



## Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 07:26 AM JST

PDB ID : 7DXA / pdb\_00007dxa  
EMDB ID : EMD-30902  
Title : PSII intermediate Psb28-RC47  
Authors : Sui, S.F.; Shen, J.R.; Han, G.Y.; Xiao, Y.N.; Huang, G.Q.  
Deposited on : 2021-01-18  
Resolution : 3.14 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](mailto: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>.

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

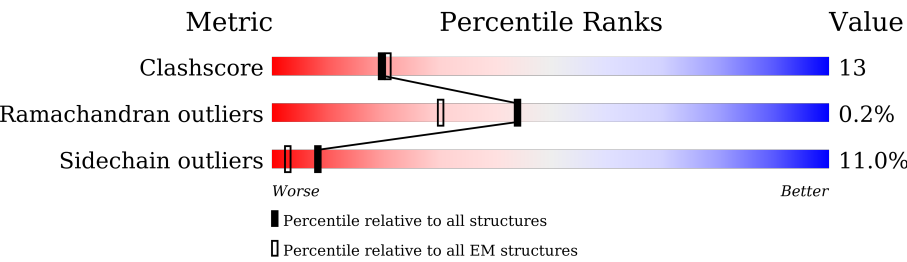
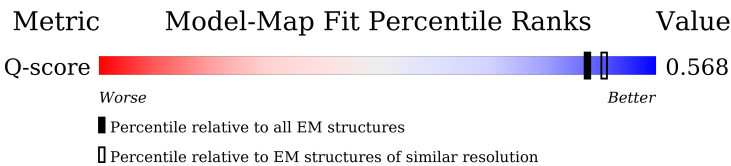
EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 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 3.14 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<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14483 ( 2.64 - 3.64 )                                    |

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  $\geq 3$ , 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     | 116    | <div><div></div><div>52%34%9%6%</div></div>  |
| 2   | B     | 56     | <div><div></div><div>68%14%7%11%</div></div> |
| 3   | a     | 360    | <div><div></div><div>64%15%.17%</div></div>  |
| 4   | b     | 505    | <div><div></div><div>78%18%..</div></div>    |
| 5   | d     | 342    | <div><div></div><div>76%21%..</div></div>    |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 6   | e     | 84     |                  |
| 7   | f     | 45     |                  |
| 8   | h     | 65     |                  |
| 9   | i     | 38     |                  |
| 10  | l     | 37     |                  |
| 11  | m     | 36     |                  |
| 12  | t     | 32     |                  |
| 13  | x     | 40     |                  |
| 14  | C     | 23     |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 16  | CLA  | b     | 606 | -         | -        | X       | -                |
| 16  | CLA  | d     | 404 | X         | -        | -       | -                |
| 19  | CL   | a     | 408 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 15162 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 reaction center Psb28 protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | A     | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 875   | 549 | 153 | 168 | 5 |         |       |

- Molecule 2 is a protein called Tsl0063 protein.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 2   | B     | 50       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 365   | 237 | 65 | 63 |         |       |

- Molecule 3 is a protein called Photosystem II protein D1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | a     | 298      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2311  | 1520 | 382 | 394 | 15 |         |       |

- Molecule 4 is a protein called Photosystem II CP47 reaction center protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | b     | 494      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3886  | 2554 | 646 | 673 | 13 |         |       |

- Molecule 5 is a protein called Photosystem II D2 protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | d     | 339      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2694  | 1787 | 439 | 456 | 12 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 6   | e     | 63       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 509   | 334 | 81 | 94 |         |       |

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | f     | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 219   | 149 | 36 | 33 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | h     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 493   | 330 | 79 | 82 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | i     | 29       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 231   | 162 | 30 | 38 | 1 |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 11  | m     | 31       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 244   | 165 | 36 | 43 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12  | t     | 30       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 254   | 179 | 36 | 37 | 2 |         |       |

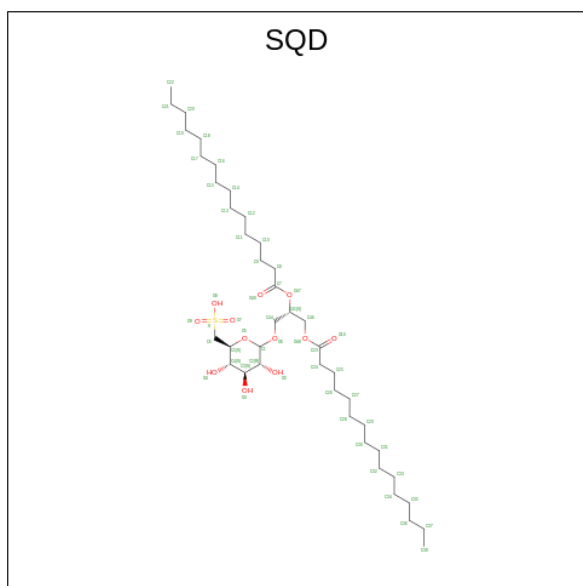
- Molecule 13 is a protein called Photosystem II reaction center protein X.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 13  | x     | 36       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 261   | 177 | 39 | 45 |         |       |

- Molecule 14 is a protein called unidentified transmembrane protein.

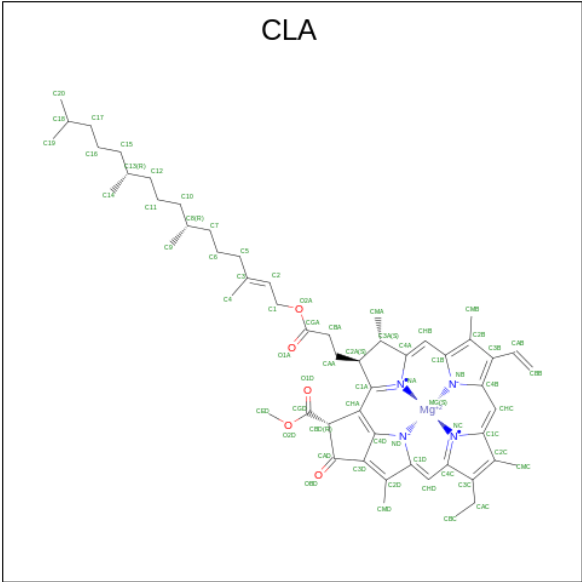
| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 14  | C     | 23       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 115   | 69 | 23 | 23 |         |       |

- Molecule 15 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 15  | a     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 26    | 13 | 12 | 1 |         |
| 15  | l     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 47    | 34 | 12 | 1 |         |

- Molecule 16 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



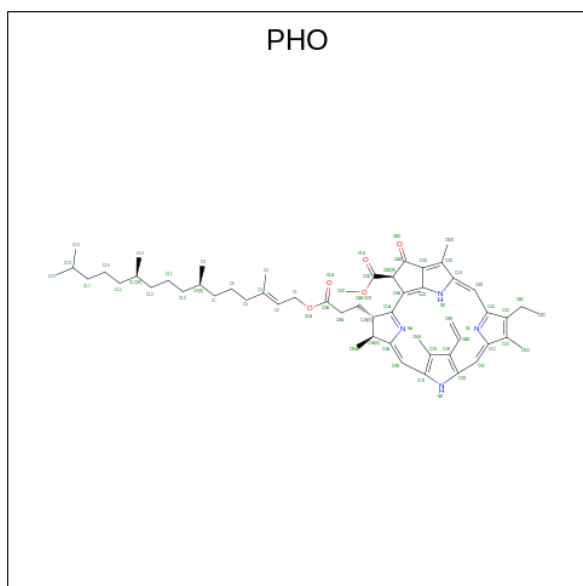
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 16  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 16  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 16  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 16  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 16  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 16  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 16  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 16  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 16  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 16  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 16  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 16  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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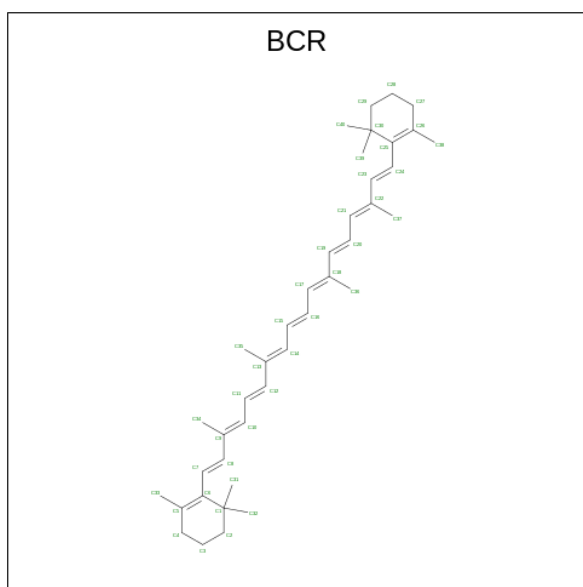
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 16  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 16  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 16  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 16  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 16  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 16  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 16  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 16  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |

- Molecule 17 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 17  | a     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 17  | a     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).

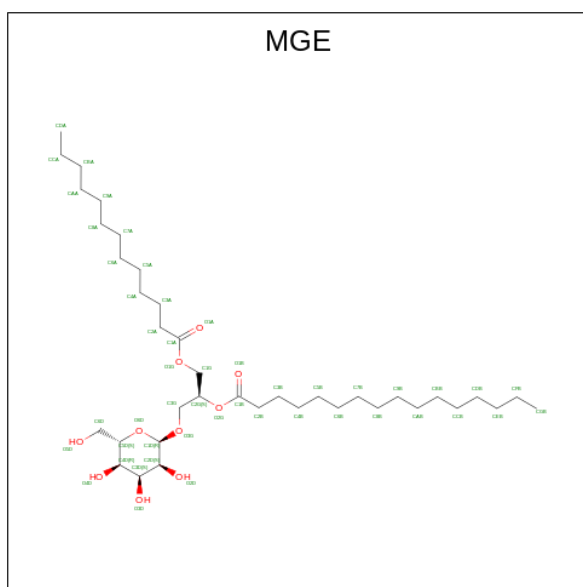


| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 18  | a     | 1        | Total C<br>40 40 | 0       |
| 18  | b     | 1        | Total C<br>40 40 | 0       |
| 18  | b     | 1        | Total C<br>40 40 | 0       |
| 18  | b     | 1        | Total C<br>40 40 | 0       |
| 18  | d     | 1        | Total C<br>40 40 | 0       |
| 18  | h     | 1        | Total C<br>40 40 | 0       |

- Molecule 19 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 19  | a     | 1        | Total Cl<br>1 1 | 0       |

- Molecule 20 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: C<sub>38</sub>H<sub>72</sub>O<sub>10</sub>).

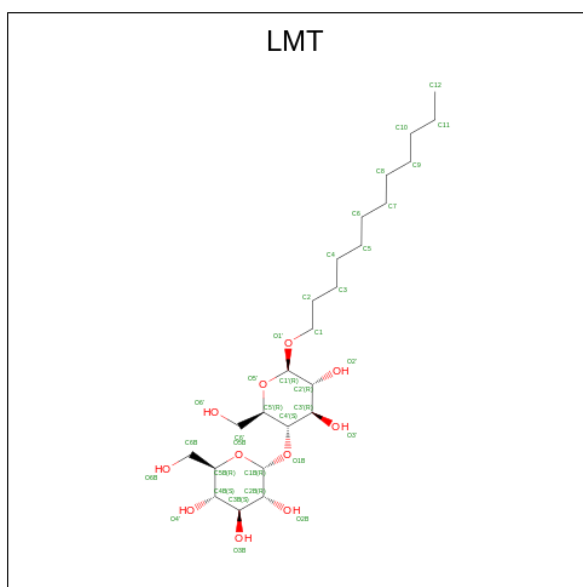


| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 20  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 20  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 20  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 20  | d     | 1        | Total | C  | O  | 0       |
|     |       |          | 47    | 37 | 10 |         |
| 20  | d     | 1        | Total | C  | O  | 0       |
|     |       |          | 41    | 31 | 10 |         |
| 20  | d     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 20  | m     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |

- Molecule 21 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 21  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 36    | 31 | 5 |         |
| 21  | x     | 1        | Total | C  | O | 0       |
|     |       |          | 17    | 16 | 1 |         |

- Molecule 22 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).

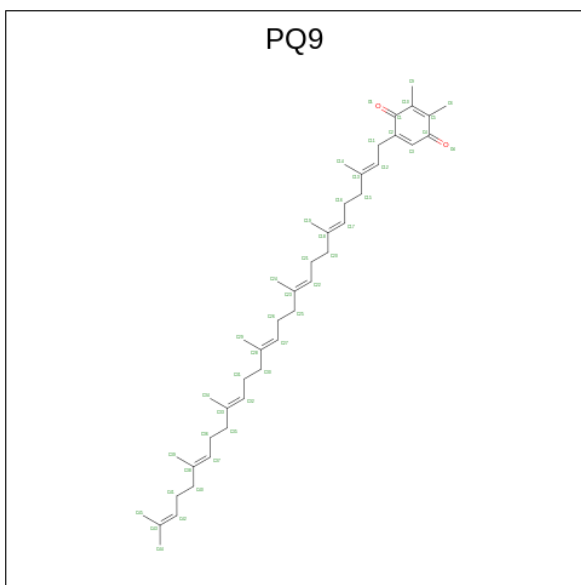


| Mol | Chain | Residues | Atoms       |         |         | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 22  | b     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 22  | d     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 22  | t     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |

- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

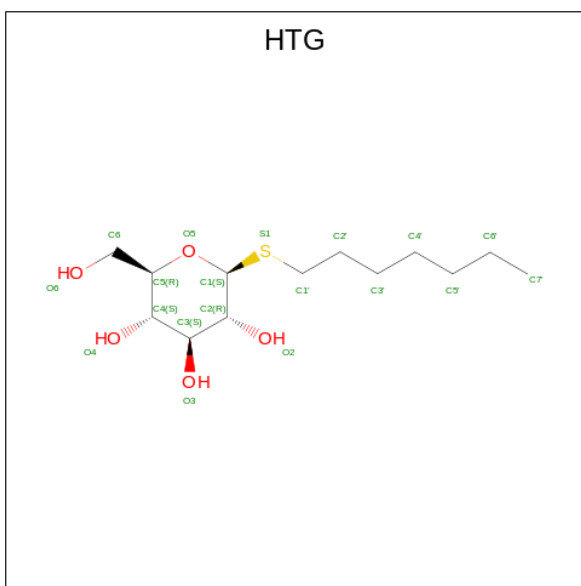
| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 23  | d     | 1        | Total Fe<br>1 1 | 0       |

- Molecule 24 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (CCD ID: PQ9) (formula:  $C_{43}H_{64}O_2$ ).



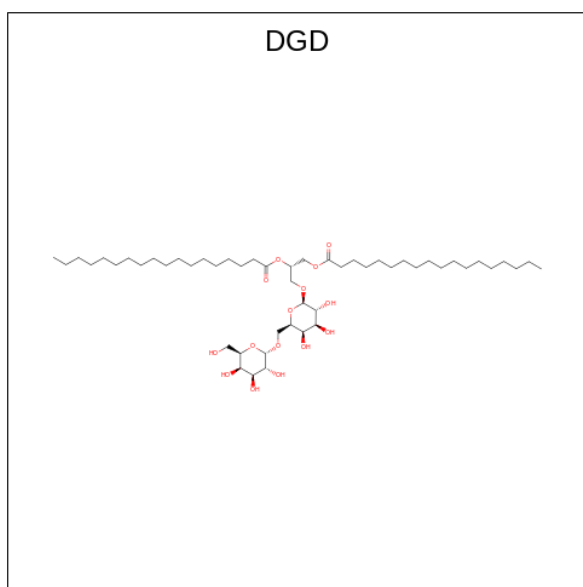
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 24  | d     | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 43 | 2 |         |

- Molecule 25 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula:  $C_{13}H_{26}O_5S$ ).



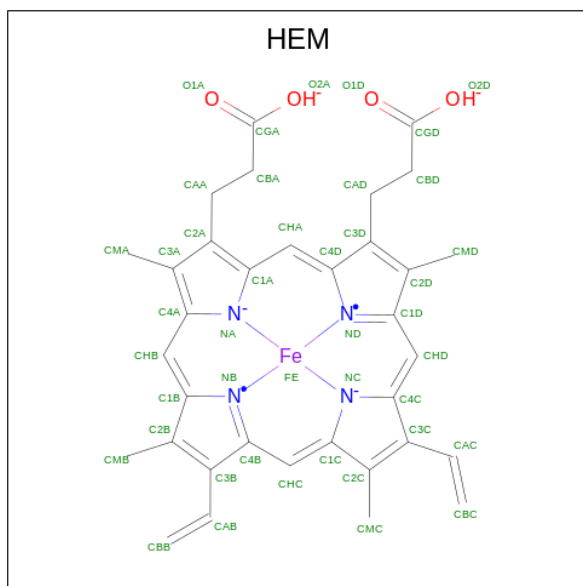
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 25  | d     | 1        | Total | C  | O | S | 0       |
|     |       |          | 16    | 10 | 5 | 1 |         |

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 26  | d     | 1        | Total | C  | O  | 0       |
|     |       |          | 54    | 39 | 15 |         |

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

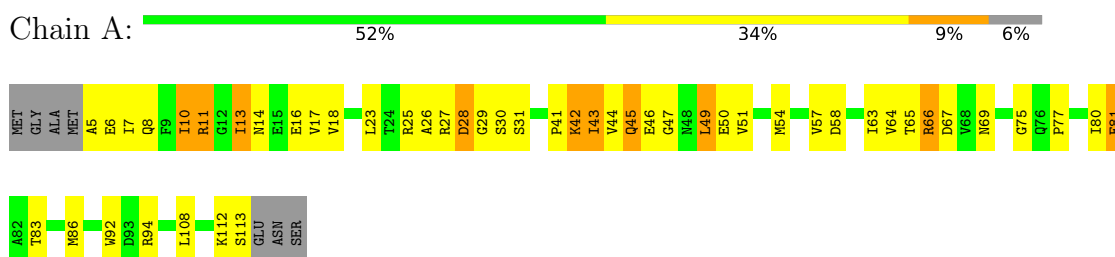


| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 27  | e     | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |

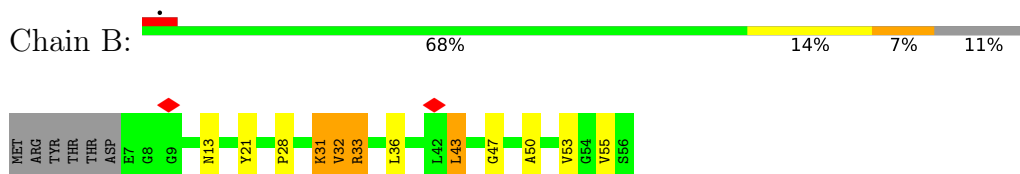
### 3 Residue-property plots

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.

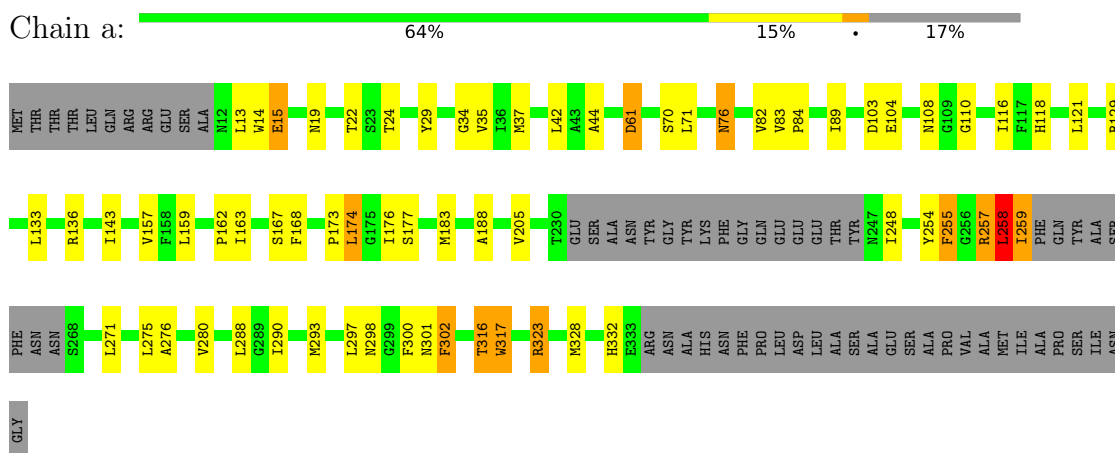
- Molecule 1: Photosystem II reaction center Psb28 protein



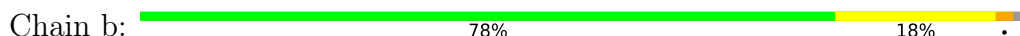
- Molecule 2: Tsl0063 protein

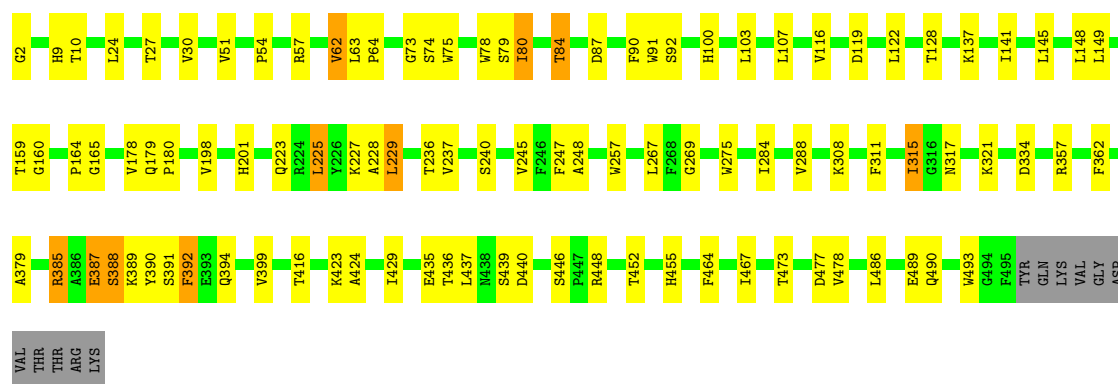


- Molecule 3: Photosystem II protein D1

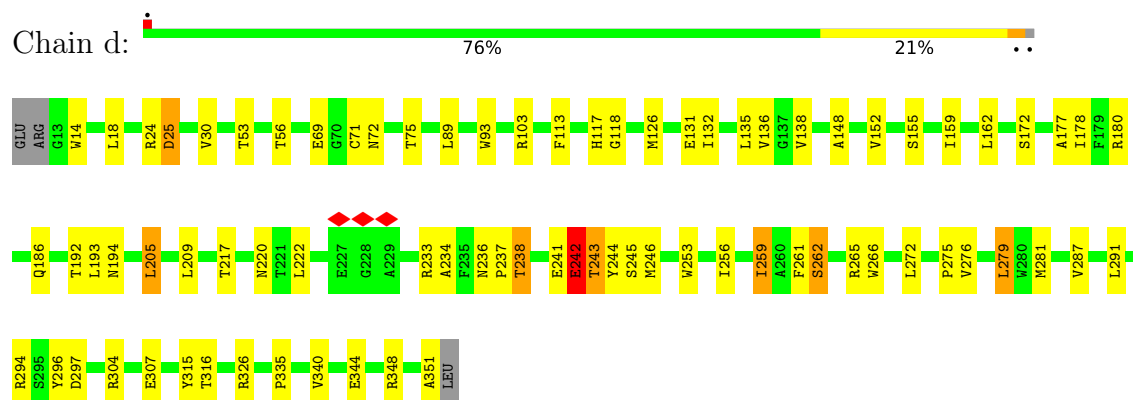


- Molecule 4: Photosystem II CP47 reaction center protein

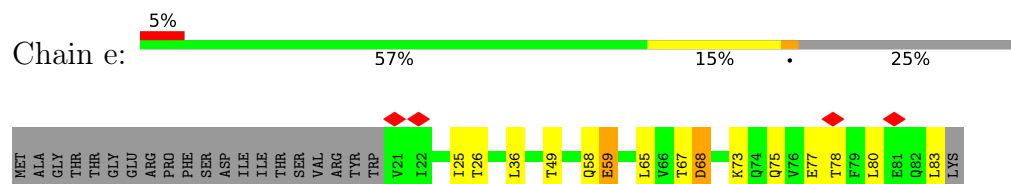




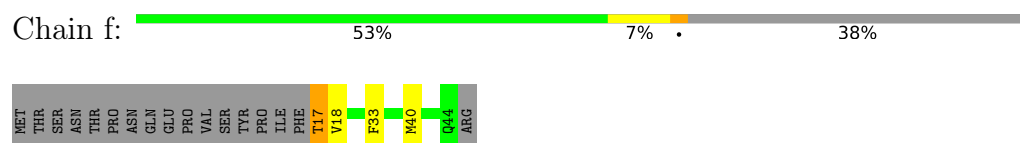
• Molecule 5: Photosystem II D2 protein



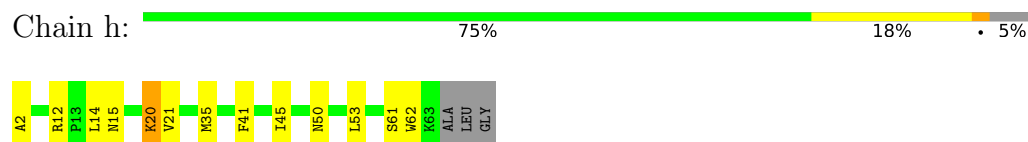
• Molecule 6: Cytochrome b559 subunit alpha



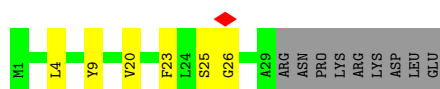
• Molecule 7: Cytochrome b559 subunit beta



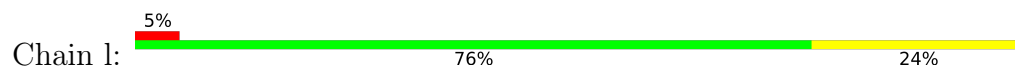
• Molecule 8: Photosystem II reaction center protein H



• Molecule 9: Photosystem II reaction center protein I



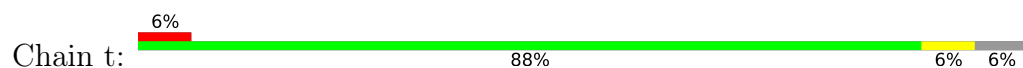
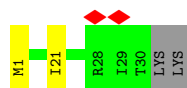
- Molecule 10: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein M



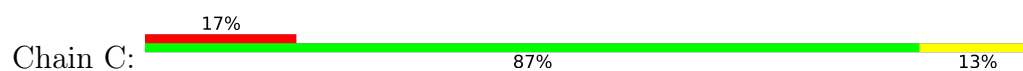
- Molecule 12: Photosystem II reaction center protein T



- Molecule 13: Photosystem II reaction center protein X



- Molecule 14: unidentified transmembrane protein



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 241790                                  | 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 ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.236                                   | Depositor |
| Minimum map value                    | -0.149                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.006                                   | Depositor |
| Recommended contour level            | 0.022                                   | Depositor |
| Map size (Å)                         | 261.308, 261.308, 261.308               | wwPDB     |
| Map dimensions                       | 200, 200, 200                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.30654, 1.30654, 1.30654               | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQ9, MGE, LMT, UNL, SQD, PHO, BCR, CL, HTG, DGD, FE2, HEM, CLA

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     | 0.61         | 0/892   | 0.85        | 0/1202         |
| 2   | B     | 0.38         | 0/371   | 0.71        | 0/505          |
| 3   | a     | 0.49         | 0/2383  | 0.77        | 3/3249 (0.1%)  |
| 4   | b     | 0.48         | 0/4025  | 0.72        | 2/5486 (0.0%)  |
| 5   | d     | 0.51         | 0/2789  | 0.74        | 0/3803         |
| 6   | e     | 0.36         | 0/523   | 0.79        | 3/714 (0.4%)   |
| 7   | f     | 0.36         | 0/225   | 0.73        | 0/308          |
| 8   | h     | 0.45         | 0/506   | 0.82        | 0/690          |
| 9   | i     | 0.31         | 0/237   | 0.70        | 0/322          |
| 10  | l     | 0.40         | 0/311   | 0.66        | 0/422          |
| 11  | m     | 0.36         | 0/248   | 0.85        | 0/339          |
| 12  | t     | 0.30         | 0/263   | 0.52        | 0/356          |
| 13  | x     | 0.28         | 0/264   | 0.61        | 0/358          |
| 14  | C     | 0.40         | 0/114   | 0.99        | 0/158          |
| All | All   | 0.48         | 0/13151 | 0.75        | 8/17912 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 5   | d     | 0                   | 1                   |
| 6   | e     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 4   | b     | 435 | GLU  | CA-C-N | 6.04 | 133.08      | 121.54   |
| 4   | b     | 435 | GLU  | C-N-CA | 6.04 | 133.08      | 121.54   |
| 6   | e     | 67  | THR  | CA-C-N | 5.66 | 129.75      | 121.31   |
| 6   | e     | 67  | THR  | C-N-CA | 5.66 | 129.75      | 121.31   |
| 3   | a     | 258 | LEU  | CA-C-N | 5.38 | 131.39      | 121.70   |
| 3   | a     | 258 | LEU  | C-N-CA | 5.38 | 131.39      | 121.70   |
| 3   | a     | 110 | GLY  | N-CA-C | 5.36 | 121.63      | 115.09   |
| 6   | e     | 68  | ASP  | N-CA-C | 5.17 | 117.59      | 110.35   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 5   | d     | 93  | TRP  | Peptide |
| 6   | e     | 68  | ASP  | Peptide |

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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     | 875   | 0        | 839      | 64      | 0            |
| 2   | B     | 365   | 0        | 386      | 34      | 0            |
| 3   | a     | 2311  | 0        | 2244     | 64      | 0            |
| 4   | b     | 3886  | 0        | 3741     | 76      | 0            |
| 5   | d     | 2694  | 0        | 2588     | 75      | 0            |
| 6   | e     | 509   | 0        | 499      | 7       | 0            |
| 7   | f     | 219   | 0        | 228      | 3       | 0            |
| 8   | h     | 493   | 0        | 513      | 14      | 0            |
| 9   | i     | 231   | 0        | 243      | 1       | 0            |
| 10  | l     | 304   | 0        | 316      | 6       | 0            |
| 11  | m     | 244   | 0        | 256      | 13      | 0            |
| 12  | t     | 254   | 0        | 257      | 9       | 0            |
| 13  | x     | 261   | 0        | 291      | 4       | 0            |
| 14  | C     | 115   | 0        | 114      | 10      | 0            |
| 15  | a     | 26    | 0        | 16       | 0       | 0            |
| 15  | l     | 47    | 0        | 61       | 2       | 0            |
| 16  | a     | 165   | 0        | 150      | 10      | 0            |
| 16  | b     | 973   | 0        | 1017     | 73      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16  | d     | 176   | 0        | 172      | 18      | 0            |
| 17  | a     | 128   | 0        | 148      | 11      | 0            |
| 18  | a     | 40    | 0        | 56       | 4       | 0            |
| 18  | b     | 120   | 0        | 168      | 21      | 0            |
| 18  | d     | 40    | 0        | 56       | 4       | 0            |
| 18  | h     | 40    | 0        | 56       | 4       | 0            |
| 19  | a     | 1     | 0        | 0        | 2       | 0            |
| 20  | a     | 48    | 0        | 72       | 0       | 0            |
| 20  | b     | 96    | 0        | 144      | 3       | 0            |
| 20  | d     | 136   | 0        | 193      | 14      | 0            |
| 20  | m     | 48    | 0        | 72       | 2       | 0            |
| 21  | b     | 36    | 0        | 0        | 0       | 0            |
| 21  | x     | 17    | 0        | 0        | 1       | 0            |
| 22  | b     | 35    | 0        | 46       | 0       | 0            |
| 22  | d     | 35    | 0        | 46       | 1       | 0            |
| 22  | t     | 35    | 0        | 46       | 1       | 0            |
| 23  | d     | 1     | 0        | 0        | 0       | 0            |
| 24  | d     | 45    | 0        | 64       | 6       | 0            |
| 25  | d     | 16    | 0        | 17       | 6       | 0            |
| 26  | d     | 54    | 0        | 66       | 1       | 0            |
| 27  | e     | 43    | 0        | 30       | 0       | 0            |
| All | All   | 15162 | 0        | 15211    | 381     | 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 13.

