



Full wwPDB EM Validation Report ⓘ

Nov 12, 2025 – 02:44 AM JST

PDB ID : 8ZSQ / pdb_00008zsq
EMDB ID : EMD-60424
Title : Respirasome closed state 1 bound by metformin (SC-MetC1)
Authors : Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.
Deposited on : 2024-06-05
Resolution : 2.86 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

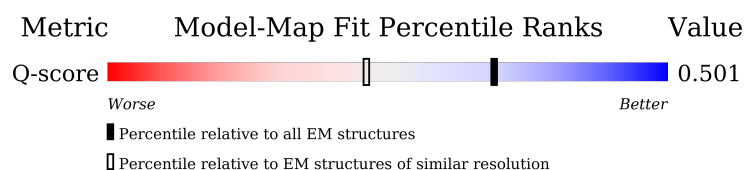
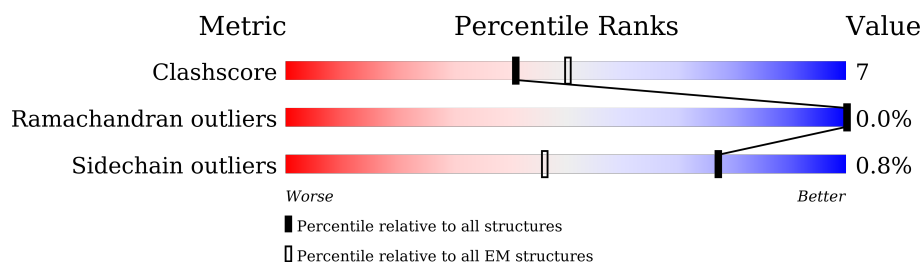
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 Å.

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









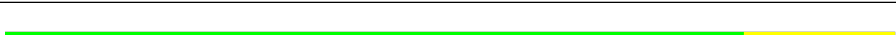
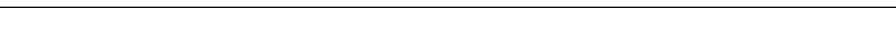
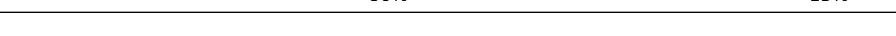
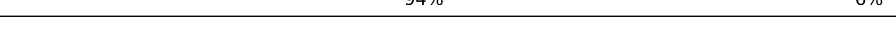
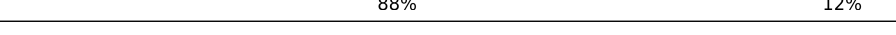
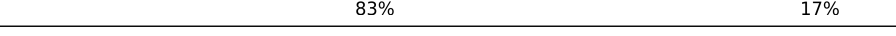













| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore | 210492 | 15764 | - |
| Ramachandran outliers | 207382 | 16835 | - |
| Sidechain outliers | 206894 | 16415 | - |
| Q-score | - | 25397 | 12017 (2.36 - 3.36) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 4L | 98 | 78% 22% |
| 2 | 5A | 102 | 84% 15% . |
| 3 | 5B | 95 | 80% 19% . |
| 4 | 6A | 75 | 81% 19% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | 6B | 82 |  |
| 6 | 6C | 70 |  |
| 7 | 7A | 57 |  |
| 8 | 7B | 50 |  |
| 9 | 7C | 47 |  |
| 10 | 8B | 43 |  |
| 11 | A1 | 70 |  |
| 12 | A2 | 85 |  |
| 13 | A3 | 83 |  |
| 14 | A5 | 112 |  |
| 15 | A6 | 114 |  |
| 16 | A7 | 112 |  |
| 17 | A8 | 171 |  |
| 18 | A9 | 341 |  |
| 19 | AB | 87 |  |
| 19 | AC | 87 |  |
| 20 | AK | 321 |  |
| 21 | AL | 140 |  |
| 22 | AM | 144 |  |
| 23 | AN | 142 |  |
| 24 | B1 | 56 |  |
| 25 | B2 | 67 |  |
| 26 | B3 | 80 |  |
| 27 | B4 | 128 |  |
| 28 | B5 | 138 |  |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29 | B6 | 126 | |
| 30 | B7 | 125 | |
| 31 | B8 | 156 | |
| 32 | B9 | 178 | |
| 33 | BK | 174 | |
| 34 | BL | 99 | |
| 35 | C1 | 514 | |
| 36 | C2 | 228 | |
| 37 | C3 | 260 | |
| 38 | C4 | 138 | |
| 39 | CA | 49 | |
| 40 | CB | 121 | |
| 41 | N1 | 318 | |
| 42 | N2 | 347 | |
| 43 | N3 | 115 | |
| 44 | N4 | 459 | |
| 45 | N5 | 603 | |
| 46 | N6 | 174 | |
| 47 | QA | 419 | |
| 47 | Qa | 419 | |
| 48 | QB | 446 | |
| 48 | Qb | 446 | |
| 49 | QC | 379 | |
| 49 | Qc | 379 | |
| 50 | QD | 241 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 50 | Qd | 241 |  |
| 51 | QE | 274 |  |
| 51 | QK | 274 |  |
| 51 | Qe | 274 |  |
| 52 | QF | 67 |  |
| 52 | Qf | 67 |  |
| 53 | QG | 101 |  |
| 53 | Qg | 101 |  |
| 54 | QH | 79 |  |
| 54 | Qh | 79 |  |
| 55 | QI | 62 |  |
| 55 | Qi | 62 |  |
| 56 | QJ | 52 |  |
| 56 | Qj | 52 |  |
| 57 | S1 | 689 |  |
| 58 | S2 | 430 |  |
| 59 | S3 | 208 |  |
| 60 | S4 | 124 |  |
| 61 | S5 | 105 |  |
| 62 | S6 | 96 |  |
| 63 | S7 | 156 |  |
| 64 | S8 | 176 |  |
| 65 | V1 | 431 |  |
| 66 | V2 | 217 |  |
| 67 | V3 | 42 |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 82 | FES | QE | 303 | - | - | X | - |
| 82 | FES | Qe | 303 | - | - | X | - |

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 117589 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 1 | 4L | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 748 | 493 | 113 | 128 | 14 | | |

- Molecule 2 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | 5A | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 825 | 528 | 139 | 156 | 2 | | |

- Molecule 3 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | 5B | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 724 | 449 | 128 | 141 | 6 | | |

- Molecule 4 is a protein called Cytochrome c oxidase subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | 6A | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 620 | 401 | 118 | 100 | 1 | | |

- Molecule 5 is a protein called Cytochrome c oxidase subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5 | 6B | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 684 | 431 | 125 | 123 | 5 | | |

- Molecule 6 is a protein called Cytochrome c oxidase subunit 6C.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 6 | 6C | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 574 | 375 | 101 | 95 | 3 | | |

- Molecule 7 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7 | 7A | 57 | Total | C | N | O | S | 0 | 0 |
| | | | 447 | 287 | 76 | 81 | 3 | | |

- Molecule 8 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8 | 7B | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 392 | 254 | 66 | 71 | 1 | | |

- Molecule 9 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9 | 7C | 47 | Total | C | N | O | S | 0 | 0 |
| | | | 387 | 257 | 65 | 63 | 2 | | |

- Molecule 10 is a protein called Cytochrome c oxidase subunit 8.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10 | 8B | 43 | Total | C | N | O | 0 | 0 |
| | | | 338 | 222 | 57 | 59 | | |

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 11 | A1 | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 562 | 361 | 101 | 94 | 6 | | |

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | A2 | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 686 | 431 | 128 | 125 | 2 | | |

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | A3 | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 643 | 417 | 110 | 115 | 1 | | |

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | A5 | 112 | Total | C | N | O | S | 0 | 0 |
| | | | 910 | 588 | 154 | 165 | 3 | | |

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | A6 | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 967 | 617 | 178 | 167 | 5 | | |

- Molecule 16 is a protein called Complex I-B14.5a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | A7 | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 780 | 491 | 147 | 139 | 3 | | |

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 17 | A8 | 171 | Total | C | N | O | S | 0 | 0 |
| | | | 1398 | 887 | 250 | 251 | 10 | | |

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 18 | A9 | 341 | Total | C | N | O | S | 0 | 0 |
| | | | 2743 | 1777 | 480 | 477 | 9 | | |

- Molecule 19 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | AB | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 624 | 402 | 93 | 124 | 5 | | |
| 19 | AC | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 702 | 452 | 103 | 142 | 5 | | |

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20 | AK | 321 | Total | C | N | O | S | 0 | 0 |
| | | | 2601 | 1655 | 444 | 492 | 10 | | |

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21 | AL | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1021 | 651 | 174 | 190 | 6 | | |

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | AM | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1204 | 770 | 218 | 212 | 4 | | |

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | AN | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1173 | 755 | 203 | 206 | 9 | | |

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 24 | B1 | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 479 | 311 | 88 | 79 | 1 | | |

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 25 | B2 | 67 | Total | C | N | O | S | 0 | 0 |
| | | | 584 | 385 | 95 | 103 | 1 | | |

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26 | B3 | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 641 | 418 | 108 | 114 | 1 | | |

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | B4 | 128 | Total | C | N | O | S | 0 | 0 |
| | | | 1062 | 691 | 182 | 189 | | | |

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | B5 | 138 | Total | C | N | O | S | 0 | 0 |
| | | | 1151 | 754 | 195 | 199 | 3 | | |

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | B6 | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 882 | 577 | 156 | 148 | 1 | | |

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 30 | B7 | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 1068 | 663 | 204 | 190 | 11 | | |

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | B8 | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1315 | 853 | 213 | 241 | 8 | | |

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | B9 | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1534 | 982 | 279 | 265 | 8 | | |

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | BK | 174 | Total | C | N | O | S | 0 | 0 |
| | | | 1456 | 913 | 264 | 271 | 8 | | |

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | BL | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 828 | 531 | 137 | 156 | 4 | | |

- Molecule 35 is a protein called Cytochrome c oxidase subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 35 | C1 | 514 | Total | C | N | O | S | 0 | 0 |
| | | | 4024 | 2692 | 625 | 675 | 32 | | |

- Molecule 36 is a protein called Cytochrome c oxidase subunit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 36 | C2 | 228 | Total | C | N | O | S | 0 | 0 |
| | | | 1833 | 1193 | 282 | 340 | 18 | | |

- Molecule 37 is a protein called Cytochrome c oxidase subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 37 | C3 | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 2103 | 1403 | 337 | 353 | 10 | | |

- Molecule 38 is a protein called Cytochrome c oxidase subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | C4 | 138 | Total | C | N | O | S | 0 | 0 |
| | | | 1153 | 751 | 188 | 210 | 4 | | |

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 39 | CA | 49 | Total | C | N | O | 0 | 0 |
| | | | 417 | 276 | 71 | 70 | | |

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40 | CB | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 1000 | 650 | 173 | 171 | 6 | | |

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 41 | N1 | 318 | Total | C | N | O | S | 0 | 0 |
| | | | 2508 | 1678 | 385 | 424 | 21 | | |

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 42 | N2 | 347 | Total | C | N | O | S | 0 | 0 |
| | | | 2710 | 1782 | 420 | 462 | 46 | | |

- Molecule 43 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43 | N3 | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 914 | 615 | 134 | 158 | 7 | | |

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 44 | N4 | 459 | Total | C | N | O | S | 0 | 0 |
| | | | 3631 | 2412 | 572 | 609 | 38 | | |

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 45 | N5 | 603 | Total | C | N | O | S | 0 | 0 |
| | | | 4785 | 3173 | 741 | 820 | 51 | | |

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 46 | N6 | 174 | Total | C | N | O | S | 0 | 0 |
| | | | 1329 | 892 | 189 | 236 | 12 | | |

- Molecule 47 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 47 | QA | 419 | Total | C | N | O | S | 0 | 0 |
| | | | 3147 | 1971 | 557 | 611 | 8 | | |
| 47 | Qa | 419 | Total | C | N | O | S | 0 | 0 |
| | | | 3147 | 1971 | 557 | 611 | 8 | | |

- Molecule 48 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 48 | QB | 446 | Total | C | N | O | S | 0 | 0 |
| | | | 3459 | 2161 | 605 | 674 | 19 | | |
| 48 | Qb | 433 | Total | C | N | O | S | 0 | 0 |
| | | | 3367 | 2103 | 592 | 653 | 19 | | |

- Molecule 49 is a protein called Cytochrome b.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 49 | QC | 379 | Total | C | N | O | S | 0 | 0 |
| | | | 3025 | 2031 | 471 | 502 | 21 | | |
| 49 | Qc | 379 | Total | C | N | O | S | 0 | 0 |
| | | | 3025 | 2031 | 471 | 502 | 21 | | |

- Molecule 50 is a protein called Cytochrome c1, heme protein, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 50 | QD | 241 | Total | C | N | O | S | 0 | 0 |
| | | | 1921 | 1225 | 330 | 350 | 16 | | |
| 50 | Qd | 239 | Total | C | N | O | S | 0 | 0 |
| | | | 1904 | 1215 | 327 | 346 | 16 | | |

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51 | QE | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1517 | 955 | 265 | 290 | 7 | | |
| 51 | QK | 73 | Total | C | N | O | S | 0 | 0 |
| | | | 520 | 328 | 98 | 92 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51 | Qe | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1517 | 955 | 265 | 290 | 7 | | |

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52 | QF | 67 | Total | C | N | O | S | 0 | 0 |
| | | | 552 | 336 | 100 | 111 | 5 | | |
| 52 | Qf | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 528 | 320 | 97 | 106 | 5 | | |

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53 | QG | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 893 | 572 | 157 | 162 | 2 | | |
| 53 | Qg | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 893 | 572 | 157 | 162 | 2 | | |

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54 | QH | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 662 | 432 | 121 | 107 | 2 | | |
| 54 | Qh | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 666 | 434 | 122 | 108 | 2 | | |

- Molecule 55 is a protein called Complex III subunit 9.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 55 | QI | 62 | Total | C | N | O | 0 | 0 |
| | | | 507 | 331 | 90 | 86 | | |
| 55 | Qi | 60 | Total | C | N | O | 0 | 0 |
| | | | 493 | 322 | 87 | 84 | | |

- Molecule 56 is a protein called Cytochrome b-c1 complex subunit 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 56 | QJ | 49 | Total | C | N | O | S | 0 | 0 |
| | | | 405 | 269 | 71 | 63 | 2 | | |
| 56 | Qj | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 421 | 281 | 74 | 65 | 1 | | |

- Molecule 57 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 57 | S1 | 689 | Total | C | N | O | S | 0 | 0 |
| | | | 5290 | 3317 | 922 | 1012 | 39 | | |

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 58 | S2 | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3459 | 2212 | 594 | 629 | 24 | | |

- Molecule 59 is a protein called Complex I-30kD.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 59 | S3 | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1738 | 1124 | 298 | 314 | 2 | | |

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60 | S4 | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 1007 | 637 | 179 | 188 | 3 | | |

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61 | S5 | 105 | Total | C | N | O | S | 0 | 0 |
| | | | 867 | 550 | 161 | 150 | 6 | | |

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62 | S6 | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 741 | 452 | 140 | 146 | 3 | | |

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 63 | S7 | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1248 | 794 | 227 | 213 | 14 | | |

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 64 | S8 | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1412 | 887 | 243 | 269 | 13 | | |

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 65 | V1 | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3316 | 2092 | 592 | 612 | 20 | | |

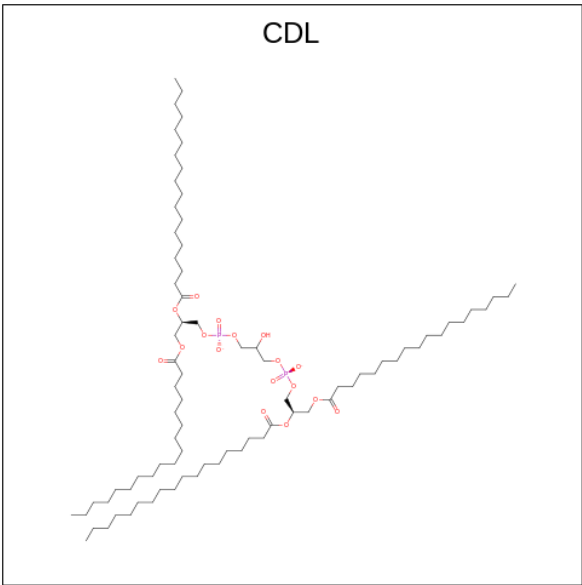
- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 66 | V2 | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1671 | 1065 | 281 | 315 | 10 | | |

- Molecule 67 is a protein called NADH:ubiquinone oxidoreductase subunit V3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 67 | V3 | 42 | Total | C | N | O | S | 0 | 0 |
| | | | 355 | 219 | 67 | 68 | 1 | | |

- Molecule 68 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 68 | 4L | 1 | Total | C | O | P | 0 |
| | | | 92 | 73 | 17 | 2 | |
| 68 | 7A | 1 | Total | C | O | P | 0 |
| | | | 91 | 72 | 17 | 2 | |
| 68 | A7 | 1 | Total | C | O | P | 0 |
| | | | 51 | 32 | 17 | 2 | |
| 68 | A8 | 1 | Total | C | O | P | 0 |
| | | | 83 | 64 | 17 | 2 | |
| 68 | AK | 1 | Total | C | O | P | 0 |
| | | | 68 | 49 | 17 | 2 | |
| 68 | AL | 1 | Total | C | O | P | 0 |
| | | | 94 | 75 | 17 | 2 | |
| 68 | B4 | 1 | Total | C | O | P | 0 |
| | | | 80 | 61 | 17 | 2 | |
| 68 | B5 | 1 | Total | C | O | P | 0 |
| | | | 100 | 81 | 17 | 2 | |
| 68 | C3 | 1 | Total | C | O | P | 0 |
| | | | 87 | 68 | 17 | 2 | |
| 68 | C3 | 1 | Total | C | O | P | 0 |
| | | | 83 | 64 | 17 | 2 | |
| 68 | CB | 1 | Total | C | O | P | 0 |
| | | | 100 | 81 | 17 | 2 | |
| 68 | N1 | 1 | Total | C | O | P | 0 |
| | | | 78 | 59 | 17 | 2 | |
| 68 | N4 | 1 | Total | C | O | P | 0 |
| | | | 62 | 43 | 17 | 2 | |
| 68 | N5 | 1 | Total | C | O | P | 0 |
| | | | 89 | 70 | 17 | 2 | |

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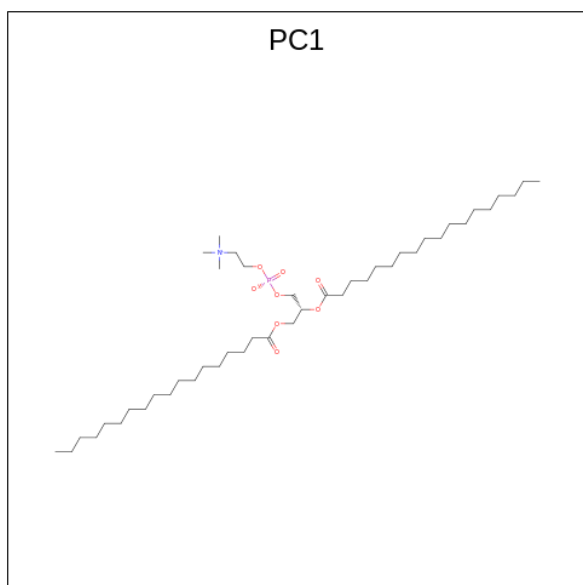
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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 68 | N5 | 1 | Total | C | O | P | 0 |
| | | | 100 | 81 | 17 | 2 | |
| 68 | QB | 1 | Total | C | O | P | 0 |
| | | | 64 | 45 | 17 | 2 | |
| 68 | QC | 1 | Total | C | O | P | 0 |
| | | | 55 | 36 | 17 | 2 | |
| 68 | QD | 1 | Total | C | O | P | 0 |
| | | | 64 | 45 | 17 | 2 | |
| 68 | QH | 1 | Total | C | O | P | 0 |
| | | | 61 | 42 | 17 | 2 | |
| 68 | QH | 1 | Total | C | O | P | 0 |
| | | | 64 | 45 | 17 | 2 | |
| 68 | Qb | 1 | Total | C | O | P | 0 |
| | | | 64 | 45 | 17 | 2 | |

- Molecule 69 is ZINC ION (CCD ID: ZN) (formula: Zn).

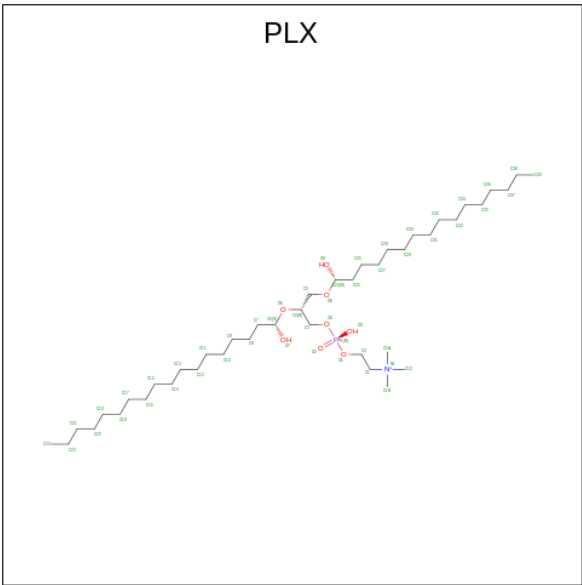
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 69 | 5B | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 69 | S6 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 70 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



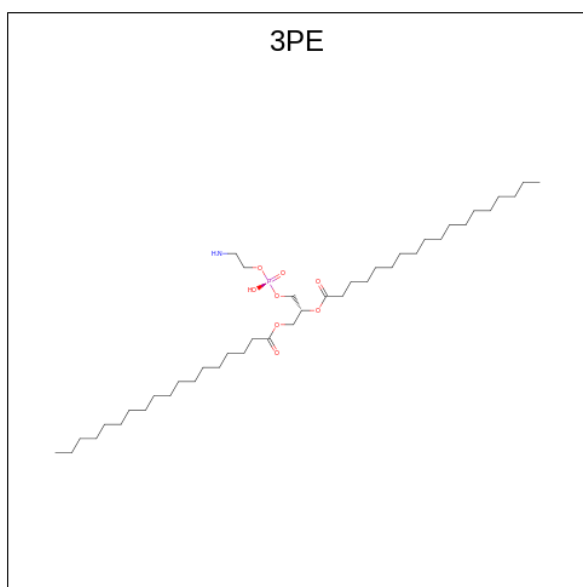
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 70 | 6A | 1 | Total | C | N | O | P | 0 |
| | | | 45 | 35 | 1 | 8 | 1 | |
| 70 | C1 | 1 | Total | C | N | O | P | 0 |
| | | | 33 | 23 | 1 | 8 | 1 | |
| 70 | C1 | 1 | Total | C | N | O | P | 0 |
| | | | 46 | 36 | 1 | 8 | 1 | |
| 70 | C1 | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 44 | 1 | 8 | 1 | |
| 70 | C1 | 1 | Total | C | N | O | P | 0 |
| | | | 50 | 40 | 1 | 8 | 1 | |
| 70 | C3 | 1 | Total | C | N | O | P | 0 |
| | | | 44 | 34 | 1 | 8 | 1 | |
| 70 | C3 | 1 | Total | C | N | O | P | 0 |
| | | | 49 | 39 | 1 | 8 | 1 | |
| 70 | C3 | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 44 | 1 | 8 | 1 | |
| 70 | C3 | 1 | Total | C | N | O | P | 0 |
| | | | 43 | 33 | 1 | 8 | 1 | |
| 70 | N1 | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 38 | 1 | 8 | 1 | |
| 70 | N3 | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 44 | 1 | 8 | 1 | |
| 70 | QB | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 70 | Qb | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 38 | 1 | 8 | 1 | |
| 70 | Qc | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 44 | 1 | 8 | 1 | |
| 70 | Qh | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 44 | 1 | 8 | 1 | |

- Molecule 71 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P).



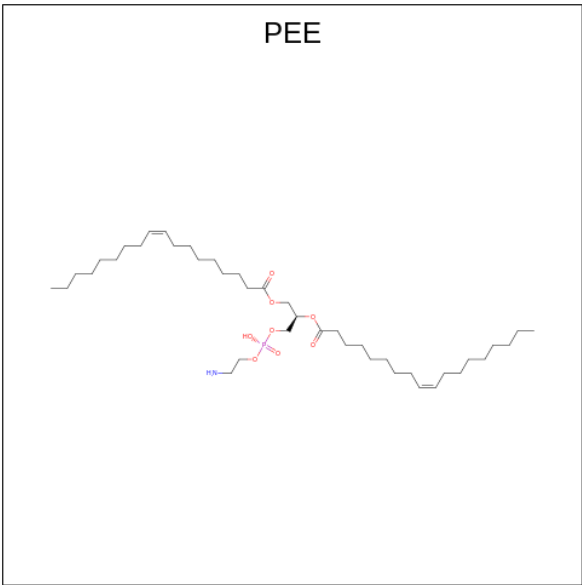
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 71 | 6C | 1 | Total | C | N | O | P | 0 |
| | | | 43 | 33 | 1 | 8 | 1 | |
| 71 | AL | 1 | Total | C | N | O | P | 0 |
| | | | 47 | 37 | 1 | 8 | 1 | |
| 71 | AM | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 71 | B1 | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 71 | CB | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 71 | N4 | 1 | Total | C | N | O | P | 0 |
| | | | 49 | 39 | 1 | 8 | 1 | |
| 71 | N6 | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 71 | QI | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 71 | Qi | 1 | Total | C | N | O | P | 0 |
| | | | 46 | 36 | 1 | 8 | 1 | |
| 71 | S7 | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |

- Molecule 72 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 72 | 7A | 1 | Total | C | N | O | P | 0 |
| | | | 43 | 33 | 1 | 8 | 1 | |
| 72 | B8 | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 22 | 1 | 8 | 1 | |
| 72 | C1 | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 72 | C1 | 1 | Total | C | N | O | P | 0 |
| | | | 46 | 36 | 1 | 8 | 1 | |
| 72 | CA | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 72 | CB | 1 | Total | C | N | O | P | 0 |
| | | | 46 | 36 | 1 | 8 | 1 | |
| 72 | N5 | 1 | Total | C | N | O | P | 0 |
| | | | 46 | 36 | 1 | 8 | 1 | |
| 72 | QE | 1 | Total | C | N | O | P | 0 |
| | | | 44 | 34 | 1 | 8 | 1 | |
| 72 | QJ | 1 | Total | C | N | O | P | 0 |
| | | | 34 | 24 | 1 | 8 | 1 | |
| 72 | Qc | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 38 | 1 | 8 | 1 | |
| 72 | Qj | 1 | Total | C | N | O | P | 0 |
| | | | 29 | 19 | 1 | 8 | 1 | |
| 72 | S7 | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |

- Molecule 73 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



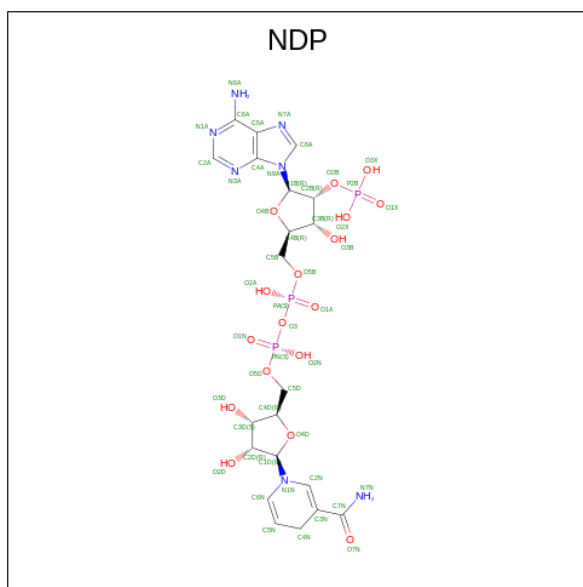
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 73 | 7C | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 73 | A9 | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 73 | N1 | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 21 | 1 | 8 | 1 | |
| 73 | N3 | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 73 | N4 | 1 | Total | C | N | O | P | 0 |
| | | | 49 | 39 | 1 | 8 | 1 | |
| 73 | N5 | 1 | Total | C | N | O | P | 0 |
| | | | 46 | 36 | 1 | 8 | 1 | |
| 73 | N5 | 1 | Total | C | N | O | P | 0 |
| | | | 40 | 30 | 1 | 8 | 1 | |
| 73 | N5 | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 73 | QB | 1 | Total | C | N | O | P | 0 |
| | | | 34 | 24 | 1 | 8 | 1 | |
| 73 | QC | 1 | Total | C | N | O | P | 0 |
| | | | 40 | 30 | 1 | 8 | 1 | |
| 73 | QE | 1 | Total | C | N | O | P | 0 |
| | | | 47 | 37 | 1 | 8 | 1 | |
| 73 | Qc | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |
| 73 | Qe | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 73 | Qe | 1 | Total | C | N | O | P | 0 |
| | | | 24 | 14 | 1 | 8 | 1 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 73 | S2 | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 38 | 1 | 8 | 1 | |
| 73 | S8 | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |

- Molecule 74 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 74 | A9 | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | |

- Molecule 75 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



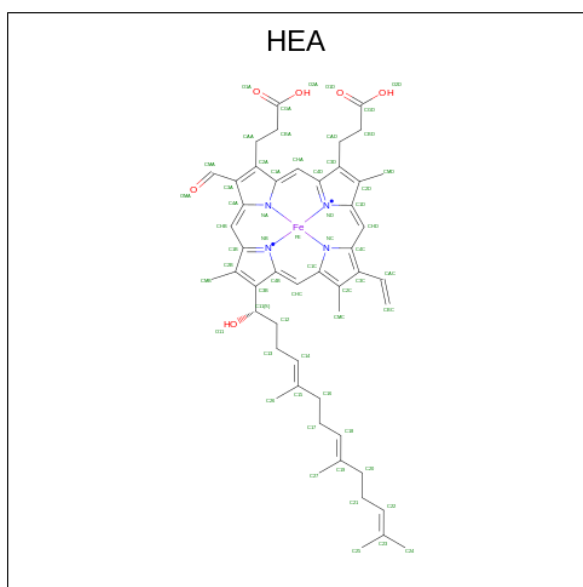
| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|--------|---------|
| 75 | AB | 1 | Total 36 | C 25 | N 2 | O 7 | P 1 | S 1 | 0 |
| 75 | AC | 1 | Total 36 | C 25 | N 2 | O 7 | P 1 | S 1 | 0 |

- Molecule 76 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 76 | AK | 1 | Total 27 | C 10 | N 5 | O 10 | P 2 | 0 |

- Molecule 77 is HEME-A (CCD ID: HEA) (formula: $\text{C}_{49}\text{H}_{56}\text{FeN}_4\text{O}_6$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 77 | C1 | 1 | Total 60 | C 49 | Fe 1 | N 4 | O 6 | 0 |
| 77 | C1 | 1 | Total 60 | C 49 | Fe 1 | N 4 | O 6 | 0 |

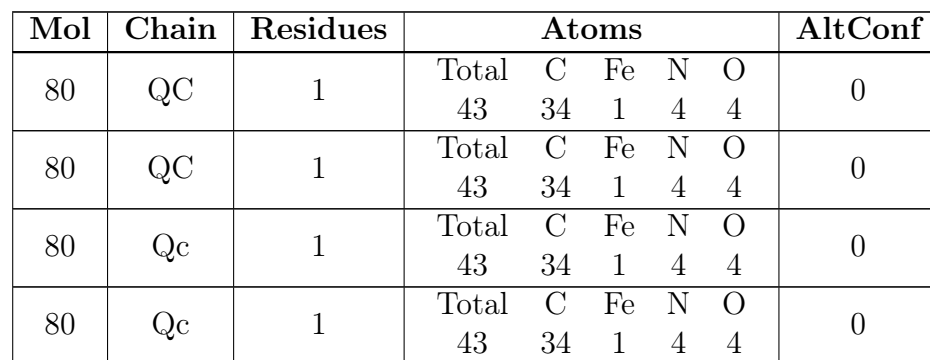
- Molecule 78 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 78 | C1 | 1 | Total | Cu | 0 |
| | | | 1 | 1 | |
| 78 | C2 | 2 | Total | Cu | 0 |
| | | | 2 | 2 | |

- Molecule 79 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 79 | C1 | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 79 | S1 | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

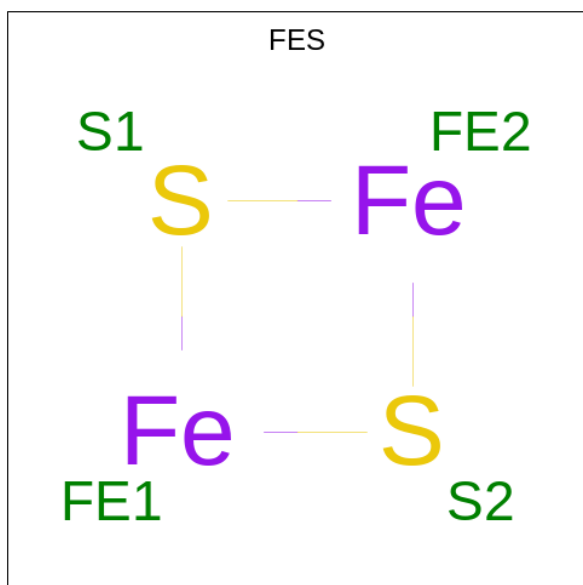
- Molecule 80 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



- # HEC
-
- The chemical structure of HEC (Hydroxyethylchlorin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure is labeled with various atoms and bonds, including O1A, O2A, O1D, O2D, O, OH, CGA, CGD, CAA, CBA, CAD, CBD, CMA, C3A, C3B, C3C, C3D, C3E, C3F, C3G, C3H, C3I, C3J, C3K, C3L, C3M, C3N, C3O, C3P, C3Q, C3R, C3S, C3T, C3U, C3V, C3W, C3X, C3Y, C3Z, C3AA, C3AB, C3AC, C3AD, C3AE, C3AF, C3AG, C3AH, C3AI, C3AJ, C3AK, C3AL, C3AM, C3AN, C3AO, C3AP, C3AQ, C3AR, C3AS, C3AT, C3AU, C3AV, C3AW, C3AX, C3AY, C3AZ, C3BA, C3BB, C3BC, C3BD, C3BE, C3BF, C3BG, C3BH, C3BI, C3BJ, C3BK, C3BL, C3BM, C3BN, C3BO, C3BP, C3BQ, C3BR, C3BS, C3BT, C3BU, C3BV, C3BW, C3BX, C3BY, C3BZ, C3CA, C3CB, C3CC, C3CD, C3CE, C3CF, C3CG, C3CH, C3CI, C3CJ, C3CK, C3CL, C3CM, C3CN, C3CO, C3CP, C3CQ, C3CR, C3CS, C3CT, C3CU, C3CV, C3CW, C3CX, C3CY, C3CZ, C3DA, C3DB, C3DC, C3DD, C3DE, C3DF, C3DG, C3DH, C3DI, C3DJ, C3DK, C3DL, C3DM, C3DN, C3DO, C3DP, C3DQ, C3DR, C3DS, C3DT, C3DU, C3DV, C3DW, C3DX, C3DY, C3DZ, C3EA, C3EB, C3EC, C3ED, C3EE, C3EF, C3EG, C3EH, C3EI, C3EJ, C3EK, C3EL, C3EM, C3EN, C3EO, C3EP, C3EQ, C3ER, C3ES, C3ET, C3EU, C3EV, C3EW, C3EX, C3EY, C3EZ, C3FA, C3FB, C3FC, C3FD, C3FE, C3FF, C3FG, C3FH, C3FI, C3FJ, C3FK, C3FL, C3FM, C3FN, C3FO, C3FP, C3FQ, C3FR, C3FS, C3FT, C3FU, C3FV, C3FW, C3FX, C3FY, C3FZ, C3GA, C3GB, C3GC, C3GD, C3GE, C3GF, C3GG, C3GH, C3GI, C3GJ, C3GK, C3GL, C3GM, C3GN, C3GO, C3GP, C3GQ, C3GR, C3GS, C3GT, C3GU, C3GV, C3GW, C3GX, C3GY, C3GZ, C3HA, C3HB, C3HC, C3HD, C3HE, C3HF, C3HG, C3HH, C3HI, C3HJ, C3HK, C3HL, C3HM, C3HN, C3HO, C3HP, C3HQ, C3HR, C3HS, C3HT, C3HU, C3HV, C3HW, C3HX, C3HY, C3HZ, C3IA, C3IB, C3IC, C3ID, C3IE, C3IF, C3IG, C3IH, C3II, C3IJ, C3IK, C3IL, C3IM, C3IN, C3IO, C3IP, C3IQ, C3IR, C3IS, C3IT, C3IU, C3IV, C3IW, C3IX, C3IY, C3IZ, C3JA, C3JB, C3JC, C3JD, C3JE, C3JF, C3JG, C3JH, C3JI, C3JJ, C3JK, C3JL, C3JM, C3JN, C3JO, C3JP, C3JQ, C3JR, C3JS, C3JT, C3JU, C3JV, C3JW, C3JX, C3JY, C3JZ, C3KA, C3KB, C3KC, C3KD, C3KE, C3KF, C3KG, C3KH, C3KI, C3KJ, C3KK, C3KL, C3KM, C3KN, C3KO, C3KP, C3KQ, C3KR, C3KS, C3KT, C3KU, C3KV, C3KW, C3KX, C3KY, C3KZ, C3LA, C3LB, C3LC, C3LD, C3LE, C3LF, C3LG, C3LH, C3LI, C3LJ, C3LK, C3LL, C3LM, C3LN, C3LO, C3LP, C3LQ, C3LR, C3LS, C3LT, C3LU, C3LV, C3LW, C3LX, C3LY, C3LZ, C3MA, C3MB, C3MC, C3MD, C3ME, C3MF, C3MG, C3MH, C3MI, C3MJ, C3MK, C3ML, C3MN, C3MO, C3MP, C3MQ, C3MR, C3MS, C3MT, C3MU, C3MV, C3MW, C3MX, C3MY, C3MZ, C3NA, C3NB, C3NC, C3ND, C3NE, C3NF, C3NG, C3NH, C3NI, C3NJ, C3NK, C3NL, C3NM, C3NO, C3NP, C3NQ, C3NR, C3NS, C3NT, C3NU, C3NV, C3NW, C3NX, C3NY, C3NZ, C3OA, C3OB, C3OC, C3OD, C3OE, C3OF, C3OG, C3OH, C3OI, C3OJ, C3OK, C3OL, C3OM, C3ON, C3OO, C3OP, C3OQ, C3OR, C3OS, C3OT, C3OU, C3OV, C3OW, C3OX, C3OY, C3OZ, C3PA, C3PB, C3PC, C3PD, C3PE, C3PF, C3PG, C3PH, C3PI, C3PJ, C3PK, C3PL, C3PM, C3PN, C3PO, C3PP, C3PQ, C3PR, C3PS, C3PT, C3PU, C3PV, C3PW, C3PX, C3PY, C3PZ, C3QA, C3QB, C3QC, C3QD, C3QE, C3QF, C3QG, C3QH, C3QI, C3QJ, C3QK, C3QL, C3QM, C3QN, C3QO, C3QP, C3QQ, C3QR, C3QS, C3QT, C3QU, C3QV, C3QW, C3QX, C3QY, C3QZ, C3RA, C3RB, C3RC, C3RD, C3RE, C3RF, C3RG, C3RH, C3RI, C3RJ, C3RK, C3RL, C3RM, C3RN, C3RO, C3RP, C3RQ, C3RR, C3RS, C3RT, C3RU, C3RV, C3RW, C3RX, C3RY, C3RZ, C3SA, C3SB, C3SC, C3SD, C3SE, C3SF, C3SG, C3SH, C3SI, C3SJ, C3SK, C3SL, C3SM, C3SN, C3SO, C3SP, C3SQ, C3SR, C3SS, C3ST, C3SU, C3SV, C3SW, C3SX, C3SY, C3SZ, C3TA, C3TB, C3TC, C3TD, C3TE, C3TF, C3TG, C3TH, C3TI, C3TJ, C3TK, C3TL, C3TM, C3TN, C3TO, C3TP, C3TQ, C3TR, C3TS, C3TT, C3TU, C3TV, C3TW, C3TX, C3TY, C3TZ, C3UA, C3UB, C3UC, C3UD, C3UE, C3UF, C3UG, C3UH, C3UI, C3UJ, C3UK, C3UL, C3UM, C3UN, C3UO, C3UP, C3UQ, C3UR, C3US, C3UT, C3UU, C3UV, C3UW, C3UX, C3UY, C3UZ, C3VA, C3VB, C3VC, C3VD, C3VE, C3VF, C3VG, C3VH, C3VI, C3VJ, C3VK, C3VL, C3VM, C3VN, C3VO, C3VP, C3VQ, C3VR, C3VS, C3VT, C3VU, C3VV, C3VW, C3VX, C3VY, C3VZ, C3WA, C3WB, C3WC, C3WD, C3WE, C3WF, C3WG, C3WH, C3WI, C3WJ, C3WK, C3WL, C3WM, C3WN, C3WO, C3WP, C3WQ, C3WR, C3WS, C3WT, C3WU, C3WV, C3WW, C3WX, C3WY, C3WZ, C3XA, C3XB, C3XC, C3XD, C3XE, C3XF, C3XG, C3XH, C3XI, C3XJ, C3XK, C3XL, C3XM, C3XN, C3XO, C3XP, C3XQ, C3XR, C3XS, C3XT, C3XU, C3XV, C3XW, C3XX, C3XY, C3XZ, C3YA, C3YB, C3YC, C3YD, C3YE, C3YF, C3YG, C3YH, C3YI, C3YJ, C3YK, C3YL, C3YM, C3YN, C3YO, C3YP, C3YQ, C3YR, C3YS, C3YT, C3YU, C3YV, C3YW, C3YX, C3YY, C3YZ, C3ZA, C3ZB, C3ZC, C3ZD, C3ZE, C3ZF, C3ZG, C3ZH, C3ZI, C3ZJ, C3ZK, C3ZL, C3ZM, C3ZN, C3ZO, C3ZP, C3ZQ, C3ZR, C3ZS, C3ZT, C3ZU, C3ZV, C3ZW, C3ZX, C3ZY, C3ZZ.

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 81 | QD | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 |
| 81 | Qd | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 |

- Molecule 82 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



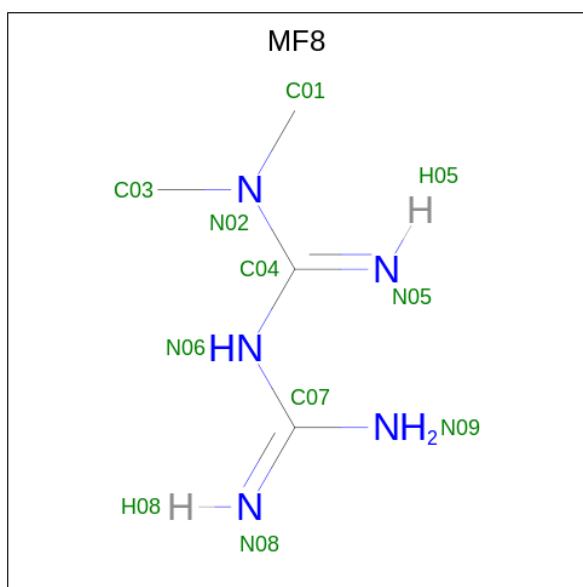
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 82 | QE | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |
| 82 | Qe | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |
| 82 | S1 | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |
| 82 | V2 | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |

- Molecule 83 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



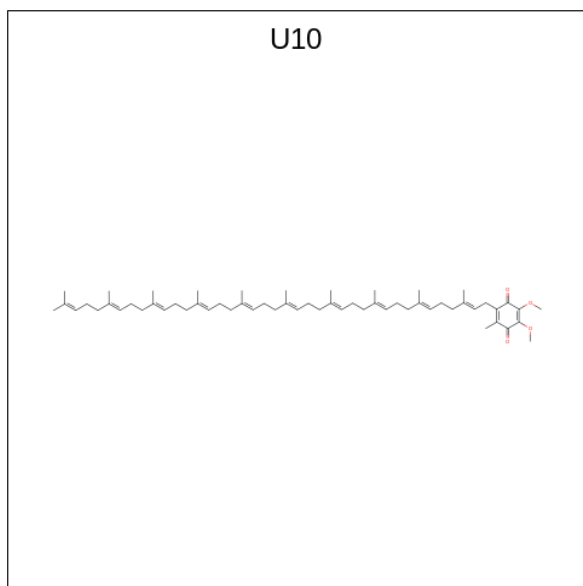
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 83 | S1 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 83 | S1 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 83 | S7 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 83 | S8 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 83 | S8 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 83 | V1 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |

- Molecule 84 is Metformin (CCD ID: MF8) (formula: $C_4H_{11}N_5$) (labeled as "Ligand of Interest" by depositor).



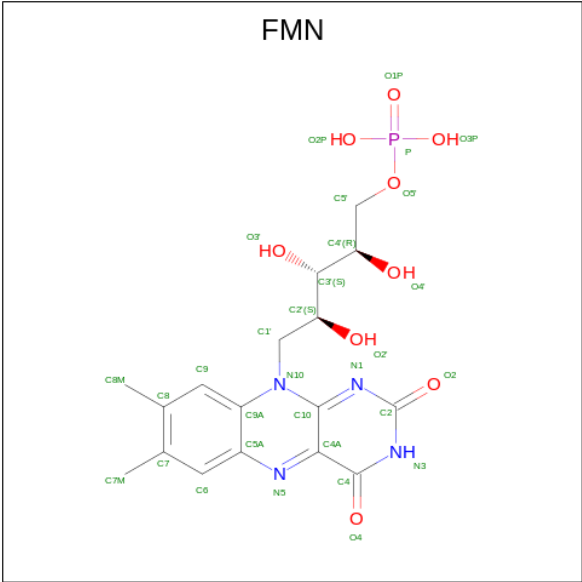
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 84 | S2 | 1 | Total | C | N | 0 |
| | | | 9 | 4 | 5 | |

- Molecule 85 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 85 | S7 | 1 | Total | C | O | 0 |
| | | | 63 | 59 | 4 | |

- Molecule 86 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).

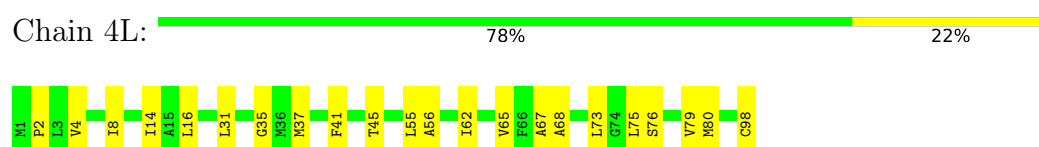


| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 86 | V1 | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | |

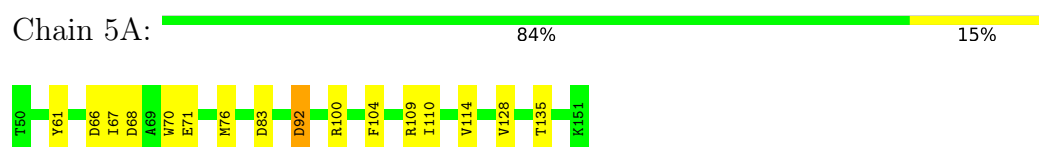
3 Residue-property plots [i](#)

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

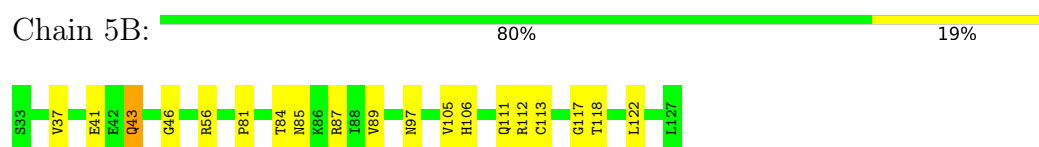
- Molecule 1: NADH-ubiquinone oxidoreductase chain 4L



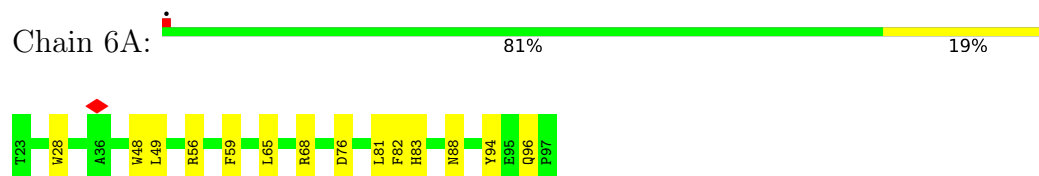
- Molecule 2: Cytochrome c oxidase subunit 5A, mitochondrial



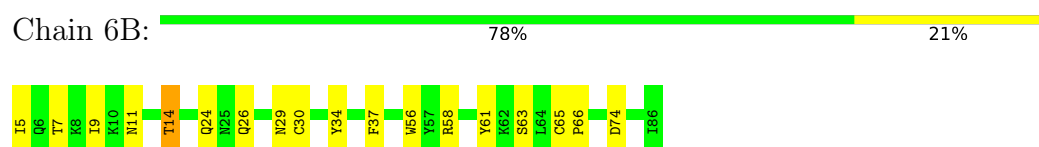
- Molecule 3: Cytochrome c oxidase subunit 5B, mitochondrial



- Molecule 4: Cytochrome c oxidase subunit



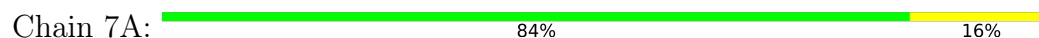
- Molecule 5: Cytochrome c oxidase subunit



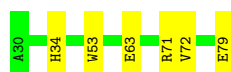
- Molecule 6: Cytochrome c oxidase subunit 6C



- Molecule 7: Cytochrome c oxidase subunit 7A1, mitochondrial



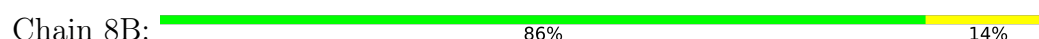
- Molecule 8: Cytochrome c oxidase subunit 7B, mitochondrial



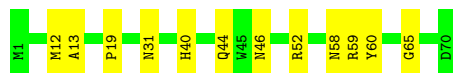
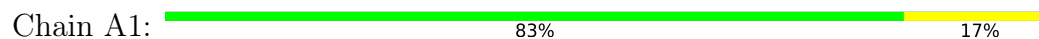
- Molecule 9: Cytochrome c oxidase subunit 7C, mitochondrial



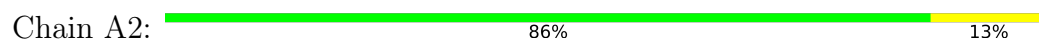
- Molecule 10: Cytochrome c oxidase subunit 8



- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2




- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain A3:  94% 6%




- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain A5:  88% 12%




- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain A6:  83% 17%




- Molecule 16: Complex I-B14.5a

Chain A7:  74% 12% 13%




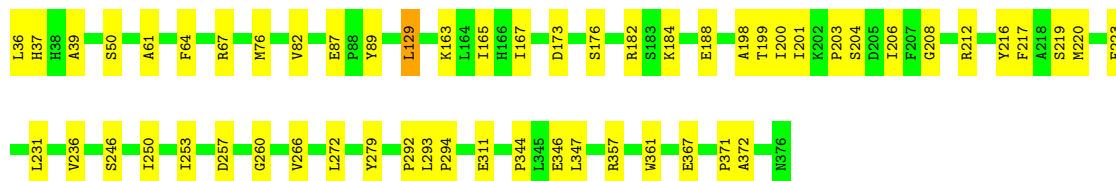
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8:  85% 15%



- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain A9:  84% 16%



- Molecule 19: Acyl carrier protein

Chain AB:  70% 18% 11%





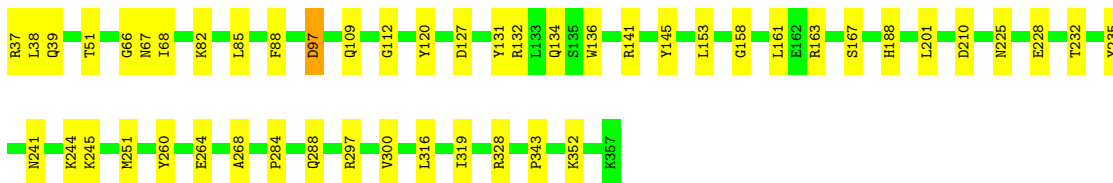
- Molecule 19: Acyl carrier protein

Chain AC: 86% 13%



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain AK: 85% 15%



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain AL: 90% 10%



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AM: 89% 10%



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain AN: 83% 17%




- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain B1: 80% 20%




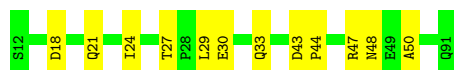
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain B2:  82% 18%



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain B3:  85% 15%



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain B4:  92% 8%



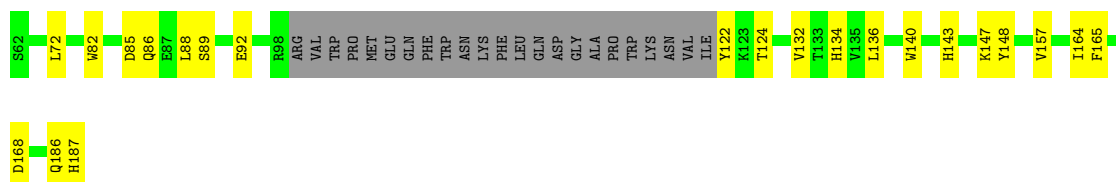
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain B5:  90% 10%




- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain B6:  64% 17% 18%



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain B7:  81% 19%



- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain B8:  91% 9%



- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain B9:  87% 13%




- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain BK:  86% 14%




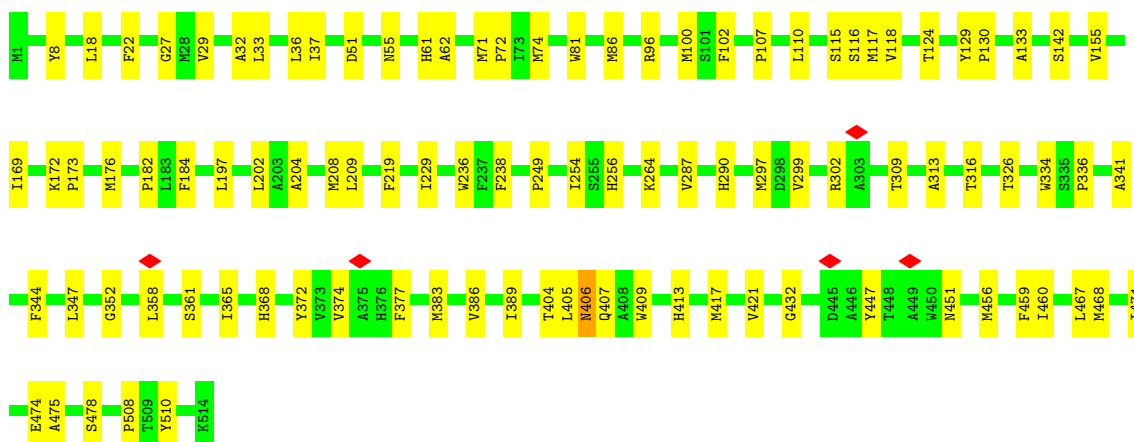
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain BL:  89% 11%



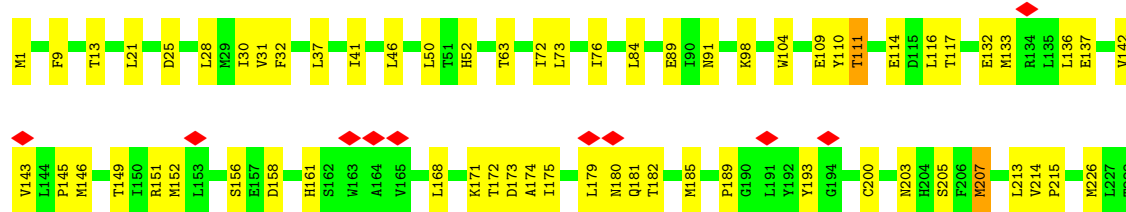
- Molecule 35: Cytochrome c oxidase subunit 1

Chain C1:  81% 19%

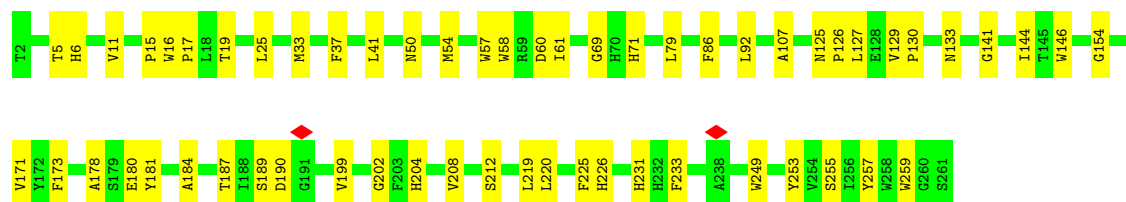
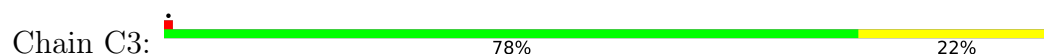


- Molecule 36: Cytochrome c oxidase subunit 2

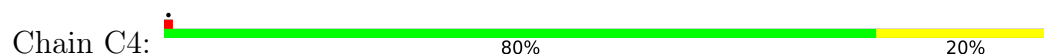
Chain C2:  72% 27%



• Molecule 37: Cytochrome c oxidase subunit 3



• Molecule 38: Cytochrome c oxidase subunit 4



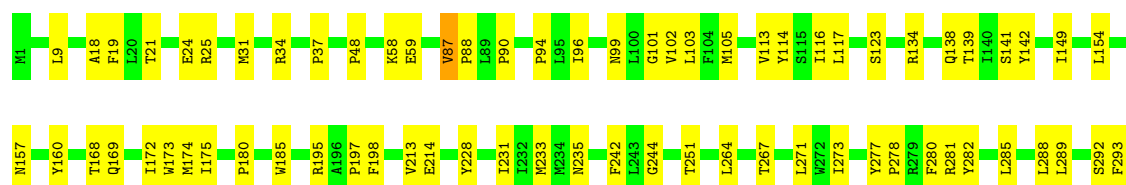
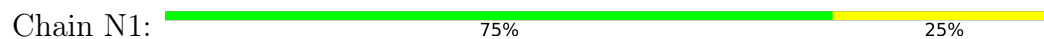
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



• Molecule 40: NADH dehydrogenase [ubiquinone] 1 subunit C2



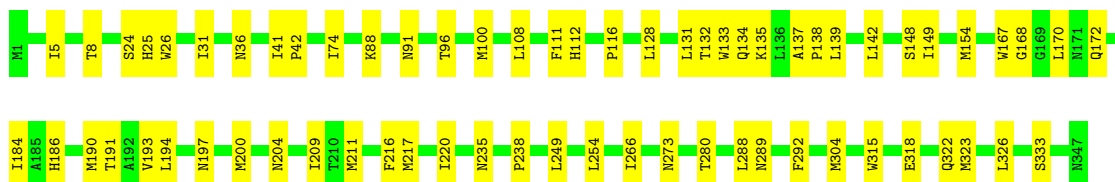
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1





• Molecule 42: NADH-ubiquinone oxidoreductase chain 2

Chain N2: 81% 19%



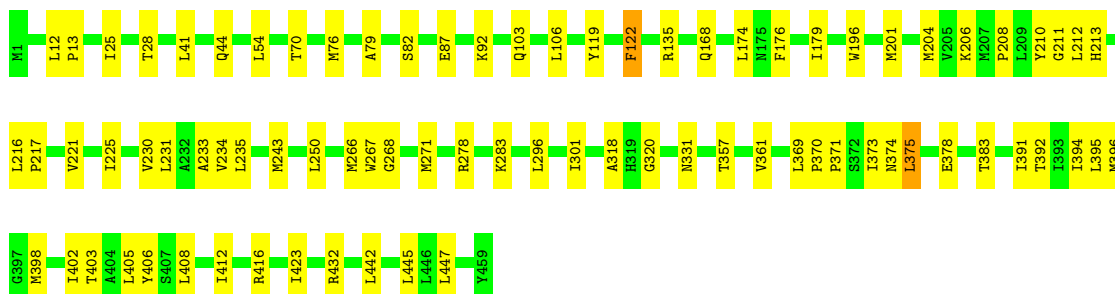
• Molecule 43: NADH-ubiquinone oxidoreductase chain 3

Chain N3: 83% 17%



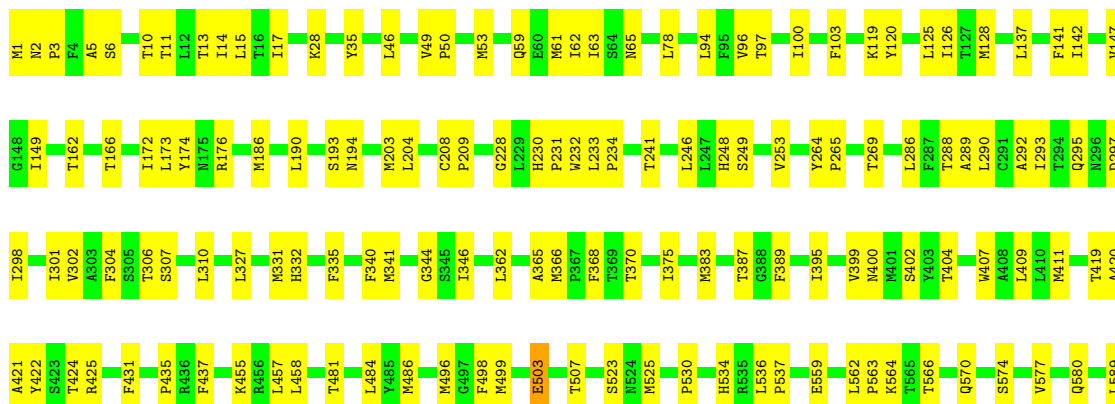
• Molecule 44: NADH-ubiquinone oxidoreductase chain 4

Chain N4: 82% 17%



• Molecule 45: NADH-ubiquinone oxidoreductase chain 5

Chain N5: 76% 24%





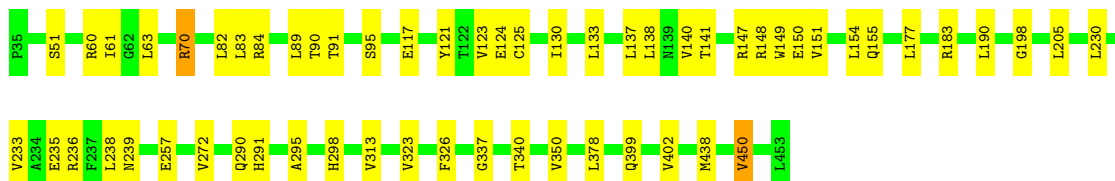
- Molecule 46: NADH-ubiquinone oxidoreductase chain 6

Chain N6: 80% 20%



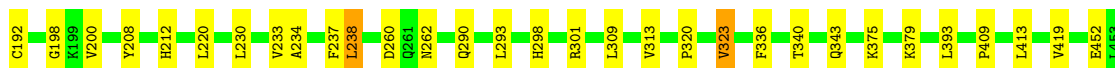
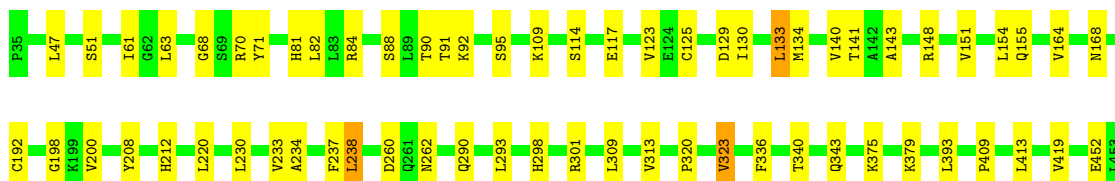
- Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain QA: 86% 13%



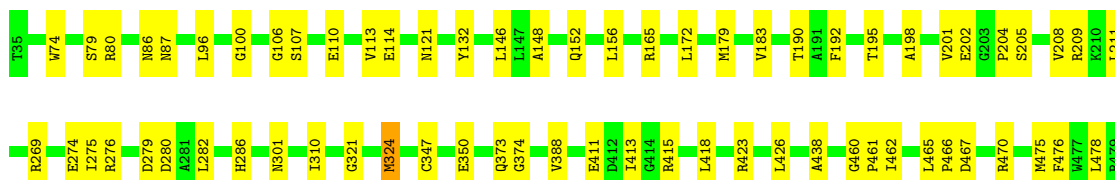
- Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain Qa: 85% 15%



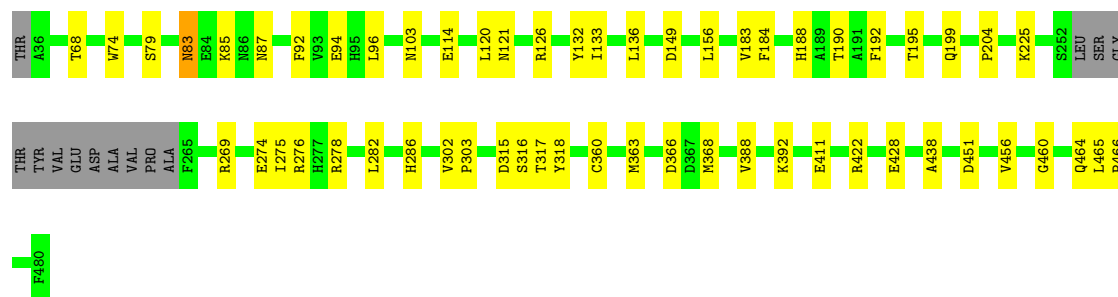
- Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain QB: 85% 15%



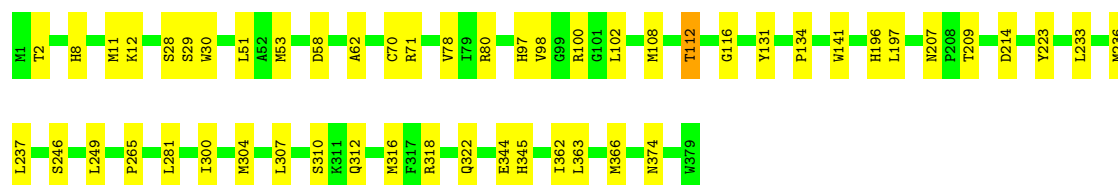
- Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain Qb: 84% 13%



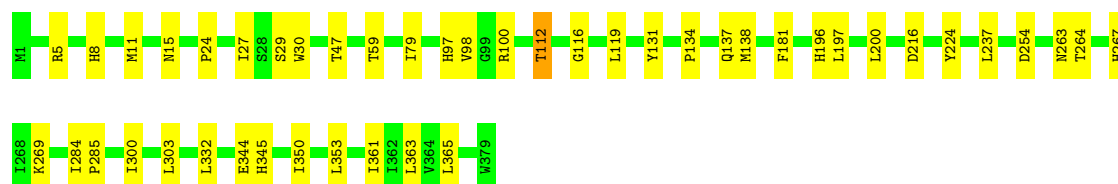
- Molecule 49: Cytochrome b

Chain QC: 86% 13%



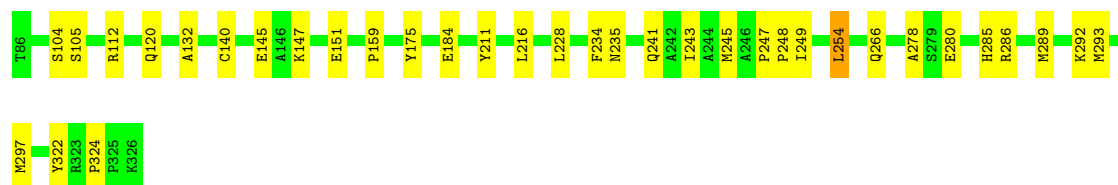
- Molecule 49: Cytochrome b

Chain Qc: 88% 12%



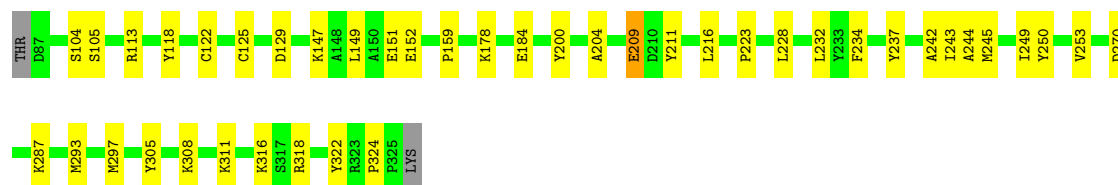
- Molecule 50: Cytochrome c1, heme protein, mitochondrial

Chain QD: 85% 14%



- Molecule 50: Cytochrome c1, heme protein, mitochondrial

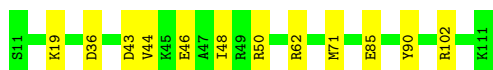
Chain Qd: 82% 17%





- Molecule 53: Cytochrome b-c1 complex subunit 7

Chain QG: 88% 12%



- Molecule 53: Cytochrome b-c1 complex subunit 7

Chain Qg: 87% 12%



- Molecule 54: Cytochrome b-c1 complex subunit 8

Chain QH: 80% 19%



- Molecule 54: Cytochrome b-c1 complex subunit 8

Chain Qh: 87% 13%



- Molecule 55: Complex III subunit 9

Chain QI: 90% 8%



- Molecule 55: Complex III subunit 9

Chain Qi: 89% 8%



- Molecule 56: Cytochrome b-c1 complex subunit 10

Chain QJ: 81% 13% 6%



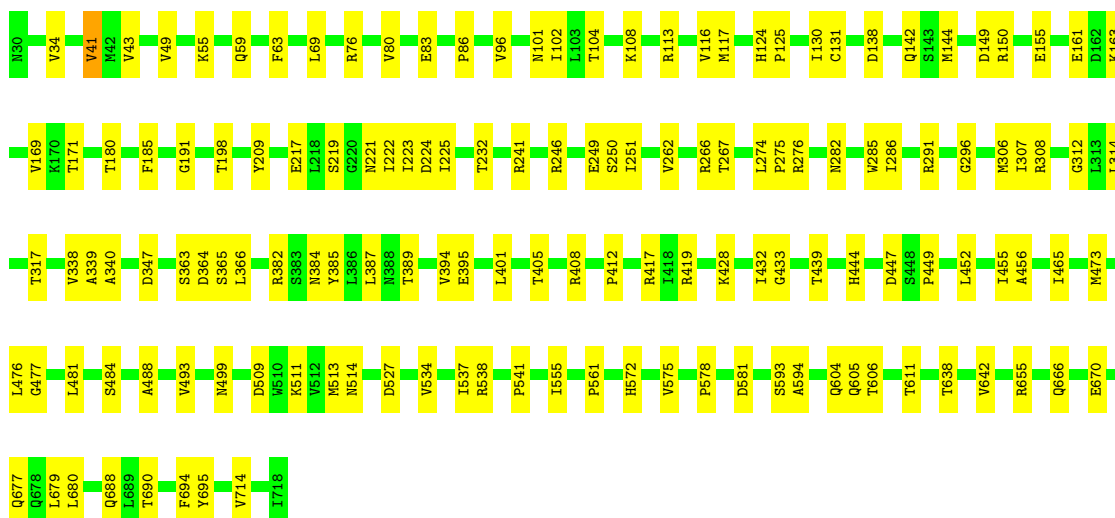
- Molecule 56: Cytochrome b-c1 complex subunit 10

Chain Qj: 83% 13% ..



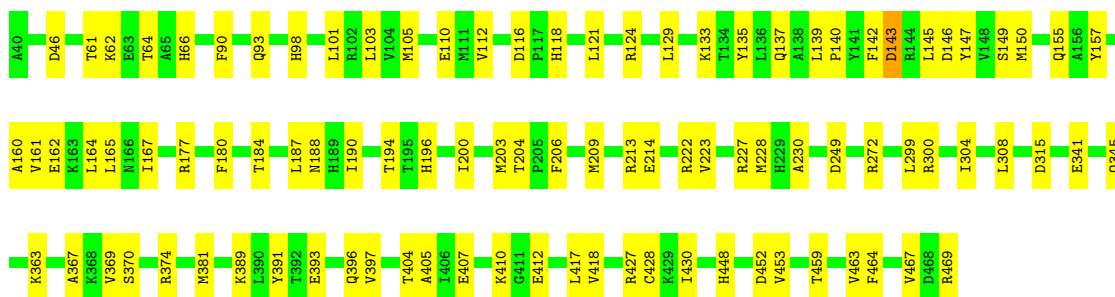
- Molecule 57: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain S1: 79% 21%



- Molecule 58: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain S2: 78% 22%



- Molecule 59: Complex I-30kD

Chain S3: 86% 14%



- Molecule 60: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain S4:  85% 15%



- Molecule 61: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain S5:  92% 8%




- Molecule 62: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain S6:  91% 9%



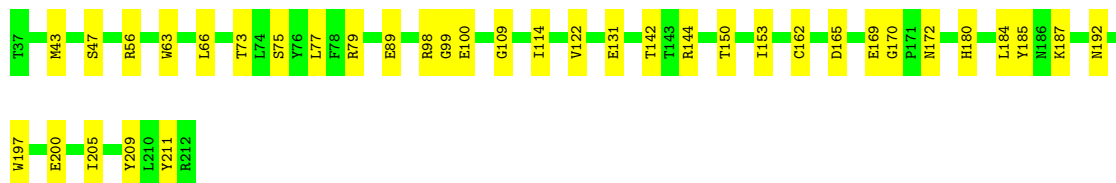
- Molecule 63: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain S7:  79% 19%




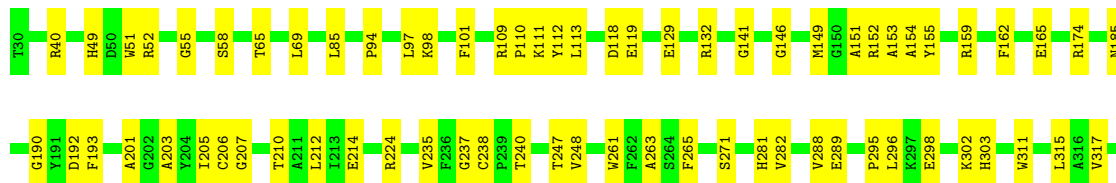
- Molecule 64: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

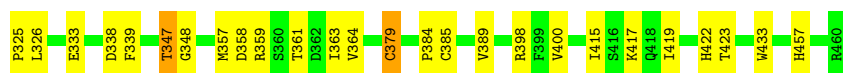
Chain S8:  80% 20%



- Molecule 65: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain V1:  78% 22%





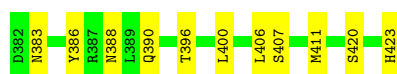
- Molecule 66: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain V2: 86% 13%



- Molecule 67: NADH:ubiquinone oxidoreductase subunit V3

Chain V3: 74% 26%



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 320129 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 51.9 | Depositor |
| Minimum defocus (nm) | 600 | Depositor |
| Maximum defocus (nm) | 1800 | Depositor |
| Magnification | 105000 | Depositor |
| Image detector | FEI FALCON IV (4k x 4k) | Depositor |
| Maximum map value | 46.884 | Depositor |
| Minimum map value | -34.576 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 1.006 | Depositor |
| Recommended contour level | 0.05 | Depositor |
| Map size (Å) | 576.0, 576.0, 576.0 | wwPDB |
| Map dimensions | 480, 480, 480 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.2, 1.2, 1.2 | Depositor |

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEE, HEC, PC1, ZN, HEA, 2MR, MG, 3PE, SF4, ADP, CDL, HEM, U10, MF8, ZMP, FMN, PLX, NDP, CU, FES

