



Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 11:28 am GMT

PDB ID : 7NHQ
EMDB ID : EMD-12337
Title : Structure of PSII-I prime (PSII with Psb28, and Psb34)
Authors : Zabret, J.; Bohn, S.; Schuller, S.K.; Arnolds, O.; Chan, A.; Tajkhorshid, E.;
Stoll, R.; Engel, B.D.; Rudack, T.; Schuller, J.M.; Nowaczyk, M.M.
Deposited on : 2021-02-11
Resolution : 2.68 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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

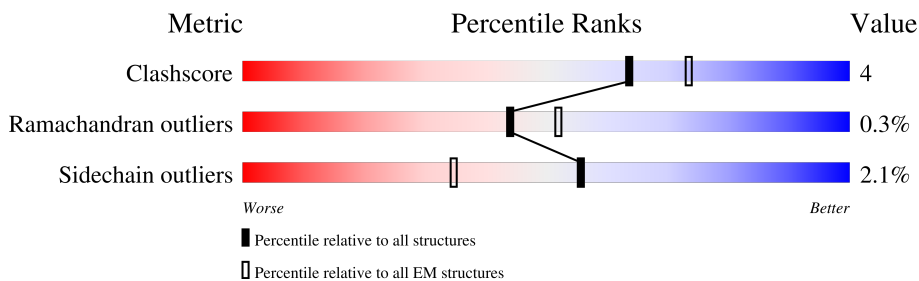
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.68 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) |
|-----------------------|--------------------------|--------------------------|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 360 | |
| 2 | B | 510 | |
| 3 | C | 461 | |
| 4 | D | 352 | |
| 5 | E | 84 | |
| 6 | F | 45 | |
| 7 | H | 66 | |
| 8 | I | 38 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 9 | K | 46 | |
| 10 | L | 37 | |
| 11 | M | 36 | |
| 12 | T | 32 | |
| 13 | X | 41 | |
| 14 | y | 46 | |
| 15 | Z | 62 | |
| 16 | 2 | 116 | |
| 17 | 3 | 56 | |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 21 | PHO | A | 404 | X | - | - | - |
| 21 | PHO | D | 406 | X | - | - | - |
| 22 | CLA | A | 405 | X | - | - | - |
| 22 | CLA | A | 406 | X | - | - | - |
| 22 | CLA | B | 601 | X | - | - | - |
| 22 | CLA | B | 602 | X | - | - | - |
| 22 | CLA | B | 603 | X | - | - | - |
| 22 | CLA | B | 604 | X | - | - | - |
| 22 | CLA | B | 605 | X | - | - | - |
| 22 | CLA | B | 606 | X | - | - | - |
| 22 | CLA | B | 607 | X | - | - | - |
| 22 | CLA | B | 609 | X | - | - | - |
| 22 | CLA | B | 610 | X | - | - | - |
| 22 | CLA | B | 611 | X | - | - | - |
| 22 | CLA | B | 612 | X | - | - | - |
| 22 | CLA | B | 613 | X | - | - | - |
| 22 | CLA | B | 614 | X | - | - | - |
| 22 | CLA | B | 615 | X | - | - | - |
| 22 | CLA | B | 616 | X | - | - | - |
| 22 | CLA | C | 504 | X | - | - | - |
| 22 | CLA | C | 505 | X | - | - | - |
| 22 | CLA | C | 506 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22 | CLA | C | 507 | X | - | - | - |
| 22 | CLA | C | 508 | X | - | - | - |
| 22 | CLA | C | 509 | X | - | - | - |
| 22 | CLA | C | 510 | X | - | - | - |
| 22 | CLA | C | 511 | X | - | - | - |
| 22 | CLA | C | 512 | X | - | - | - |
| 22 | CLA | C | 513 | X | - | - | - |
| 22 | CLA | C | 514 | X | - | - | - |
| 22 | CLA | C | 517 | X | - | - | - |
| 22 | CLA | D | 402 | X | - | - | - |
| 22 | CLA | D | 407 | X | - | - | - |
| 22 | CLA | D | 408 | X | - | - | - |

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 20946 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 Photosystem II protein D1 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 1 | A | 335 | 2627 | 1720 | 432 | 460 | 15 | 0 | 0 |

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | B | 496 | 3909 | 2569 | 649 | 678 | 13 | 0 | 0 |

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 3 | C | 432 | 3345 | 2197 | 561 | 575 | 12 | 0 | 0 |

- Molecule 4 is a protein called Photosystem II D2 protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 4 | D | 341 | 2717 | 1800 | 444 | 461 | 12 | 0 | 0 |

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 5 | E | 77 | 635 | 417 | 103 | 115 | 0 | 0 |

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 6 | F | 38 | 307 | 207 | 50 | 49 | 1 | 0 | 0 |

- Molecule 7 is a protein called Photosystem II reaction center protein H.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 7 | H | 65 | 511 | 341 | 82 | 86 | 2 | 0 | 0 |

- Molecule 8 is a protein called Photosystem II reaction center protein I.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 8 | I | 26 | 211 | 150 | 27 | 33 | 1 | 0 | 0 |

- Molecule 9 is a protein called Photosystem II reaction center protein K.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| | | | Total | C | N | O | | |
| 9 | K | 37 | 293 | 204 | 43 | 46 | 0 | 0 |

- Molecule 10 is a protein called Photosystem II reaction center protein L.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 10 | L | 37 | 304 | 202 | 48 | 53 | 1 | 0 | 0 |

- Molecule 11 is a protein called Photosystem II reaction center protein M.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 11 | M | 34 | 267 | 178 | 40 | 48 | 1 | 0 | 0 |

- Molecule 12 is a protein called Photosystem II reaction center protein T.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 12 | T | 28 | 241 | 170 | 34 | 35 | 2 | 0 | 0 |

- Molecule 13 is a protein called Photosystem II reaction center X protein.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| | | | Total | C | N | O | | |
| 13 | X | 35 | 254 | 172 | 38 | 44 | 0 | 0 |

- Molecule 14 is a protein called Photosystem II reaction center protein Ycf12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 14 | y | 28 | Total | C | N | O | S | 0 | 0 |
| | | | 208 | 137 | 36 | 32 | 3 | | |

- Molecule 15 is a protein called Photosystem II reaction center protein Z.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 15 | Z | 60 | Total | C | N | O | S | 0 | 0 |
| | | | 463 | 318 | 70 | 74 | 1 | | |

- Molecule 16 is a protein called Photosystem II reaction center Psb28 protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | 2 | 112 | Total | C | N | O | S | 0 | 0 |
| | | | 897 | 562 | 156 | 173 | 6 | | |

- Molecule 17 is a protein called Tsl0063 protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 17 | 3 | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 419 | 269 | 74 | 75 | 1 | | |

- Molecule 18 is FE (III) ION (three-letter code: FE) (formula: Fe).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 18 | A | 1 | Total | Fe | 0 |
| | | | 1 | 1 | |

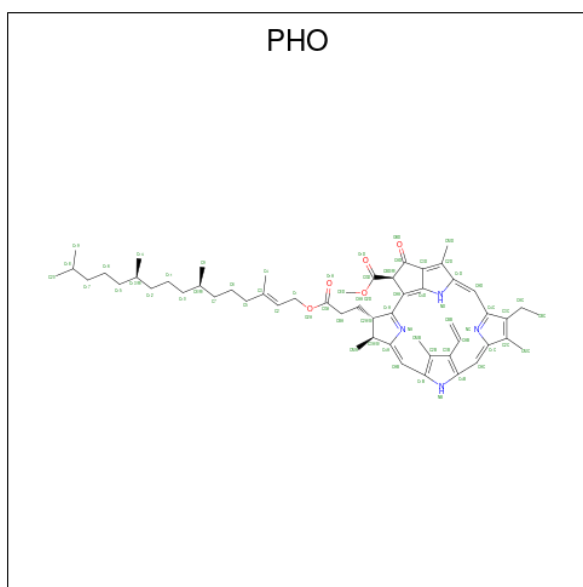
- Molecule 19 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 19 | A | 1 | Total | Mn | 0 |
| | | | 1 | 1 | |

- Molecule 20 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

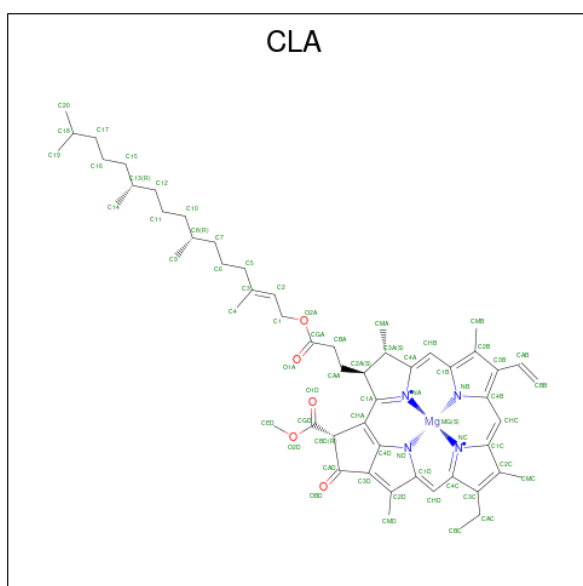
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 20 | A | 1 | Total | Cl | 0 |
| | | | 1 | 1 | |

- Molecule 21 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 21 | A | 1 | Total | C | N | O | 0 |
| | | | 64 | 55 | 4 | 5 | |
| 21 | D | 1 | Total | C | N | O | 0 |
| | | | 64 | 55 | 4 | 5 | |

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|-----|----|---|----|---------|
| 22 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 130 | 110 | 2 | 8 | 10 | |
| 22 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 130 | 110 | 2 | 8 | 10 | |

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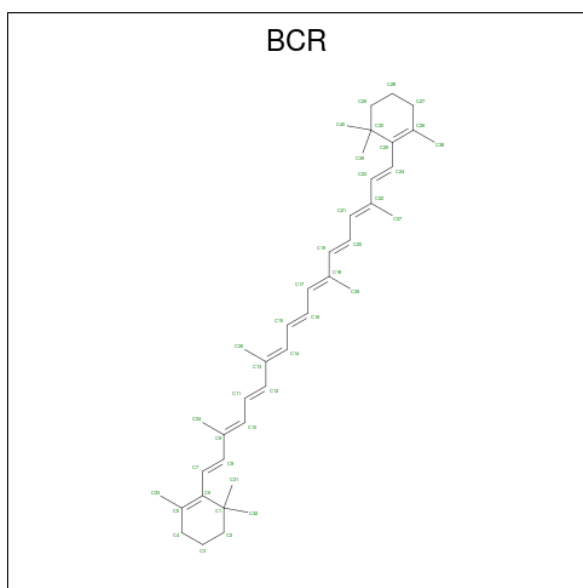
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|---------------|----------|----------|---------|---------|---------|
| | | | Total | C | Mg | N | O | |
| 22 | B | 1 | Total 1040 | C 880 | Mg 16 | N 64 | O 80 | 0 |
| 22 | B | 1 | Total 1040 | C 880 | Mg 16 | N 64 | O 80 | 0 |
| 22 | B | 1 | Total 1040 | C 880 | Mg 16 | N 64 | O 80 | 0 |
| 22 | B | 1 | Total 1040 | C 880 | Mg 16 | N 64 | O 80 | 0 |
| 22 | B | 1 | Total 1040 | C 880 | Mg 16 | N 64 | O 80 | 0 |
| 22 | B | 1 | Total 1040 | C 880 | Mg 16 | N 64 | O 80 | 0 |
| 22 | B | 1 | Total 1040 | C 880 | Mg 16 | N 64 | O 80 | 0 |
| 22 | B | 1 | Total 1040 | C 880 | Mg 16 | N 64 | O 80 | 0 |
| 22 | B | 1 | Total 1040 | C 880 | Mg 16 | N 64 | O 80 | 0 |
| 22 | B | 1 | Total 1040 | C 880 | Mg 16 | N 64 | O 80 | 0 |
| 22 | B | 1 | Total 1040 | C 880 | Mg 16 | N 64 | O 80 | 0 |
| 22 | B | 1 | Total 1040 | C 880 | Mg 16 | N 64 | O 80 | 0 |
| 22 | B | 1 | Total 1040 | C 880 | Mg 16 | N 64 | O 80 | 0 |
| 22 | B | 1 | Total 1040 | C 880 | Mg 16 | N 64 | O 80 | 0 |
| 22 | B | 1 | Total 1040 | C 880 | Mg 16 | N 64 | O 80 | 0 |
| 22 | B | 1 | Total 1040 | C 880 | Mg 16 | N 64 | O 80 | 0 |
| 22 | B | 1 | Total 1040 | C 880 | Mg 16 | N 64 | O 80 | 0 |
| 22 | C | 1 | Total 845 | C 715 | Mg 13 | N 52 | O 65 | 0 |
| 22 | C | 1 | Total 845 | C 715 | Mg 13 | N 52 | O 65 | 0 |
| 22 | C | 1 | Total 845 | C 715 | Mg 13 | N 52 | O 65 | 0 |
| 22 | C | 1 | Total 845 | C 715 | Mg 13 | N 52 | O 65 | 0 |
| 22 | C | 1 | Total 845 | C 715 | Mg 13 | N 52 | O 65 | 0 |

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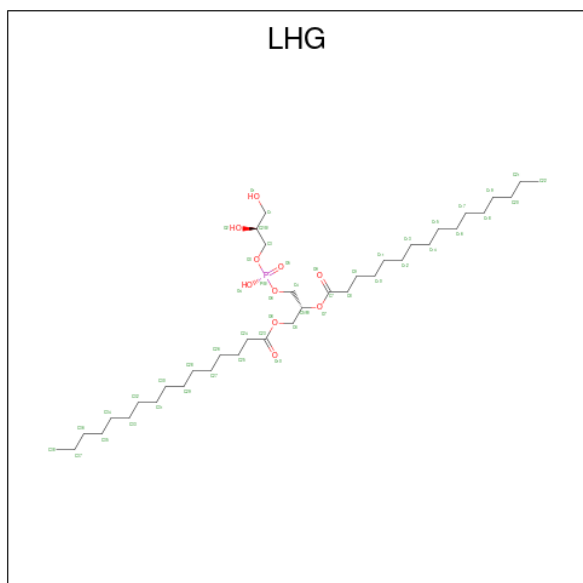
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|--------------|----------|----------|---------|---------|---------|
| | | | Total | C | Mg | N | O | |
| 22 | C | 1 | Total 845 | C 715 | Mg 13 | N 52 | O 65 | 0 |
| 22 | C | 1 | Total 845 | C 715 | Mg 13 | N 52 | O 65 | 0 |
| 22 | C | 1 | Total 845 | C 715 | Mg 13 | N 52 | O 65 | 0 |
| 22 | C | 1 | Total 845 | C 715 | Mg 13 | N 52 | O 65 | 0 |
| 22 | C | 1 | Total 845 | C 715 | Mg 13 | N 52 | O 65 | 0 |
| 22 | C | 1 | Total 845 | C 715 | Mg 13 | N 52 | O 65 | 0 |
| 22 | C | 1 | Total 845 | C 715 | Mg 13 | N 52 | O 65 | 0 |
| 22 | C | 1 | Total 845 | C 715 | Mg 13 | N 52 | O 65 | 0 |
| 22 | D | 1 | Total 260 | C 220 | Mg 4 | N 16 | O 20 | 0 |
| 22 | D | 1 | Total 260 | C 220 | Mg 4 | N 16 | O 20 | 0 |
| 22 | D | 1 | Total 260 | C 220 | Mg 4 | N 16 | O 20 | 0 |
| 22 | D | 1 | Total 260 | C 220 | Mg 4 | N 16 | O 20 | 0 |

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



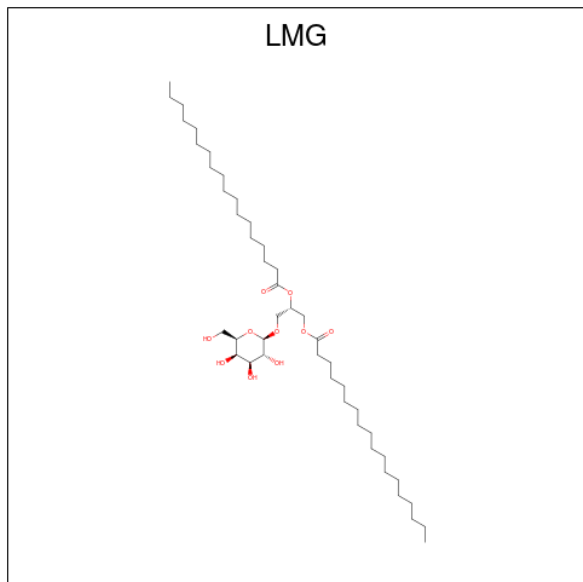
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 23 | A | 1 | Total 40 | C 40 | 0 |
| 23 | B | 1 | Total 120 | C 120 | 0 |
| 23 | B | 1 | Total 120 | C 120 | 0 |
| 23 | B | 1 | Total 120 | C 120 | 0 |
| 23 | C | 1 | Total 120 | C 120 | 0 |
| 23 | C | 1 | Total 120 | C 120 | 0 |
| 23 | C | 1 | Total 120 | C 120 | 0 |
| 23 | F | 1 | Total 40 | C 40 | 0 |
| 23 | H | 1 | Total 40 | C 40 | 0 |
| 23 | K | 1 | Total 40 | C 40 | 0 |

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



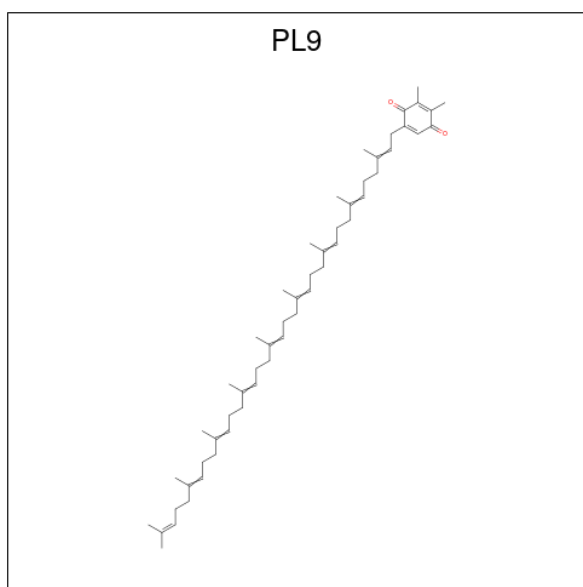
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|
| 24 | A | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



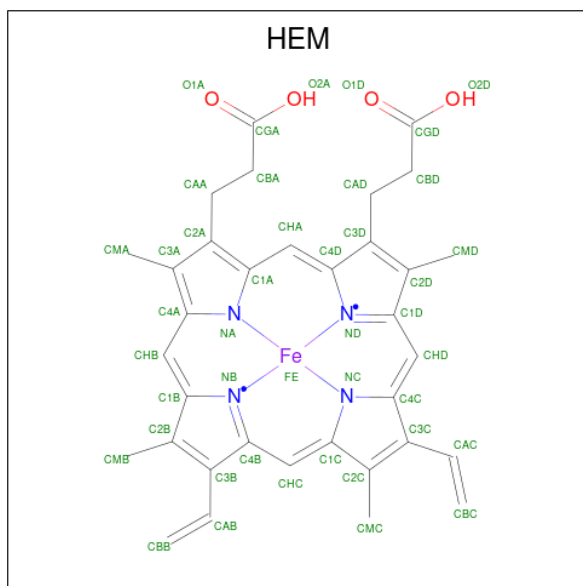
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|----|---------|
| | | | Total | C | O | |
| 25 | C | 1 | 110 | 90 | 20 | 0 |
| 25 | C | 1 | 110 | 90 | 20 | 0 |
| 25 | D | 1 | 110 | 90 | 20 | 0 |
| 25 | D | 1 | 110 | 90 | 20 | 0 |
| 25 | F | 1 | 55 | 45 | 10 | 0 |
| 25 | I | 1 | 55 | 45 | 10 | 0 |
| 25 | 3 | 1 | 55 | 45 | 10 | 0 |

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 26 | D | 1 | Total | C | O | 0 |
| | | | 55 | 53 | 2 | |

- Molecule 27 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

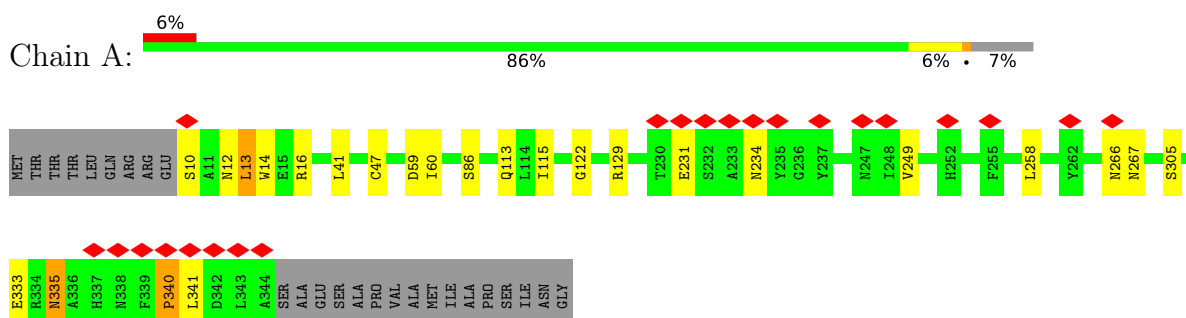


| Mol | Chain | Residues | Atoms | | | | AltConf | |
|-----|-------|----------|-------|----|----|---|---------|---|
| 27 | E | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |

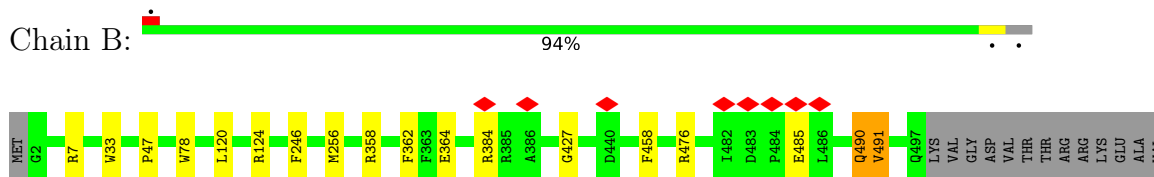
3 Residue-property plots [i](#)

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.

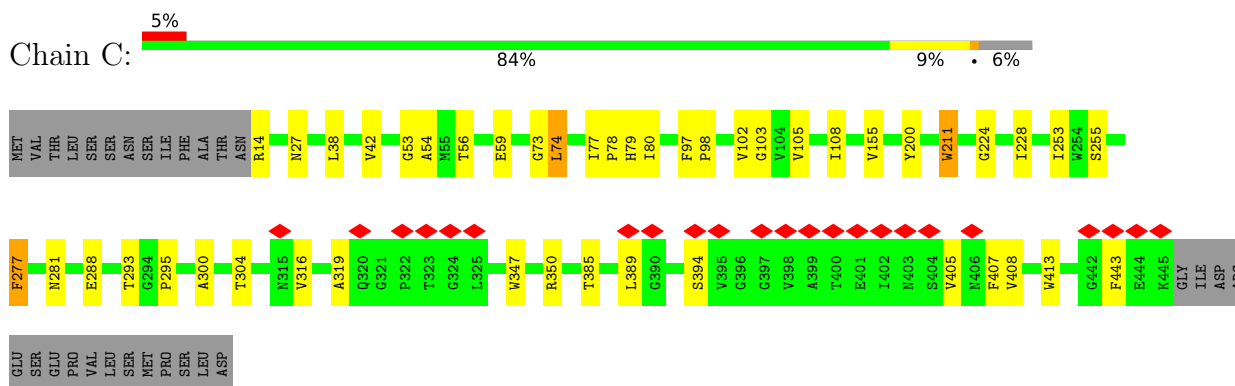
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein

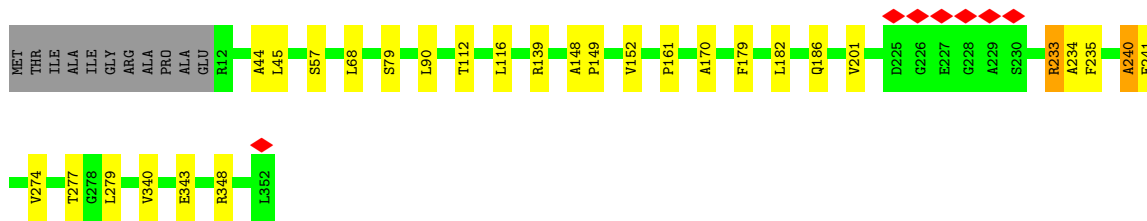


- Molecule 3: Photosystem II CP43 reaction center protein

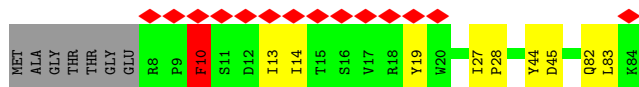
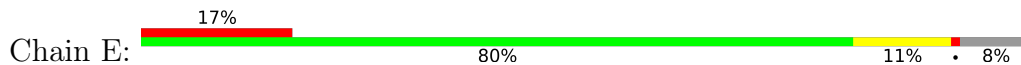


- Molecule 4: Photosystem II D2 protein

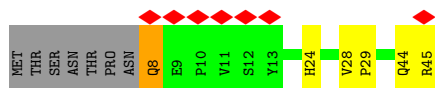




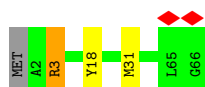
• Molecule 5: Cytochrome b559 subunit alpha



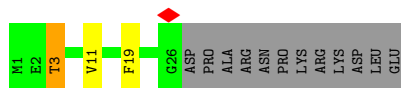
• Molecule 6: Cytochrome b559 subunit beta



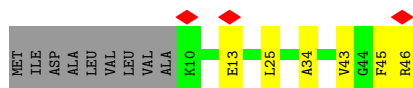
• Molecule 7: Photosystem II reaction center protein H



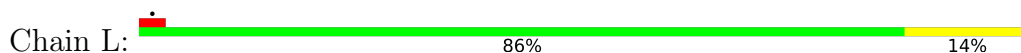
• Molecule 8: Photosystem II reaction center protein I

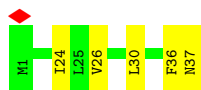


• Molecule 9: Photosystem II reaction center protein K

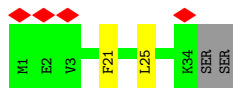
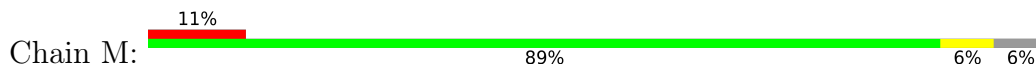


• Molecule 10: Photosystem II reaction center protein L

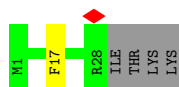
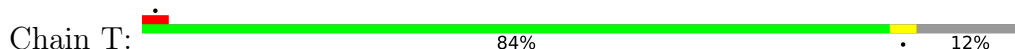




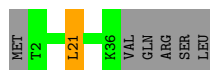
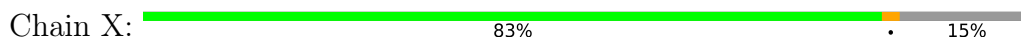
- Molecule 11: Photosystem II reaction center protein M



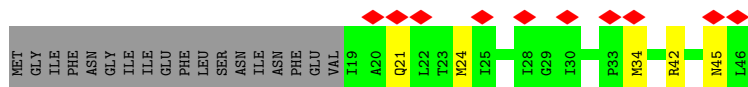
- Molecule 12: Photosystem II reaction center protein T



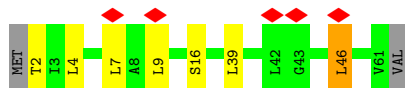
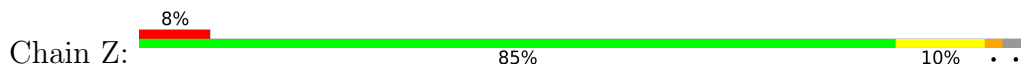
- Molecule 13: Photosystem II reaction center X protein



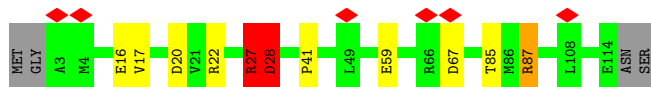
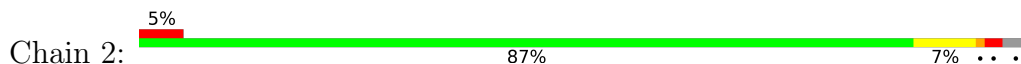
- Molecule 14: Photosystem II reaction center protein Ycf12



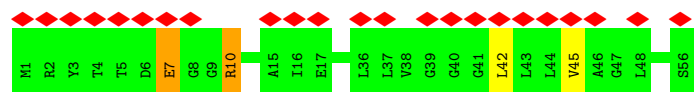
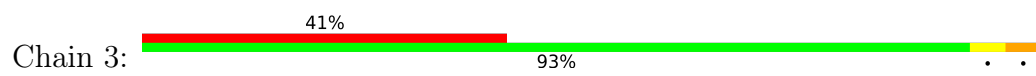
- Molecule 15: Photosystem II reaction center protein Z



- Molecule 16: Photosystem II reaction center Psb28 protein



- Molecule 17: Tsl0063 protein



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 91479 | 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 ($e^-/\text{\AA}^2$) | 55 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.065 | Depositor |
| Minimum map value | -0.030 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.002 | Depositor |
| Recommended contour level | 0.006 | Depositor |
| Map size (\AA) | 283.4, 283.4, 283.4 | wwPDB |
| Map dimensions | 260, 260, 260 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.09, 1.09, 1.09 | Depositor |

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, CLA, FE, PHO, MN, HEM, CL, PL9, LMG, LHG

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.43 | 0/2712 | 0.75 | 1/3700 (0.0%) |
| 2 | B | 0.45 | 0/4049 | 0.76 | 2/5519 (0.0%) |
| 3 | C | 0.44 | 0/3456 | 0.75 | 5/4706 (0.1%) |
| 4 | D | 0.43 | 0/2812 | 0.77 | 1/3832 (0.0%) |
| 5 | E | 0.44 | 0/654 | 0.80 | 1/891 (0.1%) |
| 6 | F | 0.57 | 0/317 | 0.96 | 1/433 (0.2%) |
| 7 | H | 0.41 | 0/524 | 0.81 | 1/713 (0.1%) |
| 8 | I | 0.52 | 0/216 | 0.91 | 0/292 |
| 9 | K | 0.50 | 0/303 | 0.72 | 0/416 |
| 10 | L | 0.43 | 0/311 | 0.79 | 0/422 |
| 11 | M | 0.46 | 0/270 | 0.83 | 0/367 |
| 12 | T | 0.55 | 0/250 | 0.84 | 1/338 (0.3%) |
| 13 | X | 0.48 | 0/257 | 0.97 | 1/348 (0.3%) |
| 14 | y | 0.52 | 0/209 | 1.01 | 1/279 (0.4%) |
| 15 | Z | 0.48 | 0/474 | 0.99 | 3/649 (0.5%) |
| 16 | 2 | 0.52 | 0/914 | 0.93 | 0/1231 |
| 17 | 3 | 0.57 | 1/426 (0.2%) | 1.11 | 3/578 (0.5%) |
| All | All | 0.45 | 1/18154 (0.0%) | 0.80 | 21/24714 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 2 | B | 0 | 3 |
| 4 | D | 0 | 1 |
| 5 | E | 0 | 1 |
| 14 | y | 0 | 1 |
| 16 | 2 | 0 | 2 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| All | All | 0 | 9 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 17 | 3 | 7 | GLU | CB-CG | -5.73 | 1.41 | 1.52 |

All (21) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 17 | 3 | 7 | GLU | CA-CB-CG | 9.35 | 133.98 | 113.40 |
| 15 | Z | 46 | LEU | CB-CG-CD1 | 7.83 | 124.31 | 111.00 |
| 1 | A | 249 | VAL | CG1-CB-CG2 | -7.13 | 99.49 | 110.90 |
| 4 | D | 45 | LEU | CA-CB-CG | 6.99 | 131.37 | 115.30 |
| 5 | E | 10 | PHE | CB-CG-CD1 | -6.88 | 115.98 | 120.80 |
| 17 | 3 | 7 | GLU | CB-CA-C | -6.74 | 96.93 | 110.40 |
| 3 | C | 443 | PHE | CB-CG-CD1 | 6.53 | 125.37 | 120.80 |
| 3 | C | 443 | PHE | CB-CG-CD2 | -6.41 | 116.31 | 120.80 |
| 7 | H | 3 | ARG | NE-CZ-NH1 | 6.17 | 123.38 | 120.30 |
| 14 | y | 34 | MET | CA-CB-CG | 6.12 | 123.70 | 113.30 |
| 15 | Z | 9 | LEU | CB-CG-CD1 | -6.10 | 100.63 | 111.00 |
| 3 | C | 14 | ARG | NE-CZ-NH2 | -5.93 | 117.33 | 120.30 |
| 12 | T | 17 | PHE | CB-CG-CD1 | 5.70 | 124.79 | 120.80 |
| 13 | X | 21 | LEU | CB-CG-CD2 | -5.62 | 101.44 | 111.00 |
| 15 | Z | 39 | LEU | CA-CB-CG | 5.60 | 128.18 | 115.30 |
| 2 | B | 490 | GLN | CA-CB-CG | 5.59 | 125.71 | 113.40 |
| 3 | C | 14 | ARG | NE-CZ-NH1 | 5.50 | 123.05 | 120.30 |
| 17 | 3 | 7 | GLU | CB-CG-CD | 5.47 | 128.97 | 114.20 |
| 6 | F | 8 | GLN | CA-CB-CG | 5.44 | 125.36 | 113.40 |
| 2 | B | 491 | VAL | N-CA-CB | -5.44 | 99.54 | 111.50 |
| 3 | C | 211 | TRP | N-CA-C | 5.12 | 124.83 | 111.00 |

There are no chirality outliers.

All (9) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 16 | 2 | 27 | ARG | Peptide |
| 16 | 2 | 67 | ASP | Sidechain |
| 1 | A | 335 | ASN | Sidechain |
| 2 | B | 364 | GLU | Sidechain |
| 2 | B | 485 | GLU | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 2 | B | 490 | GLN | Mainchain |
| 4 | D | 233 | ARG | Peptide |
| 5 | E | 10 | PHE | Sidechain |
| 14 | y | 45 | ASN | Peptide |

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2627 | 0 | 2524 | 14 | 0 |
| 2 | B | 3909 | 0 | 3763 | 8 | 0 |
| 3 | C | 3345 | 0 | 3273 | 33 | 0 |
| 4 | D | 2717 | 0 | 2621 | 19 | 0 |
| 5 | E | 635 | 0 | 625 | 5 | 0 |
| 6 | F | 307 | 0 | 312 | 4 | 0 |
| 7 | H | 511 | 0 | 532 | 2 | 0 |
| 8 | I | 211 | 0 | 227 | 2 | 0 |
| 9 | K | 293 | 0 | 305 | 7 | 0 |
| 10 | L | 304 | 0 | 316 | 4 | 0 |
| 11 | M | 267 | 0 | 289 | 2 | 0 |
| 12 | T | 241 | 0 | 244 | 0 | 0 |
| 13 | X | 254 | 0 | 282 | 0 | 0 |
| 14 | y | 208 | 0 | 237 | 0 | 0 |
| 15 | Z | 463 | 0 | 495 | 2 | 0 |
| 16 | 2 | 897 | 0 | 859 | 4 | 0 |
| 17 | 3 | 419 | 0 | 438 | 4 | 0 |
| 18 | A | 1 | 0 | 0 | 0 | 0 |
| 19 | A | 1 | 0 | 0 | 0 | 0 |
| 20 | A | 1 | 0 | 0 | 0 | 0 |
| 21 | A | 64 | 0 | 73 | 2 | 0 |
| 21 | D | 64 | 0 | 73 | 3 | 0 |
| 22 | A | 130 | 0 | 140 | 2 | 0 |
| 22 | B | 1040 | 0 | 1121 | 32 | 0 |
| 22 | C | 845 | 0 | 909 | 22 | 0 |
| 22 | D | 260 | 0 | 279 | 10 | 0 |
| 23 | A | 40 | 0 | 56 | 1 | 0 |
| 23 | B | 120 | 0 | 168 | 3 | 0 |
| 23 | C | 120 | 0 | 168 | 8 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 23 | F | 40 | 0 | 56 | 1 | 0 |
| 23 | H | 40 | 0 | 56 | 15 | 0 |
| 23 | K | 40 | 0 | 56 | 11 | 0 |
| 24 | A | 49 | 0 | 74 | 0 | 0 |
| 25 | 3 | 55 | 0 | 86 | 2 | 0 |
| 25 | C | 110 | 0 | 172 | 0 | 0 |
| 25 | D | 110 | 0 | 172 | 2 | 0 |
| 25 | F | 55 | 0 | 86 | 0 | 0 |
| 25 | I | 55 | 0 | 86 | 2 | 0 |
| 26 | D | 55 | 0 | 80 | 4 | 0 |
| 27 | E | 43 | 0 | 30 | 3 | 0 |
| All | All | 20946 | 0 | 21283 | 181 | 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 4.

