.24 | 0.25 | 0.32 |
| 5 | 0 | 4 | 11 | 27 | 34 | 76 | 0.38 | 1.25 | 0.24 | 0.32 |
| 6 | 0 | 5 | 20 | 28 | 32 | 85 | 0.38 | 1.38 | 0.27 | 0.3 |
| 7 | 0 | 4 | 15 | 31 | 39 | 89 | 0.42 | 1.32 | 0.29 | 0.36 |
| 8 | 0 | 4 | 16 | 28 | 38 | 86 | 0.4 | 1.33 | 0.25 | 0.36 |
| 9 | 0 | 4 | 14 | 28 | 33 | 79 | 0.4 | 1.49 | 0.29 | 0.31 |
| 10 | 0 | 5 | 19 | 29 | 34 | 87 | 0.37 | 1.2 | 0.25 | 0.27 |

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2266(IR:834, SQ:279, MR:455, LR:365, IC:333) restraints are not violated in the ensemble.

| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 0 | 0 | 7 | 5 | 17 | 29 | 1 | 10.0 |
| 0 | 0 | 3 | 3 | 9 | 15 | 2 | 20.0 |
| 0 | 0 | 4 | 6 | 6 | 16 | 3 | 30.0 |

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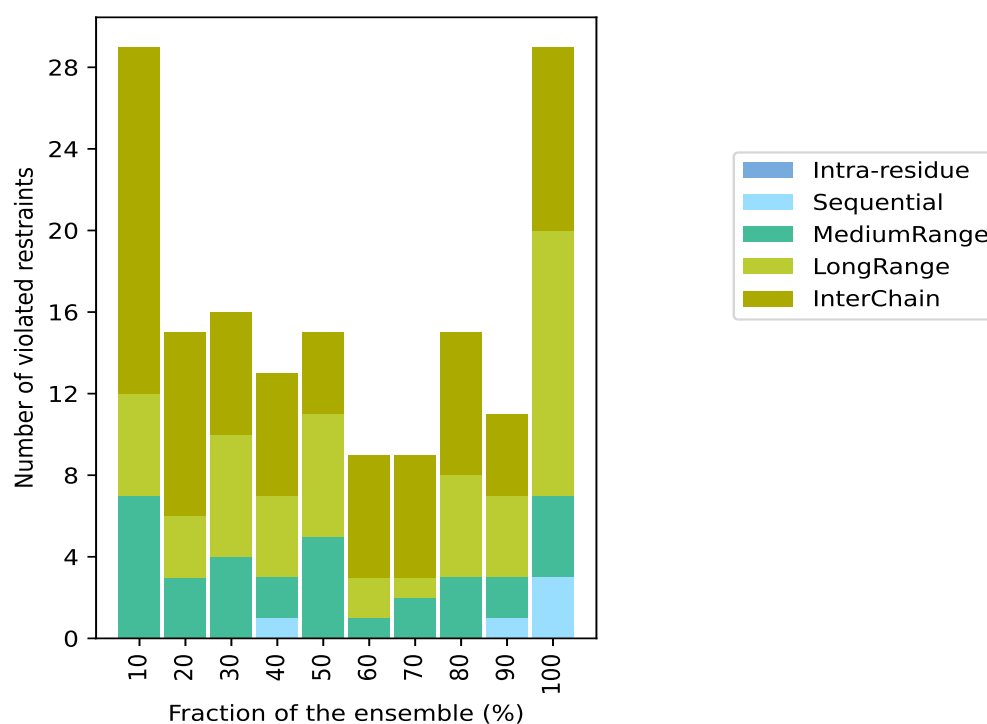
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| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 0 | 1 | 2 | 4 | 6 | 13 | 4 | 40.0 |
| 0 | 0 | 5 | 6 | 4 | 15 | 5 | 50.0 |
| 0 | 0 | 1 | 2 | 6 | 9 | 6 | 60.0 |
| 0 | 0 | 2 | 1 | 6 | 9 | 7 | 70.0 |
| 0 | 0 | 3 | 5 | 7 | 15 | 8 | 80.0 |
| 0 | 1 | 2 | 4 | 4 | 11 | 9 | 90.0 |
| 0 | 3 | 4 | 13 | 9 | 29 | 10 | 100.0 |

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

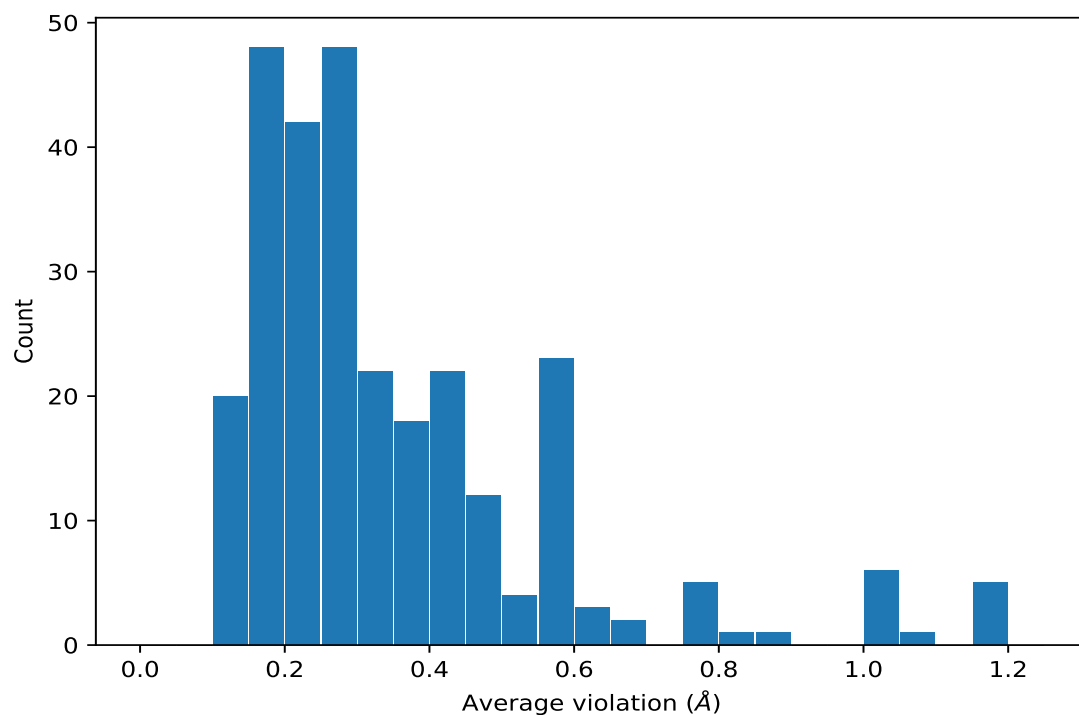


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-------------------|---------------------|----------|---------------------|------------|
| (1,1096) | 1:171:H:THR:CG2 | 1:152:H:ASP:CB | 10 | 1.16 | 0.23 | 1.22 |
| (1,1096) | 1:171:J:THR:CG2 | 1:152:J:ASP:CB | 10 | 1.16 | 0.23 | 1.22 |
| (1,1096) | 1:171:L:THR:CG2 | 1:152:L:ASP:CB | 10 | 1.16 | 0.23 | 1.22 |
| (1,1096) | 1:171:K:THR:CG2 | 1:152:K:ASP:CB | 10 | 1.16 | 0.23 | 1.22 |
| (1,1096) | 1:171:I:THR:CG2 | 1:152:I:ASP:CB | 10 | 1.16 | 0.23 | 1.22 |
| (1,2172) | 2:301:H:IHP:P1 | 1:158:H:LYS:HA | 10 | 1.05 | 0.09 | 1.03 |
| (1,833) | 1:221:J:VAL:CG2 | 1:230:J:VAL:CG2 | 10 | 1.03 | 0.24 | 1.07 |
| (1,833) | 1:221:I:VAL:CG2 | 1:230:I:VAL:CG1 | 10 | 1.03 | 0.24 | 1.07 |
| (1,833) | 1:221:G:VAL:CG2 | 1:230:G:VAL:CG2 | 10 | 1.03 | 0.24 | 1.07 |
| (1,833) | 1:221:I:VAL:CG2 | 1:230:I:VAL:CG2 | 10 | 1.03 | 0.24 | 1.07 |
| (1,833) | 1:221:H:VAL:CG2 | 1:230:H:VAL:CG1 | 10 | 1.03 | 0.24 | 1.07 |
| (1,833) | 1:221:G:VAL:CG2 | 1:230:G:VAL:CG1 | 10 | 1.03 | 0.24 | 1.07 |
| (1,2118) | 2:301:H:IHP:P4 | 1:158:J:LYS:HA | 10 | 0.89 | 0.24 | 0.96 |
| (1,2207) | 2:301:H:IHP:O35 | 3:302:H:A1CCZ:F32 | 10 | 0.85 | 0.15 | 0.86 |
| (1,2174) | 2:301:H:IHP:P2 | 1:158:L:LYS:HA | 10 | 0.78 | 0.36 | 0.74 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-------------------|----------------|---------------------|----------|---------------------|------------|
| (1,2115) | 2:301:H:IHP:P4 | 1:158:G:LYS:HA | 10 | 0.68 | 0.21 | 0.68 |
| (1,29) | 1:219:L:GLN:CG | 1:155:K:GLN:CA | 10 | 0.63 | 0.2 | 0.58 |
| (1,2262) | 3:302:H:A1CCZ:H7A | 1:232:H:ALA:CA | 10 | 0.59 | 0.21 | 0.68 |
| (1,2262) | 3:302:H:A1CCZ:H7B | 1:232:H:ALA:CA | 10 | 0.59 | 0.21 | 0.68 |
| (1,412) | 1:202:L:LEU:CG | 1:194:L:ALA:CA | 10 | 0.57 | 0.2 | 0.55 |
| (1,412) | 1:202:K:LEU:CG | 1:194:K:ALA:CA | 10 | 0.57 | 0.2 | 0.55 |
| (1,412) | 1:202:I:LEU:CG | 1:194:I:ALA:CA | 10 | 0.57 | 0.2 | 0.55 |
| (1,412) | 1:202:H:LEU:CG | 1:194:H:ALA:CA | 10 | 0.57 | 0.2 | 0.55 |
| (1,1638) | 1:155:J:GLN:CB | 1:197:J:ASP:CB | 10 | 0.56 | 0.16 | 0.52 |
| (1,1638) | 1:155:I:GLN:CB | 1:197:I:ASP:CB | 10 | 0.56 | 0.16 | 0.52 |
| (1,1582) | 1:153:I:ILE:CG1 | 1:172:I:LEU:CA | 10 | 0.55 | 0.08 | 0.57 |
| (1,1582) | 1:153:K:ILE:CG1 | 1:172:K:LEU:CA | 10 | 0.55 | 0.08 | 0.57 |
| (1,1582) | 1:153:G:ILE:CG1 | 1:172:G:LEU:CA | 10 | 0.55 | 0.08 | 0.57 |
| (1,1582) | 1:153:H:ILE:CG1 | 1:172:H:LEU:CA | 10 | 0.55 | 0.08 | 0.57 |
| (1,1582) | 1:153:L:ILE:CG1 | 1:172:L:LEU:CA | 10 | 0.55 | 0.08 | 0.57 |
| (1,278) | 1:155:H:GLN:CB | 1:196:H:PRO:CA | 10 | 0.55 | 0.13 | 0.6 |
| (1,278) | 1:155:K:GLN:CB | 1:196:K:PRO:CA | 10 | 0.55 | 0.13 | 0.6 |
| (1,278) | 1:155:G:GLN:CB | 1:196:G:PRO:CA | 10 | 0.55 | 0.13 | 0.6 |
| (1,278) | 1:155:J:GLN:CB | 1:196:J:PRO:CA | 10 | 0.55 | 0.13 | 0.6 |
| (1,1318) | 1:172:K:LEU:CD1 | 1:183:K:ASN:CB | 10 | 0.55 | 0.19 | 0.53 |
| (1,1318) | 1:172:J:LEU:CD1 | 1:183:J:ASN:CB | 10 | 0.55 | 0.19 | 0.53 |
| (1,1318) | 1:172:G:LEU:CD1 | 1:183:G:ASN:CB | 10 | 0.55 | 0.19 | 0.53 |
| (1,636) | 1:150:J:ILE:CD1 | 1:186:J:THR:CB | 10 | 0.52 | 0.15 | 0.49 |
| (1,636) | 1:150:K:ILE:CD1 | 1:186:K:THR:CB | 10 | 0.52 | 0.15 | 0.49 |
| (1,636) | 1:150:I:ILE:CD1 | 1:186:I:THR:CB | 10 | 0.52 | 0.15 | 0.49 |
| (1,1339) | 1:201:I:ILE:CG1 | 1:214:I:MET:CA | 10 | 0.49 | 0.09 | 0.5 |
| (1,1339) | 1:201:L:ILE:CG1 | 1:214:L:MET:CA | 10 | 0.49 | 0.09 | 0.5 |
| (1,987) | 1:235:K:MET:CB | 1:230:K:VAL:CA | 10 | 0.46 | 0.07 | 0.48 |
| (1,987) | 1:235:G:MET:CB | 1:230:G:VAL:CA | 10 | 0.46 | 0.07 | 0.48 |
| (1,987) | 1:235:J:MET:CB | 1:230:J:VAL:CA | 10 | 0.46 | 0.07 | 0.48 |
| (1,987) | 1:235:H:MET:CB | 1:230:H:VAL:CA | 10 | 0.46 | 0.07 | 0.48 |
| (1,75) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 10 | 0.46 | 0.18 | 0.42 |
| (1,1438) | 1:172:K:LEU:CG | 1:183:K:ASN:CA | 10 | 0.45 | 0.14 | 0.48 |
| (1,1438) | 1:172:J:LEU:CG | 1:183:J:ASN:CA | 10 | 0.45 | 0.14 | 0.48 |
| (1,1438) | 1:172:L:LEU:CG | 1:183:L:ASN:CA | 10 | 0.45 | 0.14 | 0.48 |
| (1,1150) | 1:192:H:GLN:CA | 1:164:H:TYR:CZ | 10 | 0.44 | 0.07 | 0.44 |
| (1,1150) | 1:192:I:GLN:CA | 1:164:I:TYR:CZ | 10 | 0.44 | 0.07 | 0.44 |
| (1,1648) | 1:160:H:PRO:CG | 1:161:H:PHE:CG | 10 | 0.43 | 0.05 | 0.44 |
| (1,1648) | 1:160:K:PRO:CG | 1:161:K:PHE:CG | 10 | 0.43 | 0.05 | 0.44 |
| (1,1648) | 1:160:L:PRO:CG | 1:161:L:PHE:CG | 10 | 0.43 | 0.05 | 0.44 |
| (1,1648) | 1:160:G:PRO:CG | 1:161:G:PHE:CG | 10 | 0.43 | 0.05 | 0.44 |
| (1,658) | 1:235:G:MET:CB | 1:233:G:GLU:CG | 10 | 0.42 | 0.06 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,658) | 1:235:H:MET:CB | 1:233:H:GLU:CG | 10 | 0.42 | 0.06 | 0.41 |
| (1,658) | 1:235:I:MET:CB | 1:233:I:GLU:CG | 10 | 0.42 | 0.06 | 0.41 |
| (1,1) | 1:162:G:ARG:CG | 1:154:L:ARG:CA | 10 | 0.37 | 0.15 | 0.39 |
| (1,384) | 1:185:J:MET:CG | 1:151:J:LEU:CB | 10 | 0.35 | 0.16 | 0.38 |
| (1,384) | 1:185:L:MET:CG | 1:151:L:LEU:CB | 10 | 0.35 | 0.16 | 0.38 |
| (1,218) | 1:179:G:GLN:CB | 1:177:G:ALA:CA | 10 | 0.31 | 0.03 | 0.3 |
| (1,218) | 1:179:K:GLN:CB | 1:177:K:ALA:CA | 10 | 0.31 | 0.03 | 0.3 |
| (1,689) | 1:201:J:ILE:CD1 | 1:202:J:LEU:C | 10 | 0.3 | 0.04 | 0.31 |
| (1,689) | 1:201:K:ILE:CD1 | 1:202:K:LEU:C | 10 | 0.3 | 0.04 | 0.31 |
| (1,689) | 1:201:I:ILE:CD1 | 1:202:I:LEU:C | 10 | 0.3 | 0.04 | 0.31 |
| (1,689) | 1:201:H:ILE:CD1 | 1:202:H:LEU:C | 10 | 0.3 | 0.04 | 0.31 |
| (1,968) | 1:221:I:VAL:CG2 | 1:219:I:GLN:CG | 10 | 0.3 | 0.1 | 0.32 |
| (1,968) | 1:221:K:VAL:CG2 | 1:219:K:GLN:CG | 10 | 0.3 | 0.1 | 0.32 |
| (1,968) | 1:221:G:VAL:CG2 | 1:219:G:GLN:CG | 10 | 0.3 | 0.1 | 0.32 |
| (1,389) | 1:210:K:THR:CG2 | 1:211:K:LEU:CG | 10 | 0.23 | 0.05 | 0.22 |
| (1,389) | 1:210:H:THR:CG2 | 1:211:H:LEU:CG | 10 | 0.23 | 0.05 | 0.22 |
| (1,389) | 1:210:J:THR:CG2 | 1:211:J:LEU:CG | 10 | 0.23 | 0.05 | 0.22 |
| (1,1533) | 1:190:H:LEU:CG | 1:187:H:GLU:CB | 10 | 0.22 | 0.07 | 0.22 |
| (1,1533) | 1:190:K:LEU:CG | 1:187:K:GLU:CB | 10 | 0.22 | 0.07 | 0.22 |
| (1,1533) | 1:190:L:LEU:CG | 1:187:L:GLU:CB | 10 | 0.22 | 0.07 | 0.22 |
| (1,1533) | 1:190:I:LEU:CG | 1:187:I:GLU:CB | 10 | 0.22 | 0.07 | 0.22 |
| (1,2277) | 3:302:H:A1CCZ:H9A | 1:232:I:ALA:CA | 9 | 0.77 | 0.22 | 0.78 |
| (1,2277) | 3:302:H:A1CCZ:H9B | 1:232:I:ALA:CA | 9 | 0.77 | 0.22 | 0.78 |
| (1,685) | 1:187:J:GLU:CB | 1:184:J:TRP:CE2 | 9 | 0.51 | 0.15 | 0.49 |
| (1,169) | 1:165:K:VAL:CG2 | 1:202:K:LEU:CG | 9 | 0.44 | 0.1 | 0.45 |
| (1,2258) | 3:302:H:A1CCZ:H11 | 1:232:H:ALA:CA | 9 | 0.42 | 0.16 | 0.4 |
| (1,2293) | 3:302:H:A1CCZ:F33 | 1:160:H:PRO:CA | 9 | 0.42 | 0.14 | 0.39 |
| (1,540) | 1:230:K:VAL:CG2 | 1:221:K:VAL:CA | 9 | 0.35 | 0.13 | 0.44 |
| (1,540) | 1:230:J:VAL:CG1 | 1:221:J:VAL:CA | 9 | 0.35 | 0.13 | 0.44 |
| (1,540) | 1:230:H:VAL:CG1 | 1:221:H:VAL:CA | 9 | 0.35 | 0.13 | 0.44 |
| (1,540) | 1:230:J:VAL:CG2 | 1:221:J:VAL:CA | 9 | 0.35 | 0.13 | 0.44 |
| (1,540) | 1:230:I:VAL:CG2 | 1:221:I:VAL:CA | 9 | 0.35 | 0.13 | 0.44 |
| (1,540) | 1:230:H:VAL:CG2 | 1:221:H:VAL:CA | 9 | 0.35 | 0.13 | 0.44 |
| (1,227) | 1:198:H:CYS:CB | 1:199:H:LYS:CE | 9 | 0.3 | 0.07 | 0.29 |
| (1,227) | 1:198:J:CYS:CB | 1:199:J:LYS:CE | 9 | 0.3 | 0.07 | 0.29 |
| (1,227) | 1:198:G:CYS:CB | 1:199:G:LYS:CE | 9 | 0.3 | 0.07 | 0.29 |
| (1,1233) | 1:190:H:LEU:CD1 | 1:166:H:ASP:CA | 9 | 0.27 | 0.06 | 0.28 |
| (1,1233) | 1:190:K:LEU:CD1 | 1:166:K:ASP:CA | 9 | 0.27 | 0.06 | 0.28 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE2 | 9 | 0.26 | 0.08 | 0.24 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE3 | 9 | 0.26 | 0.08 | 0.24 |
| (1,267) | 1:188:K:THR:CG2 | 1:185:K:MET:CB | 9 | 0.26 | 0.08 | 0.24 |
| (1,297) | 1:244:L:ILE:CG1 | 1:237:L:GLN:CA | 9 | 0.17 | 0.03 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-------------------|--------------------|---------------------|----------|---------------------|------------|
| (1,297) | 1:244:H:ILE:CG1 | 1:237:H:GLN:CA | 9 | 0.17 | 0.03 | 0.15 |
| (1,297) | 1:244:I:ILE:CG1 | 1:237:I:GLN:CA | 9 | 0.17 | 0.03 | 0.15 |
| (1,297) | 1:244:J:ILE:CG1 | 1:237:J:GLN:CA | 9 | 0.17 | 0.03 | 0.15 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD2 | 8 | 0.75 | 0.13 | 0.78 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD3 | 8 | 0.75 | 0.13 | 0.78 |
| (1,2225) | 3:302:H:A1CCZ:F33 | 1:159:H:GLU:CB | 8 | 0.7 | 0.09 | 0.69 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12A | 8 | 0.56 | 0.24 | 0.55 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12B | 8 | 0.56 | 0.24 | 0.55 |
| (1,1013) | 1:189:I:LEU:CA | 1:153:I:ILE:C | 8 | 0.4 | 0.19 | 0.3 |
| (1,1013) | 1:189:K:LEU:CA | 1:153:K:ILE:C | 8 | 0.4 | 0.19 | 0.3 |
| (1,1013) | 1:189:H:LEU:CA | 1:153:H:ILE:C | 8 | 0.4 | 0.19 | 0.3 |
| (1,1013) | 1:189:L:LEU:CA | 1:153:L:ILE:C | 8 | 0.4 | 0.19 | 0.3 |
| (1,365) | 1:196:H:PRO:CD | 1:200:H:THR:CB | 8 | 0.39 | 0.1 | 0.41 |
| (1,365) | 1:196:K:PRO:CD | 1:200:K:THR:CB | 8 | 0.39 | 0.1 | 0.41 |
| (1,365) | 1:196:J:PRO:CD | 1:200:J:THR:CB | 8 | 0.39 | 0.1 | 0.41 |
| (1,365) | 1:196:I:PRO:CD | 1:200:I:THR:CB | 8 | 0.39 | 0.1 | 0.41 |
| (1,1377) | 1:205:I:LEU:CD1 | 1:210:I:THR:CA | 8 | 0.36 | 0.13 | 0.33 |
| (1,1377) | 1:205:J:LEU:CD1 | 1:210:J:THR:CA | 8 | 0.36 | 0.13 | 0.33 |
| (1,1377) | 1:205:L:LEU:CD1 | 1:210:L:THR:CA | 8 | 0.36 | 0.13 | 0.33 |
| (1,1377) | 1:205:K:LEU:CD1 | 1:210:K:THR:CA | 8 | 0.36 | 0.13 | 0.33 |
| (1,74) | 1:231:J:LEU:N | 1:228:K:ALA:CB | 8 | 0.35 | 0.08 | 0.4 |
| (1,5) | 1:162:I:ARG:CG | 1:154:H:ARG:CA | 8 | 0.34 | 0.15 | 0.4 |
| (1,78) | 1:219:J:GLN:CG | 1:195:I:ASN:CA | 8 | 0.31 | 0.11 | 0.33 |
| (1,561) | 1:201:H:ILE:CG1 | 1:205:H:LEU:CA | 8 | 0.3 | 0.04 | 0.3 |
| (1,561) | 1:201:L:ILE:CG1 | 1:205:L:LEU:CA | 8 | 0.3 | 0.04 | 0.3 |
| (1,561) | 1:201:J:ILE:CG1 | 1:205:J:LEU:CA | 8 | 0.3 | 0.04 | 0.3 |
| (1,387) | 1:194:J:ALA:CB | 1:154:J:ARG:CG | 8 | 0.29 | 0.12 | 0.25 |
| (1,387) | 1:194:L:ALA:CB | 1:154:L:ARG:CG | 8 | 0.29 | 0.12 | 0.25 |
| (1,387) | 1:194:K:ALA:CB | 1:154:K:ARG:CG | 8 | 0.29 | 0.12 | 0.25 |
| (1,387) | 1:194:I:ALA:CB | 1:154:I:ARG:CG | 8 | 0.29 | 0.12 | 0.25 |
| (1,673) | 1:165:G:VAL:CG2 | 1:163:G:ASP:CB | 8 | 0.22 | 0.08 | 0.22 |
| (1,673) | 1:165:H:VAL:CG2 | 1:163:H:ASP:CB | 8 | 0.22 | 0.08 | 0.22 |
| (1,673) | 1:165:J:VAL:CG2 | 1:163:J:ASP:CB | 8 | 0.22 | 0.08 | 0.22 |
| (1,673) | 1:165:K:VAL:CG2 | 1:163:K:ASP:CB | 8 | 0.22 | 0.08 | 0.22 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE2 | 8 | 0.22 | 0.07 | 0.24 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE3 | 8 | 0.22 | 0.07 | 0.24 |
| (1,1100) | 1:190:H:LEU:CD1 | 1:169:H:TYR:CB | 8 | 0.2 | 0.08 | 0.19 |
| (1,1100) | 1:190:G:LEU:CD1 | 1:169:G:TYR:CB | 8 | 0.2 | 0.08 | 0.19 |
| (1,1100) | 1:190:K:LEU:CD1 | 1:169:K:TYR:CB | 8 | 0.2 | 0.08 | 0.19 |
| (1,936) | 1:172:I:LEU:CD1 | 1:189:I:LEU:CB | 8 | 0.16 | 0.05 | 0.15 |
| (1,936) | 1:172:H:LEU:CD1 | 1:189:H:LEU:CB | 8 | 0.16 | 0.05 | 0.15 |
| (1,936) | 1:172:K:LEU:CD1 | 1:189:K:LEU:CB | 8 | 0.16 | 0.05 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-------------------|--------------------|---------------------|----------|---------------------|------------|
| (1,2296) | 3:302:H:A1CCZ:F32 | 1:196:H:PRO:CG | 7 | 0.59 | 0.3 | 0.7 |
| (2,92) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:H12A | 7 | 0.39 | 0.2 | 0.42 |
| (2,92) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:H12B | 7 | 0.39 | 0.2 | 0.42 |
| (1,2204) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:F32 | 7 | 0.35 | 0.24 | 0.27 |
| (1,414) | 1:201:I:ILE:CG2 | 1:197:I:ASP:CB | 7 | 0.31 | 0.1 | 0.35 |
| (1,414) | 1:201:H:ILE:CG2 | 1:197:H:ASP:CB | 7 | 0.31 | 0.1 | 0.35 |
| (1,414) | 1:201:J:ILE:CG2 | 1:197:J:ASP:CB | 7 | 0.31 | 0.1 | 0.35 |
| (1,2308) | 3:302:H:A1CCZ:F31 | 1:228:H:ALA:CA | 7 | 0.25 | 0.11 | 0.19 |
| (1,1220) | 1:214:J:MET:CG | 1:191:J:VAL:CB | 7 | 0.24 | 0.06 | 0.28 |
| (1,1220) | 1:214:I:MET:CG | 1:191:I:VAL:CB | 7 | 0.24 | 0.06 | 0.28 |
| (1,1220) | 1:214:K:MET:CG | 1:191:K:VAL:CB | 7 | 0.24 | 0.06 | 0.28 |
| (1,3) | 1:162:K:ARG:CG | 1:154:J:ARG:CA | 7 | 0.24 | 0.12 | 0.21 |
| (1,8) | 1:195:I:ASN:CA | 1:219:J:GLN:CA | 7 | 0.22 | 0.09 | 0.22 |
| (1,1381) | 1:217:I:ALA:CB | 1:221:I:VAL:CG2 | 7 | 0.21 | 0.08 | 0.22 |
| (1,1381) | 1:217:L:ALA:CB | 1:221:L:VAL:CG2 | 7 | 0.21 | 0.08 | 0.22 |
| (1,1381) | 1:217:K:ALA:CB | 1:221:K:VAL:CG2 | 7 | 0.21 | 0.08 | 0.22 |
| (1,2196) | 2:301:H:IHP:O41 | 3:302:H:A1CCZ:F32 | 6 | 0.42 | 0.28 | 0.34 |
| (1,1481) | 1:194:I:ALA:CB | 1:202:I:LEU:CB | 6 | 0.36 | 0.1 | 0.38 |
| (1,1481) | 1:194:J:ALA:CB | 1:202:J:LEU:CB | 6 | 0.36 | 0.1 | 0.38 |
| (1,1481) | 1:194:L:ALA:CB | 1:202:L:LEU:CB | 6 | 0.36 | 0.1 | 0.38 |
| (1,1481) | 1:194:H:ALA:CB | 1:202:H:LEU:CB | 6 | 0.36 | 0.1 | 0.38 |
| (1,73) | 1:231:I:LEU:N | 1:228:J:ALA:CB | 6 | 0.28 | 0.13 | 0.24 |
| (1,4) | 1:162:J:ARG:CG | 1:154:I:ARG:CA | 6 | 0.28 | 0.11 | 0.26 |
| (1,25) | 1:232:L:ALA:CB | 1:238:K:VAL:CB | 6 | 0.27 | 0.05 | 0.29 |
| (1,2163) | 2:301:H:IHP:P1 | 1:224:J:PRO:HG2 | 6 | 0.25 | 0.18 | 0.18 |
| (1,2163) | 2:301:H:IHP:P1 | 1:224:J:PRO:HG3 | 6 | 0.25 | 0.18 | 0.18 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ1 | 6 | 0.2 | 0.1 | 0.18 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ2 | 6 | 0.2 | 0.1 | 0.18 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ3 | 6 | 0.2 | 0.1 | 0.18 |
| (1,808) | 1:191:L:VAL:CG1 | 1:193:L:ASN:CA | 6 | 0.19 | 0.08 | 0.16 |
| (1,808) | 1:191:K:VAL:CG1 | 1:193:K:ASN:CA | 6 | 0.19 | 0.08 | 0.16 |
| (1,166) | 1:219:H:GLN:CG | 1:160:H:PRO:CA | 6 | 0.18 | 0.04 | 0.18 |
| (1,166) | 1:219:J:GLN:CG | 1:160:J:PRO:CA | 6 | 0.18 | 0.04 | 0.18 |
| (2,8) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H9A | 5 | 0.63 | 0.35 | 0.59 |
| (2,8) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H9B | 5 | 0.63 | 0.35 | 0.59 |
| (1,2250) | 3:302:H:A1CCZ:F32 | 1:198:H:CYS:CA | 5 | 0.32 | 0.15 | 0.29 |
| (1,945) | 1:150:J:ILE:CD1 | 1:193:J:ASN:CG | 5 | 0.25 | 0.07 | 0.27 |
| (1,945) | 1:150:G:ILE:CD1 | 1:193:G:ASN:CG | 5 | 0.25 | 0.07 | 0.27 |
| (1,2210) | 2:301:H:IHP:O45 | 3:302:H:A1CCZ:F32 | 5 | 0.25 | 0.13 | 0.18 |
| (1,580) | 1:153:K:ILE:CD1 | 1:193:K:ASN:CG | 5 | 0.22 | 0.04 | 0.23 |
| (1,580) | 1:153:L:ILE:CD1 | 1:193:L:ASN:CG | 5 | 0.22 | 0.04 | 0.23 |
| (1,248) | 1:156:J:GLY:CA | 1:196:J:PRO:CD | 5 | 0.19 | 0.1 | 0.13 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-------------------|--------------------|---------------------|----------|---------------------|------------|
| (1,248) | 1:156:L:GLY:CA | 1:196:L:PRO:CD | 5 | 0.19 | 0.1 | 0.13 |
| (1,248) | 1:156:I:GLY:CA | 1:196:I:PRO:CD | 5 | 0.19 | 0.1 | 0.13 |
| (1,248) | 1:156:K:GLY:CA | 1:196:K:PRO:CD | 5 | 0.19 | 0.1 | 0.13 |
| (1,1313) | 1:190:G:LEU:CD1 | 1:202:G:LEU:CG | 5 | 0.18 | 0.06 | 0.19 |
| (1,1313) | 1:190:K:LEU:CD1 | 1:202:K:LEU:CG | 5 | 0.18 | 0.06 | 0.19 |
| (1,1313) | 1:190:L:LEU:CD1 | 1:202:L:LEU:CG | 5 | 0.18 | 0.06 | 0.19 |
| (1,505) | 1:174:J:ALA:CA | 1:148:J:THR:CA | 5 | 0.17 | 0.03 | 0.17 |
| (1,505) | 1:174:K:ALA:CA | 1:148:K:THR:CA | 5 | 0.17 | 0.03 | 0.17 |
| (1,505) | 1:174:I:ALA:CA | 1:148:I:THR:CA | 5 | 0.17 | 0.03 | 0.17 |
| (1,423) | 1:190:G:LEU:CG | 1:193:G:ASN:C | 5 | 0.17 | 0.06 | 0.14 |
| (1,423) | 1:190:K:LEU:CG | 1:193:K:ASN:C | 5 | 0.17 | 0.06 | 0.14 |
| (1,539) | 1:187:J:GLU:CB | 1:184:J:TRP:CZ3 | 5 | 0.16 | 0.02 | 0.17 |
| (1,539) | 1:187:G:GLU:CB | 1:184:G:TRP:CZ3 | 5 | 0.16 | 0.02 | 0.17 |
| (1,539) | 1:187:L:GLU:CB | 1:184:L:TRP:CZ3 | 5 | 0.16 | 0.02 | 0.17 |
| (1,1620) | 1:190:G:LEU:CD1 | 1:194:G:ALA:C | 5 | 0.16 | 0.03 | 0.15 |
| (1,1620) | 1:190:H:LEU:CD1 | 1:194:H:ALA:C | 5 | 0.16 | 0.03 | 0.15 |
| (1,76) | 1:219:L:GLN:CG | 1:195:K:ASN:CA | 5 | 0.16 | 0.08 | 0.12 |
| (1,640) | 1:190:L:LEU:CD1 | 1:193:L:ASN:C | 5 | 0.16 | 0.03 | 0.16 |
| (1,640) | 1:190:I:LEU:CD1 | 1:193:I:ASN:C | 5 | 0.16 | 0.03 | 0.16 |
| (1,640) | 1:190:G:LEU:CD1 | 1:193:G:ASN:C | 5 | 0.16 | 0.03 | 0.16 |
| (1,989) | 1:221:I:VAL:CG1 | 1:223:I:GLY:CA | 5 | 0.16 | 0.04 | 0.15 |
| (1,989) | 1:221:K:VAL:CG1 | 1:223:K:GLY:CA | 5 | 0.16 | 0.04 | 0.15 |
| (1,1591) | 1:175:I:GLU:CB | 1:185:I:MET:CB | 5 | 0.16 | 0.03 | 0.14 |
| (1,1591) | 1:175:L:GLU:CB | 1:185:L:MET:CB | 5 | 0.16 | 0.03 | 0.14 |
| (1,1591) | 1:175:K:GLU:CB | 1:185:K:MET:CB | 5 | 0.16 | 0.03 | 0.14 |
| (1,2221) | 3:302:H:A1CCZ:F33 | 1:224:H:PRO:CG | 4 | 0.42 | 0.1 | 0.44 |
| (2,12) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H12A | 4 | 0.37 | 0.13 | 0.36 |
| (2,12) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H12B | 4 | 0.37 | 0.13 | 0.36 |
| (1,420) | 1:202:L:LEU:CD1 | 1:199:L:LYS:CD | 4 | 0.36 | 0.12 | 0.38 |
| (1,2197) | 2:301:H:IHP:O41 | 3:302:H:A1CCZ:F33 | 4 | 0.33 | 0.1 | 0.38 |
| (1,1497) | 1:165:K:VAL:CG2 | 1:214:K:MET:CA | 4 | 0.29 | 0.04 | 0.29 |
| (1,1497) | 1:165:H:VAL:CG2 | 1:214:H:MET:CA | 4 | 0.29 | 0.04 | 0.29 |
| (1,48) | 1:221:K:VAL:CG1 | 1:224:L:PRO:CD | 4 | 0.26 | 0.04 | 0.26 |
| (1,48) | 1:221:K:VAL:CG2 | 1:224:L:PRO:CD | 4 | 0.26 | 0.04 | 0.26 |
| (1,2284) | 3:302:H:A1CCZ:F32 | 1:157:H:PRO:CG | 4 | 0.25 | 0.06 | 0.28 |
| (1,204) | 1:150:H:ILE:CD1 | 1:189:H:LEU:CA | 4 | 0.25 | 0.1 | 0.21 |
| (1,204) | 1:150:K:ILE:CD1 | 1:189:K:LEU:CA | 4 | 0.25 | 0.1 | 0.21 |
| (1,1519) | 1:167:K:ARG:CD | 1:171:K:THR:CA | 4 | 0.16 | 0.05 | 0.14 |
| (1,1519) | 1:167:G:ARG:CD | 1:171:G:THR:CA | 4 | 0.16 | 0.05 | 0.14 |
| (1,1519) | 1:167:I:ARG:CD | 1:171:I:THR:CA | 4 | 0.16 | 0.05 | 0.14 |
| (1,1519) | 1:167:H:ARG:CD | 1:171:H:THR:CA | 4 | 0.16 | 0.05 | 0.14 |
| (1,1473) | 1:153:J:ILE:CG2 | 1:165:J:VAL:C | 4 | 0.14 | 0.03 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-------------------|--------------------|---------------------|----------|---------------------|------------|
| (1,1473) | 1:153:I:ILE:CG2 | 1:165:I:VAL:C | 4 | 0.14 | 0.03 | 0.15 |
| (1,2133) | 2:301:H:IHP:P4 | 1:158:L:LYS:HZ1 | 4 | 0.14 | 0.03 | 0.13 |
| (1,2133) | 2:301:H:IHP:P4 | 1:158:L:LYS:HZ2 | 4 | 0.14 | 0.03 | 0.13 |
| (1,2133) | 2:301:H:IHP:P4 | 1:158:L:LYS:HZ3 | 4 | 0.14 | 0.03 | 0.13 |
| (1,1172) | 1:244:L:ILE:CG1 | 1:237:L:GLN:CB | 4 | 0.13 | 0.02 | 0.13 |
| (1,1123) | 1:211:J:LEU:CD1 | 1:210:J:THR:CB | 4 | 0.12 | 0.01 | 0.12 |
| (1,1123) | 1:211:L:LEU:CD1 | 1:210:L:THR:CB | 4 | 0.12 | 0.01 | 0.12 |
| (1,77) | 1:219:K:GLN:CG | 1:195:J:ASN:CA | 3 | 0.35 | 0.01 | 0.34 |
| (1,11) | 1:195:L:ASN:CA | 1:219:G:GLN:CA | 3 | 0.31 | 0.11 | 0.35 |
| (1,1385) | 1:151:J:LEU:CG | 1:189:J:LEU:CB | 3 | 0.27 | 0.01 | 0.28 |
| (1,1385) | 1:151:G:LEU:CG | 1:189:G:LEU:CB | 3 | 0.27 | 0.01 | 0.28 |
| (1,2190) | 2:301:H:IHP:O21 | 3:302:H:A1CCZ:F32 | 3 | 0.25 | 0.06 | 0.23 |
| (1,2233) | 3:302:H:A1CCZ:F32 | 1:195:H:ASN:CA | 3 | 0.25 | 0.07 | 0.24 |
| (1,1469) | 1:214:J:MET:CB | 1:205:J:LEU:CA | 3 | 0.25 | 0.11 | 0.21 |
| (1,1469) | 1:214:I:MET:CB | 1:205:I:LEU:CA | 3 | 0.25 | 0.11 | 0.21 |
| (1,2251) | 3:302:H:A1CCZ:F33 | 1:198:H:CYS:CA | 3 | 0.22 | 0.05 | 0.22 |
| (1,831) | 1:150:K:ILE:CD1 | 1:190:K:LEU:CA | 3 | 0.2 | 0.06 | 0.21 |
| (1,756) | 1:191:K:VAL:CG1 | 1:194:K:ALA:C | 3 | 0.19 | 0.03 | 0.2 |
| (1,756) | 1:191:L:VAL:CG1 | 1:194:L:ALA:C | 3 | 0.19 | 0.03 | 0.2 |
| (1,1514) | 1:193:J:ASN:CB | 1:188:J:THR:C | 3 | 0.18 | 0.05 | 0.17 |
| (1,1514) | 1:193:L:ASN:CB | 1:188:L:THR:C | 3 | 0.18 | 0.05 | 0.17 |
| (1,442) | 1:228:H:ALA:CB | 1:224:H:PRO:CG | 3 | 0.17 | 0.03 | 0.19 |
| (1,442) | 1:228:K:ALA:CB | 1:224:K:PRO:CG | 3 | 0.17 | 0.03 | 0.19 |
| (1,442) | 1:228:L:ALA:CB | 1:224:L:PRO:CG | 3 | 0.17 | 0.03 | 0.19 |
| (1,1237) | 1:155:H:GLN:CA | 1:160:H:PRO:CA | 3 | 0.15 | 0.05 | 0.11 |
| (1,206) | 1:160:J:PRO:CA | 1:164:J:TYR:CD2 | 3 | 0.14 | 0.04 | 0.12 |
| (1,206) | 1:160:L:PRO:CA | 1:164:L:TYR:CD2 | 3 | 0.14 | 0.04 | 0.12 |
| (1,206) | 1:160:I:PRO:CA | 1:164:I:TYR:CD2 | 3 | 0.14 | 0.04 | 0.12 |
| (1,399) | 1:150:J:ILE:CD1 | 1:190:J:LEU:CD1 | 3 | 0.13 | 0.02 | 0.14 |
| (1,399) | 1:150:K:ILE:CD1 | 1:190:K:LEU:CD1 | 3 | 0.13 | 0.02 | 0.14 |
| (1,1650) | 1:204:H:ALA:CB | 1:206:H:GLY:C | 3 | 0.13 | 0.01 | 0.13 |
| (1,1650) | 1:204:J:ALA:CB | 1:206:J:GLY:C | 3 | 0.13 | 0.01 | 0.13 |
| (1,24) | 1:232:G:ALA:CB | 1:238:L:VAL:CB | 3 | 0.12 | 0.02 | 0.11 |
| (2,16) | 2:301:H:IHP:O43 | 3:302:H:A1CCZ:H12A | 2 | 0.47 | 0.13 | 0.47 |
| (2,16) | 2:301:H:IHP:O43 | 3:302:H:A1CCZ:H12B | 2 | 0.47 | 0.13 | 0.47 |
| (1,2141) | 2:301:H:IHP:P6 | 1:158:I:LYS:HA | 2 | 0.43 | 0.1 | 0.43 |
| (1,2135) | 2:301:H:IHP:P4 | 1:227:H:LYS:HZ1 | 2 | 0.42 | 0.01 | 0.42 |
| (1,2135) | 2:301:H:IHP:P4 | 1:227:H:LYS:HZ2 | 2 | 0.42 | 0.01 | 0.42 |
| (1,2135) | 2:301:H:IHP:P4 | 1:227:H:LYS:HZ3 | 2 | 0.42 | 0.01 | 0.42 |
| (1,2191) | 2:301:H:IHP:O21 | 3:302:H:A1CCZ:F33 | 2 | 0.34 | 0.05 | 0.34 |
| (1,2122) | 2:301:H:IHP:P4 | 1:158:J:LYS:HE2 | 2 | 0.3 | 0.05 | 0.3 |
| (1,2122) | 2:301:H:IHP:P4 | 1:158:J:LYS:HE3 | 2 | 0.3 | 0.05 | 0.3 |

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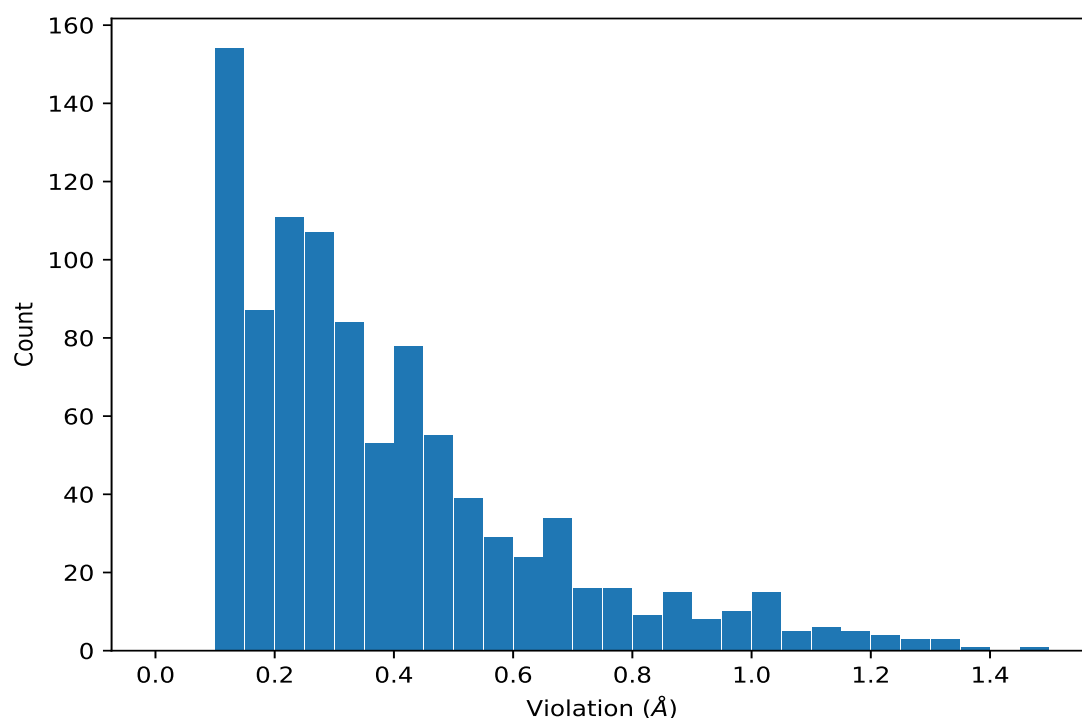
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2292) | 3:302:H:A1CCZ:F32 | 1:160:H:PRO:CA | 2 | 0.29 | 0.14 | 0.29 |
| (1,2157) | 2:301:H:IHP:P3 | 1:158:L:LYS:HA | 2 | 0.27 | 0.1 | 0.27 |
| (1,1205) | 1:153:K:ILE:CB | 1:193:K:ASN:CA | 2 | 0.24 | 0.04 | 0.24 |
| (1,1205) | 1:153:J:ILE:CB | 1:193:J:ASN:CA | 2 | 0.24 | 0.04 | 0.24 |
| (1,6) | 1:162:H:ARG:CG | 1:154:G:ARG:CA | 2 | 0.24 | 0.04 | 0.24 |
| (1,974) | 1:153:J:ILE:CD1 | 1:151:J:LEU:C | 2 | 0.23 | 0.02 | 0.23 |
| (1,974) | 1:153:I:ILE:CD1 | 1:151:I:LEU:C | 2 | 0.23 | 0.02 | 0.23 |
| (1,2169) | 2:301:H:IHP:P1 | 1:224:J:PRO:HD2 | 2 | 0.22 | 0.11 | 0.22 |
| (1,2169) | 2:301:H:IHP:P1 | 1:224:J:PRO:HD3 | 2 | 0.22 | 0.11 | 0.22 |
| (1,1203) | 1:191:K:VAL:CG1 | 1:194:K:ALA:CA | 2 | 0.2 | 0.05 | 0.2 |
| (1,1203) | 1:191:L:VAL:CG1 | 1:194:L:ALA:CA | 2 | 0.2 | 0.05 | 0.2 |
| (1,1297) | 1:218:G:CYS:CB | 1:226:G:HIS:CD2 | 2 | 0.2 | 0.05 | 0.2 |
| (1,1297) | 1:218:J:CYS:CB | 1:226:J:HIS:CD2 | 2 | 0.2 | 0.05 | 0.2 |
| (1,915) | 1:235:G:MET:CB | 1:239:G:THR:CA | 2 | 0.14 | 0.01 | 0.14 |
| (1,560) | 1:201:I:ILE:CD1 | 1:161:I:PHE:CD1 | 2 | 0.12 | 0.0 | 0.12 |
| (1,560) | 1:201:K:ILE:CD1 | 1:161:K:PHE:CD1 | 2 | 0.12 | 0.0 | 0.12 |