All (381) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:28:PRO:HA     | 2:B:31:LYS:CG     | 1.25                     | 1.62              |
| 16:b:606:CLA:H71  | 18:b:619:BCR:C34  | 1.52                     | 1.39              |
| 16:b:606:CLA:C7   | 18:b:619:BCR:H342 | 1.60                     | 1.29              |
| 16:b:607:CLA:H191 | 20:d:409:MGE:C6A  | 1.63                     | 1.29              |
| 2:B:28:PRO:HA     | 2:B:31:LYS:CD     | 1.71                     | 1.20              |
| 5:d:14:TRP:CB     | 25:d:411:HTG:H61  | 1.73                     | 1.19              |
| 2:B:28:PRO:CA     | 2:B:31:LYS:CG     | 2.20                     | 1.19              |
| 16:b:607:CLA:H201 | 20:d:409:MGE:C6A  | 1.74                     | 1.18              |
| 1:A:50:GLU:OE1    | 5:d:236:ASN:HB2   | 1.41                     | 1.17              |
| 2:B:28:PRO:HA     | 2:B:31:LYS:HG2    | 1.20                     | 1.13              |
| 5:d:14:TRP:HB3    | 25:d:411:HTG:C6   | 1.79                     | 1.12              |
| 16:b:602:CLA:H43  | 8:h:45:ILE:HG22   | 1.33                     | 1.10              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:28:PRO:HA    | 2:B:31:LYS:HG3    | 1.27                     | 1.06              |
| 5:d:14:TRP:HB3   | 25:d:411:HTG:H61  | 1.08                     | 1.05              |
| 4:b:385:ARG:NH1  | 5:d:351:ALA:O     | 1.88                     | 1.05              |
| 3:a:257:ARG:CZ   | 3:a:257:ARG:HA    | 1.88                     | 1.03              |
| 1:A:16:GLU:OE1   | 1:A:42:LYS:NZ     | 1.93                     | 1.01              |
| 2:B:28:PRO:O     | 2:B:32:VAL:HG12   | 1.61                     | 1.01              |
| 16:b:607:CLA:C19 | 20:d:409:MGE:C6A  | 2.40                     | 0.99              |
| 2:B:28:PRO:CA    | 2:B:31:LYS:CD     | 2.40                     | 0.95              |
| 3:a:257:ARG:HH21 | 3:a:257:ARG:HG3   | 1.31                     | 0.95              |
| 1:A:66:ARG:O     | 3:a:255:PHE:CE2   | 2.19                     | 0.95              |
| 1:A:6:GLU:CD     | 1:A:14:ASN:HB3    | 1.90                     | 0.95              |
| 16:b:607:CLA:C20 | 20:d:409:MGE:C6A  | 2.47                     | 0.91              |
| 11:m:8:PHE:CE2   | 12:t:1:MET:HG3    | 2.06                     | 0.91              |
| 1:A:66:ARG:O     | 3:a:255:PHE:HE2   | 1.53                     | 0.91              |
| 5:d:241:GLU:OE2  | 5:d:244:TYR:OH    | 1.90                     | 0.89              |
| 2:B:28:PRO:C     | 2:B:31:LYS:HG3    | 1.97                     | 0.88              |
| 1:A:6:GLU:OE1    | 1:A:14:ASN:HB3    | 1.74                     | 0.88              |
| 16:b:606:CLA:H2  | 18:b:619:BCR:H321 | 1.55                     | 0.88              |
| 16:b:602:CLA:C4  | 8:h:45:ILE:HG22   | 2.04                     | 0.87              |
| 2:B:50:ALA:HB3   | 14:C:36:ALA:CB    | 2.04                     | 0.86              |
| 4:b:388:SER:HB3  | 4:b:394:GLN:HE22  | 1.40                     | 0.86              |
| 11:m:8:PHE:HE2   | 12:t:1:MET:HG3    | 1.40                     | 0.86              |
| 5:d:238:THR:HG21 | 5:d:242:GLU:OE2   | 1.75                     | 0.85              |
| 1:A:5:ALA:N      | 1:A:58:ASP:HA     | 1.93                     | 0.84              |
| 1:A:25:ARG:HE    | 1:A:29:GLY:HA2    | 1.42                     | 0.83              |
| 3:a:332:HIS:HD2  | 19:a:408:CL:CL    | 1.98                     | 0.83              |
| 16:b:606:CLA:H71 | 18:b:619:BCR:H342 | 0.83                     | 0.83              |
| 2:B:28:PRO:HB3   | 2:B:31:LYS:HD2    | 1.59                     | 0.82              |
| 16:b:602:CLA:H43 | 8:h:45:ILE:CG2    | 2.09                     | 0.81              |
| 2:B:28:PRO:CA    | 2:B:31:LYS:HG3    | 1.95                     | 0.81              |
| 5:d:14:TRP:CB    | 25:d:411:HTG:C6   | 2.50                     | 0.80              |
| 16:b:607:CLA:C18 | 20:d:409:MGE:C6A  | 2.60                     | 0.80              |
| 2:B:28:PRO:O     | 2:B:31:LYS:HG3    | 1.83                     | 0.79              |
| 2:B:28:PRO:O     | 2:B:32:VAL:CG1    | 2.31                     | 0.79              |
| 4:b:90:PHE:CE2   | 16:b:606:CLA:H162 | 2.18                     | 0.78              |
| 5:d:238:THR:CG2  | 5:d:242:GLU:OE2   | 2.32                     | 0.78              |
| 2:B:50:ALA:HB3   | 14:C:36:ALA:HB2   | 1.66                     | 0.77              |
| 4:b:165:GLY:HA3  | 4:b:179:GLN:O     | 1.84                     | 0.77              |
| 3:a:257:ARG:HA   | 3:a:257:ARG:NE    | 1.96                     | 0.77              |
| 16:b:606:CLA:C5  | 18:b:619:BCR:H342 | 2.14                     | 0.77              |
| 2:B:28:PRO:CB    | 2:B:31:LYS:CD     | 2.64                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:b:100:HIS:ND1   | 16:b:606:CLA:C4   | 2.48                     | 0.76              |
| 1:A:6:GLU:OE2     | 1:A:14:ASN:CG     | 2.30                     | 0.75              |
| 16:b:606:CLA:H71  | 18:b:619:BCR:C9   | 2.18                     | 0.73              |
| 1:A:6:GLU:OE2     | 1:A:14:ASN:HB3    | 1.88                     | 0.73              |
| 11:m:8:PHE:CE2    | 12:t:1:MET:HE2    | 2.24                     | 0.73              |
| 2:B:28:PRO:CA     | 2:B:31:LYS:HG2    | 2.05                     | 0.72              |
| 5:d:246:MET:CE    | 5:d:261:PHE:O     | 2.37                     | 0.72              |
| 1:A:44:VAL:HG13   | 1:A:77:PRO:HB2    | 1.72                     | 0.72              |
| 16:b:608:CLA:HBB1 | 5:d:126:MET:HE2   | 1.72                     | 0.71              |
| 16:a:402:CLA:H202 | 17:a:404:PHO:H43  | 1.71                     | 0.71              |
| 2:B:50:ALA:CB     | 14:C:36:ALA:HB2   | 2.19                     | 0.71              |
| 4:b:62:VAL:HG13   | 16:b:605:CLA:HED3 | 1.73                     | 0.71              |
| 2:B:28:PRO:CB     | 2:B:31:LYS:HD2    | 2.21                     | 0.70              |
| 4:b:62:VAL:CG1    | 16:b:605:CLA:HED3 | 2.21                     | 0.70              |
| 16:b:615:CLA:H2   | 16:b:616:CLA:HBB2 | 1.72                     | 0.70              |
| 4:b:148:LEU:HD23  | 16:b:604:CLA:H191 | 1.73                     | 0.69              |
| 16:b:606:CLA:H52  | 18:b:619:BCR:HC7  | 1.75                     | 0.69              |
| 3:a:257:ARG:HE    | 5:d:136:VAL:CG2   | 2.06                     | 0.69              |
| 1:A:69:ASN:ND2    | 1:A:81:GLU:OE1    | 2.26                     | 0.69              |
| 2:B:50:ALA:HB3    | 14:C:36:ALA:HB1   | 1.75                     | 0.69              |
| 2:B:28:PRO:HB3    | 2:B:31:LYS:CD     | 2.22                     | 0.69              |
| 3:a:293:MET:HE1   | 3:a:298:ASN:HB3   | 1.75                     | 0.69              |
| 11:m:8:PHE:CZ     | 12:t:1:MET:HE2    | 2.27                     | 0.69              |
| 1:A:43:ILE:HD12   | 1:A:43:ILE:O      | 1.92                     | 0.69              |
| 4:b:391:SER:CB    | 4:b:394:GLN:OE1   | 2.42                     | 0.68              |
| 1:A:66:ARG:HD3    | 5:d:135:LEU:O     | 1.94                     | 0.66              |
| 3:a:183:MET:SD    | 16:d:401:CLA:HAC1 | 2.35                     | 0.66              |
| 3:a:257:ARG:HH21  | 3:a:257:ARG:CG    | 2.09                     | 0.65              |
| 16:b:606:CLA:C6   | 18:b:619:BCR:H342 | 2.24                     | 0.65              |
| 1:A:11:ARG:CB     | 1:A:11:ARG:HH21   | 2.10                     | 0.65              |
| 2:B:43:LEU:HB3    | 14:C:43:ALA:HB2   | 1.79                     | 0.65              |
| 1:A:6:GLU:OE2     | 1:A:14:ASN:CB     | 2.46                     | 0.64              |
| 1:A:66:ARG:O      | 3:a:255:PHE:CZ    | 2.50                     | 0.64              |
| 3:a:293:MET:HE1   | 3:a:298:ASN:CA    | 2.27                     | 0.64              |
| 17:a:404:PHO:H162 | 16:d:401:CLA:H143 | 1.80                     | 0.64              |
| 16:b:606:CLA:H2   | 18:b:619:BCR:C32  | 2.27                     | 0.63              |
| 4:b:100:HIS:ND1   | 16:b:606:CLA:H42  | 2.14                     | 0.62              |
| 1:A:66:ARG:CB     | 3:a:255:PHE:HZ    | 2.12                     | 0.62              |
| 1:A:11:ARG:HH21   | 1:A:11:ARG:CG     | 2.12                     | 0.62              |
| 4:b:100:HIS:CE1   | 16:b:606:CLA:H43  | 2.35                     | 0.62              |
| 5:d:14:TRP:HB2    | 25:d:411:HTG:H61  | 1.74                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:a:89:ILE:HD11   | 3:a:108:ASN:HB3   | 1.80                     | 0.62              |
| 4:b:247:PHE:HE1   | 16:b:602:CLA:H102 | 1.64                     | 0.62              |
| 1:A:41:PRO:O      | 1:A:45:GLN:HG2    | 2.00                     | 0.62              |
| 1:A:44:VAL:CG1    | 1:A:77:PRO:HB2    | 2.29                     | 0.61              |
| 16:b:607:CLA:H2   | 20:b:620:MGE:H6A1 | 1.82                     | 0.61              |
| 1:A:8:GLN:NE2     | 1:A:13:ILE:O      | 2.34                     | 0.61              |
| 2:B:28:PRO:CA     | 2:B:31:LYS:HD2    | 2.27                     | 0.61              |
| 5:d:186:GLN:HB2   | 16:d:404:CLA:HBC1 | 1.82                     | 0.61              |
| 3:a:257:ARG:HE    | 5:d:136:VAL:HG22  | 1.67                     | 0.60              |
| 4:b:149:LEU:HB2   | 16:b:604:CLA:H171 | 1.83                     | 0.60              |
| 4:b:100:HIS:ND1   | 16:b:606:CLA:H43  | 2.17                     | 0.60              |
| 1:A:5:ALA:N       | 1:A:58:ASP:CA     | 2.58                     | 0.59              |
| 3:a:293:MET:HE1   | 3:a:298:ASN:HA    | 1.83                     | 0.59              |
| 5:d:217:THR:HG21  | 5:d:253:TRP:HE1   | 1.66                     | 0.59              |
| 4:b:64:PRO:HB3    | 4:b:267:LEU:HB3   | 1.83                     | 0.59              |
| 1:A:51:VAL:HG12   | 3:a:255:PHE:HB2   | 1.85                     | 0.59              |
| 16:a:402:CLA:HBC3 | 16:a:402:CLA:HMC3 | 1.83                     | 0.59              |
| 1:A:81:GLU:O      | 1:A:81:GLU:HG2    | 2.02                     | 0.59              |
| 18:d:407:BCR:H271 | 20:d:408:MGE:H231 | 1.85                     | 0.58              |
| 16:a:402:CLA:C20  | 17:a:404:PHO:H43  | 2.33                     | 0.58              |
| 3:a:76:ASN:OD1    | 3:a:76:ASN:N      | 2.37                     | 0.58              |
| 3:a:257:ARG:NE    | 5:d:136:VAL:CG2   | 2.66                     | 0.58              |
| 3:a:332:HIS:CD2   | 19:a:408:CL:CL    | 2.88                     | 0.58              |
| 5:d:241:GLU:OE2   | 5:d:244:TYR:CZ    | 2.57                     | 0.57              |
| 3:a:276:ALA:O     | 3:a:280:VAL:HG23  | 2.04                     | 0.57              |
| 4:b:455:HIS:HE1   | 16:b:607:CLA:HBB2 | 1.69                     | 0.57              |
| 1:A:41:PRO:O      | 1:A:45:GLN:CG     | 2.53                     | 0.57              |
| 2:B:28:PRO:CB     | 2:B:31:LYS:HD3    | 2.33                     | 0.57              |
| 3:a:29:TYR:O      | 3:a:129:ARG:NH1   | 2.38                     | 0.57              |
| 3:a:29:TYR:OH     | 3:a:136:ARG:NH1   | 2.38                     | 0.57              |
| 1:A:42:LYS:HA     | 1:A:45:GLN:HG3    | 1.86                     | 0.57              |
| 3:a:293:MET:HE1   | 3:a:298:ASN:CB    | 2.34                     | 0.57              |
| 6:e:77:GLU:HA     | 6:e:80:LEU:HB2    | 1.87                     | 0.57              |
| 3:a:254:TYR:HA    | 5:d:237:PRO:HG2   | 1.87                     | 0.56              |
| 1:A:46:GLU:HA     | 5:d:233:ARG:HD3   | 1.87                     | 0.56              |
| 3:a:255:PHE:N     | 5:d:237:PRO:HG3   | 2.20                     | 0.56              |
| 1:A:43:ILE:HD11   | 5:d:233:ARG:HH11  | 1.70                     | 0.56              |
| 2:B:28:PRO:CA     | 2:B:31:LYS:HD3    | 2.34                     | 0.56              |
| 4:b:9:HIS:ND1     | 16:b:613:CLA:O1A  | 2.38                     | 0.56              |
| 15:l:101:SQD:H141 | 20:m:101:MGE:H7B1 | 1.86                     | 0.56              |
| 2:B:36:LEU:HB3    | 14:C:50:ALA:HB2   | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:23:LEU:HB2    | 4:b:493:TRP:HB2   | 1.87                     | 0.56              |
| 20:d:410:MGE:H9A2 | 12:t:21:ILE:HD11  | 1.88                     | 0.56              |
| 4:b:247:PHE:CE1   | 16:b:602:CLA:H121 | 2.41                     | 0.55              |
| 16:b:615:CLA:H2   | 16:b:616:CLA:CBB  | 2.36                     | 0.55              |
| 1:A:66:ARG:CA     | 3:a:255:PHE:CZ    | 2.89                     | 0.55              |
| 4:b:148:LEU:HD23  | 16:b:604:CLA:C19  | 2.35                     | 0.55              |
| 4:b:311:PHE:O     | 4:b:317:ASN:ND2   | 2.40                     | 0.55              |
| 1:A:66:ARG:HA     | 3:a:255:PHE:CZ    | 2.41                     | 0.55              |
| 3:a:302:PHE:N     | 3:a:302:PHE:CD1   | 2.73                     | 0.55              |
| 5:d:56:THR:HB     | 6:e:49:THR:HG23   | 1.88                     | 0.55              |
| 4:b:229:LEU:HD21  | 16:b:609:CLA:H43  | 1.87                     | 0.55              |
| 5:d:241:GLU:OE2   | 5:d:244:TYR:CE1   | 2.60                     | 0.55              |
| 3:a:257:ARG:HG3   | 3:a:257:ARG:NH2   | 2.09                     | 0.55              |
| 1:A:26:ALA:C      | 1:A:28:ASP:H      | 2.14                     | 0.55              |
| 13:x:21:LEU:HD11  | 21:x:101:UNL:C38  | 2.37                     | 0.55              |
| 1:A:49:LEU:O      | 5:d:233:ARG:NH1   | 2.38                     | 0.54              |
| 16:a:402:CLA:HMC1 | 16:d:404:CLA:HAC2 | 1.88                     | 0.54              |
| 10:l:12:LEU:H     | 11:m:29:THR:HG21  | 1.71                     | 0.54              |
| 1:A:10:ILE:HD11   | 1:A:43:ILE:CD1    | 2.38                     | 0.54              |
| 16:b:604:CLA:H43  | 16:b:605:CLA:H2   | 1.90                     | 0.54              |
| 17:a:404:PHO:H72  | 16:d:401:CLA:H201 | 1.90                     | 0.54              |
| 1:A:10:ILE:HG21   | 1:A:49:LEU:HB3    | 1.90                     | 0.54              |
| 16:a:402:CLA:CMC  | 16:d:404:CLA:HAC2 | 2.37                     | 0.54              |
| 3:a:44:ALA:HB2    | 3:a:118:HIS:HB2   | 1.90                     | 0.54              |
| 3:a:84:PRO:HD3    | 3:a:173:PRO:HB3   | 1.90                     | 0.54              |
| 3:a:257:ARG:HA    | 3:a:257:ARG:NH2   | 2.23                     | 0.54              |
| 4:b:269:GLY:O     | 4:b:448:ARG:NH1   | 2.40                     | 0.54              |
| 4:b:100:HIS:CE1   | 16:b:606:CLA:C4   | 2.91                     | 0.54              |
| 4:b:164:PRO:HD3   | 16:b:606:CLA:O1D  | 2.08                     | 0.53              |
| 15:l:101:SQD:H45  | 20:m:101:MGE:H4A1 | 1.90                     | 0.53              |
| 16:b:607:CLA:HMC2 | 18:b:618:BCR:H323 | 1.88                     | 0.53              |
| 4:b:486:LEU:HG    | 4:b:490:GLN:NE2   | 2.22                     | 0.53              |
| 3:a:257:ARG:HD3   | 5:d:132:ILE:HG23  | 1.90                     | 0.53              |
| 3:a:76:ASN:HD22   | 10:l:33:SER:HB3   | 1.74                     | 0.53              |
| 16:b:606:CLA:C7   | 18:b:619:BCR:C34  | 2.43                     | 0.53              |
| 16:b:613:CLA:HBB1 | 16:b:613:CLA:HMB1 | 1.90                     | 0.53              |
| 4:b:9:HIS:CE1     | 16:b:613:CLA:O1A  | 2.62                     | 0.53              |
| 4:b:149:LEU:HD22  | 16:b:604:CLA:H152 | 1.90                     | 0.53              |
| 4:b:477:ASP:OD1   | 4:b:477:ASP:N     | 2.41                     | 0.52              |
| 16:b:608:CLA:H191 | 5:d:89:LEU:HD13   | 1.91                     | 0.52              |
| 3:a:176:ILE:CD1   | 16:d:401:CLA:HMA3 | 2.39                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:a:403:CLA:CMC  | 16:d:404:CLA:H2   | 2.39                     | 0.52              |
| 16:a:403:CLA:HMC1 | 16:d:404:CLA:H2   | 1.91                     | 0.52              |
| 2:B:21:TYR:CE2    | 8:h:20:LYS:NZ     | 2.77                     | 0.52              |
| 1:A:50:GLU:CD     | 5:d:236:ASN:HB2   | 2.27                     | 0.52              |
| 4:b:464:PHE:HA    | 4:b:467:ILE:HD12  | 1.92                     | 0.52              |
| 1:A:6:GLU:OE2     | 1:A:14:ASN:ND2    | 2.43                     | 0.51              |
| 4:b:27:THR:HG22   | 4:b:107:LEU:HD13  | 1.91                     | 0.51              |
| 4:b:388:SER:HA    | 5:d:344:GLU:OE1   | 2.10                     | 0.51              |
| 20:b:622:MGE:H8B2 | 10:l:19:LEU:HD22  | 1.92                     | 0.51              |
| 5:d:222:LEU:HD23  | 5:d:243:THR:O     | 2.10                     | 0.51              |
| 8:h:61:SER:OG     | 8:h:62:TRP:N      | 2.44                     | 0.51              |
| 16:b:610:CLA:H152 | 16:b:610:CLA:H203 | 1.92                     | 0.51              |
| 13:x:2:THR:OG1    | 13:x:3:ILE:N      | 2.44                     | 0.51              |
| 16:d:401:CLA:H42  | 24:d:406:PQ9:H22  | 1.91                     | 0.51              |
| 3:a:257:ARG:NE    | 3:a:257:ARG:CA    | 2.73                     | 0.51              |
| 4:b:91:TRP:CZ2    | 16:b:606:CLA:H18  | 2.45                     | 0.51              |
| 5:d:262:SER:H     | 20:d:410:MGE:H2D  | 1.76                     | 0.51              |
| 3:a:61:ASP:OD1    | 3:a:61:ASP:N      | 2.45                     | 0.50              |
| 5:d:246:MET:HE1   | 24:d:406:PQ9:H93  | 1.93                     | 0.50              |
| 16:b:604:CLA:HMC1 | 16:b:611:CLA:H191 | 1.92                     | 0.50              |
| 3:a:183:MET:HG2   | 16:d:401:CLA:HBC1 | 1.94                     | 0.50              |
| 4:b:2:GLY:N       | 10:l:9:PRO:O      | 2.44                     | 0.50              |
| 1:A:11:ARG:CG     | 1:A:11:ARG:NH2    | 2.73                     | 0.50              |
| 5:d:304:ARG:HH22  | 22:d:402:LMT:H3O1 | 1.58                     | 0.49              |
| 1:A:8:GLN:HB2     | 1:A:13:ILE:O      | 2.12                     | 0.49              |
| 3:a:34:GLY:HA2    | 3:a:37:MET:HB3    | 1.94                     | 0.49              |
| 3:a:42:LEU:HD23   | 18:a:407:BCR:H12C | 1.94                     | 0.49              |
| 11:m:8:PHE:CE2    | 12:t:1:MET:CE     | 2.94                     | 0.49              |
| 11:m:8:PHE:HD1    | 11:m:8:PHE:O      | 1.95                     | 0.49              |
| 16:b:606:CLA:C7   | 18:b:619:BCR:C9   | 2.85                     | 0.49              |
| 20:d:410:MGE:H8B2 | 20:d:410:MGE:H6A2 | 1.94                     | 0.49              |
| 1:A:26:ALA:C      | 1:A:28:ASP:N      | 2.71                     | 0.49              |
| 5:d:148:ALA:HB2   | 5:d:276:VAL:HG13  | 1.95                     | 0.49              |
| 1:A:66:ARG:C      | 3:a:255:PHE:CE2   | 2.88                     | 0.49              |
| 4:b:57:ARG:NH2    | 4:b:317:ASN:OD1   | 2.46                     | 0.49              |
| 4:b:160:GLY:HA3   | 4:b:180:PRO:HB3   | 1.94                     | 0.49              |
| 8:h:53:LEU:HA     | 13:x:6:SER:HB3    | 1.95                     | 0.48              |
| 4:b:379:ALA:HA    | 4:b:390:TYR:HB3   | 1.95                     | 0.48              |
| 1:A:44:VAL:HG12   | 1:A:44:VAL:O      | 2.12                     | 0.48              |
| 4:b:24:LEU:HG     | 16:b:615:CLA:HED2 | 1.94                     | 0.48              |
| 11:m:8:PHE:CD1    | 11:m:8:PHE:C      | 2.92                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:a:143:ILE:HG13  | 5:d:220:ASN:HD22  | 1.78                     | 0.48              |
| 3:a:162:PRO:HB3   | 3:a:168:PHE:HA    | 1.95                     | 0.48              |
| 3:a:129:ARG:NH2   | 5:d:256:ILE:O     | 2.47                     | 0.48              |
| 16:a:402:CLA:H202 | 17:a:404:PHO:C4   | 2.42                     | 0.48              |
| 5:d:296:TYR:OH    | 5:d:326:ARG:NH2   | 2.40                     | 0.48              |
| 2:B:21:TYR:OH     | 8:h:20:LYS:NZ     | 2.46                     | 0.48              |
| 4:b:145:LEU:HD22  | 16:b:604:CLA:H162 | 1.94                     | 0.48              |
| 5:d:155:SER:HB2   | 5:d:287:VAL:HG23  | 1.95                     | 0.48              |
| 4:b:78:TRP:HA     | 4:b:84:THR:HA     | 1.96                     | 0.48              |
| 5:d:238:THR:HG21  | 5:d:242:GLU:CD    | 2.39                     | 0.48              |
| 7:f:17:THR:OG1    | 7:f:18:VAL:N      | 2.44                     | 0.48              |
| 5:d:205:LEU:HB3   | 16:d:401:CLA:H11  | 1.95                     | 0.47              |
| 11:m:8:PHE:CD2    | 12:t:1:MET:HG3    | 2.48                     | 0.47              |
| 17:a:405:PHO:HBC1 | 5:d:275:PRO:HB2   | 1.96                     | 0.47              |
| 12:t:1:MET:N      | 22:t:101:LMT:O6'  | 2.44                     | 0.47              |
| 18:a:407:BCR:H24C | 18:a:407:BCR:H371 | 1.69                     | 0.47              |
| 5:d:242:GLU:O     | 5:d:242:GLU:HG2   | 2.14                     | 0.47              |
| 5:d:246:MET:CE    | 24:d:406:PQ9:H93  | 2.44                     | 0.47              |
| 17:a:404:PHO:H193 | 16:d:401:CLA:H142 | 1.95                     | 0.47              |
| 6:e:25:ILE:HG12   | 6:e:26:THR:HG22   | 1.96                     | 0.47              |
| 1:A:11:ARG:NH2    | 1:A:11:ARG:HG2    | 2.29                     | 0.47              |
| 1:A:43:ILE:CD1    | 5:d:233:ARG:HH11  | 2.28                     | 0.47              |
| 3:a:82:VAL:HB     | 3:a:174:LEU:HD12  | 1.97                     | 0.47              |
| 3:a:15:GLU:O      | 3:a:19:ASN:ND2    | 2.47                     | 0.47              |
| 4:b:225:LEU:HA    | 4:b:228:ALA:HB3   | 1.97                     | 0.47              |
| 4:b:275:TRP:CE2   | 4:b:315:ILE:HD13  | 2.50                     | 0.47              |
| 5:d:265:ARG:NH2   | 20:d:409:MGE:O4D  | 2.48                     | 0.47              |
| 9:i:25:SER:OG     | 9:i:26:GLY:N      | 2.47                     | 0.47              |
| 1:A:66:ARG:CG     | 3:a:255:PHE:CZ    | 2.98                     | 0.47              |
| 18:a:407:BCR:H341 | 18:a:407:BCR:H11C | 1.65                     | 0.47              |
| 4:b:391:SER:HB3   | 4:b:394:GLN:OE1   | 2.14                     | 0.47              |
| 17:a:405:PHO:H61  | 5:d:118:GLY:HA2   | 1.97                     | 0.47              |
| 5:d:113:PHE:O     | 5:d:117:HIS:ND1   | 2.48                     | 0.46              |
| 1:A:51:VAL:HG12   | 3:a:255:PHE:CB    | 2.45                     | 0.46              |
| 3:a:13:LEU:C      | 3:a:15:GLU:N      | 2.73                     | 0.46              |
| 3:a:316:THR:OG1   | 3:a:317:TRP:N     | 2.48                     | 0.46              |
| 4:b:9:HIS:CD2     | 16:b:612:CLA:HBB2 | 2.50                     | 0.46              |
| 1:A:43:ILE:HD11   | 5:d:233:ARG:NH1   | 2.31                     | 0.46              |
| 5:d:25:ASP:OD1    | 5:d:25:ASP:N      | 2.41                     | 0.46              |
| 5:d:71:CYS:HB3    | 5:d:75:THR:HB     | 1.97                     | 0.46              |
| 3:a:13:LEU:C      | 3:a:15:GLU:H      | 2.24                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:d:172:SER:HB2   | 5:d:177:ALA:HB1   | 1.97                     | 0.46              |
| 1:A:44:VAL:HG13   | 1:A:77:PRO:CB     | 2.42                     | 0.45              |
| 4:b:141:ILE:HD11  | 8:h:14:LEU:HD22   | 1.98                     | 0.45              |
| 8:h:12:ARG:NH1    | 8:h:15:ASN:O      | 2.45                     | 0.45              |
| 1:A:31:SER:HB3    | 4:b:490:GLN:HE22  | 1.81                     | 0.45              |
| 16:b:606:CLA:C5   | 18:b:619:BCR:C34  | 2.92                     | 0.45              |
| 5:d:103:ARG:HG2   | 6:e:73:LYS:HG2    | 1.98                     | 0.45              |
| 16:d:404:CLA:H41  | 16:d:404:CLA:H61  | 1.64                     | 0.45              |
| 2:B:33:ARG:O      | 14:C:50:ALA:HB1   | 2.16                     | 0.45              |
| 4:b:391:SER:OG    | 4:b:392:PHE:N     | 2.48                     | 0.45              |
| 5:d:297:ASP:OD1   | 5:d:297:ASP:N     | 2.49                     | 0.45              |
| 2:B:47:GLY:O      | 14:C:36:ALA:HB1   | 2.17                     | 0.45              |
| 4:b:73:GLY:HA2    | 4:b:79:SER:HA     | 1.97                     | 0.45              |
| 5:d:89:LEU:HG     | 8:h:50:ASN:HD22   | 1.81                     | 0.45              |
| 3:a:183:MET:CG    | 16:d:401:CLA:HBC1 | 2.47                     | 0.45              |
| 4:b:79:SER:OG     | 4:b:80:ILE:N      | 2.49                     | 0.45              |
| 4:b:237:VAL:HG11  | 16:b:610:CLA:H201 | 1.99                     | 0.45              |
| 16:b:610:CLA:H203 | 16:b:610:CLA:C15  | 2.46                     | 0.45              |
| 11:m:8:PHE:O      | 11:m:8:PHE:CD1    | 2.70                     | 0.45              |
| 2:B:55:VAL:HB     | 4:b:159:THR:HG21  | 1.98                     | 0.44              |
| 4:b:74:SER:HA     | 4:b:92:SER:HB2    | 1.99                     | 0.44              |
| 1:A:67:ASP:OD2    | 1:A:83:THR:HB     | 2.17                     | 0.44              |
| 2:B:31:LYS:HE3    | 2:B:31:LYS:HB2    | 1.55                     | 0.44              |
| 4:b:74:SER:OG     | 4:b:75:TRP:N      | 2.49                     | 0.44              |
| 5:d:296:TYR:O     | 5:d:315:TYR:OH    | 2.34                     | 0.44              |
| 16:d:401:CLA:H203 | 16:d:401:CLA:H162 | 1.69                     | 0.44              |
| 1:A:42:LYS:HE3    | 1:A:42:LYS:HB2    | 1.59                     | 0.44              |
| 24:d:406:PQ9:H352 | 10:l:30:LEU:HD22  | 1.98                     | 0.44              |
| 4:b:80:ILE:HD13   | 4:b:80:ILE:HA     | 1.84                     | 0.44              |
| 5:d:53:THR:HG22   | 7:f:40:MET:HE1    | 1.99                     | 0.44              |
| 4:b:455:HIS:HE1   | 16:b:607:CLA:CBB  | 2.30                     | 0.44              |
| 3:a:259:ILE:H     | 3:a:259:ILE:HG13  | 1.48                     | 0.43              |
| 18:b:619:BCR:H361 | 18:b:619:BCR:H20C | 1.80                     | 0.43              |
| 5:d:152:VAL:HG21  | 5:d:279:LEU:HD13  | 2.00                     | 0.43              |
| 8:h:20:LYS:HZ3    | 8:h:20:LYS:HB2    | 1.83                     | 0.43              |
| 4:b:122:LEU:HD21  | 16:b:615:CLA:HBC2 | 1.99                     | 0.43              |
| 1:A:66:ARG:CA     | 3:a:255:PHE:HZ    | 2.30                     | 0.43              |
| 3:a:14:TRP:O      | 3:a:14:TRP:CG     | 2.70                     | 0.43              |
| 1:A:10:ILE:HD11   | 1:A:43:ILE:HD11   | 2.00                     | 0.43              |
| 8:h:41:PHE:HB2    | 18:h:101:BCR:H16C | 1.99                     | 0.43              |
| 18:b:618:BCR:H24C | 18:b:618:BCR:H371 | 1.78                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:m:8:PHE:HD1    | 11:m:8:PHE:C      | 2.26                     | 0.43              |
| 1:A:69:ASN:HD22   | 1:A:81:GLU:CD     | 2.26                     | 0.43              |
| 2:B:13:ASN:HB2    | 4:b:10:THR:HB     | 2.01                     | 0.43              |
| 16:b:614:CLA:H62  | 16:b:614:CLA:H41  | 1.35                     | 0.43              |
| 16:b:615:CLA:H92  | 16:b:615:CLA:H61  | 1.81                     | 0.43              |
| 5:d:236:ASN:N     | 5:d:237:PRO:HD2   | 2.34                     | 0.43              |
| 6:e:58:GLN:HG2    | 6:e:59:GLU:HG3    | 2.00                     | 0.43              |
| 11:m:8:PHE:CE2    | 12:t:1:MET:CG     | 2.93                     | 0.43              |
| 1:A:75:GLY:HA2    | 5:d:242:GLU:O     | 2.18                     | 0.42              |
| 16:b:606:CLA:H52  | 18:b:619:BCR:H342 | 1.99                     | 0.42              |
| 18:d:407:BCR:H15C | 18:d:407:BCR:H351 | 1.89                     | 0.42              |
| 18:a:407:BCR:H15C | 18:a:407:BCR:H351 | 1.80                     | 0.42              |
| 5:d:72:ASN:HA     | 20:d:408:MGE:H1D  | 2.01                     | 0.42              |
| 5:d:262:SER:O     | 5:d:262:SER:OG    | 2.37                     | 0.42              |
| 5:d:266:TRP:CD1   | 20:d:410:MGE:H1D  | 2.55                     | 0.42              |
| 4:b:257:TRP:HB2   | 4:b:452:THR:HG21  | 2.01                     | 0.42              |
| 6:e:75:GLN:O      | 6:e:78:THR:HB     | 2.19                     | 0.42              |
| 4:b:236:THR:HB    | 4:b:473:THR:HG21  | 2.01                     | 0.42              |
| 18:d:407:BCR:H11C | 18:d:407:BCR:H341 | 1.93                     | 0.42              |
| 16:a:402:CLA:H51  | 17:a:404:PHO:C4B  | 2.50                     | 0.42              |
| 4:b:30:VAL:HG12   | 16:b:605:CLA:HHD  | 2.02                     | 0.42              |
| 18:b:618:BCR:H20C | 18:b:618:BCR:H361 | 1.83                     | 0.42              |
| 20:b:622:MGE:H7A1 | 11:m:18:PRO:HB3   | 2.02                     | 0.42              |
| 4:b:227:LYS:HE2   | 4:b:227:LYS:HB3   | 1.85                     | 0.42              |
| 8:h:35:MET:HG2    | 18:h:101:BCR:H312 | 2.02                     | 0.42              |
| 1:A:64:VAL:HG21   | 1:A:66:ARG:HH21   | 1.84                     | 0.42              |
| 4:b:247:PHE:CE1   | 16:b:602:CLA:H102 | 2.50                     | 0.42              |
| 16:b:608:CLA:H162 | 16:d:405:CLA:H3A  | 2.01                     | 0.42              |
| 17:a:404:PHO:H61  | 17:a:404:PHO:H41  | 1.78                     | 0.42              |
| 4:b:248:ALA:HA    | 16:b:603:CLA:H42  | 2.02                     | 0.42              |
| 16:b:606:CLA:H72  | 18:b:619:BCR:H311 | 2.01                     | 0.42              |
| 5:d:335:PRO:HB2   | 6:e:65:LEU:HD11   | 2.00                     | 0.42              |
| 2:B:36:LEU:HB3    | 14:C:50:ALA:CB    | 2.50                     | 0.42              |
| 4:b:57:ARG:NH1    | 4:b:334:ASP:OD1   | 2.53                     | 0.42              |
| 5:d:14:TRP:HB3    | 25:d:411:HTG:O6   | 2.16                     | 0.42              |
| 4:b:51:VAL:HG13   | 4:b:308:LYS:HB2   | 2.02                     | 0.42              |
| 4:b:247:PHE:HD1   | 16:b:602:CLA:H142 | 1.84                     | 0.41              |
| 16:b:607:CLA:H172 | 5:d:281:MET:HE2   | 2.01                     | 0.41              |
| 4:b:119:ASP:OD1   | 8:h:2:ALA:N       | 2.53                     | 0.41              |
| 4:b:424:ALA:HB2   | 4:b:429:ILE:HD11  | 2.02                     | 0.41              |
| 5:d:246:MET:HE1   | 5:d:261:PHE:O     | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:d:410:MGE:H4A2 | 10:l:22:LEU:HD22  | 2.02                     | 0.41              |
| 3:a:258:LEU:H     | 3:a:258:LEU:HG    | 1.56                     | 0.41              |
| 3:a:257:ARG:CG    | 3:a:257:ARG:NH2   | 2.73                     | 0.41              |
| 4:b:247:PHE:CD1   | 16:b:602:CLA:H121 | 2.55                     | 0.41              |
| 18:d:407:BCR:H363 | 7:f:33:PHE:HB3    | 2.03                     | 0.41              |
| 1:A:66:ARG:CB     | 3:a:255:PHE:CZ    | 2.99                     | 0.41              |
| 18:h:101:BCR:H15C | 18:h:101:BCR:H351 | 1.83                     | 0.41              |
| 5:d:24:ARG:HH12   | 13:x:35:ASP:HB3   | 1.84                     | 0.41              |
| 24:d:406:PQ9:H193 | 20:d:410:MGE:H7B1 | 2.02                     | 0.41              |
| 5:d:246:MET:HE3   | 5:d:261:PHE:O     | 2.19                     | 0.41              |
| 2:B:50:ALA:HB1    | 14:C:36:ALA:HB2   | 1.99                     | 0.41              |
| 3:a:188:ALA:HB2   | 3:a:328:MET:HB2   | 2.02                     | 0.41              |
| 5:d:162:LEU:HD11  | 26:d:412:DGD:HA32 | 2.02                     | 0.41              |
| 5:d:233:ARG:NH2   | 5:d:234:ALA:O     | 2.54                     | 0.41              |
| 1:A:86:MET:HG2    | 1:A:92:TRP:HE3    | 1.85                     | 0.41              |
| 16:a:402:CLA:HBB1 | 16:a:402:CLA:HMB1 | 2.02                     | 0.41              |
| 4:b:388:SER:HB3   | 4:b:394:GLN:NE2   | 2.22                     | 0.41              |
| 5:d:304:ARG:HE    | 5:d:304:ARG:HB3   | 1.62                     | 0.41              |
| 24:d:406:PQ9:H191 | 24:d:406:PQ9:H211 | 1.87                     | 0.41              |
| 1:A:113:SER:N     | 4:b:493:TRP:O     | 2.54                     | 0.41              |
| 3:a:258:LEU:HB2   | 3:a:259:ILE:H     | 1.62                     | 0.41              |
| 4:b:223:GLN:HG2   | 4:b:227:LYS:HE3   | 2.02                     | 0.41              |
| 5:d:259:ILE:HA    | 5:d:259:ILE:HD12  | 1.85                     | 0.40              |
| 16:d:404:CLA:HBB1 | 16:d:404:CLA:CHC  | 2.51                     | 0.40              |
| 4:b:54:PRO:HD2    | 4:b:57:ARG:HB2    | 2.03                     | 0.40              |
| 4:b:423:LYS:HA    | 4:b:423:LYS:HD2   | 1.92                     | 0.40              |
| 17:a:405:PHO:H71  | 17:a:405:PHO:H112 | 1.77                     | 0.40              |
| 16:b:603:CLA:HAB  | 16:b:605:CLA:H171 | 2.03                     | 0.40              |
| 18:b:619:BCR:H24C | 18:b:619:BCR:H371 | 1.77                     | 0.40              |
| 5:d:159:ILE:HG21  | 5:d:287:VAL:HG22  | 2.03                     | 0.40              |
| 1:A:66:ARG:HB3    | 3:a:255:PHE:HZ    | 1.85                     | 0.40              |
| 3:a:323:ARG:HD3   | 3:a:323:ARG:HA    | 1.85                     | 0.40              |
| 4:b:103:LEU:HD22  | 16:b:606:CLA:H41  | 2.04                     | 0.40              |
| 4:b:103:LEU:HD22  | 16:b:606:CLA:H51  | 2.03                     | 0.40              |
| 18:b:617:BCR:H11C | 18:b:617:BCR:H341 | 1.88                     | 0.40              |
| 1:A:17:VAL:HG21   | 1:A:41:PRO:HA     | 2.04                     | 0.40              |
| 1:A:44:VAL:HG13   | 1:A:77:PRO:CG     | 2.52                     | 0.40              |
| 1:A:49:LEU:HD12   | 1:A:49:LEU:HA     | 1.78                     | 0.40              |
| 3:a:257:ARG:CD    | 5:d:132:ILE:HG23  | 2.51                     | 0.40              |
| 16:b:601:CLA:HMB2 | 18:h:101:BCR:H391 | 2.04                     | 0.40              |
| 16:b:606:CLA:H72  | 18:b:619:BCR:C7   | 2.52                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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     | 107/116 (92%)   | 91 (85%)   | 15 (14%) | 1 (1%)   | 14          | 41  |
| 2   | B     | 48/56 (86%)     | 47 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 3   | a     | 292/360 (81%)   | 272 (93%)  | 20 (7%)  | 0        | 100         | 100 |
| 4   | b     | 492/505 (97%)   | 466 (95%)  | 25 (5%)  | 1 (0%)   | 43          | 70  |
| 5   | d     | 337/342 (98%)   | 323 (96%)  | 13 (4%)  | 1 (0%)   | 36          | 64  |
| 6   | e     | 61/84 (73%)     | 53 (87%)   | 8 (13%)  | 0        | 100         | 100 |
| 7   | f     | 26/45 (58%)     | 26 (100%)  | 0        | 0        | 100         | 100 |
| 8   | h     | 60/65 (92%)     | 57 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 9   | i     | 27/38 (71%)     | 26 (96%)   | 1 (4%)   | 0        | 100         | 100 |
| 10  | l     | 35/37 (95%)     | 33 (94%)   | 2 (6%)   | 0        | 100         | 100 |
| 11  | m     | 29/36 (81%)     | 27 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| 12  | t     | 28/32 (88%)     | 27 (96%)   | 1 (4%)   | 0        | 100         | 100 |
| 13  | x     | 34/40 (85%)     | 34 (100%)  | 0        | 0        | 100         | 100 |
| 14  | C     | 21/23 (91%)     | 20 (95%)   | 1 (5%)   | 0        | 100         | 100 |
| All | All   | 1597/1779 (90%) | 1502 (94%) | 92 (6%)  | 3 (0%)   | 44          | 70  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | d     | 242 | GLU  |
| 1   | A     | 47  | GLY  |
| 4   | b     | 387 | GLU  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |     |
|-----|-------|-----------------|------------|-----------|-------------|-----|
| 1   | A     | 92/97 (95%)     | 70 (76%)   | 22 (24%)  | 1           | 3   |
| 2   | B     | 36/42 (86%)     | 31 (86%)   | 5 (14%)   | 3           | 14  |
| 3   | a     | 237/290 (82%)   | 200 (84%)  | 37 (16%)  | 2           | 11  |
| 4   | b     | 392/403 (97%)   | 357 (91%)  | 35 (9%)   | 9           | 29  |
| 5   | d     | 272/277 (98%)   | 245 (90%)  | 27 (10%)  | 7           | 26  |
| 6   | e     | 55/73 (75%)     | 52 (94%)   | 3 (6%)    | 19          | 46  |
| 7   | f     | 22/39 (56%)     | 21 (96%)   | 1 (4%)    | 24          | 52  |
| 8   | h     | 53/54 (98%)     | 51 (96%)   | 2 (4%)    | 29          | 56  |
| 9   | i     | 26/35 (74%)     | 22 (85%)   | 4 (15%)   | 2           | 11  |
| 10  | l     | 35/35 (100%)    | 32 (91%)   | 3 (9%)    | 10          | 31  |
| 11  | m     | 28/33 (85%)     | 26 (93%)   | 2 (7%)    | 13          | 37  |
| 12  | t     | 26/29 (90%)     | 26 (100%)  | 0         | 100         | 100 |
| 13  | x     | 29/33 (88%)     | 27 (93%)   | 2 (7%)    | 14          | 38  |
| All | All   | 1303/1440 (90%) | 1160 (89%) | 143 (11%) | 8           | 21  |

All (143) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | ILE  |
| 1   | A     | 10  | ILE  |
| 1   | A     | 11  | ARG  |
| 1   | A     | 13  | ILE  |
| 1   | A     | 18  | VAL  |
| 1   | A     | 27  | ARG  |
| 1   | A     | 28  | ASP  |
| 1   | A     | 30  | SER  |
| 1   | A     | 42  | LYS  |
| 1   | A     | 43  | ILE  |
| 1   | A     | 45  | GLN  |
| 1   | A     | 49  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 54  | MET  |
| 1   | A     | 57  | VAL  |
| 1   | A     | 63  | ILE  |
| 1   | A     | 65  | THR  |
| 1   | A     | 66  | ARG  |
| 1   | A     | 80  | ILE  |
| 1   | A     | 81  | GLU  |
| 1   | A     | 94  | ARG  |
| 1   | A     | 108 | LEU  |
| 1   | A     | 112 | LYS  |
| 2   | B     | 31  | LYS  |
| 2   | B     | 32  | VAL  |
| 2   | B     | 33  | ARG  |
| 2   | B     | 43  | LEU  |
| 2   | B     | 53  | VAL  |
| 3   | a     | 15  | GLU  |
| 3   | a     | 22  | THR  |
| 3   | a     | 24  | THR  |
| 3   | a     | 35  | VAL  |
| 3   | a     | 61  | ASP  |
| 3   | a     | 70  | SER  |
| 3   | a     | 71  | LEU  |
| 3   | a     | 76  | ASN  |
| 3   | a     | 83  | VAL  |
| 3   | a     | 103 | ASP  |
| 3   | a     | 104 | GLU  |
| 3   | a     | 116 | ILE  |
| 3   | a     | 121 | LEU  |
| 3   | a     | 133 | LEU  |
| 3   | a     | 157 | VAL  |
| 3   | a     | 159 | LEU  |
| 3   | a     | 163 | ILE  |
| 3   | a     | 167 | SER  |
| 3   | a     | 174 | LEU  |
| 3   | a     | 177 | SER  |
| 3   | a     | 205 | VAL  |
| 3   | a     | 248 | ILE  |
| 3   | a     | 255 | PHE  |
| 3   | a     | 257 | ARG  |
| 3   | a     | 258 | LEU  |
| 3   | a     | 259 | ILE  |
| 3   | a     | 271 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | a     | 275 | LEU  |
| 3   | a     | 288 | LEU  |
| 3   | a     | 290 | ILE  |
| 3   | a     | 297 | LEU  |
| 3   | a     | 300 | PHE  |
| 3   | a     | 301 | ASN  |
| 3   | a     | 302 | PHE  |
| 3   | a     | 316 | THR  |
| 3   | a     | 317 | TRP  |
| 3   | a     | 323 | ARG  |
| 4   | b     | 62  | VAL  |
| 4   | b     | 63  | LEU  |
| 4   | b     | 80  | ILE  |
| 4   | b     | 84  | THR  |
| 4   | b     | 87  | ASP  |
| 4   | b     | 116 | VAL  |
| 4   | b     | 128 | THR  |
| 4   | b     | 137 | LYS  |
| 4   | b     | 178 | VAL  |
| 4   | b     | 198 | VAL  |
| 4   | b     | 201 | HIS  |
| 4   | b     | 225 | LEU  |
| 4   | b     | 229 | LEU  |
| 4   | b     | 240 | SER  |
| 4   | b     | 245 | VAL  |
| 4   | b     | 284 | ILE  |
| 4   | b     | 288 | VAL  |
| 4   | b     | 315 | ILE  |
| 4   | b     | 321 | LYS  |
| 4   | b     | 357 | ARG  |
| 4   | b     | 362 | PHE  |
| 4   | b     | 385 | ARG  |
| 4   | b     | 387 | GLU  |
| 4   | b     | 388 | SER  |
| 4   | b     | 389 | LYS  |
| 4   | b     | 392 | PHE  |
| 4   | b     | 399 | VAL  |
| 4   | b     | 416 | THR  |
| 4   | b     | 436 | THR  |
| 4   | b     | 437 | LEU  |
| 4   | b     | 439 | SER  |
| 4   | b     | 440 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | b     | 446 | SER  |
| 4   | b     | 478 | VAL  |
| 4   | b     | 489 | GLU  |
| 5   | d     | 18  | LEU  |
| 5   | d     | 25  | ASP  |
| 5   | d     | 30  | VAL  |
| 5   | d     | 69  | GLU  |
| 5   | d     | 131 | GLU  |
| 5   | d     | 138 | VAL  |
| 5   | d     | 178 | ILE  |
| 5   | d     | 180 | ARG  |
| 5   | d     | 192 | THR  |
| 5   | d     | 193 | LEU  |
| 5   | d     | 194 | ASN  |
| 5   | d     | 205 | LEU  |
| 5   | d     | 209 | LEU  |
| 5   | d     | 238 | THR  |
| 5   | d     | 242 | GLU  |
| 5   | d     | 243 | THR  |
| 5   | d     | 245 | SER  |
| 5   | d     | 259 | ILE  |
| 5   | d     | 262 | SER  |
| 5   | d     | 272 | LEU  |
| 5   | d     | 279 | LEU  |
| 5   | d     | 291 | LEU  |
| 5   | d     | 294 | ARG  |
| 5   | d     | 307 | GLU  |
| 5   | d     | 316 | THR  |
| 5   | d     | 340 | VAL  |
| 5   | d     | 348 | ARG  |
| 6   | e     | 36  | LEU  |
| 6   | e     | 59  | GLU  |
| 6   | e     | 83  | LEU  |
| 7   | f     | 17  | THR  |
| 8   | h     | 20  | LYS  |
| 8   | h     | 21  | VAL  |
| 9   | i     | 4   | LEU  |
| 9   | i     | 9   | TYR  |
| 9   | i     | 20  | VAL  |
| 9   | i     | 23  | PHE  |
| 10  | l     | 7   | ARG  |
| 10  | l     | 13  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | l     | 32  | SER  |
| 11  | m     | 6   | LEU  |
| 11  | m     | 16  | LEU  |
| 13  | x     | 14  | LEU  |
| 13  | x     | 23  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 33  | GLN  |
| 1   | A     | 69  | ASN  |
| 1   | A     | 76  | GLN  |
| 2   | B     | 30  | GLN  |
| 3   | a     | 19  | ASN  |
| 3   | a     | 118 | HIS  |
| 3   | a     | 165 | GLN  |
| 3   | a     | 187 | GLN  |
| 3   | a     | 190 | HIS  |
| 3   | a     | 272 | HIS  |
| 3   | a     | 296 | ASN  |
| 3   | a     | 301 | ASN  |
| 3   | a     | 322 | ASN  |
| 3   | a     | 332 | HIS  |
| 4   | b     | 58  | GLN  |
| 4   | b     | 179 | GLN  |
| 4   | b     | 223 | GLN  |
| 4   | b     | 289 | GLN  |
| 4   | b     | 331 | ASN  |
| 4   | b     | 338 | GLN  |
| 4   | b     | 395 | GLN  |
| 4   | b     | 455 | HIS  |
| 4   | b     | 490 | GLN  |
| 5   | d     | 98  | GLN  |
| 5   | d     | 129 | GLN  |
| 5   | d     | 164 | GLN  |
| 5   | d     | 194 | ASN  |
| 5   | d     | 236 | ASN  |
| 5   | d     | 250 | ASN  |
| 5   | d     | 332 | GLN  |
| 10  | l     | 4   | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 50 ligands modelled in this entry, 2 are monoatomic and 2 are unknown - leaving 46 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 |
| 16  | CLA  | b     | 610 | -    | 69,73,73     | 2.16 | 18 (26%) | 83,113,113  | 2.65 | 25 (30%) |
| 24  | PQ9  | d     | 406 | -    | 45,45,45     | 0.75 | 1 (2%)   | 56,57,57    | 1.44 | 10 (17%) |
| 16  | CLA  | a     | 402 | 3    | 69,73,73     | 1.92 | 17 (24%) | 83,113,113  | 2.43 | 28 (33%) |
| 16  | CLA  | b     | 607 | -    | 69,73,73     | 2.32 | 18 (26%) | 83,113,113  | 2.12 | 26 (31%) |
| 22  | LMT  | t     | 101 | -    | 36,36,36     | 0.46 | 0        | 47,47,47    | 1.09 | 4 (8%)   |
| 16  | CLA  | b     | 603 | -    | 69,73,73     | 2.08 | 19 (27%) | 83,113,113  | 2.70 | 29 (34%) |
| 16  | CLA  | b     | 612 | 4    | 69,73,73     | 2.22 | 18 (26%) | 83,113,113  | 2.58 | 27 (32%) |
| 18  | BCR  | b     | 617 | -    | 41,41,41     | 0.76 | 0        | 56,56,56    | 1.70 | 16 (28%) |
| 27  | HEM  | e     | 101 | -    | 50,50,50     | 1.56 | 8 (16%)  | 66,82,82    | 1.72 | 13 (19%) |
| 17  | PHO  | a     | 404 | -    | 58,69,69     | 2.00 | 10 (17%) | 56,99,99    | 2.03 | 12 (21%) |
| 15  | SQD  | a     | 401 | -    | 25,26,54     | 1.70 | 4 (16%)  | 34,37,65    | 5.07 | 11 (32%) |
| 20  | MGE  | b     | 620 | -    | 48,48,48     | 0.96 | 2 (4%)   | 56,56,56    | 1.37 | 5 (8%)   |
| 18  | BCR  | a     | 407 | -    | 41,41,41     | 0.72 | 0        | 56,56,56    | 2.37 | 20 (35%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 16  | CLA  | b     | 611 | -    | 69,73,73     | 2.06 | 16 (23%) | 83,113,113  | 2.37 | 30 (36%) |
| 18  | BCR  | h     | 101 | -    | 41,41,41     | 0.81 | 0        | 56,56,56    | 2.03 | 16 (28%) |
| 22  | LMT  | d     | 402 | -    | 36,36,36     | 0.41 | 0        | 47,47,47    | 0.87 | 1 (2%)   |
| 20  | MGE  | a     | 409 | -    | 48,48,48     | 0.98 | 2 (4%)   | 56,56,56    | 1.05 | 4 (7%)   |
| 20  | MGE  | b     | 622 | -    | 48,48,48     | 0.96 | 2 (4%)   | 56,56,56    | 1.38 | 8 (14%)  |
| 16  | CLA  | d     | 405 | -    | 54,58,73     | 2.15 | 16 (29%) | 65,95,113   | 4.50 | 32 (49%) |
| 16  | CLA  | b     | 614 | -    | 56,60,73     | 2.10 | 16 (28%) | 67,97,113   | 3.24 | 38 (56%) |
| 16  | CLA  | d     | 404 | -    | 65,69,73     | 1.95 | 12 (18%) | 78,108,113  | 4.10 | 36 (46%) |
| 16  | CLA  | b     | 609 | -    | 69,73,73     | 2.39 | 22 (31%) | 83,113,113  | 2.09 | 23 (27%) |
| 17  | PHO  | a     | 405 | 3    | 58,69,69     | 1.96 | 9 (15%)  | 56,99,99    | 2.07 | 16 (28%) |
| 20  | MGE  | d     | 410 | 5    | 48,48,48     | 0.98 | 3 (6%)   | 56,56,56    | 1.56 | 11 (19%) |
| 20  | MGE  | m     | 101 | -    | 48,48,48     | 1.01 | 3 (6%)   | 56,56,56    | 1.10 | 3 (5%)   |
| 16  | CLA  | b     | 604 | -    | 69,73,73     | 2.13 | 20 (28%) | 83,113,113  | 2.58 | 28 (33%) |
| 15  | SQD  | l     | 101 | -    | 46,47,54     | 1.31 | 4 (8%)   | 55,58,65    | 3.92 | 10 (18%) |
| 20  | MGE  | d     | 408 | -    | 47,47,48     | 0.96 | 2 (4%)   | 55,55,56    | 1.20 | 6 (10%)  |
| 18  | BCR  | b     | 619 | -    | 41,41,41     | 0.73 | 0        | 56,56,56    | 1.99 | 16 (28%) |
| 26  | DGD  | d     | 412 | -    | 55,55,67     | 0.93 | 2 (3%)   | 69,69,81    | 1.18 | 4 (5%)   |
| 16  | CLA  | b     | 615 | 4    | 69,73,73     | 2.06 | 18 (26%) | 83,113,113  | 2.57 | 30 (36%) |
| 18  | BCR  | d     | 407 | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 1.60 | 12 (21%) |
| 16  | CLA  | a     | 406 | -    | 54,58,73     | 2.23 | 15 (27%) | 65,95,113   | 4.73 | 35 (53%) |
| 16  | CLA  | b     | 602 | -    | 69,73,73     | 2.14 | 17 (24%) | 83,113,113  | 2.33 | 29 (34%) |
| 16  | CLA  | b     | 605 | -    | 69,73,73     | 1.99 | 18 (26%) | 83,113,113  | 2.61 | 29 (34%) |
| 16  | CLA  | d     | 401 | -    | 69,73,73     | 2.00 | 21 (30%) | 83,113,113  | 2.37 | 26 (31%) |
| 16  | CLA  | b     | 608 | -    | 69,73,73     | 2.12 | 18 (26%) | 83,113,113  | 2.21 | 24 (28%) |
| 16  | CLA  | a     | 403 | -    | 54,58,73     | 2.10 | 11 (20%) | 65,95,113   | 4.74 | 35 (53%) |
| 16  | CLA  | b     | 616 | 4    | 50,54,73     | 2.54 | 19 (38%) | 60,90,113   | 2.88 | 26 (43%) |
| 18  | BCR  | b     | 618 | -    | 41,41,41     | 0.68 | 0        | 56,56,56    | 1.87 | 16 (28%) |
| 16  | CLA  | b     | 606 | -    | 69,73,73     | 2.32 | 20 (28%) | 83,113,113  | 2.56 | 28 (33%) |
| 25  | HTG  | d     | 411 | -    | 16,16,19     | 1.18 | 2 (12%)  | 20,21,24    | 1.68 | 1 (5%)   |
| 22  | LMT  | b     | 623 | -    | 36,36,36     | 0.44 | 0        | 47,47,47    | 0.84 | 1 (2%)   |
| 20  | MGE  | d     | 409 | -    | 41,41,48     | 1.06 | 2 (4%)   | 49,49,56    | 1.46 | 9 (18%)  |
| 16  | CLA  | b     | 613 | 4    | 58,62,73     | 2.12 | 18 (31%) | 69,99,113   | 2.60 | 24 (34%) |
| 16  | CLA  | b     | 601 | -    | 45,49,73     | 2.43 | 17 (37%) | 54,84,113   | 4.99 | 29 (53%) |