All (181) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:B:609:CLA:C4B | 23:H:101:BCR:H333 | 1.79 | 1.12 |
| 23:C:515:BCR:H353 | 23:K:101:BCR:H332 | 1.25 | 1.08 |
| 22:B:609:CLA:C3B | 23:H:101:BCR:H333 | 1.95 | 0.96 |
| 23:K:101:BCR:C38 | 23:K:101:BCR:H23C | 2.02 | 0.90 |
| 23:H:101:BCR:C38 | 23:H:101:BCR:H23C | 2.03 | 0.89 |
| 22:B:602:CLA:HED2 | 22:B:603:CLA:H43 | 1.57 | 0.87 |
| 23:C:515:BCR:C35 | 23:K:101:BCR:H332 | 2.05 | 0.86 |
| 1:A:341:LEU:HD13 | 3:C:385:THR:HA | 1.62 | 0.82 |
| 23:C:515:BCR:H353 | 23:K:101:BCR:C33 | 2.08 | 0.80 |
| 4:D:116:LEU:HD13 | 22:D:408:CLA:HBA1 | 1.65 | 0.78 |
| 22:B:602:CLA:HBA2 | 22:B:602:CLA:HMA2 | 1.69 | 0.74 |
| 22:C:517:CLA:HMB1 | 22:C:517:CLA:HBB1 | 1.69 | 0.74 |
| 23:H:101:BCR:H23C | 23:H:101:BCR:H382 | 1.69 | 0.74 |
| 22:B:607:CLA:H142 | 22:B:607:CLA:H101 | 1.71 | 0.72 |
| 23:K:101:BCR:H23C | 23:K:101:BCR:H382 | 1.69 | 0.72 |
| 1:A:341:LEU:CD1 | 3:C:385:THR:HA | 2.21 | 0.70 |
| 22:B:609:CLA:C3B | 23:H:101:BCR:C33 | 2.69 | 0.69 |
| 6:F:45:ARG:OXT | 6:F:45:ARG:HD2 | 1.92 | 0.69 |
| 27:E:101:HEM:HMB2 | 27:E:101:HEM:HBB2 | 1.75 | 0.69 |
| 9:K:34:ALA:HB1 | 23:K:101:BCR:H21C | 1.75 | 0.69 |
| 3:C:59:GLU:HG3 | 3:C:74:LEU:HD12 | 1.75 | 0.67 |
| 22:C:511:CLA:HMA3 | 22:C:517:CLA:HMA1 | 1.77 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:D:402:CLA:H41 | 22:D:402:CLA:H92 | 1.78 | 0.65 |
| 22:C:503:CLA:HMA1 | 23:C:516:BCR:H401 | 1.82 | 0.62 |
| 3:C:408:VAL:HG13 | 3:C:413:TRP:HE1 | 1.64 | 0.61 |
| 22:B:601:CLA:HMA3 | 23:H:101:BCR:H382 | 1.83 | 0.60 |
| 26:D:405:PL9:H352 | 10:L:26:VAL:HG12 | 1.83 | 0.59 |
| 2:B:33:TRP:HE1 | 22:B:607:CLA:HBC2 | 1.67 | 0.59 |
| 22:B:609:CLA:NB | 23:H:101:BCR:H333 | 2.18 | 0.59 |
| 21:A:404:PHO:HMB1 | 21:A:404:PHO:HBB1 | 1.84 | 0.59 |
| 22:C:504:CLA:H42 | 22:C:505:CLA:H172 | 1.85 | 0.59 |
| 16:2:85:THR:O | 16:2:87:ARG:NH1 | 2.36 | 0.59 |
| 4:D:116:LEU:HD13 | 22:D:408:CLA:CBA | 2.32 | 0.57 |
| 22:C:511:CLA:HAA2 | 22:C:517:CLA:HMB2 | 1.87 | 0.56 |
| 17:3:42:LEU:O | 17:3:45:VAL:HG12 | 2.04 | 0.56 |
| 3:C:288:GLU:N | 3:C:288:GLU:OE1 | 2.39 | 0.56 |
| 17:3:42:LEU:HA | 17:3:45:VAL:HG12 | 1.86 | 0.56 |
| 22:B:603:CLA:HAB | 22:B:605:CLA:H171 | 1.88 | 0.56 |
| 3:C:293:THR:HG22 | 3:C:295:PRO:HD2 | 1.87 | 0.54 |
| 3:C:102:VAL:HG21 | 22:C:505:CLA:HMA3 | 1.90 | 0.54 |
| 5:E:27:ILE:HB | 5:E:28:PRO:HD3 | 1.89 | 0.54 |
| 22:C:505:CLA:HMD2 | 22:C:505:CLA:H191 | 1.89 | 0.54 |
| 3:C:108:ILE:HD11 | 23:C:518:BCR:H10C | 1.90 | 0.53 |
| 22:C:509:CLA:H72 | 22:C:509:CLA:H41 | 1.90 | 0.53 |
| 23:K:101:BCR:H23C | 23:K:101:BCR:H383 | 1.89 | 0.53 |
| 4:D:161:PRO:HG3 | 4:D:170:ALA:HB2 | 1.91 | 0.52 |
| 22:D:402:CLA:HAA1 | 22:D:402:CLA:CGD | 2.40 | 0.52 |
| 9:K:34:ALA:HB1 | 23:K:101:BCR:C21 | 2.39 | 0.52 |
| 22:B:614:CLA:HAA1 | 22:B:614:CLA:CGD | 2.39 | 0.52 |
| 1:A:231:GLU:HB2 | 1:A:234:ASN:OD1 | 2.10 | 0.52 |
| 22:A:406:CLA:HBB1 | 22:A:406:CLA:HMB1 | 1.91 | 0.52 |
| 22:C:510:CLA:CMA | 22:C:511:CLA:HMC3 | 2.41 | 0.51 |
| 1:A:12:ASN:O | 1:A:14:TRP:N | 2.43 | 0.51 |
| 22:B:604:CLA:H72 | 22:B:604:CLA:H41 | 1.92 | 0.51 |
| 3:C:405:VAL:HG22 | 3:C:407:PHE:H | 1.76 | 0.51 |
| 4:D:148:ALA:HB3 | 4:D:149:PRO:HD3 | 1.92 | 0.51 |
| 3:C:253:ILE:HG22 | 3:C:255:SER:H | 1.76 | 0.51 |
| 4:D:233:ARG:HA | 4:D:234:ALA:O | 2.11 | 0.51 |
| 22:B:609:CLA:C2B | 23:H:101:BCR:H333 | 2.38 | 0.51 |
| 25:D:403:LMG:H453 | 10:L:24:ILE:HD12 | 1.94 | 0.50 |
| 27:E:101:HEM:HBB2 | 27:E:101:HEM:CMB | 2.41 | 0.50 |
| 9:K:25:LEU:CD2 | 23:K:101:BCR:H322 | 2.41 | 0.50 |
| 23:B:619:BCR:C8 | 23:B:619:BCR:H331 | 2.41 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:D:405:PL9:H202 | 26:D:405:PL9:H162 | 1.93 | 0.50 |
| 6:F:28:VAL:HG23 | 6:F:29:PRO:HD3 | 1.93 | 0.50 |
| 1:A:59:ASP:O | 1:A:86:SER:HB3 | 2.11 | 0.49 |
| 4:D:234:ALA:HA | 4:D:235:PHE:HB2 | 1.94 | 0.49 |
| 23:B:617:BCR:H392 | 23:B:617:BCR:H23C | 1.95 | 0.49 |
| 4:D:240:ALA:O | 4:D:241:GLU:HB2 | 2.12 | 0.49 |
| 22:C:503:CLA:H203 | 22:C:509:CLA:HMB3 | 1.95 | 0.49 |
| 1:A:341:LEU:CD1 | 3:C:385:THR:HG22 | 2.43 | 0.48 |
| 22:B:608:CLA:HBA1 | 22:B:608:CLA:HBD | 1.95 | 0.48 |
| 3:C:389:LEU:O | 3:C:408:VAL:HG23 | 2.13 | 0.48 |
| 21:D:406:PHO:HBB1 | 21:D:406:PHO:HMB1 | 1.95 | 0.48 |
| 9:K:43:VAL:HG12 | 9:K:43:VAL:O | 2.13 | 0.48 |
| 22:B:609:CLA:H41 | 7:H:31:MET:SD | 2.54 | 0.48 |
| 22:B:613:CLA:OBD | 22:B:614:CLA:HHC | 2.14 | 0.48 |
| 4:D:279:LEU:HD22 | 22:D:407:CLA:HBA2 | 1.96 | 0.48 |
| 22:D:408:CLA:HAA1 | 22:D:408:CLA:CGD | 2.44 | 0.48 |
| 22:B:613:CLA:OBD | 22:B:614:CLA:CAB | 2.62 | 0.47 |
| 11:M:21:PHE:CE1 | 11:M:25:LEU:HD11 | 2.48 | 0.47 |
| 4:D:201:VAL:HG11 | 22:D:401:CLA:C3D | 2.44 | 0.47 |
| 5:E:14:ILE:HD12 | 5:E:19:TYR:CZ | 2.49 | 0.47 |
| 23:H:101:BCR:C8 | 23:H:101:BCR:H311 | 2.44 | 0.47 |
| 21:D:406:PHO:HMB1 | 21:D:406:PHO:CBB | 2.45 | 0.47 |
| 3:C:316:VAL:HB | 3:C:319:ALA:HB3 | 1.97 | 0.47 |
| 1:A:340:PRO:O | 1:A:341:LEU:HG | 2.15 | 0.47 |
| 23:K:101:BCR:C8 | 23:K:101:BCR:H311 | 2.42 | 0.47 |
| 22:B:609:CLA:HHC | 22:B:609:CLA:HBB1 | 1.96 | 0.47 |
| 4:D:57:SER:HB3 | 4:D:79:SER:OG | 2.15 | 0.47 |
| 22:B:609:CLA:O2A | 22:B:610:CLA:HMC3 | 2.15 | 0.46 |
| 1:A:13:LEU:HA | 1:A:16:ARG:HE | 1.79 | 0.46 |
| 22:B:612:CLA:H93 | 22:B:612:CLA:CGA | 2.45 | 0.46 |
| 3:C:77:ILE:N | 3:C:78:PRO:CD | 2.78 | 0.46 |
| 3:C:53:GLY:O | 3:C:56:THR:HG22 | 2.16 | 0.46 |
| 4:D:343:GLU:H | 4:D:343:GLU:CD | 2.18 | 0.46 |
| 22:B:610:CLA:HAA1 | 22:B:610:CLA:CGD | 2.46 | 0.46 |
| 22:C:510:CLA:HMA3 | 22:C:511:CLA:HMC3 | 1.97 | 0.46 |
| 1:A:341:LEU:HD12 | 3:C:385:THR:HG22 | 1.97 | 0.46 |
| 3:C:56:THR:CG2 | 3:C:103:GLY:HA2 | 2.45 | 0.46 |
| 23:H:101:BCR:H23C | 23:H:101:BCR:H383 | 1.91 | 0.46 |
| 22:A:406:CLA:HMA2 | 22:A:406:CLA:HBA2 | 1.98 | 0.46 |
| 2:B:47:PRO:HG3 | 2:B:78:TRP:CD2 | 2.51 | 0.45 |
| 3:C:79:HIS:CE1 | 22:C:504:CLA:HAA2 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:B:601:CLA:HMC3 | 23:H:101:BCR:H15C | 1.98 | 0.45 |
| 3:C:42:VAL:HG23 | 22:C:513:CLA:HED1 | 1.97 | 0.45 |
| 5:E:10:PHE:HA | 5:E:13:ILE:HB | 1.99 | 0.45 |
| 26:D:405:PL9:H371 | 10:L:30:LEU:HB2 | 1.98 | 0.45 |
| 3:C:224:GLY:O | 3:C:228:ILE:HG13 | 2.16 | 0.45 |
| 16:2:28:ASP:N | 16:2:28:ASP:OD1 | 2.50 | 0.45 |
| 17:3:10:ARG:CZ | 25:3:101:LMG:HC4 | 2.47 | 0.45 |
| 23:A:407:BCR:C8 | 23:A:407:BCR:H331 | 2.47 | 0.44 |
| 4:D:340:VAL:HG23 | 4:D:340:VAL:O | 2.17 | 0.44 |
| 3:C:200:TYR:O | 3:C:211:TRP:O | 2.36 | 0.44 |
| 23:C:515:BCR:H371 | 23:C:515:BCR:H24C | 1.78 | 0.44 |
| 8:I:11:VAL:HG12 | 25:I:101:LMG:H273 | 2.00 | 0.44 |
| 15:Z:4:LEU:HA | 15:Z:7:LEU:HG | 2.00 | 0.44 |
| 3:C:277:PHE:CE1 | 3:C:281:ASN:ND2 | 2.85 | 0.44 |
| 4:D:152:VAL:HG21 | 22:D:407:CLA:HBA1 | 1.98 | 0.44 |
| 5:E:82:GLN:O | 5:E:83:LEU:HB2 | 2.17 | 0.44 |
| 22:C:503:CLA:CMB | 22:C:503:CLA:H93 | 2.48 | 0.44 |
| 22:B:603:CLA:HMB1 | 22:B:603:CLA:CBB | 2.48 | 0.44 |
| 3:C:155:VAL:HG21 | 22:C:513:CLA:HMA1 | 2.00 | 0.44 |
| 22:D:401:CLA:HMA2 | 25:3:101:LMG:H271 | 2.00 | 0.44 |
| 22:B:609:CLA:C1B | 23:H:101:BCR:H333 | 2.48 | 0.43 |
| 1:A:41:LEU:CD1 | 1:A:122:GLY:HA3 | 2.48 | 0.43 |
| 1:A:60:ILE:HA | 1:A:86:SER:HA | 2.00 | 0.43 |
| 22:B:612:CLA:HAA2 | 22:B:613:CLA:HMB2 | 1.99 | 0.43 |
| 22:B:615:CLA:HBA1 | 22:B:615:CLA:HMA2 | 2.00 | 0.43 |
| 22:C:514:CLA:HAA1 | 22:C:514:CLA:CGD | 2.48 | 0.43 |
| 22:C:517:CLA:HAA1 | 22:C:517:CLA:CGD | 2.48 | 0.43 |
| 22:B:604:CLA:H93 | 22:B:606:CLA:HMB1 | 2.00 | 0.43 |
| 1:A:258:LEU:HD12 | 1:A:258:LEU:N | 2.33 | 0.43 |
| 4:D:179:PHE:HA | 4:D:182:LEU:HD12 | 2.01 | 0.43 |
| 11:M:21:PHE:CZ | 11:M:25:LEU:HD11 | 2.53 | 0.43 |
| 2:B:458:PHE:CE1 | 22:B:613:CLA:H101 | 2.53 | 0.43 |
| 22:B:609:CLA:HMA2 | 22:B:609:CLA:HBA2 | 2.00 | 0.43 |
| 22:D:407:CLA:HBB1 | 22:D:407:CLA:HHC | 2.01 | 0.43 |
| 9:K:45:PHE:C | 9:K:46:ARG:O | 2.57 | 0.43 |
| 2:B:120:LEU:HA | 7:H:3:ARG:H | 1.83 | 0.43 |
| 23:F:102:BCR:C8 | 23:F:102:BCR:H331 | 2.48 | 0.42 |
| 16:2:17:VAL:HG21 | 16:2:41:PRO:HA | 2.01 | 0.42 |
| 23:H:101:BCR:HC31 | 23:H:101:BCR:H323 | 1.82 | 0.42 |
| 9:K:43:VAL:O | 9:K:43:VAL:CG1 | 2.67 | 0.42 |
| 2:B:384:ARG:HH12 | 4:D:348:ARG:HH11 | 1.67 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:300:ALA:O | 3:C:304:THR:HG22 | 2.20 | 0.42 |
| 23:H:101:BCR:C38 | 23:H:101:BCR:C23 | 2.82 | 0.42 |
| 22:B:603:CLA:H92 | 22:B:605:CLA:H122 | 2.01 | 0.42 |
| 3:C:77:ILE:HA | 3:C:80:ILE:HD12 | 2.01 | 0.42 |
| 4:D:274:VAL:HG22 | 26:D:405:PL9:H253 | 2.01 | 0.42 |
| 3:C:73:GLY:HA3 | 22:C:506:CLA:HBA1 | 2.01 | 0.42 |
| 8:I:3:THR:HG21 | 25:I:101:LMG:HC1 | 2.02 | 0.42 |
| 3:C:102:VAL:HA | 3:C:105:VAL:HG22 | 2.01 | 0.42 |
| 16:2:27:ARG:O | 16:2:28:ASP:O | 2.38 | 0.42 |
| 3:C:228:ILE:HD11 | 23:C:516:BCR:H392 | 2.02 | 0.42 |
| 1:A:47:CYS:SG | 1:A:115:ILE:HG13 | 2.59 | 0.42 |
| 2:B:124:ARG:HH11 | 2:B:124:ARG:HG3 | 1.85 | 0.42 |
| 22:C:505:CLA:HMD2 | 22:C:505:CLA:C19 | 2.49 | 0.42 |
| 3:C:56:THR:HG21 | 3:C:103:GLY:HA2 | 2.03 | 0.41 |
| 3:C:347:TRP:CD1 | 3:C:347:TRP:N | 2.89 | 0.41 |
| 4:D:68:LEU:HD11 | 5:E:44:TYR:CE2 | 2.55 | 0.41 |
| 2:B:7:ARG:HA | 22:B:611:CLA:HBA1 | 2.01 | 0.41 |
| 10:L:36:PHE:O | 10:L:37:ASN:O | 2.38 | 0.41 |
| 23:B:617:BCR:C8 | 23:B:617:BCR:H331 | 2.51 | 0.41 |
| 22:C:511:CLA:H202 | 22:C:513:CLA:HMD2 | 2.02 | 0.41 |
| 4:D:44:ALA:HB1 | 21:D:406:PHO:H92 | 2.01 | 0.41 |
| 1:A:129:ARG:HH12 | 25:D:404:LMG:H441 | 1.86 | 0.41 |
| 23:C:516:BCR:H20C | 23:C:516:BCR:H361 | 1.87 | 0.41 |
| 23:K:101:BCR:H331 | 23:K:101:BCR:HC7 | 1.50 | 0.41 |
| 17:3:42:LEU:HA | 17:3:45:VAL:CG1 | 2.51 | 0.41 |
| 21:A:404:PHO:HMB1 | 21:A:404:PHO:CBB | 2.51 | 0.41 |
| 2:B:358:ARG:CZ | 2:B:427:GLY:HA2 | 2.51 | 0.41 |
| 22:B:609:CLA:C1B | 23:H:101:BCR:HC42 | 2.51 | 0.41 |
| 27:E:101:HEM:C4D | 6:F:24:HIS:HE1 | 2.39 | 0.41 |
| 15:Z:2:THR:CG2 | 15:Z:4:LEU:HD23 | 2.51 | 0.41 |
| 3:C:27:ASN:OD1 | 22:C:510:CLA:H42 | 2.21 | 0.40 |
| 3:C:97:PHE:HB3 | 3:C:98:PRO:HD3 | 2.03 | 0.40 |
| 22:C:503:CLA:H2 | 22:C:504:CLA:OBD | 2.22 | 0.40 |
| 3:C:54:ALA:HB1 | 9:K:25:LEU:HB3 | 2.04 | 0.40 |
| 4:D:90:LEU:HD12 | 4:D:112:THR:HG21 | 2.04 | 0.40 |
| 6:F:44:GLN:CD | 6:F:44:GLN:H | 2.25 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | A | 333/360 (92%) | 314 (94%) | 17 (5%) | 2 (1%) | 25 | 47 |
| 2 | B | 494/510 (97%) | 470 (95%) | 23 (5%) | 1 (0%) | 47 | 71 |
| 3 | C | 430/461 (93%) | 405 (94%) | 25 (6%) | 0 | 100 | 100 |
| 4 | D | 339/352 (96%) | 321 (95%) | 17 (5%) | 1 (0%) | 41 | 64 |
| 5 | E | 75/84 (89%) | 71 (95%) | 4 (5%) | 0 | 100 | 100 |
| 6 | F | 36/45 (80%) | 32 (89%) | 4 (11%) | 0 | 100 | 100 |
| 7 | H | 63/66 (96%) | 57 (90%) | 5 (8%) | 1 (2%) | 9 | 22 |
| 8 | I | 24/38 (63%) | 24 (100%) | 0 | 0 | 100 | 100 |
| 9 | K | 35/46 (76%) | 33 (94%) | 2 (6%) | 0 | 100 | 100 |
| 10 | L | 35/37 (95%) | 34 (97%) | 1 (3%) | 0 | 100 | 100 |
| 11 | M | 32/36 (89%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 12 | T | 26/32 (81%) | 24 (92%) | 2 (8%) | 0 | 100 | 100 |
| 13 | X | 33/41 (80%) | 32 (97%) | 1 (3%) | 0 | 100 | 100 |
| 14 | y | 26/46 (56%) | 22 (85%) | 4 (15%) | 0 | 100 | 100 |
| 15 | Z | 58/62 (94%) | 57 (98%) | 1 (2%) | 0 | 100 | 100 |
| 16 | 2 | 110/116 (95%) | 102 (93%) | 6 (6%) | 2 (2%) | 8 | 19 |
| 17 | 3 | 54/56 (96%) | 53 (98%) | 1 (2%) | 0 | 100 | 100 |
| All | All | 2203/2388 (92%) | 2083 (95%) | 113 (5%) | 7 (0%) | 44 | 64 |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 491 | VAL |
| 4 | D | 240 | ALA |
| 16 | 2 | 28 | ASP |
| 1 | A | 13 | LEU |
| 16 | 2 | 27 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 340 | PRO |
| 7 | H | 18 | TYR |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1 | A | 271/291 (93%) | 264 (97%) | 7 (3%) | 46 | 73 |
| 2 | B | 395/407 (97%) | 391 (99%) | 4 (1%) | 76 | 90 |
| 3 | C | 335/362 (92%) | 330 (98%) | 5 (2%) | 65 | 84 |
| 4 | D | 276/283 (98%) | 273 (99%) | 3 (1%) | 73 | 89 |
| 5 | E | 69/73 (94%) | 68 (99%) | 1 (1%) | 67 | 85 |
| 6 | F | 32/39 (82%) | 31 (97%) | 1 (3%) | 40 | 67 |
| 7 | H | 54/55 (98%) | 54 (100%) | 0 | 100 | 100 |
| 8 | I | 24/35 (69%) | 22 (92%) | 2 (8%) | 11 | 23 |
| 9 | K | 30/37 (81%) | 29 (97%) | 1 (3%) | 38 | 64 |
| 10 | L | 35/35 (100%) | 35 (100%) | 0 | 100 | 100 |
| 11 | M | 31/33 (94%) | 31 (100%) | 0 | 100 | 100 |
| 12 | T | 25/29 (86%) | 25 (100%) | 0 | 100 | 100 |
| 13 | X | 28/34 (82%) | 27 (96%) | 1 (4%) | 35 | 61 |
| 14 | y | 21/37 (57%) | 18 (86%) | 3 (14%) | 3 | 7 |
| 15 | Z | 50/52 (96%) | 48 (96%) | 2 (4%) | 31 | 57 |
| 16 | 2 | 94/97 (97%) | 88 (94%) | 6 (6%) | 17 | 36 |
| 17 | 3 | 42/42 (100%) | 40 (95%) | 2 (5%) | 25 | 49 |
| All | All | 1812/1941 (93%) | 1774 (98%) | 38 (2%) | 56 | 78 |

All (38) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 10 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 113 | GLN |
| 1 | A | 266 | ASN |
| 1 | A | 267 | ASN |
| 1 | A | 305 | SER |
| 1 | A | 333 | GLU |
| 1 | A | 335 | ASN |
| 2 | B | 246 | PHE |
| 2 | B | 256 | MET |
| 2 | B | 362 | PHE |
| 2 | B | 476 | ARG |
| 3 | C | 38 | LEU |
| 3 | C | 74 | LEU |
| 3 | C | 277 | PHE |
| 3 | C | 350 | ARG |
| 3 | C | 394 | SER |
| 4 | D | 139 | ARG |
| 4 | D | 186 | GLN |
| 4 | D | 277 | THR |
| 5 | E | 45 | ASP |
| 6 | F | 8 | GLN |
| 8 | I | 3 | THR |
| 8 | I | 19 | PHE |
| 9 | K | 13 | GLU |
| 13 | X | 21 | LEU |
| 14 | y | 21 | GLN |
| 14 | y | 24 | MET |
| 14 | y | 42 | ARG |
| 15 | Z | 16 | SER |
| 15 | Z | 46 | LEU |
| 16 | 2 | 16 | GLU |
| 16 | 2 | 20 | ASP |
| 16 | 2 | 22 | ARG |
| 16 | 2 | 28 | ASP |
| 16 | 2 | 59 | GLU |
| 16 | 2 | 87 | ARG |
| 17 | 3 | 7 | GLU |
| 17 | 3 | 10 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 92 | HIS |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 3 are monoatomic - leaving 57 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 |
| 23 | BCR | C | 515 | - | 41,41,41 | 1.01 | 2 (4%) | 56,56,56 | 1.45 | 12 (21%) |
| 22 | CLA | B | 602 | - | 65,73,73 | 1.62 | 9 (13%) | 76,113,113 | 2.53 | 21 (27%) |
| 22 | CLA | B | 601 | - | 65,73,73 | 1.66 | 10 (15%) | 76,113,113 | 2.54 | 19 (25%) |
| 25 | LMG | C | 501 | - | 55,55,55 | 0.91 | 0 | 63,63,63 | 1.13 | 5 (7%) |
| 22 | CLA | B | 604 | - | 65,73,73 | 1.61 | 9 (13%) | 76,113,113 | 2.77 | 19 (25%) |
| 23 | BCR | K | 101 | - | 41,41,41 | 2.83 | 10 (24%) | 56,56,56 | 3.77 | 31 (55%) |
| 22 | CLA | B | 613 | - | 65,73,73 | 1.72 | 10 (15%) | 76,113,113 | 2.81 | 25 (32%) |
| 23 | BCR | A | 407 | - | 41,41,41 | 0.91 | 2 (4%) | 56,56,56 | 1.08 | 3 (5%) |
| 27 | HEM | E | 101 | 6,5 | 41,50,50 | 1.45 | 3 (7%) | 45,82,82 | 1.08 | 1 (2%) |
| 22 | CLA | B | 605 | - | 65,73,73 | 1.50 | 11 (16%) | 76,113,113 | 2.35 | 17 (22%) |
| 22 | CLA | B | 608 | - | 65,73,73 | 1.72 | 11 (16%) | 76,113,113 | 2.62 | 23 (30%) |
| 26 | PL9 | D | 405 | - | 55,55,55 | 1.12 | 3 (5%) | 68,69,69 | 1.41 | 11 (16%) |
| 22 | CLA | B | 614 | - | 65,73,73 | 1.73 | 12 (18%) | 76,113,113 | 2.65 | 23 (30%) |
| 22 | CLA | B | 616 | - | 65,73,73 | 1.80 | 12 (18%) | 76,113,113 | 3.08 | 22 (28%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 25 | LMG | I | 101 | - | 55,55,55 | 0.98 | 2 (3%) | 63,63,63 | 1.09 | 3 (4%) |
| 22 | CLA | C | 504 | - | 65,73,73 | 1.59 | 12 (18%) | 76,113,113 | 2.19 | 17 (22%) |
| 23 | BCR | B | 618 | - | 41,41,41 | 1.00 | 1 (2%) | 56,56,56 | 1.14 | 5 (8%) |
| 25 | LMG | D | 403 | - | 55,55,55 | 0.96 | 2 (3%) | 63,63,63 | 1.05 | 3 (4%) |
| 23 | BCR | B | 619 | - | 41,41,41 | 0.92 | 2 (4%) | 56,56,56 | 1.26 | 8 (14%) |
| 22 | CLA | A | 406 | - | 65,73,73 | 1.57 | 9 (13%) | 76,113,113 | 2.27 | 19 (25%) |
| 25 | LMG | D | 404 | - | 55,55,55 | 0.97 | 2 (3%) | 63,63,63 | 1.08 | 4 (6%) |
| 22 | CLA | D | 401 | - | 65,73,73 | 1.55 | 9 (13%) | 76,113,113 | 2.13 | 22 (28%) |
| 22 | CLA | C | 514 | - | 65,73,73 | 1.77 | 10 (15%) | 76,113,113 | 2.35 | 19 (25%) |
| 23 | BCR | C | 516 | - | 41,41,41 | 0.93 | 1 (2%) | 56,56,56 | 1.20 | 9 (16%) |
| 23 | BCR | H | 101 | - | 41,41,41 | 3.05 | 11 (26%) | 56,56,56 | 3.99 | 30 (53%) |
| 24 | LHG | A | 408 | - | 48,48,48 | 0.82 | 1 (2%) | 51,54,54 | 0.90 | 2 (3%) |
| 23 | BCR | F | 102 | - | 41,41,41 | 0.84 | 0 | 56,56,56 | 1.18 | 8 (14%) |
| 22 | CLA | B | 606 | - | 65,73,73 | 1.57 | 11 (16%) | 76,113,113 | 2.30 | 26 (34%) |
| 22 | CLA | B | 609 | - | 65,73,73 | 1.79 | 9 (13%) | 76,113,113 | 2.75 | 20 (26%) |
| 22 | CLA | A | 405 | - | 65,73,73 | 1.62 | 9 (13%) | 76,113,113 | 2.18 | 21 (27%) |
| 22 | CLA | B | 615 | - | 65,73,73 | 1.71 | 8 (12%) | 76,113,113 | 2.64 | 23 (30%) |
| 22 | CLA | C | 507 | - | 65,73,73 | 1.83 | 13 (20%) | 76,113,113 | 2.82 | 25 (32%) |
| 22 | CLA | C | 511 | - | 65,73,73 | 1.64 | 9 (13%) | 76,113,113 | 2.64 | 21 (27%) |
| 22 | CLA | C | 513 | - | 65,73,73 | 1.65 | 9 (13%) | 76,113,113 | 2.80 | 24 (31%) |
| 22 | CLA | B | 610 | - | 65,73,73 | 1.67 | 13 (20%) | 76,113,113 | 2.84 | 24 (31%) |
| 22 | CLA | B | 607 | - | 65,73,73 | 1.58 | 9 (13%) | 76,113,113 | 2.23 | 25 (32%) |
| 22 | CLA | C | 503 | - | 65,73,73 | 1.69 | 11 (16%) | 76,113,113 | 1.90 | 24 (31%) |
| 25 | LMG | 3 | 101 | - | 55,55,55 | 0.92 | 1 (1%) | 63,63,63 | 1.08 | 5 (7%) |
| 22 | CLA | C | 505 | - | 65,73,73 | 1.58 | 10 (15%) | 76,113,113 | 2.90 | 27 (35%) |
| 22 | CLA | C | 509 | - | 65,73,73 | 1.61 | 11 (16%) | 76,113,113 | 2.49 | 15 (19%) |
| 22 | CLA | D | 402 | - | 65,73,73 | 1.62 | 10 (15%) | 76,113,113 | 2.44 | 26 (34%) |
| 22 | CLA | B | 611 | - | 65,73,73 | 1.70 | 9 (13%) | 76,113,113 | 2.42 | 23 (30%) |
| 25 | LMG | F | 101 | - | 55,55,55 | 1.02 | 2 (3%) | 63,63,63 | 1.00 | 3 (4%) |
| 22 | CLA | C | 510 | 22 | 65,73,73 | 1.79 | 13 (20%) | 76,113,113 | 2.70 | 22 (28%) |
| 21 | PHO | A | 404 | - | 51,69,69 | 1.04 | 5 (9%) | 47,99,99 | 1.22 | 5 (10%) |
| 22 | CLA | D | 408 | - | 65,73,73 | 1.67 | 9 (13%) | 76,113,113 | 2.08 | 16 (21%) |
| 23 | BCR | C | 518 | - | 41,41,41 | 0.99 | 2 (4%) | 56,56,56 | 1.53 | 13 (23%) |
| 22 | CLA | C | 517 | 22 | 65,73,73 | 1.76 | 12 (18%) | 76,113,113 | 2.94 | 28 (36%) |
| 22 | CLA | C | 512 | - | 65,73,73 | 1.79 | 11 (16%) | 76,113,113 | 2.75 | 23 (30%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | CLA | D | 407 | - | 65,73,73 | 1.62 | 10 (15%) | 76,113,113 | 2.05 | 21 (27%) |
| 23 | BCR | B | 617 | - | 41,41,41 | 0.98 | 2 (4%) | 56,56,56 | 1.27 | 7 (12%) |
| 25 | LMG | C | 502 | - | 55,55,55 | 1.06 | 3 (5%) | 63,63,63 | 0.99 | 5 (7%) |
| 21 | PHO | D | 406 | - | 51,69,69 | 1.08 | 5 (9%) | 47,99,99 | 1.28 | 6 (12%) |
| 22 | CLA | C | 508 | - | 65,73,73 | 1.78 | 12 (18%) | 76,113,113 | 2.13 | 18 (23%) |
| 22 | CLA | B | 612 | - | 65,73,73 | 1.66 | 15 (23%) | 76,113,113 | 2.88 | 26 (34%) |
| 22 | CLA | B | 603 | - | 65,73,73 | 1.54 | 8 (12%) | 76,113,113 | 2.33 | 20 (26%) |
| 22 | CLA | C | 506 | - | 65,73,73 | 1.57 | 12 (18%) | 76,113,113 | 2.44 | 18 (23%) |

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 |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 23 | BCR | C | 515 | - | - | 9/29/63/63 | 0/2/2/2 |
| 22 | CLA | B | 602 | - | 2/2/15/20 | 11/37/115/115 | - |
| 22 | CLA | B | 601 | - | 3/3/15/20 | 9/37/115/115 | - |
| 25 | LMG | C | 501 | - | - | 18/50/70/70 | 0/1/1/1 |
| 22 | CLA | B | 604 | - | 1/1/15/20 | 7/37/115/115 | - |
| 23 | BCR | K | 101 | - | - | 15/29/63/63 | 0/2/2/2 |
| 22 | CLA | B | 613 | - | 3/3/15/20 | 8/37/115/115 | - |
| 23 | BCR | A | 407 | - | - | 8/29/63/63 | 0/2/2/2 |
| 27 | HEM | E | 101 | 6,5 | - | 4/12/54/54 | - |
| 22 | CLA | B | 605 | - | 2/2/15/20 | 9/37/115/115 | - |
| 22 | CLA | B | 608 | - | - | 6/37/115/115 | - |
| 26 | PL9 | D | 405 | - | - | 14/53/73/73 | 0/1/1/1 |
| 22 | CLA | B | 614 | - | 3/3/15/20 | 9/37/115/115 | - |
| 22 | CLA | B | 616 | - | 4/4/15/20 | 9/37/115/115 | - |
| 25 | LMG | I | 101 | - | - | 5/50/70/70 | 0/1/1/1 |
| 22 | CLA | C | 504 | - | 2/2/15/20 | 13/37/115/115 | - |
| 23 | BCR | B | 618 | - | - | 5/29/63/63 | 0/2/2/2 |
| 25 | LMG | D | 403 | - | - | 5/50/70/70 | 0/1/1/1 |
| 23 | BCR | B | 619 | - | - | 6/29/63/63 | 0/2/2/2 |
| 22 | CLA | A | 406 | - | 2/2/15/20 | 10/37/115/115 | - |
| 25 | LMG | D | 404 | - | - | 11/50/70/70 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22 | CLA | D | 401 | - | - | 13/37/115/115 | - |
| 22 | CLA | C | 514 | - | 3/3/15/20 | 10/37/115/115 | - |
| 23 | BCR | C | 516 | - | - | 14/29/63/63 | 0/2/2/2 |
| 23 | BCR | H | 101 | - | - | 15/29/63/63 | 0/2/2/2 |
| 24 | LHG | A | 408 | - | - | 7/53/53/53 | - |
| 23 | BCR | F | 102 | - | - | 3/29/63/63 | 0/2/2/2 |
| 22 | CLA | B | 606 | - | 2/2/15/20 | 14/37/115/115 | - |
| 22 | CLA | B | 609 | - | 2/2/15/20 | 7/37/115/115 | - |
| 22 | CLA | A | 405 | - | 2/2/15/20 | 12/37/115/115 | - |
| 22 | CLA | B | 615 | - | 3/3/15/20 | 10/37/115/115 | - |
| 22 | CLA | C | 507 | - | 2/2/15/20 | 11/37/115/115 | - |
| 22 | CLA | C | 511 | - | 3/3/15/20 | 9/37/115/115 | - |
| 22 | CLA | C | 513 | - | 3/3/15/20 | 4/37/115/115 | - |
| 22 | CLA | B | 610 | - | 2/2/15/20 | 9/37/115/115 | - |
| 22 | CLA | B | 607 | - | 2/2/15/20 | 12/37/115/115 | - |
| 22 | CLA | C | 503 | - | - | 7/37/115/115 | - |
| 25 | LMG | 3 | 101 | - | - | 8/50/70/70 | 0/1/1/1 |
| 22 | CLA | C | 505 | - | 1/1/15/20 | 17/37/115/115 | - |
| 22 | CLA | C | 509 | - | 2/2/15/20 | 8/37/115/115 | - |
| 22 | CLA | D | 402 | - | 2/2/15/20 | 9/37/115/115 | - |
| 22 | CLA | B | 611 | - | 1/1/15/20 | 13/37/115/115 | - |
| 25 | LMG | F | 101 | - | - | 7/50/70/70 | 0/1/1/1 |
| 22 | CLA | C | 510 | 22 | 1/1/15/20 | 12/37/115/115 | - |
| 21 | PHO | A | 404 | - | 1/1/17/22 | 7/37/103/103 | 0/5/6/6 |
| 22 | CLA | D | 408 | - | 3/3/15/20 | 5/37/115/115 | - |
| 23 | BCR | C | 518 | - | - | 9/29/63/63 | 0/2/2/2 |
| 22 | CLA | C | 517 | 22 | 3/3/15/20 | 11/37/115/115 | - |
| 22 | CLA | C | 512 | - | 1/1/15/20 | 9/37/115/115 | - |
| 22 | CLA | D | 407 | - | 2/2/15/20 | 9/37/115/115 | - |
| 23 | BCR | B | 617 | - | - | 14/29/63/63 | 0/2/2/2 |
| 25 | LMG | C | 502 | - | - | 7/50/70/70 | 0/1/1/1 |
| 21 | PHO | D | 406 | - | 1/1/17/22 | 6/37/103/103 | 0/5/6/6 |
| 22 | CLA | C | 508 | - | 1/1/15/20 | 3/37/115/115 | - |
| 22 | CLA | B | 612 | - | 4/4/15/20 | 12/37/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|-------|
| 22 | CLA | B | 603 | - | 3/3/15/20 | 10/37/115/115 | - |
| 22 | CLA | C | 506 | - | 3/3/15/20 | 11/37/115/115 | - |