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|-------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | 4L | 0.15 | 0/759 | 0.29 | 0/1029 |
| 2 | 5A | 0.09 | 0/843 | 0.23 | 0/1145 |
| 3 | 5B | 0.12 | 0/739 | 0.30 | 0/1002 |
| 4 | 6A | 0.10 | 0/648 | 0.23 | 0/888 |
| 5 | 6B | 0.11 | 0/704 | 0.26 | 0/951 |
| 6 | 6C | 0.10 | 0/587 | 0.25 | 0/781 |
| 7 | 7A | 0.11 | 0/457 | 0.23 | 0/620 |
| 8 | 7B | 0.10 | 0/405 | 0.26 | 0/555 |
| 9 | 7C | 0.11 | 0/400 | 0.22 | 0/536 |
| 10 | 8B | 0.11 | 0/349 | 0.23 | 0/477 |
| 11 | A1 | 0.14 | 0/577 | 0.32 | 0/777 |
| 12 | A2 | 0.10 | 0/697 | 0.25 | 0/938 |
| 13 | A3 | 0.10 | 0/664 | 0.23 | 0/912 |
| 14 | A5 | 0.13 | 0/929 | 0.23 | 0/1258 |
| 15 | A6 | 0.14 | 0/991 | 0.29 | 0/1335 |
| 16 | A7 | 0.12 | 0/798 | 0.26 | 0/1079 |
| 17 | A8 | 0.11 | 0/1436 | 0.25 | 0/1938 |
| 18 | A9 | 0.14 | 0/2820 | 0.27 | 0/3823 |
| 19 | AB | 0.10 | 0/633 | 0.23 | 0/851 |
| 19 | AC | 0.13 | 0/714 | 0.23 | 0/965 |
| 20 | AK | 0.12 | 0/2661 | 0.27 | 0/3602 |
| 21 | AL | 0.12 | 0/1042 | 0.21 | 0/1411 |
| 22 | AM | 0.10 | 0/1245 | 0.23 | 0/1694 |
| 23 | AN | 0.14 | 0/1204 | 0.27 | 0/1624 |
| 24 | B1 | 0.13 | 0/491 | 0.28 | 0/663 |
| 25 | B2 | 0.12 | 0/610 | 0.23 | 0/836 |
| 26 | B3 | 0.12 | 0/660 | 0.25 | 0/892 |
| 27 | B4 | 0.14 | 0/1092 | 0.26 | 0/1481 |
| 28 | B5 | 0.15 | 0/1184 | 0.28 | 0/1603 |
| 29 | B6 | 0.15 | 0/910 | 0.33 | 0/1237 |
| 30 | B7 | 0.12 | 0/1092 | 0.25 | 0/1459 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 31 | B8 | 0.13 | 0/1371 | 0.26 | 0/1875 |
| 32 | B9 | 0.14 | 0/1590 | 0.27 | 0/2155 |
| 33 | BK | 0.13 | 0/1489 | 0.25 | 0/2008 |
| 34 | BL | 0.13 | 0/851 | 0.27 | 0/1155 |
| 35 | C1 | 0.14 | 0/4164 | 0.28 | 0/5689 |
| 36 | C2 | 0.12 | 0/1880 | 0.28 | 0/2564 |
| 37 | C3 | 0.13 | 0/2186 | 0.26 | 0/2991 |
| 38 | C4 | 0.12 | 0/1187 | 0.26 | 0/1606 |
| 39 | CA | 0.10 | 0/430 | 0.19 | 0/581 |
| 40 | CB | 0.13 | 0/1031 | 0.26 | 0/1394 |
| 41 | N1 | 0.18 | 0/2581 | 0.35 | 0/3529 |
| 42 | N2 | 0.17 | 0/2773 | 0.33 | 0/3768 |
| 43 | N3 | 0.16 | 0/938 | 0.28 | 0/1281 |
| 44 | N4 | 0.17 | 0/3723 | 0.31 | 0/5078 |
| 45 | N5 | 0.16 | 0/4914 | 0.34 | 0/6683 |
| 46 | N6 | 0.14 | 0/1364 | 0.31 | 0/1850 |
| 47 | QA | 0.15 | 0/3200 | 0.29 | 0/4333 |
| 47 | Qa | 0.15 | 0/3200 | 0.29 | 0/4333 |
| 48 | QB | 0.15 | 0/3531 | 0.30 | 0/4793 |
| 48 | Qb | 0.14 | 0/3436 | 0.27 | 0/4659 |
| 49 | QC | 0.17 | 0/3123 | 0.31 | 0/4269 |
| 49 | Qc | 0.17 | 0/3123 | 0.32 | 0/4269 |
| 50 | QD | 0.15 | 0/1979 | 0.26 | 0/2684 |
| 50 | Qd | 0.15 | 0/1962 | 0.27 | 0/2663 |
| 51 | QE | 0.12 | 0/1550 | 0.25 | 0/2098 |
| 51 | QK | 0.11 | 0/528 | 0.27 | 0/716 |
| 51 | Qe | 0.12 | 0/1550 | 0.27 | 0/2098 |
| 52 | QF | 0.11 | 0/558 | 0.22 | 0/747 |
| 52 | Qf | 0.13 | 0/534 | 0.25 | 0/714 |
| 53 | QG | 0.14 | 0/913 | 0.25 | 0/1223 |
| 53 | Qg | 0.14 | 0/913 | 0.27 | 0/1223 |
| 54 | QH | 0.14 | 0/684 | 0.30 | 0/926 |
| 54 | Qh | 0.14 | 0/688 | 0.28 | 0/931 |
| 55 | QI | 0.11 | 0/520 | 0.20 | 0/701 |
| 55 | Qi | 0.16 | 0/506 | 0.27 | 0/683 |
| 56 | QJ | 0.10 | 0/420 | 0.22 | 0/576 |
| 56 | Qj | 0.14 | 0/437 | 0.31 | 0/598 |
| 57 | S1 | 0.15 | 0/5378 | 0.32 | 2/7287 (0.0%) |
| 58 | S2 | 0.18 | 0/3538 | 0.31 | 0/4796 |
| 59 | S3 | 0.15 | 0/1789 | 0.29 | 0/2436 |
| 60 | S4 | 0.14 | 0/1030 | 0.27 | 0/1391 |
| 61 | S5 | 0.11 | 0/889 | 0.23 | 0/1190 |
| 62 | S6 | 0.13 | 0/755 | 0.29 | 0/1018 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 63 | S7 | 0.17 | 0/1279 | 0.30 | 0/1730 |
| 64 | S8 | 0.16 | 0/1443 | 0.29 | 0/1952 |
| 65 | V1 | 0.15 | 0/3391 | 0.31 | 0/4583 |
| 66 | V2 | 0.14 | 0/1711 | 0.30 | 0/2328 |
| 67 | V3 | 0.11 | 0/365 | 0.27 | 0/493 |
| All | All | 0.14 | 0/115736 | 0.29 | 2/157010 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 57 | S1 | 364 | ASP | CA-C-N | -5.03 | 114.77 | 122.21 |
| 57 | S1 | 364 | ASP | C-N-CA | -5.03 | 114.77 | 122.21 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 4L | 748 | 0 | 799 | 23 | 0 |
| 2 | 5A | 825 | 0 | 823 | 12 | 0 |
| 3 | 5B | 724 | 0 | 705 | 15 | 0 |
| 4 | 6A | 620 | 0 | 589 | 16 | 0 |
| 5 | 6B | 684 | 0 | 649 | 12 | 0 |
| 6 | 6C | 574 | 0 | 590 | 7 | 0 |
| 7 | 7A | 447 | 0 | 443 | 13 | 0 |
| 8 | 7B | 392 | 0 | 372 | 4 | 0 |
| 9 | 7C | 387 | 0 | 385 | 13 | 0 |
| 10 | 8B | 338 | 0 | 342 | 6 | 0 |
| 11 | A1 | 562 | 0 | 557 | 9 | 0 |
| 12 | A2 | 686 | 0 | 699 | 8 | 0 |
| 13 | A3 | 643 | 0 | 642 | 5 | 0 |
| 14 | A5 | 910 | 0 | 950 | 8 | 0 |
| 15 | A6 | 967 | 0 | 972 | 14 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16 | A7 | 780 | 0 | 808 | 9 | 0 |
| 17 | A8 | 1398 | 0 | 1372 | 20 | 0 |
| 18 | A9 | 2743 | 0 | 2762 | 33 | 0 |
| 19 | AB | 624 | 0 | 625 | 10 | 0 |
| 19 | AC | 702 | 0 | 694 | 9 | 0 |
| 20 | AK | 2601 | 0 | 2566 | 28 | 0 |
| 21 | AL | 1021 | 0 | 1025 | 13 | 0 |
| 22 | AM | 1204 | 0 | 1162 | 15 | 0 |
| 23 | AN | 1173 | 0 | 1166 | 20 | 0 |
| 24 | B1 | 479 | 0 | 486 | 8 | 0 |
| 25 | B2 | 584 | 0 | 529 | 10 | 0 |
| 26 | B3 | 641 | 0 | 620 | 8 | 0 |
| 27 | B4 | 1062 | 0 | 1072 | 7 | 0 |
| 28 | B5 | 1151 | 0 | 1164 | 13 | 0 |
| 29 | B6 | 882 | 0 | 899 | 20 | 0 |
| 30 | B7 | 1068 | 0 | 1043 | 22 | 0 |
| 31 | B8 | 1315 | 0 | 1208 | 11 | 0 |
| 32 | B9 | 1534 | 0 | 1470 | 21 | 0 |
| 33 | BK | 1456 | 0 | 1426 | 23 | 0 |
| 34 | BL | 828 | 0 | 788 | 8 | 0 |
| 35 | C1 | 4024 | 0 | 4005 | 82 | 0 |
| 36 | C2 | 1833 | 0 | 1843 | 45 | 0 |
| 37 | C3 | 2103 | 0 | 2034 | 50 | 0 |
| 38 | C4 | 1153 | 0 | 1130 | 20 | 0 |
| 39 | CA | 417 | 0 | 422 | 4 | 0 |
| 40 | CB | 1000 | 0 | 994 | 13 | 0 |
| 41 | N1 | 2508 | 0 | 2607 | 60 | 0 |
| 42 | N2 | 2710 | 0 | 2874 | 46 | 0 |
| 43 | N3 | 914 | 0 | 951 | 18 | 0 |
| 44 | N4 | 3631 | 0 | 3839 | 55 | 0 |
| 45 | N5 | 4785 | 0 | 4933 | 98 | 0 |
| 46 | N6 | 1329 | 0 | 1326 | 31 | 0 |
| 47 | QA | 3147 | 0 | 3129 | 40 | 0 |
| 47 | Qa | 3147 | 0 | 3129 | 40 | 0 |
| 48 | QB | 3459 | 0 | 3350 | 45 | 0 |
| 48 | Qb | 3367 | 0 | 3262 | 34 | 0 |
| 49 | QC | 3025 | 0 | 3090 | 38 | 0 |
| 49 | Qc | 3025 | 0 | 3090 | 35 | 0 |
| 50 | QD | 1921 | 0 | 1867 | 26 | 0 |
| 50 | Qd | 1904 | 0 | 1849 | 32 | 0 |
| 51 | QE | 1517 | 0 | 1500 | 33 | 0 |
| 51 | QK | 520 | 0 | 554 | 9 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 51 | Qe | 1517 | 0 | 1500 | 21 | 0 |
| 52 | QF | 552 | 0 | 536 | 7 | 0 |
| 52 | Qf | 528 | 0 | 510 | 6 | 0 |
| 53 | QG | 893 | 0 | 888 | 8 | 0 |
| 53 | Qg | 893 | 0 | 888 | 10 | 0 |
| 54 | QH | 662 | 0 | 660 | 12 | 0 |
| 54 | Qh | 666 | 0 | 663 | 9 | 0 |
| 55 | QI | 507 | 0 | 509 | 5 | 0 |
| 55 | Qi | 493 | 0 | 491 | 5 | 0 |
| 56 | QJ | 405 | 0 | 405 | 6 | 0 |
| 56 | Qj | 421 | 0 | 418 | 5 | 0 |
| 57 | S1 | 5290 | 0 | 5321 | 92 | 0 |
| 58 | S2 | 3459 | 0 | 3396 | 68 | 0 |
| 59 | S3 | 1738 | 0 | 1693 | 18 | 0 |
| 60 | S4 | 1007 | 0 | 1008 | 17 | 0 |
| 61 | S5 | 867 | 0 | 871 | 9 | 0 |
| 62 | S6 | 741 | 0 | 701 | 7 | 0 |
| 63 | S7 | 1248 | 0 | 1254 | 31 | 0 |
| 64 | S8 | 1412 | 0 | 1363 | 30 | 0 |
| 65 | V1 | 3316 | 0 | 3272 | 56 | 0 |
| 66 | V2 | 1671 | 0 | 1673 | 20 | 0 |
| 67 | V3 | 355 | 0 | 329 | 10 | 0 |
| 68 | 4L | 92 | 0 | 137 | 8 | 0 |
| 68 | 7A | 91 | 0 | 132 | 6 | 0 |
| 68 | A7 | 51 | 0 | 46 | 1 | 0 |
| 68 | A8 | 83 | 0 | 113 | 7 | 0 |
| 68 | AK | 68 | 0 | 80 | 3 | 0 |
| 68 | AL | 94 | 0 | 138 | 7 | 0 |
| 68 | B4 | 80 | 0 | 107 | 4 | 0 |
| 68 | B5 | 100 | 0 | 156 | 6 | 0 |
| 68 | C3 | 170 | 0 | 240 | 7 | 0 |
| 68 | CB | 100 | 0 | 156 | 4 | 0 |
| 68 | N1 | 78 | 0 | 103 | 4 | 0 |
| 68 | N4 | 62 | 0 | 68 | 2 | 0 |
| 68 | N5 | 189 | 0 | 284 | 15 | 0 |
| 68 | QB | 64 | 0 | 72 | 3 | 0 |
| 68 | QC | 55 | 0 | 54 | 2 | 0 |
| 68 | QD | 64 | 0 | 72 | 1 | 0 |
| 68 | QH | 125 | 0 | 138 | 7 | 0 |
| 68 | Qb | 64 | 0 | 72 | 2 | 0 |
| 69 | 5B | 1 | 0 | 0 | 0 | 0 |
| 69 | S6 | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 70 | 6A | 45 | 0 | 64 | 11 | 0 |
| 70 | C1 | 183 | 0 | 274 | 14 | 0 |
| 70 | C3 | 190 | 0 | 291 | 13 | 0 |
| 70 | N1 | 48 | 0 | 73 | 3 | 0 |
| 70 | N3 | 54 | 0 | 88 | 1 | 0 |
| 70 | QB | 51 | 0 | 79 | 2 | 0 |
| 70 | Qb | 48 | 0 | 73 | 2 | 0 |
| 70 | Qc | 54 | 0 | 88 | 4 | 0 |
| 70 | Qh | 54 | 0 | 88 | 1 | 0 |
| 71 | 6C | 43 | 0 | 67 | 1 | 0 |
| 71 | AL | 47 | 0 | 75 | 2 | 0 |
| 71 | AM | 51 | 0 | 83 | 6 | 0 |
| 71 | B1 | 52 | 0 | 88 | 1 | 0 |
| 71 | CB | 52 | 0 | 88 | 3 | 0 |
| 71 | N4 | 49 | 0 | 79 | 4 | 0 |
| 71 | N6 | 52 | 0 | 88 | 1 | 0 |
| 71 | QI | 52 | 0 | 88 | 2 | 0 |
| 71 | Qi | 46 | 0 | 73 | 5 | 0 |
| 71 | S7 | 52 | 0 | 88 | 6 | 0 |
| 72 | 7A | 43 | 0 | 60 | 6 | 0 |
| 72 | B8 | 32 | 0 | 38 | 0 | 0 |
| 72 | C1 | 85 | 0 | 124 | 1 | 0 |
| 72 | CA | 51 | 0 | 82 | 1 | 0 |
| 72 | CB | 46 | 0 | 69 | 1 | 0 |
| 72 | N5 | 46 | 0 | 69 | 1 | 0 |
| 72 | QE | 44 | 0 | 65 | 1 | 0 |
| 72 | QJ | 34 | 0 | 42 | 1 | 0 |
| 72 | Qc | 48 | 0 | 73 | 2 | 0 |
| 72 | Qj | 29 | 0 | 32 | 0 | 0 |
| 72 | S7 | 51 | 0 | 82 | 2 | 0 |
| 73 | 7C | 51 | 0 | 82 | 5 | 0 |
| 73 | A9 | 39 | 0 | 52 | 4 | 0 |
| 73 | N1 | 31 | 0 | 36 | 0 | 0 |
| 73 | N3 | 51 | 0 | 82 | 4 | 0 |
| 73 | N4 | 49 | 0 | 75 | 5 | 0 |
| 73 | N5 | 137 | 0 | 205 | 4 | 0 |
| 73 | QB | 34 | 0 | 42 | 1 | 0 |
| 73 | QC | 40 | 0 | 54 | 1 | 0 |
| 73 | QE | 47 | 0 | 71 | 2 | 0 |
| 73 | Qc | 42 | 0 | 61 | 1 | 0 |
| 73 | Qe | 75 | 0 | 104 | 8 | 0 |
| 73 | S2 | 48 | 0 | 73 | 4 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 73 | S8 | 51 | 0 | 82 | 7 | 0 |
| 74 | A9 | 48 | 0 | 26 | 1 | 0 |
| 75 | AB | 36 | 0 | 47 | 2 | 0 |
| 75 | AC | 36 | 0 | 47 | 4 | 0 |
| 76 | AK | 27 | 0 | 12 | 3 | 0 |
| 77 | C1 | 120 | 0 | 108 | 18 | 0 |
| 78 | C1 | 1 | 0 | 0 | 0 | 0 |
| 78 | C2 | 2 | 0 | 0 | 0 | 0 |
| 79 | C1 | 1 | 0 | 0 | 0 | 0 |
| 79 | S1 | 1 | 0 | 0 | 0 | 0 |
| 80 | QC | 86 | 0 | 60 | 8 | 0 |
| 80 | Qc | 86 | 0 | 60 | 7 | 0 |
| 81 | QD | 43 | 0 | 30 | 2 | 0 |
| 81 | Qd | 43 | 0 | 32 | 4 | 0 |
| 82 | QE | 4 | 0 | 0 | 2 | 0 |
| 82 | Qe | 4 | 0 | 0 | 2 | 0 |
| 82 | S1 | 4 | 0 | 0 | 0 | 0 |
| 82 | V2 | 4 | 0 | 0 | 0 | 0 |
| 83 | S1 | 16 | 0 | 0 | 1 | 0 |
| 83 | S7 | 8 | 0 | 0 | 1 | 0 |
| 83 | S8 | 16 | 0 | 0 | 1 | 0 |
| 83 | V1 | 8 | 0 | 0 | 0 | 0 |
| 84 | S2 | 9 | 0 | 0 | 0 | 0 |
| 85 | S7 | 63 | 0 | 90 | 6 | 0 |
| 86 | V1 | 31 | 0 | 19 | 1 | 0 |
| All | All | 117589 | 0 | 118918 | 1583 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1583) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:BK:140:GLN:O | 33:BK:144:SER:HB2 | 1.73 | 0.88 |
| 1:4L:37:MET:HG2 | 1:4L:67:ALA:HB2 | 1.62 | 0.81 |
| 49:QC:98:VAL:HG22 | 80:QC:402:HEM:HBC2 | 1.64 | 0.80 |
| 49:QC:237:LEU:HB2 | 50:QD:297:MET:HE2 | 1.64 | 0.80 |
| 68:4L:201:CDL:H521 | 46:N6:88:THR:HG23 | 1.65 | 0.78 |
| 29:B6:88:LEU:HD22 | 29:B6:92:GLU:HG2 | 1.64 | 0.78 |
| 49:Qc:98:VAL:HG22 | 80:Qc:403:HEM:HBC2 | 1.66 | 0.77 |
| 21:AL:140:LYS:H | 42:N2:273:ASN:HD22 | 1.32 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:S2:272:ARG:HH11 | 73:S8:303:PEE:H2 | 1.52 | 0.74 |
| 57:S1:149:ASP:HB2 | 58:S2:367:ALA:HB3 | 1.68 | 0.74 |
| 26:B3:27:THR:HG22 | 26:B3:29:LEU:H | 1.53 | 0.74 |
| 35:C1:447:TYR:O | 35:C1:451:ASN:ND2 | 2.21 | 0.73 |
| 20:AK:120:TYR:HH | 76:AK:401:ADP:HO2' | 1.30 | 0.73 |
| 42:N2:88:LYS:HG3 | 42:N2:148:SER:HB3 | 1.68 | 0.73 |
| 1:4L:68:ALA:HB3 | 43:N3:67:LEU:HD11 | 1.69 | 0.73 |
| 66:V2:68:LYS:NZ | 67:V3:407:SER:OG | 2.22 | 0.72 |
| 30:B7:29:TYR:O | 30:B7:104:ARG:NH2 | 2.23 | 0.71 |
| 36:C2:104:TRP:HA | 36:C2:207:MET:HG2 | 1.73 | 0.71 |
| 45:N5:5:ALA:HB2 | 45:N5:61:MET:HE1 | 1.72 | 0.71 |
| 37:C3:129:VAL:HG11 | 37:C3:180:GLU:HG3 | 1.71 | 0.70 |
| 47:Qa:81:HIS:HD2 | 47:Qa:192:CYS:H | 1.37 | 0.70 |
| 57:S1:124:HIS:HD2 | 58:S2:381:MET:HE2 | 1.57 | 0.70 |
| 47:Qa:155:GLN:HE22 | 47:Qa:200:VAL:HB | 1.57 | 0.69 |
| 68:7A:102:CDL:H421 | 73:7C:101:PEE:H31 | 1.74 | 0.69 |
| 49:Qc:138:MET:HG2 | 49:Qc:254:ASP:HB2 | 1.75 | 0.69 |
| 5:6B:9:ILE:HG12 | 5:6B:56:TRP:HB2 | 1.75 | 0.69 |
| 12:A2:24:CYS:N | 12:A2:58:CYS:SG | 2.66 | 0.69 |
| 36:C2:132:GLU:HB3 | 36:C2:137:GLU:HG3 | 1.72 | 0.69 |
| 68:N5:703:CDL:H591 | 68:N5:703:CDL:H642 | 1.75 | 0.69 |
| 57:S1:493:VAL:HG23 | 57:S1:513:MET:HE1 | 1.75 | 0.69 |
| 1:4L:14:ILE:HG12 | 68:4L:201:CDL:H781 | 1.75 | 0.68 |
| 8:7B:53:TRP:HE1 | 38:C4:111:ILE:HG22 | 1.58 | 0.68 |
| 18:A9:188:GLU:HG3 | 18:A9:200:ILE:HD13 | 1.76 | 0.68 |
| 18:A9:212:ARG:NH1 | 18:A9:311:GLU:OE2 | 2.27 | 0.68 |
| 19:AC:114:ASP:OD1 | 32:B9:87:ARG:NH2 | 2.26 | 0.68 |
| 49:QC:246:SER:HB2 | 49:QC:249:LEU:HB2 | 1.75 | 0.68 |
| 20:AK:141:ARG:NH2 | 76:AK:401:ADP:N7 | 2.41 | 0.68 |
| 48:QB:100:GLY:HA2 | 48:QB:106:GLY:H | 1.59 | 0.68 |
| 50:QD:266:GLN:HE22 | 52:Qf:91:LYS:H | 1.42 | 0.68 |
| 57:S1:419:ARG:NH1 | 57:S1:439:THR:O | 2.26 | 0.67 |
| 35:C1:107:PRO:HB3 | 37:C3:25:LEU:HB2 | 1.75 | 0.67 |
| 18:A9:173:ASP:HB3 | 18:A9:176:SER:HB2 | 1.75 | 0.67 |
| 43:N3:37:TYR:OH | 58:S2:93:GLN:NE2 | 2.27 | 0.67 |
| 44:N4:391:ILE:HG23 | 44:N4:394:ILE:HD12 | 1.76 | 0.67 |
| 15:A6:42:SER:HB3 | 60:S4:52:LEU:HB3 | 1.75 | 0.67 |
| 45:N5:100:ILE:HG21 | 45:N5:246:LEU:HB2 | 1.77 | 0.67 |
| 63:S7:188:LYS:HB2 | 63:S7:191:ARG:HB2 | 1.74 | 0.67 |
| 47:Qa:155:GLN:NE2 | 47:Qa:200:VAL:O | 2.27 | 0.67 |
| 51:Qe:190:VAL:HG21 | 51:Qe:250:ARG:HH22 | 1.59 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:A8:301:CDL:H112 | 40:CB:32:ARG:HG2 | 1.76 | 0.67 |
| 33:BK:2:PRO:O | 33:BK:7:LYS:NZ | 2.28 | 0.67 |
| 3:5B:113:CYS:HB3 | 3:5B:118:THR:HG22 | 1.76 | 0.66 |
| 65:V1:40:ARG:NH1 | 65:V1:289:GLU:O | 2.27 | 0.66 |
| 44:N4:371:PRO:HD2 | 68:N5:703:CDL:H391 | 1.77 | 0.66 |
| 41:N1:102:VAL:HG11 | 41:N1:154:LEU:HD11 | 1.76 | 0.66 |
| 41:N1:141:SER:HB2 | 41:N1:289:LEU:HD12 | 1.78 | 0.66 |
| 42:N2:108:LEU:HD11 | 42:N2:191:THR:HG21 | 1.76 | 0.66 |
| 50:Qd:125:CYS:SG | 81:Qd:401:HEC:HAC | 2.35 | 0.66 |
| 13:A3:151:VAL:O | 17:A8:207:LYS:NZ | 2.27 | 0.66 |
| 15:A6:89:VAL:HG22 | 75:AB:201:ZMP:H2 | 1.76 | 0.66 |
| 57:S1:266:ARG:HD2 | 57:S1:267:THR:HG23 | 1.77 | 0.66 |
| 50:QD:280:GLU:OE2 | 50:QD:286:ARG:NH1 | 2.28 | 0.66 |
| 75:AC:201:ZMP:H14 | 32:B9:102:ALA:HB1 | 1.77 | 0.66 |
| 45:N5:126:ILE:HG21 | 68:N5:703:CDL:H621 | 1.77 | 0.66 |
| 51:QK:24:GLY:HA3 | 47:Qa:109:LYS:HE3 | 1.76 | 0.66 |
| 58:S2:300:ARG:NH2 | 58:S2:407:GLU:OE2 | 2.29 | 0.66 |
| 65:V1:235:VAL:HG12 | 65:V1:240:THR:HG21 | 1.78 | 0.66 |
| 12:A2:59:SER:HB2 | 57:S1:655:ARG:HD3 | 1.78 | 0.66 |
| 20:AK:66:GLY:O | 20:AK:163:ARG:NH2 | 2.29 | 0.65 |
| 15:A6:66:TYR:O | 15:A6:86:ARG:NH1 | 2.29 | 0.65 |
| 49:QC:316:MET:HE3 | 73:QC:403:PEE:H11 | 1.79 | 0.65 |
| 57:S1:433:GLY:HA2 | 57:S1:447:ASP:HA | 1.78 | 0.65 |
| 21:AL:140:LYS:O | 42:N2:273:ASN:ND2 | 2.30 | 0.65 |
| 36:C2:89:GLU:O | 36:C2:91:ASN:ND2 | 2.30 | 0.65 |
| 70:6A:101:PC1:H321 | 37:C3:202:GLY:HA3 | 1.77 | 0.65 |
| 27:B4:15:PRO:HG2 | 27:B4:18:LEU:HB2 | 1.78 | 0.65 |
| 52:QF:56:ARG:NH1 | 52:QF:65:GLU:OE2 | 2.29 | 0.65 |
| 72:C1:609:3PE:H372 | 72:C1:609:3PE:H282 | 1.77 | 0.64 |
| 58:S2:374:ARG:NH2 | 64:S8:165:ASP:OD1 | 2.29 | 0.64 |
| 9:7C:42:THR:HG21 | 10:8B:45:VAL:HG12 | 1.79 | 0.64 |
| 18:A9:346:GLU:HG2 | 18:A9:371:PRO:HB3 | 1.80 | 0.64 |
| 2:5A:114:VAL:HG11 | 2:5A:128:VAL:HG11 | 1.79 | 0.64 |
| 65:V1:112:TYR:HB2 | 65:V1:240:THR:HG22 | 1.79 | 0.64 |
| 41:N1:58:LYS:HE2 | 63:S7:125:PRO:HG2 | 1.80 | 0.64 |
| 47:Qa:82:LEU:HD11 | 47:Qa:154:LEU:HB3 | 1.80 | 0.63 |
| 35:C1:51:ASP:O | 35:C1:55:ASN:ND2 | 2.31 | 0.63 |
| 57:S1:250:SER:HB2 | 57:S1:606:THR:HG23 | 1.80 | 0.63 |
| 65:V1:111:LYS:HB2 | 65:V1:151:ALA:HA | 1.78 | 0.63 |
| 4:6A:81:LEU:HB3 | 70:6A:101:PC1:H12 | 1.80 | 0.63 |
| 15:A6:88:LYS:NZ | 15:A6:132:PHE:O | 2.29 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:QC:214:ASP:OD1 | 54:Qh:3:ARG:NH2 | 2.31 | 0.63 |
| 70:6A:101:PC1:H112 | 37:C3:187:THR:HA | 1.81 | 0.63 |
| 6:6C:69:GLY:HA3 | 8:7B:79:GLU:HG3 | 1.78 | 0.63 |
| 35:C1:129:TYR:OH | 35:C1:236:TRP:NE1 | 2.31 | 0.63 |
| 52:Qf:60:ARG:NH1 | 54:Qh:78:TYR:O | 2.31 | 0.63 |
| 57:S1:308:ARG:NH1 | 57:S1:312:GLY:O | 2.31 | 0.63 |
| 33:BK:107:GLN:HE22 | 45:N5:194:ASN:HD22 | 1.46 | 0.63 |
| 41:N1:173:TRP:HB3 | 41:N1:175:ILE:HG22 | 1.80 | 0.63 |
| 22:AM:106:ARG:HB2 | 22:AM:109:ILE:HG13 | 1.81 | 0.63 |
| 44:N4:369:LEU:HD21 | 45:N5:149:ILE:HD13 | 1.81 | 0.63 |
| 59:S3:89:HIS:ND1 | 59:S3:91:ASP:OD1 | 2.26 | 0.62 |
| 15:A6:78:LEU:HD22 | 15:A6:130:MET:HE3 | 1.81 | 0.62 |
| 38:C4:41:ARG:NH1 | 38:C4:43:ASP:OD1 | 2.32 | 0.62 |
| 47:QA:121:TYR:HB3 | 47:QA:137:LEU:HD11 | 1.81 | 0.62 |
| 47:Qa:81:HIS:CD2 | 47:Qa:192:CYS:H | 2.17 | 0.62 |
| 59:S3:187:ILE:HG23 | 59:S3:188:LEU:HG | 1.80 | 0.62 |
| 65:V1:94:PRO:HB2 | 65:V1:97:LEU:HB2 | 1.82 | 0.62 |
| 18:A9:61:ALA:HB3 | 18:A9:82:VAL:HG13 | 1.82 | 0.62 |
| 29:B6:85:ASP:OD2 | 32:B9:167:TRP:NE1 | 2.27 | 0.62 |
| 70:C1:605:PC1:H241 | 70:C3:301:PC1:H241 | 1.82 | 0.62 |
| 58:S2:61:THR:H | 58:S2:64:THR:HG1 | 1.47 | 0.62 |
| 36:C2:116:LEU:HD11 | 36:C2:226:MET:HB3 | 1.81 | 0.62 |
| 59:S3:83:GLU:OE1 | 59:S3:142:ARG:NH2 | 2.30 | 0.62 |
| 37:C3:178:ALA:HB2 | 70:C3:306:PC1:H2B2 | 1.81 | 0.62 |
| 45:N5:295:GLN:O | 45:N5:425:ARG:NH1 | 2.33 | 0.62 |
| 57:S1:246:ARG:HH22 | 60:S4:123:ASN:HD21 | 1.48 | 0.62 |
| 60:S4:109:ASN:ND2 | 60:S4:111:LEU:O | 2.33 | 0.62 |
| 35:C1:27:GLY:HA3 | 77:C1:601:HEA:H273 | 1.82 | 0.61 |
| 58:S2:90:PHE:HB3 | 58:S2:103:LEU:HB3 | 1.82 | 0.61 |
| 30:B7:92:HIS:ND1 | 45:N5:481:THR:OG1 | 2.29 | 0.61 |
| 44:N4:87:GLU:O | 44:N4:92:LYS:NZ | 2.28 | 0.61 |
| 47:Qa:84:ARG:NH1 | 47:Qa:114:SER:OG | 2.32 | 0.61 |
| 18:A9:87:GLU:HG3 | 18:A9:89:TYR:H | 1.65 | 0.61 |
| 36:C2:173:ASP:O | 36:C2:180:ASN:ND2 | 2.32 | 0.61 |
| 58:S2:155:GLN:NE2 | 58:S2:315:ASP:OD2 | 2.28 | 0.61 |
| 65:V1:110:PRO:HB3 | 65:V1:152:ARG:HD3 | 1.81 | 0.61 |
| 24:B1:57:TRP:NE1 | 28:B5:134:GLU:OE1 | 2.25 | 0.61 |
| 47:Qa:70:ARG:HD2 | 47:Qa:117:GLU:HG2 | 1.83 | 0.61 |
| 58:S2:188:ASN:OD1 | 58:S2:410:LYS:NZ | 2.29 | 0.61 |
| 41:N1:87:VAL:HG11 | 43:N3:6:THR:HG21 | 1.80 | 0.61 |
| 48:QB:411:GLU:OE2 | 48:QB:415:ARG:NH2 | 2.33 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 64:S8:63:TRP:HE1 | 73:S8:303:PEE:H13 | 1.64 | 0.61 |
| 65:V1:109:ARG:NH1 | 65:V1:237:GLY:O | 2.33 | 0.61 |
| 3:5B:89:VAL:HG22 | 35:C1:510:TYR:HB3 | 1.83 | 0.61 |
| 9:7C:62:LYS:NZ | 35:C1:117:MET:O | 2.33 | 0.61 |
| 43:N3:68:GLU:HG3 | 43:N3:98:LEU:HD13 | 1.82 | 0.61 |
| 49:Qc:137:GLN:NE2 | 49:Qc:263:ASN:O | 2.33 | 0.61 |
| 57:S1:161:GLU:OE2 | 66:V2:42:ARG:NH1 | 2.33 | 0.61 |
| 49:Qc:284:ILE:HD11 | 70:Qc:405:PC1:H241 | 1.83 | 0.61 |
| 58:S2:222:ARG:NH1 | 58:S2:249:ASP:OD2 | 2.23 | 0.61 |
| 66:V2:38:LEU:O | 66:V2:124:ARG:NH2 | 2.34 | 0.61 |
| 66:V2:108:PRO:HB2 | 66:V2:111:ARG:HG2 | 1.82 | 0.61 |
| 1:4L:31:LEU:HD21 | 46:N6:67:VAL:HG11 | 1.81 | 0.61 |
| 34:BL:95:PHE:O | 34:BL:99:LEU:HB2 | 2.01 | 0.61 |
| 35:C1:51:ASP:OD1 | 35:C1:55:ASN:ND2 | 2.34 | 0.61 |
| 48:QB:374:GLY:HA3 | 70:QB:503:PC1:H151 | 1.83 | 0.61 |
| 49:QC:233:LEU:HG | 50:QD:297:MET:HE1 | 1.83 | 0.61 |
| 41:N1:99:ASN:N | 70:N1:402:PC1:O12 | 2.26 | 0.60 |
| 41:N1:103:LEU:HD13 | 46:N6:55:MET:HE3 | 1.83 | 0.60 |
| 50:Qd:147:LYS:NZ | 50:Qd:151:GLU:OE2 | 2.34 | 0.60 |
| 22:AM:34:ARG:NH2 | 64:S8:89:GLU:OE2 | 2.34 | 0.60 |
| 43:N3:70:ALA:HB2 | 46:N6:59:ILE:HD11 | 1.82 | 0.60 |
| 49:QC:71:ARG:NH2 | 50:QD:278:ALA:O | 2.34 | 0.60 |
| 35:C1:155:VAL:HG11 | 70:C1:610:PC1:H3B1 | 1.83 | 0.60 |
| 35:C1:169:ILE:O | 35:C1:172:LYS:NZ | 2.34 | 0.60 |
| 51:QE:177:ARG:HH12 | 51:QE:233:GLY:HA2 | 1.65 | 0.60 |
| 49:Qc:100:ARG:NH2 | 80:Qc:403:HEM:O1A | 2.34 | 0.60 |
| 51:Qe:204:ARG:NH2 | 51:Qe:258:LEU:O | 2.27 | 0.60 |
| 65:V1:52:ARG:HH21 | 67:V3:390:GLN:HG2 | 1.66 | 0.60 |
| 65:V1:263:ALA:HA | 65:V1:271:SER:HB3 | 1.84 | 0.60 |
| 48:Qb:121:ASN:ND2 | 48:Qb:132:TYR:OH | 2.35 | 0.60 |
| 70:C1:608:PC1:H391 | 70:C1:608:PC1:H2A2 | 1.84 | 0.60 |
| 9:7C:59:GLN:NE2 | 35:C1:116:SER:O | 2.34 | 0.60 |
| 37:C3:220:LEU:HG | 68:C3:304:CDL:H751 | 1.84 | 0.60 |
| 5:6B:66:PRO:HD3 | 36:C2:179:LEU:HD11 | 1.84 | 0.60 |
| 41:N1:34:ARG:HG2 | 63:S7:82:PRO:HA | 1.83 | 0.60 |
| 51:QE:207:LYS:HE3 | 51:QE:210:TRP:HD1 | 1.66 | 0.60 |
| 3:5B:43:GLN:NE2 | 37:C3:225:PHE:O | 2.27 | 0.60 |
| 66:V2:187:GLN:HE21 | 66:V2:190:ASP:HA | 1.66 | 0.60 |
| 1:4L:65:VAL:HA | 43:N3:67:LEU:HD22 | 1.84 | 0.59 |
| 44:N4:403:THR:HA | 44:N4:406:TYR:CE2 | 2.37 | 0.59 |
| 47:QA:399:GLN:HA | 47:QA:402:VAL:HG22 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:6B:7:THR:O | 5:6B:11:ASN:ND2 | 2.35 | 0.59 |
| 12:A2:89:ARG:O | 12:A2:93:ASN:ND2 | 2.35 | 0.59 |
| 29:B6:132:VAL:O | 29:B6:136:LEU:HB3 | 2.02 | 0.59 |
| 72:7A:101:3PE:H292 | 45:N5:484:LEU:HD23 | 1.83 | 0.59 |
| 51:Qe:187:GLU:OE1 | 51:Qe:248:ARG:NH2 | 2.35 | 0.59 |
| 73:7C:101:PEE:H38 | 35:C1:22:PHE:HD1 | 1.67 | 0.59 |
| 19:AB:116:VAL:HG12 | 19:AB:120:MET:HE2 | 1.84 | 0.59 |
| 70:N3:202:PC1:H151 | 72:S7:204:3PE:H31 | 1.84 | 0.59 |
| 50:QD:216:LEU:HB3 | 50:QD:249:ILE:HD11 | 1.84 | 0.59 |
| 51:QE:234:TYR:HB2 | 51:QE:243:TYR:HB2 | 1.84 | 0.59 |
| 48:Qb:276:ARG:NH2 | 48:Qb:466:PRO:O | 2.35 | 0.59 |
| 20:AK:109:GLN:OE1 | 20:AK:328:ARG:NH1 | 2.34 | 0.59 |
| 42:N2:42:PRO:HG2 | 46:N6:167:VAL:HG22 | 1.84 | 0.59 |
| 42:N2:289:ASN:HA | 42:N2:292:PHE:CE2 | 2.38 | 0.59 |
| 44:N4:231:LEU:HD23 | 44:N4:235:LEU:HD12 | 1.85 | 0.59 |
| 57:S1:69:LEU:O | 60:S4:158:LYS:NZ | 2.32 | 0.59 |
| 66:V2:85:LEU:HD13 | 67:V3:400:LEU:HD22 | 1.83 | 0.59 |
| 35:C1:347:LEU:HD13 | 35:C1:383:MET:HB3 | 1.83 | 0.59 |
| 44:N4:447:LEU:HD11 | 71:N4:502:PLX:H381 | 1.85 | 0.59 |
| 47:QA:84:ARG:NH2 | 47:QA:190:LEU:O | 2.33 | 0.59 |
| 44:N4:445:LEU:HD22 | 68:N5:703:CDL:H401 | 1.84 | 0.59 |
| 33:BK:60:ARG:NH1 | 33:BK:62:TYR:OH | 2.35 | 0.59 |
| 68:C3:304:CDL:H231 | 68:C3:304:CDL:H352 | 1.84 | 0.59 |
| 35:C1:254:ILE:HD12 | 35:C1:341:ALA:HA | 1.85 | 0.58 |
| 58:S2:162:GLU:OE2 | 58:S2:177:ARG:NH2 | 2.34 | 0.58 |
| 64:S8:205:ILE:O | 64:S8:209:TYR:HB3 | 2.02 | 0.58 |
| 48:QB:165:ARG:NH1 | 48:QB:208:VAL:O | 2.36 | 0.58 |
| 49:Qc:119:LEU:HD13 | 80:Qc:403:HEM:HBB2 | 1.85 | 0.58 |
| 57:S1:405:THR:HB | 57:S1:477:GLY:HA3 | 1.84 | 0.58 |
| 65:V1:296:LEU:HD21 | 65:V1:317:VAL:HG11 | 1.85 | 0.58 |
| 34:BL:150:PRO:HG3 | 40:CB:115:LEU:HD22 | 1.85 | 0.58 |
| 35:C1:406:ASN:ND2 | 70:C1:608:PC1:O14 | 2.36 | 0.58 |
| 57:S1:488:ALA:HB2 | 57:S1:677:GLN:HG3 | 1.85 | 0.58 |
| 57:S1:666:GLN:NE2 | 57:S1:670:GLU:OE2 | 2.36 | 0.58 |
| 25:B2:57:ARG:NH1 | 25:B2:61:PHE:O | 2.36 | 0.58 |
| 50:QD:105:SER:OG | 55:Qi:44:TYR:OH | 2.21 | 0.58 |
| 54:QH:37:ASN:ND2 | 68:QH:102:CDL:OB4 | 2.35 | 0.58 |
| 65:V1:118:ASP:HB3 | 65:V1:207:GLY:HA2 | 1.85 | 0.58 |
| 10:8B:36:PRO:HB3 | 70:C1:608:PC1:H261 | 1.84 | 0.58 |
| 53:QG:36:ASP:OD1 | 53:QG:90:TYR:OH | 2.16 | 0.58 |
| 58:S2:308:LEU:HB2 | 58:S2:407:GLU:HB2 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 63:S7:85:ASP:HB3 | 63:S7:88:ARG:HB3 | 1.86 | 0.58 |
| 65:V1:338:ASP:OD1 | 65:V1:339:PHE:N | 2.37 | 0.58 |
| 21:AL:140:LYS:H | 42:N2:273:ASN:ND2 | 2.01 | 0.58 |
| 37:C3:204:HIS:CE1 | 37:C3:249:TRP:HB2 | 2.39 | 0.58 |
| 49:QC:207:ASN:OD1 | 49:QC:209:THR:OG1 | 2.21 | 0.58 |
| 57:S1:198:THR:HG21 | 57:S1:209:TYR:HB2 | 1.85 | 0.58 |
| 42:N2:170:LEU:HD11 | 42:N2:288:LEU:HD22 | 1.86 | 0.57 |
| 48:QB:195:THR:HG21 | 48:QB:269:ARG:H | 1.68 | 0.57 |
| 44:N4:392:THR:O | 44:N4:396:MET:HG2 | 2.04 | 0.57 |
| 48:QB:478:LEU:HB3 | 68:QB:501:CDL:H522 | 1.86 | 0.57 |
| 49:QC:236:MET:HE3 | 71:Qi:301:PLX:H202 | 1.86 | 0.57 |
| 57:S1:534:VAL:HG22 | 57:S1:537:ILE:HB | 1.85 | 0.57 |
| 18:A9:279:TYR:HB2 | 18:A9:372:ALA:HB2 | 1.86 | 0.57 |
| 45:N5:249:SER:HA | 45:N5:306:THR:HG21 | 1.85 | 0.57 |
| 47:QA:151:VAL:O | 47:QA:155:GLN:HG2 | 2.05 | 0.57 |
| 48:QB:301:ASN:ND2 | 48:QB:347:CYS:SG | 2.78 | 0.57 |
| 57:S1:282:ASN:ND2 | 57:S1:285:TRP:O | 2.37 | 0.57 |
| 45:N5:362:LEU:HA | 45:N5:365:ALA:HB3 | 1.85 | 0.57 |
| 68:N5:703:CDL:H541 | 68:N5:703:CDL:HA4 | 1.86 | 0.57 |
| 48:QB:113:VAL:HG12 | 48:QB:146:LEU:HD13 | 1.85 | 0.57 |
| 50:QD:104:SER:HA | 55:Qi:48:ASN:HD21 | 1.68 | 0.57 |
| 71:QI:301:PLX:H341 | 56:QJ:31:GLY:HA3 | 1.85 | 0.57 |
| 65:V1:113:LEU:O | 65:V1:154:ALA:HA | 2.05 | 0.57 |
| 14:A5:48:THR:HA | 14:A5:51:ILE:HG12 | 1.86 | 0.57 |
| 40:CB:52:ARG:NH1 | 42:N2:318:GLU:OE1 | 2.37 | 0.57 |
| 44:N4:383:THR:HG21 | 45:N5:190:LEU:HD22 | 1.86 | 0.57 |
| 70:6A:101:PC1:H142 | 37:C3:181:TYR:O | 2.05 | 0.57 |
| 47:Qa:151:VAL:O | 47:Qa:155:GLN:HG2 | 2.05 | 0.57 |
| 48:Qb:360:CYS:SG | 48:Qb:368:MET:HG3 | 2.45 | 0.57 |
| 60:S4:75:ARG:NH1 | 60:S4:119:ASP:OD1 | 2.35 | 0.57 |
| 11:A1:46:ASN:ND2 | 46:N6:132:ASP:OD2 | 2.38 | 0.57 |
| 15:A6:81:SER:OG | 18:A9:367:GLU:OE2 | 2.22 | 0.57 |
| 48:QB:121:ASN:ND2 | 48:QB:132:TYR:OH | 2.38 | 0.57 |
| 50:Qd:118:TYR:HA | 50:Qd:122:CYS:SG | 2.45 | 0.57 |
| 65:V1:112:TYR:O | 65:V1:240:THR:HA | 2.05 | 0.57 |
| 7:7A:66:TYR:HE1 | 72:7A:101:3PE:H2A2 | 1.68 | 0.57 |
| 41:N1:197:PRO:HB2 | 41:N1:280:PHE:HD1 | 1.70 | 0.57 |
| 73:N4:501:PEE:H46 | 73:S2:501:PEE:H37 | 1.87 | 0.57 |
| 53:Qg:14:LEU:HD12 | 53:Qg:17:ILE:HD11 | 1.86 | 0.57 |
| 66:V2:182:ASN:HB3 | 66:V2:194:GLU:HB3 | 1.86 | 0.57 |
| 44:N4:445:LEU:HB3 | 68:N5:703:CDL:H452 | 1.85 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:N5:419:THR:HA | 45:N5:422:TYR:CE2 | 2.40 | 0.56 |
| 49:Qc:285:PRO:HG2 | 70:Qc:405:PC1:H3E2 | 1.87 | 0.56 |
| 63:S7:86:MET:HB2 | 63:S7:91:VAL:HB | 1.87 | 0.56 |
| 3:5B:105:VAL:HA | 3:5B:111:GLN:HG3 | 1.87 | 0.56 |
| 37:C3:58:TRP:HD1 | 37:C3:61:ILE:HD12 | 1.70 | 0.56 |
| 38:C4:90:PHE:HA | 38:C4:93:MET:HG2 | 1.87 | 0.56 |
| 73:N5:701:PEE:H36 | 68:N5:703:CDL:H231 | 1.87 | 0.56 |
| 51:Qe:196:ARG:NH1 | 51:Qe:254:ALA:O | 2.39 | 0.56 |
| 58:S2:140:PRO:HB2 | 63:S7:142:TYR:CE2 | 2.40 | 0.56 |
| 58:S2:464:PHE:HA | 58:S2:467:VAL:HB | 1.86 | 0.56 |
| 60:S4:112:MET:HG3 | 64:S8:184:LEU:HD23 | 1.87 | 0.56 |
| 63:S7:66:THR:HG22 | 85:S7:201:U10:H3M2 | 1.87 | 0.56 |
| 9:7C:31:VAL:HG13 | 9:7C:37:LEU:HD22 | 1.87 | 0.56 |
| 17:A8:146:ASP:OD1 | 17:A8:149:ARG:NH2 | 2.38 | 0.56 |
| 22:AM:88:ARG:HD3 | 64:S8:200:GLU:HG3 | 1.86 | 0.56 |
| 70:N1:402:PC1:H112 | 70:N1:402:PC1:H32 | 1.87 | 0.56 |
| 51:QE:160:PRO:HD2 | 51:QE:163:LYS:HG2 | 1.87 | 0.56 |
| 47:Qa:91:THR:HG21 | 47:Qa:140:VAL:HA | 1.86 | 0.56 |
| 30:B7:29:TYR:OH | 30:B7:111:ARG:NH2 | 2.36 | 0.56 |
| 42:N2:112:HIS:O | 42:N2:116:PRO:HD2 | 2.05 | 0.56 |
| 42:N2:131:LEU:O | 42:N2:135:LYS:HG2 | 2.06 | 0.56 |
| 44:N4:211:GLY:H | 44:N4:213:HIS:HD2 | 1.52 | 0.56 |
| 57:S1:49:VAL:HG13 | 57:S1:102:ILE:HD13 | 1.87 | 0.56 |
| 58:S2:140:PRO:HA | 58:S2:143:ASP:HB2 | 1.88 | 0.56 |
| 59:S3:128:ILE:HB | 59:S3:145:THR:HG23 | 1.87 | 0.56 |
| 51:QK:1:MET:O | 51:QK:7:ARG:NH1 | 2.38 | 0.56 |
| 51:Qe:244:ASP:OD2 | 51:Qe:250:ARG:NH2 | 2.39 | 0.56 |
| 29:B6:165:PHE:O | 29:B6:168:ASP:HB2 | 2.05 | 0.56 |
| 68:N1:401:CDL:H791 | 46:N6:16:GLY:HA2 | 1.88 | 0.56 |
| 47:QA:148:ARG:NH2 | 53:QG:50:ARG:O | 2.38 | 0.56 |
| 47:Qa:320:PRO:HG2 | 47:Qa:343:GLN:HE21 | 1.71 | 0.56 |
| 48:Qb:366:ASP:H | 48:Qb:464:GLN:HE21 | 1.53 | 0.56 |
| 52:Qf:38:GLU:OE2 | 52:Qf:78:ARG:NH1 | 2.39 | 0.56 |
| 23:AN:51:MET:HE2 | 41:N1:311:THR:HB | 1.87 | 0.56 |
| 33:BK:114:GLN:HG3 | 45:N5:203:MET:HG2 | 1.87 | 0.56 |
| 55:QI:48:ASN:HD21 | 50:Qd:104:SER:HA | 1.71 | 0.56 |
| 57:S1:389:THR:OG1 | 57:S1:511:LYS:O | 2.23 | 0.56 |
| 42:N2:142:LEU:HB3 | 42:N2:194:LEU:HD21 | 1.87 | 0.56 |
| 57:S1:433:GLY:O | 57:S1:444:HIS:NE2 | 2.34 | 0.56 |
| 35:C1:358:LEU:HB3 | 77:C1:602:HEA:HMA | 1.87 | 0.56 |
| 4:6A:82:PHE:O | 70:6A:101:PC1:H143 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:A8:301:CDL:H572 | 68:A8:301:CDL:H532 | 1.88 | 0.55 |
| 68:A8:301:CDL:H782 | 72:CB:202:3PE:H281 | 1.87 | 0.55 |
| 36:C2:151:ARG:HG3 | 36:C2:181:GLN:HG3 | 1.89 | 0.55 |
| 48:QB:80:ARG:NH2 | 48:QB:350:GLU:OE1 | 2.39 | 0.55 |
| 47:Qa:164:VAL:HG21 | 48:Qb:317:THR:HG21 | 1.88 | 0.55 |
| 57:S1:163:LYS:O | 57:S1:171:THR:OG1 | 2.25 | 0.55 |
| 23:AN:144:THR:HB | 41:N1:96:ILE:HG23 | 1.89 | 0.55 |
| 36:C2:189:PRO:HA | 36:C2:213:LEU:HB2 | 1.87 | 0.55 |
| 47:Qa:260:ASP:OD2 | 47:Qa:262:ASN:ND2 | 2.39 | 0.55 |
| 35:C1:197:LEU:HA | 37:C3:92:LEU:HD13 | 1.88 | 0.55 |
| 35:C1:383:MET:HE3 | 35:C1:421:VAL:HG23 | 1.89 | 0.55 |
| 49:Qc:353:LEU:HD12 | 72:Qc:404:3PE:H351 | 1.88 | 0.55 |
| 51:Qe:239:HIS:HB2 | 82:Qe:303:FES:S2 | 2.46 | 0.55 |
| 64:S8:47:SER:O | 64:S8:56:ARG:NH2 | 2.40 | 0.55 |
| 64:S8:100:GLU:OE1 | 64:S8:172:ASN:ND2 | 2.37 | 0.55 |
| 57:S1:191:GLY:HA3 | 57:S1:439:THR:HB | 1.89 | 0.55 |
| 6:6C:60:LYS:NZ | 6:6C:64:GLU:OE2 | 2.30 | 0.55 |
| 45:N5:6:SER:O | 45:N5:10:THR:OG1 | 2.19 | 0.55 |
| 45:N5:331:MET:HB3 | 45:N5:387:THR:HG22 | 1.89 | 0.55 |
| 54:Qh:49:VAL:HG12 | 70:Qh:101:PC1:H131 | 1.88 | 0.55 |
| 57:S1:688:GLN:HE21 | 57:S1:694:PHE:HA | 1.71 | 0.55 |
| 12:A2:65:LEU:HD11 | 12:A2:91:LEU:HD13 | 1.89 | 0.55 |
| 35:C1:264:LYS:NZ | 35:C1:326:THR:O | 2.36 | 0.55 |
| 50:Qd:211:TYR:OH | 81:Qd:401:HEC:O1A | 2.15 | 0.55 |
| 63:S7:62:LEU:O | 63:S7:91:VAL:HA | 2.06 | 0.55 |
| 37:C3:16:TRP:NE1 | 37:C3:60:ASP:OD2 | 2.35 | 0.55 |
| 42:N2:36:ASN:OD1 | 42:N2:134:GLN:NE2 | 2.29 | 0.55 |
| 49:QC:197:LEU:HD11 | 80:QC:402:HEM:HMA3 | 1.89 | 0.55 |
| 48:Qb:274:GLU:HG3 | 48:Qb:456:VAL:HB | 1.88 | 0.55 |
| 58:S2:101:LEU:HB2 | 58:S2:464:PHE:CZ | 2.42 | 0.55 |
| 63:S7:55:ASN:ND2 | 63:S7:187:GLU:O | 2.35 | 0.55 |
| 20:AK:82:LYS:HZ2 | 20:AK:268:ALA:HB3 | 1.72 | 0.55 |
| 50:QD:228:LEU:HD11 | 50:QD:234:PHE:HB2 | 1.89 | 0.55 |
| 58:S2:146:ASP:OD2 | 58:S2:149:SER:OG | 2.24 | 0.54 |
| 65:V1:295:PRO:HG2 | 65:V1:298:GLU:HB2 | 1.90 | 0.54 |
| 41:N1:123:SER:HB3 | 41:N1:214:GLU:HG3 | 1.89 | 0.54 |
| 49:QC:362:ILE:HG23 | 49:QC:366:MET:HE2 | 1.87 | 0.54 |
| 57:S1:484:SER:HB2 | 57:S1:680:LEU:HD11 | 1.88 | 0.54 |
| 18:A9:212:ARG:O | 18:A9:216:TYR:N | 2.32 | 0.54 |
| 22:AM:78:ASP:OD1 | 22:AM:78:ASP:N | 2.37 | 0.54 |
| 41:N1:134:ARG:NH2 | 58:S2:110:GLU:OE2 | 2.36 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:5B:46:GLY:HA3 | 37:C3:69:GLY:HA3 | 1.88 | 0.54 |
| 5:6B:24:GLN:OE1 | 35:C1:302:ARG:NH1 | 2.41 | 0.54 |
| 35:C1:508:PRO:HG3 | 37:C3:6:HIS:HB3 | 1.88 | 0.54 |
| 47:QA:233:VAL:HG22 | 47:QA:236:ARG:HH12 | 1.72 | 0.54 |
| 48:Qb:422:ARG:NH2 | 48:Qb:428:GLU:OE1 | 2.39 | 0.54 |
| 49:Qc:332:LEU:HD11 | 73:Qc:401:PEE:H44 | 1.90 | 0.54 |
| 57:S1:340:ALA:HB3 | 57:S1:366:LEU:HD23 | 1.90 | 0.54 |
| 58:S2:137:GLN:O | 63:S7:142:TYR:OH | 2.26 | 0.54 |
| 14:A5:44:TYR:O | 14:A5:48:THR:HG22 | 2.08 | 0.54 |
| 48:Qb:388:VAL:HG21 | 48:Qb:438:ALA:HA | 1.88 | 0.54 |
| 50:Qd:122:CYS:SG | 81:Qd:401:HEC:HAB | 2.47 | 0.54 |
| 19:AB:82:ARG:HH21 | 19:AB:125:GLU:HG3 | 1.72 | 0.54 |
| 41:N1:31:MET:HG2 | 64:S8:77:LEU:HB2 | 1.90 | 0.54 |
| 51:QE:187:GLU:OE1 | 51:QE:248:ARG:NH2 | 2.40 | 0.54 |
| 20:AK:145:TYR:OH | 20:AK:201:LEU:O | 2.18 | 0.54 |
| 22:AM:55:PHE:CZ | 22:AM:58:ARG:HG3 | 2.43 | 0.54 |
| 54:QH:37:ASN:OD1 | 54:QH:40:ARG:NH2 | 2.36 | 0.54 |
| 57:S1:593:SER:HA | 57:S1:606:THR:O | 2.07 | 0.54 |
| 36:C2:104:TRP:CG | 36:C2:203:ASN:HB2 | 2.42 | 0.54 |
| 68:Qb:501:CDL:HA32 | 70:Qb:502:PC1:H151 | 1.89 | 0.54 |
| 50:Qd:293:MET:HA | 73:Qc:302:PEE:H49 | 1.90 | 0.54 |
| 64:S8:63:TRP:HB3 | 64:S8:66:LEU:HD12 | 1.89 | 0.54 |
| 18:A9:206:ILE:HG13 | 74:A9:401:NDP:H42N | 1.90 | 0.54 |
| 20:AK:210:ASP:OD1 | 20:AK:244:LYS:NZ | 2.32 | 0.54 |
| 59:S3:132:LEU:HB2 | 59:S3:141:ILE:HG22 | 1.90 | 0.54 |
| 8:7B:71:ARG:HG3 | 8:7B:72:VAL:HG23 | 1.89 | 0.53 |
| 35:C1:374:VAL:HA | 35:C1:377:PHE:CE2 | 2.42 | 0.53 |
| 63:S7:69:LEU:HB2 | 63:S7:107:GLY:HA3 | 1.89 | 0.53 |
| 35:C1:299:VAL:HG23 | 36:C2:84:LEU:HG | 1.90 | 0.53 |
| 41:N1:288:LEU:HD11 | 73:S8:303:PEE:H8 | 1.88 | 0.53 |
| 58:S2:430:ILE:HB | 58:S2:469:ARG:HD2 | 1.90 | 0.53 |
| 45:N5:400:ASN:HB3 | 45:N5:486:MET:HE3 | 1.90 | 0.53 |
| 38:C4:115:ALA:HA | 38:C4:118:LEU:HD12 | 1.90 | 0.53 |
| 48:QB:476:PHE:O | 73:QB:502:PEE:N | 2.41 | 0.53 |
| 58:S2:214:GLU:OE2 | 58:S2:227:ARG:NH2 | 2.41 | 0.53 |
| 28:B5:163:ARG:NH1 | 40:CB:102:ASP:OD2 | 2.29 | 0.53 |
| 32:B9:143:GLU:O | 32:B9:164:ARG:NH2 | 2.42 | 0.53 |
| 17:A8:219:TYR:OH | 28:B5:189:ASN:ND2 | 2.35 | 0.53 |
| 34:BL:129:ARG:NH1 | 34:BL:136:LEU:O | 2.33 | 0.53 |
| 35:C1:130:PRO:HG3 | 35:C1:209:LEU:HD13 | 1.91 | 0.53 |
| 47:QA:60:ARG:NH1 | 47:QA:124:GLU:OE1 | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:QA:70:ARG:HD2 | 47:QA:117:GLU:HG2 | 1.91 | 0.53 |
| 50:QD:120:GLN:HB2 | 50:QD:254:LEU:HD11 | 1.89 | 0.53 |
| 49:QC:8:HIS:HB3 | 49:QC:11:MET:HB2 | 1.90 | 0.53 |
| 70:Qb:502:PC1:H2A2 | 73:Qe:301:PEE:H76 | 1.90 | 0.53 |
| 37:C3:126:PRO:HB3 | 37:C3:257:TYR:HB3 | 1.91 | 0.53 |
| 45:N5:421:ALA:O | 45:N5:424:THR:OG1 | 2.26 | 0.53 |
| 48:QB:165:ARG:HD3 | 48:QB:209:ARG:HA | 1.91 | 0.53 |
| 19:AC:105:MET:HE3 | 19:AC:139:MET:HE1 | 1.89 | 0.53 |
| 34:BL:89:VAL:HG21 | 44:N4:25:ILE:HG23 | 1.90 | 0.53 |
| 35:C1:173:PRO:HD2 | 35:C1:176:MET:HE2 | 1.90 | 0.53 |
| 37:C3:226:HIS:HE1 | 70:C3:303:PC1:H3A1 | 1.72 | 0.53 |
| 38:C4:155:GLY:H | 38:C4:158:ALA:HB3 | 1.74 | 0.53 |
| 68:CB:203:CDL:H422 | 68:CB:203:CDL:H812 | 1.90 | 0.53 |
| 48:QB:79:SER:OG | 48:QB:201:VAL:HA | 2.09 | 0.53 |
| 80:QC:401:HEM:HMC1 | 80:QC:401:HEM:HBC2 | 1.91 | 0.53 |
| 47:Qa:68:GLY:O | 47:Qa:208:TYR:OH | 2.27 | 0.53 |
| 4:6A:68:ARG:NH1 | 37:C3:189:SER:OG | 2.42 | 0.53 |
| 29:B6:85:ASP:O | 32:B9:163:LYS:NZ | 2.42 | 0.53 |
| 36:C2:161:HIS:HB2 | 36:C2:174:ALA:HB3 | 1.91 | 0.53 |
| 45:N5:103:PHE:HB2 | 45:N5:341:MET:HE3 | 1.91 | 0.53 |
| 47:Qa:155:GLN:HB3 | 47:Qa:198:GLY:HA2 | 1.90 | 0.53 |
| 48:Qb:103:ASN:ND2 | 48:Qb:149:ASP:OD2 | 2.40 | 0.53 |
| 7:7A:77:PRO:HG3 | 9:7C:62:LYS:HG3 | 1.90 | 0.52 |
| 1:4L:37:MET:HG2 | 1:4L:67:ALA:CB | 2.37 | 0.52 |
| 1:4L:75:LEU:O | 1:4L:79:VAL:HG13 | 2.10 | 0.52 |
| 41:N1:139:THR:HA | 41:N1:142:TYR:CE2 | 2.44 | 0.52 |
| 43:N3:66:ASP:O | 43:N3:69:ILE:HG13 | 2.09 | 0.52 |
| 16:A7:14:TRP:O | 23:AN:28:ARG:NH1 | 2.42 | 0.52 |
| 50:QD:211:TYR:OH | 81:QD:401:HEC:O2A | 2.19 | 0.52 |
| 57:S1:104:THR:O | 57:S1:113:ARG:NH2 | 2.41 | 0.52 |
| 65:V1:281:HIS:ND1 | 65:V1:358:ASP:OD1 | 2.42 | 0.52 |
| 3:5B:106:HIS:NE2 | 38:C4:34:ALA:O | 2.31 | 0.52 |
| 35:C1:86:MET:HB3 | 35:C1:182:PRO:HG2 | 1.90 | 0.52 |
| 36:C2:30:ILE:HD13 | 36:C2:76:ILE:HG12 | 1.92 | 0.52 |
| 41:N1:174:MET:HB2 | 41:N1:242:PHE:HA | 1.91 | 0.52 |
| 51:QE:209:GLU:HG3 | 51:QE:210:TRP:CD1 | 2.44 | 0.52 |
| 29:B6:89:SER:HB2 | 29:B6:92:GLU:HB2 | 1.90 | 0.52 |
| 29:B6:143:HIS:CD2 | 33:BK:45:VAL:HG21 | 2.44 | 0.52 |
| 47:QA:61:ILE:HG12 | 47:QA:130:ILE:HD11 | 1.92 | 0.52 |
| 4:6A:83:HIS:HA | 70:6A:101:PC1:H132 | 1.90 | 0.52 |
| 30:B7:96:VAL:HA | 30:B7:99:MET:HE3 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:S1:452:LEU:HD21 | 57:S1:493:VAL:HG13 | 1.92 | 0.52 |
| 68:4L:201:CDL:H181 | 45:N5:589:LEU:HD11 | 1.91 | 0.52 |
| 3:5B:112:ARG:HA | 3:5B:118:THR:O | 2.09 | 0.52 |
| 28:B5:83:ALA:HA | 68:B5:201:CDL:H162 | 1.90 | 0.52 |
| 36:C2:109:GLU:HG2 | 36:C2:117:THR:HG23 | 1.92 | 0.52 |
| 43:N3:79:SER:HA | 43:N3:87:MET:HE2 | 1.91 | 0.52 |
| 44:N4:318:ALA:HB2 | 44:N4:373:ILE:HG13 | 1.92 | 0.52 |
| 46:N6:86:ASN:HD22 | 46:N6:89:VAL:HG23 | 1.74 | 0.52 |
| 57:S1:347:ASP:OD1 | 57:S1:347:ASP:N | 2.43 | 0.52 |
| 65:V1:311:TRP:NE1 | 65:V1:333:GLU:OE1 | 2.38 | 0.52 |
| 10:8B:43:LEU:HD12 | 70:C1:608:PC1:H2B1 | 1.91 | 0.52 |
| 77:C1:602:HEA:HHC | 77:C1:602:HEA:H122 | 1.91 | 0.52 |
| 45:N5:248:HIS:O | 45:N5:253:VAL:HG22 | 2.10 | 0.52 |
| 47:QA:323:VAL:HG23 | 47:QA:340:THR:HG22 | 1.91 | 0.52 |
| 48:QB:107:SER:HA | 48:QB:110:GLU:HG2 | 1.90 | 0.52 |
| 72:QJ:101:3PE:H322 | 73:Qe:301:PEE:H49 | 1.92 | 0.52 |
| 17:A8:107:HIS:HB3 | 17:A8:197:PRO:HD2 | 1.92 | 0.52 |
| 29:B6:140:TRP:HD1 | 33:BK:41:VAL:HG13 | 1.75 | 0.52 |
| 41:N1:231:ILE:O | 41:N1:235:ASN:ND2 | 2.42 | 0.52 |
| 73:N4:501:PEE:H53 | 73:N4:501:PEE:H24 | 1.92 | 0.52 |
| 50:QD:322:TYR:CE2 | 50:QD:324:PRO:HG3 | 2.45 | 0.52 |
| 57:S1:456:ALA:O | 57:S1:499:ASN:ND2 | 2.43 | 0.52 |
| 65:V1:364:VAL:HG12 | 65:V1:400:VAL:HG12 | 1.92 | 0.52 |
| 18:A9:163:LYS:NZ | 18:A9:253:ILE:O | 2.37 | 0.52 |
| 35:C1:406:ASN:HB3 | 35:C1:409:TRP:HB2 | 1.91 | 0.52 |
| 71:N6:201:PLX:H151 | 71:N6:201:PLX:H332 | 1.91 | 0.52 |
| 65:V1:326:LEU:HD22 | 65:V1:363:ILE:HD11 | 1.92 | 0.52 |
| 6:6C:45:ARG:NH1 | 36:C2:25:ASP:OD2 | 2.42 | 0.51 |
| 44:N4:82:SER:HB2 | 44:N4:432:ARG:CZ | 2.40 | 0.51 |
| 41:N1:24:GLU:HA | 41:N1:271:LEU:HD13 | 1.93 | 0.51 |
| 42:N2:280:THR:HG21 | 73:N4:501:PEE:H19 | 1.93 | 0.51 |
| 49:Qc:24:PRO:O | 49:Qc:224:TYR:OH | 2.16 | 0.51 |
| 65:V1:113:LEU:HD13 | 65:V1:149:MET:HE1 | 1.93 | 0.51 |
| 49:QC:300:ILE:HD11 | 49:QC:363:LEU:HD21 | 1.93 | 0.51 |
| 35:C1:358:LEU:C | 77:C1:602:HEA:HMA | 2.36 | 0.51 |
| 47:QA:82:LEU:HD11 | 47:QA:154:LEU:HB3 | 1.92 | 0.51 |
| 49:QC:97:HIS:HD2 | 80:QC:402:HEM:C1C | 2.28 | 0.51 |
| 54:QH:29:HIS:HB2 | 54:QH:33:LYS:HE2 | 1.92 | 0.51 |
| 17:A8:196:ARG:NH2 | 23:AN:63:GLU:OE2 | 2.43 | 0.51 |
| 20:AK:241:ASN:HB3 | 20:AK:245:LYS:HE2 | 1.91 | 0.51 |
| 35:C1:309:THR:HG22 | 77:C1:602:HEA:HMB1 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:QC:29:SER:OG | 68:QC:404:CDL:OB9 | 2.25 | 0.51 |
| 41:N1:25:ARG:HD3 | 41:N1:37:PRO:HG2 | 1.93 | 0.51 |
| 42:N2:211:MET:HG2 | 42:N2:333:SER:HB2 | 1.93 | 0.51 |
| 49:QC:112:THR:HG22 | 49:QC:196:HIS:CE1 | 2.45 | 0.51 |
| 49:Qc:8:HIS:HB3 | 49:Qc:11:MET:HB2 | 1.91 | 0.51 |
| 58:S2:190:ILE:HG23 | 58:S2:209:MET:HB3 | 1.93 | 0.51 |
| 1:4L:55:LEU:H | 61:S5:25:GLN:HE22 | 1.59 | 0.51 |
| 11:A1:40:HIS:N | 11:A1:44:GLN:OE1 | 2.44 | 0.51 |
| 68:AL:201:CDL:H532 | 45:N5:577:VAL:HG22 | 1.93 | 0.51 |
| 41:N1:160:TYR:OH | 43:N3:73:LEU:O | 2.28 | 0.51 |
| 45:N5:530:PRO:O | 45:N5:534:HIS:HB2 | 2.10 | 0.51 |
| 48:QB:192:PHE:HB3 | 48:QB:195:THR:OG1 | 2.10 | 0.51 |
| 53:Qg:46:GLU:OE2 | 53:Qg:49:ARG:NH1 | 2.38 | 0.51 |
| 65:V1:205:ILE:HG12 | 65:V1:379:CYS:HB3 | 1.92 | 0.51 |
| 1:4L:98:CYS:HB3 | 45:N5:580:GLN:HB2 | 1.93 | 0.51 |
| 18:A9:204:SER:HB2 | 18:A9:266:VAL:HG12 | 1.92 | 0.51 |
| 30:B7:103:GLU:O | 30:B7:107:ARG:HG2 | 2.11 | 0.51 |
| 44:N4:375:LEU:HD11 | 45:N5:141:PHE:HE2 | 1.75 | 0.51 |
| 46:N6:82:VAL:HG12 | 46:N6:85:SER:HB2 | 1.92 | 0.51 |
| 26:B3:33:GLN:NE2 | 26:B3:43:ASP:OD1 | 2.44 | 0.51 |
| 28:B5:139:ILE:HG23 | 44:N4:54:LEU:HD23 | 1.92 | 0.51 |
| 40:CB:13:LEU:HD21 | 61:S5:4:PHE:HB3 | 1.93 | 0.51 |
| 42:N2:167:TRP:HB3 | 45:N5:574:SER:HA | 1.92 | 0.51 |
| 45:N5:97:THR:HG21 | 45:N5:125:LEU:HD22 | 1.93 | 0.51 |
| 54:QH:25:ARG:NH1 | 51:Qe:92:ARG:O | 2.44 | 0.51 |
| 70:6A:101:PC1:H153 | 37:C3:184:ALA:HB3 | 1.93 | 0.51 |
| 45:N5:228:GLY:H | 45:N5:230:HIS:HD2 | 1.58 | 0.51 |
| 45:N5:399:VAL:HG12 | 45:N5:409:LEU:HD13 | 1.92 | 0.51 |
| 49:Qc:237:LEU:HD13 | 50:Qd:297:MET:HG2 | 1.93 | 0.51 |
| 45:N5:368:PHE:HZ | 45:N5:455:LYS:HG3 | 1.76 | 0.50 |
| 47:QA:155:GLN:HE21 | 47:QA:198:GLY:H | 1.59 | 0.50 |
| 18:A9:64:PHE:O | 18:A9:67:ARG:HG2 | 2.11 | 0.50 |
| 25:B2:65:THR:HB | 25:B2:68:GLN:HG2 | 1.92 | 0.50 |
| 68:B5:201:CDL:H191 | 68:B5:201:CDL:H762 | 1.93 | 0.50 |
| 35:C1:254:ILE:HG13 | 35:C1:344:PHE:CD2 | 2.46 | 0.50 |
| 41:N1:213:VAL:HG13 | 41:N1:214:GLU:HG2 | 1.93 | 0.50 |
| 42:N2:139:LEU:HD13 | 42:N2:190:MET:HE1 | 1.93 | 0.50 |
| 46:N6:113:VAL:HG13 | 46:N6:118:LYS:HG2 | 1.93 | 0.50 |
| 57:S1:395:GLU:OE2 | 57:S1:417:ARG:NH1 | 2.44 | 0.50 |
| 62:S6:61:GLU:OE2 | 64:S8:192:ASN:ND2 | 2.34 | 0.50 |
| 65:V1:129:GLU:OE2 | 65:V1:132:ARG:NH2 | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:V1:162:PHE:HB3 | 65:V1:165:GLU:HB2 | 1.93 | 0.50 |
| 3:5B:37:VAL:HB | 37:C3:154:GLY:HA2 | 1.94 | 0.50 |
| 21:AL:35:ILE:HD12 | 68:AL:201:CDL:H811 | 1.92 | 0.50 |
| 29:B6:186:GLN:O | 29:B6:187:HIS:ND1 | 2.44 | 0.50 |
| 45:N5:253:VAL:HG23 | 45:N5:310:LEU:HD21 | 1.93 | 0.50 |
| 48:QB:192:PHE:O | 48:QB:198:ALA:HB2 | 2.11 | 0.50 |
| 51:QE:196:ARG:NH2 | 51:QE:252:GLY:O | 2.24 | 0.50 |
| 5:6B:30:CYS:HB2 | 5:6B:65:CYS:SG | 2.52 | 0.50 |
| 29:B6:147:LYS:NZ | 33:BK:42:ASP:OD1 | 2.39 | 0.50 |
| 73:N4:501:PEE:H32 | 68:N4:503:CDL:H381 | 1.92 | 0.50 |
| 47:Qa:148:ARG:NH2 | 53:Qg:50:ARG:O | 2.44 | 0.50 |
| 57:S1:251:ILE:HG21 | 57:S1:604:GLN:HB3 | 1.92 | 0.50 |
| 58:S2:393:GLU:OE2 | 58:S2:396:GLN:NE2 | 2.45 | 0.50 |
| 65:V1:203:ALA:HB3 | 65:V1:206:CYS:HB2 | 1.92 | 0.50 |
| 50:QD:132:ALA:HA | 50:QD:175:TYR:HA | 1.92 | 0.50 |
| 50:QD:147:LYS:NZ | 50:QD:151:GLU:OE2 | 2.44 | 0.50 |
| 57:S1:34:VAL:HG23 | 57:S1:41:VAL:HG13 | 1.92 | 0.50 |
| 57:S1:389:THR:HG21 | 57:S1:473:MET:HE2 | 1.93 | 0.50 |
| 65:V1:385:CYS:O | 65:V1:389:VAL:HB | 2.12 | 0.50 |
| 35:C1:347:LEU:HD13 | 35:C1:383:MET:HE2 | 1.94 | 0.50 |
| 43:N3:42:ASP:OD1 | 63:S7:119:LYS:NZ | 2.44 | 0.50 |
| 49:QC:78:VAL:HG11 | 51:QE:135:GLN:HE22 | 1.77 | 0.50 |
| 49:QC:304:MET:HE1 | 49:QC:366:MET:HE1 | 1.94 | 0.50 |
| 50:Qd:129:ASP:OD1 | 50:Qd:178:LYS:NZ | 2.42 | 0.50 |
| 51:Qe:204:ARG:NE | 51:Qe:246:SER:O | 2.43 | 0.50 |
| 41:N1:138:GLN:HG3 | 41:N1:285:LEU:HD21 | 1.94 | 0.50 |
| 45:N5:562:LEU:HB3 | 45:N5:563:PRO:HD3 | 1.92 | 0.50 |
| 54:QH:67:PHE:HE1 | 49:Qc:344:GLU:HG3 | 1.75 | 0.50 |
| 47:Qa:298:HIS:HB2 | 48:Qb:114:GLU:HG2 | 1.94 | 0.50 |
| 57:S1:149:ASP:OD2 | 57:S1:150:ARG:NH2 | 2.44 | 0.50 |
| 35:C1:37:ILE:CG2 | 77:C1:601:HEA:HMA | 2.42 | 0.50 |
| 49:QC:8:HIS:O | 49:QC:12:LYS:N | 2.38 | 0.50 |
| 68:A7:201:CDL:HA61 | 68:A7:201:CDL:H521 | 1.93 | 0.50 |
| 20:AK:225:ASN:HB3 | 20:AK:228:GLU:HG2 | 1.94 | 0.50 |
| 21:AL:124:LEU:HD11 | 73:N4:501:PEE:H70 | 1.93 | 0.50 |
| 42:N2:24:SER:OG | 61:S5:15:ASP:OD1 | 2.25 | 0.50 |
| 43:N3:56:PHE:O | 46:N6:70:TYR:OH | 2.30 | 0.50 |
| 49:QC:344:GLU:HG3 | 54:Qh:67:PHE:HE1 | 1.77 | 0.50 |
| 50:QD:159:PRO:HB2 | 50:Qd:184:GLU:HG3 | 1.94 | 0.50 |
| 47:Qa:61:ILE:HG12 | 47:Qa:130:ILE:HD11 | 1.93 | 0.50 |
| 63:S7:108:THR:HA | 63:S7:136:CYS:HB3 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:6A:56:ARG:HH21 | 4:6A:94:TYR:HB3 | 1.76 | 0.49 |
| 46:N6:17:PHE:HA | 46:N6:20:PHE:CE2 | 2.46 | 0.49 |
| 47:QA:90:THR:HG23 | 47:QA:95:SER:HA | 1.94 | 0.49 |
| 48:QB:274:GLU:HG2 | 54:Qh:18:SER:HB2 | 1.92 | 0.49 |
| 51:QE:220:LEU:HD12 | 51:QE:239:HIS:CE1 | 2.47 | 0.49 |
| 51:Qe:267:SER:HB3 | 51:Qe:270:LEU:HB3 | 1.93 | 0.49 |
| 57:S1:387:LEU:HD12 | 57:S1:514:ASN:HB3 | 1.93 | 0.49 |
| 65:V1:357:MET:HB3 | 65:V1:361:THR:HG21 | 1.93 | 0.49 |
| 13:A3:127:ALA:HB2 | 41:N1:312:ALA:HA | 1.94 | 0.49 |
| 17:A8:95:VAL:HG12 | 17:A8:97:VAL:HG22 | 1.94 | 0.49 |
| 47:QA:298:HIS:HB2 | 48:QB:114:GLU:HG2 | 1.93 | 0.49 |
| 47:Qa:47:LEU:HD21 | 47:Qa:234:ALA:HB1 | 1.92 | 0.49 |
| 2:5A:76:MET:HE2 | 2:5A:110:ILE:HG12 | 1.94 | 0.49 |
| 7:7A:54:ARG:HH12 | 68:7A:102:CDL:HB61 | 1.78 | 0.49 |
| 11:A1:12:MET:HE3 | 41:N1:264:LEU:HD22 | 1.95 | 0.49 |
| 18:A9:293:LEU:HD12 | 18:A9:294:PRO:HD2 | 1.92 | 0.49 |
| 44:N4:41:LEU:O | 44:N4:44:GLN:NE2 | 2.45 | 0.49 |
| 68:QH:102:CDL:HB32 | 68:QH:102:CDL:HA22 | 1.93 | 0.49 |
| 11:A1:58:ASN:O | 11:A1:59:ARG:NH1 | 2.41 | 0.49 |
| 17:A8:201:GLU:HA | 17:A8:204:LYS:HD3 | 1.95 | 0.49 |
| 68:AL:201:CDL:H401 | 68:AL:201:CDL:H771 | 1.94 | 0.49 |
| 37:C3:178:ALA:HB1 | 68:C3:305:CDL:H122 | 1.94 | 0.49 |
| 44:N4:266:MET:HB3 | 44:N4:395:LEU:HD13 | 1.94 | 0.49 |
| 50:Qd:322:TYR:CZ | 50:Qd:324:PRO:HG3 | 2.46 | 0.49 |
| 57:S1:449:PRO:HB2 | 57:S1:679:LEU:HD13 | 1.94 | 0.49 |
| 65:V1:288:VAL:HG21 | 65:V1:303:HIS:CD2 | 2.47 | 0.49 |
| 4:6A:56:ARG:NH2 | 4:6A:96:GLN:O | 2.45 | 0.49 |
| 5:6B:63:SER:HA | 36:C2:111:THR:HG23 | 1.94 | 0.49 |
| 17:A8:160:THR:HA | 17:A8:163:TRP:CD1 | 2.47 | 0.49 |
| 21:AL:81:ARG:HH11 | 21:AL:89:ASN:HD21 | 1.61 | 0.49 |
| 36:C2:149:THR:OG1 | 36:C2:185:MET:SD | 2.67 | 0.49 |
| 57:S1:246:ARG:HH12 | 60:S4:123:ASN:HD22 | 1.60 | 0.49 |
| 58:S2:121:LEU:HD23 | 63:S7:113:MET:SD | 2.53 | 0.49 |
| 65:V1:119:GLU:O | 65:V1:159:ARG:NH1 | 2.45 | 0.49 |
| 23:AN:93:GLU:HG3 | 61:S5:98:HIS:CD2 | 2.47 | 0.49 |
| 37:C3:33:MET:O | 37:C3:37:PHE:N | 2.44 | 0.49 |
| 71:N4:502:PLX:H192 | 68:N5:703:CDL:H611 | 1.94 | 0.49 |
| 50:Qd:149:LEU:O | 50:Qd:152:GLU:HG2 | 2.13 | 0.49 |
| 51:Qe:145:ASP:OD1 | 51:Qe:145:ASP:N | 2.42 | 0.49 |
| 51:Qe:228:ALA:HB3 | 51:Qe:235:TYR:HB3 | 1.95 | 0.49 |
| 58:S2:227:ARG:NH1 | 63:S7:75:GLU:OE1 | 2.44 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:A9:50:SER:OG | 59:S3:225:GLU:OE2 | 2.30 | 0.49 |
| 32:B9:87:ARG:NH1 | 32:B9:91:ASP:OD2 | 2.46 | 0.49 |
| 36:C2:72:ILE:O | 36:C2:76:ILE:HG13 | 2.13 | 0.49 |
| 36:C2:156:SER:HB2 | 36:C2:174:ALA:HB1 | 1.95 | 0.49 |
| 42:N2:304:MET:HE3 | 44:N4:135:ARG:HH22 | 1.76 | 0.49 |
| 44:N4:296:LEU:HD21 | 44:N4:378:GLU:HG3 | 1.95 | 0.49 |
| 47:QA:89:LEU:HD22 | 47:QA:150:GLU:HB3 | 1.94 | 0.49 |
| 57:S1:83:GLU:HB2 | 57:S1:101:ASN:HB3 | 1.94 | 0.49 |
| 41:N1:281:ARG:NH1 | 58:S2:452:ASP:OD1 | 2.46 | 0.49 |
| 44:N4:369:LEU:HD23 | 68:N5:703:CDL:H362 | 1.95 | 0.49 |
| 48:QB:373:GLN:NE2 | 48:QB:475:MET:SD | 2.86 | 0.49 |
| 48:Qb:83:ASN:HD22 | 48:Qb:85:LYS:H | 1.61 | 0.49 |
| 49:Qc:47:THR:HG23 | 49:Qc:79:ILE:HG23 | 1.93 | 0.49 |
| 57:S1:538:ARG:HG2 | 57:S1:555:ILE:HD11 | 1.95 | 0.49 |
| 58:S2:90:PHE:HB2 | 58:S2:105:MET:HE2 | 1.93 | 0.49 |
| 58:S2:190:ILE:HG21 | 58:S2:213:ARG:HG3 | 1.95 | 0.49 |
| 11:A1:52:ARG:NH1 | 11:A1:58:ASN:OD1 | 2.44 | 0.49 |
| 20:AK:97:ASP:N | 20:AK:97:ASP:OD1 | 2.45 | 0.49 |
| 24:B1:47:ARG:NH2 | 24:B1:53:GLU:OE2 | 2.46 | 0.49 |
| 36:C2:137:GLU:OE2 | 38:C4:144:ARG:NH1 | 2.44 | 0.49 |
| 57:S1:339:ALA:HA | 57:S1:365:SER:HB2 | 1.93 | 0.49 |
| 58:S2:194:THR:HG21 | 58:S2:209:MET:HB2 | 1.94 | 0.49 |
| 67:V3:420:SER:HB3 | 67:V3:423:HIS:ND1 | 2.27 | 0.49 |
| 1:4L:73:LEU:HD21 | 42:N2:41:ILE:HG13 | 1.95 | 0.49 |
| 17:A8:84:LEU:O | 23:AN:88:ARG:NH1 | 2.46 | 0.49 |
| 17:A8:86:THR:OG1 | 17:A8:88:GLU:OE1 | 2.27 | 0.49 |
| 45:N5:119:LYS:NZ | 68:N5:703:CDL:OA3 | 2.39 | 0.49 |
| 53:QG:71:MET:HE2 | 50:Qd:316:LYS:HD3 | 1.95 | 0.49 |
| 48:Qb:126:ARG:NH1 | 48:Qb:199:GLN:O | 2.46 | 0.49 |
| 57:S1:307:ILE:HG23 | 57:S1:317:THR:HG21 | 1.94 | 0.49 |
| 21:AL:67:GLY:HA2 | 68:AL:201:CDL:H221 | 1.93 | 0.48 |
| 70:C1:610:PC1:H111 | 37:C3:11:VAL:HG21 | 1.95 | 0.48 |
| 45:N5:15:LEU:HD11 | 45:N5:94:LEU:HD21 | 1.94 | 0.48 |
| 51:Qe:201:ASP:OD1 | 51:Qe:201:ASP:N | 2.41 | 0.48 |
| 59:S3:61:PHE:HZ | 59:S3:106:ALA:HB2 | 1.78 | 0.48 |
| 15:A6:66:TYR:CE2 | 15:A6:86:ARG:HD3 | 2.48 | 0.48 |
| 30:B7:17:PRO:HB3 | 30:B7:105:GLU:HG2 | 1.95 | 0.48 |
| 37:C3:219:LEU:HD23 | 68:C3:304:CDL:H761 | 1.95 | 0.48 |
| 41:N1:59:GLU:HG3 | 43:N3:27:LEU:HD13 | 1.94 | 0.48 |
| 42:N2:96:THR:HG22 | 42:N2:100:MET:HE2 | 1.95 | 0.48 |
| 42:N2:197:ASN:HD22 | 42:N2:200:MET:HG2 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:QB:465:LEU:HD12 | 48:QB:466:PRO:HD2 | 1.93 | 0.48 |
| 15:A6:90:ARG:HE | 15:A6:94:MET:HE2 | 1.78 | 0.48 |
| 17:A8:178:ARG:NH1 | 17:A8:181:GLN:OE1 | 2.43 | 0.48 |
| 18:A9:220:MET:HG2 | 73:A9:402:PEE:H17 | 1.96 | 0.48 |
| 18:A9:257:ASP:OD1 | 18:A9:257:ASP:N | 2.46 | 0.48 |
| 20:AK:297:ARG:HA | 20:AK:300:VAL:HG22 | 1.95 | 0.48 |
| 23:AN:98:MET:HE3 | 23:AN:101:VAL:HG21 | 1.94 | 0.48 |
| 68:B4:201:CDL:OA7 | 54:Qh:39:LEU:HD13 | 2.14 | 0.48 |
| 33:BK:142:ARG:NH1 | 33:BK:143:TYR:OH | 2.46 | 0.48 |
| 36:C2:28:LEU:HA | 36:C2:31:VAL:HG22 | 1.95 | 0.48 |
| 43:N3:33:LYS:O | 63:S7:98:ARG:NH1 | 2.37 | 0.48 |
| 45:N5:65:ASN:HD21 | 45:N5:78:LEU:HD23 | 1.78 | 0.48 |
| 52:QF:34:ARG:O | 52:QF:38:GLU:HG2 | 2.12 | 0.48 |
| 63:S7:75:GLU:HB2 | 63:S7:133:MET:HE1 | 1.95 | 0.48 |
| 71:AL:202:PLX:H1A2 | 71:AL:202:PLX:H21 | 1.58 | 0.48 |
| 22:AM:144:TYR:OH | 57:S1:581:ASP:OD1 | 2.24 | 0.48 |
| 35:C1:358:LEU:CB | 77:C1:602:HEA:HMA | 2.44 | 0.48 |
| 35:C1:413:HIS:CE1 | 35:C1:468:MET:HB2 | 2.48 | 0.48 |
| 44:N4:233:ALA:HA | 44:N4:320:GLY:HA2 | 1.95 | 0.48 |
| 48:QB:190:THR:HG22 | 48:QB:275:ILE:HG23 | 1.95 | 0.48 |
| 68:4L:201:CDL:H262 | 68:4L:201:CDL:H371 | 1.95 | 0.48 |
| 9:7C:56:VAL:HG21 | 35:C1:36:LEU:HD13 | 1.94 | 0.48 |
| 27:B4:26:SER:OG | 27:B4:28:GLU:OE1 | 2.28 | 0.48 |
| 33:BK:74:ILE:HG23 | 33:BK:156:LEU:HD22 | 1.96 | 0.48 |
| 37:C3:54:MET:HB3 | 37:C3:58:TRP:CZ3 | 2.48 | 0.48 |
| 38:C4:44:TYR:OH | 38:C4:48:ASP:OD1 | 2.30 | 0.48 |
| 41:N1:113:VAL:HG13 | 41:N1:139:THR:HG21 | 1.95 | 0.48 |
| 44:N4:12:LEU:HB2 | 44:N4:13:PRO:HD3 | 1.95 | 0.48 |
| 45:N5:368:PHE:CZ | 45:N5:455:LYS:HG3 | 2.49 | 0.48 |
| 48:QB:205:SER:HA | 48:QB:208:VAL:HG12 | 1.96 | 0.48 |
| 56:QJ:14:ALA:O | 56:QJ:18:ILE:HG12 | 2.13 | 0.48 |
| 47:Qa:375:LYS:NZ | 47:Qa:419:VAL:O | 2.32 | 0.48 |
| 51:Qe:262:THR:HB | 51:Qe:274:GLY:O | 2.13 | 0.48 |
| 57:S1:43:VAL:HG12 | 57:S1:55:LYS:HD2 | 1.94 | 0.48 |
| 57:S1:338:VAL:HB | 57:S1:363:SER:CB | 2.43 | 0.48 |
| 59:S3:145:THR:OG1 | 59:S3:146:TYR:N | 2.46 | 0.48 |
| 16:A7:109:ASP:OD2 | 23:AN:21:TYR:OH | 2.30 | 0.48 |
| 42:N2:26:TRP:HB3 | 42:N2:74:ILE:HD13 | 1.96 | 0.48 |
| 45:N5:241:THR:HG21 | 45:N5:344:GLY:HA3 | 1.94 | 0.48 |
| 47:Qa:237:PHE:CE2 | 47:Qa:238:LEU:HD12 | 2.48 | 0.48 |
| 48:Qb:302:VAL:HB | 48:Qb:303:PRO:HD3 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:S2:129:LEU:O | 58:S2:133:LYS:HG2 | 2.13 | 0.48 |
| 62:S6:108:THR:HG22 | 62:S6:119:ARG:HD3 | 1.94 | 0.48 |
| 64:S8:75:SER:O | 64:S8:79:ARG:HG3 | 2.14 | 0.48 |
| 23:AN:95:ALA:HA | 23:AN:106:VAL:HG11 | 1.96 | 0.48 |
| 28:B5:53:ARG:NH2 | 29:B6:89:SER:O | 2.45 | 0.48 |
| 45:N5:536:LEU:HB3 | 45:N5:537:PRO:HD3 | 1.96 | 0.48 |
| 68:QH:102:CDL:OA3 | 50:Qd:305:TYR:OH | 2.28 | 0.48 |
| 55:QI:50:GLY:H | 55:QI:55:HIS:CD2 | 2.32 | 0.48 |
| 17:A8:115:LYS:HB3 | 17:A8:116:PRO:HD3 | 1.96 | 0.48 |
| 33:BK:73:ASP:OD1 | 33:BK:73:ASP:N | 2.44 | 0.48 |
| 36:C2:152:MET:HB2 | 36:C2:182:THR:HB | 1.95 | 0.48 |
| 42:N2:42:PRO:HG3 | 46:N6:167:VAL:HG13 | 1.95 | 0.48 |
| 47:QA:438:MET:HB2 | 47:QA:450:VAL:HG13 | 1.94 | 0.48 |
| 53:QG:43:ASP:OD2 | 53:QG:102:ARG:NH1 | 2.47 | 0.48 |
| 47:Qa:409:PRO:O | 47:Qa:413:LEU:HG | 2.13 | 0.48 |
| 65:V1:174:ARG:HA | 67:V3:406:LEU:HD21 | 1.94 | 0.48 |
| 3:5B:84:THR:OG1 | 3:5B:85:ASN:N | 2.47 | 0.48 |
| 68:B5:201:CDL:HB21 | 73:N5:701:PEE:H49 | 1.95 | 0.48 |
| 49:Qc:5:ARG:HH11 | 49:Qc:15:ASN:ND2 | 2.12 | 0.48 |
| 60:S4:70:GLU:O | 60:S4:74:THR:OG1 | 2.28 | 0.48 |
| 63:S7:56:TRP:CE2 | 71:S7:203:PLX:H101 | 2.49 | 0.48 |
| 65:V1:185:ASN:OD1 | 65:V1:190:GLY:N | 2.42 | 0.48 |
| 2:5A:61:TYR:OH | 2:5A:71:GLU:O | 2.31 | 0.48 |
| 40:CB:107:ASP:OD1 | 40:CB:107:ASP:N | 2.47 | 0.48 |
| 44:N4:106:LEU:HD13 | 44:N4:234:VAL:HG11 | 1.96 | 0.48 |
| 48:QB:74:TRP:CZ2 | 48:QB:411:GLU:HA | 2.48 | 0.48 |
| 66:V2:111:ARG:NH1 | 66:V2:114:GLU:OE2 | 2.47 | 0.48 |
| 1:4L:4:VAL:O | 1:4L:8:ILE:HG12 | 2.14 | 0.47 |
| 4:6A:88:ASN:ND2 | 70:6A:101:PC1:H151 | 2.29 | 0.47 |
| 6:6C:63:GLU:O | 6:6C:67:LYS:NZ | 2.44 | 0.47 |
| 14:A5:38:ILE:O | 14:A5:45:ARG:NH1 | 2.47 | 0.47 |
| 19:AC:119:ILE:HG21 | 19:AC:135:ALA:HB1 | 1.95 | 0.47 |
| 55:Qi:38:GLN:NE2 | 56:Qj:47:TYR:OH | 2.47 | 0.47 |
| 56:Qj:42:LEU:HA | 56:Qj:45:VAL:HG22 | 1.96 | 0.47 |
| 60:S4:112:MET:O | 64:S8:144:ARG:NH1 | 2.36 | 0.47 |
| 85:S7:201:U10:H401 | 85:S7:201:U10:H422 | 1.66 | 0.47 |
| 44:N4:196:TRP:CD1 | 44:N4:250:LEU:HB3 | 2.48 | 0.47 |
| 23:AN:49:SER:HB2 | 41:N1:172:ILE:HD13 | 1.95 | 0.47 |
| 68:C3:304:CDL:H802 | 68:C3:305:CDL:H273 | 1.96 | 0.47 |
| 47:Qa:71:TYR:HB3 | 47:Qa:212:HIS:CE1 | 2.50 | 0.47 |
| 47:Qa:313:VAL:HG21 | 47:Qa:323:VAL:HG11 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:S1:274:LEU:HD21 | 60:S4:87:MET:HE2 | 1.96 | 0.47 |
| 58:S2:299:LEU:HD22 | 58:S2:304:ILE:HD12 | 1.97 | 0.47 |
| 68:7A:102:CDL:H232 | 68:7A:102:CDL:H822 | 1.96 | 0.47 |
| 9:7C:60:LEU:HD23 | 10:8B:64:TYR:HB2 | 1.96 | 0.47 |
| 28:B5:94:GLY:O | 33:BK:61:TYR:OH | 2.29 | 0.47 |
| 29:B6:148:TYR:CE1 | 33:BK:49:ARG:HG2 | 2.49 | 0.47 |
| 70:C1:610:PC1:H341 | 70:C1:610:PC1:H2A2 | 1.95 | 0.47 |
| 36:C2:98:LYS:HZ3 | 36:C2:111:THR:HG21 | 1.80 | 0.47 |
| 36:C2:145:PRO:HA | 36:C2:214:VAL:O | 2.14 | 0.47 |
| 44:N4:210:TYR:CG | 44:N4:268:GLY:HA3 | 2.49 | 0.47 |
| 65:V1:210:THR:HB | 65:V1:224:ARG:H | 1.80 | 0.47 |
| 65:V1:325:PRO:HG3 | 65:V1:433:TRP:HB3 | 1.95 | 0.47 |
| 9:7C:52:PRO:HG2 | 35:C1:32:ALA:HB3 | 1.97 | 0.47 |
| 18:A9:129:LEU:HD23 | 18:A9:167:ILE:HG13 | 1.97 | 0.47 |
| 36:C2:110:TYR:HB2 | 36:C2:116:LEU:HB3 | 1.96 | 0.47 |
| 44:N4:79:ALA:O | 44:N4:82:SER:HB3 | 2.15 | 0.47 |
| 50:QD:292:LYS:HD2 | 73:QE:301:PEE:H3 | 1.96 | 0.47 |
| 51:Qe:126:ALA:HA | 73:Qe:301:PEE:H74 | 1.96 | 0.47 |
| 65:V1:347:THR:HG22 | 65:V1:348:GLY:H | 1.80 | 0.47 |
| 20:AK:316:LEU:HB2 | 20:AK:319:ILE:HG12 | 1.96 | 0.47 |
| 36:C2:161:HIS:CE1 | 36:C2:200:CYS:SG | 3.06 | 0.47 |
| 37:C3:173:PHE:CE1 | 37:C3:208:VAL:HG21 | 2.49 | 0.47 |
| 42:N2:25:HIS:HB2 | 61:S5:15:ASP:HB2 | 1.97 | 0.47 |
| 68:QB:501:CDL:H512 | 70:QB:503:PC1:H361 | 1.96 | 0.47 |
| 48:Qb:68:THR:HG22 | 48:Qb:136:LEU:HD23 | 1.96 | 0.47 |
| 57:S1:217:GLU:HG3 | 57:S1:412:PRO:HB3 | 1.95 | 0.47 |
| 5:6B:14:THR:HG23 | 36:C2:151:ARG:HH12 | 1.80 | 0.47 |
| 12:A2:18:GLU:HG2 | 12:A2:68:ARG:HB3 | 1.96 | 0.47 |
| 13:A3:160:GLY:HA3 | 17:A8:204:LYS:HE3 | 1.97 | 0.47 |
| 17:A8:124:ARG:NE | 23:AN:80:ASP:OD2 | 2.44 | 0.47 |
| 75:AC:201:ZMP:H11A | 32:B9:58:VAL:HG23 | 1.97 | 0.47 |
| 35:C1:74:MET:HE3 | 35:C1:389:ILE:HG13 | 1.97 | 0.47 |
| 41:N1:113:VAL:O | 41:N1:116:ILE:HG12 | 2.14 | 0.47 |
| 43:N3:35:SER:O | 63:S7:98:ARG:NH2 | 2.47 | 0.47 |
| 44:N4:82:SER:HB2 | 44:N4:432:ARG:NH1 | 2.30 | 0.47 |
| 44:N4:211:GLY:H | 44:N4:213:HIS:CD2 | 2.31 | 0.47 |
| 45:N5:292:ALA:HB2 | 45:N5:304:PHE:HB3 | 1.97 | 0.47 |
| 45:N5:366:MET:O | 45:N5:370:THR:OG1 | 2.25 | 0.47 |
| 49:QC:29:SER:HB2 | 68:QD:402:CDL:H142 | 1.97 | 0.47 |
| 51:QE:143:SER:OG | 51:QE:145:ASP:OD1 | 2.31 | 0.47 |
| 48:Qb:87:ASN:HD22 | 48:Qb:204:PRO:HD3 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:Qb:96:LEU:HD13 | 48:Qb:156:LEU:HD22 | 1.96 | 0.47 |
| 66:V2:149:LEU:HD11 | 66:V2:160:VAL:HG23 | 1.95 | 0.47 |
| 18:A9:165:ILE:HD13 | 18:A9:199:THR:HB | 1.97 | 0.47 |
| 34:BL:77:ASP:OD1 | 34:BL:78:LYS:N | 2.48 | 0.47 |
| 40:CB:106:LYS:NZ | 40:CB:107:ASP:OD1 | 2.37 | 0.47 |
| 44:N4:201:MET:HE1 | 44:N4:212:LEU:HD11 | 1.96 | 0.47 |
| 44:N4:361:VAL:HG22 | 68:N5:703:CDL:H311 | 1.96 | 0.47 |
| 51:QE:177:ARG:HB3 | 51:QE:211:VAL:HG13 | 1.96 | 0.47 |
| 52:QF:60:ARG:HD3 | 52:QF:63:THR:HG21 | 1.96 | 0.47 |
| 47:Qa:301:ARG:NH2 | 48:Qb:94:GLU:OE2 | 2.46 | 0.47 |
| 50:Qd:311:LYS:HD3 | 50:Qd:311:LYS:HA | 1.75 | 0.47 |
| 53:Qg:44:VAL:O | 53:Qg:48:ILE:HG12 | 2.15 | 0.47 |
| 57:S1:575:VAL:C | 57:S1:578:PRO:HD2 | 2.39 | 0.47 |
| 1:4L:76:SER:O | 1:4L:79:VAL:HG22 | 2.14 | 0.47 |
| 18:A9:231:LEU:HD13 | 18:A9:292:PRO:HG3 | 1.95 | 0.47 |
| 25:B2:108:ASP:OD1 | 30:B7:107:ARG:NH1 | 2.47 | 0.47 |
| 35:C1:352:GLY:HA3 | 77:C1:602:HEA:C14 | 2.45 | 0.47 |
| 44:N4:76:MET:SD | 44:N4:230:VAL:HB | 2.55 | 0.47 |
| 45:N5:49:VAL:HB | 45:N5:50:PRO:HD3 | 1.97 | 0.47 |
| 45:N5:566:THR:O | 45:N5:570:GLN:HG2 | 2.15 | 0.47 |
| 47:QA:138:LEU:HD12 | 47:QA:233:VAL:HG12 | 1.97 | 0.47 |
| 35:C1:405:LEU:HD23 | 35:C1:475:ALA:HB2 | 1.97 | 0.47 |
| 36:C2:13:THR:HB | 36:C2:168:LEU:HD23 | 1.97 | 0.47 |
| 44:N4:267:TRP:O | 44:N4:271:MET:HG2 | 2.15 | 0.47 |
| 47:QA:313:VAL:HG11 | 47:QA:350:VAL:HG13 | 1.97 | 0.47 |
| 48:QB:110:GLU:HA | 48:QB:113:VAL:HG22 | 1.97 | 0.47 |
| 47:Qa:125:CYS:HB3 | 47:Qa:133:LEU:HD22 | 1.97 | 0.47 |
| 57:S1:222:ILE:HA | 57:S1:225:ILE:HG12 | 1.97 | 0.47 |
| 58:S2:167:ILE:HD13 | 58:S2:369:VAL:HG11 | 1.97 | 0.47 |
| 59:S3:89:HIS:CG | 59:S3:90:PRO:HD2 | 2.50 | 0.47 |
| 59:S3:118:ASP:OD2 | 59:S3:125:ARG:NH2 | 2.45 | 0.47 |
| 67:V3:386:TYR:CZ | 67:V3:388:ASN:HB3 | 2.50 | 0.47 |
| 16:A7:62:GLU:OE2 | 59:S3:44:ARG:NH1 | 2.44 | 0.46 |
| 35:C1:336:PRO:HD3 | 35:C1:407:GLN:HG3 | 1.98 | 0.46 |
| 41:N1:90:PRO:HB3 | 41:N1:94:PRO:HD3 | 1.96 | 0.46 |
| 42:N2:149:ILE:HD13 | 42:N2:154:MET:HE3 | 1.96 | 0.46 |
| 44:N4:168:GLN:HB2 | 44:N4:174:LEU:HG | 1.96 | 0.46 |
| 49:Qc:303:LEU:HD11 | 70:Qc:405:PC1:H122 | 1.97 | 0.46 |
| 52:Qf:40:ILE:HG13 | 52:Qf:43:CYS:H | 1.80 | 0.46 |
| 65:V1:235:VAL:H | 65:V1:240:THR:HG21 | 1.80 | 0.46 |
| 71:CB:201:PLX:H171 | 61:S5:9:ARG:HH22 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:N2:112:HIS:HB2 | 42:N2:184:ILE:HD13 | 1.97 | 0.46 |
| 44:N4:408:LEU:HD12 | 45:N5:172:ILE:HG21 | 1.97 | 0.46 |
| 47:QA:154:LEU:HD23 | 47:QA:154:LEU:HA | 1.78 | 0.46 |
| 50:QD:184:GLU:HG3 | 50:Qd:159:PRO:HB2 | 1.97 | 0.46 |
| 47:Qa:290:GLN:HB2 | 47:Qa:336:PHE:HE1 | 1.80 | 0.46 |
| 62:S6:36:GLU:OE2 | 62:S6:60:LYS:NZ | 2.41 | 0.46 |
| 65:V1:384:PRO:HG2 | 65:V1:422:HIS:O | 2.15 | 0.46 |
| 1:4L:35:GLY:HA3 | 46:N6:20:PHE:CZ | 2.51 | 0.46 |
| 1:4L:65:VAL:HG11 | 46:N6:157:THR:HG23 | 1.97 | 0.46 |
| 9:7C:41:MET:HG2 | 73:7C:101:PEE:H62 | 1.97 | 0.46 |
| 31:B8:108:ASP:HB3 | 31:B8:111:MET:HG2 | 1.98 | 0.46 |
| 36:C2:133:MET:HB2 | 36:C2:136:LEU:HB2 | 1.98 | 0.46 |
| 45:N5:327:LEU:O | 45:N5:331:MET:HG2 | 2.15 | 0.46 |
| 50:QD:243:ILE:HG12 | 50:QD:245:MET:H | 1.81 | 0.46 |
| 51:QE:154:ILE:HD13 | 51:QE:176:VAL:HG21 | 1.98 | 0.46 |
| 68:QH:102:CDL:HA32 | 50:Qd:308:LYS:HE3 | 1.95 | 0.46 |
| 51:QK:34:LEU:HD23 | 51:QK:34:LEU:H | 1.79 | 0.46 |
| 47:Qa:68:GLY:H | 47:Qa:71:TYR:HD2 | 1.63 | 0.46 |
| 57:S1:219:SER:O | 57:S1:222:ILE:HG12 | 2.15 | 0.46 |
| 58:S2:145:LEU:HD13 | 58:S2:430:ILE:HG21 | 1.97 | 0.46 |
| 58:S2:418:VAL:HB | 58:S2:427:ARG:HB3 | 1.96 | 0.46 |
| 64:S8:142:THR:O | 64:S8:187:LYS:NZ | 2.49 | 0.46 |
| 38:C4:142:THR:HG23 | 38:C4:156:PHE:HZ | 1.80 | 0.46 |
| 42:N2:132:THR:HG23 | 42:N2:209:ILE:HG12 | 1.98 | 0.46 |
| 45:N5:288:THR:HG21 | 45:N5:307:SER:HB3 | 1.97 | 0.46 |
| 15:A6:48:SER:O | 15:A6:50:ASP:N | 2.49 | 0.46 |
| 19:AB:140:CYS:HB2 | 19:AB:143:GLU:HG3 | 1.98 | 0.46 |
| 30:B7:22:MET:HE1 | 30:B7:102:PHE:CD2 | 2.51 | 0.46 |
| 35:C1:8:TYR:CZ | 37:C3:15:PRO:HB3 | 2.51 | 0.46 |
| 35:C1:368:HIS:O | 36:C2:171:LYS:NZ | 2.42 | 0.46 |
| 68:CB:203:CDL:H342 | 68:CB:203:CDL:H191 | 1.98 | 0.46 |
| 65:V1:65:THR:O | 65:V1:69:LEU:HG | 2.16 | 0.46 |
| 66:V2:144:ASN:HB3 | 66:V2:147:SER:OG | 2.16 | 0.46 |
| 4:6A:59:PHE:HB2 | 4:6A:94:TYR:CE2 | 2.50 | 0.46 |
| 5:6B:5:ILE:HG13 | 5:6B:7:THR:H | 1.80 | 0.46 |
| 31:B8:62:TYR:OH | 31:B8:74:ASP:O | 2.21 | 0.46 |
| 36:C2:146:MET:HE2 | 36:C2:215:PRO:HG3 | 1.96 | 0.46 |
| 45:N5:402:SER:HB2 | 45:N5:404:THR:HG23 | 1.97 | 0.46 |
| 45:N5:435:PRO:HB3 | 45:N5:437:PHE:CZ | 2.51 | 0.46 |
| 48:QB:467:ASP:HB3 | 48:QB:470:ARG:HG2 | 1.97 | 0.46 |
| 51:QE:123:VAL:HG13 | 55:Qi:29:ALA:HA | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:S2:467:VAL:O | 58:S2:469:ARG:NH1 | 2.49 | 0.46 |
| 65:V1:55:GLY:O | 65:V1:58:SER:OG | 2.20 | 0.46 |
| 3:5B:41:GLU:HG2 | 3:5B:56:ARG:NH2 | 2.29 | 0.46 |
| 15:A6:88:LYS:NZ | 15:A6:133:PHE:HA | 2.31 | 0.46 |
| 16:A7:112:TYR:HE2 | 64:S8:43:MET:HE2 | 1.80 | 0.46 |
| 18:A9:219:SER:HB3 | 73:A9:402:PEE:H1 | 1.98 | 0.46 |
| 71:AM:201:PLX:H341 | 71:AM:201:PLX:H372 | 1.70 | 0.46 |
| 34:BL:72:ASP:OD1 | 34:BL:72:ASP:N | 2.38 | 0.46 |
| 41:N1:273:ILE:HG23 | 41:N1:277:TYR:HD2 | 1.81 | 0.46 |
| 45:N5:346:ILE:HD11 | 45:N5:431:PHE:CZ | 2.51 | 0.46 |
| 47:QA:235:GLU:O | 47:QA:239:ASN:ND2 | 2.48 | 0.46 |
| 50:QD:112:ARG:NH2 | 50:QD:145:GLU:OE1 | 2.49 | 0.46 |
| 50:Qd:104:SER:O | 50:Qd:287:LYS:NZ | 2.49 | 0.46 |
| 65:V1:49:HIS:NE2 | 67:V3:383:ASN:OD1 | 2.49 | 0.46 |
| 68:A8:301:CDL:HB61 | 40:CB:29:THR:HB | 1.98 | 0.46 |
| 18:A9:176:SER:O | 18:A9:182:ARG:NE | 2.47 | 0.46 |
| 18:A9:223:PHE:HB3 | 73:A9:402:PEE:H28 | 1.98 | 0.46 |
| 68:AK:402:CDL:H342 | 68:AK:402:CDL:H142 | 1.96 | 0.46 |
| 35:C1:202:LEU:HD22 | 35:C1:238:PHE:CE2 | 2.51 | 0.46 |
| 47:QA:272:VAL:HA | 47:QA:337:GLY:HA3 | 1.97 | 0.46 |
| 49:QC:141:TRP:CD1 | 49:QC:265:PRO:HD3 | 2.50 | 0.46 |
| 64:S8:131:GLU:HB2 | 64:S8:144:ARG:HB3 | 1.97 | 0.46 |
| 15:A6:92:MET:HB2 | 75:AB:201:ZMP:H4A | 1.97 | 0.46 |
| 68:B4:201:CDL:HA31 | 54:Qh:43:ARG:HH22 | 1.81 | 0.46 |
| 32:B9:52:LEU:O | 32:B9:57:LYS:NZ | 2.47 | 0.46 |
| 37:C3:126:PRO:HA | 37:C3:130:PRO:HG2 | 1.97 | 0.46 |
| 71:CB:201:PLX:H131 | 71:CB:201:PLX:H101 | 1.73 | 0.46 |
| 41:N1:301:CYS:O | 41:N1:305:ILE:HG13 | 2.16 | 0.46 |
| 68:N1:401:CDL:H721 | 68:N1:401:CDL:H341 | 1.98 | 0.46 |
| 44:N4:216:LEU:HB3 | 44:N4:217:PRO:HD3 | 1.97 | 0.46 |
| 68:QH:102:CDL:H331 | 68:QH:102:CDL:H721 | 1.98 | 0.46 |
| 71:QI:301:PLX:H1A3 | 71:QI:301:PLX:H22 | 1.64 | 0.46 |
| 57:S1:476:LEU:HD21 | 57:S1:481:LEU:HD21 | 1.97 | 0.46 |
| 57:S1:509:ASP:OD1 | 57:S1:509:ASP:N | 2.47 | 0.46 |
| 58:S2:180:PHE:CZ | 58:S2:223:VAL:HG11 | 2.51 | 0.46 |
| 21:AL:110:ILE:HG12 | 73:N5:702:PEE:H14 | 1.97 | 0.46 |
| 35:C1:219:PHE:HZ | 37:C3:199:VAL:HG21 | 1.81 | 0.46 |
| 35:C1:334:TRP:HH2 | 36:C2:46:LEU:HD13 | 1.81 | 0.46 |
| 36:C2:9:PHE:HB2 | 36:C2:21:LEU:HD21 | 1.97 | 0.46 |
| 48:QB:321:GLY:HA2 | 48:QB:324:MET:HE2 | 1.98 | 0.46 |
| 49:QC:312:GLN:HG3 | 53:Qg:37:THR:HG22 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 63:S7:84:TYR:CE1 | 63:S7:171:GLU:HG3 | 2.50 | 0.46 |
| 8:7B:34:HIS:CE1 | 38:C4:99:GLU:HG3 | 2.51 | 0.45 |
| 16:A7:39:PRO:HG3 | 64:S8:211:TYR:CZ | 2.52 | 0.45 |
| 17:A8:160:THR:HA | 17:A8:163:TRP:NE1 | 2.31 | 0.45 |
| 30:B7:12:ASP:OD1 | 30:B7:14:SER:OG | 2.29 | 0.45 |
| 35:C1:124:THR:HG21 | 35:C1:133:ALA:HB2 | 1.97 | 0.45 |
| 35:C1:297:MET:O | 35:C1:302:ARG:NH1 | 2.47 | 0.45 |
| 77:C1:602:HEA:H271 | 77:C1:602:HEA:H211 | 1.63 | 0.45 |
| 37:C3:107:ALA:HB3 | 70:C3:301:PC1:H121 | 1.97 | 0.45 |
| 44:N4:398:MET:O | 44:N4:402:ILE:HG13 | 2.15 | 0.45 |
| 45:N5:496:MET:HE1 | 68:N5:704:CDL:H431 | 1.99 | 0.45 |
| 48:QB:276:ARG:NH2 | 48:QB:466:PRO:O | 2.49 | 0.45 |
| 48:Qb:282:LEU:HD12 | 48:Qb:460:GLY:HA2 | 1.97 | 0.45 |
| 52:Qf:28:ASP:HB3 | 52:Qf:29:PRO:HD3 | 1.98 | 0.45 |
| 58:S2:410:LYS:HE2 | 58:S2:463:VAL:HG23 | 1.97 | 0.45 |
| 6:6C:15:LEU:HD13 | 36:C2:50:LEU:HB2 | 1.99 | 0.45 |
| 6:6C:73:SER:HB3 | 36:C2:143:VAL:HG21 | 1.98 | 0.45 |
| 42:N2:137:ALA:HB3 | 42:N2:138:PRO:HD3 | 1.98 | 0.45 |
| 42:N2:168:GLY:O | 42:N2:172:GLN:HG2 | 2.15 | 0.45 |
| 48:QB:388:VAL:HG21 | 48:QB:438:ALA:HA | 1.98 | 0.45 |
| 47:Qa:323:VAL:HG12 | 47:Qa:340:THR:HG22 | 1.96 | 0.45 |
| 50:Qd:228:LEU:HD11 | 50:Qd:234:PHE:HB2 | 1.98 | 0.45 |
| 59:S3:119:VAL:HG12 | 59:S3:121:THR:HG22 | 1.98 | 0.45 |
| 68:4L:201:CDL:HA61 | 21:AL:49:PHE:HA | 1.98 | 0.45 |
| 68:A8:301:CDL:H192 | 40:CB:34:VAL:HG12 | 1.97 | 0.45 |
| 35:C1:372:TYR:N | 35:C1:432:GLY:HA3 | 2.30 | 0.45 |
| 41:N1:309:ILE:HD11 | 43:N3:87:MET:HE1 | 1.98 | 0.45 |
| 45:N5:298:ILE:O | 45:N5:302:VAL:HG23 | 2.16 | 0.45 |
| 50:QD:112:ARG:HB2 | 50:QD:140:CYS:HB2 | 1.98 | 0.45 |
| 51:QE:151:LYS:HB3 | 51:QE:272:ILE:HD11 | 1.99 | 0.45 |
| 57:S1:275:PRO:HG3 | 57:S1:286:ILE:HG12 | 1.98 | 0.45 |
| 58:S2:140:PRO:HB2 | 63:S7:142:TYR:HE2 | 1.80 | 0.45 |
| 58:S2:194:THR:HB | 58:S2:206:PHE:HA | 1.98 | 0.45 |
| 2:5A:67:ILE:HG22 | 2:5A:100:ARG:HH12 | 1.82 | 0.45 |
| 15:A6:127:THR:HG23 | 59:S3:219:VAL:O | 2.16 | 0.45 |
| 71:AM:201:PLX:H82 | 71:S7:203:PLX:H72 | 1.99 | 0.45 |
| 30:B7:107:ARG:HA | 30:B7:110:GLN:HG2 | 1.97 | 0.45 |
| 33:BK:115:GLN:HG2 | 45:N5:62:ILE:HG12 | 1.98 | 0.45 |
| 47:QA:123:VAL:HB | 47:QA:133:LEU:HD23 | 1.98 | 0.45 |
| 47:QA:155:GLN:HB3 | 47:QA:198:GLY:HA2 | 1.97 | 0.45 |
| 50:QD:285:HIS:O | 50:QD:289:MET:HG3 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:Qb:501:CDL:H122 | 68:Qb:501:CDL:HB4 | 1.98 | 0.45 |
| 62:S6:70:LEU:HD13 | 64:S8:109:GLY:HA3 | 1.99 | 0.45 |
| 63:S7:59:ARG:HG3 | 63:S7:181:GLN:HB3 | 1.98 | 0.45 |
| 68:7A:102:CDL:H822 | 68:7A:102:CDL:H201 | 1.99 | 0.45 |
| 24:B1:50:ARG:HB2 | 24:B1:53:GLU:HG2 | 1.98 | 0.45 |
| 30:B7:37:ARG:NH1 | 31:B8:160:GLN:OE1 | 2.39 | 0.45 |
| 54:QH:11:MET:HE2 | 48:Qb:278:ARG:HD3 | 1.97 | 0.45 |
| 51:QK:64:LEU:HA | 51:QK:77:ARG:O | 2.16 | 0.45 |
| 47:Qa:379:LYS:HG2 | 47:Qa:413:LEU:HD22 | 1.99 | 0.45 |
| 57:S1:224:ASP:OD2 | 57:S1:291:ARG:NH2 | 2.47 | 0.45 |
| 1:4L:55:LEU:HD13 | 61:S5:17:TRP:HE3 | 1.82 | 0.45 |
| 20:AK:51:THR:HG21 | 20:AK:153:LEU:HD22 | 1.98 | 0.45 |
| 20:AK:85:LEU:HD22 | 20:AK:158:GLY:HA3 | 1.99 | 0.45 |
| 41:N1:114:TYR:OH | 46:N6:61:LEU:O | 2.23 | 0.45 |
| 41:N1:117:LEU:HD11 | 46:N6:65:LEU:HD12 | 1.97 | 0.45 |
| 42:N2:193:VAL:HG21 | 42:N2:266:ILE:HG12 | 1.99 | 0.45 |
| 51:QE:193:SER:OG | 51:QE:194:GLN:OE1 | 2.34 | 0.45 |
| 49:Qc:200:LEU:CD2 | 80:Qc:403:HEM:HAA1 | 2.46 | 0.45 |
| 49:Qc:361:ILE:HG12 | 49:Qc:365:LEU:HD12 | 1.97 | 0.45 |
| 63:S7:107:GLY:HA2 | 83:S7:202:SF4:S4 | 2.57 | 0.45 |
| 65:V1:141:GLY:HA3 | 65:V1:248:VAL:O | 2.15 | 0.45 |
| 75:AC:201:ZMP:H5A | 32:B9:109:ALA:HB1 | 1.99 | 0.45 |
| 20:AK:343:PRO:HB2 | 39:CA:34:PRO:HB3 | 1.98 | 0.45 |
| 40:CB:2:THR:HB | 40:CB:5:SER:HB3 | 1.98 | 0.45 |
| 42:N2:220:ILE:HG22 | 42:N2:323:MET:HE1 | 1.99 | 0.45 |
| 73:N3:201:PEE:H22 | 73:N3:201:PEE:H27 | 1.72 | 0.45 |
| 47:QA:51:SER:OG | 47:QA:230:LEU:HD12 | 2.17 | 0.45 |
| 48:QB:86:ASN:HA | 48:QB:211:LEU:HD21 | 1.97 | 0.45 |
| 51:QE:211:VAL:HG21 | 51:QE:246:SER:HA | 1.97 | 0.45 |
| 71:Qi:301:PLX:H1A3 | 71:Qi:301:PLX:H22 | 1.63 | 0.45 |
| 57:S1:169:VAL:HG22 | 57:S1:223:ILE:HD11 | 1.97 | 0.45 |
| 57:S1:262:VAL:HG23 | 57:S1:276:ARG:HB2 | 1.99 | 0.45 |
| 57:S1:296:GLY:O | 57:S1:572:HIS:NE2 | 2.41 | 0.45 |
| 57:S1:385:TYR:OH | 57:S1:527:ASP:OD1 | 2.31 | 0.45 |
| 3:5B:81:PRO:O | 3:5B:87:ARG:NH1 | 2.48 | 0.45 |
| 68:7A:102:CDL:H111 | 68:7A:102:CDL:H722 | 1.98 | 0.45 |
| 22:AM:60:ARG:HH22 | 22:AM:95:ASP:HA | 1.82 | 0.45 |
| 26:B3:18:ASP:O | 26:B3:21:GLN:HG2 | 2.17 | 0.45 |
| 37:C3:171:VAL:HG22 | 68:C3:305:CDL:H232 | 1.98 | 0.45 |
| 49:QC:70:CYS:SG | 49:QC:80:ARG:HD2 | 2.57 | 0.45 |
| 51:QE:228:ALA:HB3 | 51:QE:235:TYR:HB3 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 60:S4:131:LYS:NZ | 60:S4:132:GLU:OE2 | 2.48 | 0.45 |
| 1:4L:79:VAL:HG12 | 46:N6:74:MET:HE3 | 1.98 | 0.45 |
| 4:6A:59:PHE:HB2 | 4:6A:94:TYR:HE2 | 1.81 | 0.45 |
| 35:C1:361:SER:O | 35:C1:365:ILE:HG12 | 2.16 | 0.45 |
| 35:C1:383:MET:HG2 | 35:C1:421:VAL:HB | 1.99 | 0.45 |
| 45:N5:265:PRO:O | 45:N5:269:THR:HG23 | 2.15 | 0.45 |
| 52:QF:65:GLU:HG3 | 54:QH:73:LYS:NZ | 2.32 | 0.45 |
| 58:S2:203:MET:O | 58:S2:206:PHE:HB3 | 2.16 | 0.45 |
| 58:S2:272:ARG:NH1 | 73:S8:303:PEE:H2 | 2.27 | 0.45 |
| 63:S7:188:LYS:HB3 | 63:S7:191:ARG:HE | 1.82 | 0.45 |
| 37:C3:181:TYR:HE2 | 70:C3:306:PC1:H271 | 1.82 | 0.45 |
| 37:C3:204:HIS:NE2 | 37:C3:249:TRP:HB2 | 2.32 | 0.45 |
| 48:Qb:315:ASP:OD1 | 48:Qb:316:SER:N | 2.50 | 0.45 |
| 49:Qc:300:ILE:HD11 | 49:Qc:363:LEU:HD21 | 1.99 | 0.45 |
| 58:S2:160:ALA:HA | 58:S2:404:THR:HG21 | 1.99 | 0.45 |
| 73:S2:501:PEE:H34 | 73:S2:501:PEE:H27 | 1.73 | 0.45 |
| 65:V1:261:TRP:NE1 | 65:V1:265:PHE:HE2 | 2.13 | 0.45 |
| 4:6A:65:LEU:HD22 | 37:C3:190:ASP:HB3 | 1.99 | 0.44 |
| 7:7A:66:TYR:HB2 | 72:7A:101:3PE:H232 | 1.99 | 0.44 |
| 19:AB:93:ILE:HD12 | 19:AB:108:LEU:HD13 | 1.99 | 0.44 |
| 19:AC:120:MET:HE1 | 32:B9:66:LEU:HB3 | 1.99 | 0.44 |
| 20:AK:112:GLY:HA2 | 20:AK:136:TRP:CD2 | 2.52 | 0.44 |
| 29:B6:143:HIS:HE1 | 45:N5:1:MET:HB2 | 1.82 | 0.44 |
| 35:C1:409:TRP:HB3 | 35:C1:471:ILE:HG12 | 1.98 | 0.44 |
| 71:N4:502:PLX:H191 | 68:N5:703:CDL:H242 | 1.98 | 0.44 |
| 53:QG:19:LYS:NZ | 53:QG:85:GLU:OE2 | 2.40 | 0.44 |
| 47:Qa:90:THR:HG23 | 47:Qa:95:SER:HA | 1.98 | 0.44 |
| 48:Qb:192:PHE:O | 48:Qb:195:THR:OG1 | 2.31 | 0.44 |
| 58:S2:187:LEU:HD23 | 58:S2:213:ARG:HG2 | 1.99 | 0.44 |
| 1:4L:62:ILE:HG21 | 42:N2:31:ILE:HD11 | 1.99 | 0.44 |
| 22:AM:75:TRP:HE1 | 71:AM:201:PLX:H11 | 1.82 | 0.44 |
| 24:B1:29:ARG:NH2 | 71:B1:101:PLX:O2 | 2.51 | 0.44 |
| 68:B4:201:CDL:HA62 | 68:B4:201:CDL:H521 | 1.98 | 0.44 |
| 33:BK:107:GLN:NE2 | 45:N5:194:ASN:HD22 | 2.14 | 0.44 |
| 34:BL:90:VAL:HG22 | 44:N4:28:THR:HG21 | 1.98 | 0.44 |
| 42:N2:111:PHE:HA | 45:N5:591:PHE:CE1 | 2.52 | 0.44 |
| 73:N5:705:PEE:H76 | 73:N5:705:PEE:H71 | 1.70 | 0.44 |
| 46:N6:39:VAL:O | 46:N6:43:ILE:HG13 | 2.18 | 0.44 |
| 47:QA:91:THR:HG21 | 47:QA:140:VAL:HA | 1.99 | 0.44 |
| 49:QC:307:LEU:HD11 | 49:QC:363:LEU:HD23 | 1.98 | 0.44 |
| 48:Qb:388:VAL:O | 48:Qb:392:LYS:HG3 | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:Qe:133:VAL:HG12 | 73:Qe:301:PEE:H57 | 1.99 | 0.44 |
| 20:AK:134:GLN:HE22 | 76:AK:401:ADP:HN62 | 1.65 | 0.44 |
| 30:B7:44:GLN:NE2 | 30:B7:48:ASP:OD1 | 2.50 | 0.44 |
| 30:B7:103:GLU:OE2 | 30:B7:106:ARG:NH2 | 2.43 | 0.44 |
| 51:Qe:201:ASP:C | 51:Qe:203:GLU:H | 2.25 | 0.44 |
| 19:AB:140:CYS:O | 19:AB:144:ILE:HG12 | 2.16 | 0.44 |
| 70:C1:610:PC1:H321 | 70:C1:610:PC1:H291 | 2.00 | 0.44 |
| 36:C2:111:THR:O | 36:C2:111:THR:OG1 | 2.29 | 0.44 |
| 44:N4:204:MET:O | 44:N4:208:PRO:HA | 2.18 | 0.44 |
| 45:N5:3:PRO:HB2 | 45:N5:53:MET:HE1 | 1.99 | 0.44 |
| 64:S8:100:GLU:OE2 | 64:S8:185:TYR:OH | 2.33 | 0.44 |
| 66:V2:245:VAL:HG13 | 66:V2:249:LEU:HD13 | 1.99 | 0.44 |
| 3:5B:41:GLU:HG2 | 3:5B:56:ARG:HH22 | 1.83 | 0.44 |
| 18:A9:246:SER:O | 18:A9:250:ILE:HG12 | 2.17 | 0.44 |
| 36:C2:158:ASP:OD1 | 36:C2:158:ASP:N | 2.50 | 0.44 |
| 46:N6:129:ASP:HB2 | 61:S5:32:ARG:NH1 | 2.32 | 0.44 |
| 54:QH:19:LEU:HG | 54:QH:20:SER:H | 1.81 | 0.44 |
| 57:S1:131:CYS:O | 57:S1:241:ARG:NH1 | 2.33 | 0.44 |
| 73:S2:501:PEE:H71 | 73:S2:501:PEE:H76 | 1.79 | 0.44 |
| 65:V1:192:ASP:HB3 | 67:V3:411:MET:SD | 2.58 | 0.44 |
| 24:B1:32:ASP:OD1 | 28:B5:135:LYS:NZ | 2.38 | 0.44 |
| 70:C3:301:PC1:H142 | 70:C3:301:PC1:H111 | 1.83 | 0.44 |
| 41:N1:169:GLN:HB3 | 41:N1:244:GLY:HA3 | 1.98 | 0.44 |
| 44:N4:221:VAL:HA | 44:N4:283:LYS:HD3 | 1.98 | 0.44 |
| 46:N6:82:VAL:HG22 | 46:N6:83:TRP:H | 1.83 | 0.44 |
| 47:Qa:134:MET:SD | 47:Qa:233:VAL:HG21 | 2.57 | 0.44 |
| 50:Qd:216:LEU:HB3 | 50:Qd:249:ILE:HD11 | 1.98 | 0.44 |
| 57:S1:124:HIS:CG | 57:S1:125:PRO:HD2 | 2.53 | 0.44 |
| 57:S1:155:GLU:OE2 | 65:V1:398:ARG:NH2 | 2.41 | 0.44 |
| 1:4L:55:LEU:HD23 | 1:4L:55:LEU:HA | 1.87 | 0.44 |
| 12:A2:85:ASP:OD1 | 12:A2:85:ASP:N | 2.51 | 0.44 |
| 17:A8:157:GLU:HB2 | 17:A8:158:PRO:HD3 | 2.00 | 0.44 |
| 25:B2:79:MET:SD | 45:N5:375:ILE:HG12 | 2.58 | 0.44 |
| 72:CA:101:3PE:H261 | 72:CA:101:3PE:H2A2 | 1.99 | 0.44 |
| 40:CB:51:ARG:CZ | 42:N2:322:GLN:HG2 | 2.48 | 0.44 |
| 45:N5:407:TRP:O | 45:N5:411:MET:HG2 | 2.17 | 0.44 |
| 46:N6:24:PRO:HG3 | 46:N6:83:TRP:CE2 | 2.52 | 0.44 |
| 51:QE:241:SER:OG | 82:QE:303:FES:S1 | 2.69 | 0.44 |
| 49:Qc:24:PRO:HB2 | 49:Qc:27:ILE:HG23 | 1.99 | 0.44 |
| 57:S1:43:VAL:HG21 | 57:S1:96:VAL:HG21 | 1.99 | 0.44 |
| 57:S1:338:VAL:O | 57:S1:365:SER:HB2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:S1:401:LEU:HD11 | 57:S1:432:ILE:HG13 | 1.99 | 0.44 |
| 5:6B:58:ARG:HA | 5:6B:61:TYR:CD1 | 2.53 | 0.44 |
| 9:7C:18:HIS:CD2 | 9:7C:18:HIS:H | 2.35 | 0.44 |
| 18:A9:64:PHE:HZ | 18:A9:208:GLY:HA3 | 1.83 | 0.44 |
| 42:N2:235:ASN:O | 42:N2:315:TRP:NE1 | 2.51 | 0.44 |
| 51:QE:156:LEU:HB3 | 51:QE:210:TRP:CZ2 | 2.53 | 0.44 |
| 55:QI:48:ASN:ND2 | 50:Qd:105:SER:H | 2.16 | 0.44 |
| 50:Qd:209:GLU:H | 50:Qd:209:GLU:HG2 | 1.48 | 0.44 |
| 57:S1:76:ARG:O | 57:S1:116:VAL:HG21 | 2.18 | 0.44 |
| 57:S1:180:THR:N | 83:S1:802:SF4:S4 | 2.85 | 0.44 |
| 71:S7:203:PLX:H393 | 71:S7:203:PLX:H362 | 1.84 | 0.44 |
| 64:S8:153:ILE:HG12 | 83:S8:302:SF4:S1 | 2.58 | 0.44 |
| 66:V2:93:LEU:HD12 | 66:V2:122:TYR:HB3 | 2.00 | 0.44 |
| 1:4L:2:PRO:HG3 | 46:N6:127:ILE:HD13 | 1.98 | 0.44 |
| 68:B4:201:CDL:H1 | 68:B4:201:CDL:H512 | 2.00 | 0.44 |
| 35:C1:352:GLY:HA3 | 77:C1:602:HEA:H162 | 1.99 | 0.44 |
| 41:N1:87:VAL:HG22 | 41:N1:88:PRO:HD3 | 2.00 | 0.44 |
| 41:N1:293:PHE:HE1 | 73:S8:303:PEE:H7 | 1.83 | 0.44 |
| 47:QA:147:ARG:HD3 | 47:QA:149:TRP:CZ2 | 2.52 | 0.44 |
| 48:QB:310:ILE:HD11 | 48:QB:388:VAL:HA | 1.99 | 0.44 |
| 54:QH:20:SER:O | 54:QH:24:GLN:HG2 | 2.18 | 0.44 |
| 48:Qb:120:LEU:HD13 | 48:Qb:133:ILE:HG12 | 2.00 | 0.44 |
| 48:Qb:195:THR:HG21 | 48:Qb:269:ARG:H | 1.83 | 0.44 |
| 48:Qb:225:LYS:HE2 | 48:Qb:225:LYS:HB3 | 1.79 | 0.44 |
| 49:Qc:216:ASP:CG | 50:Qd:318:ARG:HH22 | 2.26 | 0.44 |
| 53:Qg:79:GLU:H | 53:Qg:79:GLU:HG3 | 1.48 | 0.44 |
| 56:Qj:41:ILE:H | 56:Qj:41:ILE:HD12 | 1.83 | 0.44 |
| 2:5A:104:PHE:N | 38:C4:66:GLU:OE2 | 2.48 | 0.43 |
| 7:7A:60:CYS:SG | 37:C3:19:THR:HG23 | 2.58 | 0.43 |
| 72:7A:101:3PE:H342 | 72:7A:101:3PE:H291 | 2.00 | 0.43 |
| 11:A1:31:ASN:OD1 | 11:A1:60:TYR:OH | 2.23 | 0.43 |
| 14:A5:59:VAL:HG23 | 14:A5:68:LEU:HD21 | 1.99 | 0.43 |
| 14:A5:75:GLY:O | 16:A7:103:ARG:NH2 | 2.50 | 0.43 |
| 68:AK:402:CDL:H382 | 42:N2:133:TRP:HZ3 | 1.83 | 0.43 |
| 24:B1:30:ARG:O | 24:B1:33:GLU:HG2 | 2.18 | 0.43 |
| 29:B6:82:TRP:O | 29:B6:86:GLN:HG2 | 2.18 | 0.43 |
| 29:B6:122:TYR:HD2 | 29:B6:124:THR:H | 1.66 | 0.43 |
| 35:C1:287:VAL:O | 35:C1:290:HIS:HD2 | 2.00 | 0.43 |
| 41:N1:233:MET:HE3 | 41:N1:233:MET:HB3 | 1.88 | 0.43 |
| 48:QB:148:ALA:O | 48:QB:152:GLN:HB2 | 2.18 | 0.43 |
| 56:QJ:9:ARG:HD3 | 53:Qg:109:ALA:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:S1:594:ALA:O | 57:S1:605:GLN:HA | 2.17 | 0.43 |
| 2:5A:70:TRP:CH2 | 3:5B:117:GLY:HA2 | 2.53 | 0.43 |
| 73:N3:201:PEE:H30 | 73:N3:201:PEE:H36 | 1.70 | 0.43 |
| 45:N5:174:TYR:CD2 | 45:N5:232:TRP:HB3 | 2.53 | 0.43 |
| 45:N5:559:GLU:O | 45:N5:564:LYS:HB2 | 2.18 | 0.43 |
| 50:Qd:244:ALA:HB3 | 81:Qd:401:HEC:HBD2 | 2.00 | 0.43 |
| 58:S2:374:ARG:NH1 | 64:S8:162:CYS:O | 2.38 | 0.43 |
| 5:6B:37:PHE:CE1 | 5:6B:58:ARG:HB2 | 2.54 | 0.43 |
| 20:AK:37:ARG:C | 20:AK:39:GLN:H | 2.25 | 0.43 |
| 20:AK:127:ASP:O | 20:AK:132:ARG:NH1 | 2.50 | 0.43 |
| 35:C1:96:ARG:NE | 70:C1:610:PC1:O14 | 2.44 | 0.43 |
| 41:N1:157:ASN:OD1 | 41:N1:168:THR:OG1 | 2.28 | 0.43 |
| 42:N2:249:LEU:HD22 | 42:N2:254:LEU:HD12 | 2.00 | 0.43 |
| 45:N5:120:TYR:OH | 68:N5:703:CDL:OA4 | 2.33 | 0.43 |
| 46:N6:77:GLU:N | 46:N6:77:GLU:OE1 | 2.51 | 0.43 |
| 68:QB:501:CDL:H572 | 71:Qi:301:PLX:H291 | 2.00 | 0.43 |
| 52:QF:71:LEU:HD22 | 50:Qd:223:PRO:HG3 | 2.01 | 0.43 |
| 53:Qg:36:ASP:OD1 | 53:Qg:90:TYR:OH | 2.20 | 0.43 |
| 57:S1:611:THR:HG21 | 60:S4:105:GLU:HA | 2.00 | 0.43 |
| 65:V1:146:GLY:HA3 | 65:V1:193:PHE:CE1 | 2.52 | 0.43 |
| 2:5A:92:ASP:OD1 | 2:5A:135:THR:OG1 | 2.36 | 0.43 |
| 13:A3:110:ILE:HD11 | 73:S8:303:PEE:H36 | 2.01 | 0.43 |
| 16:A7:28:TYR:CZ | 22:AM:55:PHE:HB3 | 2.54 | 0.43 |
| 18:A9:198:ALA:O | 18:A9:260:GLY:HA2 | 2.18 | 0.43 |
| 38:C4:70:TRP:HA | 38:C4:73:LEU:HG | 2.00 | 0.43 |
| 49:QC:97:HIS:CD2 | 80:QC:402:HEM:NC | 2.86 | 0.43 |
| 49:QC:131:TYR:O | 49:QC:134:PRO:HD2 | 2.18 | 0.43 |
| 58:S2:150:MET:SD | 58:S2:228:MET:HB2 | 2.58 | 0.43 |
| 7:7A:54:ARG:HD2 | 45:N5:499:MET:HE2 | 2.00 | 0.43 |
| 16:A7:42:PRO:HG3 | 23:AN:6:VAL:HG11 | 1.99 | 0.43 |
| 68:A8:301:CDL:H202 | 68:A8:301:CDL:H781 | 2.01 | 0.43 |
| 19:AC:128:PHE:HZ | 19:AC:148:ILE:HG12 | 1.82 | 0.43 |
| 75:AC:201:ZMP:H11A | 32:B9:58:VAL:CG2 | 2.49 | 0.43 |
| 26:B3:47:ARG:HA | 26:B3:50:ALA:HB3 | 1.99 | 0.43 |
| 30:B7:15:LYS:HG2 | 30:B7:113:LYS:HG3 | 2.01 | 0.43 |
| 35:C1:71:MET:HB2 | 35:C1:72:PRO:HD3 | 2.01 | 0.43 |
| 41:N1:21:THR:HG21 | 85:S7:201:U10:H311 | 2.01 | 0.43 |
| 41:N1:295:PRO:HB3 | 73:N3:201:PEE:H26 | 2.00 | 0.43 |
| 68:N1:401:CDL:H511 | 46:N6:83:TRP:HZ3 | 1.84 | 0.43 |
| 44:N4:405:LEU:HD21 | 45:N5:173:LEU:HD12 | 1.99 | 0.43 |
| 45:N5:162:THR:O | 45:N5:166:THR:HG23 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:N6:24:PRO:O | 46:N6:81:GLU:HB2 | 2.19 | 0.43 |
| 50:QD:105:SER:H | 55:Qi:48:ASN:ND2 | 2.16 | 0.43 |
| 51:QE:239:HIS:HB2 | 82:QE:303:FES:S1 | 2.59 | 0.43 |
| 51:QK:20:ARG:HH11 | 51:QK:23:ALA:HA | 1.84 | 0.43 |
| 49:Qc:350:ILE:HG12 | 72:Qc:404:3PE:H352 | 1.99 | 0.43 |
| 51:Qe:241:SER:OG | 82:Qe:303:FES:S2 | 2.56 | 0.43 |
| 58:S2:149:SER:HA | 58:S2:184:THR:HG22 | 2.00 | 0.43 |
| 63:S7:53:LEU:HD13 | 71:S7:203:PLX:H322 | 2.00 | 0.43 |
| 7:7A:29:LYS:HZ2 | 70:C3:303:PC1:H3F2 | 1.84 | 0.43 |
| 72:7A:101:3PE:H3C2 | 37:C3:41:LEU:HB2 | 2.01 | 0.43 |
| 9:7C:36:ARG:HH22 | 73:7C:101:PEE:H3 | 1.84 | 0.43 |
| 14:A5:9:THR:HG23 | 14:A5:16:VAL:HG22 | 2.01 | 0.43 |
| 23:AN:24:ASN:ND2 | 23:AN:24:ASN:O | 2.51 | 0.43 |
| 32:B9:123:ILE:HD13 | 32:B9:129:GLY:HA3 | 2.01 | 0.43 |
| 77:C1:601:HEA:H212 | 77:C1:601:HEA:H271 | 1.52 | 0.43 |
| 44:N4:70:THR:HA | 44:N4:103:GLN:HE21 | 1.83 | 0.43 |
| 44:N4:357:THR:O | 44:N4:361:VAL:HG23 | 2.19 | 0.43 |
| 57:S1:338:VAL:HB | 57:S1:363:SER:HB2 | 2.00 | 0.43 |
| 57:S1:638:THR:O | 57:S1:642:VAL:HG23 | 2.19 | 0.43 |
| 37:C3:212:SER:HB2 | 68:C3:305:CDL:H242 | 2.00 | 0.43 |
| 44:N4:243:MET:HB3 | 44:N4:301:ILE:HG21 | 2.00 | 0.43 |
| 45:N5:233:LEU:HB3 | 45:N5:234:PRO:HD3 | 2.00 | 0.43 |
| 45:N5:289:ALA:O | 45:N5:293:ILE:HG23 | 2.19 | 0.43 |
| 48:QB:467:ASP:OD2 | 49:QC:223:TYR:OH | 2.28 | 0.43 |
| 49:QC:318:ARG:O | 49:QC:322:GLN:HG3 | 2.19 | 0.43 |
| 70:Qc:405:PC1:H2E1 | 70:Qc:405:PC1:H3D2 | 2.00 | 0.43 |
| 58:S2:150:MET:HE3 | 58:S2:150:MET:HB2 | 1.93 | 0.43 |
| 65:V1:315:LEU:HB2 | 65:V1:359:ARG:HA | 2.00 | 0.43 |
| 1:4L:16:LEU:HD23 | 68:4L:201:CDL:H862 | 2.01 | 0.43 |
| 20:AK:38:LEU:O | 20:AK:39:GLN:HG2 | 2.18 | 0.43 |
| 20:AK:88:PHE:HB2 | 20:AK:161:LEU:HD23 | 2.00 | 0.43 |
| 71:AL:202:PLX:H131 | 68:N4:503:CDL:H121 | 2.01 | 0.43 |
| 27:B4:48:LEU:HB3 | 32:B9:208:LEU:HD13 | 2.01 | 0.43 |
| 41:N1:180:PRO:HB3 | 73:S8:303:PEE:H21 | 2.01 | 0.43 |
| 42:N2:135:LYS:O | 42:N2:139:LEU:HD12 | 2.19 | 0.43 |
| 47:QA:123:VAL:HG13 | 47:QA:137:LEU:HD13 | 1.99 | 0.43 |
| 47:Qa:51:SER:HB3 | 47:Qa:230:LEU:HD12 | 2.00 | 0.43 |
| 49:Qc:30:TRP:HB3 | 49:Qc:100:ARG:HG3 | 2.00 | 0.43 |
| 57:S1:144:MET:HG3 | 58:S2:389:LYS:HG3 | 2.00 | 0.43 |
| 58:S2:147:TYR:CB | 63:S7:71:CYS:HB3 | 2.49 | 0.43 |
| 63:S7:196:ARG:NE | 72:S7:204:3PE:O14 | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:V1:384:PRO:HB2 | 65:V1:423:THR:HG22 | 2.00 | 0.43 |
| 6:6C:37:TYR:CZ | 36:C2:28:LEU:HD23 | 2.53 | 0.43 |
| 12:A2:57:GLU:O | 57:S1:655:ARG:NH2 | 2.51 | 0.43 |
| 23:AN:68:ARG:O | 23:AN:72:MET:HG3 | 2.18 | 0.43 |
| 30:B7:22:MET:HE1 | 30:B7:102:PHE:HD2 | 1.84 | 0.43 |
| 33:BK:107:GLN:HE22 | 45:N5:194:ASN:ND2 | 2.14 | 0.43 |
| 35:C1:37:ILE:HG22 | 77:C1:601:HEA:HMA | 2.01 | 0.43 |
| 37:C3:133:ASN:HB3 | 37:C3:173:PHE:HE2 | 1.82 | 0.43 |
| 41:N1:142:TYR:CD1 | 41:N1:142:TYR:C | 2.97 | 0.43 |
| 45:N5:96:VAL:O | 45:N5:100:ILE:HG12 | 2.19 | 0.43 |
| 45:N5:172:ILE:O | 45:N5:176:ARG:HG2 | 2.18 | 0.43 |
| 47:QA:89:LEU:HD11 | 47:QA:154:LEU:HD12 | 2.00 | 0.43 |
| 47:QA:177:LEU:HD21 | 47:QA:272:VAL:HG11 | 2.01 | 0.43 |
| 47:QA:291:HIS:CD2 | 47:QA:378:LEU:HD13 | 2.54 | 0.43 |
| 49:QC:102:LEU:HD22 | 49:QC:304:MET:HE2 | 2.00 | 0.43 |
| 47:Qa:63:LEU:HD23 | 47:Qa:141:THR:HG21 | 2.00 | 0.43 |
| 57:S1:428:LYS:HE2 | 57:S1:465:ILE:HD13 | 2.00 | 0.43 |
| 57:S1:695:TYR:HE2 | 57:S1:714:VAL:HG11 | 1.84 | 0.43 |
| 65:V1:85:LEU:HD21 | 65:V1:247:THR:HG23 | 2.00 | 0.43 |
| 68:4L:201:CDL:H191 | 68:4L:201:CDL:H152 | 2.00 | 0.43 |
| 18:A9:201:ILE:HG22 | 18:A9:203:PRO:HD3 | 2.01 | 0.43 |
| 19:AC:112:SER:HB2 | 32:B9:59:LEU:HD21 | 2.00 | 0.43 |
| 22:AM:61:TRP:HB3 | 64:S8:89:GLU:HG2 | 2.01 | 0.43 |
| 35:C1:229:ILE:HD11 | 36:C2:175:ILE:HG12 | 2.01 | 0.43 |
| 35:C1:313:ALA:HB3 | 36:C2:73:LEU:HD11 | 1.99 | 0.43 |
| 70:C1:610:PC1:H371 | 37:C3:50:ASN:HD21 | 1.83 | 0.43 |
| 68:N1:401:CDL:H752 | 68:N1:401:CDL:H782 | 1.83 | 0.43 |
| 45:N5:2:ASN:ND2 | 45:N5:59:GLN:OE1 | 2.52 | 0.43 |
| 45:N5:341:MET:SD | 45:N5:457:LEU:HD12 | 2.59 | 0.43 |
| 51:QE:125:VAL:HG21 | 71:Qi:301:PLX:H101 | 2.00 | 0.43 |
| 51:QE:178:HIS:CE1 | 51:QE:209:GLU:HB2 | 2.54 | 0.43 |
| 55:QI:11:TYR:OH | 48:Qb:451:ASP:OD2 | 2.29 | 0.43 |
| 73:Qe:301:PEE:H48 | 73:Qe:301:PEE:H13 | 2.00 | 0.43 |
| 57:S1:246:ARG:HH12 | 60:S4:123:ASN:ND2 | 2.17 | 0.43 |
| 62:S6:39:THR:HG22 | 62:S6:62:VAL:HG22 | 2.01 | 0.43 |
| 65:V1:415:ILE:O | 65:V1:419:ILE:HG13 | 2.19 | 0.43 |
| 7:7A:54:ARG:HE | 45:N5:503:GLU:HG2 | 1.84 | 0.42 |
| 7:7A:75:SER:HA | 35:C1:118:VAL:HA | 2.00 | 0.42 |
| 13:A3:135:PRO:HB2 | 23:AN:69:ILE:HD11 | 2.01 | 0.42 |
| 18:A9:236:VAL:HG22 | 18:A9:272:LEU:HD23 | 2.01 | 0.42 |
| 44:N4:412:ILE:HA | 44:N4:416:ARG:HD2 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:N5:375:ILE:HD12 | 45:N5:458:LEU:HD11 | 2.01 | 0.42 |
| 48:Qb:74:TRP:CZ2 | 48:Qb:411:GLU:HA | 2.54 | 0.42 |
| 57:S1:394:VAL:HA | 57:S1:473:MET:HE1 | 2.01 | 0.42 |
| 60:S4:133:ASP:N | 60:S4:133:ASP:OD1 | 2.52 | 0.42 |
| 4:6A:88:ASN:OD1 | 70:6A:101:PC1:H141 | 2.19 | 0.42 |
| 71:AM:201:PLX:H182 | 41:N1:19:PHE:HZ | 1.84 | 0.42 |
| 28:B5:71:MET:HE3 | 44:N4:442:LEU:HD11 | 2.01 | 0.42 |
| 38:C4:39:VAL:HG22 | 38:C4:41:ARG:HG3 | 2.01 | 0.42 |
| 41:N1:197:PRO:HB3 | 41:N1:278:PRO:O | 2.18 | 0.42 |
| 42:N2:91:ASN:HD21 | 46:N6:117:PHE:HE1 | 1.67 | 0.42 |
| 45:N5:503:GLU:O | 45:N5:507:THR:HG23 | 2.20 | 0.42 |
| 58:S2:405:ALA:HB1 | 58:S2:412:GLU:HG3 | 2.01 | 0.42 |
| 65:V1:112:TYR:CD1 | 65:V1:153:ALA:HB3 | 2.54 | 0.42 |
| 66:V2:59:ASN:HD21 | 66:V2:89:GLN:HB2 | 1.84 | 0.42 |
| 19:AC:112:SER:HB3 | 32:B9:59:LEU:HD11 | 2.02 | 0.42 |
| 20:AK:328:ARG:HH21 | 34:BL:58:ASP:CG | 2.27 | 0.42 |
| 25:B2:59:ARG:HH12 | 26:B3:48:ASN:HA | 1.83 | 0.42 |
| 25:B2:65:THR:HG22 | 25:B2:67:SER:H | 1.84 | 0.42 |
| 30:B7:95:TYR:CZ | 31:B8:156:VAL:HG11 | 2.55 | 0.42 |
| 39:CA:55:TRP:O | 39:CA:59:ILE:HG12 | 2.19 | 0.42 |
| 47:QA:125:CYS:HB3 | 47:QA:133:LEU:HD22 | 2.01 | 0.42 |
| 47:QA:183:ARG:NH1 | 47:Qa:452:GLU:OE1 | 2.52 | 0.42 |
| 48:QB:426:LEU:HD12 | 48:QB:426:LEU:HA | 1.87 | 0.42 |
| 51:QE:178:HIS:HB2 | 51:QE:210:TRP:CZ3 | 2.54 | 0.42 |
| 57:S1:476:LEU:HD22 | 57:S1:493:VAL:HG21 | 2.01 | 0.42 |
| 58:S2:112:VAL:HG21 | 58:S2:453:VAL:HG21 | 2.02 | 0.42 |
| 19:AC:90:TYR:CE1 | 26:B3:44:PRO:HB2 | 2.54 | 0.42 |
| 21:AL:36:VAL:HG22 | 68:AL:201:CDL:H742 | 2.01 | 0.42 |
| 25:B2:64:LEU:HD13 | 25:B2:69:LEU:HD21 | 2.01 | 0.42 |
| 28:B5:75:ILE:HD12 | 68:B5:201:CDL:H871 | 2.00 | 0.42 |
| 29:B6:157:VAL:HG22 | 45:N5:63:ILE:HG23 | 2.01 | 0.42 |
| 32:B9:119:PRO:HB3 | 45:N5:525:MET:HE2 | 2.01 | 0.42 |
| 37:C3:141:GLY:O | 37:C3:144:ILE:HG22 | 2.19 | 0.42 |
| 41:N1:101:GLY:O | 41:N1:105:MET:HG3 | 2.19 | 0.42 |
| 51:QE:178:HIS:HE1 | 51:QE:209:GLU:HB2 | 1.83 | 0.42 |
| 53:QG:36:ASP:OD2 | 53:QG:62:ARG:NH1 | 2.50 | 0.42 |
| 49:Qc:97:HIS:HD2 | 80:Qc:403:HEM:C1C | 2.37 | 0.42 |
| 49:Qc:112:THR:HG22 | 49:Qc:196:HIS:CE1 | 2.54 | 0.42 |
| 58:S2:62:LYS:O | 58:S2:66:HIS:ND1 | 2.48 | 0.42 |
| 59:S3:120:PRO:HB3 | 60:S4:137:PHE:CE1 | 2.55 | 0.42 |
| 64:S8:100:GLU:O | 64:S8:170:GLY:N | 2.46 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:V1:98:LYS:O | 65:V1:101:PHE:HB2 | 2.19 | 0.42 |
| 66:V2:59:ASN:ND2 | 66:V2:89:GLN:HB2 | 2.34 | 0.42 |
| 17:A8:246:PHE:HE1 | 68:A8:301:CDL:H341 | 1.83 | 0.42 |
| 20:AK:284:PRO:O | 20:AK:288:GLN:HG2 | 2.20 | 0.42 |
| 28:B5:90:ASN:ND2 | 68:B5:201:CDL:OA7 | 2.42 | 0.42 |
| 29:B6:134:HIS:NE2 | 45:N5:35:TYR:OH | 2.36 | 0.42 |
| 38:C4:149:LYS:HB3 | 38:C4:152:PRO:HB3 | 2.01 | 0.42 |
| 41:N1:293:PHE:O | 41:N1:297:THR:OG1 | 2.34 | 0.42 |
| 47:QA:290:GLN:HG2 | 47:QA:295:ALA:HB2 | 2.01 | 0.42 |
| 48:QB:179:MET:HE1 | 48:QB:282:LEU:HD13 | 2.01 | 0.42 |
| 52:QF:56:ARG:O | 52:QF:60:ARG:HG3 | 2.19 | 0.42 |
| 54:QH:49:VAL:O | 54:QH:52:PRO:HD2 | 2.19 | 0.42 |
| 51:QK:71:ASN:OD1 | 51:QK:71:ASN:N | 2.52 | 0.42 |
| 48:Qb:79:SER:HB3 | 48:Qb:126:ARG:HA | 2.02 | 0.42 |
| 5:6B:34:TYR:OH | 5:6B:74:ASP:OD1 | 2.24 | 0.42 |
| 33:BK:35:LYS:HE3 | 33:BK:35:LYS:HB3 | 1.90 | 0.42 |
| 35:C1:33:LEU:O | 35:C1:37:ILE:HG13 | 2.19 | 0.42 |
| 45:N5:290:LEU:O | 45:N5:523:SER:OG | 2.37 | 0.42 |
| 49:Qc:267:HIS:CD2 | 49:Qc:269:LYS:HG2 | 2.54 | 0.42 |
| 58:S2:230:ALA:O | 64:S8:98:ARG:NH2 | 2.52 | 0.42 |
| 64:S8:99:GLY:O | 64:S8:169:GLU:HG2 | 2.19 | 0.42 |
| 65:V1:51:TRP:CD1 | 67:V3:388:ASN:HD22 | 2.38 | 0.42 |
| 73:7C:101:PEE:H34 | 73:7C:101:PEE:H40 | 1.76 | 0.42 |
| 14:A5:104:VAL:HG23 | 59:S3:71:LYS:HG2 | 2.00 | 0.42 |
| 17:A8:202:LEU:HD13 | 23:AN:70:ALA:HB2 | 2.01 | 0.42 |
| 23:AN:141:ILE:HA | 70:N1:402:PC1:H153 | 2.01 | 0.42 |
| 25:B2:90:ASP:OD1 | 25:B2:90:ASP:N | 2.52 | 0.42 |
| 36:C2:37:LEU:O | 36:C2:41:ILE:HG12 | 2.20 | 0.42 |
| 42:N2:190:MET:HG2 | 42:N2:204:ASN:HB3 | 2.02 | 0.42 |
| 42:N2:217:MET:HE2 | 42:N2:326:LEU:HB2 | 2.02 | 0.42 |
| 45:N5:137:LEU:HD13 | 45:N5:186:MET:HG2 | 2.02 | 0.42 |
| 48:QB:172:LEU:HD21 | 48:QB:202:GLU:HB3 | 2.02 | 0.42 |
| 51:QE:241:SER:HA | 51:QE:252:GLY:HA3 | 2.02 | 0.42 |
| 52:QF:79:ASP:OD2 | 50:Qd:237:TYR:OH | 2.29 | 0.42 |
| 47:Qa:237:PHE:HE2 | 47:Qa:238:LEU:HD12 | 1.84 | 0.42 |
| 47:Qa:293:LEU:HB3 | 47:Qa:309:LEU:HG | 2.00 | 0.42 |
| 49:Qc:267:HIS:HD2 | 49:Qc:269:LYS:HG2 | 1.84 | 0.42 |
| 54:Qh:20:SER:O | 54:Qh:24:GLN:HG2 | 2.19 | 0.42 |
| 58:S2:341:GLU:O | 58:S2:345:GLN:HG2 | 2.19 | 0.42 |
| 63:S7:63:TRP:HH2 | 85:S7:201:U10:H303 | 1.85 | 0.42 |
| 1:4L:56:ALA:HA | 61:S5:18:MET:HE3 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:5A:83:ASP:HB2 | 36:C2:52:HIS:ND1 | 2.34 | 0.42 |
| 15:A6:48:SER:OG | 15:A6:106:ASP:OD1 | 2.35 | 0.42 |
| 19:AB:78:ALA:HA | 19:AB:81:ASP:OD2 | 2.20 | 0.42 |
| 29:B6:132:VAL:O | 29:B6:136:LEU:CB | 2.67 | 0.42 |
| 77:C1:601:HEA:CMA | 77:C1:601:HEA:HBA2 | 2.50 | 0.42 |
| 70:C1:610:PC1:H2C1 | 70:C3:302:PC1:H3D2 | 2.01 | 0.42 |
| 43:N3:73:LEU:HD23 | 43:N3:73:LEU:HA | 1.88 | 0.42 |
| 44:N4:370:PRO:HB2 | 45:N5:142:ILE:HA | 2.01 | 0.42 |
| 46:N6:3:MET:HB3 | 46:N6:5:ILE:HG12 | 2.02 | 0.42 |
| 46:N6:24:PRO:HG2 | 46:N6:28:TYR:HB2 | 2.01 | 0.42 |
| 47:QA:138:LEU:HD22 | 47:QA:238:LEU:HD21 | 2.01 | 0.42 |
| 49:QC:116:GLY:HA3 | 80:QC:402:HEM:C3C | 2.55 | 0.42 |
| 50:QD:248:PRO:HB2 | 81:QD:401:HEC:HBB2 | 2.00 | 0.42 |
| 51:QE:130:LYS:HA | 72:QE:302:3PE:H2A1 | 2.01 | 0.42 |
| 48:Qb:184:PHE:O | 48:Qb:188:HIS:HD2 | 2.02 | 0.42 |
| 48:Qb:465:LEU:HD12 | 48:Qb:466:PRO:HD2 | 2.02 | 0.42 |
| 57:S1:138:ASP:HB3 | 57:S1:142:GLN:HE21 | 1.83 | 0.42 |
| 57:S1:541:PRO:HB3 | 57:S1:561:PRO:HD3 | 2.02 | 0.42 |
| 58:S2:164:LEU:HD23 | 58:S2:164:LEU:HA | 1.91 | 0.42 |
| 65:V1:214:GLU:OE2 | 65:V1:224:ARG:NE | 2.26 | 0.42 |
| 2:5A:68:ASP:OD1 | 2:5A:68:ASP:N | 2.52 | 0.42 |
| 9:7C:52:PRO:HG3 | 35:C1:29:VAL:HG13 | 2.02 | 0.42 |
| 21:AL:107:SER:HB3 | 21:AL:110:ILE:HB | 2.02 | 0.42 |
| 27:B4:25:ILE:HG21 | 27:B4:30:ARG:CZ | 2.50 | 0.42 |
| 30:B7:99:MET:HG3 | 31:B8:156:VAL:HG12 | 2.01 | 0.42 |
| 37:C3:125:ASN:HD21 | 37:C3:127:LEU:HB2 | 1.84 | 0.42 |
| 68:CB:203:CDL:HA31 | 42:N2:238:PRO:HG2 | 2.02 | 0.42 |
| 44:N4:225:ILE:HD13 | 44:N4:331:ASN:HB2 | 2.01 | 0.42 |
| 44:N4:318:ALA:HB1 | 44:N4:374:ASN:CG | 2.45 | 0.42 |
| 45:N5:10:THR:O | 45:N5:14:ILE:HG23 | 2.20 | 0.42 |
| 45:N5:264:TYR:CG | 45:N5:265:PRO:HD3 | 2.55 | 0.42 |
| 45:N5:383:MET:O | 45:N5:389:PHE:HB2 | 2.19 | 0.42 |
| 48:QB:413:ILE:HG12 | 48:QB:423:ARG:HD2 | 2.01 | 0.42 |
| 50:QD:247:PRO:HA | 50:QD:248:PRO:HD3 | 1.86 | 0.42 |
| 54:Qh:49:VAL:O | 54:Qh:52:PRO:HD2 | 2.19 | 0.42 |
| 58:S2:142:PHE:HZ | 58:S2:428:CYS:HG | 1.68 | 0.42 |
| 59:S3:147:THR:HB | 59:S3:153:ILE:HD11 | 2.01 | 0.42 |
| 71:6C:101:PLX:H21 | 71:6C:101:PLX:H1C3 | 1.86 | 0.42 |
| 11:A1:19:PRO:HB3 | 41:N1:9:LEU:HD12 | 2.00 | 0.42 |
| 23:AN:88:ARG:O | 23:AN:92:GLU:HG2 | 2.19 | 0.42 |
| 30:B7:4:HIS:NE2 | 31:B8:155:PRO:HD3 | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:B9:218:GLU:HG2 | 32:B9:219:ARG:HG2 | 2.02 | 0.42 |
| 35:C1:184:PHE:H | 35:C1:256:HIS:CE1 | 2.37 | 0.42 |
| 68:QH:102:CDL:OA7 | 49:Qc:29:SER:OG | 2.37 | 0.42 |
| 48:Qb:315:ASP:HB3 | 48:Qb:318:TYR:CE1 | 2.54 | 0.42 |
| 50:Qd:113:ARG:NH1 | 50:Qd:270:ASP:OD1 | 2.53 | 0.42 |
| 50:Qd:250:TYR:H | 50:Qd:253:VAL:CG2 | 2.33 | 0.42 |
| 57:S1:49:VAL:HG11 | 57:S1:80:VAL:HG21 | 2.02 | 0.42 |
| 58:S2:391:TYR:HD1 | 64:S8:122:VAL:HG21 | 1.84 | 0.42 |
| 66:V2:88:ARG:HH11 | 67:V3:396:THR:HG23 | 1.85 | 0.42 |
| 18:A9:37:HIS:CD2 | 18:A9:39:ALA:H | 2.37 | 0.41 |
| 68:AK:402:CDL:H162 | 68:AK:402:CDL:H361 | 2.01 | 0.41 |
| 22:AM:85:GLU:HG2 | 22:AM:86:TRP:H | 1.85 | 0.41 |
| 24:B1:42:SER:O | 24:B1:46:LYS:HB2 | 2.20 | 0.41 |
| 25:B2:59:ARG:NH2 | 26:B3:48:ASN:OD1 | 2.44 | 0.41 |
| 26:B3:24:ILE:O | 26:B3:30:GLU:HB3 | 2.20 | 0.41 |
| 30:B7:92:HIS:O | 30:B7:96:VAL:HG13 | 2.20 | 0.41 |
| 31:B8:164:ASN:HA | 31:B8:181:VAL:HB | 2.01 | 0.41 |
| 32:B9:147:ASP:HB3 | 32:B9:164:ARG:HH12 | 1.84 | 0.41 |
| 35:C1:316:THR:HG21 | 77:C1:602:HEA:C14 | 2.51 | 0.41 |
| 42:N2:186:HIS:O | 42:N2:190:MET:HG3 | 2.20 | 0.41 |
| 45:N5:11:THR:HG22 | 45:N5:46:LEU:HB3 | 2.01 | 0.41 |
| 47:QA:63:LEU:HD23 | 47:QA:141:THR:HG21 | 2.02 | 0.41 |
| 48:QB:279:ASP:H | 48:QB:460:GLY:HA3 | 1.85 | 0.41 |
| 62:S6:104:LYS:HE2 | 62:S6:104:LYS:HB2 | 1.82 | 0.41 |
| 63:S7:94:ARG:HD3 | 85:S7:201:U10:H253 | 2.01 | 0.41 |
| 2:5A:70:TRP:HH2 | 3:5B:117:GLY:HA2 | 1.85 | 0.41 |
| 10:8B:27:ALA:HB2 | 35:C1:404:THR:HG21 | 2.02 | 0.41 |
| 11:A1:13:ALA:HB2 | 41:N1:264:LEU:HD11 | 2.01 | 0.41 |
| 17:A8:200:GLY:N | 23:AN:66:GLU:OE2 | 2.45 | 0.41 |
| 19:AB:134:ASP:HA | 19:AB:137:LYS:HE2 | 2.00 | 0.41 |
| 22:AM:127:TYR:OH | 62:S6:61:GLU:O | 2.27 | 0.41 |
| 71:AM:201:PLX:H271 | 71:S7:203:PLX:H111 | 2.02 | 0.41 |
| 32:B9:144:TRP:HA | 32:B9:147:ASP:OD2 | 2.20 | 0.41 |
| 36:C2:104:TRP:CD2 | 36:C2:203:ASN:HB2 | 2.56 | 0.41 |
| 72:N5:706:3PE:H3D1 | 72:N5:706:3PE:H391 | 2.02 | 0.41 |
| 48:QB:74:TRP:HB3 | 48:QB:418:LEU:HD11 | 2.02 | 0.41 |
| 49:QC:30:TRP:HB3 | 49:QC:100:ARG:HG3 | 2.02 | 0.41 |
| 51:QE:169:TRP:HZ2 | 51:QE:274:GLY:HA2 | 1.84 | 0.41 |
| 57:S1:130:ILE:HG23 | 64:S8:114:ILE:HD12 | 2.02 | 0.41 |
| 57:S1:382:ARG:C | 57:S1:384:ASN:H | 2.28 | 0.41 |
| 57:S1:432:ILE:HD11 | 57:S1:455:ILE:HD12 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:V1:155:TYR:OH | 66:V2:69:ASN:O | 2.26 | 0.41 |
| 66:V2:137:THR:HG22 | 66:V2:138:THR:H | 1.85 | 0.41 |
| 18:A9:357:ARG:HD3 | 18:A9:361:TRP:O | 2.20 | 0.41 |
| 31:B8:162:PRO:HB2 | 31:B8:163:TYR:CD2 | 2.54 | 0.41 |
| 35:C1:352:GLY:HA2 | 77:C1:602:HEA:H121 | 2.02 | 0.41 |
| 36:C2:30:ILE:HG21 | 36:C2:76:ILE:HD11 | 2.02 | 0.41 |
| 39:CA:47:THR:HG23 | 40:CB:65:LEU:HD22 | 2.01 | 0.41 |
| 45:N5:420:ALA:HB1 | 45:N5:498:PHE:CD1 | 2.55 | 0.41 |
| 50:QD:235:ASN:O | 50:QD:241:GLN:HA | 2.21 | 0.41 |
| 49:Qc:131:TYR:O | 49:Qc:134:PRO:HD2 | 2.19 | 0.41 |
| 85:S7:201:U10:H271 | 85:S7:201:U10:H251 | 1.70 | 0.41 |
| 20:AK:260:TYR:HB3 | 20:AK:264:GLU:HB2 | 2.02 | 0.41 |
| 22:AM:84:PRO:HB3 | 64:S8:197:TRP:CE3 | 2.55 | 0.41 |
| 29:B6:72:LEU:HD23 | 29:B6:72:LEU:HA | 1.92 | 0.41 |
| 31:B8:96:ASP:OD1 | 31:B8:96:ASP:N | 2.50 | 0.41 |
| 35:C1:386:VAL:HG11 | 77:C1:601:HEA:H261 | 2.03 | 0.41 |
| 37:C3:253:TYR:HA | 37:C3:257:TYR:HD1 | 1.85 | 0.41 |
| 37:C3:255:SER:O | 37:C3:259:TRP:HB3 | 2.21 | 0.41 |
| 41:N1:18:ALA:HB1 | 41:N1:48:PRO:HB3 | 2.01 | 0.41 |
| 44:N4:122:PHE:HE2 | 44:N4:206:LYS:HG3 | 1.85 | 0.41 |
| 71:N4:502:PLX:H22 | 71:N4:502:PLX:H1A3 | 1.79 | 0.41 |
| 45:N5:28:LYS:HD3 | 45:N5:28:LYS:HA | 1.91 | 0.41 |
| 45:N5:193:SER:OG | 45:N5:204:LEU:HD12 | 2.20 | 0.41 |
| 48:QB:183:VAL:HG21 | 48:QB:286:HIS:HB3 | 2.02 | 0.41 |
| 53:QG:46:GLU:OE2 | 53:QG:50:ARG:NH2 | 2.50 | 0.41 |
| 47:Qa:123:VAL:HB | 47:Qa:133:LEU:HD23 | 2.01 | 0.41 |
| 51:Qe:199:GLN:HE22 | 51:Qe:204:ARG:HH11 | 1.67 | 0.41 |
| 57:S1:408:ARG:HD2 | 57:S1:439:THR:HG23 | 2.02 | 0.41 |
| 58:S2:135:TYR:HE1 | 58:S2:417:LEU:HD21 | 1.86 | 0.41 |
| 58:S2:363:LYS:HD3 | 58:S2:370:SER:HB2 | 2.01 | 0.41 |
| 65:V1:119:GLU:HA | 86:V1:502:FMN:HM71 | 2.02 | 0.41 |
| 73:A9:402:PEE:H26 | 73:A9:402:PEE:H32 | 1.80 | 0.41 |
| 22:AM:144:TYR:HD1 | 22:AM:144:TYR:H | 1.68 | 0.41 |
| 30:B7:34:ARG:HH21 | 31:B8:186:ILE:HB | 1.86 | 0.41 |
| 35:C1:460:ILE:HG12 | 38:C4:114:THR:HG21 | 2.02 | 0.41 |
| 44:N4:176:PHE:HA | 44:N4:179:ILE:HG12 | 2.02 | 0.41 |
| 47:QA:155:GLN:NE2 | 47:QA:198:GLY:H | 2.17 | 0.41 |
| 47:QA:257:GLU:HG3 | 47:QA:438:MET:HB3 | 2.02 | 0.41 |
| 51:QE:155:LYS:HZ2 | 51:QE:158:ASP:CG | 2.29 | 0.41 |
| 47:Qa:92:LYS:HB2 | 47:Qa:143:ALA:HB1 | 2.02 | 0.41 |
| 48:Qb:183:VAL:HG21 | 48:Qb:286:HIS:HB3 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:Qe:153:GLU:HG2 | 51:Qe:272:ILE:HG12 | 2.02 | 0.41 |
| 58:S2:116:ASP:OD2 | 58:S2:118:HIS:NE2 | 2.54 | 0.41 |
| 59:S3:157:VAL:HG21 | 59:S3:182:PRO:HD3 | 2.01 | 0.41 |
| 4:6A:81:LEU:HD22 | 70:6A:101:PC1:H221 | 2.02 | 0.41 |
| 5:6B:26:GLN:NE2 | 5:6B:29:ASN:HD22 | 2.18 | 0.41 |
| 18:A9:76:MET:HE2 | 18:A9:76:MET:HB3 | 1.90 | 0.41 |
| 19:AC:140:CYS:HB3 | 19:AC:143:GLU:HG3 | 2.03 | 0.41 |
| 20:AK:131:TYR:OH | 20:AK:188:HIS:ND1 | 2.34 | 0.41 |
| 21:AL:39:TYR:CZ | 68:AL:201:CDL:H592 | 2.56 | 0.41 |
| 36:C2:1:MET:HB3 | 36:C2:193:TYR:CD1 | 2.56 | 0.41 |
| 71:CB:201:PLX:H302 | 71:CB:201:PLX:H271 | 1.88 | 0.41 |
| 41:N1:307:LEU:HB3 | 41:N1:308:PRO:HD3 | 2.03 | 0.41 |
| 42:N2:5:ILE:O | 42:N2:8:THR:HG22 | 2.20 | 0.41 |
| 45:N5:174:TYR:HD2 | 45:N5:232:TRP:HB3 | 1.86 | 0.41 |
| 48:QB:96:LEU:HD13 | 48:QB:156:LEU:HD22 | 2.01 | 0.41 |
| 48:QB:280:ASP:HA | 48:QB:461:PRO:HB3 | 2.02 | 0.41 |
| 50:QD:293:MET:HA | 73:QE:301:PEE:H49 | 2.02 | 0.41 |
| 51:QE:223:VAL:HG23 | 49:Qc:264:THR:HG23 | 2.02 | 0.41 |
| 48:Qb:190:THR:HB | 48:Qb:275:ILE:HG13 | 2.02 | 0.41 |
| 51:Qe:220:LEU:HD12 | 51:Qe:239:HIS:CE1 | 2.55 | 0.41 |
| 2:5A:66:ASP:OD1 | 2:5A:66:ASP:N | 2.52 | 0.41 |
| 3:5B:105:VAL:HG12 | 3:5B:122:LEU:HB2 | 2.02 | 0.41 |
| 7:7A:68:LEU:HD21 | 35:C1:110:LEU:HD11 | 2.01 | 0.41 |
| 68:AL:201:CDL:H322 | 68:AL:201:CDL:H352 | 1.90 | 0.41 |
| 27:B4:4:PRO:HD2 | 32:B9:115:TYR:CE1 | 2.56 | 0.41 |
| 27:B4:77:TYR:OH | 45:N5:564:LYS:HG2 | 2.21 | 0.41 |
| 33:BK:74:ILE:O | 40:CB:111:TYR:HB2 | 2.21 | 0.41 |
| 70:C1:610:PC1:H381 | 70:C1:610:PC1:H352 | 1.97 | 0.41 |
| 38:C4:149:LYS:O | 38:C4:152:PRO:HD3 | 2.20 | 0.41 |
| 41:N1:198:PHE:CD1 | 41:N1:285:LEU:HD13 | 2.55 | 0.41 |
| 44:N4:119:TYR:HA | 44:N4:122:PHE:HD1 | 1.84 | 0.41 |
| 51:QE:196:ARG:NH1 | 51:QE:254:ALA:O | 2.54 | 0.41 |
| 51:QE:207:LYS:HG2 | 51:QE:209:GLU:HG2 | 2.01 | 0.41 |
| 56:QJ:23:MET:O | 56:QJ:27:VAL:HG23 | 2.20 | 0.41 |
| 49:Qc:197:LEU:HD11 | 80:Qc:403:HEM:HMA2 | 2.03 | 0.41 |
| 50:Qd:232:LEU:HD13 | 50:Qd:242:ALA:HB1 | 2.02 | 0.41 |
| 57:S1:534:VAL:HG23 | 57:S1:537:ILE:HD12 | 2.03 | 0.41 |
| 2:5A:109:ARG:NH2 | 38:C4:82:TYR:OH | 2.45 | 0.41 |
| 28:B5:113:PHE:O | 28:B5:119:ARG:NH1 | 2.48 | 0.41 |
| 28:B5:133:TYR:OH | 33:BK:87:GLU:OE1 | 2.34 | 0.41 |
| 35:C1:62:ALA:HB2 | 77:C1:601:HEA:HBD1 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:C1:417:MET:O | 35:C1:421:VAL:HG22 | 2.21 | 0.41 |
| 37:C3:79:LEU:HB3 | 37:C3:233:PHE:CE2 | 2.56 | 0.41 |
| 37:C3:173:PHE:HD1 | 37:C3:208:VAL:HG11 | 1.86 | 0.41 |
| 45:N5:15:LEU:HD23 | 45:N5:15:LEU:HA | 1.93 | 0.41 |
| 49:QC:53:MET:HE2 | 49:Qc:181:PHE:CE1 | 2.56 | 0.41 |
| 49:QC:58:ASP:O | 49:QC:62:ALA:N | 2.51 | 0.41 |
| 51:QK:21:GLY:O | 47:Qa:88:SER:OG | 2.35 | 0.41 |
| 51:Qe:88:PHE:O | 51:Qe:92:ARG:HG3 | 2.21 | 0.41 |
| 52:Qf:42:LYS:HE2 | 52:Qf:42:LYS:HB3 | 1.92 | 0.41 |
| 58:S2:46:ASP:OD1 | 58:S2:46:ASP:N | 2.53 | 0.41 |
| 58:S2:448:HIS:HB3 | 58:S2:452:ASP:HB2 | 2.03 | 0.41 |
| 63:S7:85:ASP:O | 63:S7:88:ARG:HB3 | 2.20 | 0.41 |
| 1:4L:80:MET:SD | 46:N6:172:THR:HA | 2.60 | 0.41 |
| 4:6A:76:ASP:OD1 | 4:6A:76:ASP:N | 2.54 | 0.41 |
| 4:6A:88:ASN:CG | 70:6A:101:PC1:H131 | 2.45 | 0.41 |
| 7:7A:29:LYS:NZ | 70:C3:303:PC1:H3F2 | 2.36 | 0.41 |
| 7:7A:69:TYR:CE2 | 72:7A:101:3PE:H281 | 2.56 | 0.41 |
| 20:AK:352:LYS:HE2 | 20:AK:352:LYS:HB2 | 1.92 | 0.41 |
| 21:AL:45:PRO:HA | 21:AL:46:PRO:HD3 | 1.92 | 0.41 |
| 29:B6:164:ILE:HB | 30:B7:48:ASP:HB3 | 2.02 | 0.41 |
| 31:B8:110:ASP:HB3 | 44:N4:278:ARG:NH1 | 2.36 | 0.41 |
| 32:B9:146:LEU:HD21 | 32:B9:160:TYR:HE2 | 1.85 | 0.41 |
| 35:C1:18:LEU:HB3 | 35:C1:102:PHE:CZ | 2.55 | 0.41 |
| 35:C1:33:LEU:HB3 | 35:C1:61:HIS:HB2 | 2.02 | 0.41 |
| 35:C1:459:PHE:HB3 | 38:C4:114:THR:HG23 | 2.03 | 0.41 |
| 36:C2:32:PHE:HD1 | 36:C2:32:PHE:HA | 1.74 | 0.41 |
| 37:C3:231:HIS:HB3 | 70:C3:302:PC1:H133 | 2.01 | 0.41 |
| 41:N1:267:THR:O | 41:N1:271:LEU:HG | 2.21 | 0.41 |
| 42:N2:128:LEU:HD12 | 42:N2:216:PHE:HB3 | 2.03 | 0.41 |
| 45:N5:13:THR:O | 45:N5:17:ILE:HG13 | 2.21 | 0.41 |
| 45:N5:230:HIS:N | 45:N5:231:PRO:HD3 | 2.36 | 0.41 |
| 47:QA:82:LEU:HD23 | 47:QA:205:LEU:HD11 | 2.02 | 0.41 |
| 48:QB:179:MET:O | 48:QB:183:VAL:HG23 | 2.21 | 0.41 |
| 49:QC:51:LEU:HD13 | 80:QC:401:HEM:HBD1 | 2.03 | 0.41 |
| 49:Qc:5:ARG:HH11 | 49:Qc:15:ASN:HD21 | 1.68 | 0.41 |
| 73:Qe:301:PEE:H81 | 73:Qe:301:PEE:H75 | 1.87 | 0.41 |
| 56:Qj:2:LEU:HD22 | 56:Qj:4:ARG:HG2 | 2.02 | 0.41 |
| 57:S1:86:PRO:O | 57:S1:108:LYS:NZ | 2.53 | 0.41 |
| 58:S2:165:LEU:HD21 | 58:S2:397:VAL:HG22 | 2.02 | 0.41 |
| 73:S2:501:PEE:H13 | 73:S2:501:PEE:H1 | 1.77 | 0.41 |
| 64:S8:98:ARG:HB3 | 64:S8:169:GLU:CD | 2.46 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:V1:110:PRO:HD2 | 65:V1:238:CYS:SG | 2.60 | 0.41 |
| 65:V1:201:ALA:HB3 | 66:V2:119:TYR:CD1 | 2.55 | 0.41 |
| 66:V2:152:ILE:HG21 | 66:V2:171:LEU:HD13 | 2.02 | 0.41 |
| 11:A1:65:GLY:HA2 | 17:A8:97:VAL:HG12 | 2.02 | 0.41 |
| 19:AB:137:LYS:HE3 | 19:AB:137:LYS:HB2 | 1.93 | 0.41 |
| 20:AK:67:ASN:ND2 | 20:AK:68:ILE:H | 2.19 | 0.41 |
| 35:C1:37:ILE:HG21 | 77:C1:601:HEA:HMA | 2.03 | 0.41 |
| 41:N1:288:LEU:O | 41:N1:292:SER:HB2 | 2.20 | 0.41 |
| 45:N5:264:TYR:CD2 | 45:N5:265:PRO:HD3 | 2.56 | 0.41 |
| 49:Qc:237:LEU:HB2 | 50:Qd:297:MET:HG2 | 2.02 | 0.41 |
| 66:V2:237:PRO:HA | 66:V2:238:PRO:HD3 | 1.95 | 0.41 |
| 15:A6:63:ARG:HH12 | 19:AB:132:ASP:HA | 1.86 | 0.40 |
| 23:AN:36:PHE:O | 23:AN:40:ILE:HG12 | 2.21 | 0.40 |
| 33:BK:99:ASP:OD2 | 33:BK:142:ARG:NH1 | 2.54 | 0.40 |
| 35:C1:468:MET:HE2 | 35:C1:468:MET:HB3 | 1.97 | 0.40 |
| 70:C3:302:PC1:H272 | 70:C3:302:PC1:H241 | 1.84 | 0.40 |
| 68:CB:203:CDL:H851 | 68:CB:203:CDL:H242 | 2.03 | 0.40 |
| 45:N5:128:MET:HE2 | 45:N5:147:VAL:HG11 | 2.02 | 0.40 |
| 45:N5:297:ASP:O | 45:N5:301:ILE:HG13 | 2.21 | 0.40 |
| 48:QB:324:MET:HE2 | 48:QB:324:MET:HB2 | 1.90 | 0.40 |
| 54:QH:6:GLY:HA3 | 48:Qb:363:MET:SD | 2.61 | 0.40 |
| 57:S1:185:PHE:CZ | 57:S1:221:ASN:HB2 | 2.56 | 0.40 |
| 57:S1:306:MET:HE2 | 57:S1:314:LEU:HB3 | 2.03 | 0.40 |
| 64:S8:150:THR:HG21 | 64:S8:180:HIS:CD2 | 2.56 | 0.40 |
| 68:4L:201:CDL:H172 | 68:4L:201:CDL:H211 | 2.03 | 0.40 |
| 4:6A:48:TRP:HE3 | 4:6A:49:LEU:HD12 | 1.86 | 0.40 |
| 9:7C:49:PHE:HE2 | 10:8B:54:ALA:HB2 | 1.85 | 0.40 |
| 68:B5:201:CDL:H362 | 33:BK:45:VAL:HG12 | 2.03 | 0.40 |
| 35:C1:74:MET:SD | 35:C1:249:PRO:HG2 | 2.61 | 0.40 |
| 35:C1:474:GLU:OE2 | 35:C1:478:SER:OG | 2.37 | 0.40 |
| 70:C1:610:PC1:H131 | 37:C3:71:HIS:NE2 | 2.35 | 0.40 |
| 39:CA:31:ILE:HG23 | 39:CA:32:ARG:HG3 | 2.03 | 0.40 |
| 41:N1:228:TYR:HA | 41:N1:231:ILE:HD12 | 2.03 | 0.40 |
| 43:N3:90:MET:SD | 46:N6:151:THR:HG23 | 2.61 | 0.40 |
| 45:N5:208:CYS:HA | 45:N5:209:PRO:HD3 | 1.78 | 0.40 |
| 45:N5:395:ILE:O | 45:N5:399:VAL:HG23 | 2.21 | 0.40 |
| 48:QB:100:GLY:HA2 | 48:QB:106:GLY:N | 2.30 | 0.40 |
| 49:QC:97:HIS:CD2 | 80:QC:402:HEM:C1C | 3.09 | 0.40 |
| 68:QH:102:CDL:H721 | 68:QH:102:CDL:H311 | 2.02 | 0.40 |
| 55:QI:9:ARG:O | 55:QI:13:LEU:HB2 | 2.21 | 0.40 |
| 57:S1:249:GLU:OE1 | 60:S4:78:ARG:NH2 | 2.37 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 63:S7:53:LEU:HB2 | 71:S7:203:PLX:H301 | 2.03 | 0.40 |
| 68:7A:102:CDL:H811 | 68:7A:102:CDL:H782 | 1.77 | 0.40 |
| 19:AB:115:GLN:O | 19:AB:119:ILE:HG12 | 2.21 | 0.40 |
| 20:AK:232:THR:HG23 | 20:AK:235:TYR:H | 1.86 | 0.40 |
| 71:AM:201:PLX:H182 | 41:N1:19:PHE:CZ | 2.57 | 0.40 |
| 27:B4:59:VAL:HG22 | 44:N4:423:ILE:HG12 | 2.02 | 0.40 |
| 35:C1:100:MET:N | 37:C3:17:PRO:HB3 | 2.36 | 0.40 |
| 35:C1:115:SER:OG | 35:C1:142:SER:O | 2.38 | 0.40 |
| 35:C1:204:ALA:O | 35:C1:208:MET:HG3 | 2.21 | 0.40 |
| 37:C3:57:TRP:O | 37:C3:61:ILE:HG13 | 2.22 | 0.40 |
| 38:C4:148:MET:HG3 | 38:C4:150:VAL:HG23 | 2.03 | 0.40 |
| 41:N1:195:ARG:HD3 | 41:N1:231:ILE:HD11 | 2.02 | 0.40 |
| 54:QH:72:ARG:HD3 | 54:QH:72:ARG:HA | 1.93 | 0.40 |
| 56:Qj:23:MET:O | 56:Qj:27:VAL:HG23 | 2.22 | 0.40 |
| 57:S1:59:GLN:NE2 | 60:S4:89:SER:O | 2.53 | 0.40 |
| 58:S2:98:HIS:HB2 | 58:S2:464:PHE:HE2 | 1.86 | 0.40 |
| 59:S3:213:ASP:HB3 | 59:S3:216:VAL:HG22 | 2.03 | 0.40 |
| 4:6A:28:TRP:HB3 | 37:C3:146:TRP:HB2 | 2.03 | 0.40 |
| 7:7A:48:THR:HG21 | 70:C3:303:PC1:H2A2 | 2.03 | 0.40 |
| 16:A7:12:ARG:HB3 | 16:A7:20:LEU:HD12 | 2.02 | 0.40 |
| 35:C1:409:TRP:CZ3 | 35:C1:467:LEU:HD11 | 2.56 | 0.40 |
| 73:N3:201:PEE:H49 | 73:N3:201:PEE:H8 | 1.71 | 0.40 |
| 45:N5:332:HIS:HA | 45:N5:335:PHE:CZ | 2.57 | 0.40 |
| 47:QA:326:PHE:HA | 51:QK:61:GLY:HA2 | 2.03 | 0.40 |
| 49:QC:28:SER:HB2 | 68:QC:404:CDL:HB22 | 2.03 | 0.40 |
| 49:QC:310:SER:HA | 49:QC:374:ASN:HD21 | 1.85 | 0.40 |
| 51:QE:125:VAL:HG11 | 71:Qi:301:PLX:H122 | 2.02 | 0.40 |
| 51:QE:176:VAL:HG22 | 51:QE:212:ILE:HG12 | 2.03 | 0.40 |
| 49:Qc:116:GLY:HA3 | 80:Qc:403:HEM:C3C | 2.56 | 0.40 |
| 50:Qd:200:TYR:O | 50:Qd:204:ALA:CB | 2.69 | 0.40 |
| 73:Qe:301:PEE:H62 | 73:Qe:301:PEE:H68 | 1.80 | 0.40 |
| 57:S1:63:PHE:HZ | 57:S1:117:MET:HE1 | 1.87 | 0.40 |
| 58:S2:139:LEU:HB3 | 58:S2:140:PRO:HD3 | 2.03 | 0.40 |
| 1:4L:41:PHE:O | 1:4L:45:THR:HG22 | 2.21 | 0.40 |
| 12:A2:46:LYS:HE3 | 12:A2:46:LYS:HB2 | 1.85 | 0.40 |
| 14:A5:49:GLU:O | 14:A5:53:ASN:ND2 | 2.55 | 0.40 |
| 18:A9:217:PHE:HA | 18:A9:220:MET:HE2 | 2.04 | 0.40 |
| 18:A9:344:PRO:HG2 | 18:A9:347:LEU:HD13 | 2.04 | 0.40 |
| 22:AM:85:GLU:H | 22:AM:85:GLU:CD | 2.30 | 0.40 |
| 24:B1:43:LEU:O | 33:BK:69:ARG:HD2 | 2.22 | 0.40 |
| 25:B2:101:PRO:HD2 | 30:B7:99:MET:HE1 | 2.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:BK:43:ARG:HB2 | 33:BK:44:PRO:HD3 | 2.03 | 0.40 |
| 35:C1:456:MET:HA | 38:C4:118:LEU:HD21 | 2.03 | 0.40 |
| 37:C3:86:PHE:HZ | 70:C3:302:PC1:H3C1 | 1.87 | 0.40 |
| 41:N1:149:ILE:HG21 | 41:N1:185:TRP:HB2 | 2.03 | 0.40 |
| 43:N3:97:LEU:HD23 | 43:N3:97:LEU:HA | 1.91 | 0.40 |
| 45:N5:293:ILE:HD11 | 68:N5:704:CDL:H721 | 2.04 | 0.40 |
| 47:QA:83:LEU:HD23 | 47:QA:83:LEU:HA | 1.90 | 0.40 |
| 48:QB:87:ASN:HD22 | 48:QB:204:PRO:HD3 | 1.86 | 0.40 |
| 53:QG:44:VAL:O | 53:QG:48:ILE:HG12 | 2.22 | 0.40 |
| 56:QJ:4:ARG:HA | 53:Qg:110:LYS:HD3 | 2.02 | 0.40 |
| 56:QJ:18:ILE:HD13 | 56:QJ:18:ILE:HA | 1.89 | 0.40 |
| 51:QK:34:LEU:HA | 51:QK:35:PRO:HD3 | 1.97 | 0.40 |
| 50:Qd:243:ILE:HG12 | 50:Qd:245:MET:H | 1.85 | 0.40 |
| 53:Qg:46:GLU:HA | 53:Qg:49:ARG:HG2 | 2.03 | 0.40 |
| 58:S2:157:TYR:O | 58:S2:161:VAL:HG23 | 2.22 | 0.40 |
| 58:S2:196:HIS:O | 58:S2:200:ILE:HG12 | 2.21 | 0.40 |
| 65:V1:302:LYS:HE3 | 65:V1:303:HIS:CE1 | 2.56 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1 | 4L | 96/98 (98%) | 94 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | 5A | 100/102 (98%) | 100 (100%) | 0 | 0 | 100 | 100 |
| 3 | 5B | 93/95 (98%) | 91 (98%) | 2 (2%) | 0 | 100 | 100 |
| 4 | 6A | 73/75 (97%) | 71 (97%) | 2 (3%) | 0 | 100 | 100 |
| 5 | 6B | 80/82 (98%) | 78 (98%) | 2 (2%) | 0 | 100 | 100 |
| 6 | 6C | 68/70 (97%) | 68 (100%) | 0 | 0 | 100 | 100 |
| 7 | 7A | 55/57 (96%) | 55 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|------------|---------|----------|-------------|-----|
| 8 | 7B | 48/50 (96%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |
| 9 | 7C | 45/47 (96%) | 44 (98%) | 1 (2%) | 0 | 100 | 100 |
| 10 | 8B | 41/43 (95%) | 41 (100%) | 0 | 0 | 100 | 100 |
| 11 | A1 | 68/70 (97%) | 68 (100%) | 0 | 0 | 100 | 100 |
| 12 | A2 | 83/85 (98%) | 79 (95%) | 4 (5%) | 0 | 100 | 100 |
| 13 | A3 | 81/83 (98%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |
| 14 | A5 | 110/112 (98%) | 108 (98%) | 2 (2%) | 0 | 100 | 100 |
| 15 | A6 | 112/114 (98%) | 108 (96%) | 3 (3%) | 1 (1%) | 14 | 29 |
| 16 | A7 | 93/112 (83%) | 91 (98%) | 2 (2%) | 0 | 100 | 100 |
| 17 | A8 | 169/171 (99%) | 165 (98%) | 4 (2%) | 0 | 100 | 100 |
| 18 | A9 | 339/341 (99%) | 331 (98%) | 8 (2%) | 0 | 100 | 100 |
| 19 | AB | 75/87 (86%) | 74 (99%) | 1 (1%) | 0 | 100 | 100 |
| 19 | AC | 85/87 (98%) | 85 (100%) | 0 | 0 | 100 | 100 |
| 20 | AK | 319/321 (99%) | 310 (97%) | 9 (3%) | 0 | 100 | 100 |
| 21 | AL | 138/140 (99%) | 138 (100%) | 0 | 0 | 100 | 100 |
| 22 | AM | 142/144 (99%) | 141 (99%) | 1 (1%) | 0 | 100 | 100 |
| 23 | AN | 140/142 (99%) | 132 (94%) | 8 (6%) | 0 | 100 | 100 |
| 24 | B1 | 54/56 (96%) | 54 (100%) | 0 | 0 | 100 | 100 |
| 25 | B2 | 65/67 (97%) | 64 (98%) | 1 (2%) | 0 | 100 | 100 |
| 26 | B3 | 78/80 (98%) | 77 (99%) | 1 (1%) | 0 | 100 | 100 |
| 27 | B4 | 126/128 (98%) | 124 (98%) | 2 (2%) | 0 | 100 | 100 |
| 28 | B5 | 136/138 (99%) | 135 (99%) | 1 (1%) | 0 | 100 | 100 |
| 29 | B6 | 99/126 (79%) | 94 (95%) | 5 (5%) | 0 | 100 | 100 |
| 30 | B7 | 123/125 (98%) | 118 (96%) | 5 (4%) | 0 | 100 | 100 |
| 31 | B8 | 154/156 (99%) | 151 (98%) | 3 (2%) | 0 | 100 | 100 |
| 32 | B9 | 176/178 (99%) | 174 (99%) | 2 (1%) | 0 | 100 | 100 |
| 33 | BK | 172/174 (99%) | 171 (99%) | 1 (1%) | 0 | 100 | 100 |
| 34 | BL | 97/99 (98%) | 89 (92%) | 8 (8%) | 0 | 100 | 100 |
| 35 | C1 | 512/514 (100%) | 498 (97%) | 14 (3%) | 0 | 100 | 100 |
| 36 | C2 | 226/228 (99%) | 219 (97%) | 7 (3%) | 0 | 100 | 100 |
| 37 | C3 | 258/260 (99%) | 252 (98%) | 6 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 38 | C4 | 136/138 (99%) | 131 (96%) | 5 (4%) | 0 | 100 | 100 |
| 39 | CA | 47/49 (96%) | 46 (98%) | 1 (2%) | 0 | 100 | 100 |
| 40 | CB | 119/121 (98%) | 118 (99%) | 1 (1%) | 0 | 100 | 100 |
| 41 | N1 | 316/318 (99%) | 309 (98%) | 7 (2%) | 0 | 100 | 100 |
| 42 | N2 | 345/347 (99%) | 337 (98%) | 8 (2%) | 0 | 100 | 100 |
| 43 | N3 | 113/115 (98%) | 112 (99%) | 1 (1%) | 0 | 100 | 100 |
| 44 | N4 | 457/459 (100%) | 448 (98%) | 9 (2%) | 0 | 100 | 100 |
| 45 | N5 | 601/603 (100%) | 576 (96%) | 25 (4%) | 0 | 100 | 100 |
| 46 | N6 | 172/174 (99%) | 163 (95%) | 9 (5%) | 0 | 100 | 100 |
| 47 | QA | 417/419 (100%) | 407 (98%) | 10 (2%) | 0 | 100 | 100 |
| 47 | Qa | 417/419 (100%) | 408 (98%) | 9 (2%) | 0 | 100 | 100 |
| 48 | QB | 444/446 (100%) | 431 (97%) | 13 (3%) | 0 | 100 | 100 |
| 48 | Qb | 429/446 (96%) | 424 (99%) | 5 (1%) | 0 | 100 | 100 |
| 49 | QC | 377/379 (100%) | 374 (99%) | 3 (1%) | 0 | 100 | 100 |
| 49 | Qc | 377/379 (100%) | 372 (99%) | 5 (1%) | 0 | 100 | 100 |
| 50 | QD | 239/241 (99%) | 231 (97%) | 8 (3%) | 0 | 100 | 100 |
| 50 | Qd | 237/241 (98%) | 233 (98%) | 4 (2%) | 0 | 100 | 100 |
| 51 | QE | 194/274 (71%) | 189 (97%) | 5 (3%) | 0 | 100 | 100 |
| 51 | QK | 69/274 (25%) | 69 (100%) | 0 | 0 | 100 | 100 |
| 51 | Qe | 194/274 (71%) | 189 (97%) | 5 (3%) | 0 | 100 | 100 |
| 52 | QF | 65/67 (97%) | 64 (98%) | 1 (2%) | 0 | 100 | 100 |
| 52 | Qf | 62/67 (92%) | 62 (100%) | 0 | 0 | 100 | 100 |
| 53 | QG | 99/101 (98%) | 98 (99%) | 1 (1%) | 0 | 100 | 100 |
| 53 | Qg | 99/101 (98%) | 98 (99%) | 1 (1%) | 0 | 100 | 100 |
| 54 | QH | 76/79 (96%) | 74 (97%) | 2 (3%) | 0 | 100 | 100 |
| 54 | Qh | 77/79 (98%) | 77 (100%) | 0 | 0 | 100 | 100 |
| 55 | QI | 60/62 (97%) | 60 (100%) | 0 | 0 | 100 | 100 |
| 55 | Qi | 58/62 (94%) | 58 (100%) | 0 | 0 | 100 | 100 |
| 56 | QJ | 47/52 (90%) | 46 (98%) | 1 (2%) | 0 | 100 | 100 |
| 56 | Qj | 49/52 (94%) | 46 (94%) | 3 (6%) | 0 | 100 | 100 |
| 57 | S1 | 687/689 (100%) | 663 (96%) | 24 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 58 | S2 | 427/430 (99%) | 413 (97%) | 14 (3%) | 0 | 100 | 100 |
| 59 | S3 | 206/208 (99%) | 197 (96%) | 9 (4%) | 0 | 100 | 100 |
| 60 | S4 | 122/124 (98%) | 120 (98%) | 2 (2%) | 0 | 100 | 100 |
| 61 | S5 | 103/105 (98%) | 102 (99%) | 1 (1%) | 0 | 100 | 100 |
| 62 | S6 | 94/96 (98%) | 92 (98%) | 2 (2%) | 0 | 100 | 100 |
| 63 | S7 | 154/156 (99%) | 149 (97%) | 5 (3%) | 0 | 100 | 100 |
| 64 | S8 | 174/176 (99%) | 170 (98%) | 4 (2%) | 0 | 100 | 100 |
| 65 | V1 | 429/431 (100%) | 411 (96%) | 18 (4%) | 0 | 100 | 100 |
| 66 | V2 | 215/217 (99%) | 209 (97%) | 6 (3%) | 0 | 100 | 100 |
| 67 | V3 | 40/42 (95%) | 37 (92%) | 3 (8%) | 0 | 100 | 100 |
| All | All | 13972/14569 (96%) | 13630 (98%) | 341 (2%) | 1 (0%) | 100 | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | A6 | 49 | ARG |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1 | 4L | 85/85 (100%) | 85 (100%) | 0 | 100 | 100 |
| 2 | 5A | 89/89 (100%) | 88 (99%) | 1 (1%) | 70 | 85 |
| 3 | 5B | 80/80 (100%) | 78 (98%) | 2 (2%) | 42 | 68 |
| 4 | 6A | 66/66 (100%) | 66 (100%) | 0 | 100 | 100 |
| 5 | 6B | 73/73 (100%) | 72 (99%) | 1 (1%) | 62 | 82 |
| 6 | 6C | 57/57 (100%) | 57 (100%) | 0 | 100 | 100 |
| 7 | 7A | 48/48 (100%) | 48 (100%) | 0 | 100 | 100 |
| 8 | 7B | 39/39 (100%) | 38 (97%) | 1 (3%) | 41 | 67 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 9 | 7C | 40/40 (100%) | 39 (98%) | 1 (2%) | 42 | 68 |
| 10 | 8B | 37/37 (100%) | 37 (100%) | 0 | 100 | 100 |
| 11 | A1 | 58/58 (100%) | 58 (100%) | 0 | 100 | 100 |
| 12 | A2 | 76/76 (100%) | 75 (99%) | 1 (1%) | 65 | 83 |
| 13 | A3 | 69/69 (100%) | 69 (100%) | 0 | 100 | 100 |
| 14 | A5 | 99/99 (100%) | 98 (99%) | 1 (1%) | 73 | 87 |
| 15 | A6 | 107/107 (100%) | 107 (100%) | 0 | 100 | 100 |
| 16 | A7 | 87/97 (90%) | 83 (95%) | 4 (5%) | 23 | 44 |
| 17 | A8 | 153/153 (100%) | 153 (100%) | 0 | 100 | 100 |
| 18 | A9 | 295/295 (100%) | 292 (99%) | 3 (1%) | 73 | 87 |
| 19 | AB | 71/80 (89%) | 71 (100%) | 0 | 100 | 100 |
| 19 | AC | 80/80 (100%) | 79 (99%) | 1 (1%) | 65 | 83 |
| 20 | AK | 284/284 (100%) | 281 (99%) | 3 (1%) | 70 | 85 |
| 21 | AL | 101/101 (100%) | 100 (99%) | 1 (1%) | 73 | 87 |
| 22 | AM | 130/130 (100%) | 128 (98%) | 2 (2%) | 60 | 81 |
| 23 | AN | 123/123 (100%) | 123 (100%) | 0 | 100 | 100 |
| 24 | B1 | 53/53 (100%) | 53 (100%) | 0 | 100 | 100 |
| 25 | B2 | 62/62 (100%) | 62 (100%) | 0 | 100 | 100 |
| 26 | B3 | 62/62 (100%) | 62 (100%) | 0 | 100 | 100 |
| 27 | B4 | 113/113 (100%) | 113 (100%) | 0 | 100 | 100 |
| 28 | B5 | 121/121 (100%) | 121 (100%) | 0 | 100 | 100 |
| 29 | B6 | 98/119 (82%) | 98 (100%) | 0 | 100 | 100 |
| 30 | B7 | 112/112 (100%) | 112 (100%) | 0 | 100 | 100 |
| 31 | B8 | 141/141 (100%) | 141 (100%) | 0 | 100 | 100 |
| 32 | B9 | 159/159 (100%) | 159 (100%) | 0 | 100 | 100 |
| 33 | BK | 155/155 (100%) | 155 (100%) | 0 | 100 | 100 |
| 34 | BL | 91/91 (100%) | 91 (100%) | 0 | 100 | 100 |
| 35 | C1 | 425/425 (100%) | 423 (100%) | 2 (0%) | 86 | 94 |
| 36 | C2 | 212/212 (100%) | 205 (97%) | 7 (3%) | 33 | 59 |
| 37 | C3 | 224/224 (100%) | 223 (100%) | 1 (0%) | 89 | 95 |
| 38 | C4 | 123/123 (100%) | 122 (99%) | 1 (1%) | 79 | 90 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 39 | CA | 45/45 (100%) | 45 (100%) | 0 | 100 | 100 |
| 40 | CB | 108/108 (100%) | 108 (100%) | 0 | 100 | 100 |
| 41 | N1 | 275/275 (100%) | 272 (99%) | 3 (1%) | 70 | 85 |
| 42 | N2 | 311/311 (100%) | 311 (100%) | 0 | 100 | 100 |
| 43 | N3 | 100/100 (100%) | 99 (99%) | 1 (1%) | 73 | 87 |
| 44 | N4 | 410/410 (100%) | 408 (100%) | 2 (0%) | 86 | 94 |
| 45 | N5 | 537/537 (100%) | 534 (99%) | 3 (1%) | 84 | 92 |
| 46 | N6 | 140/140 (100%) | 139 (99%) | 1 (1%) | 81 | 91 |
| 47 | QA | 330/330 (100%) | 328 (99%) | 2 (1%) | 84 | 92 |
| 47 | Qa | 330/330 (100%) | 323 (98%) | 7 (2%) | 48 | 72 |
| 48 | QB | 372/372 (100%) | 370 (100%) | 2 (0%) | 86 | 94 |
| 48 | Qb | 362/372 (97%) | 360 (99%) | 2 (1%) | 84 | 92 |
| 49 | QC | 332/332 (100%) | 327 (98%) | 5 (2%) | 60 | 81 |
| 49 | Qc | 332/332 (100%) | 329 (99%) | 3 (1%) | 75 | 88 |
| 50 | QD | 206/206 (100%) | 205 (100%) | 1 (0%) | 86 | 94 |
| 50 | Qd | 204/206 (99%) | 203 (100%) | 1 (0%) | 86 | 94 |
| 51 | QE | 166/225 (74%) | 165 (99%) | 1 (1%) | 84 | 92 |
| 51 | QK | 55/225 (24%) | 54 (98%) | 1 (2%) | 54 | 76 |
| 51 | Qe | 166/225 (74%) | 166 (100%) | 0 | 100 | 100 |
| 52 | QF | 64/64 (100%) | 63 (98%) | 1 (2%) | 58 | 79 |
| 52 | Qf | 61/64 (95%) | 61 (100%) | 0 | 100 | 100 |
| 53 | QG | 93/93 (100%) | 93 (100%) | 0 | 100 | 100 |
| 53 | Qg | 93/93 (100%) | 92 (99%) | 1 (1%) | 70 | 85 |
| 54 | QH | 70/70 (100%) | 70 (100%) | 0 | 100 | 100 |
| 54 | Qh | 70/70 (100%) | 70 (100%) | 0 | 100 | 100 |
| 55 | QI | 50/50 (100%) | 49 (98%) | 1 (2%) | 50 | 73 |
| 55 | Qi | 49/50 (98%) | 48 (98%) | 1 (2%) | 50 | 73 |
| 56 | QJ | 40/42 (95%) | 40 (100%) | 0 | 100 | 100 |
| 56 | Qj | 41/42 (98%) | 40 (98%) | 1 (2%) | 44 | 69 |
| 57 | S1 | 579/579 (100%) | 576 (100%) | 3 (0%) | 86 | 94 |
| 58 | S2 | 370/370 (100%) | 367 (99%) | 3 (1%) | 79 | 90 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|-------------|-----|
| 59 | S3 | 190/190 (100%) | 188 (99%) | 2 (1%) | 70 | 85 |
| 60 | S4 | 112/112 (100%) | 110 (98%) | 2 (2%) | 54 | 76 |
| 61 | S5 | 93/93 (100%) | 93 (100%) | 0 | 100 | 100 |
| 62 | S6 | 79/79 (100%) | 79 (100%) | 0 | 100 | 100 |
| 63 | S7 | 132/132 (100%) | 130 (98%) | 2 (2%) | 60 | 81 |
| 64 | S8 | 151/151 (100%) | 150 (99%) | 1 (1%) | 81 | 91 |
| 65 | V1 | 344/344 (100%) | 338 (98%) | 6 (2%) | 56 | 78 |
| 66 | V2 | 183/183 (100%) | 181 (99%) | 2 (1%) | 70 | 85 |
| 67 | V3 | 41/41 (100%) | 41 (100%) | 0 | 100 | 100 |
| All | All | 12184/12531 (97%) | 12090 (99%) | 94 (1%) | 77 | 90 |