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-------------------|----------|---------------|
| (1,1096) | 1:171:I:THR:CG2 | 1:152:I:ASP:CB | 9 | 1.49 |
| (1,2174) | 2:301:H:IHP:P2 | 1:158:L:LYS:HA | 6 | 1.38 |
| (1,1096) | 1:171:J:THR:CG2 | 1:152:J:ASP:CB | 8 | 1.33 |
| (1,833) | 1:221:G:VAL:CG2 | 1:230:G:VAL:CG1 | 9 | 1.33 |
| (1,1096) | 1:171:I:THR:CG2 | 1:152:I:ASP:CB | 7 | 1.32 |
| (1,2174) | 2:301:H:IHP:P2 | 1:158:L:LYS:HA | 7 | 1.28 |
| (1,2172) | 2:301:H:IHP:P1 | 1:158:H:LYS:HA | 5 | 1.25 |
| (1,1096) | 1:171:J:THR:CG2 | 1:152:J:ASP:CB | 2 | 1.25 |
| (1,1096) | 1:171:L:THR:CG2 | 1:152:L:ASP:CB | 3 | 1.24 |
| (1,833) | 1:221:G:VAL:CG2 | 1:230:G:VAL:CG2 | 4 | 1.24 |
| (1,2118) | 2:301:H:IHP:P4 | 1:158:J:LYS:HA | 5 | 1.21 |
| (1,833) | 1:221:I:VAL:CG2 | 1:230:I:VAL:CG2 | 6 | 1.21 |
| (1,1096) | 1:171:H:THR:CG2 | 1:152:H:ASP:CB | 10 | 1.2 |
| (1,833) | 1:221:J:VAL:CG2 | 1:230:J:VAL:CG2 | 1 | 1.19 |
| (1,2172) | 2:301:H:IHP:P1 | 1:158:H:LYS:HA | 10 | 1.18 |
| (1,2207) | 2:301:H:IHP:O35 | 3:302:H:A1CCZ:F32 | 6 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,2118) | 2:301:H:IHP:P4 | 1:158:J:LYS:HA | 6 | 1.16 |
| (1,29) | 1:219:L:GLN:CG | 1:155:K:GLN:CA | 7 | 1.15 |
| (1,2174) | 2:301:H:IHP:P2 | 1:158:L:LYS:HA | 8 | 1.12 |
| (1,2162) | 2:301:H:IHP:P1 | 1:224:I:PRO:HG2 | 7 | 1.12 |
| (1,2162) | 2:301:H:IHP:P1 | 1:224:I:PRO:HG3 | 7 | 1.12 |
| (1,2118) | 2:301:H:IHP:P4 | 1:158:J:LYS:HA | 7 | 1.11 |
| (1,833) | 1:221:J:VAL:CG2 | 1:230:J:VAL:CG2 | 3 | 1.11 |
| (1,2277) | 3:302:H:A1CCZ:H9A | 1:232:I:ALA:CA | 9 | 1.05 |
| (1,2277) | 3:302:H:A1CCZ:H9B | 1:232:I:ALA:CA | 9 | 1.05 |
| (1,2172) | 2:301:H:IHP:P1 | 1:158:H:LYS:HA | 1 | 1.05 |
| (1,1096) | 1:171:H:THR:CG2 | 1:152:H:ASP:CB | 1 | 1.05 |
| (1,1096) | 1:171:H:THR:CG2 | 1:152:H:ASP:CB | 5 | 1.05 |
| (1,2172) | 2:301:H:IHP:P1 | 1:158:H:LYS:HA | 2 | 1.04 |
| (1,2172) | 2:301:H:IHP:P1 | 1:158:H:LYS:HA | 3 | 1.04 |
| (2,8) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H9A | 1 | 1.03 |
| (2,8) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H9B | 1 | 1.03 |
| (1,2118) | 2:301:H:IHP:P4 | 1:158:J:LYS:HA | 10 | 1.03 |
| (1,833) | 1:221:J:VAL:CG2 | 1:230:J:VAL:CG2 | 10 | 1.03 |
| (2,8) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H9A | 5 | 1.02 |
| (2,8) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H9B | 5 | 1.02 |
| (1,2172) | 2:301:H:IHP:P1 | 1:158:H:LYS:HA | 8 | 1.02 |
| (1,1096) | 1:171:K:THR:CG2 | 1:152:K:ASP:CB | 4 | 1.02 |
| (1,2172) | 2:301:H:IHP:P1 | 1:158:H:LYS:HA | 7 | 1.01 |
| (1,2115) | 2:301:H:IHP:P4 | 1:158:G:LYS:HA | 3 | 1.01 |
| (1,833) | 1:221:H:VAL:CG2 | 1:230:H:VAL:CG1 | 8 | 1.01 |
| (1,2296) | 3:302:H:A1CCZ:F32 | 1:196:H:PRO:CG | 10 | 1.0 |
| (1,412) | 1:202:L:LEU:CG | 1:194:L:ALA:CA | 4 | 1.0 |
| (1,2277) | 3:302:H:A1CCZ:H9A | 1:232:I:ALA:CA | 2 | 0.99 |
| (1,2277) | 3:302:H:A1CCZ:H9B | 1:232:I:ALA:CA | 2 | 0.99 |
| (1,2172) | 2:301:H:IHP:P1 | 1:158:H:LYS:HA | 4 | 0.99 |
| (1,833) | 1:221:I:VAL:CG2 | 1:230:I:VAL:CG1 | 2 | 0.99 |
| (1,2277) | 3:302:H:A1CCZ:H9A | 1:232:I:ALA:CA | 4 | 0.98 |
| (1,2277) | 3:302:H:A1CCZ:H9B | 1:232:I:ALA:CA | 4 | 0.98 |
| (1,2172) | 2:301:H:IHP:P1 | 1:158:H:LYS:HA | 9 | 0.98 |
| (1,2115) | 2:301:H:IHP:P4 | 1:158:G:LYS:HA | 9 | 0.97 |
| (1,1318) | 1:172:G:LEU:CD1 | 1:183:G:ASN:CB | 7 | 0.97 |
| (1,2118) | 2:301:H:IHP:P4 | 1:158:J:LYS:HA | 9 | 0.96 |
| (1,2207) | 2:301:H:IHP:O35 | 3:302:H:A1CCZ:F32 | 9 | 0.95 |
| (1,2118) | 2:301:H:IHP:P4 | 1:158:J:LYS:HA | 2 | 0.95 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12A | 4 | 0.94 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12B | 4 | 0.94 |
| (1,2172) | 2:301:H:IHP:P1 | 1:158:H:LYS:HA | 6 | 0.93 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,75) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 7 | 0.92 |
| (1,2207) | 2:301:H:IHP:O35 | 3:302:H:A1CCZ:F32 | 4 | 0.91 |
| (1,2204) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:F32 | 6 | 0.9 |
| (1,2207) | 2:301:H:IHP:O35 | 3:302:H:A1CCZ:F32 | 10 | 0.89 |
| (1,2196) | 2:301:H:IHP:O41 | 3:302:H:A1CCZ:F32 | 5 | 0.89 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD2 | 9 | 0.89 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD3 | 9 | 0.89 |
| (1,2296) | 3:302:H:A1CCZ:F32 | 1:196:H:PRO:CG | 1 | 0.88 |
| (1,2277) | 3:302:H:A1CCZ:H9A | 1:232:I:ALA:CA | 1 | 0.88 |
| (1,2277) | 3:302:H:A1CCZ:H9B | 1:232:I:ALA:CA | 1 | 0.88 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD2 | 10 | 0.88 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD3 | 10 | 0.88 |
| (1,2225) | 3:302:H:A1CCZ:F33 | 1:159:H:GLU:CB | 3 | 0.87 |
| (1,2115) | 2:301:H:IHP:P4 | 1:158:G:LYS:HA | 4 | 0.87 |
| (1,2207) | 2:301:H:IHP:O35 | 3:302:H:A1CCZ:F32 | 2 | 0.86 |
| (1,2207) | 2:301:H:IHP:O35 | 3:302:H:A1CCZ:F32 | 5 | 0.86 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD2 | 2 | 0.86 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD3 | 2 | 0.86 |
| (1,2207) | 2:301:H:IHP:O35 | 3:302:H:A1CCZ:F32 | 3 | 0.84 |
| (1,685) | 1:187:J:GLU:CB | 1:184:J:TRP:CE2 | 8 | 0.84 |
| (1,1638) | 1:155:J:GLN:CB | 1:197:J:ASP:CB | 8 | 0.83 |
| (1,2262) | 3:302:H:A1CCZ:H7A | 1:232:H:ALA:CA | 4 | 0.81 |
| (1,2262) | 3:302:H:A1CCZ:H7B | 1:232:H:ALA:CA | 4 | 0.81 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD2 | 1 | 0.81 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD3 | 1 | 0.81 |
| (1,2174) | 2:301:H:IHP:P2 | 1:158:L:LYS:HA | 9 | 0.8 |
| (1,412) | 1:202:I:LEU:CG | 1:194:I:ALA:CA | 3 | 0.8 |
| (1,2225) | 3:302:H:A1CCZ:F33 | 1:159:H:GLU:CB | 9 | 0.79 |
| (1,636) | 1:150:K:ILE:CD1 | 1:186:K:THR:CB | 3 | 0.79 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12A | 3 | 0.78 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12B | 3 | 0.78 |
| (1,2277) | 3:302:H:A1CCZ:H9A | 1:232:I:ALA:CA | 10 | 0.78 |
| (1,2277) | 3:302:H:A1CCZ:H9B | 1:232:I:ALA:CA | 10 | 0.78 |
| (1,2115) | 2:301:H:IHP:P4 | 1:158:G:LYS:HA | 1 | 0.78 |
| (2,92) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:H12A | 8 | 0.77 |
| (2,92) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:H12B | 8 | 0.77 |
| (1,2296) | 3:302:H:A1CCZ:F32 | 1:196:H:PRO:CG | 7 | 0.77 |
| (1,2258) | 3:302:H:A1CCZ:H11 | 1:232:H:ALA:CA | 6 | 0.77 |
| (1,29) | 1:219:L:GLN:CG | 1:155:K:GLN:CA | 1 | 0.77 |
| (1,2262) | 3:302:H:A1CCZ:H7A | 1:232:H:ALA:CA | 7 | 0.76 |
| (1,2262) | 3:302:H:A1CCZ:H7B | 1:232:H:ALA:CA | 7 | 0.76 |
| (1,2174) | 2:301:H:IHP:P2 | 1:158:L:LYS:HA | 10 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,1638) | 1:155:J:GLN:CB | 1:197:J:ASP:CB | 1 | 0.75 |
| (1,2207) | 2:301:H:IHP:O35 | 3:302:H:A1CCZ:F32 | 7 | 0.74 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD2 | 3 | 0.74 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD3 | 3 | 0.74 |
| (1,636) | 1:150:J:ILE:CD1 | 1:186:J:THR:CB | 1 | 0.74 |
| (1,2262) | 3:302:H:A1CCZ:H7A | 1:232:H:ALA:CA | 10 | 0.73 |
| (1,2262) | 3:302:H:A1CCZ:H7B | 1:232:H:ALA:CA | 10 | 0.73 |
| (1,1318) | 1:172:J:LEU:CD1 | 1:183:J:ASN:CB | 3 | 0.73 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12A | 1 | 0.72 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12B | 1 | 0.72 |
| (1,2262) | 3:302:H:A1CCZ:H7A | 1:232:H:ALA:CA | 3 | 0.72 |
| (1,2262) | 3:302:H:A1CCZ:H7B | 1:232:H:ALA:CA | 3 | 0.72 |
| (1,2174) | 2:301:H:IHP:P2 | 1:158:L:LYS:HA | 3 | 0.72 |
| (1,1013) | 1:189:H:LEU:CA | 1:153:H:ILE:C | 7 | 0.72 |
| (1,2225) | 3:302:H:A1CCZ:F33 | 1:159:H:GLU:CB | 8 | 0.71 |
| (1,2118) | 2:301:H:IHP:P4 | 1:158:J:LYS:HA | 1 | 0.71 |
| (1,1638) | 1:155:J:GLN:CB | 1:197:J:ASP:CB | 7 | 0.71 |
| (1,2296) | 3:302:H:A1CCZ:F32 | 1:196:H:PRO:CG | 8 | 0.7 |
| (1,2225) | 3:302:H:A1CCZ:F33 | 1:159:H:GLU:CB | 2 | 0.7 |
| (1,2168) | 2:301:H:IHP:P1 | 1:224:I:PRO:HD2 | 7 | 0.7 |
| (1,2168) | 2:301:H:IHP:P1 | 1:224:I:PRO:HD3 | 7 | 0.7 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD2 | 8 | 0.7 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD3 | 8 | 0.7 |
| (1,2115) | 2:301:H:IHP:P4 | 1:158:G:LYS:HA | 2 | 0.7 |
| (1,384) | 1:185:L:MET:CG | 1:151:L:LEU:CB | 8 | 0.7 |
| (1,2277) | 3:302:H:A1CCZ:H9A | 1:232:I:ALA:CA | 3 | 0.69 |
| (1,2277) | 3:302:H:A1CCZ:H9B | 1:232:I:ALA:CA | 3 | 0.69 |
| (1,2262) | 3:302:H:A1CCZ:H7A | 1:232:H:ALA:CA | 2 | 0.69 |
| (1,2262) | 3:302:H:A1CCZ:H7B | 1:232:H:ALA:CA | 2 | 0.69 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD2 | 4 | 0.69 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD3 | 4 | 0.69 |
| (1,29) | 1:219:L:GLN:CG | 1:155:K:GLN:CA | 4 | 0.69 |
| (1,1) | 1:162:G:ARG:CG | 1:154:L:ARG:CA | 7 | 0.69 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12A | 2 | 0.68 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12B | 2 | 0.68 |
| (1,2277) | 3:302:H:A1CCZ:H9A | 1:232:I:ALA:CA | 8 | 0.68 |
| (1,2277) | 3:302:H:A1CCZ:H9B | 1:232:I:ALA:CA | 8 | 0.68 |
| (1,2225) | 3:302:H:A1CCZ:F33 | 1:159:H:GLU:CB | 10 | 0.68 |
| (1,2196) | 2:301:H:IHP:O41 | 3:302:H:A1CCZ:F32 | 6 | 0.68 |
| (1,2262) | 3:302:H:A1CCZ:H7A | 1:232:H:ALA:CA | 1 | 0.67 |
| (1,2262) | 3:302:H:A1CCZ:H7B | 1:232:H:ALA:CA | 1 | 0.67 |
| (1,1582) | 1:153:G:ILE:CG1 | 1:172:G:LEU:CA | 7 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,1318) | 1:172:K:LEU:CD1 | 1:183:K:ASN:CB | 9 | 0.67 |
| (1,2225) | 3:302:H:A1CCZ:F33 | 1:159:H:GLU:CB | 4 | 0.66 |
| (1,2207) | 2:301:H:IHP:O35 | 3:302:H:A1CCZ:F32 | 1 | 0.66 |
| (1,1438) | 1:172:K:LEU:CG | 1:183:K:ASN:CA | 9 | 0.66 |
| (1,1339) | 1:201:I:ILE:CG1 | 1:214:I:MET:CA | 6 | 0.66 |
| (1,412) | 1:202:H:LEU:CG | 1:194:H:ALA:CA | 8 | 0.66 |
| (1,2115) | 2:301:H:IHP:P4 | 1:158:G:LYS:HA | 10 | 0.65 |
| (1,636) | 1:150:K:ILE:CD1 | 1:186:K:THR:CB | 9 | 0.65 |
| (1,278) | 1:155:G:GLN:CB | 1:196:G:PRO:CA | 3 | 0.65 |
| (1,2293) | 3:302:H:A1CCZ:F33 | 1:160:H:PRO:CA | 3 | 0.64 |
| (1,2163) | 2:301:H:IHP:P1 | 1:224:J:PRO:HG2 | 6 | 0.64 |
| (1,2163) | 2:301:H:IHP:P1 | 1:224:J:PRO:HG3 | 6 | 0.64 |
| (1,685) | 1:187:J:GLU:CB | 1:184:J:TRP:CE2 | 4 | 0.64 |
| (1,278) | 1:155:G:GLN:CB | 1:196:G:PRO:CA | 6 | 0.64 |
| (1,278) | 1:155:J:GLN:CB | 1:196:J:PRO:CA | 10 | 0.64 |
| (1,2293) | 3:302:H:A1CCZ:F33 | 1:160:H:PRO:CA | 7 | 0.63 |
| (1,2174) | 2:301:H:IHP:P2 | 1:158:L:LYS:HA | 5 | 0.63 |
| (1,1013) | 1:189:H:LEU:CA | 1:153:H:ILE:C | 8 | 0.63 |
| (1,278) | 1:155:G:GLN:CB | 1:196:G:PRO:CA | 8 | 0.63 |
| (1,169) | 1:165:K:VAL:CG2 | 1:202:K:LEU:CG | 6 | 0.63 |
| (1,2207) | 2:301:H:IHP:O35 | 3:302:H:A1CCZ:F32 | 8 | 0.62 |
| (1,2153) | 2:301:H:IHP:P3 | 1:157:H:PRO:HD2 | 8 | 0.62 |
| (1,2153) | 2:301:H:IHP:P3 | 1:157:H:PRO:HD3 | 8 | 0.62 |
| (1,1638) | 1:155:J:GLN:CB | 1:197:J:ASP:CB | 3 | 0.62 |
| (1,1582) | 1:153:G:ILE:CG1 | 1:172:G:LEU:CA | 4 | 0.62 |
| (1,1582) | 1:153:H:ILE:CG1 | 1:172:H:LEU:CA | 5 | 0.62 |
| (1,29) | 1:219:L:GLN:CG | 1:155:K:GLN:CA | 6 | 0.62 |
| (1,2262) | 3:302:H:A1CCZ:H7A | 1:232:H:ALA:CA | 9 | 0.61 |
| (1,2262) | 3:302:H:A1CCZ:H7B | 1:232:H:ALA:CA | 9 | 0.61 |
| (1,2225) | 3:302:H:A1CCZ:F33 | 1:159:H:GLU:CB | 1 | 0.61 |
| (1,1096) | 1:171:H:THR:CG2 | 1:152:H:ASP:CB | 6 | 0.61 |
| (1,412) | 1:202:K:LEU:CG | 1:194:K:ALA:CA | 2 | 0.61 |
| (1,29) | 1:219:L:GLN:CG | 1:155:K:GLN:CA | 3 | 0.61 |
| (2,16) | 2:301:H:IHP:O43 | 3:302:H:A1CCZ:H12A | 4 | 0.6 |
| (2,16) | 2:301:H:IHP:O43 | 3:302:H:A1CCZ:H12B | 4 | 0.6 |
| (1,2258) | 3:302:H:A1CCZ:H11 | 1:232:H:ALA:CA | 7 | 0.6 |
| (1,2118) | 2:301:H:IHP:P4 | 1:158:J:LYS:HA | 3 | 0.6 |
| (1,2118) | 2:301:H:IHP:P4 | 1:158:J:LYS:HA | 8 | 0.6 |
| (1,278) | 1:155:G:GLN:CB | 1:196:G:PRO:CA | 4 | 0.6 |
| (2,8) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H9A | 4 | 0.59 |
| (2,8) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H9B | 4 | 0.59 |
| (1,1582) | 1:153:K:ILE:CG1 | 1:172:K:LEU:CA | 3 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,987) | 1:235:G:MET:CB | 1:230:G:VAL:CA | 6 | 0.59 |
| (1,833) | 1:221:I:VAL:CG2 | 1:230:I:VAL:CG2 | 5 | 0.59 |
| (1,833) | 1:221:I:VAL:CG2 | 1:230:I:VAL:CG2 | 7 | 0.59 |
| (1,685) | 1:187:J:GLU:CB | 1:184:J:TRP:CE2 | 1 | 0.59 |
| (1,278) | 1:155:G:GLN:CB | 1:196:G:PRO:CA | 7 | 0.59 |
| (1,75) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 2 | 0.59 |
| (1,1582) | 1:153:I:ILE:CG1 | 1:172:I:LEU:CA | 1 | 0.58 |
| (1,1377) | 1:205:I:LEU:CD1 | 1:210:I:THR:CA | 4 | 0.58 |
| (1,412) | 1:202:H:LEU:CG | 1:194:H:ALA:CA | 10 | 0.58 |
| (1,1582) | 1:153:K:ILE:CG1 | 1:172:K:LEU:CA | 2 | 0.57 |
| (1,1438) | 1:172:K:LEU:CG | 1:183:K:ASN:CA | 6 | 0.56 |
| (1,1339) | 1:201:I:ILE:CG1 | 1:214:I:MET:CA | 7 | 0.56 |
| (1,636) | 1:150:K:ILE:CD1 | 1:186:K:THR:CB | 7 | 0.56 |
| (1,278) | 1:155:H:GLN:CB | 1:196:H:PRO:CA | 1 | 0.56 |
| (1,75) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 8 | 0.56 |
| (1,73) | 1:231:I:LEU:N | 1:228:J:ALA:CB | 5 | 0.56 |
| (1,29) | 1:219:L:GLN:CG | 1:155:K:GLN:CA | 9 | 0.56 |
| (1,2225) | 3:302:H:A1CCZ:F33 | 1:159:H:GLU:CB | 7 | 0.55 |
| (1,1013) | 1:189:K:LEU:CA | 1:153:K:ILE:C | 5 | 0.55 |
| (1,636) | 1:150:K:ILE:CD1 | 1:186:K:THR:CB | 4 | 0.55 |
| (2,12) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H12A | 4 | 0.54 |
| (2,12) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H12B | 4 | 0.54 |
| (1,2221) | 3:302:H:A1CCZ:F33 | 1:224:H:PRO:CG | 3 | 0.54 |
| (1,2115) | 2:301:H:IHP:P4 | 1:158:G:LYS:HA | 8 | 0.54 |
| (1,1438) | 1:172:J:LEU:CG | 1:183:J:ASN:CA | 3 | 0.54 |
| (1,1377) | 1:205:L:LEU:CD1 | 1:210:L:THR:CA | 7 | 0.54 |
| (1,1339) | 1:201:I:ILE:CG1 | 1:214:I:MET:CA | 8 | 0.54 |
| (1,1339) | 1:201:L:ILE:CG1 | 1:214:L:MET:CA | 9 | 0.54 |
| (1,1318) | 1:172:K:LEU:CD1 | 1:183:K:ASN:CB | 6 | 0.54 |
| (1,1318) | 1:172:J:LEU:CD1 | 1:183:J:ASN:CB | 8 | 0.54 |
| (1,1150) | 1:192:I:GLN:CA | 1:164:I:TYR:CZ | 7 | 0.54 |
| (1,987) | 1:235:J:MET:CB | 1:230:J:VAL:CA | 7 | 0.54 |
| (1,365) | 1:196:K:PRO:CD | 1:200:K:THR:CB | 6 | 0.54 |
| (1,278) | 1:155:H:GLN:CB | 1:196:H:PRO:CA | 9 | 0.54 |
| (1,2293) | 3:302:H:A1CCZ:F33 | 1:160:H:PRO:CA | 9 | 0.53 |
| (1,2250) | 3:302:H:A1CCZ:F32 | 1:198:H:CYS:CA | 8 | 0.53 |
| (1,2174) | 2:301:H:IHP:P2 | 1:158:L:LYS:HA | 4 | 0.53 |
| (1,2118) | 2:301:H:IHP:P4 | 1:158:J:LYS:HA | 4 | 0.53 |
| (1,1638) | 1:155:J:GLN:CB | 1:197:J:ASP:CB | 2 | 0.53 |
| (1,1582) | 1:153:G:ILE:CG1 | 1:172:G:LEU:CA | 10 | 0.53 |
| (1,987) | 1:235:H:MET:CB | 1:230:H:VAL:CA | 8 | 0.53 |
| (1,2141) | 2:301:H:IHP:P6 | 1:158:I:LYS:HA | 6 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,1481) | 1:194:J:ALA:CB | 1:202:J:LEU:CB | 4 | 0.52 |
| (1,1438) | 1:172:K:LEU:CG | 1:183:K:ASN:CA | 2 | 0.52 |
| (1,1318) | 1:172:K:LEU:CD1 | 1:183:K:ASN:CB | 2 | 0.52 |
| (1,1150) | 1:192:H:GLN:CA | 1:164:H:TYR:CZ | 4 | 0.52 |
| (1,1150) | 1:192:H:GLN:CA | 1:164:H:TYR:CZ | 5 | 0.52 |
| (1,412) | 1:202:L:LEU:CG | 1:194:L:ALA:CA | 7 | 0.52 |
| (1,412) | 1:202:L:LEU:CG | 1:194:L:ALA:CA | 9 | 0.52 |
| (1,387) | 1:194:J:ALA:CB | 1:154:J:ARG:CG | 5 | 0.52 |
| (1,29) | 1:219:L:GLN:CG | 1:155:K:GLN:CA | 2 | 0.52 |
| (1,1648) | 1:160:K:PRO:CG | 1:161:K:PHE:CG | 9 | 0.51 |
| (1,1318) | 1:172:K:LEU:CD1 | 1:183:K:ASN:CB | 10 | 0.51 |
| (1,658) | 1:235:H:MET:CB | 1:233:H:GLU:CG | 10 | 0.51 |
| (1,3) | 1:162:K:ARG:CG | 1:154:J:ARG:CA | 8 | 0.51 |
| (1,1638) | 1:155:J:GLN:CB | 1:197:J:ASP:CB | 4 | 0.5 |
| (1,1339) | 1:201:I:ILE:CG1 | 1:214:I:MET:CA | 4 | 0.5 |
| (1,29) | 1:219:L:GLN:CG | 1:155:K:GLN:CA | 5 | 0.5 |
| (1,5) | 1:162:I:ARG:CG | 1:154:H:ARG:CA | 9 | 0.5 |
| (1,2115) | 2:301:H:IHP:P4 | 1:158:G:LYS:HA | 7 | 0.49 |
| (1,1648) | 1:160:G:PRO:CG | 1:161:G:PHE:CG | 6 | 0.49 |
| (1,1582) | 1:153:L:ILE:CG1 | 1:172:L:LEU:CA | 6 | 0.49 |
| (1,1438) | 1:172:K:LEU:CG | 1:183:K:ASN:CA | 10 | 0.49 |
| (1,1339) | 1:201:I:ILE:CG1 | 1:214:I:MET:CA | 10 | 0.49 |
| (1,987) | 1:235:K:MET:CB | 1:230:K:VAL:CA | 5 | 0.49 |
| (1,685) | 1:187:J:GLU:CB | 1:184:J:TRP:CE2 | 2 | 0.49 |
| (1,685) | 1:187:J:GLU:CB | 1:184:J:TRP:CE2 | 6 | 0.49 |
| (1,685) | 1:187:J:GLU:CB | 1:184:J:TRP:CE2 | 7 | 0.49 |
| (1,1) | 1:162:G:ARG:CG | 1:154:L:ARG:CA | 1 | 0.49 |
| (1,2258) | 3:302:H:A1CCZ:H11 | 1:232:H:ALA:CA | 5 | 0.48 |
| (1,1438) | 1:172:J:LEU:CG | 1:183:J:ASN:CA | 8 | 0.48 |
| (1,1150) | 1:192:H:GLN:CA | 1:164:H:TYR:CZ | 8 | 0.48 |
| (1,987) | 1:235:K:MET:CB | 1:230:K:VAL:CA | 2 | 0.48 |
| (1,540) | 1:230:J:VAL:CG1 | 1:221:J:VAL:CA | 2 | 0.48 |
| (1,540) | 1:230:J:VAL:CG2 | 1:221:J:VAL:CA | 4 | 0.48 |
| (1,365) | 1:196:K:PRO:CD | 1:200:K:THR:CB | 4 | 0.48 |
| (1,169) | 1:165:K:VAL:CG2 | 1:202:K:LEU:CG | 5 | 0.48 |
| (1,78) | 1:219:J:GLN:CG | 1:195:I:ASN:CA | 4 | 0.48 |
| (2,92) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:H12A | 6 | 0.47 |
| (2,92) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:H12B | 6 | 0.47 |
| (2,92) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:H12A | 9 | 0.47 |
| (2,92) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:H12B | 9 | 0.47 |
| (1,2277) | 3:302:H:A1CCZ:H9A | 1:232:I:ALA:CA | 7 | 0.47 |
| (1,2277) | 3:302:H:A1CCZ:H9B | 1:232:I:ALA:CA | 7 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,2221) | 3:302:H:A1CCZ:F33 | 1:224:H:PRO:CG | 2 | 0.47 |
| (1,2210) | 2:301:H:IHP:O45 | 3:302:H:A1CCZ:F32 | 4 | 0.47 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD2 | 7 | 0.47 |
| (1,2143) | 2:301:H:IHP:P6 | 1:157:J:PRO:HD3 | 7 | 0.47 |
| (1,1638) | 1:155:I:GLN:CB | 1:197:I:ASP:CB | 5 | 0.47 |
| (1,987) | 1:235:K:MET:CB | 1:230:K:VAL:CA | 1 | 0.47 |
| (1,658) | 1:235:H:MET:CB | 1:233:H:GLU:CG | 6 | 0.47 |
| (1,420) | 1:202:L:LEU:CD1 | 1:199:L:LYS:CD | 1 | 0.47 |
| (1,5) | 1:162:I:ARG:CG | 1:154:H:ARG:CA | 5 | 0.47 |
| (1,4) | 1:162:J:ARG:CG | 1:154:I:ARG:CA | 7 | 0.47 |
| (1,1648) | 1:160:L:PRO:CG | 1:161:L:PHE:CG | 3 | 0.46 |
| (1,1150) | 1:192:H:GLN:CA | 1:164:H:TYR:CZ | 1 | 0.46 |
| (1,658) | 1:235:H:MET:CB | 1:233:H:GLU:CG | 3 | 0.46 |
| (1,420) | 1:202:L:LEU:CD1 | 1:199:L:LYS:CD | 3 | 0.46 |
| (1,5) | 1:162:I:ARG:CG | 1:154:H:ARG:CA | 2 | 0.46 |
| (1,2262) | 3:302:H:A1CCZ:H7A | 1:232:H:ALA:CA | 8 | 0.45 |
| (1,2262) | 3:302:H:A1CCZ:H7B | 1:232:H:ALA:CA | 8 | 0.45 |
| (1,2159) | 2:301:H:IHP:P3 | 1:159:H:GLU:H | 8 | 0.45 |
| (1,1648) | 1:160:L:PRO:CG | 1:161:L:PHE:CG | 4 | 0.45 |
| (1,1582) | 1:153:H:ILE:CG1 | 1:172:H:LEU:CA | 8 | 0.45 |
| (1,1438) | 1:172:L:LEU:CG | 1:183:L:ASN:CA | 7 | 0.45 |
| (1,658) | 1:235:G:MET:CB | 1:233:G:GLU:CG | 4 | 0.45 |
| (1,540) | 1:230:H:VAL:CG2 | 1:221:H:VAL:CA | 7 | 0.45 |
| (1,365) | 1:196:H:PRO:CD | 1:200:H:THR:CB | 2 | 0.45 |
| (1,278) | 1:155:H:GLN:CB | 1:196:H:PRO:CA | 5 | 0.45 |
| (1,169) | 1:165:K:VAL:CG2 | 1:202:K:LEU:CG | 3 | 0.45 |
| (1,169) | 1:165:K:VAL:CG2 | 1:202:K:LEU:CG | 9 | 0.45 |
| (1,169) | 1:165:K:VAL:CG2 | 1:202:K:LEU:CG | 10 | 0.45 |
| (1,75) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 10 | 0.45 |
| (1,29) | 1:219:L:GLN:CG | 1:155:K:GLN:CA | 10 | 0.45 |
| (2,12) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H12A | 1 | 0.44 |
| (2,12) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H12B | 1 | 0.44 |
| (1,2258) | 3:302:H:A1CCZ:H11 | 1:232:H:ALA:CA | 4 | 0.44 |
| (1,2250) | 3:302:H:A1CCZ:F32 | 1:198:H:CYS:CA | 7 | 0.44 |
| (1,2115) | 2:301:H:IHP:P4 | 1:158:G:LYS:HA | 6 | 0.44 |
| (1,1648) | 1:160:K:PRO:CG | 1:161:K:PHE:CG | 8 | 0.44 |
| (1,1339) | 1:201:I:ILE:CG1 | 1:214:I:MET:CA | 1 | 0.44 |
| (1,540) | 1:230:K:VAL:CG2 | 1:221:K:VAL:CA | 1 | 0.44 |
| (1,540) | 1:230:I:VAL:CG2 | 1:221:I:VAL:CA | 6 | 0.44 |
| (1,384) | 1:185:L:MET:CG | 1:151:L:LEU:CB | 9 | 0.44 |
| (1,365) | 1:196:K:PRO:CD | 1:200:K:THR:CB | 10 | 0.44 |
| (1,169) | 1:165:K:VAL:CG2 | 1:202:K:LEU:CG | 2 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,169) | 1:165:K:VAL:CG2 | 1:202:K:LEU:CG | 4 | 0.44 |
| (1,75) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 5 | 0.44 |
| (1,74) | 1:231:J:LEU:N | 1:228:K:ALA:CB | 3 | 0.44 |
| (1,5) | 1:162:I:ARG:CG | 1:154:H:ARG:CA | 7 | 0.44 |
| (1,1) | 1:162:G:ARG:CG | 1:154:L:ARG:CA | 3 | 0.44 |
| (1,2292) | 3:302:H:A1CCZ:F32 | 1:160:H:PRO:CA | 7 | 0.43 |
| (1,2204) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:F32 | 7 | 0.43 |
| (1,2135) | 2:301:H:IHP:P4 | 1:227:H:LYS:HZ1 | 6 | 0.43 |
| (1,2135) | 2:301:H:IHP:P4 | 1:227:H:LYS:HZ2 | 6 | 0.43 |
| (1,2135) | 2:301:H:IHP:P4 | 1:227:H:LYS:HZ3 | 6 | 0.43 |
| (1,1648) | 1:160:K:PRO:CG | 1:161:K:PHE:CG | 2 | 0.43 |
| (1,1638) | 1:155:I:GLN:CB | 1:197:I:ASP:CB | 10 | 0.43 |
| (1,1339) | 1:201:I:ILE:CG1 | 1:214:I:MET:CA | 2 | 0.43 |
| (1,1339) | 1:201:I:ILE:CG1 | 1:214:I:MET:CA | 3 | 0.43 |
| (1,987) | 1:235:K:MET:CB | 1:230:K:VAL:CA | 10 | 0.43 |
| (1,636) | 1:150:K:ILE:CD1 | 1:186:K:THR:CB | 6 | 0.43 |
| (1,414) | 1:201:H:ILE:CG2 | 1:197:H:ASP:CB | 5 | 0.43 |
| (1,387) | 1:194:L:ALA:CB | 1:154:L:ARG:CG | 3 | 0.43 |
| (1,29) | 1:219:L:GLN:CG | 1:155:K:GLN:CA | 8 | 0.43 |
| (2,92) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:H12A | 7 | 0.42 |
| (2,92) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:H12B | 7 | 0.42 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12A | 8 | 0.42 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12B | 8 | 0.42 |
| (1,2135) | 2:301:H:IHP:P4 | 1:227:H:LYS:HZ1 | 7 | 0.42 |
| (1,2135) | 2:301:H:IHP:P4 | 1:227:H:LYS:HZ2 | 7 | 0.42 |
| (1,2135) | 2:301:H:IHP:P4 | 1:227:H:LYS:HZ3 | 7 | 0.42 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE2 | 5 | 0.42 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE3 | 5 | 0.42 |
| (1,1638) | 1:155:I:GLN:CB | 1:197:I:ASP:CB | 6 | 0.42 |
| (1,1488) | 1:152:J:ASP:CB | 1:149:J:SER:CB | 2 | 0.42 |
| (1,1150) | 1:192:H:GLN:CA | 1:164:H:TYR:CZ | 2 | 0.42 |
| (1,968) | 1:221:K:VAL:CG2 | 1:219:K:GLN:CG | 8 | 0.42 |
| (1,685) | 1:187:J:GLU:CB | 1:184:J:TRP:CE2 | 10 | 0.42 |
| (1,658) | 1:235:I:MET:CB | 1:233:I:GLU:CG | 9 | 0.42 |
| (1,636) | 1:150:K:ILE:CD1 | 1:186:K:THR:CB | 2 | 0.42 |
| (1,412) | 1:202:L:LEU:CG | 1:194:L:ALA:CA | 6 | 0.42 |
| (1,227) | 1:198:G:CYS:CB | 1:199:G:LYS:CE | 8 | 0.42 |
| (1,204) | 1:150:K:ILE:CD1 | 1:189:K:LEU:CA | 7 | 0.42 |
| (1,74) | 1:231:J:LEU:N | 1:228:K:ALA:CB | 4 | 0.42 |
| (1,11) | 1:195:L:ASN:CA | 1:219:G:GLN:CA | 7 | 0.42 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12A | 5 | 0.41 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12B | 5 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,2308) | 3:302:H:A1CCZ:F31 | 1:228:H:ALA:CA | 3 | 0.41 |
| (1,2221) | 3:302:H:A1CCZ:F33 | 1:224:H:PRO:CG | 9 | 0.41 |
| (1,2197) | 2:301:H:IHP:O41 | 3:302:H:A1CCZ:F33 | 5 | 0.41 |
| (1,1648) | 1:160:H:PRO:CG | 1:161:H:PHE:CG | 1 | 0.41 |
| (1,1150) | 1:192:H:GLN:CA | 1:164:H:TYR:CZ | 6 | 0.41 |
| (1,968) | 1:221:K:VAL:CG2 | 1:219:K:GLN:CG | 4 | 0.41 |
| (1,636) | 1:150:K:ILE:CD1 | 1:186:K:THR:CB | 5 | 0.41 |
| (1,78) | 1:219:J:GLN:CG | 1:195:I:ASN:CA | 7 | 0.41 |
| (1,74) | 1:231:J:LEU:N | 1:228:K:ALA:CB | 10 | 0.41 |
| (1,1) | 1:162:G:ARG:CG | 1:154:L:ARG:CA | 5 | 0.41 |
| (1,2293) | 3:302:H:A1CCZ:F33 | 1:160:H:PRO:CA | 4 | 0.4 |
| (1,2258) | 3:302:H:A1CCZ:H11 | 1:232:H:ALA:CA | 2 | 0.4 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ1 | 8 | 0.4 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ2 | 8 | 0.4 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ3 | 8 | 0.4 |
| (1,1648) | 1:160:H:PRO:CG | 1:161:H:PHE:CG | 7 | 0.4 |
| (1,1582) | 1:153:H:ILE:CG1 | 1:172:H:LEU:CA | 9 | 0.4 |
| (1,1481) | 1:194:H:ALA:CB | 1:202:H:LEU:CB | 8 | 0.4 |
| (1,658) | 1:235:G:MET:CB | 1:233:G:GLU:CG | 8 | 0.4 |
| (1,384) | 1:185:J:MET:CG | 1:151:J:LEU:CB | 3 | 0.4 |
| (1,169) | 1:165:K:VAL:CG2 | 1:202:K:LEU:CG | 8 | 0.4 |
| (1,74) | 1:231:J:LEU:N | 1:228:K:ALA:CB | 1 | 0.4 |
| (1,74) | 1:231:J:LEU:N | 1:228:K:ALA:CB | 2 | 0.4 |
| (1,1) | 1:162:G:ARG:CG | 1:154:L:ARG:CA | 4 | 0.4 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12A | 10 | 0.39 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12B | 10 | 0.39 |
| (1,2293) | 3:302:H:A1CCZ:F33 | 1:160:H:PRO:CA | 8 | 0.39 |
| (1,2197) | 2:301:H:IHP:O41 | 3:302:H:A1CCZ:F33 | 1 | 0.39 |
| (1,2191) | 2:301:H:IHP:O21 | 3:302:H:A1CCZ:F33 | 2 | 0.39 |
| (1,1481) | 1:194:I:ALA:CB | 1:202:I:LEU:CB | 3 | 0.39 |
| (1,1469) | 1:214:J:MET:CB | 1:205:J:LEU:CA | 1 | 0.39 |
| (1,1318) | 1:172:J:LEU:CD1 | 1:183:J:ASN:CB | 4 | 0.39 |
| (1,1150) | 1:192:H:GLN:CA | 1:164:H:TYR:CZ | 10 | 0.39 |
| (1,987) | 1:235:K:MET:CB | 1:230:K:VAL:CA | 3 | 0.39 |
| (1,685) | 1:187:J:GLU:CB | 1:184:J:TRP:CE2 | 3 | 0.39 |
| (1,658) | 1:235:G:MET:CB | 1:233:G:GLU:CG | 2 | 0.39 |
| (1,414) | 1:201:J:ILE:CG2 | 1:197:J:ASP:CB | 9 | 0.39 |
| (1,414) | 1:201:J:ILE:CG2 | 1:197:J:ASP:CB | 10 | 0.39 |
| (1,384) | 1:185:L:MET:CG | 1:151:L:LEU:CB | 2 | 0.39 |
| (1,75) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 4 | 0.39 |
| (1,2308) | 3:302:H:A1CCZ:F31 | 1:228:H:ALA:CA | 2 | 0.38 |
| (1,2293) | 3:302:H:A1CCZ:F33 | 1:160:H:PRO:CA | 2 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,1648) | 1:160:L:PRO:CG | 1:161:L:PHE:CG | 5 | 0.38 |
| (1,1481) | 1:194:L:ALA:CB | 1:202:L:LEU:CB | 6 | 0.38 |
| (1,1233) | 1:190:H:LEU:CD1 | 1:166:H:ASP:CA | 4 | 0.38 |
| (1,658) | 1:235:G:MET:CB | 1:233:G:GLU:CG | 1 | 0.38 |
| (1,384) | 1:185:J:MET:CG | 1:151:J:LEU:CB | 1 | 0.38 |
| (1,384) | 1:185:L:MET:CG | 1:151:L:LEU:CB | 10 | 0.38 |
| (1,365) | 1:196:K:PRO:CD | 1:200:K:THR:CB | 3 | 0.38 |
| (1,267) | 1:188:K:THR:CG2 | 1:185:K:MET:CB | 6 | 0.38 |
| (1,227) | 1:198:G:CYS:CB | 1:199:G:LYS:CE | 10 | 0.38 |
| (1,1) | 1:162:G:ARG:CG | 1:154:L:ARG:CA | 8 | 0.38 |
| (1,2277) | 3:302:H:A1CCZ:H9A | 1:232:I:ALA:CA | 6 | 0.37 |
| (1,2277) | 3:302:H:A1CCZ:H9B | 1:232:I:ALA:CA | 6 | 0.37 |
| (1,2196) | 2:301:H:IHP:O41 | 3:302:H:A1CCZ:F32 | 1 | 0.37 |
| (1,2157) | 2:301:H:IHP:P3 | 1:158:L:LYS:HA | 1 | 0.37 |
| (1,1318) | 1:172:J:LEU:CD1 | 1:183:J:ASN:CB | 5 | 0.37 |
| (1,987) | 1:235:K:MET:CB | 1:230:K:VAL:CA | 4 | 0.37 |
| (1,689) | 1:201:K:ILE:CD1 | 1:202:K:LEU:C | 5 | 0.37 |
| (1,412) | 1:202:L:LEU:CG | 1:194:L:ALA:CA | 1 | 0.37 |
| (1,78) | 1:219:J:GLN:CG | 1:195:I:ASN:CA | 6 | 0.37 |
| (1,77) | 1:219:K:GLN:CG | 1:195:J:ASN:CA | 8 | 0.37 |
| (1,4) | 1:162:J:ARG:CG | 1:154:I:ARG:CA | 9 | 0.37 |
| (1,2197) | 2:301:H:IHP:O41 | 3:302:H:A1CCZ:F33 | 6 | 0.36 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE2 | 2 | 0.36 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE3 | 2 | 0.36 |
| (1,2122) | 2:301:H:IHP:P4 | 1:158:J:LYS:HE2 | 5 | 0.36 |
| (1,2122) | 2:301:H:IHP:P4 | 1:158:J:LYS:HE3 | 5 | 0.36 |
| (1,2115) | 2:301:H:IHP:P4 | 1:158:G:LYS:HA | 5 | 0.36 |
| (1,1377) | 1:205:I:LEU:CD1 | 1:210:I:THR:CA | 8 | 0.36 |
| (1,1150) | 1:192:H:GLN:CA | 1:164:H:TYR:CZ | 3 | 0.36 |
| (1,1013) | 1:189:K:LEU:CA | 1:153:K:ILE:C | 6 | 0.36 |
| (1,968) | 1:221:I:VAL:CG2 | 1:219:I:GLN:CG | 2 | 0.36 |
| (1,968) | 1:221:G:VAL:CG2 | 1:219:G:GLN:CG | 7 | 0.36 |
| (1,248) | 1:156:L:GLY:CA | 1:196:L:PRO:CD | 9 | 0.36 |
| (1,227) | 1:198:H:CYS:CB | 1:199:H:LYS:CE | 1 | 0.36 |
| (1,75) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 6 | 0.36 |
| (2,8) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H9A | 3 | 0.35 |
| (2,8) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H9B | 3 | 0.35 |
| (1,1150) | 1:192:H:GLN:CA | 1:164:H:TYR:CZ | 9 | 0.35 |
| (1,1100) | 1:190:G:LEU:CD1 | 1:169:G:TYR:CB | 5 | 0.35 |
| (1,987) | 1:235:K:MET:CB | 1:230:K:VAL:CA | 9 | 0.35 |
| (1,689) | 1:201:K:ILE:CD1 | 1:202:K:LEU:C | 10 | 0.35 |
| (1,658) | 1:235:G:MET:CB | 1:233:G:GLU:CG | 5 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,561) | 1:201:L:ILE:CG1 | 1:205:L:LEU:CA | 5 | 0.35 |
| (1,414) | 1:201:J:ILE:CG2 | 1:197:J:ASP:CB | 4 | 0.35 |
| (1,389) | 1:210:J:THR:CG2 | 1:211:J:LEU:CG | 6 | 0.35 |
| (1,267) | 1:188:K:THR:CG2 | 1:185:K:MET:CB | 5 | 0.35 |
| (1,267) | 1:188:K:THR:CG2 | 1:185:K:MET:CB | 9 | 0.35 |
| (1,218) | 1:179:K:GLN:CB | 1:177:K:ALA:CA | 7 | 0.35 |
| (1,218) | 1:179:G:GLN:CB | 1:177:G:ALA:CA | 9 | 0.35 |
| (1,218) | 1:179:G:GLN:CB | 1:177:G:ALA:CA | 10 | 0.35 |
| (1,78) | 1:219:J:GLN:CG | 1:195:I:ASN:CA | 2 | 0.35 |
| (1,33) | 1:223:J:GLY:CA | 1:157:I:PRO:CD | 4 | 0.35 |
| (1,11) | 1:195:L:ASN:CA | 1:219:G:GLN:CA | 8 | 0.35 |
| (1,8) | 1:195:I:ASN:CA | 1:219:J:GLN:CA | 6 | 0.35 |
| (1,5) | 1:162:I:ARG:CG | 1:154:H:ARG:CA | 8 | 0.35 |
| (2,16) | 2:301:H:IHP:O43 | 3:302:H:A1CCZ:H12A | 3 | 0.34 |
| (2,16) | 2:301:H:IHP:O43 | 3:302:H:A1CCZ:H12B | 3 | 0.34 |
| (1,2308) | 3:302:H:A1CCZ:F31 | 1:228:H:ALA:CA | 9 | 0.34 |
| (1,2233) | 3:302:H:A1CCZ:F32 | 1:195:H:ASN:CA | 10 | 0.34 |
| (1,2190) | 2:301:H:IHP:O21 | 3:302:H:A1CCZ:F32 | 2 | 0.34 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE2 | 1 | 0.34 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE3 | 1 | 0.34 |
| (1,1497) | 1:165:K:VAL:CG2 | 1:214:K:MET:CA | 8 | 0.34 |
| (1,1377) | 1:205:I:LEU:CD1 | 1:210:I:THR:CA | 5 | 0.34 |
| (1,945) | 1:150:G:ILE:CD1 | 1:193:G:ASN:CG | 9 | 0.34 |
| (1,808) | 1:191:L:VAL:CG1 | 1:193:L:ASN:CA | 4 | 0.34 |
| (1,636) | 1:150:I:ILE:CD1 | 1:186:I:THR:CB | 8 | 0.34 |
| (1,636) | 1:150:K:ILE:CD1 | 1:186:K:THR:CB | 10 | 0.34 |
| (1,218) | 1:179:G:GLN:CB | 1:177:G:ALA:CA | 1 | 0.34 |
| (1,77) | 1:219:K:GLN:CG | 1:195:J:ASN:CA | 4 | 0.34 |
| (1,77) | 1:219:K:GLN:CG | 1:195:J:ASN:CA | 7 | 0.34 |
| (1,75) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 1 | 0.34 |
| (1,2293) | 3:302:H:A1CCZ:F33 | 1:160:H:PRO:CA | 1 | 0.33 |
| (1,2169) | 2:301:H:IHP:P1 | 1:224:J:PRO:HD2 | 6 | 0.33 |
| (1,2169) | 2:301:H:IHP:P1 | 1:224:J:PRO:HD3 | 6 | 0.33 |
| (1,2141) | 2:301:H:IHP:P6 | 1:158:I:LYS:HA | 1 | 0.33 |
| (1,1648) | 1:160:L:PRO:CG | 1:161:L:PHE:CG | 10 | 0.33 |
| (1,1533) | 1:190:H:LEU:CG | 1:187:H:GLU:CB | 8 | 0.33 |
| (1,1438) | 1:172:K:LEU:CG | 1:183:K:ASN:CA | 1 | 0.33 |
| (1,1381) | 1:217:K:ALA:CB | 1:221:K:VAL:CG2 | 10 | 0.33 |
| (1,1233) | 1:190:H:LEU:CD1 | 1:166:H:ASP:CA | 5 | 0.33 |
| (1,968) | 1:221:K:VAL:CG2 | 1:219:K:GLN:CG | 9 | 0.33 |
| (1,689) | 1:201:J:ILE:CD1 | 1:202:J:LEU:C | 1 | 0.33 |
| (1,673) | 1:165:G:VAL:CG2 | 1:163:G:ASP:CB | 2 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,561) | 1:201:H:ILE:CG1 | 1:205:H:LEU:CA | 4 | 0.33 |
| (1,561) | 1:201:L:ILE:CG1 | 1:205:L:LEU:CA | 9 | 0.33 |
| (1,384) | 1:185:L:MET:CG | 1:151:L:LEU:CB | 7 | 0.33 |
| (1,2319) | 3:302:H:A1CCZ:F32 | 1:231:H:LEU:CB | 6 | 0.32 |
| (1,2296) | 3:302:H:A1CCZ:F32 | 1:196:H:PRO:CG | 4 | 0.32 |
| (1,2258) | 3:302:H:A1CCZ:H11 | 1:232:H:ALA:CA | 1 | 0.32 |
| (1,2174) | 2:301:H:IHP:P2 | 1:158:L:LYS:HA | 2 | 0.32 |
| (1,1638) | 1:155:I:GLN:CB | 1:197:I:ASP:CB | 9 | 0.32 |
| (1,1533) | 1:190:I:LEU:CG | 1:187:I:GLU:CB | 7 | 0.32 |
| (1,1377) | 1:205:K:LEU:CD1 | 1:210:K:THR:CA | 10 | 0.32 |
| (1,1220) | 1:214:I:MET:CG | 1:191:I:VAL:CB | 7 | 0.32 |
| (1,689) | 1:201:J:ILE:CD1 | 1:202:J:LEU:C | 4 | 0.32 |
| (1,658) | 1:235:I:MET:CB | 1:233:I:GLU:CG | 7 | 0.32 |
| (1,227) | 1:198:H:CYS:CB | 1:199:H:LYS:CE | 5 | 0.32 |
| (1,48) | 1:221:K:VAL:CG1 | 1:224:L:PRO:CD | 1 | 0.32 |
| (1,48) | 1:221:K:VAL:CG2 | 1:224:L:PRO:CD | 1 | 0.32 |
| (1,25) | 1:232:L:ALA:CB | 1:238:K:VAL:CB | 8 | 0.32 |
| (1,8) | 1:195:I:ASN:CA | 1:219:J:GLN:CA | 2 | 0.32 |
| (1,2210) | 2:301:H:IHP:O45 | 3:302:H:A1CCZ:F32 | 3 | 0.31 |
| (1,2196) | 2:301:H:IHP:O41 | 3:302:H:A1CCZ:F32 | 2 | 0.31 |
| (1,1497) | 1:165:H:VAL:CG2 | 1:214:H:MET:CA | 7 | 0.31 |
| (1,1481) | 1:194:L:ALA:CB | 1:202:L:LEU:CB | 9 | 0.31 |
| (1,1339) | 1:201:I:ILE:CG1 | 1:214:I:MET:CA | 5 | 0.31 |
| (1,1233) | 1:190:H:LEU:CD1 | 1:166:H:ASP:CA | 1 | 0.31 |
| (1,968) | 1:221:I:VAL:CG2 | 1:219:I:GLN:CG | 5 | 0.31 |
| (1,689) | 1:201:I:ILE:CD1 | 1:202:I:LEU:C | 3 | 0.31 |
| (1,689) | 1:201:K:ILE:CD1 | 1:202:K:LEU:C | 8 | 0.31 |
| (1,420) | 1:202:L:LEU:CD1 | 1:199:L:LYS:CD | 7 | 0.31 |
| (1,387) | 1:194:J:ALA:CB | 1:154:J:ARG:CG | 1 | 0.31 |
| (1,218) | 1:179:G:GLN:CB | 1:177:G:ALA:CA | 4 | 0.31 |
| (1,78) | 1:219:J:GLN:CG | 1:195:I:ASN:CA | 3 | 0.31 |
| (1,76) | 1:219:L:GLN:CG | 1:195:K:ASN:CA | 1 | 0.31 |
| (1,75) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 9 | 0.31 |
| (1,25) | 1:232:L:ALA:CB | 1:238:K:VAL:CB | 5 | 0.31 |
| (1,4) | 1:162:J:ARG:CG | 1:154:I:ARG:CA | 1 | 0.31 |
| (1,2284) | 3:302:H:A1CCZ:F32 | 1:157:H:PRO:CG | 1 | 0.3 |
| (1,2284) | 3:302:H:A1CCZ:F32 | 1:157:H:PRO:CG | 8 | 0.3 |
| (1,2204) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:F32 | 8 | 0.3 |
| (1,2191) | 2:301:H:IHP:O21 | 3:302:H:A1CCZ:F33 | 1 | 0.3 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE2 | 3 | 0.3 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE3 | 3 | 0.3 |
| (1,1100) | 1:190:H:LEU:CD1 | 1:169:H:TYR:CB | 6 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,673) | 1:165:H:VAL:CG2 | 1:163:H:ASP:CB | 6 | 0.3 |
| (1,561) | 1:201:H:ILE:CG1 | 1:205:H:LEU:CA | 3 | 0.3 |
| (1,540) | 1:230:H:VAL:CG1 | 1:221:H:VAL:CA | 3 | 0.3 |
| (1,218) | 1:179:G:GLN:CB | 1:177:G:ALA:CA | 6 | 0.3 |
| (1,25) | 1:232:L:ALA:CB | 1:238:K:VAL:CB | 10 | 0.3 |
| (2,12) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H12A | 3 | 0.29 |
| (2,12) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H12B | 3 | 0.29 |
| (1,2250) | 3:302:H:A1CCZ:F32 | 1:198:H:CYS:CA | 1 | 0.29 |
| (1,1220) | 1:214:K:MET:CG | 1:191:K:VAL:CB | 8 | 0.29 |
| (1,945) | 1:150:J:ILE:CD1 | 1:193:J:ASN:CG | 10 | 0.29 |
| (1,689) | 1:201:J:ILE:CD1 | 1:202:J:LEU:C | 6 | 0.29 |
| (1,673) | 1:165:J:VAL:CG2 | 1:163:J:ASP:CB | 10 | 0.29 |
| (1,561) | 1:201:H:ILE:CG1 | 1:205:H:LEU:CA | 1 | 0.29 |
| (1,423) | 1:190:G:LEU:CG | 1:193:G:ASN:C | 6 | 0.29 |
| (1,387) | 1:194:L:ALA:CB | 1:154:L:ARG:CG | 2 | 0.29 |
| (1,227) | 1:198:J:CYS:CB | 1:199:J:LYS:CE | 9 | 0.29 |
| (1,218) | 1:179:G:GLN:CB | 1:177:G:ALA:CA | 5 | 0.29 |
| (1,2258) | 3:302:H:A1CCZ:H11 | 1:232:H:ALA:CA | 3 | 0.28 |
| (1,2251) | 3:302:H:A1CCZ:F33 | 1:198:H:CYS:CA | 6 | 0.28 |
| (1,2174) | 2:301:H:IHP:P2 | 1:158:L:LYS:HA | 1 | 0.28 |
| (1,1385) | 1:151:J:LEU:CG | 1:189:J:LEU:CB | 2 | 0.28 |
| (1,1385) | 1:151:J:LEU:CG | 1:189:J:LEU:CB | 9 | 0.28 |
| (1,1233) | 1:190:H:LEU:CD1 | 1:166:H:ASP:CA | 2 | 0.28 |
| (1,1233) | 1:190:H:LEU:CD1 | 1:166:H:ASP:CA | 10 | 0.28 |
| (1,1220) | 1:214:J:MET:CG | 1:191:J:VAL:CB | 1 | 0.28 |
| (1,1220) | 1:214:I:MET:CG | 1:191:I:VAL:CB | 2 | 0.28 |
| (1,1205) | 1:153:J:ILE:CB | 1:193:J:ASN:CA | 1 | 0.28 |
| (1,689) | 1:201:J:ILE:CD1 | 1:202:J:LEU:C | 9 | 0.28 |
| (1,561) | 1:201:H:ILE:CG1 | 1:205:H:LEU:CA | 7 | 0.28 |
| (1,365) | 1:196:K:PRO:CD | 1:200:K:THR:CB | 5 | 0.28 |
| (1,218) | 1:179:G:GLN:CB | 1:177:G:ALA:CA | 3 | 0.28 |
| (1,218) | 1:179:G:GLN:CB | 1:177:G:ALA:CA | 8 | 0.28 |
| (1,2296) | 3:302:H:A1CCZ:F32 | 1:196:H:PRO:CG | 9 | 0.27 |
| (1,2293) | 3:302:H:A1CCZ:F33 | 1:160:H:PRO:CA | 10 | 0.27 |
| (1,2204) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:F32 | 9 | 0.27 |
| (1,1381) | 1:217:I:ALA:CB | 1:221:I:VAL:CG2 | 4 | 0.27 |
| (1,1377) | 1:205:I:LEU:CD1 | 1:210:I:THR:CA | 2 | 0.27 |
| (1,968) | 1:221:K:VAL:CG2 | 1:219:K:GLN:CG | 3 | 0.27 |
| (1,945) | 1:150:J:ILE:CD1 | 1:193:J:ASN:CG | 6 | 0.27 |
| (1,831) | 1:150:K:ILE:CD1 | 1:190:K:LEU:CA | 1 | 0.27 |
| (1,685) | 1:187:J:GLU:CB | 1:184:J:TRP:CE2 | 9 | 0.27 |
| (1,673) | 1:165:H:VAL:CG2 | 1:163:H:ASP:CB | 3 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-----------------|----------|---------------|
| (1,580) | 1:153:K:ILE:CD1 | 1:193:K:ASN:CG | 1 | 0.27 |
| (1,561) | 1:201:H:ILE:CG1 | 1:205:H:LEU:CA | 6 | 0.27 |
| (1,540) | 1:230:J:VAL:CG2 | 1:221:J:VAL:CA | 5 | 0.27 |
| (1,365) | 1:196:I:PRO:CD | 1:200:I:THR:CB | 9 | 0.27 |
| (1,267) | 1:188:K:THR:CG2 | 1:185:K:MET:CB | 10 | 0.27 |
| (1,74) | 1:231:J:LEU:N | 1:228:K:ALA:CB | 8 | 0.27 |
| (1,73) | 1:231:I:LEU:N | 1:228:J:ALA:CB | 8 | 0.27 |
| (1,48) | 1:221:K:VAL:CG1 | 1:224:L:PRO:CD | 5 | 0.27 |
| (1,48) | 1:221:K:VAL:CG2 | 1:224:L:PRO:CD | 5 | 0.27 |
| (1,25) | 1:232:L:ALA:CB | 1:238:K:VAL:CB | 1 | 0.27 |
| (1,6) | 1:162:H:ARG:CG | 1:154:G:ARG:CA | 7 | 0.27 |
| (1,3) | 1:162:K:ARG:CG | 1:154:J:ARG:CA | 2 | 0.27 |
| (1,2262) | 3:302:H:A1CCZ:H7A | 1:232:H:ALA:CA | 6 | 0.26 |
| (1,2262) | 3:302:H:A1CCZ:H7B | 1:232:H:ALA:CA | 6 | 0.26 |
| (1,2258) | 3:302:H:A1CCZ:H11 | 1:232:H:ALA:CA | 9 | 0.26 |
| (1,2221) | 3:302:H:A1CCZ:F33 | 1:224:H:PRO:CG | 4 | 0.26 |
| (1,1533) | 1:190:H:LEU:CG | 1:187:H:GLU:CB | 4 | 0.26 |
| (1,1497) | 1:165:H:VAL:CG2 | 1:214:H:MET:CA | 4 | 0.26 |
| (1,1385) | 1:151:G:LEU:CG | 1:189:G:LEU:CB | 10 | 0.26 |
| (1,1377) | 1:205:J:LEU:CD1 | 1:210:J:THR:CA | 3 | 0.26 |
| (1,689) | 1:201:K:ILE:CD1 | 1:202:K:LEU:C | 2 | 0.26 |
| (1,412) | 1:202:I:LEU:CG | 1:194:I:ALA:CA | 5 | 0.26 |
| (1,389) | 1:210:H:THR:CG2 | 1:211:H:LEU:CG | 5 | 0.26 |
| (1,365) | 1:196:J:PRO:CD | 1:200:J:THR:CB | 7 | 0.26 |
| (1,218) | 1:179:G:GLN:CB | 1:177:G:ALA:CA | 2 | 0.26 |
| (1,75) | 1:219:G:GLN:CG | 1:195:L:ASN:CA | 3 | 0.26 |
| (1,73) | 1:231:I:LEU:N | 1:228:J:ALA:CB | 9 | 0.26 |
| (1,1) | 1:162:G:ARG:CG | 1:154:L:ARG:CA | 2 | 0.26 |
| (1,2284) | 3:302:H:A1CCZ:F32 | 1:157:H:PRO:CG | 10 | 0.25 |
| (1,2258) | 3:302:H:A1CCZ:H11 | 1:232:H:ALA:CA | 10 | 0.25 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ1 | 7 | 0.25 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ2 | 7 | 0.25 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ3 | 7 | 0.25 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE2 | 4 | 0.25 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE3 | 4 | 0.25 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE2 | 10 | 0.25 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE3 | 10 | 0.25 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE2 | 4 | 0.25 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE3 | 4 | 0.25 |
| (1,2122) | 2:301:H:IHP:P4 | 1:158:J:LYS:HE2 | 1 | 0.25 |
| (1,2122) | 2:301:H:IHP:P4 | 1:158:J:LYS:HE3 | 1 | 0.25 |
| (1,1533) | 1:190:I:LEU:CG | 1:187:I:GLU:CB | 9 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,1519) | 1:167:G:ARG:CD | 1:171:G:THR:CA | 1 | 0.25 |
| (1,1514) | 1:193:J:ASN:CB | 1:188:J:THR:C | 10 | 0.25 |
| (1,1318) | 1:172:K:LEU:CD1 | 1:183:K:ASN:CB | 1 | 0.25 |
| (1,1313) | 1:190:L:LEU:CD1 | 1:202:L:LEU:CG | 6 | 0.25 |
| (1,1297) | 1:218:G:CYS:CB | 1:226:G:HIS:CD2 | 9 | 0.25 |
| (1,1203) | 1:191:K:VAL:CG1 | 1:194:K:ALA:CA | 10 | 0.25 |
| (1,1013) | 1:189:I:LEU:CA | 1:153:I:ILE:C | 1 | 0.25 |
| (1,1013) | 1:189:I:LEU:CA | 1:153:I:ILE:C | 4 | 0.25 |
| (1,974) | 1:153:J:ILE:CD1 | 1:151:J:LEU:C | 8 | 0.25 |
| (1,936) | 1:172:K:LEU:CD1 | 1:189:K:LEU:CB | 6 | 0.25 |
| (1,384) | 1:185:J:MET:CG | 1:151:J:LEU:CB | 5 | 0.25 |
| (1,297) | 1:244:H:ILE:CG1 | 1:237:H:GLN:CA | 8 | 0.25 |
| (1,166) | 1:219:H:GLN:CG | 1:160:H:PRO:CA | 2 | 0.25 |
| (1,78) | 1:219:J:GLN:CG | 1:195:I:ASN:CA | 5 | 0.25 |
| (1,8) | 1:195:I:ASN:CA | 1:219:J:GLN:CA | 4 | 0.25 |
| (1,1) | 1:162:G:ARG:CG | 1:154:L:ARG:CA | 9 | 0.25 |
| (1,2233) | 3:302:H:A1CCZ:F32 | 1:195:H:ASN:CA | 1 | 0.24 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE2 | 6 | 0.24 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE3 | 6 | 0.24 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE2 | 8 | 0.24 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE3 | 8 | 0.24 |
| (1,1497) | 1:165:K:VAL:CG2 | 1:214:K:MET:CA | 2 | 0.24 |
| (1,1381) | 1:217:I:ALA:CB | 1:221:I:VAL:CG2 | 8 | 0.24 |
| (1,1233) | 1:190:H:LEU:CD1 | 1:166:H:ASP:CA | 3 | 0.24 |
| (1,1013) | 1:189:L:LEU:CA | 1:153:L:ILE:C | 10 | 0.24 |
| (1,580) | 1:153:L:ILE:CD1 | 1:193:L:ASN:CG | 5 | 0.24 |
| (1,414) | 1:201:H:ILE:CG2 | 1:197:H:ASP:CB | 3 | 0.24 |
| (1,414) | 1:201:H:ILE:CG2 | 1:197:H:ASP:CB | 8 | 0.24 |
| (1,389) | 1:210:H:THR:CG2 | 1:211:H:LEU:CG | 2 | 0.24 |
| (1,267) | 1:188:K:THR:CG2 | 1:185:K:MET:CB | 2 | 0.24 |
| (1,227) | 1:198:H:CYS:CB | 1:199:H:LYS:CE | 3 | 0.24 |
| (1,227) | 1:198:J:CYS:CB | 1:199:J:LYS:CE | 4 | 0.24 |
| (1,74) | 1:231:J:LEU:N | 1:228:K:ALA:CB | 6 | 0.24 |
| (1,48) | 1:221:K:VAL:CG1 | 1:224:L:PRO:CD | 3 | 0.24 |
| (1,48) | 1:221:K:VAL:CG2 | 1:224:L:PRO:CD | 3 | 0.24 |
| (1,10) | 1:195:K:ASN:CA | 1:219:L:GLN:CA | 1 | 0.24 |
| (1,1) | 1:162:G:ARG:CG | 1:154:L:ARG:CA | 6 | 0.24 |
| (2,92) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:H12A | 10 | 0.23 |
| (2,92) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:H12B | 10 | 0.23 |
| (1,2190) | 2:301:H:IHP:O21 | 3:302:H:A1CCZ:F32 | 5 | 0.23 |
| (1,2163) | 2:301:H:IHP:P1 | 1:224:J:PRO:HG2 | 1 | 0.23 |
| (1,2163) | 2:301:H:IHP:P1 | 1:224:J:PRO:HG3 | 1 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,2158) | 2:301:H:IHP:P3 | 1:159:G:GLU:H | 3 | 0.23 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE2 | 5 | 0.23 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE3 | 5 | 0.23 |
| (1,1438) | 1:172:J:LEU:CG | 1:183:J:ASN:CA | 5 | 0.23 |
| (1,1313) | 1:190:G:LEU:CD1 | 1:202:G:LEU:CG | 4 | 0.23 |
| (1,808) | 1:191:K:VAL:CG1 | 1:193:K:ASN:CA | 8 | 0.23 |
| (1,580) | 1:153:K:ILE:CD1 | 1:193:K:ASN:CG | 9 | 0.23 |
| (1,378) | 1:151:L:LEU:CD1 | 1:153:L:ILE:CB | 10 | 0.23 |
| (1,267) | 1:188:K:THR:CG2 | 1:185:K:MET:CB | 3 | 0.23 |
| (1,227) | 1:198:J:CYS:CB | 1:199:J:LYS:CE | 7 | 0.23 |
| (1,48) | 1:221:K:VAL:CG1 | 1:224:L:PRO:CD | 10 | 0.23 |
| (1,48) | 1:221:K:VAL:CG2 | 1:224:L:PRO:CD | 10 | 0.23 |
| (1,3) | 1:162:K:ARG:CG | 1:154:J:ARG:CA | 1 | 0.23 |
| (2,92) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:H12A | 5 | 0.22 |
| (2,92) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:H12B | 5 | 0.22 |
| (1,2293) | 3:302:H:A1CCZ:F33 | 1:160:H:PRO:CA | 5 | 0.22 |
| (1,2251) | 3:302:H:A1CCZ:F33 | 1:198:H:CYS:CA | 8 | 0.22 |
| (1,1533) | 1:190:K:LEU:CG | 1:187:K:GLU:CB | 3 | 0.22 |
| (1,1438) | 1:172:J:LEU:CG | 1:183:J:ASN:CA | 4 | 0.22 |
| (1,1381) | 1:217:L:ALA:CB | 1:221:L:VAL:CG2 | 6 | 0.22 |
| (1,1237) | 1:155:H:GLN:CA | 1:160:H:PRO:CA | 4 | 0.22 |
| (1,1233) | 1:190:K:LEU:CD1 | 1:166:K:ASP:CA | 7 | 0.22 |
| (1,989) | 1:221:I:VAL:CG1 | 1:223:I:GLY:CA | 4 | 0.22 |
| (1,756) | 1:191:K:VAL:CG1 | 1:194:K:ALA:C | 10 | 0.22 |
| (1,689) | 1:201:H:ILE:CD1 | 1:202:H:LEU:C | 7 | 0.22 |
| (1,389) | 1:210:H:THR:CG2 | 1:211:H:LEU:CG | 9 | 0.22 |
| (1,389) | 1:210:H:THR:CG2 | 1:211:H:LEU:CG | 10 | 0.22 |
| (1,248) | 1:156:J:GLY:CA | 1:196:J:PRO:CD | 1 | 0.22 |
| (1,204) | 1:150:K:ILE:CD1 | 1:189:K:LEU:CA | 4 | 0.22 |
| (1,74) | 1:231:J:LEU:N | 1:228:K:ALA:CB | 7 | 0.22 |
| (1,25) | 1:232:L:ALA:CB | 1:238:K:VAL:CB | 4 | 0.22 |
| (1,8) | 1:195:I:ASN:CA | 1:219:J:GLN:CA | 7 | 0.22 |
| (2,12) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H12A | 2 | 0.21 |
| (2,12) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H12B | 2 | 0.21 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ1 | 9 | 0.21 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ2 | 9 | 0.21 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ3 | 9 | 0.21 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE2 | 7 | 0.21 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE3 | 7 | 0.21 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE2 | 1 | 0.21 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE3 | 1 | 0.21 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE2 | 10 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-------------------|----------|---------------|
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE3 | 10 | 0.21 |
| (1,1620) | 1:190:G:LEU:CD1 | 1:194:G:ALA:C | 10 | 0.21 |
| (1,1591) | 1:175:I:GLU:CB | 1:185:I:MET:CB | 4 | 0.21 |
| (1,1533) | 1:190:H:LEU:CG | 1:187:H:GLU:CB | 2 | 0.21 |
| (1,1469) | 1:214:I:MET:CB | 1:205:I:LEU:CA | 7 | 0.21 |
| (1,1220) | 1:214:I:MET:CG | 1:191:I:VAL:CB | 5 | 0.21 |
| (1,1100) | 1:190:H:LEU:CD1 | 1:169:H:TYR:CB | 9 | 0.21 |
| (1,974) | 1:153:I:ILE:CD1 | 1:151:I:LEU:C | 2 | 0.21 |
| (1,936) | 1:172:K:LEU:CD1 | 1:189:K:LEU:CB | 4 | 0.21 |
| (1,831) | 1:150:K:ILE:CD1 | 1:190:K:LEU:CA | 2 | 0.21 |
| (1,561) | 1:201:J:ILE:CG1 | 1:205:J:LEU:CA | 10 | 0.21 |
| (1,505) | 1:174:K:ALA:CA | 1:148:K:THR:CA | 7 | 0.21 |
| (1,389) | 1:210:K:THR:CG2 | 1:211:K:LEU:CG | 1 | 0.21 |
| (1,387) | 1:194:K:ALA:CB | 1:154:K:ARG:CG | 4 | 0.21 |
| (1,387) | 1:194:I:ALA:CB | 1:154:I:ARG:CG | 7 | 0.21 |
| (1,169) | 1:165:K:VAL:CG2 | 1:202:K:LEU:CG | 1 | 0.21 |
| (1,166) | 1:219:H:GLN:CG | 1:160:H:PRO:CA | 9 | 0.21 |
| (1,73) | 1:231:I:LEU:N | 1:228:J:ALA:CB | 10 | 0.21 |
| (1,4) | 1:162:J:ARG:CG | 1:154:I:ARG:CA | 5 | 0.21 |
| (1,3) | 1:162:K:ARG:CG | 1:154:J:ARG:CA | 5 | 0.21 |
| (1,2204) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:F32 | 4 | 0.2 |
| (1,1233) | 1:190:H:LEU:CD1 | 1:166:H:ASP:CA | 6 | 0.2 |
| (1,1220) | 1:214:K:MET:CG | 1:191:K:VAL:CB | 4 | 0.2 |
| (1,1205) | 1:153:K:ILE:CB | 1:193:K:ASN:CA | 8 | 0.2 |
| (1,1100) | 1:190:H:LEU:CD1 | 1:169:H:TYR:CB | 10 | 0.2 |
| (1,968) | 1:221:I:VAL:CG2 | 1:219:I:GLN:CG | 6 | 0.2 |
| (1,936) | 1:172:K:LEU:CD1 | 1:189:K:LEU:CB | 10 | 0.2 |
| (1,756) | 1:191:L:VAL:CG1 | 1:194:L:ALA:C | 4 | 0.2 |
| (1,640) | 1:190:G:LEU:CD1 | 1:193:G:ASN:C | 10 | 0.2 |
| (1,540) | 1:230:H:VAL:CG1 | 1:221:H:VAL:CA | 9 | 0.2 |
| (1,505) | 1:174:J:ALA:CA | 1:148:J:THR:CA | 2 | 0.2 |
| (1,442) | 1:228:L:ALA:CB | 1:224:L:PRO:CG | 7 | 0.2 |
| (1,389) | 1:210:H:THR:CG2 | 1:211:H:LEU:CG | 3 | 0.2 |
| (1,389) | 1:210:H:THR:CG2 | 1:211:H:LEU:CG | 4 | 0.2 |
| (1,278) | 1:155:K:GLN:CB | 1:196:K:PRO:CA | 2 | 0.2 |
| (1,227) | 1:198:J:CYS:CB | 1:199:J:LYS:CE | 6 | 0.2 |
| (1,206) | 1:160:I:PRO:CA | 1:164:I:TYR:CD2 | 5 | 0.2 |
| (1,204) | 1:150:H:ILE:CD1 | 1:189:H:LEU:CA | 3 | 0.2 |
| (1,166) | 1:219:H:GLN:CG | 1:160:H:PRO:CA | 6 | 0.2 |
| (1,78) | 1:219:J:GLN:CG | 1:195:I:ASN:CA | 8 | 0.2 |
| (1,73) | 1:231:I:LEU:N | 1:228:J:ALA:CB | 2 | 0.2 |
| (1,8) | 1:195:I:ASN:CA | 1:219:J:GLN:CA | 3 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,6) | 1:162:H:ARG:CG | 1:154:G:ARG:CA | 5 | 0.2 |
| (1,2308) | 3:302:H:A1CCZ:F31 | 1:228:H:ALA:CA | 8 | 0.19 |
| (1,2296) | 3:302:H:A1CCZ:F32 | 1:196:H:PRO:CG | 5 | 0.19 |
| (1,2190) | 2:301:H:IHP:O21 | 3:302:H:A1CCZ:F32 | 1 | 0.19 |
| (1,2163) | 2:301:H:IHP:P1 | 1:224:J:PRO:HG2 | 10 | 0.19 |
| (1,2163) | 2:301:H:IHP:P1 | 1:224:J:PRO:HG3 | 10 | 0.19 |
| (1,2133) | 2:301:H:IHP:P4 | 1:158:L:LYS:HZ1 | 9 | 0.19 |
| (1,2133) | 2:301:H:IHP:P4 | 1:158:L:LYS:HZ2 | 9 | 0.19 |
| (1,2133) | 2:301:H:IHP:P4 | 1:158:L:LYS:HZ3 | 9 | 0.19 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE2 | 9 | 0.19 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE3 | 9 | 0.19 |
| (1,1620) | 1:190:G:LEU:CD1 | 1:194:G:ALA:C | 4 | 0.19 |
| (1,1533) | 1:190:H:LEU:CG | 1:187:H:GLU:CB | 6 | 0.19 |
| (1,1481) | 1:194:I:ALA:CB | 1:202:I:LEU:CB | 10 | 0.19 |
| (1,1377) | 1:205:I:LEU:CD1 | 1:210:I:THR:CA | 6 | 0.19 |
| (1,1313) | 1:190:G:LEU:CD1 | 1:202:G:LEU:CG | 2 | 0.19 |
| (1,1233) | 1:190:H:LEU:CD1 | 1:166:H:ASP:CA | 8 | 0.19 |
| (1,1013) | 1:189:I:LEU:CA | 1:153:I:ILE:C | 3 | 0.19 |
| (1,539) | 1:187:J:GLU:CB | 1:184:J:TRP:CZ3 | 6 | 0.19 |
| (1,442) | 1:228:H:ALA:CB | 1:224:H:PRO:CG | 8 | 0.19 |
| (1,420) | 1:202:L:LEU:CD1 | 1:199:L:LYS:CD | 5 | 0.19 |
| (1,389) | 1:210:H:THR:CG2 | 1:211:H:LEU:CG | 8 | 0.19 |
| (1,387) | 1:194:K:ALA:CB | 1:154:K:ARG:CG | 8 | 0.19 |
| (1,297) | 1:244:H:ILE:CG1 | 1:237:H:GLN:CA | 3 | 0.19 |
| (1,267) | 1:188:K:THR:CG2 | 1:185:K:MET:CB | 4 | 0.19 |
| (1,73) | 1:231:I:LEU:N | 1:228:J:ALA:CB | 4 | 0.19 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12A | 9 | 0.18 |
| (2,14) | 2:301:H:IHP:O33 | 3:302:H:A1CCZ:H12B | 9 | 0.18 |
| (1,2275) | 3:302:H:A1CCZ:H11 | 1:231:I:LEU:CA | 7 | 0.18 |
| (1,2250) | 3:302:H:A1CCZ:F32 | 1:198:H:CYS:CA | 10 | 0.18 |
| (1,2233) | 3:302:H:A1CCZ:F32 | 1:195:H:ASN:CA | 7 | 0.18 |
| (1,2210) | 2:301:H:IHP:O45 | 3:302:H:A1CCZ:F32 | 8 | 0.18 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE2 | 6 | 0.18 |
| (1,2123) | 2:301:H:IHP:P4 | 1:158:K:LYS:HE3 | 6 | 0.18 |
| (1,1381) | 1:217:I:ALA:CB | 1:221:I:VAL:CG2 | 9 | 0.18 |
| (1,1100) | 1:190:H:LEU:CD1 | 1:169:H:TYR:CB | 1 | 0.18 |
| (1,989) | 1:221:K:VAL:CG1 | 1:223:K:GLY:CA | 10 | 0.18 |
| (1,808) | 1:191:L:VAL:CG1 | 1:193:L:ASN:CA | 6 | 0.18 |
| (1,673) | 1:165:J:VAL:CG2 | 1:163:J:ASP:CB | 4 | 0.18 |
| (1,25) | 1:232:L:ALA:CB | 1:238:K:VAL:CB | 3 | 0.18 |
| (1,5) | 1:162:I:ARG:CG | 1:154:H:ARG:CA | 10 | 0.18 |
| (1,3) | 1:162:K:ARG:CG | 1:154:J:ARG:CA | 3 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-------------------|----------|---------------|
| (1,3) | 1:162:K:ARG:CG | 1:154:J:ARG:CA | 7 | 0.18 |
| (2,8) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H9A | 2 | 0.17 |
| (2,8) | 2:301:H:IHP:O23 | 3:302:H:A1CCZ:H9B | 2 | 0.17 |
| (1,2308) | 3:302:H:A1CCZ:F31 | 1:228:H:ALA:CA | 4 | 0.17 |
| (1,2262) | 3:302:H:A1CCZ:H7A | 1:232:H:ALA:CA | 5 | 0.17 |
| (1,2262) | 3:302:H:A1CCZ:H7B | 1:232:H:ALA:CA | 5 | 0.17 |
| (1,2204) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:F32 | 10 | 0.17 |
| (1,2197) | 2:301:H:IHP:O41 | 3:302:H:A1CCZ:F33 | 2 | 0.17 |
| (1,2157) | 2:301:H:IHP:P3 | 1:158:L:LYS:HA | 6 | 0.17 |
| (1,1514) | 1:193:J:ASN:CB | 1:188:J:THR:C | 8 | 0.17 |
| (1,1473) | 1:153:I:ILE:CG2 | 1:165:I:VAL:C | 4 | 0.17 |
| (1,968) | 1:221:I:VAL:CG2 | 1:219:I:GLN:CG | 1 | 0.17 |
| (1,945) | 1:150:J:ILE:CD1 | 1:193:J:ASN:CG | 1 | 0.17 |
| (1,945) | 1:150:J:ILE:CD1 | 1:193:J:ASN:CG | 5 | 0.17 |
| (1,640) | 1:190:I:LEU:CD1 | 1:193:I:ASN:C | 2 | 0.17 |
| (1,580) | 1:153:K:ILE:CD1 | 1:193:K:ASN:CG | 3 | 0.17 |
| (1,580) | 1:153:L:ILE:CD1 | 1:193:L:ASN:CG | 4 | 0.17 |
| (1,539) | 1:187:G:GLU:CB | 1:184:G:TRP:CZ3 | 4 | 0.17 |
| (1,539) | 1:187:L:GLU:CB | 1:184:L:TRP:CZ3 | 8 | 0.17 |
| (1,505) | 1:174:K:ALA:CA | 1:148:K:THR:CA | 10 | 0.17 |
| (1,389) | 1:210:K:THR:CG2 | 1:211:K:LEU:CG | 7 | 0.17 |
| (1,387) | 1:194:K:ALA:CB | 1:154:K:ARG:CG | 10 | 0.17 |
| (1,297) | 1:244:H:ILE:CG1 | 1:237:H:GLN:CA | 5 | 0.17 |
| (1,274) | 1:156:I:GLY:CA | 1:160:I:PRO:C | 6 | 0.17 |
| (1,11) | 1:195:L:ASN:CA | 1:219:G:GLN:CA | 10 | 0.17 |
| (1,5) | 1:162:I:ARG:CG | 1:154:H:ARG:CA | 6 | 0.17 |
| (1,2284) | 3:302:H:A1CCZ:F32 | 1:157:H:PRO:CG | 4 | 0.16 |
| (1,2251) | 3:302:H:A1CCZ:F33 | 1:198:H:CYS:CA | 2 | 0.16 |
| (1,2196) | 2:301:H:IHP:O41 | 3:302:H:A1CCZ:F32 | 10 | 0.16 |
| (1,2163) | 2:301:H:IHP:P1 | 1:224:J:PRO:HG2 | 5 | 0.16 |
| (1,2163) | 2:301:H:IHP:P1 | 1:224:J:PRO:HG3 | 5 | 0.16 |
| (1,1591) | 1:175:K:GLU:CB | 1:185:K:MET:CB | 3 | 0.16 |
| (1,1563) | 1:148:G:THR:CA | 1:174:G:ALA:C | 7 | 0.16 |
| (1,1533) | 1:190:H:LEU:CG | 1:187:H:GLU:CB | 10 | 0.16 |
| (1,1473) | 1:153:J:ILE:CG2 | 1:165:J:VAL:C | 5 | 0.16 |
| (1,673) | 1:165:J:VAL:CG2 | 1:163:J:ASP:CB | 9 | 0.16 |
| (1,640) | 1:190:G:LEU:CD1 | 1:193:G:ASN:C | 9 | 0.16 |
| (1,539) | 1:187:J:GLU:CB | 1:184:J:TRP:CZ3 | 1 | 0.16 |
| (1,423) | 1:190:G:LEU:CG | 1:193:G:ASN:C | 4 | 0.16 |
| (1,399) | 1:150:K:ILE:CD1 | 1:190:K:LEU:CD1 | 4 | 0.16 |
| (1,297) | 1:244:H:ILE:CG1 | 1:237:H:GLN:CA | 10 | 0.16 |
| (1,166) | 1:219:J:GLN:CG | 1:160:J:PRO:CA | 4 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|--------------------|----------|---------------|
| (1,76) | 1:219:L:GLN:CG | 1:195:K:ASN:CA | 10 | 0.16 |
| (1,4) | 1:162:J:ARG:CG | 1:154:I:ARG:CA | 3 | 0.16 |
| (1,4) | 1:162:J:ARG:CG | 1:154:I:ARG:CA | 6 | 0.16 |
| (1,1) | 1:162:G:ARG:CG | 1:154:L:ARG:CA | 10 | 0.16 |
| (2,92) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:H12A | 3 | 0.15 |
| (2,92) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:H12B | 3 | 0.15 |
| (1,2310) | 3:302:H:A1CCZ:F31 | 1:228:I:ALA:CA | 7 | 0.15 |
| (1,2308) | 3:302:H:A1CCZ:F31 | 1:228:H:ALA:CA | 5 | 0.15 |
| (1,2294) | 3:302:H:A1CCZ:F32 | 1:196:H:PRO:CA | 7 | 0.15 |
| (1,2292) | 3:302:H:A1CCZ:F32 | 1:160:H:PRO:CA | 3 | 0.15 |
| (1,2204) | 2:301:H:IHP:O25 | 3:302:H:A1CCZ:F32 | 5 | 0.15 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE2 | 8 | 0.15 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE3 | 8 | 0.15 |
| (1,1620) | 1:190:H:LEU:CD1 | 1:194:H:ALA:C | 6 | 0.15 |
| (1,1620) | 1:190:G:LEU:CD1 | 1:194:G:ALA:C | 7 | 0.15 |
| (1,1519) | 1:167:H:ARG:CD | 1:171:H:THR:CA | 7 | 0.15 |
| (1,1297) | 1:218:J:CYS:CB | 1:226:J:HIS:CD2 | 6 | 0.15 |
| (1,1203) | 1:191:L:VAL:CG1 | 1:194:L:ALA:CA | 4 | 0.15 |
| (1,1172) | 1:244:L:ILE:CG1 | 1:237:L:GLN:CB | 1 | 0.15 |
| (1,1172) | 1:244:L:ILE:CG1 | 1:237:L:GLN:CB | 4 | 0.15 |
| (1,989) | 1:221:I:VAL:CG1 | 1:223:I:GLY:CA | 3 | 0.15 |
| (1,936) | 1:172:H:LEU:CD1 | 1:189:H:LEU:CB | 2 | 0.15 |
| (1,936) | 1:172:K:LEU:CD1 | 1:189:K:LEU:CB | 5 | 0.15 |
| (1,808) | 1:191:K:VAL:CG1 | 1:193:K:ASN:CA | 7 | 0.15 |
| (1,756) | 1:191:L:VAL:CG1 | 1:194:L:ALA:C | 3 | 0.15 |
| (1,640) | 1:190:L:LEU:CD1 | 1:193:L:ASN:C | 6 | 0.15 |
| (1,384) | 1:185:L:MET:CG | 1:151:L:LEU:CB | 6 | 0.15 |
| (1,297) | 1:244:I:ILE:CG1 | 1:237:I:GLN:CA | 4 | 0.15 |
| (1,297) | 1:244:L:ILE:CG1 | 1:237:L:GLN:CA | 6 | 0.15 |
| (1,297) | 1:244:J:ILE:CG1 | 1:237:J:GLN:CA | 9 | 0.15 |
| (1,267) | 1:188:K:THR:CG2 | 1:185:K:MET:CB | 7 | 0.15 |
| (1,204) | 1:150:H:ILE:CD1 | 1:189:H:LEU:CA | 1 | 0.15 |
| (2,93) | 2:301:H:IHP:O35 | 3:302:H:A1CCZ:H11 | 5 | 0.14 |
| (1,2308) | 3:302:H:A1CCZ:F31 | 1:228:H:ALA:CA | 1 | 0.14 |
| (1,2250) | 3:302:H:A1CCZ:F32 | 1:198:H:CYS:CA | 4 | 0.14 |
| (1,2210) | 2:301:H:IHP:O45 | 3:302:H:A1CCZ:F32 | 9 | 0.14 |
| (1,2208) | 2:301:H:IHP:O35 | 3:302:H:A1CCZ:F33 | 9 | 0.14 |
| (1,2163) | 2:301:H:IHP:P1 | 1:224:J:PRO:HG2 | 4 | 0.14 |
| (1,2163) | 2:301:H:IHP:P1 | 1:224:J:PRO:HG3 | 4 | 0.14 |
| (1,2133) | 2:301:H:IHP:P4 | 1:158:L:LYS:HZ1 | 6 | 0.14 |
| (1,2133) | 2:301:H:IHP:P4 | 1:158:L:LYS:HZ2 | 6 | 0.14 |
| (1,2133) | 2:301:H:IHP:P4 | 1:158:L:LYS:HZ3 | 6 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-------------------|----------|---------------|
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ1 | 2 | 0.14 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ2 | 2 | 0.14 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ3 | 2 | 0.14 |
| (1,1650) | 1:204:H:ALA:CB | 1:206:H:GLY:C | 1 | 0.14 |
| (1,1591) | 1:175:I:GLU:CB | 1:185:I:MET:CB | 1 | 0.14 |
| (1,1591) | 1:175:L:GLU:CB | 1:185:L:MET:CB | 7 | 0.14 |
| (1,1533) | 1:190:L:LEU:CG | 1:187:L:GLU:CB | 5 | 0.14 |
| (1,1473) | 1:153:J:ILE:CG2 | 1:165:J:VAL:C | 1 | 0.14 |
| (1,1469) | 1:214:I:MET:CB | 1:205:I:LEU:CA | 3 | 0.14 |
| (1,1313) | 1:190:G:LEU:CD1 | 1:202:G:LEU:CG | 9 | 0.14 |
| (1,1100) | 1:190:H:LEU:CD1 | 1:169:H:TYR:CB | 2 | 0.14 |
| (1,936) | 1:172:K:LEU:CD1 | 1:189:K:LEU:CB | 9 | 0.14 |
| (1,915) | 1:235:G:MET:CB | 1:239:G:THR:CA | 7 | 0.14 |
| (1,505) | 1:174:I:ALA:CA | 1:148:I:THR:CA | 8 | 0.14 |
| (1,423) | 1:190:K:LEU:CG | 1:193:K:ASN:C | 9 | 0.14 |
| (1,423) | 1:190:G:LEU:CG | 1:193:G:ASN:C | 10 | 0.14 |
| (1,414) | 1:201:I:ILE:CG2 | 1:197:I:ASP:CB | 1 | 0.14 |
| (1,399) | 1:150:K:ILE:CD1 | 1:190:K:LEU:CD1 | 3 | 0.14 |
| (1,297) | 1:244:L:ILE:CG1 | 1:237:L:GLN:CA | 2 | 0.14 |
| (1,297) | 1:244:L:ILE:CG1 | 1:237:L:GLN:CA | 7 | 0.14 |
| (1,267) | 1:188:K:THR:CG2 | 1:185:K:MET:CB | 1 | 0.14 |
| (1,166) | 1:219:J:GLN:CG | 1:160:J:PRO:CA | 8 | 0.14 |
| (1,24) | 1:232:G:ALA:CB | 1:238:L:VAL:CB | 7 | 0.14 |
| (2,94) | 2:301:H:IHP:O45 | 3:302:H:A1CCZ:H11 | 8 | 0.13 |
| (1,2210) | 2:301:H:IHP:O45 | 3:302:H:A1CCZ:F32 | 2 | 0.13 |
| (1,2196) | 2:301:H:IHP:O41 | 3:302:H:A1CCZ:F32 | 9 | 0.13 |
| (1,2163) | 2:301:H:IHP:P1 | 1:224:J:PRO:HG2 | 9 | 0.13 |
| (1,2163) | 2:301:H:IHP:P1 | 1:224:J:PRO:HG3 | 9 | 0.13 |
| (1,1650) | 1:204:J:ALA:CB | 1:206:J:GLY:C | 6 | 0.13 |
| (1,1591) | 1:175:L:GLU:CB | 1:185:L:MET:CB | 2 | 0.13 |
| (1,1533) | 1:190:H:LEU:CG | 1:187:H:GLU:CB | 1 | 0.13 |
| (1,1519) | 1:167:K:ARG:CD | 1:171:K:THR:CA | 8 | 0.13 |
| (1,1495) | 1:202:L:LEU:CG | 1:161:L:PHE:CB | 5 | 0.13 |
| (1,1220) | 1:214:I:MET:CG | 1:191:I:VAL:CB | 10 | 0.13 |
| (1,1123) | 1:211:L:LEU:CD1 | 1:210:L:THR:CB | 6 | 0.13 |
| (1,1100) | 1:190:K:LEU:CD1 | 1:169:K:TYR:CB | 7 | 0.13 |
| (1,989) | 1:221:I:VAL:CG1 | 1:223:I:GLY:CA | 9 | 0.13 |
| (1,968) | 1:221:I:VAL:CG2 | 1:219:I:GLN:CG | 10 | 0.13 |
| (1,915) | 1:235:G:MET:CB | 1:239:G:THR:CA | 1 | 0.13 |
| (1,673) | 1:165:J:VAL:CG2 | 1:163:J:ASP:CB | 5 | 0.13 |
| (1,673) | 1:165:K:VAL:CG2 | 1:163:K:ASP:CB | 8 | 0.13 |
| (1,539) | 1:187:G:GLU:CB | 1:184:G:TRP:CZ3 | 2 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-------------------|-----------------|----------|---------------|
| (1,505) | 1:174:K:ALA:CA | 1:148:K:THR:CA | 9 | 0.13 |
| (1,442) | 1:228:K:ALA:CB | 1:224:K:PRO:CG | 6 | 0.13 |
| (1,248) | 1:156:K:GLY:CA | 1:196:K:PRO:CD | 10 | 0.13 |
| (1,2133) | 2:301:H:IHP:P4 | 1:158:L:LYS:HZ1 | 3 | 0.12 |
| (1,2133) | 2:301:H:IHP:P4 | 1:158:L:LYS:HZ2 | 3 | 0.12 |
| (1,2133) | 2:301:H:IHP:P4 | 1:158:L:LYS:HZ3 | 3 | 0.12 |
| (1,2133) | 2:301:H:IHP:P4 | 1:158:L:LYS:HZ1 | 4 | 0.12 |
| (1,2133) | 2:301:H:IHP:P4 | 1:158:L:LYS:HZ2 | 4 | 0.12 |
| (1,2133) | 2:301:H:IHP:P4 | 1:158:L:LYS:HZ3 | 4 | 0.12 |
| (1,1565) | 1:214:I:MET:CG | 1:190:I:LEU:CB | 8 | 0.12 |
| (1,1514) | 1:193:L:ASN:CB | 1:188:L:THR:C | 2 | 0.12 |
| (1,1381) | 1:217:I:ALA:CB | 1:221:I:VAL:CG2 | 2 | 0.12 |
| (1,1282) | 1:217:G:ALA:CB | 1:215:G:MET:CB | 3 | 0.12 |
| (1,1123) | 1:211:L:LEU:CD1 | 1:210:L:THR:CB | 3 | 0.12 |
| (1,831) | 1:150:K:ILE:CD1 | 1:190:K:LEU:CA | 7 | 0.12 |
| (1,808) | 1:191:L:VAL:CG1 | 1:193:L:ASN:CA | 1 | 0.12 |
| (1,619) | 1:208:H:GLY:CA | 1:210:H:THR:CB | 8 | 0.12 |
| (1,560) | 1:201:I:ILE:CD1 | 1:161:I:PHE:CD1 | 4 | 0.12 |
| (1,560) | 1:201:K:ILE:CD1 | 1:161:K:PHE:CD1 | 7 | 0.12 |
| (1,423) | 1:190:G:LEU:CG | 1:193:G:ASN:C | 8 | 0.12 |
| (1,206) | 1:160:J:PRO:CA | 1:164:J:TYR:CD2 | 2 | 0.12 |
| (1,166) | 1:219:H:GLN:CG | 1:160:H:PRO:CA | 1 | 0.12 |
| (1,76) | 1:219:L:GLN:CG | 1:195:K:ASN:CA | 8 | 0.12 |
| (1,8) | 1:195:I:ASN:CA | 1:219:J:GLN:CA | 9 | 0.12 |
| (1,5) | 1:162:I:ARG:CG | 1:154:H:ARG:CA | 4 | 0.12 |
| (1,2318) | 3:302:H:A1CCZ:F31 | 1:231:H:LEU:CB | 6 | 0.11 |
| (1,2288) | 3:302:H:A1CCZ:F33 | 1:157:G:PRO:CG | 3 | 0.11 |
| (1,2169) | 2:301:H:IHP:P1 | 1:224:J:PRO:HD2 | 10 | 0.11 |
| (1,2169) | 2:301:H:IHP:P1 | 1:224:J:PRO:HD3 | 10 | 0.11 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ1 | 5 | 0.11 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ2 | 5 | 0.11 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ3 | 5 | 0.11 |
| (1,1650) | 1:204:H:ALA:CB | 1:206:H:GLY:C | 10 | 0.11 |
| (1,1620) | 1:190:G:LEU:CD1 | 1:194:G:ALA:C | 8 | 0.11 |
| (1,1519) | 1:167:I:ARG:CD | 1:171:I:THR:CA | 2 | 0.11 |
| (1,1437) | 1:211:H:LEU:CD2 | 1:209:H:ALA:CA | 6 | 0.11 |
| (1,1237) | 1:155:H:GLN:CA | 1:160:H:PRO:CA | 1 | 0.11 |
| (1,1237) | 1:155:H:GLN:CA | 1:160:H:PRO:CA | 2 | 0.11 |
| (1,1172) | 1:244:L:ILE:CG1 | 1:237:L:GLN:CB | 2 | 0.11 |
| (1,1172) | 1:244:L:ILE:CG1 | 1:237:L:GLN:CB | 3 | 0.11 |
| (1,1123) | 1:211:L:LEU:CD1 | 1:210:L:THR:CB | 10 | 0.11 |
| (1,989) | 1:221:I:VAL:CG1 | 1:223:I:GLY:CA | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,936) | 1:172:I:LEU:CD1 | 1:189:I:LEU:CB | 1 | 0.11 |
| (1,936) | 1:172:K:LEU:CD1 | 1:189:K:LEU:CB | 3 | 0.11 |
| (1,808) | 1:191:K:VAL:CG1 | 1:193:K:ASN:CA | 2 | 0.11 |
| (1,745) | 1:167:G:ARG:CB | 1:159:G:GLU:CG | 7 | 0.11 |
| (1,657) | 1:172:H:LEU:CG | 1:153:H:ILE:CB | 7 | 0.11 |
| (1,640) | 1:190:L:LEU:CD1 | 1:193:L:ASN:C | 1 | 0.11 |
| (1,540) | 1:230:H:VAL:CG1 | 1:221:H:VAL:CA | 10 | 0.11 |
| (1,384) | 1:185:J:MET:CG | 1:151:J:LEU:CB | 4 | 0.11 |
| (1,248) | 1:156:L:GLY:CA | 1:196:L:PRO:CD | 4 | 0.11 |
| (1,248) | 1:156:I:GLY:CA | 1:196:I:PRO:CD | 6 | 0.11 |
| (1,206) | 1:160:L:PRO:CA | 1:164:L:TYR:CD2 | 3 | 0.11 |
| (1,76) | 1:219:L:GLN:CG | 1:195:K:ASN:CA | 7 | 0.11 |
| (1,24) | 1:232:G:ALA:CB | 1:238:L:VAL:CB | 6 | 0.11 |
| (1,3) | 1:162:K:ARG:CG | 1:154:J:ARG:CA | 4 | 0.11 |
| (1,2140) | 2:301:H:IHP:P6 | 1:224:L:PRO:HD2 | 3 | 0.1 |
| (1,2140) | 2:301:H:IHP:P6 | 1:224:L:PRO:HD3 | 3 | 0.1 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ1 | 3 | 0.1 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ2 | 3 | 0.1 |
| (1,2132) | 2:301:H:IHP:P4 | 1:158:K:LYS:HZ3 | 3 | 0.1 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE2 | 9 | 0.1 |
| (1,2124) | 2:301:H:IHP:P4 | 1:158:L:LYS:HE3 | 9 | 0.1 |
| (1,1473) | 1:153:J:ILE:CG2 | 1:165:J:VAL:C | 6 | 0.1 |
| (1,1381) | 1:217:I:ALA:CB | 1:221:I:VAL:CG2 | 1 | 0.1 |
| (1,1313) | 1:190:K:LEU:CD1 | 1:202:K:LEU:CG | 3 | 0.1 |
| (1,1241) | 1:216:G:THR:CA | 1:212:G:GLU:CD | 7 | 0.1 |
| (1,1123) | 1:211:J:LEU:CD1 | 1:210:J:THR:CB | 1 | 0.1 |
| (1,1100) | 1:190:H:LEU:CD1 | 1:169:H:TYR:CB | 8 | 0.1 |
| (1,399) | 1:150:J:ILE:CD1 | 1:190:J:LEU:CD1 | 9 | 0.1 |
| (1,78) | 1:219:J:GLN:CG | 1:195:I:ASN:CA | 10 | 0.1 |
| (1,76) | 1:219:L:GLN:CG | 1:195:K:ASN:CA | 2 | 0.1 |
| (1,24) | 1:232:G:ALA:CB | 1:238:L:VAL:CB | 9 | 0.1 |
| (1,8) | 1:195:I:ASN:CA | 1:219:J:GLN:CA | 8 | 0.1 |