All (429) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 23 | H | 101 | BCR | C1-C6 | -9.89 | 1.40 | 1.53 |
| 23 | H | 101 | BCR | C5-C6 | -9.63 | 1.17 | 1.34 |
| 22 | B | 615 | CLA | C4B-NB | 9.42 | 1.43 | 1.35 |
| 22 | C | 514 | CLA | C4B-NB | 9.37 | 1.43 | 1.35 |
| 22 | C | 512 | CLA | C4B-NB | 9.23 | 1.43 | 1.35 |
| 23 | K | 101 | BCR | C1-C6 | -9.10 | 1.41 | 1.53 |
| 22 | D | 408 | CLA | C4B-NB | 9.08 | 1.43 | 1.35 |
| 22 | B | 609 | CLA | C4B-NB | 8.79 | 1.43 | 1.35 |
| 22 | B | 616 | CLA | C4B-NB | 8.75 | 1.43 | 1.35 |
| 22 | C | 508 | CLA | C4B-NB | 8.69 | 1.43 | 1.35 |
| 22 | A | 405 | CLA | C4B-NB | 8.66 | 1.42 | 1.35 |
| 22 | C | 511 | CLA | C4B-NB | 8.54 | 1.42 | 1.35 |
| 22 | C | 507 | CLA | C4B-NB | 8.46 | 1.42 | 1.35 |
| 22 | B | 601 | CLA | C4B-NB | 8.33 | 1.42 | 1.35 |
| 22 | C | 503 | CLA | C4B-NB | 8.32 | 1.42 | 1.35 |
| 22 | B | 607 | CLA | C4B-NB | 8.31 | 1.42 | 1.35 |
| 23 | K | 101 | BCR | C5-C6 | -8.27 | 1.20 | 1.34 |
| 22 | C | 513 | CLA | C4B-NB | 8.26 | 1.42 | 1.35 |
| 22 | B | 608 | CLA | C4B-NB | 8.24 | 1.42 | 1.35 |
| 22 | B | 604 | CLA | C4B-NB | 8.21 | 1.42 | 1.35 |
| 22 | B | 613 | CLA | C4B-NB | 8.09 | 1.42 | 1.35 |
| 22 | C | 517 | CLA | C4B-NB | 8.09 | 1.42 | 1.35 |
| 22 | D | 407 | CLA | C4B-NB | 8.06 | 1.42 | 1.35 |
| 22 | D | 401 | CLA | C4B-NB | 7.96 | 1.42 | 1.35 |
| 22 | D | 402 | CLA | C4B-NB | 7.90 | 1.42 | 1.35 |
| 22 | C | 509 | CLA | C4B-NB | 7.86 | 1.42 | 1.35 |
| 22 | B | 614 | CLA | C4B-NB | 7.86 | 1.42 | 1.35 |
| 22 | B | 611 | CLA | C4B-NB | 7.83 | 1.42 | 1.35 |
| 22 | C | 505 | CLA | C4B-NB | 7.83 | 1.42 | 1.35 |
| 22 | B | 610 | CLA | C4B-NB | 7.79 | 1.42 | 1.35 |
| 22 | C | 510 | CLA | C4B-NB | 7.76 | 1.42 | 1.35 |
| 22 | B | 606 | CLA | C4B-NB | 7.65 | 1.42 | 1.35 |
| 22 | C | 506 | CLA | C4B-NB | 7.56 | 1.42 | 1.35 |
| 23 | H | 101 | BCR | C33-C5 | -7.40 | 1.38 | 1.50 |
| 22 | B | 602 | CLA | C4B-NB | 7.38 | 1.41 | 1.35 |
| 22 | C | 504 | CLA | C4B-NB | 7.33 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | A | 406 | CLA | C4B-NB | 7.16 | 1.41 | 1.35 |
| 22 | B | 612 | CLA | C4B-NB | 7.13 | 1.41 | 1.35 |
| 22 | B | 605 | CLA | C4B-NB | 6.83 | 1.41 | 1.35 |
| 22 | B | 603 | CLA | C4B-NB | 6.71 | 1.41 | 1.35 |
| 23 | K | 101 | BCR | C33-C5 | -6.55 | 1.40 | 1.50 |
| 23 | H | 101 | BCR | C30-C25 | -6.47 | 1.44 | 1.53 |
| 23 | K | 101 | BCR | C30-C25 | -6.33 | 1.45 | 1.53 |
| 23 | H | 101 | BCR | C31-C1 | -5.30 | 1.43 | 1.53 |
| 23 | K | 101 | BCR | C31-C1 | -4.96 | 1.44 | 1.53 |
| 27 | E | 101 | HEM | C3C-C2C | -4.82 | 1.33 | 1.40 |
| 22 | C | 510 | CLA | C3D-CAD | 4.67 | 1.61 | 1.45 |
| 22 | B | 609 | CLA | C3D-C4D | 4.34 | 1.54 | 1.44 |
| 22 | B | 616 | CLA | C3D-C4D | 4.31 | 1.53 | 1.44 |
| 22 | C | 507 | CLA | C3D-CAD | 4.23 | 1.59 | 1.45 |
| 22 | C | 510 | CLA | C3D-C4D | 4.17 | 1.53 | 1.44 |
| 22 | B | 614 | CLA | C3D-CAD | 4.14 | 1.59 | 1.45 |
| 22 | C | 517 | CLA | C3D-CAD | 4.12 | 1.59 | 1.45 |
| 22 | C | 507 | CLA | C3D-C4D | 4.10 | 1.53 | 1.44 |
| 22 | B | 614 | CLA | C3D-C4D | 4.09 | 1.53 | 1.44 |
| 22 | C | 512 | CLA | C3D-C4D | 4.01 | 1.53 | 1.44 |
| 22 | B | 611 | CLA | C3D-CAD | 3.98 | 1.58 | 1.45 |
| 22 | B | 613 | CLA | C3D-CAD | 3.97 | 1.58 | 1.45 |
| 22 | C | 508 | CLA | C3D-CAD | 3.94 | 1.58 | 1.45 |
| 22 | B | 612 | CLA | CMD-C2D | -3.86 | 1.42 | 1.50 |
| 22 | B | 608 | CLA | C3D-CAD | 3.86 | 1.58 | 1.45 |
| 22 | B | 609 | CLA | C3D-CAD | 3.85 | 1.58 | 1.45 |
| 22 | B | 602 | CLA | CMD-C2D | -3.84 | 1.42 | 1.50 |
| 23 | K | 101 | BCR | C37-C22 | -3.81 | 1.43 | 1.50 |
| 23 | H | 101 | BCR | C37-C22 | -3.78 | 1.43 | 1.50 |
| 22 | C | 508 | CLA | C3D-C4D | 3.72 | 1.52 | 1.44 |
| 22 | B | 606 | CLA | CMD-C2D | -3.68 | 1.43 | 1.50 |
| 22 | C | 512 | CLA | C3D-CAD | 3.63 | 1.57 | 1.45 |
| 22 | B | 608 | CLA | C3D-C4D | 3.61 | 1.52 | 1.44 |
| 22 | B | 610 | CLA | C3D-C4D | 3.59 | 1.52 | 1.44 |
| 22 | C | 517 | CLA | C3D-C4D | 3.58 | 1.52 | 1.44 |
| 22 | B | 605 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 22 | B | 612 | CLA | CHC-C1C | 3.54 | 1.44 | 1.35 |
| 22 | C | 504 | CLA | C1D-ND | 3.53 | 1.42 | 1.37 |
| 22 | C | 508 | CLA | CHC-C1C | 3.53 | 1.44 | 1.35 |
| 22 | B | 603 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 22 | A | 405 | CLA | CHC-C1C | 3.49 | 1.43 | 1.35 |
| 22 | B | 615 | CLA | CHC-C1C | 3.49 | 1.43 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | B | 613 | CLA | C3D-C4D | 3.49 | 1.52 | 1.44 |
| 22 | C | 510 | CLA | CHC-C1C | 3.44 | 1.43 | 1.35 |
| 22 | C | 512 | CLA | CHC-C1C | 3.44 | 1.43 | 1.35 |
| 22 | B | 602 | CLA | CAA-C2A | -3.42 | 1.47 | 1.54 |
| 22 | C | 514 | CLA | C3D-C4D | 3.41 | 1.51 | 1.44 |
| 22 | B | 603 | CLA | C4D-ND | -3.41 | 1.33 | 1.37 |
| 22 | B | 615 | CLA | C1D-ND | 3.40 | 1.42 | 1.37 |
| 22 | B | 611 | CLA | C3D-C4D | 3.39 | 1.51 | 1.44 |
| 22 | C | 514 | CLA | CHC-C1C | 3.35 | 1.43 | 1.35 |
| 22 | B | 611 | CLA | CHC-C1C | 3.35 | 1.43 | 1.35 |
| 22 | B | 615 | CLA | C3D-C4D | 3.35 | 1.51 | 1.44 |
| 22 | C | 517 | CLA | CHC-C1C | 3.33 | 1.43 | 1.35 |
| 22 | C | 513 | CLA | CMD-C2D | -3.33 | 1.43 | 1.50 |
| 22 | B | 604 | CLA | C3D-C4D | 3.31 | 1.51 | 1.44 |
| 22 | C | 514 | CLA | C3D-CAD | 3.31 | 1.56 | 1.45 |
| 22 | D | 401 | CLA | CHC-C1C | 3.28 | 1.43 | 1.35 |
| 22 | C | 509 | CLA | C1D-ND | 3.28 | 1.41 | 1.37 |
| 22 | C | 507 | CLA | C1D-C2D | 3.28 | 1.51 | 1.45 |
| 22 | C | 512 | CLA | CMD-C2D | -3.28 | 1.43 | 1.50 |
| 22 | B | 616 | CLA | CMD-C2D | -3.28 | 1.43 | 1.50 |
| 22 | A | 406 | CLA | CHC-C1C | 3.27 | 1.43 | 1.35 |
| 22 | C | 511 | CLA | CHC-C1C | 3.27 | 1.43 | 1.35 |
| 22 | D | 402 | CLA | C1D-ND | 3.27 | 1.41 | 1.37 |
| 22 | B | 604 | CLA | CHC-C1C | 3.26 | 1.43 | 1.35 |
| 22 | C | 506 | CLA | C1D-ND | 3.26 | 1.41 | 1.37 |
| 22 | C | 505 | CLA | C1D-ND | 3.26 | 1.41 | 1.37 |
| 22 | B | 601 | CLA | CMD-C2D | -3.25 | 1.43 | 1.50 |
| 22 | B | 608 | CLA | CHC-C1C | 3.24 | 1.43 | 1.35 |
| 22 | A | 405 | CLA | C1D-ND | 3.23 | 1.41 | 1.37 |
| 22 | B | 616 | CLA | CHC-C1C | 3.22 | 1.43 | 1.35 |
| 22 | B | 609 | CLA | CAA-C2A | -3.21 | 1.48 | 1.54 |
| 22 | B | 608 | CLA | C1D-ND | 3.20 | 1.41 | 1.37 |
| 22 | B | 614 | CLA | CAA-C2A | -3.20 | 1.48 | 1.54 |
| 23 | B | 617 | BCR | C1-C6 | -3.19 | 1.49 | 1.53 |
| 22 | C | 510 | CLA | C1D-C2D | 3.19 | 1.51 | 1.45 |
| 22 | D | 408 | CLA | CHC-C1C | 3.17 | 1.43 | 1.35 |
| 22 | B | 610 | CLA | CMD-C2D | -3.17 | 1.44 | 1.50 |
| 22 | C | 503 | CLA | C1D-ND | 3.17 | 1.41 | 1.37 |
| 22 | B | 604 | CLA | CMD-C2D | -3.14 | 1.44 | 1.50 |
| 23 | K | 101 | BCR | C32-C1 | -3.14 | 1.47 | 1.53 |
| 22 | B | 603 | CLA | CHC-C1C | 3.14 | 1.43 | 1.35 |
| 22 | C | 507 | CLA | CHC-C1C | 3.13 | 1.43 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 27 | E | 101 | HEM | C3C-CAC | 3.13 | 1.54 | 1.47 |
| 22 | A | 406 | CLA | C1D-ND | 3.12 | 1.41 | 1.37 |
| 22 | B | 606 | CLA | CHC-C1C | 3.11 | 1.42 | 1.35 |
| 22 | B | 610 | CLA | CHC-C1C | 3.10 | 1.42 | 1.35 |
| 22 | B | 607 | CLA | CHC-C1C | 3.10 | 1.42 | 1.35 |
| 22 | B | 613 | CLA | CMD-C2D | -3.09 | 1.44 | 1.50 |
| 22 | C | 503 | CLA | CHC-C1C | 3.08 | 1.42 | 1.35 |
| 22 | B | 605 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |
| 22 | B | 602 | CLA | C3D-C4D | 3.08 | 1.51 | 1.44 |
| 22 | D | 408 | CLA | C4D-ND | -3.06 | 1.33 | 1.37 |
| 22 | B | 611 | CLA | C3B-C2B | -3.06 | 1.36 | 1.40 |
| 22 | B | 601 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 22 | B | 602 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 22 | B | 607 | CLA | CMD-C2D | -3.02 | 1.44 | 1.50 |
| 22 | C | 505 | CLA | C3D-C4D | 3.02 | 1.51 | 1.44 |
| 22 | C | 503 | CLA | C4D-ND | -3.02 | 1.33 | 1.37 |
| 22 | D | 402 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 22 | C | 505 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 22 | C | 503 | CLA | CMB-C2B | -3.02 | 1.45 | 1.51 |
| 22 | B | 611 | CLA | CMD-C2D | -3.01 | 1.44 | 1.50 |
| 22 | C | 509 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 22 | C | 509 | CLA | CMD-C2D | -3.00 | 1.44 | 1.50 |
| 22 | C | 504 | CLA | CMD-C2D | -2.99 | 1.44 | 1.50 |
| 22 | C | 513 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 22 | D | 402 | CLA | CMB-C2B | -2.99 | 1.45 | 1.51 |
| 22 | C | 514 | CLA | CAA-C2A | -2.98 | 1.48 | 1.54 |
| 22 | C | 511 | CLA | C3D-C4D | 2.98 | 1.50 | 1.44 |
| 22 | C | 507 | CLA | C1D-ND | 2.98 | 1.41 | 1.37 |
| 22 | A | 406 | CLA | C4D-ND | -2.98 | 1.33 | 1.37 |
| 22 | B | 603 | CLA | CMD-C2D | -2.97 | 1.44 | 1.50 |
| 22 | C | 503 | CLA | C3B-C2B | -2.96 | 1.36 | 1.40 |
| 22 | B | 614 | CLA | CMD-C2D | -2.96 | 1.44 | 1.50 |
| 22 | C | 509 | CLA | C3D-C4D | 2.96 | 1.50 | 1.44 |
| 22 | B | 612 | CLA | C3B-CAB | -2.95 | 1.41 | 1.47 |
| 23 | B | 619 | BCR | C1-C6 | -2.94 | 1.49 | 1.53 |
| 22 | B | 613 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 22 | C | 506 | CLA | CMB-C2B | -2.93 | 1.45 | 1.51 |
| 22 | B | 610 | CLA | C1D-ND | 2.93 | 1.41 | 1.37 |
| 22 | B | 605 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 23 | B | 618 | BCR | C30-C25 | -2.93 | 1.49 | 1.53 |
| 26 | D | 405 | PL9 | C3-C4 | -2.92 | 1.44 | 1.49 |
| 22 | D | 408 | CLA | CMD-C2D | -2.91 | 1.44 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21 | A | 404 | PHO | CAC-C3C | -2.90 | 1.47 | 1.52 |
| 22 | B | 607 | CLA | C1D-ND | 2.90 | 1.41 | 1.37 |
| 21 | D | 406 | PHO | CAC-C3C | -2.89 | 1.47 | 1.52 |
| 22 | C | 503 | CLA | CMD-C2D | -2.89 | 1.44 | 1.50 |
| 22 | C | 510 | CLA | C1D-ND | 2.89 | 1.41 | 1.37 |
| 22 | D | 407 | CLA | CMB-C2B | -2.88 | 1.45 | 1.51 |
| 22 | A | 406 | CLA | MG-ND | -2.87 | 2.00 | 2.05 |
| 22 | C | 509 | CLA | C4D-ND | -2.86 | 1.33 | 1.37 |
| 22 | B | 601 | CLA | C3D-C4D | 2.85 | 1.50 | 1.44 |
| 22 | B | 609 | CLA | CHC-C1C | 2.85 | 1.42 | 1.35 |
| 22 | B | 616 | CLA | C1D-ND | 2.85 | 1.41 | 1.37 |
| 22 | C | 513 | CLA | C3D-C4D | 2.85 | 1.50 | 1.44 |
| 23 | C | 515 | BCR | C1-C6 | -2.84 | 1.49 | 1.53 |
| 22 | C | 506 | CLA | C4D-ND | -2.84 | 1.33 | 1.37 |
| 22 | D | 401 | CLA | CMD-C2D | -2.84 | 1.44 | 1.50 |
| 22 | C | 517 | CLA | CMD-C2D | -2.84 | 1.44 | 1.50 |
| 22 | C | 511 | CLA | CMB-C2B | -2.84 | 1.45 | 1.51 |
| 22 | C | 511 | CLA | CMD-C2D | -2.83 | 1.44 | 1.50 |
| 22 | C | 505 | CLA | C4D-ND | -2.83 | 1.33 | 1.37 |
| 22 | C | 508 | CLA | C3B-C2B | -2.83 | 1.36 | 1.40 |
| 22 | D | 407 | CLA | C3D-CAD | 2.82 | 1.54 | 1.45 |
| 22 | B | 616 | CLA | C3D-CAD | 2.82 | 1.54 | 1.45 |
| 22 | B | 615 | CLA | CMD-C2D | -2.82 | 1.44 | 1.50 |
| 22 | C | 517 | CLA | C1D-C2D | 2.81 | 1.50 | 1.45 |
| 22 | C | 513 | CLA | CMB-C2B | -2.81 | 1.45 | 1.51 |
| 22 | C | 507 | CLA | CMD-C2D | -2.80 | 1.44 | 1.50 |
| 22 | B | 614 | CLA | CHC-C1C | 2.80 | 1.42 | 1.35 |
| 24 | A | 408 | LHG | P-O6 | 2.79 | 1.70 | 1.59 |
| 22 | C | 511 | CLA | C3B-C2B | -2.79 | 1.36 | 1.40 |
| 22 | C | 508 | CLA | CMB-C2B | -2.79 | 1.45 | 1.51 |
| 22 | C | 504 | CLA | C4D-ND | -2.79 | 1.33 | 1.37 |
| 22 | B | 613 | CLA | CMB-C2B | -2.78 | 1.45 | 1.51 |
| 25 | F | 101 | LMG | C4-C5 | 2.77 | 1.58 | 1.53 |
| 22 | B | 604 | CLA | C3B-C2B | -2.76 | 1.36 | 1.40 |
| 22 | B | 609 | CLA | CMD-C2D | -2.76 | 1.44 | 1.50 |
| 22 | B | 611 | CLA | CMB-C2B | -2.76 | 1.45 | 1.51 |
| 22 | B | 606 | CLA | C3B-C2B | -2.76 | 1.36 | 1.40 |
| 22 | B | 610 | CLA | MG-NC | 2.76 | 2.12 | 2.06 |
| 22 | D | 407 | CLA | CMD-C2D | -2.76 | 1.45 | 1.50 |
| 22 | A | 406 | CLA | CMD-C2D | -2.75 | 1.45 | 1.50 |
| 22 | C | 508 | CLA | CMD-C2D | -2.75 | 1.45 | 1.50 |
| 22 | A | 405 | CLA | CMD-C2D | -2.75 | 1.45 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | C | 511 | CLA | C1D-ND | 2.75 | 1.41 | 1.37 |
| 22 | B | 612 | CLA | CMB-C2B | -2.74 | 1.45 | 1.51 |
| 22 | B | 605 | CLA | CMD-C2D | -2.74 | 1.45 | 1.50 |
| 22 | C | 514 | CLA | CMD-C2D | -2.74 | 1.45 | 1.50 |
| 22 | C | 504 | CLA | C3D-C4D | 2.73 | 1.50 | 1.44 |
| 22 | C | 510 | CLA | CMD-C2D | -2.72 | 1.45 | 1.50 |
| 22 | D | 402 | CLA | C1D-C2D | 2.71 | 1.50 | 1.45 |
| 22 | C | 506 | CLA | CMD-C2D | -2.70 | 1.45 | 1.50 |
| 22 | B | 610 | CLA | C3B-C2B | -2.70 | 1.36 | 1.40 |
| 22 | C | 510 | CLA | C3B-C2B | -2.69 | 1.36 | 1.40 |
| 22 | C | 506 | CLA | CHC-C1C | 2.68 | 1.41 | 1.35 |
| 22 | C | 507 | CLA | C3B-C2B | -2.68 | 1.36 | 1.40 |
| 22 | B | 616 | CLA | CMB-C2B | -2.68 | 1.46 | 1.51 |
| 26 | D | 405 | PL9 | C46-C44 | 2.68 | 1.56 | 1.51 |
| 22 | B | 614 | CLA | CMB-C2B | -2.67 | 1.46 | 1.51 |
| 22 | B | 601 | CLA | C3B-C2B | -2.65 | 1.36 | 1.40 |
| 22 | C | 505 | CLA | CMD-C2D | -2.65 | 1.45 | 1.50 |
| 23 | C | 518 | BCR | C1-C6 | -2.64 | 1.50 | 1.53 |
| 22 | C | 517 | CLA | CAA-C2A | -2.64 | 1.49 | 1.54 |
| 22 | B | 608 | CLA | C1D-C2D | 2.64 | 1.50 | 1.45 |
| 22 | C | 517 | CLA | C1B-NB | 2.63 | 1.37 | 1.35 |
| 22 | B | 601 | CLA | CMB-C2B | -2.63 | 1.46 | 1.51 |
| 22 | C | 517 | CLA | C1D-ND | 2.63 | 1.41 | 1.37 |
| 22 | A | 406 | CLA | CMB-C2B | -2.62 | 1.46 | 1.51 |
| 22 | B | 609 | CLA | CMB-C2B | -2.62 | 1.46 | 1.51 |
| 22 | D | 408 | CLA | C1D-ND | 2.62 | 1.41 | 1.37 |
| 22 | C | 508 | CLA | C1D-ND | 2.62 | 1.41 | 1.37 |
| 22 | B | 611 | CLA | C1D-C2D | 2.60 | 1.50 | 1.45 |
| 22 | B | 612 | CLA | MG-ND | -2.60 | 2.00 | 2.05 |
| 27 | E | 101 | HEM | CAB-C3B | 2.59 | 1.54 | 1.47 |
| 22 | B | 610 | CLA | CMB-C2B | -2.58 | 1.46 | 1.51 |
| 22 | C | 503 | CLA | MG-NA | 2.58 | 2.12 | 2.06 |
| 22 | D | 408 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 22 | B | 607 | CLA | C4D-ND | -2.56 | 1.34 | 1.37 |
| 22 | B | 602 | CLA | C1D-ND | 2.56 | 1.40 | 1.37 |
| 21 | A | 404 | PHO | CBD-CGD | -2.56 | 1.49 | 1.52 |
| 22 | B | 606 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 22 | B | 612 | CLA | C3D-C4D | 2.55 | 1.49 | 1.44 |
| 22 | B | 603 | CLA | CMB-C2B | -2.55 | 1.46 | 1.51 |
| 22 | D | 401 | CLA | CMB-C2B | -2.54 | 1.46 | 1.51 |
| 22 | B | 608 | CLA | C3B-C2B | -2.54 | 1.36 | 1.40 |
| 22 | D | 407 | CLA | C1D-ND | 2.54 | 1.40 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | B | 616 | CLA | C3B-C2B | -2.53 | 1.36 | 1.40 |
| 22 | D | 402 | CLA | C3B-C2B | -2.53 | 1.36 | 1.40 |
| 23 | H | 101 | BCR | C32-C1 | -2.52 | 1.48 | 1.53 |
| 22 | C | 503 | CLA | MG-ND | -2.52 | 2.00 | 2.05 |
| 22 | C | 504 | CLA | CHC-C1C | 2.52 | 1.41 | 1.35 |
| 22 | C | 517 | CLA | CMA-C3A | -2.52 | 1.47 | 1.53 |
| 22 | B | 616 | CLA | C1B-NB | 2.51 | 1.37 | 1.35 |
| 22 | B | 602 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 22 | C | 504 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 22 | B | 609 | CLA | C1D-ND | 2.49 | 1.40 | 1.37 |
| 22 | B | 613 | CLA | C1D-C2D | 2.49 | 1.50 | 1.45 |
| 22 | C | 512 | CLA | C1D-ND | 2.49 | 1.40 | 1.37 |
| 22 | B | 614 | CLA | C3B-C2B | -2.48 | 1.36 | 1.40 |
| 22 | B | 608 | CLA | CMD-C2D | -2.47 | 1.45 | 1.50 |
| 22 | D | 402 | CLA | C3D-C4D | 2.47 | 1.49 | 1.44 |
| 22 | B | 601 | CLA | C1D-ND | 2.46 | 1.40 | 1.37 |
| 25 | C | 502 | LMG | C9-C8 | 2.45 | 1.58 | 1.50 |
| 23 | C | 518 | BCR | C30-C25 | -2.45 | 1.50 | 1.53 |
| 22 | C | 504 | CLA | MG-NA | 2.45 | 2.12 | 2.06 |
| 22 | B | 613 | CLA | C3B-C2B | -2.44 | 1.37 | 1.40 |
| 22 | D | 407 | CLA | C3D-C4D | 2.44 | 1.49 | 1.44 |
| 22 | D | 407 | CLA | CHC-C1C | 2.44 | 1.41 | 1.35 |
| 22 | B | 604 | CLA | CMB-C2B | -2.43 | 1.46 | 1.51 |
| 22 | B | 606 | CLA | MG-ND | -2.43 | 2.01 | 2.05 |
| 22 | B | 610 | CLA | MG-NA | 2.43 | 2.12 | 2.06 |
| 22 | D | 407 | CLA | C3B-C2B | -2.42 | 1.37 | 1.40 |
| 22 | B | 604 | CLA | C1D-ND | 2.41 | 1.40 | 1.37 |
| 22 | D | 401 | CLA | CMA-C3A | -2.41 | 1.48 | 1.53 |
| 22 | C | 509 | CLA | C3B-C2B | -2.41 | 1.37 | 1.40 |
| 22 | C | 507 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 22 | B | 604 | CLA | CMC-C2C | -2.40 | 1.45 | 1.50 |
| 22 | C | 510 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 22 | C | 511 | CLA | C4D-ND | -2.40 | 1.34 | 1.37 |
| 22 | B | 605 | CLA | C3D-C4D | 2.39 | 1.49 | 1.44 |
| 22 | C | 517 | CLA | C3A-C2A | -2.39 | 1.47 | 1.54 |
| 22 | C | 506 | CLA | C3D-C4D | 2.39 | 1.49 | 1.44 |
| 22 | C | 509 | CLA | CMB-C2B | -2.38 | 1.46 | 1.51 |
| 22 | B | 612 | CLA | C4D-ND | -2.38 | 1.34 | 1.37 |
| 22 | B | 607 | CLA | CMB-C2B | -2.38 | 1.46 | 1.51 |
| 22 | D | 402 | CLA | C3D-CAD | 2.38 | 1.53 | 1.45 |
| 22 | B | 603 | CLA | C3B-C2B | -2.38 | 1.37 | 1.40 |
| 22 | B | 605 | CLA | C3B-C2B | -2.37 | 1.37 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | B | 602 | CLA | C4D-ND | -2.37 | 1.34 | 1.37 |
| 22 | B | 613 | CLA | C1D-ND | 2.37 | 1.40 | 1.37 |
| 22 | B | 611 | CLA | C3B-CAB | -2.37 | 1.43 | 1.47 |
| 22 | B | 608 | CLA | CMB-C2B | -2.36 | 1.46 | 1.51 |
| 22 | B | 612 | CLA | CMA-C3A | -2.36 | 1.48 | 1.53 |
| 22 | B | 607 | CLA | MG-ND | -2.36 | 2.01 | 2.05 |
| 22 | A | 405 | CLA | C3D-C4D | 2.36 | 1.49 | 1.44 |
| 22 | B | 612 | CLA | C3A-C2A | -2.36 | 1.47 | 1.54 |
| 22 | B | 612 | CLA | C3B-C2B | -2.36 | 1.37 | 1.40 |
| 23 | C | 516 | BCR | C30-C25 | -2.35 | 1.50 | 1.53 |
| 22 | C | 507 | CLA | C4C-C3C | 2.35 | 1.49 | 1.45 |
| 21 | A | 404 | PHO | CMC-C2C | -2.35 | 1.46 | 1.51 |
| 22 | B | 605 | CLA | CMB-C2B | -2.35 | 1.46 | 1.51 |
| 22 | B | 616 | CLA | C3A-C2A | -2.35 | 1.47 | 1.54 |
| 22 | C | 514 | CLA | C3B-C2B | -2.34 | 1.37 | 1.40 |
| 22 | C | 514 | CLA | C1D-ND | 2.34 | 1.40 | 1.37 |
| 22 | B | 601 | CLA | C4D-ND | -2.32 | 1.34 | 1.37 |
| 22 | C | 513 | CLA | C1D-ND | 2.32 | 1.40 | 1.37 |
| 22 | C | 510 | CLA | C3B-CAB | -2.32 | 1.43 | 1.47 |
| 21 | D | 406 | PHO | CMB-C2B | -2.32 | 1.46 | 1.51 |
| 23 | A | 407 | BCR | C30-C25 | -2.32 | 1.50 | 1.53 |
| 22 | C | 505 | CLA | CMC-C2C | -2.31 | 1.45 | 1.50 |
| 22 | C | 517 | CLA | CMB-C2B | -2.31 | 1.46 | 1.51 |
| 22 | D | 402 | CLA | CMD-C2D | -2.30 | 1.45 | 1.50 |
| 22 | C | 503 | CLA | C3B-CAB | -2.30 | 1.43 | 1.47 |
| 25 | C | 502 | LMG | C7-C8 | 2.30 | 1.57 | 1.50 |
| 22 | C | 505 | CLA | C3B-C2B | -2.30 | 1.37 | 1.40 |
| 22 | C | 512 | CLA | C1B-NB | 2.30 | 1.37 | 1.35 |
| 22 | A | 405 | CLA | CMC-C2C | -2.29 | 1.45 | 1.50 |
| 22 | B | 609 | CLA | C1D-C2D | 2.29 | 1.49 | 1.45 |
| 21 | D | 406 | PHO | CMC-C2C | -2.28 | 1.46 | 1.51 |
| 22 | B | 615 | CLA | CMB-C2B | -2.28 | 1.46 | 1.51 |
| 22 | C | 510 | CLA | C3C-C2C | 2.28 | 1.41 | 1.36 |
| 25 | D | 404 | LMG | C3-C2 | 2.27 | 1.58 | 1.52 |
| 22 | B | 608 | CLA | C3B-CAB | -2.27 | 1.43 | 1.47 |
| 22 | C | 514 | CLA | C1D-C2D | 2.27 | 1.49 | 1.45 |
| 22 | D | 401 | CLA | C3B-C2B | -2.27 | 1.37 | 1.40 |
| 22 | C | 510 | CLA | C1B-NB | 2.26 | 1.37 | 1.35 |
| 22 | D | 408 | CLA | C3B-C2B | -2.26 | 1.37 | 1.40 |
| 22 | B | 612 | CLA | C3D-C2D | -2.26 | 1.32 | 1.39 |
| 22 | B | 614 | CLA | C2A-C1A | -2.26 | 1.47 | 1.52 |
| 22 | B | 610 | CLA | C3B-CAB | -2.25 | 1.43 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | B | 607 | CLA | CMC-C2C | -2.25 | 1.46 | 1.50 |
| 22 | B | 601 | CLA | CAA-C2A | -2.24 | 1.49 | 1.54 |
| 25 | D | 403 | LMG | C3-C2 | 2.24 | 1.58 | 1.52 |
| 22 | B | 614 | CLA | C1D-ND | 2.24 | 1.40 | 1.37 |
| 22 | C | 513 | CLA | C1B-NB | 2.23 | 1.37 | 1.35 |
| 22 | A | 406 | CLA | CAA-C2A | -2.23 | 1.50 | 1.54 |
| 22 | C | 513 | CLA | C3B-C2B | -2.22 | 1.37 | 1.40 |
| 22 | C | 504 | CLA | MG-NC | 2.22 | 2.11 | 2.06 |
| 22 | C | 505 | CLA | C3D-C2D | -2.22 | 1.33 | 1.39 |
| 21 | D | 406 | PHO | C3B-C2B | -2.22 | 1.37 | 1.40 |
| 22 | B | 606 | CLA | C4D-ND | -2.22 | 1.34 | 1.37 |
| 22 | C | 512 | CLA | C1D-C2D | 2.21 | 1.49 | 1.45 |
| 22 | C | 504 | CLA | C3B-CAB | -2.21 | 1.43 | 1.47 |
| 23 | H | 101 | BCR | C27-C26 | -2.20 | 1.46 | 1.51 |
| 22 | B | 612 | CLA | CAA-C2A | -2.20 | 1.50 | 1.54 |
| 22 | C | 509 | CLA | C3D-C2D | -2.20 | 1.33 | 1.39 |
| 25 | 3 | 101 | LMG | O7-C8 | -2.20 | 1.41 | 1.46 |
| 22 | C | 512 | CLA | CMB-C2B | -2.20 | 1.47 | 1.51 |
| 22 | D | 401 | CLA | C3B-CAB | -2.19 | 1.43 | 1.47 |
| 22 | C | 514 | CLA | CMB-C2B | -2.19 | 1.47 | 1.51 |
| 22 | B | 614 | CLA | C3B-CAB | -2.19 | 1.43 | 1.47 |
| 21 | D | 406 | PHO | CBD-CGD | -2.19 | 1.49 | 1.52 |
| 22 | C | 507 | CLA | MG-NC | 2.19 | 2.11 | 2.06 |
| 25 | D | 404 | LMG | C4-C3 | 2.19 | 1.57 | 1.52 |
| 22 | D | 402 | CLA | C3B-CAB | -2.18 | 1.43 | 1.47 |
| 22 | A | 405 | CLA | CMB-C2B | -2.18 | 1.47 | 1.51 |
| 23 | K | 101 | BCR | C27-C26 | -2.18 | 1.46 | 1.51 |
| 23 | K | 101 | BCR | C21-C22 | -2.17 | 1.32 | 1.35 |
| 22 | C | 503 | CLA | MG-NC | 2.17 | 2.11 | 2.06 |
| 22 | C | 506 | CLA | O2D-CGD | 2.17 | 1.38 | 1.33 |
| 22 | B | 604 | CLA | C4D-ND | -2.17 | 1.34 | 1.37 |
| 22 | C | 506 | CLA | MG-ND | -2.17 | 2.01 | 2.05 |
| 25 | I | 101 | LMG | C3-C2 | 2.17 | 1.57 | 1.52 |
| 22 | B | 601 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 22 | D | 407 | CLA | C1D-C2D | 2.16 | 1.49 | 1.45 |
| 22 | B | 602 | CLA | C3D-C2D | -2.16 | 1.33 | 1.39 |
| 22 | D | 408 | CLA | MG-ND | -2.16 | 2.01 | 2.05 |
| 22 | B | 610 | CLA | CMC-C2C | -2.15 | 1.46 | 1.50 |
| 22 | C | 504 | CLA | C2A-C1A | 2.14 | 1.57 | 1.52 |
| 22 | D | 401 | CLA | C3D-C4D | 2.13 | 1.49 | 1.44 |
| 21 | A | 404 | PHO | CMB-C2B | -2.13 | 1.46 | 1.51 |
| 22 | B | 610 | CLA | C4C-C3C | 2.13 | 1.48 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23 | C | 515 | BCR | C35-C13 | -2.12 | 1.46 | 1.50 |
| 22 | A | 405 | CLA | C3D-CAD | 2.12 | 1.52 | 1.45 |
| 22 | B | 606 | CLA | C1D-ND | 2.12 | 1.40 | 1.37 |
| 21 | A | 404 | PHO | CMD-C2D | -2.12 | 1.46 | 1.51 |
| 22 | C | 504 | CLA | MG-ND | -2.12 | 2.01 | 2.05 |
| 22 | B | 605 | CLA | C3B-CAB | -2.12 | 1.43 | 1.47 |
| 22 | C | 508 | CLA | C1D-C2D | 2.12 | 1.49 | 1.45 |
| 22 | C | 508 | CLA | MG-NC | 2.11 | 2.11 | 2.06 |
| 22 | A | 406 | CLA | MG-NC | 2.11 | 2.11 | 2.06 |
| 22 | C | 506 | CLA | C3B-C2B | -2.11 | 1.37 | 1.40 |
| 22 | C | 508 | CLA | C3B-CAB | -2.11 | 1.43 | 1.47 |
| 22 | B | 612 | CLA | C1D-ND | 2.11 | 1.40 | 1.37 |
| 22 | C | 510 | CLA | C4C-C3C | 2.11 | 1.48 | 1.45 |
| 22 | B | 606 | CLA | CMC-C2C | -2.11 | 1.46 | 1.50 |
| 22 | B | 616 | CLA | OBD-CAD | -2.10 | 1.18 | 1.22 |
| 22 | C | 505 | CLA | CMB-C2B | -2.10 | 1.47 | 1.51 |
| 22 | D | 407 | CLA | C4C-C3C | 2.09 | 1.48 | 1.45 |
| 22 | B | 603 | CLA | C3D-C4D | 2.09 | 1.48 | 1.44 |
| 23 | K | 101 | BCR | C36-C18 | -2.09 | 1.46 | 1.50 |
| 22 | B | 608 | CLA | C1B-NB | 2.09 | 1.37 | 1.35 |
| 26 | D | 405 | PL9 | C52-C5 | -2.09 | 1.46 | 1.50 |
| 22 | B | 607 | CLA | C3D-C2D | -2.09 | 1.33 | 1.39 |
| 22 | C | 506 | CLA | CAA-C2A | -2.09 | 1.50 | 1.54 |
| 22 | C | 512 | CLA | C3B-C2B | -2.09 | 1.37 | 1.40 |
| 23 | H | 101 | BCR | C29-C30 | -2.08 | 1.49 | 1.54 |
| 23 | B | 619 | BCR | C30-C25 | -2.08 | 1.50 | 1.53 |
| 22 | B | 610 | CLA | MG-ND | -2.08 | 2.01 | 2.05 |
| 22 | D | 401 | CLA | C1D-ND | 2.08 | 1.40 | 1.37 |
| 22 | B | 605 | CLA | CMC-C2C | -2.08 | 1.46 | 1.50 |
| 25 | F | 101 | LMG | C4-C3 | 2.08 | 1.57 | 1.52 |
| 23 | H | 101 | BCR | C36-C18 | -2.07 | 1.46 | 1.50 |
| 22 | B | 615 | CLA | MG-NC | 2.07 | 2.11 | 2.06 |
| 22 | B | 606 | CLA | C3B-CAB | -2.06 | 1.43 | 1.47 |
| 25 | C | 502 | LMG | C3-C2 | 2.06 | 1.57 | 1.52 |
| 22 | C | 508 | CLA | C3C-C2C | 2.05 | 1.41 | 1.36 |
| 23 | B | 617 | BCR | C33-C5 | -2.05 | 1.47 | 1.50 |
| 22 | B | 614 | CLA | C1D-C2D | 2.05 | 1.49 | 1.45 |
| 25 | I | 101 | LMG | C4-C3 | 2.05 | 1.57 | 1.52 |
| 23 | H | 101 | BCR | C21-C22 | -2.04 | 1.33 | 1.35 |
| 23 | A | 407 | BCR | C1-C6 | -2.04 | 1.51 | 1.53 |
| 22 | B | 615 | CLA | C3B-C2B | -2.04 | 1.37 | 1.40 |
| 22 | C | 509 | CLA | C3B-CAB | -2.04 | 1.43 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | B | 613 | CLA | CAA-C2A | -2.03 | 1.50 | 1.54 |
| 22 | B | 606 | CLA | C3D-C4D | 2.03 | 1.48 | 1.44 |
| 22 | B | 605 | CLA | C3D-C2D | -2.03 | 1.33 | 1.39 |
| 22 | C | 509 | CLA | C3C-C2C | 2.03 | 1.41 | 1.36 |
| 22 | C | 507 | CLA | C3C-C2C | 2.03 | 1.41 | 1.36 |
| 22 | B | 612 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 25 | D | 403 | LMG | C7-C8 | 2.02 | 1.56 | 1.50 |
| 22 | C | 512 | CLA | OBD-CAD | -2.02 | 1.19 | 1.22 |
| 22 | B | 616 | CLA | CMA-C3A | -2.01 | 1.48 | 1.53 |
| 22 | C | 507 | CLA | CHD-C4C | 2.01 | 1.43 | 1.39 |
| 22 | A | 405 | CLA | C1D-C2D | 2.01 | 1.49 | 1.45 |
| 22 | D | 408 | CLA | C3B-CAB | -2.01 | 1.43 | 1.47 |
| 22 | C | 511 | CLA | C3B-CAB | -2.00 | 1.43 | 1.47 |
| 22 | C | 506 | CLA | C3B-CAB | -2.00 | 1.43 | 1.47 |
| 22 | C | 513 | CLA | C3A-C2A | -2.00 | 1.48 | 1.54 |