All (94) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | 5A | 92 | ASP |
| 3 | 5B | 43 | GLN |
| 3 | 5B | 97 | ASN |
| 5 | 6B | 14 | THR |
| 8 | 7B | 63 | GLU |
| 9 | 7C | 60 | LEU |
| 12 | A2 | 85 | ASP |
| 14 | A5 | 113 | LYS |
| 16 | A7 | 5 | THR |
| 16 | A7 | 7 | VAL |
| 16 | A7 | 31 | ILE |
| 16 | A7 | 43 | VAL |
| 18 | A9 | 36 | LEU |
| 18 | A9 | 129 | LEU |
| 18 | A9 | 184 | LYS |
| 19 | AC | 112 | SER |
| 20 | AK | 97 | ASP |
| 20 | AK | 167 | SER |
| 20 | AK | 251 | MET |
| 21 | AL | 115 | CYS |
| 22 | AM | 78 | ASP |
| 22 | AM | 144 | TYR |
| 35 | C1 | 81 | TRP |
| 35 | C1 | 406 | ASN |
| 36 | C2 | 63 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | C2 | 111 | THR |
| 36 | C2 | 114 | GLU |
| 36 | C2 | 142 | VAL |
| 36 | C2 | 172 | THR |
| 36 | C2 | 205 | SER |
| 36 | C2 | 207 | MET |
| 37 | C3 | 5 | THR |
| 38 | C4 | 109 | PHE |
| 41 | N1 | 87 | VAL |
| 41 | N1 | 251 | THR |
| 41 | N1 | 282 | TYR |
| 43 | N3 | 38 | GLU |
| 44 | N4 | 122 | PHE |
| 44 | N4 | 375 | LEU |
| 45 | N5 | 286 | LEU |
| 45 | N5 | 340 | PHE |
| 45 | N5 | 503 | GLU |
| 46 | N6 | 135 | PHE |
| 47 | QA | 70 | ARG |
| 47 | QA | 450 | VAL |
| 48 | QB | 324 | MET |
| 48 | QB | 462 | ILE |
| 49 | QC | 2 | THR |
| 49 | QC | 108 | MET |
| 49 | QC | 112 | THR |
| 49 | QC | 281 | LEU |
| 49 | QC | 345 | HIS |
| 50 | QD | 254 | LEU |
| 51 | QE | 211 | VAL |
| 52 | QF | 43 | CYS |
| 55 | QI | 13 | LEU |
| 51 | QK | 14 | VAL |
| 47 | Qa | 129 | ASP |
| 47 | Qa | 133 | LEU |
| 47 | Qa | 168 | ASN |
| 47 | Qa | 220 | LEU |
| 47 | Qa | 238 | LEU |
| 47 | Qa | 323 | VAL |
| 47 | Qa | 393 | LEU |
| 48 | Qb | 83 | ASN |
| 48 | Qb | 92 | PHE |
| 49 | Qc | 59 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49 | Qc | 112 | THR |
| 49 | Qc | 345 | HIS |
| 50 | Qd | 209 | GLU |
| 53 | Qg | 79 | GLU |
| 55 | Qi | 18 | THR |
| 56 | Qj | 2 | LEU |
| 57 | S1 | 41 | VAL |
| 57 | S1 | 232 | THR |
| 57 | S1 | 690 | THR |
| 58 | S2 | 143 | ASP |
| 58 | S2 | 204 | THR |
| 58 | S2 | 459 | THR |
| 59 | S3 | 85 | GLU |
| 59 | S3 | 145 | THR |
| 60 | S4 | 86 | ASN |
| 60 | S4 | 133 | ASP |
| 63 | S7 | 71 | CYS |
| 63 | S7 | 142 | TYR |
| 64 | S8 | 73 | THR |
| 65 | V1 | 212 | LEU |
| 65 | V1 | 282 | VAL |
| 65 | V1 | 347 | THR |
| 65 | V1 | 379 | CYS |
| 65 | V1 | 417 | LYS |
| 65 | V1 | 457 | HIS |
| 66 | V2 | 137 | THR |
| 66 | V2 | 249 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (257) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 4L | 7 | ASN |
| 2 | 5A | 77 | ASN |
| 3 | 5B | 119 | HIS |
| 4 | 6A | 50 | HIS |
| 4 | 6A | 63 | HIS |
| 5 | 6B | 26 | GLN |
| 5 | 6B | 33 | ASN |
| 5 | 6B | 38 | HIS |
| 6 | 6C | 72 | GLN |
| 7 | 7A | 50 | ASN |
| 8 | 7B | 59 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | 7C | 59 | GLN |
| 11 | A1 | 61 | HIS |
| 12 | A2 | 25 | GLN |
| 12 | A2 | 73 | GLN |
| 14 | A5 | 53 | ASN |
| 14 | A5 | 71 | GLN |
| 14 | A5 | 86 | ASN |
| 15 | A6 | 84 | GLN |
| 15 | A6 | 152 | HIS |
| 16 | A7 | 9 | GLN |
| 16 | A7 | 21 | GLN |
| 16 | A7 | 25 | GLN |
| 17 | A8 | 141 | ASN |
| 17 | A8 | 142 | GLN |
| 18 | A9 | 37 | HIS |
| 18 | A9 | 72 | HIS |
| 18 | A9 | 122 | HIS |
| 18 | A9 | 154 | GLN |
| 18 | A9 | 295 | HIS |
| 18 | A9 | 323 | HIS |
| 20 | AK | 39 | GLN |
| 20 | AK | 67 | ASN |
| 20 | AK | 134 | GLN |
| 20 | AK | 151 | HIS |
| 20 | AK | 221 | GLN |
| 20 | AK | 325 | GLN |
| 21 | AL | 79 | GLN |
| 21 | AL | 89 | ASN |
| 22 | AM | 112 | ASN |
| 23 | AN | 61 | GLN |
| 23 | AN | 90 | ASN |
| 24 | B1 | 3 | ASN |
| 24 | B1 | 6 | GLN |
| 25 | B2 | 63 | GLN |
| 26 | B3 | 91 | GLN |
| 27 | B4 | 50 | GLN |
| 27 | B4 | 79 | ASN |
| 27 | B4 | 123 | GLN |
| 29 | B6 | 143 | HIS |
| 30 | B7 | 76 | ASN |
| 30 | B7 | 85 | HIS |
| 30 | B7 | 110 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | B8 | 56 | ASN |
| 31 | B8 | 115 | ASN |
| 32 | B9 | 104 | GLN |
| 32 | B9 | 117 | GLN |
| 33 | BK | 28 | ASN |
| 33 | BK | 55 | GLN |
| 33 | BK | 107 | GLN |
| 33 | BK | 161 | GLN |
| 34 | BL | 86 | ASN |
| 34 | BL | 140 | ASN |
| 35 | C1 | 12 | HIS |
| 35 | C1 | 80 | ASN |
| 35 | C1 | 138 | HIS |
| 35 | C1 | 256 | HIS |
| 35 | C1 | 328 | HIS |
| 35 | C1 | 368 | HIS |
| 35 | C1 | 413 | HIS |
| 35 | C1 | 422 | ASN |
| 35 | C1 | 503 | HIS |
| 36 | C2 | 59 | GLN |
| 36 | C2 | 91 | ASN |
| 37 | C3 | 50 | ASN |
| 37 | C3 | 103 | HIS |
| 37 | C3 | 125 | ASN |
| 37 | C3 | 148 | HIS |
| 37 | C3 | 161 | GLN |
| 37 | C3 | 222 | GLN |
| 37 | C3 | 226 | HIS |
| 38 | C4 | 98 | ASN |
| 39 | CA | 73 | ASN |
| 41 | N1 | 138 | GLN |
| 41 | N1 | 171 | HIS |
| 42 | N2 | 2 | ASN |
| 42 | N2 | 49 | ASN |
| 42 | N2 | 112 | HIS |
| 42 | N2 | 144 | GLN |
| 42 | N2 | 186 | HIS |
| 42 | N2 | 273 | ASN |
| 42 | N2 | 316 | GLN |
| 42 | N2 | 322 | GLN |
| 43 | N3 | 10 | ASN |
| 43 | N3 | 26 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44 | N4 | 103 | GLN |
| 44 | N4 | 175 | ASN |
| 44 | N4 | 213 | HIS |
| 44 | N4 | 251 | ASN |
| 44 | N4 | 338 | HIS |
| 44 | N4 | 366 | ASN |
| 45 | N5 | 2 | ASN |
| 45 | N5 | 59 | GLN |
| 45 | N5 | 109 | HIS |
| 45 | N5 | 135 | ASN |
| 45 | N5 | 136 | ASN |
| 45 | N5 | 139 | GLN |
| 45 | N5 | 199 | GLN |
| 45 | N5 | 230 | HIS |
| 45 | N5 | 248 | HIS |
| 45 | N5 | 348 | HIS |
| 45 | N5 | 447 | ASN |
| 45 | N5 | 470 | ASN |
| 45 | N5 | 518 | GLN |
| 45 | N5 | 524 | ASN |
| 45 | N5 | 580 | GLN |
| 46 | N6 | 86 | ASN |
| 47 | QA | 168 | ASN |
| 47 | QA | 176 | ASN |
| 47 | QA | 206 | HIS |
| 47 | QA | 227 | HIS |
| 47 | QA | 284 | ASN |
| 47 | QA | 291 | HIS |
| 47 | QA | 319 | GLN |
| 47 | QA | 415 | GLN |
| 47 | QA | 426 | ASN |
| 47 | QA | 443 | ASN |
| 48 | QB | 49 | GLN |
| 48 | QB | 66 | GLN |
| 48 | QB | 87 | ASN |
| 48 | QB | 152 | GLN |
| 48 | QB | 173 | GLN |
| 48 | QB | 188 | HIS |
| 48 | QB | 239 | HIS |
| 48 | QB | 249 | HIS |
| 48 | QB | 301 | ASN |
| 48 | QB | 357 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49 | QC | 32 | ASN |
| 49 | QC | 54 | HIS |
| 49 | QC | 85 | ASN |
| 49 | QC | 137 | GLN |
| 49 | QC | 255 | ASN |
| 49 | QC | 260 | ASN |
| 49 | QC | 267 | HIS |
| 49 | QC | 308 | HIS |
| 49 | QC | 322 | GLN |
| 49 | QC | 341 | GLN |
| 50 | QD | 99 | HIS |
| 50 | QD | 206 | HIS |
| 50 | QD | 251 | ASN |
| 50 | QD | 266 | GLN |
| 51 | QE | 135 | GLN |
| 51 | QE | 164 | ASN |
| 51 | QE | 186 | GLN |
| 51 | QE | 199 | GLN |
| 51 | QE | 257 | ASN |
| 52 | QF | 80 | HIS |
| 52 | QF | 88 | ASN |
| 53 | QG | 54 | ASN |
| 54 | QH | 7 | HIS |
| 55 | QI | 38 | GLN |
| 55 | QI | 48 | ASN |
| 55 | QI | 55 | HIS |
| 56 | QJ | 16 | ASN |
| 51 | QK | 31 | GLN |
| 51 | QK | 58 | GLN |
| 47 | Qa | 81 | HIS |
| 47 | Qa | 155 | GLN |
| 47 | Qa | 167 | GLN |
| 47 | Qa | 172 | GLN |
| 47 | Qa | 178 | HIS |
| 47 | Qa | 211 | ASN |
| 47 | Qa | 212 | HIS |
| 47 | Qa | 239 | ASN |
| 47 | Qa | 284 | ASN |
| 47 | Qa | 290 | GLN |
| 47 | Qa | 319 | GLN |
| 47 | Qa | 343 | GLN |
| 47 | Qa | 376 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | Qa | 408 | GLN |
| 48 | Qb | 40 | GLN |
| 48 | Qb | 43 | GLN |
| 48 | Qb | 83 | ASN |
| 48 | Qb | 160 | GLN |
| 48 | Qb | 170 | GLN |
| 48 | Qb | 188 | HIS |
| 48 | Qb | 207 | ASN |
| 48 | Qb | 239 | HIS |
| 48 | Qb | 286 | HIS |
| 48 | Qb | 313 | HIS |
| 48 | Qb | 357 | HIS |
| 48 | Qb | 464 | GLN |
| 49 | Qc | 15 | ASN |
| 49 | Qc | 54 | HIS |
| 49 | Qc | 207 | ASN |
| 49 | Qc | 260 | ASN |
| 49 | Qc | 267 | HIS |
| 49 | Qc | 352 | GLN |
| 50 | Qd | 116 | GLN |
| 50 | Qd | 190 | ASN |
| 51 | Qe | 135 | GLN |
| 51 | Qe | 186 | GLN |
| 51 | Qe | 199 | GLN |
| 51 | Qe | 239 | HIS |
| 52 | Qf | 36 | GLN |
| 52 | Qf | 55 | GLN |
| 53 | Qg | 23 | ASN |
| 54 | Qh | 13 | HIS |
| 55 | Qi | 38 | GLN |
| 55 | Qi | 48 | ASN |
| 56 | Qj | 16 | ASN |
| 57 | S1 | 39 | GLN |
| 57 | S1 | 142 | GLN |
| 57 | S1 | 260 | ASN |
| 57 | S1 | 282 | ASN |
| 57 | S1 | 331 | GLN |
| 57 | S1 | 336 | ASN |
| 57 | S1 | 425 | ASN |
| 57 | S1 | 453 | GLN |
| 57 | S1 | 498 | GLN |
| 57 | S1 | 604 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57 | S1 | 652 | ASN |
| 57 | S1 | 688 | GLN |
| 58 | S2 | 89 | ASN |
| 58 | S2 | 93 | GLN |
| 58 | S2 | 166 | ASN |
| 58 | S2 | 189 | HIS |
| 58 | S2 | 239 | HIS |
| 59 | S3 | 77 | GLN |
| 59 | S3 | 82 | ASN |
| 59 | S3 | 123 | GLN |
| 59 | S3 | 196 | HIS |
| 59 | S3 | 228 | GLN |
| 60 | S4 | 86 | ASN |
| 60 | S4 | 123 | ASN |
| 60 | S4 | 163 | ASN |
| 61 | S5 | 25 | GLN |
| 61 | S5 | 45 | HIS |
| 62 | S6 | 74 | GLN |
| 62 | S6 | 117 | GLN |
| 65 | V1 | 220 | GLN |
| 65 | V1 | 270 | ASN |
| 65 | V1 | 284 | HIS |
| 65 | V1 | 303 | HIS |
| 65 | V1 | 344 | GLN |
| 65 | V1 | 376 | HIS |
| 65 | V1 | 393 | ASN |
| 65 | V1 | 422 | HIS |
| 65 | V1 | 456 | GLN |
| 66 | V2 | 74 | HIS |
| 66 | V2 | 90 | ASN |
| 66 | V2 | 131 | HIS |
| 66 | V2 | 133 | GLN |
| 66 | V2 | 153 | GLN |
| 66 | V2 | 246 | GLN |
| 67 | V3 | 388 | ASN |
| 67 | V3 | 419 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 58 | 2MR | S2 | 124 | 58 | 10,12,13 | 2.45 | 3 (30%) | 5,13,15 | 1.01 | 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 |
|-----|------|-------|-----|------|---------|------------|-------|
| 58 | 2MR | S2 | 124 | 58 | - | 3/10/13/15 | - |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 58 | S2 | 124 | 2MR | CZ-NE | 5.20 | 1.45 | 1.34 |
| 58 | S2 | 124 | 2MR | CZ-NH2 | 5.07 | 1.44 | 1.33 |
| 58 | S2 | 124 | 2MR | CQ1-NH1 | -2.03 | 1.42 | 1.46 |