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   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 16  | CLA  | b     | 610 | -    | -         | 4/39/115/115  | -       |
| 24  | PQ9  | d     | 406 | -    | -         | 8/41/61/61    | 0/1/1/1 |
| 16  | CLA  | a     | 402 | 3    | -         | 5/39/115/115  | -       |
| 16  | CLA  | b     | 607 | -    | -         | 2/39/115/115  | -       |
| 22  | LMT  | t     | 101 | -    | -         | 7/21/61/61    | 0/2/2/2 |
| 16  | CLA  | b     | 603 | -    | -         | 4/39/115/115  | -       |
| 16  | CLA  | b     | 612 | 4    | -         | 7/39/115/115  | -       |
| 18  | BCR  | b     | 617 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 27  | HEM  | e     | 101 | -    | -         | 6/14/54/54    | -       |
| 17  | PHO  | a     | 404 | -    | -         | 13/37/103/103 | 0/5/6/6 |
| 15  | SQD  | a     | 401 | -    | -         | 4/19/39/69    | 0/1/1/1 |
| 20  | MGE  | b     | 620 | -    | -         | 13/43/63/63   | 0/1/1/1 |
| 18  | BCR  | a     | 407 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 16  | CLA  | b     | 611 | -    | -         | 6/39/115/115  | -       |
| 18  | BCR  | h     | 101 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 22  | LMT  | d     | 402 | -    | -         | 4/21/61/61    | 0/2/2/2 |
| 20  | MGE  | a     | 409 | -    | -         | 13/43/63/63   | 0/1/1/1 |
| 20  | MGE  | b     | 622 | -    | -         | 15/43/63/63   | 0/1/1/1 |
| 16  | CLA  | d     | 405 | -    | -         | 6/21/97/115   | -       |
| 16  | CLA  | d     | 404 | -    | 1/1/14/20 | 9/35/111/115  | -       |
| 16  | CLA  | b     | 614 | -    | -         | 9/24/100/115  | -       |
| 16  | CLA  | b     | 609 | -    | -         | 2/39/115/115  | -       |
| 17  | PHO  | a     | 405 | 3    | -         | 10/37/103/103 | 0/5/6/6 |
| 20  | MGE  | d     | 410 | 5    | -         | 13/43/63/63   | 0/1/1/1 |
| 20  | MGE  | m     | 101 | -    | -         | 8/43/63/63    | 0/1/1/1 |
| 16  | CLA  | b     | 604 | -    | -         | 7/39/115/115  | -       |
| 15  | SQD  | l     | 101 | -    | -         | 14/42/62/69   | 0/1/1/1 |
| 20  | MGE  | d     | 408 | -    | -         | 7/42/62/63    | 0/1/1/1 |
| 18  | BCR  | b     | 619 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 26  | DGD  | d     | 412 | -    | -         | 9/43/83/95    | 0/2/2/2 |
| 16  | CLA  | b     | 615 | 4    | -         | 9/39/115/115  | -       |
| 18  | BCR  | d     | 407 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 16  | CLA  | a     | 406 | -    | -         | 6/21/97/115   | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 16  | CLA  | b     | 602 | -    | -       | 4/39/115/115  | -       |
| 16  | CLA  | b     | 605 | -    | -       | 4/39/115/115  | -       |
| 16  | CLA  | d     | 401 | -    | -       | 5/39/115/115  | -       |
| 16  | CLA  | b     | 608 | -    | -       | 1/39/115/115  | -       |
| 16  | CLA  | a     | 403 | -    | -       | 5/21/97/115   | -       |
| 16  | CLA  | b     | 616 | 4    | -       | 2/17/93/115   | -       |
| 18  | BCR  | b     | 618 | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 16  | CLA  | b     | 606 | -    | -       | 12/39/115/115 | -       |
| 25  | HTG  | d     | 411 | -    | -       | 0/7/27/30     | 0/1/1/1 |
| 22  | LMT  | b     | 623 | -    | -       | 1/21/61/61    | 0/2/2/2 |
| 20  | MGE  | d     | 409 | -    | -       | 6/36/56/63    | 0/1/1/1 |
| 16  | CLA  | b     | 613 | 4    | -       | 0/26/102/115  | -       |
| 16  | CLA  | b     | 601 | -    | -       | 4/10/86/115   | -       |

All (440) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | b     | 612 | CLA  | MG-NA   | 10.40 | 2.31        | 2.06     |
| 16  | b     | 606 | CLA  | MG-NA   | 10.30 | 2.30        | 2.06     |
| 17  | a     | 405 | PHO  | C1B-C2B | 9.35  | 1.49        | 1.39     |
| 16  | a     | 406 | CLA  | C1D-ND  | 8.86  | 1.48        | 1.37     |
| 17  | a     | 404 | PHO  | C1B-C2B | 8.78  | 1.49        | 1.39     |
| 16  | a     | 403 | CLA  | C1D-ND  | 8.66  | 1.48        | 1.37     |
| 16  | b     | 615 | CLA  | MG-NA   | 8.37  | 2.26        | 2.06     |
| 16  | b     | 611 | CLA  | MG-NA   | 8.35  | 2.26        | 2.06     |
| 16  | d     | 404 | CLA  | C1D-ND  | 8.29  | 1.48        | 1.37     |
| 16  | b     | 604 | CLA  | MG-NA   | 8.23  | 2.25        | 2.06     |
| 16  | b     | 601 | CLA  | C1D-ND  | 7.72  | 1.47        | 1.37     |
| 16  | b     | 608 | CLA  | MG-NA   | 7.71  | 2.24        | 2.06     |
| 16  | d     | 405 | CLA  | C1D-ND  | 7.70  | 1.47        | 1.37     |
| 16  | b     | 607 | CLA  | MG-NA   | 7.14  | 2.23        | 2.06     |
| 16  | b     | 609 | CLA  | MG-NC   | 6.76  | 2.22        | 2.06     |
| 17  | a     | 404 | PHO  | C3B-C4B | 6.71  | 1.49        | 1.41     |
| 17  | a     | 405 | PHO  | C3B-C4B | 6.36  | 1.48        | 1.41     |
| 16  | a     | 402 | CLA  | MG-NA   | 6.34  | 2.21        | 2.06     |
| 16  | b     | 609 | CLA  | CHC-C1C | 6.31  | 1.51        | 1.38     |
| 16  | d     | 401 | CLA  | MG-NA   | 6.28  | 2.21        | 2.06     |
| 16  | b     | 602 | CLA  | MG-NC   | 6.17  | 2.20        | 2.06     |
| 16  | b     | 610 | CLA  | MG-NA   | 6.11  | 2.20        | 2.06     |
| 16  | b     | 607 | CLA  | C3C-C2C | 6.07  | 1.49        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | b     | 602 | CLA  | C3C-C2C | 5.98  | 1.49        | 1.36     |
| 16  | b     | 613 | CLA  | MG-NA   | 5.96  | 2.20        | 2.06     |
| 16  | b     | 616 | CLA  | MG-NA   | 5.86  | 2.20        | 2.06     |
| 16  | b     | 605 | CLA  | C1D-ND  | -5.86 | 1.30        | 1.37     |
| 16  | b     | 616 | CLA  | CHC-C1C | 5.85  | 1.50        | 1.38     |
| 16  | b     | 607 | CLA  | CHC-C1C | 5.80  | 1.50        | 1.38     |
| 16  | b     | 603 | CLA  | MG-NA   | 5.70  | 2.19        | 2.06     |
| 16  | b     | 609 | CLA  | O2D-CGD | 5.64  | 1.47        | 1.33     |
| 16  | b     | 607 | CLA  | MG-NC   | 5.62  | 2.19        | 2.06     |
| 16  | b     | 610 | CLA  | C3C-C2C | 5.59  | 1.48        | 1.36     |
| 16  | b     | 612 | CLA  | C3C-C2C | 5.57  | 1.48        | 1.36     |
| 16  | b     | 614 | CLA  | MG-NA   | 5.44  | 2.19        | 2.06     |
| 16  | b     | 609 | CLA  | C3C-C2C | 5.44  | 1.48        | 1.36     |
| 27  | e     | 101 | HEM  | FE-NB   | 5.36  | 2.11        | 1.94     |
| 16  | b     | 601 | CLA  | O2D-CGD | 5.34  | 1.46        | 1.33     |
| 16  | b     | 606 | CLA  | MG-NC   | 5.34  | 2.19        | 2.06     |
| 16  | b     | 603 | CLA  | C3C-C2C | 5.31  | 1.48        | 1.36     |
| 16  | b     | 603 | CLA  | C1D-ND  | -5.26 | 1.31        | 1.37     |
| 16  | d     | 401 | CLA  | CHC-C1C | 5.25  | 1.49        | 1.38     |
| 16  | b     | 603 | CLA  | CHC-C1C | 5.15  | 1.49        | 1.38     |
| 16  | b     | 604 | CLA  | CHC-C1C | 5.14  | 1.49        | 1.38     |
| 16  | b     | 604 | CLA  | C3C-C2C | 5.11  | 1.47        | 1.36     |
| 16  | b     | 609 | CLA  | CHD-C1D | 5.11  | 1.48        | 1.38     |
| 16  | b     | 611 | CLA  | CHD-C1D | 5.10  | 1.48        | 1.38     |
| 16  | b     | 610 | CLA  | O2D-CGD | 5.09  | 1.45        | 1.33     |
| 16  | b     | 602 | CLA  | OBD-CAD | 5.08  | 1.31        | 1.22     |
| 16  | b     | 602 | CLA  | C1D-ND  | -5.05 | 1.31        | 1.37     |
| 16  | b     | 613 | CLA  | O2D-CGD | 5.05  | 1.45        | 1.33     |
| 15  | a     | 401 | SQD  | O8-S    | 5.04  | 1.65        | 1.47     |
| 16  | b     | 605 | CLA  | MG-NA   | 5.02  | 2.18        | 2.06     |
| 15  | l     | 101 | SQD  | O8-S    | 5.02  | 1.65        | 1.47     |
| 16  | b     | 605 | CLA  | O2D-CGD | 5.01  | 1.45        | 1.33     |
| 16  | b     | 615 | CLA  | C3C-C2C | 5.00  | 1.47        | 1.36     |
| 16  | b     | 616 | CLA  | C1D-ND  | -4.97 | 1.31        | 1.37     |
| 16  | b     | 601 | CLA  | C3D-C4D | -4.95 | 1.33        | 1.44     |
| 16  | b     | 602 | CLA  | CHC-C1C | 4.94  | 1.48        | 1.38     |
| 16  | a     | 402 | CLA  | OBD-CAD | 4.92  | 1.31        | 1.22     |
| 15  | a     | 401 | SQD  | O47-C7  | 4.89  | 1.46        | 1.35     |
| 16  | d     | 404 | CLA  | O2D-CGD | 4.88  | 1.45        | 1.33     |
| 16  | b     | 605 | CLA  | CHC-C1C | 4.87  | 1.48        | 1.38     |
| 16  | b     | 616 | CLA  | C3C-C2C | 4.85  | 1.47        | 1.36     |
| 16  | b     | 605 | CLA  | C3C-C2C | 4.83  | 1.47        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | b     | 611 | CLA  | CHB-C1B | 4.82  | 1.50        | 1.39     |
| 16  | d     | 404 | CLA  | C3D-C4D | -4.80 | 1.33        | 1.44     |
| 16  | b     | 610 | CLA  | CHD-C1D | 4.80  | 1.47        | 1.38     |
| 16  | d     | 401 | CLA  | C3C-C2C | 4.78  | 1.46        | 1.36     |
| 16  | b     | 614 | CLA  | CHD-C1D | 4.77  | 1.47        | 1.38     |
| 16  | a     | 402 | CLA  | C3C-C2C | 4.77  | 1.46        | 1.36     |
| 16  | b     | 616 | CLA  | O2D-CGD | 4.75  | 1.44        | 1.33     |
| 16  | b     | 613 | CLA  | CHC-C1C | 4.75  | 1.48        | 1.38     |
| 16  | d     | 405 | CLA  | C3D-C4D | -4.74 | 1.33        | 1.44     |
| 16  | b     | 606 | CLA  | C3C-C2C | 4.74  | 1.46        | 1.36     |
| 16  | b     | 601 | CLA  | C3C-C2C | 4.72  | 1.46        | 1.36     |
| 16  | a     | 406 | CLA  | O2D-CGD | 4.71  | 1.44        | 1.33     |
| 16  | d     | 405 | CLA  | O2D-CGD | 4.71  | 1.44        | 1.33     |
| 16  | b     | 608 | CLA  | C4B-NB  | -4.70 | 1.32        | 1.37     |
| 16  | b     | 602 | CLA  | CHD-C4C | 4.67  | 1.49        | 1.39     |
| 16  | a     | 403 | CLA  | C3D-C4D | -4.67 | 1.33        | 1.44     |
| 16  | b     | 615 | CLA  | O2D-CGD | 4.61  | 1.44        | 1.33     |
| 16  | b     | 603 | CLA  | O2D-CGD | 4.58  | 1.44        | 1.33     |
| 16  | b     | 610 | CLA  | MG-ND   | -4.57 | 1.96        | 2.05     |
| 16  | b     | 607 | CLA  | CHD-C1D | 4.57  | 1.47        | 1.38     |
| 16  | a     | 406 | CLA  | C3D-C4D | -4.56 | 1.33        | 1.44     |
| 16  | a     | 403 | CLA  | O2D-CGD | 4.55  | 1.44        | 1.33     |
| 16  | b     | 615 | CLA  | OBD-CAD | 4.52  | 1.30        | 1.22     |
| 16  | b     | 606 | CLA  | CHD-C1D | 4.50  | 1.47        | 1.38     |
| 16  | b     | 615 | CLA  | CHD-C4C | 4.49  | 1.49        | 1.39     |
| 16  | b     | 611 | CLA  | O2D-CGD | 4.48  | 1.44        | 1.33     |
| 16  | a     | 402 | CLA  | C4B-NB  | -4.44 | 1.32        | 1.37     |
| 16  | b     | 606 | CLA  | O2D-CGD | 4.44  | 1.44        | 1.33     |
| 16  | b     | 614 | CLA  | O2A-CGA | 4.40  | 1.46        | 1.33     |
| 16  | d     | 405 | CLA  | O2A-CGA | 4.39  | 1.46        | 1.33     |
| 16  | b     | 609 | CLA  | MG-NB   | 4.39  | 2.14        | 2.05     |
| 16  | b     | 613 | CLA  | C3C-C2C | 4.38  | 1.46        | 1.36     |
| 20  | d     | 409 | MGE  | O2G-C1B | 4.36  | 1.46        | 1.34     |
| 16  | b     | 616 | CLA  | CHD-C1D | 4.36  | 1.46        | 1.38     |
| 16  | a     | 406 | CLA  | O2A-CGA | 4.35  | 1.46        | 1.33     |
| 16  | b     | 604 | CLA  | MG-ND   | -4.33 | 1.97        | 2.05     |
| 20  | m     | 101 | MGE  | O1G-C1A | 4.32  | 1.46        | 1.33     |
| 16  | b     | 608 | CLA  | C3C-C2C | 4.31  | 1.45        | 1.36     |
| 20  | a     | 409 | MGE  | O2G-C1B | 4.31  | 1.46        | 1.34     |
| 16  | b     | 611 | CLA  | CHC-C1C | 4.30  | 1.47        | 1.38     |
| 16  | b     | 602 | CLA  | CHD-C1D | 4.30  | 1.46        | 1.38     |
| 16  | b     | 609 | CLA  | C3B-C4B | 4.30  | 1.52        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 16  | d     | 401 | CLA  | CHD-C1D | 4.28 | 1.46        | 1.38     |
| 15  | l     | 101 | SQD  | O47-C7  | 4.24 | 1.46        | 1.34     |
| 16  | b     | 613 | CLA  | O2A-CGA | 4.23 | 1.45        | 1.33     |
| 16  | b     | 608 | CLA  | CHC-C1C | 4.23 | 1.47        | 1.38     |
| 16  | b     | 614 | CLA  | CHB-C1B | 4.22 | 1.48        | 1.39     |
| 20  | m     | 101 | MGE  | O2G-C1B | 4.22 | 1.46        | 1.34     |
| 20  | b     | 620 | MGE  | O2G-C1B | 4.22 | 1.46        | 1.34     |
| 20  | a     | 409 | MGE  | O1G-C1A | 4.21 | 1.45        | 1.33     |
| 26  | d     | 412 | DGD  | O1G-C1A | 4.20 | 1.45        | 1.33     |
| 20  | b     | 620 | MGE  | O1G-C1A | 4.18 | 1.45        | 1.33     |
| 20  | d     | 408 | MGE  | O2G-C1B | 4.16 | 1.46        | 1.34     |
| 16  | b     | 612 | CLA  | CHC-C1C | 4.16 | 1.47        | 1.38     |
| 20  | d     | 409 | MGE  | O1G-C1A | 4.15 | 1.45        | 1.33     |
| 16  | b     | 608 | CLA  | OBD-CAD | 4.14 | 1.29        | 1.22     |
| 16  | d     | 405 | CLA  | C3C-C2C | 4.14 | 1.45        | 1.36     |
| 26  | d     | 412 | DGD  | O2G-C1B | 4.13 | 1.45        | 1.34     |
| 20  | d     | 410 | MGE  | O1G-C1A | 4.13 | 1.45        | 1.33     |
| 16  | b     | 607 | CLA  | O2D-CGD | 4.11 | 1.43        | 1.33     |
| 27  | e     | 101 | HEM  | FE-NC   | 4.10 | 2.09        | 1.95     |
| 16  | a     | 406 | CLA  | C3C-C2C | 4.09 | 1.45        | 1.36     |
| 15  | l     | 101 | SQD  | O48-C23 | 4.08 | 1.45        | 1.33     |
| 16  | b     | 604 | CLA  | CHD-C1D | 4.07 | 1.46        | 1.38     |
| 20  | b     | 622 | MGE  | O2G-C1B | 4.07 | 1.45        | 1.34     |
| 16  | b     | 611 | CLA  | C3C-C2C | 4.06 | 1.45        | 1.36     |
| 16  | a     | 403 | CLA  | O2A-CGA | 4.05 | 1.45        | 1.33     |
| 16  | b     | 612 | CLA  | C1B-C2B | 4.05 | 1.52        | 1.43     |
| 16  | b     | 604 | CLA  | O2D-CGD | 4.04 | 1.43        | 1.33     |
| 16  | d     | 404 | CLA  | C3C-C2C | 4.03 | 1.45        | 1.36     |
| 16  | b     | 610 | CLA  | OBD-CAD | 4.03 | 1.29        | 1.22     |
| 16  | b     | 616 | CLA  | MG-ND   | 4.02 | 2.13        | 2.05     |
| 16  | b     | 616 | CLA  | O2A-CGA | 4.01 | 1.45        | 1.33     |
| 16  | b     | 606 | CLA  | CHB-C1B | 4.01 | 1.48        | 1.39     |
| 20  | d     | 408 | MGE  | O1G-C1A | 4.00 | 1.45        | 1.33     |
| 16  | b     | 602 | CLA  | CHB-C1B | 3.99 | 1.48        | 1.39     |
| 16  | b     | 609 | CLA  | MG-NA   | 3.99 | 2.15        | 2.06     |
| 16  | b     | 606 | CLA  | CHC-C1C | 3.97 | 1.46        | 1.38     |
| 20  | b     | 622 | MGE  | O1G-C1A | 3.97 | 1.44        | 1.33     |
| 16  | b     | 616 | CLA  | CHB-C1B | 3.97 | 1.48        | 1.39     |
| 16  | d     | 404 | CLA  | O2A-CGA | 3.96 | 1.44        | 1.33     |
| 16  | d     | 401 | CLA  | CHD-C4C | 3.96 | 1.48        | 1.39     |
| 16  | b     | 614 | CLA  | O2D-CGD | 3.95 | 1.42        | 1.33     |
| 16  | b     | 612 | CLA  | O2D-CGD | 3.95 | 1.42        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | b     | 610 | CLA  | CHC-C1C | 3.92  | 1.46        | 1.38     |
| 16  | b     | 607 | CLA  | MG-NB   | 3.92  | 2.13        | 2.05     |
| 16  | b     | 614 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 16  | b     | 610 | CLA  | C4C-C3C | 3.92  | 1.51        | 1.45     |
| 16  | b     | 607 | CLA  | C1D-ND  | -3.90 | 1.33        | 1.37     |
| 16  | b     | 616 | CLA  | CHC-C4B | 3.89  | 1.48        | 1.39     |
| 16  | a     | 402 | CLA  | MG-NB   | -3.88 | 1.98        | 2.05     |
| 20  | d     | 410 | MGE  | O2G-C1B | 3.88  | 1.45        | 1.34     |
| 16  | b     | 608 | CLA  | CHB-C1B | 3.87  | 1.48        | 1.39     |
| 16  | a     | 402 | CLA  | O2D-CGD | 3.86  | 1.42        | 1.33     |
| 25  | d     | 411 | HTG  | C1'-S1  | -3.84 | 1.76        | 1.81     |
| 16  | b     | 610 | CLA  | CHD-C4C | 3.83  | 1.48        | 1.39     |
| 16  | b     | 606 | CLA  | CHD-C4C | 3.83  | 1.48        | 1.39     |
| 16  | b     | 614 | CLA  | CHC-C4B | 3.82  | 1.48        | 1.39     |
| 16  | b     | 608 | CLA  | CHD-C1D | 3.81  | 1.45        | 1.38     |
| 16  | b     | 605 | CLA  | C3B-C4B | 3.80  | 1.51        | 1.42     |
| 16  | b     | 608 | CLA  | C3B-C4B | 3.79  | 1.51        | 1.42     |
| 16  | a     | 403 | CLA  | C3C-C2C | 3.77  | 1.44        | 1.36     |
| 16  | b     | 609 | CLA  | CHB-C1B | 3.76  | 1.47        | 1.39     |
| 16  | b     | 615 | CLA  | CHC-C1C | 3.76  | 1.46        | 1.38     |
| 16  | b     | 603 | CLA  | CHD-C1D | 3.75  | 1.45        | 1.38     |
| 16  | b     | 604 | CLA  | CHB-C1B | 3.74  | 1.47        | 1.39     |
| 16  | b     | 605 | CLA  | C1B-NB  | -3.73 | 1.33        | 1.37     |
| 16  | b     | 607 | CLA  | C3D-C2D | 3.73  | 1.49        | 1.39     |
| 16  | b     | 603 | CLA  | C1B-NB  | -3.72 | 1.33        | 1.37     |
| 16  | b     | 610 | CLA  | CHC-C4B | 3.69  | 1.47        | 1.39     |
| 16  | b     | 608 | CLA  | CHD-C4C | 3.69  | 1.47        | 1.39     |
| 16  | b     | 603 | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 16  | b     | 607 | CLA  | MG-ND   | 3.69  | 2.13        | 2.05     |
| 16  | b     | 606 | CLA  | CHC-C4B | 3.66  | 1.47        | 1.39     |
| 16  | b     | 614 | CLA  | CHC-C1C | 3.65  | 1.45        | 1.38     |
| 16  | b     | 613 | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 16  | b     | 615 | CLA  | C3D-C2D | 3.64  | 1.49        | 1.39     |
| 16  | b     | 609 | CLA  | O2A-CGA | 3.63  | 1.43        | 1.33     |
| 27  | e     | 101 | HEM  | C1B-NB  | -3.62 | 1.34        | 1.40     |
| 16  | b     | 604 | CLA  | MG-NC   | 3.62  | 2.14        | 2.06     |
| 16  | b     | 611 | CLA  | CHD-C4C | 3.60  | 1.47        | 1.39     |
| 16  | b     | 607 | CLA  | CHB-C1B | 3.60  | 1.47        | 1.39     |
| 16  | b     | 608 | CLA  | CHC-C4B | 3.60  | 1.47        | 1.39     |
| 16  | b     | 611 | CLA  | O2A-CGA | 3.60  | 1.43        | 1.33     |
| 16  | b     | 607 | CLA  | C3B-C4B | 3.60  | 1.51        | 1.42     |
| 16  | b     | 608 | CLA  | C1B-NB  | -3.57 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | b     | 612 | CLA  | CHD-C1D | 3.57  | 1.45        | 1.38     |
| 16  | b     | 613 | CLA  | C3B-C4B | 3.56  | 1.51        | 1.42     |
| 16  | b     | 614 | CLA  | C3C-C2C | 3.54  | 1.44        | 1.36     |
| 16  | b     | 612 | CLA  | CHB-C1B | 3.53  | 1.47        | 1.39     |
| 16  | b     | 601 | CLA  | CHD-C1D | 3.51  | 1.45        | 1.38     |
| 16  | b     | 603 | CLA  | C4B-NB  | -3.50 | 1.33        | 1.37     |
| 16  | b     | 608 | CLA  | O2D-CGD | 3.49  | 1.41        | 1.33     |
| 16  | b     | 613 | CLA  | CHC-C4B | 3.47  | 1.47        | 1.39     |
| 16  | b     | 601 | CLA  | CHB-C4A | -3.47 | 1.29        | 1.37     |
| 16  | b     | 610 | CLA  | CHB-C1B | 3.46  | 1.47        | 1.39     |
| 16  | b     | 607 | CLA  | C1B-C2B | 3.46  | 1.51        | 1.43     |
| 16  | b     | 602 | CLA  | C3B-C4B | 3.43  | 1.50        | 1.42     |
| 16  | b     | 610 | CLA  | MG-NC   | 3.39  | 2.14        | 2.06     |
| 16  | a     | 406 | CLA  | CHC-C1C | 3.37  | 1.45        | 1.38     |
| 17  | a     | 404 | PHO  | C4D-CHA | 3.37  | 1.45        | 1.39     |
| 16  | b     | 602 | CLA  | O2A-CGA | 3.37  | 1.43        | 1.33     |
| 16  | b     | 601 | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 16  | b     | 610 | CLA  | C1B-NB  | -3.35 | 1.33        | 1.37     |
| 16  | b     | 609 | CLA  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 16  | d     | 401 | CLA  | C1D-ND  | -3.34 | 1.33        | 1.37     |
| 16  | b     | 607 | CLA  | CHC-C4B | 3.33  | 1.46        | 1.39     |
| 16  | a     | 406 | CLA  | OBD-CAD | 3.33  | 1.28        | 1.22     |
| 16  | b     | 601 | CLA  | CHC-C1C | 3.33  | 1.45        | 1.38     |
| 16  | b     | 608 | CLA  | C1D-ND  | -3.32 | 1.33        | 1.37     |
| 16  | b     | 609 | CLA  | C1B-C2B | 3.32  | 1.51        | 1.43     |
| 16  | b     | 601 | CLA  | CHD-C4C | 3.32  | 1.46        | 1.39     |
| 17  | a     | 405 | PHO  | C1D-C2D | 3.31  | 1.43        | 1.39     |
| 16  | b     | 607 | CLA  | C1B-NB  | -3.30 | 1.33        | 1.37     |
| 17  | a     | 404 | PHO  | C1D-C2D | 3.30  | 1.43        | 1.39     |
| 16  | a     | 402 | CLA  | CHD-C4C | 3.29  | 1.46        | 1.39     |
| 16  | b     | 613 | CLA  | CHD-C1D | 3.29  | 1.44        | 1.38     |
| 16  | b     | 616 | CLA  | C4B-NB  | -3.28 | 1.33        | 1.37     |
| 17  | a     | 405 | PHO  | CAC-C3C | -3.28 | 1.45        | 1.51     |
| 16  | b     | 606 | CLA  | C3B-C4B | 3.28  | 1.50        | 1.42     |
| 16  | b     | 603 | CLA  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 16  | b     | 602 | CLA  | C1B-C2B | 3.27  | 1.50        | 1.43     |
| 16  | b     | 609 | CLA  | CHC-C4B | 3.26  | 1.46        | 1.39     |
| 16  | b     | 604 | CLA  | C3B-C4B | 3.26  | 1.50        | 1.42     |
| 17  | a     | 405 | PHO  | C4D-ND  | -3.25 | 1.34        | 1.38     |
| 16  | d     | 404 | CLA  | CHC-C1C | 3.25  | 1.45        | 1.38     |
| 16  | b     | 612 | CLA  | CHC-C4B | 3.23  | 1.46        | 1.39     |
| 16  | b     | 609 | CLA  | C4B-NB  | -3.21 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | d     | 401 | CLA  | CHB-C1B | 3.21  | 1.46        | 1.39     |
| 16  | b     | 603 | CLA  | CHD-C4C | 3.21  | 1.46        | 1.39     |
| 16  | b     | 609 | CLA  | CHD-C4C | 3.21  | 1.46        | 1.39     |
| 16  | b     | 606 | CLA  | C4D-CHA | 3.20  | 1.49        | 1.38     |
| 16  | b     | 612 | CLA  | O2A-CGA | 3.20  | 1.42        | 1.33     |
| 16  | b     | 614 | CLA  | MG-ND   | -3.19 | 1.99        | 2.05     |
| 16  | b     | 604 | CLA  | C4B-NB  | -3.16 | 1.33        | 1.37     |
| 16  | d     | 404 | CLA  | OBD-CAD | 3.16  | 1.27        | 1.22     |
| 17  | a     | 404 | PHO  | CAC-C3C | -3.14 | 1.45        | 1.51     |
| 16  | d     | 405 | CLA  | CHC-C1C | 3.14  | 1.44        | 1.38     |
| 16  | b     | 615 | CLA  | CHB-C1B | 3.13  | 1.46        | 1.39     |
| 16  | b     | 616 | CLA  | C3D-C2D | 3.13  | 1.47        | 1.39     |
| 16  | a     | 406 | CLA  | CHB-C4A | -3.13 | 1.30        | 1.37     |
| 16  | b     | 604 | CLA  | CHD-C4C | 3.12  | 1.46        | 1.39     |
| 16  | a     | 403 | CLA  | OBD-CAD | 3.11  | 1.27        | 1.22     |
| 16  | d     | 401 | CLA  | O2A-CGA | 3.11  | 1.42        | 1.33     |
| 16  | b     | 616 | CLA  | OBD-CAD | 3.11  | 1.27        | 1.22     |
| 16  | b     | 612 | CLA  | C4B-NB  | -3.08 | 1.34        | 1.37     |
| 16  | b     | 611 | CLA  | C3B-C4B | 3.07  | 1.49        | 1.42     |
| 16  | b     | 611 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 17  | a     | 404 | PHO  | CMB-C2B | -3.06 | 1.45        | 1.51     |
| 16  | b     | 609 | CLA  | C3D-C2D | 3.05  | 1.47        | 1.39     |
| 27  | e     | 101 | HEM  | C4D-ND  | -3.05 | 1.35        | 1.40     |
| 16  | b     | 612 | CLA  | C1B-NB  | -3.05 | 1.34        | 1.37     |
| 16  | b     | 615 | CLA  | CHD-C1D | 3.04  | 1.44        | 1.38     |
| 16  | b     | 609 | CLA  | C1D-ND  | -3.04 | 1.34        | 1.37     |
| 16  | b     | 612 | CLA  | C3B-C4B | 3.04  | 1.49        | 1.42     |
| 16  | d     | 405 | CLA  | CHB-C4A | -3.03 | 1.30        | 1.37     |
| 16  | b     | 603 | CLA  | C3B-C4B | 3.02  | 1.49        | 1.42     |
| 16  | d     | 405 | CLA  | OBD-CAD | 3.02  | 1.27        | 1.22     |
| 16  | b     | 602 | CLA  | C1B-NB  | -3.00 | 1.34        | 1.37     |
| 16  | d     | 401 | CLA  | OBD-CAD | 2.99  | 1.27        | 1.22     |
| 16  | b     | 607 | CLA  | CHD-C4C | 2.98  | 1.46        | 1.39     |
| 16  | a     | 403 | CLA  | CHB-C4A | -2.98 | 1.30        | 1.37     |
| 16  | b     | 616 | CLA  | C1C-C2C | 2.97  | 1.50        | 1.44     |
| 16  | b     | 612 | CLA  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 16  | b     | 611 | CLA  | C4D-CHA | 2.96  | 1.48        | 1.38     |
| 16  | b     | 616 | CLA  | CHD-C4C | 2.95  | 1.46        | 1.39     |
| 16  | a     | 402 | CLA  | CHB-C1B | 2.93  | 1.46        | 1.39     |
| 16  | b     | 606 | CLA  | C3D-C2D | 2.93  | 1.47        | 1.39     |
| 17  | a     | 404 | PHO  | CMD-C2D | -2.93 | 1.45        | 1.51     |
| 16  | b     | 603 | CLA  | C3D-C2D | 2.92  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | b     | 613 | CLA  | C1D-ND  | -2.92 | 1.34        | 1.37     |
| 16  | b     | 612 | CLA  | MG-NC   | -2.92 | 1.99        | 2.06     |
| 17  | a     | 404 | PHO  | C4D-ND  | -2.90 | 1.34        | 1.38     |
| 16  | b     | 602 | CLA  | CHC-C4B | 2.89  | 1.45        | 1.39     |
| 16  | b     | 603 | CLA  | C4D-CHA | 2.89  | 1.48        | 1.38     |
| 16  | b     | 605 | CLA  | O2A-CGA | 2.89  | 1.41        | 1.33     |
| 16  | d     | 401 | CLA  | MG-ND   | -2.88 | 2.00        | 2.05     |
| 16  | b     | 601 | CLA  | C1D-C2D | 2.88  | 1.51        | 1.45     |
| 16  | d     | 401 | CLA  | CHC-C4B | 2.88  | 1.45        | 1.39     |
| 16  | b     | 615 | CLA  | C3B-C4B | 2.86  | 1.49        | 1.42     |
| 16  | b     | 605 | CLA  | CHB-C1B | 2.86  | 1.45        | 1.39     |
| 16  | b     | 615 | CLA  | C1B-C2B | 2.86  | 1.50        | 1.43     |
| 16  | b     | 608 | CLA  | C4D-CHA | 2.86  | 1.48        | 1.38     |
| 16  | a     | 406 | CLA  | CHC-C4B | 2.86  | 1.45        | 1.39     |
| 16  | a     | 402 | CLA  | O2A-CGA | 2.86  | 1.41        | 1.33     |
| 16  | d     | 404 | CLA  | C3B-C4B | 2.85  | 1.49        | 1.42     |
| 16  | b     | 607 | CLA  | C4D-CHA | 2.85  | 1.48        | 1.38     |
| 16  | b     | 616 | CLA  | C3B-C4B | 2.85  | 1.49        | 1.42     |
| 17  | a     | 404 | PHO  | CMC-C2C | -2.85 | 1.46        | 1.50     |
| 16  | b     | 613 | CLA  | CHD-C4C | 2.84  | 1.45        | 1.39     |
| 16  | a     | 402 | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 17  | a     | 405 | PHO  | CMD-C2D | -2.83 | 1.45        | 1.51     |
| 16  | b     | 615 | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 16  | b     | 616 | CLA  | C1C-NC  | -2.82 | 1.33        | 1.37     |
| 16  | b     | 605 | CLA  | CHD-C1D | 2.82  | 1.43        | 1.38     |
| 16  | b     | 602 | CLA  | MG-NB   | 2.81  | 2.11        | 2.05     |
| 16  | b     | 613 | CLA  | C3D-C2D | 2.80  | 1.46        | 1.39     |
| 16  | b     | 609 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 16  | a     | 402 | CLA  | CHC-C1C | 2.79  | 1.44        | 1.38     |
| 16  | a     | 406 | CLA  | C3B-C4B | 2.78  | 1.49        | 1.42     |
| 16  | b     | 601 | CLA  | C4B-NB  | -2.77 | 1.34        | 1.37     |
| 16  | a     | 403 | CLA  | CHC-C1C | 2.77  | 1.44        | 1.38     |
| 16  | b     | 604 | CLA  | C3D-C2D | 2.74  | 1.46        | 1.39     |
| 16  | a     | 402 | CLA  | CHD-C1D | 2.74  | 1.43        | 1.38     |
| 16  | b     | 609 | CLA  | C4C-C3C | 2.74  | 1.49        | 1.45     |
| 16  | b     | 606 | CLA  | O2A-CGA | 2.74  | 1.41        | 1.33     |
| 16  | b     | 605 | CLA  | OBD-CAD | 2.74  | 1.27        | 1.22     |
| 16  | b     | 616 | CLA  | C4D-CHA | 2.73  | 1.48        | 1.38     |
| 16  | d     | 405 | CLA  | CHD-C1D | 2.72  | 1.43        | 1.38     |
| 16  | d     | 405 | CLA  | CHD-C4C | 2.71  | 1.45        | 1.39     |
| 16  | b     | 615 | CLA  | MG-NC   | 2.71  | 2.12        | 2.06     |
| 16  | b     | 603 | CLA  | O2A-CGA | 2.70  | 1.41        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | d     | 404 | CLA  | CHB-C4A | -2.70 | 1.31        | 1.37     |
| 16  | b     | 605 | CLA  | CHD-C4C | 2.70  | 1.45        | 1.39     |
| 16  | b     | 602 | CLA  | C4C-C3C | 2.69  | 1.49        | 1.45     |
| 16  | b     | 613 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 16  | b     | 606 | CLA  | OBD-CAD | 2.66  | 1.27        | 1.22     |
| 17  | a     | 405 | PHO  | CMC-C2C | -2.65 | 1.46        | 1.50     |
| 16  | b     | 615 | CLA  | C1D-ND  | -2.65 | 1.34        | 1.37     |
| 16  | b     | 607 | CLA  | O2A-CGA | 2.65  | 1.41        | 1.33     |
| 16  | b     | 609 | CLA  | C1B-NB  | -2.65 | 1.34        | 1.37     |
| 17  | a     | 405 | PHO  | C4D-CHA | 2.64  | 1.43        | 1.39     |
| 16  | d     | 401 | CLA  | C1B-NB  | -2.64 | 1.34        | 1.37     |
| 16  | b     | 615 | CLA  | CHC-C4B | 2.64  | 1.45        | 1.39     |
| 16  | d     | 404 | CLA  | CHC-C4B | 2.63  | 1.45        | 1.39     |
| 15  | a     | 401 | SQD  | O48-C23 | 2.63  | 1.46        | 1.33     |
| 16  | b     | 608 | CLA  | O2A-CGA | 2.63  | 1.41        | 1.33     |
| 16  | b     | 606 | CLA  | C1C-NC  | -2.62 | 1.33        | 1.37     |
| 16  | d     | 404 | CLA  | CHB-C1B | 2.62  | 1.45        | 1.39     |
| 16  | b     | 610 | CLA  | C4D-CHA | 2.61  | 1.47        | 1.38     |
| 16  | b     | 615 | CLA  | O2A-CGA | 2.61  | 1.41        | 1.33     |
| 16  | b     | 601 | CLA  | C4C-C3C | 2.61  | 1.49        | 1.45     |
| 16  | b     | 611 | CLA  | C1B-NB  | -2.61 | 1.34        | 1.37     |
| 16  | b     | 614 | CLA  | MG-NC   | 2.60  | 2.12        | 2.06     |
| 16  | b     | 605 | CLA  | CHC-C4B | 2.60  | 1.45        | 1.39     |
| 16  | a     | 402 | CLA  | CHC-C4B | 2.58  | 1.45        | 1.39     |
| 16  | b     | 606 | CLA  | MG-NB   | 2.58  | 2.10        | 2.05     |
| 16  | b     | 610 | CLA  | C4B-NB  | -2.57 | 1.34        | 1.37     |
| 16  | d     | 401 | CLA  | C1-C2   | 2.57  | 1.56        | 1.49     |
| 16  | b     | 613 | CLA  | C4C-C3C | 2.57  | 1.49        | 1.45     |
| 16  | b     | 603 | CLA  | MG-ND   | 2.56  | 2.10        | 2.05     |
| 16  | d     | 401 | CLA  | C3B-C4B | 2.55  | 1.48        | 1.42     |
| 16  | d     | 401 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 16  | b     | 610 | CLA  | C3B-C4B | 2.55  | 1.48        | 1.42     |
| 16  | b     | 611 | CLA  | C1D-ND  | -2.54 | 1.34        | 1.37     |
| 15  | l     | 101 | SQD  | C6-S    | -2.54 | 1.68        | 1.77     |
| 16  | b     | 608 | CLA  | C3D-C2D | 2.54  | 1.46        | 1.39     |
| 15  | a     | 401 | SQD  | C6-S    | -2.53 | 1.68        | 1.77     |
| 16  | a     | 402 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 16  | b     | 604 | CLA  | C4D-CHA | 2.52  | 1.47        | 1.38     |
| 16  | b     | 606 | CLA  | MG-ND   | 2.52  | 2.10        | 2.05     |
| 16  | b     | 605 | CLA  | C4B-NB  | -2.52 | 1.34        | 1.37     |
| 16  | b     | 610 | CLA  | O2A-CGA | 2.51  | 1.40        | 1.33     |
| 16  | b     | 612 | CLA  | OBD-CAD | 2.49  | 1.26        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | b     | 604 | CLA  | MG-NB   | 2.49  | 2.10        | 2.05     |
| 16  | b     | 606 | CLA  | C1C-C2C | 2.49  | 1.49        | 1.44     |
| 16  | d     | 401 | CLA  | O2D-CGD | 2.48  | 1.39        | 1.33     |
| 16  | b     | 610 | CLA  | C3D-C2D | 2.47  | 1.45        | 1.39     |
| 16  | b     | 602 | CLA  | C3D-C2D | 2.47  | 1.45        | 1.39     |
| 16  | b     | 603 | CLA  | CHC-C4B | 2.46  | 1.44        | 1.39     |
| 16  | b     | 604 | CLA  | C1C-NC  | -2.46 | 1.34        | 1.37     |
| 16  | b     | 615 | CLA  | C4D-ND  | 2.45  | 1.41        | 1.37     |
| 16  | b     | 602 | CLA  | C4D-CHA | 2.44  | 1.47        | 1.38     |
| 17  | a     | 405 | PHO  | CMB-C2B | -2.42 | 1.46        | 1.51     |
| 16  | b     | 601 | CLA  | C3D-C2D | 2.40  | 1.45        | 1.39     |
| 17  | a     | 404 | PHO  | C3B-C2B | -2.40 | 1.37        | 1.40     |
| 16  | b     | 605 | CLA  | C4D-CHA | 2.39  | 1.46        | 1.38     |
| 16  | a     | 403 | CLA  | CHD-C4C | 2.38  | 1.44        | 1.39     |
| 27  | e     | 101 | HEM  | C3C-C4C | -2.37 | 1.41        | 1.46     |
| 27  | e     | 101 | HEM  | C1C-C2C | -2.37 | 1.40        | 1.45     |
| 16  | b     | 601 | CLA  | C3A-C2A | -2.37 | 1.52        | 1.54     |
| 27  | e     | 101 | HEM  | FE-ND   | -2.37 | 1.87        | 1.94     |
| 16  | b     | 603 | CLA  | C1B-C2B | 2.37  | 1.48        | 1.43     |
| 16  | b     | 605 | CLA  | MG-NB   | 2.37  | 2.10        | 2.05     |
| 16  | d     | 405 | CLA  | CHB-C1B | 2.35  | 1.44        | 1.39     |
| 16  | a     | 406 | CLA  | CHD-C4C | 2.35  | 1.44        | 1.39     |
| 16  | b     | 614 | CLA  | C4B-NB  | -2.34 | 1.34        | 1.37     |
| 24  | d     | 406 | PQ9  | C10-C5  | 2.34  | 1.47        | 1.35     |
| 16  | d     | 405 | CLA  | CHC-C4B | 2.33  | 1.44        | 1.39     |
| 16  | b     | 612 | CLA  | CHD-C4C | 2.33  | 1.44        | 1.39     |
| 16  | b     | 605 | CLA  | C1B-C2B | 2.31  | 1.48        | 1.43     |
| 16  | d     | 405 | CLA  | C3D-C2D | 2.29  | 1.45        | 1.39     |
| 16  | b     | 612 | CLA  | C4D-CHA | 2.29  | 1.46        | 1.38     |
| 16  | d     | 405 | CLA  | C3B-C4B | 2.29  | 1.48        | 1.42     |
| 16  | b     | 613 | CLA  | C3D-C4D | -2.28 | 1.39        | 1.44     |
| 16  | b     | 615 | CLA  | C4C-C3C | 2.27  | 1.49        | 1.45     |
| 25  | d     | 411 | HTG  | C1-S1   | -2.27 | 1.77        | 1.80     |
| 16  | b     | 612 | CLA  | C1D-ND  | -2.26 | 1.35        | 1.37     |
| 16  | b     | 614 | CLA  | C4C-C3C | 2.26  | 1.48        | 1.45     |
| 16  | b     | 601 | CLA  | C1B-NB  | -2.25 | 1.35        | 1.37     |
| 16  | b     | 613 | CLA  | C1B-C2B | 2.25  | 1.48        | 1.43     |
| 16  | b     | 614 | CLA  | C4D-CHA | 2.24  | 1.46        | 1.38     |
| 16  | a     | 406 | CLA  | CHD-C1D | 2.24  | 1.42        | 1.38     |
| 16  | a     | 402 | CLA  | C3B-C4B | 2.23  | 1.48        | 1.42     |
| 16  | d     | 401 | CLA  | C4B-NB  | -2.22 | 1.35        | 1.37     |
| 16  | b     | 609 | CLA  | MG-ND   | 2.21  | 2.10        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | b     | 604 | CLA  | O2A-CGA | 2.21  | 1.39        | 1.33     |
| 16  | b     | 603 | CLA  | MG-NC   | -2.20 | 2.01        | 2.06     |
| 16  | a     | 402 | CLA  | C3D-C2D | 2.20  | 1.45        | 1.39     |
| 16  | a     | 406 | CLA  | C1D-C2D | 2.20  | 1.49        | 1.45     |
| 16  | d     | 401 | CLA  | C4D-CHA | 2.20  | 1.46        | 1.38     |
| 16  | b     | 613 | CLA  | C1B-NB  | -2.18 | 1.35        | 1.37     |
| 16  | b     | 601 | CLA  | CHB-C1B | 2.16  | 1.44        | 1.39     |
| 16  | b     | 608 | CLA  | C1B-C2B | 2.15  | 1.48        | 1.43     |
| 16  | a     | 406 | CLA  | C1B-NB  | -2.15 | 1.35        | 1.37     |
| 16  | a     | 406 | CLA  | CHB-C1B | 2.15  | 1.44        | 1.39     |
| 16  | b     | 605 | CLA  | C1C-NC  | -2.15 | 1.34        | 1.37     |
| 16  | a     | 403 | CLA  | CHD-C1D | 2.13  | 1.42        | 1.38     |
| 16  | a     | 402 | CLA  | C1C-NC  | -2.13 | 1.34        | 1.37     |
| 16  | d     | 404 | CLA  | C1B-C2B | 2.12  | 1.48        | 1.43     |
| 16  | d     | 405 | CLA  | C1D-C2D | 2.12  | 1.49        | 1.45     |
| 16  | b     | 614 | CLA  | OBD-CAD | 2.11  | 1.26        | 1.22     |
| 16  | b     | 611 | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 16  | b     | 606 | CLA  | C4C-C3C | 2.10  | 1.48        | 1.45     |
| 16  | d     | 401 | CLA  | C4C-C3C | 2.09  | 1.48        | 1.45     |
| 16  | b     | 613 | CLA  | C1-C2   | 2.08  | 1.55        | 1.49     |
| 16  | b     | 604 | CLA  | C1B-C2B | 2.08  | 1.48        | 1.43     |
| 16  | b     | 608 | CLA  | CAA-C2A | 2.08  | 1.58        | 1.54     |
| 16  | b     | 604 | CLA  | C1D-ND  | -2.07 | 1.35        | 1.37     |
| 20  | d     | 410 | MGE  | O3G-C1D | 2.07  | 1.43        | 1.40     |
| 16  | d     | 401 | CLA  | CMD-C2D | 2.07  | 1.55        | 1.50     |
| 16  | b     | 604 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 20  | m     | 101 | MGE  | O3G-C1D | 2.06  | 1.43        | 1.40     |
| 16  | b     | 606 | CLA  | C3B-C2B | 2.06  | 1.48        | 1.41     |
| 16  | b     | 609 | CLA  | O2D-CED | -2.05 | 1.40        | 1.45     |
| 16  | b     | 614 | CLA  | C3D-C2D | 2.05  | 1.44        | 1.39     |
| 16  | d     | 405 | CLA  | C1B-C2B | 2.04  | 1.48        | 1.43     |
| 16  | b     | 611 | CLA  | MG-NC   | 2.03  | 2.11        | 2.06     |
| 16  | b     | 604 | CLA  | CHC-C4B | 2.03  | 1.44        | 1.39     |
| 16  | d     | 401 | CLA  | C3D-C2D | 2.02  | 1.44        | 1.39     |
| 16  | b     | 611 | CLA  | C1B-C2B | 2.02  | 1.48        | 1.43     |
| 16  | b     | 601 | CLA  | CHC-C4B | 2.01  | 1.43        | 1.39     |
| 27  | e     | 101 | HEM  | C1D-ND  | -2.01 | 1.34        | 1.38     |
| 16  | a     | 403 | CLA  | C3D-C2D | 2.01  | 1.44        | 1.39     |
| 16  | b     | 616 | CLA  | MG-NC   | 2.01  | 2.11        | 2.06     |