All (941) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 22 | B | 604 | CLA | C4A-NA-C1A | 15.59 | 113.71 | 106.71 |
| 22 | C | 505 | CLA | C4A-NA-C1A | 15.19 | 113.53 | 106.71 |
| 23 | H | 101 | BCR | C33-C5-C6 | -13.26 | 109.64 | 124.53 |
| 22 | B | 616 | CLA | C4A-NA-C1A | 13.21 | 112.64 | 106.71 |
| 22 | B | 605 | CLA | C4A-NA-C1A | 12.70 | 112.42 | 106.71 |
| 22 | C | 517 | CLA | C4A-NA-C1A | 12.57 | 112.36 | 106.71 |
| 22 | B | 603 | CLA | C4A-NA-C1A | 12.46 | 112.31 | 106.71 |
| 22 | B | 615 | CLA | C4A-NA-C1A | 12.10 | 112.14 | 106.71 |
| 22 | C | 513 | CLA | C4A-NA-C1A | 11.74 | 111.98 | 106.71 |
| 22 | C | 512 | CLA | C4A-NA-C1A | 11.64 | 111.94 | 106.71 |
| 22 | B | 609 | CLA | C4A-NA-C1A | 11.62 | 111.93 | 106.71 |
| 22 | B | 601 | CLA | C4A-NA-C1A | 11.58 | 111.91 | 106.71 |
| 22 | B | 616 | CLA | C4D-C3D-CAD | 11.55 | 121.71 | 108.10 |
| 22 | C | 511 | CLA | C4A-NA-C1A | 11.51 | 111.88 | 106.71 |
| 22 | C | 510 | CLA | C4A-NA-C1A | 11.33 | 111.80 | 106.71 |
| 23 | K | 101 | BCR | C33-C5-C6 | -11.23 | 111.92 | 124.53 |
| 22 | C | 512 | CLA | C4D-C3D-CAD | 11.16 | 121.25 | 108.10 |
| 22 | B | 613 | CLA | C4A-NA-C1A | 10.79 | 111.56 | 106.71 |
| 22 | C | 507 | CLA | C4A-NA-C1A | 10.73 | 111.53 | 106.71 |
| 22 | B | 608 | CLA | C4A-NA-C1A | 10.53 | 111.44 | 106.71 |
| 22 | C | 509 | CLA | C4A-NA-C1A | 10.53 | 111.44 | 106.71 |
| 22 | B | 614 | CLA | C4A-NA-C1A | 10.44 | 111.40 | 106.71 |
| 22 | B | 612 | CLA | C4A-NA-C1A | 10.40 | 111.38 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 602 | CLA | C4A-NA-C1A | 10.36 | 111.36 | 106.71 |
| 22 | B | 610 | CLA | C4A-NA-C1A | 10.01 | 111.21 | 106.71 |
| 22 | C | 507 | CLA | C4D-C3D-CAD | 9.93 | 119.80 | 108.10 |
| 22 | B | 606 | CLA | C4A-NA-C1A | 9.81 | 111.12 | 106.71 |
| 22 | C | 506 | CLA | C4A-NA-C1A | 9.75 | 111.09 | 106.71 |
| 22 | C | 513 | CLA | CAA-C2A-C3A | 9.73 | 139.43 | 112.78 |
| 22 | B | 607 | CLA | C4A-NA-C1A | 9.73 | 111.08 | 106.71 |
| 22 | C | 504 | CLA | C4A-NA-C1A | 9.62 | 111.03 | 106.71 |
| 22 | D | 402 | CLA | C4A-NA-C1A | 9.60 | 111.02 | 106.71 |
| 23 | K | 101 | BCR | C37-C22-C21 | -9.48 | 109.65 | 122.92 |
| 22 | B | 609 | CLA | C3A-C2A-C1A | 9.46 | 115.51 | 101.34 |
| 23 | H | 101 | BCR | C37-C22-C23 | -9.31 | 103.41 | 118.08 |
| 22 | B | 609 | CLA | C4D-C3D-CAD | 9.30 | 119.05 | 108.10 |
| 22 | B | 610 | CLA | C3A-C2A-C1A | 9.26 | 115.21 | 101.34 |
| 23 | K | 101 | BCR | C37-C22-C23 | -9.22 | 103.55 | 118.08 |
| 23 | H | 101 | BCR | C37-C22-C21 | -9.17 | 110.08 | 122.92 |
| 22 | B | 616 | CLA | CAA-C2A-C3A | 8.97 | 137.34 | 112.78 |
| 22 | A | 405 | CLA | C4A-NA-C1A | 8.97 | 110.74 | 106.71 |
| 22 | B | 602 | CLA | C4D-C3D-CAD | 8.77 | 118.44 | 108.10 |
| 22 | B | 613 | CLA | C3A-C2A-C1A | 8.75 | 114.45 | 101.34 |
| 22 | B | 614 | CLA | C3A-C2A-C1A | 8.75 | 114.44 | 101.34 |
| 22 | B | 610 | CLA | C4D-C3D-CAD | 8.68 | 118.33 | 108.10 |
| 22 | B | 602 | CLA | C3A-C2A-C1A | 8.48 | 114.05 | 101.34 |
| 23 | H | 101 | BCR | C1-C6-C5 | -8.48 | 110.67 | 122.61 |
| 22 | D | 408 | CLA | C4A-NA-C1A | 8.46 | 110.51 | 106.71 |
| 22 | B | 612 | CLA | CAA-C2A-C3A | 8.44 | 135.88 | 112.78 |
| 22 | C | 517 | CLA | C4D-C3D-CAD | 8.37 | 117.96 | 108.10 |
| 22 | C | 509 | CLA | C4D-C3D-CAD | 8.35 | 117.94 | 108.10 |
| 22 | B | 615 | CLA | C4D-C3D-CAD | 8.33 | 117.91 | 108.10 |
| 22 | B | 601 | CLA | C4D-C3D-CAD | 8.32 | 117.91 | 108.10 |
| 22 | B | 614 | CLA | C4D-C3D-CAD | 8.32 | 117.90 | 108.10 |
| 22 | B | 601 | CLA | C3A-C2A-C1A | 8.30 | 113.77 | 101.34 |
| 22 | C | 510 | CLA | C4D-C3D-CAD | 8.29 | 117.87 | 108.10 |
| 22 | B | 611 | CLA | C4A-NA-C1A | 8.29 | 110.43 | 106.71 |
| 22 | A | 406 | CLA | C2A-C3A-C4A | -8.22 | 88.59 | 101.87 |
| 22 | C | 514 | CLA | C4A-NA-C1A | 8.22 | 110.40 | 106.71 |
| 23 | K | 101 | BCR | C1-C6-C5 | -8.19 | 111.08 | 122.61 |
| 22 | D | 401 | CLA | C4A-NA-C1A | 8.18 | 110.39 | 106.71 |
| 22 | B | 612 | CLA | C4D-C3D-CAD | 8.12 | 117.67 | 108.10 |
| 22 | C | 511 | CLA | C3A-C2A-C1A | 8.12 | 113.50 | 101.34 |
| 22 | B | 613 | CLA | C4D-C3D-CAD | 8.11 | 117.65 | 108.10 |
| 23 | H | 101 | BCR | C2-C1-C6 | 8.07 | 122.90 | 110.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | C | 506 | CLA | C3A-C2A-C1A | 7.84 | 113.08 | 101.34 |
| 22 | B | 604 | CLA | C4D-C3D-CAD | 7.84 | 117.33 | 108.10 |
| 22 | C | 517 | CLA | CAA-C2A-C3A | 7.80 | 134.13 | 112.78 |
| 22 | C | 505 | CLA | C1D-ND-C4D | -7.77 | 100.82 | 106.33 |
| 22 | D | 407 | CLA | C4A-NA-C1A | 7.75 | 110.19 | 106.71 |
| 22 | B | 611 | CLA | C4D-C3D-CAD | 7.71 | 117.19 | 108.10 |
| 22 | C | 505 | CLA | C4D-C3D-CAD | 7.53 | 116.97 | 108.10 |
| 22 | B | 606 | CLA | C4D-C3D-CAD | 7.51 | 116.94 | 108.10 |
| 23 | K | 101 | BCR | C2-C1-C6 | 7.51 | 122.04 | 110.48 |
| 22 | C | 508 | CLA | C4A-NA-C1A | 7.50 | 110.08 | 106.71 |
| 22 | B | 608 | CLA | C4D-C3D-CAD | 7.45 | 116.88 | 108.10 |
| 22 | C | 511 | CLA | C4D-C3D-CAD | 7.40 | 116.81 | 108.10 |
| 22 | C | 514 | CLA | C3A-C2A-C1A | 7.39 | 112.41 | 101.34 |
| 22 | C | 508 | CLA | C4D-C3D-CAD | 7.31 | 116.72 | 108.10 |
| 22 | C | 514 | CLA | C4D-C3D-CAD | 7.31 | 116.71 | 108.10 |
| 22 | A | 406 | CLA | C2A-C1A-CHA | 7.31 | 136.63 | 123.86 |
| 22 | C | 507 | CLA | C3A-C2A-C1A | 7.20 | 112.13 | 101.34 |
| 22 | B | 610 | CLA | C2A-C1A-CHA | 7.18 | 136.42 | 123.86 |
| 22 | B | 615 | CLA | C3A-C2A-C1A | 7.15 | 112.04 | 101.34 |
| 23 | H | 101 | BCR | C32-C1-C6 | -7.00 | 98.94 | 110.30 |
| 22 | C | 509 | CLA | C3A-C2A-C1A | 6.96 | 111.77 | 101.34 |
| 22 | B | 604 | CLA | CAA-C2A-C3A | 6.89 | 131.66 | 112.78 |
| 22 | B | 603 | CLA | C3A-C2A-C1A | 6.70 | 111.38 | 101.34 |
| 22 | A | 406 | CLA | C3A-C2A-C1A | 6.70 | 111.37 | 101.34 |
| 22 | C | 509 | CLA | C2A-C1A-CHA | 6.65 | 135.48 | 123.86 |
| 22 | C | 513 | CLA | C4D-C3D-CAD | 6.56 | 115.83 | 108.10 |
| 22 | C | 506 | CLA | C2A-C1A-CHA | 6.55 | 135.32 | 123.86 |
| 22 | C | 507 | CLA | C3D-C2D-C1D | 6.54 | 114.76 | 105.83 |
| 22 | D | 408 | CLA | CAA-C2A-C3A | 6.52 | 130.64 | 112.78 |
| 22 | A | 406 | CLA | CAA-C2A-C3A | 6.52 | 130.62 | 112.78 |
| 22 | B | 616 | CLA | C2A-C1A-CHA | 6.50 | 135.23 | 123.86 |
| 22 | B | 614 | CLA | C6-C7-C8 | -6.40 | 95.24 | 115.92 |
| 22 | C | 511 | CLA | C2A-C1A-CHA | 6.36 | 134.98 | 123.86 |
| 22 | C | 510 | CLA | C3D-C2D-C1D | 6.34 | 114.48 | 105.83 |
| 22 | C | 504 | CLA | C4D-C3D-CAD | 6.31 | 115.53 | 108.10 |
| 22 | C | 517 | CLA | CHB-C4A-NA | 6.25 | 133.15 | 124.51 |
| 22 | B | 613 | CLA | C3D-C2D-C1D | 6.23 | 114.33 | 105.83 |
| 22 | C | 512 | CLA | C3A-C2A-C1A | 6.21 | 110.64 | 101.34 |
| 22 | B | 612 | CLA | C6-C7-C8 | -6.18 | 95.96 | 115.92 |
| 22 | B | 610 | CLA | C2A-C3A-C4A | -6.15 | 91.94 | 101.87 |
| 22 | C | 513 | CLA | C2A-C1A-CHA | 6.12 | 134.56 | 123.86 |
| 22 | D | 408 | CLA | C3A-C2A-C1A | 6.10 | 110.48 | 101.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | C | 505 | CLA | C3A-C2A-C1A | 6.07 | 110.43 | 101.34 |
| 22 | B | 611 | CLA | C3D-C2D-C1D | 6.05 | 114.09 | 105.83 |
| 22 | D | 402 | CLA | C3A-C2A-C1A | 6.02 | 110.36 | 101.34 |
| 22 | B | 616 | CLA | CMA-C3A-C4A | 6.00 | 127.89 | 111.77 |
| 22 | C | 512 | CLA | C3D-C2D-C1D | 5.96 | 113.96 | 105.83 |
| 22 | B | 605 | CLA | C4D-C3D-CAD | 5.84 | 114.98 | 108.10 |
| 22 | B | 614 | CLA | C3D-C2D-C1D | 5.82 | 113.78 | 105.83 |
| 22 | B | 604 | CLA | CHB-C4A-NA | 5.80 | 132.53 | 124.51 |
| 22 | B | 604 | CLA | CMA-C3A-C2A | 5.80 | 137.22 | 113.83 |
| 22 | B | 608 | CLA | C6-C7-C8 | -5.79 | 97.19 | 115.92 |
| 22 | C | 508 | CLA | CBA-CAA-C2A | 5.77 | 130.91 | 113.86 |
| 22 | B | 612 | CLA | C2A-C1A-CHA | 5.77 | 133.94 | 123.86 |
| 22 | C | 517 | CLA | C3D-C2D-C1D | 5.75 | 113.68 | 105.83 |
| 22 | B | 613 | CLA | C2A-C1A-CHA | 5.73 | 133.88 | 123.86 |
| 22 | B | 601 | CLA | C2A-C1A-CHA | 5.73 | 133.87 | 123.86 |
| 22 | B | 610 | CLA | CBA-CAA-C2A | 5.70 | 130.70 | 113.86 |
| 22 | C | 517 | CLA | CMA-C3A-C2A | 5.68 | 136.74 | 113.83 |
| 22 | C | 514 | CLA | C6-C7-C8 | -5.68 | 97.56 | 115.92 |
| 22 | D | 402 | CLA | CAA-C2A-C3A | 5.66 | 128.28 | 112.78 |
| 23 | H | 101 | BCR | C2-C3-C4 | -5.66 | 98.74 | 111.38 |
| 23 | K | 101 | BCR | C2-C3-C4 | -5.65 | 98.76 | 111.38 |
| 22 | B | 602 | CLA | C2A-C1A-CHA | 5.63 | 133.70 | 123.86 |
| 22 | C | 507 | CLA | C6-C7-C8 | -5.60 | 97.83 | 115.92 |
| 22 | B | 609 | CLA | C2A-C1A-CHA | 5.59 | 133.63 | 123.86 |
| 22 | C | 506 | CLA | C4D-C3D-CAD | 5.58 | 114.68 | 108.10 |
| 22 | C | 504 | CLA | CBA-CAA-C2A | 5.58 | 130.32 | 113.86 |
| 22 | C | 510 | CLA | C3D-C4D-ND | 5.57 | 119.24 | 110.24 |
| 22 | B | 609 | CLA | C3D-C2D-C1D | 5.55 | 113.41 | 105.83 |
| 22 | C | 503 | CLA | C4A-NA-C1A | 5.51 | 109.18 | 106.71 |
| 23 | H | 101 | BCR | C31-C1-C6 | -5.50 | 101.38 | 110.30 |
| 22 | B | 610 | CLA | CAC-C3C-C4C | 5.49 | 131.93 | 124.81 |
| 23 | K | 101 | BCR | C32-C1-C6 | -5.48 | 101.42 | 110.30 |
| 22 | D | 407 | CLA | C2D-C1D-ND | -5.47 | 106.08 | 110.10 |
| 23 | K | 101 | BCR | C31-C1-C6 | -5.45 | 101.46 | 110.30 |
| 22 | C | 513 | CLA | CMA-C3A-C2A | 5.44 | 135.77 | 113.83 |
| 22 | B | 613 | CLA | C2D-C1D-ND | -5.39 | 106.13 | 110.10 |
| 22 | B | 612 | CLA | CMA-C3A-C2A | 5.38 | 135.54 | 113.83 |
| 22 | C | 507 | CLA | C2D-C1D-ND | -5.37 | 106.15 | 110.10 |
| 22 | C | 509 | CLA | C2A-C3A-C4A | -5.35 | 93.23 | 101.87 |
| 22 | D | 402 | CLA | C2A-C3A-C4A | -5.34 | 93.24 | 101.87 |
| 22 | D | 401 | CLA | C4D-C3D-CAD | 5.33 | 114.38 | 108.10 |
| 22 | C | 503 | CLA | C4D-C3D-CAD | 5.31 | 114.35 | 108.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | D | 408 | CLA | CBA-CAA-C2A | 5.29 | 129.49 | 113.86 |
| 22 | B | 611 | CLA | C2D-C1D-ND | -5.29 | 106.20 | 110.10 |
| 22 | B | 610 | CLA | OBD-CAD-C3D | 5.24 | 141.13 | 128.52 |
| 22 | B | 607 | CLA | C4D-C3D-CAD | 5.21 | 114.23 | 108.10 |
| 22 | B | 615 | CLA | O2A-C1-C2 | -5.21 | 94.96 | 108.64 |
| 22 | C | 510 | CLA | CHB-C4A-NA | 5.20 | 131.71 | 124.51 |
| 22 | C | 517 | CLA | C3D-C4D-ND | 5.15 | 118.56 | 110.24 |
| 22 | B | 608 | CLA | CMA-C3A-C2A | 5.15 | 134.59 | 113.83 |
| 22 | A | 405 | CLA | C3A-C2A-C1A | 5.14 | 109.04 | 101.34 |
| 22 | A | 406 | CLA | C4A-NA-C1A | 5.13 | 109.01 | 106.71 |
| 22 | D | 402 | CLA | CBA-CAA-C2A | 5.12 | 128.99 | 113.86 |
| 22 | B | 616 | CLA | OBD-CAD-C3D | 5.07 | 140.73 | 128.52 |
| 22 | B | 602 | CLA | OBD-CAD-C3D | 5.04 | 140.65 | 128.52 |
| 22 | C | 510 | CLA | CBA-CAA-C2A | 5.03 | 128.72 | 113.86 |
| 22 | A | 405 | CLA | C4D-C3D-CAD | 5.01 | 114.01 | 108.10 |
| 22 | C | 508 | CLA | C3D-C4D-ND | 5.01 | 118.34 | 110.24 |
| 22 | C | 506 | CLA | O2D-CGD-CBD | 5.00 | 120.16 | 111.27 |
| 22 | C | 506 | CLA | C2A-C3A-C4A | -5.00 | 93.80 | 101.87 |
| 22 | B | 615 | CLA | C2A-C1A-CHA | 4.99 | 132.59 | 123.86 |
| 22 | A | 405 | CLA | CAA-C2A-C3A | 4.98 | 126.41 | 112.78 |
| 23 | H | 101 | BCR | C1-C6-C7 | 4.98 | 129.86 | 115.78 |
| 22 | B | 610 | CLA | C6-C7-C8 | -4.96 | 99.88 | 115.92 |
| 22 | B | 608 | CLA | C3D-C2D-C1D | 4.94 | 112.58 | 105.83 |
| 22 | B | 616 | CLA | C3D-C2D-C1D | 4.91 | 112.53 | 105.83 |
| 22 | C | 512 | CLA | C3D-C4D-ND | 4.90 | 118.16 | 110.24 |
| 22 | B | 614 | CLA | C3D-C4D-ND | 4.89 | 118.14 | 110.24 |
| 22 | B | 609 | CLA | C2A-C3A-C4A | -4.87 | 94.00 | 101.87 |
| 22 | C | 507 | CLA | C3D-C4D-ND | 4.86 | 118.10 | 110.24 |
| 22 | C | 510 | CLA | C2D-C1D-ND | -4.86 | 106.52 | 110.10 |
| 22 | C | 513 | CLA | CMA-C3A-C4A | 4.86 | 124.82 | 111.77 |
| 22 | C | 507 | CLA | CAA-C2A-C3A | 4.85 | 126.06 | 112.78 |
| 22 | B | 611 | CLA | C3D-C4D-ND | 4.84 | 118.06 | 110.24 |
| 22 | C | 514 | CLA | C3D-C2D-C1D | 4.83 | 112.42 | 105.83 |
| 22 | B | 603 | CLA | C2A-C1A-CHA | 4.81 | 132.27 | 123.86 |
| 22 | C | 510 | CLA | C11-C10-C8 | 4.81 | 131.47 | 115.92 |
| 22 | C | 512 | CLA | C1D-ND-C4D | -4.81 | 102.92 | 106.33 |
| 22 | B | 612 | CLA | CHB-C4A-NA | 4.79 | 131.14 | 124.51 |
| 22 | C | 513 | CLA | CHB-C4A-NA | 4.75 | 131.08 | 124.51 |
| 22 | C | 511 | CLA | OBD-CAD-C3D | 4.75 | 139.94 | 128.52 |
| 23 | H | 101 | BCR | C23-C22-C21 | 4.71 | 126.17 | 118.94 |
| 22 | C | 511 | CLA | C2A-C3A-C4A | -4.71 | 94.26 | 101.87 |
| 22 | B | 615 | CLA | OBD-CAD-C3D | 4.71 | 139.86 | 128.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 607 | CLA | C2A-C1A-CHA | 4.70 | 132.08 | 123.86 |
| 22 | B | 608 | CLA | C3D-C4D-ND | 4.68 | 117.81 | 110.24 |
| 22 | D | 407 | CLA | C3D-C2D-C1D | 4.66 | 112.19 | 105.83 |
| 22 | C | 508 | CLA | C3D-C2D-C1D | 4.66 | 112.19 | 105.83 |
| 23 | K | 101 | BCR | C1-C6-C7 | 4.65 | 128.94 | 115.78 |
| 22 | B | 611 | CLA | O2A-C1-C2 | 4.64 | 120.82 | 108.64 |
| 22 | B | 607 | CLA | C3A-C2A-C1A | 4.63 | 108.27 | 101.34 |
| 22 | B | 607 | CLA | CAA-C2A-C1A | 4.60 | 127.06 | 111.97 |
| 22 | C | 509 | CLA | OBD-CAD-C3D | 4.60 | 139.58 | 128.52 |
| 22 | B | 612 | CLA | CMA-C3A-C4A | 4.59 | 124.11 | 111.77 |
| 22 | B | 603 | CLA | C4D-C3D-CAD | 4.58 | 113.50 | 108.10 |
| 22 | A | 406 | CLA | CBA-CAA-C2A | 4.58 | 127.38 | 113.86 |
| 22 | C | 506 | CLA | CAA-C2A-C3A | 4.58 | 125.31 | 112.78 |
| 22 | C | 517 | CLA | O2D-CGD-CBD | 4.58 | 119.40 | 111.27 |
| 22 | C | 503 | CLA | CBA-CAA-C2A | 4.57 | 127.36 | 113.86 |
| 23 | K | 101 | BCR | C23-C22-C21 | 4.55 | 125.93 | 118.94 |
| 22 | B | 616 | CLA | CMA-C3A-C2A | 4.54 | 132.14 | 113.83 |
| 22 | D | 407 | CLA | C4D-C3D-CAD | 4.52 | 113.42 | 108.10 |
| 22 | C | 513 | CLA | OBD-CAD-C3D | 4.52 | 139.40 | 128.52 |
| 22 | B | 601 | CLA | CAA-C2A-C3A | 4.52 | 125.15 | 112.78 |
| 22 | C | 506 | CLA | O2D-CGD-O1D | -4.51 | 115.02 | 123.84 |
| 22 | D | 401 | CLA | CHB-C4A-NA | 4.51 | 130.75 | 124.51 |
| 22 | B | 610 | CLA | CAA-C2A-C3A | 4.47 | 125.03 | 112.78 |
| 22 | C | 509 | CLA | CAA-C2A-C3A | 4.46 | 124.99 | 112.78 |
| 22 | B | 612 | CLA | OBD-CAD-C3D | 4.46 | 139.24 | 128.52 |
| 22 | C | 504 | CLA | O2D-CGD-O1D | -4.45 | 115.13 | 123.84 |
| 22 | D | 402 | CLA | C2A-C1A-CHA | 4.45 | 131.63 | 123.86 |
| 22 | B | 605 | CLA | C3A-C2A-C1A | 4.39 | 107.91 | 101.34 |
| 22 | C | 505 | CLA | OBD-CAD-C3D | 4.38 | 139.05 | 128.52 |
| 22 | C | 514 | CLA | C3D-C4D-ND | 4.36 | 117.30 | 110.24 |
| 22 | B | 616 | CLA | C1D-ND-C4D | -4.35 | 103.25 | 106.33 |
| 22 | B | 608 | CLA | CAA-C2A-C3A | 4.34 | 124.67 | 112.78 |
| 22 | B | 613 | CLA | C3D-C4D-ND | 4.33 | 117.25 | 110.24 |
| 22 | C | 507 | CLA | CBA-CAA-C2A | 4.30 | 126.55 | 113.86 |
| 22 | B | 616 | CLA | CHB-C4A-NA | 4.29 | 130.44 | 124.51 |
| 23 | H | 101 | BCR | C33-C5-C4 | 4.29 | 121.86 | 113.62 |
| 23 | K | 101 | BCR | C36-C18-C17 | -4.26 | 116.96 | 122.92 |
| 22 | B | 601 | CLA | CBA-CAA-C2A | 4.26 | 126.43 | 113.86 |
| 23 | H | 101 | BCR | C36-C18-C17 | -4.25 | 116.98 | 122.92 |
| 22 | B | 604 | CLA | C2A-C1A-CHA | 4.22 | 131.24 | 123.86 |
| 22 | B | 608 | CLA | CAA-C2A-C1A | 4.19 | 125.71 | 111.97 |
| 22 | C | 508 | CLA | C1D-ND-C4D | -4.18 | 103.36 | 106.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 608 | CLA | CHB-C4A-NA | 4.17 | 130.28 | 124.51 |
| 22 | C | 510 | CLA | CMA-C3A-C2A | 4.17 | 130.66 | 113.83 |
| 22 | C | 510 | CLA | CBC-CAC-C3C | 4.14 | 123.84 | 112.43 |
| 22 | B | 603 | CLA | CAA-C2A-C3A | 4.12 | 124.05 | 112.78 |
| 22 | B | 613 | CLA | C2A-C3A-C4A | -4.11 | 95.23 | 101.87 |
| 22 | C | 513 | CLA | C11-C10-C8 | 4.11 | 129.21 | 115.92 |
| 22 | C | 505 | CLA | C2D-C1D-ND | 4.09 | 113.12 | 110.10 |
| 22 | C | 514 | CLA | CAA-C2A-C3A | 4.09 | 123.97 | 112.78 |
| 22 | B | 605 | CLA | CAA-C2A-C1A | 4.08 | 125.34 | 111.97 |
| 22 | C | 517 | CLA | C2A-C1A-CHA | 4.08 | 130.99 | 123.86 |
| 22 | B | 604 | CLA | OBD-CAD-C3D | 4.07 | 138.31 | 128.52 |
| 22 | B | 609 | CLA | C3D-C4D-ND | 4.06 | 116.81 | 110.24 |
| 23 | K | 101 | BCR | C20-C21-C22 | -4.06 | 121.52 | 127.31 |
| 22 | B | 608 | CLA | C9-C8-C10 | 4.05 | 125.95 | 111.29 |
| 22 | B | 614 | CLA | C2A-C1A-CHA | 4.04 | 130.93 | 123.86 |
| 26 | D | 405 | PL9 | C7-C3-C4 | 4.03 | 120.16 | 116.88 |
| 22 | C | 511 | CLA | CAA-C2A-C3A | 4.03 | 123.81 | 112.78 |
| 22 | C | 504 | CLA | C2A-C1A-CHA | 4.01 | 130.87 | 123.86 |
| 26 | D | 405 | PL9 | C36-C34-C33 | -4.01 | 113.00 | 121.12 |
| 22 | B | 612 | CLA | CBA-CAA-C2A | 4.00 | 125.67 | 113.86 |
| 22 | D | 401 | CLA | C2A-C3A-C4A | 4.00 | 108.33 | 101.87 |
| 22 | B | 611 | CLA | C6-C7-C8 | -3.99 | 103.02 | 115.92 |
| 22 | C | 506 | CLA | CBA-CAA-C2A | 3.99 | 125.64 | 113.86 |
| 22 | B | 613 | CLA | O2A-C1-C2 | -3.98 | 98.17 | 108.64 |
| 22 | C | 517 | CLA | C2D-C1D-ND | -3.98 | 107.17 | 110.10 |
| 22 | B | 606 | CLA | C3A-C2A-C1A | 3.97 | 107.29 | 101.34 |
| 22 | C | 517 | CLA | C6-C7-C8 | -3.97 | 103.09 | 115.92 |
| 23 | H | 101 | BCR | C4-C5-C6 | 3.96 | 128.48 | 122.73 |
| 22 | B | 609 | CLA | CGD-CBD-CAD | -3.96 | 97.92 | 110.73 |
| 22 | C | 504 | CLA | C3A-C2A-C1A | 3.95 | 107.26 | 101.34 |
| 23 | K | 101 | BCR | C39-C30-C25 | -3.95 | 103.89 | 110.30 |
| 22 | B | 616 | CLA | C11-C10-C8 | 3.94 | 128.66 | 115.92 |
| 23 | B | 618 | BCR | C2-C1-C6 | 3.94 | 116.54 | 110.48 |
| 22 | C | 505 | CLA | C2A-C1A-CHA | 3.93 | 130.73 | 123.86 |
| 22 | C | 505 | CLA | C6-C5-C3 | 3.92 | 123.74 | 113.45 |
| 23 | H | 101 | BCR | C7-C8-C9 | -3.92 | 120.32 | 126.23 |
| 22 | D | 408 | CLA | C2A-C1A-CHA | 3.91 | 130.70 | 123.86 |
| 22 | B | 615 | CLA | CAA-C2A-C3A | 3.91 | 123.47 | 112.78 |
| 23 | H | 101 | BCR | C39-C30-C25 | -3.88 | 104.00 | 110.30 |
| 22 | B | 615 | CLA | C11-C10-C8 | -3.88 | 103.38 | 115.92 |
| 22 | B | 608 | CLA | C2A-C1A-CHA | 3.88 | 130.64 | 123.86 |
| 22 | B | 611 | CLA | CMA-C3A-C2A | -3.87 | 98.20 | 113.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 612 | CLA | O2D-CGD-O1D | -3.87 | 116.27 | 123.84 |
| 22 | C | 513 | CLA | O2D-CGD-O1D | -3.87 | 116.27 | 123.84 |
| 22 | C | 506 | CLA | OBD-CAD-C3D | 3.87 | 137.83 | 128.52 |
| 22 | B | 609 | CLA | CAA-C2A-C3A | 3.87 | 123.37 | 112.78 |
| 22 | D | 407 | CLA | CAA-C2A-C3A | 3.87 | 123.36 | 112.78 |
| 22 | C | 505 | CLA | CMD-C2D-C1D | 3.84 | 131.49 | 124.71 |
| 22 | B | 616 | CLA | C3D-C4D-ND | 3.84 | 116.46 | 110.24 |
| 22 | B | 603 | CLA | CAA-C2A-C1A | 3.84 | 124.54 | 111.97 |
| 22 | C | 507 | CLA | CGD-CBD-CAD | -3.83 | 98.32 | 110.73 |
| 22 | C | 512 | CLA | CAA-C2A-C3A | 3.83 | 123.26 | 112.78 |
| 22 | B | 606 | CLA | CBA-CAA-C2A | 3.83 | 125.16 | 113.86 |
| 22 | B | 611 | CLA | CAC-C3C-C4C | 3.82 | 129.76 | 124.81 |
| 22 | B | 614 | CLA | C11-C10-C8 | 3.81 | 128.23 | 115.92 |
| 22 | B | 615 | CLA | CAA-C2A-C1A | 3.80 | 124.44 | 111.97 |
| 22 | D | 407 | CLA | CAA-C2A-C1A | 3.79 | 124.39 | 111.97 |
| 23 | H | 101 | BCR | C20-C21-C22 | -3.77 | 121.94 | 127.31 |
| 22 | C | 510 | CLA | C1B-CHB-C4A | -3.76 | 122.66 | 130.12 |
| 22 | C | 514 | CLA | CGD-CBD-CAD | -3.75 | 98.59 | 110.73 |
| 22 | B | 605 | CLA | OBD-CAD-C3D | 3.74 | 137.53 | 128.52 |
| 22 | B | 612 | CLA | C3B-C4B-NB | -3.74 | 104.37 | 109.21 |
| 22 | C | 513 | CLA | CBA-CAA-C2A | 3.74 | 124.91 | 113.86 |
| 22 | B | 608 | CLA | CBA-CAA-C2A | 3.74 | 124.90 | 113.86 |
| 22 | C | 504 | CLA | OBD-CAD-C3D | 3.73 | 137.51 | 128.52 |
| 22 | C | 517 | CLA | CMA-C3A-C4A | 3.73 | 121.80 | 111.77 |
| 22 | C | 504 | CLA | O2D-CGD-CBD | 3.73 | 117.89 | 111.27 |
| 24 | A | 408 | LHG | O4-P-O5 | 3.73 | 130.68 | 112.24 |
| 22 | C | 503 | CLA | C11-C10-C8 | 3.73 | 127.97 | 115.92 |
| 22 | D | 407 | CLA | CMA-C3A-C2A | -3.73 | 98.79 | 113.83 |
| 22 | B | 604 | CLA | C1D-ND-C4D | -3.72 | 103.69 | 106.33 |
| 22 | B | 608 | CLA | CMB-C2B-C1B | -3.71 | 122.76 | 128.46 |
| 22 | B | 605 | CLA | O2D-CGD-O1D | -3.71 | 116.58 | 123.84 |
| 22 | D | 402 | CLA | C4D-C3D-CAD | 3.71 | 112.47 | 108.10 |
| 22 | B | 606 | CLA | O2D-CGD-O1D | -3.70 | 116.60 | 123.84 |
| 22 | A | 405 | CLA | C2D-C1D-ND | -3.70 | 107.38 | 110.10 |
| 23 | K | 101 | BCR | C4-C5-C6 | 3.69 | 128.09 | 122.73 |
| 22 | B | 601 | CLA | OBD-CAD-C3D | 3.69 | 137.40 | 128.52 |
| 23 | K | 101 | BCR | C7-C8-C9 | -3.68 | 120.67 | 126.23 |
| 22 | B | 602 | CLA | CAC-C3C-C4C | 3.68 | 129.59 | 124.81 |
| 22 | B | 602 | CLA | C2A-C3A-C4A | -3.68 | 95.92 | 101.87 |
| 22 | D | 402 | CLA | C2D-C1D-ND | -3.67 | 107.40 | 110.10 |
| 22 | C | 511 | CLA | CAC-C3C-C4C | 3.66 | 129.56 | 124.81 |
| 22 | B | 605 | CLA | CMA-C3A-C2A | -3.66 | 99.06 | 113.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | C | 512 | CLA | CMD-C2D-C3D | -3.65 | 119.21 | 127.61 |
| 22 | B | 616 | CLA | CMD-C2D-C3D | -3.65 | 119.21 | 127.61 |
| 22 | D | 401 | CLA | CBA-CAA-C2A | 3.65 | 124.63 | 113.86 |
| 22 | B | 602 | CLA | CAA-C2A-C3A | 3.64 | 122.73 | 112.78 |
| 22 | B | 613 | CLA | C4D-CHA-C1A | -3.63 | 116.83 | 121.25 |
| 21 | D | 406 | PHO | C9-C8-C7 | 3.62 | 124.39 | 111.29 |
| 22 | B | 612 | CLA | CAA-C2A-C1A | 3.62 | 123.83 | 111.97 |
| 22 | B | 612 | CLA | O2A-C1-C2 | -3.60 | 99.18 | 108.64 |
| 21 | A | 404 | PHO | CMB-C2B-C3B | 3.60 | 131.41 | 124.68 |
| 22 | C | 503 | CLA | CMB-C2B-C1B | -3.60 | 122.94 | 128.46 |
| 22 | B | 609 | CLA | C2D-C1D-ND | -3.59 | 107.45 | 110.10 |
| 22 | A | 405 | CLA | C3D-C2D-C1D | 3.59 | 110.73 | 105.83 |
| 22 | D | 402 | CLA | C6-C7-C8 | -3.58 | 104.34 | 115.92 |
| 22 | C | 503 | CLA | CAA-C2A-C3A | 3.58 | 122.57 | 112.78 |
| 22 | A | 406 | CLA | CMB-C2B-C1B | -3.56 | 122.98 | 128.46 |
| 23 | K | 101 | BCR | C16-C17-C18 | -3.56 | 122.23 | 127.31 |
| 23 | C | 515 | BCR | C35-C13-C14 | -3.56 | 117.94 | 122.92 |
| 22 | D | 401 | CLA | O2A-C1-C2 | -3.56 | 99.29 | 108.64 |
| 23 | H | 101 | BCR | C16-C17-C18 | -3.55 | 122.24 | 127.31 |
| 23 | H | 101 | BCR | C23-C24-C25 | -3.54 | 117.25 | 127.20 |
| 22 | D | 401 | CLA | CMA-C3A-C2A | 3.54 | 128.11 | 113.83 |
| 22 | C | 514 | CLA | C2A-C1A-CHA | 3.54 | 130.05 | 123.86 |
| 22 | B | 605 | CLA | CMD-C2D-C1D | 3.53 | 130.93 | 124.71 |
| 22 | D | 401 | CLA | C3D-C4D-ND | 3.53 | 115.94 | 110.24 |
| 22 | C | 513 | CLA | C1B-CHB-C4A | -3.52 | 123.14 | 130.12 |
| 22 | B | 608 | CLA | CMA-C3A-C4A | 3.52 | 121.24 | 111.77 |
| 22 | A | 405 | CLA | CAC-C3C-C4C | 3.52 | 129.37 | 124.81 |
| 23 | K | 101 | BCR | C23-C24-C25 | -3.50 | 117.36 | 127.20 |
| 22 | A | 405 | CLA | CAA-C2A-C1A | 3.50 | 123.46 | 111.97 |
| 22 | B | 607 | CLA | CAA-C2A-C3A | 3.50 | 122.37 | 112.78 |
| 22 | B | 608 | CLA | C1B-CHB-C4A | -3.50 | 123.18 | 130.12 |
| 22 | B | 601 | CLA | C2A-C3A-C4A | -3.49 | 96.24 | 101.87 |
| 22 | C | 512 | CLA | CAA-C2A-C1A | 3.48 | 123.39 | 111.97 |
| 22 | B | 603 | CLA | OBD-CAD-C3D | 3.48 | 136.90 | 128.52 |
| 22 | B | 616 | CLA | C1B-CHB-C4A | -3.48 | 123.22 | 130.12 |
| 23 | C | 518 | BCR | C37-C22-C21 | -3.48 | 118.05 | 122.92 |
| 22 | C | 511 | CLA | CMB-C2B-C1B | -3.47 | 123.13 | 128.46 |
| 22 | C | 514 | CLA | C11-C10-C8 | 3.47 | 127.13 | 115.92 |
| 22 | C | 508 | CLA | CMA-C3A-C2A | -3.47 | 99.84 | 113.83 |
| 22 | B | 612 | CLA | C1B-CHB-C4A | -3.46 | 123.26 | 130.12 |
| 23 | B | 619 | BCR | C32-C1-C6 | -3.45 | 104.70 | 110.30 |
| 22 | B | 606 | CLA | C2A-C1A-CHA | 3.45 | 129.89 | 123.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | D | 408 | CLA | C2A-C3A-C4A | -3.45 | 96.30 | 101.87 |
| 22 | B | 606 | CLA | C6-C5-C3 | 3.44 | 122.47 | 113.45 |
| 22 | C | 509 | CLA | CAA-C2A-C1A | 3.44 | 123.24 | 111.97 |
| 22 | B | 612 | CLA | CMB-C2B-C1B | -3.43 | 123.19 | 128.46 |
| 22 | D | 401 | CLA | CAA-C2A-C1A | 3.43 | 123.22 | 111.97 |
| 22 | B | 616 | CLA | CBA-CAA-C2A | 3.43 | 123.98 | 113.86 |
| 22 | C | 512 | CLA | OBD-CAD-C3D | 3.43 | 136.77 | 128.52 |
| 22 | B | 605 | CLA | C2A-C1A-CHA | 3.42 | 129.84 | 123.86 |
| 22 | D | 401 | CLA | C3D-C2D-C1D | 3.42 | 110.50 | 105.83 |
| 22 | B | 607 | CLA | O2D-CGD-O1D | -3.41 | 117.16 | 123.84 |
| 23 | C | 518 | BCR | C35-C13-C14 | -3.41 | 118.14 | 122.92 |
| 22 | C | 504 | CLA | C6-C7-C8 | 3.41 | 126.95 | 115.92 |
| 22 | B | 601 | CLA | C11-C10-C8 | 3.41 | 126.95 | 115.92 |
| 22 | C | 511 | CLA | O2A-C1-C2 | -3.41 | 99.67 | 108.64 |
| 22 | C | 514 | CLA | CBA-CAA-C2A | 3.40 | 123.91 | 113.86 |
| 22 | D | 402 | CLA | O2D-CGD-O1D | -3.40 | 117.19 | 123.84 |
| 22 | B | 613 | CLA | CAA-C2A-C3A | 3.40 | 122.08 | 112.78 |
| 22 | C | 507 | CLA | C2A-C1A-CHA | 3.40 | 129.80 | 123.86 |
| 23 | C | 515 | BCR | C30-C25-C26 | -3.39 | 117.84 | 122.61 |
| 22 | B | 614 | CLA | C2A-C3A-C4A | -3.38 | 96.41 | 101.87 |
| 22 | B | 607 | CLA | C6-C7-C8 | 3.38 | 126.84 | 115.92 |
| 22 | B | 605 | CLA | CHB-C4A-NA | 3.38 | 129.19 | 124.51 |
| 22 | B | 602 | CLA | C3D-C2D-C1D | 3.37 | 110.43 | 105.83 |
| 22 | D | 401 | CLA | CMA-C3A-C4A | 3.36 | 120.81 | 111.77 |
| 22 | C | 503 | CLA | C3A-C2A-C1A | 3.36 | 106.37 | 101.34 |
| 22 | B | 606 | CLA | CAA-C2A-C1A | 3.34 | 122.90 | 111.97 |
| 22 | D | 407 | CLA | C3D-C4D-ND | 3.33 | 115.62 | 110.24 |
| 22 | B | 613 | CLA | CAC-C3C-C4C | 3.32 | 129.12 | 124.81 |
| 23 | K | 101 | BCR | C33-C5-C4 | 3.32 | 119.99 | 113.62 |
| 22 | C | 517 | CLA | O2D-CGD-O1D | -3.32 | 117.35 | 123.84 |
| 22 | C | 517 | CLA | C1B-CHB-C4A | -3.31 | 123.55 | 130.12 |
| 22 | B | 615 | CLA | C1-O2A-CGA | 3.31 | 125.12 | 116.44 |
| 23 | K | 101 | BCR | C16-C15-C14 | -3.30 | 116.70 | 123.47 |
| 22 | D | 402 | CLA | CMB-C2B-C1B | -3.30 | 123.39 | 128.46 |
| 22 | B | 604 | CLA | O2D-CGD-O1D | -3.30 | 117.39 | 123.84 |
| 23 | H | 101 | BCR | C38-C26-C25 | 3.30 | 128.23 | 124.53 |
| 22 | D | 402 | CLA | C3D-C4D-ND | 3.29 | 115.56 | 110.24 |
| 23 | H | 101 | BCR | C16-C15-C14 | -3.28 | 116.75 | 123.47 |
| 22 | B | 611 | CLA | C11-C10-C8 | 3.28 | 126.53 | 115.92 |
| 22 | C | 517 | CLA | CAA-C2A-C1A | 3.28 | 122.72 | 111.97 |
| 22 | C | 511 | CLA | CAA-C2A-C1A | 3.27 | 122.68 | 111.97 |
| 22 | B | 612 | CLA | O2D-CGD-CBD | 3.27 | 117.07 | 111.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | D | 408 | CLA | C6-C7-C8 | 3.26 | 126.47 | 115.92 |
| 22 | C | 503 | CLA | CAA-C2A-C1A | 3.26 | 122.67 | 111.97 |
| 22 | B | 613 | CLA | C9-C8-C10 | 3.25 | 123.08 | 111.29 |
| 23 | H | 101 | BCR | C29-C28-C27 | -3.25 | 104.11 | 111.38 |
| 22 | C | 511 | CLA | C4-C3-C5 | 3.25 | 120.74 | 115.27 |
| 22 | C | 505 | CLA | CHB-C4A-NA | 3.25 | 129.00 | 124.51 |
| 22 | B | 606 | CLA | OBD-CAD-C3D | 3.24 | 136.33 | 128.52 |
| 22 | C | 512 | CLA | C2A-C1A-CHA | 3.24 | 129.53 | 123.86 |
| 22 | C | 512 | CLA | C11-C10-C8 | 3.24 | 126.40 | 115.92 |
| 23 | B | 617 | BCR | C1-C6-C5 | -3.24 | 118.05 | 122.61 |
| 22 | C | 508 | CLA | C3A-C2A-C1A | 3.24 | 106.19 | 101.34 |
| 22 | C | 506 | CLA | CMB-C2B-C1B | -3.24 | 123.49 | 128.46 |
| 22 | C | 505 | CLA | CAA-C2A-C3A | 3.23 | 121.63 | 112.78 |
| 23 | K | 101 | BCR | C29-C28-C27 | -3.23 | 104.16 | 111.38 |
| 22 | C | 504 | CLA | CAA-C2A-C1A | 3.23 | 122.55 | 111.97 |
| 21 | A | 404 | PHO | C9-C8-C7 | 3.22 | 122.97 | 111.29 |
| 22 | C | 503 | CLA | CMD-C2D-C1D | 3.22 | 130.40 | 124.71 |
| 22 | B | 606 | CLA | C7-C6-C5 | -3.22 | 104.61 | 113.36 |
| 22 | B | 614 | CLA | C1D-ND-C4D | -3.22 | 104.05 | 106.33 |
| 22 | B | 614 | CLA | C2D-C1D-ND | -3.22 | 107.73 | 110.10 |
| 22 | C | 517 | CLA | C1D-ND-C4D | -3.22 | 104.05 | 106.33 |
| 25 | C | 501 | LMG | C3-C4-C5 | -3.21 | 104.51 | 110.24 |
| 22 | C | 508 | CLA | CAA-C2A-C3A | 3.21 | 121.56 | 112.78 |
| 23 | H | 101 | BCR | C38-C26-C27 | -3.21 | 107.46 | 113.62 |
| 22 | B | 612 | CLA | CMB-C2B-C3B | 3.20 | 130.67 | 124.68 |
| 22 | D | 402 | CLA | CHD-C1D-ND | -3.20 | 121.51 | 124.45 |
| 22 | B | 608 | CLA | C2D-C1D-ND | -3.20 | 107.74 | 110.10 |
| 22 | C | 507 | CLA | C2A-C3A-C4A | -3.20 | 96.70 | 101.87 |
| 22 | C | 509 | CLA | CMD-C2D-C1D | 3.19 | 130.34 | 124.71 |
| 22 | B | 616 | CLA | C6-C7-C8 | 3.19 | 126.23 | 115.92 |
| 23 | K | 101 | BCR | C38-C26-C27 | -3.19 | 107.49 | 113.62 |
| 22 | D | 402 | CLA | C4-C3-C2 | -3.19 | 115.50 | 123.68 |
| 22 | C | 505 | CLA | C6-C7-C8 | -3.19 | 105.62 | 115.92 |
| 22 | B | 610 | CLA | C3D-C2D-C1D | 3.19 | 110.18 | 105.83 |
| 22 | B | 607 | CLA | OBD-CAD-C3D | 3.18 | 136.17 | 128.52 |
| 23 | K | 101 | BCR | C38-C26-C25 | 3.17 | 128.09 | 124.53 |
| 22 | B | 612 | CLA | C3D-C2D-C1D | 3.15 | 110.13 | 105.83 |
| 22 | A | 405 | CLA | C9-C8-C10 | 3.15 | 122.71 | 111.29 |
| 23 | C | 518 | BCR | C12-C13-C14 | 3.15 | 123.78 | 118.94 |
| 22 | D | 408 | CLA | C3B-C4B-NB | -3.14 | 105.16 | 109.21 |
| 22 | C | 505 | CLA | O2A-C1-C2 | 3.13 | 116.86 | 108.64 |
| 22 | B | 614 | CLA | CAA-C2A-C3A | 3.12 | 121.33 | 112.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 608 | CLA | C1D-ND-C4D | -3.11 | 104.13 | 106.33 |
| 22 | B | 611 | CLA | C3A-C2A-C1A | 3.11 | 105.99 | 101.34 |
| 22 | C | 510 | CLA | O1D-CGD-CBD | 3.10 | 130.84 | 124.48 |
| 22 | C | 514 | CLA | C1D-ND-C4D | -3.10 | 104.14 | 106.33 |
| 22 | D | 401 | CLA | C9-C8-C7 | 3.09 | 122.49 | 111.29 |
| 22 | B | 611 | CLA | C1-C2-C3 | 3.09 | 131.39 | 126.04 |
| 22 | D | 401 | CLA | C1D-ND-C4D | -3.09 | 104.14 | 106.33 |
| 22 | C | 507 | CLA | C4D-CHA-C1A | -3.09 | 117.49 | 121.25 |
| 22 | B | 615 | CLA | CMD-C2D-C1D | 3.08 | 130.15 | 124.71 |
| 22 | D | 408 | CLA | C9-C8-C7 | 3.08 | 122.45 | 111.29 |
| 22 | C | 512 | CLA | CBA-CAA-C2A | 3.07 | 122.94 | 113.86 |
| 22 | C | 511 | CLA | CBA-CAA-C2A | 3.07 | 122.92 | 113.86 |
| 22 | D | 401 | CLA | C1B-CHB-C4A | -3.06 | 124.05 | 130.12 |
| 22 | B | 602 | CLA | CBA-CAA-C2A | 3.06 | 122.89 | 113.86 |
| 22 | D | 402 | CLA | C3D-C2D-C1D | 3.06 | 110.01 | 105.83 |
| 22 | B | 604 | CLA | C6-C7-C8 | 3.05 | 125.79 | 115.92 |
| 22 | B | 604 | CLA | CBA-CAA-C2A | 3.05 | 122.86 | 113.86 |
| 22 | B | 615 | CLA | CBA-CAA-C2A | 3.05 | 122.85 | 113.86 |
| 22 | B | 614 | CLA | CMD-C2D-C1D | -3.04 | 119.35 | 124.71 |
| 22 | C | 510 | CLA | C2A-C3A-C4A | 3.04 | 106.78 | 101.87 |
| 22 | B | 612 | CLA | C9-C8-C10 | 3.04 | 122.30 | 111.29 |
| 22 | B | 606 | CLA | CMA-C3A-C4A | 3.04 | 119.94 | 111.77 |
| 23 | B | 617 | BCR | C39-C30-C25 | 3.04 | 115.22 | 110.30 |
| 22 | D | 408 | CLA | O2D-CGD-O1D | -3.03 | 117.91 | 123.84 |
| 22 | B | 608 | CLA | CMB-C2B-C3B | 3.03 | 130.35 | 124.68 |
| 22 | D | 408 | CLA | C4D-C3D-CAD | 3.03 | 111.67 | 108.10 |
| 22 | D | 407 | CLA | CAC-C3C-C4C | 3.03 | 128.74 | 124.81 |
| 22 | B | 601 | CLA | C9-C8-C10 | 3.03 | 122.26 | 111.29 |
| 22 | B | 612 | CLA | CAC-C3C-C4C | 3.03 | 128.74 | 124.81 |
| 25 | 3 | 101 | LMG | C1-C2-C3 | -3.03 | 103.69 | 110.00 |
| 22 | B | 602 | CLA | CMB-C2B-C1B | -3.02 | 123.82 | 128.46 |
| 23 | C | 518 | BCR | C30-C25-C26 | -3.01 | 118.37 | 122.61 |
| 22 | B | 607 | CLA | C11-C10-C8 | 3.01 | 125.64 | 115.92 |
| 22 | B | 603 | CLA | C1B-CHB-C4A | -3.00 | 124.17 | 130.12 |
| 22 | B | 608 | CLA | C11-C10-C8 | 3.00 | 125.62 | 115.92 |
| 22 | B | 606 | CLA | CHB-C4A-NA | 3.00 | 128.66 | 124.51 |
| 22 | C | 510 | CLA | C1D-ND-C4D | -2.99 | 104.21 | 106.33 |
| 22 | B | 613 | CLA | CHD-C4C-C3C | 2.99 | 129.23 | 124.84 |
| 22 | C | 504 | CLA | CMA-C3A-C4A | 2.98 | 119.79 | 111.77 |
| 22 | C | 513 | CLA | O2D-CGD-CBD | 2.97 | 116.55 | 111.27 |
| 23 | K | 101 | BCR | C24-C23-C22 | -2.97 | 121.75 | 126.23 |
| 22 | A | 405 | CLA | C3D-C4D-ND | 2.97 | 115.04 | 110.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 406 | CLA | O2A-C1-C2 | -2.96 | 100.85 | 108.64 |
| 22 | C | 512 | CLA | O1D-CGD-CBD | 2.96 | 130.54 | 124.48 |
| 22 | C | 517 | CLA | C4D-CHA-C1A | -2.96 | 117.65 | 121.25 |
| 23 | C | 515 | BCR | C33-C5-C6 | -2.95 | 121.21 | 124.53 |
| 22 | A | 406 | CLA | C2D-C1D-ND | -2.95 | 107.93 | 110.10 |
| 22 | D | 401 | CLA | CMB-C2B-C1B | -2.95 | 123.93 | 128.46 |
| 23 | H | 101 | BCR | C24-C23-C22 | -2.94 | 121.79 | 126.23 |
| 22 | C | 513 | CLA | CMB-C2B-C1B | -2.94 | 123.94 | 128.46 |
| 22 | B | 603 | CLA | CMD-C2D-C1D | 2.94 | 129.89 | 124.71 |
| 22 | A | 405 | CLA | O2A-C1-C2 | -2.93 | 100.92 | 108.64 |
| 22 | B | 613 | CLA | CHB-C4A-NA | 2.93 | 128.57 | 124.51 |
| 22 | B | 605 | CLA | C6-C7-C8 | 2.93 | 125.39 | 115.92 |
| 22 | D | 402 | CLA | O2A-C1-C2 | -2.93 | 100.94 | 108.64 |
| 25 | 3 | 101 | LMG | C1-O6-C5 | -2.93 | 107.94 | 113.69 |
| 22 | B | 611 | CLA | CBA-CAA-C2A | 2.93 | 122.51 | 113.86 |
| 22 | B | 607 | CLA | C9-C8-C7 | 2.93 | 121.89 | 111.29 |
| 23 | C | 518 | BCR | C2-C1-C6 | 2.93 | 114.98 | 110.48 |
| 22 | B | 606 | CLA | CAC-C3C-C4C | 2.93 | 128.61 | 124.81 |
| 22 | B | 616 | CLA | CAA-C2A-C1A | 2.92 | 121.56 | 111.97 |
| 22 | B | 605 | CLA | C11-C10-C8 | 2.92 | 125.36 | 115.92 |
| 22 | D | 401 | CLA | C6-C7-C8 | 2.92 | 125.35 | 115.92 |
| 22 | C | 517 | CLA | CHD-C1D-ND | -2.91 | 121.78 | 124.45 |
| 22 | B | 604 | CLA | C9-C8-C7 | 2.90 | 121.81 | 111.29 |
| 23 | F | 102 | BCR | C31-C1-C6 | 2.90 | 115.01 | 110.30 |
| 22 | B | 615 | CLA | C9-C8-C7 | 2.90 | 121.80 | 111.29 |
| 22 | B | 614 | CLA | O2A-C1-C2 | -2.90 | 101.01 | 108.64 |
| 22 | B | 614 | CLA | C10-C8-C7 | 2.89 | 127.34 | 112.13 |
| 22 | C | 511 | CLA | O2D-CGD-O1D | -2.89 | 118.19 | 123.84 |
| 22 | C | 503 | CLA | C9-C8-C7 | 2.88 | 121.72 | 111.29 |
| 22 | C | 503 | CLA | O2A-C1-C2 | 2.87 | 116.18 | 108.64 |
| 26 | D | 405 | PL9 | C35-C34-C36 | 2.87 | 120.10 | 115.27 |
| 22 | D | 402 | CLA | CAA-C2A-C1A | 2.86 | 121.35 | 111.97 |
| 22 | C | 513 | CLA | C4D-CHA-C1A | -2.86 | 117.77 | 121.25 |
| 22 | B | 602 | CLA | C4-C3-C5 | 2.86 | 120.08 | 115.27 |
| 22 | C | 506 | CLA | CAA-C2A-C1A | 2.85 | 121.32 | 111.97 |
| 22 | C | 513 | CLA | C3D-C2D-C1D | 2.85 | 109.72 | 105.83 |
| 23 | B | 619 | BCR | C39-C30-C25 | 2.85 | 114.92 | 110.30 |
| 22 | C | 512 | CLA | C4D-CHA-C1A | -2.84 | 117.79 | 121.25 |
| 22 | C | 507 | CLA | CMD-C2D-C3D | -2.83 | 121.10 | 127.61 |
| 22 | B | 609 | CLA | CBA-CAA-C2A | 2.83 | 122.22 | 113.86 |
| 25 | C | 502 | LMG | C6-C5-C4 | -2.83 | 106.38 | 113.00 |
| 22 | B | 606 | CLA | C3D-C2D-C1D | 2.83 | 109.69 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | C | 503 | CLA | O2D-CGD-O1D | -2.82 | 118.32 | 123.84 |
| 22 | D | 407 | CLA | CGD-CBD-CAD | -2.82 | 101.59 | 110.73 |
| 22 | B | 604 | CLA | O1D-CGD-CBD | 2.82 | 130.25 | 124.48 |
| 21 | D | 406 | PHO | C6-C7-C8 | 2.81 | 125.01 | 115.92 |
| 22 | B | 613 | CLA | C4-C3-C5 | 2.81 | 120.00 | 115.27 |
| 22 | B | 602 | CLA | C9-C8-C10 | 2.81 | 121.45 | 111.29 |
| 23 | H | 101 | BCR | C21-C20-C19 | -2.81 | 114.46 | 123.22 |
| 22 | B | 611 | CLA | CAA-C2A-C3A | 2.80 | 120.45 | 112.78 |
| 27 | E | 101 | HEM | C4B-CHC-C1C | 2.80 | 126.25 | 122.56 |
| 23 | K | 101 | BCR | C21-C20-C19 | -2.79 | 114.51 | 123.22 |
| 22 | C | 512 | CLA | C2A-C3A-C4A | -2.79 | 97.36 | 101.87 |
| 22 | B | 613 | CLA | CAA-C2A-C1A | 2.79 | 121.12 | 111.97 |
| 23 | H | 101 | BCR | C8-C9-C10 | -2.79 | 114.66 | 118.94 |
| 25 | C | 501 | LMG | C1-C2-C3 | -2.79 | 104.19 | 110.00 |
| 22 | C | 511 | CLA | CAA-CBA-CGA | -2.78 | 105.13 | 113.25 |
| 22 | C | 513 | CLA | C10-C8-C7 | 2.78 | 126.74 | 112.13 |
| 22 | C | 507 | CLA | CAA-C2A-C1A | 2.78 | 121.07 | 111.97 |
| 22 | C | 504 | CLA | C9-C8-C7 | 2.77 | 121.33 | 111.29 |
| 22 | B | 615 | CLA | O2D-CGD-O1D | -2.77 | 118.43 | 123.84 |
| 23 | C | 515 | BCR | C40-C30-C25 | 2.77 | 114.79 | 110.30 |
| 22 | D | 407 | CLA | C3A-C2A-C1A | 2.76 | 105.47 | 101.34 |
| 22 | C | 514 | CLA | C2D-C1D-ND | -2.76 | 108.07 | 110.10 |
| 22 | B | 601 | CLA | C6-C5-C3 | 2.76 | 120.68 | 113.45 |
| 22 | A | 405 | CLA | C4D-CHA-C1A | -2.75 | 117.90 | 121.25 |
| 22 | B | 611 | CLA | CHB-C4A-NA | 2.75 | 128.32 | 124.51 |
| 22 | B | 606 | CLA | C9-C8-C7 | 2.75 | 121.25 | 111.29 |
| 23 | F | 102 | BCR | C35-C13-C14 | -2.75 | 119.08 | 122.92 |
| 23 | K | 101 | BCR | C8-C9-C10 | -2.74 | 114.73 | 118.94 |
| 22 | C | 509 | CLA | O2D-CGD-O1D | -2.74 | 118.48 | 123.84 |
| 22 | C | 508 | CLA | C9-C8-C10 | 2.73 | 121.19 | 111.29 |
| 22 | A | 406 | CLA | C9-C8-C7 | 2.73 | 121.18 | 111.29 |
| 22 | B | 609 | CLA | CHB-C4A-NA | 2.73 | 128.29 | 124.51 |
| 23 | H | 101 | BCR | C32-C1-C31 | 2.72 | 116.89 | 108.53 |
| 22 | D | 401 | CLA | C9-C8-C10 | 2.72 | 121.14 | 111.29 |
| 22 | C | 505 | CLA | C3D-C4D-ND | 2.72 | 114.64 | 110.24 |
| 22 | C | 509 | CLA | CMD-C2D-C3D | -2.72 | 121.36 | 127.61 |
| 22 | C | 512 | CLA | C2D-C1D-ND | -2.72 | 108.10 | 110.10 |
| 22 | B | 609 | CLA | OBD-CAD-C3D | 2.71 | 135.04 | 128.52 |
| 22 | C | 507 | CLA | CHD-C1D-C2D | 2.71 | 131.16 | 125.48 |
| 22 | B | 607 | CLA | C2D-C1D-ND | -2.71 | 108.11 | 110.10 |
| 22 | C | 513 | CLA | CAA-C2A-C1A | 2.71 | 120.84 | 111.97 |
| 23 | H | 101 | BCR | C3-C4-C5 | 2.70 | 118.91 | 114.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | K | 101 | BCR | C3-C4-C5 | 2.70 | 118.90 | 114.08 |
| 22 | B | 612 | CLA | C4D-CHA-C1A | -2.70 | 117.96 | 121.25 |
| 22 | B | 611 | CLA | C9-C8-C7 | 2.70 | 121.06 | 111.29 |
| 23 | B | 617 | BCR | C7-C6-C5 | 2.69 | 127.99 | 121.46 |
| 22 | D | 407 | CLA | CBA-CAA-C2A | 2.69 | 121.81 | 113.86 |
| 22 | B | 601 | CLA | C6-C7-C8 | 2.69 | 124.61 | 115.92 |
| 22 | B | 615 | CLA | CMD-C2D-C3D | -2.69 | 121.43 | 127.61 |
| 22 | B | 616 | CLA | C10-C8-C7 | 2.69 | 126.27 | 112.13 |
| 22 | B | 607 | CLA | CMB-C2B-C1B | -2.69 | 124.33 | 128.46 |
| 26 | D | 405 | PL9 | C46-C44-C43 | 2.68 | 126.54 | 121.12 |
| 22 | A | 406 | CLA | C11-C10-C8 | 2.68 | 124.59 | 115.92 |
| 22 | B | 601 | CLA | C9-C8-C7 | 2.68 | 121.00 | 111.29 |
| 22 | C | 503 | CLA | CMA-C3A-C4A | 2.67 | 118.96 | 111.77 |
| 22 | B | 610 | CLA | C3B-C4B-NB | -2.67 | 105.75 | 109.21 |
| 22 | D | 402 | CLA | C3C-C4C-NC | -2.67 | 107.57 | 110.57 |
| 22 | D | 402 | CLA | C4-C3-C5 | 2.67 | 119.77 | 115.27 |
| 22 | C | 505 | CLA | C5-C3-C2 | 2.67 | 126.52 | 121.12 |
| 22 | C | 504 | CLA | CMB-C2B-C1B | -2.67 | 124.36 | 128.46 |
| 21 | D | 406 | PHO | C1B-NB-C4B | 2.67 | 112.57 | 107.09 |
| 23 | B | 618 | BCR | C12-C13-C14 | 2.67 | 123.03 | 118.94 |
| 22 | C | 512 | CLA | CMA-C3A-C4A | 2.66 | 118.93 | 111.77 |
| 23 | C | 515 | BCR | C15-C14-C13 | -2.66 | 123.52 | 127.31 |
| 22 | C | 507 | CLA | C9-C8-C10 | 2.66 | 120.91 | 111.29 |
| 22 | C | 505 | CLA | CMD-C2D-C3D | -2.65 | 121.51 | 127.61 |
| 22 | A | 406 | CLA | CMB-C2B-C3B | 2.65 | 129.63 | 124.68 |
| 22 | B | 610 | CLA | CMB-C2B-C1B | -2.65 | 124.40 | 128.46 |
| 22 | D | 407 | CLA | CHD-C4C-C3C | 2.64 | 128.72 | 124.84 |
| 22 | C | 509 | CLA | CBA-CAA-C2A | 2.64 | 121.66 | 113.86 |
| 22 | B | 602 | CLA | CMD-C2D-C3D | -2.64 | 121.54 | 127.61 |
| 22 | C | 507 | CLA | CBC-CAC-C3C | 2.64 | 119.70 | 112.43 |
| 22 | B | 613 | CLA | O1D-CGD-CBD | 2.64 | 129.88 | 124.48 |
| 22 | A | 405 | CLA | CGD-CBD-CAD | -2.64 | 102.20 | 110.73 |
| 22 | C | 504 | CLA | CMD-C2D-C1D | 2.63 | 129.35 | 124.71 |
| 23 | B | 619 | BCR | C2-C1-C6 | 2.63 | 114.53 | 110.48 |
| 22 | A | 405 | CLA | O1D-CGD-CBD | 2.63 | 129.86 | 124.48 |
| 22 | B | 609 | CLA | C11-C10-C8 | 2.61 | 124.37 | 115.92 |
| 22 | C | 507 | CLA | CHB-C4A-NA | 2.61 | 128.13 | 124.51 |
| 22 | A | 405 | CLA | C6-C7-C8 | 2.61 | 124.36 | 115.92 |
| 22 | B | 613 | CLA | CMB-C2B-C1B | -2.61 | 124.45 | 128.46 |
| 22 | B | 609 | CLA | C4D-CHA-C1A | -2.61 | 118.07 | 121.25 |
| 22 | B | 615 | CLA | CHB-C4A-NA | 2.60 | 128.11 | 124.51 |
| 22 | C | 517 | CLA | CMD-C2D-C3D | -2.60 | 121.64 | 127.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 603 | CLA | CHB-C4A-NA | 2.60 | 128.10 | 124.51 |
| 22 | B | 610 | CLA | CBC-CAC-C3C | 2.59 | 119.58 | 112.43 |
| 22 | B | 603 | CLA | O2D-CGD-O1D | -2.59 | 118.77 | 123.84 |
| 22 | B | 615 | CLA | C1D-ND-C4D | -2.59 | 104.49 | 106.33 |
| 22 | C | 512 | CLA | C9-C8-C7 | 2.59 | 120.67 | 111.29 |
| 23 | B | 619 | BCR | C33-C5-C6 | -2.59 | 121.62 | 124.53 |
| 22 | C | 503 | CLA | C3B-C4B-NB | -2.58 | 105.87 | 109.21 |
| 22 | B | 615 | CLA | O2D-CGD-CBD | 2.58 | 115.86 | 111.27 |
| 22 | C | 505 | CLA | C1B-CHB-C4A | -2.58 | 125.01 | 130.12 |
| 22 | B | 609 | CLA | CAC-C3C-C4C | 2.58 | 128.16 | 124.81 |
| 23 | H | 101 | BCR | C24-C25-C26 | 2.58 | 127.71 | 121.46 |
| 22 | C | 505 | CLA | O2D-CGD-O1D | -2.58 | 118.80 | 123.84 |
| 23 | K | 101 | BCR | C32-C1-C31 | 2.58 | 116.44 | 108.53 |
| 23 | B | 619 | BCR | C27-C26-C25 | 2.57 | 126.47 | 122.73 |
| 22 | C | 508 | CLA | C3B-C4B-NB | -2.57 | 105.89 | 109.21 |
| 22 | D | 408 | CLA | C6-C5-C3 | 2.57 | 120.20 | 113.45 |
| 22 | B | 613 | CLA | C11-C10-C8 | 2.57 | 124.21 | 115.92 |
| 22 | B | 611 | CLA | CHD-C1D-C2D | 2.57 | 130.86 | 125.48 |
| 22 | C | 503 | CLA | OBD-CAD-C3D | 2.56 | 134.68 | 128.52 |
| 23 | B | 619 | BCR | C31-C1-C6 | 2.56 | 114.45 | 110.30 |
| 22 | C | 505 | CLA | O1D-CGD-CBD | 2.56 | 129.72 | 124.48 |
| 22 | B | 607 | CLA | CMD-C2D-C1D | 2.56 | 129.22 | 124.71 |
| 22 | C | 506 | CLA | CMD-C2D-C1D | 2.56 | 129.22 | 124.71 |
| 22 | C | 510 | CLA | C6-C7-C8 | 2.55 | 124.17 | 115.92 |
| 22 | B | 606 | CLA | C6-C7-C8 | 2.55 | 124.16 | 115.92 |
| 22 | C | 517 | CLA | C9-C8-C10 | 2.54 | 120.50 | 111.29 |
| 22 | A | 406 | CLA | C3B-C4B-NB | -2.54 | 105.92 | 109.21 |
| 22 | A | 405 | CLA | C4-C3-C2 | -2.54 | 117.16 | 123.68 |
| 22 | D | 402 | CLA | CHD-C1D-C2D | 2.54 | 130.81 | 125.48 |
| 22 | B | 612 | CLA | C2D-C1D-ND | -2.54 | 108.23 | 110.10 |
| 22 | C | 514 | CLA | C2A-C3A-C4A | -2.53 | 97.78 | 101.87 |
| 23 | B | 618 | BCR | C27-C26-C25 | 2.53 | 126.40 | 122.73 |
| 22 | C | 509 | CLA | C6-C7-C8 | 2.52 | 124.08 | 115.92 |
| 22 | B | 610 | CLA | CHD-C4C-NC | -2.52 | 120.23 | 124.20 |
| 22 | A | 405 | CLA | CHB-C4A-NA | 2.52 | 128.00 | 124.51 |
| 22 | D | 407 | CLA | C9-C8-C10 | 2.52 | 120.41 | 111.29 |
| 22 | C | 514 | CLA | C4D-CHA-C1A | -2.52 | 118.19 | 121.25 |
| 22 | B | 607 | CLA | O1D-CGD-CBD | 2.51 | 129.63 | 124.48 |
| 22 | B | 609 | CLA | C9-C8-C10 | 2.51 | 120.39 | 111.29 |
| 22 | D | 401 | CLA | C2D-C1D-ND | -2.51 | 108.25 | 110.10 |
| 23 | K | 101 | BCR | C24-C25-C26 | 2.51 | 127.54 | 121.46 |
| 22 | D | 407 | CLA | C2C-C1C-NC | 2.50 | 112.31 | 109.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23 | C | 518 | BCR | C15-C14-C13 | -2.50 | 123.75 | 127.31 |
| 25 | D | 403 | LMG | O6-C1-O1 | -2.49 | 104.07 | 109.97 |
| 22 | B | 603 | CLA | C5-C3-C2 | -2.49 | 116.08 | 121.12 |
| 22 | B | 602 | CLA | CMB-C2B-C3B | 2.49 | 129.34 | 124.68 |
| 25 | D | 404 | LMG | C1-O6-C5 | -2.49 | 108.81 | 113.69 |
| 22 | D | 402 | CLA | C9-C8-C7 | 2.49 | 120.29 | 111.29 |
| 22 | B | 614 | CLA | CHB-C4A-NA | 2.49 | 127.95 | 124.51 |
| 22 | C | 505 | CLA | O2A-CGA-O1A | -2.48 | 117.33 | 123.59 |
| 22 | C | 505 | CLA | CHD-C1D-ND | -2.48 | 122.18 | 124.45 |
| 22 | C | 517 | CLA | CMB-C2B-C1B | -2.48 | 124.66 | 128.46 |
| 23 | C | 516 | BCR | C27-C26-C25 | 2.47 | 126.31 | 122.73 |
| 22 | C | 508 | CLA | CMB-C2B-C1B | -2.46 | 124.68 | 128.46 |
| 22 | B | 602 | CLA | O2D-CGD-O1D | -2.46 | 119.02 | 123.84 |
| 22 | C | 507 | CLA | CHD-C4C-C3C | 2.46 | 128.46 | 124.84 |
| 22 | B | 606 | CLA | CMA-C3A-C2A | -2.46 | 103.91 | 113.83 |
| 22 | C | 512 | CLA | O2D-CGD-CBD | -2.45 | 106.91 | 111.27 |
| 22 | B | 612 | CLA | C9-C8-C7 | 2.45 | 120.17 | 111.29 |
| 22 | C | 510 | CLA | C10-C8-C7 | 2.45 | 125.01 | 112.13 |
| 22 | B | 607 | CLA | C4D-CHA-C1A | -2.45 | 118.27 | 121.25 |
| 23 | C | 516 | BCR | C8-C7-C6 | -2.45 | 120.33 | 127.20 |
| 23 | C | 515 | BCR | C27-C26-C25 | 2.44 | 126.28 | 122.73 |
| 22 | A | 406 | CLA | C1D-ND-C4D | 2.44 | 108.07 | 106.33 |
| 23 | A | 407 | BCR | C29-C30-C25 | 2.44 | 114.24 | 110.48 |
| 23 | B | 617 | BCR | C24-C23-C22 | -2.44 | 122.55 | 126.23 |
| 22 | C | 510 | CLA | CHD-C1D-C2D | 2.43 | 130.59 | 125.48 |
| 22 | C | 517 | CLA | CHD-C1D-C2D | 2.43 | 130.58 | 125.48 |
| 25 | D | 403 | LMG | C1-O6-C5 | -2.43 | 108.91 | 113.69 |
| 22 | B | 601 | CLA | CBC-CAC-C3C | 2.43 | 119.14 | 112.43 |
| 23 | C | 518 | BCR | C8-C9-C10 | 2.43 | 122.67 | 118.94 |
| 22 | B | 603 | CLA | C6-C5-C3 | 2.43 | 119.83 | 113.45 |
| 23 | C | 516 | BCR | C39-C30-C25 | 2.43 | 114.24 | 110.30 |
| 25 | F | 101 | LMG | O2-C2-C1 | -2.43 | 104.15 | 110.05 |
| 22 | C | 503 | CLA | CMB-C2B-C3B | 2.43 | 129.22 | 124.68 |
| 22 | C | 510 | CLA | CAA-CBA-CGA | 2.42 | 120.34 | 113.25 |
| 22 | B | 612 | CLA | CMD-C2D-C3D | -2.42 | 122.05 | 127.61 |
| 22 | C | 510 | CLA | CMA-C3A-C4A | 2.42 | 118.28 | 111.77 |
| 22 | B | 604 | CLA | C1B-CHB-C4A | -2.42 | 125.33 | 130.12 |
| 22 | C | 511 | CLA | C6-C7-C8 | 2.42 | 123.73 | 115.92 |
| 25 | C | 502 | LMG | O6-C1-O1 | -2.41 | 104.26 | 109.97 |
| 22 | D | 407 | CLA | O1D-CGD-CBD | 2.41 | 129.42 | 124.48 |
| 23 | C | 516 | BCR | C19-C18-C17 | 2.41 | 122.64 | 118.94 |
| 22 | B | 611 | CLA | CMA-C3A-C4A | 2.41 | 118.24 | 111.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | 3 | 101 | LMG | O6-C5-C6 | 2.40 | 112.41 | 106.44 |
| 22 | C | 513 | CLA | C2A-C3A-C4A | -2.40 | 97.99 | 101.87 |
| 26 | D | 405 | PL9 | O1-C4-C3 | -2.40 | 118.08 | 120.72 |
| 22 | B | 615 | CLA | O2A-CGA-O1A | -2.40 | 117.53 | 123.59 |
| 22 | C | 509 | CLA | C1B-CHB-C4A | -2.40 | 125.37 | 130.12 |
| 22 | C | 514 | CLA | C9-C8-C7 | 2.39 | 119.96 | 111.29 |
| 22 | B | 606 | CLA | CMD-C2D-C3D | -2.39 | 122.11 | 127.61 |
| 22 | B | 605 | CLA | CBA-CAA-C2A | 2.39 | 120.92 | 113.86 |
| 22 | C | 505 | CLA | CGD-CBD-CAD | 2.39 | 118.47 | 110.73 |
| 22 | B | 608 | CLA | CBC-CAC-C3C | 2.39 | 119.01 | 112.43 |
| 22 | B | 606 | CLA | O1D-CGD-CBD | 2.38 | 129.36 | 124.48 |
| 22 | C | 509 | CLA | C9-C8-C7 | 2.38 | 119.92 | 111.29 |
| 22 | A | 406 | CLA | O1D-CGD-CBD | 2.38 | 129.36 | 124.48 |
| 23 | A | 407 | BCR | C2-C1-C6 | 2.38 | 114.14 | 110.48 |
| 22 | A | 405 | CLA | CMA-C3A-C2A | -2.38 | 104.24 | 113.83 |
| 22 | B | 603 | CLA | CMA-C3A-C2A | -2.37 | 104.28 | 113.83 |
| 22 | B | 605 | CLA | C1B-CHB-C4A | -2.37 | 125.43 | 130.12 |
| 23 | C | 516 | BCR | C36-C18-C17 | -2.37 | 119.61 | 122.92 |
| 22 | B | 603 | CLA | C9-C8-C7 | 2.36 | 119.84 | 111.29 |
| 22 | A | 405 | CLA | C9-C8-C7 | 2.36 | 119.83 | 111.29 |
| 25 | C | 501 | LMG | O6-C1-O1 | -2.36 | 104.39 | 109.97 |
| 26 | D | 405 | PL9 | C45-C44-C46 | -2.35 | 111.31 | 115.27 |
| 23 | C | 516 | BCR | C31-C1-C6 | 2.34 | 114.10 | 110.30 |
| 22 | B | 610 | CLA | CHD-C1D-ND | 2.34 | 126.61 | 124.45 |
| 23 | F | 102 | BCR | C27-C26-C25 | 2.34 | 126.13 | 122.73 |
| 22 | B | 611 | CLA | C3B-C4B-NB | -2.34 | 106.19 | 109.21 |
| 26 | D | 405 | PL9 | C37-C38-C39 | -2.33 | 122.05 | 127.66 |
| 22 | B | 605 | CLA | C1D-ND-C4D | -2.33 | 104.68 | 106.33 |
| 22 | C | 506 | CLA | C6-C5-C3 | 2.33 | 119.57 | 113.45 |
| 22 | B | 611 | CLA | CBC-CAC-C3C | 2.33 | 118.84 | 112.43 |
| 22 | C | 503 | CLA | CMD-C2D-C3D | -2.32 | 122.27 | 127.61 |
| 23 | B | 617 | BCR | C15-C16-C17 | -2.32 | 118.71 | 123.47 |
| 25 | D | 404 | LMG | O1-C7-C8 | -2.32 | 105.29 | 110.90 |
| 22 | C | 514 | CLA | C10-C8-C7 | 2.32 | 124.34 | 112.13 |
| 22 | B | 604 | CLA | C3D-C2D-C1D | 2.32 | 109.00 | 105.83 |
| 22 | B | 613 | CLA | CHD-C1D-C2D | 2.32 | 130.34 | 125.48 |
| 22 | C | 514 | CLA | CHB-C4A-NA | 2.31 | 127.71 | 124.51 |
| 22 | B | 610 | CLA | C1B-CHB-C4A | -2.31 | 125.54 | 130.12 |
| 25 | F | 101 | LMG | O6-C1-O1 | -2.31 | 104.50 | 109.97 |
| 22 | C | 503 | CLA | C1-C2-C3 | 2.31 | 130.04 | 126.04 |
| 22 | A | 405 | CLA | CBA-CAA-C2A | 2.31 | 120.68 | 113.86 |
| 22 | C | 511 | CLA | CMB-C2B-C3B | 2.31 | 128.99 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | C | 501 | LMG | C8-O7-C10 | 2.31 | 123.47 | 117.79 |
| 23 | A | 407 | BCR | C30-C25-C26 | -2.30 | 119.37 | 122.61 |
| 22 | B | 610 | CLA | C4C-C3C-C2C | -2.30 | 103.54 | 106.90 |
| 22 | B | 605 | CLA | CMD-C2D-C3D | -2.30 | 122.32 | 127.61 |
| 22 | C | 513 | CLA | C6-C7-C8 | 2.29 | 123.33 | 115.92 |
| 22 | C | 513 | CLA | CAC-C3C-C4C | 2.29 | 127.78 | 124.81 |
| 22 | C | 508 | CLA | CAA-C2A-C1A | 2.29 | 119.47 | 111.97 |
| 22 | B | 616 | CLA | CMB-C2B-C1B | -2.29 | 124.95 | 128.46 |
| 22 | B | 610 | CLA | C2D-C1D-ND | -2.29 | 108.42 | 110.10 |
| 22 | B | 604 | CLA | C6-C5-C3 | 2.28 | 119.45 | 113.45 |
| 22 | C | 508 | CLA | CMA-C3A-C4A | 2.28 | 117.91 | 111.77 |
| 25 | I | 101 | LMG | C1-O6-C5 | -2.28 | 109.21 | 113.69 |
| 22 | B | 615 | CLA | C9-C8-C10 | 2.28 | 119.55 | 111.29 |
| 22 | C | 517 | CLA | CAA-CBA-CGA | -2.28 | 106.59 | 113.25 |
| 22 | D | 402 | CLA | CAC-C3C-C4C | 2.28 | 127.76 | 124.81 |
| 23 | F | 102 | BCR | C39-C30-C25 | 2.28 | 113.99 | 110.30 |
| 25 | C | 502 | LMG | O2-C2-C1 | -2.27 | 104.53 | 110.05 |
| 22 | C | 513 | CLA | CBC-CAC-C3C | -2.27 | 106.18 | 112.43 |
| 22 | B | 614 | CLA | CMB-C2B-C1B | -2.27 | 124.98 | 128.46 |
| 22 | C | 510 | CLA | OBD-CAD-C3D | 2.26 | 133.96 | 128.52 |
| 22 | D | 402 | CLA | CMB-C2B-C3B | 2.26 | 128.91 | 124.68 |
| 22 | B | 613 | CLA | CAC-C3C-C2C | -2.26 | 123.67 | 127.53 |
| 23 | B | 618 | BCR | C1-C6-C5 | -2.26 | 119.43 | 122.61 |
| 25 | C | 501 | LMG | C1-O6-C5 | -2.26 | 109.26 | 113.69 |
| 23 | C | 518 | BCR | C38-C26-C25 | -2.25 | 122.00 | 124.53 |
| 22 | C | 513 | CLA | CGD-CBD-CAD | 2.25 | 118.04 | 110.73 |
| 22 | D | 401 | CLA | CMB-C2B-C3B | 2.25 | 128.89 | 124.68 |
| 22 | C | 510 | CLA | C9-C8-C10 | 2.25 | 119.43 | 111.29 |
| 22 | B | 603 | CLA | C9-C8-C10 | 2.25 | 119.43 | 111.29 |
| 23 | C | 516 | BCR | C30-C25-C26 | -2.24 | 119.45 | 122.61 |
| 23 | C | 515 | BCR | C29-C30-C25 | 2.24 | 113.93 | 110.48 |
| 24 | A | 408 | LHG | O8-C23-C24 | 2.24 | 118.94 | 111.91 |
| 23 | C | 518 | BCR | C36-C18-C17 | -2.24 | 119.79 | 122.92 |
| 22 | B | 613 | CLA | CMA-C3A-C4A | -2.24 | 105.76 | 111.77 |
| 22 | D | 402 | CLA | C1B-CHB-C4A | -2.23 | 125.69 | 130.12 |
| 22 | D | 401 | CLA | CAC-C3C-C4C | 2.23 | 127.71 | 124.81 |
| 22 | B | 610 | CLA | CMB-C2B-C3B | 2.23 | 128.85 | 124.68 |
| 23 | F | 102 | BCR | C8-C7-C6 | -2.23 | 120.94 | 127.20 |
| 22 | B | 601 | CLA | CMD-C2D-C1D | 2.23 | 128.64 | 124.71 |
| 23 | C | 518 | BCR | C27-C26-C25 | 2.23 | 125.96 | 122.73 |
| 22 | C | 503 | CLA | O1D-CGD-CBD | 2.23 | 129.04 | 124.48 |
| 22 | C | 517 | CLA | CMB-C2B-C3B | 2.22 | 128.83 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 614 | CLA | CGD-CBD-CAD | -2.22 | 103.55 | 110.73 |
| 22 | B | 607 | CLA | C5-C3-C2 | -2.22 | 116.63 | 121.12 |
| 22 | B | 616 | CLA | C9-C8-C7 | 2.22 | 119.32 | 111.29 |
| 25 | I | 101 | LMG | C32-C31-C30 | -2.22 | 103.18 | 114.42 |
| 22 | B | 611 | CLA | C1B-CHB-C4A | -2.21 | 125.73 | 130.12 |
| 22 | B | 607 | CLA | O2A-C1-C2 | -2.21 | 102.82 | 108.64 |
| 22 | D | 407 | CLA | CMD-C2D-C1D | -2.21 | 120.82 | 124.71 |
| 22 | B | 601 | CLA | O2D-CGD-O1D | -2.21 | 119.52 | 123.84 |
| 22 | B | 610 | CLA | CAA-C2A-C1A | 2.21 | 119.21 | 111.97 |
| 22 | A | 406 | CLA | C6-C7-C8 | 2.21 | 123.05 | 115.92 |
| 22 | C | 506 | CLA | CMB-C2B-C3B | 2.21 | 128.81 | 124.68 |
| 22 | B | 607 | CLA | C2A-C3A-C4A | -2.21 | 98.31 | 101.87 |
| 22 | B | 607 | CLA | CAC-C3C-C4C | 2.20 | 127.67 | 124.81 |
| 22 | B | 603 | CLA | C2A-C3A-C4A | -2.20 | 98.31 | 101.87 |
| 22 | C | 512 | CLA | CGD-CBD-CAD | -2.20 | 103.62 | 110.73 |
| 22 | B | 604 | CLA | O2A-CGA-O1A | -2.20 | 118.05 | 123.59 |
| 22 | A | 405 | CLA | CBC-CAC-C3C | 2.20 | 118.48 | 112.43 |
| 22 | B | 609 | CLA | CMA-C3A-C4A | -2.19 | 105.88 | 111.77 |
| 22 | B | 601 | CLA | CMD-C2D-C3D | -2.19 | 122.57 | 127.61 |
| 26 | D | 405 | PL9 | C8-C7-C3 | 2.19 | 118.17 | 111.98 |
| 26 | D | 405 | PL9 | C40-C39-C41 | 2.19 | 118.95 | 115.27 |
| 21 | A | 404 | PHO | C9-C8-C10 | 2.19 | 119.22 | 111.29 |
| 23 | C | 518 | BCR | C33-C5-C6 | -2.18 | 122.08 | 124.53 |
| 22 | C | 512 | CLA | CHB-C4A-NA | 2.18 | 127.53 | 124.51 |
| 23 | C | 515 | BCR | C1-C6-C5 | -2.18 | 119.54 | 122.61 |
| 22 | C | 508 | CLA | C2D-C1D-ND | -2.18 | 108.50 | 110.10 |
| 22 | C | 507 | CLA | OBD-CAD-C3D | 2.18 | 133.76 | 128.52 |
| 22 | B | 606 | CLA | C4D-CHA-C1A | -2.18 | 118.60 | 121.25 |
| 22 | C | 513 | CLA | CMB-C2B-C3B | 2.18 | 128.75 | 124.68 |
| 22 | B | 605 | CLA | O1D-CGD-CBD | 2.17 | 128.93 | 124.48 |
| 22 | C | 517 | CLA | C9-C8-C7 | 2.17 | 119.16 | 111.29 |
| 22 | C | 510 | CLA | CMD-C2D-C1D | -2.17 | 120.89 | 124.71 |
| 22 | B | 606 | CLA | C1D-ND-C4D | -2.17 | 104.79 | 106.33 |
| 22 | A | 406 | CLA | CHA-C4D-ND | 2.17 | 137.04 | 132.50 |
| 22 | C | 505 | CLA | O2A-CGA-CBA | 2.17 | 118.71 | 111.91 |
| 22 | B | 601 | CLA | C3D-C2D-C1D | 2.17 | 108.79 | 105.83 |
| 22 | C | 503 | CLA | C2A-C1A-CHA | 2.16 | 127.64 | 123.86 |
| 23 | C | 518 | BCR | C34-C9-C8 | -2.16 | 114.67 | 118.08 |
| 22 | B | 606 | CLA | CAA-C2A-C3A | 2.16 | 118.70 | 112.78 |
| 25 | D | 403 | LMG | O2-C2-C1 | -2.16 | 104.80 | 110.05 |
| 22 | C | 508 | CLA | CGD-CBD-CAD | -2.16 | 103.74 | 110.73 |
| 22 | B | 606 | CLA | C5-C3-C2 | -2.16 | 116.75 | 121.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 607 | CLA | CBA-CAA-C2A | 2.16 | 120.23 | 113.86 |
| 22 | B | 614 | CLA | CMA-C3A-C4A | -2.15 | 105.99 | 111.77 |
| 22 | B | 608 | CLA | CAC-C3C-C4C | 2.15 | 127.60 | 124.81 |
| 22 | C | 511 | CLA | C10-C8-C7 | 2.15 | 123.44 | 112.13 |
| 21 | D | 406 | PHO | C11-C10-C8 | 2.15 | 122.85 | 115.92 |
| 22 | B | 608 | CLA | O1D-CGD-CBD | 2.14 | 128.87 | 124.48 |
| 23 | C | 515 | BCR | C2-C1-C6 | 2.14 | 113.78 | 110.48 |
| 23 | C | 516 | BCR | C29-C30-C25 | 2.14 | 113.78 | 110.48 |
| 22 | B | 612 | CLA | C4C-C3C-C2C | -2.14 | 103.78 | 106.90 |
| 22 | C | 505 | CLA | CED-O2D-CGD | 2.14 | 120.78 | 115.94 |
| 22 | C | 507 | CLA | C1D-ND-C4D | -2.14 | 104.82 | 106.33 |
| 22 | D | 407 | CLA | CHD-C1D-C2D | 2.14 | 129.96 | 125.48 |
| 22 | C | 512 | CLA | O2A-CGA-O1A | -2.14 | 118.20 | 123.59 |
| 23 | B | 619 | BCR | C37-C22-C21 | -2.14 | 119.93 | 122.92 |
| 22 | B | 603 | CLA | CMB-C2B-C1B | -2.14 | 125.18 | 128.46 |
| 22 | C | 504 | CLA | CMB-C2B-C3B | 2.14 | 128.67 | 124.68 |
| 22 | B | 610 | CLA | O2A-C1-C2 | -2.14 | 103.02 | 108.64 |
| 25 | D | 404 | LMG | C8-O7-C10 | 2.14 | 123.05 | 117.79 |
| 22 | D | 407 | CLA | C6-C7-C8 | 2.13 | 122.82 | 115.92 |
| 25 | 3 | 101 | LMG | C6-C5-C4 | -2.13 | 108.00 | 113.00 |
| 22 | C | 514 | CLA | C4-C3-C5 | 2.13 | 118.86 | 115.27 |
| 23 | K | 101 | BCR | C34-C9-C8 | 2.13 | 121.44 | 118.08 |
| 22 | C | 508 | CLA | C1B-CHB-C4A | -2.13 | 125.89 | 130.12 |
| 21 | A | 404 | PHO | O2D-CGD-O1D | -2.13 | 119.67 | 123.84 |
| 22 | B | 615 | CLA | C4D-CHA-C1A | -2.13 | 118.66 | 121.25 |
| 22 | C | 508 | CLA | C6-C7-C8 | 2.13 | 122.81 | 115.92 |
| 22 | B | 613 | CLA | CMD-C2D-C3D | -2.13 | 122.72 | 127.61 |
| 22 | B | 606 | CLA | C9-C8-C10 | 2.13 | 118.99 | 111.29 |
| 22 | B | 606 | CLA | O2A-CGA-O1A | -2.13 | 118.23 | 123.59 |
| 22 | C | 517 | CLA | CBA-CAA-C2A | 2.12 | 120.14 | 113.86 |
| 22 | B | 616 | CLA | C2A-C3A-C4A | -2.12 | 98.44 | 101.87 |
| 22 | B | 604 | CLA | C3D-C4D-ND | 2.12 | 113.67 | 110.24 |
| 22 | D | 401 | CLA | C3A-C2A-C1A | -2.12 | 98.16 | 101.34 |
| 22 | C | 506 | CLA | C9-C8-C7 | 2.12 | 118.97 | 111.29 |
| 22 | C | 517 | CLA | C3A-C2A-C1A | -2.12 | 98.17 | 101.34 |
| 22 | B | 614 | CLA | C4D-CHA-C1A | -2.12 | 118.67 | 121.25 |
| 22 | C | 506 | CLA | C9-C8-C10 | 2.12 | 118.96 | 111.29 |
| 22 | B | 614 | CLA | C1B-CHB-C4A | -2.12 | 125.93 | 130.12 |
| 22 | C | 507 | CLA | C1B-CHB-C4A | -2.11 | 125.93 | 130.12 |
| 22 | D | 408 | CLA | O1D-CGD-CBD | 2.11 | 128.81 | 124.48 |
| 22 | C | 505 | CLA | C9-C8-C7 | 2.11 | 118.95 | 111.29 |
| 22 | B | 607 | CLA | CHB-C4A-NA | 2.11 | 127.43 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26 | D | 405 | PL9 | C7-C3-C2 | -2.11 | 120.52 | 123.30 |
| 22 | B | 616 | CLA | O1D-CGD-CBD | 2.11 | 128.81 | 124.48 |
| 23 | C | 515 | BCR | C39-C30-C25 | -2.11 | 106.88 | 110.30 |
| 22 | C | 504 | CLA | CMD-C2D-C3D | -2.11 | 122.77 | 127.61 |
| 22 | D | 408 | CLA | CAA-C2A-C1A | 2.11 | 118.88 | 111.97 |
| 22 | B | 607 | CLA | CMB-C2B-C3B | 2.11 | 128.62 | 124.68 |
| 22 | C | 511 | CLA | CMD-C2D-C1D | 2.10 | 128.42 | 124.71 |
| 22 | B | 606 | CLA | C4-C3-C5 | 2.10 | 118.81 | 115.27 |
| 22 | B | 602 | CLA | CHB-C4A-NA | 2.10 | 127.42 | 124.51 |
| 22 | C | 503 | CLA | CMA-C3A-C2A | -2.10 | 105.35 | 113.83 |
| 22 | B | 611 | CLA | CMD-C2D-C1D | -2.10 | 121.01 | 124.71 |
| 22 | B | 614 | CLA | OBD-CAD-C3D | 2.10 | 133.57 | 128.52 |
| 23 | H | 101 | BCR | C34-C9-C8 | 2.10 | 121.39 | 118.08 |
| 23 | C | 515 | BCR | C38-C26-C27 | -2.10 | 109.58 | 113.62 |
| 22 | B | 607 | CLA | CHA-C4D-ND | 2.10 | 136.88 | 132.50 |
| 22 | A | 406 | CLA | C1B-CHB-C4A | -2.10 | 125.97 | 130.12 |
| 21 | A | 404 | PHO | C1B-NB-C4B | 2.09 | 111.39 | 107.09 |
| 22 | D | 407 | CLA | CAC-C3C-C2C | -2.09 | 123.95 | 127.53 |
| 22 | B | 609 | CLA | C1D-ND-C4D | -2.09 | 104.85 | 106.33 |
| 22 | B | 607 | CLA | CED-O2D-CGD | 2.09 | 120.67 | 115.94 |
| 22 | B | 610 | CLA | C10-C8-C7 | 2.09 | 123.12 | 112.13 |
| 25 | I | 101 | LMG | C1-C2-C3 | -2.09 | 105.64 | 110.00 |
| 22 | C | 503 | CLA | C1B-CHB-C4A | -2.09 | 125.98 | 130.12 |
| 22 | C | 507 | CLA | O1D-CGD-CBD | 2.09 | 128.76 | 124.48 |
| 22 | B | 614 | CLA | CBC-CAC-C3C | 2.09 | 118.19 | 112.43 |
| 22 | B | 611 | CLA | CAC-C3C-C2C | -2.09 | 123.96 | 127.53 |
| 23 | B | 618 | BCR | C35-C13-C14 | -2.08 | 120.00 | 122.92 |
| 22 | B | 613 | CLA | C3C-C4C-NC | -2.08 | 108.24 | 110.57 |
| 22 | C | 511 | CLA | C9-C8-C7 | 2.08 | 118.81 | 111.29 |
| 21 | D | 406 | PHO | CMC-C2C-C3C | 2.07 | 128.85 | 124.94 |
| 23 | C | 516 | BCR | C23-C24-C25 | -2.07 | 121.39 | 127.20 |
| 22 | C | 511 | CLA | C3B-C4B-NB | -2.07 | 106.54 | 109.21 |
| 22 | C | 503 | CLA | C9-C8-C10 | 2.06 | 118.76 | 111.29 |
| 22 | D | 402 | CLA | O1D-CGD-CBD | 2.06 | 128.70 | 124.48 |
| 22 | D | 408 | CLA | C9-C8-C10 | 2.06 | 118.75 | 111.29 |
| 23 | B | 617 | BCR | C8-C9-C10 | 2.06 | 122.10 | 118.94 |
| 22 | B | 603 | CLA | CMA-C3A-C4A | -2.06 | 106.24 | 111.77 |
| 22 | D | 408 | CLA | C4D-CHA-C1A | -2.06 | 118.75 | 121.25 |
| 22 | C | 517 | CLA | C3D-C4D-CHA | -2.05 | 108.03 | 112.72 |
| 26 | D | 405 | PL9 | O2-C1-C6 | 2.05 | 124.14 | 120.59 |
| 22 | B | 602 | CLA | C1B-CHB-C4A | -2.05 | 126.06 | 130.12 |
| 22 | B | 609 | CLA | CMD-C2D-C1D | -2.05 | 121.10 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 615 | CLA | CMB-C2B-C1B | -2.05 | 125.32 | 128.46 |
| 22 | B | 601 | CLA | O2D-CGD-CBD | 2.05 | 114.90 | 111.27 |
| 23 | B | 619 | BCR | C1-C6-C5 | -2.05 | 119.73 | 122.61 |
| 22 | B | 602 | CLA | O2D-CGD-CBD | 2.05 | 114.90 | 111.27 |
| 23 | K | 101 | BCR | C28-C27-C26 | -2.04 | 110.43 | 114.08 |
| 22 | D | 402 | CLA | CHB-C4A-NA | 2.04 | 127.34 | 124.51 |
| 22 | C | 505 | CLA | CBA-CAA-C2A | 2.04 | 119.89 | 113.86 |
| 25 | D | 404 | LMG | O6-C1-O1 | -2.04 | 105.15 | 109.97 |
| 23 | K | 101 | BCR | C11-C10-C9 | -2.04 | 124.40 | 127.31 |
| 25 | C | 502 | LMG | C1-C2-C3 | -2.03 | 105.76 | 110.00 |
| 23 | F | 102 | BCR | C16-C15-C14 | -2.03 | 119.31 | 123.47 |
| 23 | C | 518 | BCR | C11-C10-C9 | -2.03 | 124.41 | 127.31 |
| 25 | F | 101 | LMG | O3-C3-C2 | -2.03 | 105.66 | 110.35 |
| 22 | B | 610 | CLA | O2D-CGD-O1D | -2.03 | 119.87 | 123.84 |
| 22 | C | 505 | CLA | CMA-C3A-C2A | -2.03 | 105.65 | 113.83 |
| 22 | D | 401 | CLA | O2D-CGD-O1D | -2.02 | 119.88 | 123.84 |
| 23 | H | 101 | BCR | C28-C27-C26 | -2.02 | 110.46 | 114.08 |
| 22 | C | 506 | CLA | CHB-C4A-NA | 2.02 | 127.31 | 124.51 |
| 22 | B | 602 | CLA | C2D-C1D-ND | -2.02 | 108.61 | 110.10 |
| 23 | F | 102 | BCR | C2-C1-C6 | 2.02 | 113.59 | 110.48 |
| 22 | B | 608 | CLA | C3B-C4B-NB | -2.02 | 106.60 | 109.21 |
| 21 | D | 406 | PHO | O2D-CGD-O1D | -2.02 | 119.89 | 123.84 |
| 22 | D | 407 | CLA | CHB-C4A-NA | 2.02 | 127.30 | 124.51 |
| 22 | C | 507 | CLA | C11-C10-C8 | 2.02 | 122.43 | 115.92 |
| 22 | C | 504 | CLA | C2C-C1C-NC | 2.02 | 111.86 | 109.97 |
| 23 | C | 515 | BCR | C35-C13-C12 | 2.02 | 121.25 | 118.08 |
| 22 | B | 604 | CLA | C10-C8-C7 | 2.01 | 122.71 | 112.13 |
| 22 | B | 615 | CLA | C2A-C3A-C4A | -2.01 | 98.62 | 101.87 |
| 22 | B | 603 | CLA | CMD-C2D-C3D | -2.01 | 122.99 | 127.61 |
| 25 | C | 502 | LMG | O6-C5-C6 | 2.01 | 111.43 | 106.44 |
| 22 | C | 503 | CLA | CHA-C4D-ND | 2.01 | 136.70 | 132.50 |
| 22 | A | 406 | CLA | C4D-C3D-CAD | 2.01 | 110.46 | 108.10 |
| 23 | B | 617 | BCR | C34-C9-C10 | -2.00 | 120.11 | 122.92 |
| 22 | B | 602 | CLA | CAC-C3C-C2C | -2.00 | 124.10 | 127.53 |
| 25 | 3 | 101 | LMG | O6-C1-O1 | -2.00 | 105.23 | 109.97 |
| 23 | F | 102 | BCR | C37-C22-C21 | -2.00 | 120.12 | 122.92 |