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 58 | S2 | 124 | 2MR | NE-CD-CG-CB |
| 58 | S2 | 124 | 2MR | CA-CB-CG-CD |
| 58 | S2 | 124 | 2MR | C-CA-CB-CG |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 106 ligands modelled in this entry, 7 are monoatomic - leaving 99 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 72 | 3PE | C1 | 609 | - | 45,45,50 | 0.32 | 0 | 48,50,55 | 0.28 | 0 |
| 83 | SF4 | S1 | 802 | 57 | 0,12,12 | - | - | - | | |
| 81 | HEC | Qd | 401 | 50 | 32,50,50 | 2.03 | 5 (15%) | 24,82,82 | 2.25 | 13 (54%) |
| 83 | SF4 | S1 | 801 | 57 | 0,12,12 | - | - | - | | |
| 70 | PC1 | Qh | 101 | - | 53,53,53 | 0.30 | 0 | 59,61,61 | 0.26 | 0 |
| 82 | FES | V2 | 301 | 66 | 0,4,4 | - | - | - | | |
| 73 | PEE | N5 | 702 | - | 39,39,50 | 1.49 | 5 (12%) | 41,44,55 | 1.22 | 2 (4%) |
| 68 | CDL | 7A | 102 | - | 90,90,99 | 0.31 | 0 | 96,102,111 | 0.28 | 0 |
| 86 | FMN | V1 | 502 | - | 33,33,33 | 0.23 | 0 | 48,50,50 | 0.41 | 0 |
| 77 | HEA | C1 | 601 | 35 | 57,67,67 | 2.01 | 18 (31%) | 61,103,103 | 2.68 | 29 (47%) |
| 80 | HEM | Qc | 402 | 49 | 41,50,50 | 1.20 | 3 (7%) | 45,82,82 | 1.69 | 8 (17%) |
| 70 | PC1 | C1 | 608 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.32 | 0 |
| 70 | PC1 | C3 | 302 | - | 48,48,53 | 0.31 | 0 | 54,56,61 | 0.37 | 0 |
| 71 | PLX | B1 | 101 | - | 51,51,51 | 1.11 | 4 (7%) | 55,59,59 | 0.89 | 1 (1%) |
| 73 | PEE | S2 | 501 | - | 47,47,50 | 1.35 | 5 (10%) | 50,52,55 | 1.20 | 4 (8%) |
| 72 | 3PE | Qj | 101 | - | 28,28,50 | 0.39 | 0 | 31,33,55 | 0.36 | 0 |
| 68 | CDL | N5 | 704 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.27 | 0 |
| 68 | CDL | QH | 101 | - | 60,60,99 | 0.38 | 0 | 66,72,111 | 0.32 | 0 |
| 72 | 3PE | 7A | 101 | - | 42,42,50 | 0.33 | 0 | 45,47,55 | 0.28 | 0 |
| 72 | 3PE | C1 | 607 | - | 38,38,50 | 0.35 | 0 | 41,43,55 | 0.37 | 0 |
| 70 | PC1 | QB | 503 | - | 50,50,53 | 0.30 | 0 | 56,58,61 | 0.36 | 0 |
| 70 | PC1 | C3 | 306 | - | 42,42,53 | 0.32 | 0 | 48,50,61 | 0.29 | 0 |
| 72 | 3PE | CA | 101 | - | 50,50,50 | 0.31 | 0 | 53,55,55 | 0.28 | 0 |
| 74 | NDP | A9 | 401 | - | 45,52,52 | 0.54 | 0 | 53,80,80 | 0.53 | 1 (1%) |
| 68 | CDL | B4 | 201 | - | 79,79,99 | 0.33 | 0 | 85,91,111 | 0.32 | 0 |
| 68 | CDL | QC | 404 | - | 54,54,99 | 0.40 | 0 | 60,66,111 | 0.36 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 81 | HEC | QD | 401 | 50 | 32,50,50 | 1.99 | 4 (12%) | 24,82,82 | 2.41 | 15 (62%) |
| 73 | PEE | S8 | 303 | - | 50,50,50 | 1.32 | 5 (10%) | 53,55,55 | 1.20 | 3 (5%) |
| 70 | PC1 | C1 | 610 | - | 49,49,53 | 0.30 | 0 | 55,57,61 | 0.35 | 0 |
| 82 | FES | QE | 303 | 51 | 0,4,4 | - | - | - | - | - |
| 73 | PEE | N5 | 705 | - | 50,50,50 | 1.31 | 5 (10%) | 53,55,55 | 1.16 | 3 (5%) |
| 68 | CDL | A8 | 301 | - | 82,82,99 | 0.33 | 0 | 88,94,111 | 0.33 | 0 |
| 68 | CDL | N4 | 503 | - | 61,61,99 | 0.37 | 0 | 67,73,111 | 0.35 | 0 |
| 75 | ZMP | AB | 201 | 19 | 29,35,36 | 0.69 | 1 (3%) | 34,42,45 | 0.77 | 1 (2%) |
| 76 | ADP | AK | 401 | - | 24,29,29 | 0.95 | 1 (4%) | 29,45,45 | 1.40 | 4 (13%) |
| 73 | PEE | N5 | 701 | - | 45,45,50 | 1.39 | 5 (11%) | 48,50,55 | 1.18 | 3 (6%) |
| 70 | PC1 | N3 | 202 | - | 53,53,53 | 0.30 | 0 | 59,61,61 | 0.29 | 0 |
| 71 | PLX | CB | 201 | - | 51,51,51 | 1.10 | 3 (5%) | 55,59,59 | 0.88 | 1 (1%) |
| 73 | PEE | QB | 502 | - | 33,33,50 | 1.41 | 4 (12%) | 36,38,55 | 1.14 | 2 (5%) |
| 68 | CDL | C3 | 305 | - | 82,82,99 | 0.32 | 0 | 88,94,111 | 0.27 | 0 |
| 73 | PEE | QE | 301 | - | 46,46,50 | 1.36 | 5 (10%) | 49,51,55 | 1.24 | 5 (10%) |
| 83 | SF4 | V1 | 501 | 65 | 0,12,12 | - | - | - | - | - |
| 73 | PEE | N3 | 201 | - | 50,50,50 | 1.32 | 5 (10%) | 53,55,55 | 1.15 | 3 (5%) |
| 68 | CDL | B5 | 201 | - | 99,99,99 | 0.31 | 0 | 105,111,111 | 0.37 | 0 |
| 70 | PC1 | C1 | 606 | - | 45,45,53 | 0.31 | 0 | 51,53,61 | 0.31 | 0 |
| 73 | PEE | A9 | 402 | - | 38,38,50 | 1.48 | 5 (13%) | 41,43,55 | 1.23 | 3 (7%) |
| 70 | PC1 | C3 | 303 | - | 53,53,53 | 0.31 | 0 | 59,61,61 | 0.43 | 0 |
| 73 | PEE | Qe | 302 | - | 23,23,50 | 1.42 | 3 (13%) | 26,28,55 | 1.34 | 3 (11%) |
| 72 | 3PE | QE | 302 | - | 43,43,50 | 0.32 | 0 | 46,48,55 | 0.31 | 0 |
| 72 | 3PE | CB | 202 | - | 45,45,50 | 0.32 | 0 | 48,50,55 | 0.29 | 0 |
| 80 | HEM | QC | 402 | 49 | 41,50,50 | 1.23 | 3 (7%) | 45,82,82 | 1.70 | 8 (17%) |
| 75 | ZMP | AC | 201 | 19 | 29,35,36 | 0.65 | 1 (3%) | 34,42,45 | 0.78 | 1 (2%) |
| 68 | CDL | QB | 501 | - | 63,63,99 | 0.37 | 0 | 69,75,111 | 0.38 | 0 |
| 68 | CDL | N1 | 401 | - | 77,77,99 | 0.34 | 0 | 83,89,111 | 0.30 | 0 |
| 72 | 3PE | S7 | 204 | - | 50,50,50 | 0.32 | 0 | 53,55,55 | 0.37 | 0 |
| 73 | PEE | N4 | 501 | - | 48,48,50 | 1.34 | 5 (10%) | 51,53,55 | 1.23 | 2 (3%) |
| 73 | PEE | QC | 403 | - | 39,39,50 | 1.31 | 4 (10%) | 42,44,55 | 1.19 | 3 (7%) |
| 68 | CDL | CB | 203 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.27 | 0 |
| 71 | PLX | 6C | 101 | - | 42,42,51 | 1.17 | 4 (9%) | 46,50,59 | 0.85 | 1 (2%) |
| 84 | MF8 | S2 | 502 | - | 7,8,8 | 1.06 | 0 | 7,10,10 | 1.40 | 1 (14%) |
| 70 | PC1 | 6A | 101 | - | 44,44,53 | 0.32 | 0 | 50,52,61 | 0.31 | 0 |
| 70 | PC1 | Qb | 502 | - | 47,47,53 | 0.31 | 0 | 53,55,61 | 0.36 | 0 |
| 73 | PEE | Qc | 401 | - | 41,41,50 | 1.28 | 4 (9%) | 44,46,55 | 1.17 | 3 (6%) |
| 70 | PC1 | C1 | 605 | - | 32,32,53 | 0.36 | 0 | 38,40,61 | 0.35 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 71 | PLX | AL | 202 | - | 46,46,51 | 1.16 | 5 (10%) | 50,54,59 | 0.87 | 1 (2%) |
| 70 | PC1 | C3 | 301 | - | 43,43,53 | 0.31 | 0 | 49,51,61 | 0.30 | 0 |
| 71 | PLX | AM | 201 | - | 50,50,51 | 1.12 | 4 (8%) | 54,58,59 | 0.85 | 1 (1%) |
| 83 | SF4 | S7 | 202 | 63 | 0,12,12 | - | - | - | - | - |
| 73 | PEE | N1 | 403 | - | 30,30,50 | 1.28 | 3 (10%) | 33,35,55 | 1.15 | 2 (6%) |
| 68 | CDL | A7 | 201 | - | 50,50,99 | 0.40 | 0 | 56,62,111 | 0.33 | 0 |
| 72 | 3PE | Qc | 404 | - | 47,47,50 | 0.31 | 0 | 50,52,55 | 0.29 | 0 |
| 70 | PC1 | Qc | 405 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.33 | 0 |
| 72 | 3PE | N5 | 706 | - | 45,45,50 | 0.33 | 0 | 48,50,55 | 0.29 | 0 |
| 73 | PEE | Qe | 301 | - | 50,50,50 | 1.32 | 5 (10%) | 53,55,55 | 1.19 | 3 (5%) |
| 80 | HEM | Qc | 403 | 49 | 41,50,50 | 1.23 | 3 (7%) | 45,82,82 | 1.69 | 8 (17%) |
| 68 | CDL | C3 | 304 | - | 86,86,99 | 0.32 | 0 | 92,98,111 | 0.28 | 0 |
| 68 | CDL | AK | 402 | - | 67,67,99 | 0.36 | 0 | 73,79,111 | 0.38 | 0 |
| 71 | PLX | N4 | 502 | - | 48,48,51 | 1.13 | 4 (8%) | 52,56,59 | 0.91 | 2 (3%) |
| 71 | PLX | N6 | 201 | - | 51,51,51 | 1.11 | 4 (7%) | 55,59,59 | 0.86 | 1 (1%) |
| 70 | PC1 | N1 | 402 | - | 47,47,53 | 0.31 | 0 | 53,55,61 | 0.30 | 0 |
| 68 | CDL | Qb | 501 | - | 63,63,99 | 0.37 | 0 | 69,75,111 | 0.35 | 0 |
| 68 | CDL | AL | 201 | - | 93,93,99 | 0.31 | 0 | 99,105,111 | 0.31 | 0 |
| 82 | FES | Qe | 303 | 51 | 0,4,4 | - | - | - | - | - |
| 71 | PLX | Qi | 301 | - | 45,45,51 | 1.18 | 6 (13%) | 49,53,59 | 0.82 | 1 (2%) |
| 68 | CDL | 4L | 201 | - | 91,91,99 | 0.32 | 0 | 97,103,111 | 0.36 | 0 |
| 71 | PLX | QI | 301 | - | 51,51,51 | 1.11 | 4 (7%) | 55,59,59 | 0.87 | 1 (1%) |
| 85 | U10 | S7 | 201 | - | 63,63,63 | 2.17 | 21 (33%) | 76,79,79 | 1.68 | 21 (27%) |
| 80 | HEM | QC | 401 | 49 | 41,50,50 | 1.20 | 4 (9%) | 45,82,82 | 1.74 | 9 (20%) |
| 68 | CDL | N5 | 703 | - | 88,88,99 | 0.31 | 0 | 94,100,111 | 0.31 | 0 |
| 83 | SF4 | S8 | 301 | 64 | 0,12,12 | - | - | - | - | - |
| 68 | CDL | QD | 402 | - | 63,63,99 | 0.37 | 0 | 69,75,111 | 0.39 | 0 |
| 82 | FES | S1 | 803 | 57 | 0,4,4 | - | - | - | - | - |
| 68 | CDL | QH | 102 | - | 63,63,99 | 0.37 | 0 | 69,75,111 | 0.35 | 0 |
| 72 | 3PE | QJ | 101 | - | 33,33,50 | 0.37 | 0 | 36,38,55 | 0.34 | 0 |
| 72 | 3PE | B8 | 201 | - | 31,31,50 | 0.37 | 0 | 34,36,55 | 0.34 | 0 |
| 77 | HEA | C1 | 602 | 35 | 57,67,67 | 2.04 | 18 (31%) | 61,103,103 | 2.64 | 26 (42%) |
| 83 | SF4 | S8 | 302 | 64 | 0,12,12 | - | - | - | - | - |
| 73 | PEE | 7C | 101 | - | 50,50,50 | 1.33 | 5 (10%) | 53,55,55 | 1.16 | 4 (7%) |
| 71 | PLX | S7 | 203 | - | 51,51,51 | 1.11 | 3 (5%) | 55,59,59 | 0.88 | 2 (3%) |

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 |
|-----|------|-------|-----|------|---------|----------------|---------|
| 72 | 3PE | C1 | 609 | - | - | 15/49/49/54 | - |
| 83 | SF4 | S1 | 802 | 57 | - | - | 0/6/5/5 |
| 81 | HEC | Qd | 401 | 50 | - | 5/10/54/54 | - |
| 83 | SF4 | S1 | 801 | 57 | - | - | 0/6/5/5 |
| 70 | PC1 | Qh | 101 | - | - | 5/57/57/57 | - |
| 82 | FES | V2 | 301 | 66 | - | - | 0/1/1/1 |
| 73 | PEE | N5 | 702 | - | - | 20/43/43/54 | - |
| 68 | CDL | 7A | 102 | - | - | 18/101/101/110 | - |
| 86 | FMN | V1 | 502 | - | - | 0/18/18/18 | 0/3/3/3 |
| 77 | HEA | C1 | 601 | 35 | - | 10/32/76/76 | - |
| 80 | HEM | Qc | 402 | 49 | - | 7/12/54/54 | - |
| 70 | PC1 | C1 | 608 | - | - | 14/57/57/57 | - |
| 70 | PC1 | C3 | 302 | - | - | 16/52/52/57 | - |
| 71 | PLX | B1 | 101 | - | - | 18/55/55/55 | - |
| 73 | PEE | S2 | 501 | - | - | 30/51/51/54 | - |
| 72 | 3PE | Qj | 101 | - | - | 7/32/32/54 | - |
| 68 | CDL | N5 | 704 | - | - | 19/110/110/110 | - |
| 68 | CDL | QH | 101 | - | - | 11/71/71/110 | - |
| 72 | 3PE | 7A | 101 | - | - | 13/46/46/54 | - |
| 72 | 3PE | C1 | 607 | - | - | 13/42/42/54 | - |
| 70 | PC1 | QB | 503 | - | - | 8/54/54/57 | - |
| 70 | PC1 | C3 | 306 | - | - | 8/46/46/57 | - |
| 72 | 3PE | CA | 101 | - | - | 10/54/54/54 | - |
| 74 | NDP | A9 | 401 | - | - | 6/30/77/77 | 0/5/5/5 |
| 68 | CDL | B4 | 201 | - | - | 21/90/90/110 | - |
| 68 | CDL | QC | 404 | - | - | 19/65/65/110 | - |
| 81 | HEC | QD | 401 | 50 | - | 2/10/54/54 | - |
| 73 | PEE | S8 | 303 | - | - | 24/54/54/54 | - |
| 70 | PC1 | C1 | 610 | - | - | 7/53/53/57 | - |
| 82 | FES | QE | 303 | 51 | - | - | 0/1/1/1 |
| 73 | PEE | N5 | 705 | - | - | 27/54/54/54 | - |
| 68 | CDL | A8 | 301 | - | - | 20/93/93/110 | - |
| 68 | CDL | N4 | 503 | - | - | 22/72/72/110 | - |
| 75 | ZMP | AB | 201 | 19 | - | 8/40/42/43 | - |
| 76 | ADP | AK | 401 | - | - | 4/12/32/32 | 0/3/3/3 |
| 73 | PEE | N5 | 701 | - | - | 26/49/49/54 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------------|---------|
| 70 | PC1 | N3 | 202 | - | - | 15/57/57/57 | - |
| 71 | PLX | CB | 201 | - | - | 26/55/55/55 | - |
| 73 | PEE | QB | 502 | - | - | 22/37/37/54 | - |
| 68 | CDL | C3 | 305 | - | - | 11/93/93/110 | - |
| 73 | PEE | QE | 301 | - | - | 24/50/50/54 | - |
| 83 | SF4 | V1 | 501 | 65 | - | - | 0/6/5/5 |
| 73 | PEE | N3 | 201 | - | - | 26/54/54/54 | - |
| 68 | CDL | B5 | 201 | - | - | 17/110/110/110 | - |
| 70 | PC1 | C1 | 606 | - | - | 7/49/49/57 | - |
| 73 | PEE | A9 | 402 | - | - | 20/42/42/54 | - |
| 70 | PC1 | C3 | 303 | - | - | 14/57/57/57 | - |
| 73 | PEE | Qe | 302 | - | - | 9/27/27/54 | - |
| 72 | 3PE | QE | 302 | - | - | 7/47/47/54 | - |
| 72 | 3PE | CB | 202 | - | - | 12/49/49/54 | - |
| 80 | HEM | QC | 402 | 49 | - | 4/12/54/54 | - |
| 75 | ZMP | AC | 201 | 19 | - | 19/40/42/43 | - |
| 68 | CDL | QB | 501 | - | - | 15/74/74/110 | - |
| 68 | CDL | N1 | 401 | - | - | 14/88/88/110 | - |
| 72 | 3PE | S7 | 204 | - | - | 12/54/54/54 | - |
| 73 | PEE | N4 | 501 | - | - | 24/52/52/54 | - |
| 73 | PEE | QC | 403 | - | - | 14/43/43/54 | - |
| 68 | CDL | CB | 203 | - | - | 25/110/110/110 | - |
| 71 | PLX | 6C | 101 | - | - | 16/46/46/55 | - |
| 84 | MF8 | S2 | 502 | - | - | 5/8/8/8 | - |
| 70 | PC1 | 6A | 101 | - | - | 10/48/48/57 | - |
| 70 | PC1 | Qb | 502 | - | - | 12/51/51/57 | - |
| 73 | PEE | Qc | 401 | - | - | 27/45/45/54 | - |
| 70 | PC1 | C1 | 605 | - | - | 8/36/36/57 | - |
| 71 | PLX | AL | 202 | - | - | 19/50/50/55 | - |
| 70 | PC1 | C3 | 301 | - | - | 12/47/47/57 | - |
| 71 | PLX | AM | 201 | - | - | 20/54/54/55 | - |
| 83 | SF4 | S7 | 202 | 63 | - | - | 0/6/5/5 |
| 73 | PEE | N1 | 403 | - | - | 22/34/34/54 | - |
| 68 | CDL | A7 | 201 | - | - | 12/61/61/110 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------------|---------|
| 72 | 3PE | Qc | 404 | - | - | 10/51/51/54 | - |
| 70 | PC1 | Qc | 405 | - | - | 11/57/57/57 | - |
| 72 | 3PE | N5 | 706 | - | - | 12/49/49/54 | - |
| 73 | PEE | Qe | 301 | - | - | 28/54/54/54 | - |
| 80 | HEM | Qc | 403 | 49 | - | 9/12/54/54 | - |
| 68 | CDL | C3 | 304 | - | - | 13/97/97/110 | - |
| 68 | CDL | AK | 402 | - | - | 18/78/78/110 | - |
| 71 | PLX | N4 | 502 | - | - | 17/52/52/55 | - |
| 71 | PLX | N6 | 201 | - | - | 22/55/55/55 | - |
| 70 | PC1 | N1 | 402 | - | - | 14/51/51/57 | - |
| 68 | CDL | Qb | 501 | - | - | 18/74/74/110 | - |
| 68 | CDL | AL | 201 | - | - | 25/104/104/110 | - |
| 82 | FES | Qe | 303 | 51 | - | - | 0/1/1/1 |
| 71 | PLX | Qi | 301 | - | - | 24/49/49/55 | - |
| 68 | CDL | 4L | 201 | - | - | 22/102/102/110 | - |
| 71 | PLX | QI | 301 | - | - | 15/55/55/55 | - |
| 85 | U10 | S7 | 201 | - | - | 22/63/87/87 | 0/1/1/1 |
| 80 | HEM | QC | 401 | 49 | - | 7/12/54/54 | - |
| 68 | CDL | N5 | 703 | - | - | 23/99/99/110 | - |
| 83 | SF4 | S8 | 301 | 64 | - | - | 0/6/5/5 |
| 68 | CDL | QD | 402 | - | - | 17/74/74/110 | - |
| 82 | FES | S1 | 803 | 57 | - | - | 0/1/1/1 |
| 68 | CDL | QH | 102 | - | - | 21/74/74/110 | - |
| 72 | 3PE | QJ | 101 | - | - | 10/37/37/54 | - |
| 72 | 3PE | B8 | 201 | - | - | 8/35/35/54 | - |
| 77 | HEA | C1 | 602 | 35 | - | 12/32/76/76 | - |
| 83 | SF4 | S8 | 302 | 64 | - | - | 0/6/5/5 |
| 73 | PEE | 7C | 101 | - | - | 16/54/54/54 | - |
| 71 | PLX | S7 | 203 | - | - | 22/55/55/55 | - |

All (196) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 85 | S7 | 201 | U10 | C6-C1 | 10.34 | 1.54 | 1.35 |
| 81 | Qd | 401 | HEC | C3C-C2C | -6.55 | 1.33 | 1.40 |
| 81 | QD | 401 | HEC | C3C-C2C | -6.22 | 1.34 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 81 | QD | 401 | HEC | C2B-C3B | -6.06 | 1.34 | 1.40 |
| 81 | Qd | 401 | HEC | C2B-C3B | -5.84 | 1.34 | 1.40 |
| 77 | C1 | 602 | HEA | C3B-C2B | 5.37 | 1.46 | 1.34 |
| 77 | C1 | 601 | HEA | C3B-C2B | 5.05 | 1.46 | 1.34 |
| 77 | C1 | 601 | HEA | C3A-C2A | 5.03 | 1.47 | 1.40 |
| 77 | C1 | 601 | HEA | C4B-NB | -4.69 | 1.32 | 1.40 |
| 77 | C1 | 602 | HEA | C3A-C2A | 4.65 | 1.46 | 1.40 |
| 77 | C1 | 602 | HEA | CHC-C4B | 4.60 | 1.46 | 1.35 |
| 77 | C1 | 602 | HEA | CHD-C1D | 4.43 | 1.46 | 1.35 |
| 85 | S7 | 201 | U10 | C4-C3 | 4.28 | 1.53 | 1.36 |
| 77 | C1 | 601 | HEA | CHC-C4B | 4.25 | 1.45 | 1.35 |
| 77 | C1 | 602 | HEA | C3C-C2C | 4.25 | 1.46 | 1.40 |
| 77 | C1 | 601 | HEA | C3D-C2D | 4.12 | 1.45 | 1.36 |
| 73 | N5 | 701 | PEE | C18-C19 | 4.05 | 1.55 | 1.31 |
| 73 | A9 | 402 | PEE | C18-C19 | 4.05 | 1.55 | 1.31 |
| 73 | Qe | 301 | PEE | C18-C19 | 4.05 | 1.55 | 1.31 |
| 73 | N5 | 702 | PEE | C18-C19 | 4.05 | 1.55 | 1.31 |
| 73 | QE | 301 | PEE | C18-C19 | 4.05 | 1.55 | 1.31 |
| 73 | 7C | 101 | PEE | C18-C19 | 4.04 | 1.55 | 1.31 |
| 73 | N3 | 201 | PEE | C18-C19 | 4.04 | 1.55 | 1.31 |
| 73 | N5 | 705 | PEE | C18-C19 | 4.04 | 1.55 | 1.31 |
| 73 | S8 | 303 | PEE | C18-C19 | 4.03 | 1.55 | 1.31 |
| 73 | S2 | 501 | PEE | C18-C19 | 4.03 | 1.55 | 1.31 |
| 73 | QC | 403 | PEE | C18-C19 | 4.02 | 1.55 | 1.31 |
| 73 | N4 | 501 | PEE | C18-C19 | 4.02 | 1.55 | 1.31 |
| 73 | Qc | 401 | PEE | C18-C19 | 4.01 | 1.55 | 1.31 |
| 73 | S8 | 303 | PEE | C39-C38 | 3.96 | 1.54 | 1.31 |
| 73 | N5 | 702 | PEE | C39-C38 | 3.96 | 1.54 | 1.31 |
| 73 | N4 | 501 | PEE | C39-C38 | 3.96 | 1.54 | 1.31 |
| 73 | Qe | 301 | PEE | C39-C38 | 3.96 | 1.54 | 1.31 |
| 77 | C1 | 601 | HEA | C3C-C2C | 3.95 | 1.45 | 1.40 |
| 73 | S2 | 501 | PEE | C39-C38 | 3.94 | 1.54 | 1.31 |
| 73 | QE | 301 | PEE | C39-C38 | 3.94 | 1.54 | 1.31 |
| 73 | QB | 502 | PEE | C39-C38 | 3.93 | 1.54 | 1.31 |
| 73 | 7C | 101 | PEE | C39-C38 | 3.93 | 1.54 | 1.31 |
| 73 | N3 | 201 | PEE | C39-C38 | 3.93 | 1.54 | 1.31 |
| 73 | N5 | 705 | PEE | C39-C38 | 3.92 | 1.54 | 1.31 |
| 73 | N5 | 701 | PEE | C39-C38 | 3.92 | 1.54 | 1.31 |
| 73 | A9 | 402 | PEE | C39-C38 | 3.88 | 1.54 | 1.28 |
| 77 | C1 | 602 | HEA | C4B-NB | -3.81 | 1.33 | 1.40 |
| 80 | Qc | 403 | HEM | C4D-ND | -3.78 | 1.33 | 1.40 |
| 77 | C1 | 602 | HEA | C1D-ND | -3.66 | 1.34 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 80 | QC | 402 | HEM | C4D-ND | -3.65 | 1.34 | 1.40 |
| 81 | Qd | 401 | HEC | CBC-CAC | -3.64 | 1.35 | 1.49 |
| 77 | C1 | 602 | HEA | C3D-C2D | 3.59 | 1.44 | 1.36 |
| 77 | C1 | 601 | HEA | C1D-ND | -3.58 | 1.34 | 1.40 |
| 80 | Qc | 402 | HEM | C4D-ND | -3.54 | 1.34 | 1.40 |
| 80 | QC | 401 | HEM | C4D-ND | -3.54 | 1.34 | 1.40 |
| 81 | QD | 401 | HEC | CBC-CAC | -3.41 | 1.36 | 1.49 |
| 77 | C1 | 601 | HEA | CHD-C1D | 3.36 | 1.43 | 1.35 |
| 73 | N1 | 403 | PEE | O3-C30 | 3.28 | 1.42 | 1.33 |
| 73 | N3 | 201 | PEE | O3-C30 | 3.28 | 1.42 | 1.33 |
| 73 | Qe | 301 | PEE | O3-C30 | 3.26 | 1.42 | 1.33 |
| 80 | Qc | 403 | HEM | C1B-NB | -3.26 | 1.34 | 1.40 |
| 73 | QB | 502 | PEE | O3-C30 | 3.25 | 1.42 | 1.33 |
| 73 | N5 | 701 | PEE | O3-C30 | 3.25 | 1.42 | 1.33 |
| 73 | Qc | 401 | PEE | O3-C30 | 3.25 | 1.42 | 1.33 |
| 73 | 7C | 101 | PEE | O3-C30 | 3.23 | 1.42 | 1.33 |
| 73 | QC | 403 | PEE | O3-C30 | 3.22 | 1.42 | 1.33 |
| 73 | N5 | 702 | PEE | O3-C30 | 3.20 | 1.42 | 1.33 |
| 73 | Qe | 302 | PEE | O3-C30 | 3.19 | 1.42 | 1.33 |
| 73 | S2 | 501 | PEE | O3-C30 | 3.19 | 1.42 | 1.33 |
| 73 | A9 | 402 | PEE | O3-C30 | 3.19 | 1.42 | 1.33 |
| 73 | S8 | 303 | PEE | O3-C30 | 3.17 | 1.42 | 1.33 |
| 77 | C1 | 602 | HEA | C1B-NB | -3.16 | 1.32 | 1.38 |
| 73 | N4 | 501 | PEE | O3-C30 | 3.15 | 1.42 | 1.33 |
| 77 | C1 | 602 | HEA | FE-NB | 3.15 | 2.12 | 1.96 |
| 73 | QE | 301 | PEE | O3-C30 | 3.14 | 1.42 | 1.33 |
| 80 | QC | 402 | HEM | C1B-NB | -3.12 | 1.34 | 1.40 |
| 73 | N5 | 705 | PEE | O3-C30 | 3.11 | 1.42 | 1.33 |
| 77 | C1 | 601 | HEA | FE-NB | 3.08 | 2.12 | 1.96 |
| 80 | Qc | 402 | HEM | C1B-NB | -3.04 | 1.35 | 1.40 |
| 71 | S7 | 203 | PLX | O6-C4 | -3.02 | 1.40 | 1.44 |
| 71 | CB | 201 | PLX | O6-C4 | -2.99 | 1.40 | 1.44 |
| 71 | N4 | 502 | PLX | O6-C4 | -2.98 | 1.40 | 1.44 |
| 71 | Qi | 301 | PLX | O6-C4 | -2.98 | 1.40 | 1.44 |
| 85 | S7 | 201 | U10 | C41-C39 | 2.98 | 1.57 | 1.51 |
| 80 | QC | 401 | HEM | C1B-NB | -2.96 | 1.35 | 1.40 |
| 71 | B1 | 101 | PLX | O6-C4 | -2.94 | 1.40 | 1.44 |
| 85 | S7 | 201 | U10 | C7-C8 | 2.91 | 1.54 | 1.50 |
| 71 | 6C | 101 | PLX | O6-C4 | -2.90 | 1.40 | 1.44 |
| 71 | AL | 202 | PLX | O6-C4 | -2.89 | 1.40 | 1.44 |
| 73 | QB | 502 | PEE | O2-C10 | 2.88 | 1.42 | 1.34 |
| 71 | AM | 201 | PLX | O6-C4 | -2.87 | 1.40 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 71 | N6 | 201 | PLX | O6-C4 | -2.85 | 1.40 | 1.44 |
| 71 | QI | 301 | PLX | O6-C4 | -2.80 | 1.40 | 1.44 |
| 77 | C1 | 601 | HEA | C1B-NB | -2.79 | 1.33 | 1.38 |
| 85 | S7 | 201 | U10 | C7-C6 | 2.73 | 1.55 | 1.51 |
| 73 | 7C | 101 | PEE | O2-C10 | 2.71 | 1.42 | 1.34 |
| 85 | S7 | 201 | U10 | C26-C24 | 2.69 | 1.56 | 1.51 |
| 73 | S8 | 303 | PEE | O2-C10 | 2.69 | 1.41 | 1.34 |
| 73 | Qe | 301 | PEE | O2-C10 | 2.68 | 1.41 | 1.34 |
| 73 | N5 | 702 | PEE | O2-C10 | 2.66 | 1.41 | 1.34 |
| 73 | Qe | 302 | PEE | O2-C10 | 2.64 | 1.41 | 1.34 |
| 85 | S7 | 201 | U10 | C31-C29 | 2.64 | 1.56 | 1.51 |
| 85 | S7 | 201 | U10 | C21-C19 | 2.64 | 1.56 | 1.51 |
| 80 | Qc | 403 | HEM | C1D-ND | -2.63 | 1.33 | 1.38 |
| 73 | S2 | 501 | PEE | O2-C10 | 2.63 | 1.41 | 1.34 |
| 75 | AB | 201 | ZMP | C9-C10 | -2.62 | 1.48 | 1.50 |
| 73 | N5 | 701 | PEE | O2-C10 | 2.61 | 1.41 | 1.34 |
| 73 | QE | 301 | PEE | O2-C10 | 2.60 | 1.41 | 1.34 |
| 73 | N3 | 201 | PEE | O2-C10 | 2.60 | 1.41 | 1.34 |
| 80 | QC | 402 | HEM | C1D-ND | -2.58 | 1.33 | 1.38 |
| 73 | N5 | 705 | PEE | O2-C10 | 2.58 | 1.41 | 1.34 |
| 73 | N4 | 501 | PEE | O2-C2 | -2.57 | 1.40 | 1.46 |
| 73 | N1 | 403 | PEE | O2-C10 | 2.57 | 1.41 | 1.34 |
| 73 | QC | 403 | PEE | O2-C2 | -2.57 | 1.40 | 1.46 |
| 73 | QE | 301 | PEE | O2-C2 | -2.56 | 1.40 | 1.46 |
| 73 | N5 | 705 | PEE | O2-C2 | -2.55 | 1.40 | 1.46 |
| 73 | A9 | 402 | PEE | O2-C10 | 2.55 | 1.41 | 1.34 |
| 73 | Qc | 401 | PEE | O2-C2 | -2.55 | 1.40 | 1.46 |
| 80 | QC | 401 | HEM | C1D-ND | -2.54 | 1.33 | 1.38 |
| 73 | N1 | 403 | PEE | O2-C2 | -2.54 | 1.40 | 1.46 |
| 73 | Qe | 302 | PEE | O2-C2 | -2.53 | 1.40 | 1.46 |
| 73 | S8 | 303 | PEE | O2-C2 | -2.52 | 1.40 | 1.46 |
| 73 | Qc | 401 | PEE | O2-C10 | 2.51 | 1.41 | 1.34 |
| 81 | Qd | 401 | HEC | CBB-CAB | -2.50 | 1.40 | 1.49 |
| 80 | Qc | 402 | HEM | C1D-ND | -2.50 | 1.33 | 1.38 |
| 73 | N4 | 501 | PEE | O2-C10 | 2.49 | 1.41 | 1.34 |
| 73 | S2 | 501 | PEE | O2-C2 | -2.49 | 1.40 | 1.46 |
| 73 | QC | 403 | PEE | O2-C10 | 2.48 | 1.41 | 1.34 |
| 73 | A9 | 402 | PEE | O2-C2 | -2.48 | 1.40 | 1.46 |
| 73 | Qe | 301 | PEE | O2-C2 | -2.47 | 1.40 | 1.46 |
| 77 | C1 | 602 | HEA | C4D-ND | -2.47 | 1.33 | 1.38 |
| 73 | N5 | 702 | PEE | O2-C2 | -2.47 | 1.40 | 1.46 |
| 75 | AC | 201 | ZMP | C9-C10 | -2.43 | 1.48 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 73 | N5 | 701 | PEE | O2-C2 | -2.43 | 1.40 | 1.46 |
| 73 | N3 | 201 | PEE | O2-C2 | -2.43 | 1.40 | 1.46 |
| 85 | S7 | 201 | U10 | C36-C34 | 2.43 | 1.56 | 1.51 |
| 85 | S7 | 201 | U10 | O5-C5 | -2.42 | 1.18 | 1.23 |
| 77 | C1 | 601 | HEA | O2D-CGD | -2.42 | 1.22 | 1.30 |
| 77 | C1 | 601 | HEA | C4B-C3B | 2.41 | 1.48 | 1.44 |
| 76 | AK | 401 | ADP | C5-C4 | 2.41 | 1.47 | 1.40 |
| 73 | 7C | 101 | PEE | O2-C2 | -2.40 | 1.40 | 1.46 |
| 85 | S7 | 201 | U10 | C46-C44 | 2.38 | 1.56 | 1.51 |
| 77 | C1 | 602 | HEA | O2D-CGD | -2.38 | 1.22 | 1.30 |
| 77 | C1 | 602 | HEA | C1C-NC | -2.35 | 1.31 | 1.36 |
| 85 | S7 | 201 | U10 | C51-C49 | 2.34 | 1.56 | 1.51 |
| 77 | C1 | 601 | HEA | O2A-CGA | -2.33 | 1.22 | 1.30 |
| 85 | S7 | 201 | U10 | O2-C2 | -2.33 | 1.18 | 1.23 |
| 81 | QD | 401 | HEC | CBB-CAB | -2.32 | 1.40 | 1.49 |
| 85 | S7 | 201 | U10 | C11-C9 | 2.31 | 1.56 | 1.51 |
| 85 | S7 | 201 | U10 | C6-C5 | 2.30 | 1.53 | 1.46 |
| 71 | Qi | 301 | PLX | C1B-N1 | -2.27 | 1.43 | 1.50 |
| 71 | QI | 301 | PLX | C1B-N1 | -2.22 | 1.43 | 1.50 |
| 77 | C1 | 602 | HEA | O2A-CGA | -2.22 | 1.23 | 1.30 |
| 71 | B1 | 101 | PLX | C1B-N1 | -2.20 | 1.43 | 1.50 |
| 77 | C1 | 601 | HEA | CAA-C2A | -2.20 | 1.48 | 1.52 |
| 71 | AL | 202 | PLX | C1B-N1 | -2.17 | 1.43 | 1.50 |
| 71 | Qi | 301 | PLX | C1A-N1 | -2.17 | 1.43 | 1.50 |
| 85 | S7 | 201 | U10 | C16-C14 | 2.16 | 1.55 | 1.51 |
| 71 | N6 | 201 | PLX | C1B-N1 | -2.16 | 1.43 | 1.50 |
| 71 | N4 | 502 | PLX | C1B-N1 | -2.15 | 1.43 | 1.50 |
| 71 | S7 | 203 | PLX | C1B-N1 | -2.13 | 1.43 | 1.50 |
| 71 | CB | 201 | PLX | C1B-N1 | -2.13 | 1.43 | 1.50 |
| 85 | S7 | 201 | U10 | C27-C28 | 2.12 | 1.57 | 1.50 |
| 71 | QI | 301 | PLX | C1A-N1 | -2.12 | 1.43 | 1.50 |
| 85 | S7 | 201 | U10 | O3-C3M | -2.11 | 1.40 | 1.45 |
| 71 | 6C | 101 | PLX | C1B-N1 | -2.11 | 1.43 | 1.50 |
| 77 | C1 | 602 | HEA | FE-ND | 2.11 | 2.07 | 1.96 |
| 71 | AM | 201 | PLX | C1B-N1 | -2.10 | 1.43 | 1.50 |
| 77 | C1 | 602 | HEA | CAA-C2A | -2.10 | 1.48 | 1.52 |
| 77 | C1 | 602 | HEA | C1C-CHC | 2.08 | 1.46 | 1.41 |
| 77 | C1 | 602 | HEA | C4C-NC | -2.08 | 1.31 | 1.36 |
| 85 | S7 | 201 | U10 | C22-C23 | 2.08 | 1.57 | 1.50 |
| 71 | 6C | 101 | PLX | P1-O4 | 2.08 | 1.67 | 1.59 |
| 73 | QB | 502 | PEE | O2-C2 | -2.08 | 1.41 | 1.46 |
| 71 | CB | 201 | PLX | C1A-N1 | -2.07 | 1.44 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 85 | S7 | 201 | U10 | C42-C43 | 2.06 | 1.57 | 1.50 |
| 71 | AL | 202 | PLX | C1A-N1 | -2.06 | 1.44 | 1.50 |
| 71 | AM | 201 | PLX | P1-O4 | 2.06 | 1.67 | 1.59 |
| 77 | C1 | 601 | HEA | C1C-CHC | 2.06 | 1.46 | 1.41 |
| 77 | C1 | 601 | HEA | CHB-C1B | 2.06 | 1.47 | 1.41 |
| 80 | QC | 401 | HEM | CHB-C1B | 2.05 | 1.40 | 1.35 |
| 71 | S7 | 203 | PLX | C1A-N1 | -2.05 | 1.44 | 1.50 |
| 71 | N4 | 502 | PLX | C1A-N1 | -2.04 | 1.44 | 1.50 |
| 71 | N6 | 201 | PLX | C1A-N1 | -2.04 | 1.44 | 1.50 |
| 85 | S7 | 201 | U10 | O4-C4M | -2.04 | 1.40 | 1.45 |
| 71 | AL | 202 | PLX | P1-O4 | 2.03 | 1.67 | 1.59 |
| 77 | C1 | 601 | HEA | FE-ND | 2.03 | 2.06 | 1.96 |
| 81 | Qd | 401 | HEC | CMD-C2D | 2.03 | 1.55 | 1.51 |
| 71 | Qi | 301 | PLX | C7-C6 | 2.03 | 1.55 | 1.50 |
| 77 | C1 | 601 | HEA | CHA-C4D | 2.03 | 1.46 | 1.41 |
| 71 | N6 | 201 | PLX | P1-O4 | 2.03 | 1.67 | 1.59 |
| 71 | N4 | 502 | PLX | P1-O4 | 2.03 | 1.67 | 1.59 |
| 71 | AL | 202 | PLX | C7-C6 | 2.02 | 1.55 | 1.50 |
| 71 | B1 | 101 | PLX | C1A-N1 | -2.02 | 1.44 | 1.50 |
| 71 | Qi | 301 | PLX | P1-O4 | 2.02 | 1.67 | 1.59 |
| 71 | AM | 201 | PLX | C7-C6 | 2.01 | 1.55 | 1.50 |
| 71 | QI | 301 | PLX | P1-O3 | -2.01 | 1.45 | 1.55 |
| 71 | 6C | 101 | PLX | C1A-N1 | -2.01 | 1.44 | 1.50 |
| 71 | B1 | 101 | PLX | P1-O4 | 2.01 | 1.67 | 1.59 |
| 71 | Qi | 301 | PLX | P1-O3 | -2.00 | 1.45 | 1.55 |

All (205) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 77 | C1 | 601 | HEA | CAD-CBD-CGD | -7.00 | 98.54 | 113.60 |
| 77 | C1 | 602 | HEA | CAD-CBD-CGD | -6.96 | 98.63 | 113.60 |
| 77 | C1 | 601 | HEA | C3D-C4D-ND | 6.30 | 116.46 | 110.36 |
| 77 | C1 | 602 | HEA | C2D-C1D-ND | 5.64 | 116.52 | 109.84 |
| 77 | C1 | 602 | HEA | C1D-C2D-C3D | -5.62 | 101.05 | 106.96 |
| 77 | C1 | 601 | HEA | C13-C12-C11 | -5.35 | 106.32 | 114.35 |
| 77 | C1 | 602 | HEA | CAA-CBA-CGA | -5.24 | 99.07 | 113.76 |
| 77 | C1 | 602 | HEA | C3D-C4D-ND | 5.18 | 115.37 | 110.36 |
| 77 | C1 | 602 | HEA | C13-C12-C11 | -5.16 | 106.60 | 114.35 |
| 77 | C1 | 601 | HEA | C2D-C1D-ND | 5.05 | 115.82 | 109.84 |
| 77 | C1 | 601 | HEA | CHB-C1B-C2B | -4.85 | 117.40 | 124.98 |
| 80 | QC | 401 | HEM | CHC-C4B-NB | 4.81 | 129.66 | 124.43 |
| 80 | Qc | 402 | HEM | CHC-C4B-NB | 4.67 | 129.50 | 124.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 77 | C1 | 601 | HEA | CAA-CBA-CGA | -4.62 | 100.81 | 113.76 |
| 73 | Qe | 301 | PEE | O2-C10-C11 | 4.47 | 121.14 | 111.50 |
| 73 | S8 | 303 | PEE | O2-C10-C11 | 4.46 | 121.12 | 111.50 |
| 77 | C1 | 601 | HEA | C2B-C1B-NB | 4.43 | 115.19 | 109.88 |
| 80 | QC | 402 | HEM | CHC-C4B-NB | 4.43 | 129.25 | 124.43 |
| 77 | C1 | 601 | HEA | C1D-C2D-C3D | -4.38 | 102.35 | 106.96 |
| 80 | Qc | 403 | HEM | CHC-C4B-NB | 4.36 | 129.16 | 124.43 |
| 77 | C1 | 602 | HEA | CHB-C1B-C2B | -4.29 | 118.28 | 124.98 |
| 73 | N4 | 501 | PEE | O2-C10-C11 | 4.24 | 120.64 | 111.50 |
| 80 | QC | 402 | HEM | C4D-ND-C1D | 4.21 | 109.42 | 105.07 |
| 77 | C1 | 601 | HEA | CHA-C4D-C3D | -4.20 | 118.66 | 124.84 |
| 73 | Qe | 302 | PEE | O2-C10-C11 | 4.15 | 120.45 | 111.50 |
| 81 | QD | 401 | HEC | CMD-C2D-C1D | -4.10 | 122.17 | 128.46 |
| 73 | QE | 301 | PEE | O2-C10-C11 | 4.09 | 120.31 | 111.50 |
| 73 | S2 | 501 | PEE | O2-C10-C11 | 4.08 | 120.29 | 111.50 |
| 73 | N5 | 702 | PEE | O2-C10-C11 | 4.08 | 120.29 | 111.50 |
| 80 | QC | 401 | HEM | CHB-C1B-NB | 4.01 | 129.34 | 124.38 |
| 73 | QC | 403 | PEE | O2-C10-C11 | 4.00 | 120.12 | 111.50 |
| 77 | C1 | 602 | HEA | C2B-C1B-NB | 3.99 | 114.66 | 109.88 |
| 73 | 7C | 101 | PEE | O2-C10-C11 | 3.95 | 120.02 | 111.50 |
| 73 | N3 | 201 | PEE | O2-C10-C11 | 3.95 | 120.01 | 111.50 |
| 77 | C1 | 602 | HEA | C4B-C3B-C2B | -3.95 | 100.67 | 107.41 |
| 73 | N5 | 701 | PEE | O2-C10-C11 | 3.94 | 119.98 | 111.50 |
| 73 | A9 | 402 | PEE | O2-C10-C11 | 3.93 | 119.98 | 111.50 |
| 77 | C1 | 602 | HEA | C3B-C4B-NB | 3.93 | 114.50 | 109.84 |
| 73 | N1 | 403 | PEE | O2-C10-C11 | 3.91 | 119.92 | 111.50 |
| 80 | Qc | 402 | HEM | CHB-C1B-NB | 3.90 | 129.20 | 124.38 |
| 77 | C1 | 601 | HEA | CMC-C2C-C3C | 3.83 | 131.84 | 124.68 |
| 85 | S7 | 201 | U10 | C7-C8-C9 | -3.82 | 120.43 | 126.79 |
| 77 | C1 | 602 | HEA | CMC-C2C-C3C | 3.81 | 131.81 | 124.68 |
| 80 | Qc | 403 | HEM | CHB-C1B-NB | 3.81 | 129.08 | 124.38 |
| 73 | N5 | 705 | PEE | O2-C10-C11 | 3.77 | 119.62 | 111.50 |
| 73 | Qc | 401 | PEE | O2-C10-C11 | 3.73 | 119.54 | 111.50 |
| 77 | C1 | 602 | HEA | C3C-C4C-NC | 3.71 | 114.01 | 109.21 |
| 80 | Qc | 403 | HEM | C4D-ND-C1D | 3.71 | 108.90 | 105.07 |
| 81 | Qd | 401 | HEC | CMB-C2B-C1B | -3.63 | 122.89 | 128.46 |
| 81 | Qd | 401 | HEC | CMD-C2D-C1D | -3.63 | 122.89 | 128.46 |
| 80 | QC | 402 | HEM | CHB-C1B-NB | 3.61 | 128.85 | 124.38 |
| 80 | QC | 401 | HEM | C4D-ND-C1D | 3.60 | 108.79 | 105.07 |
| 81 | QD | 401 | HEC | CMC-C2C-C3C | 3.57 | 130.02 | 125.82 |
| 81 | Qd | 401 | HEC | CMB-C2B-C3B | 3.50 | 129.94 | 125.82 |
| 80 | Qc | 402 | HEM | C4D-ND-C1D | 3.49 | 108.68 | 105.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 81 | QD | 401 | HEC | CMB-C2B-C3B | 3.47 | 129.90 | 125.82 |
| 81 | QD | 401 | HEC | CMB-C2B-C1B | -3.47 | 123.13 | 128.46 |
| 77 | C1 | 601 | HEA | C3C-C4C-NC | 3.45 | 113.68 | 109.21 |
| 77 | C1 | 601 | HEA | C3B-C4B-NB | 3.39 | 113.86 | 109.84 |
| 80 | QC | 401 | HEM | C1B-NB-C4B | 3.35 | 108.53 | 105.07 |
| 84 | S2 | 502 | MF8 | C07-N06-C04 | 3.33 | 131.84 | 124.55 |
| 73 | Qe | 302 | PEE | O3-C30-C31 | 3.32 | 120.10 | 111.38 |
| 76 | AK | 401 | ADP | PA-O3A-PB | -3.32 | 121.42 | 132.83 |
| 73 | QB | 502 | PEE | O2-C10-C11 | 3.30 | 118.61 | 111.50 |
| 80 | Qc | 403 | HEM | C1B-NB-C4B | 3.26 | 108.44 | 105.07 |
| 85 | S7 | 201 | U10 | C22-C23-C24 | -3.23 | 119.87 | 127.66 |
| 76 | AK | 401 | ADP | N3-C2-N1 | -3.21 | 123.66 | 128.68 |
| 85 | S7 | 201 | U10 | C17-C18-C19 | -3.21 | 119.94 | 127.66 |
| 80 | QC | 402 | HEM | C1B-NB-C4B | 3.16 | 108.34 | 105.07 |
| 77 | C1 | 601 | HEA | C4B-C3B-C2B | -3.16 | 102.01 | 107.41 |
| 77 | C1 | 602 | HEA | CHA-C4D-C3D | -3.09 | 120.29 | 124.84 |
| 81 | Qd | 401 | HEC | CMC-C2C-C3C | 3.09 | 129.45 | 125.82 |
| 77 | C1 | 602 | HEA | C27-C19-C20 | 3.05 | 120.40 | 115.27 |
| 80 | Qc | 402 | HEM | C1B-NB-C4B | 3.04 | 108.21 | 105.07 |
| 85 | S7 | 201 | U10 | C12-C13-C14 | -3.03 | 120.36 | 127.66 |
| 85 | S7 | 201 | U10 | C30-C29-C31 | 3.01 | 120.33 | 115.27 |
| 81 | Qd | 401 | HEC | C4C-C3C-C2C | 2.98 | 109.57 | 106.35 |
| 81 | QD | 401 | HEC | CBD-CAD-C3D | 2.98 | 117.70 | 112.62 |
| 77 | C1 | 601 | HEA | CMB-C2B-C1B | -2.97 | 120.51 | 125.04 |
| 85 | S7 | 201 | U10 | C47-C48-C49 | -2.94 | 120.57 | 127.66 |
| 77 | C1 | 601 | HEA | CMB-C2B-C3B | 2.93 | 135.93 | 130.34 |
| 85 | S7 | 201 | U10 | C45-C44-C46 | 2.92 | 120.19 | 115.27 |
| 80 | QC | 401 | HEM | CHA-C4D-ND | 2.89 | 127.96 | 124.38 |
| 85 | S7 | 201 | U10 | C20-C19-C21 | 2.88 | 120.12 | 115.27 |
| 81 | QD | 401 | HEC | CMC-C2C-C1C | -2.88 | 124.04 | 128.46 |
| 73 | Qc | 401 | PEE | O3-C30-C31 | 2.88 | 120.94 | 111.91 |
| 85 | S7 | 201 | U10 | C42-C43-C44 | -2.88 | 120.74 | 127.66 |
| 81 | QD | 401 | HEC | C4C-C3C-C2C | 2.85 | 109.43 | 106.35 |
| 77 | C1 | 602 | HEA | C13-C14-C15 | -2.84 | 120.81 | 127.66 |
| 80 | Qc | 402 | HEM | CHA-C4D-ND | 2.84 | 127.89 | 124.38 |
| 73 | QE | 301 | PEE | O3-C30-C31 | 2.84 | 120.82 | 111.91 |
| 81 | QD | 401 | HEC | CBA-CAA-C2A | 2.83 | 117.38 | 112.60 |
| 80 | QC | 401 | HEM | CHD-C1D-ND | 2.82 | 127.50 | 124.43 |
| 85 | S7 | 201 | U10 | C37-C38-C39 | -2.82 | 120.88 | 127.66 |
| 80 | QC | 402 | HEM | CHD-C1D-ND | 2.81 | 127.49 | 124.43 |
| 81 | QD | 401 | HEC | O1D-CGD-CBD | -2.79 | 114.12 | 123.08 |
| 85 | S7 | 201 | U10 | C32-C33-C34 | -2.79 | 120.94 | 127.66 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 81 | Qd | 401 | HEC | O1D-CGD-CBD | -2.79 | 114.13 | 123.08 |
| 77 | C1 | 601 | HEA | C1D-ND-C4D | -2.79 | 102.20 | 105.07 |
| 85 | S7 | 201 | U10 | C50-C49-C51 | 2.78 | 119.95 | 115.27 |
| 77 | C1 | 601 | HEA | C27-C19-C20 | 2.78 | 119.94 | 115.27 |
| 85 | S7 | 201 | U10 | C10-C9-C11 | 2.75 | 119.90 | 115.27 |
| 77 | C1 | 601 | HEA | C17-C18-C19 | -2.75 | 121.03 | 127.66 |
| 80 | QC | 402 | HEM | CHA-C4D-ND | 2.75 | 127.78 | 124.38 |
| 77 | C1 | 601 | HEA | C13-C14-C15 | -2.75 | 121.04 | 127.66 |
| 73 | N5 | 705 | PEE | O3-C30-C31 | 2.74 | 120.49 | 111.91 |
| 77 | C1 | 602 | HEA | C17-C18-C19 | -2.73 | 121.08 | 127.66 |
| 77 | C1 | 602 | HEA | CMD-C2D-C1D | 2.73 | 129.19 | 125.04 |
| 77 | C1 | 602 | HEA | CHC-C4B-NB | -2.72 | 121.02 | 124.38 |
| 77 | C1 | 601 | HEA | CHB-C1B-NB | 2.72 | 127.39 | 124.43 |
| 85 | S7 | 201 | U10 | C40-C39-C41 | 2.72 | 119.84 | 115.27 |
| 73 | QB | 502 | PEE | O3-C30-C31 | 2.71 | 120.42 | 111.91 |
| 77 | C1 | 601 | HEA | C1B-C2B-C3B | -2.71 | 103.56 | 106.80 |
| 73 | N4 | 501 | PEE | O3-C30-C31 | 2.70 | 120.38 | 111.91 |
| 77 | C1 | 601 | HEA | CMD-C2D-C1D | 2.70 | 129.15 | 125.04 |
| 80 | Qc | 403 | HEM | CHA-C4D-ND | 2.68 | 127.69 | 124.38 |
| 85 | S7 | 201 | U10 | C35-C34-C36 | 2.68 | 119.77 | 115.27 |
| 73 | S2 | 501 | PEE | O3-C30-C31 | 2.68 | 120.30 | 111.91 |
| 76 | AK | 401 | ADP | C3'-C2'-C1' | 2.68 | 105.01 | 100.98 |
| 80 | Qc | 403 | HEM | CHD-C1D-ND | 2.67 | 127.33 | 124.43 |
| 73 | QC | 403 | PEE | O3-C30-C31 | 2.66 | 120.26 | 111.91 |
| 73 | N1 | 403 | PEE | O3-C30-C31 | 2.66 | 120.25 | 111.91 |
| 77 | C1 | 601 | HEA | C4D-C3D-C2D | -2.61 | 103.09 | 106.90 |
| 76 | AK | 401 | ADP | C4-C5-N7 | -2.61 | 106.68 | 109.40 |
| 85 | S7 | 201 | U10 | C27-C28-C29 | -2.61 | 121.37 | 127.66 |
| 85 | S7 | 201 | U10 | C25-C24-C26 | 2.61 | 119.66 | 115.27 |
| 81 | Qd | 401 | HEC | CMA-C3A-C2A | 2.60 | 129.84 | 124.94 |
| 73 | 7C | 101 | PEE | O3-C30-C31 | 2.59 | 120.05 | 111.91 |
| 73 | S8 | 303 | PEE | O3-C30-C31 | 2.58 | 120.02 | 111.91 |
| 73 | Qe | 301 | PEE | O3-C30-C31 | 2.57 | 119.96 | 111.91 |
| 73 | N3 | 201 | PEE | O3-C30-C31 | 2.56 | 119.95 | 111.91 |
| 77 | C1 | 602 | HEA | CMB-C2B-C1B | -2.56 | 121.14 | 125.04 |
| 73 | A9 | 402 | PEE | O3-C30-C31 | 2.55 | 119.91 | 111.91 |
| 85 | S7 | 201 | U10 | C15-C14-C16 | 2.55 | 119.56 | 115.27 |
| 73 | N5 | 702 | PEE | O3-C30-C31 | 2.54 | 119.89 | 111.91 |
| 73 | A9 | 402 | PEE | C37-C38-C39 | -2.54 | 109.59 | 126.84 |
| 77 | C1 | 601 | HEA | C26-C15-C16 | 2.54 | 119.54 | 115.27 |
| 81 | Qd | 401 | HEC | C2B-C3B-C4B | 2.50 | 109.05 | 106.35 |
| 73 | N5 | 701 | PEE | O3-C30-C31 | 2.50 | 119.75 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 81 | Qd | 401 | HEC | O1A-CGA-CBA | -2.48 | 115.12 | 123.08 |
| 81 | QD | 401 | HEC | CMA-C3A-C2A | 2.47 | 129.59 | 124.94 |
| 81 | QD | 401 | HEC | O1A-CGA-CBA | -2.46 | 115.18 | 123.08 |
| 80 | Qc | 402 | HEM | CHD-C1D-ND | 2.45 | 127.09 | 124.43 |
| 80 | Qc | 403 | HEM | CAD-CBD-CGD | -2.45 | 108.33 | 113.60 |
| 75 | AC | 201 | ZMP | O1-C10-C9 | -2.44 | 121.11 | 123.99 |
| 81 | Qd | 401 | HEC | CMC-C2C-C1C | -2.43 | 124.73 | 128.46 |
| 77 | C1 | 602 | HEA | C1D-ND-C4D | -2.42 | 102.57 | 105.07 |
| 77 | C1 | 602 | HEA | CHB-C1B-NB | 2.41 | 127.05 | 124.43 |
| 85 | S7 | 201 | U10 | C1M-C1-C6 | -2.37 | 120.53 | 124.40 |
| 85 | S7 | 201 | U10 | C56-C54-C55 | 2.37 | 119.83 | 114.60 |
| 74 | A9 | 401 | NDP | C5A-C6A-N6A | 2.36 | 123.94 | 120.35 |
| 77 | C1 | 601 | HEA | C27-C19-C18 | -2.36 | 117.63 | 123.68 |
| 80 | QC | 401 | HEM | CAD-CBD-CGD | -2.33 | 108.59 | 113.60 |
| 80 | Qc | 402 | HEM | CHB-C1B-C2B | -2.33 | 120.28 | 126.72 |
| 81 | Qd | 401 | HEC | CBD-CAD-C3D | 2.31 | 116.56 | 112.62 |
| 81 | QD | 401 | HEC | CMD-C2D-C3D | 2.30 | 129.29 | 124.94 |
| 71 | B1 | 101 | PLX | O3-P1-O2 | -2.28 | 100.98 | 112.24 |
| 80 | QC | 401 | HEM | CHB-C1B-C2B | -2.27 | 120.43 | 126.72 |
| 71 | 6C | 101 | PLX | O3-P1-O2 | -2.27 | 101.01 | 112.24 |
| 71 | CB | 201 | PLX | O3-P1-O2 | -2.27 | 101.03 | 112.24 |
| 80 | Qc | 402 | HEM | CAD-CBD-CGD | -2.27 | 108.72 | 113.60 |
| 71 | N6 | 201 | PLX | O3-P1-O2 | -2.25 | 101.11 | 112.24 |
| 71 | AL | 202 | PLX | O3-P1-O2 | -2.25 | 101.12 | 112.24 |
| 80 | Qc | 403 | HEM | CHB-C1B-C2B | -2.24 | 120.52 | 126.72 |
| 71 | AM | 201 | PLX | O3-P1-O2 | -2.24 | 101.17 | 112.24 |
| 81 | Qd | 401 | HEC | O2A-CGA-O1A | 2.24 | 128.88 | 123.30 |
| 77 | C1 | 602 | HEA | O1D-CGD-CBD | -2.24 | 115.90 | 123.08 |
| 71 | QI | 301 | PLX | O3-P1-O2 | -2.23 | 101.23 | 112.24 |
| 81 | QD | 401 | HEC | C1D-C2D-C3D | 2.23 | 108.54 | 107.00 |
| 71 | N4 | 502 | PLX | O3-P1-O2 | -2.22 | 101.25 | 112.24 |
| 81 | QD | 401 | HEC | O2A-CGA-O1A | 2.20 | 128.79 | 123.30 |
| 71 | Qi | 301 | PLX | O3-P1-O2 | -2.20 | 101.35 | 112.24 |
| 71 | S7 | 203 | PLX | O3-P1-O2 | -2.20 | 101.36 | 112.24 |
| 77 | C1 | 601 | HEA | CAA-C2A-C3A | 2.19 | 132.27 | 126.86 |
| 80 | QC | 402 | HEM | CHB-C1B-C2B | -2.19 | 120.65 | 126.72 |
| 80 | QC | 401 | HEM | CBA-CAA-C2A | -2.18 | 108.89 | 112.62 |
| 77 | C1 | 601 | HEA | OMA-CMA-C3A | -2.18 | 120.15 | 124.91 |
| 77 | C1 | 601 | HEA | CHC-C4B-NB | -2.18 | 121.69 | 124.38 |
| 77 | C1 | 602 | HEA | CHD-C1D-C2D | -2.18 | 120.70 | 126.72 |
| 77 | C1 | 602 | HEA | O1A-CGA-CBA | -2.16 | 116.14 | 123.08 |
| 73 | Qe | 302 | PEE | C2-O2-C10 | -2.14 | 112.53 | 117.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 73 | QE | 301 | PEE | C2-O2-C10 | -2.13 | 112.55 | 117.79 |
| 81 | Qd | 401 | HEC | CMD-C2D-C3D | 2.12 | 128.93 | 124.94 |
| 85 | S7 | 201 | U10 | C52-C53-C54 | -2.10 | 120.58 | 127.75 |
| 77 | C1 | 602 | HEA | C26-C15-C16 | 2.09 | 118.78 | 115.27 |
| 81 | QD | 401 | HEC | C2B-C3B-C4B | 2.07 | 108.59 | 106.35 |
| 71 | N4 | 502 | PLX | C26-C25-C24 | -2.07 | 108.59 | 113.38 |
| 77 | C1 | 601 | HEA | O1D-CGD-CBD | -2.07 | 116.44 | 123.08 |
| 73 | Qc | 401 | PEE | C17-C18-C19 | -2.06 | 108.90 | 124.73 |
| 77 | C1 | 602 | HEA | C27-C19-C18 | -2.06 | 118.39 | 123.68 |
| 73 | QC | 403 | PEE | C17-C18-C19 | -2.06 | 108.95 | 124.73 |
| 73 | S2 | 501 | PEE | C20-C19-C18 | -2.05 | 109.01 | 124.73 |
| 73 | S8 | 303 | PEE | C17-C18-C19 | -2.04 | 109.05 | 124.73 |
| 73 | Qe | 301 | PEE | C17-C18-C19 | -2.04 | 109.05 | 124.73 |
| 73 | QE | 301 | PEE | C40-C39-C38 | -2.04 | 109.09 | 124.73 |
| 80 | QC | 402 | HEM | CMC-C2C-C3C | 2.03 | 128.49 | 124.68 |
| 73 | S2 | 501 | PEE | C37-C38-C39 | -2.03 | 109.15 | 124.73 |
| 73 | N5 | 705 | PEE | C37-C38-C39 | -2.03 | 109.17 | 124.73 |
| 75 | AB | 201 | ZMP | C15-C14-C13 | -2.03 | 108.98 | 112.36 |
| 73 | N5 | 701 | PEE | C37-C38-C39 | -2.02 | 109.21 | 124.73 |
| 73 | 7C | 101 | PEE | C40-C39-C38 | -2.02 | 109.23 | 124.73 |
| 73 | 7C | 101 | PEE | C20-C19-C18 | -2.02 | 109.25 | 124.73 |
| 73 | N3 | 201 | PEE | C37-C38-C39 | -2.01 | 109.28 | 124.73 |
| 73 | QE | 301 | PEE | C20-C19-C18 | -2.01 | 109.34 | 124.73 |
| 71 | S7 | 203 | PLX | C8-C7-C6 | -2.00 | 108.75 | 113.38 |

There are no chirality outliers.