10 Dihedral-angle violation analysis [i](#)

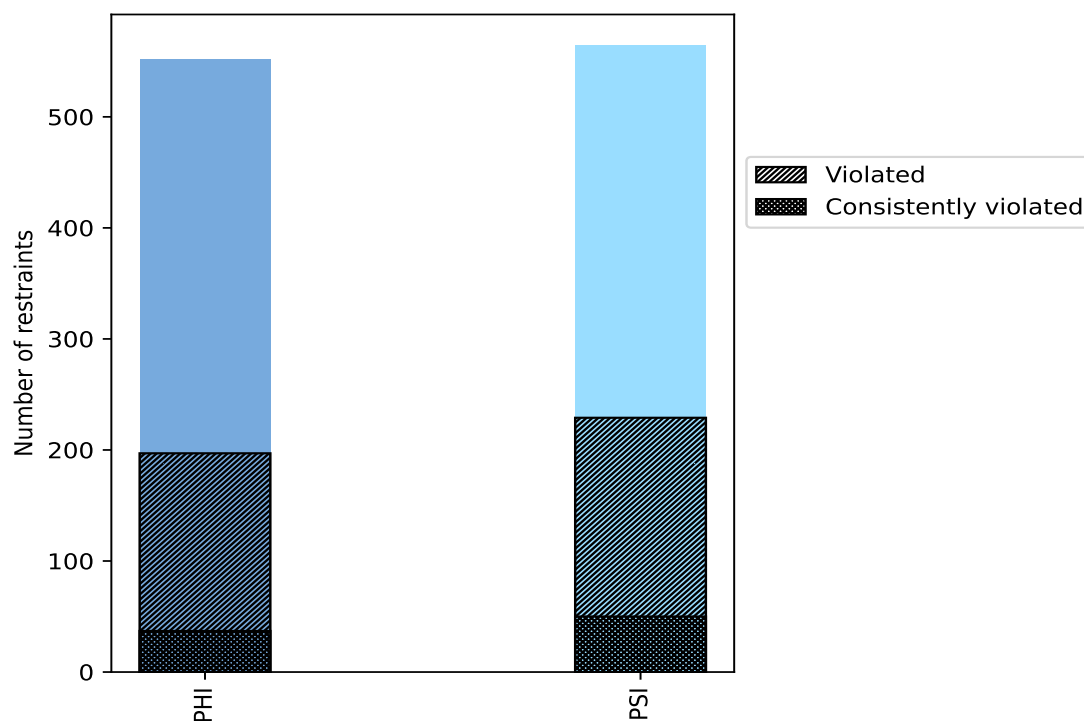
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

| Angle type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| PHI | 552 | 49.5 | 197 | 35.7 | 17.7 | 37 | 6.7 | 3.3 |
| PSI | 564 | 50.5 | 229 | 40.6 | 20.5 | 50 | 8.9 | 4.5 |
| Total | 1116 | 100.0 | 426 | 38.2 | 38.2 | 87 | 7.8 | 7.8 |

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



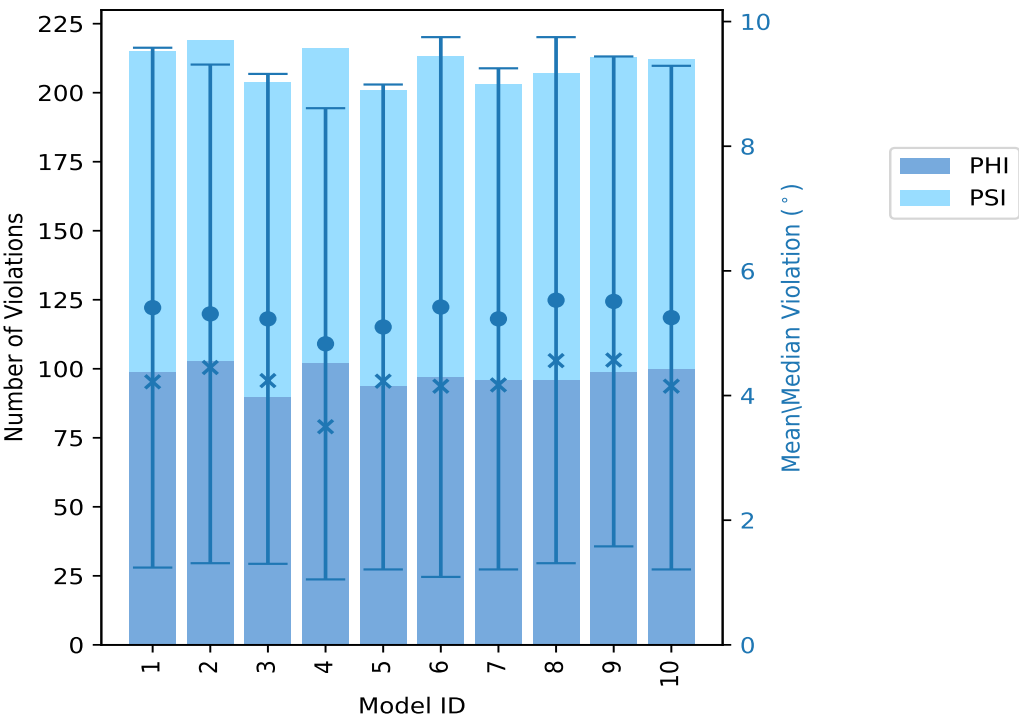
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

| Model ID | Number of violations | | | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
| | PHI | PSI | Total | | | | |
| 1 | 99 | 116 | 215 | 5.41 | 28.06 | 4.17 | 4.22 |
| 2 | 103 | 116 | 219 | 5.31 | 21.78 | 4.0 | 4.45 |
| 3 | 90 | 114 | 204 | 5.23 | 28.32 | 3.93 | 4.24 |
| 4 | 102 | 114 | 216 | 4.83 | 27.69 | 3.78 | 3.5 |
| 5 | 94 | 107 | 201 | 5.1 | 21.91 | 3.89 | 4.23 |
| 6 | 97 | 116 | 213 | 5.42 | 26.76 | 4.33 | 4.15 |
| 7 | 96 | 107 | 203 | 5.23 | 27.99 | 4.02 | 4.17 |
| 8 | 96 | 111 | 207 | 5.53 | 28.43 | 4.22 | 4.56 |
| 9 | 99 | 114 | 213 | 5.51 | 22.44 | 3.93 | 4.57 |
| 10 | 100 | 112 | 212 | 5.25 | 28.71 | 4.04 | 4.15 |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

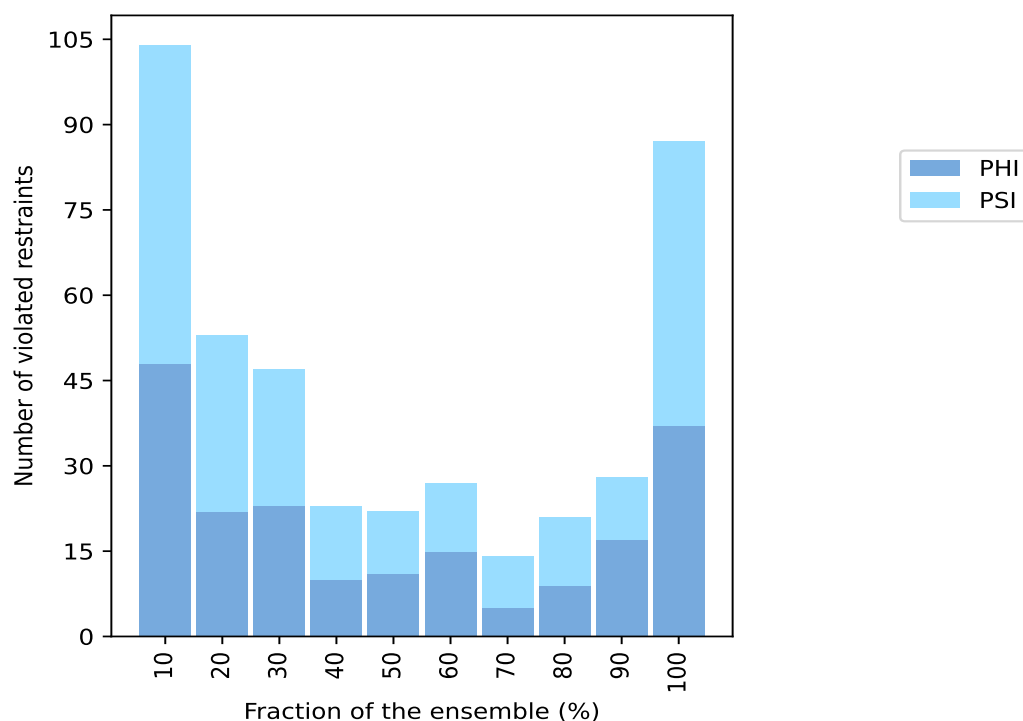
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI | PSI | Total | Count ¹ | % |
| 48 | 56 | 104 | 1 | 10.0 |
| 22 | 31 | 53 | 2 | 20.0 |
| 23 | 24 | 47 | 3 | 30.0 |
| 10 | 13 | 23 | 4 | 40.0 |
| 11 | 11 | 22 | 5 | 50.0 |
| 15 | 12 | 27 | 6 | 60.0 |
| 5 | 9 | 14 | 7 | 70.0 |
| 9 | 12 | 21 | 8 | 80.0 |
| 17 | 11 | 28 | 9 | 90.0 |
| 37 | 50 | 87 | 10 | 100.0 |