All (75) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 21 | A | 404 | PHO | C8 |
| 21 | D | 406 | PHO | C8 |

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| Mol | Chain | Res | Type | Atom |
|------------|--------------|------------|-------------|-------------|
| 22 | A | 405 | CLA | C2A |
| 22 | A | 405 | CLA | ND |
| 22 | A | 406 | CLA | C2A |
| 22 | A | 406 | CLA | ND |
| 22 | B | 601 | CLA | ND |
| 22 | B | 601 | CLA | C2A |
| 22 | B | 601 | CLA | C8 |
| 22 | B | 602 | CLA | ND |
| 22 | B | 602 | CLA | C2A |
| 22 | B | 603 | CLA | C2A |
| 22 | B | 603 | CLA | ND |
| 22 | B | 603 | CLA | C8 |
| 22 | B | 604 | CLA | ND |
| 22 | B | 605 | CLA | ND |
| 22 | B | 605 | CLA | C8 |
| 22 | B | 606 | CLA | ND |
| 22 | B | 606 | CLA | C8 |
| 22 | B | 607 | CLA | ND |
| 22 | B | 607 | CLA | C8 |
| 22 | B | 609 | CLA | C2A |
| 22 | B | 609 | CLA | ND |
| 22 | B | 610 | CLA | C2A |
| 22 | B | 610 | CLA | ND |
| 22 | B | 611 | CLA | ND |
| 22 | B | 612 | CLA | C2A |
| 22 | B | 612 | CLA | C8 |
| 22 | B | 612 | CLA | ND |
| 22 | B | 612 | CLA | C3A |
| 22 | B | 613 | CLA | ND |
| 22 | B | 613 | CLA | C2A |
| 22 | B | 613 | CLA | C8 |
| 22 | B | 614 | CLA | ND |
| 22 | B | 614 | CLA | C2A |
| 22 | B | 614 | CLA | C8 |
| 22 | B | 615 | CLA | C2A |
| 22 | B | 615 | CLA | ND |
| 22 | B | 615 | CLA | C8 |
| 22 | B | 616 | CLA | ND |
| 22 | B | 616 | CLA | C2A |
| 22 | B | 616 | CLA | C8 |
| 22 | B | 616 | CLA | C3A |
| 22 | C | 504 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22 | C | 504 | CLA | C8 |
| 22 | C | 505 | CLA | C8 |
| 22 | C | 506 | CLA | ND |
| 22 | C | 506 | CLA | C2A |
| 22 | C | 506 | CLA | C8 |
| 22 | C | 507 | CLA | C2A |
| 22 | C | 507 | CLA | ND |
| 22 | C | 508 | CLA | C8 |
| 22 | C | 509 | CLA | C2A |
| 22 | C | 509 | CLA | ND |
| 22 | C | 510 | CLA | C8 |
| 22 | C | 511 | CLA | C2A |
| 22 | C | 511 | CLA | ND |
| 22 | C | 511 | CLA | C8 |
| 22 | C | 512 | CLA | ND |
| 22 | C | 513 | CLA | ND |
| 22 | C | 513 | CLA | C2A |
| 22 | C | 513 | CLA | C3A |
| 22 | C | 514 | CLA | ND |
| 22 | C | 514 | CLA | C2A |
| 22 | C | 514 | CLA | C8 |
| 22 | C | 517 | CLA | ND |
| 22 | C | 517 | CLA | C3A |
| 22 | C | 517 | CLA | C8 |
| 22 | D | 402 | CLA | C2A |
| 22 | D | 402 | CLA | ND |
| 22 | D | 407 | CLA | ND |
| 22 | D | 407 | CLA | C8 |
| 22 | D | 408 | CLA | C2A |
| 22 | D | 408 | CLA | ND |
| 22 | D | 408 | CLA | C8 |