All (1349) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 68 | 4L | 201 | CDL | CA2-OA2-PA1-OA3 |
| 68 | 4L | 201 | CDL | CB2-OB2-PB2-OB3 |
| 68 | 4L | 201 | CDL | CB2-OB2-PB2-OB4 |
| 68 | 4L | 201 | CDL | CB2-OB2-PB2-OB5 |
| 68 | 7A | 102 | CDL | CA2-OA2-PA1-OA3 |
| 68 | 7A | 102 | CDL | CA2-OA2-PA1-OA4 |
| 68 | 7A | 102 | CDL | CA2-OA2-PA1-OA5 |
| 68 | 7A | 102 | CDL | CB3-OB5-PB2-OB3 |
| 68 | A7 | 201 | CDL | CB2-OB2-PB2-OB3 |
| 68 | A7 | 201 | CDL | CB3-OB5-PB2-OB2 |
| 68 | A7 | 201 | CDL | CB3-OB5-PB2-OB3 |
| 68 | A7 | 201 | CDL | CB3-OB5-PB2-OB4 |
| 68 | A8 | 301 | CDL | CA2-OA2-PA1-OA3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 68 | A8 | 301 | CDL | CA2-OA2-PA1-OA4 |
| 68 | A8 | 301 | CDL | CA2-OA2-PA1-OA5 |
| 68 | A8 | 301 | CDL | CB3-OB5-PB2-OB4 |
| 68 | AK | 402 | CDL | CA2-OA2-PA1-OA3 |
| 68 | AK | 402 | CDL | CA2-OA2-PA1-OA4 |
| 68 | AK | 402 | CDL | CA3-OA5-PA1-OA3 |
| 68 | AK | 402 | CDL | CA3-OA5-PA1-OA4 |
| 68 | AK | 402 | CDL | CB2-OB2-PB2-OB3 |
| 68 | AK | 402 | CDL | CB2-OB2-PB2-OB4 |
| 68 | AK | 402 | CDL | CB2-OB2-PB2-OB5 |
| 68 | AL | 201 | CDL | CA2-OA2-PA1-OA3 |
| 68 | AL | 201 | CDL | CB3-OB5-PB2-OB3 |
| 68 | AL | 201 | CDL | CB3-OB5-PB2-OB4 |
| 68 | B4 | 201 | CDL | CA3-OA5-PA1-OA3 |
| 68 | B4 | 201 | CDL | CB2-OB2-PB2-OB3 |
| 68 | B5 | 201 | CDL | CA2-OA2-PA1-OA3 |
| 68 | B5 | 201 | CDL | CB3-OB5-PB2-OB2 |
| 68 | C3 | 304 | CDL | CA2-OA2-PA1-OA3 |
| 68 | C3 | 304 | CDL | CA2-OA2-PA1-OA4 |
| 68 | C3 | 304 | CDL | CA2-OA2-PA1-OA5 |
| 68 | C3 | 304 | CDL | CA3-OA5-PA1-OA4 |
| 68 | C3 | 305 | CDL | CA2-OA2-PA1-OA4 |
| 68 | C3 | 305 | CDL | CA3-OA5-PA1-OA3 |
| 68 | CB | 203 | CDL | CA2-OA2-PA1-OA3 |
| 68 | CB | 203 | CDL | CB2-OB2-PB2-OB3 |
| 68 | N1 | 401 | CDL | CB2-OB2-PB2-OB4 |
| 68 | N4 | 503 | CDL | CA2-OA2-PA1-OA3 |
| 68 | N5 | 703 | CDL | CA2-OA2-PA1-OA3 |
| 68 | N5 | 703 | CDL | CA3-OA5-PA1-OA2 |
| 68 | N5 | 703 | CDL | CA3-OA5-PA1-OA3 |
| 68 | N5 | 703 | CDL | CA3-OA5-PA1-OA4 |
| 68 | N5 | 703 | CDL | CB2-OB2-PB2-OB3 |
| 68 | N5 | 703 | CDL | CB2-OB2-PB2-OB4 |
| 68 | N5 | 703 | CDL | CB3-OB5-PB2-OB3 |
| 68 | QB | 501 | CDL | CA2-OA2-PA1-OA3 |
| 68 | QB | 501 | CDL | CA3-OA5-PA1-OA4 |
| 68 | QC | 404 | CDL | CA2-OA2-PA1-OA4 |
| 68 | QC | 404 | CDL | CA3-OA5-PA1-OA2 |
| 68 | QC | 404 | CDL | CA3-OA5-PA1-OA3 |
| 68 | QC | 404 | CDL | CA3-OA5-PA1-OA4 |
| 68 | QC | 404 | CDL | OA6-CA4-CA6-OA8 |
| 68 | QC | 404 | CDL | CB2-OB2-PB2-OB3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 68 | QC | 404 | CDL | CB3-OB5-PB2-OB3 |
| 68 | QC | 404 | CDL | CB3-OB5-PB2-OB4 |
| 68 | QD | 402 | CDL | CA2-OA2-PA1-OA3 |
| 68 | QD | 402 | CDL | CA2-OA2-PA1-OA4 |
| 68 | QD | 402 | CDL | CA2-OA2-PA1-OA5 |
| 68 | QD | 402 | CDL | CA3-OA5-PA1-OA3 |
| 68 | QD | 402 | CDL | CB3-OB5-PB2-OB2 |
| 68 | QD | 402 | CDL | CB3-OB5-PB2-OB3 |
| 68 | QD | 402 | CDL | CB3-OB5-PB2-OB4 |
| 68 | QH | 101 | CDL | CA2-OA2-PA1-OA3 |
| 68 | QH | 102 | CDL | CA2-OA2-PA1-OA3 |
| 68 | QH | 102 | CDL | CA3-OA5-PA1-OA2 |
| 68 | QH | 102 | CDL | CA3-OA5-PA1-OA3 |
| 68 | QH | 102 | CDL | CA3-OA5-PA1-OA4 |
| 68 | QH | 102 | CDL | CB2-OB2-PB2-OB4 |
| 68 | Qb | 501 | CDL | CA2-OA2-PA1-OA3 |
| 68 | Qb | 501 | CDL | CB2-OB2-PB2-OB5 |
| 68 | Qb | 501 | CDL | CB3-OB5-PB2-OB2 |
| 68 | Qb | 501 | CDL | CB3-OB5-PB2-OB3 |
| 68 | Qb | 501 | CDL | CB3-OB5-PB2-OB4 |
| 68 | Qb | 501 | CDL | OB5-CB3-CB4-OB6 |
| 70 | 6A | 101 | PC1 | C11-O13-P-O14 |
| 70 | C1 | 606 | PC1 | C11-O13-P-O12 |
| 70 | C1 | 606 | PC1 | C11-O13-P-O14 |
| 70 | C1 | 606 | PC1 | C11-O13-P-O11 |
| 70 | C1 | 610 | PC1 | C11-O13-P-O12 |
| 70 | C1 | 610 | PC1 | C11-O13-P-O14 |
| 70 | C1 | 610 | PC1 | C11-O13-P-O11 |
| 70 | C3 | 301 | PC1 | C11-O13-P-O14 |
| 70 | C3 | 302 | PC1 | C11-O13-P-O14 |
| 70 | C3 | 302 | PC1 | C1-O11-P-O12 |
| 70 | C3 | 302 | PC1 | C1-O11-P-O14 |
| 70 | C3 | 302 | PC1 | C1-O11-P-O13 |
| 70 | C3 | 303 | PC1 | C1-O11-P-O12 |
| 70 | C3 | 303 | PC1 | C1-O11-P-O14 |
| 70 | C3 | 303 | PC1 | C1-O11-P-O13 |
| 70 | N1 | 402 | PC1 | C11-O13-P-O12 |
| 70 | N1 | 402 | PC1 | C11-O13-P-O14 |
| 70 | N1 | 402 | PC1 | C11-O13-P-O11 |
| 70 | N1 | 402 | PC1 | C1-O11-P-O12 |
| 70 | N1 | 402 | PC1 | C1-O11-P-O14 |
| 70 | Qc | 405 | PC1 | C1-O11-P-O14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 71 | 6C | 101 | PLX | O7-C6-O6-C4 |
| 71 | AL | 202 | PLX | O7-C6-C7-C8 |
| 71 | AL | 202 | PLX | O7-C6-O6-C4 |
| 71 | AL | 202 | PLX | C3-O4-P1-O2 |
| 71 | AL | 202 | PLX | C25-C24-O8-C5 |
| 71 | AL | 202 | PLX | O9-C24-C25-C26 |
| 71 | AM | 201 | PLX | O7-C6-O6-C4 |
| 71 | AM | 201 | PLX | C2-O1-P1-O4 |
| 71 | AM | 201 | PLX | C2-O1-P1-O2 |
| 71 | AM | 201 | PLX | N1-C1-C2-O1 |
| 71 | B1 | 101 | PLX | O7-C6-O6-C4 |
| 71 | B1 | 101 | PLX | C3-O4-P1-O2 |
| 71 | B1 | 101 | PLX | C3-O4-P1-O3 |
| 71 | B1 | 101 | PLX | C2-O1-P1-O2 |
| 71 | B1 | 101 | PLX | C2-O1-P1-O3 |
| 71 | CB | 201 | PLX | O7-C6-O6-C4 |
| 71 | CB | 201 | PLX | C2-O1-P1-O2 |
| 71 | CB | 201 | PLX | O9-C24-O8-C5 |
| 71 | CB | 201 | PLX | O9-C24-C25-C26 |
| 71 | N4 | 502 | PLX | O7-C6-O6-C4 |
| 71 | N4 | 502 | PLX | C5-C4-O6-C6 |
| 71 | N4 | 502 | PLX | C3-O4-P1-O2 |
| 71 | N4 | 502 | PLX | C3-O4-P1-O3 |
| 71 | N6 | 201 | PLX | O7-C6-O6-C4 |
| 71 | N6 | 201 | PLX | N1-C1-C2-O1 |
| 71 | N6 | 201 | PLX | O8-C24-C25-C26 |
| 71 | N6 | 201 | PLX | O9-C24-C25-C26 |
| 71 | QI | 301 | PLX | C2-O1-P1-O2 |
| 71 | QI | 301 | PLX | O9-C24-O8-C5 |
| 71 | QI | 301 | PLX | O9-C24-C25-C26 |
| 71 | Qi | 301 | PLX | O7-C6-C7-C8 |
| 71 | Qi | 301 | PLX | O7-C6-O6-C4 |
| 71 | Qi | 301 | PLX | C2-O1-P1-O2 |
| 71 | Qi | 301 | PLX | O9-C24-O8-C5 |
| 71 | Qi | 301 | PLX | O9-C24-C25-C26 |
| 71 | S7 | 203 | PLX | O7-C6-C7-C8 |
| 71 | S7 | 203 | PLX | C2-O1-P1-O3 |
| 71 | S7 | 203 | PLX | O9-C24-C25-C26 |
| 72 | B8 | 201 | 3PE | C1-O11-P-O13 |
| 72 | B8 | 201 | 3PE | O13-C11-C12-N |
| 72 | C1 | 609 | 3PE | C1-O11-P-O12 |
| 72 | C1 | 609 | 3PE | C1-O11-P-O13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 72 | C1 | 609 | 3PE | C1-O11-P-O14 |
| 72 | C1 | 609 | 3PE | C11-O13-P-O12 |
| 72 | C1 | 609 | 3PE | C11-O13-P-O14 |
| 72 | C1 | 609 | 3PE | O13-C11-C12-N |
| 72 | CB | 202 | 3PE | C1-O11-P-O12 |
| 72 | CB | 202 | 3PE | C11-O13-P-O12 |
| 72 | CB | 202 | 3PE | C11-O13-P-O14 |
| 72 | N5 | 706 | 3PE | C1-O11-P-O12 |
| 72 | N5 | 706 | 3PE | C1-O11-P-O13 |
| 72 | N5 | 706 | 3PE | C1-O11-P-O14 |
| 72 | N5 | 706 | 3PE | O13-C11-C12-N |
| 72 | QE | 302 | 3PE | O13-C11-C12-N |
| 72 | QJ | 101 | 3PE | C11-O13-P-O12 |
| 72 | QJ | 101 | 3PE | C11-O13-P-O14 |
| 72 | QJ | 101 | 3PE | O13-C11-C12-N |
| 72 | Qc | 404 | 3PE | C11-O13-P-O11 |
| 72 | Qc | 404 | 3PE | C11-O13-P-O12 |
| 72 | Qc | 404 | 3PE | C11-O13-P-O14 |
| 72 | Qc | 404 | 3PE | O13-C11-C12-N |
| 72 | Qj | 101 | 3PE | C11-O13-P-O12 |
| 72 | Qj | 101 | 3PE | C11-O13-P-O14 |
| 72 | Qj | 101 | 3PE | O13-C11-C12-N |
| 72 | S7 | 204 | 3PE | C1-O11-P-O12 |
| 72 | S7 | 204 | 3PE | C1-O11-P-O14 |
| 72 | S7 | 204 | 3PE | O13-C11-C12-N |
| 73 | A9 | 402 | PEE | C11-C10-O2-C2 |
| 73 | A9 | 402 | PEE | C1-O3P-P-O1P |
| 73 | A9 | 402 | PEE | C4-O4P-P-O3P |
| 73 | A9 | 402 | PEE | C4-O4P-P-O2P |
| 73 | N1 | 403 | PEE | C1-O3P-P-O2P |
| 73 | N1 | 403 | PEE | C1-O3P-P-O1P |
| 73 | N1 | 403 | PEE | C4-O4P-P-O3P |
| 73 | N1 | 403 | PEE | C4-O4P-P-O2P |
| 73 | N1 | 403 | PEE | C4-O4P-P-O1P |
| 73 | N3 | 201 | PEE | C17-C18-C19-C20 |
| 73 | N3 | 201 | PEE | C1-O3P-P-O2P |
| 73 | N3 | 201 | PEE | C4-O4P-P-O3P |
| 73 | N3 | 201 | PEE | C31-C30-O3-C3 |
| 73 | N4 | 501 | PEE | C1-O3P-P-O2P |
| 73 | N4 | 501 | PEE | C1-O3P-P-O1P |
| 73 | N4 | 501 | PEE | O4P-C4-C5-N |
| 73 | N4 | 501 | PEE | C37-C38-C39-C40 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 73 | N5 | 702 | PEE | C11-C10-O2-C2 |
| 73 | N5 | 702 | PEE | C1-O3P-P-O2P |
| 73 | N5 | 702 | PEE | C1-O3P-P-O1P |
| 73 | N5 | 702 | PEE | C1-O3P-P-O4P |
| 73 | N5 | 702 | PEE | C37-C38-C39-C40 |
| 73 | N5 | 705 | PEE | C1-O3P-P-O2P |
| 73 | N5 | 705 | PEE | C4-O4P-P-O2P |
| 73 | N5 | 705 | PEE | C4-O4P-P-O1P |
| 73 | QB | 502 | PEE | C4-O4P-P-O2P |
| 73 | QB | 502 | PEE | C4-O4P-P-O1P |
| 73 | QB | 502 | PEE | O5-C30-O3-C3 |
| 73 | QB | 502 | PEE | C31-C30-O3-C3 |
| 73 | QC | 403 | PEE | O2-C2-C3-O3 |
| 73 | QE | 301 | PEE | C1-O3P-P-O2P |
| 73 | QE | 301 | PEE | C1-O3P-P-O1P |
| 73 | QE | 301 | PEE | C4-O4P-P-O1P |
| 73 | Qc | 401 | PEE | O4P-C4-C5-N |
| 73 | Qe | 301 | PEE | C11-C10-O2-C2 |
| 73 | Qe | 301 | PEE | O4-C10-O2-C2 |
| 73 | Qe | 301 | PEE | C1-O3P-P-O2P |
| 73 | Qe | 301 | PEE | C4-O4P-P-O1P |
| 73 | S2 | 501 | PEE | C11-C10-O2-C2 |
| 73 | S2 | 501 | PEE | O4-C10-O2-C2 |
| 73 | S2 | 501 | PEE | C1-O3P-P-O1P |
| 73 | S2 | 501 | PEE | C4-O4P-P-O3P |
| 73 | S2 | 501 | PEE | C4-O4P-P-O2P |
| 73 | S2 | 501 | PEE | C4-O4P-P-O1P |
| 73 | S2 | 501 | PEE | O4P-C4-C5-N |
| 73 | S8 | 303 | PEE | O4-C10-O2-C2 |
| 73 | S8 | 303 | PEE | O3P-C1-C2-O2 |
| 73 | S8 | 303 | PEE | C1-O3P-P-O1P |
| 73 | S8 | 303 | PEE | C1-O3P-P-O4P |
| 75 | AC | 201 | ZMP | C17-C18-C21-O5 |
| 75 | AC | 201 | ZMP | N2-C16-C17-O4 |
| 75 | AC | 201 | ZMP | C12-C11-S1-C10 |
| 75 | AC | 201 | ZMP | O1-C10-S1-C11 |
| 75 | AC | 201 | ZMP | C9-C10-S1-C11 |
| 75 | AC | 201 | ZMP | S1-C10-C9-C8 |
| 75 | AC | 201 | ZMP | C7-C8-C9-C10 |
| 76 | AK | 401 | ADP | C5'-O5'-PA-O2A |
| 76 | AK | 401 | ADP | C5'-O5'-PA-O3A |
| 77 | C1 | 601 | HEA | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 77 | C1 | 601 | HEA | C17-C18-C19-C27 |
| 77 | C1 | 601 | HEA | C27-C19-C20-C21 |
| 77 | C1 | 602 | HEA | C18-C19-C20-C21 |
| 77 | C1 | 602 | HEA | C27-C19-C20-C21 |
| 80 | QC | 401 | HEM | C2B-C3B-CAB-CBB |
| 80 | QC | 402 | HEM | C2B-C3B-CAB-CBB |
| 80 | Qc | 403 | HEM | C1A-C2A-CAA-CBA |
| 80 | Qc | 403 | HEM | C3A-C2A-CAA-CBA |
| 80 | Qc | 403 | HEM | C2B-C3B-CAB-CBB |
| 80 | Qc | 403 | HEM | C4B-C3B-CAB-CBB |
| 85 | S7 | 201 | U10 | C9-C11-C12-C13 |
| 85 | S7 | 201 | U10 | C18-C19-C21-C22 |
| 85 | S7 | 201 | U10 | C20-C19-C21-C22 |
| 85 | S7 | 201 | U10 | C23-C24-C26-C27 |
| 85 | S7 | 201 | U10 | C25-C24-C26-C27 |
| 85 | S7 | 201 | U10 | C34-C36-C37-C38 |
| 85 | S7 | 201 | U10 | C38-C39-C41-C42 |
| 85 | S7 | 201 | U10 | C40-C39-C41-C42 |
| 73 | N3 | 201 | PEE | O5-C30-O3-C3 |
| 73 | Qe | 301 | PEE | O5-C30-O3-C3 |
| 73 | Qe | 301 | PEE | C31-C30-O3-C3 |
| 73 | N1 | 403 | PEE | O5-C30-O3-C3 |
| 73 | N4 | 501 | PEE | O5-C30-O3-C3 |
| 73 | N5 | 702 | PEE | O5-C30-O3-C3 |
| 73 | Qc | 401 | PEE | O5-C30-O3-C3 |
| 73 | A9 | 402 | PEE | O4-C10-O2-C2 |
| 73 | N5 | 702 | PEE | O4-C10-O2-C2 |
| 73 | N5 | 705 | PEE | O4-C10-O2-C2 |
| 73 | N4 | 501 | PEE | C31-C30-O3-C3 |
| 73 | Qc | 401 | PEE | C31-C30-O3-C3 |
| 73 | N5 | 705 | PEE | C11-C10-O2-C2 |
| 73 | S8 | 303 | PEE | C11-C10-O2-C2 |
| 85 | S7 | 201 | U10 | C35-C34-C36-C37 |
| 73 | N1 | 403 | PEE | C31-C30-O3-C3 |
| 73 | N5 | 702 | PEE | C31-C30-O3-C3 |
| 73 | N5 | 701 | PEE | C17-C18-C19-C20 |
| 73 | N5 | 701 | PEE | C37-C38-C39-C40 |
| 73 | N5 | 705 | PEE | C37-C38-C39-C40 |
| 73 | S8 | 303 | PEE | C37-C38-C39-C40 |
| 77 | C1 | 602 | HEA | C17-C18-C19-C27 |
| 77 | C1 | 601 | HEA | C17-C18-C19-C20 |
| 77 | C1 | 602 | HEA | C17-C18-C19-C20 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 73 | A9 | 402 | PEE | O5-C30-O3-C3 |
| 68 | A7 | 201 | CDL | O1-C1-CA2-OA2 |
| 73 | A9 | 402 | PEE | C31-C30-O3-C3 |
| 73 | 7C | 101 | PEE | C21-C22-C23-C24 |
| 68 | AL | 201 | CDL | C1-CA2-OA2-PA1 |
| 77 | C1 | 601 | HEA | C15-C16-C17-C18 |
| 77 | C1 | 602 | HEA | C19-C20-C21-C22 |
| 85 | S7 | 201 | U10 | C19-C21-C22-C23 |
| 85 | S7 | 201 | U10 | C29-C31-C32-C33 |
| 85 | S7 | 201 | U10 | C49-C51-C52-C53 |
| 68 | A8 | 301 | CDL | CA2-C1-CB2-OB2 |
| 70 | C1 | 605 | PC1 | C11-C12-N-C14 |
| 70 | C3 | 303 | PC1 | C11-C12-N-C14 |
| 68 | A8 | 301 | CDL | O1-C1-CB2-OB2 |
| 68 | B4 | 201 | CDL | O1-C1-CA2-OA2 |
| 73 | N1 | 403 | PEE | C10-C11-C12-C13 |
| 73 | 7C | 101 | PEE | O2-C2-C3-O3 |
| 77 | C1 | 601 | HEA | C18-C19-C20-C21 |
| 85 | S7 | 201 | U10 | C33-C34-C36-C37 |
| 80 | Qc | 403 | HEM | C2A-CAA-CBA-CGA |
| 73 | N3 | 201 | PEE | C10-C11-C12-C13 |
| 73 | QC | 403 | PEE | C10-C11-C12-C13 |
| 73 | Qc | 401 | PEE | C30-C31-C32-C33 |
| 73 | N5 | 702 | PEE | C30-C31-C32-C33 |
| 73 | Qe | 302 | PEE | C10-C11-C12-C13 |
| 70 | C1 | 608 | PC1 | C2-C1-O11-P |
| 72 | 7A | 101 | 3PE | C2-C1-O11-P |
| 70 | C1 | 605 | PC1 | C11-C12-N-C13 |
| 70 | C3 | 303 | PC1 | C11-C12-N-C13 |
| 73 | N1 | 403 | PEE | C30-C31-C32-C33 |
| 72 | 7A | 101 | 3PE | C31-C32-C33-C34 |
| 77 | C1 | 601 | HEA | C19-C20-C21-C22 |
| 85 | S7 | 201 | U10 | C14-C16-C17-C18 |
| 73 | QE | 301 | PEE | C10-C11-C12-C13 |
| 68 | N1 | 401 | CDL | O1-C1-CB2-OB2 |
| 73 | N1 | 403 | PEE | C33-C34-C35-C36 |
| 73 | Qc | 401 | PEE | C17-C18-C19-C20 |
| 68 | 4L | 201 | CDL | CA2-OA2-PA1-OA5 |
| 68 | 4L | 201 | CDL | CA3-OA5-PA1-OA2 |
| 68 | 7A | 102 | CDL | CB2-OB2-PB2-OB5 |
| 68 | A8 | 301 | CDL | CB2-OB2-PB2-OB5 |
| 68 | A8 | 301 | CDL | CB3-OB5-PB2-OB2 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 68 | AK | 402 | CDL | CA2-OA2-PA1-OA5 |
| 68 | AK | 402 | CDL | CA3-OA5-PA1-OA2 |
| 68 | AL | 201 | CDL | CA2-OA2-PA1-OA5 |
| 68 | AL | 201 | CDL | CB3-OB5-PB2-OB2 |
| 68 | B4 | 201 | CDL | CA2-OA2-PA1-OA5 |
| 68 | B5 | 201 | CDL | CA3-OA5-PA1-OA2 |
| 68 | C3 | 304 | CDL | CA3-OA5-PA1-OA2 |
| 68 | C3 | 305 | CDL | CA2-OA2-PA1-OA5 |
| 68 | CB | 203 | CDL | CA2-OA2-PA1-OA5 |
| 68 | CB | 203 | CDL | CB2-OB2-PB2-OB5 |
| 68 | CB | 203 | CDL | CB3-OB5-PB2-OB2 |
| 68 | N1 | 401 | CDL | CB2-OB2-PB2-OB5 |
| 68 | N1 | 401 | CDL | CB3-OB5-PB2-OB2 |
| 68 | N4 | 503 | CDL | CA2-OA2-PA1-OA5 |
| 68 | N4 | 503 | CDL | CA3-OA5-PA1-OA2 |
| 68 | N4 | 503 | CDL | CB2-OB2-PB2-OB5 |
| 68 | N5 | 703 | CDL | CA2-OA2-PA1-OA5 |
| 68 | N5 | 703 | CDL | CB2-OB2-PB2-OB5 |
| 68 | N5 | 703 | CDL | CB3-OB5-PB2-OB2 |
| 68 | QB | 501 | CDL | CA2-OA2-PA1-OA5 |
| 68 | QB | 501 | CDL | CA3-OA5-PA1-OA2 |
| 68 | QC | 404 | CDL | CB3-OB5-PB2-OB2 |
| 68 | QH | 102 | CDL | CB2-OB2-PB2-OB5 |
| 68 | QH | 102 | CDL | CB3-OB5-PB2-OB2 |
| 68 | Qb | 501 | CDL | CA2-OA2-PA1-OA5 |
| 70 | 6A | 101 | PC1 | C11-O13-P-O11 |
| 70 | C1 | 605 | PC1 | C11-O13-P-O11 |
| 70 | C1 | 606 | PC1 | C1-O11-P-O13 |
| 70 | C1 | 608 | PC1 | C1-O11-P-O13 |
| 70 | C3 | 301 | PC1 | C11-O13-P-O11 |
| 70 | C3 | 302 | PC1 | C11-O13-P-O11 |
| 70 | N1 | 402 | PC1 | C1-O11-P-O13 |
| 70 | N3 | 202 | PC1 | C11-O13-P-O11 |
| 70 | N3 | 202 | PC1 | C1-O11-P-O13 |
| 70 | Qc | 405 | PC1 | C1-O11-P-O13 |
| 71 | B1 | 101 | PLX | C3-O4-P1-O1 |
| 71 | B1 | 101 | PLX | C2-O1-P1-O4 |
| 71 | CB | 201 | PLX | C2-O1-P1-O4 |
| 71 | N4 | 502 | PLX | C3-O4-P1-O1 |
| 71 | N6 | 201 | PLX | C3-O4-P1-O1 |
| 71 | QI | 301 | PLX | C2-O1-P1-O4 |
| 71 | S7 | 203 | PLX | C2-O1-P1-O4 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 72 | 7A | 101 | 3PE | C1-O11-P-O13 |
| 72 | 7A | 101 | 3PE | C11-O13-P-O11 |
| 72 | B8 | 201 | 3PE | C11-O13-P-O11 |
| 72 | C1 | 609 | 3PE | C11-O13-P-O11 |
| 72 | CA | 101 | 3PE | C11-O13-P-O11 |
| 72 | CB | 202 | 3PE | C11-O13-P-O11 |
| 72 | QE | 302 | 3PE | C1-O11-P-O13 |
| 72 | QJ | 101 | 3PE | C11-O13-P-O11 |
| 72 | Qc | 404 | 3PE | C1-O11-P-O13 |
| 72 | Qj | 101 | 3PE | C11-O13-P-O11 |
| 72 | S7 | 204 | 3PE | C1-O11-P-O13 |
| 73 | N1 | 403 | PEE | C1-O3P-P-O4P |
| 73 | N3 | 201 | PEE | C1-O3P-P-O4P |
| 73 | N4 | 501 | PEE | C1-O3P-P-O4P |
| 73 | N5 | 701 | PEE | C4-O4P-P-O3P |
| 73 | QB | 502 | PEE | C4-O4P-P-O3P |
| 73 | QC | 403 | PEE | C4-O4P-P-O3P |
| 73 | QE | 301 | PEE | C1-O3P-P-O4P |
| 73 | Qc | 401 | PEE | C1-O3P-P-O4P |
| 73 | Qe | 301 | PEE | C1-O3P-P-O4P |
| 73 | Qe | 301 | PEE | C4-O4P-P-O3P |
| 68 | A7 | 201 | CDL | CB2-C1-CA2-OA2 |
| 68 | B4 | 201 | CDL | CB2-C1-CA2-OA2 |
| 68 | N1 | 401 | CDL | CA2-C1-CB2-OB2 |
| 85 | S7 | 201 | U10 | C45-C44-C46-C47 |
| 73 | S8 | 303 | PEE | C31-C30-O3-C3 |
| 73 | N5 | 705 | PEE | C33-C34-C35-C36 |
| 71 | AL | 202 | PLX | O6-C6-C7-C8 |
| 71 | AM | 201 | PLX | O6-C6-C7-C8 |
| 71 | S7 | 203 | PLX | O6-C6-C7-C8 |
| 71 | S7 | 203 | PLX | O8-C24-C25-C26 |
| 71 | N4 | 502 | PLX | C9-C10-C11-C12 |
| 71 | S7 | 203 | PLX | C7-C8-C9-C10 |
| 73 | N3 | 201 | PEE | C32-C33-C34-C35 |
| 73 | N5 | 702 | PEE | C14-C15-C16-C17 |
| 71 | AL | 202 | PLX | C29-C30-C31-C32 |
| 71 | AM | 201 | PLX | C12-C13-C14-C15 |
| 71 | CB | 201 | PLX | C29-C30-C31-C32 |
| 71 | Qi | 301 | PLX | C26-C27-C28-C29 |
| 73 | N5 | 701 | PEE | C21-C22-C23-C24 |
| 73 | Qc | 401 | PEE | C31-C32-C33-C34 |
| 75 | AC | 201 | ZMP | C19-C18-C21-O5 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 75 | AC | 201 | ZMP | C20-C18-C21-O5 |
| 71 | B1 | 101 | PLX | C29-C30-C31-C32 |
| 71 | N6 | 201 | PLX | C34-C35-C36-C37 |
| 71 | S7 | 203 | PLX | C13-C14-C15-C16 |
| 73 | N5 | 701 | PEE | C31-C32-C33-C34 |
| 73 | N5 | 702 | PEE | C12-C13-C14-C15 |
| 73 | N5 | 702 | PEE | C11-C12-C13-C14 |
| 73 | N5 | 702 | PEE | C10-C11-C12-C13 |
| 71 | Qi | 301 | PLX | C18-C19-C20-C21 |
| 72 | C1 | 609 | 3PE | C25-C26-C27-C28 |
| 73 | N3 | 201 | PEE | C33-C34-C35-C36 |
| 73 | N4 | 501 | PEE | C23-C24-C25-C26 |
| 73 | N5 | 701 | PEE | C12-C13-C14-C15 |
| 70 | Qb | 502 | PC1 | C36-C37-C38-C39 |
| 71 | B1 | 101 | PLX | C25-C26-C27-C28 |
| 73 | 7C | 101 | PEE | C12-C13-C14-C15 |
| 73 | N5 | 701 | PEE | C14-C15-C16-C17 |
| 73 | QC | 403 | PEE | C21-C22-C23-C24 |
| 71 | QI | 301 | PLX | C29-C30-C31-C32 |
| 68 | N4 | 503 | CDL | CA7-C31-C32-C33 |
| 70 | N3 | 202 | PC1 | C23-C24-C25-C26 |
| 71 | Qi | 301 | PLX | C25-C26-C27-C28 |
| 72 | C1 | 607 | 3PE | C2C-C2D-C2E-C2F |
| 73 | Qc | 401 | PEE | C33-C34-C35-C36 |
| 73 | S8 | 303 | PEE | C33-C34-C35-C36 |
| 68 | N1 | 401 | CDL | C76-C77-C78-C79 |
| 71 | AL | 202 | PLX | C12-C13-C14-C15 |
| 73 | A9 | 402 | PEE | C12-C13-C14-C15 |
| 68 | 4L | 201 | CDL | C39-C40-C41-C42 |
| 68 | CB | 203 | CDL | C32-C33-C34-C35 |
| 71 | CB | 201 | PLX | C31-C32-C33-C34 |
| 73 | N1 | 403 | PEE | C12-C13-C14-C15 |
| 73 | N5 | 701 | PEE | C32-C33-C34-C35 |
| 73 | QE | 301 | PEE | C32-C33-C34-C35 |
| 73 | S2 | 501 | PEE | C11-C12-C13-C14 |
| 75 | AC | 201 | ZMP | C1-C22-C23-C24 |
| 73 | N3 | 201 | PEE | C22-C23-C24-C25 |
| 73 | N5 | 705 | PEE | C14-C15-C16-C17 |
| 73 | Qe | 301 | PEE | C33-C34-C35-C36 |
| 73 | N4 | 501 | PEE | C11-C10-O2-C2 |
| 73 | QE | 301 | PEE | C11-C10-O2-C2 |
| 73 | N1 | 403 | PEE | C13-C14-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 73 | S2 | 501 | PEE | C20-C21-C22-C23 |
| 73 | N4 | 501 | PEE | C35-C36-C37-C38 |
| 73 | N4 | 501 | PEE | C39-C40-C41-C42 |
| 73 | QB | 502 | PEE | C35-C36-C37-C38 |
| 70 | C3 | 301 | PC1 | C29-C2A-C2B-C2C |
| 70 | C3 | 306 | PC1 | C29-C2A-C2B-C2C |
| 71 | N4 | 502 | PLX | C16-C17-C18-C19 |
| 73 | Qe | 301 | PEE | C14-C15-C16-C17 |
| 75 | AB | 201 | ZMP | C2-C1-C22-C23 |
| 70 | C3 | 303 | PC1 | C11-C12-N-C15 |
| 85 | S7 | 201 | U10 | C39-C41-C42-C43 |
| 72 | CA | 101 | 3PE | C2A-C2B-C2C-C2D |
| 73 | 7C | 101 | PEE | C11-C12-C13-C14 |
| 72 | 7A | 101 | 3PE | O13-C11-C12-N |
| 73 | QE | 301 | PEE | O4P-C4-C5-N |
| 68 | CB | 203 | CDL | C38-C39-C40-C41 |
| 71 | QI | 301 | PLX | C7-C8-C9-C10 |
| 73 | S8 | 303 | PEE | C11-C12-C13-C14 |
| 68 | CB | 203 | CDL | C22-C23-C24-C25 |
| 68 | A8 | 301 | CDL | C38-C39-C40-C41 |
| 68 | N4 | 503 | CDL | C13-C14-C15-C16 |
| 73 | Qc | 401 | PEE | C22-C23-C24-C25 |
| 71 | CB | 201 | PLX | C7-C8-C9-C10 |
| 73 | N3 | 201 | PEE | C21-C22-C23-C24 |
| 68 | AL | 201 | CDL | C52-C53-C54-C55 |
| 68 | N5 | 704 | CDL | C22-C23-C24-C25 |
| 73 | Qe | 302 | PEE | C11-C12-C13-C14 |
| 68 | AL | 201 | CDL | C33-C34-C35-C36 |
| 73 | S8 | 303 | PEE | O5-C30-O3-C3 |
| 71 | AM | 201 | PLX | O9-C24-C25-C26 |
| 71 | B1 | 101 | PLX | O9-C24-C25-C26 |
| 68 | N5 | 704 | CDL | C72-C73-C74-C75 |
| 68 | QB | 501 | CDL | C51-C52-C53-C54 |
| 68 | QH | 102 | CDL | C51-C52-C53-C54 |
| 73 | N3 | 201 | PEE | C35-C36-C37-C38 |
| 73 | N5 | 701 | PEE | C15-C16-C17-C18 |
| 72 | C1 | 607 | 3PE | C2E-C2F-C2G-C2H |
| 70 | Qh | 101 | PC1 | C35-C36-C37-C38 |
| 73 | QE | 301 | PEE | C12-C13-C14-C15 |
| 68 | QH | 101 | CDL | C31-C32-C33-C34 |
| 72 | N5 | 706 | 3PE | C35-C36-C37-C38 |
| 73 | N1 | 403 | PEE | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 73 | Qc | 401 | PEE | C12-C13-C14-C15 |
| 73 | Qe | 301 | PEE | C22-C23-C24-C25 |
| 70 | C1 | 605 | PC1 | C11-C12-N-C15 |
| 70 | C3 | 302 | PC1 | C11-C12-N-C15 |
| 68 | CB | 203 | CDL | C78-C79-C80-C81 |
| 80 | QC | 401 | HEM | C3D-CAD-CBD-CGD |
| 73 | QE | 301 | PEE | C11-C12-C13-C14 |
| 73 | N5 | 702 | PEE | C18-C19-C20-C21 |
| 73 | A9 | 402 | PEE | C35-C36-C37-C38 |
| 73 | S2 | 501 | PEE | C19-C20-C21-C22 |
| 73 | N4 | 501 | PEE | O4-C10-O2-C2 |
| 73 | N5 | 701 | PEE | O4-C10-O2-C2 |
| 73 | QE | 301 | PEE | O4-C10-O2-C2 |
| 72 | S7 | 204 | 3PE | C21-C22-C23-C24 |
| 73 | S2 | 501 | PEE | C31-C30-O3-C3 |
| 75 | AC | 201 | ZMP | C22-C23-C24-C25 |
| 72 | QJ | 101 | 3PE | C24-C25-C26-C27 |
| 73 | S2 | 501 | PEE | C14-C15-C16-C17 |
| 68 | N5 | 703 | CDL | C60-C61-C62-C63 |
| 73 | Qc | 401 | PEE | C32-C33-C34-C35 |
| 72 | C1 | 607 | 3PE | C27-C28-C29-C2A |
| 80 | Qc | 402 | HEM | C2B-C3B-CAB-CBB |
| 71 | AL | 202 | PLX | C33-C34-C35-C36 |
| 71 | Qi | 301 | PLX | C13-C14-C15-C16 |
| 73 | 7C | 101 | PEE | C31-C32-C33-C34 |
| 73 | S8 | 303 | PEE | C22-C23-C24-C25 |
| 68 | CB | 203 | CDL | C61-C62-C63-C64 |
| 73 | N5 | 701 | PEE | C11-C12-C13-C14 |
| 68 | 4L | 201 | CDL | CA5-C11-C12-C13 |
| 73 | N5 | 701 | PEE | C11-C10-O2-C2 |
| 73 | Qe | 302 | PEE | C11-C10-O2-C2 |
| 71 | CB | 201 | PLX | O4-C3-C4-O6 |
| 71 | Qi | 301 | PLX | O4-C3-C4-O6 |
| 73 | Qe | 302 | PEE | O3P-C1-C2-O2 |
| 68 | N1 | 401 | CDL | C31-C32-C33-C34 |
| 73 | N4 | 501 | PEE | C22-C23-C24-C25 |
| 73 | S8 | 303 | PEE | C13-C14-C15-C16 |
| 75 | AB | 201 | ZMP | C22-C23-C24-C25 |
| 80 | QC | 401 | HEM | C4B-C3B-CAB-CBB |
| 80 | QC | 402 | HEM | C4B-C3B-CAB-CBB |
| 71 | N4 | 502 | PLX | C29-C30-C31-C32 |
| 75 | AB | 201 | ZMP | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 73 | Qe | 302 | PEE | O4-C10-O2-C2 |
| 68 | A8 | 301 | CDL | OB6-CB4-CB6-OB8 |
| 70 | C1 | 608 | PC1 | O21-C2-C3-O31 |
| 71 | 6C | 101 | PLX | O6-C4-C5-O8 |
| 72 | QJ | 101 | 3PE | O21-C2-C3-O31 |
| 68 | N5 | 703 | CDL | C59-C60-C61-C62 |
| 71 | N4 | 502 | PLX | C11-C12-C13-C14 |
| 73 | Qe | 301 | PEE | C12-C13-C14-C15 |
| 70 | Qh | 101 | PC1 | C11-C12-N-C14 |
| 75 | AC | 201 | ZMP | C6-C7-C8-C9 |
| 75 | AC | 201 | ZMP | C3-C4-C5-C6 |
| 73 | 7C | 101 | PEE | C35-C36-C37-C38 |
| 73 | N5 | 701 | PEE | C35-C36-C37-C38 |
| 73 | N5 | 705 | PEE | C35-C36-C37-C38 |
| 73 | S2 | 501 | PEE | C15-C16-C17-C18 |
| 73 | S8 | 303 | PEE | C35-C36-C37-C38 |
| 85 | S7 | 201 | U10 | C43-C44-C46-C47 |
| 73 | N4 | 501 | PEE | C11-C12-C13-C14 |
| 73 | QE | 301 | PEE | C33-C34-C35-C36 |
| 73 | N4 | 501 | PEE | C17-C18-C19-C20 |
| 73 | A9 | 402 | PEE | C33-C34-C35-C36 |
| 73 | S2 | 501 | PEE | C40-C41-C42-C43 |
| 73 | N5 | 702 | PEE | C33-C34-C35-C36 |
| 75 | AC | 201 | ZMP | C1-C2-C3-C4 |
| 73 | QE | 301 | PEE | C16-C17-C18-C19 |
| 68 | 7A | 102 | CDL | CA3-OA5-PA1-OA2 |
| 68 | AL | 201 | CDL | CB2-OB2-PB2-OB5 |
| 68 | B5 | 201 | CDL | CA2-OA2-PA1-OA5 |
| 68 | QC | 404 | CDL | CB2-OB2-PB2-OB5 |
| 68 | QH | 101 | CDL | CA2-OA2-PA1-OA5 |
| 70 | C3 | 301 | PC1 | C1-O11-P-O13 |
| 71 | AL | 202 | PLX | C3-O4-P1-O1 |
| 71 | Qi | 301 | PLX | C2-O1-P1-O4 |
| 73 | N5 | 705 | PEE | C1-O3P-P-O4P |
| 73 | N5 | 705 | PEE | C4-O4P-P-O3P |
| 73 | S2 | 501 | PEE | C1-O3P-P-O4P |
| 72 | QJ | 101 | 3PE | C26-C27-C28-C29 |
| 70 | C3 | 301 | PC1 | C2-C1-O11-P |
| 68 | 7A | 102 | CDL | OB5-CB3-CB4-CB6 |
| 68 | QD | 402 | CDL | OA5-CA3-CA4-CA6 |
| 70 | C3 | 301 | PC1 | O11-C1-C2-C3 |
| 73 | Qc | 401 | PEE | O3P-C1-C2-C3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 73 | S2 | 501 | PEE | C42-C43-C44-C45 |
| 75 | AC | 201 | ZMP | C14-C15-N2-C16 |
| 73 | Qe | 301 | PEE | C10-C11-C12-C13 |
| 73 | N5 | 705 | PEE | C21-C22-C23-C24 |
| 73 | QB | 502 | PEE | C32-C33-C34-C35 |
| 75 | AC | 201 | ZMP | C2-C3-C4-C5 |
| 73 | Qe | 301 | PEE | C35-C36-C37-C38 |
| 68 | B5 | 201 | CDL | CB2-C1-CA2-OA2 |
| 72 | CB | 202 | 3PE | C21-C22-C23-C24 |
| 73 | S2 | 501 | PEE | O5-C30-O3-C3 |
| 70 | Qc | 405 | PC1 | C3A-C3B-C3C-C3D |
| 68 | A8 | 301 | CDL | CB3-CB4-CB6-OB8 |
| 68 | N4 | 503 | CDL | CA3-CA4-CA6-OA8 |
| 68 | QC | 404 | CDL | CA3-CA4-CA6-OA8 |
| 68 | QH | 102 | CDL | CA3-CA4-CA6-OA8 |
| 70 | C1 | 608 | PC1 | C39-C3A-C3B-C3C |
| 70 | C3 | 306 | PC1 | C1-C2-C3-O31 |
| 73 | N1 | 403 | PEE | C1-C2-C3-O3 |
| 73 | N5 | 701 | PEE | C1-C2-C3-O3 |
| 73 | QB | 502 | PEE | C1-C2-C3-O3 |
| 73 | Qc | 401 | PEE | C1-C2-C3-O3 |
| 71 | S7 | 203 | PLX | C32-C33-C34-C35 |
| 70 | QB | 503 | PC1 | C29-C2A-C2B-C2C |
| 73 | N5 | 702 | PEE | C32-C33-C34-C35 |
| 73 | S2 | 501 | PEE | C21-C22-C23-C24 |
| 71 | N6 | 201 | PLX | O6-C6-C7-C8 |
| 75 | AB | 201 | ZMP | O3-C16-C17-O4 |
| 75 | AC | 201 | ZMP | O3-C16-C17-O4 |
| 73 | QC | 403 | PEE | C12-C13-C14-C15 |
| 73 | S8 | 303 | PEE | C21-C22-C23-C24 |
| 73 | QC | 403 | PEE | C16-C17-C18-C19 |
| 68 | B5 | 201 | CDL | C21-C22-C23-C24 |
| 73 | N5 | 701 | PEE | C33-C34-C35-C36 |
| 73 | 7C | 101 | PEE | C39-C40-C41-C42 |
| 73 | N5 | 705 | PEE | C19-C20-C21-C22 |
| 75 | AC | 201 | ZMP | C22-C1-C2-C3 |
| 73 | QE | 301 | PEE | C40-C41-C42-C43 |
| 73 | N5 | 701 | PEE | C30-C31-C32-C33 |
| 70 | Qc | 405 | PC1 | C28-C29-C2A-C2B |
| 68 | CB | 203 | CDL | C63-C64-C65-C66 |
| 72 | CA | 101 | 3PE | C35-C36-C37-C38 |
| 68 | B4 | 201 | CDL | C80-C81-C82-C83 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 73 | Qe | 301 | PEE | C38-C39-C40-C41 |
| 73 | S2 | 501 | PEE | C38-C39-C40-C41 |
| 71 | CB | 201 | PLX | C11-C12-C13-C14 |
| 68 | C3 | 304 | CDL | OB5-CB3-CB4-OB6 |
| 73 | N1 | 403 | PEE | O3P-C1-C2-O2 |
| 70 | C3 | 302 | PC1 | C11-C12-N-C13 |
| 71 | QI | 301 | PLX | C34-C35-C36-C37 |
| 73 | QC | 403 | PEE | C14-C15-C16-C17 |
| 73 | Qe | 301 | PEE | C41-C42-C43-C44 |
| 73 | A9 | 402 | PEE | C31-C32-C33-C34 |
| 71 | N4 | 502 | PLX | C34-C35-C36-C37 |
| 73 | S8 | 303 | PEE | O2-C2-C3-O3 |
| 71 | QI | 301 | PLX | C16-C17-C18-C19 |
| 73 | N3 | 201 | PEE | C42-C43-C44-C45 |
| 68 | N1 | 401 | CDL | C75-C76-C77-C78 |
| 71 | Qi | 301 | PLX | C29-C30-C31-C32 |
| 70 | N3 | 202 | PC1 | C32-C33-C34-C35 |
| 73 | S8 | 303 | PEE | C34-C35-C36-C37 |
| 71 | S7 | 203 | PLX | C14-C15-C16-C17 |
| 74 | A9 | 401 | NDP | PN-O3-PA-O1A |
| 73 | A9 | 402 | PEE | C11-C12-C13-C14 |
| 70 | Qc | 405 | PC1 | C2D-C2E-C2F-C2G |
| 68 | A8 | 301 | CDL | C11-C12-C13-C14 |
| 68 | N5 | 704 | CDL | C17-C18-C19-C20 |
| 73 | A9 | 402 | PEE | C17-C18-C19-C20 |
| 73 | S2 | 501 | PEE | C18-C19-C20-C21 |
| 73 | S2 | 501 | PEE | C16-C17-C18-C19 |
| 68 | AL | 201 | CDL | OB5-CB3-CB4-CB6 |
| 68 | C3 | 304 | CDL | OB5-CB3-CB4-CB6 |
| 68 | QB | 501 | CDL | OB5-CB3-CB4-CB6 |
| 70 | C1 | 608 | PC1 | O11-C1-C2-C3 |
| 71 | 6C | 101 | PLX | O4-C3-C4-C5 |
| 71 | CB | 201 | PLX | O4-C3-C4-C5 |
| 71 | Qi | 301 | PLX | O4-C3-C4-C5 |
| 72 | 7A | 101 | 3PE | O11-C1-C2-C3 |
| 73 | A9 | 402 | PEE | O3P-C1-C2-C3 |
| 73 | QB | 502 | PEE | O3P-C1-C2-C3 |
| 73 | QC | 403 | PEE | O3P-C1-C2-C3 |
| 73 | Qe | 301 | PEE | O3P-C1-C2-C3 |
| 73 | Qe | 302 | PEE | O3P-C1-C2-C3 |
| 68 | QB | 501 | CDL | CA7-C31-C32-C33 |
| 72 | CA | 101 | 3PE | O13-C11-C12-N |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 71 | N6 | 201 | PLX | C7-C8-C9-C10 |
| 72 | Qc | 404 | 3PE | C3A-C3B-C3C-C3D |
| 73 | N4 | 501 | PEE | C24-C25-C26-C27 |
| 73 | QE | 301 | PEE | C14-C15-C16-C17 |
| 68 | 7A | 102 | CDL | C78-C79-C80-C81 |
| 73 | 7C | 101 | PEE | C41-C42-C43-C44 |
| 73 | N3 | 201 | PEE | C40-C41-C42-C43 |
| 71 | AL | 202 | PLX | C32-C33-C34-C35 |
| 71 | CB | 201 | PLX | C20-C21-C22-C23 |
| 72 | CB | 202 | 3PE | C39-C3A-C3B-C3C |
| 68 | QD | 402 | CDL | CA4-CA3-OA5-PA1 |
| 68 | QH | 102 | CDL | CA4-CA3-OA5-PA1 |
| 70 | C3 | 303 | PC1 | C2-C1-O11-P |
| 70 | N1 | 402 | PC1 | C2-C1-O11-P |
| 71 | N6 | 201 | PLX | C35-C36-C37-C38 |
| 73 | N5 | 705 | PEE | C24-C25-C26-C27 |
| 68 | CB | 203 | CDL | C81-C82-C83-C84 |
| 71 | 6C | 101 | PLX | C13-C14-C15-C16 |
| 71 | AM | 201 | PLX | C25-C26-C27-C28 |
| 71 | Qi | 301 | PLX | C19-C20-C21-C22 |
| 72 | QJ | 101 | 3PE | C33-C34-C35-C36 |
| 80 | Qc | 402 | HEM | C3D-CAD-CBD-CGD |
| 68 | 4L | 201 | CDL | C15-C16-C17-C18 |
| 68 | Qb | 501 | CDL | C54-C55-C56-C57 |
| 68 | QD | 402 | CDL | CA3-CA4-CA6-OA8 |
| 70 | C1 | 608 | PC1 | C1-C2-C3-O31 |
| 71 | N4 | 502 | PLX | C3-C4-C5-O8 |
| 71 | N6 | 201 | PLX | C3-C4-C5-O8 |
| 72 | QJ | 101 | 3PE | C1-C2-C3-O31 |
| 73 | 7C | 101 | PEE | C1-C2-C3-O3 |
| 73 | N5 | 705 | PEE | C1-C2-C3-O3 |
| 73 | Qe | 302 | PEE | C1-C2-C3-O3 |
| 73 | N5 | 701 | PEE | C22-C23-C24-C25 |
| 73 | N3 | 201 | PEE | C11-C12-C13-C14 |
| 75 | AB | 201 | ZMP | N2-C16-C17-C18 |
| 68 | N1 | 401 | CDL | C13-C14-C15-C16 |
| 73 | Qc | 401 | PEE | C35-C36-C37-C38 |
| 68 | B4 | 201 | CDL | CA3-OA5-PA1-OA2 |
| 68 | C3 | 305 | CDL | CA3-OA5-PA1-OA2 |
| 71 | B1 | 101 | PLX | C5-C4-O6-C6 |
| 71 | CB | 201 | PLX | C3-C4-O6-C6 |
| 71 | N6 | 201 | PLX | C5-C4-O6-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 72 | CA | 101 | 3PE | C1-O11-P-O13 |
| 73 | N5 | 702 | PEE | C4-O4P-P-O3P |
| 70 | Qh | 101 | PC1 | C38-C39-C3A-C3B |
| 71 | CB | 201 | PLX | O7-C6-C7-C8 |
| 68 | CB | 203 | CDL | C33-C34-C35-C36 |
| 75 | AB | 201 | ZMP | C3-C4-C5-C6 |
| 68 | 7A | 102 | CDL | OB5-CB3-CB4-OB6 |
| 68 | A8 | 301 | CDL | OB5-CB3-CB4-OB6 |
| 68 | B4 | 201 | CDL | OB5-CB3-CB4-OB6 |
| 68 | B5 | 201 | CDL | OB5-CB3-CB4-OB6 |
| 71 | AM | 201 | PLX | O4-C3-C4-O6 |
| 71 | QI | 301 | PLX | O4-C3-C4-O6 |
| 72 | 7A | 101 | 3PE | O11-C1-C2-O21 |
| 73 | N5 | 701 | PEE | O3P-C1-C2-O2 |
| 73 | QB | 502 | PEE | O3P-C1-C2-O2 |
| 73 | Qe | 301 | PEE | O3P-C1-C2-O2 |
| 73 | Qc | 401 | PEE | C23-C24-C25-C26 |
| 73 | S2 | 501 | PEE | C35-C36-C37-C38 |
| 73 | QE | 301 | PEE | C34-C35-C36-C37 |
| 68 | QH | 102 | CDL | C73-C74-C75-C76 |
| 68 | QD | 402 | CDL | OA6-CA4-CA6-OA8 |
| 70 | C3 | 306 | PC1 | O21-C2-C3-O31 |
| 71 | N6 | 201 | PLX | O6-C4-C5-O8 |
| 71 | Qi | 301 | PLX | O6-C4-C5-O8 |
| 72 | S7 | 204 | 3PE | O21-C2-C3-O31 |
| 73 | N5 | 701 | PEE | O2-C2-C3-O3 |
| 73 | Qe | 302 | PEE | O2-C2-C3-O3 |
| 68 | 7A | 102 | CDL | C37-C38-C39-C40 |
| 72 | Qc | 404 | 3PE | C25-C26-C27-C28 |
| 73 | N3 | 201 | PEE | C20-C21-C22-C23 |
| 73 | Qe | 301 | PEE | C31-C32-C33-C34 |
| 71 | S7 | 203 | PLX | C35-C36-C37-C38 |
| 71 | AM | 201 | PLX | C31-C32-C33-C34 |
| 71 | CB | 201 | PLX | C9-C10-C11-C12 |
| 68 | A8 | 301 | CDL | C17-C18-C19-C20 |
| 68 | AK | 402 | CDL | C53-C54-C55-C56 |
| 68 | B5 | 201 | CDL | C17-C18-C19-C20 |
| 73 | N4 | 501 | PEE | C32-C33-C34-C35 |
| 68 | A7 | 201 | CDL | C1-CA2-OA2-PA1 |
| 68 | AK | 402 | CDL | C1-CA2-OA2-PA1 |
| 68 | N4 | 503 | CDL | CB4-CB3-OB5-PB2 |
| 68 | N5 | 703 | CDL | C1-CB2-OB2-PB2 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 68 | QH | 101 | CDL | CB4-CB3-OB5-PB2 |
| 71 | 6C | 101 | PLX | C4-C3-O4-P1 |
| 76 | AK | 401 | ADP | C4'-C5'-O5'-PA |
| 68 | B4 | 201 | CDL | C74-C75-C76-C77 |
| 68 | C3 | 304 | CDL | C74-C75-C76-C77 |
| 71 | N6 | 201 | PLX | C26-C27-C28-C29 |
| 70 | Qh | 101 | PC1 | C11-C12-N-C15 |
| 73 | N1 | 403 | PEE | C14-C15-C16-C17 |
| 73 | N5 | 705 | PEE | C22-C23-C24-C25 |
| 68 | N5 | 704 | CDL | C51-C52-C53-C54 |
| 73 | QC | 403 | PEE | C30-C31-C32-C33 |
| 75 | AC | 201 | ZMP | O1-C10-C9-C8 |
| 71 | CB | 201 | PLX | O8-C24-C25-C26 |
| 71 | QI | 301 | PLX | O8-C24-C25-C26 |
| 71 | Qi | 301 | PLX | O6-C6-C7-C8 |
| 68 | B5 | 201 | CDL | OB5-CB3-CB4-CB6 |
| 68 | N4 | 503 | CDL | OB5-CB3-CB4-CB6 |
| 68 | Qb | 501 | CDL | OB5-CB3-CB4-CB6 |
| 71 | N6 | 201 | PLX | O4-C3-C4-C5 |
| 73 | S8 | 303 | PEE | O3P-C1-C2-C3 |
| 77 | C1 | 602 | HEA | C26-C15-C16-C17 |
| 68 | 4L | 201 | CDL | C23-C24-C25-C26 |
| 73 | S2 | 501 | PEE | C44-C45-C46-C47 |
| 73 | N5 | 702 | PEE | C31-C32-C33-C34 |
| 72 | C1 | 607 | 3PE | O21-C21-C22-C23 |
| 73 | QB | 502 | PEE | C1-C2-O2-C10 |
| 68 | 4L | 201 | CDL | C76-C77-C78-C79 |
| 68 | CB | 203 | CDL | CB3-CB4-CB6-OB8 |
| 68 | N4 | 503 | CDL | C1-CA2-OA2-PA1 |
| 68 | N4 | 503 | CDL | CA4-CA3-OA5-PA1 |
| 71 | 6C | 101 | PLX | C3-C4-C5-O8 |
| 71 | AM | 201 | PLX | C3-C4-C5-O8 |
| 71 | N4 | 502 | PLX | C4-C3-O4-P1 |
| 71 | Qi | 301 | PLX | C3-C4-C5-O8 |
| 72 | S7 | 204 | 3PE | C1-C2-C3-O31 |
| 73 | QC | 403 | PEE | C1-C2-C3-O3 |
| 68 | AK | 402 | CDL | OA5-CA3-CA4-OA6 |
| 68 | AL | 201 | CDL | OB5-CB3-CB4-OB6 |
| 68 | N4 | 503 | CDL | OB5-CB3-CB4-OB6 |
| 68 | QB | 501 | CDL | OA5-CA3-CA4-OA6 |
| 70 | C1 | 608 | PC1 | O11-C1-C2-O21 |
| 70 | C3 | 301 | PC1 | O11-C1-C2-O21 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 70 | QB | 503 | PC1 | O11-C1-C2-O21 |
| 71 | 6C | 101 | PLX | O4-C3-C4-O6 |
| 73 | A9 | 402 | PEE | O3P-C1-C2-O2 |
| 73 | QC | 403 | PEE | O3P-C1-C2-O2 |
| 73 | Qc | 401 | PEE | O3P-C1-C2-O2 |
| 80 | Qc | 402 | HEM | C4B-C3B-CAB-CBB |
| 84 | S2 | 502 | MF8 | N06-C04-N02-C01 |
| 71 | S7 | 203 | PLX | C6-C7-C8-C9 |
| 68 | Qb | 501 | CDL | CB5-C51-C52-C53 |
| 68 | N5 | 704 | CDL | C59-C60-C61-C62 |
| 73 | Qe | 301 | PEE | C11-C12-C13-C14 |
| 68 | B4 | 201 | CDL | C78-C79-C80-C81 |
| 72 | C1 | 609 | 3PE | C2A-C2B-C2C-C2D |
| 68 | N4 | 503 | CDL | OA6-CA4-CA6-OA8 |
| 68 | QH | 102 | CDL | OA6-CA4-CA6-OA8 |
| 68 | Qb | 501 | CDL | OB6-CB4-CB6-OB8 |
| 71 | AL | 202 | PLX | O6-C4-C5-O8 |
| 71 | AM | 201 | PLX | O6-C4-C5-O8 |
| 73 | N5 | 705 | PEE | O2-C2-C3-O3 |
| 73 | QB | 502 | PEE | O2-C2-C3-O3 |
| 73 | Qc | 401 | PEE | O2-C2-C3-O3 |
| 71 | B1 | 101 | PLX | C31-C32-C33-C34 |
| 68 | CB | 203 | CDL | C77-C78-C79-C80 |
| 70 | N1 | 402 | PC1 | C11-C12-N-C15 |
| 70 | C3 | 303 | PC1 | C37-C38-C39-C3A |
| 70 | Qb | 502 | PC1 | C23-C24-C25-C26 |
| 73 | QB | 502 | PEE | O4-C10-O2-C2 |
| 73 | Qc | 401 | PEE | C11-C12-C13-C14 |
| 73 | S8 | 303 | PEE | C42-C43-C44-C45 |
| 73 | A9 | 402 | PEE | C10-C11-C12-C13 |
| 71 | 6C | 101 | PLX | C14-C15-C16-C17 |
| 71 | CB | 201 | PLX | C28-C29-C30-C31 |
| 71 | N4 | 502 | PLX | C31-C32-C33-C34 |
| 72 | CA | 101 | 3PE | C27-C28-C29-C2A |
| 72 | N5 | 706 | 3PE | C3A-C3B-C3C-C3D |
| 68 | N5 | 703 | CDL | CA7-C31-C32-C33 |
| 71 | CB | 201 | PLX | C15-C16-C17-C18 |
| 71 | QI | 301 | PLX | C11-C10-C9-C8 |
| 68 | B4 | 201 | CDL | CB2-OB2-PB2-OB5 |
| 68 | C3 | 305 | CDL | CB3-OB5-PB2-OB2 |
| 68 | QH | 101 | CDL | CA3-OA5-PA1-OA2 |
| 68 | QH | 102 | CDL | CA2-OA2-PA1-OA5 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 70 | C1 | 608 | PC1 | C11-O13-P-O11 |
| 70 | C3 | 303 | PC1 | C11-O13-P-O11 |
| 71 | N6 | 201 | PLX | C2-O1-P1-O4 |
| 72 | CB | 202 | 3PE | C1-O11-P-O13 |
| 68 | B5 | 201 | CDL | O1-C1-CA2-OA2 |
| 68 | B5 | 201 | CDL | CB4-CB3-OB5-PB2 |
| 72 | QE | 302 | 3PE | C2-C1-O11-P |
| 72 | Qj | 101 | 3PE | C2-C1-O11-P |
| 73 | 7C | 101 | PEE | C2-C1-O3P-P |
| 73 | S2 | 501 | PEE | C2-C1-O3P-P |
| 68 | 4L | 201 | CDL | CA2-OA2-PA1-OA4 |
| 68 | 4L | 201 | CDL | CA3-OA5-PA1-OA3 |
| 68 | 4L | 201 | CDL | CA3-OA5-PA1-OA4 |
| 68 | 7A | 102 | CDL | CA3-OA5-PA1-OA3 |
| 68 | 7A | 102 | CDL | CA3-OA5-PA1-OA4 |
| 68 | 7A | 102 | CDL | CB2-OB2-PB2-OB3 |
| 68 | 7A | 102 | CDL | CB2-OB2-PB2-OB4 |
| 68 | A8 | 301 | CDL | CB2-OB2-PB2-OB3 |
| 68 | AL | 201 | CDL | CA2-OA2-PA1-OA4 |
| 68 | B4 | 201 | CDL | CA2-OA2-PA1-OA3 |
| 68 | B4 | 201 | CDL | CB2-OB2-PB2-OB4 |
| 68 | B5 | 201 | CDL | CA2-OA2-PA1-OA4 |
| 68 | B5 | 201 | CDL | CA3-OA5-PA1-OA3 |
| 68 | B5 | 201 | CDL | CA3-OA5-PA1-OA4 |
| 68 | B5 | 201 | CDL | CB3-OB5-PB2-OB3 |
| 68 | C3 | 304 | CDL | CA3-OA5-PA1-OA3 |
| 68 | CB | 203 | CDL | CA2-OA2-PA1-OA4 |
| 68 | CB | 203 | CDL | CB3-OB5-PB2-OB3 |
| 68 | N1 | 401 | CDL | CB3-OB5-PB2-OB3 |
| 68 | N4 | 503 | CDL | CA2-OA2-PA1-OA4 |
| 68 | N4 | 503 | CDL | CA3-OA5-PA1-OA3 |
| 68 | N4 | 503 | CDL | CA3-OA5-PA1-OA4 |
| 68 | N4 | 503 | CDL | CB2-OB2-PB2-OB3 |
| 68 | N5 | 703 | CDL | CA2-OA2-PA1-OA4 |
| 68 | N5 | 703 | CDL | CB3-OB5-PB2-OB4 |
| 68 | QB | 501 | CDL | CA2-OA2-PA1-OA4 |
| 68 | QC | 404 | CDL | CB2-OB2-PB2-OB4 |
| 68 | QH | 101 | CDL | CA2-OA2-PA1-OA4 |
| 68 | QH | 102 | CDL | CA2-OA2-PA1-OA4 |
| 68 | QH | 102 | CDL | CB3-OB5-PB2-OB3 |
| 68 | QH | 102 | CDL | CB3-OB5-PB2-OB4 |
| 68 | Qb | 501 | CDL | CA2-OA2-PA1-OA4 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 68 | Qb | 501 | CDL | CB2-OB2-PB2-OB4 |
| 70 | 6A | 101 | PC1 | C11-O13-P-O12 |
| 70 | C1 | 605 | PC1 | C11-O13-P-O12 |
| 70 | C1 | 605 | PC1 | C11-O13-P-O14 |
| 70 | C1 | 606 | PC1 | C1-O11-P-O14 |
| 70 | C1 | 608 | PC1 | C1-O11-P-O14 |
| 70 | C3 | 301 | PC1 | C11-O13-P-O12 |
| 70 | C3 | 301 | PC1 | C1-O11-P-O12 |
| 70 | C3 | 302 | PC1 | C11-O13-P-O12 |
| 70 | N1 | 402 | PC1 | C11-C12-N-C14 |
| 70 | N3 | 202 | PC1 | C11-O13-P-O14 |
| 70 | N3 | 202 | PC1 | C1-O11-P-O12 |
| 70 | N3 | 202 | PC1 | C1-O11-P-O14 |
| 70 | Qc | 405 | PC1 | C1-O11-P-O12 |
| 71 | AL | 202 | PLX | C3-O4-P1-O3 |
| 71 | AM | 201 | PLX | C3-O4-P1-O2 |
| 71 | CB | 201 | PLX | C2-C1-N1-C1C |
| 71 | CB | 201 | PLX | C2-C1-N1-C1A |
| 71 | N6 | 201 | PLX | C3-O4-P1-O2 |
| 71 | N6 | 201 | PLX | C3-O4-P1-O3 |
| 71 | QI | 301 | PLX | C2-O1-P1-O3 |
| 71 | Qi | 301 | PLX | C2-O1-P1-O3 |
| 71 | S7 | 203 | PLX | C2-O1-P1-O2 |
| 72 | 7A | 101 | 3PE | C1-O11-P-O12 |
| 72 | 7A | 101 | 3PE | C1-O11-P-O14 |
| 72 | 7A | 101 | 3PE | C11-O13-P-O14 |
| 72 | B8 | 201 | 3PE | C1-O11-P-O12 |
| 72 | B8 | 201 | 3PE | C11-O13-P-O12 |
| 72 | B8 | 201 | 3PE | C11-O13-P-O14 |
| 72 | CA | 101 | 3PE | C11-O13-P-O14 |
| 72 | CB | 202 | 3PE | C1-O11-P-O14 |
| 72 | QE | 302 | 3PE | C1-O11-P-O14 |
| 72 | Qc | 404 | 3PE | C1-O11-P-O12 |
| 72 | Qc | 404 | 3PE | C1-O11-P-O14 |
| 73 | A9 | 402 | PEE | C4-O4P-P-O1P |
| 73 | N3 | 201 | PEE | C1-O3P-P-O1P |
| 73 | N5 | 701 | PEE | C4-O4P-P-O2P |
| 73 | N5 | 701 | PEE | C4-O4P-P-O1P |
| 73 | N5 | 705 | PEE | C1-O3P-P-O1P |
| 73 | QC | 403 | PEE | C4-O4P-P-O2P |
| 73 | QC | 403 | PEE | C4-O4P-P-O1P |
| 73 | Qc | 401 | PEE | C1-O3P-P-O2P |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 73 | Qe | 301 | PEE | C1-O3P-P-O1P |
| 73 | Qe | 301 | PEE | C4-O4P-P-O2P |
| 73 | Qe | 302 | PEE | C1-O3P-P-O1P |
| 73 | S2 | 501 | PEE | C1-O3P-P-O2P |
| 73 | S8 | 303 | PEE | C4-O4P-P-O2P |
| 68 | N5 | 704 | CDL | CB5-C51-C52-C53 |
| 68 | 4L | 201 | CDL | OB5-CB3-CB4-CB6 |
| 68 | A8 | 301 | CDL | OB5-CB3-CB4-CB6 |
| 70 | QB | 503 | PC1 | O11-C1-C2-C3 |
| 70 | Qb | 502 | PC1 | O11-C1-C2-C3 |
| 73 | N1 | 403 | PEE | O3P-C1-C2-C3 |
| 73 | N5 | 701 | PEE | O3P-C1-C2-C3 |
| 73 | N5 | 705 | PEE | C12-C13-C14-C15 |
| 73 | Qe | 301 | PEE | C13-C14-C15-C16 |
| 70 | C1 | 608 | PC1 | O21-C21-C22-C23 |
| 73 | Qe | 301 | PEE | C37-C38-C39-C40 |
| 71 | 6C | 101 | PLX | C25-C24-O8-C5 |
| 71 | B1 | 101 | PLX | C1-C2-O1-P1 |
| 71 | N4 | 502 | PLX | C25-C24-O8-C5 |
| 71 | N6 | 201 | PLX | C25-C24-O8-C5 |
| 71 | S7 | 203 | PLX | C25-C24-O8-C5 |
| 72 | 7A | 101 | 3PE | C12-C11-O13-P |
| 72 | CA | 101 | 3PE | C12-C11-O13-P |
| 72 | CB | 202 | 3PE | C12-C11-O13-P |
| 72 | QE | 302 | 3PE | O31-C31-C32-C33 |
| 68 | B4 | 201 | CDL | CA7-C31-C32-C33 |
| 70 | QB | 503 | PC1 | C21-C22-C23-C24 |
| 68 | QB | 501 | CDL | OB5-CB3-CB4-OB6 |
| 68 | QD | 402 | CDL | OA5-CA3-CA4-OA6 |
| 70 | C3 | 303 | PC1 | O11-C1-C2-O21 |
| 70 | Qb | 502 | PC1 | O11-C1-C2-O21 |
| 81 | Qd | 401 | HEC | C3D-CAD-CBD-CGD |
| 71 | AL | 202 | PLX | C7-C8-C9-C10 |
| 71 | B1 | 101 | PLX | C14-C15-C16-C17 |
| 73 | QB | 502 | PEE | C31-C32-C33-C34 |
| 70 | C3 | 302 | PC1 | C11-C12-N-C14 |
| 68 | Qb | 501 | CDL | CB3-CB4-CB6-OB8 |
| 70 | 6A | 101 | PC1 | O13-C11-C12-N |
| 70 | C1 | 605 | PC1 | O13-C11-C12-N |
| 70 | C1 | 606 | PC1 | O13-C11-C12-N |
| 70 | C1 | 608 | PC1 | O13-C11-C12-N |
| 70 | C3 | 302 | PC1 | O13-C11-C12-N |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 70 | C3 | 303 | PC1 | O13-C11-C12-N |
| 70 | C3 | 306 | PC1 | O13-C11-C12-N |
| 70 | N3 | 202 | PC1 | O13-C11-C12-N |
| 70 | Qc | 405 | PC1 | O13-C11-C12-N |
| 71 | 6C | 101 | PLX | N1-C1-C2-O1 |
| 71 | B1 | 101 | PLX | N1-C1-C2-O1 |
| 71 | CB | 201 | PLX | C3-C4-C5-O8 |
| 73 | N4 | 501 | PEE | C1-C2-C3-O3 |
| 73 | QE | 301 | PEE | C1-C2-C3-O3 |
| 73 | Qe | 301 | PEE | C32-C33-C34-C35 |
| 77 | C1 | 601 | HEA | C1A-C2A-CAA-CBA |
| 71 | CB | 201 | PLX | O6-C4-C5-O8 |
| 71 | N4 | 502 | PLX | O6-C4-C5-O8 |
| 73 | N4 | 501 | PEE | O2-C2-C3-O3 |
| 73 | QE | 301 | PEE | O2-C2-C3-O3 |
| 68 | C3 | 304 | CDL | C54-C55-C56-C57 |
| 73 | N4 | 501 | PEE | C12-C13-C14-C15 |
| 73 | Qc | 401 | PEE | C16-C17-C18-C19 |
| 68 | B4 | 201 | CDL | C34-C35-C36-C37 |
| 68 | B5 | 201 | CDL | C1-CA2-OA2-PA1 |
| 68 | CB | 203 | CDL | CB4-CB3-OB5-PB2 |
| 68 | N5 | 704 | CDL | CA4-CA3-OA5-PA1 |
| 70 | C3 | 302 | PC1 | C37-C38-C39-C3A |
| 68 | CB | 203 | CDL | C12-C13-C14-C15 |
| 71 | AL | 202 | PLX | O8-C24-C25-C26 |
| 71 | Qi | 301 | PLX | O8-C24-C25-C26 |
| 85 | S7 | 201 | U10 | C24-C26-C27-C28 |
| 73 | N4 | 501 | PEE | C10-C11-C12-C13 |
| 84 | S2 | 502 | MF8 | N06-C04-N02-C03 |
| 70 | Qh | 101 | PC1 | C11-C12-N-C13 |
| 71 | AM | 201 | PLX | C27-C28-C29-C30 |
| 71 | S7 | 203 | PLX | C12-C13-C14-C15 |
| 68 | QC | 404 | CDL | O1-C1-CA2-OA2 |
| 73 | QB | 502 | PEE | C11-C10-O2-C2 |
| 73 | S2 | 501 | PEE | C33-C34-C35-C36 |
| 74 | A9 | 401 | NDP | C2D-C1D-N1N-C6N |
| 70 | C1 | 610 | PC1 | C22-C23-C24-C25 |
| 72 | C1 | 607 | 3PE | C24-C25-C26-C27 |
| 73 | QE | 301 | PEE | C21-C22-C23-C24 |
| 70 | C3 | 303 | PC1 | C1-C2-O21-C21 |
| 73 | S8 | 303 | PEE | C3-C2-O2-C10 |
| 68 | N5 | 704 | CDL | OB5-CB3-CB4-CB6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 71 | AM | 201 | PLX | O4-C3-C4-C5 |
| 77 | C1 | 602 | HEA | C11-C12-C13-C14 |
| 73 | N3 | 201 | PEE | C30-C31-C32-C33 |
| 70 | C1 | 608 | PC1 | C38-C39-C3A-C3B |
| 68 | AL | 201 | CDL | CB4-CB3-OB5-PB2 |
| 68 | B4 | 201 | CDL | C73-C74-C75-C76 |
| 68 | 4L | 201 | CDL | OB5-CB3-CB4-OB6 |
| 68 | N5 | 704 | CDL | OB5-CB3-CB4-OB6 |
| 71 | N6 | 201 | PLX | O4-C3-C4-O6 |
| 72 | Qj | 101 | 3PE | O31-C31-C32-C33 |
| 71 | CB | 201 | PLX | C2-C1-N1-C1B |
| 74 | A9 | 401 | NDP | O4D-C1D-N1N-C6N |
| 70 | C1 | 606 | PC1 | C31-C32-C33-C34 |
| 71 | AL | 202 | PLX | C11-C10-C9-C8 |
| 71 | B1 | 101 | PLX | C11-C12-C13-C14 |
| 70 | 6A | 101 | PC1 | C21-C22-C23-C24 |
| 73 | N1 | 403 | PEE | O2-C2-C3-O3 |
| 68 | 7A | 102 | CDL | CB3-OB5-PB2-OB2 |
| 68 | A7 | 201 | CDL | CA2-OA2-PA1-OA5 |
| 68 | A7 | 201 | CDL | CB2-OB2-PB2-OB5 |
| 68 | AL | 201 | CDL | CA3-OA5-PA1-OA2 |
| 68 | C3 | 304 | CDL | CB2-OB2-PB2-OB5 |
| 68 | CB | 203 | CDL | CA3-OA5-PA1-OA2 |
| 68 | N1 | 401 | CDL | CA2-OA2-PA1-OA5 |
| 68 | N5 | 704 | CDL | CA3-OA5-PA1-OA2 |
| 70 | 6A | 101 | PC1 | C1-O11-P-O13 |
| 70 | C3 | 306 | PC1 | C11-O13-P-O11 |
| 70 | C3 | 306 | PC1 | C1-O11-P-O13 |
| 70 | QB | 503 | PC1 | C1-O11-P-O13 |
| 71 | 6C | 101 | PLX | C2-O1-P1-O4 |
| 71 | N4 | 502 | PLX | C2-O1-P1-O4 |
| 71 | S7 | 203 | PLX | C3-O4-P1-O1 |
| 72 | C1 | 607 | 3PE | C11-O13-P-O11 |
| 73 | 7C | 101 | PEE | C1-O3P-P-O4P |
| 73 | QC | 403 | PEE | C1-O3P-P-O4P |
| 70 | N3 | 202 | PC1 | C22-C23-C24-C25 |
| 73 | S8 | 303 | PEE | C1-C2-C3-O3 |
| 71 | 6C | 101 | PLX | C6-C7-C8-C9 |
| 68 | N1 | 401 | CDL | C73-C74-C75-C76 |
| 68 | N4 | 503 | CDL | C72-C71-CB7-OB8 |
| 68 | 7A | 102 | CDL | CB4-CB3-OB5-PB2 |
| 70 | C3 | 302 | PC1 | C2-C1-O11-P |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 73 | N3 | 201 | PEE | C2-C1-O3P-P |
| 80 | Qc | 403 | HEM | CAA-CBA-CGA-O1A |
| 84 | S2 | 502 | MF8 | N08-C07-N06-C04 |
| 73 | N3 | 201 | PEE | C41-C42-C43-C44 |
| 73 | N5 | 705 | PEE | C18-C19-C20-C21 |
| 68 | AL | 201 | CDL | C36-C37-C38-C39 |
| 73 | S8 | 303 | PEE | C14-C15-C16-C17 |
| 76 | AK | 401 | ADP | O4'-C4'-C5'-O5' |
| 85 | S7 | 201 | U10 | C44-C46-C47-C48 |
| 72 | C1 | 607 | 3PE | O13-C11-C12-N |
| 68 | B4 | 201 | CDL | C12-C13-C14-C15 |
| 68 | N5 | 703 | CDL | C36-C37-C38-C39 |
| 73 | N5 | 701 | PEE | C13-C14-C15-C16 |
| 80 | QC | 401 | HEM | CAA-CBA-CGA-O2A |
| 71 | QI | 301 | PLX | C12-C13-C14-C15 |
| 75 | AB | 201 | ZMP | C2-C3-C4-C5 |
| 73 | S8 | 303 | PEE | C15-C16-C17-C18 |
| 75 | AB | 201 | ZMP | O3-C16-C17-C18 |
| 70 | N3 | 202 | PC1 | C26-C27-C28-C29 |
| 71 | S7 | 203 | PLX | C11-C10-C9-C8 |
| 71 | Qi | 301 | PLX | C24-C25-C26-C27 |
| 80 | Qc | 403 | HEM | CAD-CBD-CGD-O1D |
| 68 | AL | 201 | CDL | OB6-CB4-CB6-OB8 |
| 70 | Qc | 405 | PC1 | O21-C2-C3-O31 |
| 70 | C3 | 306 | PC1 | C2-C1-O11-P |
| 72 | C1 | 607 | 3PE | C2-C1-O11-P |
| 85 | S7 | 201 | U10 | C5-C4-O4-C4M |
| 68 | 7A | 102 | CDL | C81-C82-C83-C84 |
| 71 | AM | 201 | PLX | C9-C10-C11-C12 |
| 73 | QE | 301 | PEE | C15-C16-C17-C18 |
| 68 | QC | 404 | CDL | C31-C32-C33-C34 |
| 70 | Qb | 502 | PC1 | C35-C36-C37-C38 |
| 71 | N4 | 502 | PLX | C33-C34-C35-C36 |
| 71 | QI | 301 | PLX | C13-C14-C15-C16 |
| 70 | Qc | 405 | PC1 | C1-C2-C3-O31 |
| 71 | AL | 202 | PLX | C3-C4-C5-O8 |
| 70 | N3 | 202 | PC1 | C28-C29-C2A-C2B |
| 72 | QE | 302 | 3PE | C23-C24-C25-C26 |
| 80 | QC | 402 | HEM | CAA-CBA-CGA-O1A |
| 72 | C1 | 609 | 3PE | C33-C34-C35-C36 |
| 72 | N5 | 706 | 3PE | C22-C23-C24-C25 |
| 73 | 7C | 101 | PEE | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 80 | Qc | 402 | HEM | CAD-CBD-CGD-O1D |
| 73 | QE | 301 | PEE | C31-C32-C33-C34 |
| 68 | 4L | 201 | CDL | CA6-CA4-OA6-CA5 |
| 68 | AL | 201 | CDL | CA6-CA4-OA6-CA5 |
| 68 | Qb | 501 | CDL | CA3-CA4-OA6-CA5 |
| 70 | C3 | 302 | PC1 | C3-C2-O21-C21 |
| 72 | S7 | 204 | 3PE | C3-C2-O21-C21 |
| 70 | N1 | 402 | PC1 | C11-C12-N-C13 |
| 68 | QD | 402 | CDL | CA3-OA5-PA1-OA2 |
| 71 | AM | 201 | PLX | C5-C4-O6-C6 |
| 84 | S2 | 502 | MF8 | N05-C04-N02-C01 |
| 71 | N6 | 201 | PLX | C25-C26-C27-C28 |
| 68 | C3 | 304 | CDL | C72-C71-CB7-OB8 |
| 70 | C1 | 605 | PC1 | C32-C33-C34-C35 |
| 68 | QD | 402 | CDL | OB5-CB3-CB4-OB6 |
| 77 | C1 | 601 | HEA | CAD-CBD-CGD-O1D |
| 71 | S7 | 203 | PLX | C25-C26-C27-C28 |
| 71 | QI | 301 | PLX | O4-C3-C4-C5 |
| 70 | N3 | 202 | PC1 | C38-C39-C3A-C3B |
| 80 | Qc | 403 | HEM | CAA-CBA-CGA-O2A |
| 71 | N6 | 201 | PLX | C10-C11-C12-C13 |
| 73 | QB | 502 | PEE | C33-C34-C35-C36 |
| 70 | C3 | 302 | PC1 | C32-C33-C34-C35 |
| 68 | CB | 203 | CDL | OB6-CB4-CB6-OB8 |
| 70 | C3 | 302 | PC1 | O21-C2-C3-O31 |
| 80 | QC | 402 | HEM | CAA-CBA-CGA-O2A |
| 68 | C3 | 305 | CDL | C57-C58-C59-C60 |
| 73 | QE | 301 | PEE | C22-C23-C24-C25 |
| 80 | QC | 401 | HEM | CAA-CBA-CGA-O1A |
| 80 | Qc | 402 | HEM | CAA-CBA-CGA-O2A |
| 81 | Qd | 401 | HEC | CAA-CBA-CGA-O2A |
| 80 | Qc | 403 | HEM | CAD-CBD-CGD-O2D |
| 77 | C1 | 602 | HEA | CAD-CBD-CGD-O2D |
| 71 | Qi | 301 | PLX | C15-C16-C17-C18 |
| 70 | C3 | 301 | PC1 | C2A-C2B-C2C-C2D |
| 73 | N5 | 705 | PEE | O5-C30-O3-C3 |
| 68 | CB | 203 | CDL | C72-C71-CB7-OB8 |
| 70 | Qb | 502 | PC1 | O21-C21-C22-C23 |
| 73 | A9 | 402 | PEE | C18-C19-C20-C21 |
| 68 | N1 | 401 | CDL | C12-C13-C14-C15 |
| 72 | N5 | 706 | 3PE | C1-C2-C3-O31 |
| 72 | C1 | 609 | 3PE | C3B-C3C-C3D-C3E |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 73 | N5 | 705 | PEE | C17-C18-C19-C20 |
| 73 | QB | 502 | PEE | C37-C38-C39-C40 |
| 73 | Qe | 301 | PEE | C30-C31-C32-C33 |
| 80 | Qc | 402 | HEM | CAA-CBA-CGA-O1A |
| 71 | CB | 201 | PLX | C11-C10-C9-C8 |
| 73 | N4 | 501 | PEE | C33-C34-C35-C36 |
| 73 | N5 | 702 | PEE | O3P-C1-C2-O2 |
| 74 | A9 | 401 | NDP | C2D-C1D-N1N-C2N |
| 68 | AL | 201 | CDL | C52-C51-CB5-OB6 |
| 71 | AM | 201 | PLX | O8-C24-C25-C26 |
| 81 | Qd | 401 | HEC | CAA-CBA-CGA-O1A |
| 72 | CA | 101 | 3PE | C29-C2A-C2B-C2C |
| 68 | B4 | 201 | CDL | OB5-CB3-CB4-CB6 |
| 68 | C3 | 305 | CDL | OB5-CB3-CB4-CB6 |
| 72 | S7 | 204 | 3PE | O11-C1-C2-C3 |
| 68 | QD | 402 | CDL | C52-C51-CB5-OB6 |
| 73 | N5 | 705 | PEE | O4P-C4-C5-N |
| 68 | QH | 101 | CDL | C72-C73-C74-C75 |
| 71 | 6C | 101 | PLX | C18-C19-C20-C21 |
| 68 | 4L | 201 | CDL | C79-C80-C81-C82 |
| 70 | N3 | 202 | PC1 | C29-C2A-C2B-C2C |
| 70 | Qb | 502 | PC1 | C22-C23-C24-C25 |
| 71 | S7 | 203 | PLX | O6-C4-C5-O8 |
| 71 | B1 | 101 | PLX | C30-C31-C32-C33 |
| 72 | 7A | 101 | 3PE | C32-C33-C34-C35 |
| 71 | S7 | 203 | PLX | C27-C28-C29-C30 |
| 73 | N5 | 705 | PEE | C31-C30-O3-C3 |
| 73 | N1 | 403 | PEE | O2-C10-C11-C12 |
| 85 | S7 | 201 | U10 | C50-C49-C51-C52 |
| 68 | AK | 402 | CDL | C72-C73-C74-C75 |
| 72 | Qj | 101 | 3PE | C33-C34-C35-C36 |
| 73 | A9 | 402 | PEE | C1-O3P-P-O4P |
| 73 | S8 | 303 | PEE | C4-O4P-P-O3P |
| 68 | C3 | 305 | CDL | C12-C11-CA5-OA6 |
| 70 | C3 | 301 | PC1 | O31-C31-C32-C33 |
| 72 | B8 | 201 | 3PE | O21-C21-C22-C23 |
| 72 | C1 | 609 | 3PE | O21-C21-C22-C23 |
| 73 | QE | 301 | PEE | C37-C38-C39-C40 |
| 80 | QC | 401 | HEM | CAD-CBD-CGD-O1D |
| 73 | N4 | 501 | PEE | O2-C10-C11-C12 |
| 73 | QB | 502 | PEE | O2-C10-C11-C12 |
| 73 | S2 | 501 | PEE | O2-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 73 | 7C | 101 | PEE | C38-C39-C40-C41 |
| 73 | N5 | 701 | PEE | C16-C17-C18-C19 |
| 73 | N5 | 702 | PEE | C36-C37-C38-C39 |
| 73 | Qc | 401 | PEE | C13-C14-C15-C16 |
| 81 | QD | 401 | HEC | CAD-CBD-CGD-O2D |
| 68 | AK | 402 | CDL | CA6-CA4-OA6-CA5 |
| 68 | B5 | 201 | CDL | CB3-CB4-OB6-CB5 |
| 68 | N4 | 503 | CDL | CB6-CB4-OB6-CB5 |
| 68 | QB | 501 | CDL | CA6-CA4-OA6-CA5 |
| 68 | QD | 402 | CDL | CB6-CB4-OB6-CB5 |
| 68 | QH | 102 | CDL | CA3-CA4-OA6-CA5 |
| 70 | QB | 503 | PC1 | C3-C2-O21-C21 |
| 70 | Qb | 502 | PC1 | C3-C2-O21-C21 |
| 72 | C1 | 607 | 3PE | C3-C2-O21-C21 |
| 72 | Qc | 404 | 3PE | C39-C3A-C3B-C3C |
| 74 | A9 | 401 | NDP | O4D-C1D-N1N-C2N |
| 73 | N3 | 201 | PEE | O2-C10-C11-C12 |
| 81 | Qd | 401 | HEC | CAD-CBD-CGD-O1D |
| 71 | Qi | 301 | PLX | C16-C17-C18-C19 |
| 68 | A7 | 201 | CDL | C72-C71-CB7-OB8 |
| 73 | N5 | 705 | PEE | O3-C30-C31-C32 |
| 68 | N5 | 704 | CDL | C1-CA2-OA2-PA1 |
| 71 | AL | 202 | PLX | C7-C6-O6-C4 |
| 77 | C1 | 601 | HEA | CAD-CBD-CGD-O2D |
| 68 | QC | 404 | CDL | OB5-CB3-CB4-OB6 |
| 68 | QH | 102 | CDL | OB5-CB3-CB4-OB6 |
| 68 | N5 | 703 | CDL | C12-C11-CA5-OA6 |
| 68 | QB | 501 | CDL | C32-C31-CA7-OA8 |
| 72 | CB | 202 | 3PE | O31-C31-C32-C33 |
| 73 | N5 | 701 | PEE | O2-C10-C11-C12 |
| 73 | Qc | 401 | PEE | O2-C10-C11-C12 |
| 77 | C1 | 602 | HEA | CAD-CBD-CGD-O1D |
| 80 | Qc | 402 | HEM | CAD-CBD-CGD-O2D |
| 68 | N5 | 704 | CDL | C42-C43-C44-C45 |
| 74 | A9 | 401 | NDP | O4B-C4B-C5B-O5B |
| 68 | C3 | 304 | CDL | CA5-C11-C12-C13 |
| 73 | Qe | 301 | PEE | C18-C19-C20-C21 |
| 68 | 7A | 102 | CDL | C57-C58-C59-C60 |
| 73 | Qc | 401 | PEE | C2-C3-O3-C30 |
| 68 | AL | 201 | CDL | C32-C31-CA7-OA8 |
| 68 | A8 | 301 | CDL | OA5-CA3-CA4-CA6 |
| 68 | AK | 402 | CDL | OA5-CA3-CA4-CA6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 77 | C1 | 602 | HEA | C2D-C3D-CAD-CBD |
| 81 | QD | 401 | HEC | CAD-CBD-CGD-O1D |
| 68 | A8 | 301 | CDL | C33-C34-C35-C36 |
| 73 | 7C | 101 | PEE | C14-C15-C16-C17 |
| 73 | N3 | 201 | PEE | C23-C24-C25-C26 |
| 68 | N5 | 704 | CDL | OA6-CA4-CA6-OA8 |
| 68 | N5 | 704 | CDL | OB6-CB4-CB6-OB8 |
| 70 | Qb | 502 | PC1 | O21-C2-C3-O31 |
| 72 | CB | 202 | 3PE | O21-C2-C3-O31 |
| 72 | N5 | 706 | 3PE | O21-C2-C3-O31 |
| 71 | Qi | 301 | PLX | C6-C7-C8-C9 |
| 68 | N5 | 703 | CDL | C61-C62-C63-C64 |
| 68 | AL | 201 | CDL | C12-C11-CA5-OA6 |
| 68 | QC | 404 | CDL | C52-C51-CB5-OB6 |
| 68 | QH | 101 | CDL | C32-C31-CA7-OA8 |
| 68 | QH | 102 | CDL | C32-C31-CA7-OA8 |
| 70 | C1 | 610 | PC1 | O21-C21-C22-C23 |
| 70 | N1 | 402 | PC1 | O21-C21-C22-C23 |
| 70 | Qc | 405 | PC1 | O21-C21-C22-C23 |
| 72 | S7 | 204 | 3PE | C3B-C3C-C3D-C3E |
| 81 | Qd | 401 | HEC | CAD-CBD-CGD-O2D |
| 68 | QH | 101 | CDL | CA4-CA3-OA5-PA1 |
| 73 | Qe | 301 | PEE | C2-C1-O3P-P |
| 73 | Qc | 401 | PEE | O4-C10-O2-C2 |
| 68 | N5 | 704 | CDL | C72-C71-CB7-OB8 |
| 70 | Qb | 502 | PC1 | O31-C31-C32-C33 |
| 80 | QC | 401 | HEM | CAD-CBD-CGD-O2D |
| 68 | CB | 203 | CDL | CB5-C51-C52-C53 |
| 85 | S7 | 201 | U10 | C3-C4-O4-C4M |
| 70 | C3 | 303 | PC1 | C2B-C2C-C2D-C2E |
| 71 | S7 | 203 | PLX | C15-C16-C17-C18 |
| 71 | B1 | 101 | PLX | C15-C16-C17-C18 |
| 70 | C3 | 301 | PC1 | O32-C31-C32-C33 |
| 73 | N3 | 201 | PEE | O4-C10-C11-C12 |
| 68 | N5 | 703 | CDL | C12-C11-CA5-OA7 |
| 73 | N1 | 403 | PEE | O4-C10-C11-C12 |
| 68 | A7 | 201 | CDL | C72-C71-CB7-OB9 |
| 68 | AL | 201 | CDL | C12-C11-CA5-OA7 |
| 68 | C3 | 305 | CDL | C12-C11-CA5-OA7 |
| 72 | C1 | 609 | 3PE | O22-C21-C22-C23 |
| 72 | CB | 202 | 3PE | O32-C31-C32-C33 |
| 73 | N5 | 705 | PEE | O5-C30-C31-C32 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 68 | 4L | 201 | CDL | C52-C51-CB5-OB6 |
| 68 | B4 | 201 | CDL | C12-C11-CA5-OA6 |
| 70 | N1 | 402 | PC1 | C2F-C2G-C2H-C2I |
| 72 | QJ | 101 | 3PE | C23-C24-C25-C26 |
| 73 | QE | 301 | PEE | C4-O4P-P-O3P |
| 71 | AM | 201 | PLX | C30-C31-C32-C33 |
| 71 | Qi | 301 | PLX | C27-C28-C29-C30 |
| 68 | AL | 201 | CDL | C32-C31-CA7-OA9 |
| 68 | N5 | 704 | CDL | C72-C71-CB7-OB9 |
| 72 | B8 | 201 | 3PE | O22-C21-C22-C23 |
| 71 | AL | 202 | PLX | C14-C15-C16-C17 |
| 68 | N5 | 703 | CDL | C72-C71-CB7-OB8 |
| 72 | N5 | 706 | 3PE | O21-C21-C22-C23 |
| 68 | QH | 102 | CDL | C32-C31-CA7-OA9 |
| 70 | Qb | 502 | PC1 | O32-C31-C32-C33 |
| 68 | A7 | 201 | CDL | CA2-OA2-PA1-OA3 |
| 68 | CB | 203 | CDL | CB2-OB2-PB2-OB4 |
| 68 | N4 | 503 | CDL | CB3-OB5-PB2-OB3 |
| 68 | N5 | 704 | CDL | CB3-OB5-PB2-OB3 |
| 68 | QC | 404 | CDL | CA2-OA2-PA1-OA3 |
| 68 | Qb | 501 | CDL | CA3-OA5-PA1-OA3 |
| 70 | C1 | 608 | PC1 | C11-O13-P-O12 |
| 70 | C1 | 608 | PC1 | C1-O11-P-O12 |
| 70 | C3 | 306 | PC1 | C1-O11-P-O14 |
| 71 | 6C | 101 | PLX | C2-O1-P1-O2 |
| 71 | N6 | 201 | PLX | C2-O1-P1-O2 |
| 72 | C1 | 607 | 3PE | C11-O13-P-O14 |
| 72 | S7 | 204 | 3PE | C11-O13-P-O14 |
| 73 | QB | 502 | PEE | C1-O3P-P-O1P |
| 73 | Qc | 401 | PEE | C4-O4P-P-O2P |
| 72 | C1 | 607 | 3PE | O22-C21-C22-C23 |
| 73 | QB | 502 | PEE | O4-C10-C11-C12 |
| 73 | S2 | 501 | PEE | O4-C10-C11-C12 |
| 70 | 6A | 101 | PC1 | C34-C35-C36-C37 |
| 77 | C1 | 602 | HEA | CAA-CBA-CGA-O2A |
| 68 | QC | 404 | CDL | C52-C51-CB5-OB7 |
| 73 | N4 | 501 | PEE | O4-C10-C11-C12 |
| 73 | N5 | 701 | PEE | O4-C10-C11-C12 |
| 73 | Qc | 401 | PEE | O4-C10-C11-C12 |
| 84 | S2 | 502 | MF8 | N09-C07-N06-C04 |
| 68 | N4 | 503 | CDL | C34-C35-C36-C37 |
| 72 | CA | 101 | 3PE | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 68 | Qb | 501 | CDL | C72-C71-CB7-OB8 |
| 68 | B4 | 201 | CDL | C12-C11-CA5-OA7 |
| 73 | Qc | 401 | PEE | C11-C10-O2-C2 |
| 68 | AL | 201 | CDL | CA3-CA4-OA6-CA5 |
| 68 | N4 | 503 | CDL | CB3-CB4-OB6-CB5 |
| 68 | QB | 501 | CDL | CA3-CA4-OA6-CA5 |
| 68 | QH | 102 | CDL | CA6-CA4-OA6-CA5 |
| 68 | Qb | 501 | CDL | CA6-CA4-OA6-CA5 |
| 70 | 6A | 101 | PC1 | C12-C11-O13-P |
| 70 | C3 | 302 | PC1 | C1-C2-O21-C21 |
| 70 | N1 | 402 | PC1 | C12-C11-O13-P |
| 70 | QB | 503 | PC1 | C1-C2-O21-C21 |
| 70 | Qb | 502 | PC1 | C1-C2-O21-C21 |
| 71 | AM | 201 | PLX | C1-C2-O1-P1 |
| 72 | C1 | 607 | 3PE | C1-C2-O21-C21 |
| 72 | N5 | 706 | 3PE | C12-C11-O13-P |
| 72 | QE | 302 | 3PE | C12-C11-O13-P |
| 72 | S7 | 204 | 3PE | C1-C2-O21-C21 |
| 73 | N1 | 403 | PEE | C5-C4-O4P-P |
| 73 | N3 | 201 | PEE | C5-C4-O4P-P |
| 68 | QB | 501 | CDL | C32-C31-CA7-OA9 |
| 73 | 7C | 101 | PEE | C13-C14-C15-C16 |
| 68 | AK | 402 | CDL | C12-C11-CA5-OA6 |
| 72 | 7A | 101 | 3PE | O21-C21-C22-C23 |
| 73 | A9 | 402 | PEE | O2-C10-C11-C12 |
| 68 | B4 | 201 | CDL | C33-C34-C35-C36 |
| 68 | N5 | 704 | CDL | C11-C12-C13-C14 |
| 71 | CB | 201 | PLX | C17-C18-C19-C20 |
| 70 | 6A | 101 | PC1 | C25-C26-C27-C28 |
| 73 | QB | 502 | PEE | C11-C12-C13-C14 |
| 70 | Qc | 405 | PC1 | C21-C22-C23-C24 |
| 68 | QD | 402 | CDL | C71-C72-C73-C74 |
| 73 | QB | 502 | PEE | C36-C37-C38-C39 |
| 68 | QH | 101 | CDL | C12-C11-CA5-OA6 |
| 72 | C1 | 609 | 3PE | O31-C31-C32-C33 |
| 73 | N3 | 201 | PEE | O3-C30-C31-C32 |
| 70 | C1 | 610 | PC1 | C3E-C3F-C3G-C3H |
| 71 | 6C | 101 | PLX | C7-C8-C9-C10 |
| 73 | S2 | 501 | PEE | C43-C44-C45-C46 |
| 73 | 7C | 101 | PEE | C33-C34-C35-C36 |
| 68 | C3 | 305 | CDL | C32-C31-CA7-OA8 |
| 71 | 6C | 101 | PLX | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 68 | C3 | 305 | CDL | C32-C31-CA7-OA9 |
| 70 | N1 | 402 | PC1 | O22-C21-C22-C23 |
| 70 | QB | 503 | PC1 | C3A-C3B-C3C-C3D |
| 68 | QC | 404 | CDL | CA4-CA3-OA5-PA1 |
| 68 | N1 | 401 | CDL | CB5-C51-C52-C53 |
| 70 | C3 | 303 | PC1 | C21-C22-C23-C24 |
| 71 | S7 | 203 | PLX | O4-C3-C4-O6 |
| 68 | 4L | 201 | CDL | C12-C11-CA5-OA7 |
| 68 | N5 | 703 | CDL | C72-C71-CB7-OB9 |
| 70 | C1 | 610 | PC1 | O22-C21-C22-C23 |
| 72 | C1 | 609 | 3PE | O32-C31-C32-C33 |
| 68 | CB | 203 | CDL | C39-C40-C41-C42 |
| 70 | N3 | 202 | PC1 | C3B-C3C-C3D-C3E |
| 68 | 4L | 201 | CDL | C12-C11-CA5-OA6 |
| 73 | N5 | 705 | PEE | C31-C32-C33-C34 |
| 72 | N5 | 706 | 3PE | O22-C21-C22-C23 |
| 77 | C1 | 602 | HEA | CAA-CBA-CGA-O1A |
| 68 | 4L | 201 | CDL | C32-C31-CA7-OA8 |
| 68 | N5 | 704 | CDL | C52-C51-CB5-OB6 |
| 68 | A8 | 301 | CDL | C54-C55-C56-C57 |
| 68 | QB | 501 | CDL | C73-C74-C75-C76 |
| 70 | N3 | 202 | PC1 | C36-C37-C38-C39 |
| 68 | QH | 101 | CDL | C12-C11-CA5-OA7 |
| 73 | N3 | 201 | PEE | O5-C30-C31-C32 |
| 68 | A8 | 301 | CDL | C22-C23-C24-C25 |
| 71 | CB | 201 | PLX | C24-C25-C26-C27 |
| 68 | AK | 402 | CDL | C72-C71-CB7-OB8 |
| 68 | N5 | 703 | CDL | C52-C51-CB5-OB6 |
| 70 | 6A | 101 | PC1 | O31-C31-C32-C33 |
| 68 | AL | 201 | CDL | C32-C33-C34-C35 |
| 68 | AL | 201 | CDL | C34-C35-C36-C37 |
| 72 | C1 | 607 | 3PE | C2A-C2B-C2C-C2D |
| 73 | S2 | 501 | PEE | C31-C32-C33-C34 |
| 68 | AK | 402 | CDL | C32-C31-CA7-OA8 |