¹ Number of models with violations

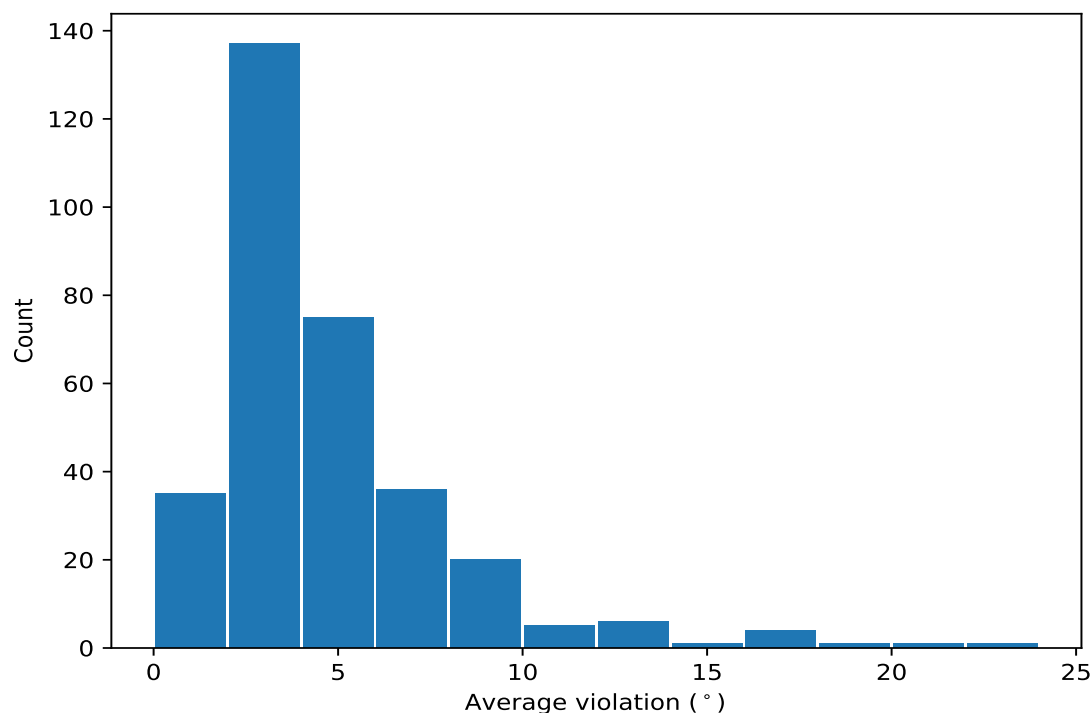
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|----------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 10 | 23.43 | 4.67 | 24.34 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 10 | 20.64 | 5.45 | 21.29 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 10 | 17.69 | 2.63 | 16.67 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 10 | 17.37 | 0.85 | 17.56 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 10 | 13.18 | 3.13 | 13.54 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 10 | 12.83 | 1.55 | 13.0 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 10 | 12.4 | 1.7 | 13.06 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 10 | 12.14 | 4.05 | 10.38 |
| (1,448) | 1:187:J:GLU:C | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 10 | 10.9 | 3.49 | 10.0 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 10 | 10.55 | 0.43 | 10.4 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 10 | 9.91 | 1.53 | 9.84 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 10 | 9.59 | 0.92 | 9.42 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 10 | 9.46 | 4.91 | 8.59 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|----------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 10 | 9.28 | 2.86 | 9.07 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 10 | 9.22 | 3.56 | 9.43 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 10 | 9.16 | 0.58 | 9.16 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 10 | 8.93 | 2.76 | 8.88 |
| (1,61) | 1:152:G:ASP:N | 1:152:G:ASP:CA | 1:152:G:ASP:C | 1:153:G:ILE:N | 10 | 8.86 | 1.57 | 9.24 |
| (1,445) | 1:187:G:GLU:C | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 10 | 8.51 | 1.33 | 8.68 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 10 | 8.51 | 1.25 | 8.19 |
| (1,794) | 1:219:H:GLN:C | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 10 | 8.14 | 1.59 | 7.93 |
| (1,1026) | 1:239:L:THR:C | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 10 | 8.06 | 1.38 | 8.64 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 10 | 7.8 | 0.92 | 7.94 |
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 10 | 7.78 | 3.39 | 8.64 |
| (1,632) | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 1:205:H:LEU:N | 10 | 7.65 | 2.51 | 7.7 |
| (1,482) | 1:190:H:LEU:C | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 10 | 7.65 | 3.73 | 6.98 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 10 | 7.5 | 1.66 | 7.39 |
| (1,558) | 1:197:L:ASP:C | 1:198:L:CYS:N | 1:198:L:CYS:CA | 1:198:L:CYS:C | 10 | 7.36 | 1.0 | 7.3 |
| (1,1024) | 1:239:J:THR:C | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 10 | 7.22 | 1.89 | 7.3 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 10 | 7.18 | 0.4 | 7.28 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 10 | 7.04 | 1.15 | 6.96 |
| (1,804) | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 1:221:L:VAL:N | 10 | 6.97 | 2.38 | 6.97 |
| (1,116) | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 1:159:H:GLU:N | 10 | 6.79 | 2.14 | 6.04 |
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 10 | 6.74 | 3.5 | 6.52 |
| (1,27) | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 1:148:I:THR:N | 10 | 6.7 | 2.02 | 7.01 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 10 | 6.5 | 1.84 | 5.88 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 10 | 6.47 | 0.69 | 6.38 |
| (1,446) | 1:187:H:GLU:C | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 10 | 6.46 | 3.16 | 4.8 |
| (1,28) | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 1:148:J:THR:N | 10 | 6.4 | 3.21 | 5.63 |
| (1,312) | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 1:175:L:GLU:N | 10 | 6.34 | 3.0 | 6.42 |
| (1,1025) | 1:239:K:THR:C | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 10 | 6.25 | 1.29 | 6.31 |
| (1,1030) | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 1:241:J:THR:N | 10 | 6.23 | 2.34 | 5.87 |
| (1,450) | 1:187:L:GLU:C | 1:188:L:THR:N | 1:188:L:THR:CA | 1:188:L:THR:C | 10 | 6.02 | 1.93 | 6.3 |
| (1,1021) | 1:239:G:THR:C | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 10 | 5.92 | 0.88 | 6.06 |
| (1,1032) | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 1:241:L:THR:N | 10 | 5.92 | 1.46 | 6.11 |
| (1,423) | 1:185:I:MET:C | 1:186:I:THR:N | 1:186:I:THR:CA | 1:186:I:THR:C | 10 | 5.9 | 2.34 | 6.13 |
| (1,1031) | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 1:241:K:THR:N | 10 | 5.86 | 1.79 | 5.9 |
| (1,89) | 1:154:K:ARG:C | 1:155:K:GLN:N | 1:155:K:GLN:CA | 1:155:K:GLN:C | 10 | 5.82 | 1.72 | 5.58 |
| (1,1014) | 1:238:L:VAL:C | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 10 | 5.8 | 1.09 | 5.62 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 10 | 5.44 | 1.04 | 5.24 |
| (1,120) | 1:158:L:LYS:N | 1:158:L:LYS:CA | 1:158:L:LYS:C | 1:159:L:GLU:N | 10 | 5.43 | 1.8 | 5.67 |
| (1,1023) | 1:239:I:THR:C | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 10 | 5.42 | 1.53 | 5.35 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 10 | 5.37 | 1.3 | 5.24 |
| (1,1111) | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1:243:G:THR:N | 10 | 5.35 | 0.77 | 5.36 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 10 | 5.33 | 1.36 | 4.94 |
| (1,1020) | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 1:240:L:ASN:N | 10 | 5.14 | 1.24 | 5.72 |
| (1,59) | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 1:152:K:ASP:N | 10 | 5.09 | 1.66 | 5.03 |
| (1,674) | 1:209:H:ALA:C | 1:210:H:THR:N | 1:210:H:THR:CA | 1:210:H:THR:C | 10 | 5.08 | 1.42 | 5.38 |
| (1,1029) | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 1:241:I:THR:N | 10 | 4.95 | 1.34 | 4.73 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 10 | 4.89 | 1.8 | 4.63 |
| (1,1027) | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1:241:G:THR:N | 10 | 4.81 | 1.32 | 4.38 |
| (1,380) | 1:182:H:LYS:N | 1:182:H:LYS:CA | 1:182:H:LYS:C | 1:183:H:ASN:N | 10 | 4.77 | 2.19 | 3.99 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 10 | 4.45 | 0.57 | 4.42 |
| (1,1022) | 1:239:H:THR:C | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 10 | 4.44 | 0.82 | 4.24 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|----------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,1028) | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 1:241:H:THR:N | 10 | 4.33 | 1.34 | 4.63 |
| (1,1009) | 1:238:G:VAL:C | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 10 | 4.27 | 2.09 | 3.62 |
| (1,434) | 1:186:H:THR:C | 1:187:H:GLU:N | 1:187:H:GLU:CA | 1:187:H:GLU:C | 10 | 4.25 | 2.42 | 3.46 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 10 | 4.19 | 1.2 | 4.17 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 10 | 4.13 | 1.4 | 3.92 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 10 | 3.95 | 1.14 | 3.87 |
| (1,1010) | 1:238:H:VAL:C | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 10 | 3.95 | 0.67 | 3.76 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 10 | 3.85 | 1.4 | 4.14 |
| (1,1018) | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 1:240:J:ASN:N | 10 | 3.71 | 1.75 | 4.27 |
| (1,889) | 1:228:G:ALA:C | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 10 | 3.69 | 0.82 | 3.87 |
| (1,1044) | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1:242:L:ALA:N | 10 | 3.2 | 1.21 | 3.35 |
| (1,60) | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 1:152:L:ASP:N | 10 | 3.09 | 1.99 | 3.05 |
| (1,1013) | 1:238:K:VAL:C | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 10 | 3.08 | 0.56 | 3.0 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 10 | 2.92 | 1.33 | 2.8 |
| (1,451) | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 1:189:G:LEU:N | 10 | 2.91 | 0.89 | 2.84 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 10 | 2.83 | 0.96 | 2.94 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 10 | 2.67 | 1.33 | 2.7 |
| (1,37) | 1:148:G:THR:C | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 10 | 2.54 | 1.14 | 2.42 |
| (1,973) | 1:235:G:MET:C | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 10 | 2.35 | 0.85 | 2.28 |
| (1,1016) | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 1:240:H:ASN:N | 10 | 2.33 | 0.71 | 2.16 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 10 | 2.31 | 0.99 | 2.5 |
| (1,1015) | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 1:240:G:ASN:N | 10 | 2.23 | 0.73 | 2.2 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 10 | 2.23 | 0.46 | 2.19 |
| (1,65) | 1:152:K:ASP:N | 1:152:K:ASP:CA | 1:152:K:ASP:C | 1:153:K:ILE:N | 9 | 13.59 | 7.57 | 15.65 |
| (1,891) | 1:228:I:ALA:C | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 9 | 9.73 | 1.43 | 10.12 |
| (1,30) | 1:147:L:PRO:N | 1:147:L:PRO:CA | 1:147:L:PRO:C | 1:148:L:THR:N | 9 | 9.28 | 3.47 | 10.55 |
| (1,36) | 1:147:L:PRO:C | 1:148:L:THR:N | 1:148:L:THR:CA | 1:148:L:THR:C | 9 | 8.27 | 3.56 | 8.53 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 9 | 8.25 | 3.43 | 9.87 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 9 | 8.12 | 2.57 | 8.73 |
| (1,483) | 1:190:I:LEU:C | 1:191:I:VAL:N | 1:191:I:VAL:CA | 1:191:I:VAL:C | 9 | 6.59 | 2.61 | 5.89 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 9 | 6.52 | 3.21 | 7.43 |
| (1,309) | 1:174:I:ALA:N | 1:174:I:ALA:CA | 1:174:I:ALA:C | 1:175:I:GLU:N | 9 | 6.08 | 2.4 | 6.77 |
| (1,33) | 1:147:I:PRO:C | 1:148:I:THR:N | 1:148:I:THR:CA | 1:148:I:THR:C | 9 | 5.57 | 1.25 | 5.47 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 9 | 5.4 | 2.1 | 5.41 |
| (1,798) | 1:219:L:GLN:C | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 9 | 5.37 | 1.86 | 5.38 |
| (1,1104) | 1:207:L:PRO:N | 1:207:L:PRO:CA | 1:207:L:PRO:C | 1:208:L:GLY:N | 9 | 4.76 | 0.38 | 4.79 |
| (1,320) | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 1:178:H:SER:N | 9 | 4.71 | 1.47 | 4.4 |
| (1,26) | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 1:148:H:THR:N | 9 | 4.0 | 2.01 | 3.34 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 9 | 3.72 | 3.29 | 2.18 |
| (1,426) | 1:185:L:MET:C | 1:186:L:THR:N | 1:186:L:THR:CA | 1:186:L:THR:C | 9 | 3.58 | 1.89 | 3.27 |
| (1,998) | 1:237:H:GLN:C | 1:238:H:VAL:N | 1:238:H:VAL:CA | 1:238:H:VAL:C | 9 | 3.44 | 1.5 | 3.86 |
| (1,1011) | 1:238:I:VAL:C | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 9 | 3.26 | 1.1 | 3.11 |
| (1,449) | 1:187:K:GLU:C | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 9 | 3.18 | 1.55 | 3.29 |
| (1,305) | 1:173:K:ARG:C | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 9 | 3.03 | 1.38 | 2.61 |
| (1,1103) | 1:207:K:PRO:N | 1:207:K:PRO:CA | 1:207:K:PRO:C | 1:208:K:GLY:N | 9 | 3.02 | 0.33 | 2.99 |
| (1,1019) | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 1:240:K:ASN:N | 9 | 2.65 | 0.85 | 2.7 |
| (1,1037) | 1:240:K:ASN:C | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 9 | 2.6 | 1.26 | 1.97 |
| (1,894) | 1:228:L:ALA:C | 1:229:L:ARG:N | 1:229:L:ARG:CA | 1:229:L:ARG:C | 9 | 2.47 | 1.13 | 1.79 |
| (1,1012) | 1:238:J:VAL:C | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 9 | 2.38 | 1.14 | 2.04 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 9 | 2.35 | 0.97 | 2.2 |
| (1,85) | 1:154:G:ARG:C | 1:155:G:GLN:N | 1:155:G:GLN:CA | 1:155:G:GLN:C | 9 | 2.0 | 0.52 | 1.76 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|----------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,66) | 1:152:L:ASP:N | 1:152:L:ASP:CA | 1:152:L:ASP:C | 1:153:L:ILE:N | 8 | 8.68 | 4.4 | 10.07 |
| (1,858) | 1:225:L:GLY:C | 1:226:L:HIS:N | 1:226:L:HIS:CA | 1:226:L:HIS:C | 8 | 7.75 | 0.78 | 8.22 |
| (1,893) | 1:228:K:ALA:C | 1:229:K:ARG:N | 1:229:K:ARG:CA | 1:229:K:ARG:C | 8 | 7.08 | 1.78 | 7.26 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 8 | 6.16 | 3.29 | 5.24 |
| (1,62) | 1:152:H:ASP:N | 1:152:H:ASP:CA | 1:152:H:ASP:C | 1:153:H:ILE:N | 8 | 5.62 | 2.14 | 5.78 |
| (1,815) | 1:221:K:VAL:N | 1:221:K:VAL:CA | 1:221:K:VAL:C | 1:222:K:GLY:N | 8 | 5.03 | 1.32 | 5.14 |
| (1,32) | 1:147:H:PRO:C | 1:148:H:THR:N | 1:148:H:THR:CA | 1:148:H:THR:C | 8 | 4.63 | 2.49 | 4.62 |
| (1,57) | 1:151:I:LEU:N | 1:151:I:LEU:CA | 1:151:I:LEU:C | 1:152:I:ASP:N | 8 | 4.54 | 2.23 | 4.54 |
| (1,70) | 1:153:J:ILE:N | 1:153:J:ILE:CA | 1:153:J:ILE:C | 1:154:J:ARG:N | 8 | 4.47 | 1.36 | 4.92 |
| (1,813) | 1:221:I:VAL:N | 1:221:I:VAL:CA | 1:221:I:VAL:C | 1:222:I:GLY:N | 8 | 4.04 | 2.8 | 2.44 |
| (1,675) | 1:209:I:ALA:C | 1:210:I:THR:N | 1:210:I:THR:CA | 1:210:I:THR:C | 8 | 3.85 | 0.81 | 3.74 |
| (1,1002) | 1:237:L:GLN:C | 1:238:L:VAL:N | 1:238:L:VAL:CA | 1:238:L:VAL:C | 8 | 3.72 | 0.82 | 4.11 |
| (1,669) | 1:209:I:ALA:N | 1:209:I:ALA:CA | 1:209:I:ALA:C | 1:210:I:THR:N | 8 | 3.47 | 1.33 | 3.32 |
| (1,1017) | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 1:240:I:ASN:N | 8 | 3.22 | 0.89 | 3.36 |
| (1,307) | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 1:175:G:GLU:N | 8 | 3.04 | 1.7 | 2.78 |
| (1,895) | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 1:230:G:VAL:N | 8 | 2.97 | 1.27 | 3.46 |
| (1,1038) | 1:240:L:ASN:C | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 8 | 2.89 | 1.11 | 2.78 |
| (1,444) | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 1:188:L:THR:N | 8 | 2.56 | 1.08 | 2.37 |
| (1,175) | 1:163:G:ASP:N | 1:163:G:ASP:CA | 1:163:G:ASP:C | 1:164:G:TYR:N | 8 | 2.23 | 0.89 | 2.14 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 8 | 2.19 | 0.46 | 2.48 |
| (1,1034) | 1:240:H:ASN:C | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 8 | 1.85 | 0.66 | 1.62 |
| (1,500) | 1:192:H:GLN:N | 1:192:H:GLN:CA | 1:192:H:GLN:C | 1:193:H:ASN:N | 7 | 11.75 | 3.62 | 11.25 |
| (1,47) | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 1:150:K:ILE:N | 7 | 8.12 | 4.22 | 7.28 |
| (1,310) | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 1:175:J:GLU:N | 7 | 7.11 | 2.07 | 6.32 |
| (1,317) | 1:176:K:GLN:C | 1:177:K:ALA:N | 1:177:K:ALA:CA | 1:177:K:ALA:C | 7 | 7.06 | 0.76 | 7.37 |
| (1,676) | 1:209:J:ALA:C | 1:210:J:THR:N | 1:210:J:THR:CA | 1:210:J:THR:C | 7 | 6.53 | 2.22 | 7.38 |
| (1,501) | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 1:193:I:ASN:N | 7 | 6.48 | 2.17 | 6.09 |
| (1,796) | 1:219:J:GLN:C | 1:220:J:GLY:N | 1:220:J:GLY:CA | 1:220:J:GLY:C | 7 | 4.77 | 1.8 | 5.21 |
| (1,800) | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1:221:H:VAL:N | 7 | 4.59 | 1.42 | 4.52 |
| (1,316) | 1:176:J:GLN:C | 1:177:J:ALA:N | 1:177:J:ALA:CA | 1:177:J:ALA:C | 7 | 4.5 | 1.87 | 4.66 |
| (1,447) | 1:187:I:GLU:C | 1:188:I:THR:N | 1:188:I:THR:CA | 1:188:I:THR:C | 7 | 4.28 | 2.54 | 2.76 |
| (1,803) | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 1:221:K:VAL:N | 7 | 4.22 | 2.74 | 2.88 |
| (1,441) | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 1:188:I:THR:N | 7 | 4.16 | 1.71 | 4.2 |
| (1,634) | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 1:205:J:LEU:N | 7 | 3.05 | 1.07 | 2.86 |
| (1,896) | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 1:230:H:VAL:N | 7 | 3.04 | 1.19 | 2.83 |
| (1,54) | 1:150:L:ILE:C | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 6 | 18.31 | 4.82 | 16.81 |
| (1,63) | 1:152:I:ASP:N | 1:152:I:ASP:CA | 1:152:I:ASP:C | 1:153:I:ILE:N | 6 | 11.65 | 5.76 | 14.98 |
| (1,53) | 1:150:K:ILE:C | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 6 | 10.68 | 5.16 | 9.6 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 6 | 5.94 | 1.46 | 6.04 |
| (1,652) | 1:207:J:PRO:C | 1:208:J:GLY:N | 1:208:J:GLY:CA | 1:208:J:GLY:C | 6 | 4.8 | 3.37 | 4.69 |
| (1,827) | 1:223:K:GLY:N | 1:223:K:GLY:CA | 1:223:K:GLY:C | 1:224:K:PRO:N | 6 | 4.75 | 1.95 | 4.63 |
| (1,911) | 1:230:K:VAL:N | 1:230:K:VAL:CA | 1:230:K:VAL:C | 1:231:K:LEU:N | 6 | 4.66 | 2.18 | 4.74 |
| (1,677) | 1:209:K:ALA:C | 1:210:K:THR:N | 1:210:K:THR:CA | 1:210:K:THR:C | 6 | 4.41 | 1.48 | 4.81 |
| (1,90) | 1:154:L:ARG:C | 1:155:L:GLN:N | 1:155:L:GLN:CA | 1:155:L:GLN:C | 6 | 4.33 | 2.77 | 3.86 |
| (1,314) | 1:176:H:GLN:C | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 6 | 4.33 | 2.16 | 3.53 |
| (1,410) | 1:184:H:TRP:C | 1:185:H:MET:N | 1:185:H:MET:CA | 1:185:H:MET:C | 6 | 4.16 | 2.69 | 3.76 |
| (1,1077) | 1:175:I:GLU:N | 1:175:I:GLU:CA | 1:175:I:GLU:C | 1:176:I:GLN:N | 6 | 3.97 | 0.89 | 3.72 |
| (1,764) | 1:217:H:ALA:N | 1:217:H:ALA:CA | 1:217:H:ALA:C | 1:218:H:CYS:N | 6 | 3.67 | 1.67 | 3.08 |
| (1,42) | 1:148:L:THR:C | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 6 | 3.46 | 1.38 | 3.22 |
| (1,88) | 1:154:J:ARG:C | 1:155:J:GLN:N | 1:155:J:GLN:CA | 1:155:J:GLN:C | 6 | 3.42 | 1.52 | 3.24 |
| (1,229) | 1:167:G:ARG:C | 1:168:G:PHE:N | 1:168:G:PHE:CA | 1:168:G:PHE:C | 6 | 3.31 | 0.8 | 3.11 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|----------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,442) | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 1:188:J:THR:N | 6 | 3.14 | 1.59 | 2.94 |
| (1,540) | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 1:197:L:ASP:N | 6 | 3.08 | 0.76 | 3.26 |
| (1,1041) | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 1:242:I:ALA:N | 6 | 3.05 | 0.51 | 3.14 |
| (1,274) | 1:171:J:THR:N | 1:171:J:THR:CA | 1:171:J:THR:C | 1:172:J:LEU:N | 6 | 2.84 | 1.09 | 2.46 |
| (1,1073) | 1:174:K:ALA:C | 1:175:K:GLU:N | 1:175:K:GLU:CA | 1:175:K:GLU:C | 6 | 2.74 | 1.01 | 2.68 |
| (1,104) | 1:157:H:PRO:N | 1:157:H:PRO:CA | 1:157:H:PRO:C | 1:158:H:LYS:N | 6 | 2.73 | 1.76 | 2.22 |
| (1,326) | 1:177:H:ALA:C | 1:178:H:SER:N | 1:178:H:SER:CA | 1:178:H:SER:C | 6 | 2.58 | 1.56 | 1.76 |
| (1,728) | 1:214:H:MET:N | 1:214:H:MET:CA | 1:214:H:MET:C | 1:215:H:MET:N | 6 | 2.42 | 0.97 | 2.12 |
| (1,1035) | 1:240:I:ASN:C | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 6 | 2.38 | 0.98 | 1.9 |
| (1,988) | 1:236:J:SER:C | 1:237:J:GLN:N | 1:237:J:GLN:CA | 1:237:J:GLN:C | 6 | 1.76 | 0.61 | 1.64 |
| (1,1054) | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 1:244:J:ILE:N | 6 | 1.24 | 0.11 | 1.28 |
| (1,51) | 1:150:I:ILE:C | 1:151:I:LEU:N | 1:151:I:LEU:CA | 1:151:I:LEU:C | 5 | 17.46 | 5.51 | 15.91 |
| (1,515) | 1:193:K:ASN:N | 1:193:K:ASN:CA | 1:193:K:ASN:C | 1:194:K:ALA:N | 5 | 8.9 | 7.72 | 7.2 |
| (1,897) | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 1:230:I:VAL:N | 5 | 5.3 | 1.4 | 5.26 |
| (1,868) | 1:226:J:HIS:C | 1:227:J:LYS:N | 1:227:J:LYS:CA | 1:227:J:LYS:C | 5 | 4.78 | 3.43 | 3.21 |
| (1,178) | 1:163:J:ASP:N | 1:163:J:ASP:CA | 1:163:J:ASP:C | 1:164:J:TYR:N | 5 | 3.59 | 0.39 | 3.73 |
| (1,87) | 1:154:I:ARG:C | 1:155:I:GLN:N | 1:155:I:GLN:CA | 1:155:I:GLN:C | 5 | 3.4 | 0.88 | 3.13 |
| (1,68) | 1:153:H:ILE:N | 1:153:H:ILE:CA | 1:153:H:ILE:C | 1:154:H:ARG:N | 5 | 3.4 | 2.14 | 2.5 |
| (1,243) | 1:168:I:PHE:C | 1:169:I:TYR:N | 1:169:I:TYR:CA | 1:169:I:TYR:C | 5 | 2.98 | 0.91 | 2.79 |
| (1,849) | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 1:226:I:HIS:N | 5 | 2.93 | 1.11 | 2.84 |
| (1,118) | 1:158:J:LYS:N | 1:158:J:LYS:CA | 1:158:J:LYS:C | 1:159:J:GLU:N | 5 | 2.93 | 0.81 | 2.63 |
| (1,107) | 1:157:K:PRO:N | 1:157:K:PRO:CA | 1:157:K:PRO:C | 1:158:K:LYS:N | 5 | 2.86 | 1.16 | 2.7 |
| (1,921) | 1:231:I:LEU:N | 1:231:I:LEU:CA | 1:231:I:LEU:C | 1:232:I:ALA:N | 5 | 2.82 | 1.18 | 2.79 |
| (1,1033) | 1:240:G:ASN:C | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 5 | 2.78 | 0.93 | 3.25 |
| (1,1036) | 1:240:J:ASN:C | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 5 | 2.69 | 1.21 | 3.05 |
| (1,396) | 1:183:L:ASN:N | 1:183:L:ASN:CA | 1:183:L:ASN:C | 1:184:L:TRP:N | 5 | 2.5 | 1.25 | 2.32 |
| (1,155) | 1:161:K:PHE:N | 1:161:K:PHE:CA | 1:161:K:PHE:C | 1:162:K:ARG:N | 5 | 2.49 | 1.13 | 2.12 |
| (1,230) | 1:167:H:ARG:C | 1:168:H:PHE:N | 1:168:H:PHE:CA | 1:168:H:PHE:C | 5 | 2.25 | 0.64 | 1.89 |
| (1,716) | 1:213:H:GLU:N | 1:213:H:GLU:CA | 1:213:H:GLU:C | 1:214:H:MET:N | 5 | 2.15 | 0.92 | 2.15 |
| (1,174) | 1:162:L:ARG:C | 1:163:L:ASP:N | 1:163:L:ASP:CA | 1:163:L:ASP:C | 5 | 2.1 | 0.37 | 2.24 |
| (1,626) | 1:203:H:LYS:C | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 5 | 1.87 | 0.5 | 1.91 |
| (1,758) | 1:216:H:THR:C | 1:217:H:ALA:N | 1:217:H:ALA:CA | 1:217:H:ALA:C | 5 | 1.87 | 0.73 | 1.52 |
| (1,433) | 1:186:G:THR:C | 1:187:G:GLU:N | 1:187:G:GLU:CA | 1:187:G:GLU:C | 5 | 1.78 | 0.45 | 1.81 |
| (1,40) | 1:148:J:THR:C | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 4 | 13.18 | 4.42 | 13.71 |
| (1,140) | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 1:161:H:PHE:N | 4 | 7.43 | 1.16 | 7.87 |
| (1,424) | 1:185:J:MET:C | 1:186:J:THR:N | 1:186:J:THR:CA | 1:186:J:THR:C | 4 | 6.88 | 3.81 | 5.63 |
| (1,912) | 1:230:L:VAL:N | 1:230:L:VAL:CA | 1:230:L:VAL:C | 1:231:L:LEU:N | 4 | 5.86 | 0.72 | 5.57 |
| (1,903) | 1:229:I:ARG:C | 1:230:I:VAL:N | 1:230:I:VAL:CA | 1:230:I:VAL:C | 4 | 4.71 | 1.25 | 4.41 |
| (1,34) | 1:147:J:PRO:C | 1:148:J:THR:N | 1:148:J:THR:CA | 1:148:J:THR:C | 4 | 4.38 | 1.6 | 4.59 |
| (1,767) | 1:217:K:ALA:N | 1:217:K:ALA:CA | 1:217:K:ALA:C | 1:218:K:CYS:N | 4 | 4.1 | 1.85 | 4.23 |
| (1,759) | 1:216:I:THR:C | 1:217:I:ALA:N | 1:217:I:ALA:CA | 1:217:I:ALA:C | 4 | 3.7 | 1.8 | 2.78 |
| (1,519) | 1:194:I:ALA:C | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 4 | 3.54 | 2.69 | 2.64 |
| (1,974) | 1:235:H:MET:C | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 4 | 3.09 | 1.38 | 3.23 |
| (1,381) | 1:182:I:LYS:N | 1:182:I:LYS:CA | 1:182:I:LYS:C | 1:183:I:ASN:N | 4 | 2.99 | 0.5 | 3.24 |
| (1,947) | 1:233:K:GLU:N | 1:233:K:GLU:CA | 1:233:K:GLU:C | 1:234:K:ALA:N | 4 | 2.88 | 1.39 | 2.48 |
| (1,975) | 1:235:I:MET:C | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 4 | 2.86 | 1.97 | 1.92 |
| (1,416) | 1:185:H:MET:N | 1:185:H:MET:CA | 1:185:H:MET:C | 1:186:H:THR:N | 4 | 2.73 | 0.78 | 2.99 |
| (1,518) | 1:194:H:ALA:C | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 4 | 2.69 | 1.37 | 2.68 |
| (1,1080) | 1:175:L:GLU:N | 1:175:L:GLU:CA | 1:175:L:GLU:C | 1:176:L:GLN:N | 4 | 2.58 | 1.24 | 2.09 |
| (1,802) | 1:220:J:GLY:N | 1:220:J:GLY:CA | 1:220:J:GLY:C | 1:221:J:VAL:N | 4 | 2.51 | 0.65 | 2.62 |
| (1,692) | 1:211:H:LEU:N | 1:211:H:LEU:CA | 1:211:H:LEU:C | 1:212:H:GLU:N | 4 | 1.98 | 0.93 | 1.66 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|----------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,435) | 1:186:I:THR:C | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 4 | 1.94 | 0.38 | 1.99 |
| (1,828) | 1:223:L:GLY:N | 1:223:L:GLY:CA | 1:223:L:GLY:C | 1:224:L:PRO:N | 4 | 1.83 | 0.65 | 1.73 |
| (1,308) | 1:174:H:ALA:N | 1:174:H:ALA:CA | 1:174:H:ALA:C | 1:175:H:GLU:N | 4 | 1.64 | 0.5 | 1.52 |
| (1,156) | 1:161:L:PHE:N | 1:161:L:PHE:CA | 1:161:L:PHE:C | 1:162:L:ARG:N | 4 | 1.59 | 0.37 | 1.66 |
| (1,237) | 1:168:I:PHE:N | 1:168:I:PHE:CA | 1:168:I:PHE:C | 1:169:I:TYR:N | 4 | 1.39 | 0.32 | 1.33 |
| (1,856) | 1:225:J:GLY:C | 1:226:J:HIS:N | 1:226:J:HIS:CA | 1:226:J:HIS:C | 3 | 15.24 | 1.44 | 16.07 |
| (1,477) | 1:190:I:LEU:N | 1:190:I:LEU:CA | 1:190:I:LEU:C | 1:191:I:VAL:N | 3 | 7.71 | 4.81 | 8.31 |
| (1,808) | 1:220:J:GLY:C | 1:221:J:VAL:N | 1:221:J:VAL:CA | 1:221:J:VAL:C | 3 | 7.53 | 2.48 | 7.21 |
| (1,990) | 1:236:L:SER:C | 1:237:L:GLN:N | 1:237:L:GLN:CA | 1:237:L:GLN:C | 3 | 6.57 | 3.8 | 7.94 |
| (1,645) | 1:205:I:LEU:N | 1:205:I:LEU:CA | 1:205:I:LEU:C | 1:206:I:GLY:N | 3 | 5.96 | 2.8 | 7.13 |
| (1,86) | 1:154:H:ARG:C | 1:155:H:GLN:N | 1:155:H:GLN:CA | 1:155:H:GLN:C | 3 | 5.93 | 0.4 | 5.66 |
| (1,522) | 1:194:L:ALA:C | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 3 | 5.22 | 3.04 | 4.49 |
| (1,508) | 1:192:J:GLN:C | 1:193:J:ASN:N | 1:193:J:ASN:CA | 1:193:J:ASN:C | 3 | 4.97 | 2.41 | 5.9 |
| (1,556) | 1:197:J:ASP:C | 1:198:J:CYS:N | 1:198:J:CYS:CA | 1:198:J:CYS:C | 3 | 4.86 | 0.63 | 4.65 |
| (1,225) | 1:167:I:ARG:N | 1:167:I:ARG:CA | 1:167:I:ARG:C | 1:168:I:PHE:N | 3 | 4.81 | 0.82 | 4.91 |
| (1,484) | 1:190:J:LEU:C | 1:191:J:VAL:N | 1:191:J:VAL:CA | 1:191:J:VAL:C | 3 | 4.62 | 2.69 | 2.86 |
| (1,839) | 1:224:K:PRO:N | 1:224:K:PRO:CA | 1:224:K:PRO:C | 1:225:K:GLY:N | 3 | 4.58 | 2.41 | 5.94 |
| (1,29) | 1:147:K:PRO:N | 1:147:K:PRO:CA | 1:147:K:PRO:C | 1:148:K:THR:N | 3 | 4.07 | 2.18 | 3.74 |
| (1,436) | 1:186:J:THR:C | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 3 | 3.96 | 1.08 | 3.26 |
| (1,580) | 1:199:J:LYS:C | 1:200:J:THR:N | 1:200:J:THR:CA | 1:200:J:THR:C | 3 | 3.94 | 1.84 | 2.91 |
| (1,269) | 1:170:K:LYS:C | 1:171:K:THR:N | 1:171:K:THR:CA | 1:171:K:THR:C | 3 | 3.9 | 0.86 | 3.52 |
| (1,119) | 1:158:K:LYS:N | 1:158:K:LYS:CA | 1:158:K:LYS:C | 1:159:K:GLU:N | 3 | 3.82 | 0.76 | 3.89 |
| (1,825) | 1:223:I:GLY:N | 1:223:I:GLY:CA | 1:223:I:GLY:C | 1:224:I:PRO:N | 3 | 3.77 | 2.46 | 2.21 |
| (1,231) | 1:167:I:ARG:C | 1:168:I:PHE:N | 1:168:I:PHE:CA | 1:168:I:PHE:C | 3 | 3.67 | 1.45 | 3.94 |
| (1,978) | 1:235:L:MET:C | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 3 | 3.65 | 1.8 | 3.61 |
| (1,1079) | 1:175:K:GLU:N | 1:175:K:GLU:CA | 1:175:K:GLU:C | 1:176:K:GLN:N | 3 | 3.58 | 0.48 | 3.37 |
| (1,814) | 1:221:J:VAL:N | 1:221:J:VAL:CA | 1:221:J:VAL:C | 1:222:J:GLY:N | 3 | 3.41 | 0.43 | 3.5 |
| (1,640) | 1:204:J:ALA:C | 1:205:J:LEU:N | 1:205:J:LEU:CA | 1:205:J:LEU:C | 3 | 3.25 | 0.51 | 3.12 |
| (1,404) | 1:184:H:TRP:N | 1:184:H:TRP:CA | 1:184:H:TRP:C | 1:185:H:MET:N | 3 | 3.14 | 1.87 | 2.38 |
| (1,906) | 1:229:L:ARG:C | 1:230:L:VAL:N | 1:230:L:VAL:CA | 1:230:L:VAL:C | 3 | 3.14 | 0.47 | 3.45 |
| (1,495) | 1:191:I:VAL:C | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 3 | 3.0 | 0.6 | 2.72 |
| (1,820) | 1:222:J:GLY:N | 1:222:J:GLY:CA | 1:222:J:GLY:C | 1:223:J:GLY:N | 3 | 2.99 | 0.56 | 3.32 |
| (1,823) | 1:223:G:GLY:N | 1:223:G:GLY:CA | 1:223:G:GLY:C | 1:224:G:PRO:N | 3 | 2.6 | 1.0 | 2.96 |
| (1,384) | 1:182:L:LYS:N | 1:182:L:LYS:CA | 1:182:L:LYS:C | 1:183:L:ASN:N | 3 | 2.53 | 1.1 | 2.49 |
| (1,492) | 1:191:L:VAL:N | 1:191:L:VAL:CA | 1:191:L:VAL:C | 1:192:L:GLN:N | 3 | 2.51 | 1.09 | 2.22 |
| (1,476) | 1:190:H:LEU:N | 1:190:H:LEU:CA | 1:190:H:LEU:C | 1:191:H:VAL:N | 3 | 2.46 | 1.52 | 1.51 |
| (1,72) | 1:153:L:ILE:N | 1:153:L:ILE:CA | 1:153:L:ILE:C | 1:154:L:ARG:N | 3 | 2.42 | 1.1 | 1.81 |
| (1,242) | 1:168:H:PHE:C | 1:169:H:TYR:N | 1:169:H:TYR:CA | 1:169:H:TYR:C | 3 | 2.22 | 0.56 | 2.38 |
| (1,71) | 1:153:K:ILE:N | 1:153:K:ILE:CA | 1:153:K:ILE:C | 1:154:K:ARG:N | 3 | 2.18 | 0.66 | 1.72 |
| (1,907) | 1:230:G:VAL:N | 1:230:G:VAL:CA | 1:230:G:VAL:C | 1:231:G:LEU:N | 3 | 2.17 | 1.42 | 1.23 |
| (1,284) | 1:172:H:LEU:N | 1:172:H:LEU:CA | 1:172:H:LEU:C | 1:173:H:ARG:N | 3 | 2.11 | 0.24 | 2.17 |
| (1,693) | 1:211:I:LEU:N | 1:211:I:LEU:CA | 1:211:I:LEU:C | 1:212:I:GLU:N | 3 | 2.07 | 0.51 | 1.72 |
| (1,636) | 1:204:L:ALA:N | 1:204:L:ALA:CA | 1:204:L:ALA:C | 1:205:L:LEU:N | 3 | 2.06 | 1.05 | 1.49 |
| (1,182) | 1:163:H:ASP:C | 1:164:H:TYR:N | 1:164:H:TYR:CA | 1:164:H:TYR:C | 3 | 1.99 | 0.7 | 1.92 |
| (1,658) | 1:208:J:GLY:N | 1:208:J:GLY:CA | 1:208:J:GLY:C | 1:209:J:ALA:N | 3 | 1.99 | 0.68 | 1.55 |
| (1,20) | 1:146:H:SER:C | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 3 | 1.91 | 0.14 | 1.98 |
| (1,172) | 1:162:J:ARG:C | 1:163:J:ASP:N | 1:163:J:ASP:CA | 1:163:J:ASP:C | 3 | 1.85 | 0.52 | 2.02 |
| (1,455) | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 1:189:K:LEU:N | 3 | 1.73 | 0.27 | 1.6 |
| (1,536) | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 1:197:H:ASP:N | 3 | 1.6 | 0.32 | 1.53 |
| (1,1094) | 1:206:H:GLY:C | 1:207:H:PRO:N | 1:207:H:PRO:CA | 1:207:H:PRO:C | 3 | 1.48 | 0.6 | 1.09 |
| (1,318) | 1:176:L:GLN:C | 1:177:L:ALA:N | 1:177:L:ALA:CA | 1:177:L:ALA:C | 3 | 1.43 | 0.08 | 1.45 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|----------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,52) | 1:150:J:ILE:C | 1:151:J:LEU:N | 1:151:J:LEU:CA | 1:151:J:LEU:C | 3 | 1.09 | 0.08 | 1.06 |
| (1,50) | 1:150:H:ILE:C | 1:151:H:LEU:N | 1:151:H:LEU:CA | 1:151:H:LEU:C | 2 | 17.82 | 3.6 | 17.82 |
| (1,795) | 1:219:I:GLN:C | 1:220:I:GLY:N | 1:220:I:GLY:CA | 1:220:I:GLY:C | 2 | 5.8 | 2.11 | 5.8 |
| (1,516) | 1:193:L:ASN:N | 1:193:L:ASN:CA | 1:193:L:ASN:C | 1:194:L:ALA:N | 2 | 5.65 | 0.96 | 5.65 |
| (1,513) | 1:193:I:ASN:N | 1:193:I:ASN:CA | 1:193:I:ASN:C | 1:194:I:ALA:N | 2 | 5.62 | 1.76 | 5.62 |
| (1,615) | 1:202:I:LEU:C | 1:203:I:LYS:N | 1:203:I:LYS:CA | 1:203:I:LYS:C | 2 | 5.0 | 0.58 | 5.0 |
| (1,843) | 1:224:I:PRO:C | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 2 | 4.98 | 2.4 | 4.98 |
| (1,538) | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 1:197:J:ASP:N | 2 | 4.78 | 0.46 | 4.78 |
| (1,488) | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 1:192:H:GLN:N | 2 | 4.5 | 1.76 | 4.5 |
| (1,857) | 1:225:K:GLY:C | 1:226:K:HIS:N | 1:226:K:HIS:CA | 1:226:K:HIS:C | 2 | 4.38 | 1.31 | 4.38 |
| (1,900) | 1:229:L:ARG:N | 1:229:L:ARG:CA | 1:229:L:ARG:C | 1:230:L:VAL:N | 2 | 3.99 | 0.46 | 3.99 |
| (1,845) | 1:224:K:PRO:C | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 2 | 3.94 | 2.74 | 3.94 |
| (1,832) | 1:223:J:GLY:C | 1:224:J:PRO:N | 1:224:J:PRO:CA | 1:224:J:PRO:C | 2 | 3.79 | 0.66 | 3.79 |
| (1,873) | 1:227:I:LYS:N | 1:227:I:LYS:CA | 1:227:I:LYS:C | 1:228:I:ALA:N | 2 | 3.79 | 2.3 | 3.79 |
| (1,694) | 1:211:J:LEU:N | 1:211:J:LEU:CA | 1:211:J:LEU:C | 1:212:J:GLU:N | 2 | 3.78 | 2.68 | 3.78 |
| (1,851) | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 1:226:K:HIS:N | 2 | 3.77 | 1.74 | 3.77 |
| (1,494) | 1:191:H:VAL:C | 1:192:H:GLN:N | 1:192:H:GLN:CA | 1:192:H:GLN:C | 2 | 3.62 | 0.67 | 3.62 |
| (1,56) | 1:151:H:LEU:N | 1:151:H:LEU:CA | 1:151:H:LEU:C | 1:152:H:ASP:N | 2 | 3.46 | 1.74 | 3.46 |
| (1,741) | 1:215:I:MET:N | 1:215:I:MET:CA | 1:215:I:MET:C | 1:216:I:THR:N | 2 | 3.41 | 0.04 | 3.41 |
| (1,232) | 1:167:J:ARG:C | 1:168:J:PHE:N | 1:168:J:PHE:CA | 1:168:J:PHE:C | 2 | 3.4 | 0.64 | 3.4 |
| (1,437) | 1:186:K:THR:C | 1:187:K:GLU:N | 1:187:K:GLU:CA | 1:187:K:GLU:C | 2 | 3.33 | 1.08 | 3.33 |
| (1,188) | 1:164:H:TYR:N | 1:164:H:TYR:CA | 1:164:H:TYR:C | 1:165:H:VAL:N | 2 | 3.22 | 1.54 | 3.22 |
| (1,499) | 1:192:G:GLN:N | 1:192:G:GLN:CA | 1:192:G:GLN:C | 1:193:G:ASN:N | 2 | 3.19 | 2.01 | 3.19 |
| (1,608) | 1:202:H:LEU:N | 1:202:H:LEU:CA | 1:202:H:LEU:C | 1:203:H:LYS:N | 2 | 3.18 | 1.63 | 3.18 |
| (1,830) | 1:223:H:GLY:C | 1:224:H:PRO:N | 1:224:H:PRO:CA | 1:224:H:PRO:C | 2 | 3.07 | 0.69 | 3.07 |
| (1,58) | 1:151:J:LEU:N | 1:151:J:LEU:CA | 1:151:J:LEU:C | 1:152:J:ASP:N | 2 | 2.97 | 1.58 | 2.97 |
| (1,1101) | 1:207:I:PRO:N | 1:207:I:PRO:CA | 1:207:I:PRO:C | 1:208:I:GLY:N | 2 | 2.94 | 0.01 | 2.94 |
| (1,1072) | 1:174:J:ALA:C | 1:175:J:GLU:N | 1:175:J:GLU:CA | 1:175:J:GLU:C | 2 | 2.84 | 0.38 | 2.84 |
| (1,136) | 1:159:J:GLU:C | 1:160:J:PRO:N | 1:160:J:PRO:CA | 1:160:J:PRO:C | 2 | 2.74 | 1.38 | 2.74 |
| (1,673) | 1:209:G:ALA:C | 1:210:G:THR:N | 1:210:G:THR:CA | 1:210:G:THR:C | 2 | 2.72 | 0.86 | 2.72 |
| (1,327) | 1:177:I:ALA:C | 1:178:I:SER:N | 1:178:I:SER:CA | 1:178:I:SER:C | 2 | 2.68 | 0.13 | 2.68 |
| (1,831) | 1:223:I:GLY:C | 1:224:I:PRO:N | 1:224:I:PRO:CA | 1:224:I:PRO:C | 2 | 2.64 | 0.92 | 2.64 |
| (1,512) | 1:193:H:ASN:N | 1:193:H:ASN:CA | 1:193:H:ASN:C | 1:194:H:ALA:N | 2 | 2.56 | 1.35 | 2.56 |
| (1,478) | 1:190:J:LEU:N | 1:190:J:LEU:CA | 1:190:J:LEU:C | 1:191:J:VAL:N | 2 | 2.54 | 0.87 | 2.54 |
| (1,125) | 1:158:K:LYS:C | 1:159:K:GLU:N | 1:159:K:GLU:CA | 1:159:K:GLU:C | 2 | 2.52 | 0.77 | 2.52 |
| (1,864) | 1:226:L:HIS:N | 1:226:L:HIS:CA | 1:226:L:HIS:C | 1:227:L:LYS:N | 2 | 2.42 | 1.1 | 2.42 |
| (1,315) | 1:176:I:GLN:C | 1:177:I:ALA:N | 1:177:I:ALA:CA | 1:177:I:ALA:C | 2 | 2.36 | 0.46 | 2.36 |
| (1,454) | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 1:189:J:LEU:N | 2 | 2.32 | 0.62 | 2.32 |
| (1,663) | 1:208:I:GLY:C | 1:209:I:ALA:N | 1:209:I:ALA:CA | 1:209:I:ALA:C | 2 | 2.07 | 0.83 | 2.07 |
| (1,311) | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 1:175:K:GLU:N | 2 | 2.05 | 0.11 | 2.05 |
| (1,273) | 1:171:I:THR:N | 1:171:I:THR:CA | 1:171:I:THR:C | 1:172:I:LEU:N | 2 | 1.92 | 0.49 | 1.92 |
| (1,1056) | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 1:244:L:ILE:N | 2 | 1.78 | 0.15 | 1.78 |
| (1,191) | 1:164:K:TYR:N | 1:164:K:TYR:CA | 1:164:K:TYR:C | 1:165:K:VAL:N | 2 | 1.76 | 0.19 | 1.76 |
| (1,431) | 1:186:K:THR:N | 1:186:K:THR:CA | 1:186:K:THR:C | 1:187:K:GLU:N | 2 | 1.76 | 0.5 | 1.76 |
| (1,826) | 1:223:J:GLY:N | 1:223:J:GLY:CA | 1:223:J:GLY:C | 1:224:J:PRO:N | 2 | 1.74 | 0.02 | 1.74 |
| (1,143) | 1:160:K:PRO:N | 1:160:K:PRO:CA | 1:160:K:PRO:C | 1:161:K:PHE:N | 2 | 1.66 | 0.02 | 1.66 |
| (1,672) | 1:209:L:ALA:N | 1:209:L:ALA:CA | 1:209:L:ALA:C | 1:210:L:THR:N | 2 | 1.62 | 0.52 | 1.62 |
| (1,1053) | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 1:244:I:ILE:N | 2 | 1.46 | 0.44 | 1.46 |
| (1,699) | 1:211:I:LEU:C | 1:212:I:GLU:N | 1:212:I:GLU:CA | 1:212:I:GLU:C | 2 | 1.4 | 0.12 | 1.4 |
| (1,671) | 1:209:K:ALA:N | 1:209:K:ALA:CA | 1:209:K:ALA:C | 1:210:K:THR:N | 2 | 1.38 | 0.06 | 1.38 |
| (1,301) | 1:173:G:ARG:C | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 2 | 1.34 | 0.09 | 1.34 |

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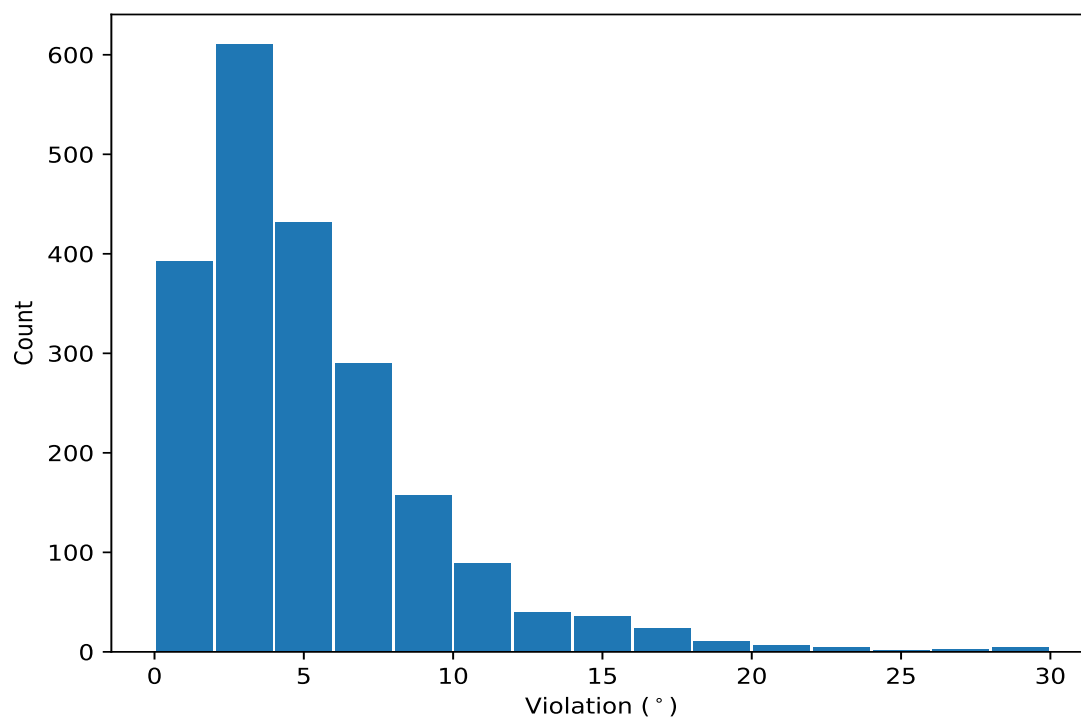
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,905) | 1:229:K:ARG:C | 1:230:K:VAL:N | 1:230:K:VAL:CA | 1:230:K:VAL:C | 2 | 1.26 | 0.04 | 1.26 |
| (1,946) | 1:233:J:GLU:N | 1:233:J:GLU:CA | 1:233:J:GLU:C | 1:234:J:ALA:N | 2 | 1.16 | 0.1 | 1.16 |
| (1,179) | 1:163:K:ASP:N | 1:163:K:ASP:CA | 1:163:K:ASP:C | 1:164:K:TYR:N | 2 | 1.13 | 0.06 | 1.13 |