All (535) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 21 | A | 404 | PHO | O2A-C1-C2-C3 |
| 22 | A | 405 | CLA | C3A-C2A-CAA-CBA |
| 22 | A | 406 | CLA | C3A-C2A-CAA-CBA |
| 22 | A | 406 | CLA | C11-C10-C8-C7 |
| 22 | B | 601 | CLA | C11-C10-C8-C9 |
| 22 | B | 602 | CLA | CHA-CBD-CGD-O1D |
| 22 | B | 602 | CLA | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | B | 603 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 603 | CLA | C2-C3-C5-C6 |
| 22 | B | 603 | CLA | C4-C3-C5-C6 |
| 22 | B | 603 | CLA | C11-C10-C8-C9 |
| 22 | B | 604 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 605 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 606 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 610 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 611 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 611 | CLA | O2A-C1-C2-C3 |
| 22 | B | 613 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 615 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 616 | CLA | C3A-C2A-CAA-CBA |
| 22 | C | 503 | CLA | O2A-C1-C2-C3 |
| 22 | C | 504 | CLA | C1A-C2A-CAA-CBA |
| 22 | C | 504 | CLA | CHA-CBD-CGD-O1D |
| 22 | C | 504 | CLA | CHA-CBD-CGD-O2D |
| 22 | C | 505 | CLA | C1A-C2A-CAA-CBA |
| 22 | C | 505 | CLA | C3A-C2A-CAA-CBA |
| 22 | C | 505 | CLA | O2A-C1-C2-C3 |
| 22 | C | 506 | CLA | C1A-C2A-CAA-CBA |
| 22 | C | 507 | CLA | C1A-C2A-CAA-CBA |
| 22 | C | 513 | CLA | C3A-C2A-CAA-CBA |
| 22 | C | 514 | CLA | O2A-C1-C2-C3 |
| 22 | C | 517 | CLA | C1A-C2A-CAA-CBA |
| 22 | C | 517 | CLA | C3A-C2A-CAA-CBA |
| 22 | D | 401 | CLA | C1A-C2A-CAA-CBA |
| 22 | D | 402 | CLA | C1A-C2A-CAA-CBA |
| 22 | D | 407 | CLA | C3A-C2A-CAA-CBA |
| 22 | D | 407 | CLA | O2A-C1-C2-C3 |
| 22 | D | 407 | CLA | C11-C10-C8-C9 |
| 22 | D | 408 | CLA | C3A-C2A-CAA-CBA |
| 23 | A | 407 | BCR | C21-C22-C23-C24 |
| 23 | A | 407 | BCR | C37-C22-C23-C24 |
| 23 | B | 617 | BCR | C7-C8-C9-C10 |
| 23 | B | 617 | BCR | C9-C10-C11-C12 |
| 23 | B | 617 | BCR | C11-C12-C13-C14 |
| 23 | B | 617 | BCR | C11-C12-C13-C35 |
| 23 | B | 617 | BCR | C15-C16-C17-C18 |
| 23 | B | 617 | BCR | C17-C18-C19-C20 |
| 23 | B | 617 | BCR | C21-C22-C23-C24 |
| 23 | B | 617 | BCR | C37-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | B | 618 | BCR | C36-C18-C19-C20 |
| 23 | B | 619 | BCR | C13-C14-C15-C16 |
| 23 | B | 619 | BCR | C36-C18-C19-C20 |
| 23 | C | 515 | BCR | C7-C8-C9-C10 |
| 23 | C | 515 | BCR | C7-C8-C9-C34 |
| 23 | C | 515 | BCR | C11-C12-C13-C14 |
| 23 | C | 515 | BCR | C11-C12-C13-C35 |
| 23 | C | 515 | BCR | C17-C18-C19-C20 |
| 23 | C | 515 | BCR | C36-C18-C19-C20 |
| 23 | C | 516 | BCR | C11-C12-C13-C14 |
| 23 | C | 516 | BCR | C11-C12-C13-C35 |
| 23 | C | 516 | BCR | C23-C24-C25-C30 |
| 23 | C | 518 | BCR | C7-C8-C9-C10 |
| 23 | C | 518 | BCR | C7-C8-C9-C34 |
| 23 | C | 518 | BCR | C15-C16-C17-C18 |
| 23 | C | 518 | BCR | C36-C18-C19-C20 |
| 23 | C | 518 | BCR | C37-C22-C23-C24 |
| 23 | F | 102 | BCR | C21-C22-C23-C24 |
| 23 | F | 102 | BCR | C37-C22-C23-C24 |
| 23 | H | 101 | BCR | C5-C6-C7-C8 |
| 23 | H | 101 | BCR | C17-C18-C19-C20 |
| 23 | H | 101 | BCR | C20-C21-C22-C37 |
| 23 | H | 101 | BCR | C23-C24-C25-C26 |
| 23 | H | 101 | BCR | C23-C24-C25-C30 |
| 23 | K | 101 | BCR | C7-C8-C9-C10 |
| 23 | K | 101 | BCR | C17-C18-C19-C20 |
| 23 | K | 101 | BCR | C20-C21-C22-C37 |
| 23 | K | 101 | BCR | C23-C24-C25-C26 |
| 23 | K | 101 | BCR | C23-C24-C25-C30 |
| 26 | D | 405 | PL9 | C35-C34-C36-C37 |
| 22 | B | 616 | CLA | CBD-CGD-O2D-CED |
| 22 | C | 507 | CLA | CBD-CGD-O2D-CED |
| 22 | C | 517 | CLA | CBD-CGD-O2D-CED |
| 22 | B | 602 | CLA | C4-C3-C5-C6 |
| 22 | B | 601 | CLA | CBD-CGD-O2D-CED |
| 22 | C | 504 | CLA | C2A-CAA-CBA-CGA |
| 22 | C | 507 | CLA | C2A-CAA-CBA-CGA |
| 22 | C | 510 | CLA | C2A-CAA-CBA-CGA |
| 23 | C | 515 | BCR | C19-C20-C21-C22 |
| 23 | C | 516 | BCR | C13-C14-C15-C16 |
| 23 | C | 518 | BCR | C13-C14-C15-C16 |
| 22 | B | 609 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 26 | D | 405 | PL9 | C33-C34-C36-C37 |
| 22 | B | 616 | CLA | O1D-CGD-O2D-CED |
| 23 | A | 407 | BCR | C19-C20-C21-C22 |
| 23 | C | 515 | BCR | C13-C14-C15-C16 |
| 23 | C | 515 | BCR | C15-C16-C17-C18 |
| 23 | C | 516 | BCR | C15-C16-C17-C18 |
| 21 | D | 406 | PHO | C8-C10-C11-C12 |
| 22 | B | 602 | CLA | C2-C3-C5-C6 |
| 22 | A | 405 | CLA | C6-C7-C8-C9 |
| 22 | A | 405 | CLA | C11-C10-C8-C9 |
| 22 | A | 406 | CLA | C6-C7-C8-C9 |
| 22 | B | 601 | CLA | C6-C7-C8-C9 |
| 22 | B | 602 | CLA | C11-C10-C8-C9 |
| 22 | B | 604 | CLA | C6-C7-C8-C9 |
| 22 | B | 608 | CLA | C11-C10-C8-C9 |
| 22 | B | 609 | CLA | C6-C7-C8-C9 |
| 22 | B | 612 | CLA | C11-C10-C8-C9 |
| 22 | B | 613 | CLA | C6-C7-C8-C9 |
| 22 | C | 503 | CLA | C6-C7-C8-C9 |
| 22 | C | 506 | CLA | C11-C10-C8-C9 |
| 22 | C | 507 | CLA | C11-C10-C8-C9 |
| 22 | C | 508 | CLA | C11-C10-C8-C9 |
| 22 | C | 509 | CLA | C6-C7-C8-C9 |
| 22 | C | 512 | CLA | C6-C7-C8-C9 |
| 22 | C | 512 | CLA | C11-C10-C8-C9 |
| 22 | D | 401 | CLA | C6-C7-C8-C9 |
| 22 | D | 401 | CLA | C11-C10-C8-C9 |
| 22 | D | 408 | CLA | C11-C10-C8-C9 |
| 23 | A | 407 | BCR | C36-C18-C19-C20 |
| 23 | B | 617 | BCR | C7-C8-C9-C34 |
| 23 | B | 617 | BCR | C36-C18-C19-C20 |
| 23 | B | 619 | BCR | C11-C12-C13-C35 |
| 23 | C | 516 | BCR | C37-C22-C23-C24 |
| 23 | H | 101 | BCR | C11-C12-C13-C35 |
| 23 | H | 101 | BCR | C37-C22-C23-C24 |
| 23 | K | 101 | BCR | C11-C12-C13-C35 |
| 23 | K | 101 | BCR | C37-C22-C23-C24 |
| 23 | A | 407 | BCR | C17-C18-C19-C20 |
| 23 | C | 516 | BCR | C7-C8-C9-C10 |
| 23 | H | 101 | BCR | C7-C8-C9-C10 |
| 23 | H | 101 | BCR | C11-C12-C13-C14 |
| 23 | K | 101 | BCR | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | B | 615 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 612 | CLA | C5-C6-C7-C8 |
| 22 | B | 605 | CLA | C3-C5-C6-C7 |
| 22 | B | 602 | CLA | C6-C7-C8-C10 |
| 22 | B | 604 | CLA | C11-C10-C8-C7 |
| 22 | B | 610 | CLA | C11-C10-C8-C7 |
| 22 | B | 614 | CLA | C11-C10-C8-C7 |
| 22 | C | 504 | CLA | C11-C10-C8-C7 |
| 22 | C | 509 | CLA | C11-C10-C8-C7 |
| 22 | C | 510 | CLA | C6-C7-C8-C10 |
| 22 | C | 513 | CLA | C6-C7-C8-C10 |
| 22 | C | 514 | CLA | C11-C10-C8-C7 |
| 22 | D | 402 | CLA | C11-C10-C8-C7 |
| 22 | B | 614 | CLA | C3-C5-C6-C7 |
| 22 | B | 615 | CLA | O1A-CGA-O2A-C1 |
| 23 | A | 407 | BCR | C9-C10-C11-C12 |
| 23 | A | 407 | BCR | C13-C14-C15-C16 |
| 23 | C | 516 | BCR | C9-C10-C11-C12 |
| 23 | F | 102 | BCR | C19-C20-C21-C22 |
| 23 | H | 101 | BCR | C19-C20-C21-C22 |
| 23 | K | 101 | BCR | C19-C20-C21-C22 |
| 22 | C | 517 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 614 | CLA | C2A-CAA-CBA-CGA |
| 23 | B | 617 | BCR | C13-C14-C15-C16 |
| 22 | A | 405 | CLA | C3-C5-C6-C7 |
| 22 | C | 507 | CLA | O1D-CGD-O2D-CED |
| 24 | A | 408 | LHG | C32-C33-C34-C35 |
| 21 | D | 406 | PHO | C4-C3-C5-C6 |
| 22 | C | 504 | CLA | C11-C10-C8-C9 |
| 22 | C | 505 | CLA | C11-C10-C8-C9 |
| 22 | C | 505 | CLA | C14-C13-C15-C16 |
| 22 | C | 506 | CLA | C11-C12-C13-C14 |
| 23 | B | 619 | BCR | C37-C22-C23-C24 |
| 23 | C | 516 | BCR | C7-C8-C9-C34 |
| 23 | H | 101 | BCR | C7-C8-C9-C34 |
| 23 | K | 101 | BCR | C7-C8-C9-C34 |
| 23 | B | 619 | BCR | C21-C22-C23-C24 |
| 24 | A | 408 | LHG | C11-C12-C13-C14 |
| 25 | D | 403 | LMG | C37-C38-C39-C40 |
| 25 | D | 404 | LMG | O6-C1-O1-C7 |
| 25 | 3 | 101 | LMG | C32-C33-C34-C35 |
| 22 | B | 601 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | B | 608 | CLA | C3A-C2A-CAA-CBA |
| 22 | C | 507 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 605 | CLA | C5-C6-C7-C8 |
| 25 | C | 502 | LMG | C15-C16-C17-C18 |
| 25 | 3 | 101 | LMG | C37-C38-C39-C40 |
| 22 | B | 601 | CLA | C4-C3-C5-C6 |
| 22 | B | 616 | CLA | C4-C3-C5-C6 |
| 22 | B | 616 | CLA | C2-C3-C5-C6 |
| 26 | D | 405 | PL9 | C13-C14-C16-C17 |
| 22 | C | 509 | CLA | C3-C5-C6-C7 |
| 23 | B | 617 | BCR | C23-C24-C25-C30 |
| 23 | H | 101 | BCR | C1-C6-C7-C8 |
| 23 | K | 101 | BCR | C1-C6-C7-C8 |
| 23 | K | 101 | BCR | C5-C6-C7-C8 |
| 25 | I | 101 | LMG | C39-C40-C41-C42 |
| 22 | B | 606 | CLA | CBA-CGA-O2A-C1 |
| 25 | C | 501 | LMG | C22-C23-C24-C25 |
| 26 | D | 405 | PL9 | C47-C48-C49-C50 |
| 26 | D | 405 | PL9 | C47-C48-C49-C51 |
| 21 | D | 406 | PHO | C2-C3-C5-C6 |
| 22 | B | 608 | CLA | C6-C7-C8-C10 |
| 22 | B | 611 | CLA | C6-C7-C8-C10 |
| 22 | B | 615 | CLA | C12-C13-C15-C16 |
| 22 | B | 616 | CLA | C6-C7-C8-C10 |
| 22 | C | 505 | CLA | C12-C13-C15-C16 |
| 22 | C | 514 | CLA | C6-C7-C8-C10 |
| 22 | C | 517 | CLA | C11-C10-C8-C7 |
| 22 | B | 606 | CLA | O1A-CGA-O2A-C1 |
| 23 | H | 101 | BCR | C9-C10-C11-C12 |
| 25 | I | 101 | LMG | C16-C17-C18-C19 |
| 22 | B | 602 | CLA | C5-C6-C7-C8 |
| 25 | C | 501 | LMG | C11-C10-O7-C8 |
| 22 | D | 401 | CLA | CBD-CGD-O2D-CED |
| 25 | D | 404 | LMG | C13-C14-C15-C16 |
| 26 | D | 405 | PL9 | C15-C14-C16-C17 |
| 21 | D | 406 | PHO | C11-C10-C8-C9 |
| 22 | B | 603 | CLA | C6-C7-C8-C9 |
| 22 | B | 603 | CLA | C11-C12-C13-C14 |
| 22 | B | 607 | CLA | C11-C10-C8-C9 |
| 22 | B | 613 | CLA | C11-C10-C8-C9 |
| 22 | B | 616 | CLA | C6-C7-C8-C9 |
| 22 | B | 604 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | B | 607 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 611 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 612 | CLA | C1A-C2A-CAA-CBA |
| 22 | C | 509 | CLA | C1A-C2A-CAA-CBA |
| 22 | C | 511 | CLA | C1A-C2A-CAA-CBA |
| 22 | C | 512 | CLA | C1A-C2A-CAA-CBA |
| 22 | D | 407 | CLA | C1A-C2A-CAA-CBA |
| 22 | D | 408 | CLA | C1A-C2A-CAA-CBA |
| 23 | K | 101 | BCR | C9-C10-C11-C12 |
| 22 | C | 505 | CLA | C4-C3-C5-C6 |
| 25 | D | 404 | LMG | O1-C7-C8-C9 |
| 24 | A | 408 | LHG | C27-C28-C29-C30 |
| 26 | D | 405 | PL9 | C46-C47-C48-C49 |
| 23 | B | 618 | BCR | C16-C17-C18-C36 |
| 25 | I | 101 | LMG | O6-C5-C6-O5 |
| 22 | A | 406 | CLA | C4-C3-C5-C6 |
| 22 | C | 505 | CLA | CBA-CGA-O2A-C1 |
| 22 | C | 517 | CLA | C8-C10-C11-C12 |
| 22 | B | 611 | CLA | C5-C6-C7-C8 |
| 25 | C | 501 | LMG | O9-C10-O7-C8 |
| 22 | A | 406 | CLA | C2-C3-C5-C6 |
| 22 | B | 605 | CLA | C6-C7-C8-C10 |
| 22 | B | 606 | CLA | C11-C12-C13-C15 |
| 22 | B | 607 | CLA | C6-C7-C8-C10 |
| 22 | B | 607 | CLA | C11-C10-C8-C7 |
| 22 | B | 612 | CLA | C6-C7-C8-C10 |
| 22 | C | 506 | CLA | C6-C7-C8-C10 |
| 22 | C | 507 | CLA | C6-C7-C8-C10 |
| 22 | C | 510 | CLA | C11-C10-C8-C7 |
| 21 | A | 404 | PHO | C6-C7-C8-C9 |
| 22 | A | 406 | CLA | C11-C10-C8-C9 |
| 22 | B | 605 | CLA | C11-C10-C8-C9 |
| 22 | B | 609 | CLA | C11-C10-C8-C9 |
| 22 | B | 615 | CLA | C14-C13-C15-C16 |
| 22 | B | 616 | CLA | C11-C10-C8-C9 |
| 22 | C | 507 | CLA | C14-C13-C15-C16 |
| 22 | C | 513 | CLA | C11-C10-C8-C9 |
| 22 | D | 402 | CLA | C6-C7-C8-C9 |
| 22 | D | 407 | CLA | C6-C7-C8-C9 |
| 23 | H | 101 | BCR | C21-C22-C23-C24 |
| 23 | K | 101 | BCR | C21-C22-C23-C24 |
| 25 | 3 | 101 | LMG | C20-C21-C22-C23 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | B | 610 | CLA | C4-C3-C5-C6 |
| 22 | B | 601 | CLA | C2-C3-C5-C6 |
| 26 | D | 405 | PL9 | C43-C44-C46-C47 |
| 25 | D | 403 | LMG | C22-C23-C24-C25 |
| 22 | B | 603 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 606 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 607 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 612 | CLA | C3A-C2A-CAA-CBA |
| 22 | D | 401 | CLA | C3A-C2A-CAA-CBA |
| 25 | D | 403 | LMG | C12-C13-C14-C15 |
| 22 | B | 604 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 610 | CLA | CBA-CGA-O2A-C1 |
| 22 | D | 401 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 602 | CLA | C8-C10-C11-C12 |
| 25 | C | 502 | LMG | C18-C19-C20-C21 |
| 25 | F | 101 | LMG | C15-C16-C17-C18 |
| 22 | B | 610 | CLA | C2-C3-C5-C6 |
| 22 | C | 505 | CLA | C2-C3-C5-C6 |
| 22 | C | 511 | CLA | C2A-CAA-CBA-CGA |
| 22 | C | 505 | CLA | O1A-CGA-O2A-C1 |
| 25 | D | 404 | LMG | O1-C7-C8-O7 |
| 25 | F | 101 | LMG | O1-C7-C8-O7 |
| 22 | B | 606 | CLA | C11-C10-C8-C9 |
| 22 | B | 611 | CLA | C11-C10-C8-C9 |
| 22 | C | 508 | CLA | C6-C7-C8-C9 |
| 22 | D | 407 | CLA | C2C-C3C-CAC-CBC |
| 24 | A | 408 | LHG | C5-C4-O6-P |
| 22 | D | 401 | CLA | O1A-CGA-O2A-C1 |
| 22 | C | 514 | CLA | C2A-CAA-CBA-CGA |
| 23 | B | 617 | BCR | C23-C24-C25-C26 |
| 23 | B | 618 | BCR | C23-C24-C25-C26 |
| 23 | B | 618 | BCR | C23-C24-C25-C30 |
| 23 | C | 516 | BCR | C1-C6-C7-C8 |
| 23 | C | 516 | BCR | C23-C24-C25-C26 |
| 25 | C | 501 | LMG | C40-C41-C42-C43 |
| 23 | B | 619 | BCR | C17-C18-C19-C20 |
| 22 | B | 610 | CLA | C2C-C3C-CAC-CBC |
| 25 | C | 501 | LMG | C29-C30-C31-C32 |
| 21 | A | 404 | PHO | C11-C10-C8-C7 |
| 22 | A | 405 | CLA | C6-C7-C8-C10 |
| 22 | A | 405 | CLA | C12-C13-C15-C16 |
| 22 | B | 601 | CLA | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | B | 602 | CLA | C12-C13-C15-C16 |
| 22 | B | 610 | CLA | C6-C7-C8-C10 |
| 22 | C | 504 | CLA | C6-C7-C8-C10 |
| 22 | C | 507 | CLA | C11-C10-C8-C7 |
| 22 | C | 507 | CLA | C12-C13-C15-C16 |
| 22 | C | 510 | CLA | C11-C12-C13-C15 |
| 22 | B | 609 | CLA | O1D-CGD-O2D-CED |
| 23 | H | 101 | BCR | C13-C14-C15-C16 |
| 23 | K | 101 | BCR | C13-C14-C15-C16 |
| 22 | D | 407 | CLA | C4C-C3C-CAC-CBC |
| 22 | B | 613 | CLA | C5-C6-C7-C8 |
| 21 | D | 406 | PHO | CAD-CBD-CGD-O2D |
| 22 | A | 406 | CLA | CAD-CBD-CGD-O2D |
| 22 | B | 609 | CLA | CAD-CBD-CGD-O2D |
| 22 | C | 503 | CLA | CAD-CBD-CGD-O2D |
| 22 | C | 511 | CLA | CAD-CBD-CGD-O2D |
| 25 | D | 404 | LMG | C9-C8-O7-C10 |
| 23 | C | 518 | BCR | C6-C7-C8-C9 |
| 26 | D | 405 | PL9 | C44-C46-C47-C48 |
| 25 | F | 101 | LMG | O1-C7-C8-C9 |
| 22 | B | 604 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 610 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 612 | CLA | C8-C10-C11-C12 |
| 22 | B | 605 | CLA | CHA-CBD-CGD-O1D |
| 22 | B | 605 | CLA | CHA-CBD-CGD-O2D |
| 22 | C | 517 | CLA | CHA-CBD-CGD-O1D |
| 22 | C | 517 | CLA | CHA-CBD-CGD-O2D |
| 22 | B | 603 | CLA | C3-C5-C6-C7 |
| 22 | C | 505 | CLA | C8-C10-C11-C12 |
| 25 | D | 404 | LMG | C22-C23-C24-C25 |
| 22 | B | 614 | CLA | C6-C7-C8-C9 |
| 22 | C | 514 | CLA | C11-C10-C8-C9 |
| 22 | C | 517 | CLA | C6-C7-C8-C9 |
| 25 | 3 | 101 | LMG | C29-C30-C31-C32 |
| 22 | C | 514 | CLA | C1A-C2A-CAA-CBA |
| 25 | C | 502 | LMG | C28-C29-C30-C31 |
| 25 | C | 501 | LMG | O6-C1-O1-C7 |
| 25 | 3 | 101 | LMG | C13-C14-C15-C16 |
| 22 | B | 605 | CLA | CAD-CBD-CGD-O1D |
| 25 | D | 404 | LMG | C39-C40-C41-C42 |
| 25 | D | 404 | LMG | C14-C15-C16-C17 |
| 22 | A | 405 | CLA | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | B | 601 | CLA | C6-C7-C8-C10 |
| 22 | B | 601 | CLA | C11-C10-C8-C7 |
| 22 | B | 604 | CLA | C6-C7-C8-C10 |
| 22 | B | 615 | CLA | C6-C7-C8-C10 |
| 22 | C | 511 | CLA | C6-C7-C8-C10 |
| 22 | C | 512 | CLA | C11-C10-C8-C7 |
| 22 | D | 401 | CLA | C6-C7-C8-C10 |
| 22 | B | 602 | CLA | C2A-CAA-CBA-CGA |
| 22 | C | 505 | CLA | C16-C17-C18-C20 |
| 25 | F | 101 | LMG | C10-C11-C12-C13 |
| 25 | D | 404 | LMG | C8-C7-O1-C1 |
| 22 | C | 504 | CLA | C3-C5-C6-C7 |
| 22 | C | 511 | CLA | C4-C3-C5-C6 |
| 22 | A | 405 | CLA | C14-C13-C15-C16 |
| 22 | C | 504 | CLA | C6-C7-C8-C9 |
| 22 | C | 510 | CLA | C11-C12-C13-C14 |
| 22 | C | 511 | CLA | C11-C10-C8-C9 |
| 23 | B | 618 | BCR | C17-C18-C19-C20 |
| 22 | C | 510 | CLA | C8-C10-C11-C12 |
| 25 | F | 101 | LMG | C7-C8-O7-C10 |
| 22 | C | 503 | CLA | C2A-CAA-CBA-CGA |
| 22 | B | 607 | CLA | C2-C1-O2A-CGA |
| 22 | C | 505 | CLA | C2-C1-O2A-CGA |
| 22 | C | 509 | CLA | C2-C1-O2A-CGA |
| 22 | B | 606 | CLA | C4-C3-C5-C6 |
| 22 | B | 611 | CLA | C4-C3-C5-C6 |
| 23 | C | 516 | BCR | C5-C6-C7-C8 |
| 22 | B | 606 | CLA | C2-C3-C5-C6 |
| 25 | D | 404 | LMG | C2-C1-O1-C7 |
| 22 | C | 504 | CLA | C10-C11-C12-C13 |
| 22 | C | 511 | CLA | C10-C11-C12-C13 |
| 25 | C | 501 | LMG | C12-C13-C14-C15 |
| 25 | C | 501 | LMG | C15-C16-C17-C18 |
| 22 | B | 609 | CLA | C11-C10-C8-C7 |
| 22 | B | 612 | CLA | C11-C12-C13-C15 |
| 22 | B | 613 | CLA | C11-C10-C8-C7 |
| 22 | C | 506 | CLA | C11-C12-C13-C15 |
| 22 | B | 608 | CLA | C6-C7-C8-C9 |
| 22 | B | 611 | CLA | C6-C7-C8-C9 |
| 22 | B | 612 | CLA | C11-C12-C13-C14 |
| 22 | C | 505 | CLA | C6-C7-C8-C9 |
| 22 | C | 514 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | C | 510 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 616 | CLA | C8-C10-C11-C12 |
| 25 | D | 404 | LMG | C40-C41-C42-C43 |
| 21 | A | 404 | PHO | C16-C17-C18-C19 |
| 22 | D | 402 | CLA | C8-C10-C11-C12 |
| 22 | B | 613 | CLA | C2-C1-O2A-CGA |
| 22 | C | 512 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 607 | CLA | C4-C3-C5-C6 |
| 22 | B | 603 | CLA | C2C-C3C-CAC-CBC |
| 22 | C | 511 | CLA | C2-C3-C5-C6 |
| 22 | B | 614 | CLA | C11-C10-C8-C9 |
| 22 | D | 408 | CLA | C6-C7-C8-C9 |
| 22 | B | 615 | CLA | C5-C6-C7-C8 |
| 27 | E | 101 | HEM | CAD-CBD-CGD-O2D |
| 25 | C | 501 | LMG | C7-C8-O7-C10 |
| 25 | C | 501 | LMG | C9-C8-O7-C10 |
| 22 | A | 405 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 609 | CLA | C1A-C2A-CAA-CBA |
| 22 | C | 513 | CLA | C1A-C2A-CAA-CBA |
| 22 | C | 505 | CLA | CAA-CBA-CGA-O2A |
| 22 | B | 606 | CLA | C6-C7-C8-C10 |
| 22 | B | 612 | CLA | C12-C13-C15-C16 |
| 22 | C | 509 | CLA | C6-C7-C8-C10 |
| 27 | E | 101 | HEM | CAD-CBD-CGD-O1D |
| 22 | C | 517 | CLA | C2A-CAA-CBA-CGA |
| 24 | A | 408 | LHG | O6-C4-C5-O7 |
| 22 | B | 607 | CLA | CBA-CGA-O2A-C1 |
| 22 | C | 506 | CLA | C13-C15-C16-C17 |
| 22 | B | 611 | CLA | C2-C3-C5-C6 |
| 25 | C | 502 | LMG | C23-C24-C25-C26 |
| 22 | B | 607 | CLA | O1A-CGA-O2A-C1 |
| 23 | C | 518 | BCR | C1-C6-C7-C8 |
| 22 | B | 607 | CLA | C2-C3-C5-C6 |
| 22 | C | 509 | CLA | C2A-CAA-CBA-CGA |
| 25 | D | 403 | LMG | C40-C41-C42-C43 |
| 24 | A | 408 | LHG | O6-C4-C5-C6 |
| 22 | D | 401 | CLA | O1D-CGD-O2D-CED |
| 26 | D | 405 | PL9 | C29-C31-C32-C33 |
| 22 | A | 405 | CLA | C11-C10-C8-C7 |
| 22 | C | 511 | CLA | C11-C10-C8-C7 |
| 22 | D | 402 | CLA | C6-C7-C8-C10 |
| 22 | D | 408 | CLA | C6-C7-C8-C10 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | C | 505 | CLA | C10-C11-C12-C13 |
| 25 | C | 501 | LMG | C2-C1-O1-C7 |
| 22 | C | 505 | CLA | CBD-CGD-O2D-CED |
| 21 | A | 404 | PHO | C16-C17-C18-C20 |
| 23 | A | 407 | BCR | C11-C10-C9-C34 |
| 22 | B | 612 | CLA | CAA-CBA-CGA-O2A |
| 21 | D | 406 | PHO | C6-C7-C8-C9 |
| 22 | B | 606 | CLA | C6-C7-C8-C9 |
| 22 | B | 606 | CLA | C11-C12-C13-C14 |
| 22 | B | 615 | CLA | C11-C10-C8-C9 |
| 22 | C | 503 | CLA | C11-C10-C8-C9 |
| 22 | C | 507 | CLA | C6-C7-C8-C9 |
| 22 | C | 504 | CLA | C3A-C2A-CAA-CBA |
| 22 | D | 402 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 613 | CLA | CAA-CBA-CGA-O2A |
| 22 | D | 402 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 404 | PHO | CAD-CBD-CGD-O2D |
| 25 | F | 101 | LMG | C9-C8-O7-C10 |
| 21 | A | 404 | PHO | C10-C11-C12-C13 |
| 22 | C | 504 | CLA | CAA-CBA-CGA-O2A |
| 22 | D | 401 | CLA | C2-C3-C5-C6 |
| 26 | D | 405 | PL9 | C39-C41-C42-C43 |
| 25 | 3 | 101 | LMG | C40-C41-C42-C43 |
| 22 | D | 402 | CLA | C13-C15-C16-C17 |
| 22 | B | 614 | CLA | CAA-CBA-CGA-O2A |
| 23 | B | 617 | BCR | C10-C11-C12-C13 |
| 22 | B | 608 | CLA | O2A-C1-C2-C3 |
| 22 | C | 509 | CLA | O2A-C1-C2-C3 |
| 22 | B | 611 | CLA | CBA-CGA-O2A-C1 |
| 25 | C | 501 | LMG | C42-C43-C44-C45 |
| 22 | B | 606 | CLA | CHA-CBD-CGD-O1D |
| 22 | B | 606 | CLA | CHA-CBD-CGD-O2D |
| 22 | C | 506 | CLA | CHA-CBD-CGD-O1D |
| 22 | C | 506 | CLA | CHA-CBD-CGD-O2D |
| 22 | C | 514 | CLA | CHA-CBD-CGD-O1D |
| 22 | C | 514 | CLA | CHA-CBD-CGD-O2D |
| 27 | E | 101 | HEM | CAA-CBA-CGA-O2A |
| 25 | C | 501 | LMG | O8-C28-C29-C30 |
| 23 | C | 516 | BCR | C12-C13-C14-C15 |
| 25 | C | 501 | LMG | O1-C7-C8-O7 |
| 22 | B | 611 | CLA | O1A-CGA-O2A-C1 |
| 25 | I | 101 | LMG | C38-C39-C40-C41 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | C | 510 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 611 | CLA | CAA-CBA-CGA-O2A |
| 22 | A | 406 | CLA | C6-C7-C8-C10 |
| 22 | B | 613 | CLA | C6-C7-C8-C10 |
| 22 | B | 614 | CLA | C11-C12-C13-C15 |
| 22 | C | 510 | CLA | C16-C17-C18-C19 |
| 22 | A | 405 | CLA | C11-C12-C13-C14 |
| 22 | B | 615 | CLA | C6-C7-C8-C9 |
| 22 | C | 506 | CLA | C6-C7-C8-C9 |
| 22 | C | 510 | CLA | C6-C7-C8-C9 |
| 22 | D | 407 | CLA | CAA-CBA-CGA-O2A |
| 25 | C | 502 | LMG | O8-C28-C29-C30 |
| 22 | C | 512 | CLA | C2A-CAA-CBA-CGA |
| 26 | D | 405 | PL9 | C16-C17-C18-C19 |
| 26 | D | 405 | PL9 | C26-C27-C28-C29 |
| 22 | B | 612 | CLA | CAA-CBA-CGA-O1A |
| 22 | B | 614 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 615 | CLA | C1A-C2A-CAA-CBA |
| 22 | C | 508 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 603 | CLA | C15-C16-C17-C18 |
| 25 | F | 101 | LMG | O6-C5-C6-O5 |
| 22 | D | 402 | CLA | CAA-CBA-CGA-O1A |
| 25 | C | 501 | LMG | O10-C28-C29-C30 |
| 25 | 3 | 101 | LMG | C30-C31-C32-C33 |
| 25 | C | 501 | LMG | O1-C7-C8-C9 |
| 22 | B | 614 | CLA | CAA-CBA-CGA-O1A |
| 25 | C | 502 | LMG | O10-C28-C29-C30 |
| 25 | I | 101 | LMG | C15-C16-C17-C18 |
| 27 | E | 101 | HEM | CAA-CBA-CGA-O1A |
| 22 | C | 514 | CLA | C16-C17-C18-C20 |
| 22 | D | 407 | CLA | CAA-CBA-CGA-O1A |
| 25 | C | 501 | LMG | O9-C10-C11-C12 |
| 22 | A | 406 | CLA | CAA-CBA-CGA-O2A |
| 25 | C | 501 | LMG | O7-C10-C11-C12 |
| 23 | C | 518 | BCR | C5-C6-C7-C8 |
| 25 | 3 | 101 | LMG | C14-C15-C16-C17 |
| 22 | C | 504 | CLA | CAA-CBA-CGA-O1A |
| 22 | C | 512 | CLA | C5-C6-C7-C8 |
| 25 | C | 502 | LMG | C38-C39-C40-C41 |
| 22 | C | 510 | CLA | CAA-CBA-CGA-O2A |
| 22 | B | 606 | CLA | CAD-CBD-CGD-O1D |
| 22 | C | 506 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | B | 602 | CLA | C14-C13-C15-C16 |
| 22 | B | 612 | CLA | C6-C7-C8-C9 |
| 22 | B | 611 | CLA | CAA-CBA-CGA-O1A |
| 22 | C | 503 | CLA | CAA-CBA-CGA-O2A |
| 22 | B | 607 | CLA | CAA-CBA-CGA-O2A |
| 22 | C | 510 | CLA | CAA-CBA-CGA-O1A |
| 25 | D | 403 | LMG | C24-C25-C26-C27 |
| 22 | B | 605 | CLA | C11-C10-C8-C7 |
| 22 | B | 608 | CLA | C11-C10-C8-C7 |
| 22 | C | 503 | CLA | C6-C7-C8-C10 |
| 22 | C | 517 | CLA | C11-C12-C13-C15 |
| 22 | D | 401 | CLA | C12-C13-C15-C16 |
| 22 | C | 512 | CLA | CAA-CBA-CGA-O2A |
| 23 | C | 516 | BCR | C21-C22-C23-C24 |
| 22 | B | 607 | CLA | CAA-CBA-CGA-O1A |
| 22 | C | 506 | CLA | CAA-CBA-CGA-O1A |
| 22 | C | 512 | CLA | CAA-CBA-CGA-O1A |
| 22 | A | 405 | CLA | CAA-CBA-CGA-O2A |
| 24 | A | 408 | LHG | C29-C30-C31-C32 |
| 22 | B | 610 | CLA | C4C-C3C-CAC-CBC |
| 22 | D | 401 | CLA | C4C-C3C-CAC-CBC |
| 22 | A | 406 | CLA | CAA-CBA-CGA-O1A |
| 22 | D | 401 | CLA | C4-C3-C5-C6 |
| 26 | D | 405 | PL9 | C45-C44-C46-C47 |

There are no ring outliers.

47 monomers are involved in 109 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23 | C | 515 | BCR | 4 | 0 |
| 22 | B | 602 | CLA | 2 | 0 |
| 22 | B | 601 | CLA | 2 | 0 |
| 22 | B | 604 | CLA | 2 | 0 |
| 23 | K | 101 | BCR | 11 | 0 |
| 22 | B | 613 | CLA | 4 | 0 |
| 23 | A | 407 | BCR | 1 | 0 |
| 27 | E | 101 | HEM | 3 | 0 |
| 22 | B | 605 | CLA | 2 | 0 |
| 22 | B | 608 | CLA | 1 | 0 |
| 26 | D | 405 | PL9 | 4 | 0 |
| 22 | B | 614 | CLA | 3 | 0 |
| 25 | I | 101 | LMG | 2 | 0 |

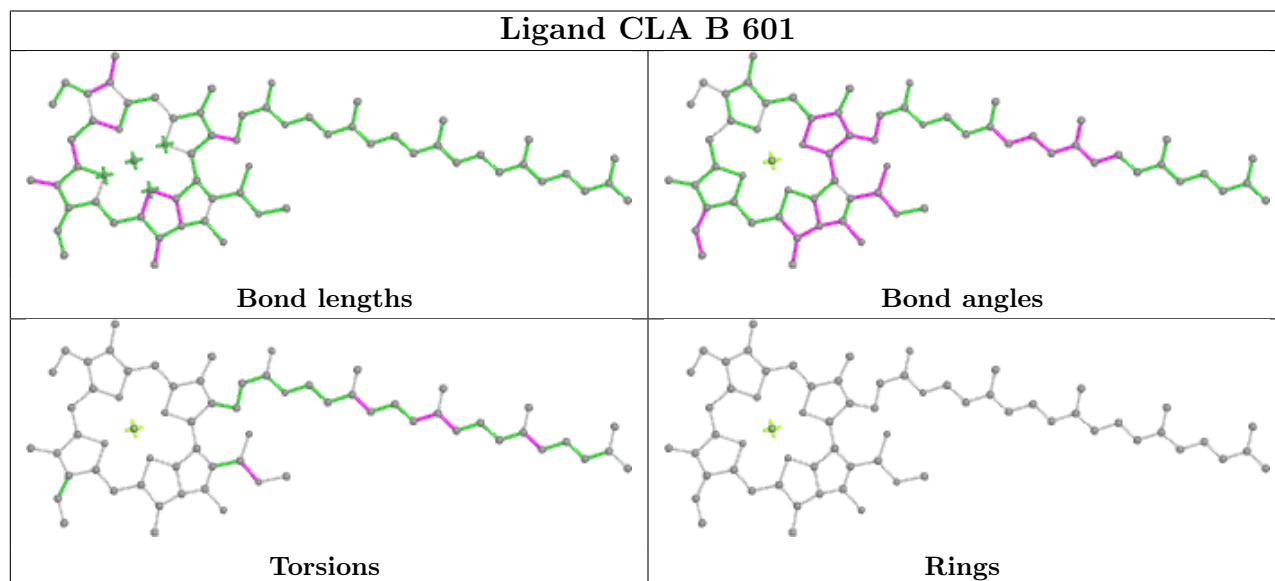
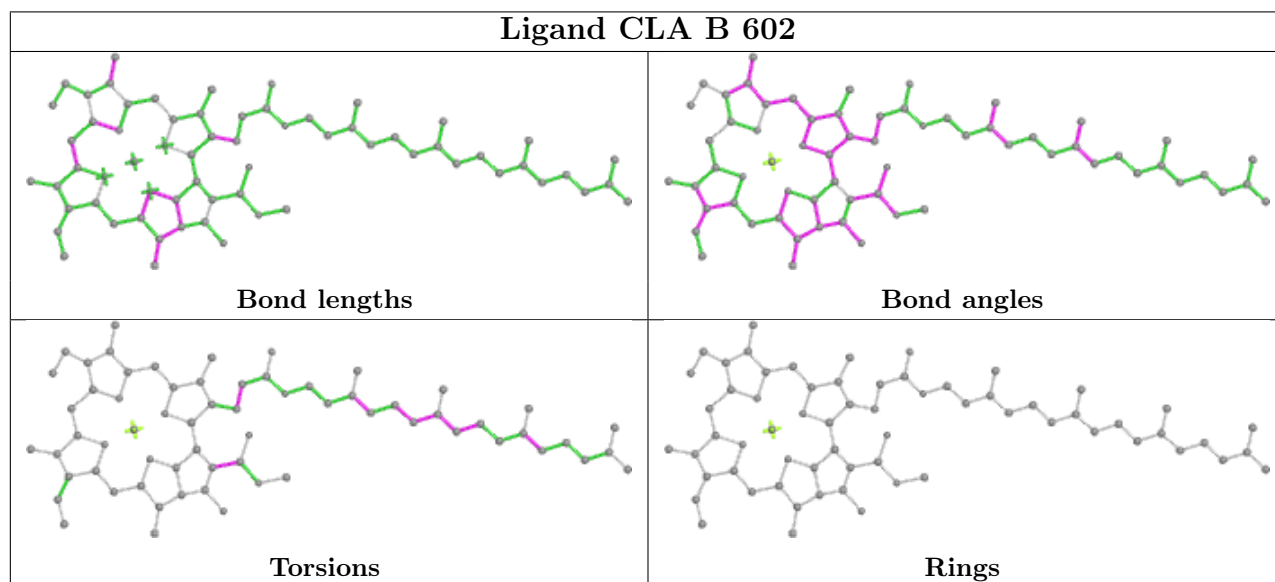
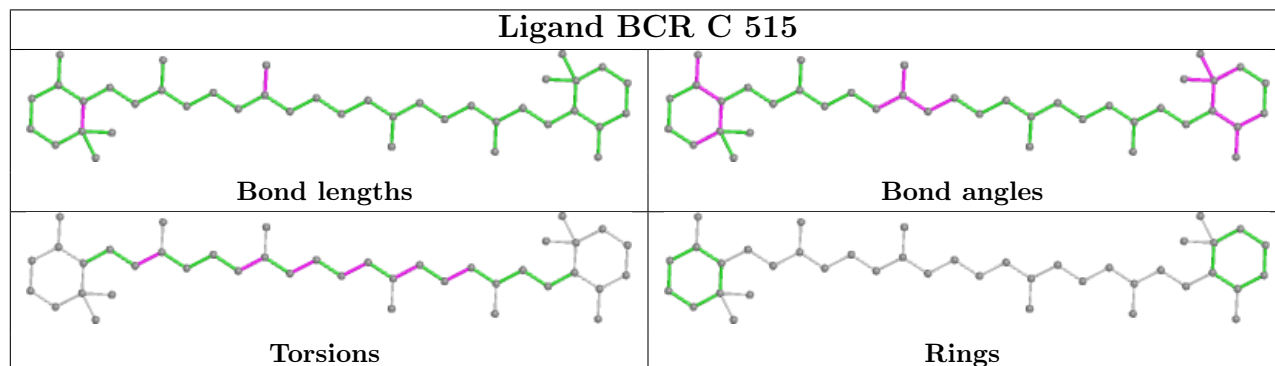
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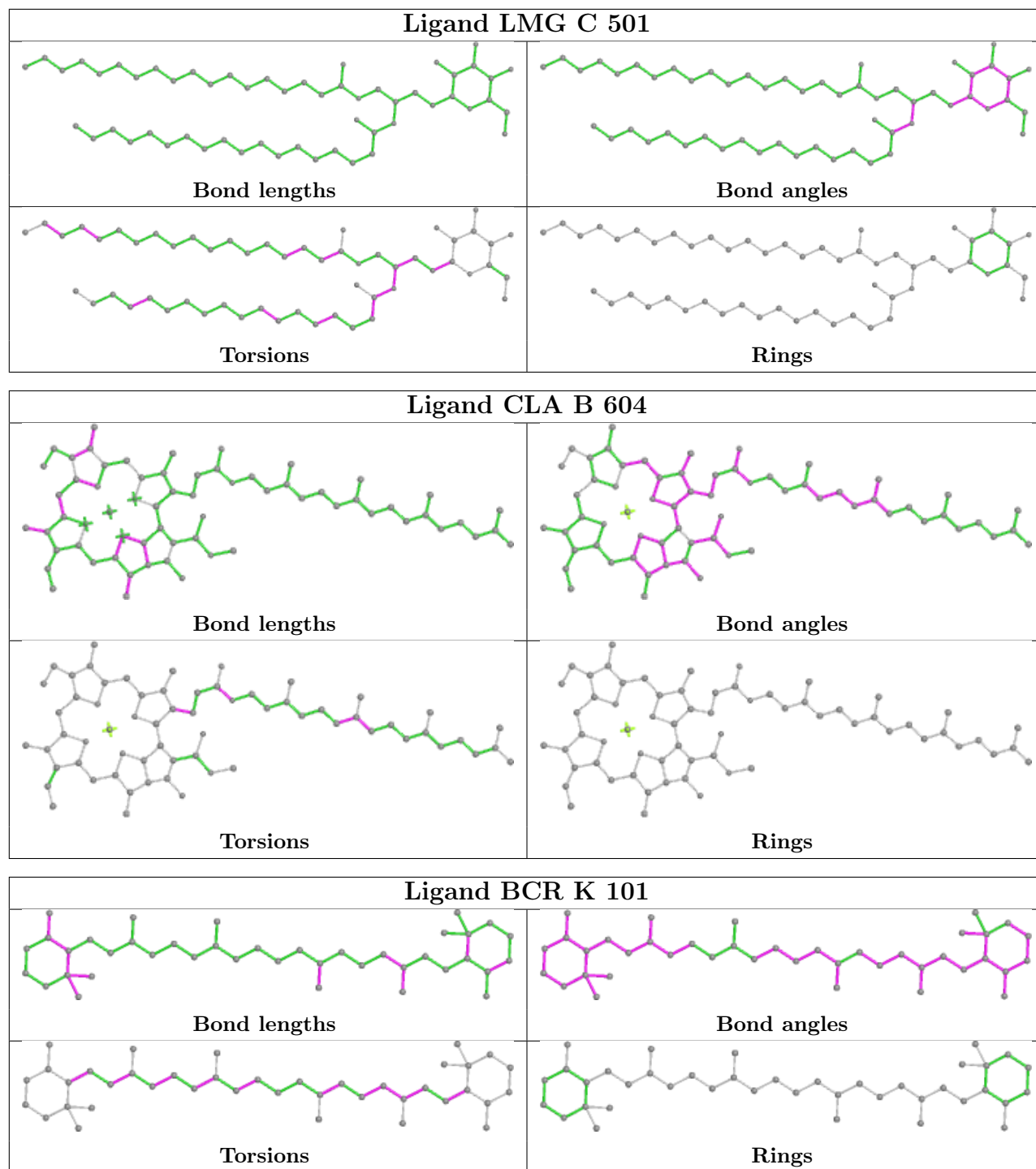
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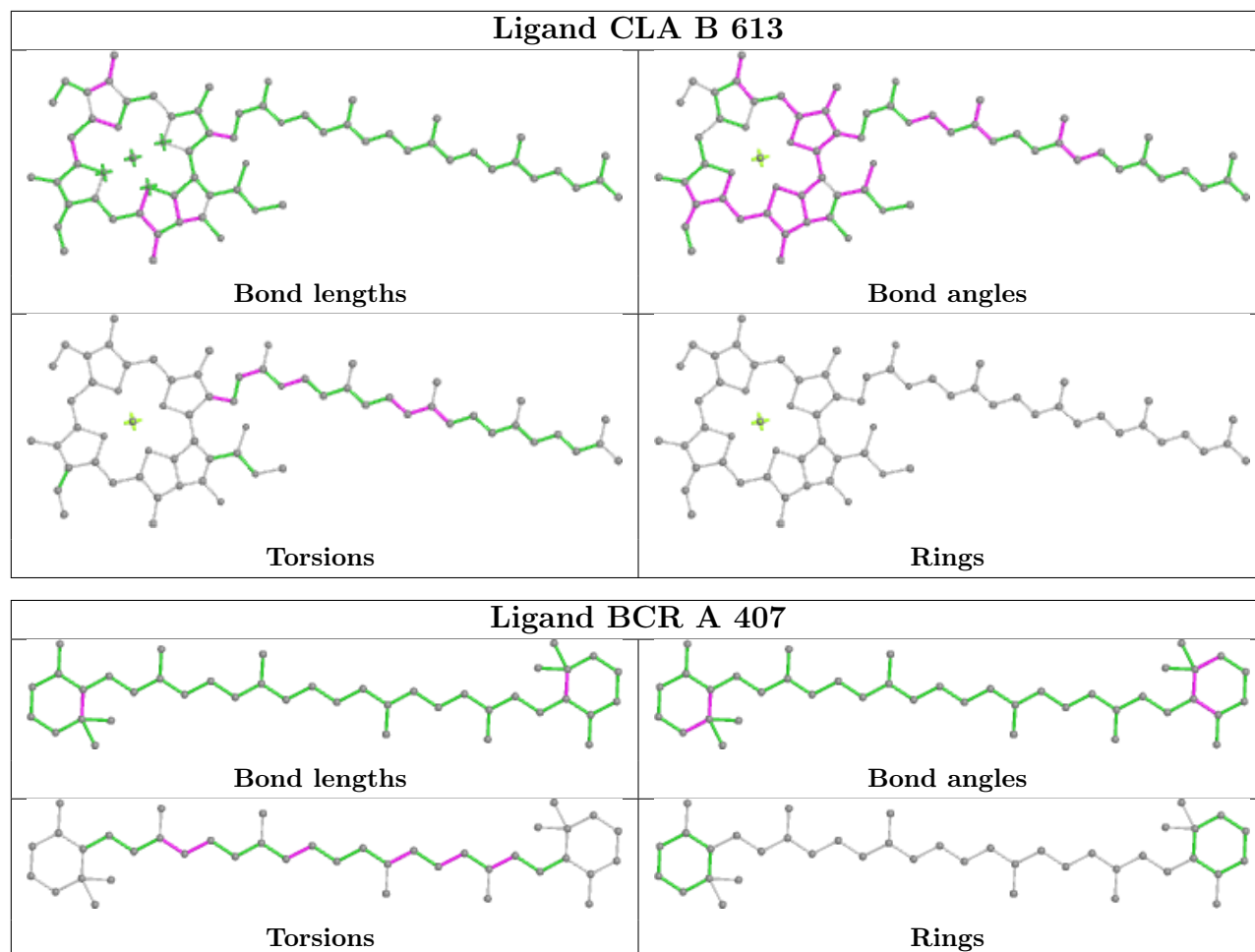
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22 | C | 504 | CLA | 3 | 0 |
| 25 | D | 403 | LMG | 1 | 0 |
| 23 | B | 619 | BCR | 1 | 0 |
| 22 | A | 406 | CLA | 2 | 0 |
| 25 | D | 404 | LMG | 1 | 0 |
| 22 | D | 401 | CLA | 2 | 0 |
| 22 | C | 514 | CLA | 1 | 0 |
| 23 | C | 516 | BCR | 3 | 0 |
| 23 | H | 101 | BCR | 15 | 0 |
| 23 | F | 102 | BCR | 1 | 0 |
| 22 | B | 606 | CLA | 1 | 0 |
| 22 | B | 609 | CLA | 11 | 0 |
| 22 | B | 615 | CLA | 1 | 0 |
| 22 | C | 511 | CLA | 5 | 0 |
| 22 | C | 513 | CLA | 3 | 0 |
| 22 | B | 610 | CLA | 2 | 0 |
| 22 | B | 607 | CLA | 2 | 0 |
| 22 | C | 503 | CLA | 4 | 0 |
| 25 | 3 | 101 | LMG | 2 | 0 |
| 22 | C | 505 | CLA | 4 | 0 |
| 22 | C | 509 | CLA | 2 | 0 |
| 22 | D | 402 | CLA | 2 | 0 |
| 22 | B | 611 | CLA | 1 | 0 |
| 22 | C | 510 | CLA | 3 | 0 |
| 21 | A | 404 | PHO | 2 | 0 |
| 22 | D | 408 | CLA | 3 | 0 |
| 23 | C | 518 | BCR | 1 | 0 |
| 22 | C | 517 | CLA | 4 | 0 |
| 22 | D | 407 | CLA | 3 | 0 |
| 23 | B | 617 | BCR | 2 | 0 |
| 21 | D | 406 | PHO | 3 | 0 |
| 22 | B | 612 | CLA | 2 | 0 |
| 22 | B | 603 | CLA | 4 | 0 |
| 22 | C | 506 | CLA | 1 | 0 |

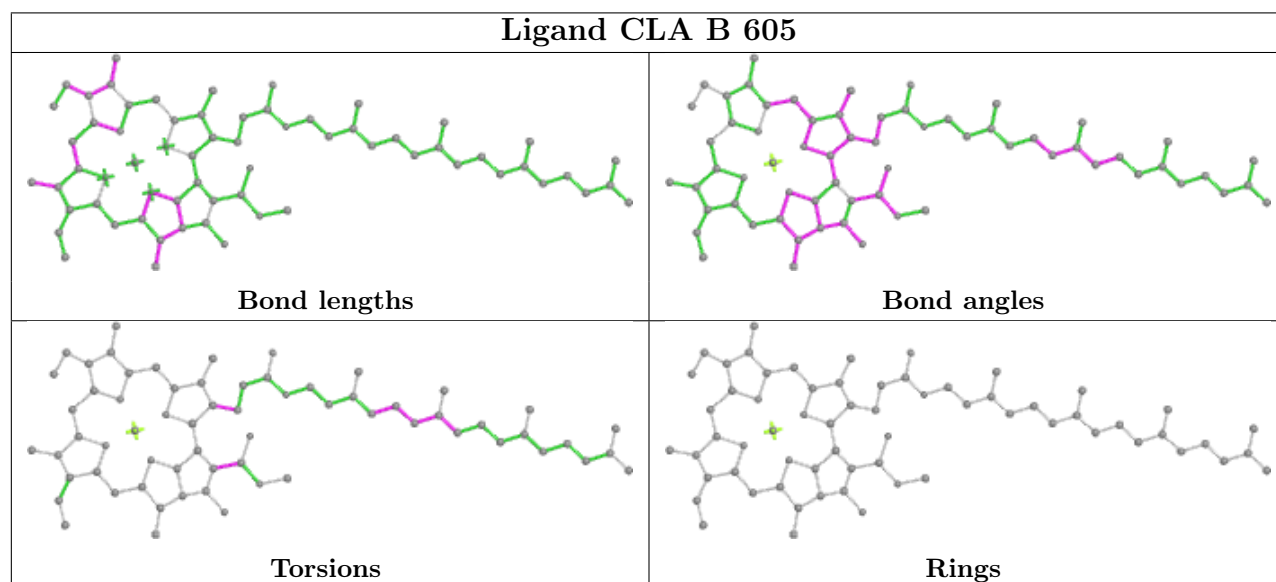
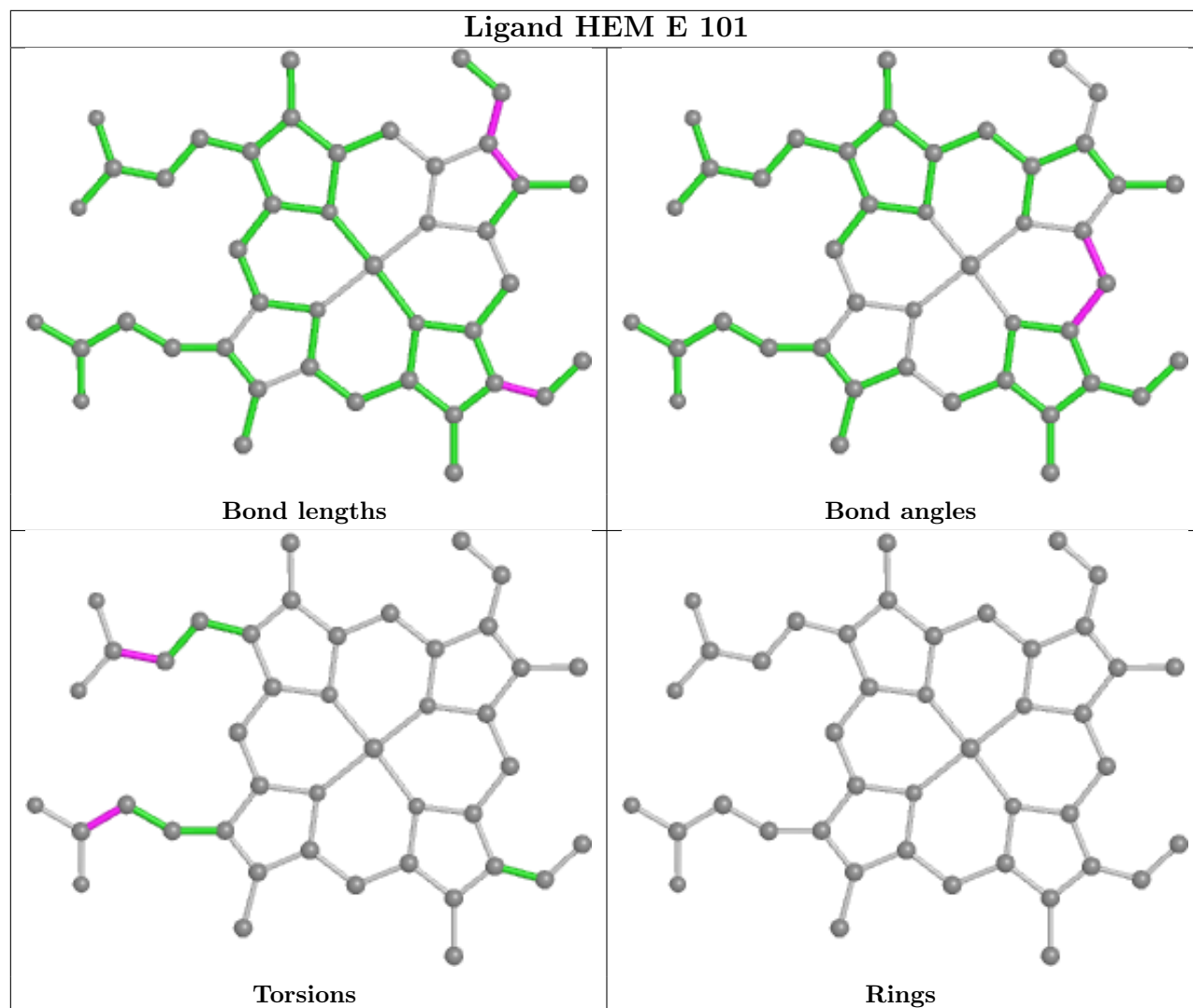
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