All (862) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 15  | a     | 401 | SQD  | O9-S-C6     | -20.30 | 82.82       | 106.94   |
| 15  | l     | 101 | SQD  | O9-S-C6     | -20.03 | 83.13       | 106.94   |
| 16  | a     | 406 | CLA  | C1D-ND-C4D  | -18.90 | 92.91       | 106.33   |
| 16  | a     | 403 | CLA  | C1D-ND-C4D  | -17.71 | 93.75       | 106.33   |
| 16  | d     | 404 | CLA  | C1D-ND-C4D  | -16.62 | 94.53       | 106.33   |
| 16  | d     | 405 | CLA  | C1D-ND-C4D  | -16.58 | 94.56       | 106.33   |
| 16  | b     | 601 | CLA  | C1D-ND-C4D  | -15.10 | 95.61       | 106.33   |
| 16  | b     | 601 | CLA  | C2B-C1B-NB  | 13.98  | 119.60      | 110.23   |
| 16  | a     | 403 | CLA  | C2B-C1B-NB  | 13.65  | 119.38      | 110.23   |
| 16  | d     | 405 | CLA  | C2B-C1B-NB  | 13.30  | 119.15      | 110.23   |
| 16  | a     | 406 | CLA  | C2B-C1B-NB  | 13.15  | 119.05      | 110.23   |
| 16  | d     | 404 | CLA  | C2B-C1B-NB  | 12.84  | 118.84      | 110.23   |
| 15  | a     | 401 | SQD  | O8-S-O9     | -11.99 | 81.97       | 111.27   |
| 16  | b     | 606 | CLA  | C4A-NA-C1A  | 11.92  | 112.06      | 106.71   |
| 15  | l     | 101 | SQD  | O8-S-O9     | -11.74 | 82.59       | 111.27   |
| 16  | a     | 403 | CLA  | C2C-C1C-NC  | 10.63  | 119.93      | 109.97   |
| 16  | a     | 406 | CLA  | C2D-C1D-ND  | 10.47  | 117.82      | 110.10   |
| 16  | d     | 404 | CLA  | C2C-C1C-NC  | 10.41  | 119.72      | 109.97   |
| 16  | b     | 601 | CLA  | CHD-C1D-ND  | -10.27 | 115.02      | 124.45   |
| 16  | a     | 403 | CLA  | C2D-C1D-ND  | 9.91   | 117.41      | 110.10   |
| 16  | b     | 604 | CLA  | C4A-NA-C1A  | 9.84   | 111.13      | 106.71   |
| 15  | l     | 101 | SQD  | O7-S-C6     | 9.80   | 118.59      | 106.94   |
| 16  | d     | 405 | CLA  | C2C-C1C-NC  | 9.67   | 119.03      | 109.97   |
| 16  | b     | 614 | CLA  | C2D-C1D-ND  | 9.29   | 116.95      | 110.10   |
| 16  | b     | 601 | CLA  | C4A-NA-C1A  | -9.27  | 102.54      | 106.71   |
| 16  | d     | 405 | CLA  | C2D-C1D-ND  | 9.25   | 116.92      | 110.10   |
| 16  | b     | 601 | CLA  | C2C-C1C-NC  | 9.07   | 118.47      | 109.97   |
| 15  | a     | 401 | SQD  | O7-S-C6     | 9.05   | 117.70      | 106.94   |
| 16  | b     | 601 | CLA  | CMD-C2D-C1D | 9.01   | 140.60      | 124.71   |
| 16  | a     | 403 | CLA  | CMD-C2D-C1D | 9.00   | 140.58      | 124.71   |
| 15  | l     | 101 | SQD  | O9-S-O7     | -8.94  | 83.02       | 113.95   |
| 16  | b     | 610 | CLA  | C2D-C1D-ND  | 8.86   | 116.64      | 110.10   |
| 16  | a     | 406 | CLA  | C2C-C1C-NC  | 8.78   | 118.19      | 109.97   |
| 16  | d     | 404 | CLA  | C2D-C1D-ND  | 8.74   | 116.55      | 110.10   |
| 16  | b     | 610 | CLA  | C4A-NA-C1A  | 8.74   | 110.64      | 106.71   |
| 16  | a     | 406 | CLA  | CMD-C2D-C1D | 8.72   | 140.08      | 124.71   |
| 16  | d     | 404 | CLA  | C3C-C4C-NC  | 8.71   | 120.34      | 110.57   |
| 16  | b     | 610 | CLA  | C2B-C1B-NB  | 8.64   | 116.03      | 110.23   |
| 15  | a     | 401 | SQD  | O9-S-O7     | -8.61  | 84.14       | 113.95   |
| 16  | b     | 601 | CLA  | C4D-CHA-C1A | -8.55  | 110.84      | 121.25   |
| 15  | a     | 401 | SQD  | O8-S-C6     | 8.53   | 119.33      | 105.74   |
| 16  | b     | 614 | CLA  | C4A-NA-C1A  | 8.52   | 110.53      | 106.71   |
| 16  | b     | 603 | CLA  | C2B-C1B-NB  | 8.46   | 115.90      | 110.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | b     | 612 | CLA  | CAC-C3C-C4C | 8.41  | 135.72      | 124.81   |
| 16  | d     | 404 | CLA  | CHD-C4C-C3C | -8.38 | 112.53      | 124.84   |
| 17  | a     | 404 | PHO  | C4D-CHA-CBD | -8.36 | 104.74      | 108.52   |
| 16  | b     | 615 | CLA  | C2B-C1B-NB  | 8.29  | 115.79      | 110.23   |
| 16  | a     | 406 | CLA  | C4A-NA-C1A  | -8.28 | 102.98      | 106.71   |
| 16  | a     | 406 | CLA  | C3C-C4C-NC  | 8.02  | 119.57      | 110.57   |
| 16  | b     | 611 | CLA  | C4A-NA-C1A  | 7.97  | 110.29      | 106.71   |
| 16  | a     | 402 | CLA  | C2D-C1D-ND  | 7.92  | 115.94      | 110.10   |
| 16  | d     | 405 | CLA  | CMD-C2D-C1D | 7.91  | 138.65      | 124.71   |
| 15  | l     | 101 | SQD  | O8-S-C6     | 7.83  | 118.22      | 105.74   |
| 16  | b     | 612 | CLA  | C4A-NA-C1A  | 7.80  | 110.21      | 106.71   |
| 16  | a     | 403 | CLA  | C3B-C4B-NB  | 7.76  | 117.71      | 110.52   |
| 16  | d     | 404 | CLA  | CMD-C2D-C1D | 7.65  | 138.19      | 124.71   |
| 16  | b     | 616 | CLA  | C2B-C1B-NB  | 7.57  | 115.31      | 110.23   |
| 16  | a     | 406 | CLA  | C4D-CHA-C1A | -7.42 | 112.22      | 121.25   |
| 16  | d     | 405 | CLA  | C3C-C4C-NC  | 7.41  | 118.89      | 110.57   |
| 16  | d     | 405 | CLA  | CHD-C1D-ND  | -7.37 | 117.68      | 124.45   |
| 16  | a     | 406 | CLA  | C3D-C4D-ND  | 7.35  | 122.14      | 110.24   |
| 17  | a     | 405 | PHO  | C4D-CHA-CBD | -7.35 | 105.19      | 108.52   |
| 16  | b     | 601 | CLA  | C3D-C4D-ND  | 7.31  | 122.06      | 110.24   |
| 16  | b     | 605 | CLA  | C2C-C1C-NC  | 7.21  | 116.72      | 109.97   |
| 16  | b     | 601 | CLA  | CHB-C1B-NB  | -7.20 | 116.63      | 124.26   |
| 16  | b     | 603 | CLA  | CHD-C1D-ND  | -7.13 | 117.90      | 124.45   |
| 18  | a     | 407 | BCR  | C7-C8-C9    | -7.11 | 115.48      | 126.23   |
| 16  | a     | 406 | CLA  | CHD-C4C-C3C | -7.10 | 114.41      | 124.84   |
| 16  | b     | 603 | CLA  | C2C-C1C-NC  | 7.10  | 116.62      | 109.97   |
| 16  | d     | 405 | CLA  | C3D-C4D-ND  | 7.08  | 121.70      | 110.24   |
| 16  | a     | 403 | CLA  | C3D-C4D-ND  | 7.04  | 121.63      | 110.24   |
| 16  | b     | 615 | CLA  | C4A-NA-C1A  | 7.00  | 109.85      | 106.71   |
| 16  | d     | 405 | CLA  | C4A-NA-C1A  | -6.96 | 103.58      | 106.71   |
| 16  | a     | 403 | CLA  | C3C-C4C-NC  | 6.94  | 118.36      | 110.57   |
| 16  | b     | 614 | CLA  | C4D-CHA-C1A | -6.94 | 112.80      | 121.25   |
| 16  | b     | 605 | CLA  | CAC-C3C-C4C | 6.93  | 133.80      | 124.81   |
| 16  | a     | 402 | CLA  | CAC-C3C-C4C | 6.92  | 133.79      | 124.81   |
| 16  | b     | 616 | CLA  | CHD-C4C-C3C | -6.83 | 114.80      | 124.84   |
| 16  | b     | 614 | CLA  | C1D-ND-C4D  | -6.71 | 101.57      | 106.33   |
| 16  | b     | 601 | CLA  | C2D-C1D-ND  | 6.69  | 115.03      | 110.10   |
| 16  | b     | 606 | CLA  | C2B-C1B-NB  | 6.68  | 114.71      | 110.23   |
| 16  | b     | 601 | CLA  | C3B-C2B-C1B | -6.67 | 99.11       | 107.16   |
| 16  | d     | 401 | CLA  | C2D-C1D-ND  | 6.63  | 114.99      | 110.10   |
| 16  | b     | 613 | CLA  | C2D-C1D-ND  | 6.59  | 114.96      | 110.10   |
| 16  | b     | 602 | CLA  | C2D-C1D-ND  | 6.54  | 114.92      | 110.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | d     | 405 | CLA  | C3B-C4B-NB  | 6.53  | 116.57      | 110.52   |
| 16  | b     | 603 | CLA  | C2D-C1D-ND  | 6.51  | 114.90      | 110.10   |
| 16  | b     | 604 | CLA  | C2C-C1C-NC  | 6.47  | 116.03      | 109.97   |
| 16  | a     | 403 | CLA  | CHD-C4C-C3C | -6.45 | 115.36      | 124.84   |
| 16  | b     | 605 | CLA  | C2D-C1D-ND  | 6.45  | 114.86      | 110.10   |
| 16  | a     | 403 | CLA  | CHD-C1D-ND  | -6.39 | 118.58      | 124.45   |
| 16  | a     | 403 | CLA  | C4A-NA-C1A  | -6.39 | 103.83      | 106.71   |
| 16  | b     | 615 | CLA  | CHC-C4B-NB  | 6.38  | 131.01      | 124.26   |
| 16  | b     | 613 | CLA  | C2B-C1B-NB  | 6.37  | 114.50      | 110.23   |
| 16  | b     | 616 | CLA  | C2D-C1D-ND  | 6.35  | 114.78      | 110.10   |
| 16  | b     | 613 | CLA  | C4A-NA-C1A  | 6.33  | 109.55      | 106.71   |
| 16  | b     | 613 | CLA  | C2C-C1C-NC  | 6.32  | 115.89      | 109.97   |
| 25  | d     | 411 | HTG  | C1'-S1-C1   | 6.29  | 111.86      | 100.09   |
| 16  | b     | 614 | CLA  | O2D-CGD-CBD | 6.28  | 122.43      | 111.27   |
| 16  | b     | 604 | CLA  | C2D-C1D-ND  | 6.25  | 114.71      | 110.10   |
| 16  | a     | 403 | CLA  | O2D-CGD-CBD | 6.25  | 122.38      | 111.27   |
| 16  | b     | 611 | CLA  | C2B-C1B-NB  | 6.24  | 114.41      | 110.23   |
| 16  | b     | 606 | CLA  | C2D-C1D-ND  | 6.23  | 114.70      | 110.10   |
| 16  | d     | 401 | CLA  | C2B-C1B-NB  | 6.19  | 114.38      | 110.23   |
| 16  | b     | 612 | CLA  | C2D-C1D-ND  | 6.18  | 114.66      | 110.10   |
| 16  | b     | 616 | CLA  | O2D-CGD-CBD | 6.17  | 122.24      | 111.27   |
| 16  | b     | 605 | CLA  | CHD-C1D-ND  | -6.14 | 118.81      | 124.45   |
| 16  | d     | 404 | CLA  | O2D-CGD-CBD | 6.11  | 122.13      | 111.27   |
| 16  | a     | 403 | CLA  | C4D-CHA-C1A | -6.10 | 113.83      | 121.25   |
| 16  | b     | 602 | CLA  | C2B-C1B-NB  | 6.09  | 114.32      | 110.23   |
| 16  | b     | 601 | CLA  | C3C-C4C-NC  | 6.09  | 117.41      | 110.57   |
| 16  | d     | 404 | CLA  | C3D-C4D-ND  | 6.07  | 120.06      | 110.24   |
| 16  | d     | 404 | CLA  | C3B-C4B-NB  | 6.02  | 116.10      | 110.52   |
| 16  | b     | 612 | CLA  | CHD-C4C-C3C | -6.02 | 116.00      | 124.84   |
| 16  | a     | 406 | CLA  | CHD-C1D-ND  | -6.01 | 118.93      | 124.45   |
| 18  | a     | 407 | BCR  | C11-C10-C9  | -6.00 | 118.74      | 127.31   |
| 16  | b     | 608 | CLA  | C2B-C1B-NB  | 5.97  | 114.24      | 110.23   |
| 16  | a     | 403 | CLA  | C1C-C2C-C3C | -5.94 | 100.71      | 106.96   |
| 16  | b     | 608 | CLA  | C2D-C1D-ND  | 5.92  | 114.47      | 110.10   |
| 16  | d     | 404 | CLA  | C4D-CHA-C1A | -5.91 | 114.05      | 121.25   |
| 17  | a     | 404 | PHO  | C2B-C1B-NB  | -5.90 | 105.45      | 109.53   |
| 16  | d     | 401 | CLA  | C2C-C1C-NC  | 5.87  | 115.47      | 109.97   |
| 16  | d     | 401 | CLA  | CHD-C4C-C3C | -5.85 | 116.24      | 124.84   |
| 16  | d     | 401 | CLA  | CHC-C4B-NB  | 5.85  | 130.45      | 124.26   |
| 16  | d     | 405 | CLA  | C4D-CHA-C1A | -5.85 | 114.13      | 121.25   |
| 16  | a     | 403 | CLA  | C3D-C2D-C1D | -5.84 | 97.86       | 105.83   |
| 17  | a     | 405 | PHO  | C2B-C1B-NB  | -5.84 | 105.50      | 109.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | b     | 609 | CLA  | C2C-C1C-NC  | 5.83  | 115.44      | 109.97   |
| 16  | b     | 615 | CLA  | C2D-C1D-ND  | 5.81  | 114.39      | 110.10   |
| 16  | a     | 406 | CLA  | C3B-C2B-C1B | -5.79 | 100.17      | 107.16   |
| 16  | d     | 405 | CLA  | O2D-CGD-CBD | 5.77  | 121.53      | 111.27   |
| 16  | a     | 406 | CLA  | C3D-C2D-C1D | -5.76 | 97.98       | 105.83   |
| 16  | b     | 614 | CLA  | C2B-C1B-NB  | 5.73  | 114.07      | 110.23   |
| 16  | b     | 615 | CLA  | C2C-C1C-NC  | 5.71  | 115.32      | 109.97   |
| 16  | d     | 405 | CLA  | C3B-C2B-C1B | -5.68 | 100.31      | 107.16   |
| 16  | b     | 603 | CLA  | CHD-C4C-C3C | -5.63 | 116.56      | 124.84   |
| 16  | d     | 404 | CLA  | C1C-C2C-C3C | -5.62 | 101.05      | 106.96   |
| 16  | a     | 403 | CLA  | C3B-C2B-C1B | -5.61 | 100.39      | 107.16   |
| 16  | d     | 405 | CLA  | CHD-C4C-C3C | -5.61 | 116.60      | 124.84   |
| 16  | d     | 405 | CLA  | C3D-C2D-C1D | -5.60 | 98.18       | 105.83   |
| 16  | b     | 608 | CLA  | C2C-C1C-NC  | 5.58  | 115.20      | 109.97   |
| 16  | b     | 612 | CLA  | C3C-C4C-NC  | 5.55  | 116.79      | 110.57   |
| 16  | b     | 604 | CLA  | C2B-C1B-NB  | 5.52  | 113.93      | 110.23   |
| 16  | b     | 616 | CLA  | C4A-NA-C1A  | 5.48  | 109.17      | 106.71   |
| 18  | h     | 101 | BCR  | C7-C8-C9    | -5.44 | 118.02      | 126.23   |
| 16  | b     | 611 | CLA  | C2D-C1D-ND  | 5.44  | 114.11      | 110.10   |
| 16  | b     | 613 | CLA  | CAC-C3C-C4C | 5.42  | 131.84      | 124.81   |
| 16  | b     | 610 | CLA  | C2C-C1C-NC  | 5.39  | 115.03      | 109.97   |
| 16  | b     | 601 | CLA  | C3B-C4B-NB  | 5.37  | 115.50      | 110.52   |
| 26  | d     | 412 | DGD  | O2G-C1B-C2B | 5.36  | 123.05      | 111.50   |
| 16  | b     | 612 | CLA  | C4D-CHA-C1A | -5.35 | 114.74      | 121.25   |
| 16  | b     | 606 | CLA  | CHD-C1D-ND  | -5.31 | 119.58      | 124.45   |
| 16  | b     | 610 | CLA  | C1D-ND-C4D  | -5.30 | 102.57      | 106.33   |
| 16  | a     | 402 | CLA  | C2B-C1B-NB  | 5.29  | 113.78      | 110.23   |
| 16  | a     | 406 | CLA  | O2D-CGD-CBD | 5.29  | 120.67      | 111.27   |
| 16  | b     | 602 | CLA  | CHD-C1D-ND  | -5.29 | 119.59      | 124.45   |
| 16  | d     | 404 | CLA  | C3D-C2D-C1D | -5.28 | 98.63       | 105.83   |
| 15  | a     | 401 | SQD  | O47-C7-C8   | 5.25  | 120.76      | 111.09   |
| 20  | b     | 620 | MGE  | O2G-C1B-C2B | 5.24  | 122.81      | 111.50   |
| 16  | b     | 609 | CLA  | CAC-C3C-C4C | 5.24  | 131.61      | 124.81   |
| 16  | b     | 601 | CLA  | C1D-CHD-C4C | -5.23 | 114.79      | 126.06   |
| 16  | b     | 612 | CLA  | C2C-C1C-NC  | 5.21  | 114.86      | 109.97   |
| 16  | b     | 603 | CLA  | CHC-C4B-NB  | 5.20  | 129.76      | 124.26   |
| 16  | a     | 402 | CLA  | C2C-C1C-NC  | 5.18  | 114.82      | 109.97   |
| 16  | b     | 615 | CLA  | C1C-C2C-C3C | -5.16 | 101.53      | 106.96   |
| 16  | b     | 603 | CLA  | C1C-C2C-C3C | -5.15 | 101.55      | 106.96   |
| 16  | b     | 611 | CLA  | C2C-C1C-NC  | 5.10  | 114.75      | 109.97   |
| 16  | a     | 402 | CLA  | C3B-C2B-C1B | -5.09 | 101.02      | 107.16   |
| 20  | d     | 410 | MGE  | O2G-C1B-C2B | 5.08  | 122.46      | 111.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | b     | 605 | CLA  | CHC-C4B-NB  | 5.06  | 129.61      | 124.26   |
| 16  | d     | 404 | CLA  | C3B-C2B-C1B | -5.05 | 101.06      | 107.16   |
| 16  | b     | 604 | CLA  | CHC-C4B-NB  | 5.03  | 129.59      | 124.26   |
| 18  | a     | 407 | BCR  | C20-C21-C22 | -4.99 | 120.19      | 127.31   |
| 16  | b     | 603 | CLA  | O2D-CGD-O1D | -4.99 | 114.09      | 123.84   |
| 27  | e     | 101 | HEM  | CHD-C1D-ND  | 4.99  | 129.84      | 124.42   |
| 16  | b     | 603 | CLA  | C4-C3-C5    | 4.98  | 123.65      | 115.27   |
| 16  | b     | 604 | CLA  | C1C-C2C-C3C | -4.97 | 101.73      | 106.96   |
| 16  | b     | 616 | CLA  | CHD-C1D-ND  | -4.96 | 119.89      | 124.45   |
| 16  | a     | 402 | CLA  | C3D-C2D-C1D | -4.95 | 99.08       | 105.83   |
| 16  | b     | 613 | CLA  | C1-C2-C3    | -4.93 | 117.52      | 126.04   |
| 17  | a     | 404 | PHO  | C2D-C1D-ND  | -4.93 | 106.12      | 109.53   |
| 16  | b     | 607 | CLA  | C2B-C1B-NB  | 4.91  | 113.53      | 110.23   |
| 27  | e     | 101 | HEM  | CHC-C4B-NB  | 4.90  | 129.74      | 124.42   |
| 18  | d     | 407 | BCR  | C7-C8-C9    | -4.89 | 118.84      | 126.23   |
| 16  | b     | 605 | CLA  | C4-C3-C5    | 4.89  | 123.50      | 115.27   |
| 16  | b     | 608 | CLA  | O2D-CGD-CBD | 4.88  | 119.94      | 111.27   |
| 16  | d     | 404 | CLA  | C1D-CHD-C4C | -4.87 | 115.56      | 126.06   |
| 16  | b     | 613 | CLA  | CHD-C4C-C3C | -4.85 | 117.71      | 124.84   |
| 16  | b     | 614 | CLA  | O2D-CGD-O1D | -4.83 | 114.39      | 123.84   |
| 16  | b     | 608 | CLA  | C1C-C2C-C3C | -4.82 | 101.89      | 106.96   |
| 16  | b     | 612 | CLA  | C4C-C3C-C2C | -4.82 | 99.88       | 106.90   |
| 16  | b     | 607 | CLA  | CHD-C4C-C3C | -4.82 | 117.76      | 124.84   |
| 16  | b     | 605 | CLA  | CHD-C4C-C3C | -4.80 | 117.79      | 124.84   |
| 16  | b     | 616 | CLA  | C3B-C2B-C1B | -4.79 | 101.37      | 107.16   |
| 16  | b     | 609 | CLA  | C2B-C1B-NB  | 4.78  | 113.44      | 110.23   |
| 16  | b     | 605 | CLA  | C3C-C4C-NC  | 4.77  | 115.92      | 110.57   |
| 16  | b     | 604 | CLA  | CAC-C3C-C4C | 4.76  | 130.98      | 124.81   |
| 16  | d     | 405 | CLA  | C1C-C2C-C3C | -4.73 | 101.98      | 106.96   |
| 16  | b     | 615 | CLA  | C3B-C2B-C1B | -4.72 | 101.46      | 107.16   |
| 16  | b     | 601 | CLA  | C3D-C2D-C1D | -4.72 | 99.39       | 105.83   |
| 16  | b     | 605 | CLA  | C2B-C1B-NB  | 4.71  | 113.39      | 110.23   |
| 16  | b     | 607 | CLA  | C2C-C1C-NC  | 4.70  | 114.38      | 109.97   |
| 16  | b     | 602 | CLA  | O2D-CGD-CBD | 4.69  | 119.61      | 111.27   |
| 16  | b     | 613 | CLA  | C3D-C2D-C1D | -4.69 | 99.44       | 105.83   |
| 20  | d     | 410 | MGE  | C1D-O6D-C5D | 4.69  | 122.89      | 113.69   |
| 18  | a     | 407 | BCR  | C24-C23-C22 | -4.67 | 119.17      | 126.23   |
| 16  | b     | 614 | CLA  | C2C-C1C-NC  | 4.67  | 114.35      | 109.97   |
| 16  | a     | 403 | CLA  | C1D-CHD-C4C | -4.66 | 116.00      | 126.06   |
| 16  | b     | 610 | CLA  | C1C-C2C-C3C | -4.64 | 102.08      | 106.96   |
| 16  | b     | 606 | CLA  | CHD-C4C-C3C | -4.63 | 118.03      | 124.84   |
| 16  | b     | 604 | CLA  | CHD-C4C-C3C | -4.61 | 118.07      | 124.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | d     | 407 | BCR  | C24-C23-C22 | -4.60 | 119.28      | 126.23   |
| 16  | b     | 616 | CLA  | C2C-C1C-NC  | 4.60  | 114.28      | 109.97   |
| 16  | b     | 603 | CLA  | C3B-C2B-C1B | -4.59 | 101.62      | 107.16   |
| 16  | b     | 608 | CLA  | CHD-C4C-C3C | -4.58 | 118.10      | 124.84   |
| 16  | b     | 611 | CLA  | C1C-C2C-C3C | -4.58 | 102.14      | 106.96   |
| 16  | b     | 609 | CLA  | O2D-CGD-CBD | 4.58  | 119.41      | 111.27   |
| 16  | b     | 607 | CLA  | CAC-C3C-C4C | 4.57  | 130.74      | 124.81   |
| 16  | b     | 614 | CLA  | C1-C2-C3    | -4.53 | 118.21      | 126.04   |
| 16  | b     | 602 | CLA  | C3B-C2B-C1B | -4.52 | 101.71      | 107.16   |
| 16  | b     | 615 | CLA  | C1D-CHD-C4C | -4.51 | 116.33      | 126.06   |
| 16  | d     | 401 | CLA  | C1D-CHD-C4C | -4.51 | 116.33      | 126.06   |
| 16  | b     | 602 | CLA  | C2C-C1C-NC  | 4.49  | 114.17      | 109.97   |
| 16  | b     | 605 | CLA  | O2D-CGD-CBD | 4.48  | 119.23      | 111.27   |
| 16  | b     | 607 | CLA  | C3D-C2D-C1D | -4.48 | 99.72       | 105.83   |
| 16  | b     | 606 | CLA  | C2C-C1C-NC  | 4.47  | 114.16      | 109.97   |
| 18  | b     | 619 | BCR  | C20-C21-C22 | -4.45 | 120.96      | 127.31   |
| 16  | b     | 607 | CLA  | C4A-NA-C1A  | 4.44  | 108.70      | 106.71   |
| 16  | b     | 612 | CLA  | CHC-C4B-NB  | 4.44  | 128.96      | 124.26   |
| 16  | b     | 609 | CLA  | C2D-C1D-ND  | 4.44  | 113.38      | 110.10   |
| 16  | a     | 402 | CLA  | CHD-C4C-C3C | -4.43 | 118.32      | 124.84   |
| 16  | b     | 610 | CLA  | C3B-C2B-C1B | -4.43 | 101.81      | 107.16   |
| 16  | b     | 602 | CLA  | O2D-CGD-O1D | -4.41 | 115.22      | 123.84   |
| 16  | b     | 604 | CLA  | C3D-C2D-C1D | -4.38 | 99.85       | 105.83   |
| 16  | b     | 616 | CLA  | C3C-C4C-NC  | 4.38  | 115.49      | 110.57   |
| 16  | b     | 607 | CLA  | C2D-C1D-ND  | 4.38  | 113.33      | 110.10   |
| 16  | b     | 605 | CLA  | CMD-C2D-C1D | 4.38  | 132.43      | 124.71   |
| 16  | a     | 406 | CLA  | C3B-C4B-NB  | 4.37  | 114.57      | 110.52   |
| 16  | d     | 401 | CLA  | C3B-C2B-C1B | -4.37 | 101.89      | 107.16   |
| 16  | b     | 601 | CLA  | O2D-CGD-CBD | 4.36  | 119.02      | 111.27   |
| 18  | b     | 619 | BCR  | C7-C8-C9    | -4.36 | 119.64      | 126.23   |
| 16  | b     | 614 | CLA  | CHD-C4C-C3C | -4.35 | 118.45      | 124.84   |
| 16  | b     | 609 | CLA  | CHC-C4B-NB  | 4.30  | 128.80      | 124.26   |
| 16  | b     | 614 | CLA  | CHC-C4B-NB  | 4.29  | 128.80      | 124.26   |
| 16  | b     | 608 | CLA  | CHD-C1D-ND  | -4.29 | 120.51      | 124.45   |
| 16  | b     | 611 | CLA  | CHD-C4C-C3C | -4.29 | 118.53      | 124.84   |
| 20  | b     | 622 | MGE  | O2G-C1B-C2B | 4.29  | 120.74      | 111.50   |
| 18  | a     | 407 | BCR  | C1-C6-C5    | -4.24 | 116.64      | 122.61   |
| 16  | b     | 605 | CLA  | C3D-C2D-C1D | -4.22 | 100.07      | 105.83   |
| 16  | a     | 406 | CLA  | C1D-CHD-C4C | -4.22 | 116.96      | 126.06   |
| 18  | h     | 101 | BCR  | C16-C17-C18 | -4.21 | 121.31      | 127.31   |
| 16  | b     | 601 | CLA  | C1C-C2C-C3C | -4.19 | 102.55      | 106.96   |
| 17  | a     | 405 | PHO  | C1C-C2C-C3C | -4.19 | 105.13      | 108.61   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | b     | 615 | CLA  | O2D-CGD-CBD | 4.17  | 118.67      | 111.27   |
| 16  | a     | 406 | CLA  | C1C-C2C-C3C | -4.15 | 102.59      | 106.96   |
| 16  | b     | 605 | CLA  | C1C-C2C-C3C | -4.14 | 102.61      | 106.96   |
| 16  | b     | 605 | CLA  | CMC-C2C-C1C | 4.14  | 131.34      | 125.04   |
| 16  | d     | 401 | CLA  | C3D-C2D-C1D | -4.13 | 100.20      | 105.83   |
| 16  | a     | 406 | CLA  | CHC-C4B-NB  | -4.13 | 119.89      | 124.26   |
| 18  | b     | 618 | BCR  | C24-C23-C22 | -4.11 | 120.02      | 126.23   |
| 16  | b     | 616 | CLA  | C3D-C2D-C1D | -4.11 | 100.22      | 105.83   |
| 16  | b     | 615 | CLA  | CHD-C4C-C3C | -4.10 | 118.81      | 124.84   |
| 16  | b     | 609 | CLA  | C4D-CHA-C1A | -4.10 | 116.26      | 121.25   |
| 16  | b     | 613 | CLA  | CHD-C1D-ND  | -4.10 | 120.69      | 124.45   |
| 16  | b     | 607 | CLA  | CHD-C1D-ND  | -4.09 | 120.69      | 124.45   |
| 20  | b     | 620 | MGE  | O1G-C1A-C2A | 4.09  | 124.75      | 111.91   |
| 16  | b     | 610 | CLA  | C3D-C2D-C1D | -4.08 | 100.27      | 105.83   |
| 16  | d     | 405 | CLA  | C1D-CHD-C4C | -4.07 | 117.29      | 126.06   |
| 16  | b     | 604 | CLA  | C3C-C4C-NC  | 4.07  | 115.13      | 110.57   |
| 15  | l     | 101 | SQD  | O47-C7-C8   | 4.07  | 120.26      | 111.50   |
| 16  | b     | 611 | CLA  | CHA-C4D-ND  | 4.06  | 141.00      | 132.50   |
| 16  | b     | 603 | CLA  | C3D-C2D-C1D | -4.06 | 100.30      | 105.83   |
| 16  | b     | 602 | CLA  | C1C-C2C-C3C | -4.04 | 102.71      | 106.96   |
| 20  | d     | 408 | MGE  | O2G-C1B-C2B | 4.03  | 120.20      | 111.50   |
| 16  | b     | 615 | CLA  | O2D-CGD-O1D | -4.02 | 115.97      | 123.84   |
| 16  | b     | 614 | CLA  | C3D-C2D-C1D | -4.01 | 100.36      | 105.83   |
| 18  | a     | 407 | BCR  | C11-C12-C13 | -4.01 | 115.15      | 126.42   |
| 16  | b     | 604 | CLA  | O2D-CGD-CBD | 4.01  | 118.39      | 111.27   |
| 16  | b     | 611 | CLA  | C1-C2-C3    | -4.01 | 119.12      | 126.04   |
| 16  | b     | 604 | CLA  | O2D-CGD-O1D | -4.00 | 116.02      | 123.84   |
| 16  | b     | 606 | CLA  | C3D-C2D-C1D | -4.00 | 100.38      | 105.83   |
| 18  | b     | 619 | BCR  | C27-C26-C25 | -3.99 | 116.94      | 122.73   |
| 16  | a     | 402 | CLA  | C1C-C2C-C3C | -3.99 | 102.77      | 106.96   |
| 16  | b     | 607 | CLA  | C1D-ND-C4D  | 3.98  | 109.16      | 106.33   |
| 16  | b     | 608 | CLA  | O2D-CGD-O1D | -3.98 | 116.05      | 123.84   |
| 18  | b     | 619 | BCR  | C24-C23-C22 | -3.97 | 120.24      | 126.23   |
| 16  | b     | 602 | CLA  | C3D-C2D-C1D | -3.96 | 100.43      | 105.83   |
| 16  | b     | 615 | CLA  | C3D-C2D-C1D | -3.96 | 100.43      | 105.83   |
| 16  | b     | 611 | CLA  | C4D-CHA-C1A | -3.95 | 116.44      | 121.25   |
| 16  | b     | 613 | CLA  | CHC-C4B-NB  | 3.95  | 128.44      | 124.26   |
| 16  | b     | 608 | CLA  | C3D-C2D-C1D | -3.95 | 100.44      | 105.83   |
| 16  | a     | 406 | CLA  | C4C-C3C-C2C | -3.94 | 101.16      | 106.90   |
| 16  | a     | 402 | CLA  | CHC-C4B-NB  | 3.94  | 128.43      | 124.26   |
| 16  | b     | 601 | CLA  | CAC-C3C-C4C | 3.93  | 129.91      | 124.81   |
| 16  | b     | 606 | CLA  | C1C-C2C-C3C | -3.93 | 102.83      | 106.96   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | b     | 616 | CLA  | CAC-C3C-C4C | 3.93  | 129.91      | 124.81   |
| 20  | m     | 101 | MGE  | O2G-C1B-C2B | 3.92  | 119.96      | 111.50   |
| 16  | b     | 605 | CLA  | C4D-CHA-C1A | -3.91 | 116.49      | 121.25   |
| 20  | d     | 409 | MGE  | O2G-C1B-C2B | 3.86  | 119.83      | 111.50   |
| 16  | b     | 612 | CLA  | C3D-C2D-C1D | -3.86 | 100.56      | 105.83   |
| 16  | d     | 401 | CLA  | C1C-C2C-C3C | -3.86 | 102.90      | 106.96   |
| 16  | b     | 611 | CLA  | O2D-CGD-CBD | 3.84  | 118.10      | 111.27   |
| 17  | a     | 405 | PHO  | CMB-C2B-C3B | 3.83  | 131.85      | 124.68   |
| 16  | b     | 611 | CLA  | C3B-C4B-NB  | 3.82  | 114.06      | 110.52   |
| 16  | b     | 613 | CLA  | CMD-C2D-C1D | 3.82  | 131.44      | 124.71   |
| 16  | b     | 609 | CLA  | CHD-C1D-ND  | -3.82 | 120.95      | 124.45   |
| 16  | a     | 403 | CLA  | CMB-C2B-C1B | 3.81  | 131.17      | 125.37   |
| 16  | b     | 607 | CLA  | CHA-C4D-ND  | 3.81  | 140.46      | 132.50   |
| 16  | a     | 402 | CLA  | CHD-C1D-ND  | -3.80 | 120.96      | 124.45   |
| 16  | b     | 612 | CLA  | O2D-CGD-O1D | -3.80 | 116.41      | 123.84   |
| 16  | b     | 602 | CLA  | CHD-C4C-C3C | -3.79 | 119.27      | 124.84   |
| 18  | b     | 619 | BCR  | C15-C14-C13 | -3.79 | 121.91      | 127.31   |
| 18  | b     | 619 | BCR  | C16-C17-C18 | -3.79 | 121.91      | 127.31   |
| 16  | b     | 609 | CLA  | C3C-C4C-NC  | 3.78  | 114.81      | 110.57   |
| 16  | b     | 609 | CLA  | C3B-C2B-C1B | -3.77 | 102.61      | 107.16   |
| 16  | d     | 401 | CLA  | CHD-C4C-NC  | 3.77  | 130.14      | 124.20   |
| 16  | b     | 615 | CLA  | CAC-C3C-C4C | 3.76  | 129.69      | 124.81   |
| 16  | b     | 604 | CLA  | CMC-C2C-C1C | 3.76  | 130.77      | 125.04   |
| 18  | b     | 618 | BCR  | C20-C21-C22 | -3.76 | 121.95      | 127.31   |
| 16  | b     | 610 | CLA  | C4D-CHA-C1A | -3.75 | 116.69      | 121.25   |
| 16  | b     | 610 | CLA  | CHD-C4C-C3C | -3.74 | 119.34      | 124.84   |
| 16  | b     | 614 | CLA  | CMD-C2D-C1D | 3.74  | 131.31      | 124.71   |
| 18  | h     | 101 | BCR  | C32-C1-C6   | 3.73  | 116.36      | 110.30   |
| 16  | b     | 614 | CLA  | O2A-CGA-O1A | -3.71 | 114.23      | 123.59   |
| 16  | a     | 402 | CLA  | CMB-C2B-C1B | 3.71  | 131.02      | 125.37   |
| 16  | b     | 612 | CLA  | C1-C2-C3    | -3.70 | 119.64      | 126.04   |
| 16  | b     | 603 | CLA  | CHD-C4C-NC  | 3.70  | 130.04      | 124.20   |
| 18  | h     | 101 | BCR  | C8-C9-C10   | 3.70  | 124.62      | 118.94   |
| 16  | b     | 614 | CLA  | C6-C5-C3    | -3.70 | 108.57      | 114.62   |
| 24  | d     | 406 | PQ9  | C39-C38-C40 | 3.70  | 121.49      | 115.27   |
| 18  | b     | 618 | BCR  | C15-C14-C13 | -3.69 | 122.04      | 127.31   |
| 16  | a     | 402 | CLA  | C1D-ND-C4D  | -3.69 | 103.72      | 106.33   |
| 16  | b     | 610 | CLA  | O2D-CGD-CBD | 3.67  | 117.79      | 111.27   |
| 16  | d     | 401 | CLA  | C4D-CHA-C1A | -3.67 | 116.78      | 121.25   |
| 16  | b     | 611 | CLA  | CBC-CAC-C3C | -3.65 | 102.37      | 112.43   |
| 16  | b     | 615 | CLA  | CMC-C2C-C1C | 3.65  | 130.59      | 125.04   |
| 16  | b     | 612 | CLA  | C2B-C1B-NB  | 3.64  | 112.67      | 110.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | h     | 101 | BCR  | C15-C14-C13 | -3.64 | 122.11      | 127.31   |
| 16  | b     | 601 | CLA  | C4C-C3C-C2C | -3.63 | 101.61      | 106.90   |
| 16  | b     | 603 | CLA  | CHA-C4D-ND  | 3.62  | 140.08      | 132.50   |
| 20  | d     | 409 | MGE  | C3G-C2G-C1G | -3.62 | 103.22      | 111.79   |
| 16  | b     | 614 | CLA  | CHD-C1D-ND  | -3.62 | 121.12      | 124.45   |
| 16  | b     | 601 | CLA  | CHC-C1C-C2C | -3.62 | 116.68      | 126.73   |
| 16  | b     | 602 | CLA  | CHA-C4D-ND  | 3.61  | 140.05      | 132.50   |
| 18  | b     | 618 | BCR  | C3-C4-C5    | -3.61 | 107.64      | 114.08   |
| 16  | d     | 404 | CLA  | C4A-NA-C1A  | -3.59 | 105.09      | 106.71   |
| 16  | b     | 603 | CLA  | CMC-C2C-C1C | 3.58  | 130.50      | 125.04   |
| 16  | b     | 604 | CLA  | CHA-C4D-ND  | 3.58  | 139.99      | 132.50   |
| 18  | h     | 101 | BCR  | C11-C10-C9  | -3.58 | 122.20      | 127.31   |
| 16  | b     | 606 | CLA  | C3B-C2B-C1B | -3.58 | 102.84      | 107.16   |
| 18  | a     | 407 | BCR  | C15-C14-C13 | -3.58 | 122.21      | 127.31   |
| 18  | b     | 619 | BCR  | C11-C10-C9  | -3.58 | 122.21      | 127.31   |
| 16  | b     | 609 | CLA  | CHD-C4C-C3C | -3.57 | 119.59      | 124.84   |
| 16  | b     | 603 | CLA  | CAC-C3C-C4C | 3.57  | 129.44      | 124.81   |
| 16  | b     | 610 | CLA  | CHC-C4B-NB  | 3.57  | 128.04      | 124.26   |
| 16  | b     | 610 | CLA  | CHD-C1D-ND  | -3.57 | 121.17      | 124.45   |
| 18  | b     | 619 | BCR  | C38-C26-C27 | 3.55  | 120.43      | 113.62   |
| 16  | b     | 602 | CLA  | CHC-C4B-NB  | 3.55  | 128.01      | 124.26   |
| 16  | b     | 614 | CLA  | C1C-C2C-C3C | -3.55 | 103.23      | 106.96   |
| 16  | b     | 611 | CLA  | O2D-CGD-O1D | -3.54 | 116.92      | 123.84   |
| 20  | d     | 410 | MGE  | C2G-O2G-C1B | -3.53 | 109.10      | 117.79   |
| 16  | a     | 406 | CLA  | C2A-C1A-CHA | -3.53 | 117.69      | 123.86   |
| 16  | b     | 608 | CLA  | C3B-C2B-C1B | -3.53 | 102.90      | 107.16   |
| 17  | a     | 404 | PHO  | C1C-C2C-C3C | -3.53 | 105.68      | 108.61   |
| 16  | b     | 612 | CLA  | C3B-C2B-C1B | -3.52 | 102.91      | 107.16   |
| 27  | e     | 101 | HEM  | C1B-NB-C4B  | 3.51  | 108.70      | 105.07   |
| 16  | d     | 405 | CLA  | C4C-C3C-C2C | -3.50 | 101.79      | 106.90   |
| 16  | b     | 604 | CLA  | C6-C5-C3    | -3.50 | 104.28      | 113.45   |
| 16  | b     | 603 | CLA  | C5-C3-C2    | -3.50 | 114.04      | 121.12   |
| 16  | b     | 616 | CLA  | CHD-C4C-NC  | 3.49  | 129.71      | 124.20   |
| 16  | a     | 403 | CLA  | CHC-C1C-C2C | -3.49 | 117.04      | 126.73   |
| 16  | b     | 611 | CLA  | C3D-C2D-C1D | -3.49 | 101.08      | 105.83   |
| 16  | d     | 404 | CLA  | C4C-C3C-C2C | -3.48 | 101.82      | 106.90   |
| 16  | b     | 616 | CLA  | O1D-CGD-CBD | -3.48 | 117.36      | 124.48   |
| 16  | b     | 606 | CLA  | O2D-CGD-CBD | 3.48  | 117.45      | 111.27   |
| 16  | a     | 403 | CLA  | CBC-CAC-C3C | -3.47 | 102.87      | 112.43   |
| 16  | b     | 608 | CLA  | C4D-CHA-C1A | -3.47 | 117.03      | 121.25   |
| 16  | d     | 401 | CLA  | CBC-CAC-C3C | -3.46 | 102.90      | 112.43   |
| 20  | d     | 409 | MGE  | C4D-C3D-C2D | 3.46  | 116.86      | 110.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | d     | 404 | CLA  | O2D-CGD-O1D | -3.45 | 117.10      | 123.84   |
| 20  | a     | 409 | MGE  | O2G-C1B-C2B | 3.44  | 118.92      | 111.50   |
| 16  | b     | 611 | CLA  | C1D-CHD-C4C | -3.44 | 118.63      | 126.06   |
| 16  | d     | 404 | CLA  | CHD-C1D-ND  | -3.44 | 121.29      | 124.45   |
| 18  | h     | 101 | BCR  | C28-C27-C26 | -3.44 | 107.94      | 114.08   |
| 18  | a     | 407 | BCR  | C21-C20-C19 | 3.43  | 133.93      | 123.22   |
| 16  | b     | 608 | CLA  | CHA-C4D-ND  | 3.43  | 139.67      | 132.50   |
| 16  | a     | 403 | CLA  | O2D-CGD-O1D | -3.42 | 117.15      | 123.84   |
| 27  | e     | 101 | HEM  | CHD-C1D-C2D | -3.40 | 119.67      | 124.98   |
| 16  | b     | 602 | CLA  | C1D-CHD-C4C | -3.40 | 118.72      | 126.06   |
| 16  | b     | 614 | CLA  | CMB-C2B-C1B | 3.40  | 130.54      | 125.37   |
| 16  | b     | 604 | CLA  | C3B-C2B-C1B | -3.40 | 103.06      | 107.16   |
| 16  | b     | 607 | CLA  | C4-C3-C5    | 3.39  | 120.98      | 115.27   |
| 16  | d     | 405 | CLA  | CMB-C2B-C1B | 3.38  | 130.52      | 125.37   |
| 16  | a     | 402 | CLA  | C7-C6-C5    | -3.38 | 104.18      | 113.36   |
| 17  | a     | 405 | PHO  | O1D-CGD-CBD | 3.38  | 130.36      | 124.74   |
| 16  | b     | 603 | CLA  | C3B-C4B-NB  | 3.38  | 113.65      | 110.52   |
| 16  | a     | 403 | CLA  | CHB-C4A-NA  | 3.37  | 129.18      | 124.51   |
| 16  | b     | 609 | CLA  | C4C-C3C-C2C | -3.37 | 101.98      | 106.90   |
| 16  | b     | 603 | CLA  | C4D-CHA-C1A | -3.36 | 117.16      | 121.25   |
| 16  | d     | 404 | CLA  | CHC-C4B-NB  | -3.36 | 120.70      | 124.26   |
| 16  | b     | 602 | CLA  | CMB-C2B-C3B | 3.36  | 134.73      | 126.59   |
| 16  | a     | 403 | CLA  | C4B-CHC-C1C | -3.36 | 118.38      | 126.34   |
| 16  | b     | 615 | CLA  | CHA-C4D-ND  | 3.35  | 139.51      | 132.50   |
| 16  | b     | 614 | CLA  | C4-C3-C2    | -3.35 | 115.08      | 123.68   |
| 16  | a     | 402 | CLA  | C1D-CHD-C4C | -3.34 | 118.84      | 126.06   |
| 16  | b     | 609 | CLA  | C1-C2-C3    | -3.34 | 120.26      | 126.04   |
| 27  | e     | 101 | HEM  | CHA-C4D-ND  | 3.33  | 128.49      | 124.37   |
| 16  | b     | 606 | CLA  | O2D-CGD-O1D | -3.32 | 117.34      | 123.84   |
| 20  | a     | 409 | MGE  | C1D-O6D-C5D | 3.32  | 120.20      | 113.69   |
| 16  | b     | 616 | CLA  | C4C-C3C-C2C | -3.31 | 102.07      | 106.90   |
| 18  | a     | 407 | BCR  | C16-C17-C18 | -3.31 | 122.59      | 127.31   |
| 16  | b     | 615 | CLA  | CMD-C2D-C3D | 3.30  | 135.22      | 127.61   |
| 16  | b     | 601 | CLA  | CMD-C2D-C3D | -3.30 | 120.01      | 127.61   |
| 20  | b     | 622 | MGE  | O1G-C1A-C2A | 3.30  | 122.27      | 111.91   |
| 16  | b     | 613 | CLA  | C1C-C2C-C3C | -3.30 | 103.49      | 106.96   |
| 16  | d     | 405 | CLA  | CHB-C4A-NA  | 3.29  | 129.06      | 124.51   |
| 16  | b     | 606 | CLA  | C4D-CHA-C1A | -3.28 | 117.25      | 121.25   |
| 16  | a     | 403 | CLA  | CHB-C1B-NB  | -3.28 | 120.78      | 124.26   |
| 18  | b     | 618 | BCR  | C15-C16-C17 | -3.27 | 116.77      | 123.47   |
| 16  | b     | 604 | CLA  | CMD-C2D-C1D | 3.27  | 130.48      | 124.71   |
| 16  | b     | 606 | CLA  | CMD-C2D-C1D | 3.26  | 130.45      | 124.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | b     | 617 | BCR  | C15-C14-C13 | -3.25 | 122.67      | 127.31   |
| 18  | b     | 617 | BCR  | C16-C17-C18 | -3.25 | 122.67      | 127.31   |
| 16  | b     | 605 | CLA  | C3B-C2B-C1B | -3.22 | 103.27      | 107.16   |
| 16  | b     | 604 | CLA  | C4D-CHA-C1A | -3.22 | 117.33      | 121.25   |
| 16  | b     | 614 | CLA  | C3B-C4B-NB  | 3.21  | 113.49      | 110.52   |
| 16  | b     | 607 | CLA  | CHC-C4B-NB  | 3.21  | 127.65      | 124.26   |
| 18  | b     | 617 | BCR  | C11-C10-C9  | -3.21 | 122.73      | 127.31   |
| 18  | b     | 618 | BCR  | C1-C6-C5    | -3.20 | 118.10      | 122.61   |
| 16  | b     | 608 | CLA  | O2A-CGA-O1A | -3.19 | 115.55      | 123.59   |
| 16  | b     | 610 | CLA  | C1D-CHD-C4C | -3.19 | 119.19      | 126.06   |