There are no ring outliers.

86 monomers are involved in 277 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 72 | C1 | 609 | 3PE | 1 | 0 |
| 83 | S1 | 802 | SF4 | 1 | 0 |
| 81 | Qd | 401 | HEC | 4 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 70 | Qh | 101 | PC1 | 1 | 0 |
| 73 | N5 | 702 | PEE | 1 | 0 |
| 68 | 7A | 102 | CDL | 6 | 0 |
| 86 | V1 | 502 | FMN | 1 | 0 |
| 77 | C1 | 601 | HEA | 8 | 0 |
| 70 | C1 | 608 | PC1 | 4 | 0 |
| 70 | C3 | 302 | PC1 | 4 | 0 |
| 71 | B1 | 101 | PLX | 1 | 0 |
| 73 | S2 | 501 | PEE | 4 | 0 |
| 68 | N5 | 704 | CDL | 2 | 0 |
| 72 | 7A | 101 | 3PE | 6 | 0 |
| 70 | QB | 503 | PC1 | 2 | 0 |
| 70 | C3 | 306 | PC1 | 2 | 0 |
| 72 | CA | 101 | 3PE | 1 | 0 |
| 74 | A9 | 401 | NDP | 1 | 0 |
| 68 | B4 | 201 | CDL | 4 | 0 |
| 68 | QC | 404 | CDL | 2 | 0 |
| 81 | QD | 401 | HEC | 2 | 0 |
| 73 | S8 | 303 | PEE | 7 | 0 |
| 70 | C1 | 610 | PC1 | 9 | 0 |
| 82 | QE | 303 | FES | 2 | 0 |
| 73 | N5 | 705 | PEE | 1 | 0 |
| 68 | A8 | 301 | CDL | 7 | 0 |
| 68 | N4 | 503 | CDL | 2 | 0 |
| 75 | AB | 201 | ZMP | 2 | 0 |
| 76 | AK | 401 | ADP | 3 | 0 |
| 73 | N5 | 701 | PEE | 2 | 0 |
| 70 | N3 | 202 | PC1 | 1 | 0 |
| 71 | CB | 201 | PLX | 3 | 0 |
| 73 | QB | 502 | PEE | 1 | 0 |
| 68 | C3 | 305 | CDL | 4 | 0 |
| 73 | QE | 301 | PEE | 2 | 0 |
| 73 | N3 | 201 | PEE | 4 | 0 |
| 68 | B5 | 201 | CDL | 6 | 0 |
| 73 | A9 | 402 | PEE | 4 | 0 |
| 70 | C3 | 303 | PC1 | 4 | 0 |
| 73 | Qe | 302 | PEE | 1 | 0 |
| 72 | QE | 302 | 3PE | 1 | 0 |
| 72 | CB | 202 | 3PE | 1 | 0 |
| 80 | QC | 402 | HEM | 6 | 0 |
| 75 | AC | 201 | ZMP | 4 | 0 |
| 68 | QB | 501 | CDL | 3 | 0 |

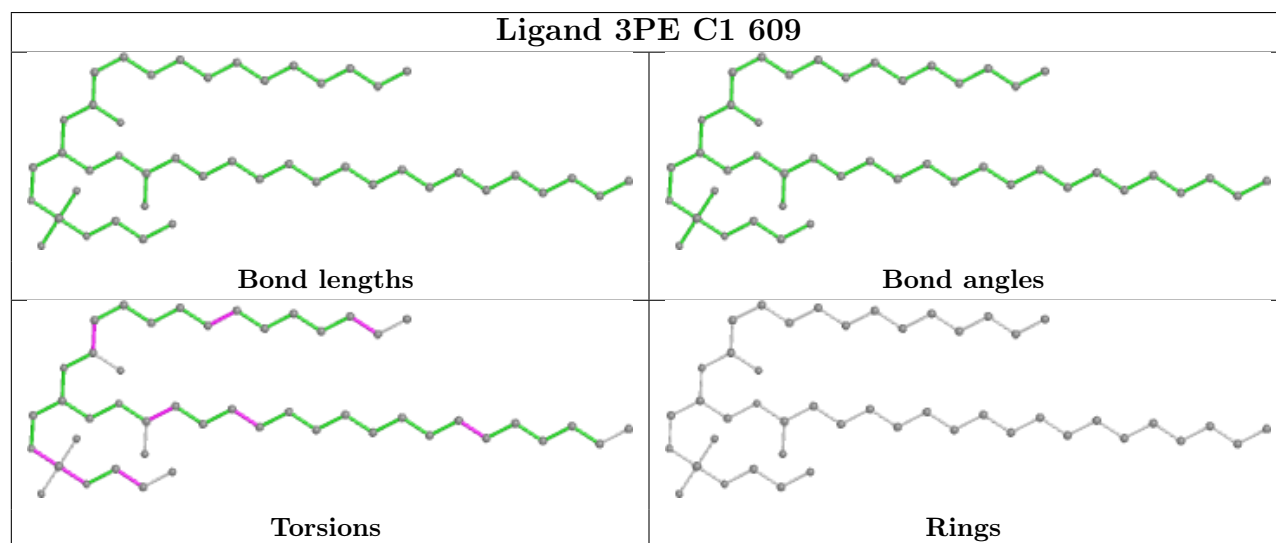
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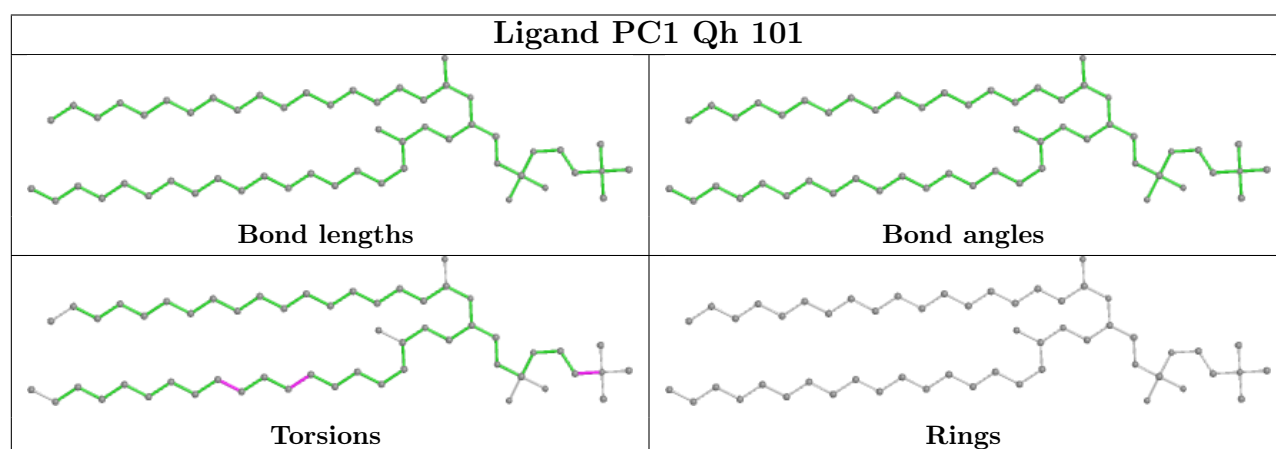
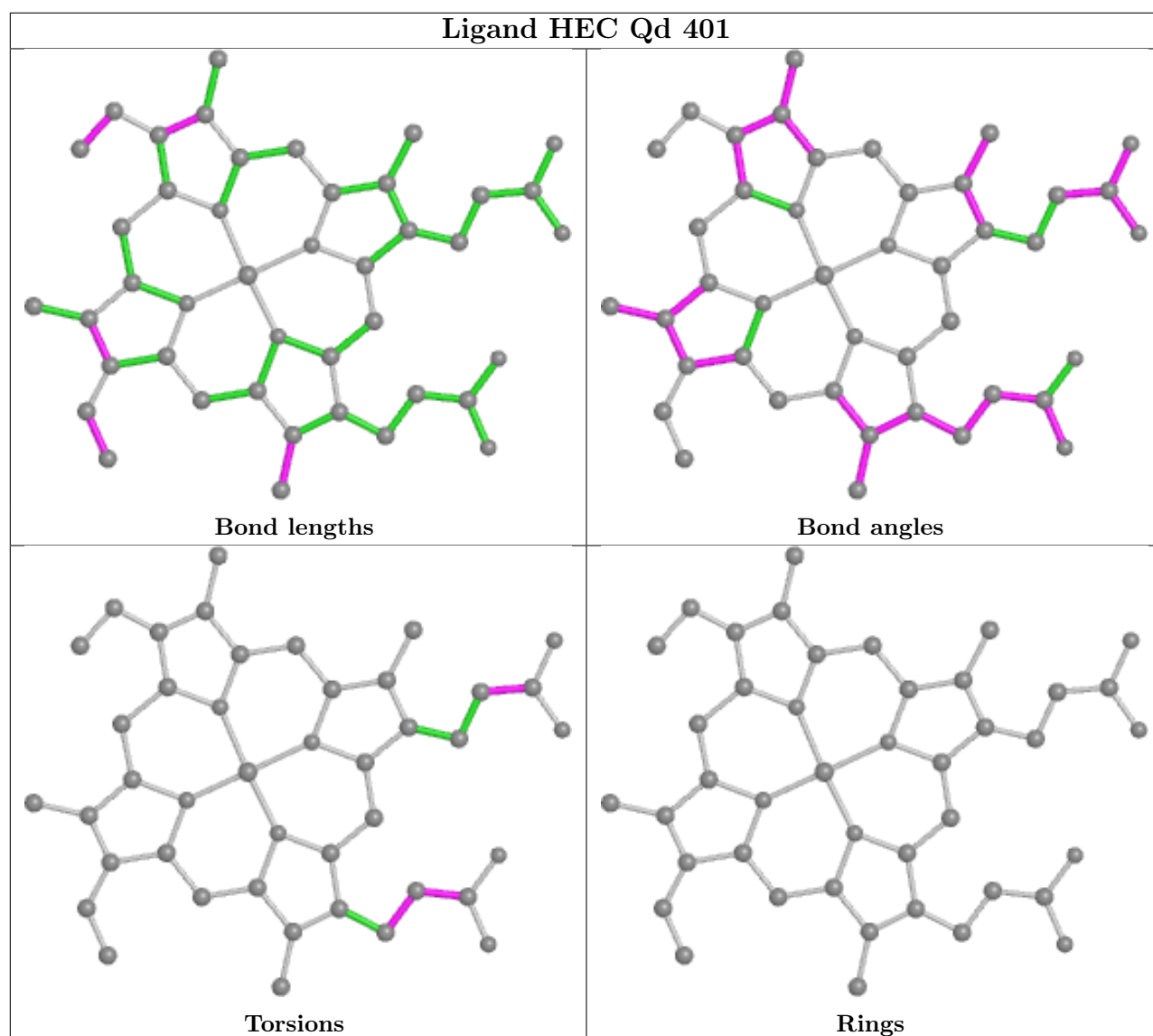
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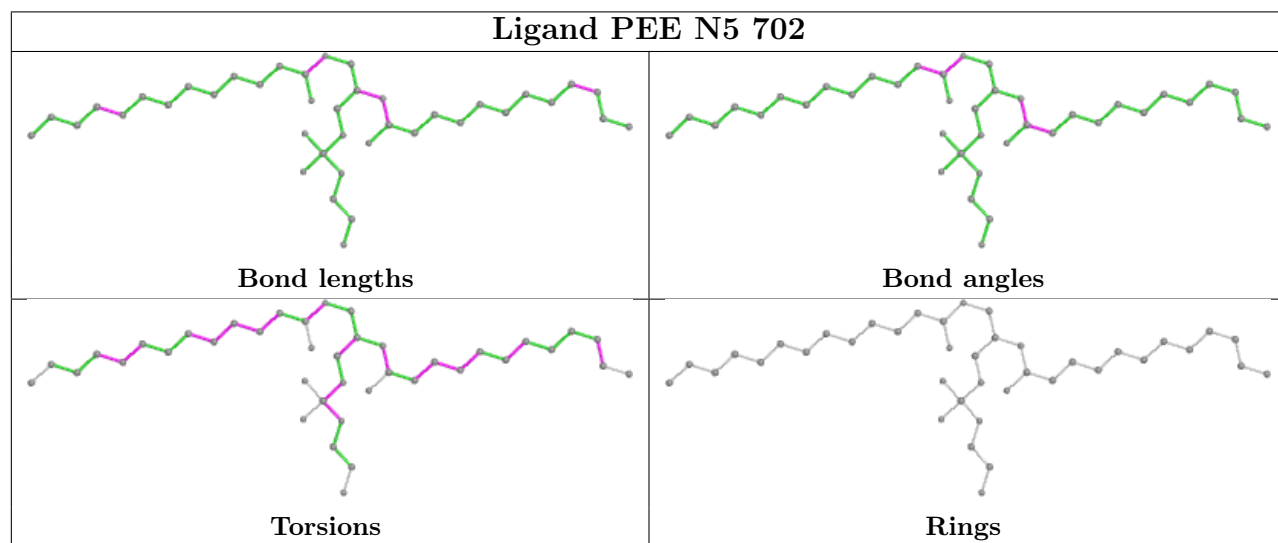
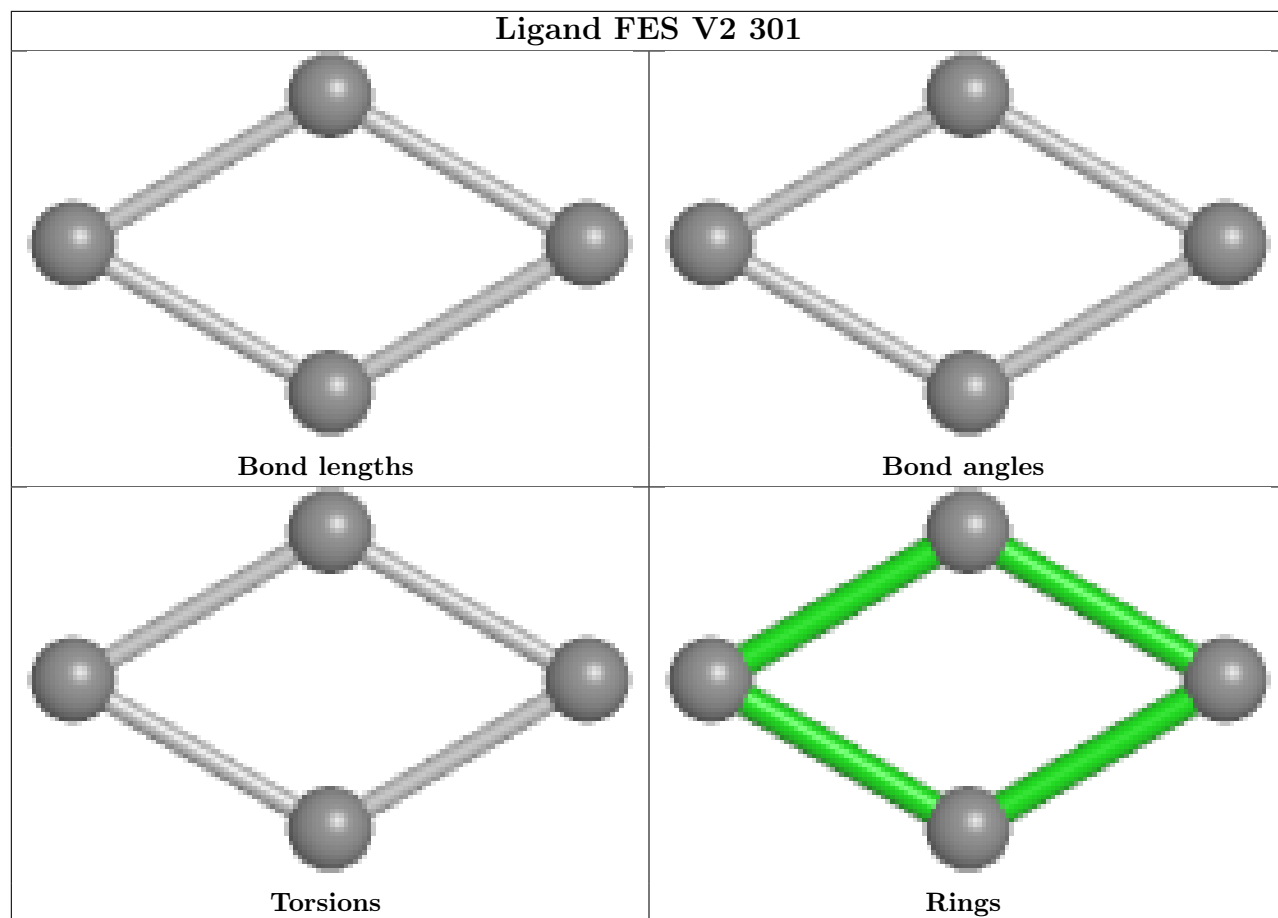
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 68 | N1 | 401 | CDL | 4 | 0 |
| 72 | S7 | 204 | 3PE | 2 | 0 |
| 73 | N4 | 501 | PEE | 5 | 0 |
| 73 | QC | 403 | PEE | 1 | 0 |
| 68 | CB | 203 | CDL | 4 | 0 |
| 71 | 6C | 101 | PLX | 1 | 0 |
| 70 | 6A | 101 | PC1 | 11 | 0 |
| 70 | Qb | 502 | PC1 | 2 | 0 |
| 73 | Qc | 401 | PEE | 1 | 0 |
| 70 | C1 | 605 | PC1 | 1 | 0 |
| 71 | AL | 202 | PLX | 2 | 0 |
| 70 | C3 | 301 | PC1 | 3 | 0 |
| 71 | AM | 201 | PLX | 6 | 0 |
| 83 | S7 | 202 | SF4 | 1 | 0 |
| 68 | A7 | 201 | CDL | 1 | 0 |
| 72 | Qc | 404 | 3PE | 2 | 0 |
| 70 | Qc | 405 | PC1 | 4 | 0 |
| 72 | N5 | 706 | 3PE | 1 | 0 |
| 73 | Qe | 301 | PEE | 7 | 0 |
| 80 | Qc | 403 | HEM | 7 | 0 |
| 68 | C3 | 304 | CDL | 4 | 0 |
| 68 | AK | 402 | CDL | 3 | 0 |
| 71 | N4 | 502 | PLX | 4 | 0 |
| 71 | N6 | 201 | PLX | 1 | 0 |
| 70 | N1 | 402 | PC1 | 3 | 0 |
| 68 | Qb | 501 | CDL | 2 | 0 |
| 68 | AL | 201 | CDL | 7 | 0 |
| 82 | Qe | 303 | FES | 2 | 0 |
| 71 | Qi | 301 | PLX | 5 | 0 |
| 68 | 4L | 201 | CDL | 8 | 0 |
| 71 | QI | 301 | PLX | 2 | 0 |
| 85 | S7 | 201 | U10 | 6 | 0 |
| 80 | QC | 401 | HEM | 2 | 0 |
| 68 | N5 | 703 | CDL | 13 | 0 |
| 68 | QD | 402 | CDL | 1 | 0 |
| 68 | QH | 102 | CDL | 7 | 0 |
| 72 | QJ | 101 | 3PE | 1 | 0 |
| 77 | C1 | 602 | HEA | 10 | 0 |
| 83 | S8 | 302 | SF4 | 1 | 0 |
| 73 | 7C | 101 | PEE | 5 | 0 |
| 71 | S7 | 203 | PLX | 6 | 0 |

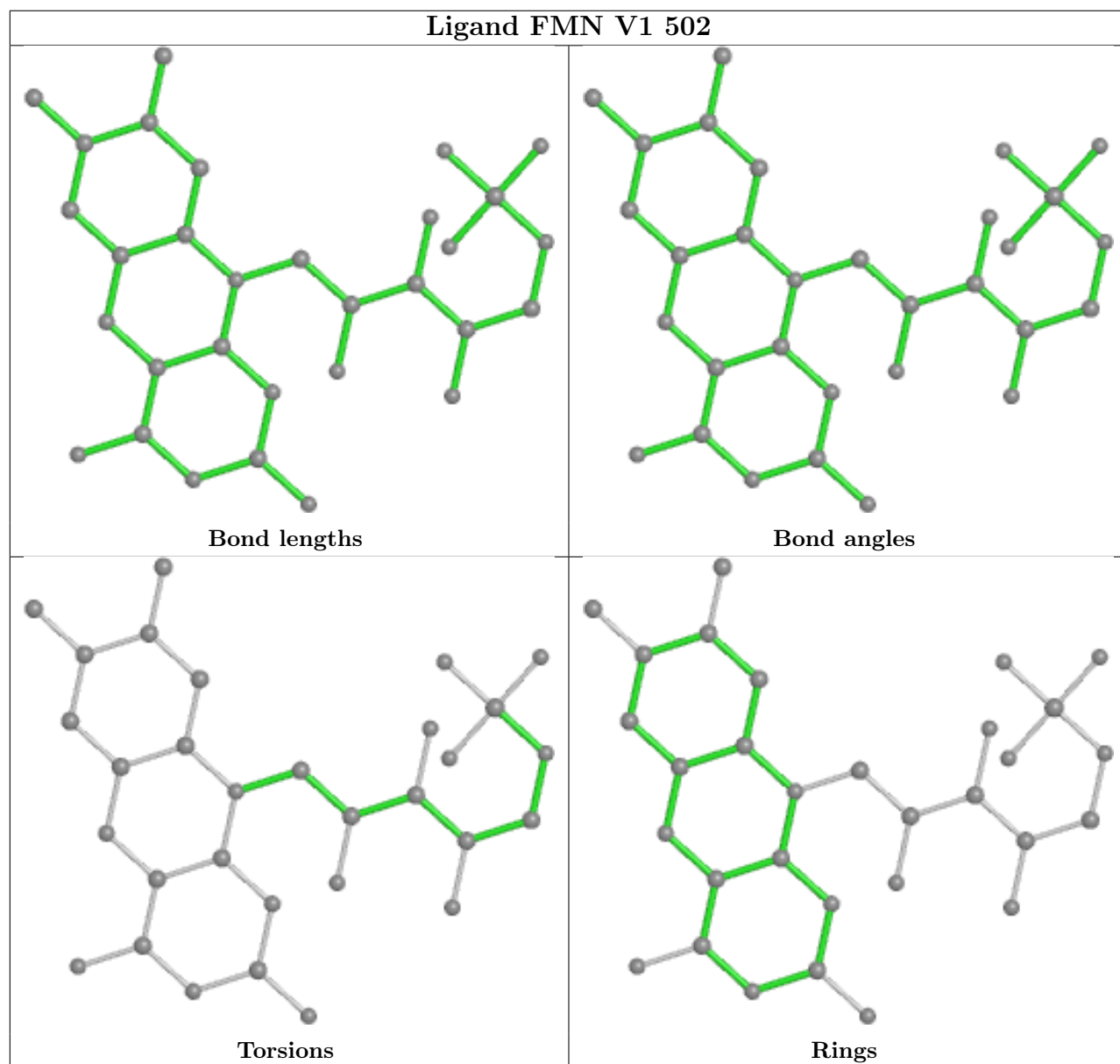
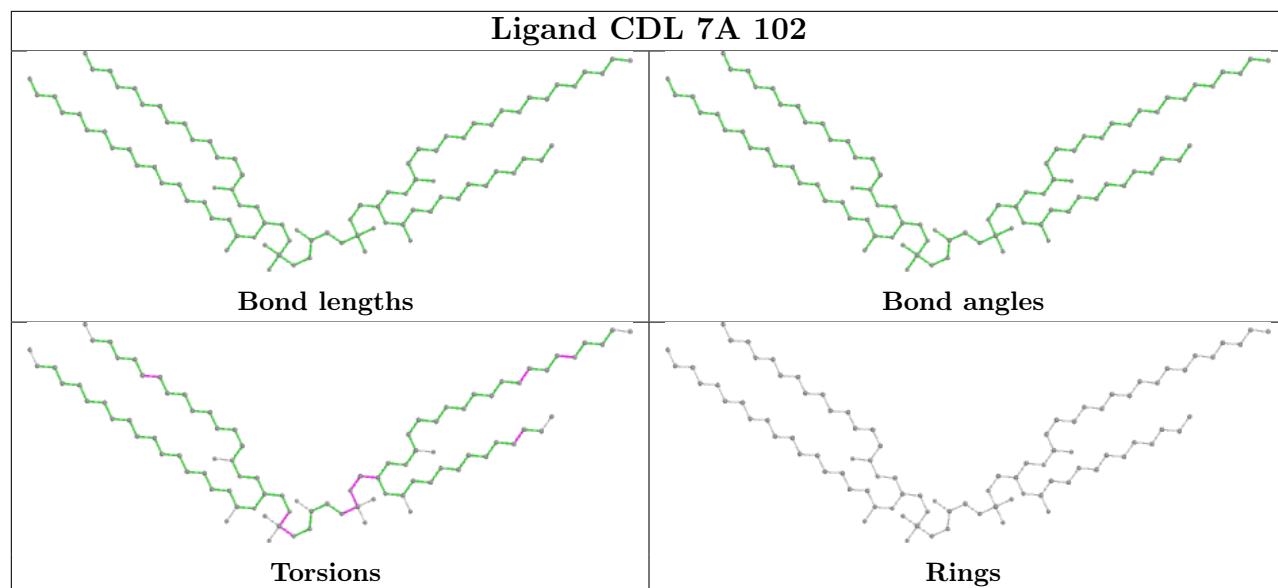
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

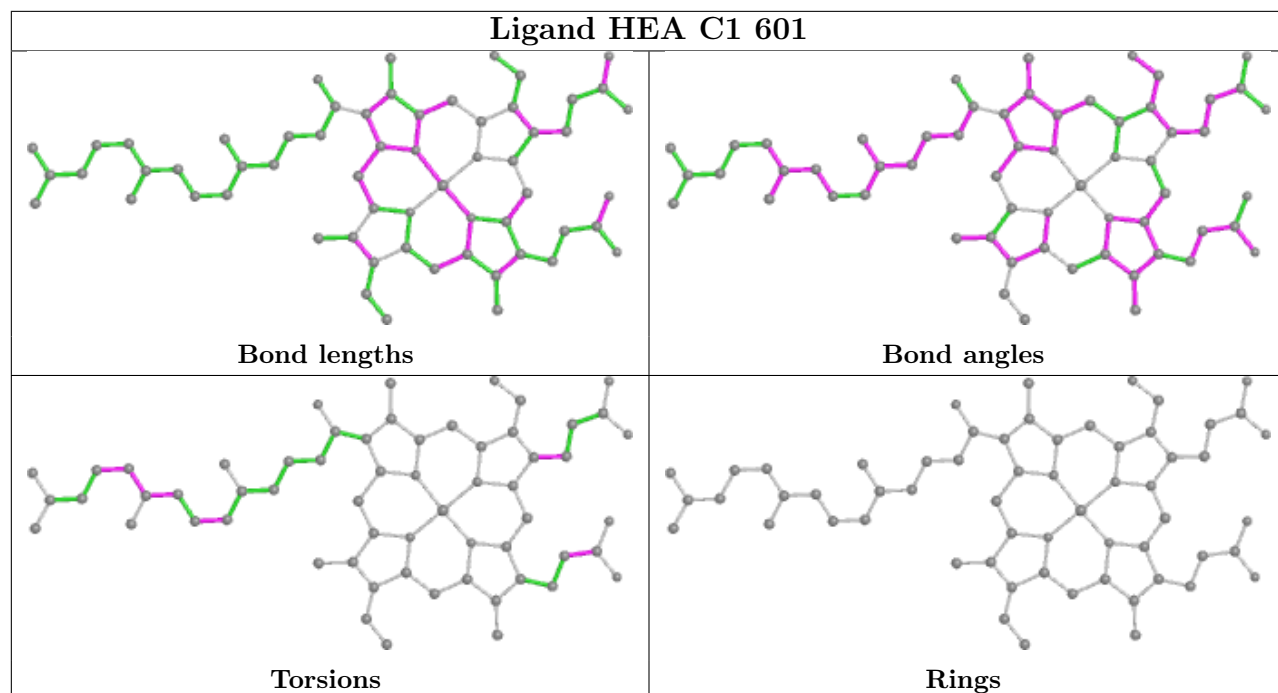




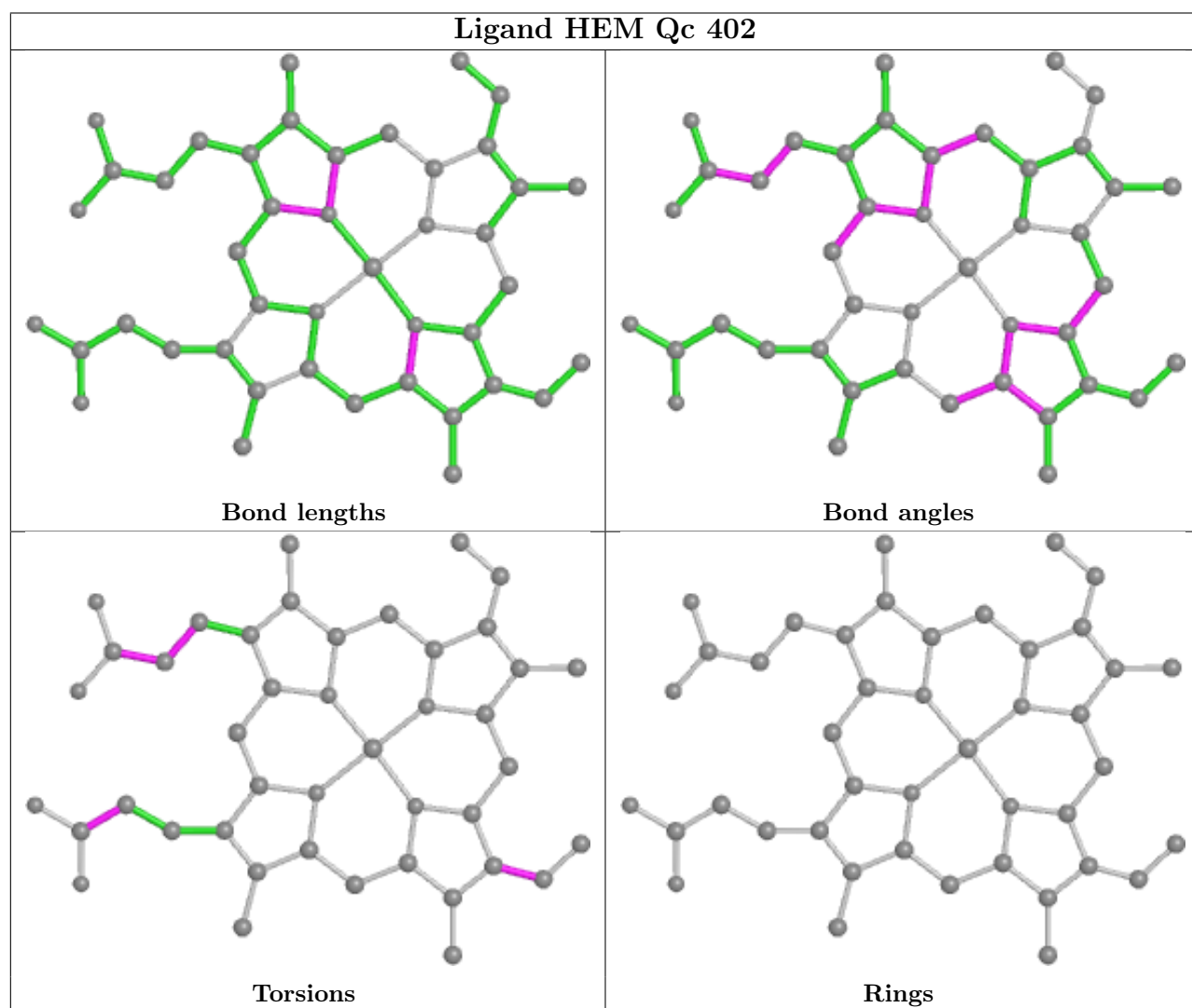


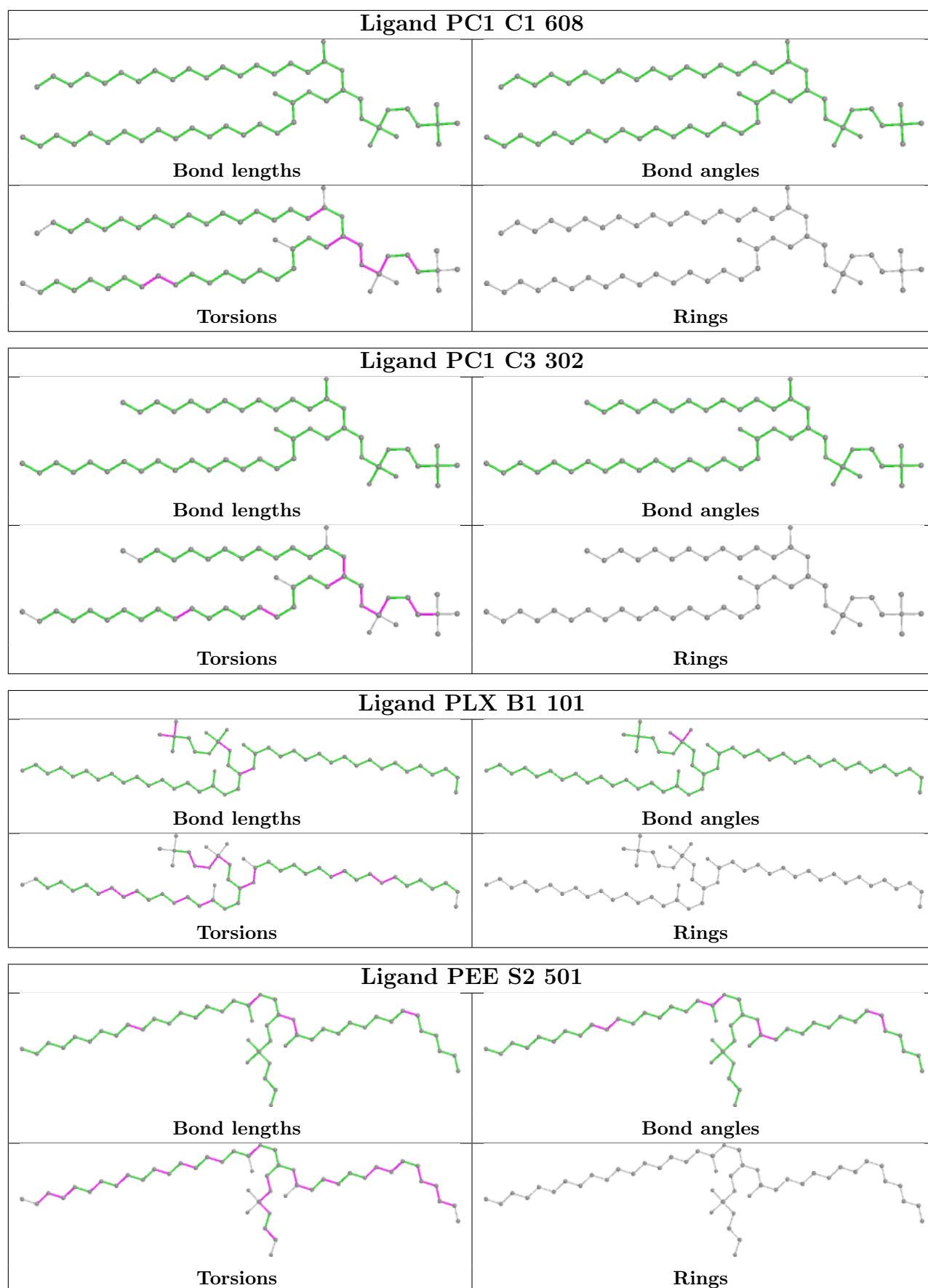


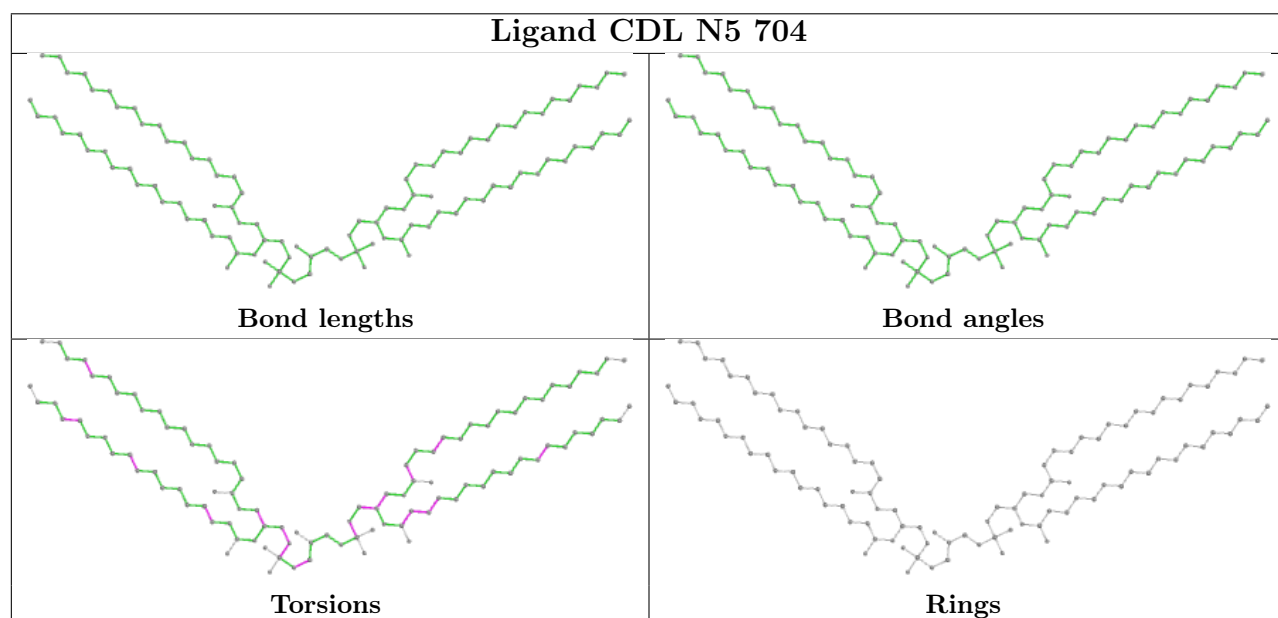
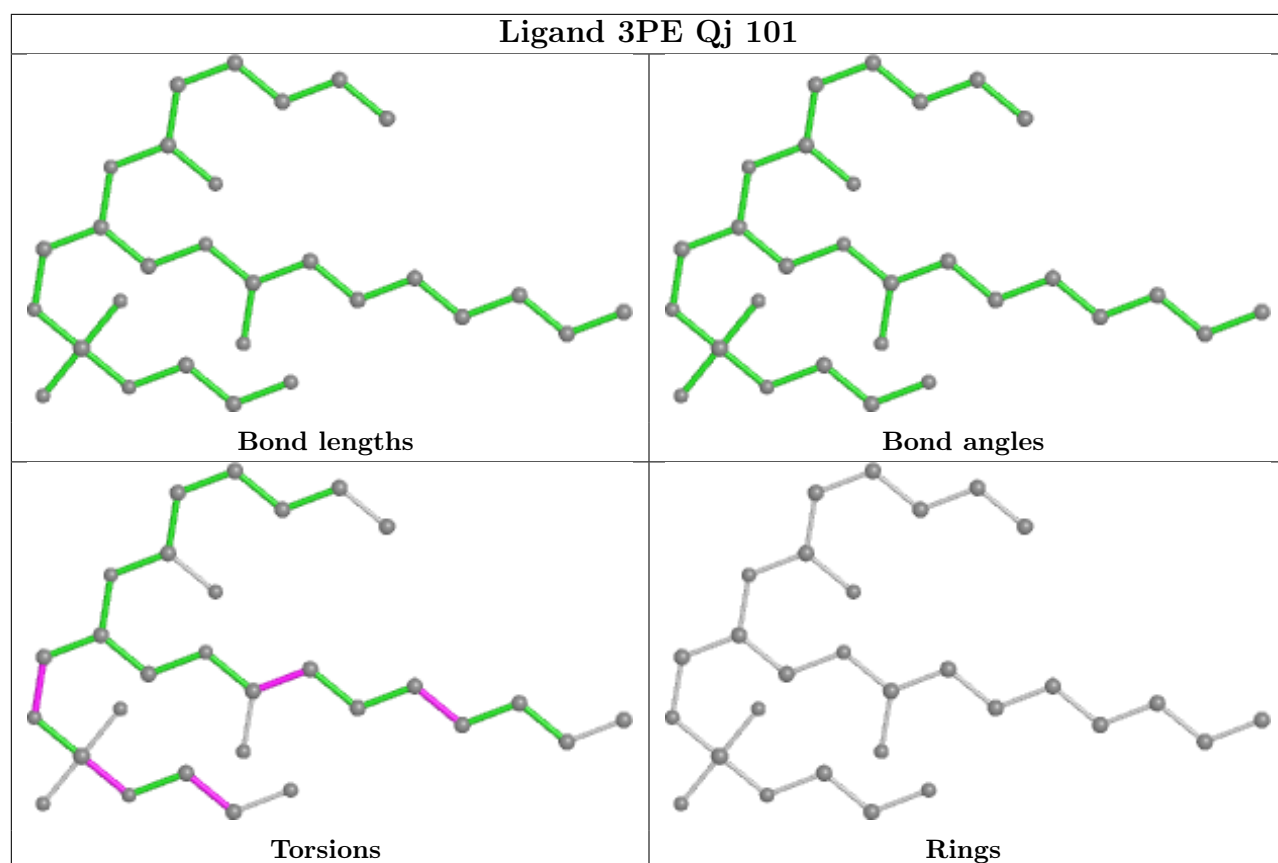
Ligand HEA C1 601

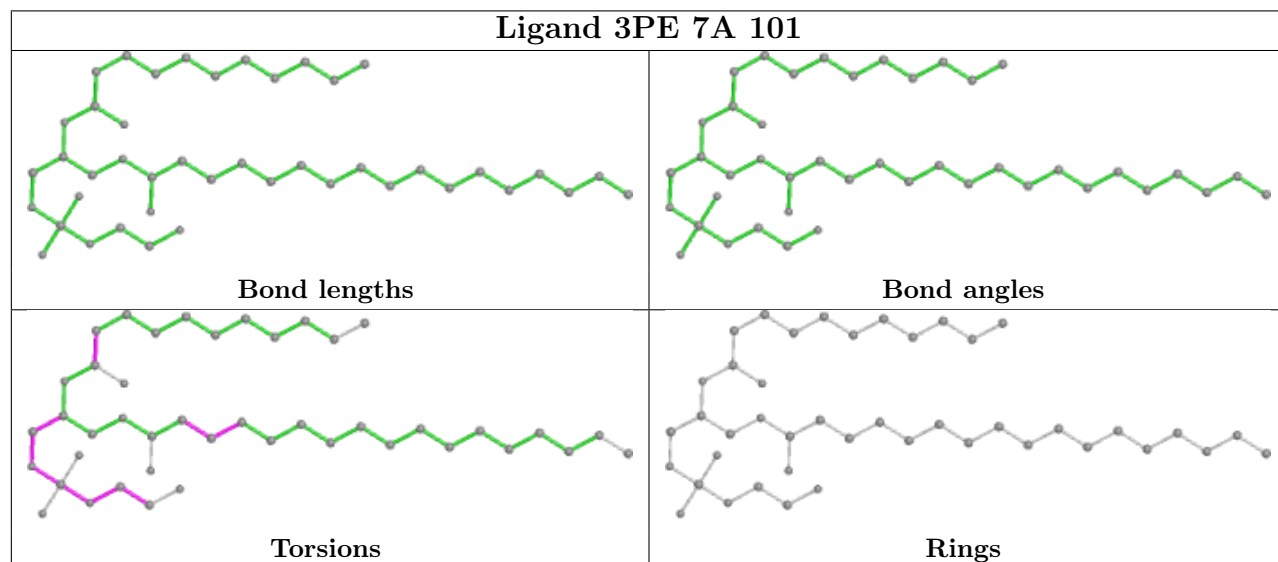
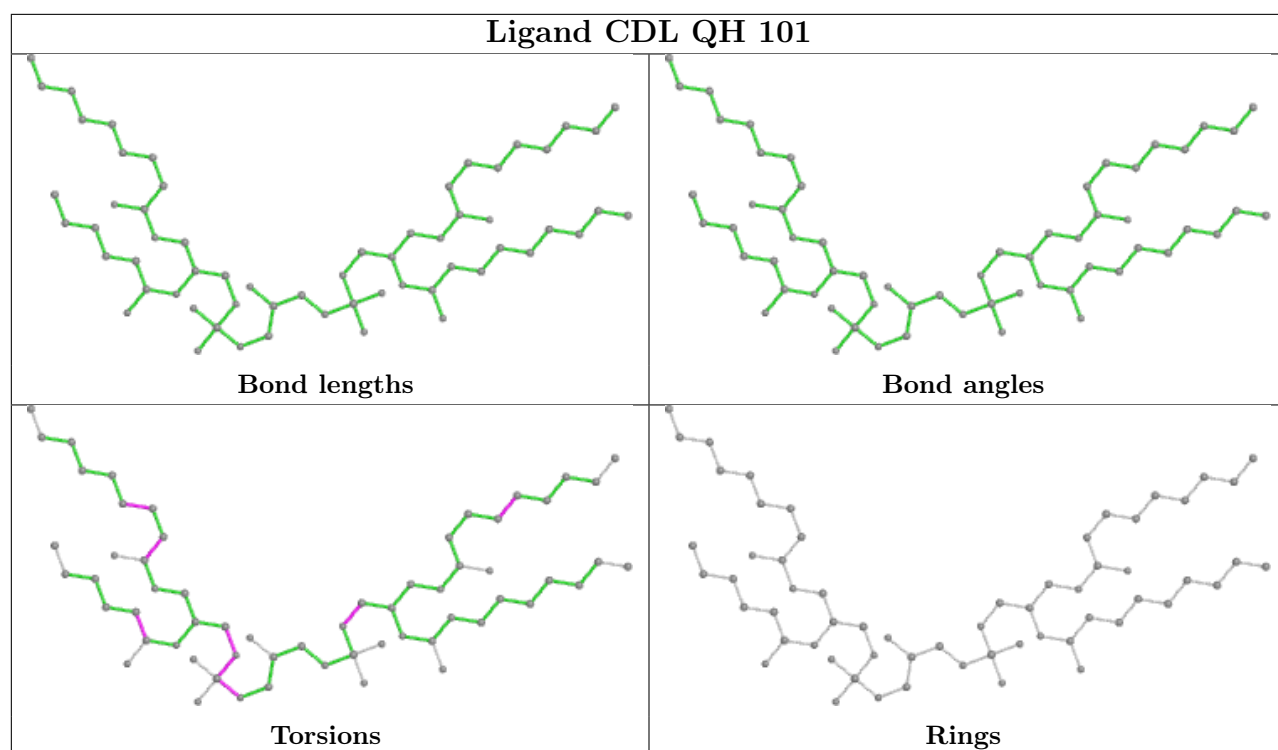


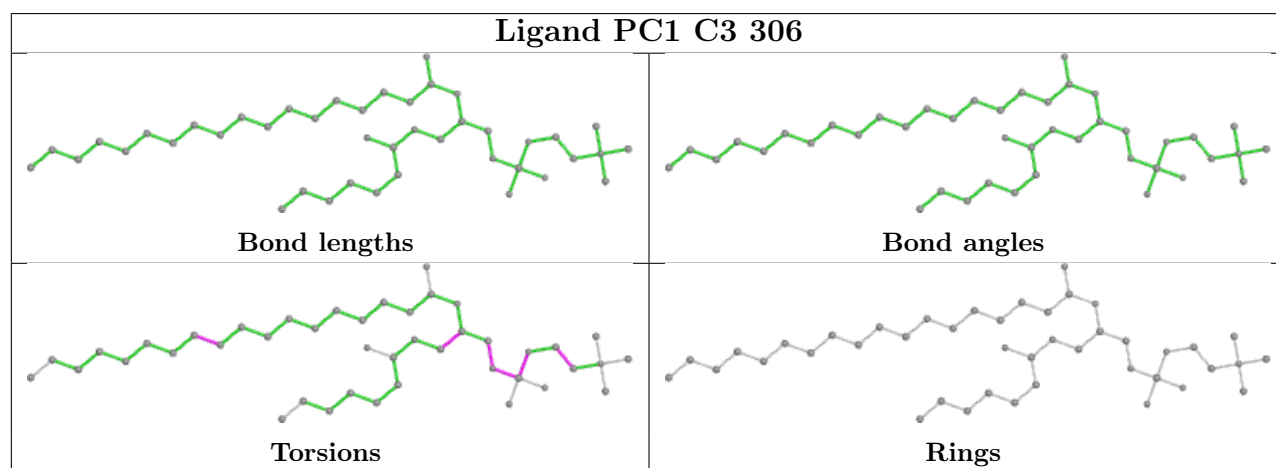
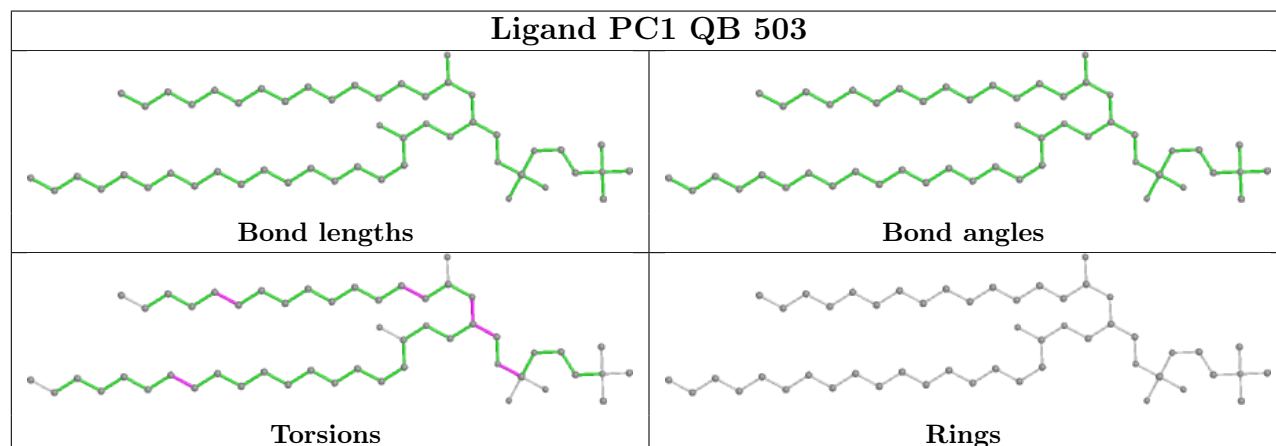
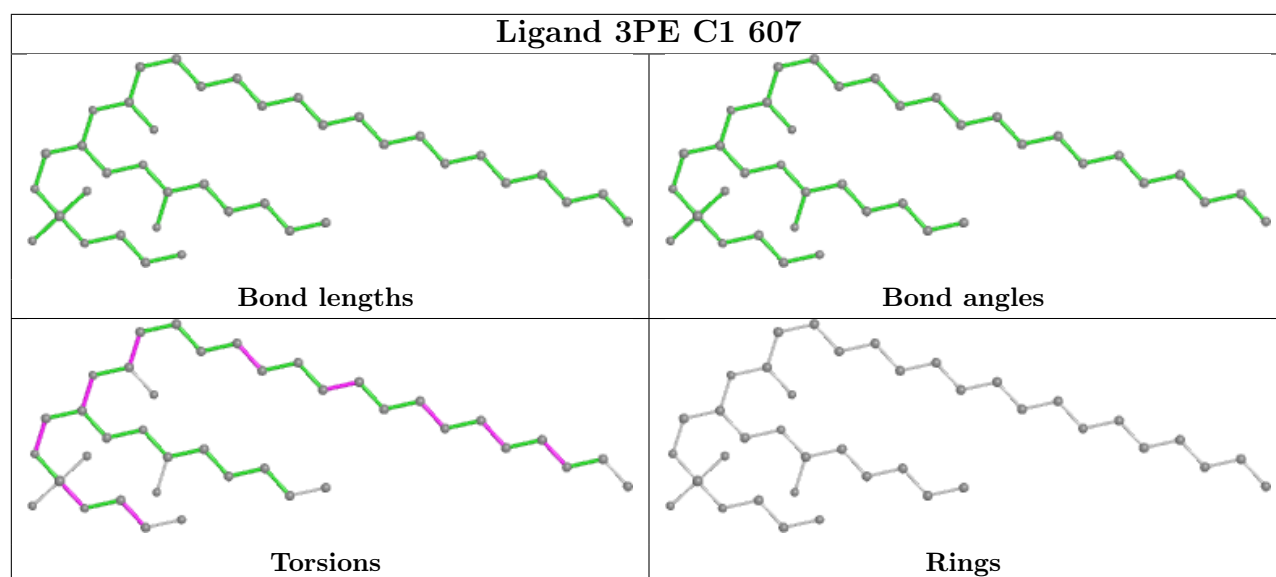
Ligand HEM Qc 402

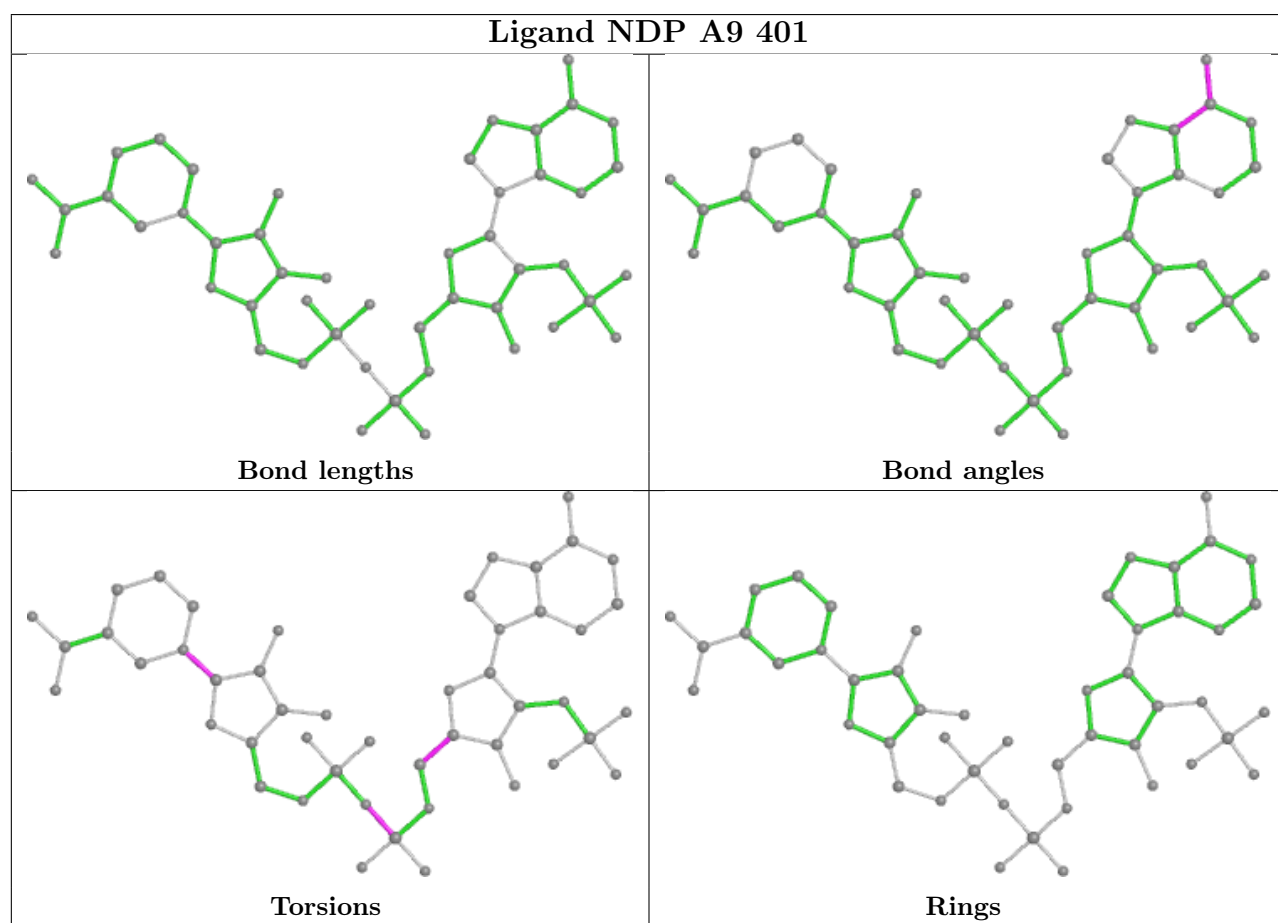
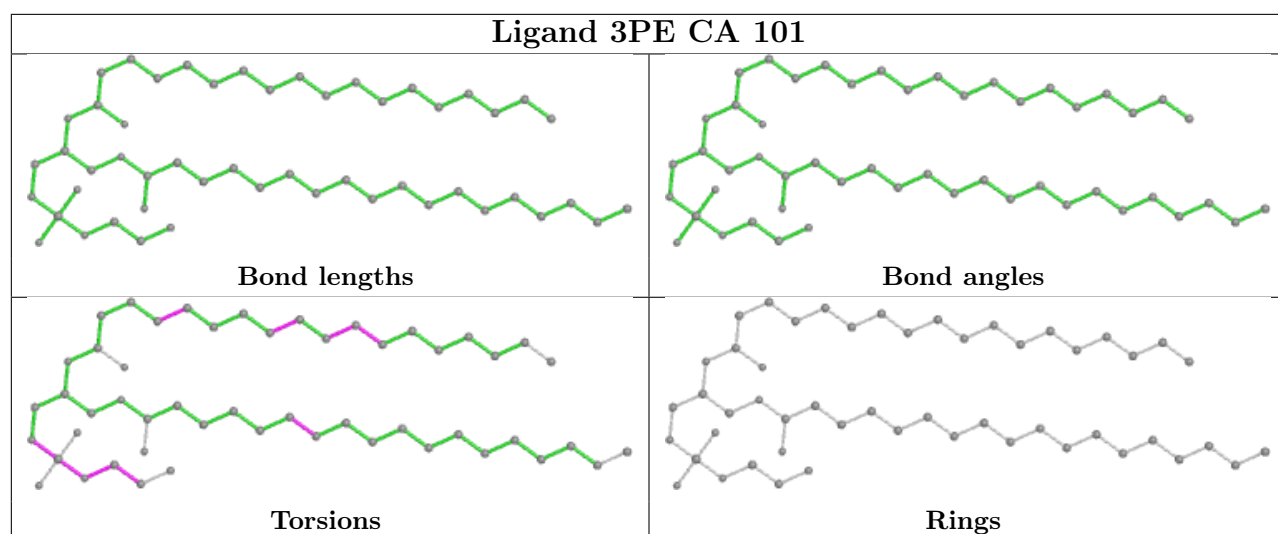


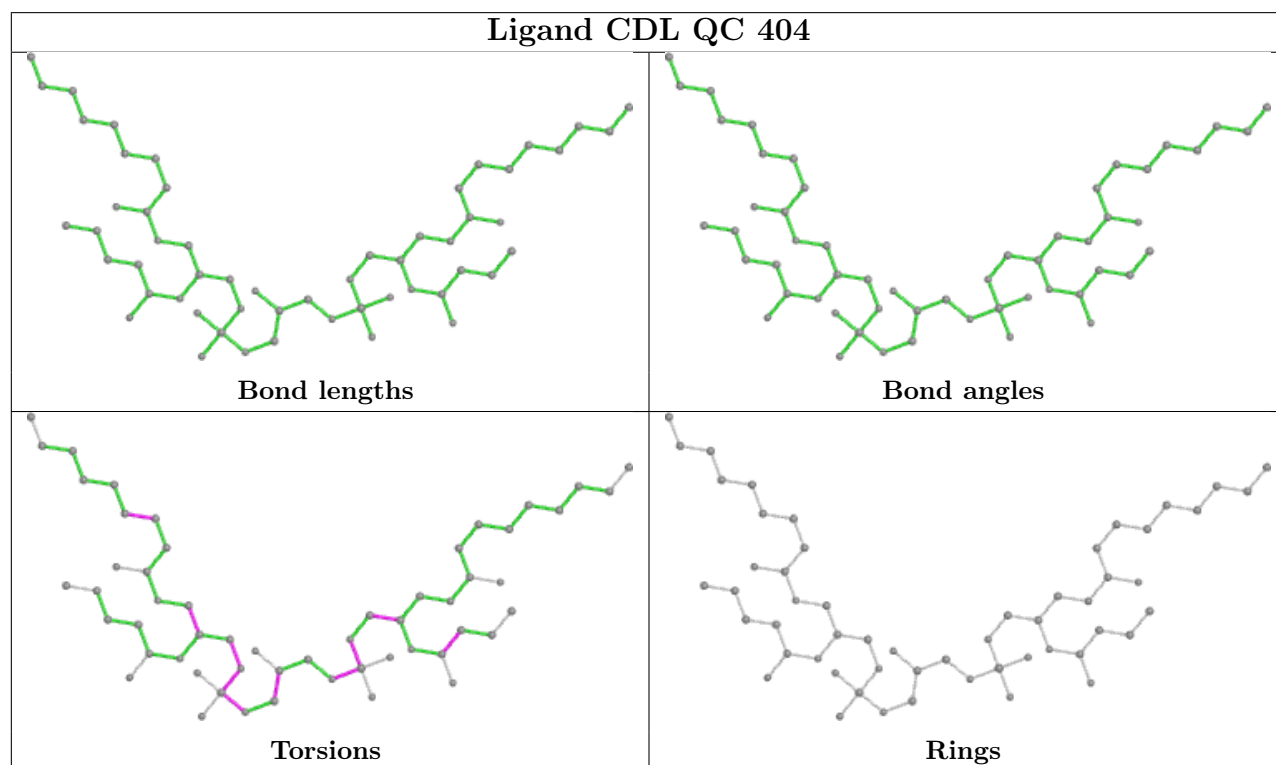
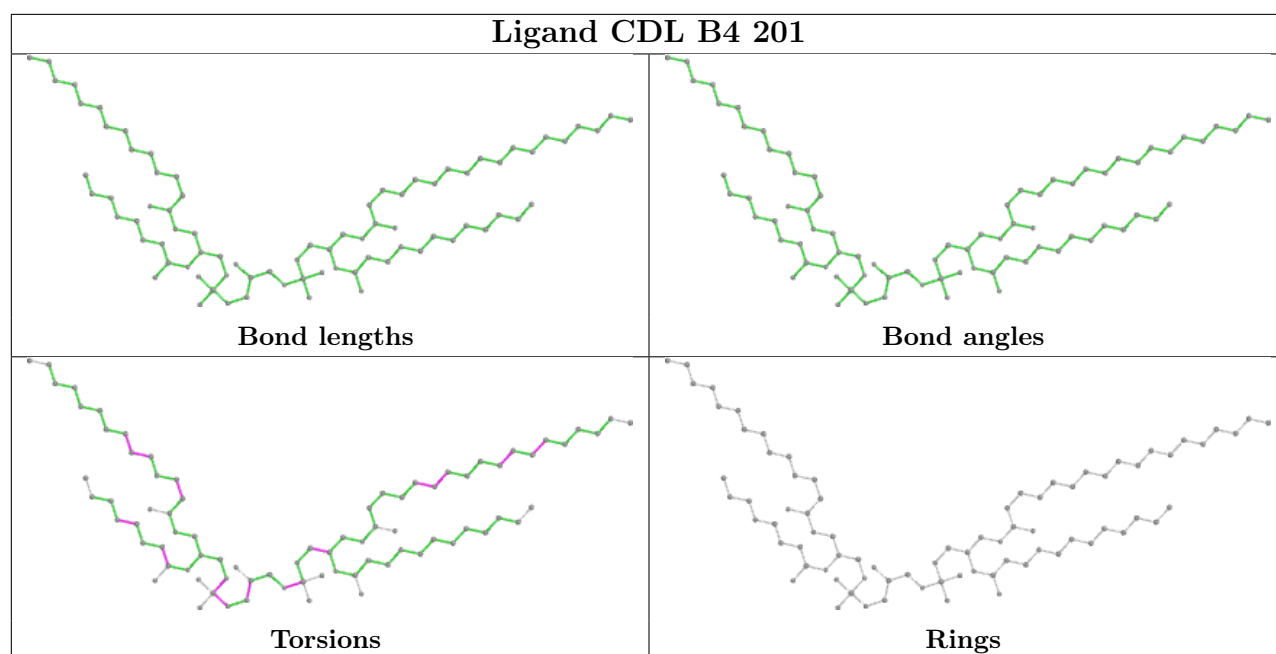




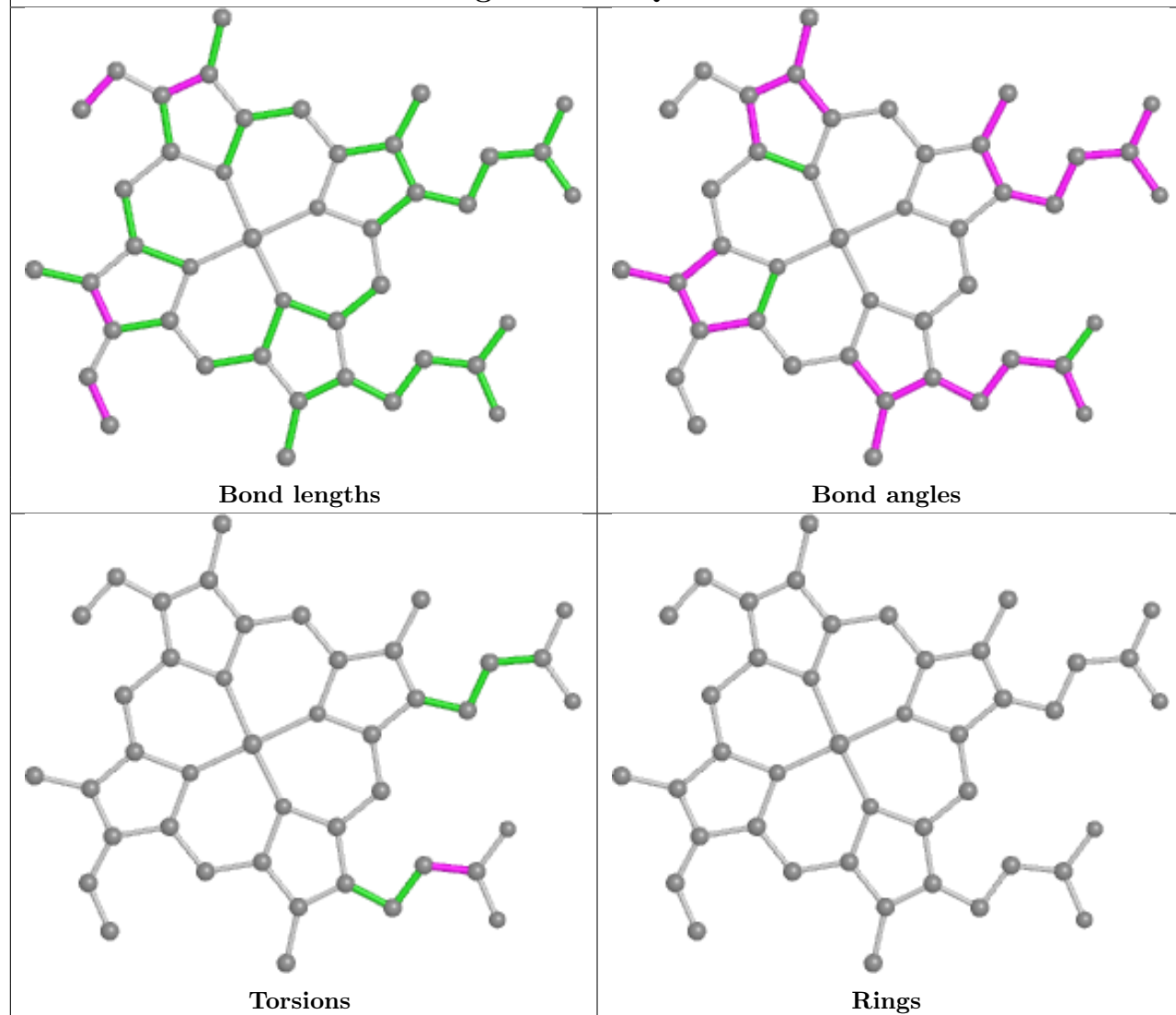




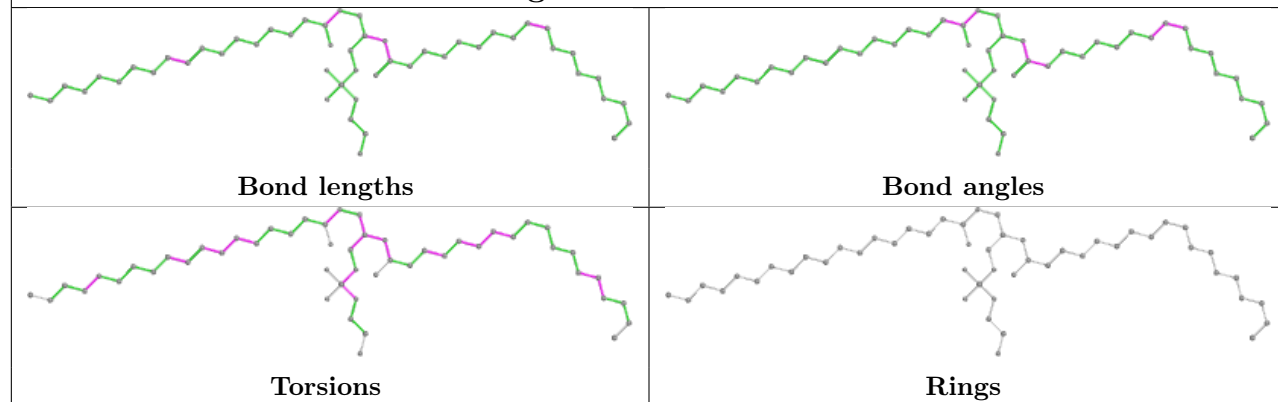


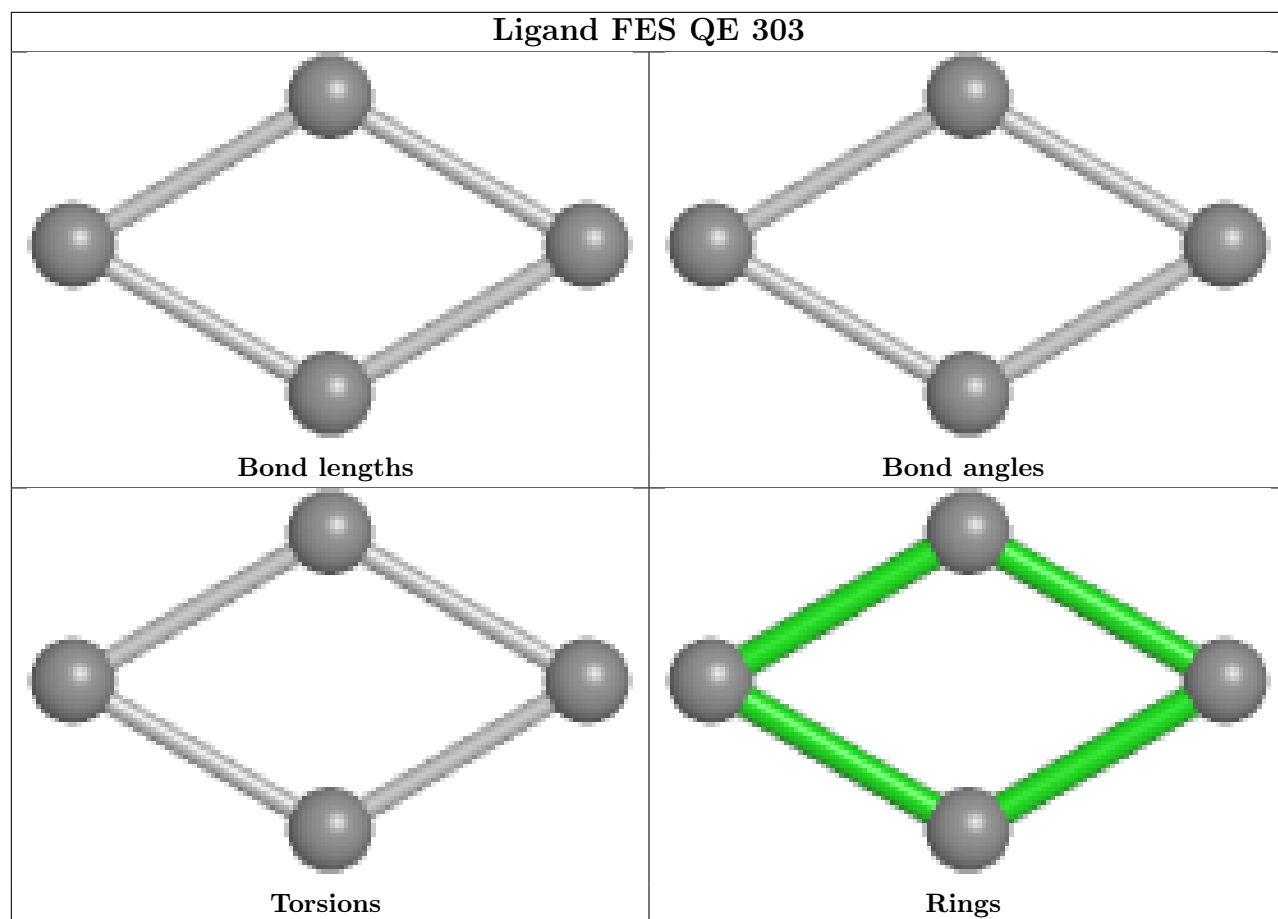
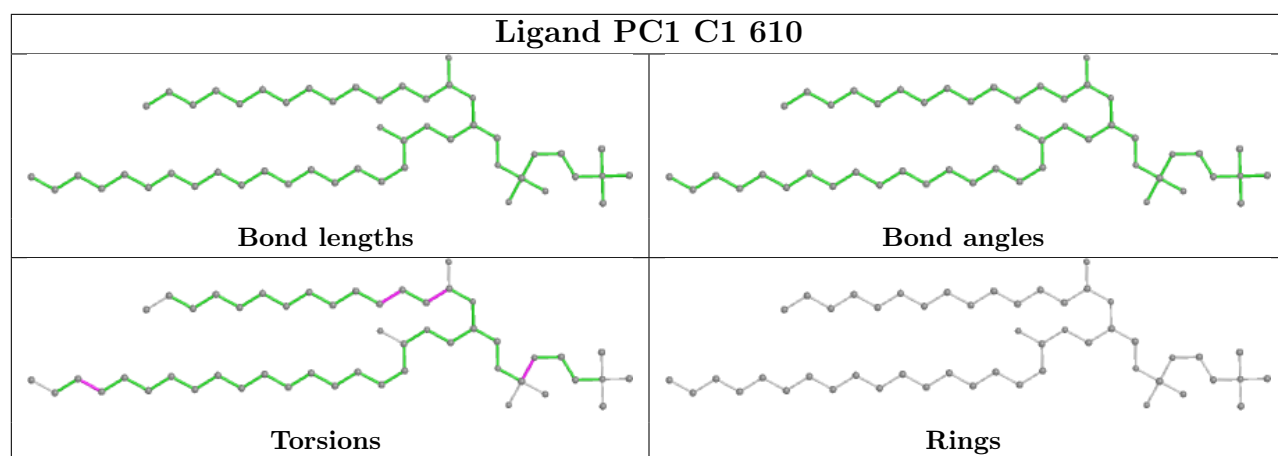