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 10 | 28.71 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 8 | 28.43 |
| (1,54) | 1:150:L:ILE:C | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 8 | 28.36 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 3 | 28.32 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 1 | 28.06 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 7 | 27.99 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 4 | 27.69 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 6 | 26.76 |
| (1,51) | 1:150:I:ILE:C | 1:151:I:LEU:N | 1:151:I:LEU:CA | 1:151:I:LEU:C | 6 | 25.79 |
| (1,65) | 1:152:K:ASP:N | 1:152:K:ASP:CA | 1:152:K:ASP:C | 1:153:K:ILE:N | 10 | 25.44 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 3 | 23.89 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 7 | 23.06 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 9 | 22.44 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 1 | 22.33 |
| (1,65) | 1:152:K:ASP:N | 1:152:K:ASP:CA | 1:152:K:ASP:C | 1:153:K:ILE:N | 9 | 22.15 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 5 | 21.91 |
| (1,515) | 1:193:K:ASN:N | 1:193:K:ASN:CA | 1:193:K:ASN:C | 1:194:K:ALA:N | 5 | 21.89 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 2 | 21.78 |
| (1,51) | 1:150:I:ILE:C | 1:151:I:LEU:N | 1:151:I:LEU:CA | 1:151:I:LEU:C | 1 | 21.65 |
| (1,50) | 1:150:H:ILE:C | 1:151:H:LEU:N | 1:151:H:LEU:CA | 1:151:H:LEU:C | 9 | 21.41 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 5 | 20.8 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 2 | 20.74 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 1 | 19.86 |
| (1,53) | 1:150:K:ILE:C | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 8 | 19.72 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 2 | 19.62 |
| (1,54) | 1:150:L:ILE:C | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 9 | 19.18 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 6 | 19.08 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 10 | 18.99 |
| (1,40) | 1:148:J:THR:C | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 6 | 18.66 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 5 | 18.64 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 7 | 18.32 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 9 | 18.3 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 9 | 18.18 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 6 | 17.92 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 3 | 17.71 |
| (1,54) | 1:150:L:ILE:C | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 2 | 17.68 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 2 | 17.63 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 2 | 17.58 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 1 | 17.55 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 8 | 17.06 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 4 | 16.99 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 4 | 16.96 |
| (1,500) | 1:192:H:GLN:N | 1:192:H:GLN:CA | 1:192:H:GLN:C | 1:193:H:ASN:N | 10 | 16.8 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 5 | 16.77 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 5 | 16.66 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 7 | 16.58 |
| (1,65) | 1:152:K:ASP:N | 1:152:K:ASP:CA | 1:152:K:ASP:C | 1:153:K:ILE:N | 8 | 16.56 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 6 | 16.55 |
| (1,63) | 1:152:I:ASP:N | 1:152:I:ASP:CA | 1:152:I:ASP:C | 1:153:I:ILE:N | 1 | 16.55 |
| (1,448) | 1:187:J:GLU:C | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 1 | 16.46 |
| (1,856) | 1:225:J:GLY:C | 1:226:J:HIS:N | 1:226:J:HIS:CA | 1:226:J:HIS:C | 8 | 16.44 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 3 | 16.27 |
| (1,65) | 1:152:K:ASP:N | 1:152:K:ASP:CA | 1:152:K:ASP:C | 1:153:K:ILE:N | 6 | 16.15 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 9 | 16.13 |
| (1,482) | 1:190:H:LEU:C | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 9 | 16.09 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,856) | 1:225:J:GLY:C | 1:226:J:HIS:N | 1:226:J:HIS:CA | 1:226:J:HIS:C | 4 | 16.07 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 8 | 16.07 |
| (1,63) | 1:152:I:ASP:N | 1:152:I:ASP:CA | 1:152:I:ASP:C | 1:153:I:ILE:N | 2 | 15.99 |
| (1,54) | 1:150:L:ILE:C | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 6 | 15.95 |
| (1,63) | 1:152:I:ASP:N | 1:152:I:ASP:CA | 1:152:I:ASP:C | 1:153:I:ILE:N | 4 | 15.94 |
| (1,51) | 1:150:I:ILE:C | 1:151:I:LEU:N | 1:151:I:LEU:CA | 1:151:I:LEU:C | 4 | 15.91 |
| (1,523) | 1:195:G:ASN:N | 1:195:G:ASN:CA | 1:195:G:ASN:C | 1:196:G:PRO:N | 10 | 15.83 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 6 | 15.81 |
| (1,65) | 1:152:K:ASP:N | 1:152:K:ASP:CA | 1:152:K:ASP:C | 1:153:K:ILE:N | 5 | 15.65 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 7 | 15.58 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 8 | 15.56 |
| (1,526) | 1:195:J:ASN:N | 1:195:J:ASN:CA | 1:195:J:ASN:C | 1:196:J:PRO:N | 10 | 15.55 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 8 | 15.5 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 2 | 15.3 |
| (1,40) | 1:148:J:THR:C | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 2 | 15.28 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 3 | 15.01 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 5 | 14.99 |
| (1,47) | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 1:150:K:ILE:N | 6 | 14.98 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 3 | 14.97 |
| (1,448) | 1:187:J:GLU:C | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 9 | 14.95 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 4 | 14.72 |
| (1,500) | 1:192:H:GLN:N | 1:192:H:GLN:CA | 1:192:H:GLN:C | 1:193:H:ASN:N | 1 | 14.68 |
| (1,528) | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 1:196:L:PRO:N | 4 | 14.56 |
| (1,30) | 1:147:L:PRO:N | 1:147:L:PRO:CA | 1:147:L:PRO:C | 1:148:L:THR:N | 2 | 14.56 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 8 | 14.55 |
| (1,54) | 1:150:L:ILE:C | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 10 | 14.54 |
| (1,65) | 1:152:K:ASP:N | 1:152:K:ASP:CA | 1:152:K:ASP:C | 1:153:K:ILE:N | 2 | 14.5 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 6 | 14.5 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 8 | 14.32 |
| (1,69) | 1:153:I:ILE:N | 1:153:I:ILE:CA | 1:153:I:ILE:C | 1:154:I:ARG:N | 1 | 14.31 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 2 | 14.31 |
| (1,50) | 1:150:H:ILE:C | 1:151:H:LEU:N | 1:151:H:LEU:CA | 1:151:H:LEU:C | 2 | 14.22 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 5 | 14.22 |
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 8 | 14.2 |
| (1,54) | 1:150:L:ILE:C | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 7 | 14.13 |
| (1,500) | 1:192:H:GLN:N | 1:192:H:GLN:CA | 1:192:H:GLN:C | 1:193:H:ASN:N | 6 | 14.11 |
| (1,63) | 1:152:I:ASP:N | 1:152:I:ASP:CA | 1:152:I:ASP:C | 1:153:I:ILE:N | 3 | 14.03 |
| (1,837) | 1:224:I:PRO:N | 1:224:I:PRO:CA | 1:224:I:PRO:C | 1:225:I:GLY:N | 7 | 14.01 |
| (1,53) | 1:150:K:ILE:C | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 10 | 13.95 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 1 | 13.83 |
| (1,36) | 1:147:L:PRO:C | 1:148:L:THR:N | 1:148:L:THR:CA | 1:148:L:THR:C | 6 | 13.72 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 7 | 13.68 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 7 | 13.67 |
| (1,47) | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 1:150:K:ILE:N | 5 | 13.65 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 6 | 13.62 |
| (1,448) | 1:187:J:GLU:C | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 8 | 13.53 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 1 | 13.46 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 4 | 13.39 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 4 | 13.37 |
| (1,66) | 1:152:L:ASP:N | 1:152:L:ASP:CA | 1:152:L:ASP:C | 1:153:L:ILE:N | 7 | 13.34 |
| (1,477) | 1:190:I:LEU:N | 1:190:I:LEU:CA | 1:190:I:LEU:C | 1:191:I:VAL:N | 1 | 13.28 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 9 | 13.23 |
| (1,856) | 1:225:J:GLY:C | 1:226:J:HIS:N | 1:226:J:HIS:CA | 1:226:J:HIS:C | 9 | 13.22 |
| (1,66) | 1:152:L:ASP:N | 1:152:L:ASP:CA | 1:152:L:ASP:C | 1:153:L:ILE:N | 6 | 13.21 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1 | 13.08 |
| (1,30) | 1:147:L:PRO:N | 1:147:L:PRO:CA | 1:147:L:PRO:C | 1:148:L:THR:N | 6 | 13.07 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 7 | 13.06 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 10 | 13.06 |
| (1,448) | 1:187:J:GLU:C | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 4 | 13.05 |
| (1,424) | 1:185:J:MET:C | 1:186:J:THR:N | 1:186:J:THR:CA | 1:186:J:THR:C | 7 | 13.02 |
| (1,51) | 1:150:I:ILE:C | 1:151:I:LEU:N | 1:151:I:LEU:CA | 1:151:I:LEU:C | 3 | 12.98 |
| (1,28) | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 1:148:J:THR:N | 6 | 12.87 |
| (1,36) | 1:147:L:PRO:C | 1:148:L:THR:N | 1:148:L:THR:CA | 1:148:L:THR:C | 2 | 12.8 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 1 | 12.64 |
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 5 | 12.63 |
| (1,515) | 1:193:K:ASN:N | 1:193:K:ASN:CA | 1:193:K:ASN:C | 1:194:K:ALA:N | 3 | 12.6 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 9 | 12.54 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 3 | 12.53 |
| (1,483) | 1:190:I:LEU:C | 1:191:I:VAL:N | 1:191:I:VAL:CA | 1:191:I:VAL:C | 1 | 12.46 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 3 | 12.37 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 10 | 12.37 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 2 | 12.25 |
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 6 | 12.23 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 2 | 12.22 |
| (1,40) | 1:148:J:THR:C | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 8 | 12.14 |
| (1,53) | 1:150:K:ILE:C | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 9 | 12.05 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 10 | 12.03 |
| (1,632) | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 1:205:H:LEU:N | 10 | 12.01 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 2 | 11.9 |
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 7 | 11.88 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 7 | 11.85 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 1 | 11.65 |
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 4 | 11.65 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 4 | 11.64 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 7 | 11.64 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 3 | 11.62 |
| (1,66) | 1:152:L:ASP:N | 1:152:L:ASP:CA | 1:152:L:ASP:C | 1:153:L:ILE:N | 10 | 11.5 |
| (1,312) | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 1:175:L:GLU:N | 6 | 11.44 |
| (1,446) | 1:187:H:GLU:C | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 9 | 11.43 |
| (1,891) | 1:228:I:ALA:C | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 3 | 11.42 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 9 | 11.42 |
| (1,891) | 1:228:I:ALA:C | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 1 | 11.4 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 10 | 11.31 |
| (1,891) | 1:228:I:ALA:C | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 4 | 11.26 |
| (1,500) | 1:192:H:GLN:N | 1:192:H:GLN:CA | 1:192:H:GLN:C | 1:193:H:ASN:N | 4 | 11.25 |
| (1,30) | 1:147:L:PRO:N | 1:147:L:PRO:CA | 1:147:L:PRO:C | 1:148:L:THR:N | 10 | 11.25 |
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 3 | 11.21 |
| (1,30) | 1:147:L:PRO:N | 1:147:L:PRO:CA | 1:147:L:PRO:C | 1:148:L:THR:N | 7 | 11.21 |
| (1,434) | 1:186:H:THR:C | 1:187:H:GLU:N | 1:187:H:GLU:CA | 1:187:H:GLU:C | 8 | 11.19 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 3 | 11.17 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 3 | 11.17 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 5 | 11.14 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1030) | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 1:241:J:THR:N | 1 | 11.13 |
| (1,446) | 1:187:H:GLU:C | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 7 | 11.13 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 7 | 11.12 |
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 9 | 11.11 |
| (1,500) | 1:192:H:GLN:N | 1:192:H:GLN:CA | 1:192:H:GLN:C | 1:193:H:ASN:N | 3 | 11.1 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 6 | 11.02 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 1 | 11.02 |
| (1,61) | 1:152:G:ASP:N | 1:152:G:ASP:CA | 1:152:G:ASP:C | 1:153:G:ILE:N | 6 | 11.02 |
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 2 | 11.0 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 10 | 11.0 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 7 | 10.99 |
| (1,51) | 1:150:I:ILE:C | 1:151:I:LEU:N | 1:151:I:LEU:CA | 1:151:I:LEU:C | 2 | 10.97 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 6 | 10.96 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 2 | 10.95 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 9 | 10.94 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 8 | 10.9 |
| (1,116) | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 1:159:H:GLU:N | 7 | 10.87 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 5 | 10.87 |
| (1,446) | 1:187:H:GLU:C | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 8 | 10.86 |
| (1,794) | 1:219:H:GLN:C | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 3 | 10.85 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 3 | 10.83 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 6 | 10.8 |
| (1,445) | 1:187:G:GLU:C | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 10 | 10.79 |
| (1,482) | 1:190:H:LEU:C | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 10 | 10.78 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 5 | 10.73 |
| (1,808) | 1:220:J:GLY:C | 1:221:J:VAL:N | 1:221:J:VAL:CA | 1:221:J:VAL:C | 4 | 10.71 |
| (1,30) | 1:147:L:PRO:N | 1:147:L:PRO:CA | 1:147:L:PRO:C | 1:148:L:THR:N | 9 | 10.55 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 4 | 10.47 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 6 | 10.45 |
| (1,43) | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1:150:G:ILE:N | 3 | 10.45 |
| (1,27) | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 1:148:I:THR:N | 1 | 10.44 |
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 10 | 10.43 |
| (1,525) | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 1:196:I:PRO:N | 4 | 10.42 |
| (1,423) | 1:185:I:MET:C | 1:186:I:THR:N | 1:186:I:THR:CA | 1:186:I:THR:C | 8 | 10.41 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 1 | 10.41 |
| (1,310) | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 1:175:J:GLU:N | 4 | 10.4 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 4 | 10.38 |
| (1,990) | 1:236:L:SER:C | 1:237:L:GLN:N | 1:237:L:GLN:CA | 1:237:L:GLN:C | 6 | 10.38 |
| (1,28) | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 1:148:J:THR:N | 2 | 10.38 |
| (1,501) | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 1:193:I:ASN:N | 1 | 10.35 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 10 | 10.32 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 9 | 10.32 |
| (1,1024) | 1:239:J:THR:C | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 1 | 10.31 |
| (1,891) | 1:228:I:ALA:C | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 2 | 10.28 |
| (1,632) | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 1:205:H:LEU:N | 2 | 10.24 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 8 | 10.21 |
| (1,482) | 1:190:H:LEU:C | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 6 | 10.2 |
| (1,36) | 1:147:L:PRO:C | 1:148:L:THR:N | 1:148:L:THR:CA | 1:148:L:THR:C | 10 | 10.19 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 5 | 10.17 |
| (1,804) | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 1:221:L:VAL:N | 8 | 10.16 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 9 | 10.15 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 1 | 10.15 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 1 | 10.13 |
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 2 | 10.13 |
| (1,891) | 1:228:I:ALA:C | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 5 | 10.12 |
| (1,66) | 1:152:L:ASP:N | 1:152:L:ASP:CA | 1:152:L:ASP:C | 1:153:L:ILE:N | 2 | 10.12 |
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 10 | 10.11 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 3 | 10.1 |
| (1,893) | 1:228:K:ALA:C | 1:229:K:ARG:N | 1:229:K:ARG:CA | 1:229:K:ARG:C | 3 | 10.08 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 7 | 10.07 |
| (1,66) | 1:152:L:ASP:N | 1:152:L:ASP:CA | 1:152:L:ASP:C | 1:153:L:ILE:N | 9 | 10.03 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 7 | 10.01 |
| (1,448) | 1:187:J:GLU:C | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 2 | 10.01 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 3 | 10.0 |
| (1,116) | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 1:159:H:GLU:N | 5 | 10.0 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 7 | 9.99 |
| (1,445) | 1:187:G:GLU:C | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 3 | 9.99 |
| (1,804) | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 1:221:L:VAL:N | 6 | 9.98 |
| (1,448) | 1:187:J:GLU:C | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 6 | 9.98 |
| (1,61) | 1:152:G:ASP:N | 1:152:G:ASP:CA | 1:152:G:ASP:C | 1:153:G:ILE:N | 4 | 9.97 |
| (1,1045) | 1:242:G:ALA:C | 1:243:G:THR:N | 1:243:G:THR:CA | 1:243:G:THR:C | 1 | 9.94 |
| (1,61) | 1:152:G:ASP:N | 1:152:G:ASP:CA | 1:152:G:ASP:C | 1:153:G:ILE:N | 10 | 9.93 |
| (1,1026) | 1:239:L:THR:C | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 8 | 9.92 |
| (1,1024) | 1:239:J:THR:C | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 7 | 9.92 |
| (1,312) | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 1:175:L:GLU:N | 7 | 9.92 |
| (1,89) | 1:154:K:ARG:C | 1:155:K:GLN:N | 1:155:K:GLN:CA | 1:155:K:GLN:C | 8 | 9.92 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 7 | 9.92 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 3 | 9.87 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 8 | 9.84 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 8 | 9.79 |
| (1,36) | 1:147:L:PRO:C | 1:148:L:THR:N | 1:148:L:THR:CA | 1:148:L:THR:C | 9 | 9.77 |
| (1,448) | 1:187:J:GLU:C | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 10 | 9.75 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 10 | 9.67 |
| (1,794) | 1:219:H:GLN:C | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 8 | 9.67 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 7 | 9.66 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 2 | 9.64 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 3 | 9.63 |
| (1,483) | 1:190:I:LEU:C | 1:191:I:VAL:N | 1:191:I:VAL:CA | 1:191:I:VAL:C | 9 | 9.63 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 6 | 9.62 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 9 | 9.61 |
| (1,794) | 1:219:H:GLN:C | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 2 | 9.6 |
| (1,558) | 1:197:L:ASP:C | 1:198:L:CYS:N | 1:198:L:CYS:CA | 1:198:L:CYS:C | 6 | 9.6 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 1 | 9.54 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 10 | 9.54 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 4 | 9.51 |
| (1,312) | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 1:175:L:GLU:N | 5 | 9.4 |
| (1,890) | 1:228:H:ALA:C | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 3 | 9.36 |
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 3 | 9.35 |
| (1,1026) | 1:239:L:THR:C | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 10 | 9.33 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 8 | 9.32 |
| (1,500) | 1:192:H:GLN:N | 1:192:H:GLN:CA | 1:192:H:GLN:C | 1:193:H:ASN:N | 7 | 9.31 |
| (1,61) | 1:152:G:ASP:N | 1:152:G:ASP:CA | 1:152:G:ASP:C | 1:153:G:ILE:N | 1 | 9.3 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,61) | 1:152:G:ASP:N | 1:152:G:ASP:CA | 1:152:G:ASP:C | 1:153:G:ILE:N | 2 | 9.29 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 5 | 9.29 |
| (1,445) | 1:187:G:GLU:C | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 1 | 9.27 |
| (1,59) | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 1:152:K:ASP:N | 8 | 9.27 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 1 | 9.25 |
| (1,522) | 1:194:L:ALA:C | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 5 | 9.25 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 5 | 9.24 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 8 | 9.22 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 10 | 9.19 |
| (1,61) | 1:152:G:ASP:N | 1:152:G:ASP:CA | 1:152:G:ASP:C | 1:153:G:ILE:N | 7 | 9.19 |
| (1,61) | 1:152:G:ASP:N | 1:152:G:ASP:CA | 1:152:G:ASP:C | 1:153:G:ILE:N | 9 | 9.19 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 2 | 9.18 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 1 | 9.18 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 5 | 9.17 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 5 | 9.17 |
| (1,1026) | 1:239:L:THR:C | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 3 | 9.17 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 6 | 9.16 |
| (1,1031) | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 1:241:K:THR:N | 5 | 9.16 |
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 4 | 9.15 |
| (1,868) | 1:226:J:HIS:C | 1:227:J:LYS:N | 1:227:J:LYS:CA | 1:227:J:LYS:C | 9 | 9.12 |
| (1,803) | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 1:221:K:VAL:N | 2 | 9.12 |
| (1,309) | 1:174:I:ALA:N | 1:174:I:ALA:CA | 1:174:I:ALA:C | 1:175:I:GLU:N | 5 | 9.12 |
| (1,1026) | 1:239:L:THR:C | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 5 | 9.11 |
| (1,314) | 1:176:H:GLN:C | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 1 | 9.11 |
| (1,813) | 1:221:I:VAL:N | 1:221:I:VAL:CA | 1:221:I:VAL:C | 1:222:I:GLY:N | 1 | 9.09 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 10 | 9.08 |
| (1,1030) | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 1:241:J:THR:N | 7 | 9.07 |
| (1,1026) | 1:239:L:THR:C | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 4 | 9.06 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 6 | 9.05 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 10 | 9.03 |
| (1,445) | 1:187:G:GLU:C | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 5 | 9.03 |
| (1,891) | 1:228:I:ALA:C | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 9 | 8.98 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 10 | 8.97 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 3 | 8.96 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 4 | 8.89 |
| (1,61) | 1:152:G:ASP:N | 1:152:G:ASP:CA | 1:152:G:ASP:C | 1:153:G:ILE:N | 3 | 8.88 |
| (1,310) | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 1:175:J:GLU:N | 10 | 8.86 |
| (1,32) | 1:147:H:PRO:C | 1:148:H:THR:N | 1:148:H:THR:CA | 1:148:H:THR:C | 9 | 8.86 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 10 | 8.83 |
| (1,652) | 1:207:J:PRO:C | 1:208:J:GLY:N | 1:208:J:GLY:CA | 1:208:J:GLY:C | 3 | 8.83 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 8 | 8.82 |
| (1,448) | 1:187:J:GLU:C | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 7 | 8.82 |
| (1,447) | 1:187:I:GLU:C | 1:188:I:THR:N | 1:188:I:THR:CA | 1:188:I:THR:C | 9 | 8.82 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 4 | 8.79 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 1 | 8.78 |
| (1,891) | 1:228:I:ALA:C | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 6 | 8.77 |
| (1,804) | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 1:221:L:VAL:N | 1 | 8.77 |
| (1,676) | 1:209:J:ALA:C | 1:210:J:THR:N | 1:210:J:THR:CA | 1:210:J:THR:C | 3 | 8.77 |
| (1,380) | 1:182:H:LYS:N | 1:182:H:LYS:CA | 1:182:H:LYS:C | 1:183:H:ASN:N | 2 | 8.75 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 5 | 8.74 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 10 | 8.73 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,445) | 1:187:G:GLU:C | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 2 | 8.73 |
| (1,57) | 1:151:I:LEU:N | 1:151:I:LEU:CA | 1:151:I:LEU:C | 1:152:I:ASP:N | 6 | 8.73 |
| (1,798) | 1:219:L:GLN:C | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 2 | 8.72 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 9 | 8.71 |
| (1,1025) | 1:239:K:THR:C | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 1 | 8.71 |
| (1,632) | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 1:205:H:LEU:N | 5 | 8.7 |
| (1,448) | 1:187:J:GLU:C | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 3 | 8.68 |
| (1,868) | 1:226:J:HIS:C | 1:227:J:LYS:N | 1:227:J:LYS:CA | 1:227:J:LYS:C | 8 | 8.67 |
| (1,28) | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 1:148:J:THR:N | 10 | 8.66 |
| (1,645) | 1:205:I:LEU:N | 1:205:I:LEU:CA | 1:205:I:LEU:C | 1:206:I:GLY:N | 4 | 8.65 |
| (1,632) | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 1:205:H:LEU:N | 9 | 8.64 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 9 | 8.63 |
| (1,62) | 1:152:H:ASP:N | 1:152:H:ASP:CA | 1:152:H:ASP:C | 1:153:H:ILE:N | 9 | 8.63 |
| (1,445) | 1:187:G:GLU:C | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 6 | 8.62 |
| (1,410) | 1:184:H:TRP:C | 1:185:H:MET:N | 1:185:H:MET:CA | 1:185:H:MET:C | 5 | 8.62 |
| (1,794) | 1:219:H:GLN:C | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 7 | 8.61 |
| (1,309) | 1:174:I:ALA:N | 1:174:I:ALA:CA | 1:174:I:ALA:C | 1:175:I:GLU:N | 7 | 8.59 |
| (1,858) | 1:225:L:GLY:C | 1:226:L:HIS:N | 1:226:L:HIS:CA | 1:226:L:HIS:C | 1 | 8.58 |
| (1,310) | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 1:175:J:GLU:N | 6 | 8.55 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 3 | 8.53 |
| (1,36) | 1:147:L:PRO:C | 1:148:L:THR:N | 1:148:L:THR:CA | 1:148:L:THR:C | 7 | 8.53 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 6 | 8.51 |
| (1,1049) | 1:242:K:ALA:C | 1:243:K:THR:N | 1:243:K:THR:CA | 1:243:K:THR:C | 2 | 8.51 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 9 | 8.49 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 4 | 8.49 |
| (1,450) | 1:187:L:GLU:C | 1:188:L:THR:N | 1:188:L:THR:CA | 1:188:L:THR:C | 1 | 8.49 |
| (1,548) | 1:197:H:ASP:N | 1:197:H:ASP:CA | 1:197:H:ASP:C | 1:198:H:CYS:N | 7 | 8.46 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 7 | 8.42 |
| (1,484) | 1:190:J:LEU:C | 1:191:J:VAL:N | 1:191:J:VAL:CA | 1:191:J:VAL:C | 9 | 8.42 |
| (1,450) | 1:187:L:GLU:C | 1:188:L:THR:N | 1:188:L:THR:CA | 1:188:L:THR:C | 8 | 8.42 |
| (1,140) | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 1:161:H:PHE:N | 1 | 8.42 |
| (1,90) | 1:154:L:ARG:C | 1:155:L:GLN:N | 1:155:L:GLN:CA | 1:155:L:GLN:C | 8 | 8.4 |
| (1,1031) | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 1:241:K:THR:N | 9 | 8.39 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 9 | 8.39 |
| (1,858) | 1:225:L:GLY:C | 1:226:L:HIS:N | 1:226:L:HIS:CA | 1:226:L:HIS:C | 2 | 8.34 |
| (1,140) | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 1:161:H:PHE:N | 4 | 8.34 |
| (1,893) | 1:228:K:ALA:C | 1:229:K:ARG:N | 1:229:K:ARG:CA | 1:229:K:ARG:C | 5 | 8.33 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 7 | 8.32 |
| (1,316) | 1:176:J:GLN:C | 1:177:J:ALA:N | 1:177:J:ALA:CA | 1:177:J:ALA:C | 5 | 8.32 |
| (1,116) | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 1:159:H:GLU:N | 2 | 8.32 |
| (1,477) | 1:190:I:LEU:N | 1:190:I:LEU:CA | 1:190:I:LEU:C | 1:191:I:VAL:N | 2 | 8.31 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 8 | 8.3 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 10 | 8.29 |
| (1,858) | 1:225:L:GLY:C | 1:226:L:HIS:N | 1:226:L:HIS:CA | 1:226:L:HIS:C | 5 | 8.29 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 3 | 8.28 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 6 | 8.28 |
| (1,858) | 1:225:L:GLY:C | 1:226:L:HIS:N | 1:226:L:HIS:CA | 1:226:L:HIS:C | 6 | 8.27 |
| (1,1026) | 1:239:L:THR:C | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 9 | 8.22 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 10 | 8.22 |
| (1,60) | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 1:152:L:ASP:N | 8 | 8.22 |
| (1,47) | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 1:150:K:ILE:N | 10 | 8.22 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,893) | 1:228:K:ALA:C | 1:229:K:ARG:N | 1:229:K:ARG:CA | 1:229:K:ARG:C | 8 | 8.21 |
| (1,1024) | 1:239:J:THR:C | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 3 | 8.16 |
| (1,858) | 1:225:L:GLY:C | 1:226:L:HIS:N | 1:226:L:HIS:CA | 1:226:L:HIS:C | 8 | 8.16 |
| (1,676) | 1:209:J:ALA:C | 1:210:J:THR:N | 1:210:J:THR:CA | 1:210:J:THR:C | 10 | 8.16 |
| (1,893) | 1:228:K:ALA:C | 1:229:K:ARG:N | 1:229:K:ARG:CA | 1:229:K:ARG:C | 4 | 8.15 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 6 | 8.14 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 3 | 8.12 |
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 10 | 8.12 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 2 | 8.1 |
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 9 | 8.09 |
| (1,1024) | 1:239:J:THR:C | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 5 | 8.07 |
| (1,62) | 1:152:H:ASP:N | 1:152:H:ASP:CA | 1:152:H:ASP:C | 1:153:H:ILE:N | 2 | 8.07 |
| (1,676) | 1:209:J:ALA:C | 1:210:J:THR:N | 1:210:J:THR:CA | 1:210:J:THR:C | 4 | 8.05 |
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 9 | 8.03 |
| (1,1046) | 1:242:H:ALA:C | 1:243:H:THR:N | 1:243:H:THR:CA | 1:243:H:THR:C | 2 | 8.02 |
| (1,911) | 1:230:K:VAL:N | 1:230:K:VAL:CA | 1:230:K:VAL:C | 1:231:K:LEU:N | 7 | 8.02 |
| (1,558) | 1:197:L:ASP:C | 1:198:L:CYS:N | 1:198:L:CYS:CA | 1:198:L:CYS:C | 1 | 8.02 |
| (1,501) | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 1:193:I:ASN:N | 8 | 8.0 |
| (1,66) | 1:152:L:ASP:N | 1:152:L:ASP:CA | 1:152:L:ASP:C | 1:153:L:ILE:N | 8 | 7.99 |
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 7 | 7.99 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 6 | 7.98 |
| (1,804) | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 1:221:L:VAL:N | 10 | 7.98 |
| (1,652) | 1:207:J:PRO:C | 1:208:J:GLY:N | 1:208:J:GLY:CA | 1:208:J:GLY:C | 4 | 7.97 |
| (1,794) | 1:219:H:GLN:C | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 4 | 7.96 |
| (1,990) | 1:236:L:SER:C | 1:237:L:GLN:N | 1:237:L:GLN:CA | 1:237:L:GLN:C | 2 | 7.94 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 1 | 7.92 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 6 | 7.91 |
| (1,795) | 1:219:I:GLN:C | 1:220:I:GLY:N | 1:220:I:GLY:CA | 1:220:I:GLY:C | 10 | 7.9 |
| (1,794) | 1:219:H:GLN:C | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 9 | 7.9 |
| (1,445) | 1:187:G:GLU:C | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 4 | 7.9 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 9 | 7.9 |
| (1,891) | 1:228:I:ALA:C | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 8 | 7.88 |
| (1,27) | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 1:148:I:THR:N | 6 | 7.88 |
| (1,590) | 1:200:H:THR:C | 1:201:H:ILE:N | 1:201:H:ILE:CA | 1:201:H:ILE:C | 10 | 7.84 |
| (1,423) | 1:185:I:MET:C | 1:186:I:THR:N | 1:186:I:THR:CA | 1:186:I:THR:C | 4 | 7.84 |
| (1,632) | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 1:205:H:LEU:N | 1 | 7.82 |
| (1,1024) | 1:239:J:THR:C | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 9 | 7.81 |
| (1,803) | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 1:221:K:VAL:N | 10 | 7.81 |
| (1,558) | 1:197:L:ASP:C | 1:198:L:CYS:N | 1:198:L:CYS:CA | 1:198:L:CYS:C | 9 | 7.77 |
| (1,519) | 1:194:I:ALA:C | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 6 | 7.77 |
| (1,317) | 1:176:K:GLN:C | 1:177:K:ALA:N | 1:177:K:ALA:CA | 1:177:K:ALA:C | 2 | 7.76 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 9 | 7.75 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 10 | 7.75 |
| (1,1032) | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 1:241:L:THR:N | 5 | 7.71 |
| (1,1023) | 1:239:I:THR:C | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 1 | 7.71 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 3 | 7.7 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 9 | 7.7 |
| (1,380) | 1:182:H:LYS:N | 1:182:H:LYS:CA | 1:182:H:LYS:C | 1:183:H:ASN:N | 9 | 7.68 |
| (1,317) | 1:176:K:GLN:C | 1:177:K:ALA:N | 1:177:K:ALA:CA | 1:177:K:ALA:C | 9 | 7.68 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 1 | 7.67 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 9 | 7.67 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1 | 7.67 |
| (1,1014) | 1:238:L:VAL:C | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 2 | 7.66 |
| (1,804) | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 1:221:L:VAL:N | 3 | 7.66 |
| (1,652) | 1:207:J:PRO:C | 1:208:J:GLY:N | 1:208:J:GLY:CA | 1:208:J:GLY:C | 6 | 7.65 |
| (1,445) | 1:187:G:GLU:C | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 8 | 7.65 |
| (1,317) | 1:176:K:GLN:C | 1:177:K:ALA:N | 1:177:K:ALA:CA | 1:177:K:ALA:C | 4 | 7.65 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 4 | 7.64 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 7 | 7.63 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 3 | 7.62 |
| (1,1030) | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 1:241:J:THR:N | 8 | 7.62 |
| (1,423) | 1:185:I:MET:C | 1:186:I:THR:N | 1:186:I:THR:CA | 1:186:I:THR:C | 9 | 7.62 |
| (1,558) | 1:197:L:ASP:C | 1:198:L:CYS:N | 1:198:L:CYS:CA | 1:198:L:CYS:C | 3 | 7.61 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 2 | 7.6 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 2 | 7.6 |
| (1,1009) | 1:238:G:VAL:C | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 9 | 7.58 |
| (1,794) | 1:219:H:GLN:C | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1 | 7.58 |
| (1,632) | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 1:205:H:LEU:N | 6 | 7.58 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 3 | 7.56 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 8 | 7.55 |
| (1,309) | 1:174:I:ALA:N | 1:174:I:ALA:CA | 1:174:I:ALA:C | 1:175:I:GLU:N | 2 | 7.55 |
| (1,120) | 1:158:L:LYS:N | 1:158:L:LYS:CA | 1:158:L:LYS:C | 1:159:L:GLU:N | 7 | 7.55 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 4 | 7.54 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 10 | 7.54 |
| (1,813) | 1:221:I:VAL:N | 1:221:I:VAL:CA | 1:221:I:VAL:C | 1:222:I:GLY:N | 5 | 7.52 |
| (1,1021) | 1:239:G:THR:C | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 9 | 7.49 |
| (1,891) | 1:228:I:ALA:C | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 10 | 7.46 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 5 | 7.45 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 6 | 7.45 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 3 | 7.44 |
| (1,120) | 1:158:L:LYS:N | 1:158:L:LYS:CA | 1:158:L:LYS:C | 1:159:L:GLU:N | 4 | 7.44 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 5 | 7.43 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 4 | 7.4 |
| (1,794) | 1:219:H:GLN:C | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 5 | 7.4 |
| (1,140) | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 1:161:H:PHE:N | 10 | 7.4 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 10 | 7.4 |
| (1,1032) | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 1:241:L:THR:N | 3 | 7.39 |
| (1,843) | 1:224:I:PRO:C | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 7 | 7.39 |
| (1,513) | 1:193:I:ASN:N | 1:193:I:ASN:CA | 1:193:I:ASN:C | 1:194:I:ALA:N | 2 | 7.39 |
| (1,120) | 1:158:L:LYS:N | 1:158:L:LYS:CA | 1:158:L:LYS:C | 1:159:L:GLU:N | 6 | 7.39 |
| (1,33) | 1:147:I:PRO:C | 1:148:I:THR:N | 1:148:I:THR:CA | 1:148:I:THR:C | 4 | 7.39 |
| (1,27) | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 1:148:I:THR:N | 3 | 7.39 |
| (1,676) | 1:209:J:ALA:C | 1:210:J:THR:N | 1:210:J:THR:CA | 1:210:J:THR:C | 2 | 7.38 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 2 | 7.37 |
| (1,1027) | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1:241:G:THR:N | 1 | 7.37 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 4 | 7.37 |
| (1,317) | 1:176:K:GLN:C | 1:177:K:ALA:N | 1:177:K:ALA:CA | 1:177:K:ALA:C | 5 | 7.37 |
| (1,827) | 1:223:K:GLY:N | 1:223:K:GLY:CA | 1:223:K:GLY:C | 1:224:K:PRO:N | 8 | 7.36 |
| (1,508) | 1:192:J:GLN:C | 1:193:J:ASN:N | 1:193:J:ASN:CA | 1:193:J:ASN:C | 8 | 7.35 |
| (1,798) | 1:219:L:GLN:C | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 7 | 7.34 |
| (1,558) | 1:197:L:ASP:C | 1:198:L:CYS:N | 1:198:L:CYS:CA | 1:198:L:CYS:C | 8 | 7.34 |
| (1,33) | 1:147:I:PRO:C | 1:148:I:THR:N | 1:148:I:THR:CA | 1:148:I:THR:C | 2 | 7.33 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1032) | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 1:241:L:THR:N | 8 | 7.32 |
| (1,632) | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 1:205:H:LEU:N | 4 | 7.32 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 3 | 7.31 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 4 | 7.31 |
| (1,858) | 1:225:L:GLY:C | 1:226:L:HIS:N | 1:226:L:HIS:CA | 1:226:L:HIS:C | 10 | 7.3 |
| (1,309) | 1:174:I:ALA:N | 1:174:I:ALA:CA | 1:174:I:ALA:C | 1:175:I:GLU:N | 3 | 7.3 |
| (1,1025) | 1:239:K:THR:C | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 8 | 7.29 |
| (1,47) | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 1:150:K:ILE:N | 9 | 7.28 |
| (1,36) | 1:147:L:PRO:C | 1:148:L:THR:N | 1:148:L:THR:CA | 1:148:L:THR:C | 8 | 7.28 |
| (1,1025) | 1:239:K:THR:C | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 9 | 7.26 |
| (1,558) | 1:197:L:ASP:C | 1:198:L:CYS:N | 1:198:L:CYS:CA | 1:198:L:CYS:C | 10 | 7.26 |
| (1,68) | 1:153:H:ILE:N | 1:153:H:ILE:CA | 1:153:H:ILE:C | 1:154:H:ARG:N | 7 | 7.26 |
| (1,62) | 1:152:H:ASP:N | 1:152:H:ASP:CA | 1:152:H:ASP:C | 1:153:H:ILE:N | 7 | 7.26 |
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 5 | 7.26 |
| (1,30) | 1:147:L:PRO:N | 1:147:L:PRO:CA | 1:147:L:PRO:C | 1:148:L:THR:N | 8 | 7.26 |
| (1,825) | 1:223:I:GLY:N | 1:223:I:GLY:CA | 1:223:I:GLY:C | 1:224:I:PRO:N | 6 | 7.24 |
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 6 | 7.24 |
| (1,445) | 1:187:G:GLU:C | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 9 | 7.22 |
| (1,26) | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 1:148:H:THR:N | 2 | 7.22 |
| (1,808) | 1:220:J:GLY:C | 1:221:J:VAL:N | 1:221:J:VAL:CA | 1:221:J:VAL:C | 8 | 7.21 |
| (1,515) | 1:193:K:ASN:N | 1:193:K:ASN:CA | 1:193:K:ASN:C | 1:194:K:ALA:N | 6 | 7.2 |
| (1,450) | 1:187:L:GLU:C | 1:188:L:THR:N | 1:188:L:THR:CA | 1:188:L:THR:C | 4 | 7.2 |
| (1,1014) | 1:238:L:VAL:C | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 1 | 7.19 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 5 | 7.18 |
| (1,1023) | 1:239:I:THR:C | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 9 | 7.18 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 5 | 7.18 |
| (1,815) | 1:221:K:VAL:N | 1:221:K:VAL:CA | 1:221:K:VAL:C | 1:222:K:GLY:N | 2 | 7.18 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 9 | 7.18 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 1 | 7.17 |
| (1,53) | 1:150:K:ILE:C | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 5 | 7.16 |
| (1,27) | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 1:148:I:THR:N | 4 | 7.16 |
| (1,441) | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 1:188:I:THR:N | 7 | 7.14 |
| (1,89) | 1:154:K:ARG:C | 1:155:K:GLN:N | 1:155:K:GLN:CA | 1:155:K:GLN:C | 10 | 7.14 |
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 1 | 7.14 |
| (1,645) | 1:205:I:LEU:N | 1:205:I:LEU:CA | 1:205:I:LEU:C | 1:206:I:GLY:N | 1 | 7.13 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 8 | 7.12 |
| (1,27) | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 1:148:I:THR:N | 2 | 7.12 |
| (1,28) | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 1:148:J:THR:N | 8 | 7.11 |
| (1,1048) | 1:242:J:ALA:C | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 5 | 7.1 |
| (1,90) | 1:154:L:ARG:C | 1:155:L:GLN:N | 1:155:L:GLN:CA | 1:155:L:GLN:C | 1 | 7.1 |
| (1,482) | 1:190:H:LEU:C | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 3 | 7.07 |
| (1,424) | 1:185:J:MET:C | 1:186:J:THR:N | 1:186:J:THR:CA | 1:186:J:THR:C | 8 | 7.06 |
| (1,912) | 1:230:L:VAL:N | 1:230:L:VAL:CA | 1:230:L:VAL:C | 1:231:L:LEU:N | 7 | 7.05 |
| (1,674) | 1:209:H:ALA:C | 1:210:H:THR:N | 1:210:H:THR:CA | 1:210:H:THR:C | 7 | 7.05 |
| (1,558) | 1:197:L:ASP:C | 1:198:L:CYS:N | 1:198:L:CYS:CA | 1:198:L:CYS:C | 4 | 7.04 |
| (1,89) | 1:154:K:ARG:C | 1:155:K:GLN:N | 1:155:K:GLN:CA | 1:155:K:GLN:C | 9 | 7.04 |
| (1,1032) | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 1:241:L:THR:N | 9 | 7.03 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 4 | 7.02 |
| (1,794) | 1:219:H:GLN:C | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 6 | 7.01 |
| (1,482) | 1:190:H:LEU:C | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 1 | 7.01 |
| (1,320) | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 1:178:H:SER:N | 8 | 7.01 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 3 | 7.0 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 4 | 6.98 |
| (1,116) | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 1:159:H:GLU:N | 8 | 6.97 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 1 | 6.96 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 2 | 6.96 |
| (1,796) | 1:219:J:GLN:C | 1:220:J:GLY:N | 1:220:J:GLY:CA | 1:220:J:GLY:C | 7 | 6.94 |
| (1,482) | 1:190:H:LEU:C | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 8 | 6.94 |
| (1,1021) | 1:239:G:THR:C | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 5 | 6.93 |
| (1,632) | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 1:205:H:LEU:N | 3 | 6.93 |
| (1,558) | 1:197:L:ASP:C | 1:198:L:CYS:N | 1:198:L:CYS:CA | 1:198:L:CYS:C | 7 | 6.93 |
| (1,527) | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 1:196:K:PRO:N | 8 | 6.93 |
| (1,1014) | 1:238:L:VAL:C | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 6 | 6.92 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 10 | 6.92 |
| (1,1023) | 1:239:I:THR:C | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 6 | 6.91 |
| (1,1029) | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 1:241:I:THR:N | 1 | 6.9 |
| (1,897) | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 1:230:I:VAL:N | 1 | 6.9 |
| (1,827) | 1:223:K:GLY:N | 1:223:K:GLY:CA | 1:223:K:GLY:C | 1:224:K:PRO:N | 6 | 6.9 |
| (1,27) | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 1:148:I:THR:N | 10 | 6.9 |
| (1,29) | 1:147:K:PRO:N | 1:147:K:PRO:CA | 1:147:K:PRO:C | 1:148:K:THR:N | 10 | 6.89 |
| (1,320) | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 1:178:H:SER:N | 6 | 6.88 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 7 | 6.87 |
| (1,483) | 1:190:I:LEU:C | 1:191:I:VAL:N | 1:191:I:VAL:CA | 1:191:I:VAL:C | 10 | 6.87 |
| (1,317) | 1:176:K:GLN:C | 1:177:K:ALA:N | 1:177:K:ALA:CA | 1:177:K:ALA:C | 6 | 6.87 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 1 | 6.86 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 1 | 6.83 |
| (1,312) | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 1:175:L:GLU:N | 2 | 6.83 |
| (1,380) | 1:182:H:LYS:N | 1:182:H:LYS:CA | 1:182:H:LYS:C | 1:183:H:ASN:N | 1 | 6.82 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 9 | 6.8 |
| (1,1024) | 1:239:J:THR:C | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 10 | 6.78 |
| (1,759) | 1:216:I:THR:C | 1:217:I:ALA:N | 1:217:I:ALA:CA | 1:217:I:ALA:C | 4 | 6.78 |
| (1,309) | 1:174:I:ALA:N | 1:174:I:ALA:CA | 1:174:I:ALA:C | 1:175:I:GLU:N | 6 | 6.77 |
| (1,1111) | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1:243:G:THR:N | 7 | 6.75 |
| (1,1009) | 1:238:G:VAL:C | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 5 | 6.74 |
| (1,897) | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 1:230:I:VAL:N | 9 | 6.74 |
| (1,33) | 1:147:I:PRO:C | 1:148:I:THR:N | 1:148:I:THR:CA | 1:148:I:THR:C | 6 | 6.74 |
| (1,447) | 1:187:I:GLU:C | 1:188:I:THR:N | 1:188:I:THR:CA | 1:188:I:THR:C | 6 | 6.73 |
| (1,903) | 1:229:I:ARG:C | 1:230:I:VAL:N | 1:230:I:VAL:CA | 1:230:I:VAL:C | 3 | 6.72 |
| (1,27) | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 1:148:I:THR:N | 5 | 6.72 |
| (1,1029) | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 1:241:I:THR:N | 8 | 6.71 |
| (1,998) | 1:237:H:GLN:C | 1:238:H:VAL:N | 1:238:H:VAL:CA | 1:238:H:VAL:C | 1 | 6.71 |
| (1,501) | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 1:193:I:ASN:N | 7 | 6.7 |
| (1,32) | 1:147:H:PRO:C | 1:148:H:THR:N | 1:148:H:THR:CA | 1:148:H:THR:C | 2 | 6.69 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 9 | 6.68 |
| (1,845) | 1:224:K:PRO:C | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 4 | 6.68 |
| (1,1026) | 1:239:L:THR:C | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 2 | 6.67 |
| (1,120) | 1:158:L:LYS:N | 1:158:L:LYS:CA | 1:158:L:LYS:C | 1:159:L:GLU:N | 10 | 6.67 |
| (1,1025) | 1:239:K:THR:C | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 10 | 6.66 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 1 | 6.66 |