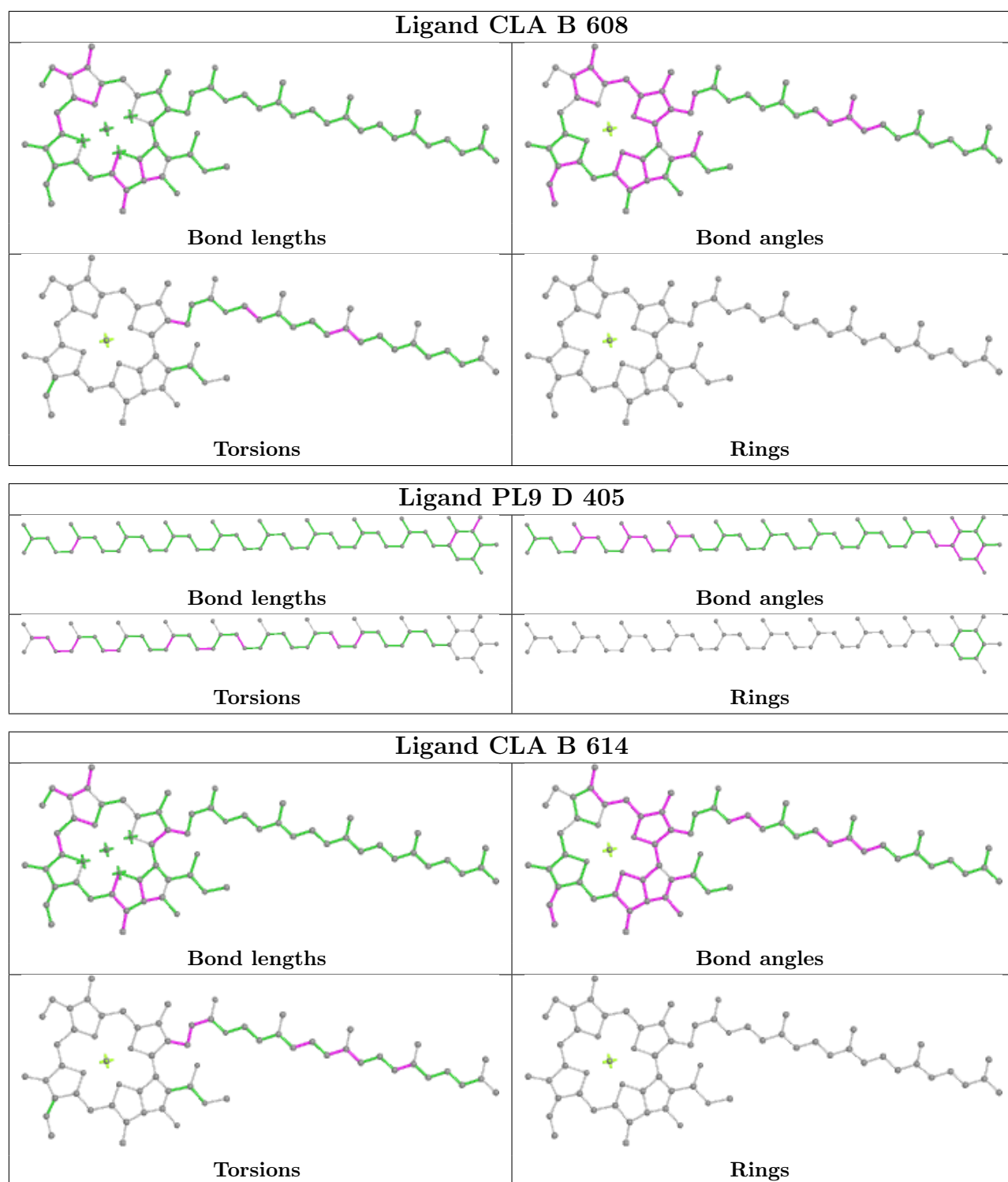
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

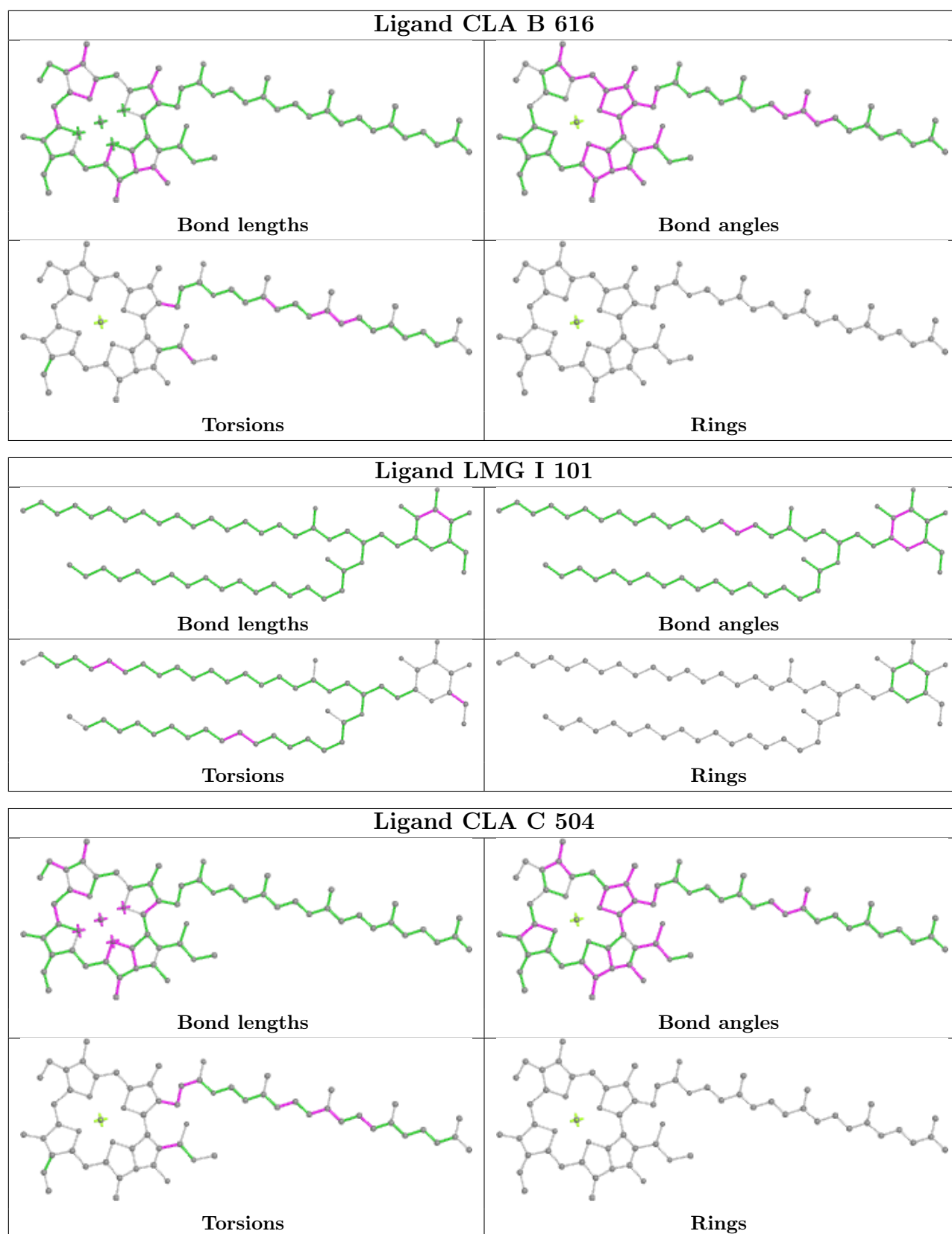


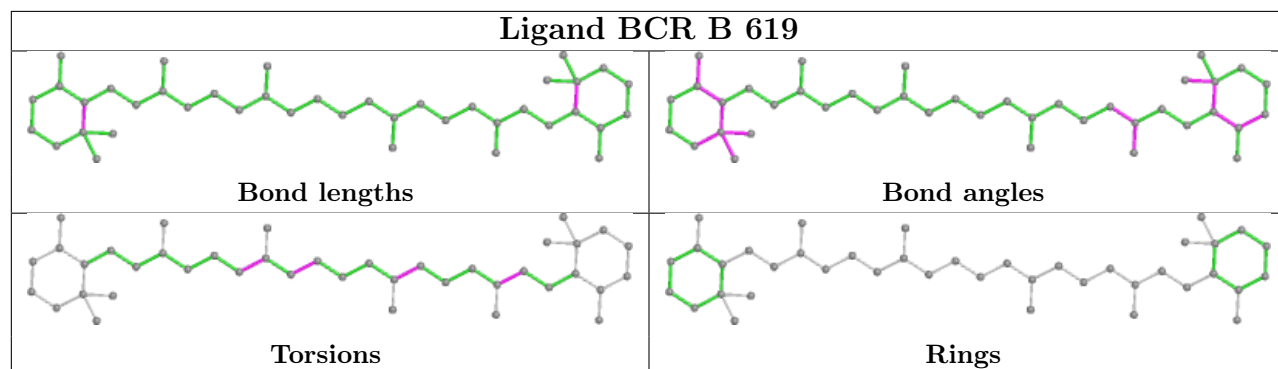
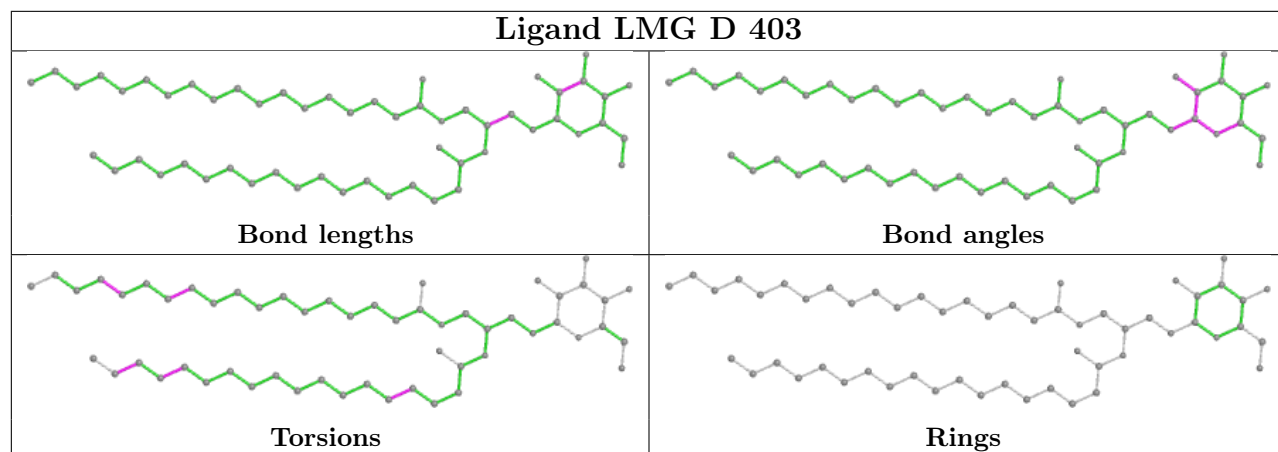
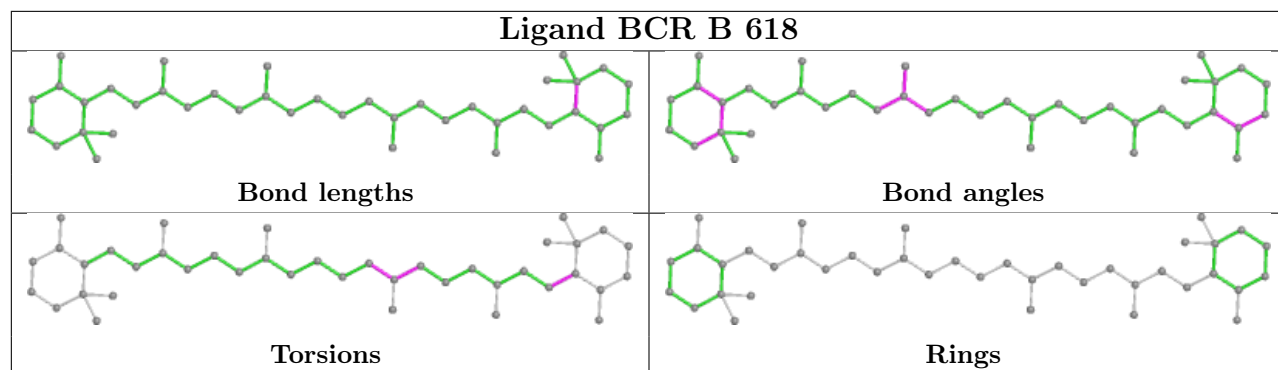


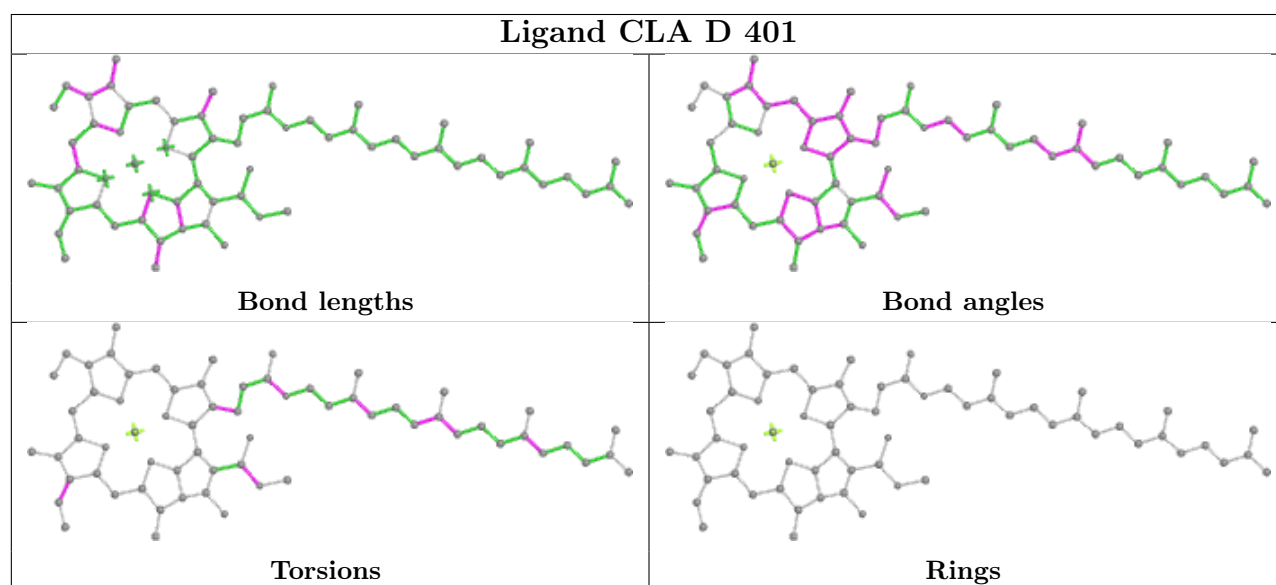
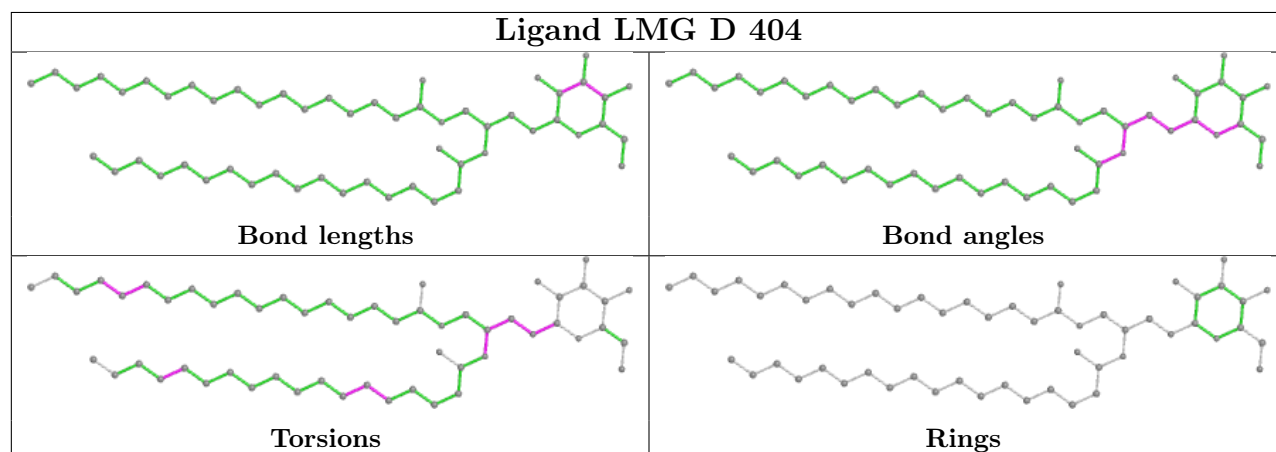
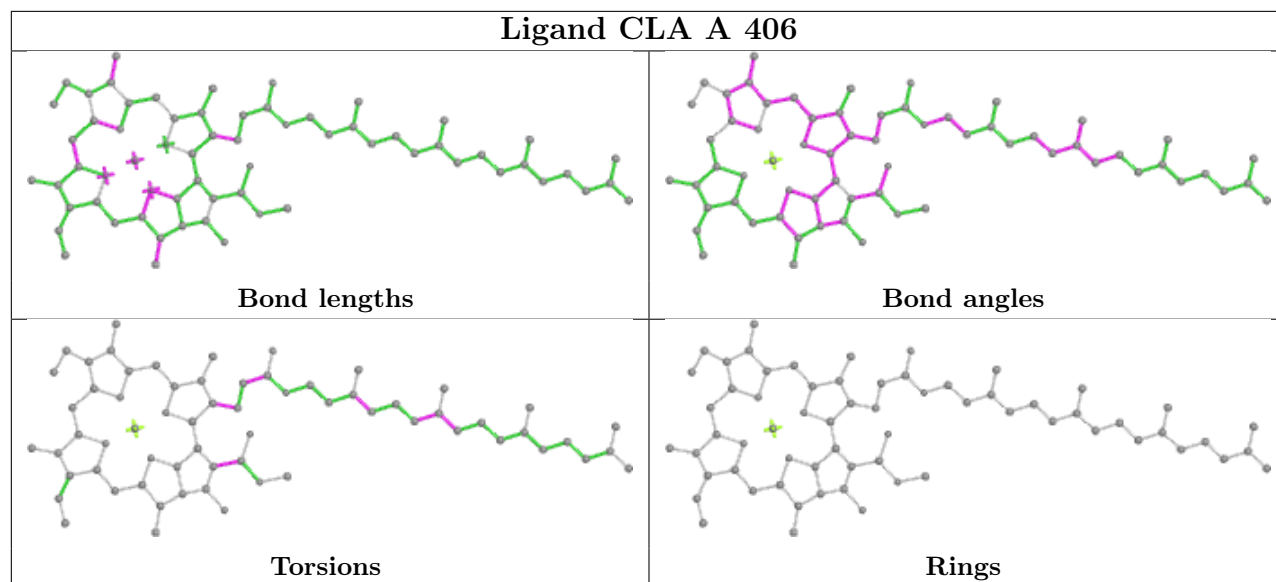


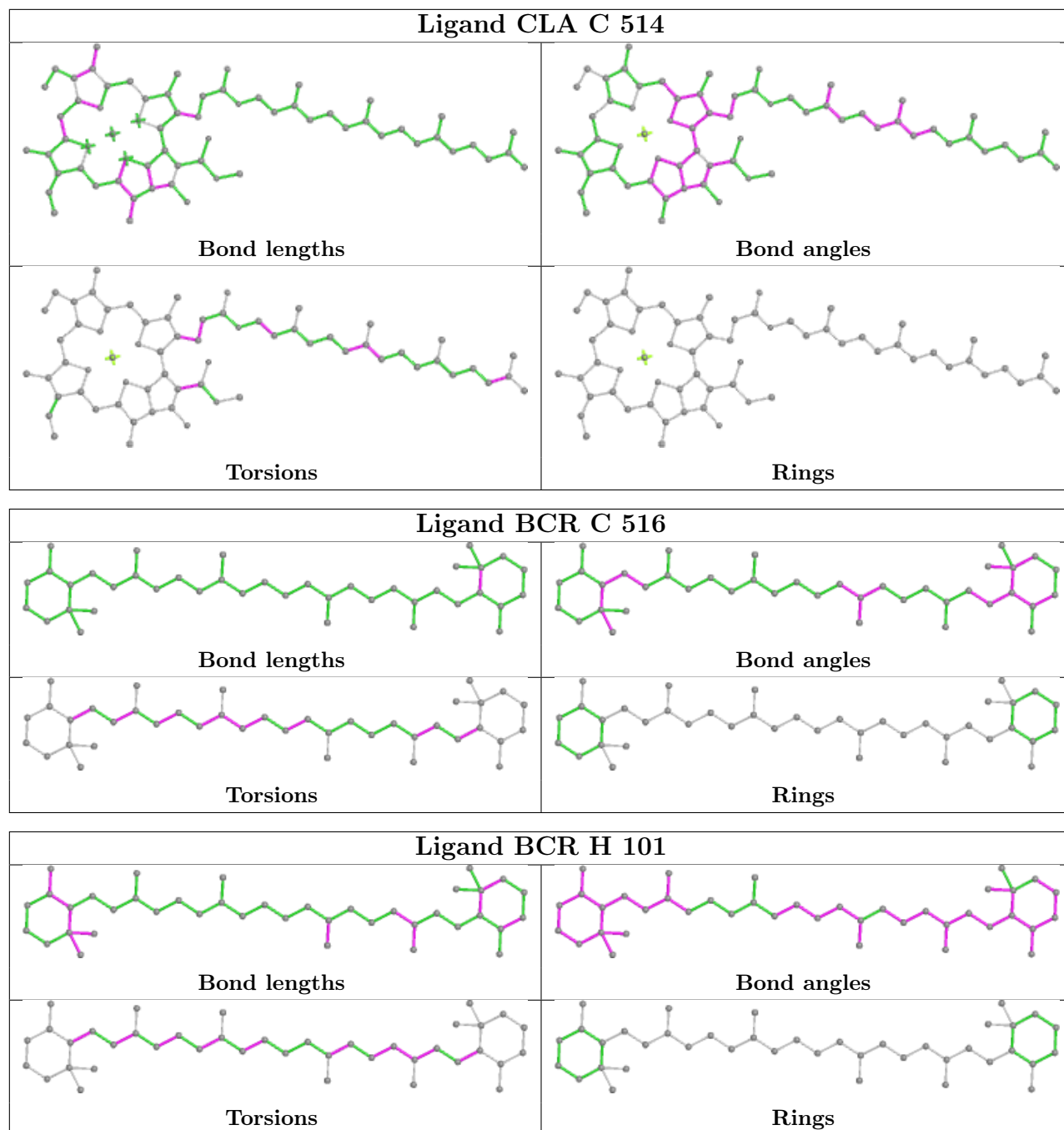


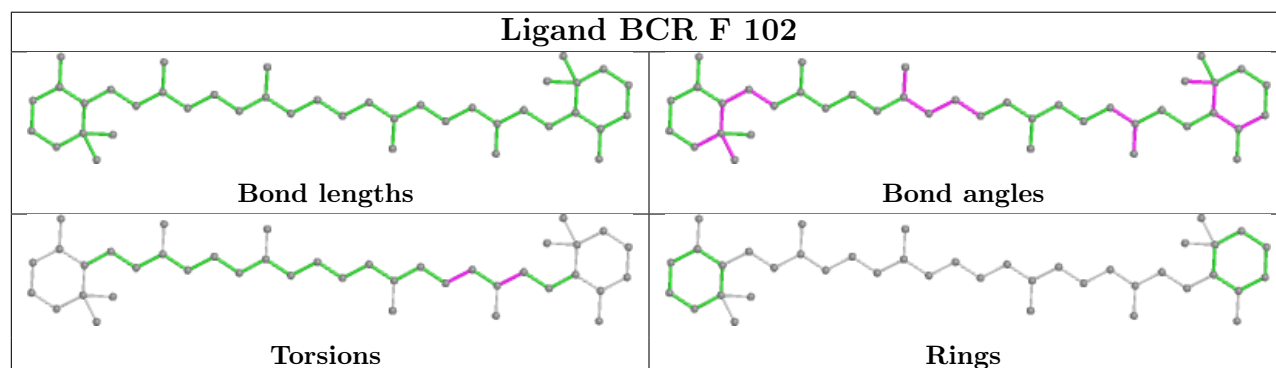
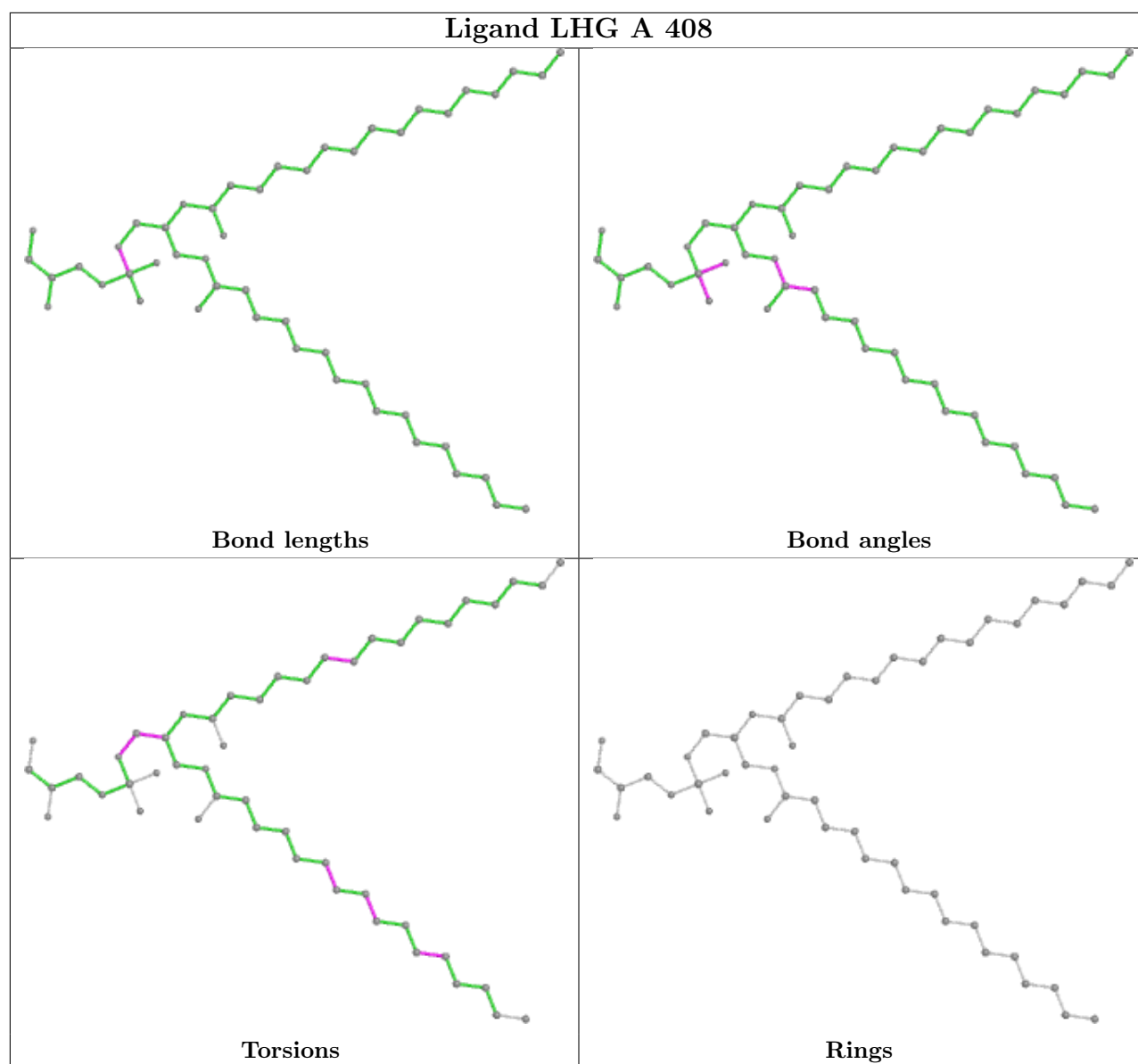