| 16  | b     | 602 | CLA  | C1-C2-C3    | -3.18 | 120.54      | 126.04   |
| 18  | h     | 101 | BCR  | C1-C6-C7    | 3.18  | 124.78      | 115.78   |
| 16  | b     | 608 | CLA  | C3C-C4C-NC  | 3.17  | 114.13      | 110.57   |
| 16  | b     | 613 | CLA  | C4D-CHA-C1A | -3.17 | 117.39      | 121.25   |
| 16  | b     | 601 | CLA  | CHA-C1A-NA  | -3.17 | 119.13      | 126.40   |
| 18  | a     | 407 | BCR  | C36-C18-C19 | 3.17  | 123.07      | 118.08   |
| 16  | b     | 615 | CLA  | C4-C3-C5    | 3.16  | 120.59      | 115.27   |
| 17  | a     | 404 | PHO  | CBA-CAA-C2A | -3.15 | 104.60      | 113.81   |
| 16  | b     | 611 | CLA  | CMC-C2C-C1C | 3.15  | 129.83      | 125.04   |
| 16  | b     | 614 | CLA  | CHB-C4A-NA  | 3.15  | 128.86      | 124.51   |
| 16  | b     | 606 | CLA  | CMC-C2C-C3C | 3.14  | 134.65      | 126.12   |
| 16  | b     | 613 | CLA  | C3C-C4C-NC  | 3.14  | 114.09      | 110.57   |
| 16  | d     | 404 | CLA  | CHC-C1C-C2C | -3.14 | 118.00      | 126.73   |
| 16  | b     | 612 | CLA  | C4-C3-C5    | 3.14  | 120.55      | 115.27   |
| 16  | b     | 605 | CLA  | CHA-C4D-ND  | 3.13  | 139.04      | 132.50   |
| 16  | d     | 405 | CLA  | CHC-C4B-NB  | -3.13 | 120.95      | 124.26   |
| 16  | d     | 404 | CLA  | CAC-C3C-C4C | 3.13  | 128.87      | 124.81   |
| 18  | b     | 617 | BCR  | C27-C26-C25 | -3.12 | 118.20      | 122.73   |
| 16  | d     | 404 | CLA  | CHB-C1B-NB  | -3.12 | 120.95      | 124.26   |
| 16  | b     | 605 | CLA  | C4C-C3C-C2C | -3.12 | 102.36      | 106.90   |
| 16  | d     | 404 | CLA  | O2A-CGA-CBA | 3.12  | 121.68      | 111.91   |
| 16  | b     | 605 | CLA  | CMB-C2B-C1B | 3.11  | 130.11      | 125.37   |
| 17  | a     | 405 | PHO  | C4-C3-C5    | 3.11  | 120.51      | 115.27   |
| 16  | b     | 610 | CLA  | CAA-CBA-CGA | -3.11 | 104.16      | 113.25   |
| 27  | e     | 101 | HEM  | CHD-C4C-NC  | 3.11  | 127.80      | 124.44   |
| 18  | b     | 618 | BCR  | C16-C17-C18 | -3.10 | 122.88      | 127.31   |
| 16  | d     | 404 | CLA  | CHB-C4A-NA  | 3.10  | 128.80      | 124.51   |
| 17  | a     | 405 | PHO  | C6-C5-C3    | 3.10  | 121.59      | 113.45   |
| 16  | b     | 612 | CLA  | O2D-CGD-CBD | 3.10  | 116.78      | 111.27   |
| 16  | d     | 401 | CLA  | CHA-C4D-ND  | 3.10  | 138.98      | 132.50   |
| 16  | b     | 605 | CLA  | C3A-C2A-C1A | -3.10 | 96.70       | 101.34   |
| 16  | d     | 401 | CLA  | C1D-ND-C4D  | -3.10 | 104.14      | 106.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | h     | 101 | BCR  | C20-C21-C22 | -3.09 | 122.90      | 127.31   |
| 20  | d     | 409 | MGE  | O1G-C1A-C2A | 3.09  | 121.60      | 111.91   |
| 16  | a     | 402 | CLA  | CMD-C2D-C1D | 3.08  | 130.15      | 124.71   |
| 27  | e     | 101 | HEM  | CHB-C1B-NB  | 3.08  | 128.17      | 124.37   |
| 16  | b     | 610 | CLA  | CMB-C2B-C1B | 3.07  | 130.05      | 125.37   |
| 16  | b     | 609 | CLA  | O2D-CGD-O1D | -3.07 | 117.84      | 123.84   |
| 16  | b     | 616 | CLA  | CHC-C4B-NB  | 3.07  | 127.51      | 124.26   |
| 16  | a     | 402 | CLA  | CAC-C3C-C2C | -3.07 | 122.28      | 127.53   |
| 16  | b     | 603 | CLA  | O2A-C1-C2   | -3.06 | 100.59      | 108.64   |
| 16  | b     | 614 | CLA  | CAC-C3C-C4C | 3.06  | 128.78      | 124.81   |
| 16  | b     | 602 | CLA  | C4-C3-C5    | 3.05  | 120.41      | 115.27   |
| 16  | b     | 614 | CLA  | C1D-CHD-C4C | -3.05 | 119.47      | 126.06   |
| 16  | d     | 405 | CLA  | O2D-CGD-O1D | -3.05 | 117.87      | 123.84   |
| 27  | e     | 101 | HEM  | CAD-CBD-CGD | -3.05 | 107.05      | 113.60   |
| 16  | b     | 607 | CLA  | C1C-C2C-C3C | -3.04 | 103.76      | 106.96   |
| 16  | b     | 614 | CLA  | CHA-C4D-ND  | 3.04  | 138.85      | 132.50   |
| 15  | l     | 101 | SQD  | O8-S-O7     | 3.04  | 118.69      | 111.27   |
| 16  | b     | 611 | CLA  | CHD-C1D-ND  | -3.03 | 121.67      | 124.45   |
| 18  | h     | 101 | BCR  | C34-C9-C10  | -3.03 | 118.67      | 122.92   |
| 16  | b     | 602 | CLA  | CMD-C2D-C3D | 3.03  | 134.59      | 127.61   |
| 18  | b     | 618 | BCR  | C33-C5-C4   | 3.03  | 119.43      | 113.62   |
| 16  | b     | 613 | CLA  | O2D-CGD-O1D | -3.02 | 117.94      | 123.84   |
| 17  | a     | 405 | PHO  | CAC-C3C-C2C | 3.01  | 132.68      | 127.53   |
| 18  | a     | 407 | BCR  | C20-C19-C18 | 3.01  | 134.86      | 126.42   |
| 16  | b     | 606 | CLA  | O2A-CGA-O1A | -3.00 | 116.01      | 123.59   |
| 16  | b     | 614 | CLA  | C3B-C2B-C1B | -3.00 | 103.53      | 107.16   |
| 16  | b     | 607 | CLA  | CMD-C2D-C1D | 3.00  | 130.00      | 124.71   |
| 18  | b     | 618 | BCR  | C11-C10-C9  | -3.00 | 123.03      | 127.31   |
| 16  | a     | 406 | CLA  | CHB-C4A-NA  | 3.00  | 128.66      | 124.51   |
| 18  | a     | 407 | BCR  | C4-C5-C6    | -3.00 | 118.38      | 122.73   |
| 16  | b     | 607 | CLA  | C3B-C2B-C1B | -2.99 | 103.55      | 107.16   |
| 18  | d     | 407 | BCR  | C11-C10-C9  | -2.99 | 123.05      | 127.31   |
| 16  | b     | 614 | CLA  | CHD-C4C-NC  | 2.99  | 128.91      | 124.20   |
| 20  | b     | 620 | MGE  | C1D-O6D-C5D | 2.99  | 119.55      | 113.69   |
| 17  | a     | 404 | PHO  | CBC-CAC-C3C | -2.98 | 108.52      | 112.88   |
| 15  | a     | 401 | SQD  | O8-S-O7     | 2.98  | 118.55      | 111.27   |
| 18  | h     | 101 | BCR  | C24-C23-C22 | -2.97 | 121.75      | 126.23   |
| 16  | b     | 613 | CLA  | C2A-C1A-CHA | -2.97 | 118.67      | 123.86   |
| 18  | b     | 618 | BCR  | C4-C5-C6    | -2.97 | 118.42      | 122.73   |
| 22  | t     | 101 | LMT  | C2'-C3'-C4' | 2.97  | 116.46      | 109.68   |
| 16  | b     | 606 | CLA  | CHD-C4C-NC  | 2.96  | 128.87      | 124.20   |
| 16  | b     | 603 | CLA  | O2D-CGD-CBD | 2.96  | 116.53      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | b     | 604 | CLA  | O2A-CGA-O1A | -2.96 | 116.11      | 123.59   |
| 16  | b     | 610 | CLA  | CHB-C4A-NA  | 2.96  | 128.60      | 124.51   |
| 16  | a     | 402 | CLA  | CHD-C4C-NC  | 2.95  | 128.85      | 124.20   |
| 16  | b     | 616 | CLA  | O2A-CGA-CBA | 2.95  | 123.88      | 112.23   |
| 16  | b     | 602 | CLA  | C2A-C3A-C4A | -2.95 | 97.11       | 101.87   |
| 16  | b     | 613 | CLA  | C1-O2A-CGA  | 2.95  | 124.17      | 116.44   |
| 16  | b     | 608 | CLA  | CAC-C3C-C4C | 2.93  | 128.62      | 124.81   |
| 18  | d     | 407 | BCR  | C16-C17-C18 | -2.93 | 123.13      | 127.31   |
| 16  | a     | 403 | CLA  | C2A-C1A-CHA | -2.93 | 118.74      | 123.86   |
| 18  | a     | 407 | BCR  | C8-C9-C10   | 2.93  | 123.44      | 118.94   |
| 16  | d     | 405 | CLA  | CMC-C2C-C1C | 2.92  | 129.49      | 125.04   |
| 16  | b     | 602 | CLA  | C4D-CHA-C1A | -2.92 | 117.69      | 121.25   |
| 16  | b     | 616 | CLA  | C1C-C2C-C3C | -2.92 | 103.89      | 106.96   |
| 16  | b     | 613 | CLA  | C3B-C2B-C1B | -2.92 | 103.64      | 107.16   |
| 16  | b     | 610 | CLA  | CHA-C4D-ND  | 2.92  | 138.60      | 132.50   |
| 16  | b     | 615 | CLA  | CHD-C4C-NC  | 2.91  | 128.79      | 124.20   |
| 16  | a     | 402 | CLA  | C4D-CHA-C1A | -2.91 | 117.71      | 121.25   |
| 16  | d     | 405 | CLA  | CHB-C1B-C2B | -2.91 | 119.03      | 127.24   |
| 16  | d     | 405 | CLA  | CAC-C3C-C4C | 2.91  | 128.58      | 124.81   |
| 15  | l     | 101 | SQD  | O48-C23-C24 | 2.89  | 120.99      | 111.91   |
| 16  | b     | 607 | CLA  | C4C-C3C-C2C | -2.89 | 102.68      | 106.90   |
| 16  | a     | 406 | CLA  | O2D-CGD-O1D | -2.89 | 118.19      | 123.84   |
| 24  | d     | 406 | PQ9  | C30-C31-C32 | 2.88  | 121.36      | 111.88   |
| 26  | d     | 412 | DGD  | O1G-C1A-C2A | 2.88  | 120.94      | 111.91   |
| 16  | a     | 406 | CLA  | CHB-C1B-C2B | -2.88 | 119.11      | 127.24   |
| 16  | b     | 605 | CLA  | CHC-C1C-NC  | -2.87 | 119.84      | 124.20   |
| 18  | h     | 101 | BCR  | C16-C15-C14 | -2.87 | 117.60      | 123.47   |
| 16  | b     | 614 | CLA  | C1-O2A-CGA  | 2.87  | 123.97      | 116.44   |
| 17  | a     | 405 | PHO  | O2D-CGD-O1D | -2.87 | 118.23      | 123.84   |
| 16  | b     | 616 | CLA  | O2D-CGD-O1D | -2.86 | 118.24      | 123.84   |
| 16  | b     | 609 | CLA  | C1C-C2C-C3C | -2.86 | 103.95      | 106.96   |
| 16  | b     | 602 | CLA  | CMA-C3A-C4A | -2.86 | 104.08      | 111.77   |
| 16  | b     | 606 | CLA  | C1D-ND-C4D  | -2.86 | 104.30      | 106.33   |
| 18  | b     | 619 | BCR  | C33-C5-C6   | -2.86 | 121.32      | 124.53   |
| 20  | d     | 410 | MGE  | O1G-C1A-C2A | 2.85  | 120.86      | 111.91   |
| 16  | b     | 605 | CLA  | C2A-C1A-CHA | -2.85 | 118.88      | 123.86   |
| 16  | b     | 607 | CLA  | CHD-C4C-NC  | 2.85  | 128.69      | 124.20   |
| 20  | d     | 408 | MGE  | C1D-O6D-C5D | 2.84  | 119.26      | 113.69   |
| 16  | b     | 612 | CLA  | C3B-C4B-NB  | 2.84  | 113.15      | 110.52   |
| 16  | a     | 403 | CLA  | CMC-C2C-C1C | 2.83  | 129.35      | 125.04   |
| 16  | b     | 614 | CLA  | C4-C3-C5    | 2.83  | 120.03      | 115.27   |
| 16  | b     | 605 | CLA  | O2D-CGD-O1D | -2.83 | 118.31      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | d     | 404 | CLA  | CMC-C2C-C1C | 2.82  | 129.34      | 125.04   |
| 18  | a     | 407 | BCR  | C36-C18-C17 | -2.82 | 118.97      | 122.92   |
| 20  | b     | 620 | MGE  | O1G-C1A-O1A | -2.81 | 116.49      | 123.59   |
| 18  | b     | 617 | BCR  | C8-C7-C6    | -2.81 | 119.30      | 127.20   |
| 16  | b     | 610 | CLA  | CMD-C2D-C1D | 2.79  | 129.63      | 124.71   |
| 16  | b     | 602 | CLA  | O2A-CGA-O1A | -2.79 | 116.56      | 123.59   |
| 16  | b     | 605 | CLA  | C4A-NA-C1A  | -2.78 | 105.45      | 106.71   |
| 16  | d     | 401 | CLA  | C4A-NA-C1A  | -2.78 | 105.45      | 106.71   |
| 15  | a     | 401 | SQD  | C45-O47-C7  | -2.78 | 112.72      | 117.90   |
| 18  | b     | 618 | BCR  | C30-C25-C26 | -2.77 | 118.71      | 122.61   |
| 16  | d     | 401 | CLA  | CMB-C2B-C1B | 2.77  | 129.59      | 125.37   |
| 16  | a     | 403 | CLA  | O2A-CGA-CBA | 2.76  | 120.58      | 111.91   |
| 16  | b     | 607 | CLA  | O2D-CGD-O1D | -2.76 | 118.44      | 123.84   |
| 16  | b     | 606 | CLA  | C3B-C4B-NB  | 2.76  | 113.08      | 110.52   |
| 16  | b     | 610 | CLA  | CHD-C4C-NC  | 2.76  | 128.55      | 124.20   |
| 16  | b     | 608 | CLA  | C3B-C4B-NB  | 2.75  | 113.07      | 110.52   |
| 18  | b     | 617 | BCR  | C30-C25-C26 | -2.75 | 118.74      | 122.61   |
| 16  | b     | 610 | CLA  | O2A-CGA-O1A | -2.74 | 116.67      | 123.59   |
| 16  | b     | 603 | CLA  | C1D-CHD-C4C | -2.74 | 120.14      | 126.06   |
| 16  | a     | 402 | CLA  | CHA-C4D-ND  | 2.74  | 138.24      | 132.50   |
| 16  | b     | 615 | CLA  | C3B-C4B-NB  | 2.74  | 113.06      | 110.52   |
| 16  | d     | 404 | CLA  | C2A-C1A-CHA | -2.74 | 119.07      | 123.86   |
| 16  | a     | 406 | CLA  | C1-C2-C3    | -2.74 | 122.32      | 126.75   |
| 16  | a     | 406 | CLA  | C4D-C3D-CAD | 2.73  | 111.31      | 108.10   |
| 16  | b     | 613 | CLA  | C3B-C4B-NB  | 2.73  | 113.05      | 110.52   |
| 18  | b     | 618 | BCR  | C8-C7-C6    | -2.73 | 119.53      | 127.20   |
| 16  | b     | 603 | CLA  | C2A-C1A-CHA | -2.73 | 119.09      | 123.86   |
| 16  | b     | 606 | CLA  | C1-O2A-CGA  | 2.73  | 123.59      | 116.44   |
| 26  | d     | 412 | DGD  | C1E-O6E-C5E | 2.73  | 119.04      | 113.69   |
| 16  | b     | 609 | CLA  | C7-C6-C5    | -2.72 | 105.96      | 113.36   |
| 16  | b     | 616 | CLA  | C2A-C1A-CHA | -2.72 | 119.10      | 123.86   |
| 16  | a     | 406 | CLA  | CMC-C2C-C1C | 2.72  | 129.18      | 125.04   |
| 16  | a     | 402 | CLA  | O2D-CGD-O1D | -2.71 | 118.53      | 123.84   |
| 16  | d     | 401 | CLA  | C3C-C4C-NC  | 2.71  | 113.61      | 110.57   |
| 20  | d     | 410 | MGE  | O6D-C1D-O3G | 2.71  | 116.39      | 109.97   |
| 24  | d     | 406 | PQ9  | C29-C28-C27 | -2.70 | 116.74      | 123.68   |
| 24  | d     | 406 | PQ9  | C19-C18-C20 | 2.70  | 119.81      | 115.27   |
| 16  | b     | 613 | CLA  | C4C-C3C-C2C | -2.70 | 102.96      | 106.90   |
| 16  | b     | 604 | CLA  | CED-O2D-CGD | 2.70  | 122.04      | 115.94   |
| 16  | b     | 614 | CLA  | C4B-CHC-C1C | -2.70 | 119.94      | 126.34   |
| 16  | b     | 611 | CLA  | C14-C13-C15 | -2.69 | 101.56      | 111.29   |
| 16  | b     | 616 | CLA  | CHA-C4D-ND  | 2.68  | 138.11      | 132.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | b     | 607 | CLA  | C4D-CHA-C1A | -2.68 | 117.99      | 121.25   |
| 16  | a     | 402 | CLA  | O2A-CGA-O1A | -2.68 | 116.83      | 123.59   |
| 24  | d     | 406 | PQ9  | C11-C12-C13 | -2.68 | 122.34      | 126.79   |
| 16  | d     | 405 | CLA  | CHC-C1C-C2C | -2.67 | 119.30      | 126.73   |
| 16  | b     | 601 | CLA  | CMB-C2B-C1B | 2.67  | 129.43      | 125.37   |
| 16  | b     | 609 | CLA  | C3D-C2D-C1D | -2.67 | 102.19      | 105.83   |
| 20  | d     | 408 | MGE  | O1G-C1A-C2A | 2.67  | 120.28      | 111.91   |
| 18  | b     | 617 | BCR  | C7-C8-C9    | -2.66 | 122.21      | 126.23   |
| 16  | b     | 603 | CLA  | C7-C6-C5    | -2.66 | 106.13      | 113.36   |
| 16  | b     | 607 | CLA  | O2D-CGD-CBD | 2.66  | 115.99      | 111.27   |
| 16  | a     | 403 | CLA  | CMD-C2D-C3D | -2.66 | 121.50      | 127.61   |
| 18  | b     | 619 | BCR  | C33-C5-C4   | 2.65  | 118.72      | 113.62   |
| 16  | a     | 406 | CLA  | CHC-C1C-C2C | -2.65 | 119.36      | 126.73   |
| 16  | b     | 614 | CLA  | CBC-CAC-C3C | -2.65 | 105.12      | 112.43   |
| 16  | b     | 615 | CLA  | CHC-C4B-C3B | -2.65 | 115.93      | 127.71   |
| 16  | b     | 609 | CLA  | CHA-C4D-ND  | 2.64  | 138.02      | 132.50   |
| 16  | a     | 406 | CLA  | CMB-C2B-C1B | 2.64  | 129.38      | 125.37   |
| 16  | b     | 612 | CLA  | O2A-CGA-CBA | 2.63  | 120.17      | 111.91   |
| 16  | b     | 615 | CLA  | CMB-C2B-C3B | 2.62  | 132.94      | 126.59   |
| 16  | a     | 403 | CLA  | CHB-C1B-C2B | -2.62 | 119.83      | 127.24   |
| 18  | h     | 101 | BCR  | C30-C25-C26 | -2.62 | 118.92      | 122.61   |
| 16  | b     | 611 | CLA  | CHC-C4B-NB  | 2.62  | 127.03      | 124.26   |
| 17  | a     | 405 | PHO  | C2D-C1D-ND  | -2.62 | 107.72      | 109.53   |
| 17  | a     | 404 | PHO  | C4-C3-C5    | 2.62  | 119.68      | 115.27   |
| 15  | a     | 401 | SQD  | C4-C3-C2    | 2.61  | 115.37      | 110.82   |
| 16  | b     | 604 | CLA  | C4C-C3C-C2C | -2.60 | 103.11      | 106.90   |
| 16  | d     | 404 | CLA  | CGD-CBD-CAD | -2.60 | 102.31      | 110.73   |
| 16  | b     | 608 | CLA  | C1D-CHD-C4C | -2.60 | 120.45      | 126.06   |
| 27  | e     | 101 | HEM  | C4C-NC-C1C  | 2.59  | 107.89      | 105.35   |
| 18  | d     | 407 | BCR  | C15-C14-C13 | -2.59 | 123.61      | 127.31   |
| 16  | a     | 406 | CLA  | O2A-CGA-CBA | 2.59  | 120.02      | 111.91   |
| 16  | d     | 405 | CLA  | O2A-CGA-CBA | 2.58  | 120.00      | 111.91   |
| 16  | b     | 615 | CLA  | CMA-C3A-C4A | -2.58 | 104.84      | 111.77   |
| 16  | b     | 613 | CLA  | O2A-CGA-CBA | 2.57  | 119.97      | 111.91   |
| 20  | d     | 409 | MGE  | C3G-O3G-C1D | -2.57 | 108.72      | 113.74   |
| 16  | b     | 614 | CLA  | CED-O2D-CGD | 2.57  | 121.74      | 115.94   |
| 18  | a     | 407 | BCR  | C28-C27-C26 | -2.56 | 109.50      | 114.08   |
| 20  | b     | 622 | MGE  | O1G-C1A-O1A | -2.56 | 117.12      | 123.59   |
| 18  | h     | 101 | BCR  | C7-C6-C5    | -2.56 | 115.26      | 121.46   |
| 16  | b     | 607 | CLA  | C3C-C4C-NC  | 2.56  | 113.44      | 110.57   |
| 16  | b     | 610 | CLA  | O2D-CGD-O1D | -2.56 | 118.84      | 123.84   |
| 16  | a     | 403 | CLA  | C1-C2-C3    | -2.55 | 122.62      | 126.75   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | b     | 618 | BCR  | C7-C8-C9    | -2.54 | 122.39      | 126.23   |
| 16  | b     | 611 | CLA  | CMD-C2D-C1D | 2.54  | 129.19      | 124.71   |
| 16  | b     | 607 | CLA  | CBC-CAC-C3C | -2.54 | 105.43      | 112.43   |
| 16  | b     | 616 | CLA  | CED-O2D-CGD | 2.54  | 121.68      | 115.94   |
| 16  | d     | 405 | CLA  | C2A-C1A-CHA | -2.54 | 119.42      | 123.86   |
| 18  | b     | 619 | BCR  | C32-C1-C6   | -2.53 | 106.19      | 110.30   |
| 16  | d     | 405 | CLA  | C4B-CHC-C1C | -2.53 | 120.33      | 126.34   |
| 20  | d     | 409 | MGE  | C3D-C4D-C5D | 2.53  | 114.76      | 110.24   |
| 16  | d     | 404 | CLA  | CMB-C2B-C1B | 2.53  | 129.22      | 125.37   |
| 16  | b     | 601 | CLA  | CHB-C4A-NA  | -2.53 | 121.02      | 124.51   |
| 18  | b     | 617 | BCR  | C38-C26-C27 | 2.53  | 118.47      | 113.62   |
| 16  | b     | 614 | CLA  | O2A-CGA-CBA | 2.53  | 119.83      | 111.91   |
| 18  | d     | 407 | BCR  | C16-C15-C14 | -2.52 | 118.31      | 123.47   |
| 18  | b     | 617 | BCR  | C21-C20-C19 | -2.52 | 115.36      | 123.22   |
| 20  | m     | 101 | MGE  | O1G-C1A-C2A | 2.52  | 119.80      | 111.91   |
| 16  | b     | 602 | CLA  | CHD-C4C-NC  | 2.51  | 128.16      | 124.20   |
| 16  | b     | 603 | CLA  | CHC-C4B-C3B | -2.51 | 116.54      | 127.71   |
| 20  | d     | 409 | MGE  | C1D-O6D-C5D | 2.51  | 118.61      | 113.69   |
| 16  | b     | 613 | CLA  | CHD-C4C-NC  | 2.50  | 128.15      | 124.20   |
| 17  | a     | 405 | PHO  | C4B-NB-C1B  | 2.50  | 112.70      | 108.83   |
| 16  | a     | 403 | CLA  | C4C-C3C-C2C | -2.50 | 103.25      | 106.90   |
| 18  | b     | 617 | BCR  | C1-C6-C5    | -2.50 | 119.09      | 122.61   |
| 16  | b     | 603 | CLA  | CMB-C2B-C3B | 2.50  | 132.63      | 126.59   |
| 16  | d     | 404 | CLA  | CHB-C1B-C2B | -2.50 | 120.19      | 127.24   |
| 16  | b     | 611 | CLA  | CHD-C4C-NC  | 2.49  | 128.13      | 124.20   |
| 17  | a     | 405 | PHO  | CBC-CAC-C3C | -2.49 | 109.23      | 112.88   |
| 18  | b     | 619 | BCR  | C1-C6-C5    | -2.49 | 119.11      | 122.61   |
| 16  | b     | 616 | CLA  | CBC-CAC-C3C | -2.49 | 105.58      | 112.43   |
| 22  | b     | 623 | LMT  | C2'-C3'-C4' | 2.48  | 115.36      | 109.68   |
| 16  | b     | 616 | CLA  | C4D-CHA-C1A | -2.48 | 118.23      | 121.25   |
| 16  | b     | 609 | CLA  | C2A-C1A-CHA | -2.48 | 119.53      | 123.86   |
| 16  | b     | 604 | CLA  | C7-C6-C5    | -2.48 | 106.63      | 113.36   |
| 16  | b     | 606 | CLA  | CBC-CAC-C3C | -2.48 | 105.60      | 112.43   |
| 16  | a     | 406 | CLA  | CMD-C2D-C3D | -2.48 | 121.92      | 127.61   |
| 18  | b     | 617 | BCR  | C4-C5-C6    | -2.48 | 119.14      | 122.73   |
| 16  | b     | 603 | CLA  | CHB-C1B-NB  | -2.47 | 121.64      | 124.26   |
| 17  | a     | 404 | PHO  | C5-C3-C2    | -2.47 | 116.12      | 121.12   |
| 18  | a     | 407 | BCR  | C33-C5-C4   | 2.47  | 118.35      | 113.62   |
| 16  | b     | 612 | CLA  | C4B-CHC-C1C | -2.46 | 120.49      | 126.34   |
| 16  | b     | 605 | CLA  | O2A-C1-C2   | -2.45 | 102.19      | 108.64   |
| 16  | b     | 615 | CLA  | O2A-CGA-O1A | -2.45 | 117.40      | 123.59   |
| 16  | b     | 606 | CLA  | CMB-C2B-C1B | 2.45  | 129.10      | 125.37   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | b     | 607 | CLA  | CGD-CBD-CAD | -2.45 | 102.80      | 110.73   |
| 16  | b     | 607 | CLA  | C7-C6-C5    | -2.45 | 106.71      | 113.36   |
| 18  | b     | 618 | BCR  | C28-C27-C26 | -2.45 | 109.71      | 114.08   |
| 18  | b     | 617 | BCR  | C40-C30-C25 | -2.44 | 106.33      | 110.30   |
| 16  | b     | 601 | CLA  | O1D-CGD-CBD | -2.44 | 119.49      | 124.48   |
| 16  | d     | 404 | CLA  | C4D-C3D-CAD | 2.44  | 110.97      | 108.10   |
| 16  | b     | 608 | CLA  | CMD-C2D-C1D | 2.44  | 129.01      | 124.71   |
| 16  | b     | 601 | CLA  | CHC-C4B-NB  | -2.44 | 121.67      | 124.26   |
| 16  | b     | 613 | CLA  | CHA-C4D-ND  | 2.44  | 137.60      | 132.50   |
| 16  | b     | 603 | CLA  | C3C-C4C-NC  | 2.44  | 113.30      | 110.57   |
| 16  | b     | 603 | CLA  | O2A-CGA-O1A | -2.44 | 117.44      | 123.59   |
| 16  | b     | 604 | CLA  | CHD-C1D-ND  | -2.44 | 122.22      | 124.45   |
| 20  | d     | 408 | MGE  | C4D-C3D-C2D | 2.43  | 115.07      | 110.82   |
| 16  | b     | 610 | CLA  | C3B-C4B-NB  | 2.43  | 112.77      | 110.52   |
| 16  | a     | 406 | CLA  | CHB-C1B-NB  | -2.43 | 121.69      | 124.26   |
| 22  | t     | 101 | LMT  | C1'-C2'-C3' | 2.43  | 115.05      | 110.00   |
| 20  | d     | 410 | MGE  | C1D-C2D-C3D | -2.43 | 104.94      | 110.00   |
| 16  | b     | 602 | CLA  | C2A-C1A-CHA | -2.42 | 119.62      | 123.86   |
| 16  | d     | 401 | CLA  | C1-O2A-CGA  | 2.42  | 122.80      | 116.44   |
| 20  | b     | 622 | MGE  | C3G-C2G-C1G | -2.42 | 106.06      | 111.79   |
| 15  | a     | 401 | SQD  | C3-C4-C5    | 2.42  | 114.55      | 110.24   |
| 24  | d     | 406 | PQ9  | C6-C5-C4    | 2.42  | 119.93      | 114.99   |
| 17  | a     | 405 | PHO  | CAA-CBA-CGA | -2.42 | 106.19      | 113.25   |
| 20  | a     | 409 | MGE  | O1G-C1A-C2A | 2.41  | 119.48      | 111.91   |
| 16  | b     | 612 | CLA  | CMB-C2B-C1B | 2.41  | 129.04      | 125.37   |
| 16  | b     | 601 | CLA  | CHD-C4C-C3C | -2.41 | 121.30      | 124.84   |
| 16  | b     | 602 | CLA  | O2A-CGA-CBA | 2.41  | 119.47      | 111.91   |
| 16  | b     | 612 | CLA  | CED-O2D-CGD | 2.40  | 121.37      | 115.94   |
| 20  | m     | 101 | MGE  | C4D-C3D-C2D | 2.40  | 115.01      | 110.82   |
| 16  | a     | 406 | CLA  | C3D-C4D-CHA | -2.39 | 107.25      | 112.72   |
| 20  | b     | 622 | MGE  | C2G-O2G-C1B | -2.39 | 111.91      | 117.79   |
| 16  | d     | 404 | CLA  | C4B-CHC-C1C | -2.39 | 120.67      | 126.34   |
| 16  | b     | 611 | CLA  | C3C-C4C-NC  | 2.38  | 113.23      | 110.57   |
| 17  | a     | 405 | PHO  | C6-C7-C8    | 2.37  | 123.59      | 115.92   |
| 17  | a     | 405 | PHO  | CMC-C2C-C3C | 2.37  | 132.56      | 126.12   |
| 20  | d     | 408 | MGE  | O3G-C1D-C2D | 2.37  | 112.00      | 108.30   |
| 16  | b     | 611 | CLA  | C7-C6-C5    | -2.36 | 106.95      | 113.36   |
| 20  | b     | 622 | MGE  | C4D-C3D-C2D | 2.35  | 114.92      | 110.82   |
| 18  | b     | 619 | BCR  | C30-C25-C26 | -2.35 | 119.31      | 122.61   |
| 16  | b     | 615 | CLA  | C11-C10-C8  | -2.34 | 108.36      | 115.92   |
| 16  | b     | 610 | CLA  | CHB-C1B-NB  | -2.34 | 121.78      | 124.26   |
| 16  | b     | 614 | CLA  | CHB-C1B-NB  | -2.34 | 121.78      | 124.26   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | d     | 401 | CLA  | CHC-C4B-C3B | -2.33 | 117.33      | 127.71   |
| 20  | b     | 622 | MGE  | C1D-O6D-C5D | 2.33  | 118.26      | 113.69   |
| 18  | b     | 617 | BCR  | C20-C21-C22 | -2.33 | 123.99      | 127.31   |
| 16  | b     | 607 | CLA  | C3B-C4B-NB  | 2.32  | 112.66      | 110.52   |
| 16  | a     | 403 | CLA  | C4D-C3D-CAD | 2.32  | 110.83      | 108.10   |
| 16  | d     | 404 | CLA  | C4-C3-C5    | 2.31  | 119.16      | 115.27   |
| 16  | d     | 405 | CLA  | CHB-C1B-NB  | -2.31 | 121.81      | 124.26   |
| 18  | h     | 101 | BCR  | C39-C30-C25 | -2.31 | 106.55      | 110.30   |
| 16  | d     | 404 | CLA  | O2A-CGA-O1A | -2.31 | 117.77      | 123.59   |
| 16  | a     | 402 | CLA  | CMC-C2C-C3C | 2.31  | 132.38      | 126.12   |
| 16  | b     | 602 | CLA  | C16-C17-C18 | -2.30 | 105.12      | 115.98   |
| 16  | b     | 614 | CLA  | C2A-C1A-CHA | -2.30 | 119.83      | 123.86   |
| 18  | a     | 407 | BCR  | C35-C13-C14 | -2.30 | 119.70      | 122.92   |
| 16  | b     | 612 | CLA  | CMC-C2C-C1C | 2.30  | 128.54      | 125.04   |
| 16  | b     | 611 | CLA  | CAC-C3C-C4C | 2.30  | 127.79      | 124.81   |
| 22  | t     | 101 | LMT  | O1B-C1B-O5B | -2.29 | 104.27      | 110.67   |
| 16  | b     | 605 | CLA  | C14-C13-C12 | -2.29 | 103.00      | 111.29   |
| 18  | d     | 407 | BCR  | C20-C21-C22 | -2.29 | 124.05      | 127.31   |
| 16  | d     | 401 | CLA  | CHD-C1D-ND  | -2.28 | 122.36      | 124.45   |
| 20  | a     | 409 | MGE  | O6D-C5D-C4D | 2.28  | 113.83      | 109.69   |
| 16  | b     | 609 | CLA  | CBC-CAC-C3C | -2.28 | 106.15      | 112.43   |
| 18  | d     | 407 | BCR  | C28-C27-C26 | -2.28 | 110.01      | 114.08   |
| 17  | a     | 404 | PHO  | O2D-CGD-O1D | -2.28 | 119.39      | 123.84   |
| 16  | a     | 402 | CLA  | C3B-C4B-NB  | 2.28  | 112.63      | 110.52   |
| 16  | b     | 614 | CLA  | C3D-C4D-CHA | -2.27 | 107.52      | 112.72   |
| 16  | b     | 602 | CLA  | CED-O2D-CGD | 2.27  | 121.07      | 115.94   |
| 16  | b     | 602 | CLA  | C3D-C4D-CHA | -2.27 | 107.54      | 112.72   |
| 16  | b     | 608 | CLA  | CHD-C4C-NC  | 2.26  | 127.77      | 124.20   |
| 18  | b     | 617 | BCR  | C16-C15-C14 | -2.26 | 118.84      | 123.47   |
| 15  | l     | 101 | SQD  | C4-C3-C2    | 2.26  | 114.77      | 110.82   |
| 22  | t     | 101 | LMT  | O1B-C1B-C2B | 2.26  | 113.95      | 108.10   |
| 16  | b     | 616 | CLA  | C1-O2A-CGA  | 2.25  | 123.52      | 116.11   |
| 16  | b     | 606 | CLA  | C3C-C4C-NC  | 2.25  | 113.09      | 110.57   |
| 16  | b     | 614 | CLA  | CHC-C4B-C3B | -2.25 | 117.70      | 127.71   |
| 16  | d     | 405 | CLA  | C1-O2A-CGA  | 2.24  | 122.33      | 116.44   |
| 16  | d     | 401 | CLA  | O2A-C1-C2   | -2.24 | 102.74      | 108.64   |
| 16  | b     | 611 | CLA  | C3B-C2B-C1B | -2.24 | 104.46      | 107.16   |
| 16  | a     | 402 | CLA  | O2A-CGA-CBA | 2.24  | 118.93      | 111.91   |
| 16  | a     | 406 | CLA  | CMA-C3A-C4A | -2.24 | 105.76      | 111.77   |
| 17  | a     | 404 | PHO  | CMB-C2B-C3B | 2.24  | 128.86      | 124.68   |
| 26  | d     | 412 | DGD  | O2G-C1B-O1B | -2.24 | 118.30      | 123.70   |
| 27  | e     | 101 | HEM  | C4D-ND-C1D  | 2.23  | 107.38      | 105.07   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | b     | 606 | CLA  | CHA-C4D-ND  | 2.23  | 137.16      | 132.50   |
| 16  | b     | 612 | CLA  | CHC-C4B-C3B | -2.23 | 117.81      | 127.71   |
| 16  | b     | 616 | CLA  | CMB-C2B-C3B | 2.22  | 131.96      | 126.59   |
| 16  | b     | 615 | CLA  | CHD-C1D-ND  | -2.22 | 122.42      | 124.45   |
| 18  | b     | 619 | BCR  | C29-C28-C27 | 2.21  | 116.31      | 111.38   |
| 16  | b     | 604 | CLA  | CHC-C4B-C3B | -2.21 | 117.90      | 127.71   |
| 16  | b     | 605 | CLA  | CAC-C3C-C2C | -2.20 | 123.76      | 127.53   |
| 16  | b     | 606 | CLA  | C4-C3-C5    | 2.20  | 118.97      | 115.27   |
| 27  | e     | 101 | HEM  | C4C-CHD-C1D | -2.20 | 121.32      | 126.06   |
| 16  | d     | 404 | CLA  | C1-C2-C3    | -2.20 | 122.25      | 126.04   |
| 16  | b     | 615 | CLA  | C1-O2A-CGA  | 2.20  | 122.20      | 116.44   |
| 16  | a     | 402 | CLA  | C1-C2-C3    | -2.19 | 122.25      | 126.04   |
| 16  | b     | 611 | CLA  | C16-C15-C13 | 2.18  | 122.97      | 115.92   |
| 18  | d     | 407 | BCR  | C21-C20-C19 | -2.18 | 116.42      | 123.22   |
| 16  | a     | 406 | CLA  | CAC-C3C-C2C | 2.17  | 131.25      | 127.53   |
| 16  | b     | 606 | CLA  | O2A-CGA-CBA | 2.17  | 118.72      | 111.91   |
| 16  | b     | 608 | CLA  | C6-C7-C8    | -2.17 | 108.91      | 115.92   |
| 16  | b     | 615 | CLA  | CBB-CAB-C3B | -2.17 | 116.83      | 127.62   |
| 20  | b     | 622 | MGE  | C3G-O3G-C1D | -2.17 | 109.50      | 113.74   |
| 18  | b     | 618 | BCR  | C33-C5-C6   | -2.16 | 122.10      | 124.53   |
| 20  | d     | 410 | MGE  | O6D-C5D-C6D | 2.16  | 111.80      | 106.44   |
| 16  | b     | 608 | CLA  | C3D-C4D-CHA | -2.16 | 107.79      | 112.72   |
| 16  | d     | 401 | CLA  | O2D-CGD-O1D | -2.15 | 119.62      | 123.84   |
| 16  | b     | 610 | CLA  | O2A-CGA-CBA | 2.15  | 118.67      | 111.91   |
| 16  | d     | 401 | CLA  | CMD-C2D-C3D | 2.15  | 132.57      | 127.61   |
| 16  | d     | 401 | CLA  | C4C-C3C-C2C | -2.15 | 103.76      | 106.90   |
| 16  | d     | 401 | CLA  | CGD-CBD-CAD | -2.15 | 103.77      | 110.73   |
| 16  | a     | 406 | CLA  | CAC-C3C-C4C | 2.15  | 127.59      | 124.81   |
| 16  | b     | 607 | CLA  | C1-C2-C3    | -2.14 | 122.34      | 126.04   |
| 16  | b     | 604 | CLA  | C3B-C4B-NB  | 2.14  | 112.50      | 110.52   |
| 27  | e     | 101 | HEM  | C1A-CHA-C4D | -2.14 | 121.26      | 126.34   |
| 24  | d     | 406 | PQ9  | C24-C23-C25 | 2.14  | 118.87      | 115.27   |
| 20  | d     | 409 | MGE  | O3D-C3D-C2D | -2.13 | 105.42      | 110.35   |
| 18  | b     | 617 | BCR  | C33-C5-C4   | 2.13  | 117.71      | 113.62   |
| 16  | b     | 604 | CLA  | C1D-CHD-C4C | -2.13 | 121.47      | 126.06   |
| 16  | b     | 611 | CLA  | C2A-C1A-CHA | -2.13 | 120.14      | 123.86   |
| 16  | b     | 609 | CLA  | CMB-C2B-C1B | 2.12  | 128.60      | 125.37   |
| 18  | d     | 407 | BCR  | C10-C11-C12 | -2.12 | 116.59      | 123.22   |
| 18  | b     | 617 | BCR  | C23-C24-C25 | -2.12 | 121.24      | 127.20   |
| 24  | d     | 406 | PQ9  | C29-C28-C30 | 2.12  | 118.84      | 115.27   |
| 20  | d     | 410 | MGE  | O1G-C1A-O1A | -2.12 | 118.25      | 123.59   |
| 16  | b     | 611 | CLA  | C3D-C4D-CHA | -2.12 | 107.88      | 112.72   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20  | d     | 409 | MGE  | O1G-C1A-O1A | -2.12 | 118.25      | 123.59   |
| 18  | b     | 619 | BCR  | C23-C24-C25 | -2.11 | 121.26      | 127.20   |
| 16  | b     | 606 | CLA  | CHC-C1C-C2C | -2.11 | 120.86      | 126.73   |
| 18  | b     | 619 | BCR  | C15-C16-C17 | -2.11 | 119.15      | 123.47   |
| 16  | d     | 401 | CLA  | OBD-CAD-C3D | -2.11 | 123.44      | 128.52   |
| 16  | b     | 605 | CLA  | C1-C2-C3    | -2.11 | 122.39      | 126.04   |
| 18  | b     | 618 | BCR  | C10-C11-C12 | -2.11 | 116.64      | 123.22   |
| 20  | d     | 408 | MGE  | C3G-O3G-C1D | -2.10 | 109.64      | 113.74   |
| 15  | a     | 401 | SQD  | O6-C1-C2    | 2.10  | 111.58      | 108.30   |
| 20  | b     | 620 | MGE  | O2G-C1B-O1B | -2.10 | 118.63      | 123.70   |
| 27  | e     | 101 | HEM  | C4B-C3B-C2B | -2.10 | 105.45      | 107.11   |
| 17  | a     | 405 | PHO  | CAC-C3C-C4C | -2.10 | 118.95      | 124.27   |
| 16  | b     | 614 | CLA  | C4D-C3D-CAD | 2.09  | 110.56      | 108.10   |
| 16  | b     | 615 | CLA  | CBC-CAC-C3C | -2.09 | 106.67      | 112.43   |
| 16  | b     | 614 | CLA  | C3D-C4D-ND  | 2.09  | 113.62      | 110.24   |
| 24  | d     | 406 | PQ9  | C14-C13-C15 | 2.09  | 118.78      | 115.27   |
| 16  | b     | 611 | CLA  | C17-C16-C15 | -2.09 | 103.65      | 113.24   |
| 18  | d     | 407 | BCR  | C33-C5-C6   | -2.09 | 122.18      | 124.53   |
| 16  | b     | 612 | CLA  | CHA-C4D-ND  | 2.09  | 136.87      | 132.50   |
| 16  | a     | 403 | CLA  | CHC-C4B-NB  | -2.08 | 122.05      | 124.26   |
| 16  | b     | 616 | CLA  | C3B-C4B-NB  | 2.08  | 112.45      | 110.52   |
| 16  | b     | 609 | CLA  | CBB-CAB-C3B | -2.08 | 117.26      | 127.62   |
| 16  | b     | 602 | CLA  | C17-C16-C15 | -2.08 | 103.67      | 113.24   |
| 16  | b     | 612 | CLA  | CMD-C2D-C1D | 2.08  | 128.38      | 124.71   |
| 18  | a     | 407 | BCR  | C34-C9-C10  | -2.07 | 120.02      | 122.92   |
| 16  | b     | 615 | CLA  | C5-C3-C2    | -2.07 | 116.92      | 121.12   |
| 20  | d     | 410 | MGE  | O6D-C5D-C4D | 2.07  | 113.45      | 109.69   |
| 16  | b     | 606 | CLA  | C4C-C3C-C2C | -2.07 | 103.88      | 106.90   |
| 16  | b     | 613 | CLA  | CHC-C4B-C3B | -2.07 | 118.51      | 127.71   |
| 16  | b     | 605 | CLA  | C5-C3-C2    | -2.07 | 116.94      | 121.12   |
| 16  | b     | 608 | CLA  | CMC-C2C-C1C | 2.06  | 128.18      | 125.04   |
| 16  | a     | 403 | CLA  | C3D-C4D-CHA | -2.06 | 108.00      | 112.72   |
| 16  | b     | 608 | CLA  | C6-C5-C3    | -2.06 | 108.04      | 113.45   |
| 16  | b     | 602 | CLA  | CHB-C1B-C2B | -2.06 | 121.41      | 127.24   |
| 17  | a     | 404 | PHO  | C6-C5-C3    | 2.06  | 118.86      | 113.45   |
| 16  | b     | 606 | CLA  | C4B-CHC-C1C | -2.06 | 121.45      | 126.34   |
| 16  | a     | 402 | CLA  | O2D-CGD-CBD | 2.06  | 114.93      | 111.27   |
| 16  | b     | 603 | CLA  | CBB-CAB-C3B | -2.06 | 117.38      | 127.62   |
| 16  | b     | 615 | CLA  | CHB-C1B-C2B | -2.06 | 121.42      | 127.24   |
| 16  | b     | 601 | CLA  | CHD-C1D-C2D | 2.06  | 129.79      | 125.48   |
| 17  | a     | 404 | PHO  | OBD-CAD-CBD | -2.05 | 122.81      | 125.82   |
| 16  | b     | 604 | CLA  | CBB-CAB-C3B | -2.05 | 117.41      | 127.62   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20  | d     | 410 | MGE  | O2G-C1B-O1B | -2.05 | 118.75      | 123.70   |
| 16  | a     | 402 | CLA  | C4C-C3C-C2C | -2.05 | 103.92      | 106.90   |
| 16  | b     | 608 | CLA  | C2A-C1A-CHA | -2.04 | 120.29      | 123.86   |
| 18  | h     | 101 | BCR  | C20-C19-C18 | -2.04 | 120.69      | 126.42   |
| 18  | a     | 407 | BCR  | C10-C11-C12 | 2.03  | 129.56      | 123.22   |
| 16  | d     | 404 | CLA  | CBC-CAC-C3C | -2.03 | 106.83      | 112.43   |
| 18  | d     | 407 | BCR  | C15-C16-C17 | -2.03 | 119.32      | 123.47   |
| 22  | d     | 402 | LMT  | C1-O1'-C1'  | -2.03 | 110.48      | 113.84   |
| 18  | a     | 407 | BCR  | C29-C28-C27 | -2.02 | 106.86      | 111.38   |
| 16  | a     | 403 | CLA  | C5-C3-C4    | 2.02  | 119.06      | 114.60   |
| 24  | d     | 406 | PQ9  | O4-C4-C5    | -2.02 | 117.10      | 120.59   |
| 16  | b     | 604 | CLA  | C6-C7-C8    | -2.01 | 109.41      | 115.92   |
| 20  | d     | 410 | MGE  | O3G-C3G-C2G | 2.01  | 115.76      | 110.90   |
| 15  | l     | 101 | SQD  | C3-C4-C5    | 2.01  | 113.83      | 110.24   |
| 16  | d     | 405 | CLA  | CMA-C3A-C4A | -2.01 | 106.36      | 111.77   |
| 16  | b     | 612 | CLA  | C1D-ND-C4D  | -2.01 | 104.91      | 106.33   |
| 16  | b     | 609 | CLA  | C4-C3-C5    | 2.01  | 118.65      | 115.27   |
| 16  | b     | 601 | CLA  | CMB-C2B-C3B | 2.01  | 131.45      | 126.59   |
| 16  | a     | 402 | CLA  | C3C-C4C-NC  | 2.01  | 112.82      | 110.57   |
| 16  | b     | 611 | CLA  | CHC-C4B-C3B | -2.00 | 118.80      | 127.71   |
| 16  | b     | 612 | CLA  | C2A-C1A-CHA | -2.00 | 120.36      | 123.86   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 16  | d     | 404 | CLA  | C8   |