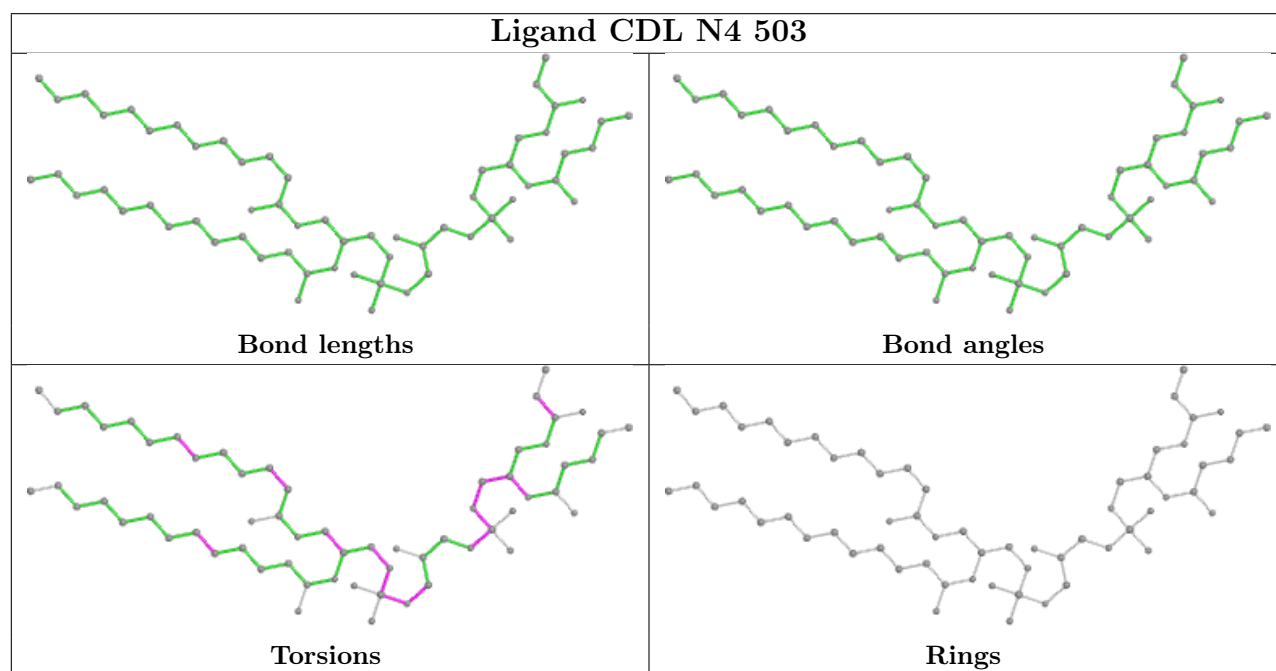
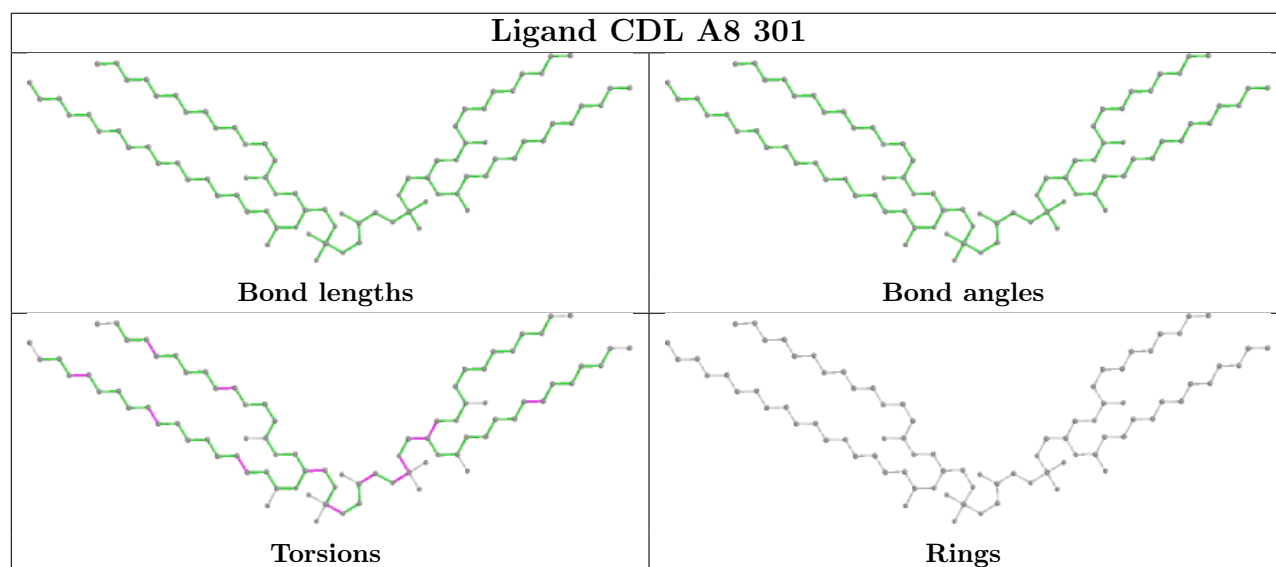
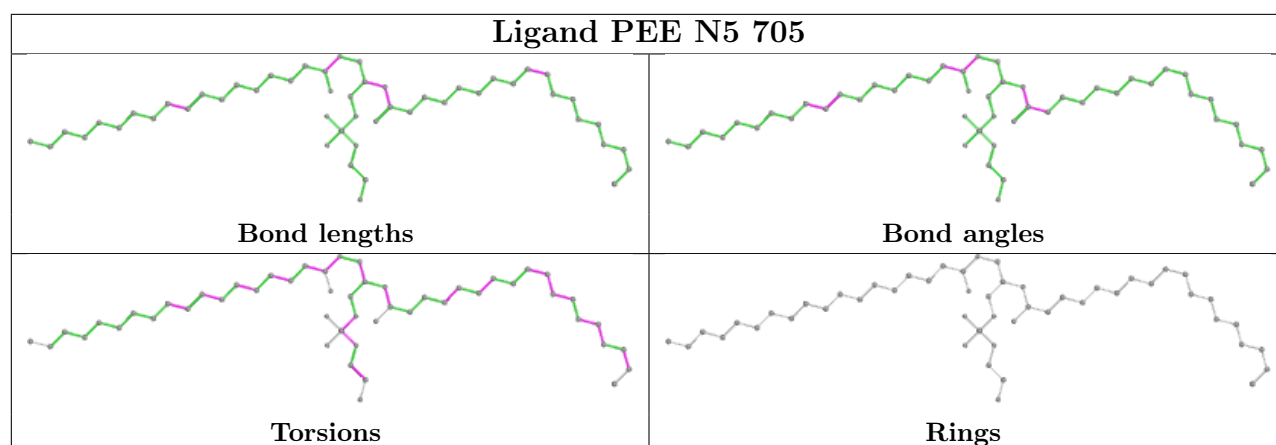
Ligand HEC QD 401



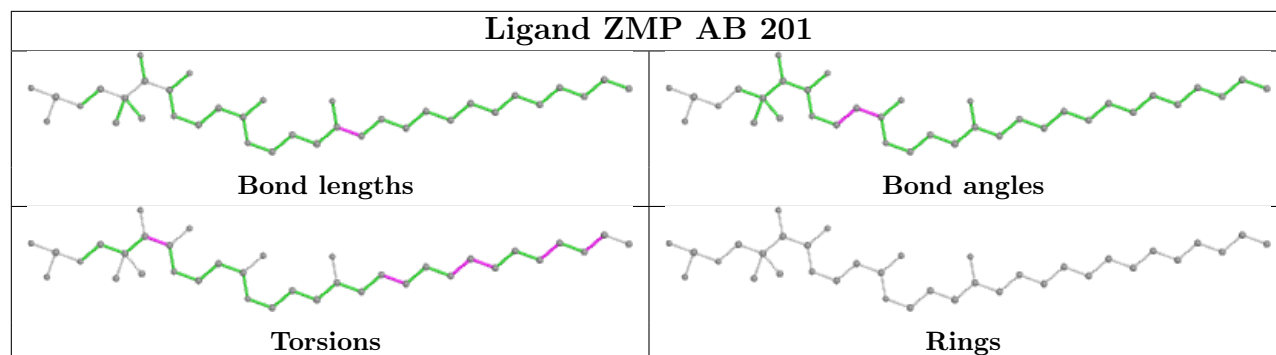
Ligand PEE S8 303



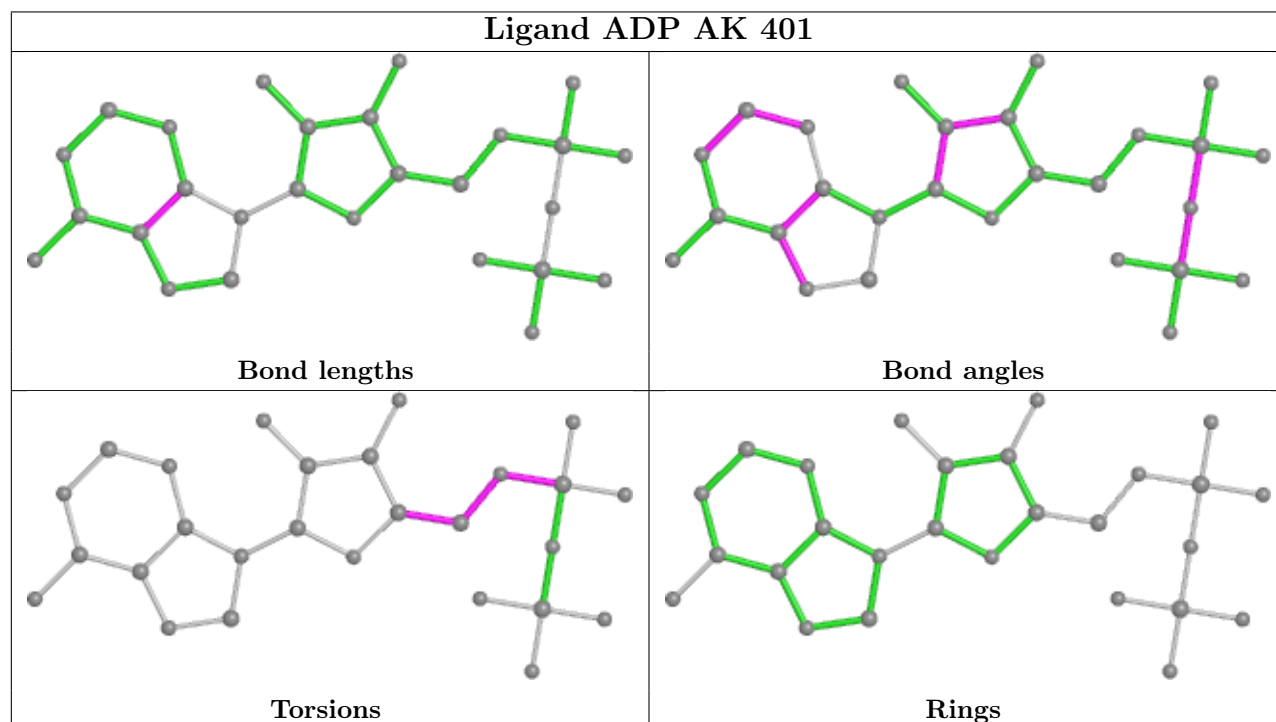




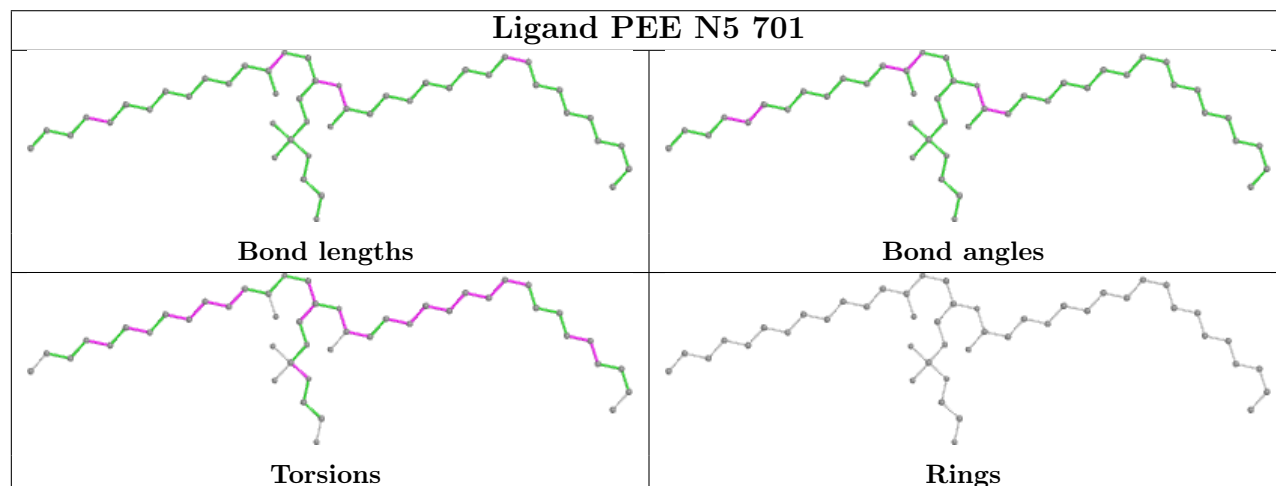
Ligand ZMP AB 201

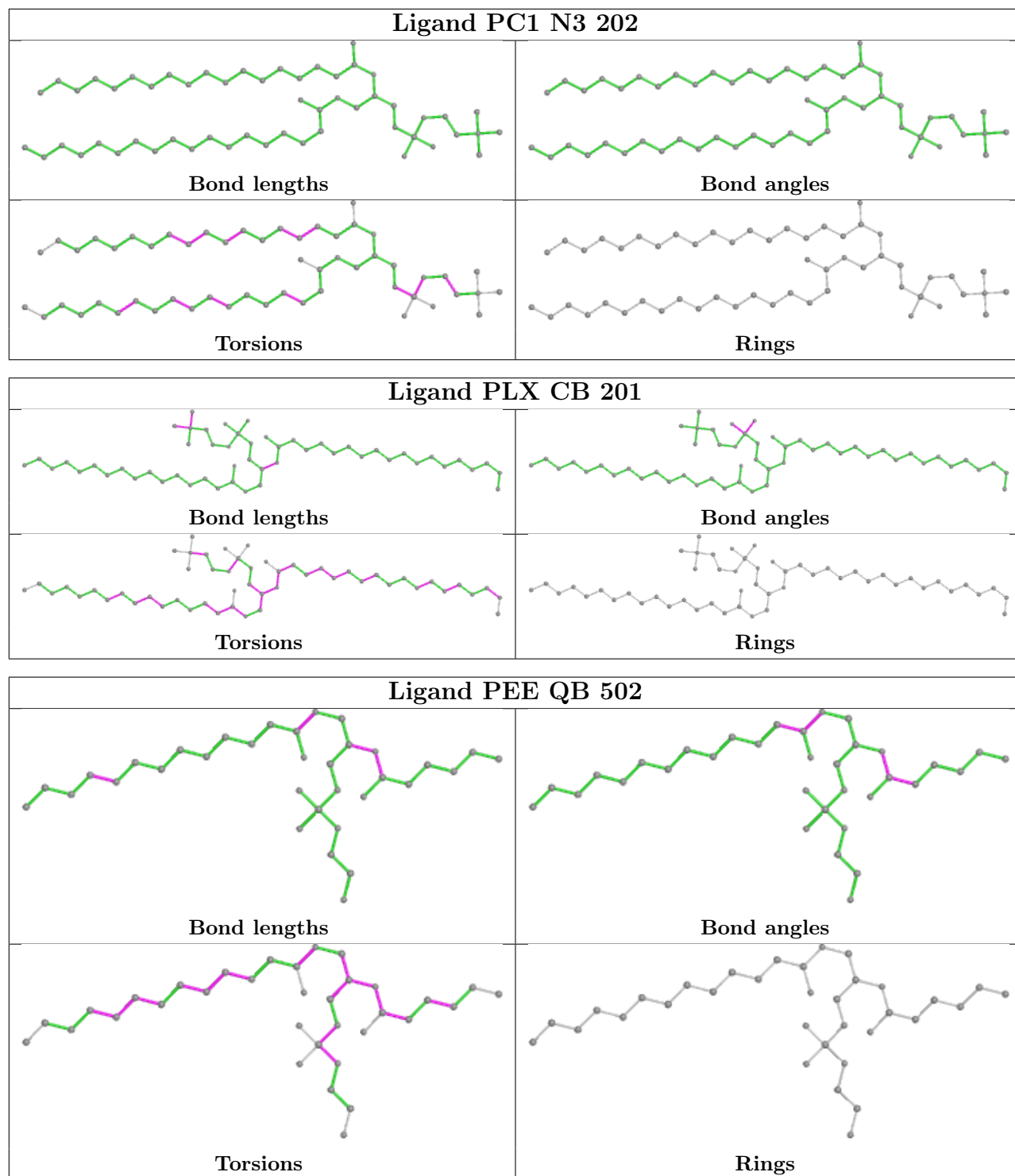


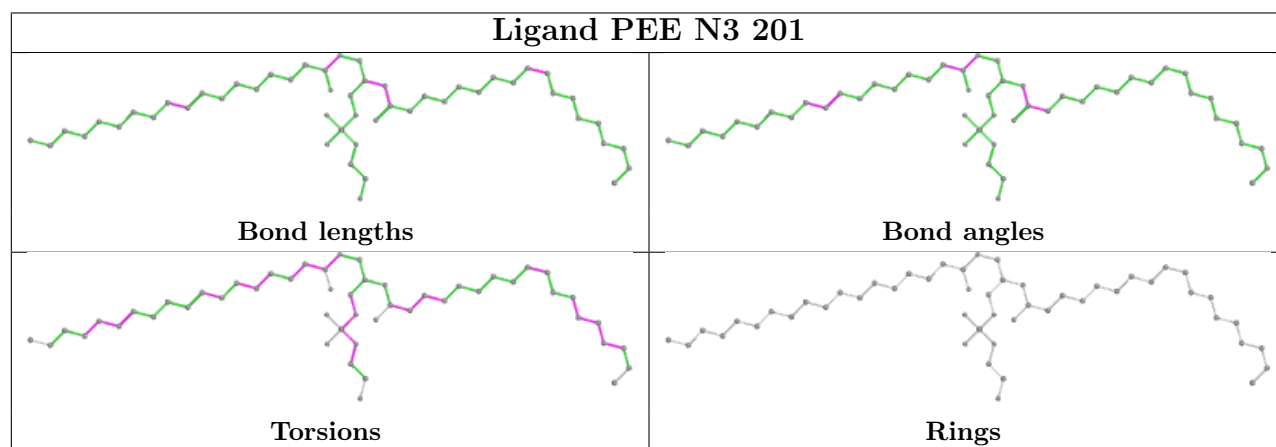
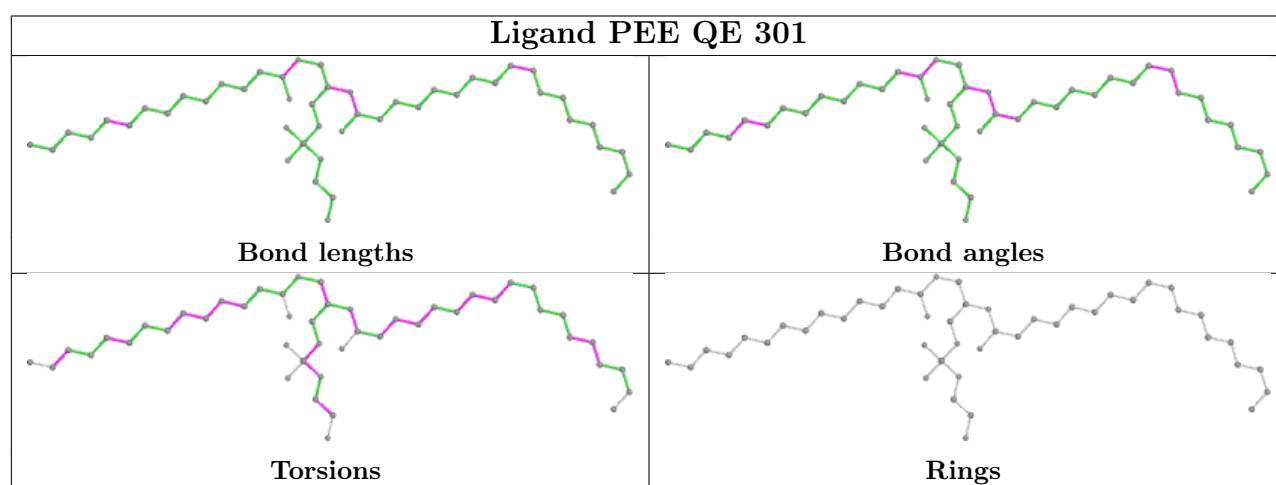
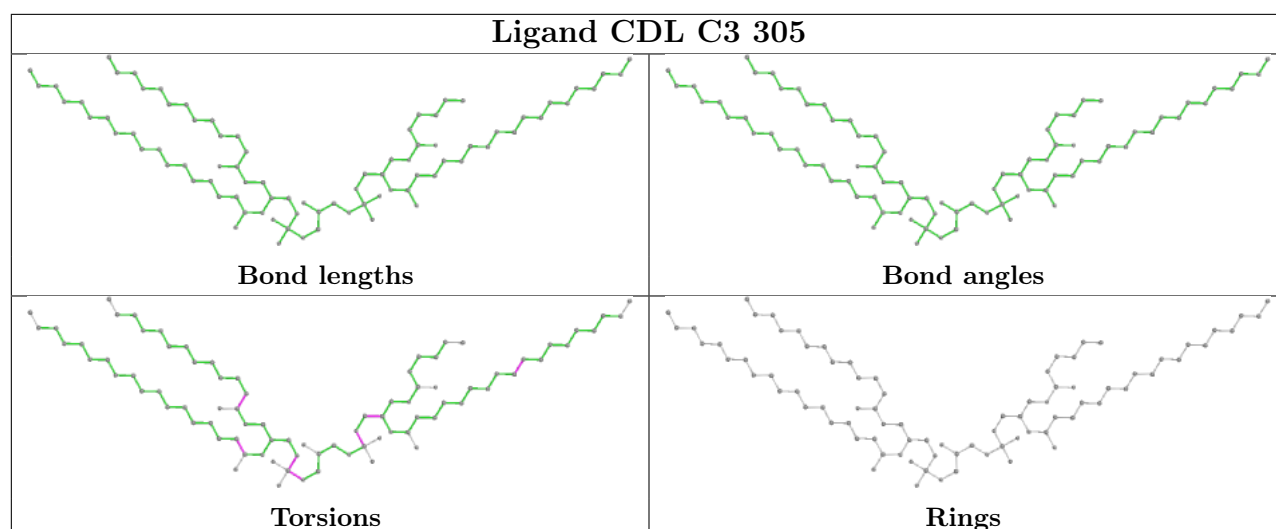
Ligand ADP AK 401

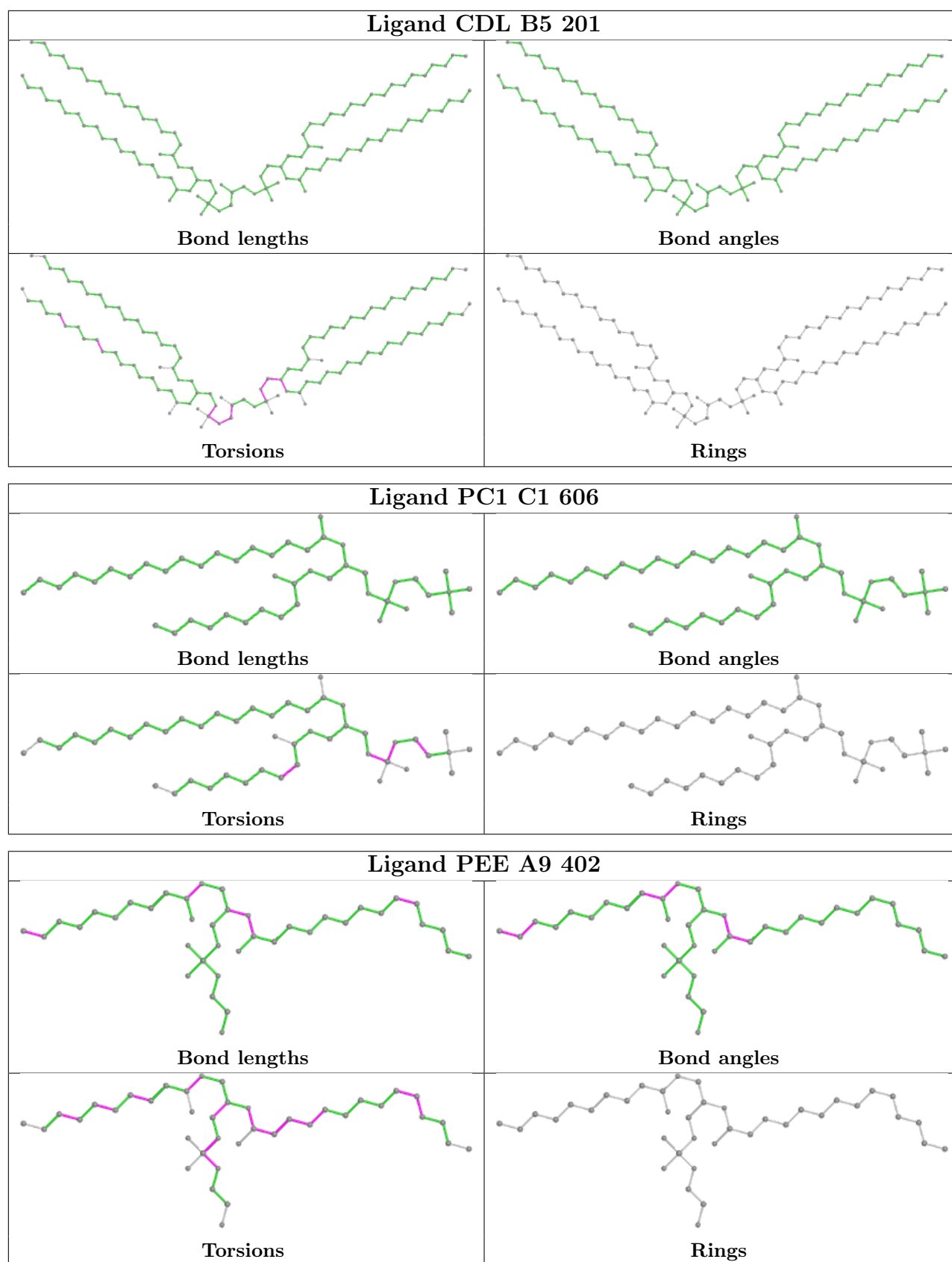


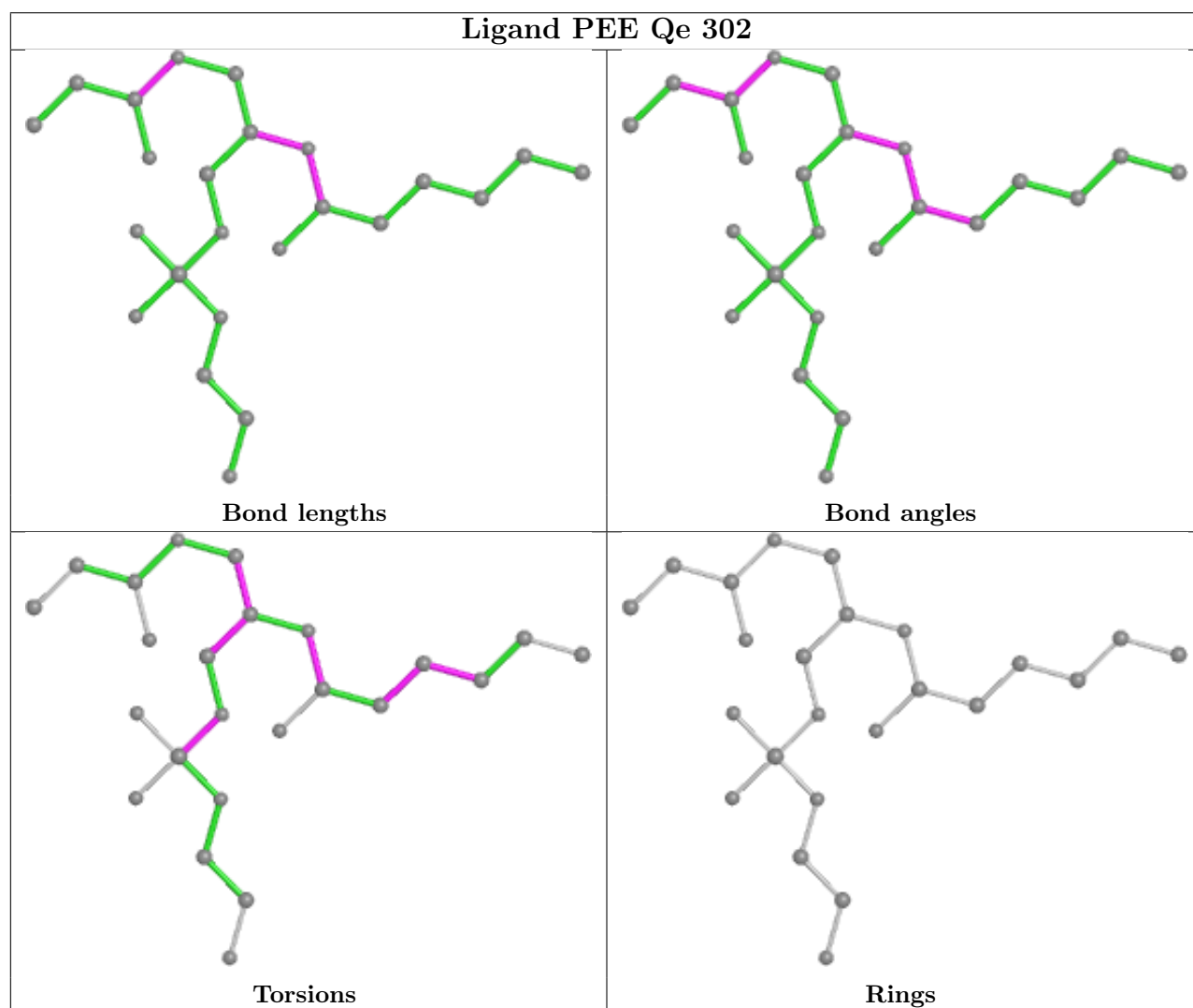
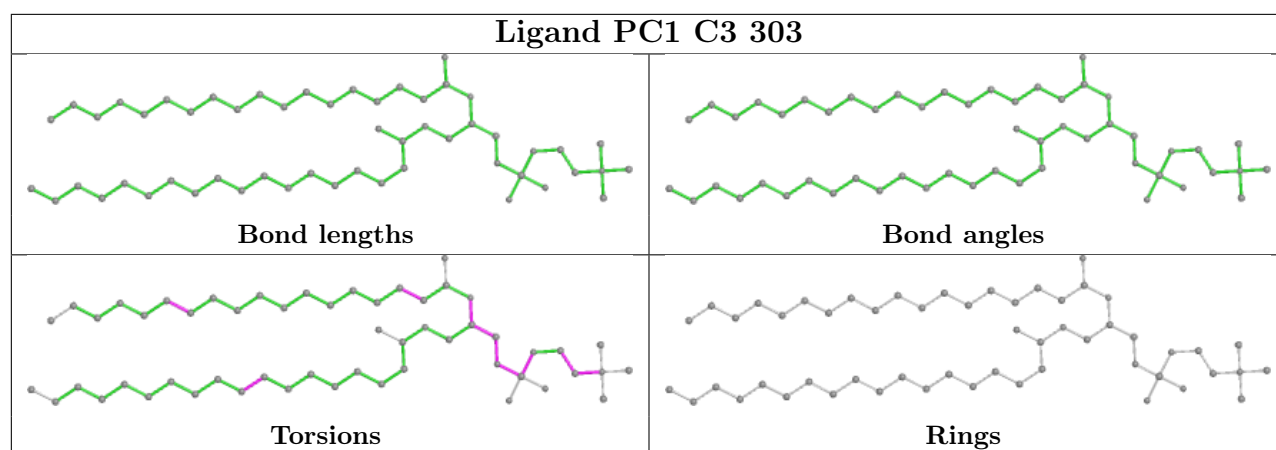
Ligand PEE N5 701

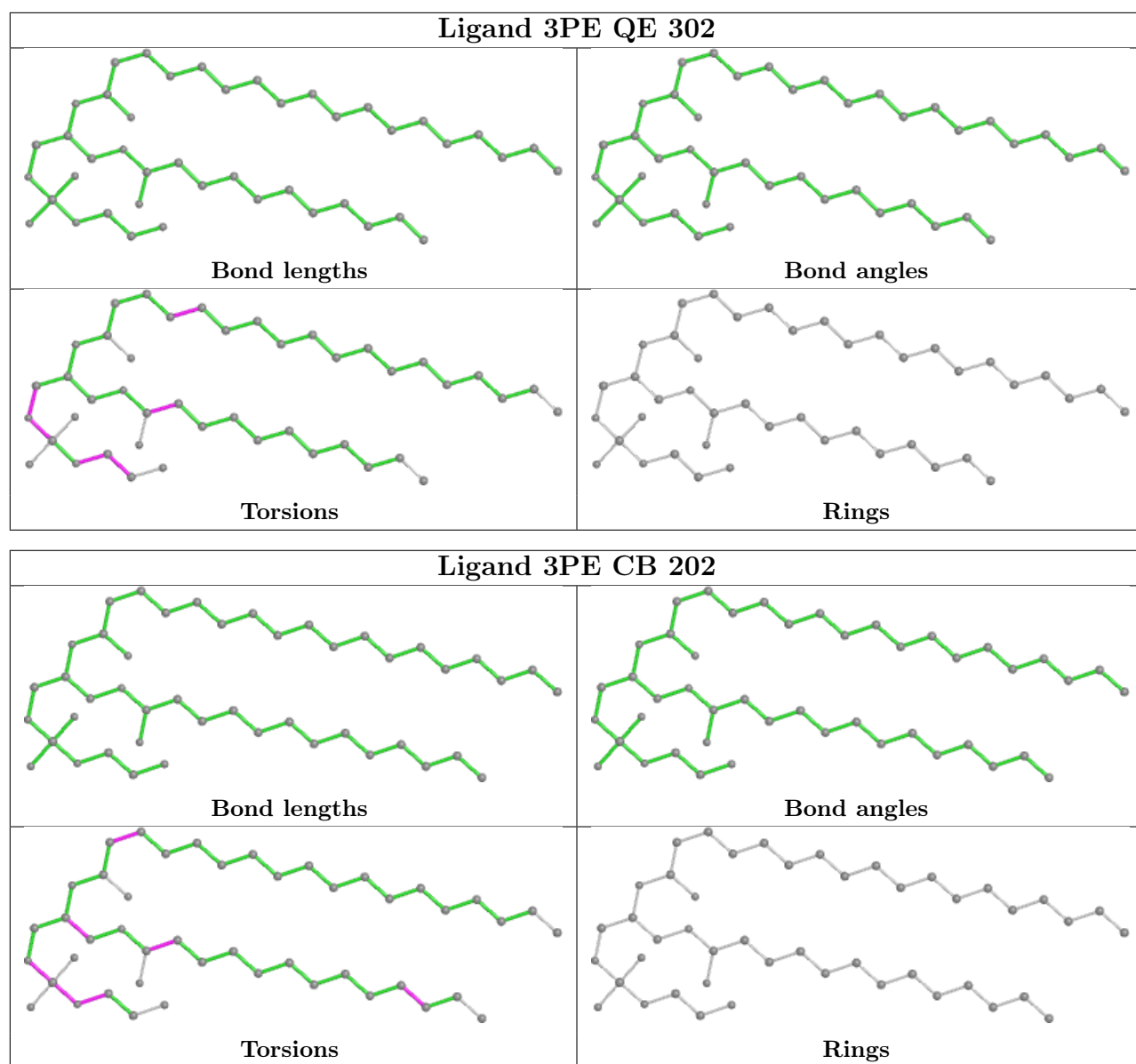




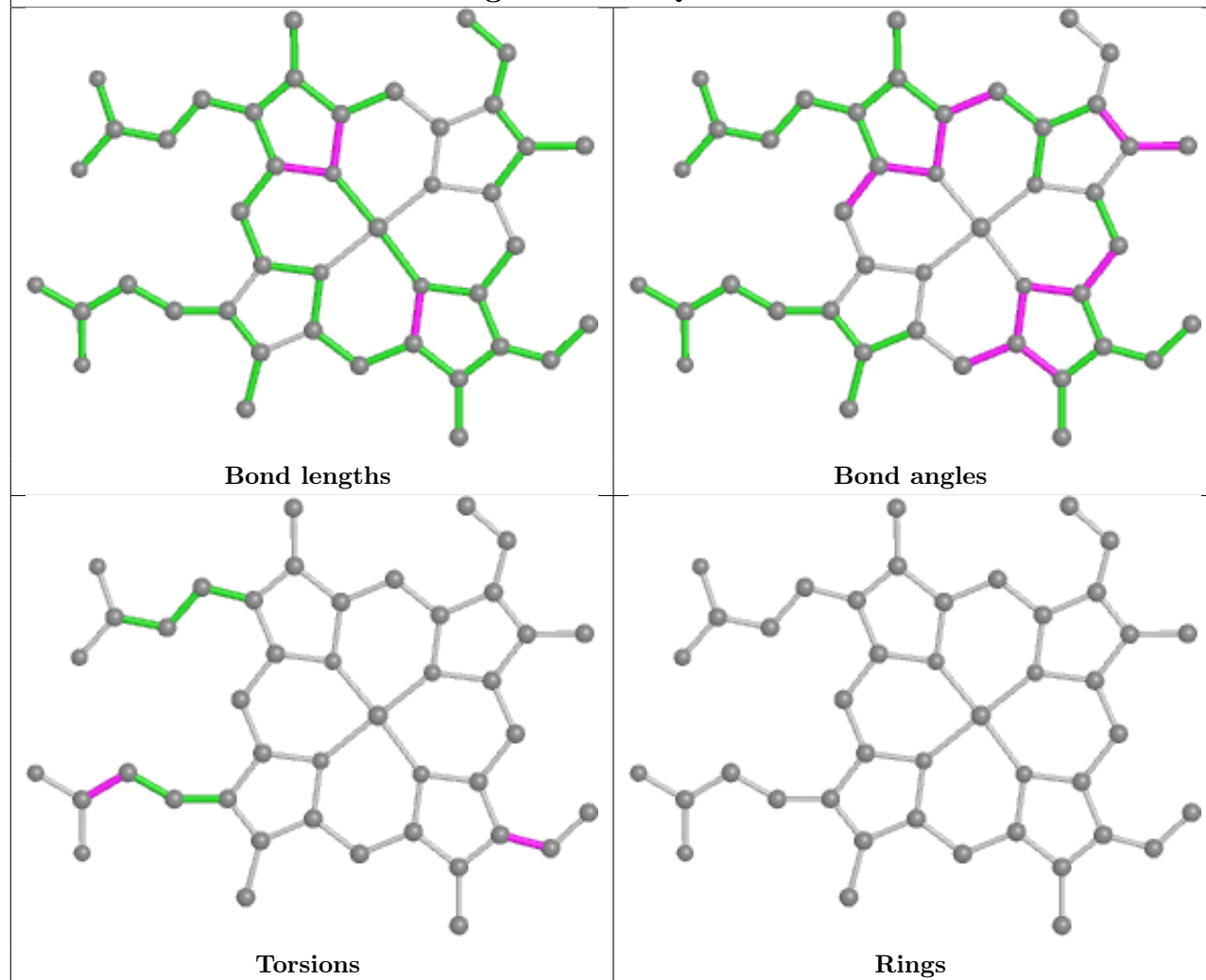




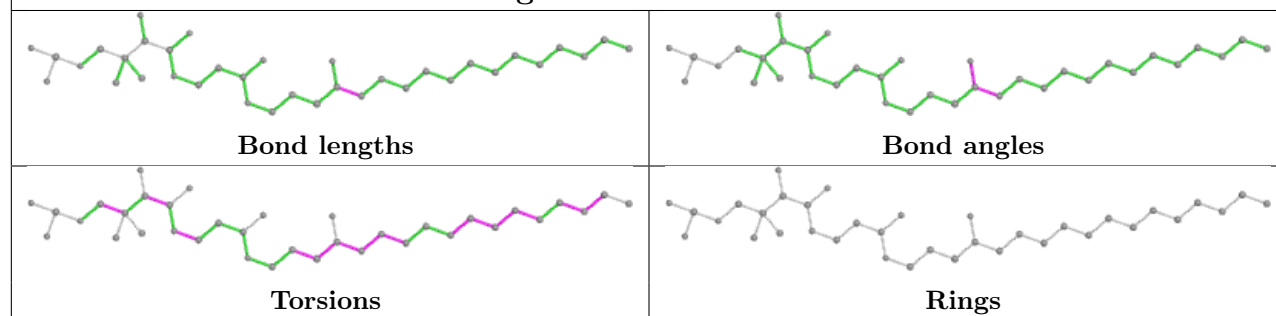


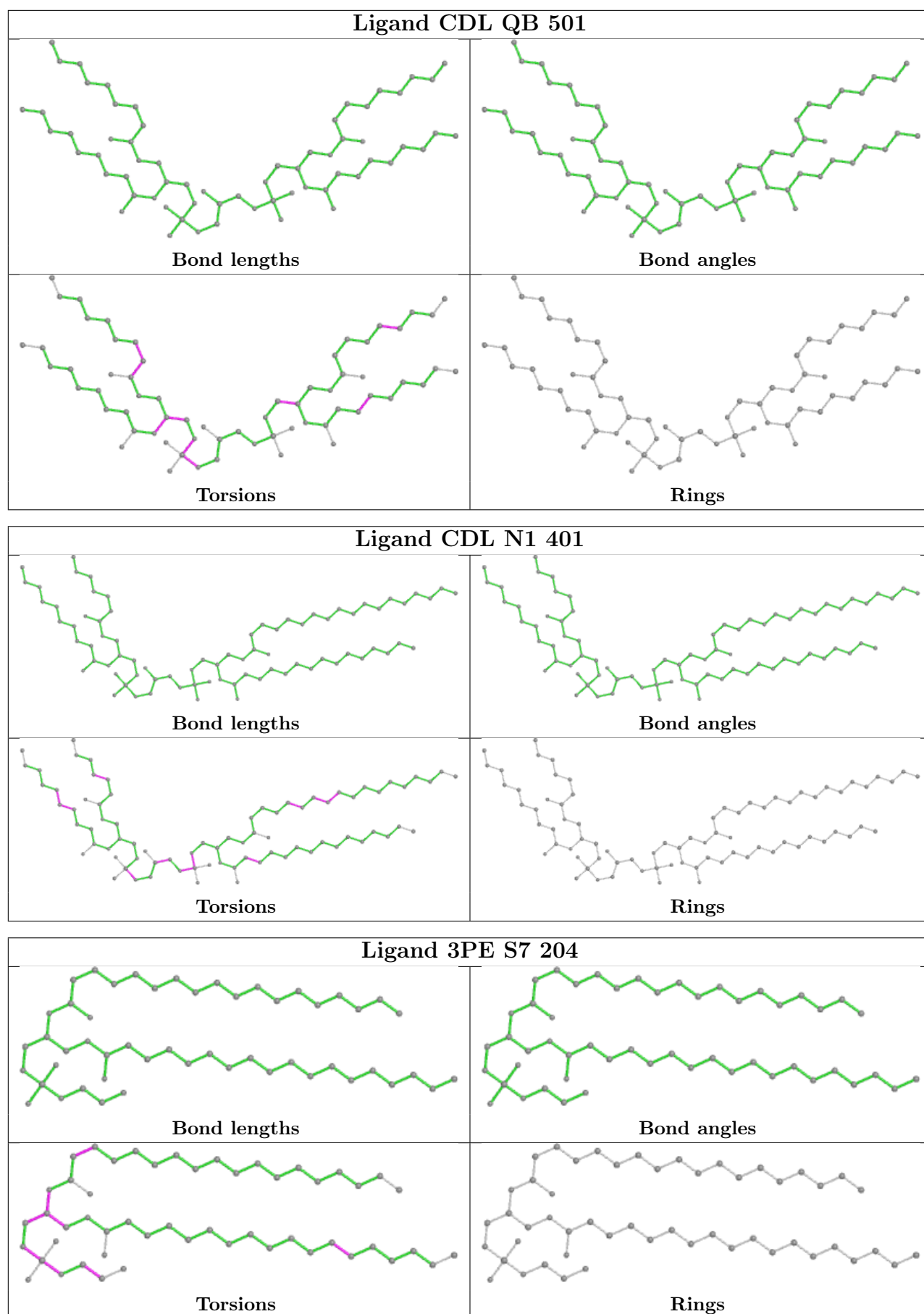


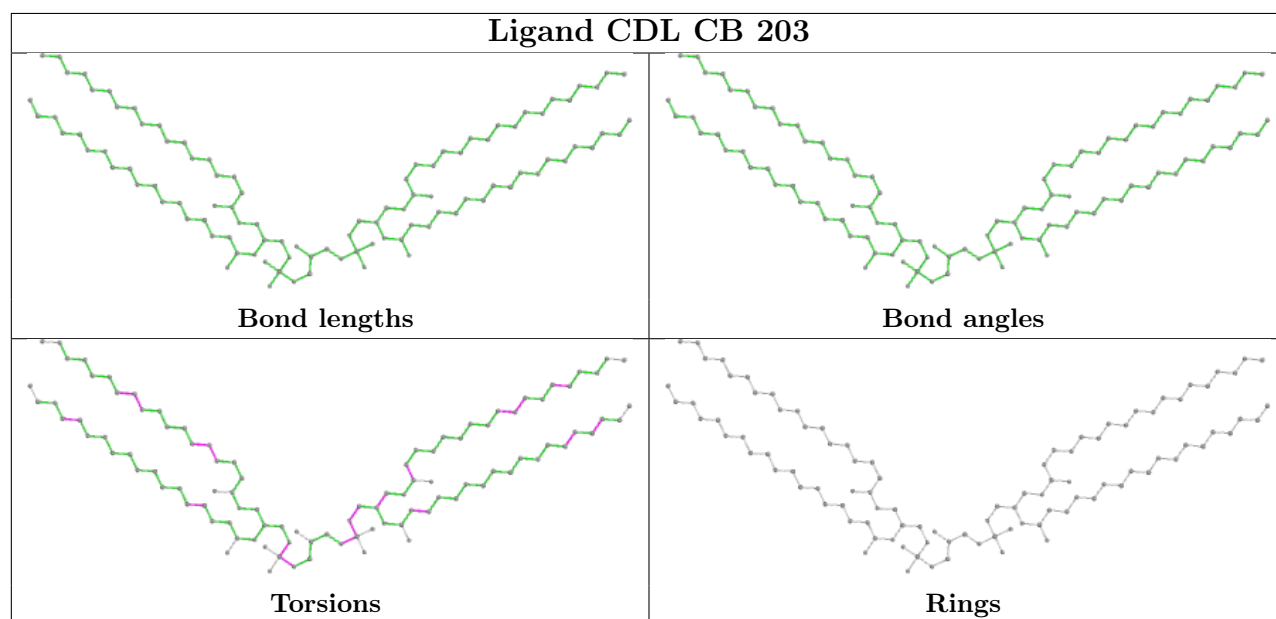
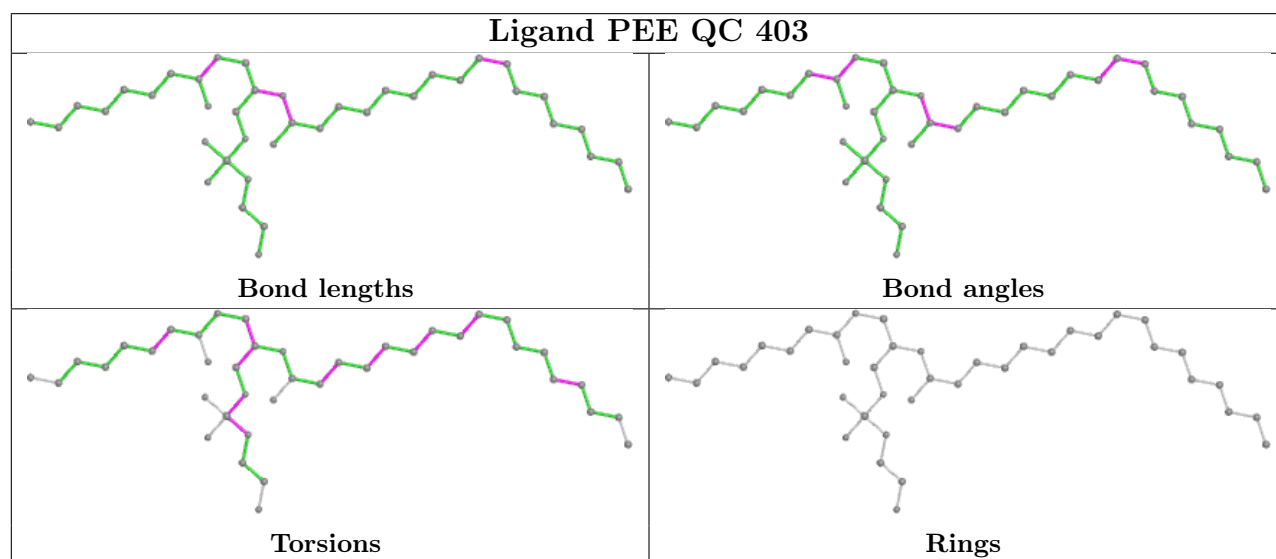
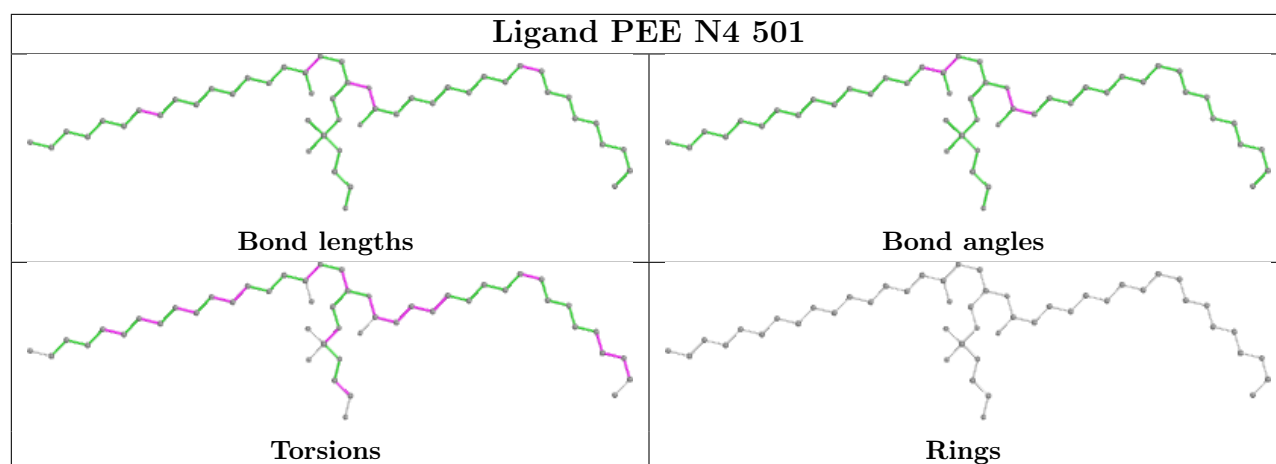
Ligand HEM QC 402

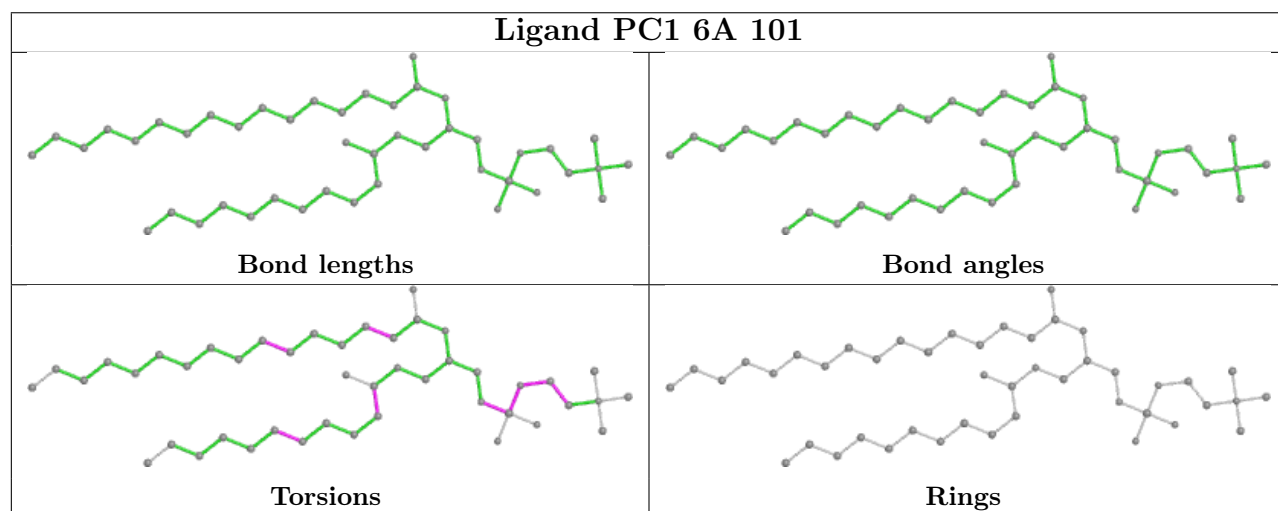
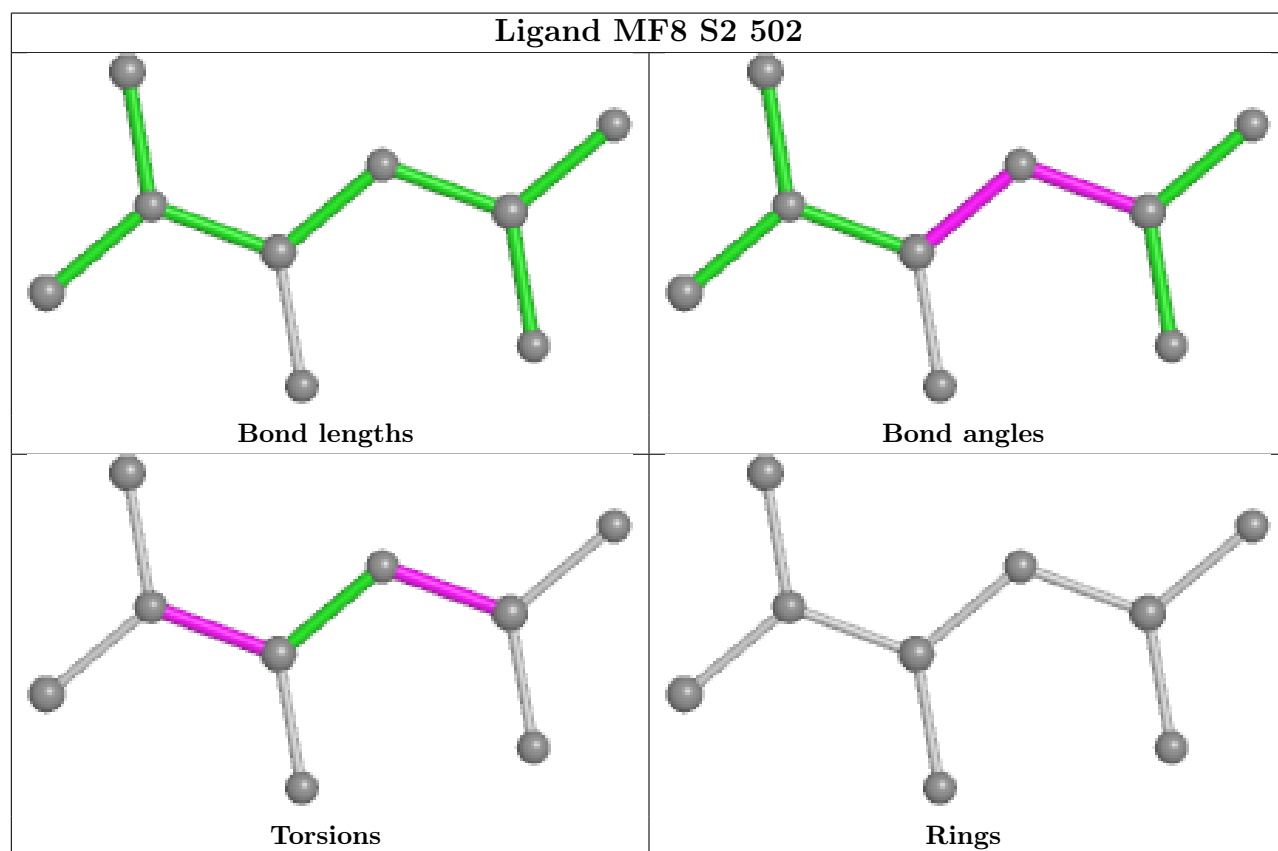
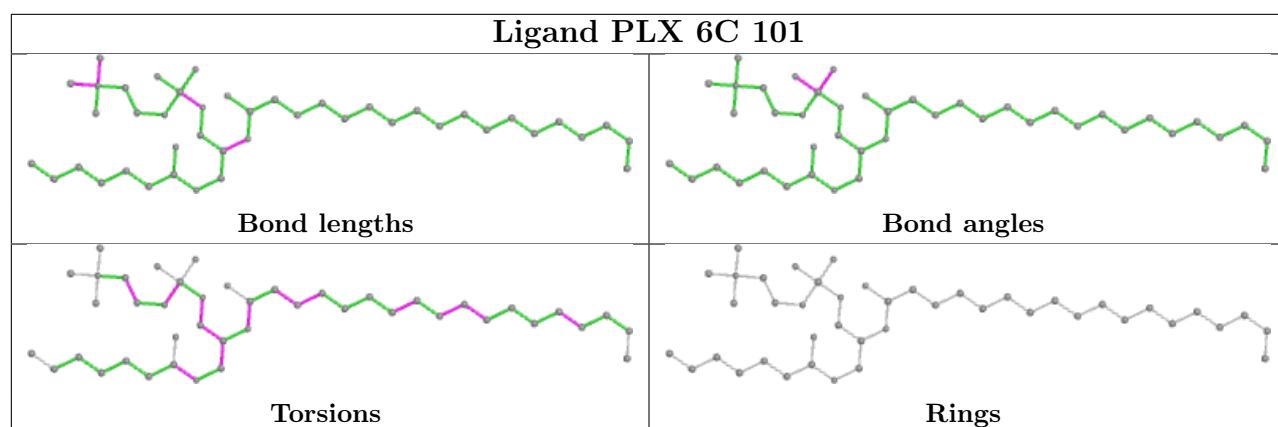


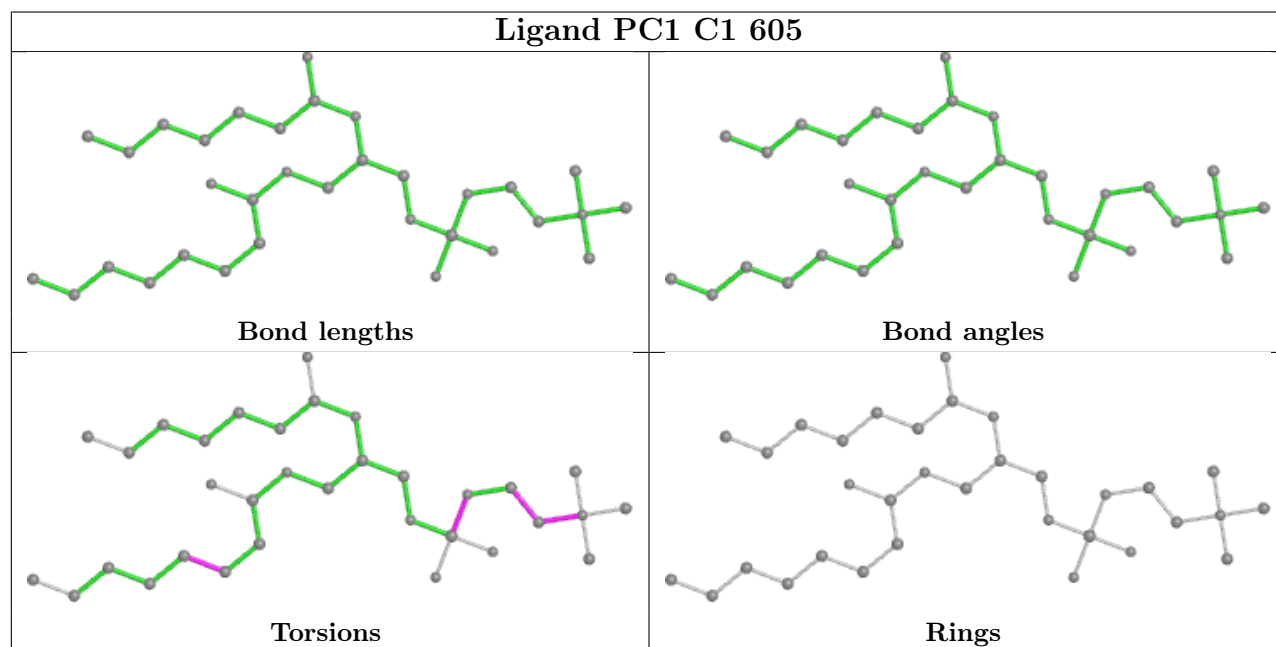
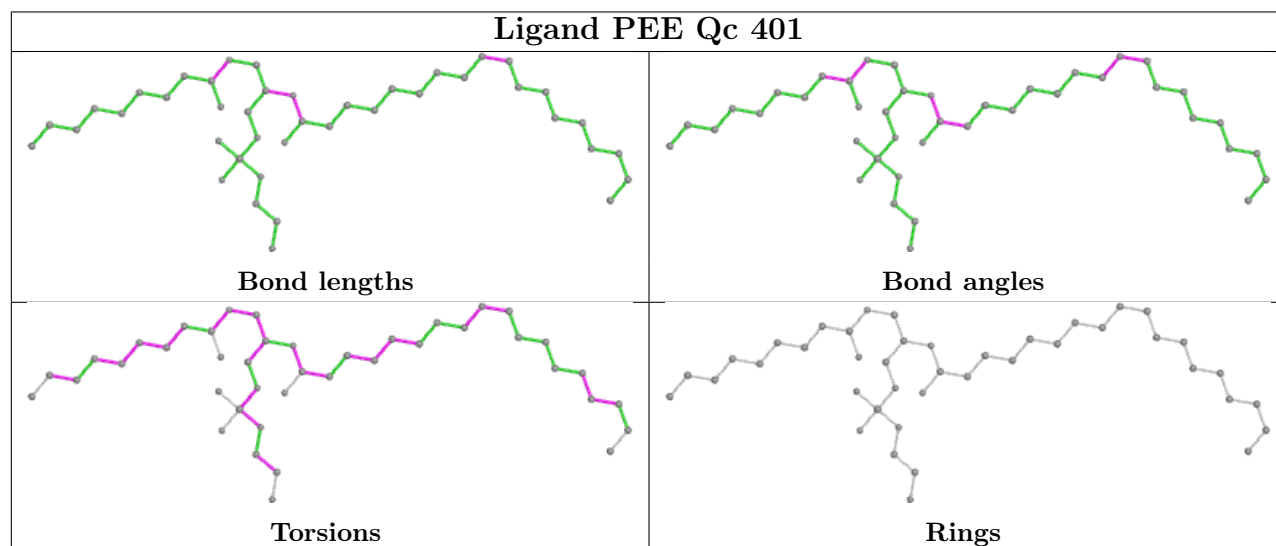
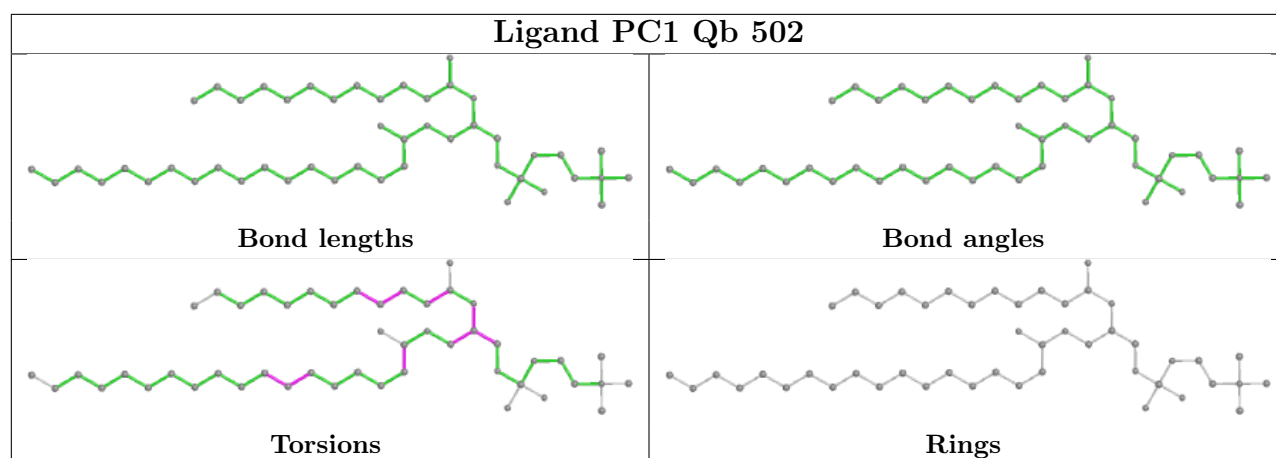
Ligand ZMP AC 201

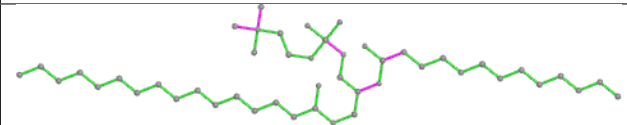
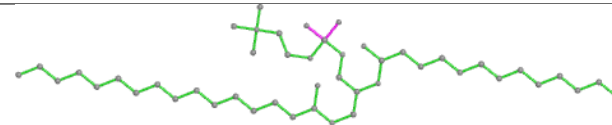
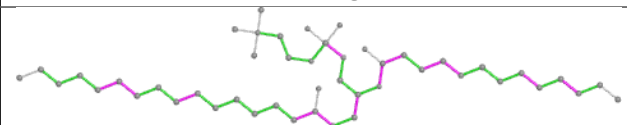
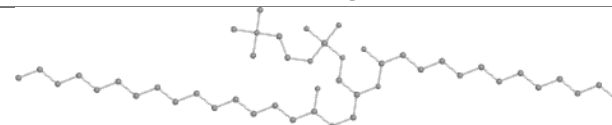


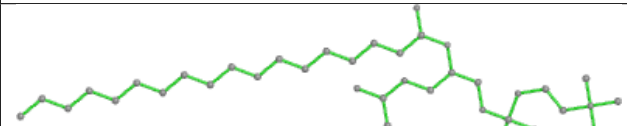
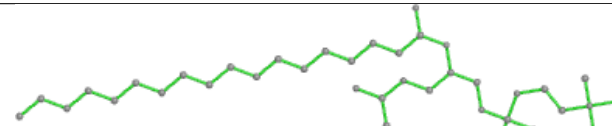
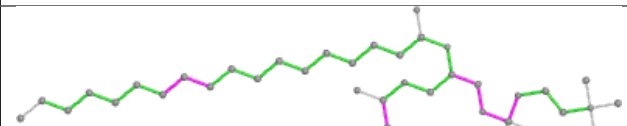
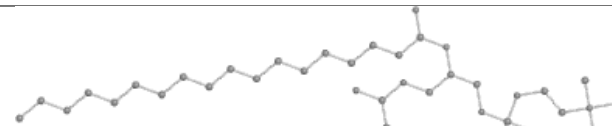


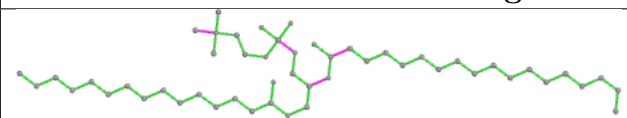
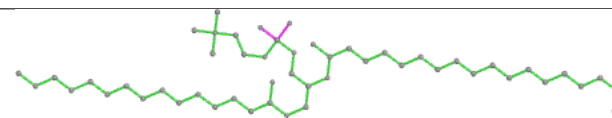
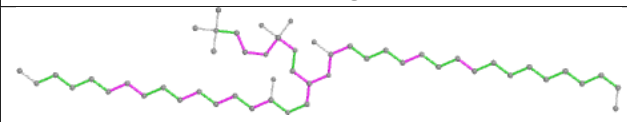
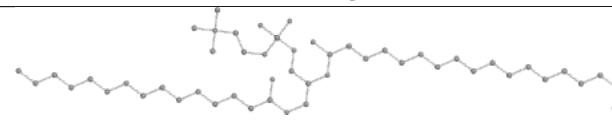


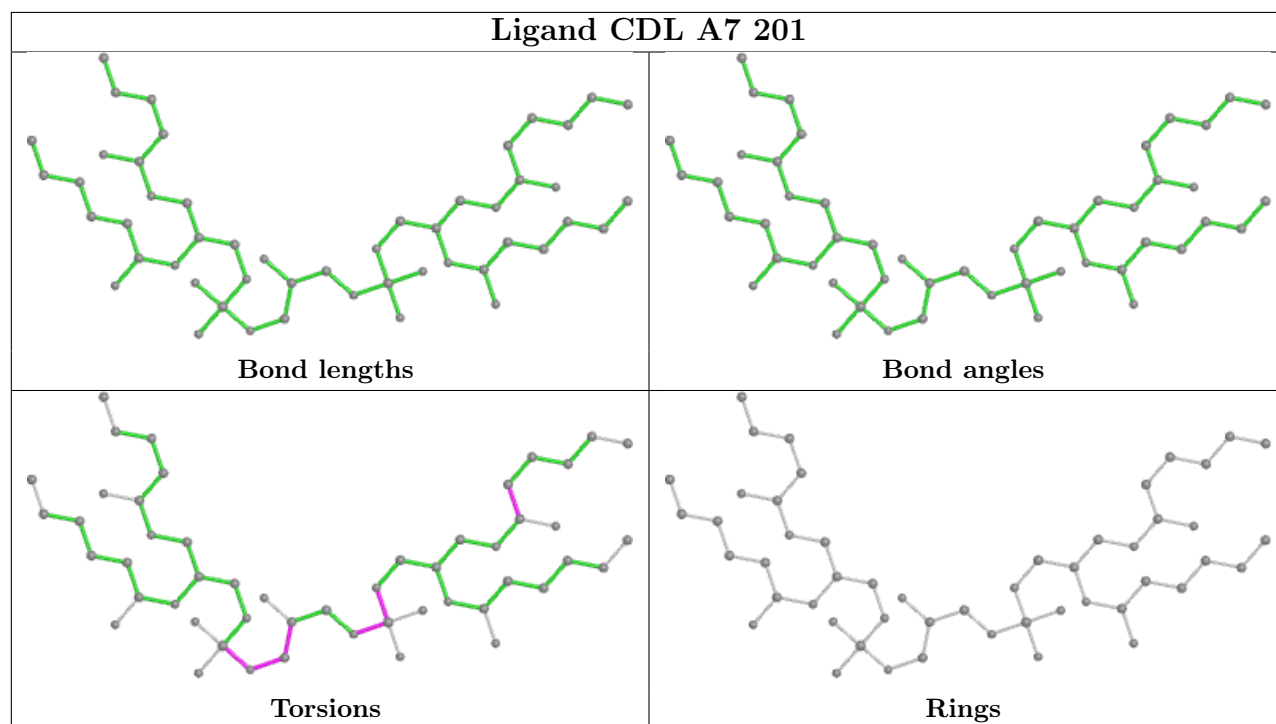
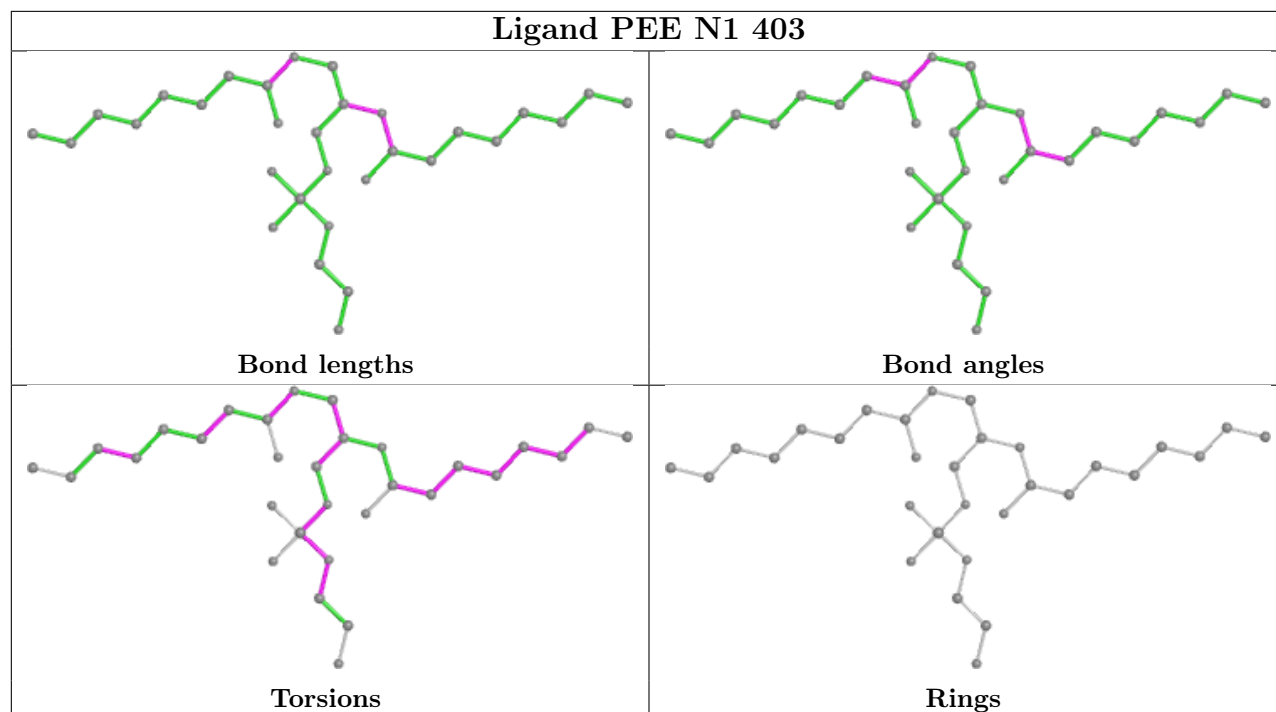


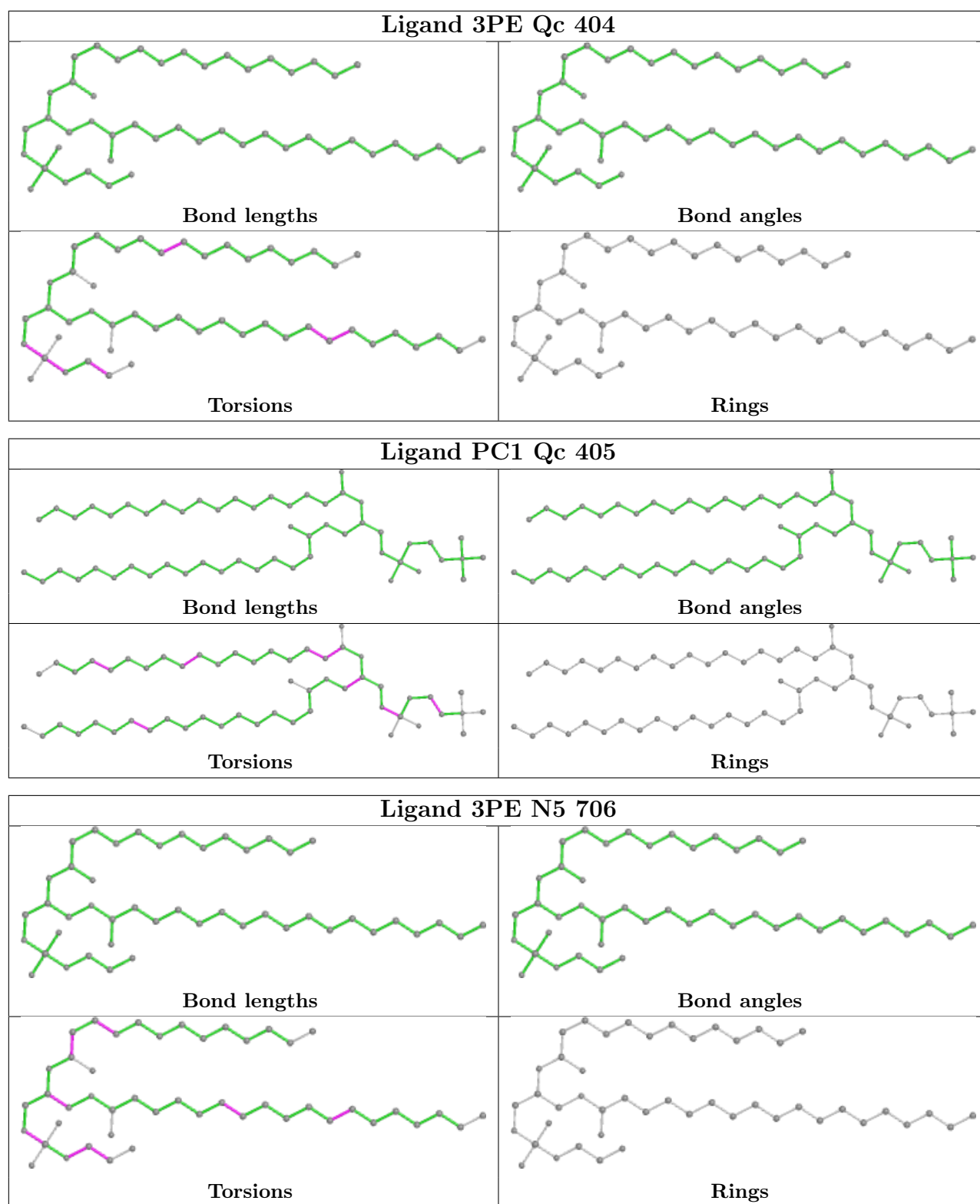


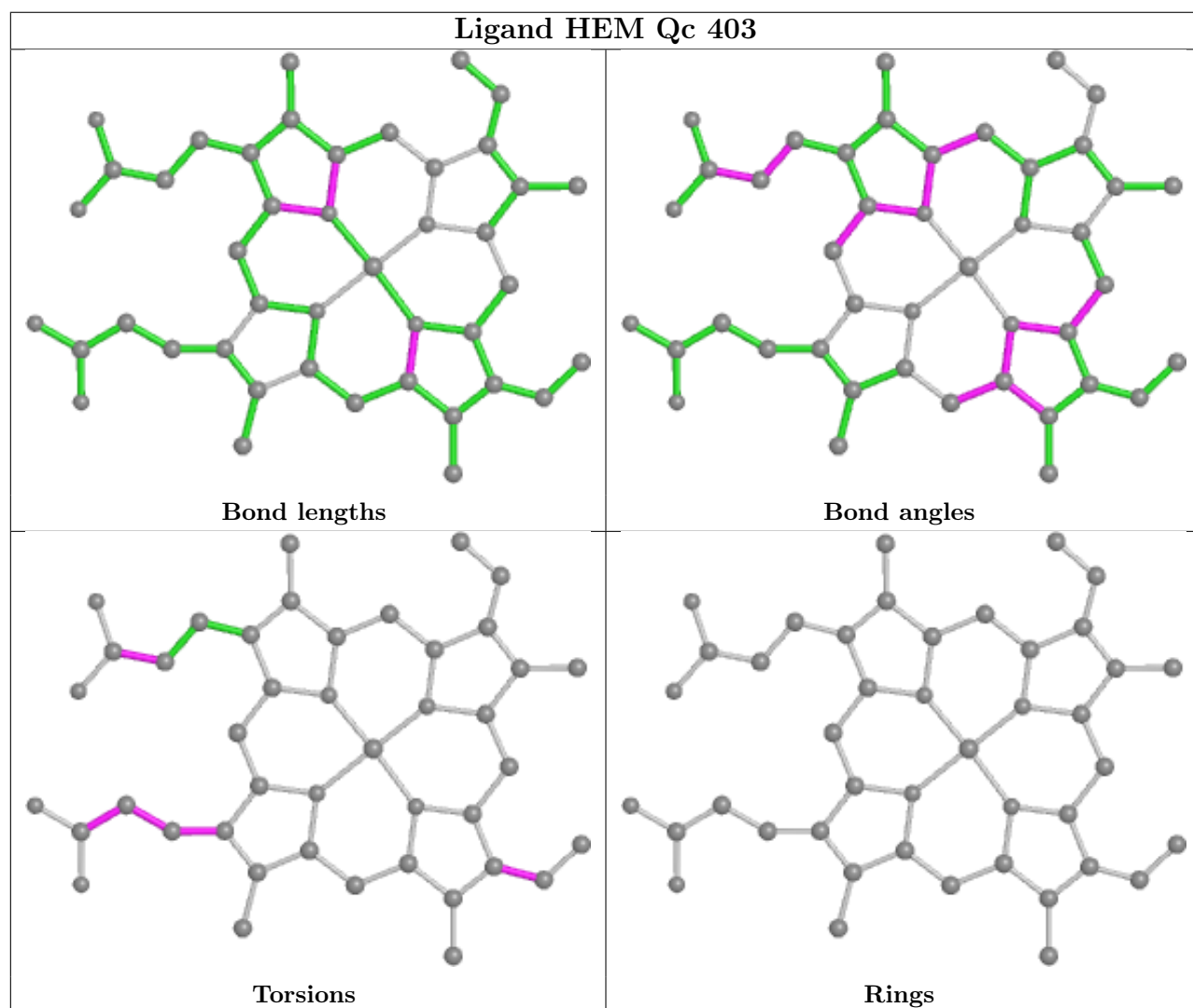
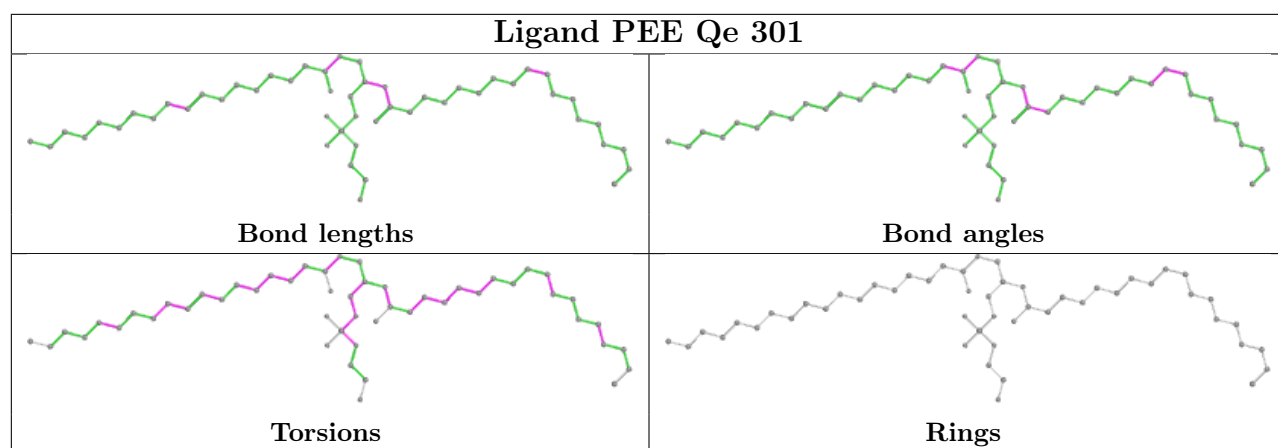
| Ligand PLX AL 202 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