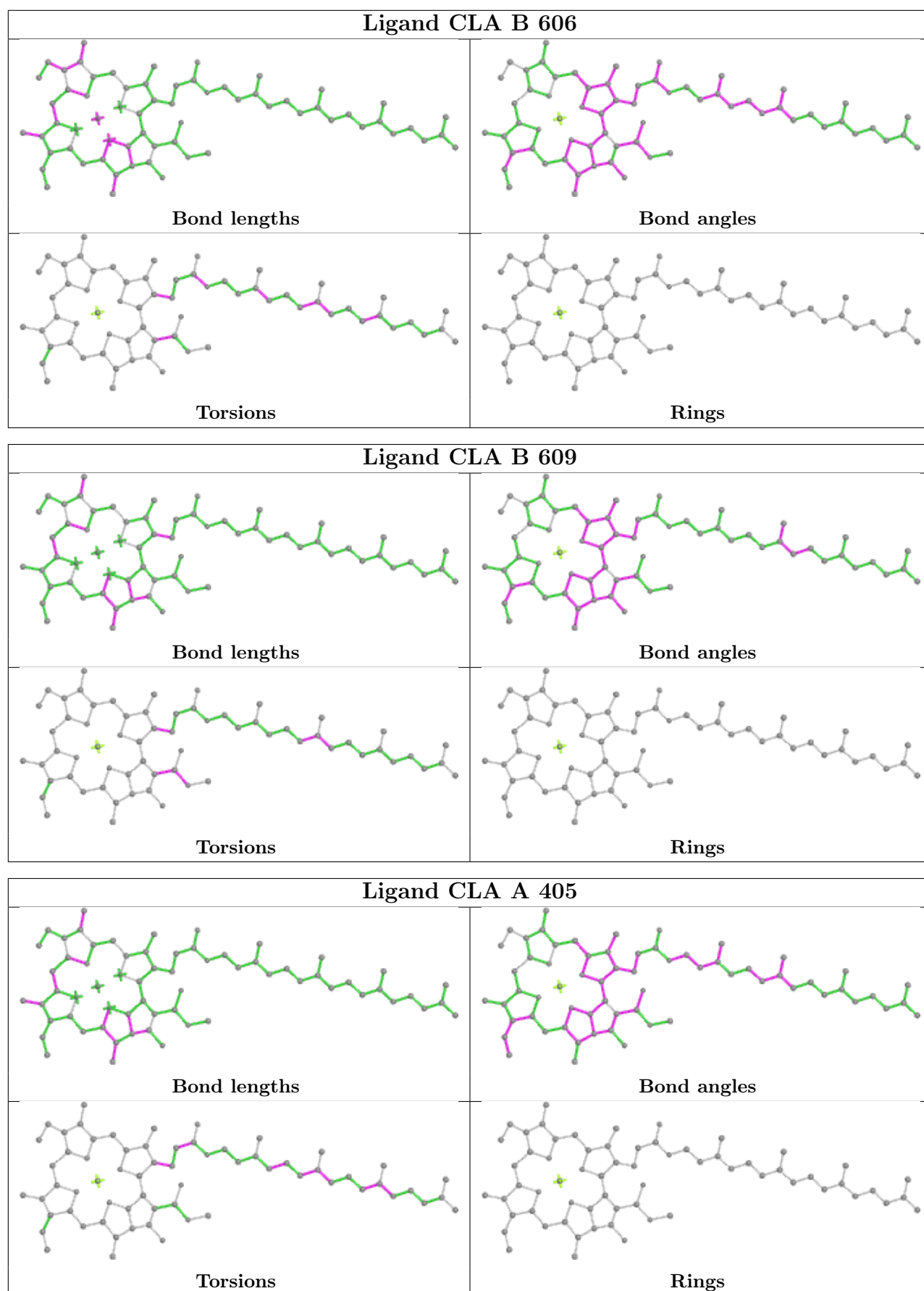


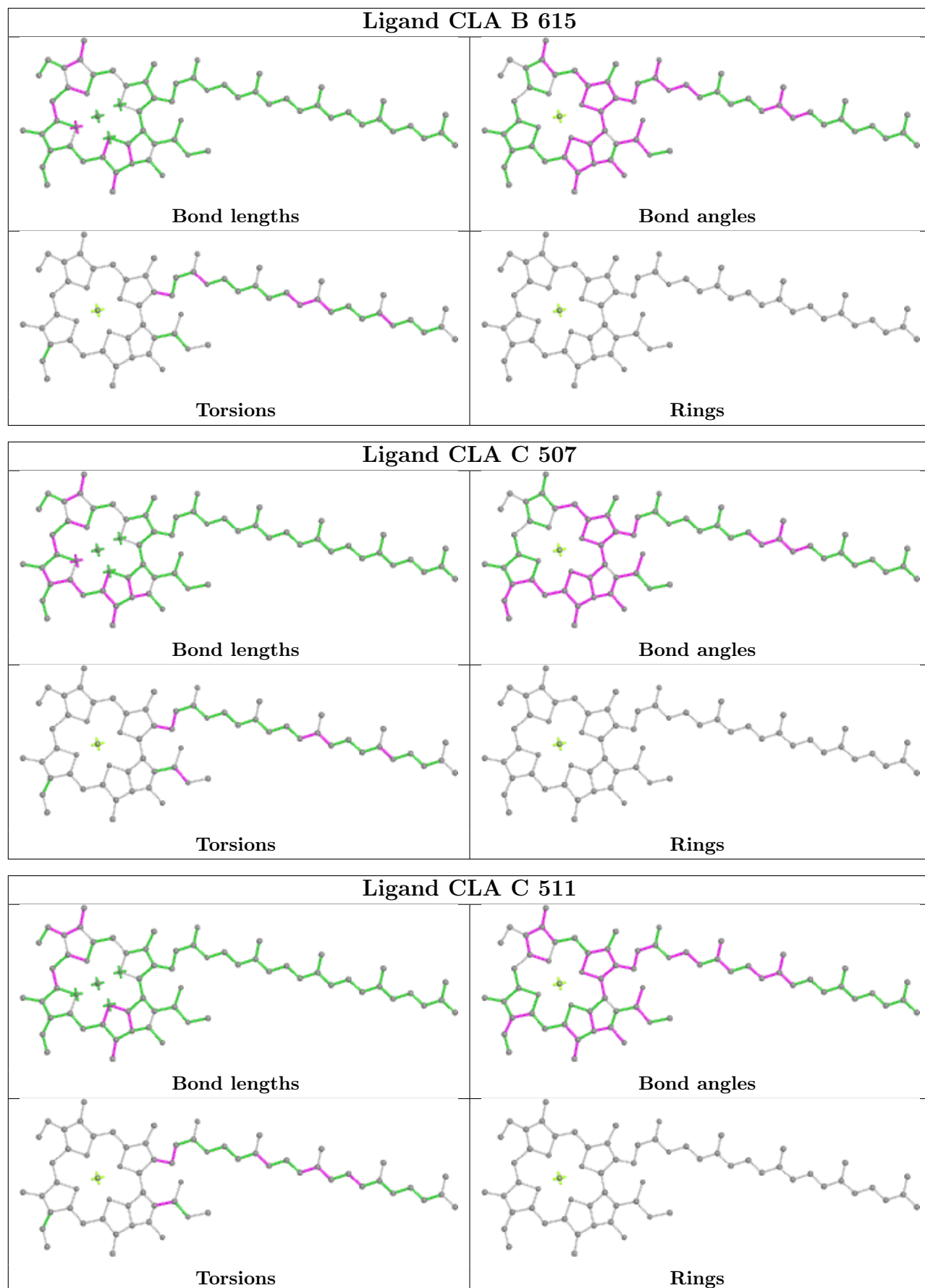


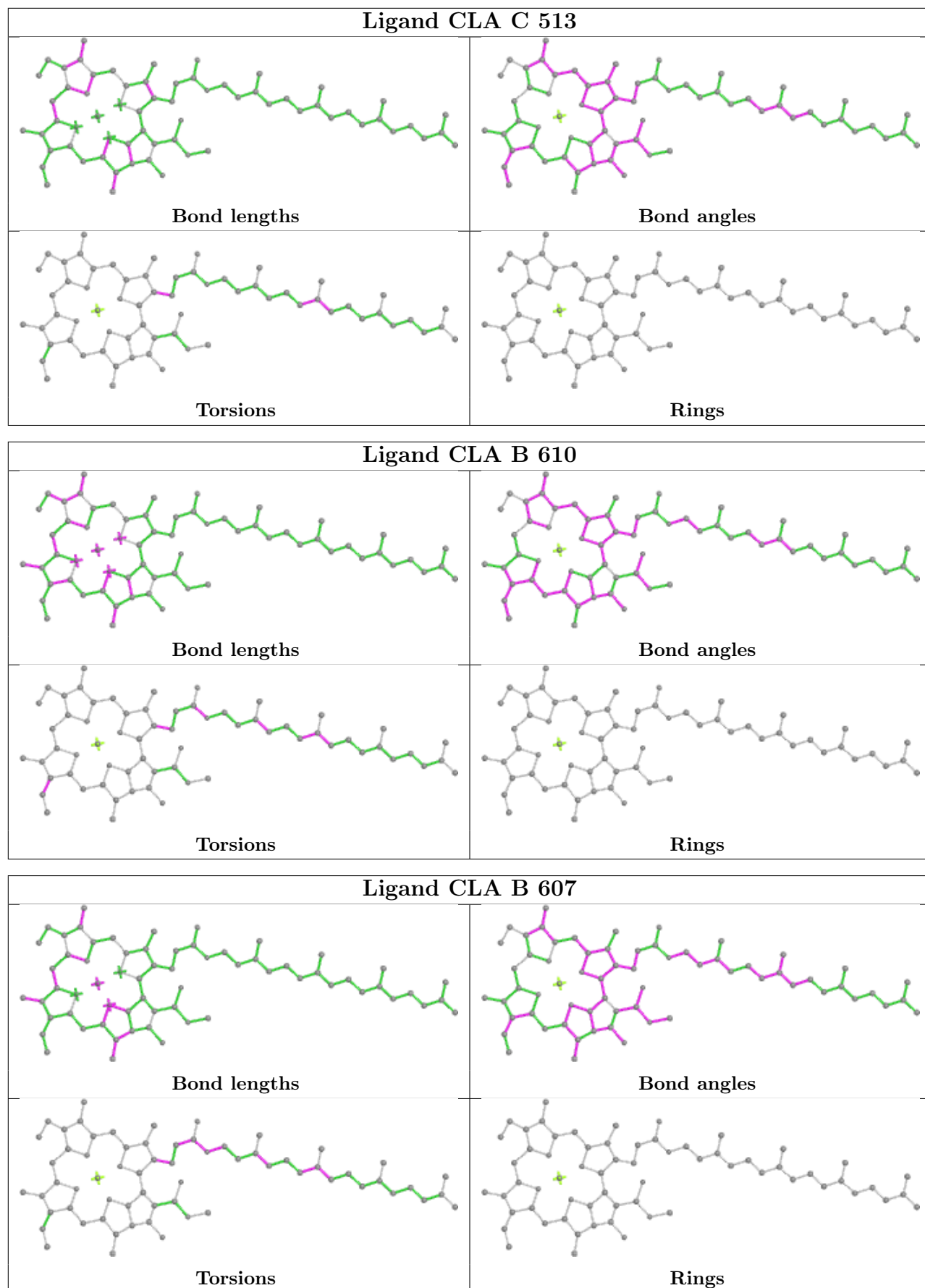


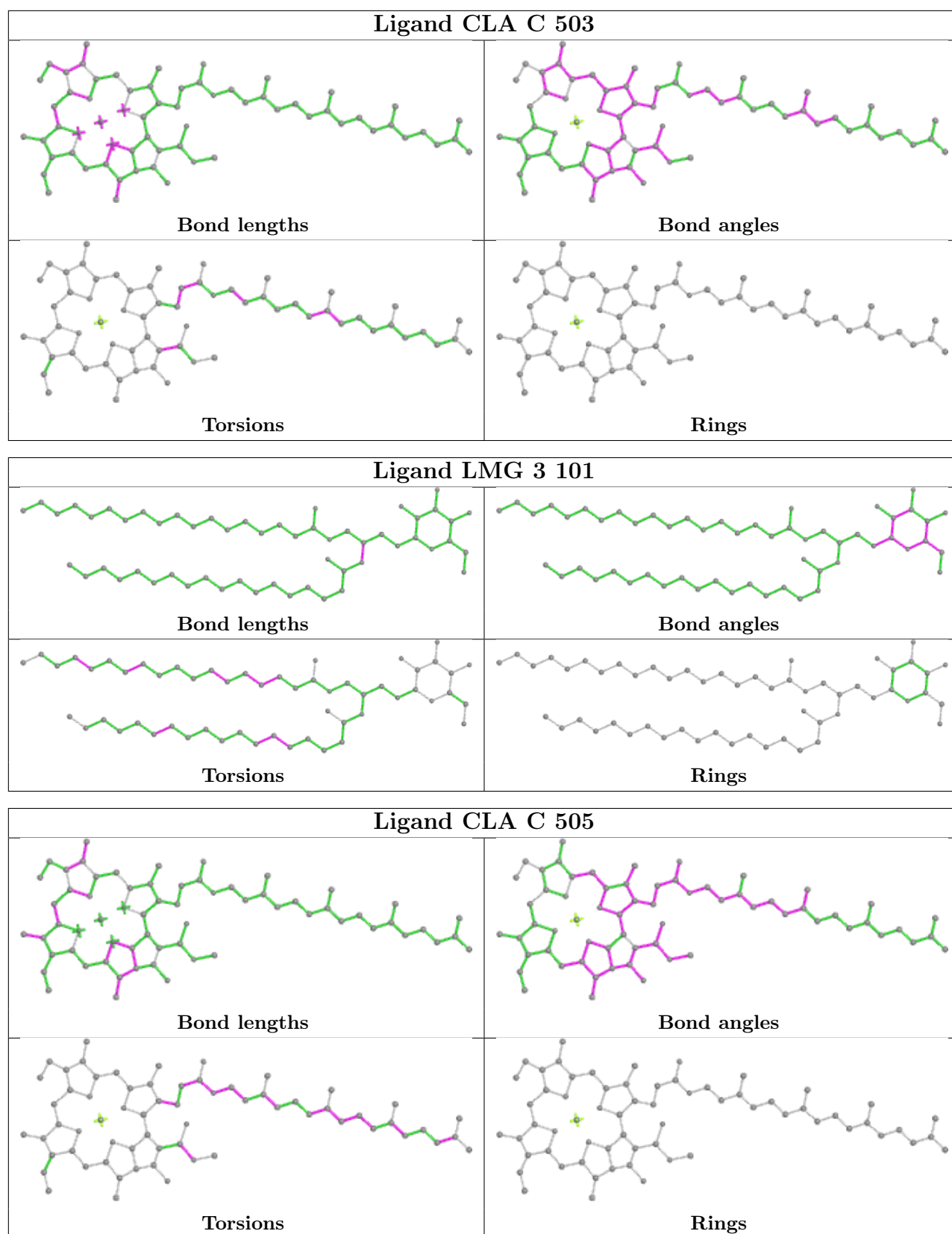


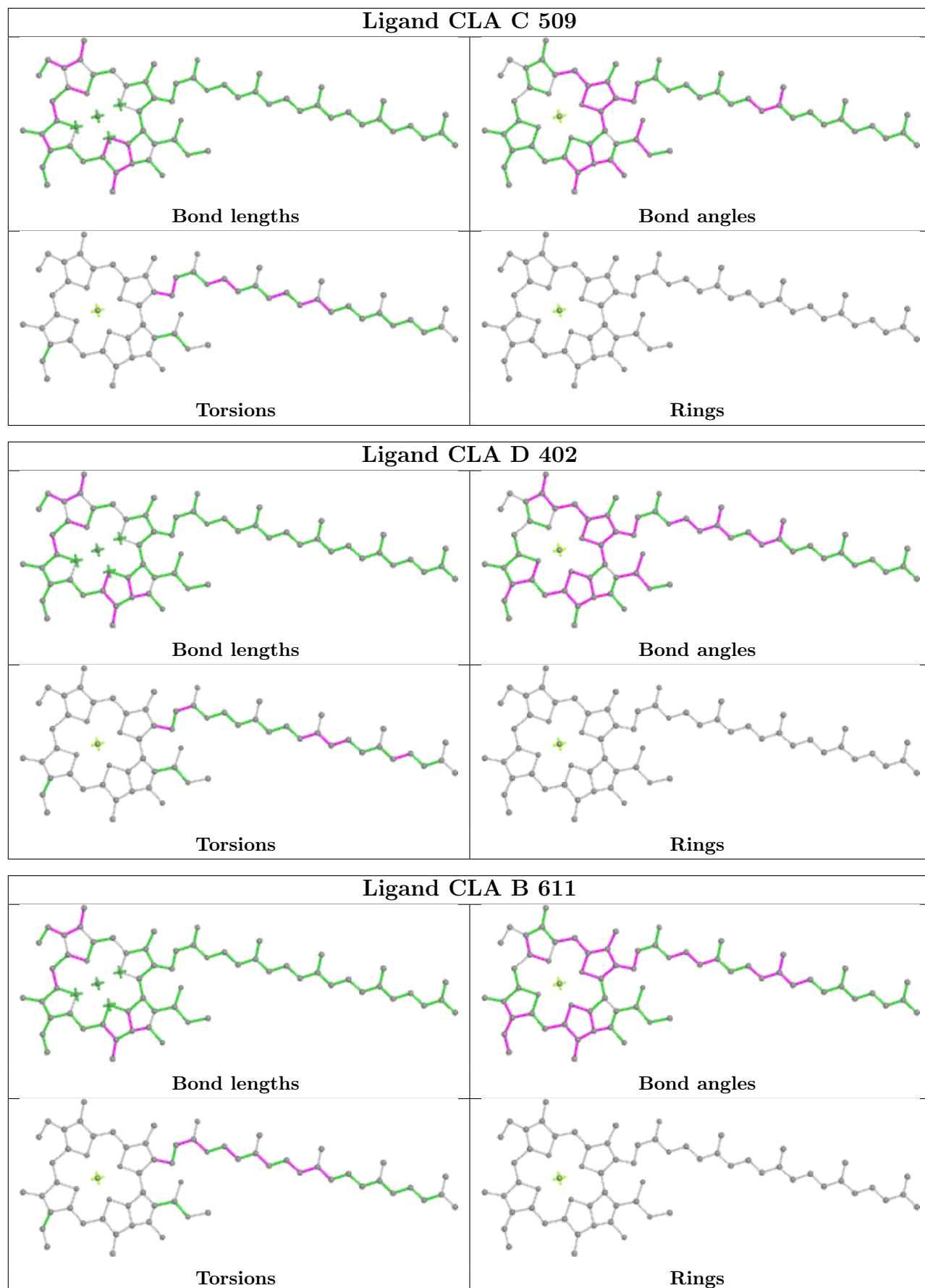


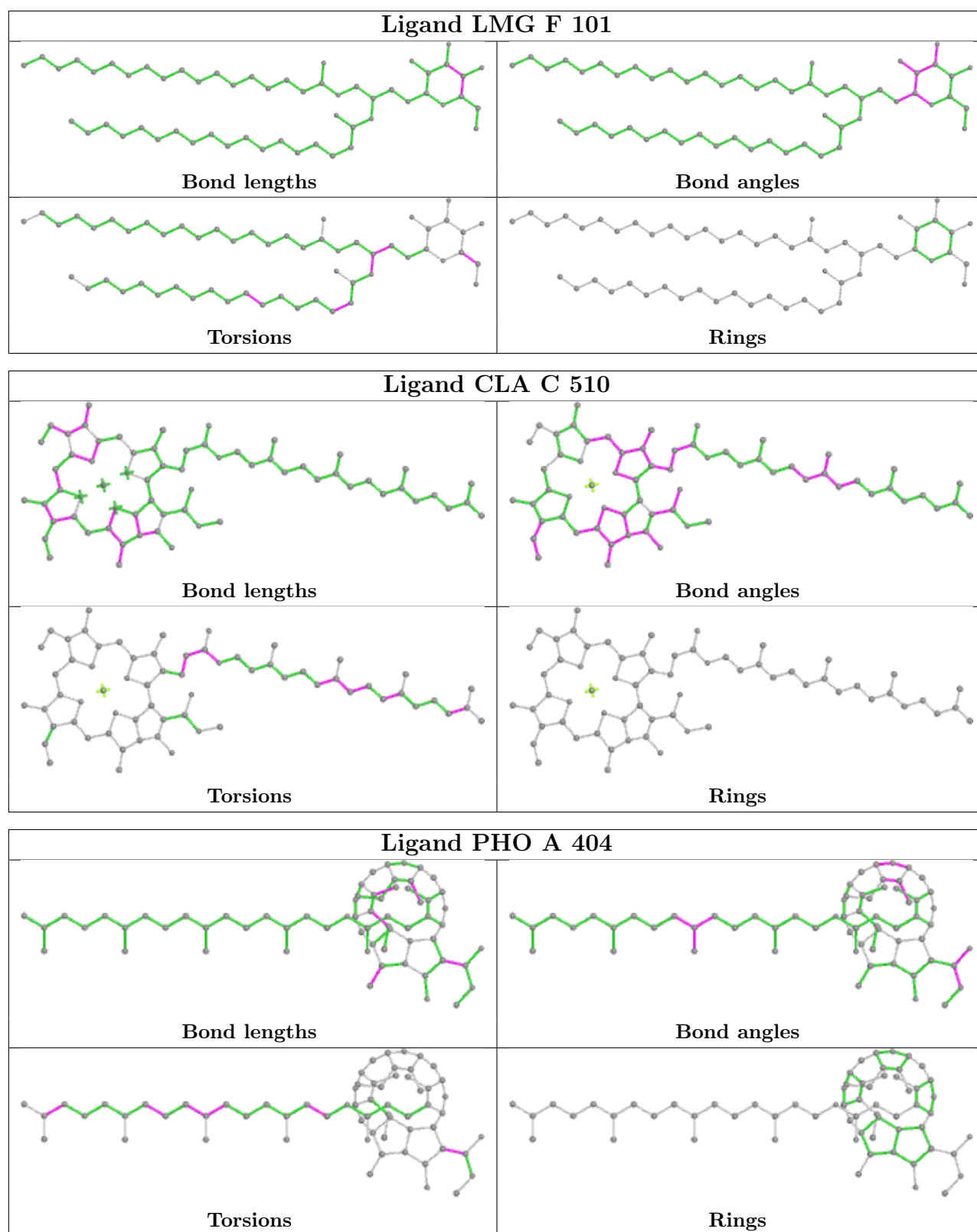


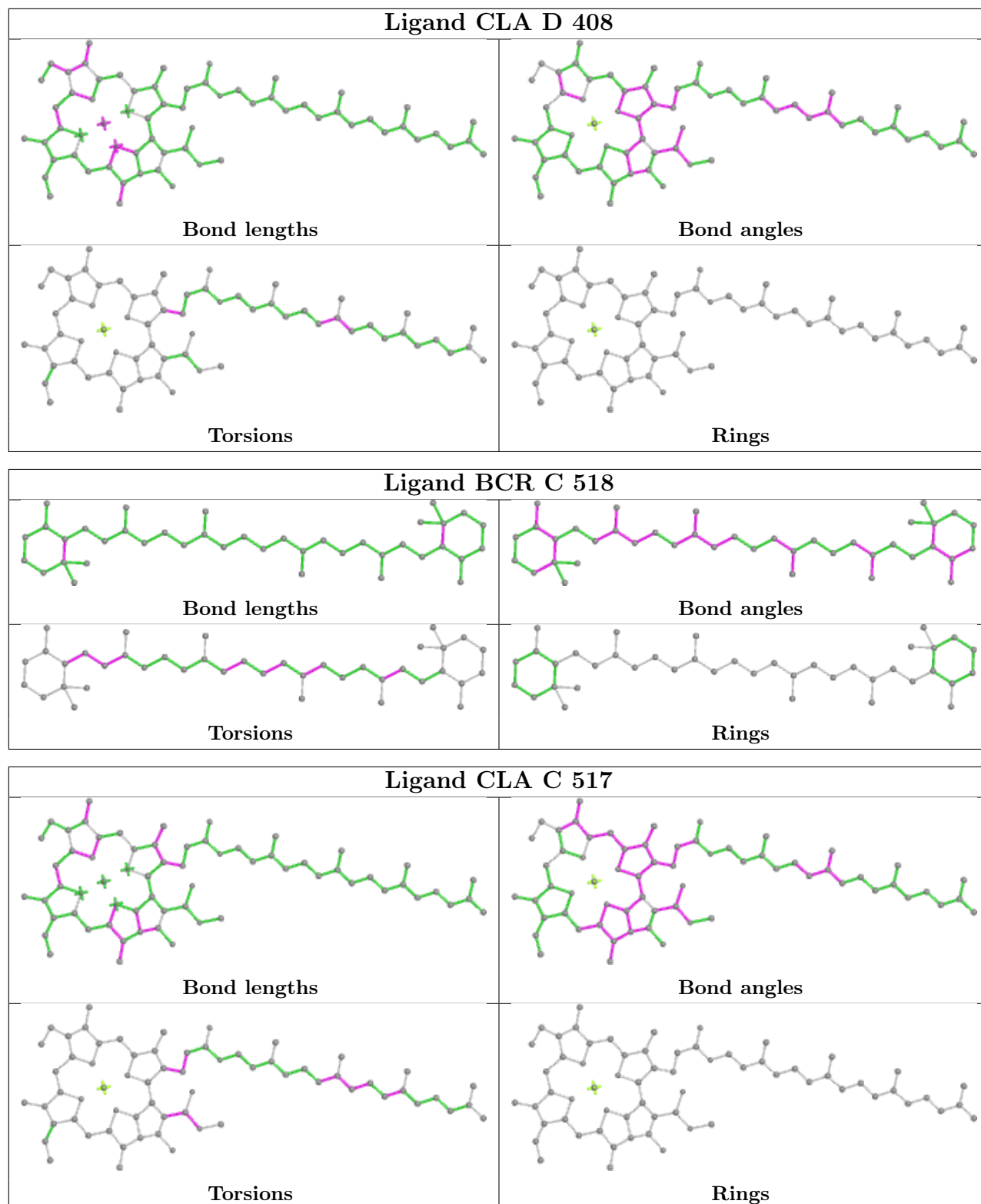


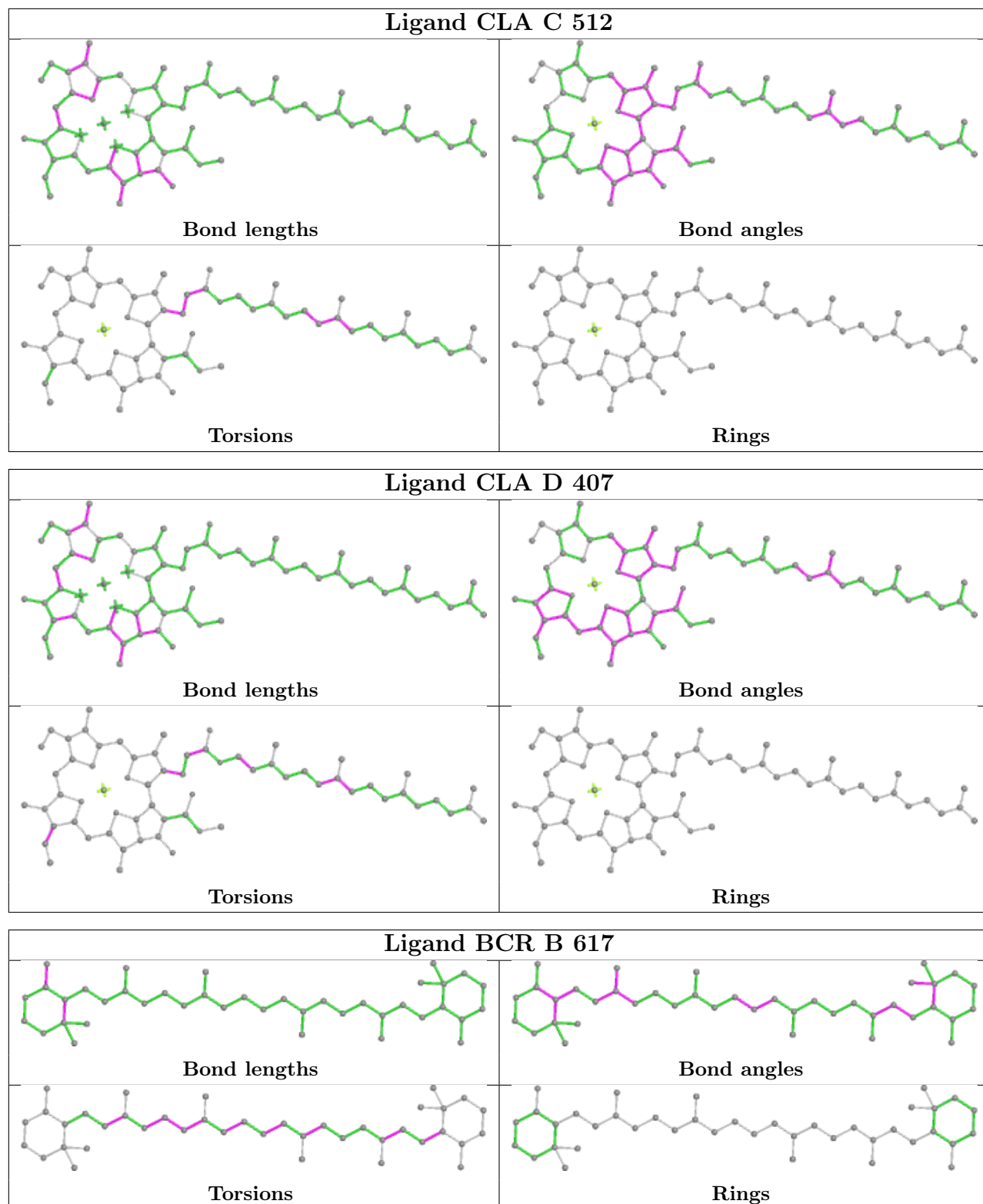


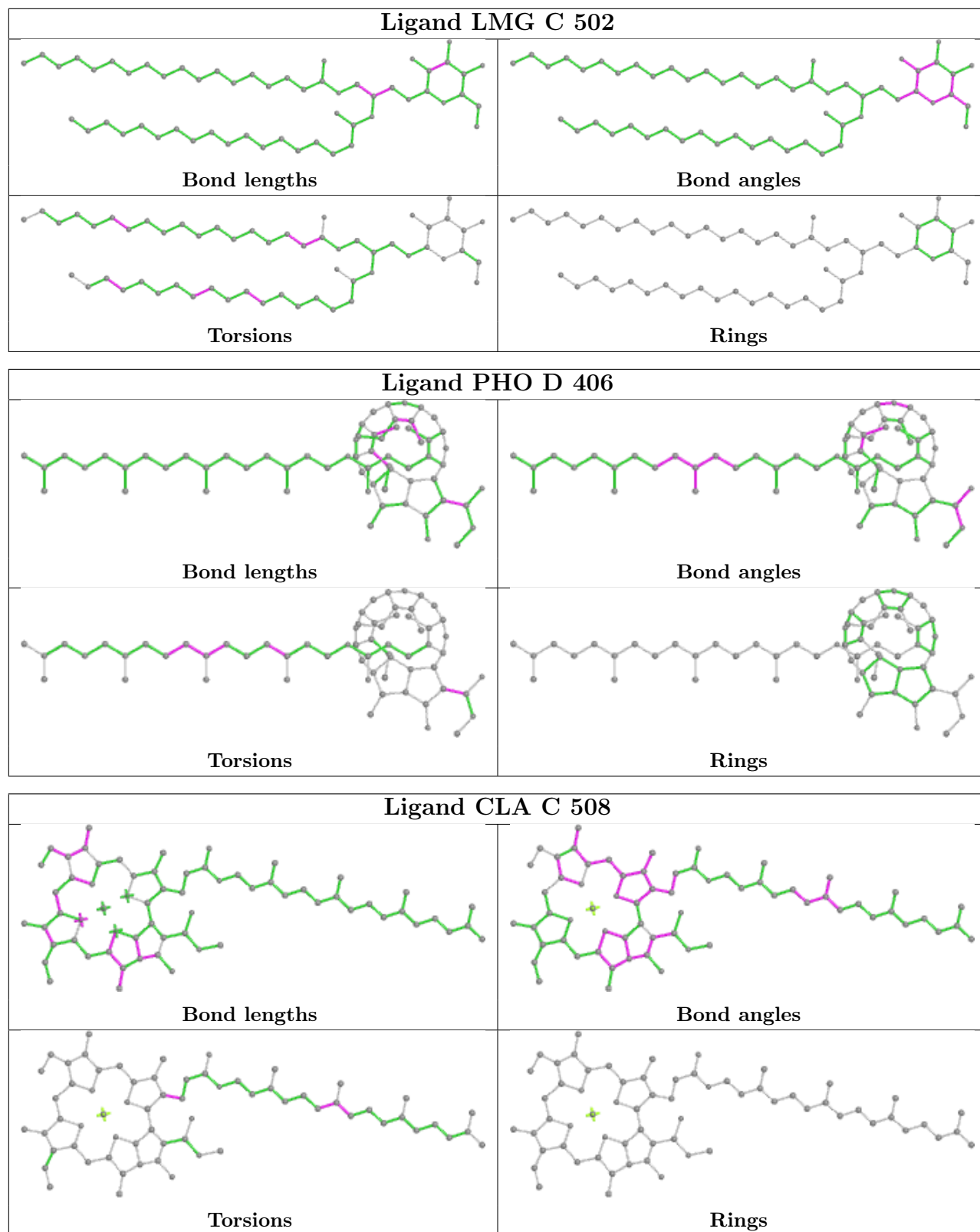


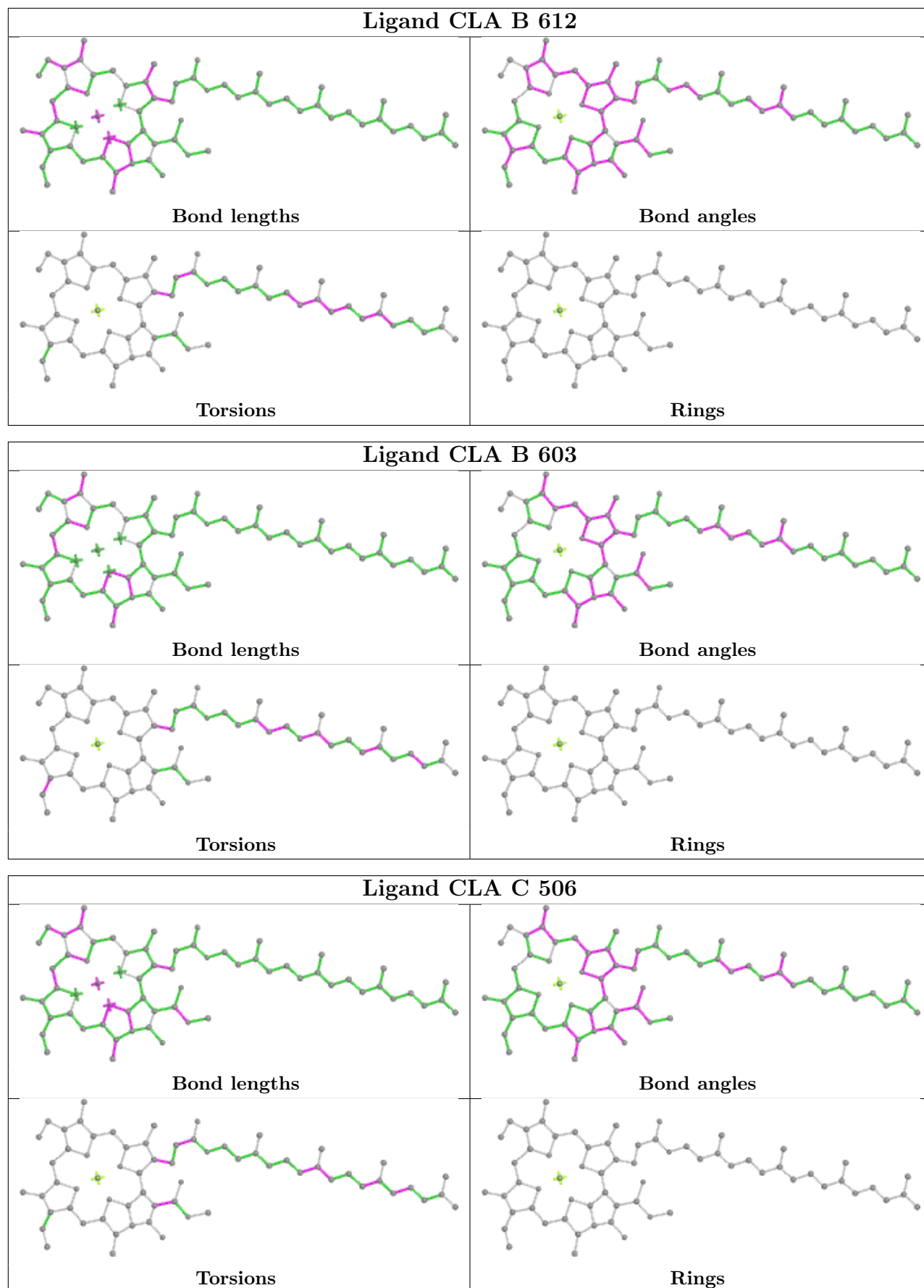












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

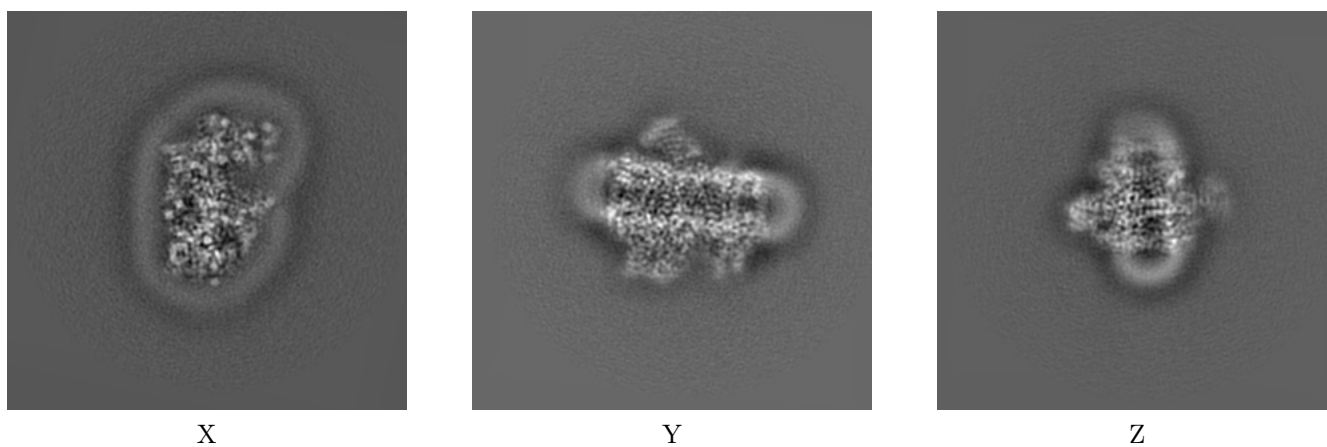
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12337. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

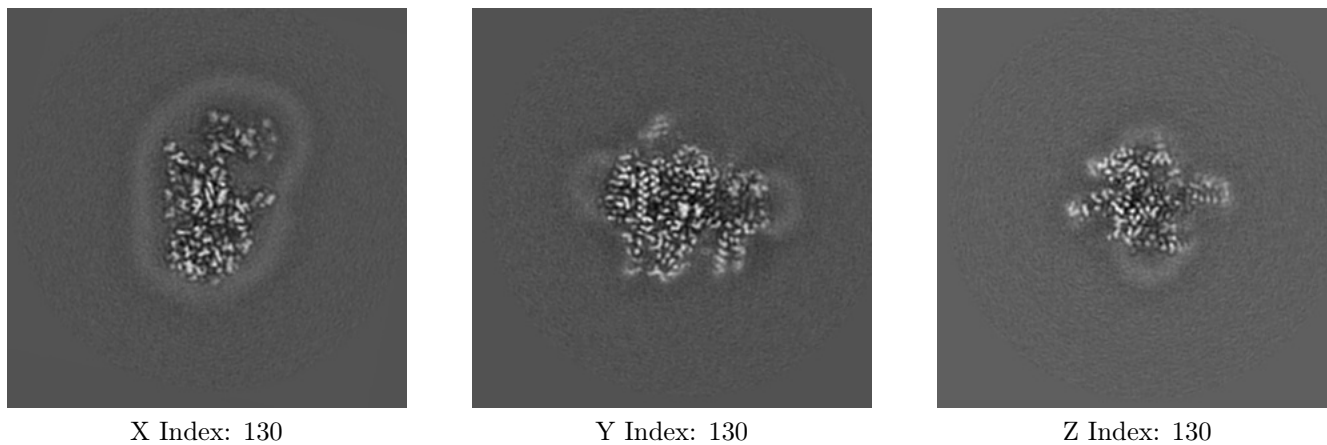
6.1.1 Primary map



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

6.2 Central slices [i](#)

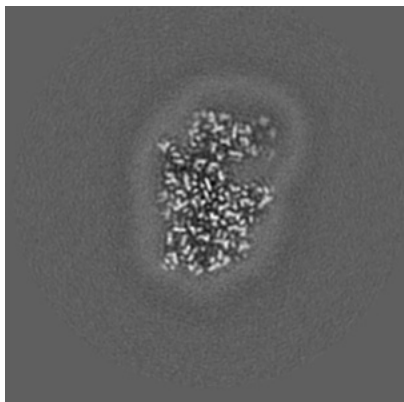
6.2.1 Primary map



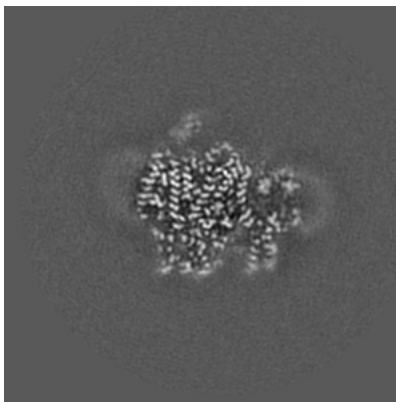
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

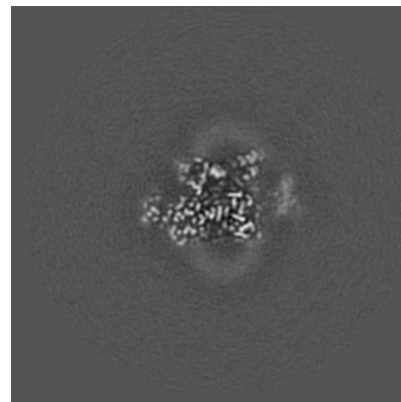
6.3.1 Primary map



X Index: 125



Y Index: 129



Z Index: 116

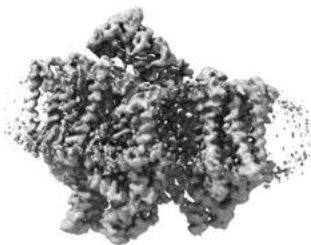
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

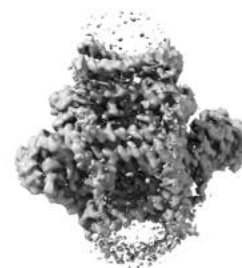
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

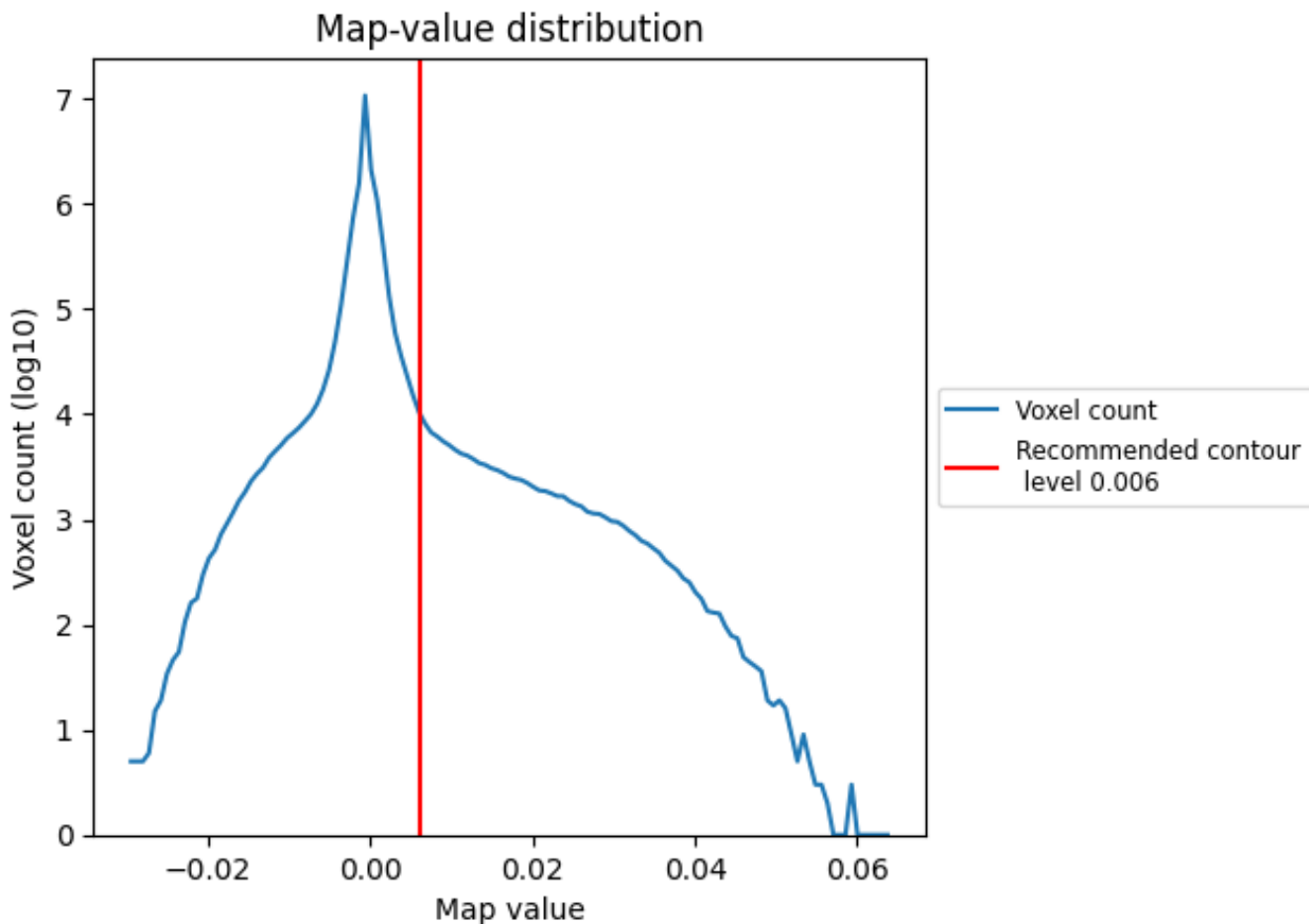
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

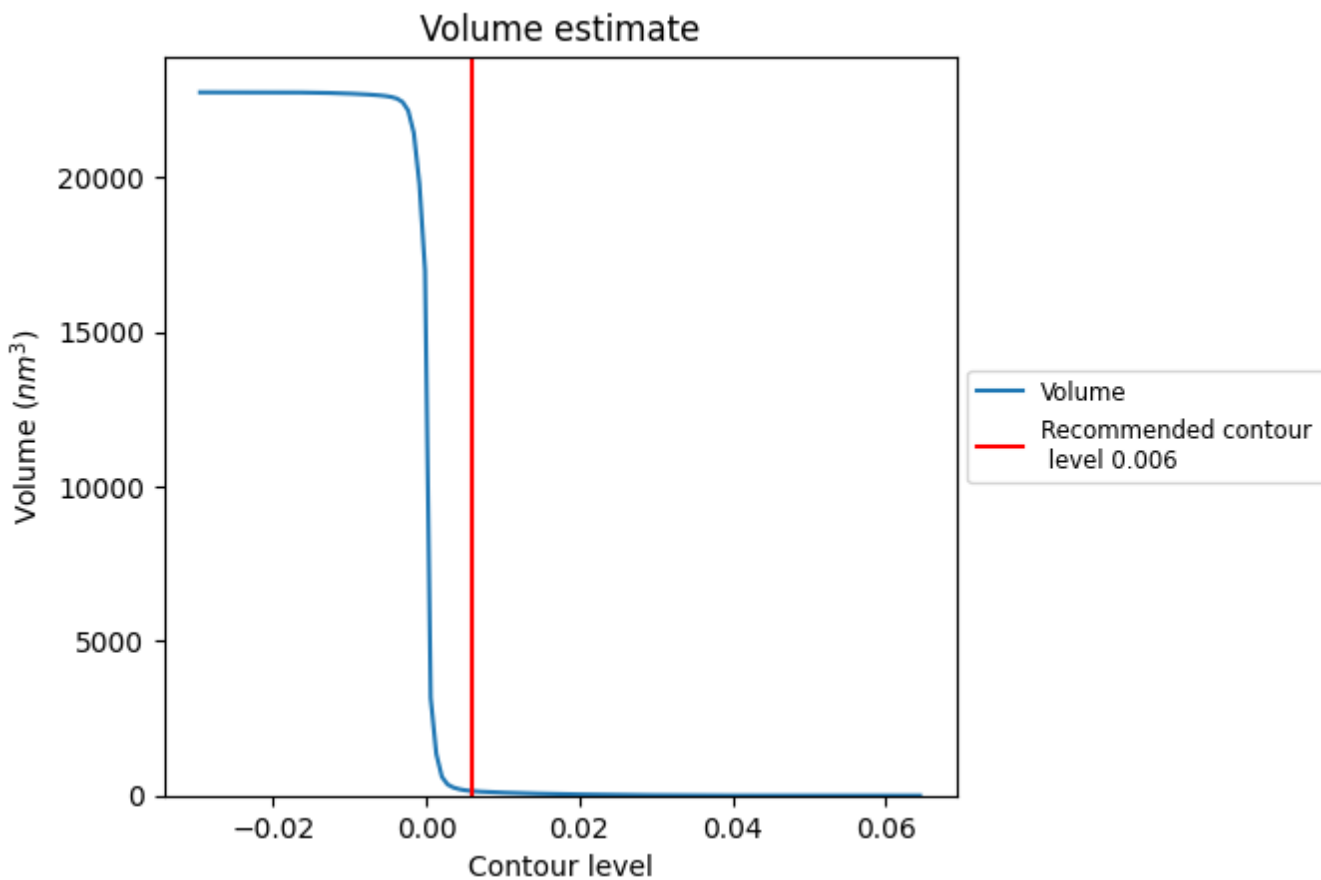
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

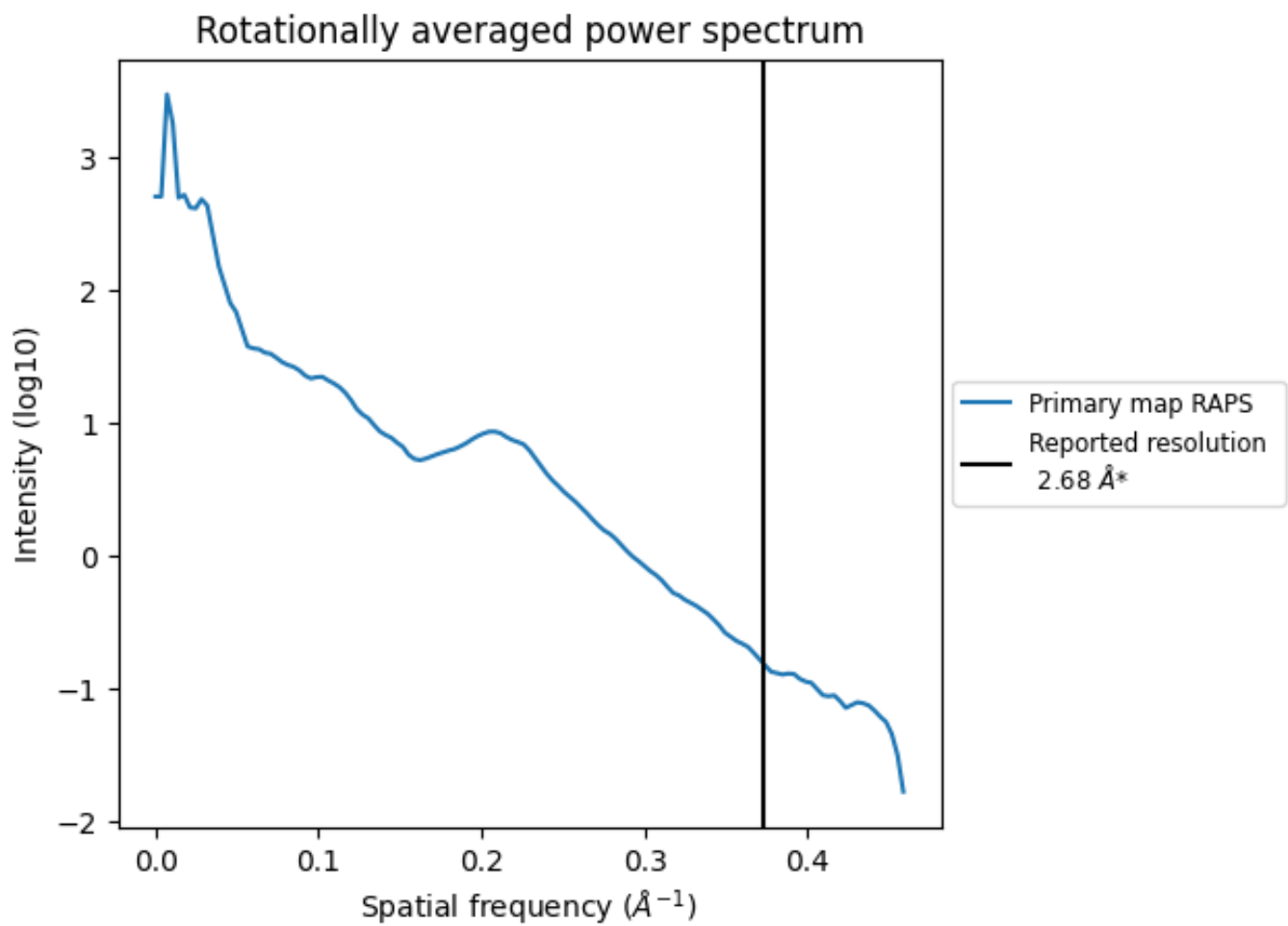
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 147 nm^3 ; this corresponds to an approximate mass of 133 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.373\AA^{-1}

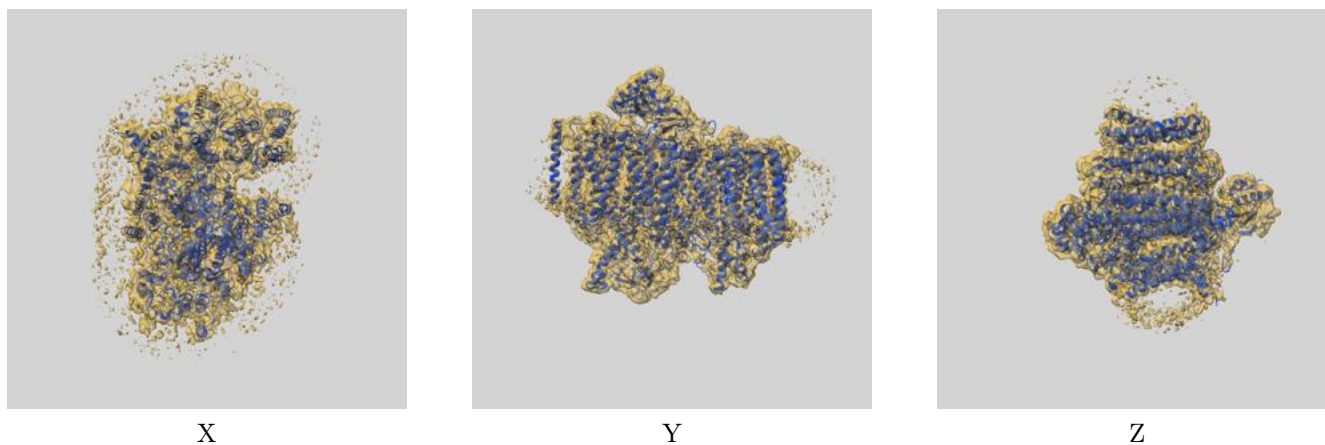
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

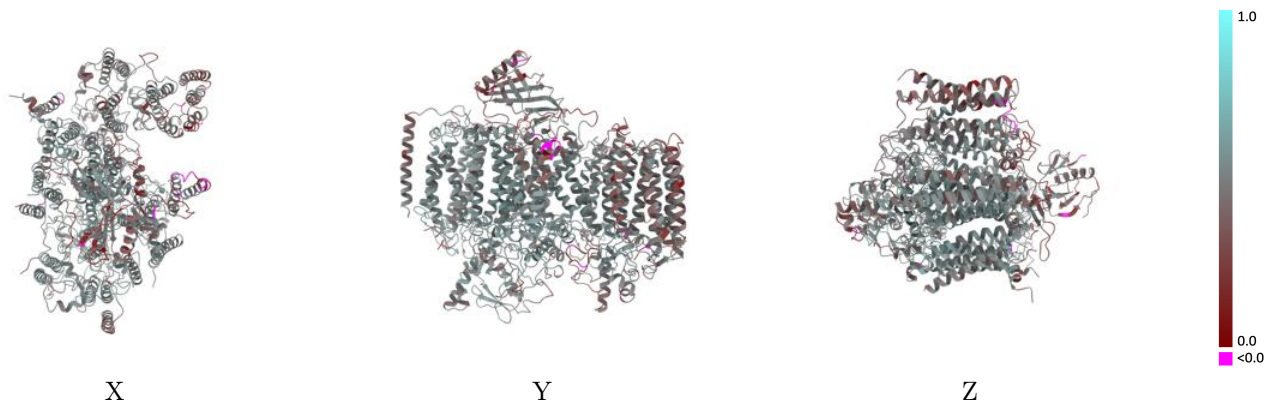
This section contains information regarding the fit between EMDB map EMD-12337 and PDB model 7NHQ. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



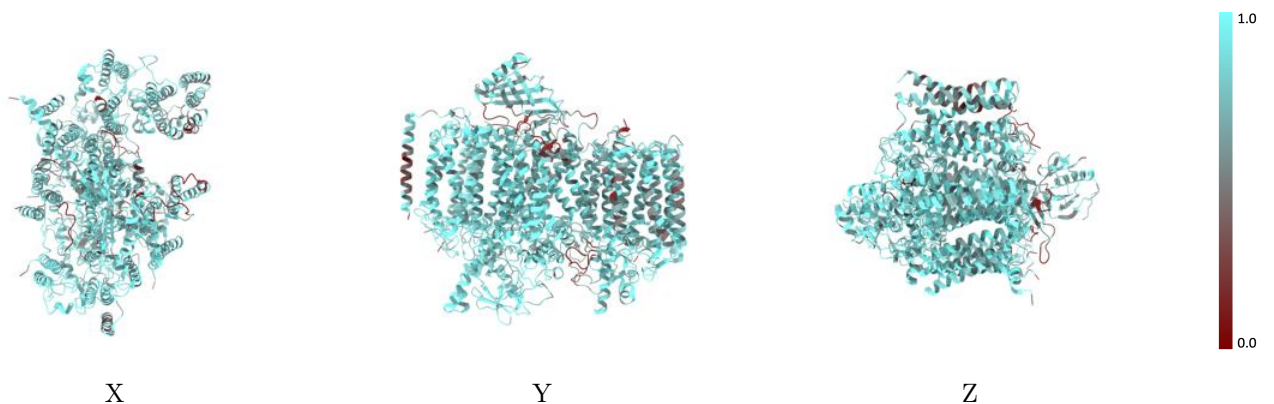
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



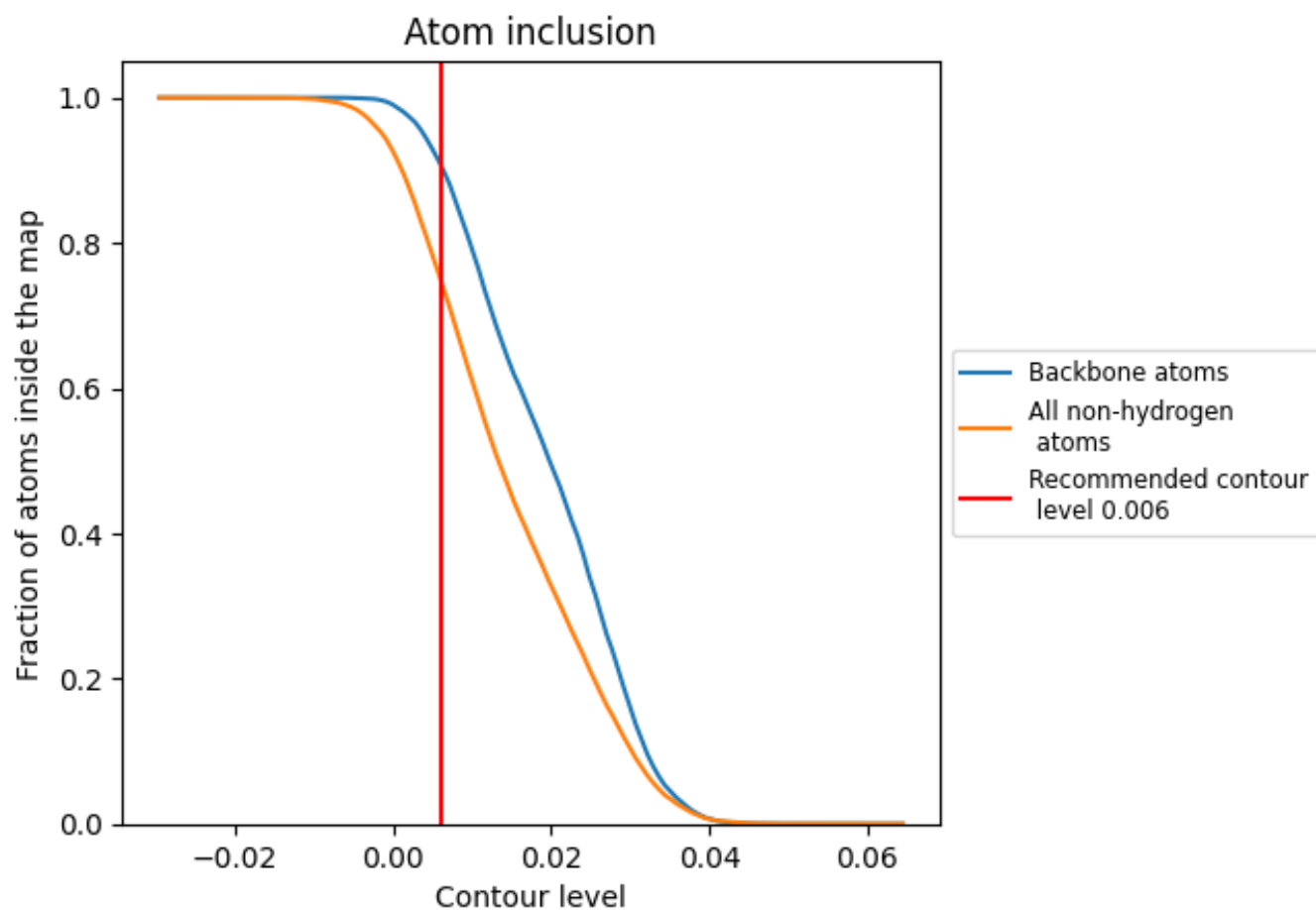
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 75% 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 (0.006) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.7511 |  0.4650 |
| 2 |  0.7494 |  0.3980 |
| 3 |  0.4989 |  0.4070 |
| A |  0.7664 |  0.4900 |
| B |  0.8124 |  0.4970 |
| C |  0.7050 |  0.4280 |
| D |  0.8149 |  0.5250 |
| E |  0.7006 |  0.3620 |
| F |  0.5682 |  0.3920 |
| H |  0.8407 |  0.4930 |
| I |  0.6226 |  0.3870 |
| K |  0.5775 |  0.3990 |
| L |  0.8020 |  0.5130 |
| M |  0.6805 |  0.4440 |
| T |  0.7415 |  0.4800 |
| X |  0.7795 |  0.4710 |
| Z |  0.6725 |  0.3760 |
| y |  0.5245 |  0.3410 |