All (294) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | a     | 401 | SQD  | O5-C5-C6-S      |
| 15  | a     | 401 | SQD  | C5-C6-S-O8      |
| 15  | l     | 101 | SQD  | C5-C6-S-O7      |
| 15  | l     | 101 | SQD  | C5-C6-S-O9      |
| 16  | a     | 403 | CLA  | C2B-C3B-CAB-CBB |
| 16  | a     | 403 | CLA  | C4B-C3B-CAB-CBB |
| 16  | a     | 406 | CLA  | C1A-C2A-CAA-CBA |
| 16  | a     | 406 | CLA  | C3A-C2A-CAA-CBA |
| 16  | b     | 601 | CLA  | C4B-C3B-CAB-CBB |
| 16  | b     | 601 | CLA  | CBD-CGD-O2D-CED |
| 16  | b     | 602 | CLA  | CHA-CBD-CGD-O1D |
| 16  | b     | 605 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | b     | 605 | CLA  | C4-C3-C5-C6     |
| 16  | b     | 606 | CLA  | CHA-CBD-CGD-O1D |
| 16  | b     | 614 | CLA  | CHA-CBD-CGD-O2D |
| 16  | b     | 614 | CLA  | CAD-CBD-CGD-O1D |
| 16  | b     | 614 | CLA  | CAD-CBD-CGD-O2D |
| 16  | b     | 614 | CLA  | C3-C5-C6-C7     |
| 16  | d     | 401 | CLA  | CHA-CBD-CGD-O2D |
| 17  | a     | 404 | PHO  | C2-C3-C5-C6     |
| 17  | a     | 404 | PHO  | C4-C3-C5-C6     |
| 17  | a     | 405 | PHO  | CBD-CGD-O2D-CED |
| 18  | a     | 407 | BCR  | C7-C8-C9-C10    |
| 18  | a     | 407 | BCR  | C7-C8-C9-C34    |
| 18  | a     | 407 | BCR  | C11-C12-C13-C14 |
| 18  | a     | 407 | BCR  | C11-C12-C13-C35 |
| 18  | a     | 407 | BCR  | C17-C18-C19-C20 |
| 18  | a     | 407 | BCR  | C36-C18-C19-C20 |
| 18  | d     | 407 | BCR  | C7-C8-C9-C34    |
| 18  | d     | 407 | BCR  | C21-C22-C23-C24 |
| 18  | d     | 407 | BCR  | C37-C22-C23-C24 |
| 18  | h     | 101 | BCR  | C5-C6-C7-C8     |
| 20  | a     | 409 | MGE  | O2G-C2G-C3G-O3G |
| 20  | b     | 620 | MGE  | O2G-C2G-C3G-O3G |
| 20  | d     | 410 | MGE  | O6D-C1D-O3G-C3G |
| 20  | m     | 101 | MGE  | C2B-C1B-O2G-C2G |
| 20  | m     | 101 | MGE  | O1B-C1B-O2G-C2G |
| 24  | d     | 406 | PQ9  | C38-C40-C41-C42 |
| 27  | e     | 101 | HEM  | C2B-C3B-CAB-CBB |
| 27  | e     | 101 | HEM  | C4B-C3B-CAB-CBB |
| 27  | e     | 101 | HEM  | C2C-C3C-CAC-CBC |
| 27  | e     | 101 | HEM  | C4C-C3C-CAC-CBC |
| 15  | a     | 401 | SQD  | C8-C7-O47-C45   |
| 17  | a     | 405 | PHO  | O1D-CGD-O2D-CED |
| 16  | d     | 405 | CLA  | CBD-CGD-O2D-CED |
| 16  | a     | 406 | CLA  | O1A-CGA-O2A-C1  |
| 16  | a     | 406 | CLA  | CBA-CGA-O2A-C1  |
| 16  | b     | 601 | CLA  | O1D-CGD-O2D-CED |
| 16  | d     | 404 | CLA  | C4-C3-C5-C6     |
| 16  | b     | 604 | CLA  | C3-C5-C6-C7     |
| 15  | a     | 401 | SQD  | O49-C7-O47-C45  |
| 16  | b     | 614 | CLA  | C4-C3-C5-C6     |
| 17  | a     | 405 | PHO  | C4-C3-C5-C6     |
| 24  | d     | 406 | PQ9  | C39-C38-C40-C41 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | b     | 614 | CLA  | C2-C3-C5-C6     |
| 17  | a     | 405 | PHO  | C2-C3-C5-C6     |
| 24  | d     | 406 | PQ9  | C37-C38-C40-C41 |
| 22  | t     | 101 | LMT  | O5'-C5'-C6'-O6' |
| 24  | d     | 406 | PQ9  | C13-C15-C16-C17 |
| 24  | d     | 406 | PQ9  | C23-C25-C26-C27 |
| 16  | d     | 405 | CLA  | O1D-CGD-O2D-CED |
| 16  | b     | 604 | CLA  | C13-C15-C16-C17 |
| 20  | m     | 101 | MGE  | C1A-C2A-C3A-C4A |
| 22  | t     | 101 | LMT  | C4'-C5'-C6'-O6' |
| 16  | d     | 404 | CLA  | C2-C3-C5-C6     |
| 18  | h     | 101 | BCR  | C7-C8-C9-C34    |
| 18  | h     | 101 | BCR  | C36-C18-C19-C20 |
| 18  | h     | 101 | BCR  | C7-C8-C9-C10    |
| 20  | d     | 410 | MGE  | C1A-C2A-C3A-C4A |
| 16  | d     | 404 | CLA  | C8-C10-C11-C12  |
| 16  | b     | 606 | CLA  | C11-C12-C13-C15 |
| 18  | h     | 101 | BCR  | C9-C10-C11-C12  |
| 16  | d     | 404 | CLA  | C10-C11-C12-C13 |
| 22  | t     | 101 | LMT  | O5'-C1'-O1'-C1  |
| 16  | b     | 603 | CLA  | C5-C6-C7-C8     |
| 17  | a     | 405 | PHO  | C5-C6-C7-C8     |
| 16  | a     | 402 | CLA  | C15-C16-C17-C18 |
| 20  | b     | 622 | MGE  | C2B-C1B-O2G-C2G |
| 20  | b     | 622 | MGE  | O1B-C1B-O2G-C2G |
| 16  | b     | 606 | CLA  | C13-C15-C16-C17 |
| 16  | b     | 615 | CLA  | C10-C11-C12-C13 |
| 20  | m     | 101 | MGE  | C5B-C6B-C7B-C8B |
| 15  | l     | 101 | SQD  | C14-C15-C16-C17 |
| 20  | d     | 410 | MGE  | C2D-C1D-O3G-C3G |
| 22  | t     | 101 | LMT  | C2'-C1'-O1'-C1  |
| 20  | d     | 408 | MGE  | C5B-C6B-C7B-C8B |
| 16  | b     | 606 | CLA  | C16-C17-C18-C19 |
| 17  | a     | 404 | PHO  | C16-C17-C18-C20 |
| 20  | b     | 620 | MGE  | C4A-C5A-C6A-C7A |
| 18  | d     | 407 | BCR  | C7-C8-C9-C10    |
| 17  | a     | 404 | PHO  | C16-C17-C18-C19 |
| 20  | d     | 410 | MGE  | C5B-C6B-C7B-C8B |
| 15  | l     | 101 | SQD  | C23-C24-C25-C26 |
| 20  | a     | 409 | MGE  | C5B-C6B-C7B-C8B |
| 16  | b     | 611 | CLA  | O1D-CGD-O2D-CED |
| 20  | d     | 410 | MGE  | C2B-C1B-O2G-C2G |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | b     | 601 | CLA  | C2B-C3B-CAB-CBB |
| 16  | b     | 608 | CLA  | C13-C15-C16-C17 |
| 16  | a     | 402 | CLA  | C2C-C3C-CAC-CBC |
| 18  | a     | 407 | BCR  | C23-C24-C25-C26 |
| 18  | a     | 407 | BCR  | C23-C24-C25-C30 |
| 18  | d     | 407 | BCR  | C1-C6-C7-C8     |
| 18  | d     | 407 | BCR  | C5-C6-C7-C8     |
| 18  | d     | 407 | BCR  | C23-C24-C25-C26 |
| 18  | d     | 407 | BCR  | C23-C24-C25-C30 |
| 18  | h     | 101 | BCR  | C1-C6-C7-C8     |
| 18  | h     | 101 | BCR  | C23-C24-C25-C26 |
| 18  | h     | 101 | BCR  | C23-C24-C25-C30 |
| 20  | a     | 409 | MGE  | C6B-C7B-C8B-C9B |
| 16  | b     | 606 | CLA  | C6-C7-C8-C10    |
| 20  | a     | 409 | MGE  | C2B-C3B-C4B-C5B |
| 20  | b     | 622 | MGE  | C1A-C2A-C3A-C4A |
| 16  | b     | 611 | CLA  | C13-C15-C16-C17 |
| 16  | b     | 612 | CLA  | C13-C15-C16-C17 |
| 16  | d     | 404 | CLA  | C5-C6-C7-C8     |
| 20  | m     | 101 | MGE  | C3A-C4A-C5A-C6A |
| 16  | b     | 603 | CLA  | CBD-CGD-O2D-CED |
| 15  | l     | 101 | SQD  | C8-C7-O47-C45   |
| 16  | d     | 401 | CLA  | C2C-C3C-CAC-CBC |
| 26  | d     | 412 | DGD  | C4B-C5B-C6B-C7B |
| 15  | l     | 101 | SQD  | O49-C7-O47-C45  |
| 20  | d     | 410 | MGE  | O1B-C1B-O2G-C2G |
| 15  | l     | 101 | SQD  | O47-C45-C46-O48 |
| 20  | d     | 408 | MGE  | O6D-C5D-C6D-O5D |
| 20  | b     | 622 | MGE  | C9B-CAB-CBB-CCB |
| 20  | m     | 101 | MGE  | C4A-C5A-C6A-C7A |
| 20  | b     | 620 | MGE  | C3B-C4B-C5B-C6B |
| 26  | d     | 412 | DGD  | O6E-C5E-C6E-O5E |
| 22  | d     | 402 | LMT  | C4B-C5B-C6B-O6B |
| 16  | b     | 606 | CLA  | C2A-CAA-CBA-CGA |
| 18  | h     | 101 | BCR  | C37-C22-C23-C24 |
| 16  | b     | 602 | CLA  | C16-C17-C18-C19 |
| 16  | b     | 606 | CLA  | C16-C17-C18-C20 |
| 15  | l     | 101 | SQD  | C18-C19-C20-C21 |
| 16  | b     | 614 | CLA  | O1D-CGD-O2D-CED |
| 15  | l     | 101 | SQD  | C44-C45-C46-O48 |
| 20  | b     | 620 | MGE  | O1G-C1G-C2G-C3G |
| 20  | b     | 620 | MGE  | C1G-C2G-C3G-O3G |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | a     | 409 | MGE  | C2A-C1A-O1G-C1G |
| 22  | b     | 623 | LMT  | C4'-C5'-C6'-O6' |
| 20  | d     | 410 | MGE  | C2G-C3G-O3G-C1D |
| 20  | b     | 622 | MGE  | CAB-CBB-CCB-CDB |
| 20  | a     | 409 | MGE  | C1B-C2B-C3B-C4B |
| 20  | d     | 410 | MGE  | O6D-C5D-C6D-O5D |
| 20  | m     | 101 | MGE  | C4B-C5B-C6B-C7B |
| 16  | b     | 602 | CLA  | C16-C17-C18-C20 |
| 20  | a     | 409 | MGE  | O1A-C1A-O1G-C1G |
| 17  | a     | 405 | PHO  | C15-C16-C17-C18 |
| 16  | b     | 606 | CLA  | C12-C13-C15-C16 |
| 17  | a     | 404 | PHO  | C6-C7-C8-C10    |
| 16  | b     | 611 | CLA  | C14-C13-C15-C16 |
| 17  | a     | 404 | PHO  | C6-C7-C8-C9     |
| 20  | a     | 409 | MGE  | C1A-C2A-C3A-C4A |
| 16  | b     | 609 | CLA  | C4B-C3B-CAB-CBB |
| 16  | b     | 612 | CLA  | C3-C5-C6-C7     |
| 16  | b     | 615 | CLA  | O1D-CGD-O2D-CED |
| 20  | d     | 409 | MGE  | C1B-C2B-C3B-C4B |
| 16  | a     | 402 | CLA  | C4C-C3C-CAC-CBC |
| 16  | b     | 615 | CLA  | C5-C6-C7-C8     |
| 20  | b     | 620 | MGE  | C8B-C9B-CAB-CBB |
| 20  | d     | 410 | MGE  | C2B-C3B-C4B-C5B |
| 16  | b     | 615 | CLA  | C16-C17-C18-C20 |
| 20  | a     | 409 | MGE  | C1G-C2G-C3G-O3G |
| 20  | b     | 622 | MGE  | C7A-C8A-C9A-CAA |
| 16  | d     | 401 | CLA  | C4C-C3C-CAC-CBC |
| 22  | t     | 101 | LMT  | C5-C6-C7-C8     |
| 16  | a     | 402 | CLA  | C16-C17-C18-C20 |
| 20  | b     | 622 | MGE  | C2A-C3A-C4A-C5A |
| 16  | d     | 405 | CLA  | C2B-C3B-CAB-CBB |
| 15  | l     | 101 | SQD  | C7-C8-C9-C10    |
| 16  | b     | 610 | CLA  | C11-C12-C13-C14 |
| 26  | d     | 412 | DGD  | C3B-C4B-C5B-C6B |
| 17  | a     | 404 | PHO  | C8-C10-C11-C12  |
| 20  | d     | 410 | MGE  | O2G-C1B-C2B-C3B |
| 20  | a     | 409 | MGE  | C7B-C8B-C9B-CAB |
| 16  | b     | 604 | CLA  | C6-C7-C8-C10    |
| 16  | b     | 611 | CLA  | C12-C13-C15-C16 |
| 16  | b     | 615 | CLA  | C16-C17-C18-C19 |
| 20  | d     | 408 | MGE  | C4B-C5B-C6B-C7B |
| 16  | b     | 604 | CLA  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | a     | 405 | PHO  | CAD-CBD-CGD-O2D |
| 17  | a     | 404 | PHO  | C15-C16-C17-C18 |
| 17  | a     | 404 | PHO  | C3-C5-C6-C7     |
| 20  | b     | 622 | MGE  | C2A-C1A-O1G-C1G |
| 22  | d     | 402 | LMT  | C5-C6-C7-C8     |
| 16  | a     | 403 | CLA  | CHA-CBD-CGD-O1D |
| 16  | a     | 403 | CLA  | CHA-CBD-CGD-O2D |
| 20  | b     | 622 | MGE  | C3B-C4B-C5B-C6B |
| 16  | b     | 606 | CLA  | C11-C12-C13-C14 |
| 20  | d     | 410 | MGE  | C9A-CAA-CBA-CCA |
| 20  | b     | 622 | MGE  | C1B-C2B-C3B-C4B |
| 16  | d     | 404 | CLA  | O1D-CGD-O2D-CED |
| 16  | d     | 405 | CLA  | C4B-C3B-CAB-CBB |
| 20  | a     | 409 | MGE  | C2A-C3A-C4A-C5A |
| 15  | l     | 101 | SQD  | O5-C5-C6-S      |
| 16  | b     | 605 | CLA  | CAD-CBD-CGD-O1D |
| 16  | b     | 607 | CLA  | CAD-CBD-CGD-O1D |
| 17  | a     | 405 | PHO  | C11-C10-C8-C7   |
| 20  | b     | 622 | MGE  | O1A-C1A-O1G-C1G |
| 16  | b     | 615 | CLA  | C13-C15-C16-C17 |
| 20  | b     | 620 | MGE  | C1A-C2A-C3A-C4A |
| 20  | b     | 620 | MGE  | C9B-CAB-CBB-CCB |
| 16  | b     | 606 | CLA  | C15-C16-C17-C18 |
| 17  | a     | 405 | PHO  | C8-C10-C11-C12  |
| 16  | b     | 604 | CLA  | C6-C7-C8-C9     |
| 16  | b     | 606 | CLA  | C14-C13-C15-C16 |
| 20  | b     | 620 | MGE  | C1B-C2B-C3B-C4B |
| 18  | a     | 407 | BCR  | C18-C19-C20-C21 |
| 17  | a     | 404 | PHO  | C5-C6-C7-C8     |
| 18  | h     | 101 | BCR  | C17-C18-C19-C20 |
| 20  | b     | 620 | MGE  | CAA-CBA-CCA-CDA |
| 20  | a     | 409 | MGE  | O6D-C5D-C6D-O5D |
| 16  | b     | 609 | CLA  | C2B-C3B-CAB-CBB |
| 26  | d     | 412 | DGD  | C6B-C7B-C8B-C9B |
| 16  | d     | 404 | CLA  | CAA-CBA-CGA-O2A |
| 16  | b     | 614 | CLA  | C2-C1-O2A-CGA   |
| 22  | d     | 402 | LMT  | O5B-C5B-C6B-O6B |
| 26  | d     | 412 | DGD  | C3A-C4A-C5A-C6A |
| 20  | b     | 620 | MGE  | O1G-C1G-C2G-O2G |
| 20  | d     | 409 | MGE  | C2B-C3B-C4B-C5B |
| 26  | d     | 412 | DGD  | C5B-C6B-C7B-C8B |
| 20  | b     | 622 | MGE  | C7B-C8B-C9B-CAB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | d     | 409 | MGE  | C8B-C9B-CAB-CBB |
| 26  | d     | 412 | DGD  | C2B-C3B-C4B-C5B |
| 24  | d     | 406 | PQ9  | C19-C18-C20-C21 |
| 16  | b     | 607 | CLA  | C3-C5-C6-C7     |
| 15  | l     | 101 | SQD  | C12-C13-C14-C15 |
| 26  | d     | 412 | DGD  | CAA-CBA-CCA-CDA |
| 16  | b     | 615 | CLA  | C14-C13-C15-C16 |
| 16  | d     | 404 | CLA  | C6-C7-C8-C9     |
| 18  | b     | 618 | BCR  | C19-C20-C21-C22 |
| 22  | d     | 402 | LMT  | C6-C7-C8-C9     |
| 20  | d     | 409 | MGE  | CAB-CBB-CCB-CDB |
| 16  | b     | 612 | CLA  | CBA-CGA-O2A-C1  |
| 18  | b     | 618 | BCR  | C13-C14-C15-C16 |
| 20  | d     | 409 | MGE  | C9B-CAB-CBB-CCB |
| 20  | d     | 408 | MGE  | C3A-C4A-C5A-C6A |
| 16  | b     | 612 | CLA  | C10-C11-C12-C13 |
| 20  | b     | 622 | MGE  | O2G-C2G-C3G-O3G |
| 20  | m     | 101 | MGE  | O1G-C1A-C2A-C3A |
| 16  | a     | 406 | CLA  | CBD-CGD-O2D-CED |
| 22  | t     | 101 | LMT  | C6-C7-C8-C9     |
| 20  | a     | 409 | MGE  | C7A-C8A-C9A-CAA |
| 27  | e     | 101 | HEM  | CAA-CBA-CGA-O1A |
| 16  | a     | 403 | CLA  | C1A-C2A-CAA-CBA |
| 16  | b     | 615 | CLA  | C12-C13-C15-C16 |
| 24  | d     | 406 | PQ9  | C17-C18-C20-C21 |
| 27  | e     | 101 | HEM  | CAA-CBA-CGA-O2A |
| 16  | b     | 610 | CLA  | C2A-CAA-CBA-CGA |
| 16  | d     | 405 | CLA  | O1A-CGA-O2A-C1  |
| 16  | d     | 401 | CLA  | C15-C16-C17-C18 |
| 16  | b     | 610 | CLA  | C16-C17-C18-C20 |
| 22  | t     | 101 | LMT  | C4-C5-C6-C7     |
| 16  | d     | 404 | CLA  | C14-C13-C15-C16 |
| 17  | a     | 404 | PHO  | C2A-CAA-CBA-CGA |
| 24  | d     | 406 | PQ9  | C24-C23-C25-C26 |
| 20  | d     | 410 | MGE  | O1B-C1B-C2B-C3B |
| 17  | a     | 404 | PHO  | CBA-CGA-O2A-C1  |
| 15  | l     | 101 | SQD  | O48-C23-C24-C25 |
| 26  | d     | 412 | DGD  | C2B-C1B-O2G-C2G |
| 16  | b     | 615 | CLA  | C3A-C2A-CAA-CBA |
| 20  | b     | 620 | MGE  | O2G-C1B-C2B-C3B |
| 16  | a     | 402 | CLA  | CAD-CBD-CGD-O2D |
| 16  | b     | 610 | CLA  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | b     | 616 | CLA  | CAD-CBD-CGD-O2D |
| 20  | d     | 408 | MGE  | CBB-CCB-CDB-CEB |
| 20  | d     | 408 | MGE  | O1G-C1A-C2A-C3A |
| 18  | h     | 101 | BCR  | C21-C22-C23-C24 |
| 16  | b     | 604 | CLA  | O2A-C1-C2-C3    |
| 17  | a     | 405 | PHO  | O2A-C1-C2-C3    |
| 16  | b     | 602 | CLA  | CHA-CBD-CGD-O2D |
| 16  | b     | 605 | CLA  | CHA-CBD-CGD-O1D |
| 16  | b     | 606 | CLA  | CHA-CBD-CGD-O2D |
| 16  | b     | 611 | CLA  | CHA-CBD-CGD-O2D |
| 16  | b     | 614 | CLA  | CHA-CBD-CGD-O1D |
| 16  | b     | 616 | CLA  | CHA-CBD-CGD-O1D |
| 17  | a     | 404 | PHO  | O1A-CGA-O2A-C1  |
| 16  | d     | 405 | CLA  | CBA-CGA-O2A-C1  |
| 16  | d     | 401 | CLA  | C11-C12-C13-C14 |
| 16  | a     | 406 | CLA  | C2A-CAA-CBA-CGA |
| 16  | b     | 603 | CLA  | C2A-CAA-CBA-CGA |
| 20  | d     | 408 | MGE  | O1A-C1A-C2A-C3A |
| 20  | b     | 620 | MGE  | O1B-C1B-C2B-C3B |
| 16  | b     | 603 | CLA  | C13-C15-C16-C17 |
| 15  | l     | 101 | SQD  | O10-C23-C24-C25 |
| 20  | b     | 622 | MGE  | O2G-C1B-C2B-C3B |
| 16  | b     | 604 | CLA  | C16-C17-C18-C19 |
| 16  | b     | 611 | CLA  | C16-C17-C18-C20 |
| 16  | b     | 612 | CLA  | C6-C7-C8-C9     |
| 16  | b     | 612 | CLA  | C11-C10-C8-C9   |
| 20  | d     | 410 | MGE  | C9B-CAB-CBB-CCB |
| 16  | b     | 612 | CLA  | C11-C10-C8-C7   |
| 20  | b     | 622 | MGE  | O1B-C1B-C2B-C3B |
| 20  | d     | 409 | MGE  | C6B-C7B-C8B-C9B |