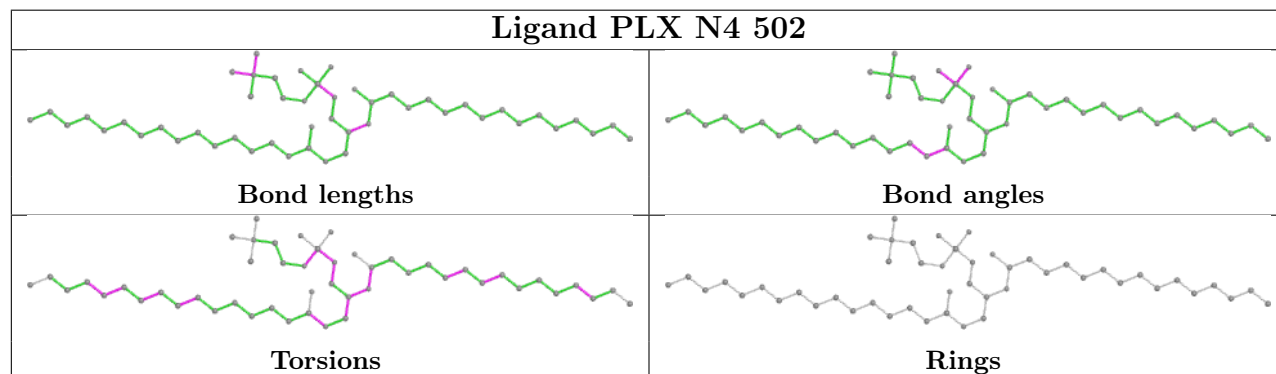
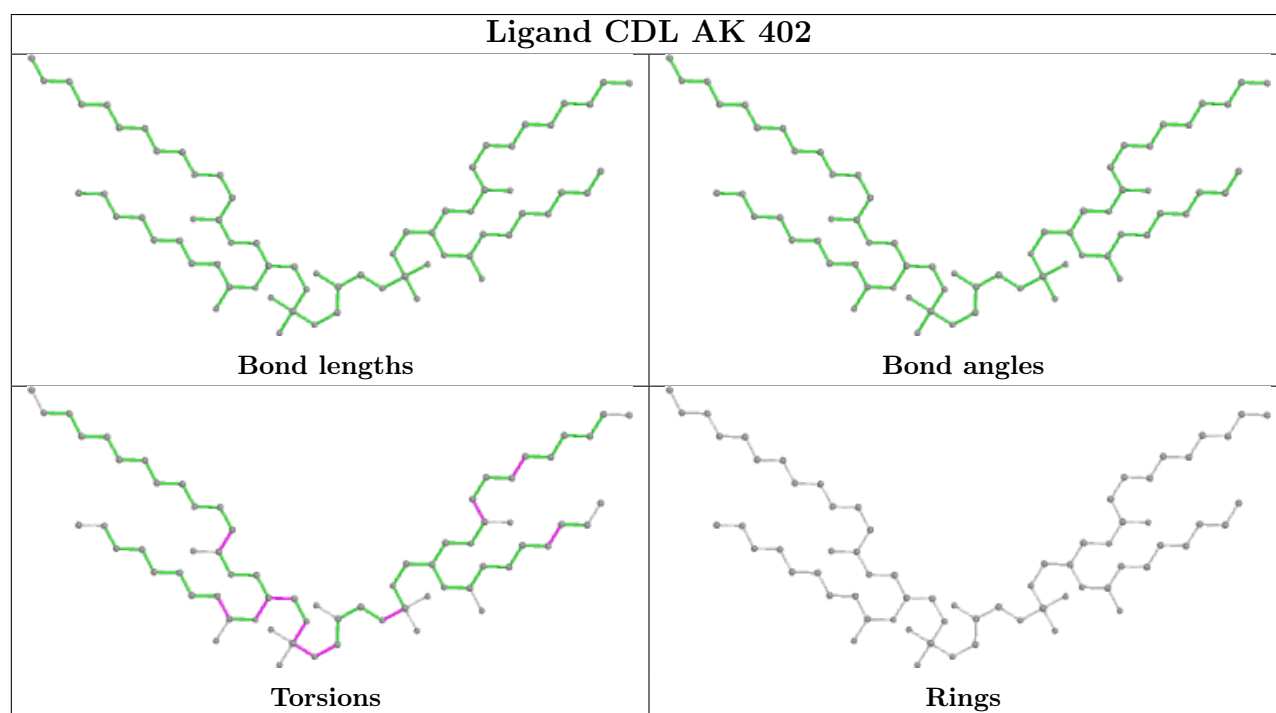
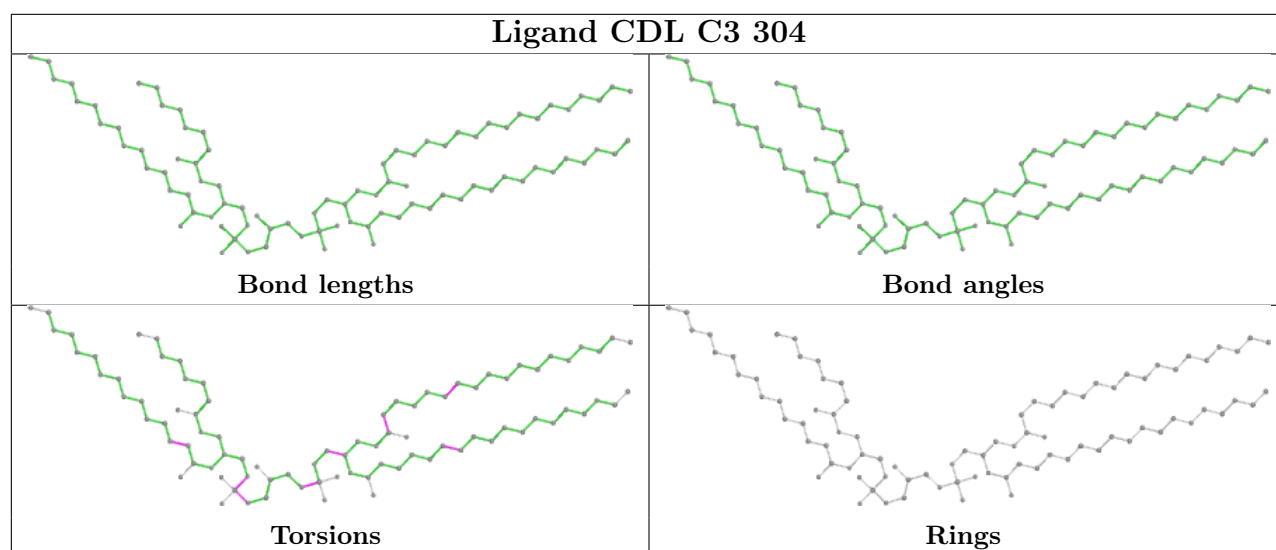
| Ligand PC1 C3 301 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

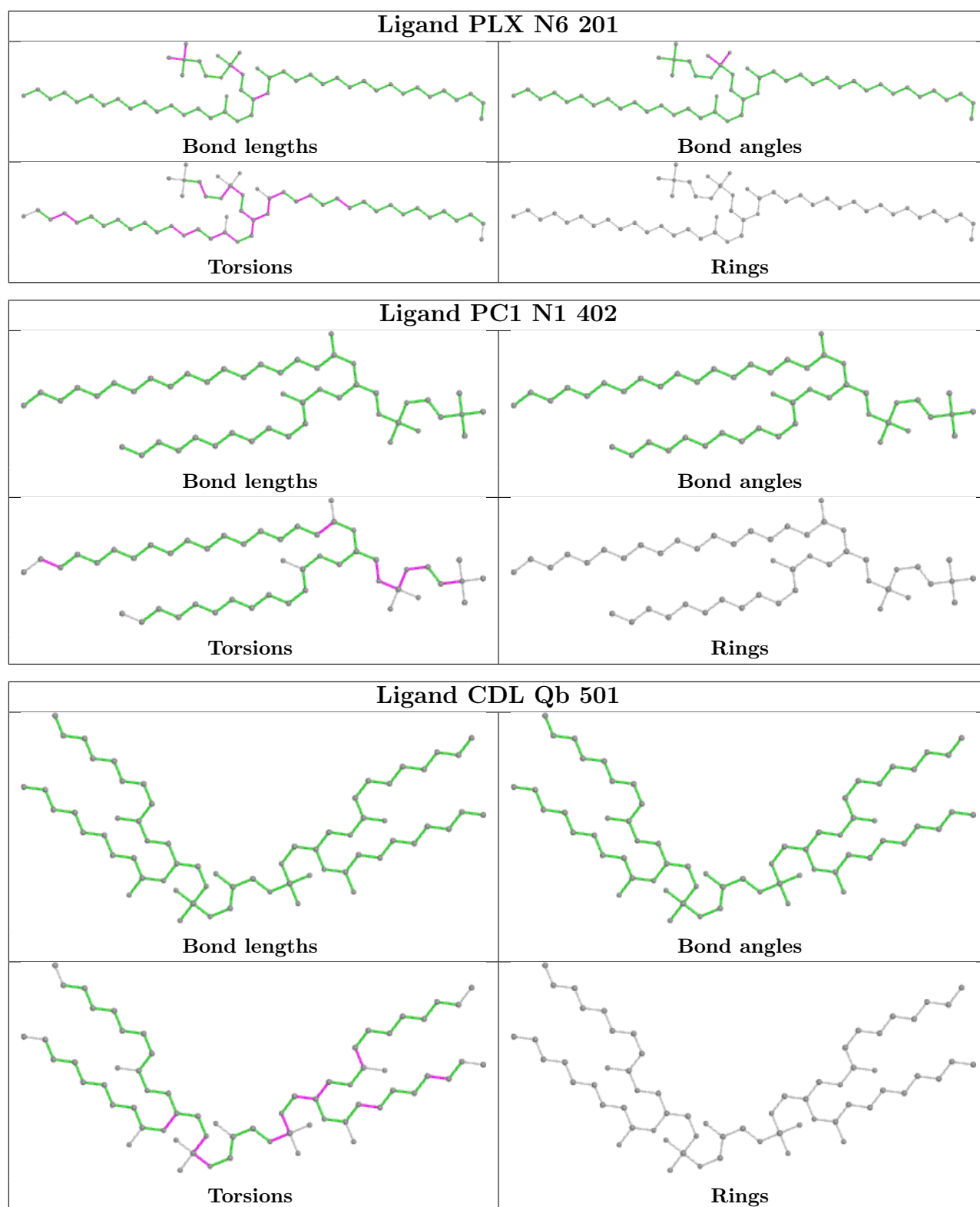
| Ligand PLX AM 201 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

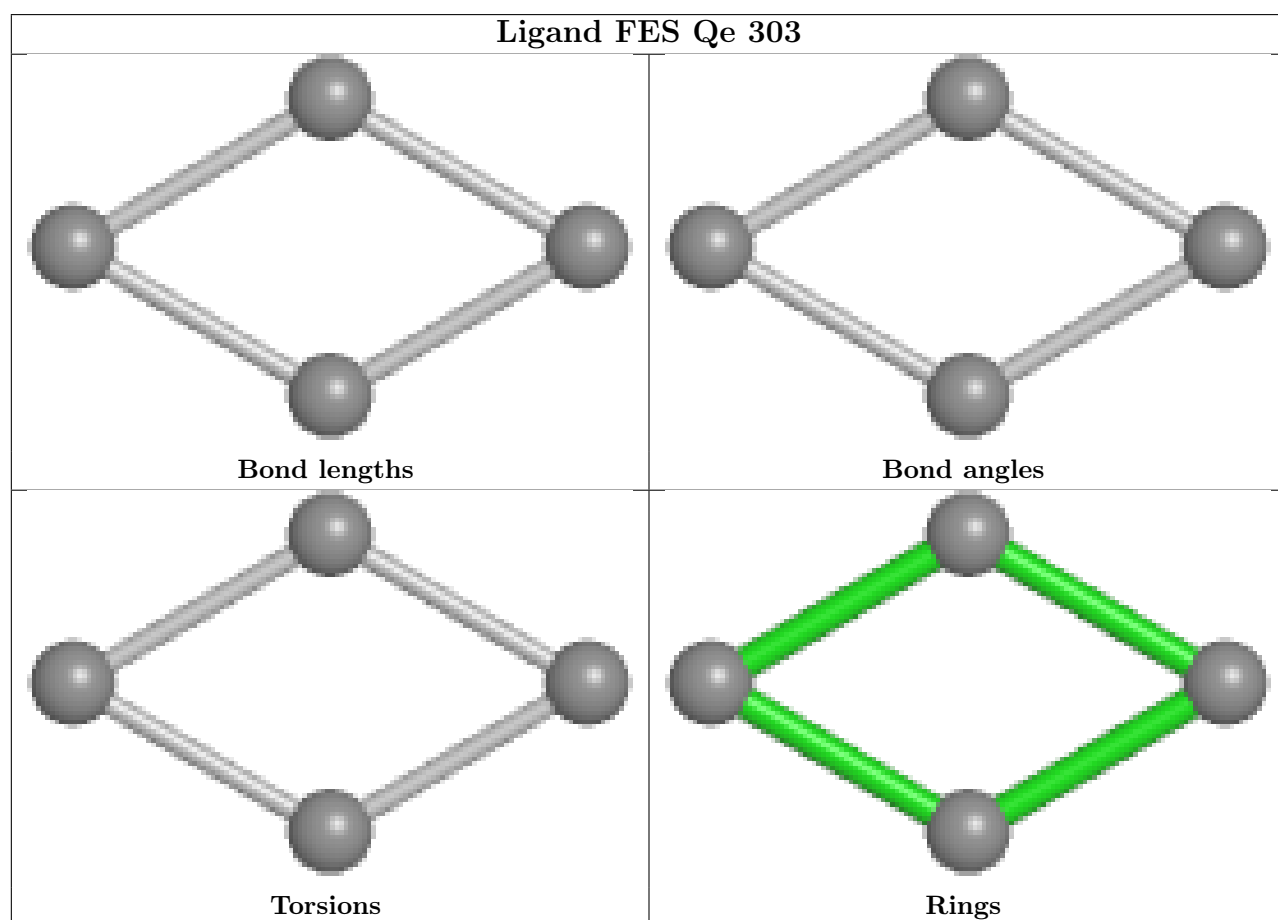
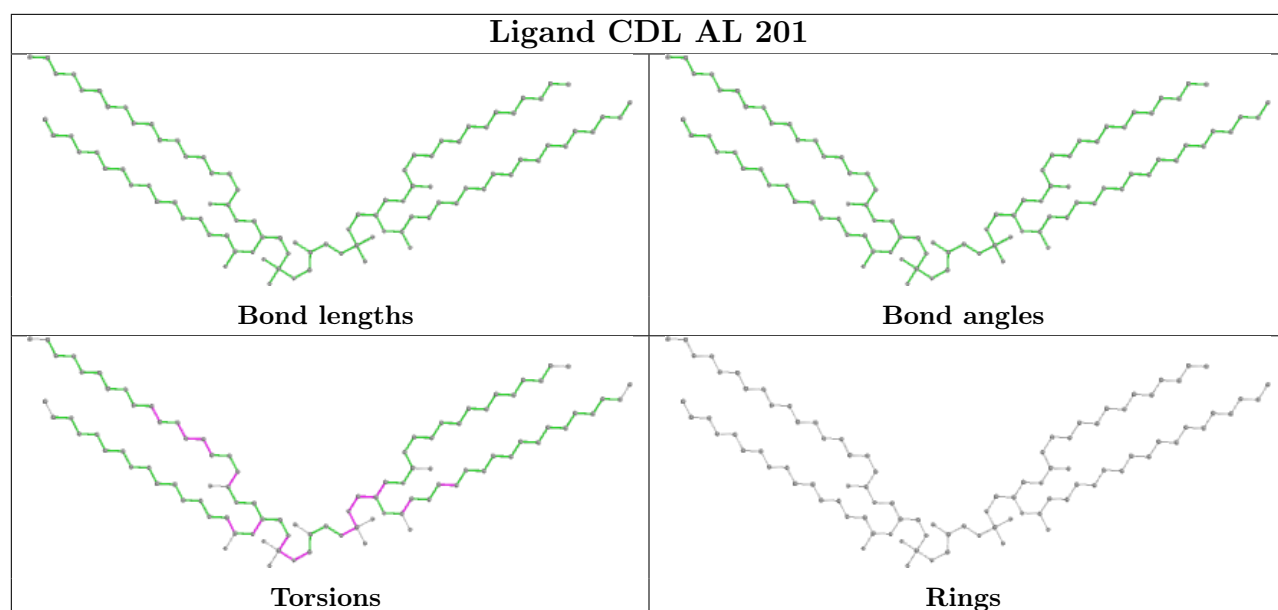


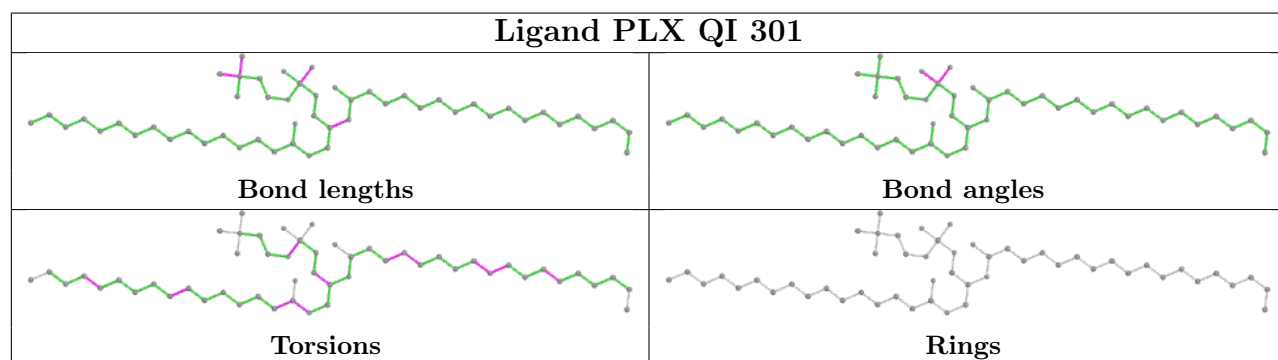
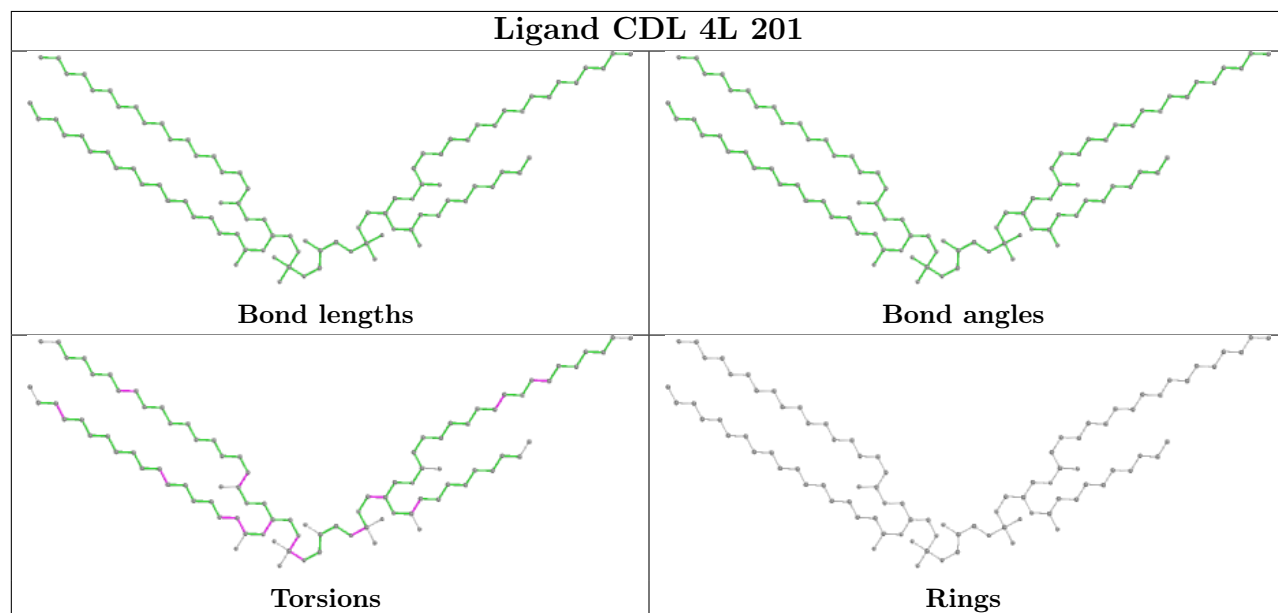
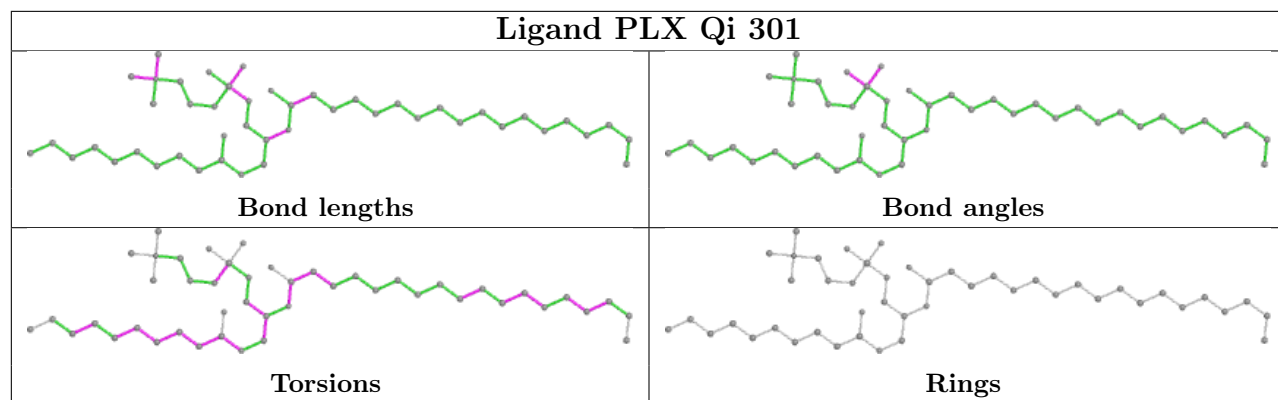


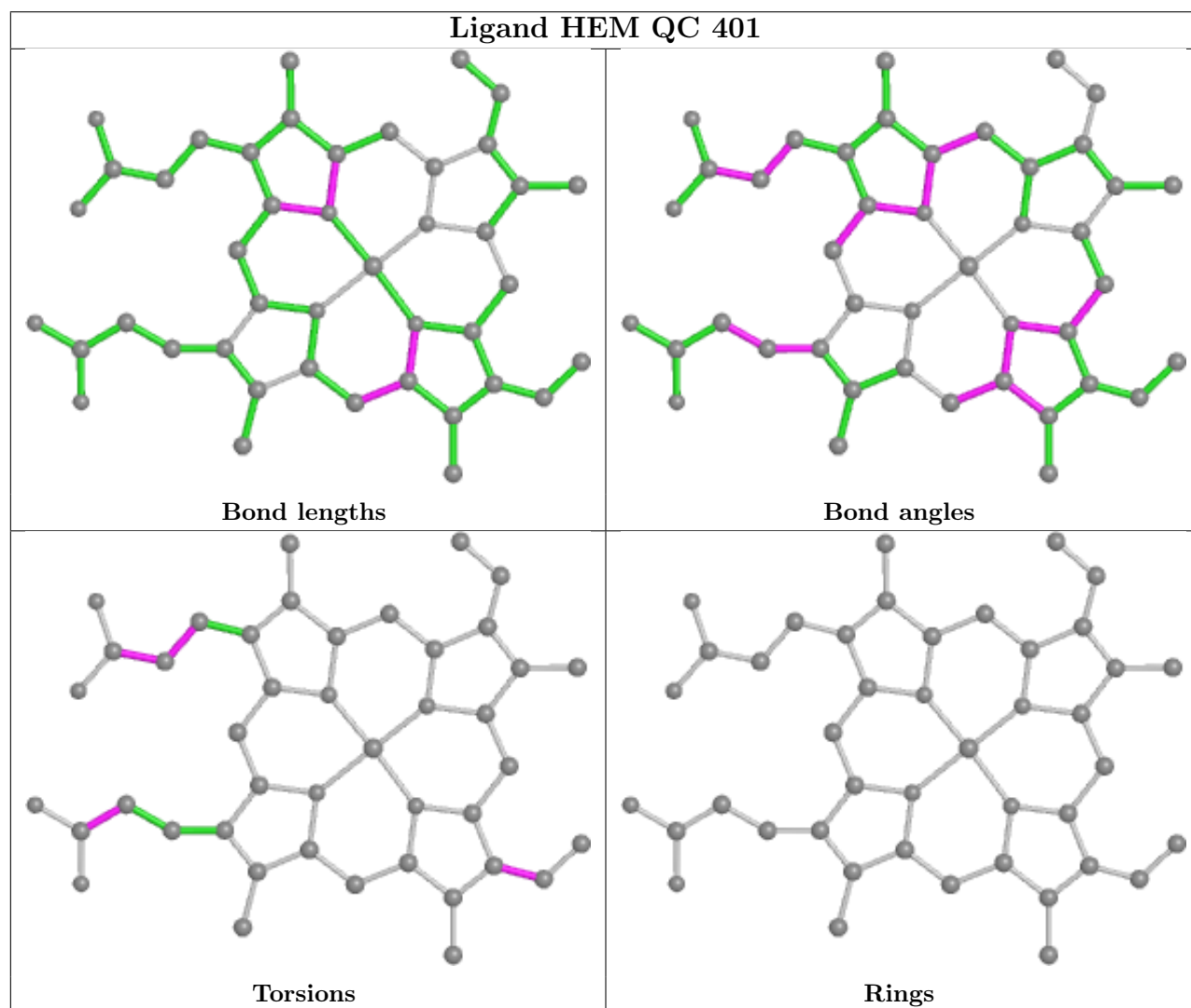
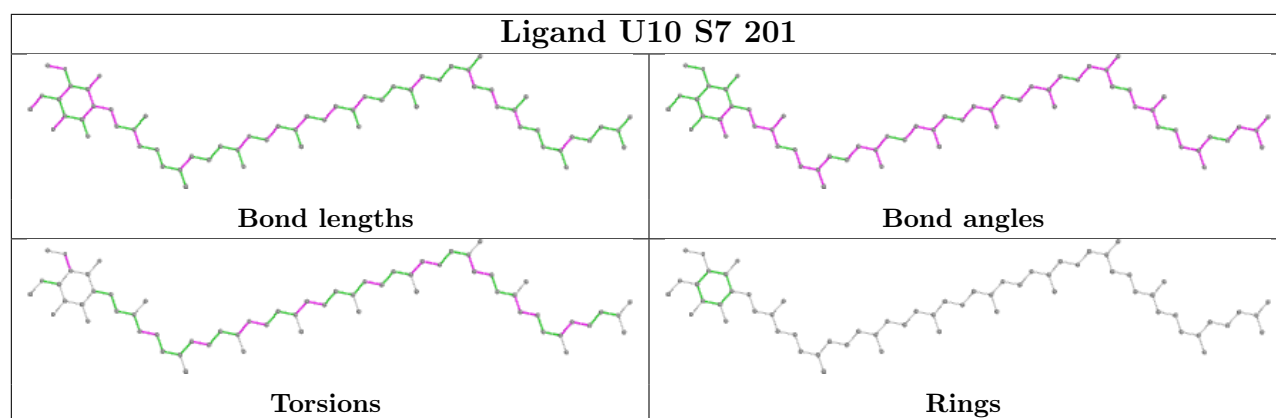


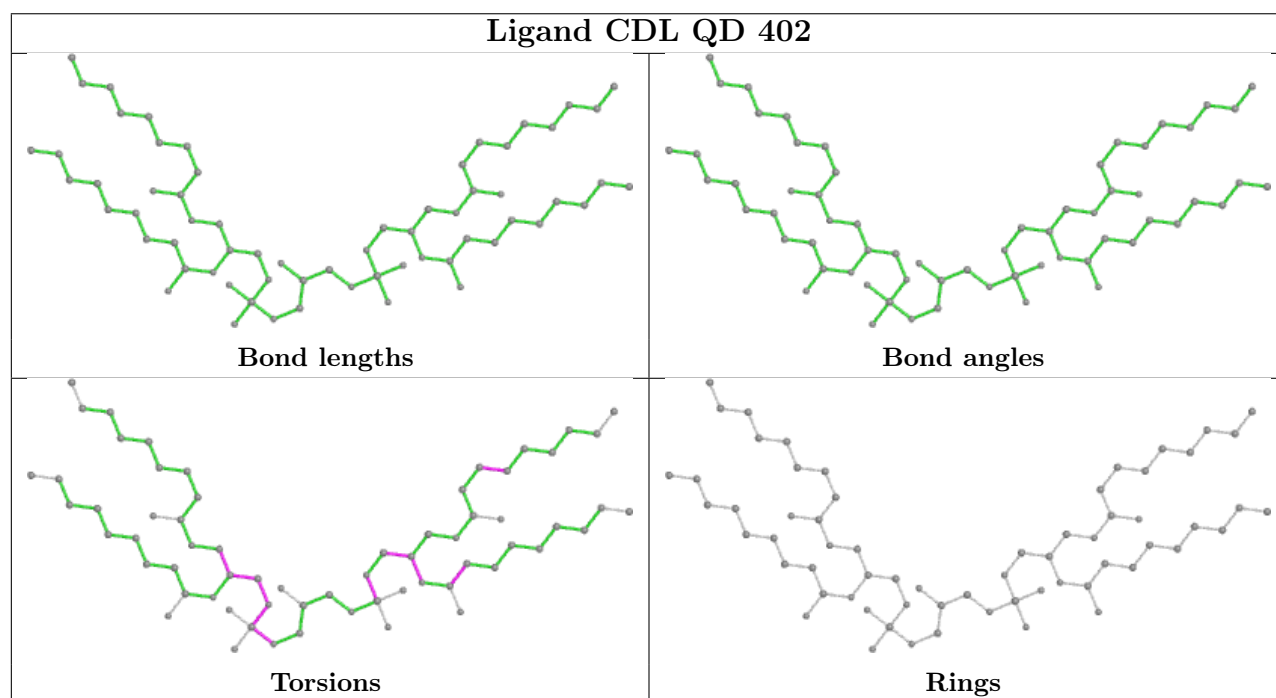
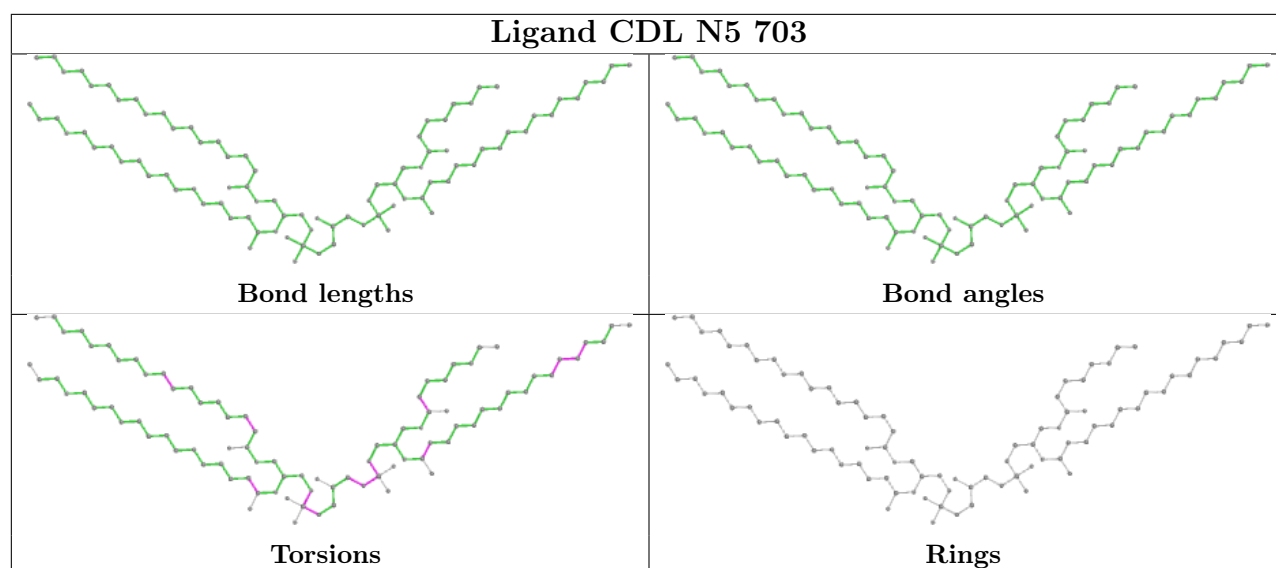


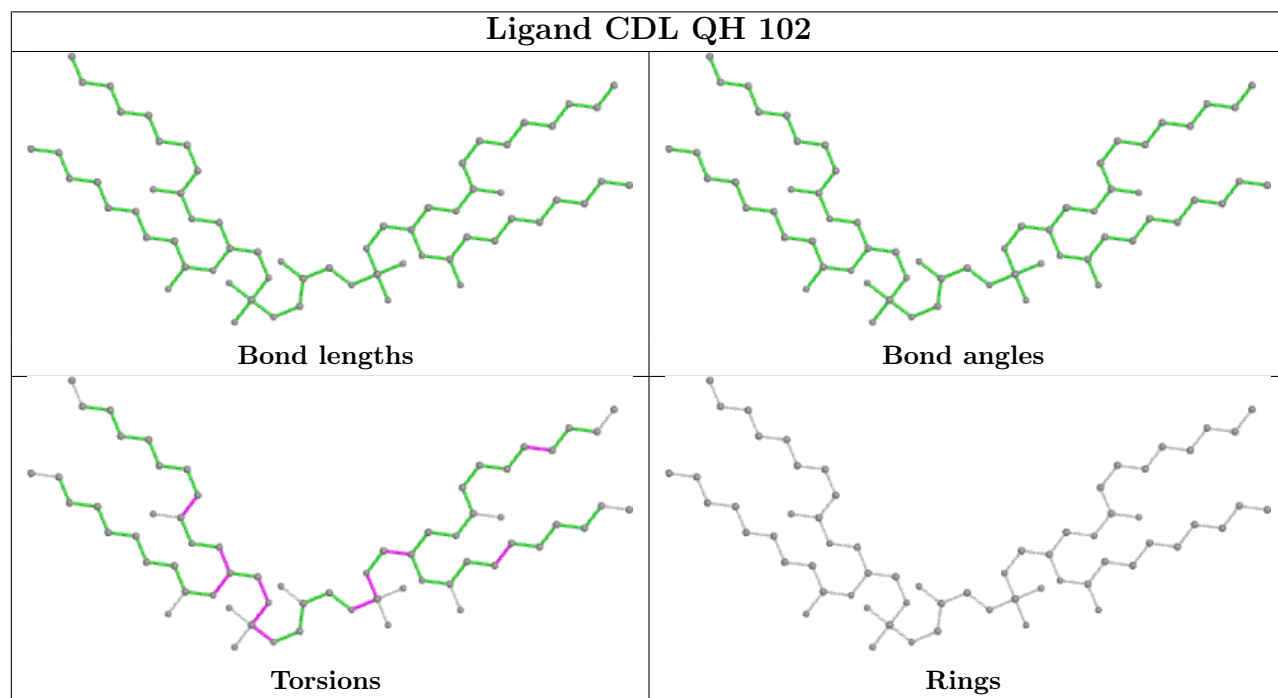
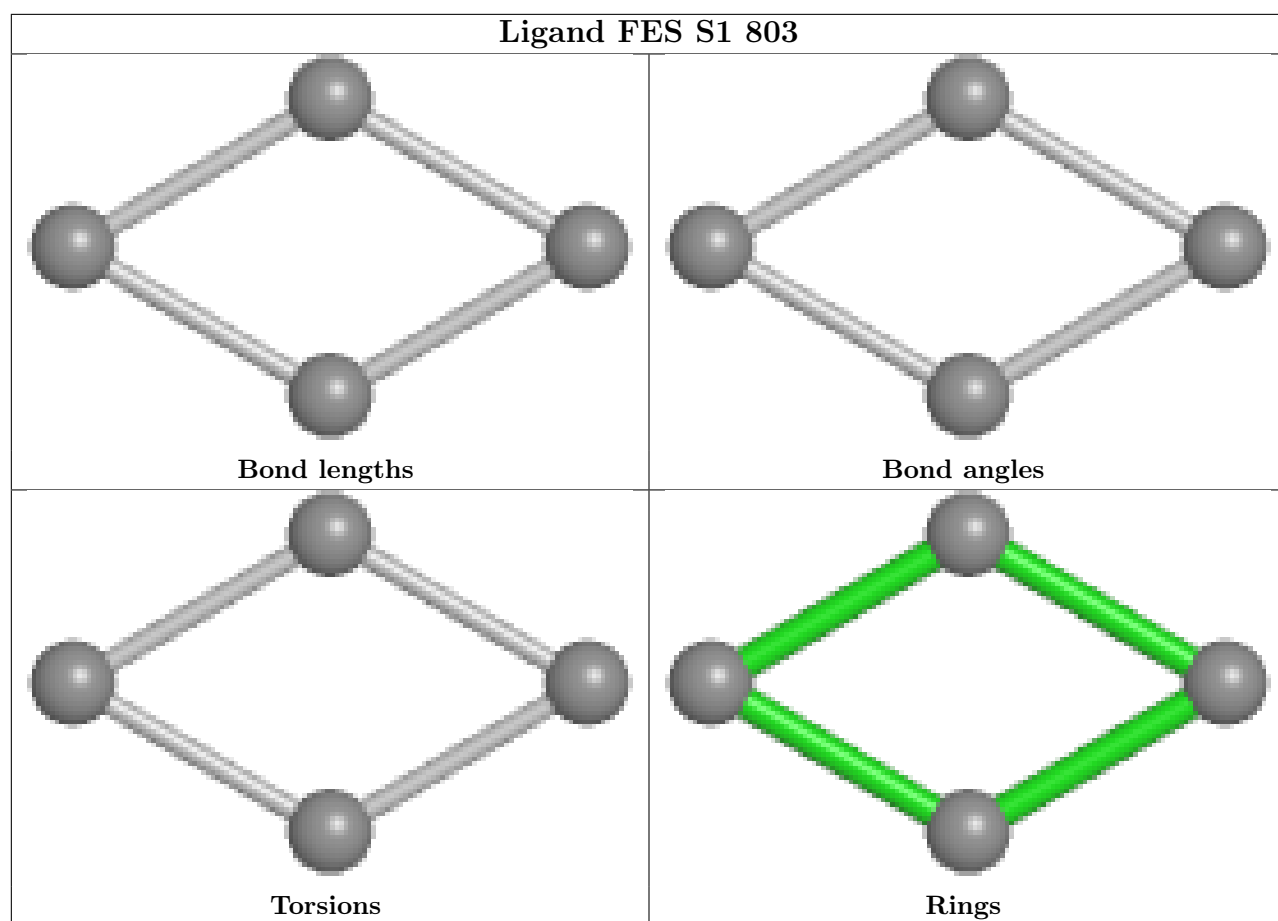


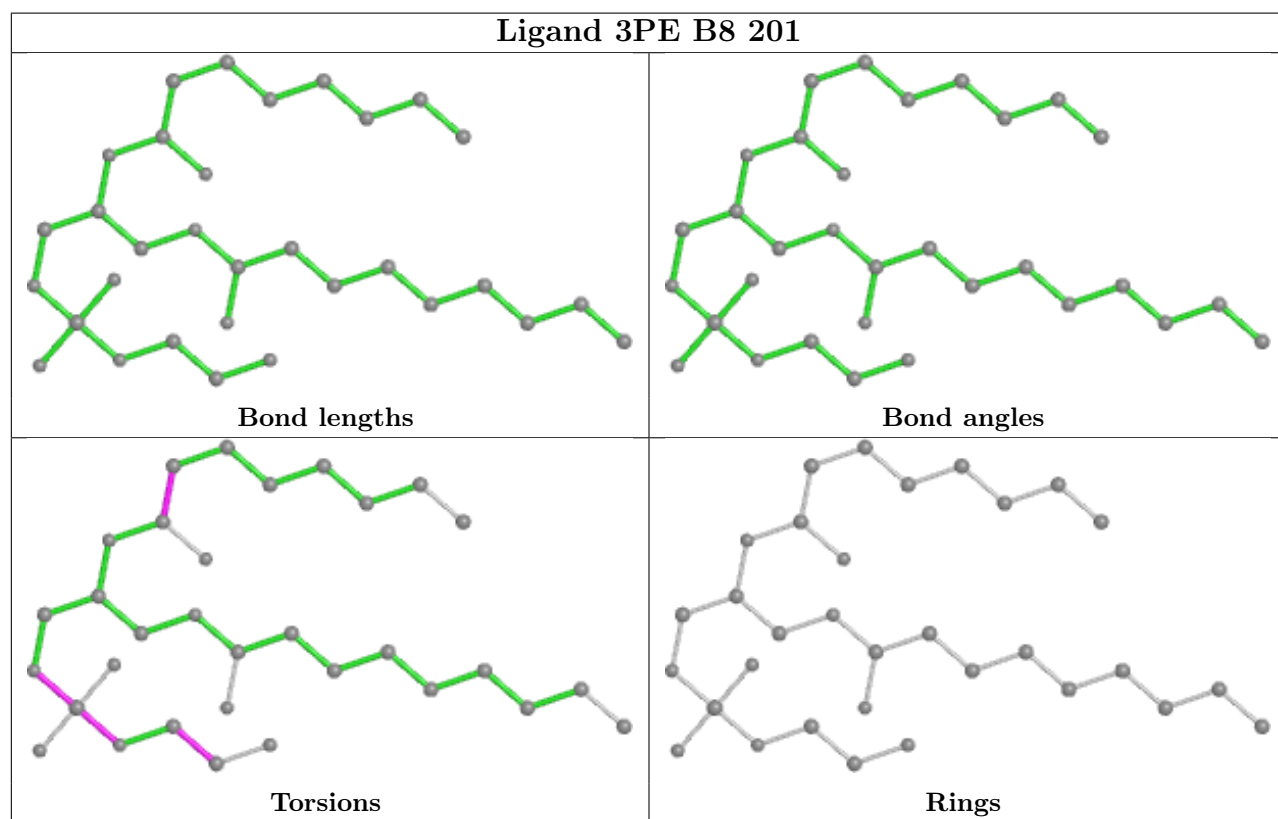
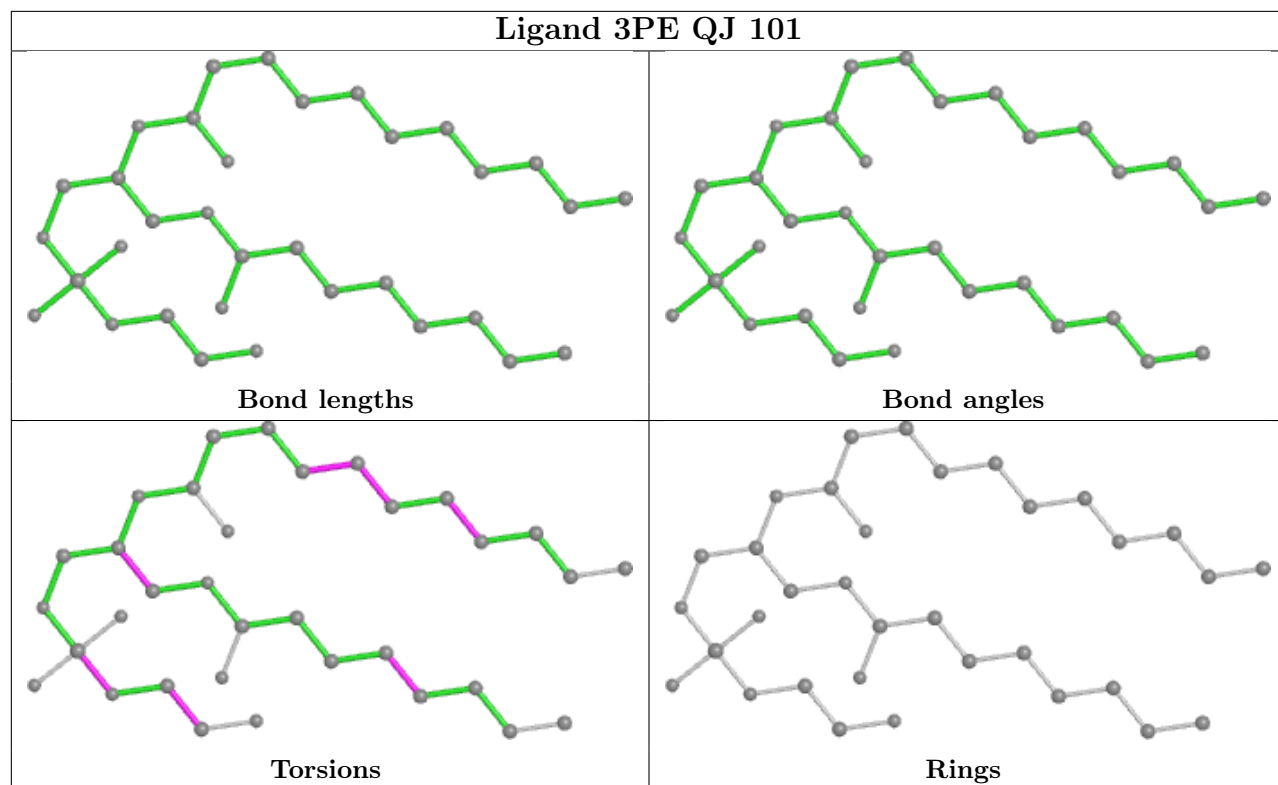


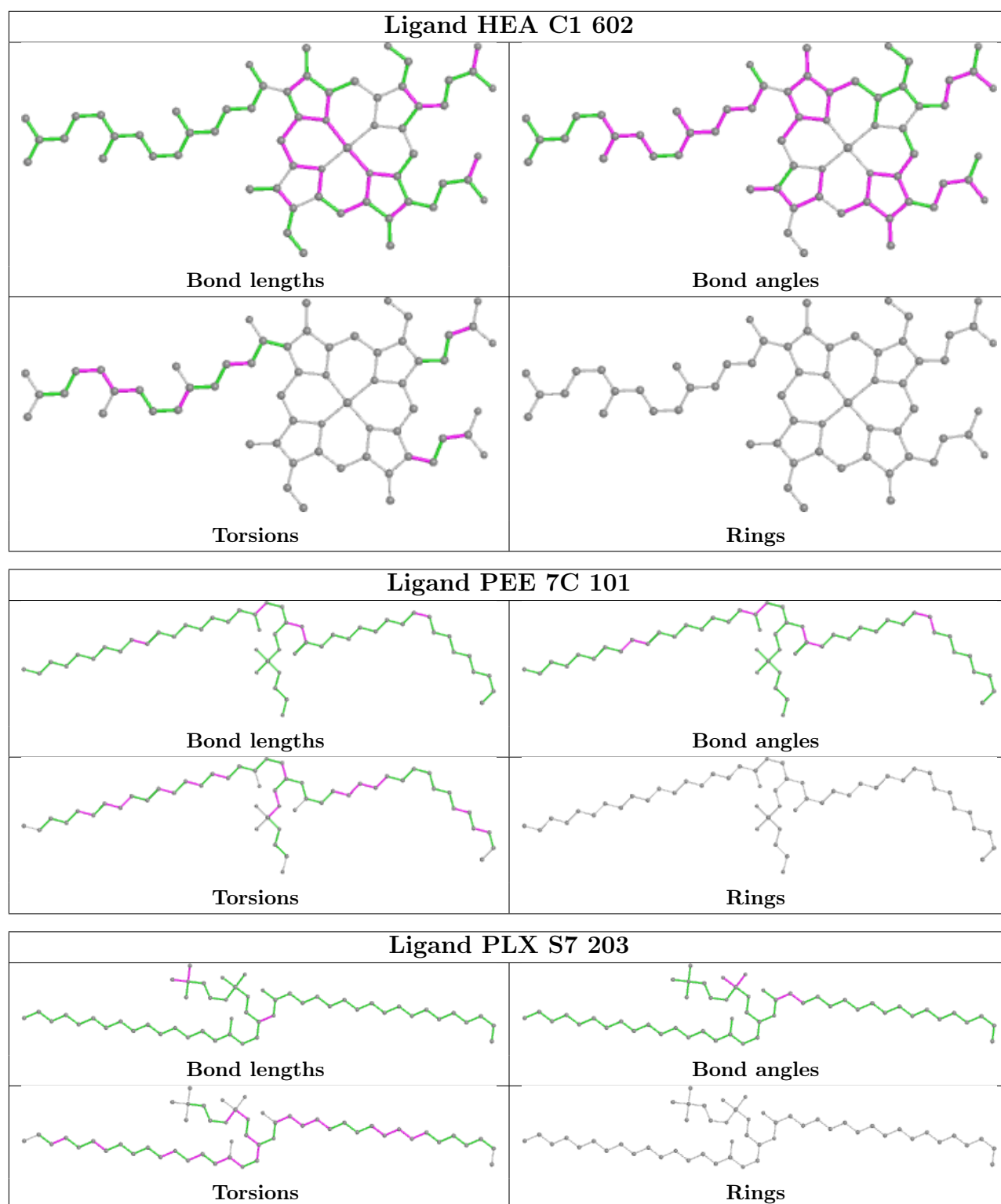












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

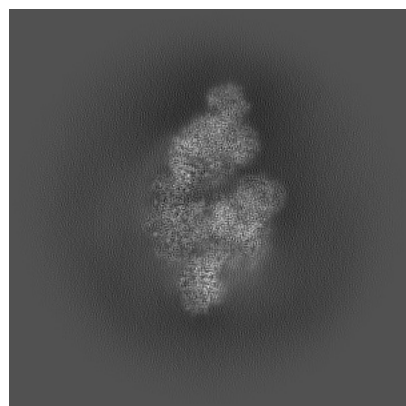
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60424. These allow visual inspection of the internal detail of the map and identification of artifacts.

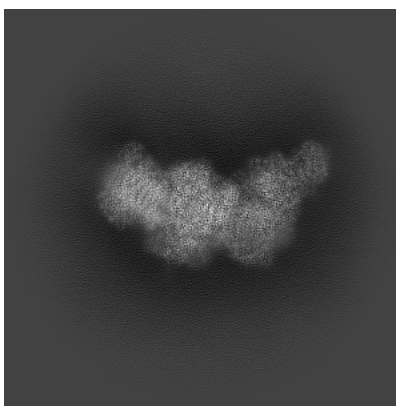
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

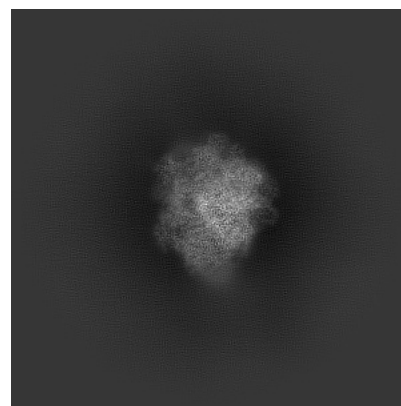
6.1.1 Primary map



X

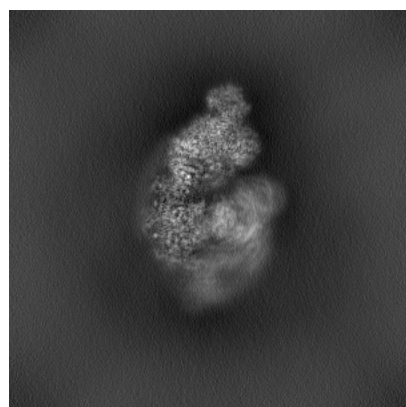


Y

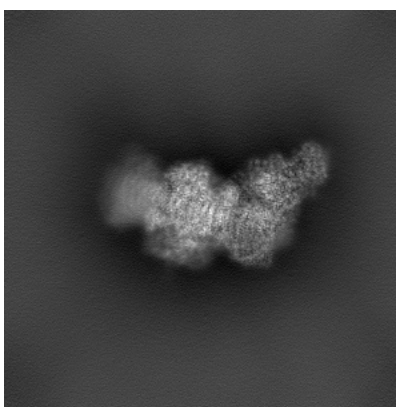


Z

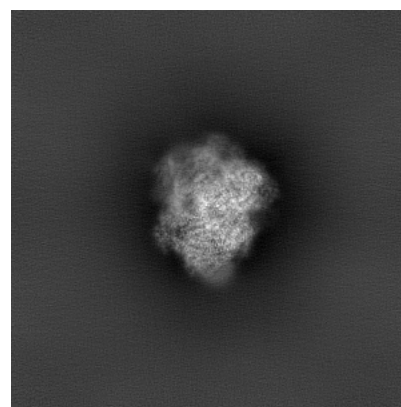
6.1.2 Raw map



X



Y

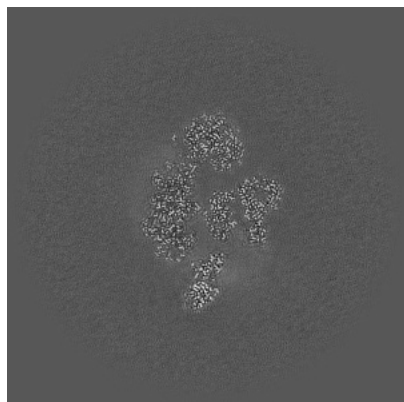


Z

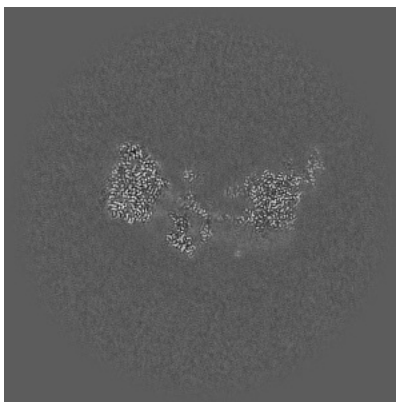
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

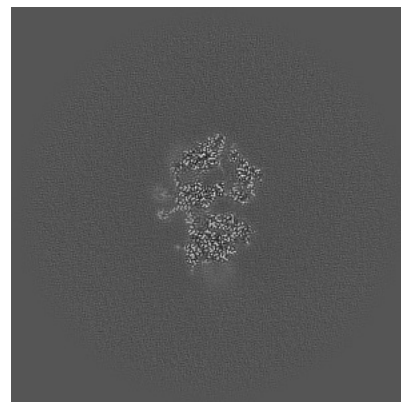
6.2.1 Primary map



X Index: 240

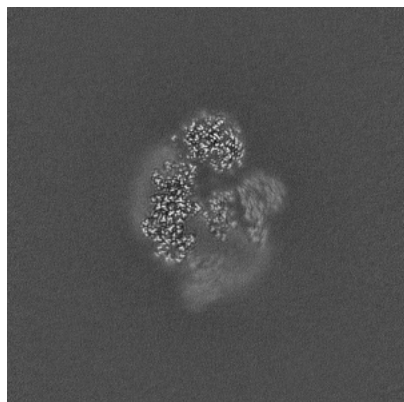


Y Index: 240

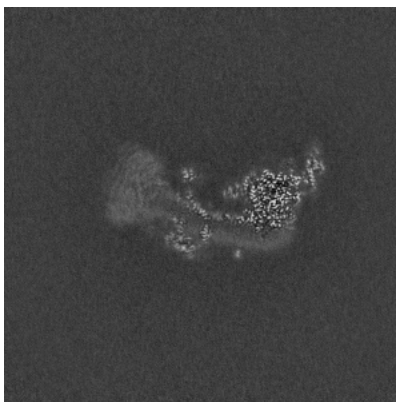


Z Index: 240

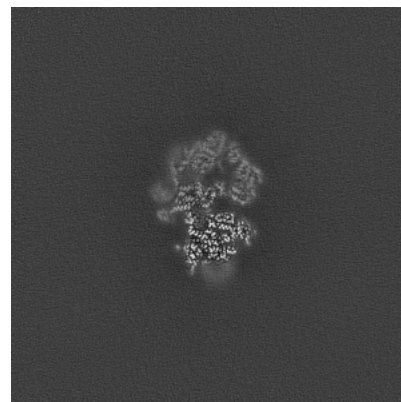
6.2.2 Raw map



X Index: 240



Y Index: 240

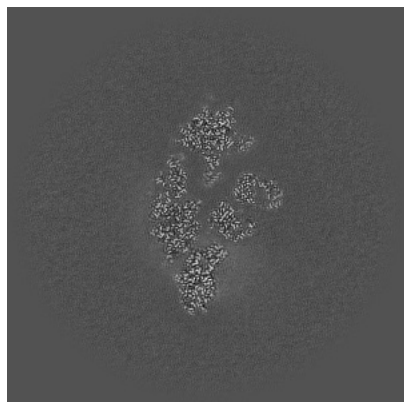


Z Index: 240

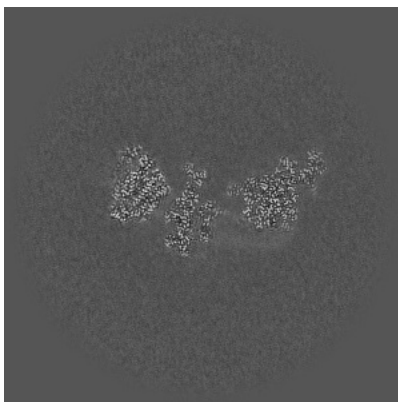
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

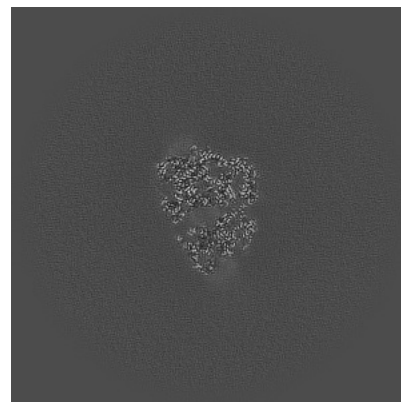
6.3.1 Primary map



X Index: 255

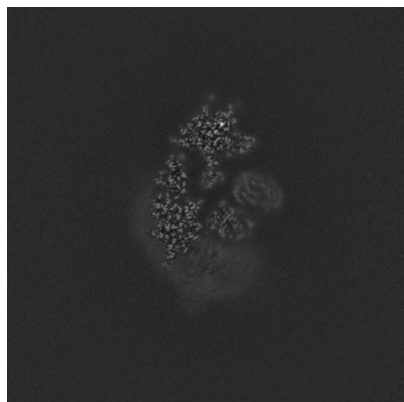


Y Index: 245

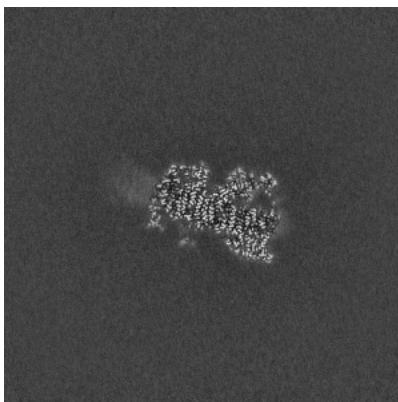


Z Index: 219

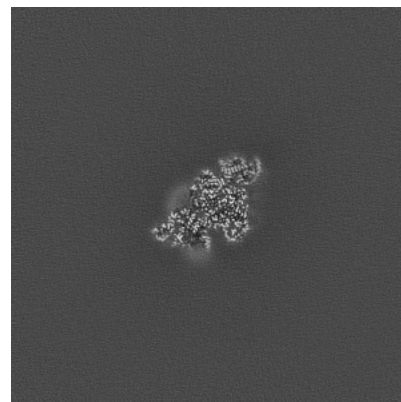
6.3.2 Raw map



X Index: 256



Y Index: 205

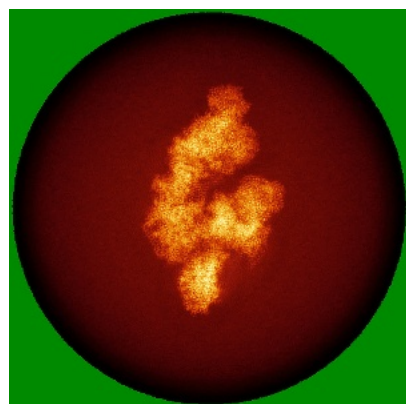


Z Index: 314

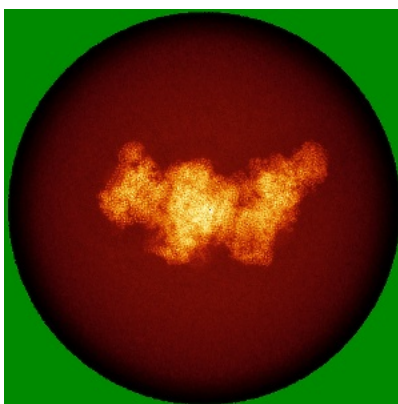
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

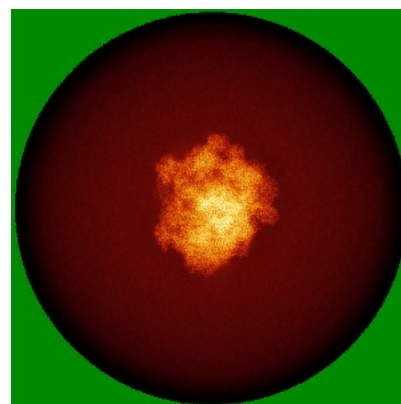
6.4.1 Primary map



X

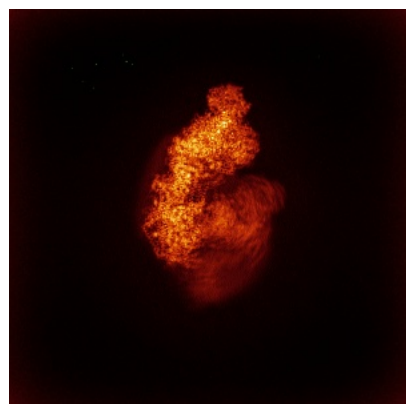


Y

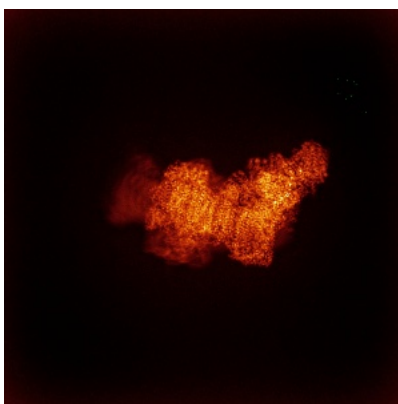


Z

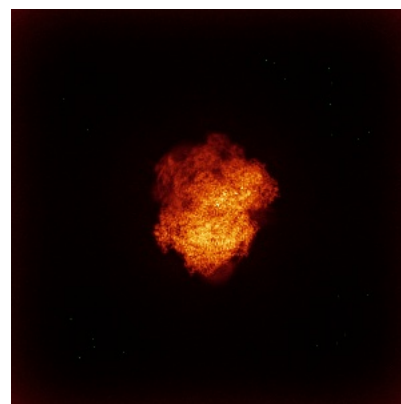
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

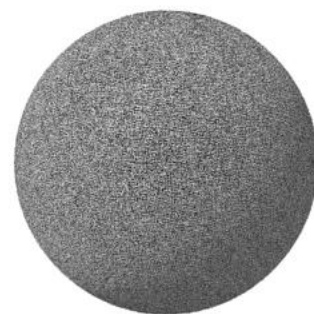
6.5.1 Primary map



X



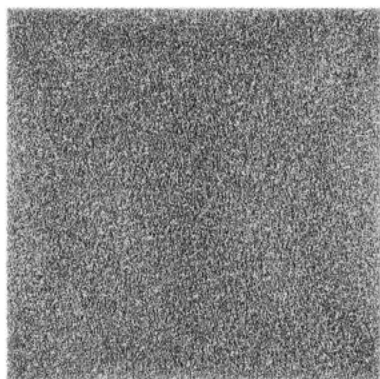
Y



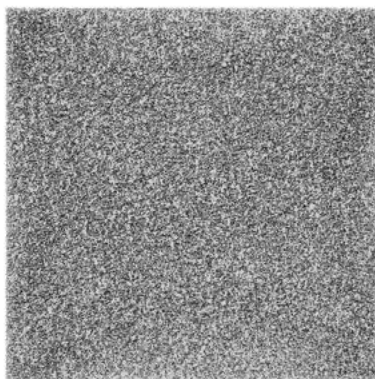
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

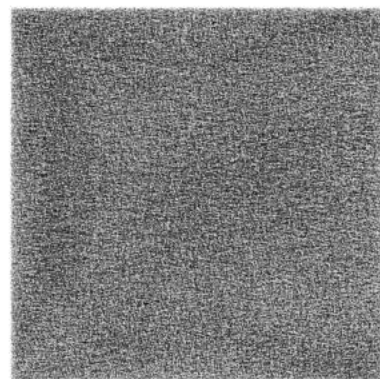
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

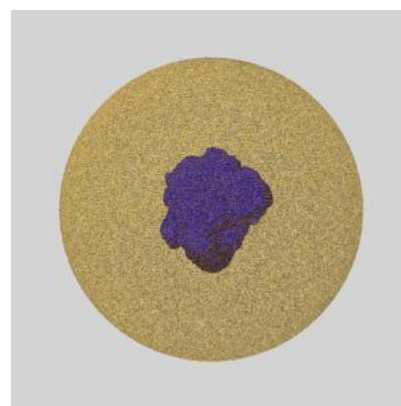
6.6.1 emd_60424_msk_1.map [i](#)



X



Y

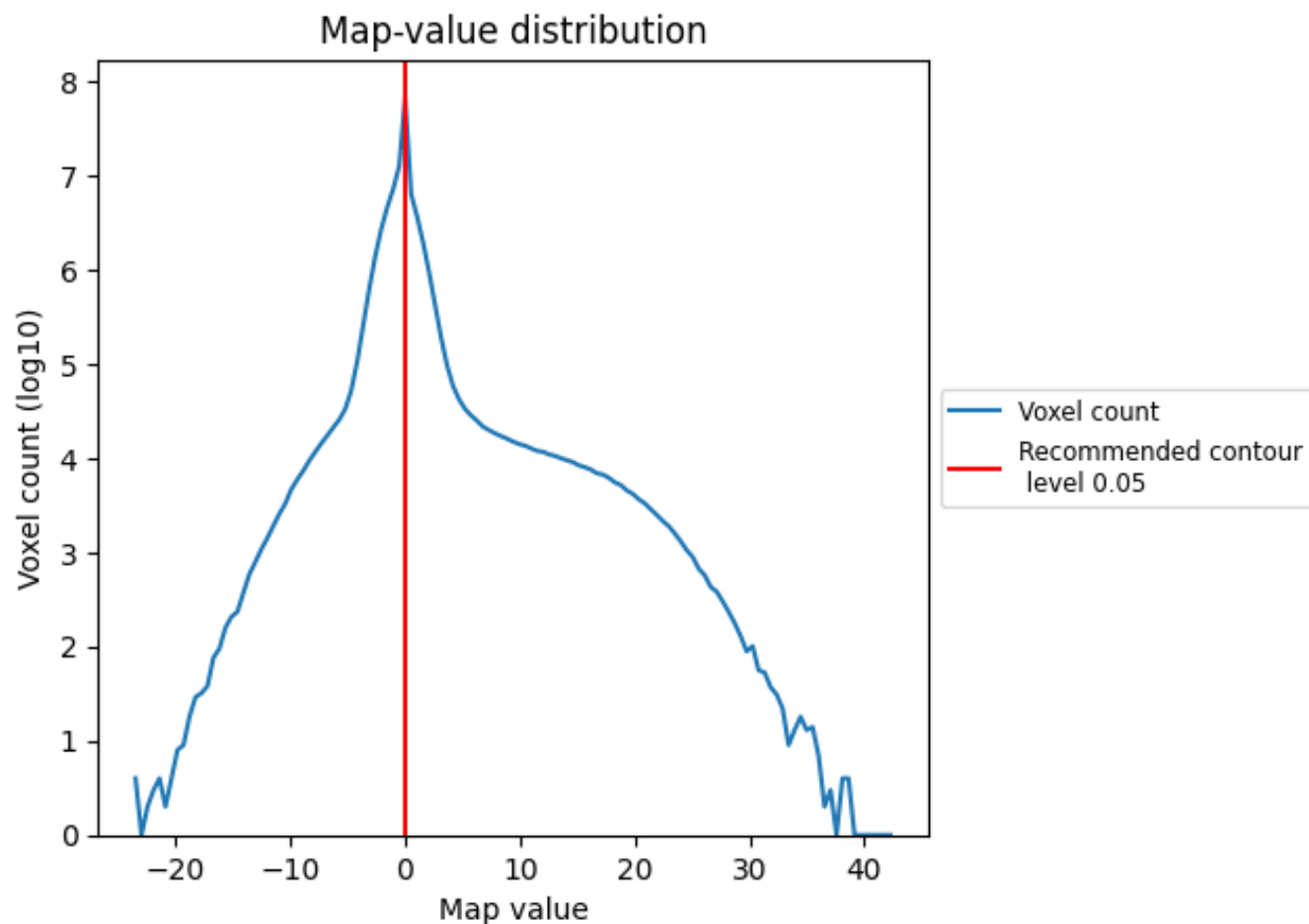


Z

7 Map analysis [i](#)

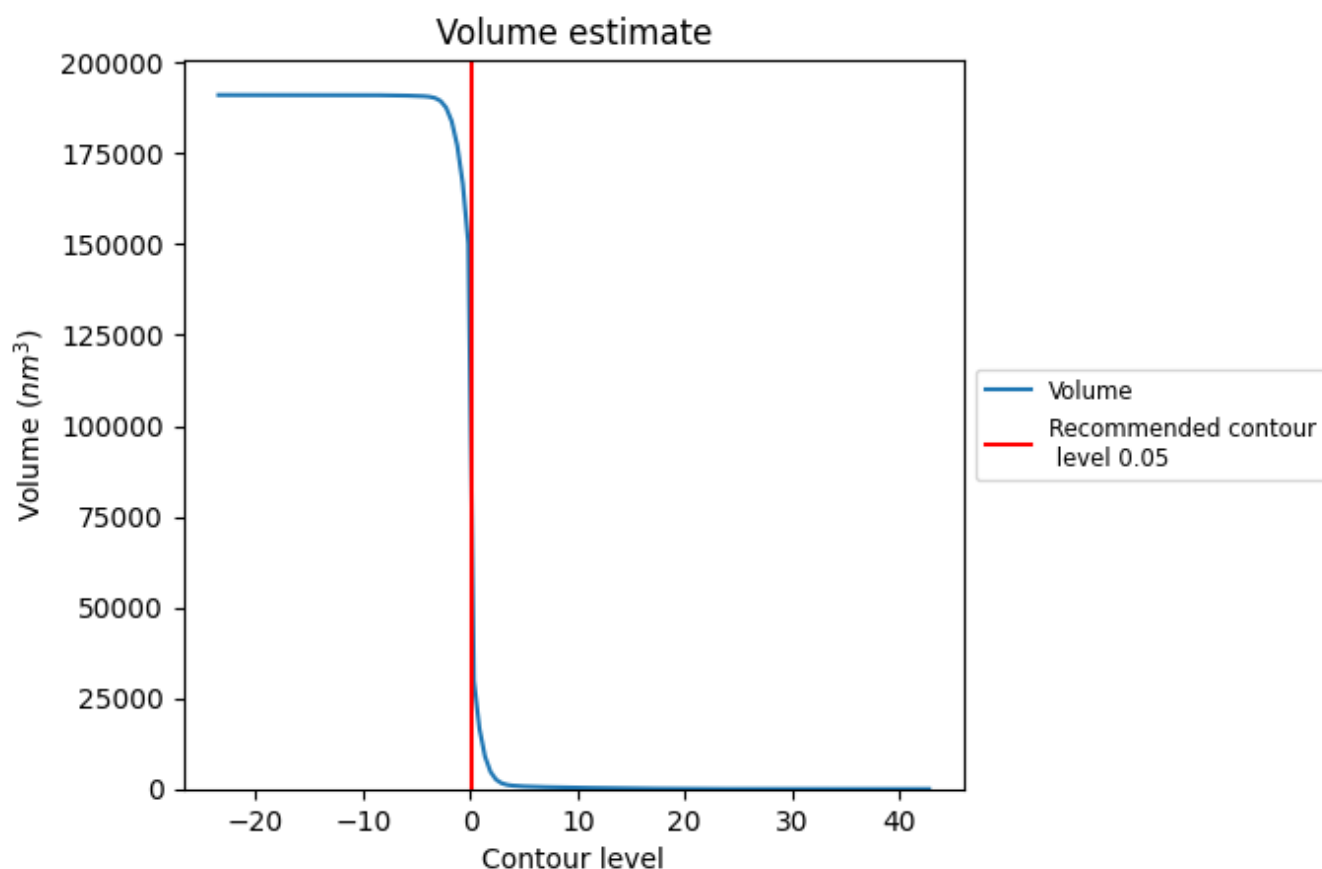
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

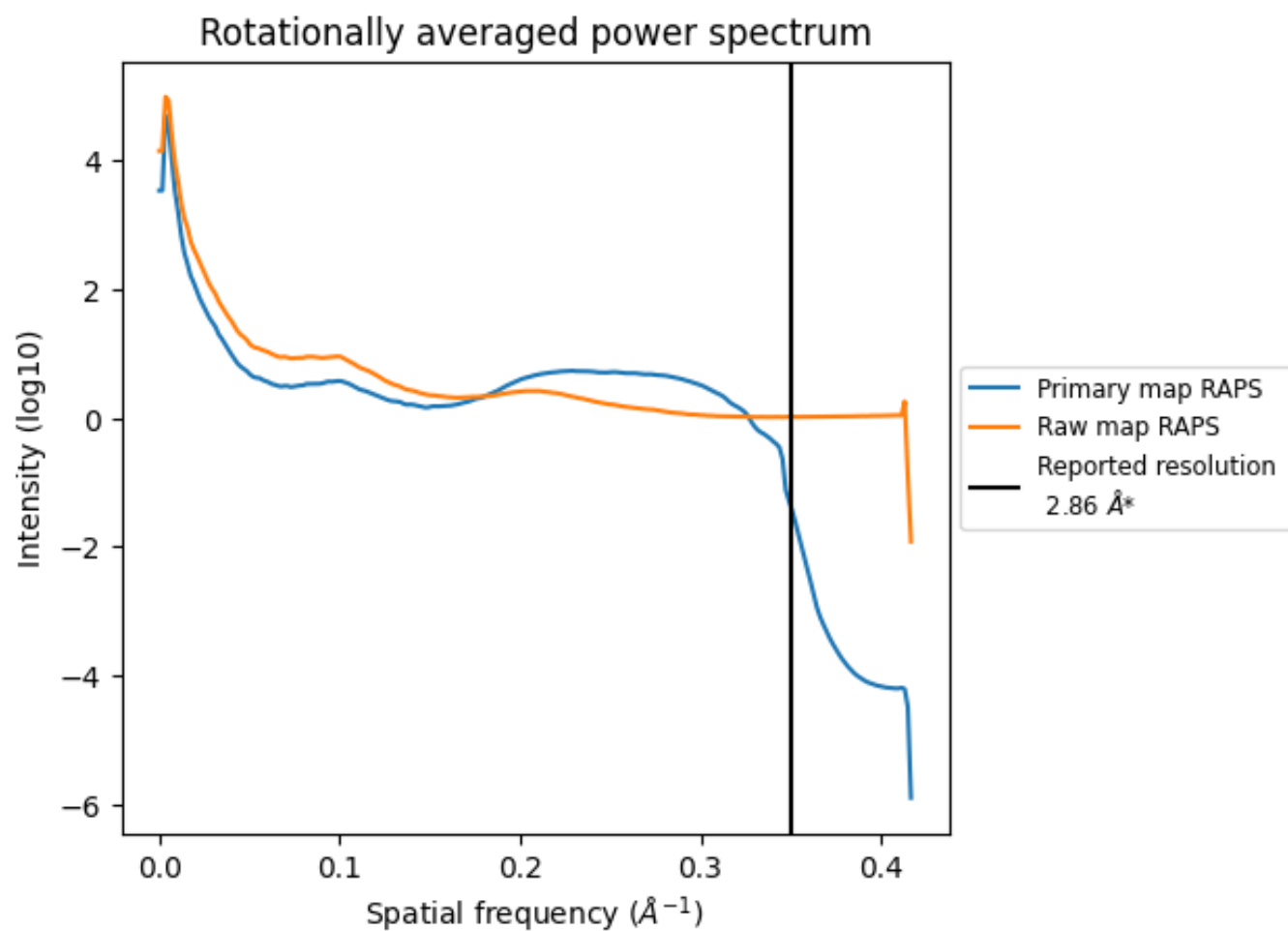
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 97381 nm^3 ; this corresponds to an approximate mass of 87967 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

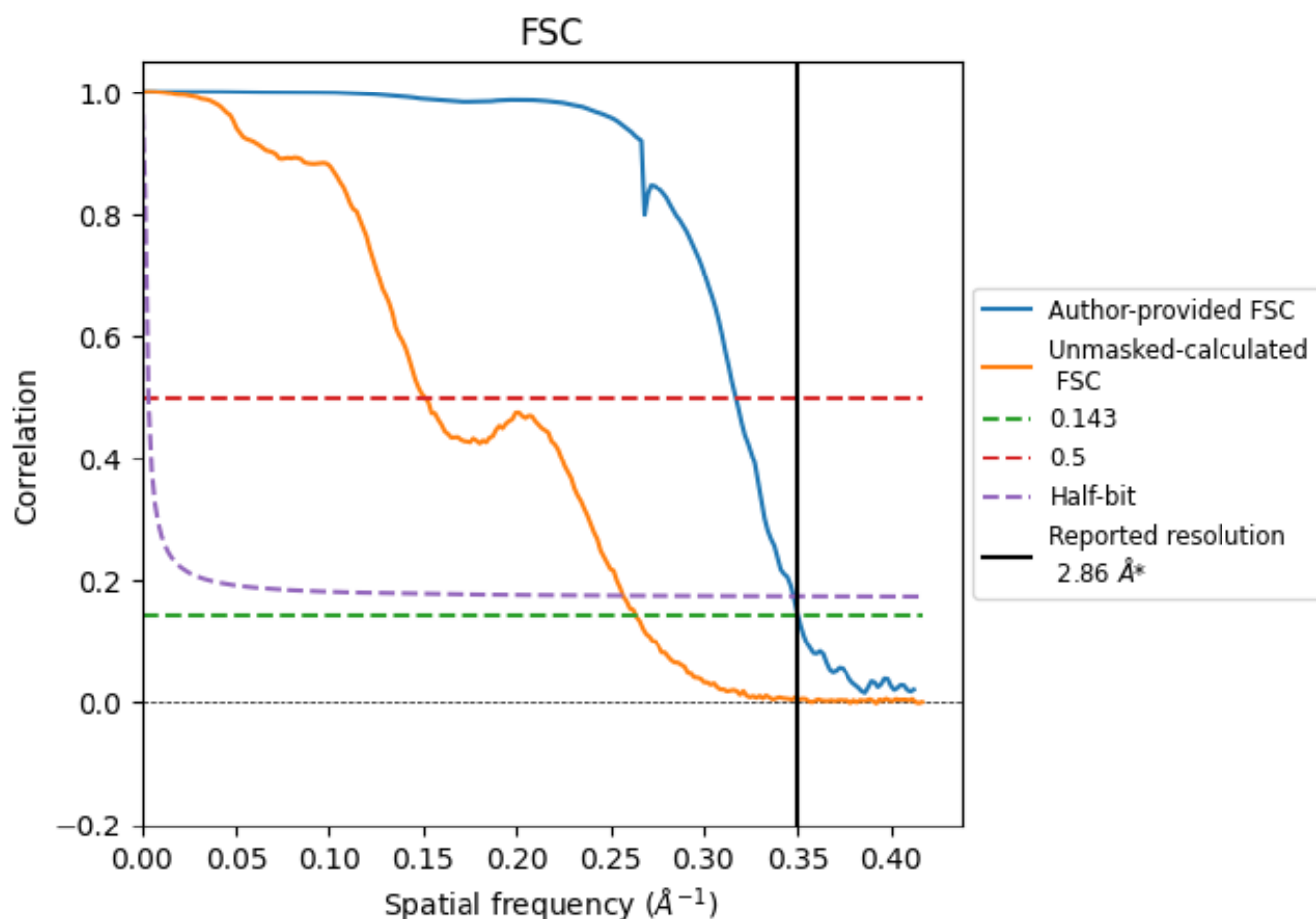


*Reported resolution corresponds to spatial frequency of 0.350 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.350 \AA^{-1}

8.2 Resolution estimates [i](#)

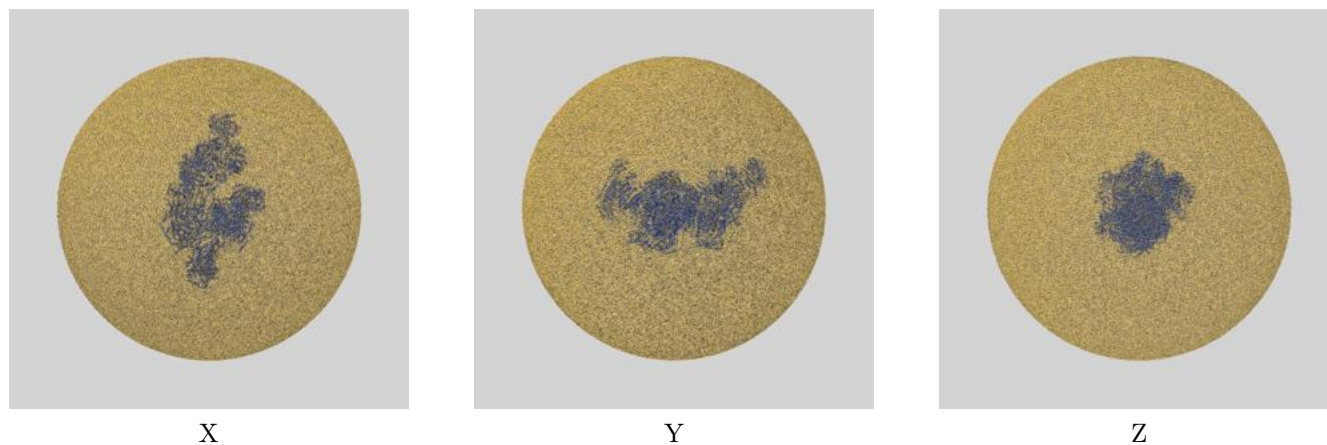
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.86 | - | - |
| Author-provided FSC curve | 2.86 | 3.15 | 2.88 |
| Unmasked-calculated* | 3.80 | 6.63 | 3.89 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 2.86 by more than 10 %

9 Map-model fit [i](#)

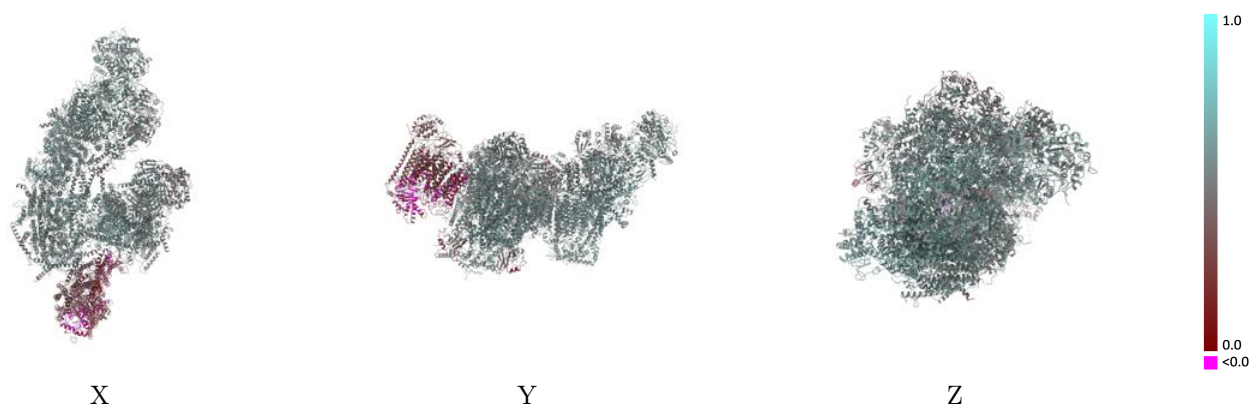
This section contains information regarding the fit between EMDB map EMD-60424 and PDB model 8ZSQ. Per-residue inclusion information can be found in [section 3](#) on [page 32](#).

9.1 Map-model overlay [i](#)



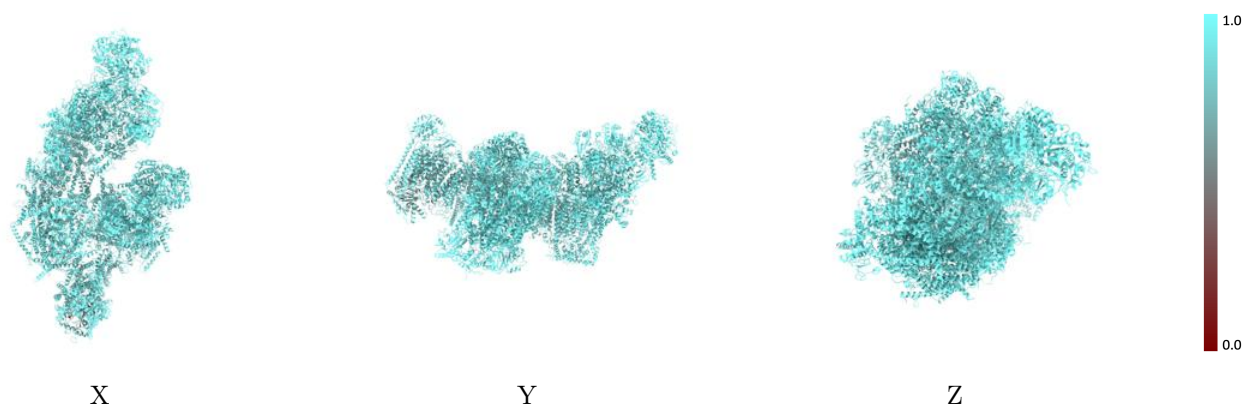
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



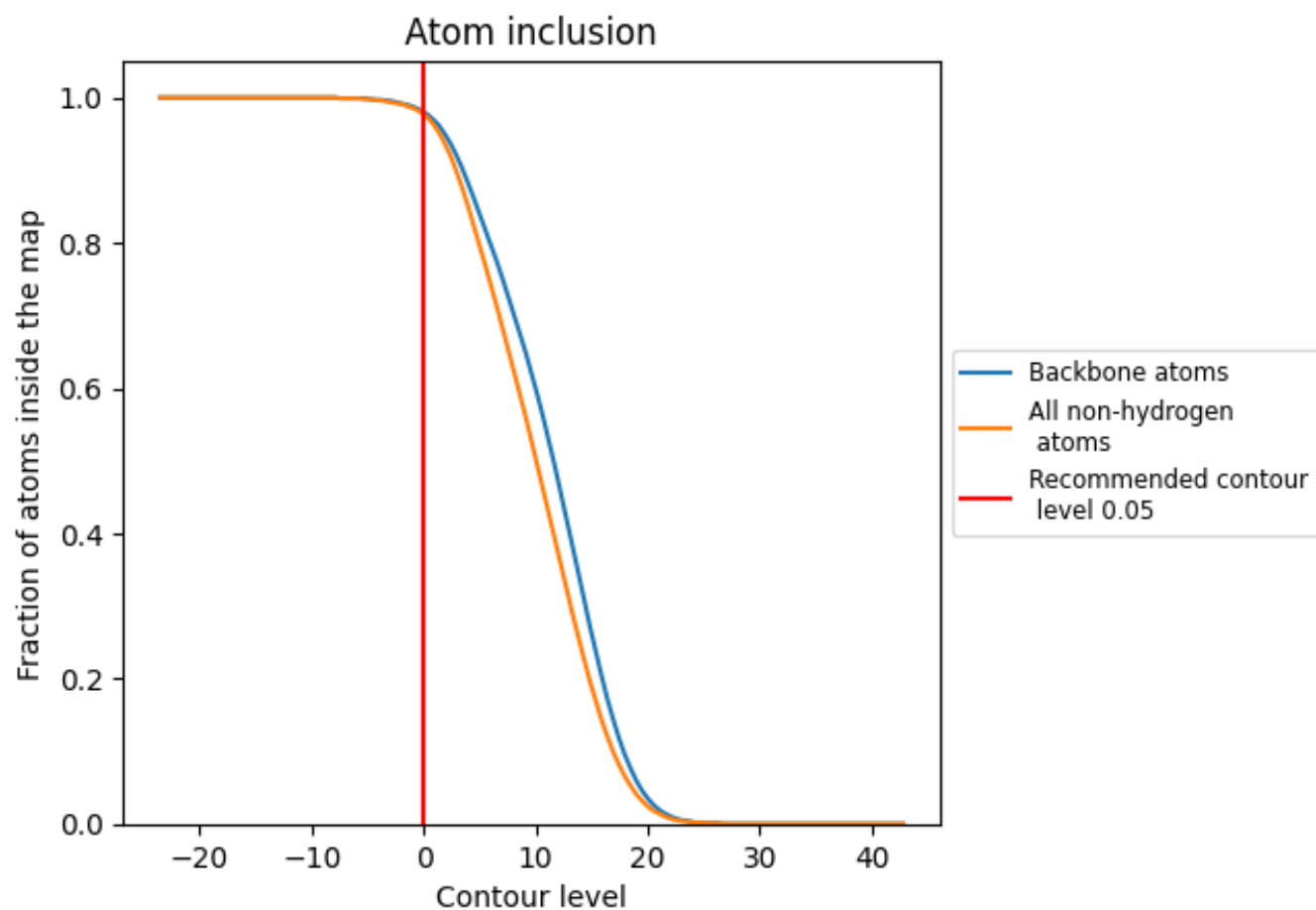
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.9770 |  0.5010 |
| 4L |  0.9980 |  0.5900 |
| 5A |  0.9340 |  0.3250 |
| 5B |  0.9410 |  0.2880 |
| 6A |  0.8750 |  0.1680 |
| 6B |  0.8540 |  0.1040 |
| 6C |  0.8800 |  0.2080 |
| 7A |  0.9620 |  0.3680 |
| 7B |  0.9370 |  0.2730 |
| 7C |  0.9260 |  0.3160 |
| 8B |  0.9460 |  0.3220 |
| A1 |  0.9980 |  0.5820 |
| A2 |  0.9900 |  0.4670 |
| A3 |  1.0000 |  0.5660 |
| A5 |  0.9910 |  0.5260 |
| A6 |  0.9930 |  0.5300 |
| A7 |  0.9990 |  0.5370 |
| A8 |  0.9990 |  0.5720 |
| A9 |  0.9970 |  0.5550 |
| AB |  0.9910 |  0.4550 |
| AC |  0.9840 |  0.5280 |
| AK |  0.9940 |  0.5360 |
| AL |  0.9990 |  0.5640 |
| AM |  0.9980 |  0.5510 |
| AN |  0.9970 |  0.5710 |
| B1 |  0.9920 |  0.5020 |
| B2 |  0.9950 |  0.5290 |
| B3 |  0.9940 |  0.4910 |
| B4 |  0.9960 |  0.5560 |
| B5 |  0.9910 |  0.5400 |
| B6 |  0.9930 |  0.4920 |
| B7 |  0.9950 |  0.5250 |
| B8 |  0.9950 |  0.5680 |
| B9 |  0.9940 |  0.5480 |
| BK |  0.9820 |  0.5200 |









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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| BL |  0.9880 |  0.5140 |
| C1 |  0.8590 |  0.2160 |
| C2 |  0.7950 |  0.1000 |
| C3 |  0.8800 |  0.2140 |
| C4 |  0.9010 |  0.2690 |
| CA |  0.9960 |  0.5340 |
| CB |  0.9950 |  0.5620 |
| N1 |  0.9940 |  0.5840 |
| N2 |  0.9950 |  0.5890 |
| N3 |  0.9990 |  0.5810 |
| N4 |  0.9900 |  0.5550 |
| N5 |  0.9920 |  0.5520 |
| N6 |  0.9900 |  0.5500 |
| QA |  0.9880 |  0.5170 |
| QB |  0.9920 |  0.5650 |
| QC |  0.9960 |  0.5870 |
| QD |  0.9970 |  0.5640 |
| QE |  0.9890 |  0.4590 |
| QF |  0.9930 |  0.4580 |
| QG |  0.9840 |  0.5110 |
| QH |  0.9800 |  0.5020 |
| QI |  0.9840 |  0.5180 |
| QJ |  0.9880 |  0.5250 |
| QK |  0.9960 |  0.5060 |
| Qa |  0.9790 |  0.5100 |
| Qb |  0.9840 |  0.5160 |
| Qc |  0.9870 |  0.5500 |
| Qd |  0.9890 |  0.5270 |
| Qe |  0.9800 |  0.4240 |
| Qf |  0.9900 |  0.5140 |
| Qg |  0.9880 |  0.5720 |
| Qh |  0.9960 |  0.5710 |
| Qi |  0.9980 |  0.5700 |
| Qj |  0.9910 |  0.5600 |
| S1 |  0.9880 |  0.5210 |
| S2 |  0.9940 |  0.5710 |
| S3 |  0.9950 |  0.5640 |
| S4 |  0.9920 |  0.5480 |
| S5 |  0.9970 |  0.5620 |
| S6 |  0.9990 |  0.5600 |
| S7 |  0.9940 |  0.5760 |
| S8 |  0.9990 |  0.5880 |

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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| V1 |  0.9920 |  0.5350 |
| V2 |  0.9950 |  0.5350 |
| V3 |  0.9970 |  0.5290 |