| (1,40) | 1:148:J:THR:C | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 4 | 6.66 |
| (1,32) | 1:147:H:PRO:C | 1:148:H:THR:N | 1:148:H:THR:CA | 1:148:H:THR:C | 5 | 6.65 |
| (1,524) | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 1:196:H:PRO:N | 9 | 6.64 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,317) | 1:176:K:GLN:C | 1:177:K:ALA:N | 1:177:K:ALA:CA | 1:177:K:ALA:C | 8 | 6.64 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 1 | 6.64 |
| (1,423) | 1:185:I:MET:C | 1:186:I:THR:N | 1:186:I:THR:CA | 1:186:I:THR:C | 1 | 6.63 |
| (1,309) | 1:174:I:ALA:N | 1:174:I:ALA:CA | 1:174:I:ALA:C | 1:175:I:GLU:N | 10 | 6.62 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 4 | 6.62 |
| (1,858) | 1:225:L:GLY:C | 1:226:L:HIS:N | 1:226:L:HIS:CA | 1:226:L:HIS:C | 4 | 6.61 |
| (1,516) | 1:193:L:ASN:N | 1:193:L:ASN:CA | 1:193:L:ASN:C | 1:194:L:ALA:N | 8 | 6.61 |
| (1,1047) | 1:242:I:ALA:C | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 8 | 6.6 |
| (1,1025) | 1:239:K:THR:C | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 5 | 6.6 |
| (1,839) | 1:224:K:PRO:N | 1:224:K:PRO:CA | 1:224:K:PRO:C | 1:225:K:GLY:N | 7 | 6.6 |
| (1,450) | 1:187:L:GLU:C | 1:188:L:THR:N | 1:188:L:THR:CA | 1:188:L:THR:C | 5 | 6.59 |
| (1,426) | 1:185:L:MET:C | 1:186:L:THR:N | 1:186:L:THR:CA | 1:186:L:THR:C | 5 | 6.58 |
| (1,1027) | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1:241:G:THR:N | 8 | 6.57 |
| (1,1029) | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 1:241:I:THR:N | 9 | 6.55 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 5 | 6.55 |
| (1,580) | 1:199:J:LYS:C | 1:200:J:THR:N | 1:200:J:THR:CA | 1:200:J:THR:C | 7 | 6.53 |
| (1,30) | 1:147:L:PRO:N | 1:147:L:PRO:CA | 1:147:L:PRO:C | 1:148:L:THR:N | 5 | 6.53 |
| (1,1020) | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 1:240:L:ASN:N | 8 | 6.52 |
| (1,116) | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 1:159:H:GLU:N | 10 | 6.51 |
| (1,800) | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1:221:H:VAL:N | 8 | 6.5 |
| (1,312) | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 1:175:L:GLU:N | 1 | 6.5 |
| (1,86) | 1:154:H:ARG:C | 1:155:H:GLN:N | 1:155:H:GLN:CA | 1:155:H:GLN:C | 5 | 6.5 |
| (1,1026) | 1:239:L:THR:C | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 7 | 6.49 |
| (1,1021) | 1:239:G:THR:C | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 7 | 6.48 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 5 | 6.48 |
| (1,858) | 1:225:L:GLY:C | 1:226:L:HIS:N | 1:226:L:HIS:CA | 1:226:L:HIS:C | 3 | 6.48 |
| (1,1026) | 1:239:L:THR:C | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 1 | 6.47 |
| (1,104) | 1:157:H:PRO:N | 1:157:H:PRO:CA | 1:157:H:PRO:C | 1:158:H:LYS:N | 7 | 6.47 |
| (1,26) | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 1:148:H:THR:N | 9 | 6.47 |
| (1,423) | 1:185:I:MET:C | 1:186:I:THR:N | 1:186:I:THR:CA | 1:186:I:THR:C | 2 | 6.46 |
| (1,28) | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 1:148:J:THR:N | 4 | 6.46 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 3 | 6.45 |
| (1,694) | 1:211:J:LEU:N | 1:211:J:LEU:CA | 1:211:J:LEU:C | 1:212:J:GLU:N | 1 | 6.45 |
| (1,449) | 1:187:K:GLU:C | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 1 | 6.44 |
| (1,1030) | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 1:241:J:THR:N | 3 | 6.41 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 5 | 6.41 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 6 | 6.4 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 9 | 6.39 |
| (1,798) | 1:219:L:GLN:C | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 9 | 6.39 |
| (1,53) | 1:150:K:ILE:C | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 6 | 6.39 |
| (1,893) | 1:228:K:ALA:C | 1:229:K:ARG:N | 1:229:K:ARG:CA | 1:229:K:ARG:C | 7 | 6.37 |
| (1,796) | 1:219:J:GLN:C | 1:220:J:GLY:N | 1:220:J:GLY:CA | 1:220:J:GLY:C | 10 | 6.37 |
| (1,815) | 1:221:K:VAL:N | 1:221:K:VAL:CA | 1:221:K:VAL:C | 1:222:K:GLY:N | 5 | 6.36 |
| (1,767) | 1:217:K:ALA:N | 1:217:K:ALA:CA | 1:217:K:ALA:C | 1:218:K:CYS:N | 4 | 6.36 |
| (1,558) | 1:197:L:ASP:C | 1:198:L:CYS:N | 1:198:L:CYS:CA | 1:198:L:CYS:C | 2 | 6.36 |
| (1,450) | 1:187:L:GLU:C | 1:188:L:THR:N | 1:188:L:THR:CA | 1:188:L:THR:C | 10 | 6.36 |
| (1,27) | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 1:148:I:THR:N | 7 | 6.36 |
| (1,312) | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 1:175:L:GLU:N | 9 | 6.35 |
| (1,1050) | 1:242:L:ALA:C | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 10 | 6.34 |
| (1,1032) | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 1:241:L:THR:N | 4 | 6.34 |
| (1,1112) | 1:242:H:ALA:N | 1:242:H:ALA:CA | 1:242:H:ALA:C | 1:243:H:THR:N | 8 | 6.33 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1020) | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 1:240:L:ASN:N | 4 | 6.33 |
| (1,446) | 1:187:H:GLU:C | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 5 | 6.33 |
| (1,1028) | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 1:241:H:THR:N | 8 | 6.32 |
| (1,310) | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 1:175:J:GLU:N | 8 | 6.32 |
| (1,1023) | 1:239:I:THR:C | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 5 | 6.31 |
| (1,1021) | 1:239:G:THR:C | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 8 | 6.31 |
| (1,1009) | 1:238:G:VAL:C | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 4 | 6.31 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 7 | 6.31 |
| (1,1031) | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 1:241:K:THR:N | 8 | 6.29 |
| (1,1020) | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 1:240:L:ASN:N | 10 | 6.29 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 6 | 6.29 |
| (1,804) | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 1:221:L:VAL:N | 4 | 6.28 |
| (1,34) | 1:147:J:PRO:C | 1:148:J:THR:N | 1:148:J:THR:CA | 1:148:J:THR:C | 6 | 6.28 |
| (1,488) | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 1:192:H:GLN:N | 8 | 6.27 |
| (1,676) | 1:209:J:ALA:C | 1:210:J:THR:N | 1:210:J:THR:CA | 1:210:J:THR:C | 8 | 6.25 |
| (1,450) | 1:187:L:GLU:C | 1:188:L:THR:N | 1:188:L:THR:CA | 1:188:L:THR:C | 9 | 6.25 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 8 | 6.24 |
| (1,975) | 1:235:I:MET:C | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 7 | 6.24 |
| (1,764) | 1:217:H:ALA:N | 1:217:H:ALA:CA | 1:217:H:ALA:C | 1:218:H:CYS:N | 6 | 6.22 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 3 | 6.21 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 7 | 6.2 |
| (1,1031) | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 1:241:K:THR:N | 2 | 6.19 |
| (1,674) | 1:209:H:ALA:C | 1:210:H:THR:N | 1:210:H:THR:CA | 1:210:H:THR:C | 10 | 6.19 |
| (1,426) | 1:185:L:MET:C | 1:186:L:THR:N | 1:186:L:THR:CA | 1:186:L:THR:C | 10 | 6.19 |
| (1,62) | 1:152:H:ASP:N | 1:152:H:ASP:CA | 1:152:H:ASP:C | 1:153:H:ILE:N | 8 | 6.19 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 1 | 6.18 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 1 | 6.17 |
| (1,1026) | 1:239:L:THR:C | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 6 | 6.17 |
| (1,1024) | 1:239:J:THR:C | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 8 | 6.17 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 2 | 6.17 |
| (1,1111) | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1:243:G:THR:N | 10 | 6.15 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 10 | 6.14 |
| (1,1009) | 1:238:G:VAL:C | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 8 | 6.11 |
| (1,310) | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 1:175:J:GLU:N | 2 | 6.11 |
| (1,1021) | 1:239:G:THR:C | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 6 | 6.1 |
| (1,1031) | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 1:241:K:THR:N | 1 | 6.09 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 1 | 6.09 |
| (1,911) | 1:230:K:VAL:N | 1:230:K:VAL:CA | 1:230:K:VAL:C | 1:231:K:LEU:N | 9 | 6.09 |
| (1,873) | 1:227:I:LYS:N | 1:227:I:LYS:CA | 1:227:I:LYS:C | 1:228:I:ALA:N | 5 | 6.09 |
| (1,501) | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 1:193:I:ASN:N | 4 | 6.09 |
| (1,61) | 1:152:G:ASP:N | 1:152:G:ASP:CA | 1:152:G:ASP:C | 1:153:G:ILE:N | 8 | 6.09 |
| (1,674) | 1:209:H:ALA:C | 1:210:H:THR:N | 1:210:H:THR:CA | 1:210:H:THR:C | 4 | 6.08 |
| (1,1020) | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 1:240:L:ASN:N | 3 | 6.05 |
| (1,482) | 1:190:H:LEU:C | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 2 | 6.05 |
| (1,70) | 1:153:J:ILE:N | 1:153:J:ILE:CA | 1:153:J:ILE:C | 1:154:J:ARG:N | 4 | 6.05 |
| (1,410) | 1:184:H:TRP:C | 1:185:H:MET:N | 1:185:H:MET:CA | 1:185:H:MET:C | 8 | 6.04 |
| (1,59) | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 1:152:K:ASP:N | 3 | 6.04 |
| (1,483) | 1:190:I:LEU:C | 1:191:I:VAL:N | 1:191:I:VAL:CA | 1:191:I:VAL:C | 5 | 6.03 |
| (1,482) | 1:190:H:LEU:C | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 4 | 6.03 |
| (1,1025) | 1:239:K:THR:C | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 2 | 6.02 |
| (1,1023) | 1:239:I:THR:C | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 8 | 6.02 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1021) | 1:239:G:THR:C | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 2 | 6.01 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 6 | 6.0 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 1 | 5.99 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 2 | 5.98 |
| (1,800) | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1:221:H:VAL:N | 6 | 5.98 |
| (1,307) | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 1:175:G:GLU:N | 3 | 5.97 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 3 | 5.97 |
| (1,1030) | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 1:241:J:THR:N | 5 | 5.95 |
| (1,839) | 1:224:K:PRO:N | 1:224:K:PRO:CA | 1:224:K:PRO:C | 1:225:K:GLY:N | 8 | 5.94 |
| (1,677) | 1:209:K:ALA:C | 1:210:K:THR:N | 1:210:K:THR:CA | 1:210:K:THR:C | 2 | 5.94 |
| (1,445) | 1:187:G:GLU:C | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 7 | 5.93 |
| (1,371) | 1:181:K:VAL:N | 1:181:K:VAL:CA | 1:181:K:VAL:C | 1:182:K:LYS:N | 1 | 5.93 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 4 | 5.93 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 10 | 5.93 |
| (1,796) | 1:219:J:GLN:C | 1:220:J:GLY:N | 1:220:J:GLY:CA | 1:220:J:GLY:C | 5 | 5.92 |
| (1,501) | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 1:193:I:ASN:N | 10 | 5.92 |
| (1,450) | 1:187:L:GLU:C | 1:188:L:THR:N | 1:188:L:THR:CA | 1:188:L:THR:C | 2 | 5.92 |
| (1,1111) | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1:243:G:THR:N | 2 | 5.91 |
| (1,804) | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 1:221:L:VAL:N | 7 | 5.91 |
| (1,1014) | 1:238:L:VAL:C | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 10 | 5.9 |
| (1,508) | 1:192:J:GLN:C | 1:193:J:ASN:N | 1:193:J:ASN:CA | 1:193:J:ASN:C | 9 | 5.9 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 7 | 5.89 |
| (1,483) | 1:190:I:LEU:C | 1:191:I:VAL:N | 1:191:I:VAL:CA | 1:191:I:VAL:C | 8 | 5.89 |
| (1,70) | 1:153:J:ILE:N | 1:153:J:ILE:CA | 1:153:J:ILE:C | 1:154:J:ARG:N | 10 | 5.89 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 5 | 5.88 |
| (1,1032) | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 1:241:L:THR:N | 10 | 5.88 |
| (1,1020) | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 1:240:L:ASN:N | 5 | 5.88 |
| (1,1014) | 1:238:L:VAL:C | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 9 | 5.88 |
| (1,978) | 1:235:L:MET:C | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 6 | 5.87 |
| (1,120) | 1:158:L:LYS:N | 1:158:L:LYS:CA | 1:158:L:LYS:C | 1:159:L:GLU:N | 1 | 5.87 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 7 | 5.86 |
| (1,804) | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 1:221:L:VAL:N | 2 | 5.85 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 3 | 5.85 |
| (1,912) | 1:230:L:VAL:N | 1:230:L:VAL:CA | 1:230:L:VAL:C | 1:231:L:LEU:N | 9 | 5.83 |
| (1,442) | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 1:188:J:THR:N | 3 | 5.83 |
| (1,57) | 1:151:I:LEU:N | 1:151:I:LEU:CA | 1:151:I:LEU:C | 1:152:I:ASP:N | 1 | 5.82 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 8 | 5.82 |
| (1,677) | 1:209:K:ALA:C | 1:210:K:THR:N | 1:210:K:THR:CA | 1:210:K:THR:C | 10 | 5.81 |
| (1,450) | 1:187:L:GLU:C | 1:188:L:THR:N | 1:188:L:THR:CA | 1:188:L:THR:C | 6 | 5.81 |
| (1,423) | 1:185:I:MET:C | 1:186:I:THR:N | 1:186:I:THR:CA | 1:186:I:THR:C | 6 | 5.8 |
| (1,1030) | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 1:241:J:THR:N | 4 | 5.79 |
| (1,1027) | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1:241:G:THR:N | 9 | 5.79 |
| (1,669) | 1:209:I:ALA:N | 1:209:I:ALA:CA | 1:209:I:ALA:C | 1:210:I:THR:N | 1 | 5.79 |
| (1,1024) | 1:239:J:THR:C | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 2 | 5.78 |
| (1,61) | 1:152:G:ASP:N | 1:152:G:ASP:CA | 1:152:G:ASP:C | 1:153:G:ILE:N | 5 | 5.78 |
| (1,813) | 1:221:I:VAL:N | 1:221:I:VAL:CA | 1:221:I:VAL:C | 1:222:I:GLY:N | 9 | 5.77 |
| (1,893) | 1:228:K:ALA:C | 1:229:K:ARG:N | 1:229:K:ARG:CA | 1:229:K:ARG:C | 2 | 5.76 |
| (1,225) | 1:167:I:ARG:N | 1:167:I:ARG:CA | 1:167:I:ARG:C | 1:168:I:PHE:N | 3 | 5.76 |
| (1,644) | 1:205:H:LEU:N | 1:205:H:LEU:CA | 1:205:H:LEU:C | 1:206:H:GLY:N | 8 | 5.75 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 7 | 5.74 |
| (1,57) | 1:151:I:LEU:N | 1:151:I:LEU:CA | 1:151:I:LEU:C | 1:152:I:ASP:N | 4 | 5.74 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,896) | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 1:230:H:VAL:N | 9 | 5.73 |
| (1,89) | 1:154:K:ARG:C | 1:155:K:GLN:N | 1:155:K:GLN:CA | 1:155:K:GLN:C | 1 | 5.73 |
| (1,556) | 1:197:J:ASP:C | 1:198:J:CYS:N | 1:198:J:CYS:CA | 1:198:J:CYS:C | 5 | 5.71 |
| (1,404) | 1:184:H:TRP:N | 1:184:H:TRP:CA | 1:184:H:TRP:C | 1:185:H:MET:N | 9 | 5.71 |
| (1,1031) | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 1:241:K:THR:N | 7 | 5.7 |
| (1,89) | 1:154:K:ARG:C | 1:155:K:GLN:N | 1:155:K:GLN:CA | 1:155:K:GLN:C | 6 | 5.7 |
| (1,857) | 1:225:K:GLY:C | 1:226:K:HIS:N | 1:226:K:HIS:CA | 1:226:K:HIS:C | 9 | 5.69 |
| (1,26) | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 1:148:H:THR:N | 5 | 5.69 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 2 | 5.67 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 9 | 5.66 |
| (1,1111) | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1:243:G:THR:N | 1 | 5.66 |
| (1,86) | 1:154:H:ARG:C | 1:155:H:GLN:N | 1:155:H:GLN:CA | 1:155:H:GLN:C | 7 | 5.66 |
| (1,764) | 1:217:H:ALA:N | 1:217:H:ALA:CA | 1:217:H:ALA:C | 1:218:H:CYS:N | 10 | 5.65 |
| (1,320) | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 1:178:H:SER:N | 9 | 5.65 |
| (1,1111) | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1:243:G:THR:N | 6 | 5.64 |
| (1,501) | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 1:193:I:ASN:N | 9 | 5.64 |
| (1,86) | 1:154:H:ARG:C | 1:155:H:GLN:N | 1:155:H:GLN:CA | 1:155:H:GLN:C | 6 | 5.64 |
| (1,1018) | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 1:240:J:ASN:N | 9 | 5.62 |
| (1,558) | 1:197:L:ASP:C | 1:198:L:CYS:N | 1:198:L:CYS:CA | 1:198:L:CYS:C | 5 | 5.62 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 2 | 5.62 |
| (1,674) | 1:209:H:ALA:C | 1:210:H:THR:N | 1:210:H:THR:CA | 1:210:H:THR:C | 8 | 5.61 |
| (1,88) | 1:154:J:ARG:C | 1:155:J:GLN:N | 1:155:J:GLN:CA | 1:155:J:GLN:C | 10 | 5.6 |
| (1,33) | 1:147:I:PRO:C | 1:148:I:THR:N | 1:148:I:THR:CA | 1:148:I:THR:C | 10 | 5.6 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 10 | 5.58 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 8 | 5.58 |
| (1,615) | 1:202:I:LEU:C | 1:203:I:LYS:N | 1:203:I:LYS:CA | 1:203:I:LYS:C | 10 | 5.58 |
| (1,116) | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 1:159:H:GLU:N | 9 | 5.58 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 2 | 5.56 |
| (1,1020) | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 1:240:L:ASN:N | 9 | 5.56 |
| (1,305) | 1:173:K:ARG:C | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 7 | 5.56 |
| (1,140) | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 1:161:H:PHE:N | 2 | 5.55 |
| (1,42) | 1:148:L:THR:C | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 7 | 5.55 |
| (1,1028) | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 1:241:H:THR:N | 9 | 5.54 |
| (1,310) | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 1:175:J:GLU:N | 3 | 5.54 |
| (1,1018) | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 1:240:J:ASN:N | 7 | 5.52 |
| (1,851) | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 1:226:K:HIS:N | 3 | 5.52 |
| (1,116) | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 1:159:H:GLU:N | 3 | 5.52 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 4 | 5.51 |
| (1,1025) | 1:239:K:THR:C | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 6 | 5.5 |
| (1,1022) | 1:239:H:THR:C | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 9 | 5.49 |
| (1,798) | 1:219:L:GLN:C | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 10 | 5.49 |
| (1,70) | 1:153:J:ILE:N | 1:153:J:ILE:CA | 1:153:J:ILE:C | 1:154:J:ARG:N | 3 | 5.49 |
| (1,436) | 1:186:J:THR:C | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 10 | 5.48 |
| (1,317) | 1:176:K:GLN:C | 1:177:K:ALA:N | 1:177:K:ALA:CA | 1:177:K:ALA:C | 10 | 5.48 |
| (1,1104) | 1:207:L:PRO:N | 1:207:L:PRO:CA | 1:207:L:PRO:C | 1:208:L:GLY:N | 3 | 5.47 |
| (1,120) | 1:158:L:LYS:N | 1:158:L:LYS:CA | 1:158:L:LYS:C | 1:159:L:GLU:N | 8 | 5.47 |
| (1,36) | 1:147:L:PRO:C | 1:148:L:THR:N | 1:148:L:THR:CA | 1:148:L:THR:C | 5 | 5.47 |
| (1,33) | 1:147:I:PRO:C | 1:148:I:THR:N | 1:148:I:THR:CA | 1:148:I:THR:C | 5 | 5.47 |
| (1,815) | 1:221:K:VAL:N | 1:221:K:VAL:CA | 1:221:K:VAL:C | 1:222:K:GLY:N | 10 | 5.45 |
| (1,89) | 1:154:K:ARG:C | 1:155:K:GLN:N | 1:155:K:GLN:CA | 1:155:K:GLN:C | 5 | 5.45 |
| (1,815) | 1:221:K:VAL:N | 1:221:K:VAL:CA | 1:221:K:VAL:C | 1:222:K:GLY:N | 3 | 5.43 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 8 | 5.43 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 3 | 5.41 |
| (1,380) | 1:182:H:LYS:N | 1:182:H:LYS:CA | 1:182:H:LYS:C | 1:183:H:ASN:N | 10 | 5.41 |
| (1,1022) | 1:239:H:THR:C | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 3 | 5.39 |
| (1,674) | 1:209:H:ALA:C | 1:210:H:THR:N | 1:210:H:THR:CA | 1:210:H:THR:C | 2 | 5.39 |
| (1,1028) | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 1:241:H:THR:N | 5 | 5.38 |
| (1,1011) | 1:238:I:VAL:C | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 7 | 5.38 |
| (1,798) | 1:219:L:GLN:C | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 6 | 5.38 |
| (1,682) | 1:210:J:THR:N | 1:210:J:THR:CA | 1:210:J:THR:C | 1:211:J:LEU:N | 3 | 5.38 |
| (1,674) | 1:209:H:ALA:C | 1:210:H:THR:N | 1:210:H:THR:CA | 1:210:H:THR:C | 1 | 5.38 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 8 | 5.38 |
| (1,979) | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1:237:G:GLN:N | 8 | 5.37 |
| (1,447) | 1:187:I:GLU:C | 1:188:I:THR:N | 1:188:I:THR:CA | 1:188:I:THR:C | 8 | 5.37 |
| (1,37) | 1:148:G:THR:C | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 5 | 5.37 |
| (1,1031) | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 1:241:K:THR:N | 10 | 5.36 |
| (1,1028) | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 1:241:H:THR:N | 7 | 5.36 |
| (1,1014) | 1:238:L:VAL:C | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 5 | 5.36 |
| (1,62) | 1:152:H:ASP:N | 1:152:H:ASP:CA | 1:152:H:ASP:C | 1:153:H:ILE:N | 3 | 5.36 |
| (1,483) | 1:190:I:LEU:C | 1:191:I:VAL:N | 1:191:I:VAL:CA | 1:191:I:VAL:C | 6 | 5.35 |
| (1,63) | 1:152:I:ASP:N | 1:152:I:ASP:CA | 1:152:I:ASP:C | 1:153:I:ILE:N | 6 | 5.35 |
| (1,34) | 1:147:J:PRO:C | 1:148:J:THR:N | 1:148:J:THR:CA | 1:148:J:THR:C | 2 | 5.35 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 6 | 5.32 |
| (1,1010) | 1:238:H:VAL:C | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 7 | 5.32 |
| (1,676) | 1:209:J:ALA:C | 1:210:J:THR:N | 1:210:J:THR:CA | 1:210:J:THR:C | 6 | 5.32 |
| (1,1025) | 1:239:K:THR:C | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 7 | 5.31 |
| (1,1022) | 1:239:H:THR:C | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 8 | 5.31 |
| (1,912) | 1:230:L:VAL:N | 1:230:L:VAL:CA | 1:230:L:VAL:C | 1:231:L:LEU:N | 6 | 5.31 |
| (1,441) | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 1:188:I:THR:N | 1 | 5.31 |
| (1,59) | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 1:152:K:ASP:N | 4 | 5.31 |
| (1,1018) | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 1:240:J:ASN:N | 3 | 5.3 |
| (1,231) | 1:167:I:ARG:C | 1:168:I:PHE:N | 1:168:I:PHE:CA | 1:168:I:PHE:C | 2 | 5.29 |
| (1,434) | 1:186:H:THR:C | 1:187:H:GLU:N | 1:187:H:GLU:CA | 1:187:H:GLU:C | 9 | 5.28 |
| (1,59) | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 1:152:K:ASP:N | 2 | 5.28 |
| (1,1025) | 1:239:K:THR:C | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 4 | 5.27 |
| (1,767) | 1:217:K:ALA:N | 1:217:K:ALA:CA | 1:217:K:ALA:C | 1:218:K:CYS:N | 8 | 5.27 |
| (1,912) | 1:230:L:VAL:N | 1:230:L:VAL:CA | 1:230:L:VAL:C | 1:231:L:LEU:N | 2 | 5.26 |
| (1,897) | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 1:230:I:VAL:N | 2 | 5.26 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 1 | 5.25 |
| (1,804) | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 1:221:L:VAL:N | 9 | 5.25 |
| (1,538) | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 1:197:J:ASP:N | 8 | 5.25 |
| (1,1028) | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 1:241:H:THR:N | 1 | 5.24 |
| (1,307) | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 1:175:G:GLU:N | 7 | 5.24 |
| (1,57) | 1:151:I:LEU:N | 1:151:I:LEU:CA | 1:151:I:LEU:C | 1:152:I:ASP:N | 3 | 5.24 |
| (1,1077) | 1:175:I:GLU:N | 1:175:I:GLU:CA | 1:175:I:GLU:C | 1:176:I:GLN:N | 6 | 5.23 |
| (1,1027) | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1:241:G:THR:N | 5 | 5.23 |
| (1,1021) | 1:239:G:THR:C | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1 | 5.23 |
| (1,1018) | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 1:240:J:ASN:N | 1 | 5.23 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 4 | 5.23 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 10 | 5.23 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 9 | 5.22 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 9 | 5.22 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,90) | 1:154:L:ARG:C | 1:155:L:GLN:N | 1:155:L:GLN:CA | 1:155:L:GLN:C | 10 | 5.22 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 1 | 5.21 |
| (1,796) | 1:219:J:GLN:C | 1:220:J:GLY:N | 1:220:J:GLY:CA | 1:220:J:GLY:C | 1 | 5.21 |
| (1,893) | 1:228:K:ALA:C | 1:229:K:ARG:N | 1:229:K:ARG:CA | 1:229:K:ARG:C | 1 | 5.2 |
| (1,499) | 1:192:G:GLN:N | 1:192:G:GLN:CA | 1:192:G:GLN:C | 1:193:G:ASN:N | 3 | 5.2 |
| (1,56) | 1:151:H:LEU:N | 1:151:H:LEU:CA | 1:151:H:LEU:C | 1:152:H:ASP:N | 2 | 5.2 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 5 | 5.19 |
| (1,1022) | 1:239:H:THR:C | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 6 | 5.18 |
| (1,320) | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 1:178:H:SER:N | 2 | 5.18 |
| (1,669) | 1:209:I:ALA:N | 1:209:I:ALA:CA | 1:209:I:ALA:C | 1:210:I:THR:N | 3 | 5.17 |
| (1,1014) | 1:238:L:VAL:C | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 7 | 5.15 |
| (1,674) | 1:209:H:ALA:C | 1:210:H:THR:N | 1:210:H:THR:CA | 1:210:H:THR:C | 3 | 5.15 |
| (1,410) | 1:184:H:TRP:C | 1:185:H:MET:N | 1:185:H:MET:CA | 1:185:H:MET:C | 9 | 5.15 |
| (1,1029) | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 1:241:I:THR:N | 5 | 5.14 |
| (1,1021) | 1:239:G:THR:C | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 3 | 5.14 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 6 | 5.14 |
| (1,33) | 1:147:I:PRO:C | 1:148:I:THR:N | 1:148:I:THR:CA | 1:148:I:THR:C | 3 | 5.13 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 9 | 5.11 |
| (1,947) | 1:233:K:GLU:N | 1:233:K:GLU:CA | 1:233:K:GLU:C | 1:234:K:ALA:N | 4 | 5.11 |
| (1,316) | 1:176:J:GLN:C | 1:177:J:ALA:N | 1:177:J:ALA:CA | 1:177:J:ALA:C | 9 | 5.09 |
| (1,269) | 1:170:K:LYS:C | 1:171:K:THR:N | 1:171:K:THR:CA | 1:171:K:THR:C | 3 | 5.09 |
| (1,70) | 1:153:J:ILE:N | 1:153:J:ILE:CA | 1:153:J:ILE:C | 1:154:J:ARG:N | 2 | 5.09 |
| (1,446) | 1:187:H:GLU:C | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 3 | 5.08 |
| (1,1111) | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1:243:G:THR:N | 3 | 5.07 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 10 | 5.07 |
| (1,1111) | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1:243:G:THR:N | 4 | 5.06 |
| (1,677) | 1:209:K:ALA:C | 1:210:K:THR:N | 1:210:K:THR:CA | 1:210:K:THR:C | 6 | 5.06 |
| (1,441) | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 1:188:I:THR:N | 2 | 5.06 |
| (1,674) | 1:209:H:ALA:C | 1:210:H:THR:N | 1:210:H:THR:CA | 1:210:H:THR:C | 5 | 5.05 |
| (1,326) | 1:177:H:ALA:C | 1:178:H:SER:N | 1:178:H:SER:CA | 1:178:H:SER:C | 1 | 5.05 |
| (1,59) | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 1:152:K:ASP:N | 6 | 5.05 |
| (1,26) | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 1:148:H:THR:N | 4 | 5.05 |
| (1,798) | 1:219:L:GLN:C | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 8 | 5.04 |
| (1,65) | 1:152:K:ASP:N | 1:152:K:ASP:CA | 1:152:K:ASP:C | 1:153:K:ILE:N | 1 | 5.04 |
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 1 | 5.04 |
| (1,500) | 1:192:H:GLN:N | 1:192:H:GLN:CA | 1:192:H:GLN:C | 1:193:H:ASN:N | 8 | 5.02 |
| (1,116) | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 1:159:H:GLU:N | 6 | 5.02 |
| (1,1014) | 1:238:L:VAL:C | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 4 | 5.01 |
| (1,87) | 1:154:I:ARG:C | 1:155:I:GLN:N | 1:155:I:GLN:CA | 1:155:I:GLN:C | 2 | 5.01 |
| (1,59) | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 1:152:K:ASP:N | 5 | 5.01 |
| (1,47) | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 1:150:K:ILE:N | 7 | 5.01 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 2 | 5.0 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 2 | 5.0 |
| (1,1032) | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 1:241:L:THR:N | 2 | 4.98 |
| (1,504) | 1:192:L:GLN:N | 1:192:L:GLN:CA | 1:192:L:GLN:C | 1:193:L:ASN:N | 5 | 4.98 |
| (1,88) | 1:154:J:ARG:C | 1:155:J:GLN:N | 1:155:J:GLN:CA | 1:155:J:GLN:C | 3 | 4.98 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 2 | 4.97 |
| (1,1104) | 1:207:L:PRO:N | 1:207:L:PRO:CA | 1:207:L:PRO:C | 1:208:L:GLY:N | 4 | 4.97 |
| (1,1104) | 1:207:L:PRO:N | 1:207:L:PRO:CA | 1:207:L:PRO:C | 1:208:L:GLY:N | 8 | 4.97 |
| (1,1010) | 1:238:H:VAL:C | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 5 | 4.96 |
| (1,30) | 1:147:L:PRO:N | 1:147:L:PRO:CA | 1:147:L:PRO:C | 1:148:L:THR:N | 3 | 4.96 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1018) | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 1:240:J:ASN:N | 5 | 4.95 |
| (1,911) | 1:230:K:VAL:N | 1:230:K:VAL:CA | 1:230:K:VAL:C | 1:231:K:LEU:N | 6 | 4.95 |
| (1,800) | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1:221:H:VAL:N | 10 | 4.95 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 6 | 4.95 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 9 | 4.94 |
| (1,1032) | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 1:241:L:THR:N | 1 | 4.94 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 9 | 4.94 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 9 | 4.94 |
| (1,1077) | 1:175:I:GLU:N | 1:175:I:GLU:CA | 1:175:I:GLU:C | 1:176:I:GLN:N | 9 | 4.93 |
| (1,225) | 1:167:I:ARG:N | 1:167:I:ARG:CA | 1:167:I:ARG:C | 1:168:I:PHE:N | 2 | 4.91 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 2 | 4.9 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 8 | 4.9 |
| (1,675) | 1:209:I:ALA:C | 1:210:I:THR:N | 1:210:I:THR:CA | 1:210:I:THR:C | 5 | 4.89 |
| (1,974) | 1:235:H:MET:C | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 8 | 4.88 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 10 | 4.87 |
| (1,1014) | 1:238:L:VAL:C | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 3 | 4.87 |
| (1,634) | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 1:205:J:LEU:N | 6 | 4.87 |
| (1,107) | 1:157:K:PRO:N | 1:157:K:PRO:CA | 1:157:K:PRO:C | 1:158:K:LYS:N | 1 | 4.87 |
| (1,827) | 1:223:K:GLY:N | 1:223:K:GLY:CA | 1:223:K:GLY:C | 1:224:K:PRO:N | 7 | 4.86 |
| (1,675) | 1:209:I:ALA:C | 1:210:I:THR:N | 1:210:I:THR:CA | 1:210:I:THR:C | 4 | 4.86 |
| (1,1030) | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 1:241:J:THR:N | 2 | 4.85 |
| (1,1029) | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 1:241:I:THR:N | 2 | 4.85 |
| (1,1024) | 1:239:J:THR:C | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 6 | 4.85 |
| (1,815) | 1:221:K:VAL:N | 1:221:K:VAL:CA | 1:221:K:VAL:C | 1:222:K:GLY:N | 9 | 4.85 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 5 | 4.85 |
| (1,316) | 1:176:J:GLN:C | 1:177:J:ALA:N | 1:177:J:ALA:CA | 1:177:J:ALA:C | 10 | 4.85 |
| (1,1037) | 1:240:K:ASN:C | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 5 | 4.84 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 4 | 4.84 |
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 8 | 4.84 |
| (1,27) | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 1:148:I:THR:N | 9 | 4.84 |
| (1,981) | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 1:237:I:GLN:N | 8 | 4.82 |
| (1,794) | 1:219:H:GLN:C | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 10 | 4.82 |
| (1,313) | 1:176:G:GLN:C | 1:177:G:ALA:N | 1:177:G:ALA:CA | 1:177:G:ALA:C | 10 | 4.82 |
| (1,608) | 1:202:H:LEU:N | 1:202:H:LEU:CA | 1:202:H:LEU:C | 1:203:H:LYS:N | 2 | 4.81 |
| (1,89) | 1:154:K:ARG:C | 1:155:K:GLN:N | 1:155:K:GLN:CA | 1:155:K:GLN:C | 2 | 4.81 |
| (1,1104) | 1:207:L:PRO:N | 1:207:L:PRO:CA | 1:207:L:PRO:C | 1:208:L:GLY:N | 7 | 4.8 |
| (1,483) | 1:190:I:LEU:C | 1:191:I:VAL:N | 1:191:I:VAL:CA | 1:191:I:VAL:C | 2 | 4.8 |
| (1,28) | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 1:148:J:THR:N | 7 | 4.8 |
| (1,1104) | 1:207:L:PRO:N | 1:207:L:PRO:CA | 1:207:L:PRO:C | 1:208:L:GLY:N | 1 | 4.79 |
| (1,1021) | 1:239:G:THR:C | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 10 | 4.79 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 4 | 4.79 |
| (1,53) | 1:150:K:ILE:C | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 2 | 4.79 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 5 | 4.77 |
| (1,451) | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 1:189:G:LEU:N | 7 | 4.77 |
| (1,632) | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 1:205:H:LEU:N | 8 | 4.76 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 2 | 4.76 |
| (1,1037) | 1:240:K:ASN:C | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 9 | 4.75 |
| (1,1011) | 1:238:I:VAL:C | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 1 | 4.75 |
| (1,983) | 1:236:K:SER:N | 1:236:K:SER:CA | 1:236:K:SER:C | 1:237:K:GLN:N | 9 | 4.75 |
| (1,396) | 1:183:L:ASN:N | 1:183:L:ASN:CA | 1:183:L:ASN:C | 1:184:L:TRP:N | 7 | 4.75 |
| (1,188) | 1:164:H:TYR:N | 1:164:H:TYR:CA | 1:164:H:TYR:C | 1:165:H:VAL:N | 9 | 4.75 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,70) | 1:153:J:ILE:N | 1:153:J:ILE:CA | 1:153:J:ILE:C | 1:154:J:ARG:N | 6 | 4.75 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 7 | 4.74 |
| (1,1032) | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 1:241:L:THR:N | 7 | 4.74 |
| (1,921) | 1:231:I:LEU:N | 1:231:I:LEU:CA | 1:231:I:LEU:C | 1:232:I:ALA:N | 9 | 4.73 |
| (1,312) | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 1:175:L:GLU:N | 10 | 4.73 |
| (1,1021) | 1:239:G:THR:C | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 4 | 4.72 |
| (1,444) | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 1:188:L:THR:N | 1 | 4.71 |
| (1,423) | 1:185:I:MET:C | 1:186:I:THR:N | 1:186:I:THR:CA | 1:186:I:THR:C | 3 | 4.71 |
| (1,120) | 1:158:L:LYS:N | 1:158:L:LYS:CA | 1:158:L:LYS:C | 1:159:L:GLU:N | 9 | 4.71 |
| (1,119) | 1:158:K:LYS:N | 1:158:K:LYS:CA | 1:158:K:LYS:C | 1:159:K:GLU:N | 1 | 4.71 |
| (1,42) | 1:148:L:THR:C | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 6 | 4.71 |
| (1,482) | 1:190:H:LEU:C | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 5 | 4.7 |
| (1,1104) | 1:207:L:PRO:N | 1:207:L:PRO:CA | 1:207:L:PRO:C | 1:208:L:GLY:N | 10 | 4.69 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 10 | 4.69 |
| (1,849) | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 1:226:I:HIS:N | 4 | 4.69 |
| (1,516) | 1:193:L:ASN:N | 1:193:L:ASN:CA | 1:193:L:ASN:C | 1:194:L:ALA:N | 7 | 4.69 |
| (1,59) | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 1:152:K:ASP:N | 10 | 4.69 |
| (1,1023) | 1:239:I:THR:C | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 2 | 4.68 |
| (1,1080) | 1:175:L:GLU:N | 1:175:L:GLU:CA | 1:175:L:GLU:C | 1:176:L:GLN:N | 5 | 4.67 |
| (1,155) | 1:161:K:PHE:N | 1:161:K:PHE:CA | 1:161:K:PHE:C | 1:162:K:ARG:N | 2 | 4.67 |
| (1,808) | 1:220:J:GLY:C | 1:221:J:VAL:N | 1:221:J:VAL:CA | 1:221:J:VAL:C | 9 | 4.66 |
| (1,316) | 1:176:J:GLN:C | 1:177:J:ALA:N | 1:177:J:ALA:CA | 1:177:J:ALA:C | 1 | 4.66 |
| (1,556) | 1:197:J:ASP:C | 1:198:J:CYS:N | 1:198:J:CYS:CA | 1:198:J:CYS:C | 8 | 4.65 |
| (1,305) | 1:173:K:ARG:C | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 1 | 4.65 |
| (1,116) | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 1:159:H:GLU:N | 1 | 4.65 |
| (1,32) | 1:147:H:PRO:C | 1:148:H:THR:N | 1:148:H:THR:CA | 1:148:H:THR:C | 4 | 4.65 |
| (1,1044) | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1:242:L:ALA:N | 2 | 4.64 |
| (1,1002) | 1:237:L:GLN:C | 1:238:L:VAL:N | 1:238:L:VAL:CA | 1:238:L:VAL:C | 1 | 4.63 |
| (1,889) | 1:228:G:ALA:C | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 3 | 4.63 |
| (1,815) | 1:221:K:VAL:N | 1:221:K:VAL:CA | 1:221:K:VAL:C | 1:222:K:GLY:N | 4 | 4.63 |
| (1,675) | 1:209:I:ALA:C | 1:210:I:THR:N | 1:210:I:THR:CA | 1:210:I:THR:C | 3 | 4.63 |
| (1,426) | 1:185:L:MET:C | 1:186:L:THR:N | 1:186:L:THR:CA | 1:186:L:THR:C | 4 | 4.63 |
| (1,894) | 1:228:L:ALA:C | 1:229:L:ARG:N | 1:229:L:ARG:CA | 1:229:L:ARG:C | 6 | 4.62 |
| (1,1029) | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 1:241:I:THR:N | 4 | 4.61 |
| (1,426) | 1:185:L:MET:C | 1:186:L:THR:N | 1:186:L:THR:CA | 1:186:L:THR:C | 9 | 4.61 |
| (1,1104) | 1:207:L:PRO:N | 1:207:L:PRO:CA | 1:207:L:PRO:C | 1:208:L:GLY:N | 2 | 4.6 |
| (1,1044) | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1:242:L:ALA:N | 1 | 4.6 |
| (1,476) | 1:190:H:LEU:N | 1:190:H:LEU:CA | 1:190:H:LEU:C | 1:191:H:VAL:N | 2 | 4.6 |
| (1,243) | 1:168:I:PHE:C | 1:169:I:TYR:N | 1:169:I:TYR:CA | 1:169:I:TYR:C | 2 | 4.6 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 5 | 4.59 |
| (1,1073) | 1:174:K:ALA:C | 1:175:K:GLU:N | 1:175:K:GLU:CA | 1:175:K:GLU:C | 8 | 4.59 |
| (1,1023) | 1:239:I:THR:C | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 7 | 4.59 |
| (1,737) | 1:214:K:MET:C | 1:215:K:MET:N | 1:215:K:MET:CA | 1:215:K:MET:C | 1 | 4.59 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 2 | 4.58 |
| (1,32) | 1:147:H:PRO:C | 1:148:H:THR:N | 1:148:H:THR:CA | 1:148:H:THR:C | 8 | 4.58 |
| (1,677) | 1:209:K:ALA:C | 1:210:K:THR:N | 1:210:K:THR:CA | 1:210:K:THR:C | 9 | 4.57 |
| (1,1017) | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 1:240:I:ASN:N | 8 | 4.56 |
| (1,1111) | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1:243:G:THR:N | 9 | 4.55 |
| (1,1104) | 1:207:L:PRO:N | 1:207:L:PRO:CA | 1:207:L:PRO:C | 1:208:L:GLY:N | 6 | 4.55 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 10 | 4.55 |
| (1,58) | 1:151:J:LEU:N | 1:151:J:LEU:CA | 1:151:J:LEU:C | 1:152:J:ASP:N | 8 | 4.55 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,911) | 1:230:K:VAL:N | 1:230:K:VAL:CA | 1:230:K:VAL:C | 1:231:K:LEU:N | 10 | 4.54 |
| (1,903) | 1:229:I:ARG:C | 1:230:I:VAL:N | 1:230:I:VAL:CA | 1:230:I:VAL:C | 8 | 4.54 |
| (1,889) | 1:228:G:ALA:C | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 8 | 4.54 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 2 | 4.54 |
| (1,1029) | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 1:241:I:THR:N | 6 | 4.53 |
| (1,1027) | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1:241:G:THR:N | 4 | 4.53 |
| (1,446) | 1:187:H:GLU:C | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 6 | 4.53 |
| (1,1036) | 1:240:J:ASN:C | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 8 | 4.52 |
| (1,800) | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1:221:H:VAL:N | 9 | 4.52 |
| (1,893) | 1:228:K:ALA:C | 1:229:K:ARG:N | 1:229:K:ARG:CA | 1:229:K:ARG:C | 10 | 4.51 |
| (1,798) | 1:219:L:GLN:C | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 1 | 4.51 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 4 | 4.51 |
| (1,796) | 1:219:J:GLN:C | 1:220:J:GLY:N | 1:220:J:GLY:CA | 1:220:J:GLY:C | 3 | 4.5 |
| (1,483) | 1:190:I:LEU:C | 1:191:I:VAL:N | 1:191:I:VAL:CA | 1:191:I:VAL:C | 3 | 4.5 |
| (1,1111) | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1:243:G:THR:N | 5 | 4.49 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 7 | 4.49 |
| (1,522) | 1:194:L:ALA:C | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 9 | 4.49 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 5 | 4.49 |
| (1,28) | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 1:148:J:THR:N | 9 | 4.49 |
| (1,1031) | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 1:241:K:THR:N | 6 | 4.48 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 3 | 4.47 |
| (1,423) | 1:185:I:MET:C | 1:186:I:THR:N | 1:186:I:THR:CA | 1:186:I:THR:C | 7 | 4.47 |
| (1,380) | 1:182:H:LYS:N | 1:182:H:LYS:CA | 1:182:H:LYS:C | 1:183:H:ASN:N | 3 | 4.47 |
| (1,1002) | 1:237:L:GLN:C | 1:238:L:VAL:N | 1:238:L:VAL:CA | 1:238:L:VAL:C | 7 | 4.45 |
| (1,900) | 1:229:L:ARG:N | 1:229:L:ARG:CA | 1:229:L:ARG:C | 1:230:L:VAL:N | 2 | 4.45 |
| (1,832) | 1:223:J:GLY:C | 1:224:J:PRO:N | 1:224:J:PRO:CA | 1:224:J:PRO:C | 3 | 4.45 |
| (1,449) | 1:187:K:GLU:C | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 4 | 4.45 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 4 | 4.44 |
| (1,326) | 1:177:H:ALA:C | 1:178:H:SER:N | 1:178:H:SER:CA | 1:178:H:SER:C | 5 | 4.44 |
| (1,615) | 1:202:I:LEU:C | 1:203:I:LYS:N | 1:203:I:LYS:CA | 1:203:I:LYS:C | 7 | 4.42 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 3 | 4.42 |
| (1,116) | 1:158:H:LYS:N | 1:158:H:LYS:CA | 1:158:H:LYS:C | 1:159:H:GLU:N | 4 | 4.42 |
| (1,437) | 1:186:K:THR:C | 1:187:K:GLU:N | 1:187:K:GLU:CA | 1:187:K:GLU:C | 3 | 4.41 |
| (1,45) | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 1:150:I:ILE:N | 6 | 4.41 |
| (1,1024) | 1:239:J:THR:C | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 4 | 4.4 |
| (1,897) | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 1:230:I:VAL:N | 3 | 4.4 |
| (1,827) | 1:223:K:GLY:N | 1:223:K:GLY:CA | 1:223:K:GLY:C | 1:224:K:PRO:N | 9 | 4.4 |
| (1,320) | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 1:178:H:SER:N | 7 | 4.4 |
| (1,895) | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 1:230:G:VAL:N | 3 | 4.39 |
| (1,274) | 1:171:J:THR:N | 1:171:J:THR:CA | 1:171:J:THR:C | 1:172:J:LEU:N | 6 | 4.39 |
| (1,229) | 1:167:G:ARG:C | 1:168:G:PHE:N | 1:168:G:PHE:CA | 1:168:G:PHE:C | 4 | 4.39 |
| (1,1030) | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 1:241:J:THR:N | 6 | 4.38 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 8 | 4.38 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 5 | 4.37 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 3 | 4.37 |
| (1,591) | 1:200:I:THR:C | 1:201:I:ILE:N | 1:201:I:ILE:CA | 1:201:I:ILE:C | 2 | 4.37 |
| (1,518) | 1:194:H:ALA:C | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 5 | 4.37 |
| (1,1002) | 1:237:L:GLN:C | 1:238:L:VAL:N | 1:238:L:VAL:CA | 1:238:L:VAL:C | 9 | 4.36 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 5 | 4.36 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 7 | 4.36 |
| (1,89) | 1:154:K:ARG:C | 1:155:K:GLN:N | 1:155:K:GLN:CA | 1:155:K:GLN:C | 3 | 4.35 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,33) | 1:147:I:PRO:C | 1:148:I:THR:N | 1:148:I:THR:CA | 1:148:I:THR:C | 1 | 4.35 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 8 | 4.34 |
| (1,1038) | 1:240:L:ASN:C | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 5 | 4.34 |
| (1,998) | 1:237:H:GLN:C | 1:238:H:VAL:N | 1:238:H:VAL:CA | 1:238:H:VAL:C | 2 | 4.34 |
| (1,889) | 1:228:G:ALA:C | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 7 | 4.34 |
| (1,895) | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 1:230:G:VAL:N | 6 | 4.33 |
| (1,446) | 1:187:H:GLU:C | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 1 | 4.33 |
| (1,1044) | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1:242:L:ALA:N | 7 | 4.32 |
| (1,1035) | 1:240:I:ASN:C | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 9 | 4.32 |
| (1,538) | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 1:197:J:ASP:N | 7 | 4.32 |
| (1,305) | 1:173:K:ARG:C | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 3 | 4.3 |
| (1,1044) | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1:242:L:ALA:N | 6 | 4.29 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 6 | 4.29 |
| (1,494) | 1:191:H:VAL:C | 1:192:H:GLN:N | 1:192:H:GLN:CA | 1:192:H:GLN:C | 7 | 4.29 |
| (1,903) | 1:229:I:ARG:C | 1:230:I:VAL:N | 1:230:I:VAL:CA | 1:230:I:VAL:C | 1 | 4.28 |
| (1,634) | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 1:205:J:LEU:N | 8 | 4.27 |
| (1,229) | 1:167:G:ARG:C | 1:168:G:PHE:N | 1:168:G:PHE:CA | 1:168:G:PHE:C | 9 | 4.27 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 10 | 4.26 |
| (1,819) | 1:222:I:GLY:N | 1:222:I:GLY:CA | 1:222:I:GLY:C | 1:223:I:GLY:N | 10 | 4.26 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 2 | 4.26 |
| (1,1022) | 1:239:H:THR:C | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 10 | 4.25 |
| (1,1111) | 1:242:G:ALA:N | 1:242:G:ALA:CA | 1:242:G:ALA:C | 1:243:G:THR:N | 8 | 4.24 |
| (1,1079) | 1:175:K:GLU:N | 1:175:K:GLU:CA | 1:175:K:GLU:C | 1:176:K:GLN:N | 3 | 4.24 |
| (1,1022) | 1:239:H:THR:C | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 5 | 4.24 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 3 | 4.24 |
| (1,889) | 1:228:G:ALA:C | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 10 | 4.24 |
| (1,797) | 1:219:K:GLN:C | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 5 | 4.24 |
| (1,1020) | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 1:240:L:ASN:N | 1 | 4.23 |
| (1,1017) | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 1:240:I:ASN:N | 5 | 4.23 |
| (1,1027) | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1:241:G:THR:N | 3 | 4.22 |
| (1,800) | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1:221:H:VAL:N | 2 | 4.22 |
| (1,556) | 1:197:J:ASP:C | 1:198:J:CYS:N | 1:198:J:CYS:CA | 1:198:J:CYS:C | 1 | 4.22 |
| (1,1023) | 1:239:I:THR:C | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 4 | 4.21 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 5 | 4.21 |
| (1,800) | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1:221:H:VAL:N | 5 | 4.21 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 9 | 4.2 |
| (1,441) | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 1:188:I:THR:N | 3 | 4.2 |
| (1,424) | 1:185:J:MET:C | 1:186:J:THR:N | 1:186:J:THR:CA | 1:186:J:THR:C | 1 | 4.2 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 4 | 4.19 |
| (1,89) | 1:154:K:ARG:C | 1:155:K:GLN:N | 1:155:K:GLN:CA | 1:155:K:GLN:C | 7 | 4.19 |
| (1,1010) | 1:238:H:VAL:C | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 6 | 4.18 |
| (1,907) | 1:230:G:VAL:N | 1:230:G:VAL:CA | 1:230:G:VAL:C | 1:231:G:LEU:N | 7 | 4.18 |
| (1,446) | 1:187:H:GLU:C | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 4 | 4.17 |
| (1,33) | 1:147:I:PRO:C | 1:148:I:THR:N | 1:148:I:THR:CA | 1:148:I:THR:C | 7 | 4.17 |
| (1,274) | 1:171:J:THR:N | 1:171:J:THR:CA | 1:171:J:THR:C | 1:172:J:LEU:N | 2 | 4.16 |
| (1,1031) | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 1:241:K:THR:N | 3 | 4.15 |
| (1,728) | 1:214:H:MET:N | 1:214:H:MET:CA | 1:214:H:MET:C | 1:215:H:MET:N | 6 | 4.15 |
| (1,1022) | 1:239:H:THR:C | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 2 | 4.14 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 3 | 4.13 |
| (1,1115) | 1:242:K:ALA:N | 1:242:K:ALA:CA | 1:242:K:ALA:C | 1:243:K:THR:N | 8 | 4.12 |
| (1,136) | 1:159:J:GLU:C | 1:160:J:PRO:N | 1:160:J:PRO:CA | 1:160:J:PRO:C | 8 | 4.12 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,44) | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 1:150:H:ILE:N | 2 | 4.12 |
| (1,1038) | 1:240:L:ASN:C | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 8 | 4.11 |
| (1,1002) | 1:237:L:GLN:C | 1:238:L:VAL:N | 1:238:L:VAL:CA | 1:238:L:VAL:C | 6 | 4.11 |
| (1,30) | 1:147:L:PRO:N | 1:147:L:PRO:CA | 1:147:L:PRO:C | 1:148:L:THR:N | 4 | 4.11 |
| (1,1012) | 1:238:J:VAL:C | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 5 | 4.1 |
| (1,1002) | 1:237:L:GLN:C | 1:238:L:VAL:N | 1:238:L:VAL:CA | 1:238:L:VAL:C | 2 | 4.1 |
| (1,999) | 1:237:I:GLN:C | 1:238:I:VAL:N | 1:238:I:VAL:CA | 1:238:I:VAL:C | 4 | 4.1 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 1 | 4.09 |