There are no ring outliers.

41 monomers are involved in 141 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 16  | b     | 610 | CLA  | 3       | 0            |
| 24  | d     | 406 | PQ9  | 6       | 0            |
| 16  | a     | 402 | CLA  | 8       | 0            |
| 16  | b     | 607 | CLA  | 10      | 0            |
| 22  | t     | 101 | LMT  | 1       | 0            |
| 16  | b     | 603 | CLA  | 2       | 0            |
| 16  | b     | 612 | CLA  | 1       | 0            |

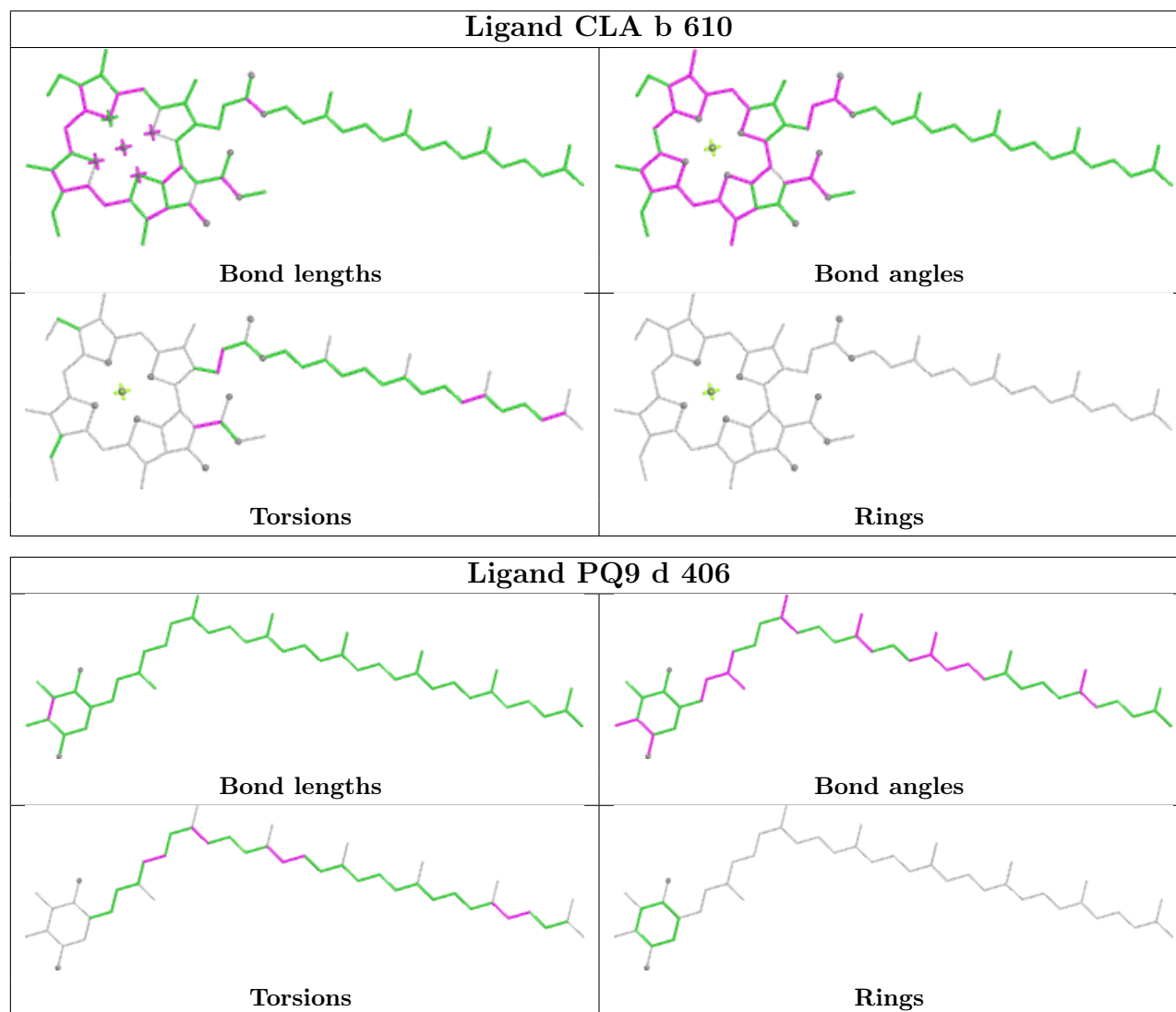
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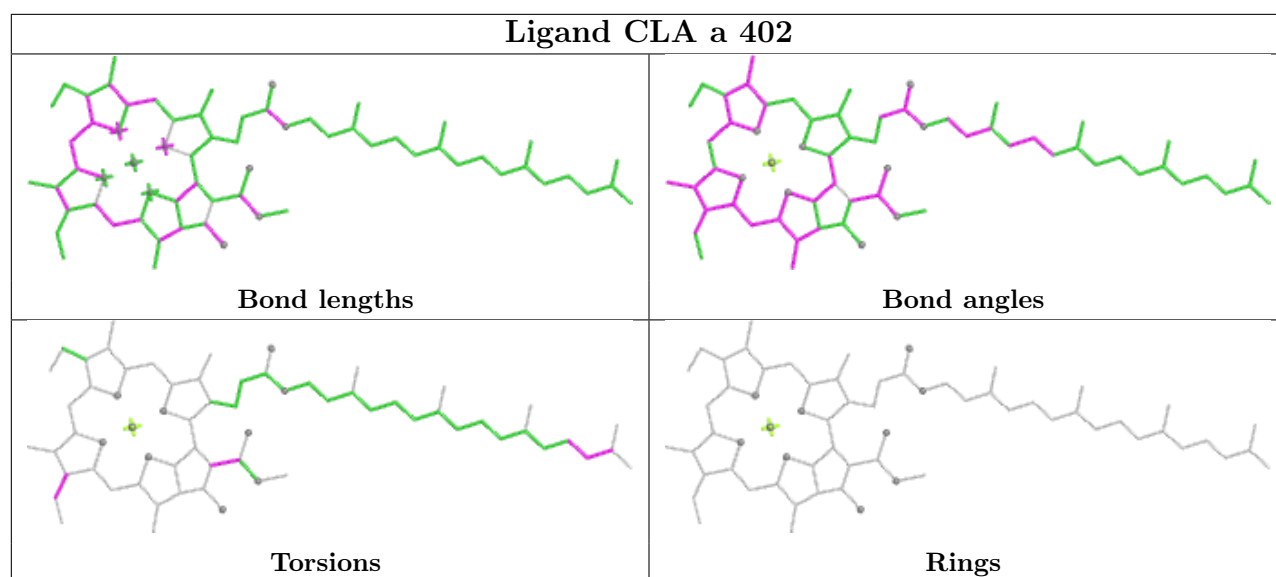
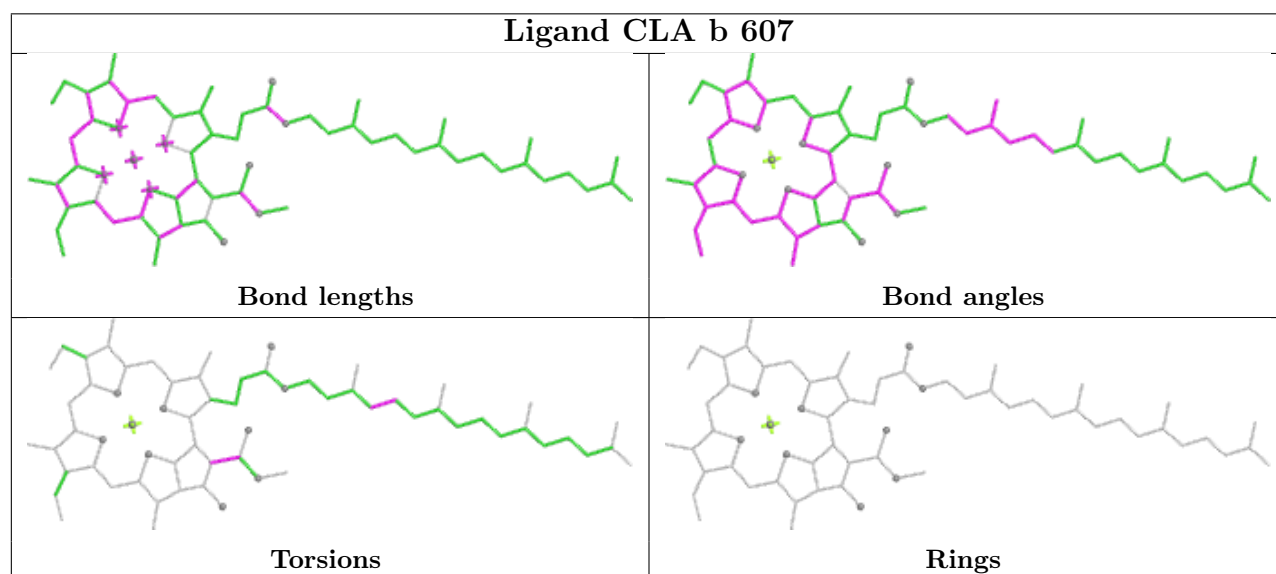
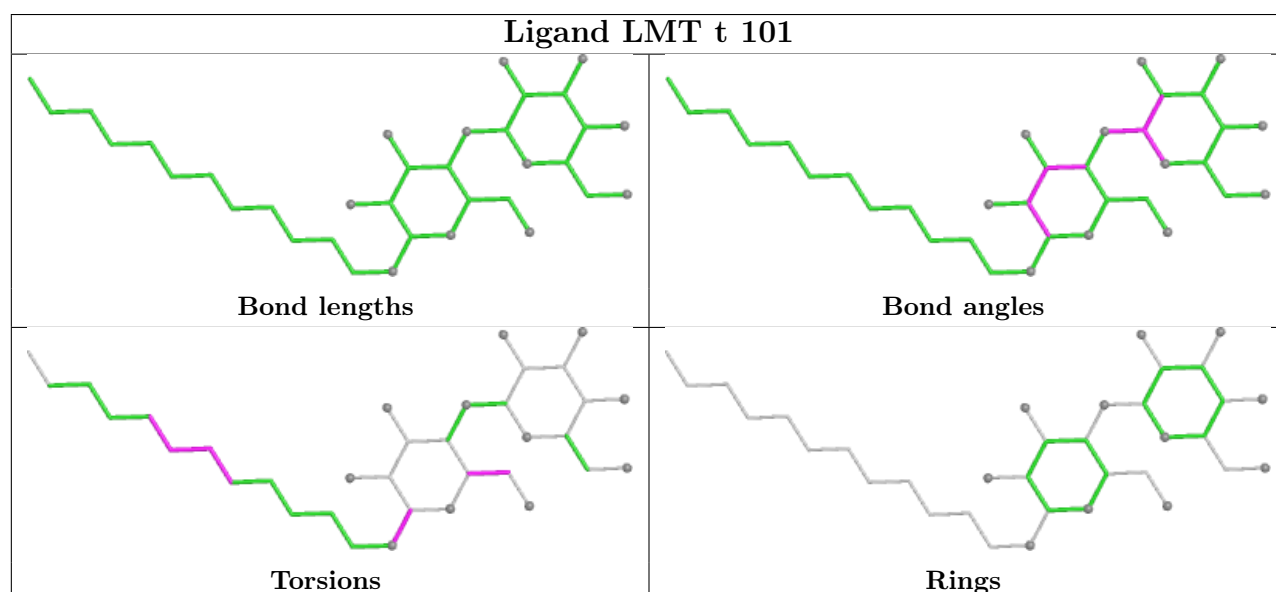
*Continued from previous page...*

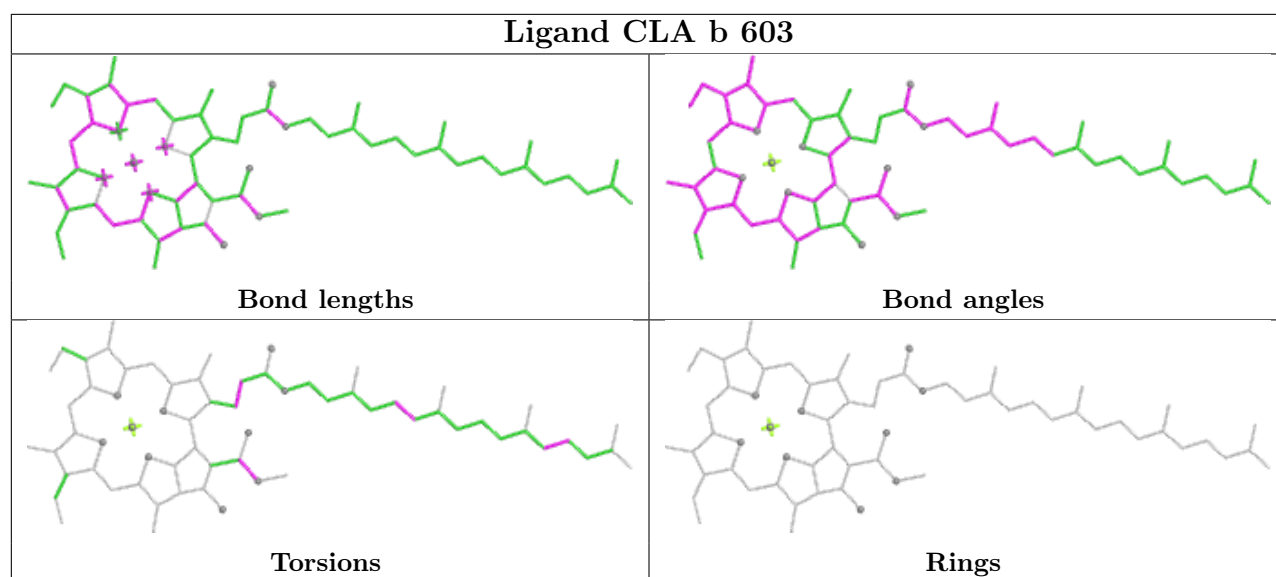
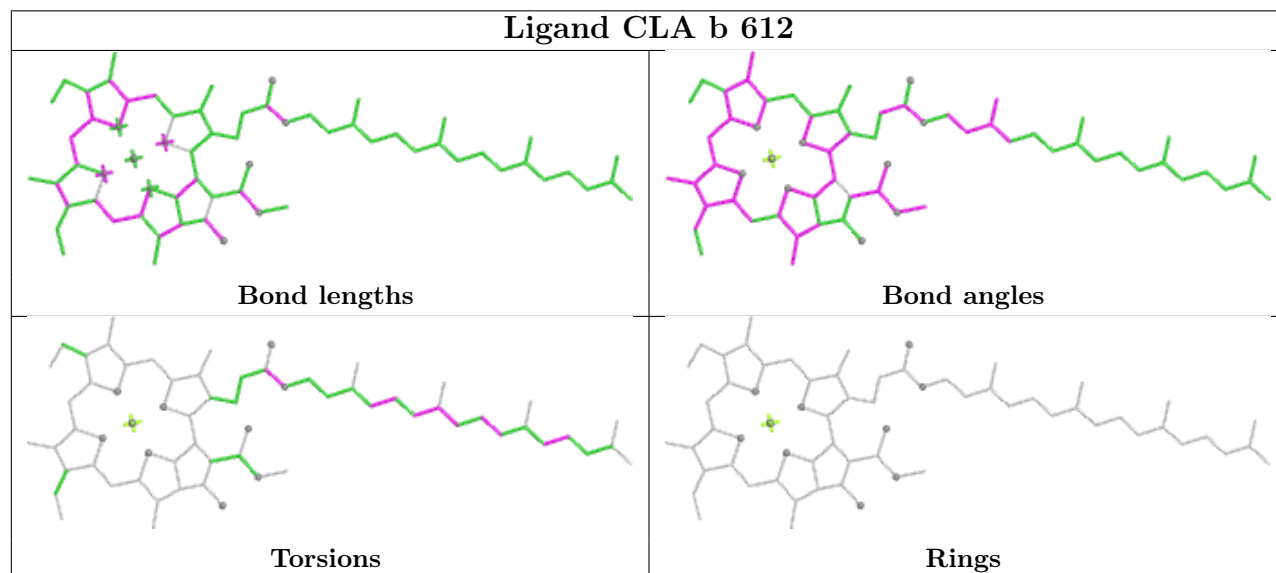
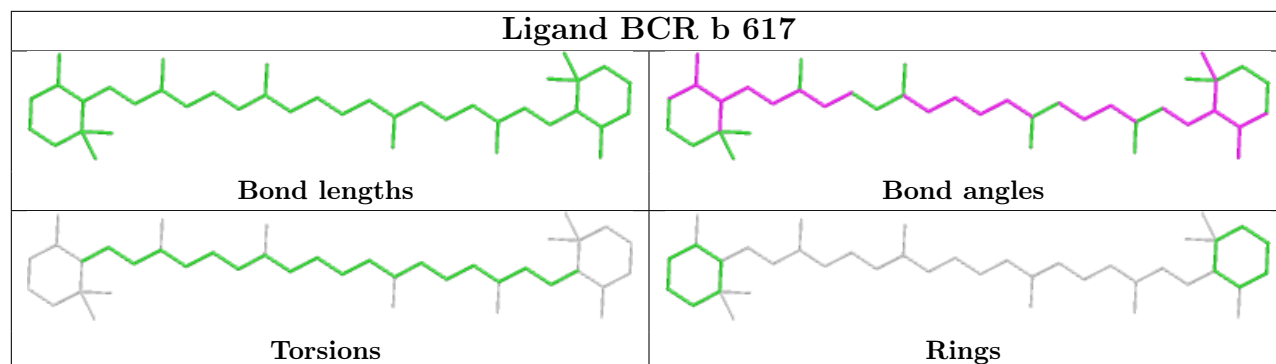
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 18  | b     | 617 | BCR  | 1       | 0            |
| 17  | a     | 404 | PHO  | 8       | 0            |
| 20  | b     | 620 | MGE  | 1       | 0            |
| 18  | a     | 407 | BCR  | 4       | 0            |
| 16  | b     | 611 | CLA  | 1       | 0            |
| 18  | h     | 101 | BCR  | 4       | 0            |
| 22  | d     | 402 | LMT  | 1       | 0            |
| 20  | b     | 622 | MGE  | 2       | 0            |
| 16  | d     | 405 | CLA  | 1       | 0            |
| 16  | b     | 614 | CLA  | 1       | 0            |
| 16  | d     | 404 | CLA  | 7       | 0            |
| 16  | b     | 609 | CLA  | 1       | 0            |
| 17  | a     | 405 | PHO  | 3       | 0            |
| 20  | d     | 410 | MGE  | 6       | 0            |
| 20  | m     | 101 | MGE  | 2       | 0            |
| 16  | b     | 604 | CLA  | 7       | 0            |
| 15  | l     | 101 | SQD  | 2       | 0            |
| 20  | d     | 408 | MGE  | 2       | 0            |
| 18  | b     | 619 | BCR  | 17      | 0            |
| 26  | d     | 412 | DGD  | 1       | 0            |
| 16  | b     | 615 | CLA  | 5       | 0            |
| 18  | d     | 407 | BCR  | 4       | 0            |
| 16  | b     | 602 | CLA  | 8       | 0            |
| 16  | b     | 605 | CLA  | 5       | 0            |
| 16  | d     | 401 | CLA  | 10      | 0            |
| 16  | b     | 608 | CLA  | 3       | 0            |
| 16  | a     | 403 | CLA  | 2       | 0            |
| 16  | b     | 616 | CLA  | 2       | 0            |
| 18  | b     | 618 | BCR  | 3       | 0            |
| 16  | b     | 606 | CLA  | 25      | 0            |
| 25  | d     | 411 | HTG  | 6       | 0            |
| 20  | d     | 409 | MGE  | 6       | 0            |
| 16  | b     | 613 | CLA  | 3       | 0            |
| 16  | b     | 601 | 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

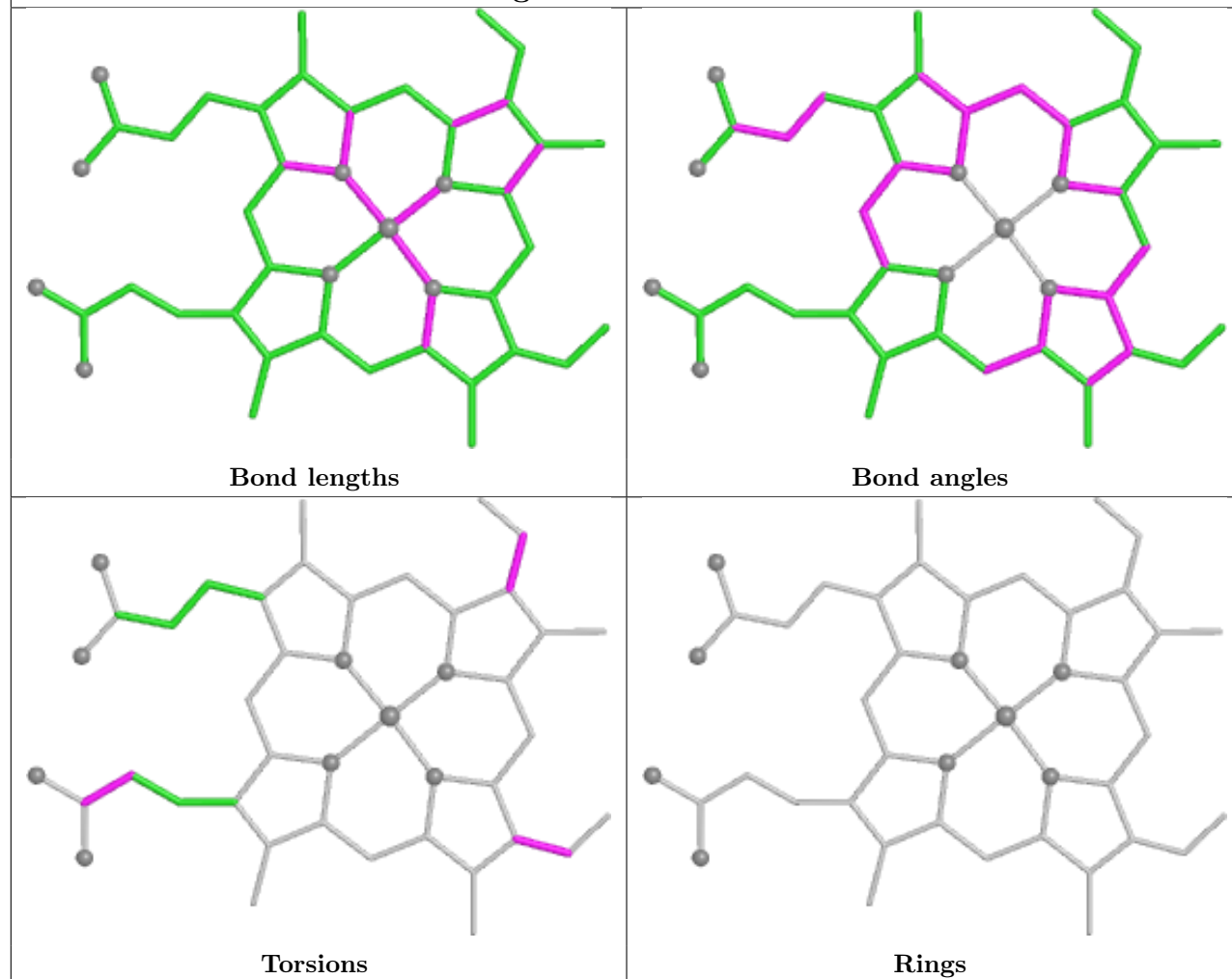
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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



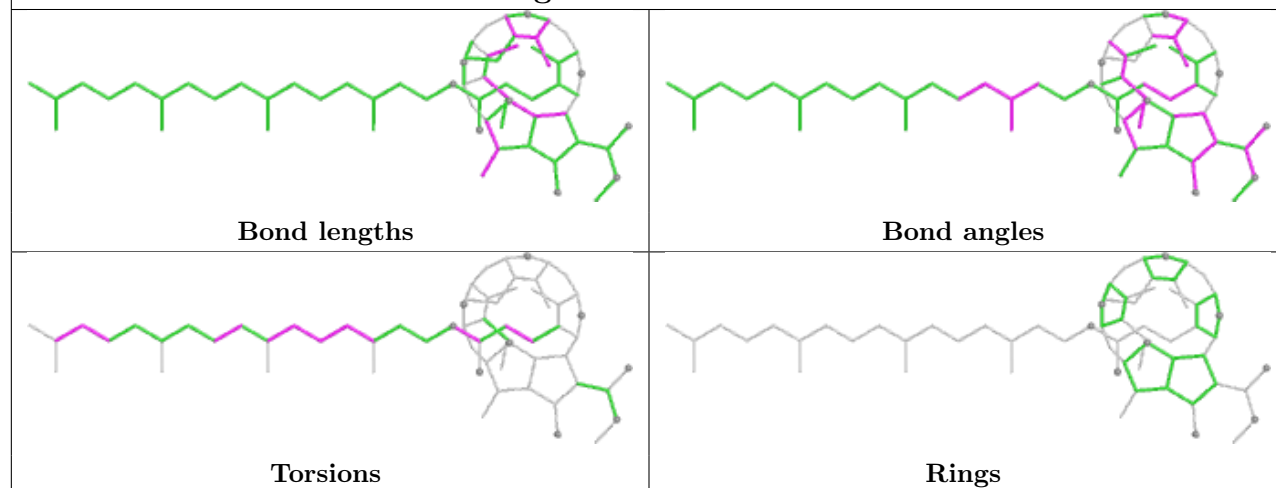


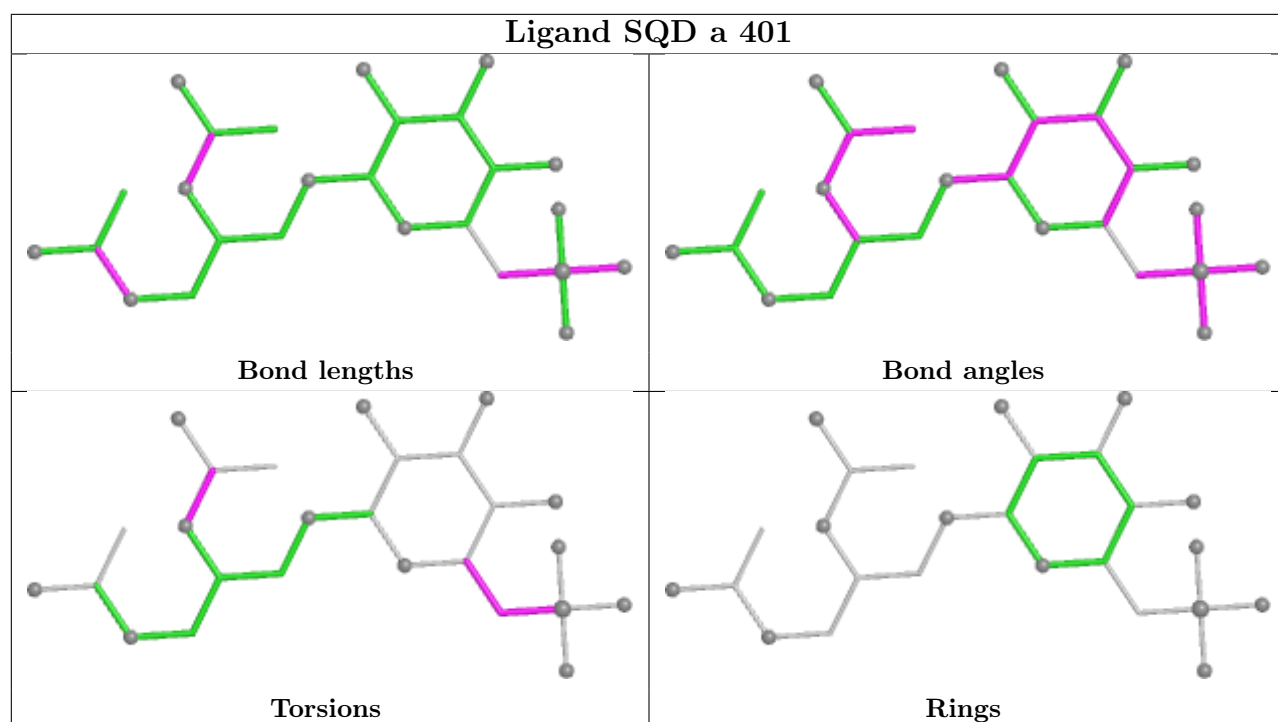
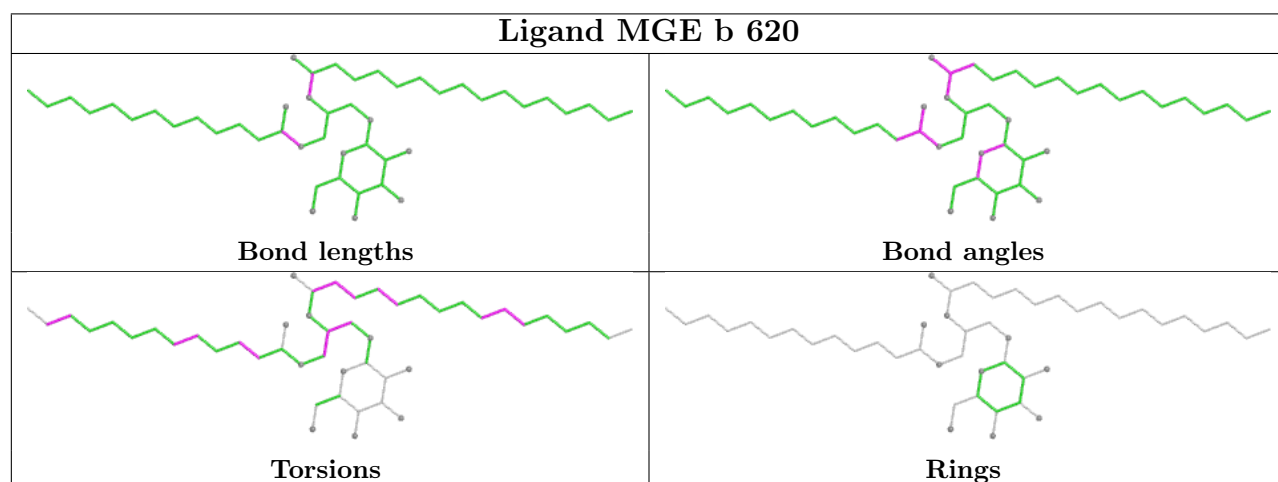
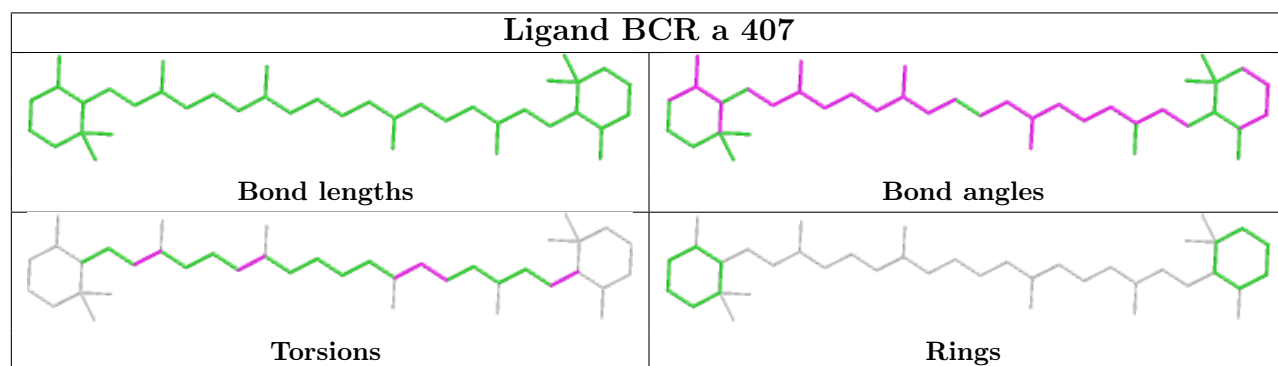