| (1,68) | 1:153:H:ILE:N | 1:153:H:ILE:CA | 1:153:H:ILE:C | 1:154:H:ARG:N | 1 | 4.09 |
| (1,1044) | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1:242:L:ALA:N | 3 | 4.08 |
| (1,1030) | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 1:241:J:THR:N | 10 | 4.06 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 1 | 4.04 |
| (1,118) | 1:158:J:LYS:N | 1:158:J:LYS:CA | 1:158:J:LYS:C | 1:159:J:GLU:N | 9 | 4.04 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 8 | 4.03 |
| (1,1010) | 1:238:H:VAL:C | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 10 | 4.03 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 9 | 4.03 |
| (1,232) | 1:167:J:ARG:C | 1:168:J:PHE:N | 1:168:J:PHE:CA | 1:168:J:PHE:C | 1 | 4.03 |
| (1,1028) | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 1:241:H:THR:N | 2 | 4.02 |
| (1,449) | 1:187:K:GLU:C | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 9 | 4.02 |
| (1,309) | 1:174:I:ALA:N | 1:174:I:ALA:CA | 1:174:I:ALA:C | 1:175:I:GLU:N | 9 | 4.02 |
| (1,47) | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 1:150:K:ILE:N | 1 | 4.02 |
| (1,1029) | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 1:241:I:THR:N | 3 | 4.01 |
| (1,1014) | 1:238:L:VAL:C | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 8 | 4.01 |
| (1,889) | 1:228:G:ALA:C | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 1 | 4.01 |
| (1,585) | 1:200:I:THR:N | 1:200:I:THR:CA | 1:200:I:THR:C | 1:201:I:ILE:N | 2 | 4.01 |
| (1,1013) | 1:238:K:VAL:C | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 5 | 4.0 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 9 | 3.99 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 6 | 3.99 |
| (1,442) | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 1:188:J:THR:N | 6 | 3.99 |
| (1,1019) | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 1:240:K:ASN:N | 8 | 3.98 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 6 | 3.98 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 4 | 3.98 |
| (1,1038) | 1:240:L:ASN:C | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 9 | 3.97 |
| (1,1013) | 1:238:K:VAL:C | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 3 | 3.97 |
| (1,492) | 1:191:L:VAL:N | 1:191:L:VAL:CA | 1:191:L:VAL:C | 1:192:L:GLN:N | 9 | 3.97 |
| (1,310) | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 1:175:J:GLU:N | 9 | 3.97 |
| (1,72) | 1:153:L:ILE:N | 1:153:L:ILE:CA | 1:153:L:ILE:C | 1:154:L:ARG:N | 3 | 3.97 |
| (1,1104) | 1:207:L:PRO:N | 1:207:L:PRO:CA | 1:207:L:PRO:C | 1:208:L:GLY:N | 5 | 3.96 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 7 | 3.96 |
| (1,998) | 1:237:H:GLN:C | 1:238:H:VAL:N | 1:238:H:VAL:CA | 1:238:H:VAL:C | 6 | 3.96 |
| (1,998) | 1:237:H:GLN:C | 1:238:H:VAL:N | 1:238:H:VAL:CA | 1:238:H:VAL:C | 10 | 3.96 |
| (1,675) | 1:209:I:ALA:C | 1:210:I:THR:N | 1:210:I:THR:CA | 1:210:I:THR:C | 1 | 3.96 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 7 | 3.96 |
| (1,519) | 1:194:I:ALA:C | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 2 | 3.96 |
| (1,474) | 1:189:L:LEU:C | 1:190:L:LEU:N | 1:190:L:LEU:CA | 1:190:L:LEU:C | 5 | 3.96 |
| (1,442) | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 1:188:J:THR:N | 10 | 3.96 |
| (1,59) | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 1:152:K:ASP:N | 1 | 3.96 |
| (1,33) | 1:147:I:PRO:C | 1:148:I:THR:N | 1:148:I:THR:CA | 1:148:I:THR:C | 9 | 3.95 |
| (1,231) | 1:167:I:ARG:C | 1:168:I:PHE:N | 1:168:I:PHE:CA | 1:168:I:PHE:C | 3 | 3.94 |
| (1,178) | 1:163:J:ASP:N | 1:163:J:ASP:CA | 1:163:J:ASP:C | 1:164:J:TYR:N | 1 | 3.94 |
| (1,60) | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 1:152:L:ASP:N | 7 | 3.94 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,540) | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 1:197:L:ASP:N | 1 | 3.93 |
| (1,320) | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 1:178:H:SER:N | 10 | 3.93 |
| (1,1022) | 1:239:H:THR:C | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 7 | 3.92 |
| (1,640) | 1:204:J:ALA:C | 1:205:J:LEU:N | 1:205:J:LEU:CA | 1:205:J:LEU:C | 2 | 3.92 |
| (1,1012) | 1:238:J:VAL:C | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 8 | 3.91 |
| (1,895) | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 1:230:G:VAL:N | 9 | 3.91 |
| (1,512) | 1:193:H:ASN:N | 1:193:H:ASN:CA | 1:193:H:ASN:C | 1:194:H:ALA:N | 9 | 3.91 |
| (1,42) | 1:148:L:THR:C | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 9 | 3.91 |
| (1,384) | 1:182:L:LYS:N | 1:182:L:LYS:CA | 1:182:L:LYS:C | 1:183:L:ASN:N | 5 | 3.9 |
| (1,89) | 1:154:K:ARG:C | 1:155:K:GLN:N | 1:155:K:GLN:CA | 1:155:K:GLN:C | 4 | 3.9 |
| (1,1019) | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 1:240:K:ASN:N | 1 | 3.89 |
| (1,120) | 1:158:L:LYS:N | 1:158:L:LYS:CA | 1:158:L:LYS:C | 1:159:L:GLU:N | 3 | 3.89 |
| (1,119) | 1:158:K:LYS:N | 1:158:K:LYS:CA | 1:158:K:LYS:C | 1:159:K:GLU:N | 10 | 3.89 |
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 8 | 3.89 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 2 | 3.88 |
| (1,1025) | 1:239:K:THR:C | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 3 | 3.88 |
| (1,1020) | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 1:240:L:ASN:N | 2 | 3.88 |
| (1,814) | 1:221:J:VAL:N | 1:221:J:VAL:CA | 1:221:J:VAL:C | 1:222:J:GLY:N | 8 | 3.88 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 6 | 3.88 |
| (1,175) | 1:163:G:ASP:N | 1:163:G:ASP:CA | 1:163:G:ASP:C | 1:164:G:TYR:N | 1 | 3.88 |
| (1,1027) | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1:241:G:THR:N | 7 | 3.87 |
| (1,998) | 1:237:H:GLN:C | 1:238:H:VAL:N | 1:238:H:VAL:CA | 1:238:H:VAL:C | 4 | 3.86 |
| (1,513) | 1:193:I:ASN:N | 1:193:I:ASN:CA | 1:193:I:ASN:C | 1:194:I:ALA:N | 6 | 3.86 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 1 | 3.85 |
| (1,1010) | 1:238:H:VAL:C | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 2 | 3.85 |
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 3 | 3.85 |
| (1,495) | 1:191:I:VAL:C | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 10 | 3.83 |
| (1,57) | 1:151:I:LEU:N | 1:151:I:LEU:CA | 1:151:I:LEU:C | 1:152:I:ASP:N | 2 | 3.83 |
| (1,34) | 1:147:J:PRO:C | 1:148:J:THR:N | 1:148:J:THR:CA | 1:148:J:THR:C | 10 | 3.83 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 1 | 3.82 |
| (1,1009) | 1:238:G:VAL:C | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 10 | 3.82 |
| (1,895) | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 1:230:G:VAL:N | 7 | 3.82 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 2 | 3.82 |
| (1,178) | 1:163:J:ASP:N | 1:163:J:ASP:CA | 1:163:J:ASP:C | 1:164:J:TYR:N | 9 | 3.81 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 2 | 3.79 |
| (1,483) | 1:190:I:LEU:C | 1:191:I:VAL:N | 1:191:I:VAL:CA | 1:191:I:VAL:C | 4 | 3.79 |
| (1,669) | 1:209:I:ALA:N | 1:209:I:ALA:CA | 1:209:I:ALA:C | 1:210:I:THR:N | 6 | 3.78 |
| (1,314) | 1:176:H:GLN:C | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 6 | 3.78 |
| (1,36) | 1:147:L:PRO:C | 1:148:L:THR:N | 1:148:L:THR:CA | 1:148:L:THR:C | 3 | 3.78 |
| (1,973) | 1:235:G:MET:C | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 4 | 3.77 |
| (1,448) | 1:187:J:GLU:C | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 5 | 3.77 |
| (1,225) | 1:167:I:ARG:N | 1:167:I:ARG:CA | 1:167:I:ARG:C | 1:168:I:PHE:N | 4 | 3.77 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 4 | 3.76 |
| (1,986) | 1:236:H:SER:C | 1:237:H:GLN:N | 1:237:H:GLN:CA | 1:237:H:GLN:C | 7 | 3.76 |
| (1,894) | 1:228:L:ALA:C | 1:229:L:ARG:N | 1:229:L:ARG:CA | 1:229:L:ARG:C | 7 | 3.76 |
| (1,830) | 1:223:H:GLY:C | 1:224:H:PRO:N | 1:224:H:PRO:CA | 1:224:H:PRO:C | 9 | 3.76 |
| (1,1077) | 1:175:I:GLU:N | 1:175:I:GLU:CA | 1:175:I:GLU:C | 1:176:I:GLN:N | 3 | 3.75 |
| (1,1020) | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 1:240:L:ASN:N | 7 | 3.74 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 7 | 3.74 |
| (1,57) | 1:151:I:LEU:N | 1:151:I:LEU:CA | 1:151:I:LEU:C | 1:152:I:ASP:N | 8 | 3.74 |
| (1,29) | 1:147:K:PRO:N | 1:147:K:PRO:CA | 1:147:K:PRO:C | 1:148:K:THR:N | 5 | 3.74 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1033) | 1:240:G:ASN:C | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 8 | 3.73 |
| (1,889) | 1:228:G:ALA:C | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 2 | 3.73 |
| (1,178) | 1:163:J:ASP:N | 1:163:J:ASP:CA | 1:163:J:ASP:C | 1:164:J:TYR:N | 10 | 3.73 |
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 7 | 3.73 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 6 | 3.72 |
| (1,1027) | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1:241:G:THR:N | 6 | 3.72 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 1 | 3.72 |
| (1,88) | 1:154:J:ARG:C | 1:155:J:GLN:N | 1:155:J:GLN:CA | 1:155:J:GLN:C | 7 | 3.72 |
| (1,1027) | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1:241:G:THR:N | 2 | 3.71 |
| (1,1077) | 1:175:I:GLU:N | 1:175:I:GLU:CA | 1:175:I:GLU:C | 1:176:I:GLN:N | 2 | 3.7 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 3 | 3.7 |
| (1,1015) | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 1:240:G:ASN:N | 9 | 3.7 |
| (1,807) | 1:220:I:GLY:C | 1:221:I:VAL:N | 1:221:I:VAL:CA | 1:221:I:VAL:C | 7 | 3.7 |
| (1,434) | 1:186:H:THR:C | 1:187:H:GLU:N | 1:187:H:GLU:CA | 1:187:H:GLU:C | 10 | 3.7 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 6 | 3.7 |
| (1,795) | 1:219:I:GLN:C | 1:220:I:GLY:N | 1:220:I:GLY:CA | 1:220:I:GLY:C | 1 | 3.69 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 9 | 3.69 |
| (1,1077) | 1:175:I:GLU:N | 1:175:I:GLU:CA | 1:175:I:GLU:C | 1:176:I:GLN:N | 5 | 3.68 |
| (1,1010) | 1:238:H:VAL:C | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 9 | 3.68 |
| (1,451) | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 1:189:G:LEU:N | 5 | 3.68 |
| (1,118) | 1:158:J:LYS:N | 1:158:J:LYS:CA | 1:158:J:LYS:C | 1:159:J:GLU:N | 3 | 3.68 |
| (1,973) | 1:235:G:MET:C | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 10 | 3.67 |
| (1,1041) | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 1:242:I:ALA:N | 6 | 3.66 |
| (1,444) | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 1:188:L:THR:N | 7 | 3.66 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 6 | 3.65 |
| (1,518) | 1:194:H:ALA:C | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 8 | 3.65 |
| (1,316) | 1:176:J:GLN:C | 1:177:J:ALA:N | 1:177:J:ALA:CA | 1:177:J:ALA:C | 6 | 3.65 |
| (1,178) | 1:163:J:ASP:N | 1:163:J:ASP:CA | 1:163:J:ASP:C | 1:164:J:TYR:N | 5 | 3.65 |
| (1,60) | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 1:152:L:ASP:N | 5 | 3.65 |
| (1,47) | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 1:150:K:ILE:N | 3 | 3.65 |
| (1,540) | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 1:197:L:ASP:N | 10 | 3.63 |
| (1,1103) | 1:207:K:PRO:N | 1:207:K:PRO:CA | 1:207:K:PRO:C | 1:208:K:GLY:N | 3 | 3.62 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 7 | 3.62 |
| (1,1116) | 1:242:L:ALA:N | 1:242:L:ALA:CA | 1:242:L:ALA:C | 1:243:L:THR:N | 10 | 3.61 |
| (1,978) | 1:235:L:MET:C | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 2 | 3.61 |
| (1,823) | 1:223:G:GLY:N | 1:223:G:GLY:CA | 1:223:G:GLY:C | 1:224:G:PRO:N | 9 | 3.61 |
| (1,314) | 1:176:H:GLN:C | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 4 | 3.6 |
| (1,1018) | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 1:240:J:ASN:N | 10 | 3.59 |
| (1,1017) | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 1:240:I:ASN:N | 1 | 3.59 |
| (1,673) | 1:209:G:ALA:C | 1:210:G:THR:N | 1:210:G:THR:CA | 1:210:G:THR:C | 10 | 3.59 |
| (1,1033) | 1:240:G:ASN:C | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 9 | 3.58 |
| (1,669) | 1:209:I:ALA:N | 1:209:I:ALA:CA | 1:209:I:ALA:C | 1:210:I:THR:N | 9 | 3.58 |
| (1,46) | 1:149:J:SER:N | 1:149:J:SER:CA | 1:149:J:SER:C | 1:150:J:ILE:N | 6 | 3.58 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 1 | 3.57 |
| (1,831) | 1:223:I:GLY:C | 1:224:I:PRO:N | 1:224:I:PRO:CA | 1:224:I:PRO:C | 1 | 3.57 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 2 | 3.57 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 3 | 3.56 |
| (1,87) | 1:154:I:ARG:C | 1:155:I:GLN:N | 1:155:I:GLN:CA | 1:155:I:GLN:C | 3 | 3.56 |
| (1,1017) | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 1:240:I:ASN:N | 9 | 3.55 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 6 | 3.54 |
| (1,849) | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 1:226:I:HIS:N | 6 | 3.54 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 4 | 3.54 |
| (1,452) | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 1:189:H:LEU:N | 8 | 3.54 |
| (1,900) | 1:229:L:ARG:N | 1:229:L:ARG:CA | 1:229:L:ARG:C | 1:230:L:VAL:N | 6 | 3.53 |
| (1,636) | 1:204:L:ALA:N | 1:204:L:ALA:CA | 1:204:L:ALA:C | 1:205:L:LEU:N | 9 | 3.53 |
| (1,434) | 1:186:H:THR:C | 1:187:H:GLU:N | 1:187:H:GLU:CA | 1:187:H:GLU:C | 7 | 3.53 |
| (1,1029) | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 1:241:I:THR:N | 10 | 3.52 |
| (1,1016) | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 1:240:H:ASN:N | 3 | 3.52 |
| (1,716) | 1:213:H:GLU:N | 1:213:H:GLU:CA | 1:213:H:GLU:C | 1:214:H:MET:N | 4 | 3.52 |
| (1,675) | 1:209:I:ALA:C | 1:210:I:THR:N | 1:210:I:THR:CA | 1:210:I:THR:C | 9 | 3.52 |
| (1,269) | 1:170:K:LYS:C | 1:171:K:THR:N | 1:171:K:THR:CA | 1:171:K:THR:C | 7 | 3.52 |
| (1,864) | 1:226:L:HIS:N | 1:226:L:HIS:CA | 1:226:L:HIS:C | 1:227:L:LYS:N | 8 | 3.51 |
| (1,540) | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 1:197:L:ASP:N | 9 | 3.51 |
| (1,380) | 1:182:H:LYS:N | 1:182:H:LYS:CA | 1:182:H:LYS:C | 1:183:H:ASN:N | 7 | 3.51 |
| (1,65) | 1:152:K:ASP:N | 1:152:K:ASP:CA | 1:152:K:ASP:C | 1:153:K:ILE:N | 7 | 3.51 |
| (1,1022) | 1:239:H:THR:C | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 1 | 3.5 |
| (1,814) | 1:221:J:VAL:N | 1:221:J:VAL:CA | 1:221:J:VAL:C | 1:222:J:GLY:N | 4 | 3.5 |
| (1,70) | 1:153:J:ILE:N | 1:153:J:ILE:CA | 1:153:J:ILE:C | 1:154:J:ARG:N | 1 | 3.5 |
| (1,1011) | 1:238:I:VAL:C | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 4 | 3.49 |
| (1,906) | 1:229:L:ARG:C | 1:230:L:VAL:N | 1:230:L:VAL:CA | 1:230:L:VAL:C | 4 | 3.49 |
| (1,307) | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 1:175:G:GLU:N | 5 | 3.49 |
| (1,1023) | 1:239:I:THR:C | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 3 | 3.48 |
| (1,692) | 1:211:H:LEU:N | 1:211:H:LEU:CA | 1:211:H:LEU:C | 1:212:H:GLU:N | 8 | 3.48 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 3 | 3.47 |
| (1,446) | 1:187:H:GLU:C | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 10 | 3.47 |
| (1,416) | 1:185:H:MET:N | 1:185:H:MET:CA | 1:185:H:MET:C | 1:186:H:THR:N | 9 | 3.47 |
| (1,1010) | 1:238:H:VAL:C | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 3 | 3.46 |
| (1,820) | 1:222:J:GLY:N | 1:222:J:GLY:CA | 1:222:J:GLY:C | 1:223:J:GLY:N | 4 | 3.46 |
| (1,434) | 1:186:H:THR:C | 1:187:H:GLU:N | 1:187:H:GLU:CA | 1:187:H:GLU:C | 1 | 3.46 |
| (1,314) | 1:176:H:GLN:C | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 10 | 3.46 |
| (1,229) | 1:167:G:ARG:C | 1:168:G:PHE:N | 1:168:G:PHE:CA | 1:168:G:PHE:C | 6 | 3.46 |
| (1,906) | 1:229:L:ARG:C | 1:230:L:VAL:N | 1:230:L:VAL:CA | 1:230:L:VAL:C | 1 | 3.45 |
| (1,741) | 1:215:I:MET:N | 1:215:I:MET:CA | 1:215:I:MET:C | 1:216:I:THR:N | 2 | 3.45 |
| (1,434) | 1:186:H:THR:C | 1:187:H:GLU:N | 1:187:H:GLU:CA | 1:187:H:GLU:C | 6 | 3.45 |
| (1,307) | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 1:175:G:GLU:N | 6 | 3.44 |
| (1,62) | 1:152:H:ASP:N | 1:152:H:ASP:CA | 1:152:H:ASP:C | 1:153:H:ILE:N | 4 | 3.44 |
| (1,1103) | 1:207:K:PRO:N | 1:207:K:PRO:CA | 1:207:K:PRO:C | 1:208:K:GLY:N | 4 | 3.43 |
| (1,1041) | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 1:242:I:ALA:N | 3 | 3.43 |
| (1,974) | 1:235:H:MET:C | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 3 | 3.43 |
| (1,1010) | 1:238:H:VAL:C | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 8 | 3.42 |
| (1,677) | 1:209:K:ALA:C | 1:210:K:THR:N | 1:210:K:THR:CA | 1:210:K:THR:C | 1 | 3.42 |
| (1,1028) | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 1:241:H:THR:N | 6 | 3.41 |
| (1,1010) | 1:238:H:VAL:C | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 4 | 3.41 |
| (1,1009) | 1:238:G:VAL:C | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 1 | 3.41 |
| (1,478) | 1:190:J:LEU:N | 1:190:J:LEU:CA | 1:190:J:LEU:C | 1:191:J:VAL:N | 9 | 3.41 |
| (1,37) | 1:148:G:THR:C | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 4 | 3.39 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 1 | 3.38 |
| (1,1079) | 1:175:K:GLU:N | 1:175:K:GLU:CA | 1:175:K:GLU:C | 1:176:K:GLN:N | 1 | 3.37 |
| (1,741) | 1:215:I:MET:N | 1:215:I:MET:CA | 1:215:I:MET:C | 1:216:I:THR:N | 7 | 3.37 |
| (1,28) | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 1:148:J:THR:N | 3 | 3.37 |
| (1,921) | 1:231:I:LEU:N | 1:231:I:LEU:CA | 1:231:I:LEU:C | 1:232:I:ALA:N | 10 | 3.36 |
| (1,894) | 1:228:L:ALA:C | 1:229:L:ARG:N | 1:229:L:ARG:CA | 1:229:L:ARG:C | 2 | 3.36 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,434) | 1:186:H:THR:C | 1:187:H:GLU:N | 1:187:H:GLU:CA | 1:187:H:GLU:C | 3 | 3.36 |
| (1,434) | 1:186:H:THR:C | 1:187:H:GLU:N | 1:187:H:GLU:CA | 1:187:H:GLU:C | 5 | 3.36 |
| (1,381) | 1:182:I:LYS:N | 1:182:I:LYS:CA | 1:182:I:LYS:C | 1:183:I:ASN:N | 9 | 3.35 |
| (1,381) | 1:182:I:LYS:N | 1:182:I:LYS:CA | 1:182:I:LYS:C | 1:183:I:ASN:N | 2 | 3.34 |
| (1,26) | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 1:148:H:THR:N | 8 | 3.34 |
| (1,380) | 1:182:H:LYS:N | 1:182:H:LYS:CA | 1:182:H:LYS:C | 1:183:H:ASN:N | 5 | 3.33 |
| (1,889) | 1:228:G:ALA:C | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 4 | 3.32 |
| (1,820) | 1:222:J:GLY:N | 1:222:J:GLY:CA | 1:222:J:GLY:C | 1:223:J:GLY:N | 8 | 3.32 |
| (1,153) | 1:161:I:PHE:N | 1:161:I:PHE:CA | 1:161:I:PHE:C | 1:162:I:ARG:N | 4 | 3.32 |
| (1,446) | 1:187:H:GLU:C | 1:188:H:THR:N | 1:188:H:THR:CA | 1:188:H:THR:C | 2 | 3.31 |
| (1,320) | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 1:178:H:SER:N | 5 | 3.31 |
| (1,1034) | 1:240:H:ASN:C | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 8 | 3.3 |
| (1,802) | 1:220:J:GLY:N | 1:220:J:GLY:CA | 1:220:J:GLY:C | 1:221:J:VAL:N | 10 | 3.3 |
| (1,449) | 1:187:K:GLU:C | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 6 | 3.3 |
| (1,423) | 1:185:I:MET:C | 1:186:I:THR:N | 1:186:I:THR:CA | 1:186:I:THR:C | 10 | 3.3 |
| (1,125) | 1:158:K:LYS:C | 1:159:K:GLU:N | 1:159:K:GLU:CA | 1:159:K:GLU:C | 7 | 3.3 |
| (1,911) | 1:230:K:VAL:N | 1:230:K:VAL:CA | 1:230:K:VAL:C | 1:231:K:LEU:N | 2 | 3.29 |
| (1,903) | 1:229:I:ARG:C | 1:230:I:VAL:N | 1:230:I:VAL:CA | 1:230:I:VAL:C | 7 | 3.29 |
| (1,449) | 1:187:K:GLU:C | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 10 | 3.29 |
| (1,1041) | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 1:242:I:ALA:N | 2 | 3.28 |
| (1,115) | 1:158:G:LYS:N | 1:158:G:LYS:CA | 1:158:G:LYS:C | 1:159:G:GLU:N | 5 | 3.28 |
| (1,1013) | 1:238:K:VAL:C | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 2 | 3.27 |
| (1,426) | 1:185:L:MET:C | 1:186:L:THR:N | 1:186:L:THR:CA | 1:186:L:THR:C | 6 | 3.27 |
| (1,320) | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 1:178:H:SER:N | 4 | 3.27 |
| (1,230) | 1:167:H:ARG:C | 1:168:H:PHE:N | 1:168:H:PHE:CA | 1:168:H:PHE:C | 9 | 3.27 |
| (1,65) | 1:152:K:ASP:N | 1:152:K:ASP:CA | 1:152:K:ASP:C | 1:153:K:ILE:N | 4 | 3.27 |
| (1,28) | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 1:148:J:THR:N | 1 | 3.27 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 2 | 3.26 |
| (1,436) | 1:186:J:THR:C | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 8 | 3.26 |
| (1,1033) | 1:240:G:ASN:C | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 5 | 3.25 |
| (1,416) | 1:185:H:MET:N | 1:185:H:MET:CA | 1:185:H:MET:C | 1:186:H:THR:N | 8 | 3.25 |
| (1,312) | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 1:175:L:GLU:N | 3 | 3.25 |
| (1,827) | 1:223:K:GLY:N | 1:223:K:GLY:CA | 1:223:K:GLY:C | 1:224:K:PRO:N | 3 | 3.24 |
| (1,424) | 1:185:J:MET:C | 1:186:J:THR:N | 1:186:J:THR:CA | 1:186:J:THR:C | 3 | 3.24 |
| (1,815) | 1:221:K:VAL:N | 1:221:K:VAL:CA | 1:221:K:VAL:C | 1:222:K:GLY:N | 8 | 3.23 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 9 | 3.23 |
| (1,59) | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 1:152:K:ASP:N | 7 | 3.23 |
| (1,243) | 1:168:I:PHE:C | 1:169:I:TYR:N | 1:169:I:TYR:CA | 1:169:I:TYR:C | 4 | 3.22 |
| (1,1073) | 1:174:K:ALA:C | 1:175:K:GLU:N | 1:175:K:GLU:CA | 1:175:K:GLU:C | 4 | 3.21 |
| (1,1072) | 1:174:J:ALA:C | 1:175:J:GLU:N | 1:175:J:GLU:CA | 1:175:J:GLU:C | 5 | 3.21 |
| (1,1011) | 1:238:I:VAL:C | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 3 | 3.21 |
| (1,897) | 1:229:I:ARG:N | 1:229:I:ARG:CA | 1:229:I:ARG:C | 1:230:I:VAL:N | 10 | 3.21 |
| (1,868) | 1:226:J:HIS:C | 1:227:J:LYS:N | 1:227:J:LYS:CA | 1:227:J:LYS:C | 1 | 3.21 |
| (1,314) | 1:176:H:GLN:C | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 5 | 3.21 |
| (1,767) | 1:217:K:ALA:N | 1:217:K:ALA:CA | 1:217:K:ALA:C | 1:218:K:CYS:N | 6 | 3.2 |
| (1,728) | 1:214:H:MET:N | 1:214:H:MET:CA | 1:214:H:MET:C | 1:215:H:MET:N | 9 | 3.2 |
| (1,441) | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 1:188:I:THR:N | 6 | 3.2 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 6 | 3.19 |
| (1,107) | 1:157:K:PRO:N | 1:157:K:PRO:CA | 1:157:K:PRO:C | 1:158:K:LYS:N | 4 | 3.19 |
| (1,1113) | 1:242:I:ALA:N | 1:242:I:ALA:CA | 1:242:I:ALA:C | 1:243:I:THR:N | 8 | 3.18 |
| (1,1017) | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 1:240:I:ASN:N | 7 | 3.18 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1016) | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 1:240:H:ASN:N | 6 | 3.18 |
| (1,1012) | 1:238:J:VAL:C | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 10 | 3.18 |
| (1,1015) | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 1:240:G:ASN:N | 5 | 3.17 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 6 | 3.17 |
| (1,764) | 1:217:H:ALA:N | 1:217:H:ALA:CA | 1:217:H:ALA:C | 1:218:H:CYS:N | 1 | 3.17 |
| (1,451) | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 1:189:G:LEU:N | 9 | 3.17 |
| (1,889) | 1:228:G:ALA:C | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 6 | 3.16 |
| (1,592) | 1:200:J:THR:C | 1:201:J:ILE:N | 1:201:J:ILE:CA | 1:201:J:ILE:C | 1 | 3.16 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 9 | 3.16 |
| (1,1010) | 1:238:H:VAL:C | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 1 | 3.15 |
| (1,1013) | 1:238:K:VAL:C | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 8 | 3.14 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 1 | 3.14 |
| (1,60) | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 1:152:L:ASP:N | 9 | 3.14 |
| (1,1079) | 1:175:K:GLU:N | 1:175:K:GLU:CA | 1:175:K:GLU:C | 1:176:K:GLN:N | 7 | 3.13 |
| (1,832) | 1:223:J:GLY:C | 1:224:J:PRO:N | 1:224:J:PRO:CA | 1:224:J:PRO:C | 10 | 3.13 |
| (1,675) | 1:209:I:ALA:C | 1:210:I:THR:N | 1:210:I:THR:CA | 1:210:I:THR:C | 6 | 3.13 |
| (1,436) | 1:186:J:THR:C | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 9 | 3.13 |
| (1,381) | 1:182:I:LYS:N | 1:182:I:LYS:CA | 1:182:I:LYS:C | 1:183:I:ASN:N | 3 | 3.13 |
| (1,87) | 1:154:I:ARG:C | 1:155:I:GLN:N | 1:155:I:GLN:CA | 1:155:I:GLN:C | 4 | 3.13 |
| (1,1103) | 1:207:K:PRO:N | 1:207:K:PRO:CA | 1:207:K:PRO:C | 1:208:K:GLY:N | 1 | 3.12 |
| (1,1036) | 1:240:J:ASN:C | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 4 | 3.12 |
| (1,803) | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 1:221:K:VAL:N | 1 | 3.12 |
| (1,798) | 1:219:L:GLN:C | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 3 | 3.12 |
| (1,640) | 1:204:J:ALA:C | 1:205:J:LEU:N | 1:205:J:LEU:CA | 1:205:J:LEU:C | 10 | 3.12 |
| (1,1103) | 1:207:K:PRO:N | 1:207:K:PRO:CA | 1:207:K:PRO:C | 1:208:K:GLY:N | 2 | 3.11 |
| (1,1027) | 1:240:G:ASN:N | 1:240:G:ASN:CA | 1:240:G:ASN:C | 1:241:G:THR:N | 10 | 3.11 |
| (1,1023) | 1:239:I:THR:C | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 10 | 3.11 |
| (1,1011) | 1:238:I:VAL:C | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 2 | 3.11 |
| (1,698) | 1:211:H:LEU:C | 1:212:H:GLU:N | 1:212:H:GLU:CA | 1:212:H:GLU:C | 8 | 3.11 |
| (1,380) | 1:182:H:LYS:N | 1:182:H:LYS:CA | 1:182:H:LYS:C | 1:183:H:ASN:N | 4 | 3.11 |
| (1,71) | 1:153:K:ILE:N | 1:153:K:ILE:CA | 1:153:K:ILE:C | 1:154:K:ARG:N | 4 | 3.11 |
| (1,895) | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 1:230:G:VAL:N | 2 | 3.1 |
| (1,502) | 1:192:J:GLN:N | 1:192:J:GLN:CA | 1:192:J:GLN:C | 1:193:J:ASN:N | 5 | 3.1 |
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 4 | 3.1 |
| (1,62) | 1:152:H:ASP:N | 1:152:H:ASP:CA | 1:152:H:ASP:C | 1:153:H:ILE:N | 10 | 3.1 |
| (1,815) | 1:221:K:VAL:N | 1:221:K:VAL:CA | 1:221:K:VAL:C | 1:222:K:GLY:N | 1 | 3.09 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 7 | 3.09 |
| (1,269) | 1:170:K:LYS:C | 1:171:K:THR:N | 1:171:K:THR:CA | 1:171:K:THR:C | 1 | 3.09 |
| (1,60) | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 1:152:L:ASP:N | 1 | 3.09 |
| (1,1012) | 1:238:J:VAL:C | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 9 | 3.08 |
| (1,85) | 1:154:G:ARG:C | 1:155:G:GLN:N | 1:155:G:GLN:CA | 1:155:G:GLN:C | 5 | 3.08 |
| (1,59) | 1:151:K:LEU:N | 1:151:K:LEU:CA | 1:151:K:LEU:C | 1:152:K:ASP:N | 9 | 3.08 |
| (1,857) | 1:225:K:GLY:C | 1:226:K:HIS:N | 1:226:K:HIS:CA | 1:226:K:HIS:C | 1 | 3.07 |
| (1,14) | 1:146:H:SER:N | 1:146:H:SER:CA | 1:146:H:SER:C | 1:147:H:PRO:N | 1 | 3.07 |
| (1,1114) | 1:242:J:ALA:N | 1:242:J:ALA:CA | 1:242:J:ALA:C | 1:243:J:THR:N | 5 | 3.06 |
| (1,1019) | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 1:240:K:ASN:N | 9 | 3.06 |
| (1,1011) | 1:238:I:VAL:C | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 8 | 3.06 |
| (1,896) | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 1:230:H:VAL:N | 5 | 3.06 |
| (1,1036) | 1:240:J:ASN:C | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 5 | 3.05 |
| (1,889) | 1:228:G:ALA:C | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 9 | 3.05 |
| (1,759) | 1:216:I:THR:C | 1:217:I:ALA:N | 1:217:I:ALA:CA | 1:217:I:ALA:C | 3 | 3.05 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,669) | 1:209:I:ALA:N | 1:209:I:ALA:CA | 1:209:I:ALA:C | 1:210:I:THR:N | 5 | 3.05 |
| (1,451) | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 1:189:G:LEU:N | 4 | 3.05 |
| (1,1030) | 1:240:J:ASN:N | 1:240:J:ASN:CA | 1:240:J:ASN:C | 1:241:J:THR:N | 9 | 3.04 |
| (1,1013) | 1:238:K:VAL:C | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 7 | 3.03 |
| (1,974) | 1:235:H:MET:C | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 9 | 3.03 |
| (1,758) | 1:216:H:THR:C | 1:217:H:ALA:N | 1:217:H:ALA:CA | 1:217:H:ALA:C | 3 | 3.03 |
| (1,540) | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 1:197:L:ASP:N | 5 | 3.02 |
| (1,168) | 1:162:L:ARG:N | 1:162:L:ARG:CA | 1:162:L:ARG:C | 1:163:L:ASP:N | 6 | 3.02 |
| (1,489) | 1:191:I:VAL:N | 1:191:I:VAL:CA | 1:191:I:VAL:C | 1:192:I:GLN:N | 3 | 3.01 |
| (1,60) | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 1:152:L:ASP:N | 4 | 3.01 |
| (1,610) | 1:202:J:LEU:N | 1:202:J:LEU:CA | 1:202:J:LEU:C | 1:203:J:LYS:N | 6 | 3.0 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 9 | 3.0 |
| (1,39) | 1:148:I:THR:C | 1:149:I:SER:N | 1:149:I:SER:CA | 1:149:I:SER:C | 6 | 3.0 |
| (1,1103) | 1:207:K:PRO:N | 1:207:K:PRO:CA | 1:207:K:PRO:C | 1:208:K:GLY:N | 10 | 2.99 |
| (1,1041) | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 1:242:I:ALA:N | 1 | 2.99 |
| (1,1028) | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 1:241:H:THR:N | 3 | 2.99 |
| (1,947) | 1:233:K:GLU:N | 1:233:K:GLU:CA | 1:233:K:GLU:C | 1:234:K:ALA:N | 6 | 2.98 |
| (1,764) | 1:217:H:ALA:N | 1:217:H:ALA:CA | 1:217:H:ALA:C | 1:218:H:CYS:N | 5 | 2.98 |
| (1,1022) | 1:239:H:THR:C | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 4 | 2.97 |
| (1,1013) | 1:238:K:VAL:C | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 1 | 2.97 |
| (1,896) | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 1:230:H:VAL:N | 2 | 2.97 |
| (1,675) | 1:209:I:ALA:C | 1:210:I:THR:N | 1:210:I:THR:CA | 1:210:I:THR:C | 7 | 2.97 |
| (1,1103) | 1:207:K:PRO:N | 1:207:K:PRO:CA | 1:207:K:PRO:C | 1:208:K:GLY:N | 7 | 2.96 |
| (1,1037) | 1:240:K:ASN:C | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 8 | 2.96 |
| (1,823) | 1:223:G:GLY:N | 1:223:G:GLY:CA | 1:223:G:GLY:C | 1:224:G:PRO:N | 10 | 2.96 |
| (1,1101) | 1:207:I:PRO:N | 1:207:I:PRO:CA | 1:207:I:PRO:C | 1:208:I:GLY:N | 2 | 2.95 |
| (1,1020) | 1:239:L:THR:N | 1:239:L:THR:CA | 1:239:L:THR:C | 1:240:L:ASN:N | 6 | 2.95 |
| (1,1016) | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 1:240:H:ASN:N | 9 | 2.95 |
| (1,796) | 1:219:J:GLN:C | 1:220:J:GLY:N | 1:220:J:GLY:CA | 1:220:J:GLY:C | 6 | 2.95 |
| (1,658) | 1:208:J:GLY:N | 1:208:J:GLY:CA | 1:208:J:GLY:C | 1:209:J:ALA:N | 5 | 2.95 |
| (1,494) | 1:191:H:VAL:C | 1:192:H:GLN:N | 1:192:H:GLN:CA | 1:192:H:GLN:C | 8 | 2.95 |
| (1,1035) | 1:240:I:ASN:C | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 8 | 2.94 |
| (1,1002) | 1:237:L:GLN:C | 1:238:L:VAL:N | 1:238:L:VAL:CA | 1:238:L:VAL:C | 5 | 2.94 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 8 | 2.94 |
| (1,454) | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 1:189:J:LEU:N | 1 | 2.94 |
| (1,1101) | 1:207:I:PRO:N | 1:207:I:PRO:CA | 1:207:I:PRO:C | 1:208:I:GLY:N | 8 | 2.93 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 7 | 2.93 |
| (1,988) | 1:236:J:SER:C | 1:237:J:GLN:N | 1:237:J:GLN:CA | 1:237:J:GLN:C | 10 | 2.92 |
| (1,486) | 1:190:L:LEU:C | 1:191:L:VAL:N | 1:191:L:VAL:CA | 1:191:L:VAL:C | 5 | 2.92 |
| (1,580) | 1:199:J:LYS:C | 1:200:J:THR:N | 1:200:J:THR:CA | 1:200:J:THR:C | 8 | 2.91 |
| (1,62) | 1:152:H:ASP:N | 1:152:H:ASP:CA | 1:152:H:ASP:C | 1:153:H:ILE:N | 6 | 2.91 |
| (1,663) | 1:208:I:GLY:C | 1:209:I:ALA:N | 1:209:I:ALA:CA | 1:209:I:ALA:C | 4 | 2.9 |
| (1,530) | 1:195:H:ASN:C | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 7 | 2.9 |
| (1,1073) | 1:174:K:ALA:C | 1:175:K:GLU:N | 1:175:K:GLU:CA | 1:175:K:GLU:C | 2 | 2.89 |
| (1,1038) | 1:240:L:ASN:C | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 10 | 2.89 |
| (1,1013) | 1:238:K:VAL:C | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 10 | 2.89 |
| (1,182) | 1:163:H:ASP:C | 1:164:H:TYR:N | 1:164:H:TYR:CA | 1:164:H:TYR:C | 4 | 2.89 |
| (1,803) | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 1:221:K:VAL:N | 9 | 2.88 |
| (1,634) | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 1:205:J:LEU:N | 10 | 2.88 |
| (1,316) | 1:176:J:GLN:C | 1:177:J:ALA:N | 1:177:J:ALA:CA | 1:177:J:ALA:C | 4 | 2.87 |
| (1,36) | 1:147:L:PRO:C | 1:148:L:THR:N | 1:148:L:THR:CA | 1:148:L:THR:C | 4 | 2.87 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1041) | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 1:242:I:ALA:N | 7 | 2.86 |
| (1,1032) | 1:240:L:ASN:N | 1:240:L:ASN:CA | 1:240:L:ASN:C | 1:241:L:THR:N | 6 | 2.86 |
| (1,813) | 1:221:I:VAL:N | 1:221:I:VAL:CA | 1:221:I:VAL:C | 1:222:I:GLY:N | 3 | 2.86 |
| (1,803) | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 1:221:K:VAL:N | 6 | 2.86 |
| (1,634) | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 1:205:J:LEU:N | 1 | 2.86 |
| (1,484) | 1:190:J:LEU:C | 1:191:J:VAL:N | 1:191:J:VAL:CA | 1:191:J:VAL:C | 1 | 2.86 |
| (1,175) | 1:163:G:ASP:N | 1:163:G:ASP:CA | 1:163:G:ASP:C | 1:164:G:TYR:N | 2 | 2.86 |
| (1,120) | 1:158:L:LYS:N | 1:158:L:LYS:CA | 1:158:L:LYS:C | 1:159:L:GLU:N | 2 | 2.86 |
| (1,119) | 1:158:K:LYS:N | 1:158:K:LYS:CA | 1:158:K:LYS:C | 1:159:K:GLU:N | 7 | 2.86 |
| (1,87) | 1:154:I:ARG:C | 1:155:I:GLN:N | 1:155:I:GLN:CA | 1:155:I:GLN:C | 1 | 2.86 |
| (1,581) | 1:199:K:LYS:C | 1:200:K:THR:N | 1:200:K:THR:CA | 1:200:K:THR:C | 2 | 2.85 |
| (1,444) | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 1:188:L:THR:N | 4 | 2.85 |
| (1,305) | 1:173:K:ARG:C | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 9 | 2.85 |
| (1,849) | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 1:226:I:HIS:N | 8 | 2.84 |
| (1,814) | 1:221:J:VAL:N | 1:221:J:VAL:CA | 1:221:J:VAL:C | 1:222:J:GLY:N | 9 | 2.84 |
| (1,451) | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 1:189:G:LEU:N | 1 | 2.84 |
| (1,451) | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 1:189:G:LEU:N | 3 | 2.84 |
| (1,178) | 1:163:J:ASP:N | 1:163:J:ASP:CA | 1:163:J:ASP:C | 1:164:J:TYR:N | 7 | 2.84 |
| (1,1013) | 1:238:K:VAL:C | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 9 | 2.83 |
| (1,896) | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 1:230:H:VAL:N | 7 | 2.83 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 5 | 2.83 |
| (1,675) | 1:209:I:ALA:C | 1:210:I:THR:N | 1:210:I:THR:CA | 1:210:I:THR:C | 10 | 2.82 |
| (1,242) | 1:168:H:PHE:C | 1:169:H:TYR:N | 1:169:H:TYR:CA | 1:169:H:TYR:C | 9 | 2.82 |
| (1,327) | 1:177:I:ALA:C | 1:178:I:SER:N | 1:178:I:SER:CA | 1:178:I:SER:C | 3 | 2.81 |
| (1,315) | 1:176:I:GLN:C | 1:177:I:ALA:N | 1:177:I:ALA:CA | 1:177:I:ALA:C | 2 | 2.81 |
| (1,37) | 1:148:G:THR:C | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 9 | 2.81 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 8 | 2.8 |
| (1,896) | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 1:230:H:VAL:N | 1 | 2.8 |
| (1,314) | 1:176:H:GLN:C | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 3 | 2.8 |
| (1,1031) | 1:240:K:ASN:N | 1:240:K:ASN:CA | 1:240:K:ASN:C | 1:241:K:THR:N | 4 | 2.79 |
| (1,1019) | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 1:240:K:ASN:N | 4 | 2.79 |
| (1,1009) | 1:238:G:VAL:C | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 2 | 2.79 |
| (1,973) | 1:235:G:MET:C | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 5 | 2.79 |
| (1,921) | 1:231:I:LEU:N | 1:231:I:LEU:CA | 1:231:I:LEU:C | 1:232:I:ALA:N | 2 | 2.79 |
| (1,693) | 1:211:I:LEU:N | 1:211:I:LEU:CA | 1:211:I:LEU:C | 1:212:I:GLU:N | 4 | 2.79 |
| (1,243) | 1:168:I:PHE:C | 1:169:I:TYR:N | 1:169:I:TYR:CA | 1:169:I:TYR:C | 8 | 2.79 |
| (1,1103) | 1:207:K:PRO:N | 1:207:K:PRO:CA | 1:207:K:PRO:C | 1:208:K:GLY:N | 5 | 2.78 |
| (1,540) | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 1:197:L:ASP:N | 7 | 2.78 |
| (1,451) | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 1:189:G:LEU:N | 8 | 2.78 |
| (1,320) | 1:177:H:ALA:N | 1:177:H:ALA:CA | 1:177:H:ALA:C | 1:178:H:SER:N | 3 | 2.78 |
| (1,716) | 1:213:H:GLU:N | 1:213:H:GLU:CA | 1:213:H:GLU:C | 1:214:H:MET:N | 8 | 2.76 |
| (1,450) | 1:187:L:GLU:C | 1:188:L:THR:N | 1:188:L:THR:CA | 1:188:L:THR:C | 3 | 2.76 |
| (1,447) | 1:187:I:GLU:C | 1:188:I:THR:N | 1:188:I:THR:CA | 1:188:I:THR:C | 4 | 2.76 |
| (1,232) | 1:167:J:ARG:C | 1:168:J:PHE:N | 1:168:J:PHE:CA | 1:168:J:PHE:C | 9 | 2.76 |
| (1,229) | 1:167:G:ARG:C | 1:168:G:PHE:N | 1:168:G:PHE:CA | 1:168:G:PHE:C | 2 | 2.76 |
| (1,104) | 1:157:H:PRO:N | 1:157:H:PRO:CA | 1:157:H:PRO:C | 1:158:H:LYS:N | 8 | 2.76 |
| (1,88) | 1:154:J:ARG:C | 1:155:J:GLN:N | 1:155:J:GLN:CA | 1:155:J:GLN:C | 2 | 2.76 |
| (1,1016) | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 1:240:H:ASN:N | 8 | 2.75 |
| (1,434) | 1:186:H:THR:C | 1:187:H:GLU:N | 1:187:H:GLU:CA | 1:187:H:GLU:C | 4 | 2.75 |
| (1,175) | 1:163:G:ASP:N | 1:163:G:ASP:CA | 1:163:G:ASP:C | 1:164:G:TYR:N | 3 | 2.75 |
| (1,488) | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 1:192:H:GLN:N | 7 | 2.74 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 2 | 2.74 |
| (1,1002) | 1:237:L:GLN:C | 1:238:L:VAL:N | 1:238:L:VAL:CA | 1:238:L:VAL:C | 4 | 2.73 |
| (1,416) | 1:185:H:MET:N | 1:185:H:MET:CA | 1:185:H:MET:C | 1:186:H:THR:N | 7 | 2.73 |
| (1,312) | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 1:175:L:GLU:N | 4 | 2.73 |
| (1,1013) | 1:238:K:VAL:C | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 4 | 2.72 |
| (1,511) | 1:193:G:ASN:N | 1:193:G:ASN:CA | 1:193:G:ASN:C | 1:194:G:ALA:N | 10 | 2.72 |
| (1,495) | 1:191:I:VAL:C | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 3 | 2.72 |
| (1,230) | 1:167:H:ARG:C | 1:168:H:PHE:N | 1:168:H:PHE:CA | 1:168:H:PHE:C | 3 | 2.72 |
| (1,894) | 1:228:L:ALA:C | 1:229:L:ARG:N | 1:229:L:ARG:CA | 1:229:L:ARG:C | 9 | 2.71 |
| (1,634) | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 1:205:J:LEU:N | 5 | 2.71 |
| (1,1019) | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 1:240:K:ASN:N | 2 | 2.7 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1 | 2.7 |
| (1,973) | 1:235:G:MET:C | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 6 | 2.7 |
| (1,828) | 1:223:L:GLY:N | 1:223:L:GLY:CA | 1:223:L:GLY:C | 1:224:L:PRO:N | 8 | 2.7 |
| (1,802) | 1:220:J:GLY:N | 1:220:J:GLY:CA | 1:220:J:GLY:C | 1:221:J:VAL:N | 2 | 2.7 |
| (1,640) | 1:204:J:ALA:C | 1:205:J:LEU:N | 1:205:J:LEU:CA | 1:205:J:LEU:C | 8 | 2.7 |
| (1,107) | 1:157:K:PRO:N | 1:157:K:PRO:CA | 1:157:K:PRO:C | 1:158:K:LYS:N | 8 | 2.7 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 10 | 2.69 |
| (1,418) | 1:185:J:MET:N | 1:185:J:MET:CA | 1:185:J:MET:C | 1:186:J:THR:N | 6 | 2.69 |
| (1,1029) | 1:240:I:ASN:N | 1:240:I:ASN:CA | 1:240:I:ASN:C | 1:241:I:THR:N | 7 | 2.68 |
| (1,501) | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 1:193:I:ASN:N | 3 | 2.68 |
| (1,380) | 1:182:H:LYS:N | 1:182:H:LYS:CA | 1:182:H:LYS:C | 1:183:H:ASN:N | 6 | 2.68 |
| (1,229) | 1:167:G:ARG:C | 1:168:G:PHE:N | 1:168:G:PHE:CA | 1:168:G:PHE:C | 1 | 2.68 |
| (1,126) | 1:158:L:LYS:C | 1:159:L:GLU:N | 1:159:L:GLU:CA | 1:159:L:GLU:C | 10 | 2.68 |
| (1,70) | 1:153:J:ILE:N | 1:153:J:ILE:CA | 1:153:J:ILE:C | 1:154:J:ARG:N | 8 | 2.67 |
| (1,37) | 1:148:G:THR:C | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 1 | 2.67 |
| (1,1038) | 1:240:L:ASN:C | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 3 | 2.66 |
| (1,1028) | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 1:241:H:THR:N | 10 | 2.64 |
| (1,1103) | 1:207:K:PRO:N | 1:207:K:PRO:CA | 1:207:K:PRO:C | 1:208:K:GLY:N | 8 | 2.63 |
| (1,396) | 1:183:L:ASN:N | 1:183:L:ASN:CA | 1:183:L:ASN:C | 1:184:L:TRP:N | 8 | 2.63 |
| (1,118) | 1:158:J:LYS:N | 1:158:J:LYS:CA | 1:158:J:LYS:C | 1:159:J:GLU:N | 10 | 2.63 |
| (1,1044) | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1:242:L:ALA:N | 10 | 2.62 |
| (1,1018) | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 1:240:J:ASN:N | 8 | 2.62 |
| (1,664) | 1:208:J:GLY:C | 1:209:J:ALA:N | 1:209:J:ALA:CA | 1:209:J:ALA:C | 5 | 2.61 |
| (1,305) | 1:173:K:ARG:C | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 10 | 2.61 |
| (1,236) | 1:168:H:PHE:N | 1:168:H:PHE:CA | 1:168:H:PHE:C | 1:169:H:TYR:N | 8 | 2.61 |
| (1,28) | 1:147:J:PRO:N | 1:147:J:PRO:CA | 1:147:J:PRO:C | 1:148:J:THR:N | 5 | 2.61 |
| (1,626) | 1:203:H:LYS:C | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 10 | 2.6 |
| (1,484) | 1:190:J:LEU:C | 1:191:J:VAL:N | 1:191:J:VAL:CA | 1:191:J:VAL:C | 6 | 2.59 |
| (1,1103) | 1:207:K:PRO:N | 1:207:K:PRO:CA | 1:207:K:PRO:C | 1:208:K:GLY:N | 9 | 2.58 |
| (1,843) | 1:224:I:PRO:C | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 4 | 2.58 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 10 | 2.58 |
| (1,48) | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1:150:L:ILE:N | 10 | 2.58 |
| (1,674) | 1:209:H:ALA:C | 1:210:H:THR:N | 1:210:H:THR:CA | 1:210:H:THR:C | 9 | 2.57 |
| (1,451) | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 1:189:G:LEU:N | 6 | 2.57 |
| (1,104) | 1:157:H:PRO:N | 1:157:H:PRO:CA | 1:157:H:PRO:C | 1:158:H:LYS:N | 10 | 2.56 |
| (1,37) | 1:148:G:THR:C | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 7 | 2.56 |
| (1,669) | 1:209:I:ALA:N | 1:209:I:ALA:CA | 1:209:I:ALA:C | 1:210:I:THR:N | 4 | 2.55 |
| (1,327) | 1:177:I:ALA:C | 1:178:I:SER:N | 1:178:I:SER:CA | 1:178:I:SER:C | 2 | 2.55 |
| (1,174) | 1:162:L:ARG:C | 1:163:L:ASP:N | 1:163:L:ASP:CA | 1:163:L:ASP:C | 10 | 2.55 |
| (1,802) | 1:220:J:GLY:N | 1:220:J:GLY:CA | 1:220:J:GLY:C | 1:221:J:VAL:N | 1 | 2.54 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,632) | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 1:205:H:LEU:N | 7 | 2.54 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 9 | 2.54 |
| (1,1077) | 1:175:I:GLU:N | 1:175:I:GLU:CA | 1:175:I:GLU:C | 1:176:I:GLN:N | 10 | 2.53 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 6 | 2.53 |
| (1,569) | 1:198:K:CYS:C | 1:199:K:LYS:N | 1:199:K:LYS:CA | 1:199:K:LYS:C | 1 | 2.53 |
| (1,42) | 1:148:L:THR:C | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 1 | 2.52 |
| (1,90) | 1:154:L:ARG:C | 1:155:L:GLN:N | 1:155:L:GLN:CA | 1:155:L:GLN:C | 4 | 2.51 |
| (1,26) | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 1:148:H:THR:N | 3 | 2.51 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 2 | 2.5 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 4 | 2.5 |
| (1,759) | 1:216:I:THR:C | 1:217:I:ALA:N | 1:217:I:ALA:CA | 1:217:I:ALA:C | 7 | 2.5 |
| (1,274) | 1:171:J:THR:N | 1:171:J:THR:CA | 1:171:J:THR:C | 1:172:J:LEU:N | 4 | 2.5 |
| (1,68) | 1:153:H:ILE:N | 1:153:H:ILE:CA | 1:153:H:ILE:C | 1:154:H:ARG:N | 10 | 2.5 |
| (1,384) | 1:182:L:LYS:N | 1:182:L:LYS:CA | 1:182:L:LYS:C | 1:183:L:ASN:N | 6 | 2.49 |
| (1,85) | 1:154:G:ARG:C | 1:155:G:GLN:N | 1:155:G:GLN:CA | 1:155:G:GLN:C | 4 | 2.49 |
| (1,1073) | 1:174:K:ALA:C | 1:175:K:GLU:N | 1:175:K:GLU:CA | 1:175:K:GLU:C | 6 | 2.47 |
| (1,1017) | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 1:240:I:ASN:N | 6 | 2.47 |
| (1,906) | 1:229:L:ARG:C | 1:230:L:VAL:N | 1:230:L:VAL:CA | 1:230:L:VAL:C | 10 | 2.47 |
| (1,120) | 1:158:L:LYS:N | 1:158:L:LYS:CA | 1:158:L:LYS:C | 1:159:L:GLU:N | 5 | 2.47 |
| (1,1072) | 1:174:J:ALA:C | 1:175:J:GLU:N | 1:175:J:GLU:CA | 1:175:J:GLU:C | 7 | 2.46 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 10 | 2.46 |
| (1,87) | 1:154:I:ARG:C | 1:155:I:GLN:N | 1:155:I:GLN:CA | 1:155:I:GLN:C | 9 | 2.46 |
| (1,1037) | 1:240:K:ASN:C | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 6 | 2.45 |
| (1,1019) | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 1:240:K:ASN:N | 10 | 2.45 |
| (1,941) | 1:232:K:ALA:C | 1:233:K:GLU:N | 1:233:K:GLU:CA | 1:233:K:GLU:C | 4 | 2.45 |
| (1,759) | 1:216:I:THR:C | 1:217:I:ALA:N | 1:217:I:ALA:CA | 1:217:I:ALA:C | 9 | 2.45 |
| (1,495) | 1:191:I:VAL:C | 1:192:I:GLN:N | 1:192:I:GLN:CA | 1:192:I:GLN:C | 9 | 2.45 |
| (1,308) | 1:174:H:ALA:N | 1:174:H:ALA:CA | 1:174:H:ALA:C | 1:175:H:GLU:N | 4 | 2.45 |
| (1,60) | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 1:152:L:ASP:N | 2 | 2.45 |
| (1,1038) | 1:240:L:ASN:C | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 4 | 2.44 |
| (1,447) | 1:187:I:GLU:C | 1:188:I:THR:N | 1:188:I:THR:CA | 1:188:I:THR:C | 5 | 2.44 |
| (1,32) | 1:147:H:PRO:C | 1:148:H:THR:N | 1:148:H:THR:CA | 1:148:H:THR:C | 7 | 2.44 |
| (1,1015) | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 1:240:G:ASN:N | 8 | 2.43 |
| (1,450) | 1:187:L:GLU:C | 1:188:L:THR:N | 1:188:L:THR:CA | 1:188:L:THR:C | 7 | 2.43 |
| (1,134) | 1:159:H:GLU:C | 1:160:H:PRO:N | 1:160:H:PRO:CA | 1:160:H:PRO:C | 7 | 2.43 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 8 | 2.42 |
| (1,1009) | 1:238:G:VAL:C | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 7 | 2.42 |
| (1,309) | 1:174:I:ALA:N | 1:174:I:ALA:CA | 1:174:I:ALA:C | 1:175:I:GLU:N | 4 | 2.42 |
| (1,1015) | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 1:240:G:ASN:N | 7 | 2.41 |
| (1,1002) | 1:237:L:GLN:C | 1:238:L:VAL:N | 1:238:L:VAL:CA | 1:238:L:VAL:C | 10 | 2.41 |
| (1,274) | 1:171:J:THR:N | 1:171:J:THR:CA | 1:171:J:THR:C | 1:172:J:LEU:N | 1 | 2.41 |
| (1,273) | 1:171:I:THR:N | 1:171:I:THR:CA | 1:171:I:THR:C | 1:172:I:LEU:N | 6 | 2.41 |
| (1,118) | 1:158:J:LYS:N | 1:158:J:LYS:CA | 1:158:J:LYS:C | 1:159:J:GLU:N | 7 | 2.41 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 7 | 2.4 |
| (1,42) | 1:148:L:THR:C | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 10 | 2.4 |
| (1,444) | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 1:188:L:THR:N | 8 | 2.39 |
| (1,434) | 1:186:H:THR:C | 1:187:H:GLU:N | 1:187:H:GLU:CA | 1:187:H:GLU:C | 2 | 2.39 |
| (1,267) | 1:170:I:LYS:C | 1:171:I:THR:N | 1:171:I:THR:CA | 1:171:I:THR:C | 6 | 2.39 |
| (1,172) | 1:162:J:ARG:C | 1:163:J:ASP:N | 1:163:J:ASP:CA | 1:163:J:ASP:C | 4 | 2.39 |
| (1,830) | 1:223:H:GLY:C | 1:224:H:PRO:N | 1:224:H:PRO:CA | 1:224:H:PRO:C | 2 | 2.38 |
| (1,798) | 1:219:L:GLN:C | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 4 | 2.38 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,758) | 1:216:H:THR:C | 1:217:H:ALA:N | 1:217:H:ALA:CA | 1:217:H:ALA:C | 8 | 2.38 |
| (1,580) | 1:199:J:LYS:C | 1:200:J:THR:N | 1:200:J:THR:CA | 1:200:J:THR:C | 5 | 2.38 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 3 | 2.38 |
| (1,433) | 1:186:G:THR:C | 1:187:G:GLU:N | 1:187:G:GLU:CA | 1:187:G:GLU:C | 6 | 2.38 |
| (1,404) | 1:184:H:TRP:N | 1:184:H:TRP:CA | 1:184:H:TRP:C | 1:185:H:MET:N | 3 | 2.38 |
| (1,242) | 1:168:H:PHE:C | 1:169:H:TYR:N | 1:169:H:TYR:CA | 1:169:H:TYR:C | 5 | 2.38 |
| (1,1078) | 1:175:J:GLU:N | 1:175:J:GLU:CA | 1:175:J:GLU:C | 1:176:J:GLN:N | 5 | 2.37 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 5 | 2.37 |
| (1,1028) | 1:240:H:ASN:N | 1:240:H:ASN:CA | 1:240:H:ASN:C | 1:241:H:THR:N | 4 | 2.37 |
| (1,993) | 1:237:I:GLN:N | 1:237:I:GLN:CA | 1:237:I:GLN:C | 1:238:I:VAL:N | 8 | 2.37 |
| (1,410) | 1:184:H:TRP:C | 1:185:H:MET:N | 1:185:H:MET:CA | 1:185:H:MET:C | 6 | 2.37 |
| (1,284) | 1:172:H:LEU:N | 1:172:H:LEU:CA | 1:172:H:LEU:C | 1:173:H:ARG:N | 6 | 2.37 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 5 | 2.36 |
| (1,863) | 1:226:K:HIS:N | 1:226:K:HIS:CA | 1:226:K:HIS:C | 1:227:K:LYS:N | 1 | 2.36 |
| (1,674) | 1:209:H:ALA:C | 1:210:H:THR:N | 1:210:H:THR:CA | 1:210:H:THR:C | 6 | 2.36 |
| (1,451) | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 1:189:G:LEU:N | 10 | 2.36 |
| (1,155) | 1:161:K:PHE:N | 1:161:K:PHE:CA | 1:161:K:PHE:C | 1:162:K:ARG:N | 1 | 2.36 |
| (1,85) | 1:154:G:ARG:C | 1:155:G:GLN:N | 1:155:G:GLN:CA | 1:155:G:GLN:C | 1 | 2.36 |
| (1,1034) | 1:240:H:ASN:C | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 5 | 2.35 |
| (1,444) | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 1:188:L:THR:N | 3 | 2.35 |
| (1,973) | 1:235:G:MET:C | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 2 | 2.34 |
| (1,773) | 1:217:K:ALA:C | 1:218:K:CYS:N | 1:218:K:CYS:CA | 1:218:K:CYS:C | 6 | 2.34 |
| (1,70) | 1:153:J:ILE:N | 1:153:J:ILE:CA | 1:153:J:ILE:C | 1:154:J:ARG:N | 5 | 2.34 |
| (1,728) | 1:214:H:MET:N | 1:214:H:MET:CA | 1:214:H:MET:C | 1:215:H:MET:N | 3 | 2.33 |
| (1,435) | 1:186:I:THR:C | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 2 | 2.33 |
| (1,174) | 1:162:L:ARG:C | 1:163:L:ASP:N | 1:163:L:ASP:CA | 1:163:L:ASP:C | 9 | 2.33 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 4 | 2.33 |
| (1,1094) | 1:206:H:GLY:C | 1:207:H:PRO:N | 1:207:H:PRO:CA | 1:207:H:PRO:C | 7 | 2.32 |
| (1,396) | 1:183:L:ASN:N | 1:183:L:ASN:CA | 1:183:L:ASN:C | 1:184:L:TRP:N | 2 | 2.32 |
| (1,227) | 1:167:K:ARG:N | 1:167:K:ARG:CA | 1:167:K:ARG:C | 1:168:K:PHE:N | 3 | 2.32 |
| (1,447) | 1:187:I:GLU:C | 1:188:I:THR:N | 1:188:I:THR:CA | 1:188:I:THR:C | 7 | 2.31 |
| (1,309) | 1:174:I:ALA:N | 1:174:I:ALA:CA | 1:174:I:ALA:C | 1:175:I:GLU:N | 8 | 2.31 |
| (1,896) | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 1:230:H:VAL:N | 4 | 2.3 |
| (1,435) | 1:186:I:THR:C | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 7 | 2.3 |
| (1,229) | 1:167:G:ARG:C | 1:168:G:PHE:N | 1:168:G:PHE:CA | 1:168:G:PHE:C | 8 | 2.3 |
| (1,37) | 1:148:G:THR:C | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 2 | 2.27 |
| (1,904) | 1:229:J:ARG:C | 1:230:J:VAL:N | 1:230:J:VAL:CA | 1:230:J:VAL:C | 4 | 2.26 |
| (1,431) | 1:186:K:THR:N | 1:186:K:THR:CA | 1:186:K:THR:C | 1:187:K:GLU:N | 7 | 2.26 |
| (1,312) | 1:174:L:ALA:N | 1:174:L:ALA:CA | 1:174:L:ALA:C | 1:175:L:GLU:N | 8 | 2.26 |
| (1,634) | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 1:205:J:LEU:N | 2 | 2.25 |
| (1,437) | 1:186:K:THR:C | 1:187:K:GLU:N | 1:187:K:GLU:CA | 1:187:K:GLU:C | 1 | 2.25 |
| (1,274) | 1:171:J:THR:N | 1:171:J:THR:CA | 1:171:J:THR:C | 1:172:J:LEU:N | 10 | 2.25 |
| (1,26) | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 1:148:H:THR:N | 7 | 2.25 |
| (1,1015) | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 1:240:G:ASN:N | 4 | 2.24 |
| (1,174) | 1:162:L:ARG:C | 1:163:L:ASP:N | 1:163:L:ASP:CA | 1:163:L:ASP:C | 8 | 2.24 |
| (1,828) | 1:223:L:GLY:N | 1:223:L:GLY:CA | 1:223:L:GLY:C | 1:224:L:PRO:N | 2 | 2.23 |
| (1,793) | 1:219:G:GLN:C | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 7 | 2.23 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 2 | 2.23 |
| (1,1017) | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 1:240:I:ASN:N | 2 | 2.22 |
| (1,492) | 1:191:L:VAL:N | 1:191:L:VAL:CA | 1:191:L:VAL:C | 1:192:L:GLN:N | 4 | 2.22 |
| (1,243) | 1:168:I:PHE:C | 1:169:I:TYR:N | 1:169:I:TYR:CA | 1:169:I:TYR:C | 9 | 2.22 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,88) | 1:154:J:ARG:C | 1:155:J:GLN:N | 1:155:J:GLN:CA | 1:155:J:GLN:C | 1 | 2.22 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 3 | 2.21 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 9 | 2.21 |
| (1,1011) | 1:238:I:VAL:C | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 9 | 2.21 |
| (1,984) | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1:237:L:GLN:N | 6 | 2.21 |
| (1,973) | 1:235:G:MET:C | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 7 | 2.21 |
| (1,825) | 1:223:I:GLY:N | 1:223:I:GLY:CA | 1:223:I:GLY:C | 1:224:I:PRO:N | 5 | 2.21 |
| (1,449) | 1:187:K:GLU:C | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 8 | 2.21 |
| (1,441) | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 1:188:I:THR:N | 10 | 2.21 |
| (1,1016) | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 1:240:H:ASN:N | 10 | 2.2 |
| (1,820) | 1:222:J:GLY:N | 1:222:J:GLY:CA | 1:222:J:GLY:C | 1:223:J:GLY:N | 1 | 2.2 |
| (1,740) | 1:215:H:MET:N | 1:215:H:MET:CA | 1:215:H:MET:C | 1:216:H:THR:N | 4 | 2.2 |
| (1,669) | 1:209:I:ALA:N | 1:209:I:ALA:CA | 1:209:I:ALA:C | 1:210:I:THR:N | 7 | 2.2 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 10 | 2.2 |
| (1,491) | 1:191:K:VAL:N | 1:191:K:VAL:CA | 1:191:K:VAL:C | 1:192:K:GLN:N | 4 | 2.19 |
| (1,305) | 1:173:K:ARG:C | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 2 | 2.19 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 1 | 2.18 |
| (1,449) | 1:187:K:GLU:C | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 7 | 2.18 |
| (1,1015) | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 1:240:G:ASN:N | 3 | 2.17 |
| (1,998) | 1:237:H:GLN:C | 1:238:H:VAL:N | 1:238:H:VAL:CA | 1:238:H:VAL:C | 9 | 2.17 |
| (1,460) | 1:188:J:THR:C | 1:189:J:LEU:N | 1:189:J:LEU:CA | 1:189:J:LEU:C | 4 | 2.17 |
| (1,284) | 1:172:H:LEU:N | 1:172:H:LEU:CA | 1:172:H:LEU:C | 1:173:H:ARG:N | 1 | 2.17 |
| (1,175) | 1:163:G:ASP:N | 1:163:G:ASP:CA | 1:163:G:ASP:C | 1:164:G:TYR:N | 4 | 2.17 |
| (1,998) | 1:237:H:GLN:C | 1:238:H:VAL:N | 1:238:H:VAL:CA | 1:238:H:VAL:C | 5 | 2.16 |
| (1,311) | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 1:175:K:GLU:N | 3 | 2.16 |
| (1,716) | 1:213:H:GLU:N | 1:213:H:GLU:CA | 1:213:H:GLU:C | 1:214:H:MET:N | 2 | 2.15 |
| (1,531) | 1:195:I:ASN:C | 1:196:I:PRO:N | 1:196:I:PRO:CA | 1:196:I:PRO:C | 7 | 2.15 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 7 | 2.15 |
| (1,433) | 1:186:G:THR:C | 1:187:G:GLU:N | 1:187:G:GLU:CA | 1:187:G:GLU:C | 5 | 2.15 |
| (1,672) | 1:209:L:ALA:N | 1:209:L:ALA:CA | 1:209:L:ALA:C | 1:210:L:THR:N | 9 | 2.14 |
| (1,532) | 1:195:J:ASN:C | 1:196:J:PRO:N | 1:196:J:PRO:CA | 1:196:J:PRO:C | 4 | 2.14 |
| (1,37) | 1:148:G:THR:C | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 6 | 2.14 |
| (1,27) | 1:147:I:PRO:N | 1:147:I:PRO:CA | 1:147:I:PRO:C | 1:148:I:THR:N | 8 | 2.14 |
| (1,426) | 1:185:L:MET:C | 1:186:L:THR:N | 1:186:L:THR:CA | 1:186:L:THR:C | 3 | 2.13 |
| (1,381) | 1:182:I:LYS:N | 1:182:I:LYS:CA | 1:182:I:LYS:C | 1:183:I:ASN:N | 1 | 2.13 |
| (1,3) | 1:144:I:GLY:C | 1:145:I:GLY:N | 1:145:I:GLY:CA | 1:145:I:GLY:C | 1 | 2.13 |
| (1,1080) | 1:175:L:GLU:N | 1:175:L:GLU:CA | 1:175:L:GLU:C | 1:176:L:GLN:N | 3 | 2.12 |
| (1,753) | 1:216:I:THR:N | 1:216:I:THR:CA | 1:216:I:THR:C | 1:217:I:ALA:N | 10 | 2.12 |
| (1,155) | 1:161:K:PHE:N | 1:161:K:PHE:CA | 1:161:K:PHE:C | 1:162:K:ARG:N | 8 | 2.12 |
| (1,1016) | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 1:240:H:ASN:N | 4 | 2.11 |
| (1,609) | 1:202:I:LEU:N | 1:202:I:LEU:CA | 1:202:I:LEU:C | 1:203:I:LYS:N | 10 | 2.11 |
| (1,455) | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 1:189:K:LEU:N | 8 | 2.11 |
| (1,307) | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 1:175:G:GLU:N | 9 | 2.11 |
| (1,250) | 1:169:J:TYR:N | 1:169:J:TYR:CA | 1:169:J:TYR:C | 1:170:J:LYS:N | 4 | 2.11 |
| (1,175) | 1:163:G:ASP:N | 1:163:G:ASP:CA | 1:163:G:ASP:C | 1:164:G:TYR:N | 8 | 2.11 |
| (1,66) | 1:152:L:ASP:N | 1:152:L:ASP:CA | 1:152:L:ASP:C | 1:153:L:ILE:N | 5 | 2.11 |
| (1,1011) | 1:238:I:VAL:C | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 10 | 2.1 |
| (1,645) | 1:205:I:LEU:N | 1:205:I:LEU:CA | 1:205:I:LEU:C | 1:206:I:GLY:N | 5 | 2.1 |
| (1,305) | 1:173:K:ARG:C | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 5 | 2.1 |
| (1,1041) | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 1:242:I:ALA:N | 9 | 2.08 |
| (1,1016) | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 1:240:H:ASN:N | 5 | 2.08 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,243) | 1:168:I:PHE:C | 1:169:I:TYR:N | 1:169:I:TYR:CA | 1:169:I:TYR:C | 3 | 2.07 |
| (1,34) | 1:147:J:PRO:C | 1:148:J:THR:N | 1:148:J:THR:CA | 1:148:J:THR:C | 7 | 2.07 |
| (1,1080) | 1:175:L:GLU:N | 1:175:L:GLU:CA | 1:175:L:GLU:C | 1:176:L:GLN:N | 4 | 2.06 |
| (1,509) | 1:192:K:GLN:C | 1:193:K:ASN:N | 1:193:K:ASN:CA | 1:193:K:ASN:C | 2 | 2.06 |
| (1,316) | 1:176:J:GLN:C | 1:177:J:ALA:N | 1:177:J:ALA:CA | 1:177:J:ALA:C | 2 | 2.06 |
| (1,1044) | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1:242:L:ALA:N | 4 | 2.05 |
| (1,1035) | 1:240:I:ASN:C | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 10 | 2.05 |
| (1,1034) | 1:240:H:ASN:C | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 9 | 2.05 |
| (1,988) | 1:236:J:SER:C | 1:237:J:GLN:N | 1:237:J:GLN:CA | 1:237:J:GLN:C | 6 | 2.05 |
| (1,849) | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 1:226:I:HIS:N | 9 | 2.05 |
| (1,85) | 1:154:G:ARG:C | 1:155:G:GLN:N | 1:155:G:GLN:CA | 1:155:G:GLN:C | 2 | 2.05 |
| (1,1012) | 1:238:J:VAL:C | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 7 | 2.04 |
| (1,63) | 1:152:I:ASP:N | 1:152:I:ASP:CA | 1:152:I:ASP:C | 1:153:I:ILE:N | 9 | 2.04 |
| (1,851) | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 1:226:K:HIS:N | 7 | 2.03 |
| (1,107) | 1:157:K:PRO:N | 1:157:K:PRO:CA | 1:157:K:PRO:C | 1:158:K:LYS:N | 9 | 2.03 |
| (1,20) | 1:146:H:SER:C | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 3 | 2.03 |
| (1,813) | 1:221:I:VAL:N | 1:221:I:VAL:CA | 1:221:I:VAL:C | 1:222:I:GLY:N | 4 | 2.02 |
| (1,692) | 1:211:H:LEU:N | 1:211:H:LEU:CA | 1:211:H:LEU:C | 1:212:H:GLU:N | 5 | 2.02 |
| (1,536) | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 1:197:H:ASP:N | 1 | 2.02 |
| (1,172) | 1:162:J:ARG:C | 1:163:J:ASP:N | 1:163:J:ASP:CA | 1:163:J:ASP:C | 8 | 2.02 |
| (1,156) | 1:161:L:PHE:N | 1:161:L:PHE:CA | 1:161:L:PHE:C | 1:162:L:ARG:N | 4 | 2.01 |
| (1,1013) | 1:238:K:VAL:C | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 6 | 2.0 |
| (1,1011) | 1:238:I:VAL:C | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 5 | 2.0 |
| (1,175) | 1:163:G:ASP:N | 1:163:G:ASP:CA | 1:163:G:ASP:C | 1:164:G:TYR:N | 6 | 2.0 |
| (1,975) | 1:235:I:MET:C | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 2 | 1.99 |
| (1,764) | 1:217:H:ALA:N | 1:217:H:ALA:CA | 1:217:H:ALA:C | 1:218:H:CYS:N | 7 | 1.99 |
| (1,764) | 1:217:H:ALA:N | 1:217:H:ALA:CA | 1:217:H:ALA:C | 1:218:H:CYS:N | 9 | 1.99 |
| (1,441) | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 1:188:I:THR:N | 5 | 1.99 |
| (1,1044) | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1:242:L:ALA:N | 9 | 1.98 |
| (1,947) | 1:233:K:GLU:N | 1:233:K:GLU:CA | 1:233:K:GLU:C | 1:234:K:ALA:N | 9 | 1.98 |
| (1,20) | 1:146:H:SER:C | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 7 | 1.98 |
| (1,1037) | 1:240:K:ASN:C | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 3 | 1.97 |
| (1,824) | 1:223:H:GLY:N | 1:223:H:GLY:CA | 1:223:H:GLY:C | 1:224:H:PRO:N | 7 | 1.97 |
| (1,1037) | 1:240:K:ASN:C | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 10 | 1.96 |
| (1,998) | 1:237:H:GLN:C | 1:238:H:VAL:N | 1:238:H:VAL:CA | 1:238:H:VAL:C | 7 | 1.96 |
| (1,803) | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 1:221:K:VAL:N | 3 | 1.96 |
| (1,245) | 1:168:K:PHE:C | 1:169:K:TYR:N | 1:169:K:TYR:CA | 1:169:K:TYR:C | 1 | 1.96 |
| (1,191) | 1:164:K:TYR:N | 1:164:K:TYR:CA | 1:164:K:TYR:C | 1:165:K:VAL:N | 8 | 1.96 |
| (1,32) | 1:147:H:PRO:C | 1:148:H:THR:N | 1:148:H:THR:CA | 1:148:H:THR:C | 10 | 1.96 |
| (1,1015) | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 1:240:G:ASN:N | 2 | 1.94 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 6 | 1.94 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 8 | 1.94 |
| (1,380) | 1:182:H:LYS:N | 1:182:H:LYS:CA | 1:182:H:LYS:C | 1:183:H:ASN:N | 8 | 1.94 |
| (1,311) | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 1:175:K:GLU:N | 7 | 1.94 |
| (1,1056) | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 1:244:L:ILE:N | 1 | 1.93 |
| (1,1017) | 1:239:I:THR:N | 1:239:I:THR:CA | 1:239:I:THR:C | 1:240:I:ASN:N | 3 | 1.93 |
| (1,521) | 1:194:K:ALA:C | 1:195:K:ASN:N | 1:195:K:ASN:CA | 1:195:K:ASN:C | 7 | 1.93 |
| (1,626) | 1:203:H:LYS:C | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 2 | 1.92 |
| (1,442) | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 1:188:J:THR:N | 2 | 1.92 |
| (1,182) | 1:163:H:ASP:C | 1:164:H:TYR:N | 1:164:H:TYR:CA | 1:164:H:TYR:C | 1 | 1.92 |
| (1,1053) | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 1:244:I:ILE:N | 3 | 1.91 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,973) | 1:235:G:MET:C | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 3 | 1.91 |
| (1,728) | 1:214:H:MET:N | 1:214:H:MET:CA | 1:214:H:MET:C | 1:215:H:MET:N | 10 | 1.91 |
| (1,626) | 1:203:H:LYS:C | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 6 | 1.91 |
| (1,522) | 1:194:L:ALA:C | 1:195:L:ASN:N | 1:195:L:ASN:CA | 1:195:L:ASN:C | 10 | 1.91 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 8 | 1.9 |
| (1,315) | 1:176:I:GLN:C | 1:177:I:ALA:N | 1:177:I:ALA:CA | 1:177:I:ALA:C | 3 | 1.9 |
| (1,633) | 1:204:I:ALA:N | 1:204:I:ALA:CA | 1:204:I:ALA:C | 1:205:I:LEU:N | 9 | 1.89 |
| (1,626) | 1:203:H:LYS:C | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 4 | 1.89 |
| (1,230) | 1:167:H:ARG:C | 1:168:H:PHE:N | 1:168:H:PHE:CA | 1:168:H:PHE:C | 8 | 1.89 |
| (1,1044) | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1:242:L:ALA:N | 8 | 1.88 |
| (1,1016) | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 1:240:H:ASN:N | 2 | 1.87 |
| (1,730) | 1:214:J:MET:N | 1:214:J:MET:CA | 1:214:J:MET:C | 1:215:J:MET:N | 4 | 1.87 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 5 | 1.87 |
| (1,118) | 1:158:J:LYS:N | 1:158:J:LYS:CA | 1:158:J:LYS:C | 1:159:J:GLU:N | 4 | 1.87 |
| (1,104) | 1:157:H:PRO:N | 1:157:H:PRO:CA | 1:157:H:PRO:C | 1:158:H:LYS:N | 3 | 1.87 |
| (1,1018) | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 1:240:J:ASN:N | 2 | 1.86 |
| (1,998) | 1:237:H:GLN:C | 1:238:H:VAL:N | 1:238:H:VAL:CA | 1:238:H:VAL:C | 3 | 1.86 |
| (1,673) | 1:209:G:ALA:C | 1:210:G:THR:N | 1:210:G:THR:CA | 1:210:G:THR:C | 5 | 1.86 |
| (1,304) | 1:173:J:ARG:C | 1:174:J:ALA:N | 1:174:J:ALA:CA | 1:174:J:ALA:C | 1 | 1.86 |
| (1,26) | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 1:148:H:THR:N | 1 | 1.86 |
| (1,889) | 1:228:G:ALA:C | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 5 | 1.85 |
| (1,825) | 1:223:I:GLY:N | 1:223:I:GLY:CA | 1:223:I:GLY:C | 1:224:I:PRO:N | 1 | 1.85 |
| (1,377) | 1:181:K:VAL:C | 1:182:K:LYS:N | 1:182:K:LYS:CA | 1:182:K:LYS:C | 1 | 1.85 |
| (1,174) | 1:162:L:ARG:C | 1:163:L:ASP:N | 1:163:L:ASP:CA | 1:163:L:ASP:C | 5 | 1.85 |
| (1,156) | 1:161:L:PHE:N | 1:161:L:PHE:CA | 1:161:L:PHE:C | 1:162:L:ARG:N | 10 | 1.85 |
| (1,1033) | 1:240:G:ASN:C | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 4 | 1.84 |
| (1,1009) | 1:238:G:VAL:C | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 3 | 1.84 |
| (1,975) | 1:235:I:MET:C | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 3 | 1.84 |
| (1,237) | 1:168:I:PHE:N | 1:168:I:PHE:CA | 1:168:I:PHE:C | 1:169:I:TYR:N | 2 | 1.84 |
| (1,1073) | 1:174:K:ALA:C | 1:175:K:GLU:N | 1:175:K:GLU:CA | 1:175:K:GLU:C | 5 | 1.83 |
| (1,921) | 1:231:I:LEU:N | 1:231:I:LEU:CA | 1:231:I:LEU:C | 1:232:I:ALA:N | 3 | 1.82 |
| (1,804) | 1:220:L:GLY:N | 1:220:L:GLY:CA | 1:220:L:GLY:C | 1:221:L:VAL:N | 5 | 1.81 |
| (1,803) | 1:220:K:GLY:N | 1:220:K:GLY:CA | 1:220:K:GLY:C | 1:221:K:VAL:N | 5 | 1.81 |
| (1,676) | 1:209:J:ALA:C | 1:210:J:THR:N | 1:210:J:THR:CA | 1:210:J:THR:C | 5 | 1.81 |
| (1,433) | 1:186:G:THR:C | 1:187:G:GLU:N | 1:187:G:GLU:CA | 1:187:G:GLU:C | 3 | 1.81 |
| (1,72) | 1:153:L:ILE:N | 1:153:L:ILE:CA | 1:153:L:ILE:C | 1:154:L:ARG:N | 1 | 1.81 |
| (1,670) | 1:209:J:ALA:N | 1:209:J:ALA:CA | 1:209:J:ALA:C | 1:210:J:THR:N | 7 | 1.8 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 4 | 1.8 |
| (1,423) | 1:185:I:MET:C | 1:186:I:THR:N | 1:186:I:THR:CA | 1:186:I:THR:C | 5 | 1.8 |
| (1,326) | 1:177:H:ALA:C | 1:178:H:SER:N | 1:178:H:SER:CA | 1:178:H:SER:C | 4 | 1.8 |
| (1,68) | 1:153:H:ILE:N | 1:153:H:ILE:CA | 1:153:H:ILE:C | 1:154:H:ARG:N | 3 | 1.8 |
| (1,894) | 1:228:L:ALA:C | 1:229:L:ARG:N | 1:229:L:ARG:CA | 1:229:L:ARG:C | 8 | 1.79 |
| (1,515) | 1:193:K:ASN:N | 1:193:K:ASN:CA | 1:193:K:ASN:C | 1:194:K:ALA:N | 8 | 1.79 |
| (1,284) | 1:172:H:LEU:N | 1:172:H:LEU:CA | 1:172:H:LEU:C | 1:173:H:ARG:N | 5 | 1.79 |
| (1,64) | 1:152:J:ASP:N | 1:152:J:ASP:CA | 1:152:J:ASP:C | 1:153:J:ILE:N | 5 | 1.79 |
| (1,5) | 1:144:K:GLY:C | 1:145:K:GLY:N | 1:145:K:GLY:CA | 1:145:K:GLY:C | 9 | 1.79 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 10 | 1.78 |
| (1,731) | 1:214:K:MET:N | 1:214:K:MET:CA | 1:214:K:MET:C | 1:215:K:MET:N | 1 | 1.78 |
| (1,442) | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 1:188:J:THR:N | 9 | 1.78 |
| (1,231) | 1:167:I:ARG:C | 1:168:I:PHE:N | 1:168:I:PHE:CA | 1:168:I:PHE:C | 4 | 1.78 |
| (1,1068) | 1:244:L:ILE:N | 1:244:L:ILE:CA | 1:244:L:ILE:C | 1:245:L:MET:N | 10 | 1.77 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,1015) | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 1:240:G:ASN:N | 6 | 1.77 |
| (1,872) | 1:227:H:LYS:N | 1:227:H:LYS:CA | 1:227:H:LYS:C | 1:228:H:ALA:N | 5 | 1.77 |
| (1,813) | 1:221:I:VAL:N | 1:221:I:VAL:CA | 1:221:I:VAL:C | 1:222:I:GLY:N | 8 | 1.77 |
| (1,472) | 1:189:J:LEU:C | 1:190:J:LEU:N | 1:190:J:LEU:CA | 1:190:J:LEU:C | 7 | 1.77 |
| (1,1035) | 1:240:I:ASN:C | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 5 | 1.76 |
| (1,1019) | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 1:240:K:ASN:N | 7 | 1.76 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 4 | 1.76 |
| (1,396) | 1:183:L:ASN:N | 1:183:L:ASN:CA | 1:183:L:ASN:C | 1:184:L:TRP:N | 3 | 1.76 |
| (1,330) | 1:177:L:ALA:C | 1:178:L:SER:N | 1:178:L:SER:CA | 1:178:L:SER:C | 6 | 1.76 |
| (1,230) | 1:167:H:ARG:C | 1:168:H:PHE:N | 1:168:H:PHE:CA | 1:168:H:PHE:C | 4 | 1.76 |
| (1,85) | 1:154:G:ARG:C | 1:155:G:GLN:N | 1:155:G:GLN:CA | 1:155:G:GLN:C | 8 | 1.76 |
| (1,1036) | 1:240:J:ASN:C | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 6 | 1.75 |
| (1,827) | 1:223:K:GLY:N | 1:223:K:GLY:CA | 1:223:K:GLY:C | 1:224:K:PRO:N | 4 | 1.75 |
| (1,826) | 1:223:J:GLY:N | 1:223:J:GLY:CA | 1:223:J:GLY:C | 1:224:J:PRO:N | 1 | 1.75 |
| (1,800) | 1:220:H:GLY:N | 1:220:H:GLY:CA | 1:220:H:GLY:C | 1:221:H:VAL:N | 3 | 1.75 |
| (1,125) | 1:158:K:LYS:C | 1:159:K:GLU:N | 1:159:K:GLU:CA | 1:159:K:GLU:C | 1 | 1.75 |
| (1,85) | 1:154:G:ARG:C | 1:155:G:GLN:N | 1:155:G:GLN:CA | 1:155:G:GLN:C | 10 | 1.75 |
| (1,57) | 1:151:I:LEU:N | 1:151:I:LEU:CA | 1:151:I:LEU:C | 1:152:I:ASP:N | 5 | 1.75 |
| (1,426) | 1:185:L:MET:C | 1:186:L:THR:N | 1:186:L:THR:CA | 1:186:L:THR:C | 7 | 1.74 |
| (1,988) | 1:236:J:SER:C | 1:237:J:GLN:N | 1:237:J:GLN:CA | 1:237:J:GLN:C | 4 | 1.73 |
| (1,652) | 1:207:J:PRO:C | 1:208:J:GLY:N | 1:208:J:GLY:CA | 1:208:J:GLY:C | 8 | 1.73 |
| (1,326) | 1:177:H:ALA:C | 1:178:H:SER:N | 1:178:H:SER:CA | 1:178:H:SER:C | 6 | 1.73 |
| (1,56) | 1:151:H:LEU:N | 1:151:H:LEU:CA | 1:151:H:LEU:C | 1:152:H:ASP:N | 5 | 1.73 |
| (1,831) | 1:223:I:GLY:C | 1:224:I:PRO:N | 1:224:I:PRO:CA | 1:224:I:PRO:C | 8 | 1.72 |
| (1,826) | 1:223:J:GLY:N | 1:223:J:GLY:CA | 1:223:J:GLY:C | 1:224:J:PRO:N | 7 | 1.72 |
| (1,693) | 1:211:I:LEU:N | 1:211:I:LEU:CA | 1:211:I:LEU:C | 1:212:I:GLU:N | 1 | 1.72 |
| (1,518) | 1:194:H:ALA:C | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 3 | 1.72 |
| (1,71) | 1:153:K:ILE:N | 1:153:K:ILE:CA | 1:153:K:ILE:C | 1:154:K:ARG:N | 6 | 1.72 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 3 | 1.71 |
| (1,410) | 1:184:H:TRP:C | 1:185:H:MET:N | 1:185:H:MET:CA | 1:185:H:MET:C | 10 | 1.71 |
| (1,117) | 1:158:I:LYS:N | 1:158:I:LYS:CA | 1:158:I:LYS:C | 1:159:I:GLU:N | 6 | 1.71 |
| (1,71) | 1:153:K:ILE:N | 1:153:K:ILE:CA | 1:153:K:ILE:C | 1:154:K:ARG:N | 5 | 1.71 |
| (1,20) | 1:146:H:SER:C | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 6 | 1.71 |
| (1,1009) | 1:238:G:VAL:C | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 6 | 1.7 |
| (1,693) | 1:211:I:LEU:N | 1:211:I:LEU:CA | 1:211:I:LEU:C | 1:212:I:GLU:N | 9 | 1.7 |
| (1,454) | 1:188:J:THR:N | 1:188:J:THR:CA | 1:188:J:THR:C | 1:189:J:LEU:N | 4 | 1.7 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 6 | 1.69 |
| (1,813) | 1:221:I:VAL:N | 1:221:I:VAL:CA | 1:221:I:VAL:C | 1:222:I:GLY:N | 2 | 1.69 |
| (1,747) | 1:215:I:MET:C | 1:216:I:THR:N | 1:216:I:THR:CA | 1:216:I:THR:C | 6 | 1.69 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 4 | 1.68 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 8 | 1.68 |
| (1,677) | 1:209:K:ALA:C | 1:210:K:THR:N | 1:210:K:THR:CA | 1:210:K:THR:C | 7 | 1.68 |
| (1,478) | 1:190:J:LEU:N | 1:190:J:LEU:CA | 1:190:J:LEU:C | 1:191:J:VAL:N | 6 | 1.68 |
| (1,444) | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 1:188:L:THR:N | 2 | 1.68 |
| (1,435) | 1:186:I:THR:C | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 1 | 1.68 |
| (1,188) | 1:164:H:TYR:N | 1:164:H:TYR:CA | 1:164:H:TYR:C | 1:165:H:VAL:N | 3 | 1.68 |
| (1,143) | 1:160:K:PRO:N | 1:160:K:PRO:CA | 1:160:K:PRO:C | 1:161:K:PHE:N | 10 | 1.68 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 9 | 1.67 |
| (1,1034) | 1:240:H:ASN:C | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1 | 1.67 |
| (1,669) | 1:209:I:ALA:N | 1:209:I:ALA:CA | 1:209:I:ALA:C | 1:210:I:THR:N | 10 | 1.67 |
| (1,508) | 1:192:J:GLN:C | 1:193:J:ASN:N | 1:193:J:ASN:CA | 1:193:J:ASN:C | 7 | 1.67 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,305) | 1:173:K:ARG:C | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 6 | 1.67 |
| (1,1037) | 1:240:K:ASN:C | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 2 | 1.66 |
| (1,444) | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 1:188:L:THR:N | 6 | 1.66 |
| (1,155) | 1:161:K:PHE:N | 1:161:K:PHE:CA | 1:161:K:PHE:C | 1:162:K:ARG:N | 3 | 1.65 |
| (1,42) | 1:148:L:THR:C | 1:149:L:SER:N | 1:149:L:SER:CA | 1:149:L:SER:C | 2 | 1.65 |
| (1,895) | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 1:230:G:VAL:N | 8 | 1.64 |
| (1,323) | 1:177:K:ALA:N | 1:177:K:ALA:CA | 1:177:K:ALA:C | 1:178:K:SER:N | 2 | 1.64 |
| (1,143) | 1:160:K:PRO:N | 1:160:K:PRO:CA | 1:160:K:PRO:C | 1:161:K:PHE:N | 2 | 1.64 |
| (1,1056) | 1:243:L:THR:N | 1:243:L:THR:CA | 1:243:L:THR:C | 1:244:L:ILE:N | 6 | 1.63 |
| (1,1019) | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 1:240:K:ASN:N | 5 | 1.63 |
| (1,449) | 1:187:K:GLU:C | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 2 | 1.63 |
| (1,155) | 1:161:K:PHE:N | 1:161:K:PHE:CA | 1:161:K:PHE:C | 1:162:K:ARG:N | 9 | 1.63 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 5 | 1.62 |
| (1,859) | 1:226:G:HIS:N | 1:226:G:HIS:CA | 1:226:G:HIS:C | 1:227:G:LYS:N | 5 | 1.62 |
| (1,596) | 1:201:H:ILE:N | 1:201:H:ILE:CA | 1:201:H:ILE:C | 1:202:H:LEU:N | 9 | 1.62 |
| (1,85) | 1:154:G:ARG:C | 1:155:G:GLN:N | 1:155:G:GLN:CA | 1:155:G:GLN:C | 6 | 1.62 |
| (1,37) | 1:148:G:THR:C | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 8 | 1.62 |
| (1,896) | 1:229:H:ARG:N | 1:229:H:ARG:CA | 1:229:H:ARG:C | 1:230:H:VAL:N | 6 | 1.61 |
| (1,894) | 1:228:L:ALA:C | 1:229:L:ARG:N | 1:229:L:ARG:CA | 1:229:L:ARG:C | 10 | 1.61 |
| (1,540) | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 1:197:L:ASP:N | 6 | 1.61 |
| (1,41) | 1:148:K:THR:C | 1:149:K:SER:N | 1:149:K:SER:CA | 1:149:K:SER:C | 1 | 1.61 |
| (1,1035) | 1:240:I:ASN:C | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 6 | 1.6 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 7 | 1.6 |
| (1,496) | 1:191:J:VAL:C | 1:192:J:GLN:N | 1:192:J:GLN:CA | 1:192:J:GLN:C | 5 | 1.6 |
| (1,482) | 1:190:H:LEU:C | 1:191:H:VAL:N | 1:191:H:VAL:CA | 1:191:H:VAL:C | 7 | 1.6 |
| (1,455) | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 1:189:K:LEU:N | 6 | 1.6 |
| (1,230) | 1:167:H:ARG:C | 1:168:H:PHE:N | 1:168:H:PHE:CA | 1:168:H:PHE:C | 2 | 1.6 |
| (1,104) | 1:157:H:PRO:N | 1:157:H:PRO:CA | 1:157:H:PRO:C | 1:158:H:LYS:N | 1 | 1.6 |
| (1,26) | 1:147:H:PRO:N | 1:147:H:PRO:CA | 1:147:H:PRO:C | 1:148:H:THR:N | 10 | 1.6 |
| (1,1044) | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 1:242:L:ALA:N | 5 | 1.59 |
| (1,1035) | 1:240:I:ASN:C | 1:241:I:THR:N | 1:241:I:THR:CA | 1:241:I:THR:C | 4 | 1.58 |
| (1,1034) | 1:240:H:ASN:C | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 10 | 1.58 |
| (1,816) | 1:221:L:VAL:N | 1:221:L:VAL:CA | 1:221:L:VAL:C | 1:222:L:GLY:N | 6 | 1.58 |
| (1,813) | 1:221:I:VAL:N | 1:221:I:VAL:CA | 1:221:I:VAL:C | 1:222:I:GLY:N | 10 | 1.58 |
| (1,767) | 1:217:K:ALA:N | 1:217:K:ALA:CA | 1:217:K:ALA:C | 1:218:K:CYS:N | 5 | 1.58 |
| (1,652) | 1:207:J:PRO:C | 1:208:J:GLY:N | 1:208:J:GLY:CA | 1:208:J:GLY:C | 9 | 1.58 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 4 | 1.58 |
| (1,533) | 1:195:K:ASN:C | 1:196:K:PRO:N | 1:196:K:PRO:CA | 1:196:K:PRO:C | 1 | 1.58 |
| (1,29) | 1:147:K:PRO:N | 1:147:K:PRO:CA | 1:147:K:PRO:C | 1:148:K:THR:N | 9 | 1.58 |
| (1,1037) | 1:240:K:ASN:C | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 7 | 1.57 |
| (1,1012) | 1:238:J:VAL:C | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 4 | 1.57 |
| (1,862) | 1:226:J:HIS:N | 1:226:J:HIS:CA | 1:226:J:HIS:C | 1:227:J:LYS:N | 4 | 1.57 |
| (1,308) | 1:174:H:ALA:N | 1:174:H:ALA:CA | 1:174:H:ALA:C | 1:175:H:GLU:N | 3 | 1.57 |
| (1,191) | 1:164:K:TYR:N | 1:164:K:TYR:CA | 1:164:K:TYR:C | 1:165:K:VAL:N | 4 | 1.57 |
| (1,988) | 1:236:J:SER:C | 1:237:J:GLN:N | 1:237:J:GLN:CA | 1:237:J:GLN:C | 7 | 1.56 |
| (1,973) | 1:235:G:MET:C | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 8 | 1.56 |
| (1,868) | 1:226:J:HIS:C | 1:227:J:LYS:N | 1:227:J:LYS:CA | 1:227:J:LYS:C | 2 | 1.56 |
| (1,1019) | 1:239:K:THR:N | 1:239:K:THR:CA | 1:239:K:THR:C | 1:240:K:ASN:N | 6 | 1.55 |
| (1,1016) | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 1:240:H:ASN:N | 7 | 1.55 |
| (1,658) | 1:208:J:GLY:N | 1:208:J:GLY:CA | 1:208:J:GLY:C | 1:209:J:ALA:N | 2 | 1.55 |
| (1,477) | 1:190:I:LEU:N | 1:190:I:LEU:CA | 1:190:I:LEU:C | 1:191:I:VAL:N | 4 | 1.55 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,426) | 1:185:L:MET:C | 1:186:L:THR:N | 1:186:L:THR:CA | 1:186:L:THR:C | 8 | 1.55 |
| (1,302) | 1:173:H:ARG:C | 1:174:H:ALA:N | 1:174:H:ALA:CA | 1:174:H:ALA:C | 7 | 1.55 |
| (1,728) | 1:214:H:MET:N | 1:214:H:MET:CA | 1:214:H:MET:C | 1:215:H:MET:N | 7 | 1.54 |
| (1,608) | 1:202:H:LEU:N | 1:202:H:LEU:CA | 1:202:H:LEU:C | 1:203:H:LYS:N | 6 | 1.54 |
| (1,237) | 1:168:I:PHE:N | 1:168:I:PHE:CA | 1:168:I:PHE:C | 1:169:I:TYR:N | 4 | 1.54 |
| (1,973) | 1:235:G:MET:C | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 9 | 1.53 |
| (1,894) | 1:228:L:ALA:C | 1:229:L:ARG:N | 1:229:L:ARG:CA | 1:229:L:ARG:C | 3 | 1.53 |
| (1,849) | 1:225:I:GLY:N | 1:225:I:GLY:CA | 1:225:I:GLY:C | 1:226:I:HIS:N | 3 | 1.53 |
| (1,536) | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 1:197:H:ASP:N | 5 | 1.53 |
| (1,239) | 1:168:K:PHE:N | 1:168:K:PHE:CA | 1:168:K:PHE:C | 1:169:K:TYR:N | 7 | 1.53 |
| (1,758) | 1:216:H:THR:C | 1:217:H:ALA:N | 1:217:H:ALA:CA | 1:217:H:ALA:C | 1 | 1.52 |
| (1,699) | 1:211:I:LEU:C | 1:212:I:GLU:N | 1:212:I:GLU:CA | 1:212:I:GLU:C | 6 | 1.52 |
| (1,634) | 1:204:J:ALA:N | 1:204:J:ALA:CA | 1:204:J:ALA:C | 1:205:J:LEU:N | 4 | 1.52 |
| (1,529) | 1:195:G:ASN:C | 1:196:G:PRO:N | 1:196:G:PRO:CA | 1:196:G:PRO:C | 1 | 1.52 |
| (1,318) | 1:176:L:GLN:C | 1:177:L:ALA:N | 1:177:L:ALA:CA | 1:177:L:ALA:C | 4 | 1.52 |
| (1,174) | 1:162:L:ARG:C | 1:163:L:ASP:N | 1:163:L:ASP:CA | 1:163:L:ASP:C | 6 | 1.52 |
| (1,796) | 1:219:J:GLN:C | 1:220:J:GLY:N | 1:220:J:GLY:CA | 1:220:J:GLY:C | 2 | 1.51 |
| (1,614) | 1:202:H:LEU:C | 1:203:H:LYS:N | 1:203:H:LYS:CA | 1:203:H:LYS:C | 8 | 1.51 |
| (1,476) | 1:190:H:LEU:N | 1:190:H:LEU:CA | 1:190:H:LEU:C | 1:191:H:VAL:N | 3 | 1.51 |
| (1,90) | 1:154:L:ARG:C | 1:155:L:GLN:N | 1:155:L:GLN:CA | 1:155:L:GLN:C | 2 | 1.51 |
| (1,447) | 1:187:I:GLU:C | 1:188:I:THR:N | 1:188:I:THR:CA | 1:188:I:THR:C | 10 | 1.5 |
| (1,37) | 1:148:G:THR:C | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 10 | 1.5 |
| (1,873) | 1:227:I:LYS:N | 1:227:I:LYS:CA | 1:227:I:LYS:C | 1:228:I:ALA:N | 2 | 1.49 |
| (1,802) | 1:220:J:GLY:N | 1:220:J:GLY:CA | 1:220:J:GLY:C | 1:221:J:VAL:N | 5 | 1.49 |
| (1,636) | 1:204:L:ALA:N | 1:204:L:ALA:CA | 1:204:L:ALA:C | 1:205:L:LEU:N | 6 | 1.49 |
| (1,563) | 1:198:K:CYS:N | 1:198:K:CYS:CA | 1:198:K:CYS:C | 1:199:K:LYS:N | 1 | 1.49 |
| (1,426) | 1:185:L:MET:C | 1:186:L:THR:N | 1:186:L:THR:CA | 1:186:L:THR:C | 2 | 1.49 |
| (1,107) | 1:157:K:PRO:N | 1:157:K:PRO:CA | 1:157:K:PRO:C | 1:158:K:LYS:N | 2 | 1.49 |
| (1,1033) | 1:240:G:ASN:C | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 10 | 1.48 |
| (1,651) | 1:207:I:PRO:C | 1:208:I:GLY:N | 1:208:I:GLY:CA | 1:208:I:GLY:C | 4 | 1.48 |
| (1,455) | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 1:189:K:LEU:N | 10 | 1.48 |
| (1,422) | 1:185:H:MET:C | 1:186:H:THR:N | 1:186:H:THR:CA | 1:186:H:THR:C | 8 | 1.48 |
| (1,85) | 1:154:G:ARG:C | 1:155:G:GLN:N | 1:155:G:GLN:CA | 1:155:G:GLN:C | 9 | 1.48 |
| (1,72) | 1:153:L:ILE:N | 1:153:L:ILE:CA | 1:153:L:ILE:C | 1:154:L:ARG:N | 4 | 1.48 |
| (1,1073) | 1:174:K:ALA:C | 1:175:K:GLU:N | 1:175:K:GLU:CA | 1:175:K:GLU:C | 9 | 1.47 |
| (1,978) | 1:235:L:MET:C | 1:236:L:SER:N | 1:236:L:SER:CA | 1:236:L:SER:C | 1 | 1.47 |
| (1,947) | 1:233:K:GLU:N | 1:233:K:GLU:CA | 1:233:K:GLU:C | 1:234:K:ALA:N | 10 | 1.47 |
| (1,435) | 1:186:I:THR:C | 1:187:I:GLU:N | 1:187:I:GLU:CA | 1:187:I:GLU:C | 6 | 1.47 |
| (1,416) | 1:185:H:MET:N | 1:185:H:MET:CA | 1:185:H:MET:C | 1:186:H:THR:N | 2 | 1.47 |
| (1,307) | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 1:175:G:GLU:N | 4 | 1.47 |
| (1,242) | 1:168:H:PHE:C | 1:169:H:TYR:N | 1:169:H:TYR:CA | 1:169:H:TYR:C | 8 | 1.47 |
| (1,150) | 1:160:L:PRO:C | 1:161:L:PHE:N | 1:161:L:PHE:CA | 1:161:L:PHE:C | 5 | 1.47 |
| (1,658) | 1:208:J:GLY:N | 1:208:J:GLY:CA | 1:208:J:GLY:C | 1:209:J:ALA:N | 10 | 1.46 |
| (1,308) | 1:174:H:ALA:N | 1:174:H:ALA:CA | 1:174:H:ALA:C | 1:175:H:GLU:N | 6 | 1.46 |
| (1,156) | 1:161:L:PHE:N | 1:161:L:PHE:CA | 1:161:L:PHE:C | 1:162:L:ARG:N | 9 | 1.46 |
| (1,1080) | 1:175:L:GLU:N | 1:175:L:GLU:CA | 1:175:L:GLU:C | 1:176:L:GLN:N | 1 | 1.45 |
| (1,895) | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 1:230:G:VAL:N | 4 | 1.45 |
| (1,318) | 1:176:L:GLN:C | 1:177:L:ALA:N | 1:177:L:ALA:CA | 1:177:L:ALA:C | 3 | 1.45 |
| (1,976) | 1:235:J:MET:C | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 7 | 1.44 |
| (1,671) | 1:209:K:ALA:N | 1:209:K:ALA:CA | 1:209:K:ALA:C | 1:210:K:THR:N | 1 | 1.44 |
| (1,273) | 1:171:I:THR:N | 1:171:I:THR:CA | 1:171:I:THR:C | 1:172:I:LEU:N | 10 | 1.44 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,57) | 1:151:I:LEU:N | 1:151:I:LEU:CA | 1:151:I:LEU:C | 1:152:I:ASP:N | 10 | 1.44 |
| (1,894) | 1:228:L:ALA:C | 1:229:L:ARG:N | 1:229:L:ARG:CA | 1:229:L:ARG:C | 1 | 1.43 |
| (1,301) | 1:173:G:ARG:C | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 3 | 1.43 |
| (1,35) | 1:147:K:PRO:C | 1:148:K:THR:N | 1:148:K:THR:CA | 1:148:K:THR:C | 6 | 1.43 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 5 | 1.42 |
| (1,1015) | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 1:240:G:ASN:N | 1 | 1.42 |
| (1,894) | 1:228:L:ALA:C | 1:229:L:ARG:N | 1:229:L:ARG:CA | 1:229:L:ARG:C | 5 | 1.42 |
| (1,728) | 1:214:H:MET:N | 1:214:H:MET:CA | 1:214:H:MET:C | 1:215:H:MET:N | 5 | 1.4 |
| (1,58) | 1:151:J:LEU:N | 1:151:J:LEU:CA | 1:151:J:LEU:C | 1:152:J:ASP:N | 5 | 1.4 |
| (1,921) | 1:231:I:LEU:N | 1:231:I:LEU:CA | 1:231:I:LEU:C | 1:232:I:ALA:N | 4 | 1.39 |
| (1,598) | 1:201:J:ILE:N | 1:201:J:ILE:CA | 1:201:J:ILE:C | 1:202:J:LEU:N | 2 | 1.39 |
| (1,85) | 1:154:G:ARG:C | 1:155:G:GLN:N | 1:155:G:GLN:CA | 1:155:G:GLN:C | 3 | 1.39 |
| (1,25) | 1:147:G:PRO:N | 1:147:G:PRO:CA | 1:147:G:PRO:C | 1:148:G:THR:N | 8 | 1.39 |
| (1,990) | 1:236:L:SER:C | 1:237:L:GLN:N | 1:237:L:GLN:CA | 1:237:L:GLN:C | 5 | 1.38 |
| (1,910) | 1:230:J:VAL:N | 1:230:J:VAL:CA | 1:230:J:VAL:C | 1:231:J:LEU:N | 6 | 1.38 |
| (1,1054) | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 1:244:J:ILE:N | 10 | 1.37 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 9 | 1.37 |
| (1,1034) | 1:240:H:ASN:C | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 4 | 1.37 |
| (1,1018) | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 1:240:J:ASN:N | 6 | 1.37 |
| (1,433) | 1:186:G:THR:C | 1:187:G:GLU:N | 1:187:G:GLU:CA | 1:187:G:GLU:C | 2 | 1.37 |
| (1,975) | 1:235:I:MET:C | 1:236:I:SER:N | 1:236:I:SER:CA | 1:236:I:SER:C | 4 | 1.36 |
| (1,307) | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 1:175:G:GLU:N | 2 | 1.36 |
| (1,136) | 1:159:J:GLU:C | 1:160:J:PRO:N | 1:160:J:PRO:CA | 1:160:J:PRO:C | 7 | 1.36 |
| (1,68) | 1:153:H:ILE:N | 1:153:H:ILE:CA | 1:153:H:ILE:C | 1:154:H:ARG:N | 4 | 1.36 |
| (1,1040) | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 1:242:H:ALA:N | 4 | 1.35 |
| (1,1038) | 1:240:L:ASN:C | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 2 | 1.35 |
| (1,1034) | 1:240:H:ASN:C | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 2 | 1.35 |
| (1,1054) | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 1:244:J:ILE:N | 5 | 1.34 |
| (1,1038) | 1:240:L:ASN:C | 1:241:L:THR:N | 1:241:L:THR:CA | 1:241:L:THR:C | 7 | 1.34 |
| (1,492) | 1:191:L:VAL:N | 1:191:L:VAL:CA | 1:191:L:VAL:C | 1:192:L:GLN:N | 6 | 1.34 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 10 | 1.33 |
| (1,519) | 1:194:I:ALA:C | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 9 | 1.33 |
| (1,442) | 1:187:J:GLU:N | 1:187:J:GLU:CA | 1:187:J:GLU:C | 1:188:J:THR:N | 7 | 1.33 |
| (1,318) | 1:176:L:GLN:C | 1:177:L:ALA:N | 1:177:L:ALA:CA | 1:177:L:ALA:C | 1 | 1.33 |
| (1,868) | 1:226:J:HIS:C | 1:227:J:LYS:N | 1:227:J:LYS:CA | 1:227:J:LYS:C | 6 | 1.32 |
| (1,864) | 1:226:L:HIS:N | 1:226:L:HIS:CA | 1:226:L:HIS:C | 1:227:L:LYS:N | 1 | 1.32 |
| (1,671) | 1:209:K:ALA:N | 1:209:K:ALA:CA | 1:209:K:ALA:C | 1:210:K:THR:N | 7 | 1.32 |
| (1,404) | 1:184:H:TRP:N | 1:184:H:TRP:CA | 1:184:H:TRP:C | 1:185:H:MET:N | 5 | 1.32 |
| (1,326) | 1:177:H:ALA:C | 1:178:H:SER:N | 1:178:H:SER:CA | 1:178:H:SER:C | 10 | 1.32 |
| (1,305) | 1:173:K:ARG:C | 1:174:K:ALA:N | 1:174:K:ALA:CA | 1:174:K:ALA:C | 4 | 1.32 |
| (1,272) | 1:171:H:THR:N | 1:171:H:THR:CA | 1:171:H:THR:C | 1:172:H:LEU:N | 2 | 1.32 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 4 | 1.31 |
| (1,274) | 1:171:J:THR:N | 1:171:J:THR:CA | 1:171:J:THR:C | 1:172:J:LEU:N | 9 | 1.31 |
| (1,1054) | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 1:244:J:ILE:N | 8 | 1.3 |
| (1,980) | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 1:237:H:GLN:N | 8 | 1.3 |
| (1,905) | 1:229:K:ARG:C | 1:230:K:VAL:N | 1:230:K:VAL:CA | 1:230:K:VAL:C | 3 | 1.3 |
| (1,692) | 1:211:H:LEU:N | 1:211:H:LEU:CA | 1:211:H:LEU:C | 1:212:H:GLU:N | 10 | 1.3 |
| (1,699) | 1:211:I:LEU:C | 1:212:I:GLU:N | 1:212:I:GLU:CA | 1:212:I:GLU:C | 9 | 1.29 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 10 | 1.28 |
| (1,758) | 1:216:H:THR:C | 1:217:H:ALA:N | 1:217:H:ALA:CA | 1:217:H:ALA:C | 9 | 1.28 |
| (1,638) | 1:204:H:ALA:C | 1:205:H:LEU:N | 1:205:H:LEU:CA | 1:205:H:LEU:C | 10 | 1.28 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,507) | 1:192:I:GLN:C | 1:193:I:ASN:N | 1:193:I:ASN:CA | 1:193:I:ASN:C | 2 | 1.28 |
| (1,1054) | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 1:244:J:ILE:N | 1 | 1.27 |
| (1,476) | 1:190:H:LEU:N | 1:190:H:LEU:CA | 1:190:H:LEU:C | 1:191:H:VAL:N | 10 | 1.27 |
| (1,270) | 1:170:L:LYS:C | 1:171:L:THR:N | 1:171:L:THR:CA | 1:171:L:THR:C | 4 | 1.27 |
| (1,1102) | 1:207:J:PRO:N | 1:207:J:PRO:CA | 1:207:J:PRO:C | 1:208:J:GLY:N | 2 | 1.26 |
| (1,946) | 1:233:J:GLU:N | 1:233:J:GLU:CA | 1:233:J:GLU:C | 1:234:J:ALA:N | 5 | 1.26 |
| (1,431) | 1:186:K:THR:N | 1:186:K:THR:CA | 1:186:K:THR:C | 1:187:K:GLU:N | 8 | 1.26 |
| (1,88) | 1:154:J:ARG:C | 1:155:J:GLN:N | 1:155:J:GLN:CA | 1:155:J:GLN:C | 8 | 1.26 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 8 | 1.25 |
| (1,1037) | 1:240:K:ASN:C | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 4 | 1.25 |
| (1,840) | 1:224:L:PRO:N | 1:224:L:PRO:CA | 1:224:L:PRO:C | 1:225:L:GLY:N | 2 | 1.25 |
| (1,663) | 1:208:I:GLY:C | 1:209:I:ALA:N | 1:209:I:ALA:CA | 1:209:I:ALA:C | 1 | 1.24 |
| (1,536) | 1:196:H:PRO:N | 1:196:H:PRO:CA | 1:196:H:PRO:C | 1:197:H:ASP:N | 10 | 1.24 |
| (1,301) | 1:173:G:ARG:C | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 7 | 1.24 |
| (1,907) | 1:230:G:VAL:N | 1:230:G:VAL:CA | 1:230:G:VAL:C | 1:231:G:LEU:N | 2 | 1.23 |
| (1,828) | 1:223:L:GLY:N | 1:223:L:GLY:CA | 1:223:L:GLY:C | 1:224:L:PRO:N | 1 | 1.23 |
| (1,823) | 1:223:G:GLY:N | 1:223:G:GLY:CA | 1:223:G:GLY:C | 1:224:G:PRO:N | 3 | 1.23 |
| (1,32) | 1:147:H:PRO:C | 1:148:H:THR:N | 1:148:H:THR:CA | 1:148:H:THR:C | 3 | 1.23 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 5 | 1.22 |
| (1,905) | 1:229:K:ARG:C | 1:230:K:VAL:N | 1:230:K:VAL:CA | 1:230:K:VAL:C | 10 | 1.22 |
| (1,444) | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 1:188:L:THR:N | 9 | 1.22 |
| (1,307) | 1:174:G:ALA:N | 1:174:G:ALA:CA | 1:174:G:ALA:C | 1:175:G:GLU:N | 8 | 1.22 |
| (1,90) | 1:154:L:ARG:C | 1:155:L:GLN:N | 1:155:L:GLN:CA | 1:155:L:GLN:C | 5 | 1.22 |
| (1,994) | 1:237:J:GLN:N | 1:237:J:GLN:CA | 1:237:J:GLN:C | 1:238:J:VAL:N | 8 | 1.21 |
| (1,845) | 1:224:K:PRO:C | 1:225:K:GLY:N | 1:225:K:GLY:CA | 1:225:K:GLY:C | 7 | 1.21 |
| (1,512) | 1:193:H:ASN:N | 1:193:H:ASN:CA | 1:193:H:ASN:C | 1:194:H:ALA:N | 6 | 1.21 |
| (1,52) | 1:150:J:ILE:C | 1:151:J:LEU:N | 1:151:J:LEU:CA | 1:151:J:LEU:C | 7 | 1.21 |
| (1,988) | 1:236:J:SER:C | 1:237:J:GLN:N | 1:237:J:GLN:CA | 1:237:J:GLN:C | 1 | 1.2 |
| (1,839) | 1:224:K:PRO:N | 1:224:K:PRO:CA | 1:224:K:PRO:C | 1:225:K:GLY:N | 4 | 1.2 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 2 | 1.2 |
| (1,384) | 1:182:L:LYS:N | 1:182:L:LYS:CA | 1:182:L:LYS:C | 1:183:L:ASN:N | 10 | 1.2 |
| (1,248) | 1:169:H:TYR:N | 1:169:H:TYR:CA | 1:169:H:TYR:C | 1:170:H:LYS:N | 2 | 1.2 |
| (1,1012) | 1:238:J:VAL:C | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 1 | 1.19 |
| (1,716) | 1:213:H:GLU:N | 1:213:H:GLU:CA | 1:213:H:GLU:C | 1:214:H:MET:N | 3 | 1.19 |
| (1,433) | 1:186:G:THR:C | 1:187:G:GLU:N | 1:187:G:GLU:CA | 1:187:G:GLU:C | 9 | 1.19 |
| (1,179) | 1:163:K:ASP:N | 1:163:K:ASP:CA | 1:163:K:ASP:C | 1:164:K:TYR:N | 7 | 1.19 |
| (1,1043) | 1:241:K:THR:N | 1:241:K:THR:CA | 1:241:K:THR:C | 1:242:K:ALA:N | 4 | 1.18 |
| (1,499) | 1:192:G:GLN:N | 1:192:G:GLN:CA | 1:192:G:GLN:C | 1:193:G:ASN:N | 8 | 1.18 |
| (1,828) | 1:223:L:GLY:N | 1:223:L:GLY:CA | 1:223:L:GLY:C | 1:224:L:PRO:N | 4 | 1.17 |
| (1,182) | 1:163:H:ASP:C | 1:164:H:TYR:N | 1:164:H:TYR:CA | 1:164:H:TYR:C | 9 | 1.17 |
| (1,1012) | 1:238:J:VAL:C | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 2 | 1.16 |
| (1,636) | 1:204:L:ALA:N | 1:204:L:ALA:CA | 1:204:L:ALA:C | 1:205:L:LEU:N | 1 | 1.16 |
| (1,60) | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 1:152:L:ASP:N | 10 | 1.16 |
| (1,1034) | 1:240:H:ASN:C | 1:241:H:THR:N | 1:241:H:THR:CA | 1:241:H:THR:C | 7 | 1.15 |
| (1,1012) | 1:238:J:VAL:C | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 6 | 1.15 |
| (1,172) | 1:162:J:ARG:C | 1:163:J:ASP:N | 1:163:J:ASP:CA | 1:163:J:ASP:C | 7 | 1.15 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 10 | 1.14 |
| (1,895) | 1:229:G:ARG:N | 1:229:G:ARG:CA | 1:229:G:ARG:C | 1:230:G:VAL:N | 1 | 1.14 |
| (1,104) | 1:157:H:PRO:N | 1:157:H:PRO:CA | 1:157:H:PRO:C | 1:158:H:LYS:N | 6 | 1.14 |
| (1,1016) | 1:239:H:THR:N | 1:239:H:THR:CA | 1:239:H:THR:C | 1:240:H:ASN:N | 1 | 1.13 |
| (1,902) | 1:229:H:ARG:C | 1:230:H:VAL:N | 1:230:H:VAL:CA | 1:230:H:VAL:C | 5 | 1.13 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,692) | 1:211:H:LEU:N | 1:211:H:LEU:CA | 1:211:H:LEU:C | 1:212:H:GLU:N | 4 | 1.13 |
| (1,326) | 1:177:H:ALA:C | 1:178:H:SER:N | 1:178:H:SER:CA | 1:178:H:SER:C | 7 | 1.13 |
| (1,1054) | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 1:244:J:ILE:N | 6 | 1.12 |
| (1,758) | 1:216:H:THR:C | 1:217:H:ALA:N | 1:217:H:ALA:CA | 1:217:H:ALA:C | 10 | 1.12 |
| (1,716) | 1:213:H:GLU:N | 1:213:H:GLU:CA | 1:213:H:GLU:C | 1:214:H:MET:N | 1 | 1.12 |
| (1,66) | 1:152:L:ASP:N | 1:152:L:ASP:CA | 1:152:L:ASP:C | 1:153:L:ILE:N | 4 | 1.12 |
| (1,555) | 1:197:I:ASP:C | 1:198:I:CYS:N | 1:198:I:CYS:CA | 1:198:I:CYS:C | 7 | 1.11 |
| (1,237) | 1:168:I:PHE:N | 1:168:I:PHE:CA | 1:168:I:PHE:C | 1:169:I:TYR:N | 3 | 1.11 |
| (1,60) | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 1:152:L:ASP:N | 3 | 1.11 |
| (1,6) | 1:144:L:GLY:C | 1:145:L:GLY:N | 1:145:L:GLY:CA | 1:145:L:GLY:C | 2 | 1.11 |
| (1,988) | 1:236:J:SER:C | 1:237:J:GLN:N | 1:237:J:GLN:CA | 1:237:J:GLN:C | 2 | 1.1 |
| (1,907) | 1:230:G:VAL:N | 1:230:G:VAL:CA | 1:230:G:VAL:C | 1:231:G:LEU:N | 6 | 1.1 |
| (1,694) | 1:211:J:LEU:N | 1:211:J:LEU:CA | 1:211:J:LEU:C | 1:212:J:GLU:N | 9 | 1.1 |
| (1,672) | 1:209:L:ALA:N | 1:209:L:ALA:CA | 1:209:L:ALA:C | 1:210:L:THR:N | 5 | 1.1 |
| (1,1094) | 1:206:H:GLY:C | 1:207:H:PRO:N | 1:207:H:PRO:CA | 1:207:H:PRO:C | 1 | 1.09 |
| (1,1075) | 1:175:G:GLU:N | 1:175:G:GLU:CA | 1:175:G:GLU:C | 1:176:G:GLN:N | 5 | 1.09 |
| (1,1015) | 1:239:G:THR:N | 1:239:G:THR:CA | 1:239:G:THR:C | 1:240:G:ASN:N | 10 | 1.09 |
| (1,449) | 1:187:K:GLU:C | 1:188:K:THR:N | 1:188:K:THR:CA | 1:188:K:THR:C | 3 | 1.09 |
| (1,60) | 1:151:L:LEU:N | 1:151:L:LEU:CA | 1:151:L:LEU:C | 1:152:L:ASP:N | 6 | 1.09 |
| (1,37) | 1:148:G:THR:C | 1:149:G:SER:N | 1:149:G:SER:CA | 1:149:G:SER:C | 3 | 1.09 |
| (1,892) | 1:228:J:ALA:C | 1:229:J:ARG:N | 1:229:J:ARG:CA | 1:229:J:ARG:C | 4 | 1.08 |
| (1,560) | 1:198:H:CYS:N | 1:198:H:CYS:CA | 1:198:H:CYS:C | 1:199:H:LYS:N | 2 | 1.08 |
| (1,519) | 1:194:I:ALA:C | 1:195:I:ASN:N | 1:195:I:ASN:CA | 1:195:I:ASN:C | 10 | 1.08 |
| (1,308) | 1:174:H:ALA:N | 1:174:H:ALA:CA | 1:174:H:ALA:C | 1:175:H:GLU:N | 10 | 1.08 |
| (1,237) | 1:168:I:PHE:N | 1:168:I:PHE:CA | 1:168:I:PHE:C | 1:169:I:TYR:N | 8 | 1.08 |
| (1,1042) | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 1:242:J:ALA:N | 9 | 1.07 |
| (1,799) | 1:220:G:GLY:N | 1:220:G:GLY:CA | 1:220:G:GLY:C | 1:221:G:VAL:N | 3 | 1.07 |
| (1,451) | 1:188:G:THR:N | 1:188:G:THR:CA | 1:188:G:THR:C | 1:189:G:LEU:N | 2 | 1.07 |
| (1,179) | 1:163:K:ASP:N | 1:163:K:ASP:CA | 1:163:K:ASP:C | 1:164:K:TYR:N | 1 | 1.07 |
| (1,1054) | 1:243:J:THR:N | 1:243:J:THR:CA | 1:243:J:THR:C | 1:244:J:ILE:N | 9 | 1.06 |
| (1,52) | 1:150:J:ILE:C | 1:151:J:LEU:N | 1:151:J:LEU:CA | 1:151:J:LEU:C | 6 | 1.06 |
| (1,1039) | 1:241:G:THR:N | 1:241:G:THR:CA | 1:241:G:THR:C | 1:242:G:ALA:N | 10 | 1.05 |
| (1,946) | 1:233:J:GLU:N | 1:233:J:GLU:CA | 1:233:J:GLU:C | 1:234:J:ALA:N | 10 | 1.05 |
| (1,410) | 1:184:H:TRP:C | 1:185:H:MET:N | 1:185:H:MET:CA | 1:185:H:MET:C | 3 | 1.05 |
| (1,396) | 1:183:L:ASN:N | 1:183:L:ASN:CA | 1:183:L:ASN:C | 1:184:L:TRP:N | 9 | 1.05 |
| (1,175) | 1:163:G:ASP:N | 1:163:G:ASP:CA | 1:163:G:ASP:C | 1:164:G:TYR:N | 5 | 1.05 |
| (1,156) | 1:161:L:PHE:N | 1:161:L:PHE:CA | 1:161:L:PHE:C | 1:162:L:ARG:N | 8 | 1.05 |
| (1,1084) | 1:175:J:GLU:C | 1:176:J:GLN:N | 1:176:J:GLN:CA | 1:176:J:GLN:C | 7 | 1.04 |
| (1,973) | 1:235:G:MET:C | 1:236:G:SER:N | 1:236:G:SER:CA | 1:236:G:SER:C | 1 | 1.04 |
| (1,911) | 1:230:K:VAL:N | 1:230:K:VAL:CA | 1:230:K:VAL:C | 1:231:K:LEU:N | 3 | 1.04 |
| (1,838) | 1:224:J:PRO:N | 1:224:J:PRO:CA | 1:224:J:PRO:C | 1:225:J:GLY:N | 6 | 1.04 |
| (1,652) | 1:207:J:PRO:C | 1:208:J:GLY:N | 1:208:J:GLY:CA | 1:208:J:GLY:C | 1 | 1.04 |
| (1,626) | 1:203:H:LYS:C | 1:204:H:ALA:N | 1:204:H:ALA:CA | 1:204:H:ALA:C | 5 | 1.04 |
| (1,562) | 1:198:J:CYS:N | 1:198:J:CYS:CA | 1:198:J:CYS:C | 1:199:J:LYS:N | 3 | 1.04 |
| (1,438) | 1:186:L:THR:C | 1:187:L:GLU:N | 1:187:L:GLU:CA | 1:187:L:GLU:C | 5 | 1.04 |
| (1,175) | 1:163:G:ASP:N | 1:163:G:ASP:CA | 1:163:G:ASP:C | 1:164:G:TYR:N | 9 | 1.04 |
| (1,275) | 1:171:K:THR:N | 1:171:K:THR:CA | 1:171:K:THR:C | 1:172:K:LEU:N | 8 | 1.03 |
| (1,38) | 1:148:H:THR:C | 1:149:H:SER:N | 1:149:H:SER:CA | 1:149:H:SER:C | 6 | 1.03 |
| (1,1094) | 1:206:H:GLY:C | 1:207:H:PRO:N | 1:207:H:PRO:CA | 1:207:H:PRO:C | 3 | 1.02 |
| (1,1053) | 1:243:I:THR:N | 1:243:I:THR:CA | 1:243:I:THR:C | 1:244:I:ILE:N | 7 | 1.02 |
| (1,1036) | 1:240:J:ASN:C | 1:241:J:THR:N | 1:241:J:THR:CA | 1:241:J:THR:C | 2 | 1.02 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|----------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,939) | 1:232:I:ALA:C | 1:233:I:GLU:N | 1:233:I:GLU:CA | 1:233:I:GLU:C | 5 | 1.02 |
| (1,534) | 1:195:L:ASN:C | 1:196:L:PRO:N | 1:196:L:PRO:CA | 1:196:L:PRO:C | 8 | 1.02 |
| (1,1018) | 1:239:J:THR:N | 1:239:J:THR:CA | 1:239:J:THR:C | 1:240:J:ASN:N | 4 | 1.01 |
| (1,982) | 1:236:J:SER:N | 1:236:J:SER:CA | 1:236:J:SER:C | 1:237:J:GLN:N | 2 | 1.01 |
| (1,974) | 1:235:H:MET:C | 1:236:H:SER:N | 1:236:H:SER:CA | 1:236:H:SER:C | 4 | 1.01 |
| (1,518) | 1:194:H:ALA:C | 1:195:H:ASN:N | 1:195:H:ASN:CA | 1:195:H:ASN:C | 7 | 1.01 |
| (1,515) | 1:193:K:ASN:N | 1:193:K:ASN:CA | 1:193:K:ASN:C | 1:194:K:ALA:N | 4 | 1.01 |
| (1,52) | 1:150:J:ILE:C | 1:151:J:LEU:N | 1:151:J:LEU:CA | 1:151:J:LEU:C | 2 | 1.01 |