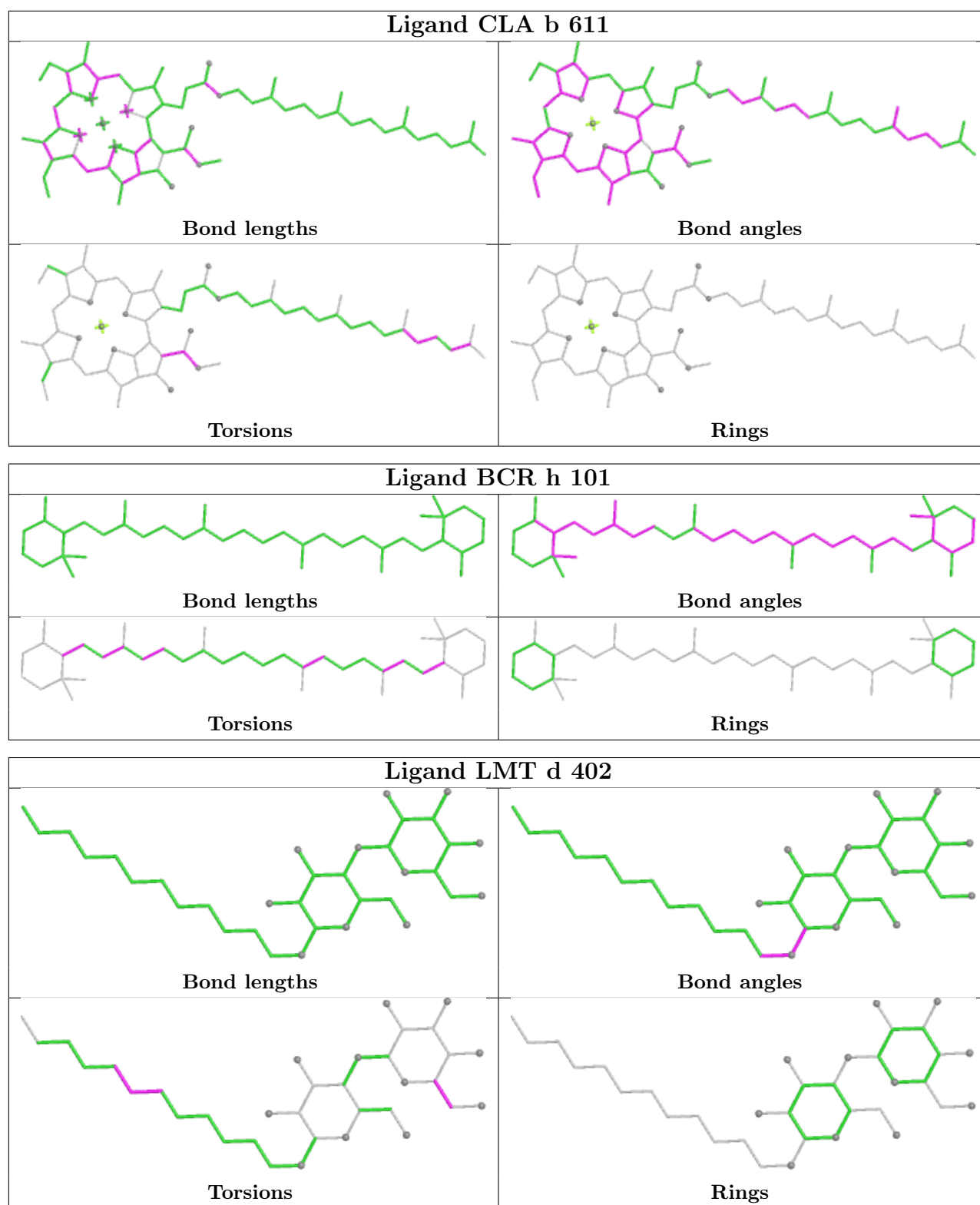
## Ligand HEM e 101

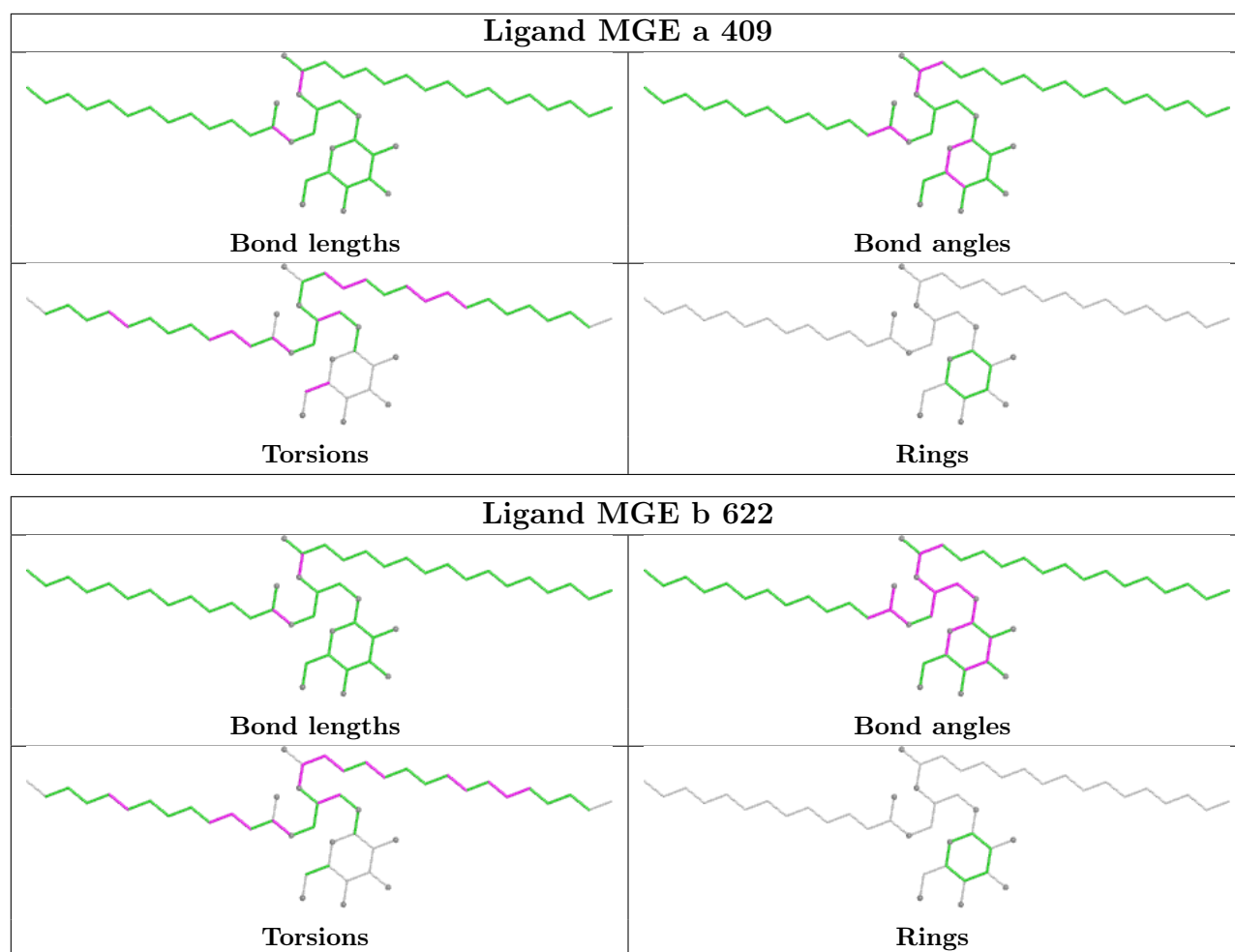


## Ligand PHO a 404

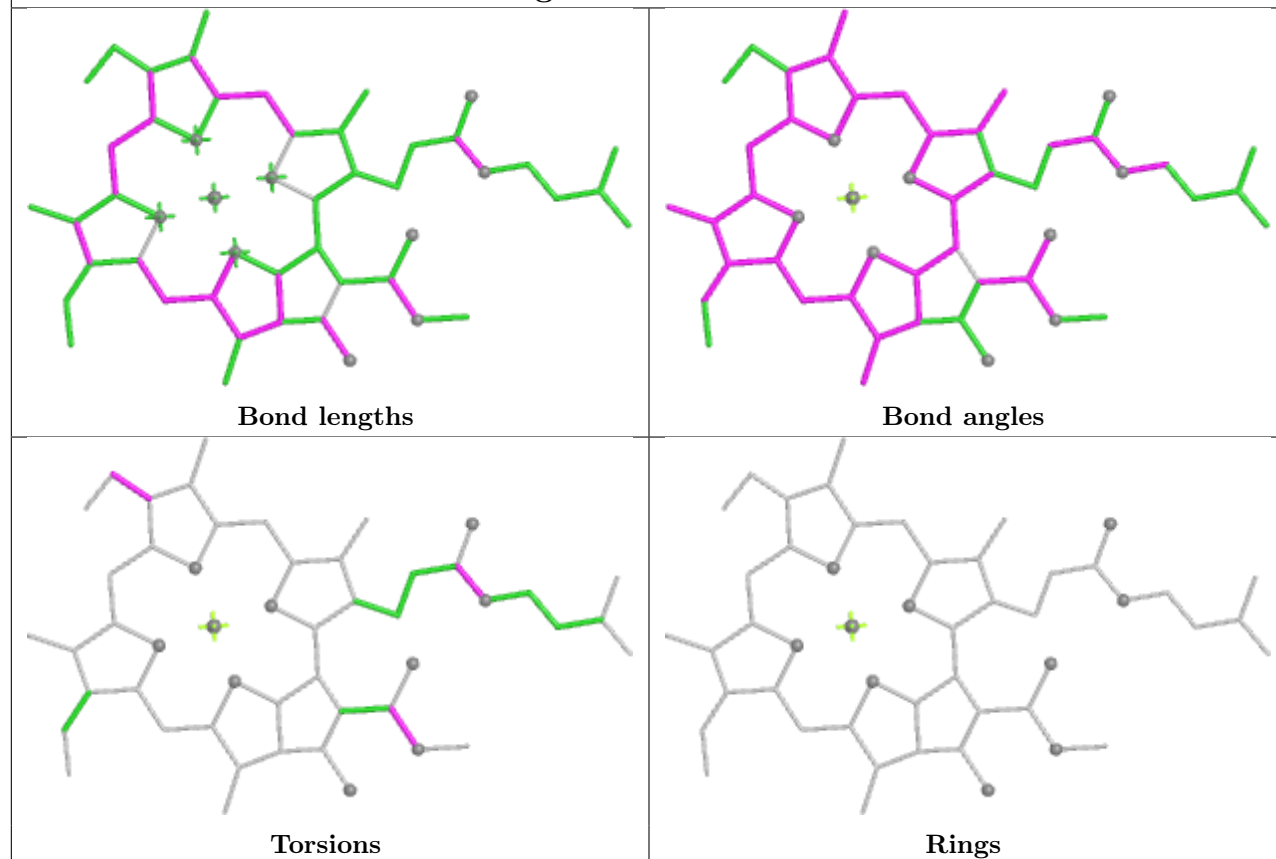




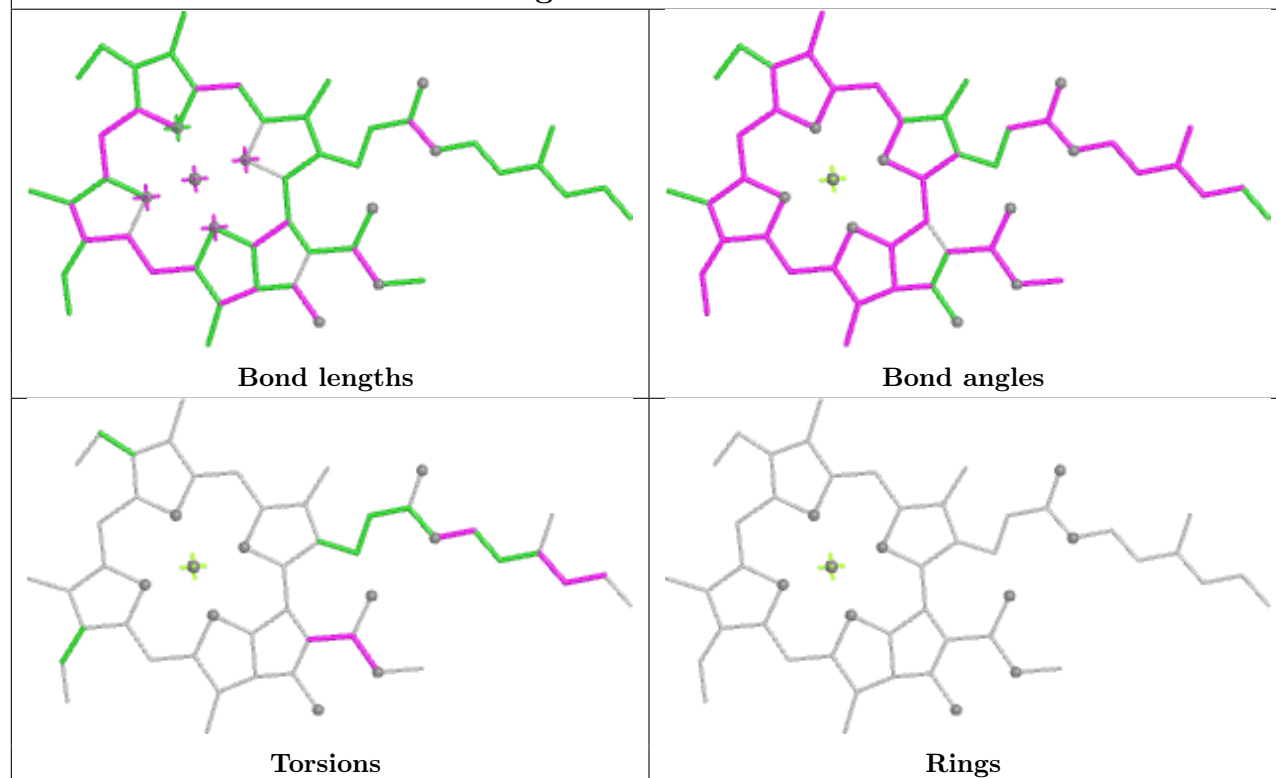


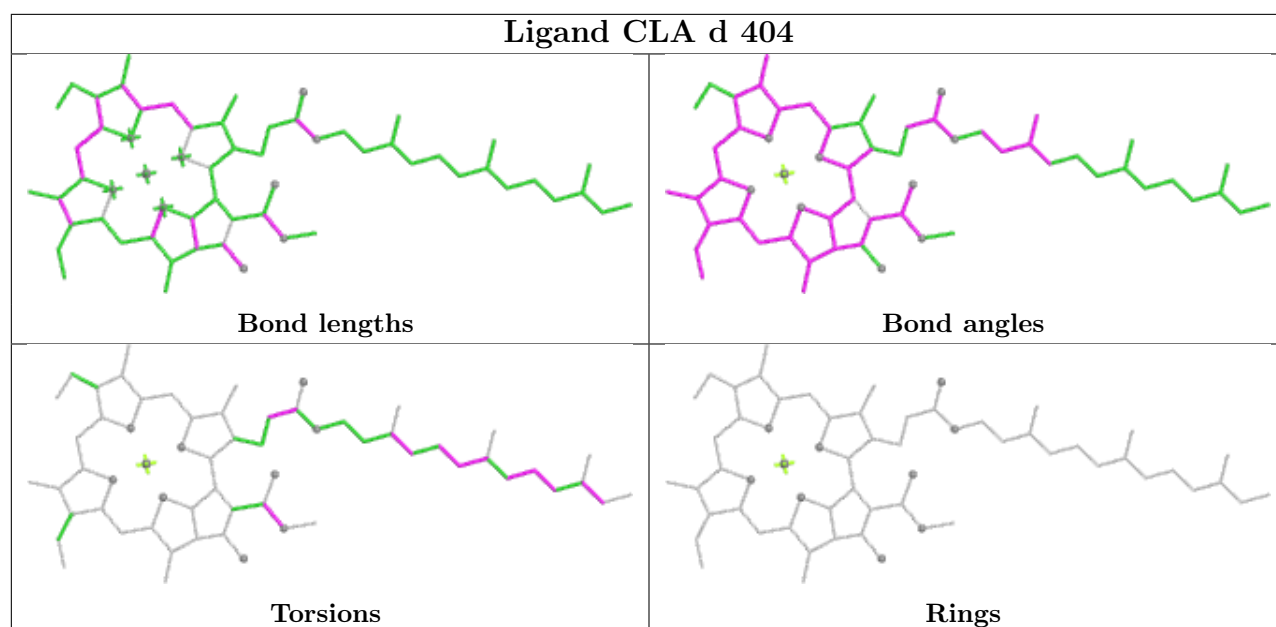
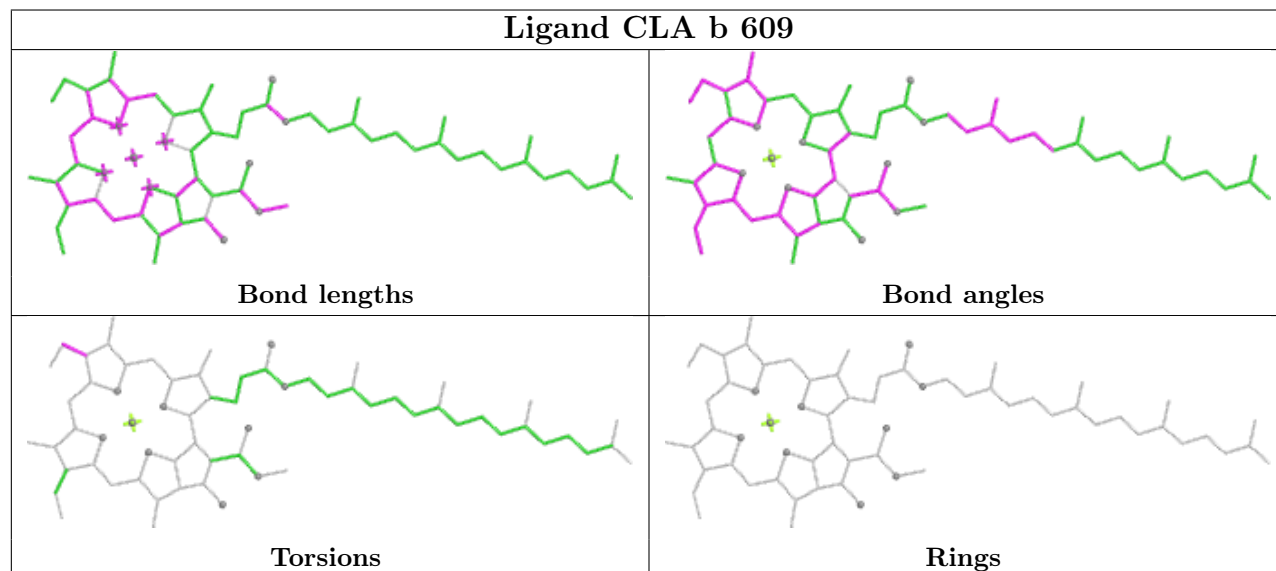
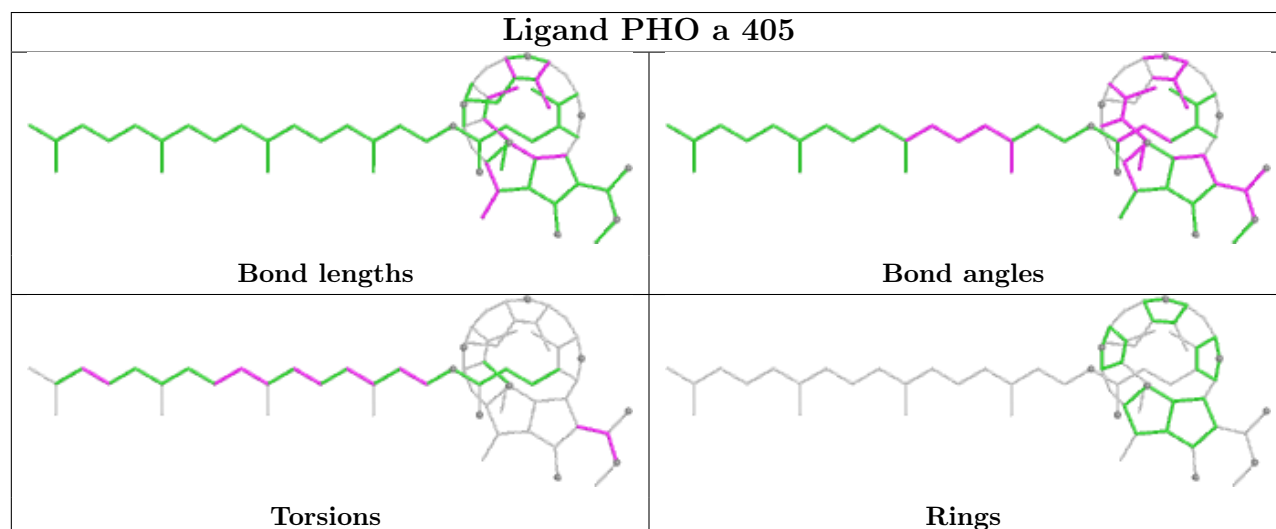


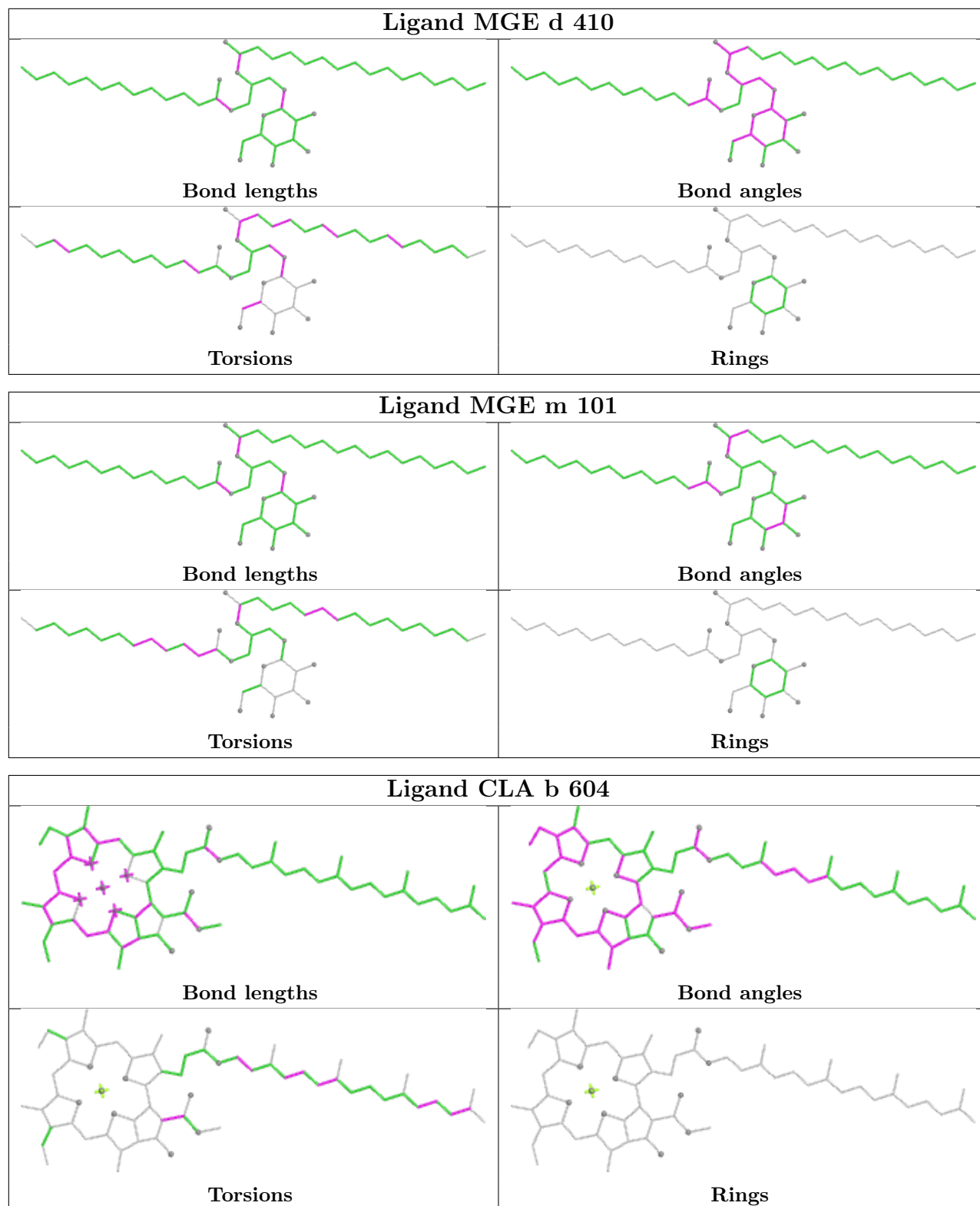
## Ligand CLA d 405

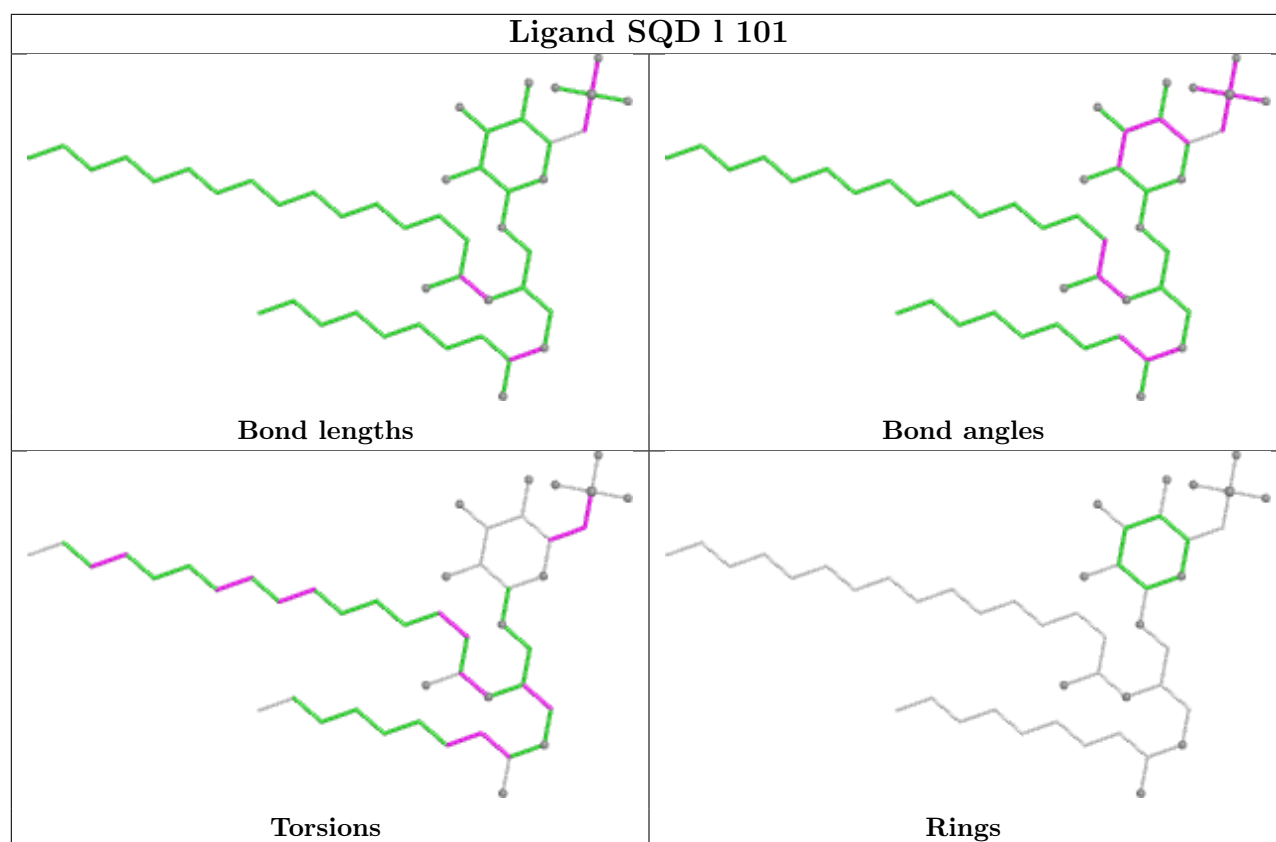
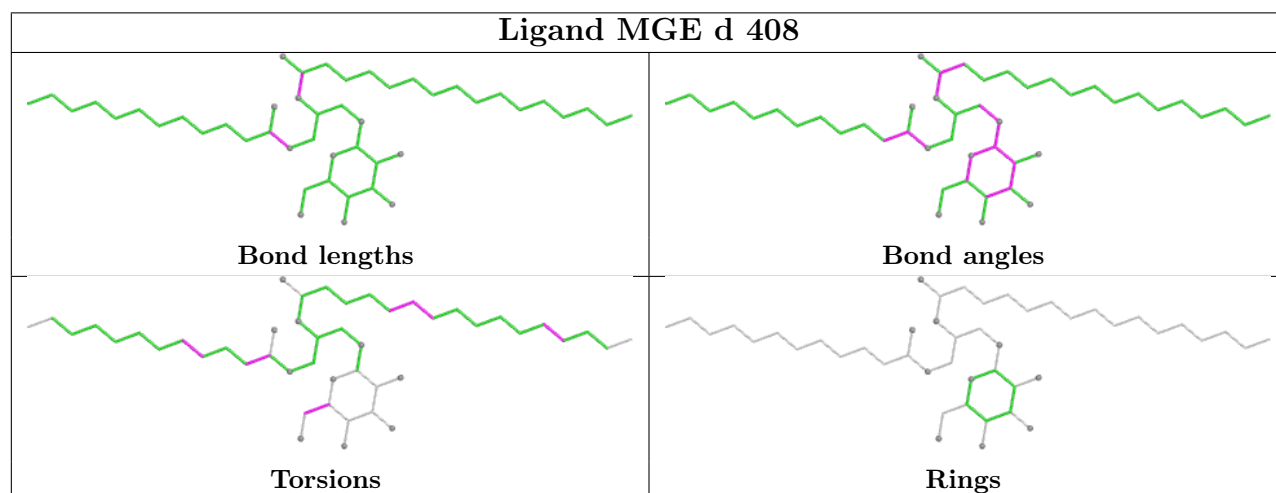
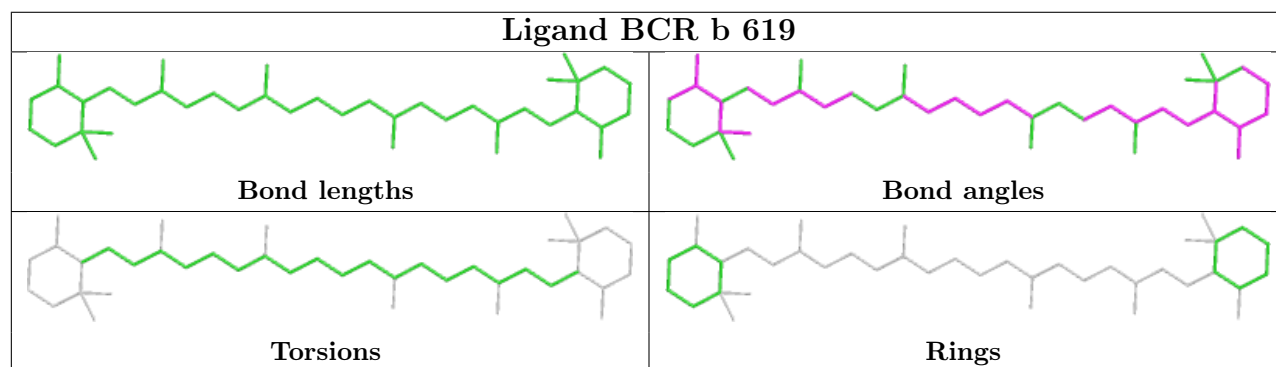


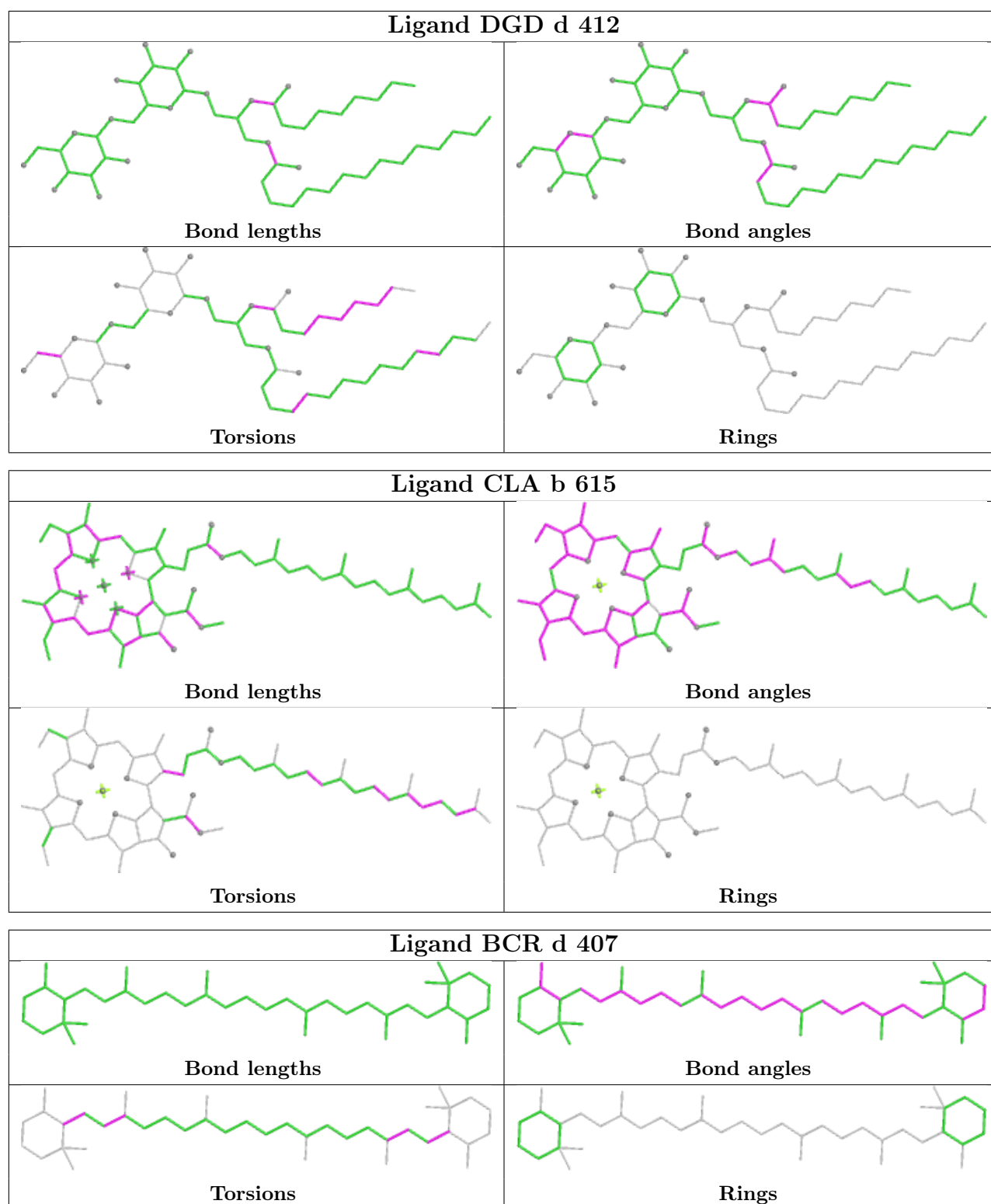
## Ligand CLA b 614



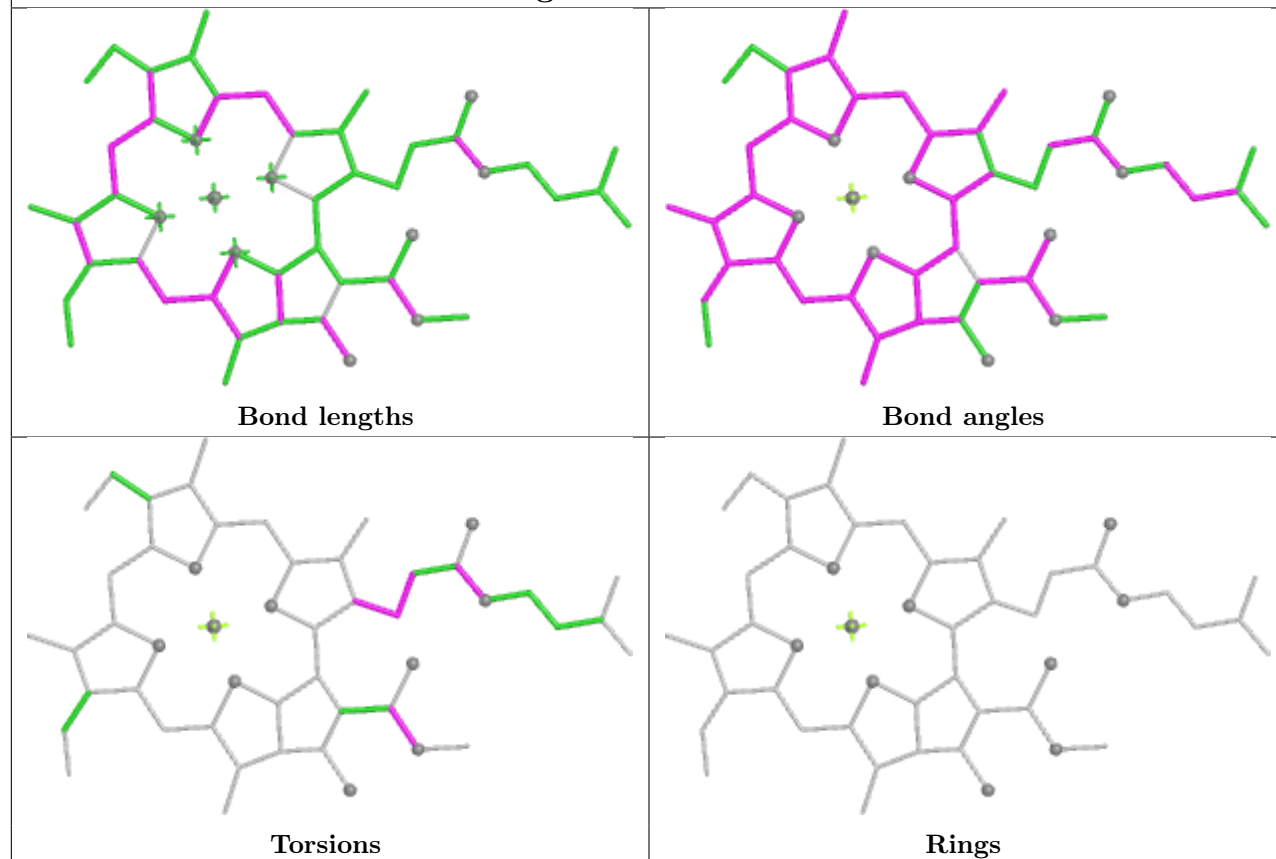




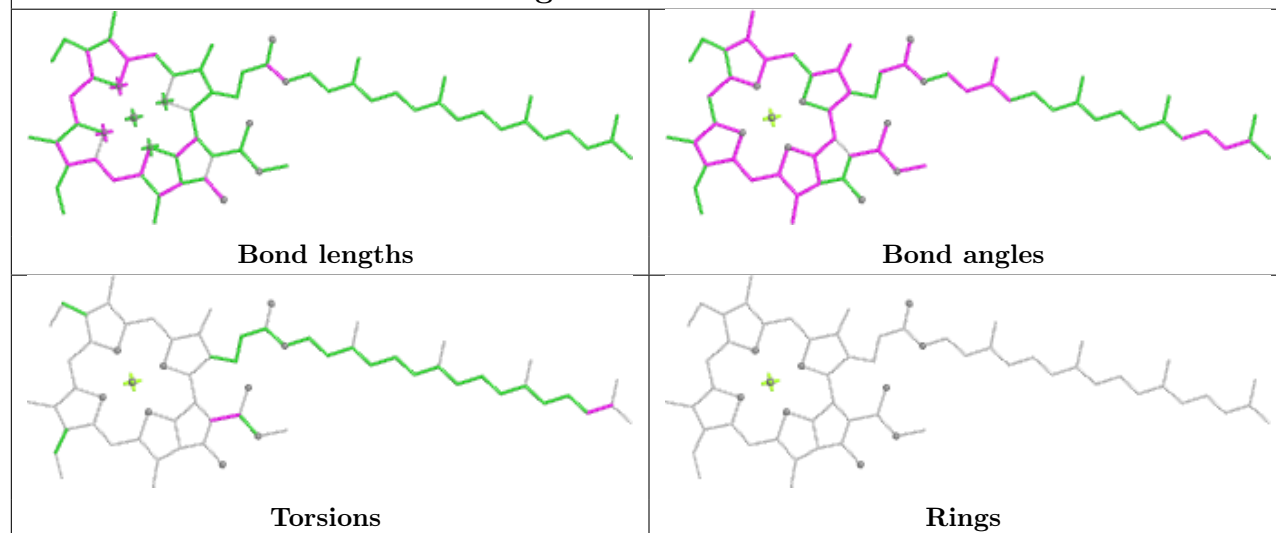


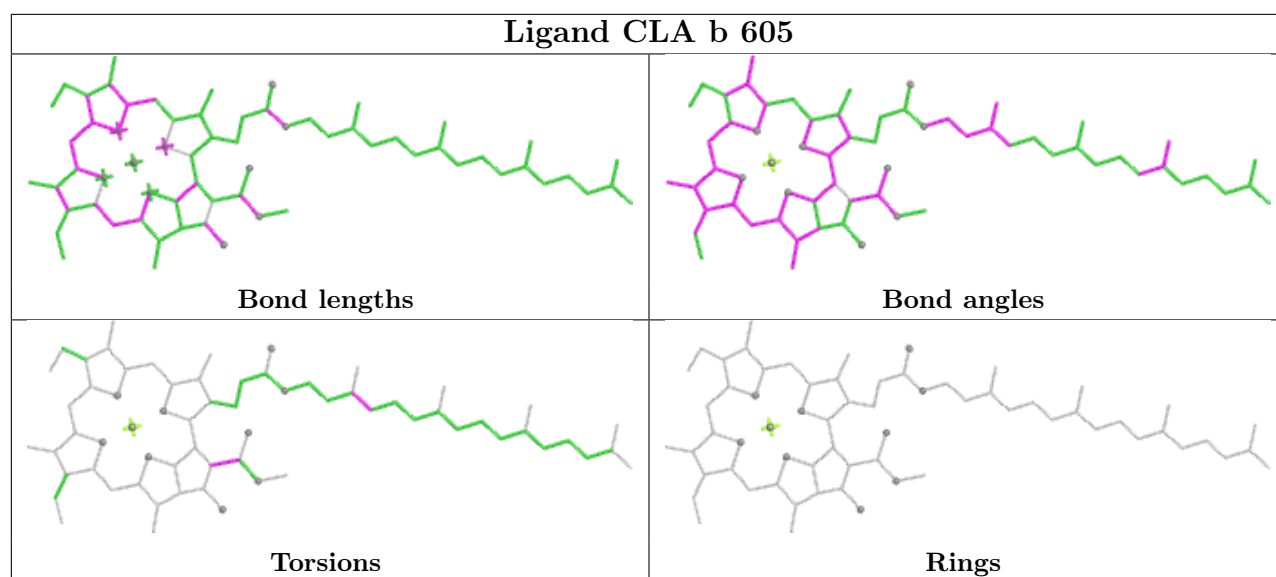
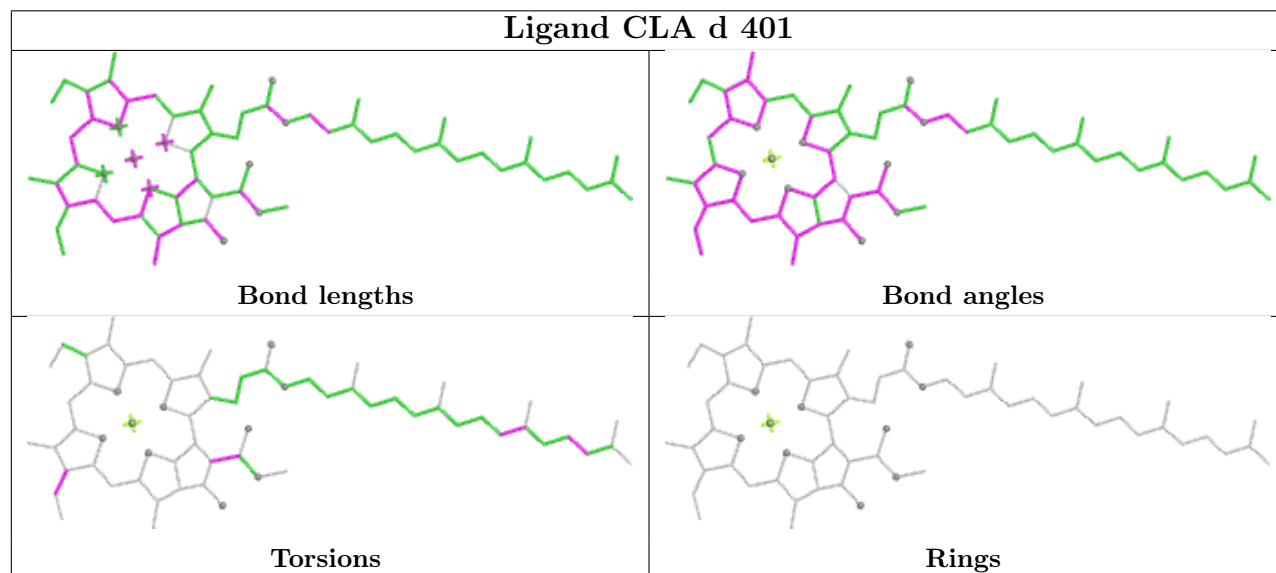
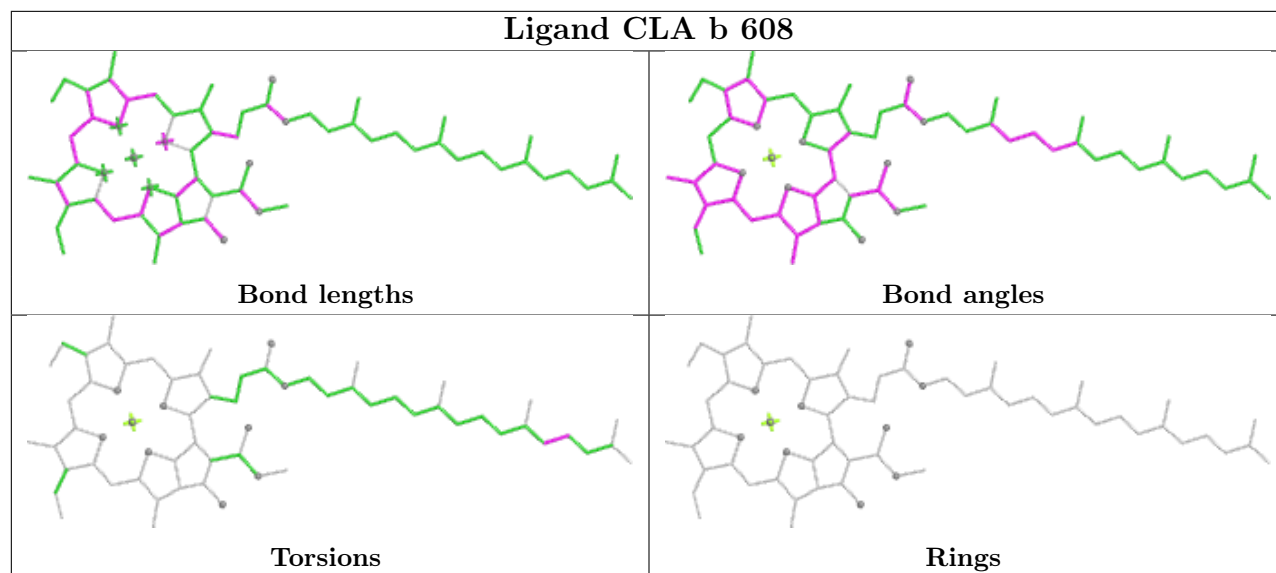


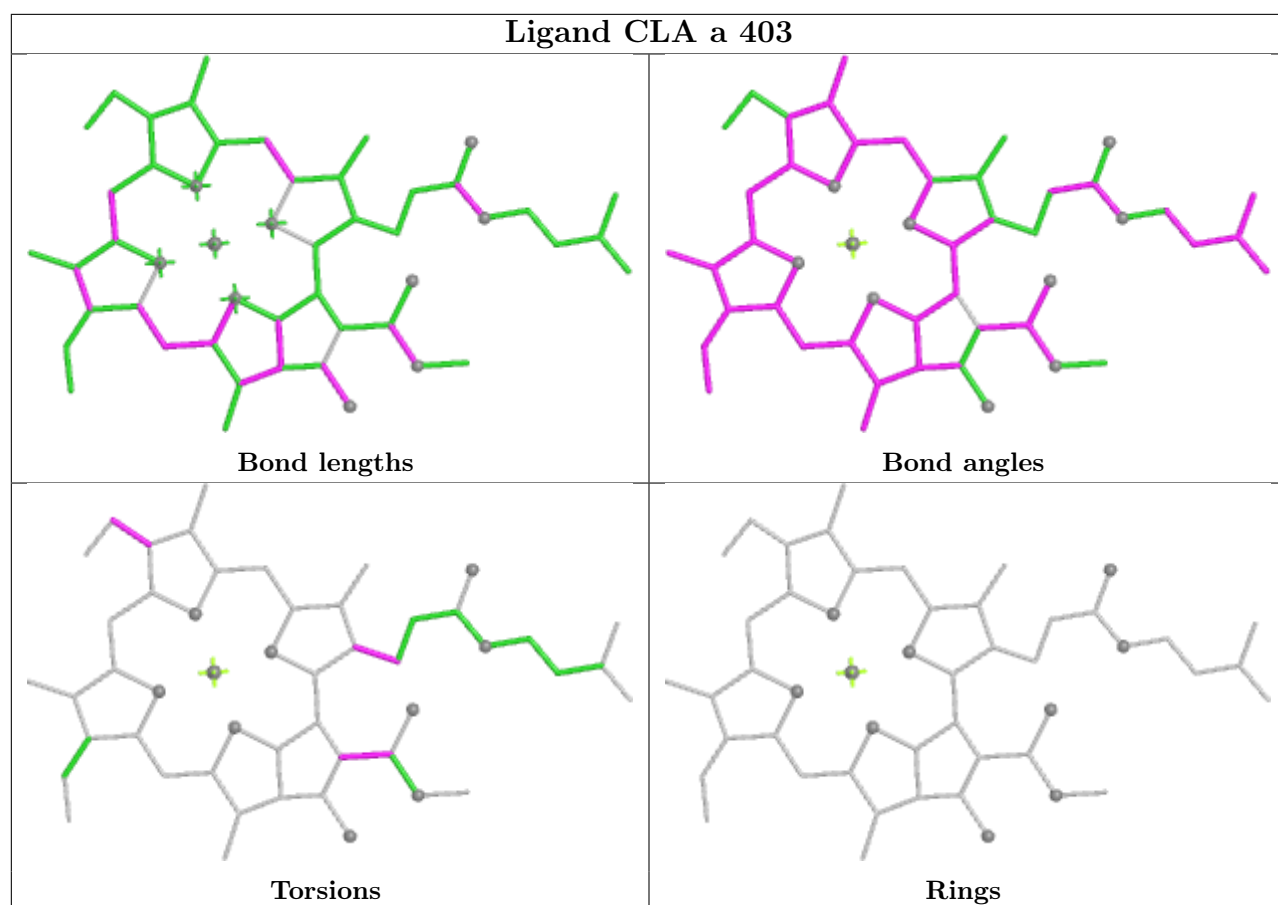
## Ligand CLA a 406

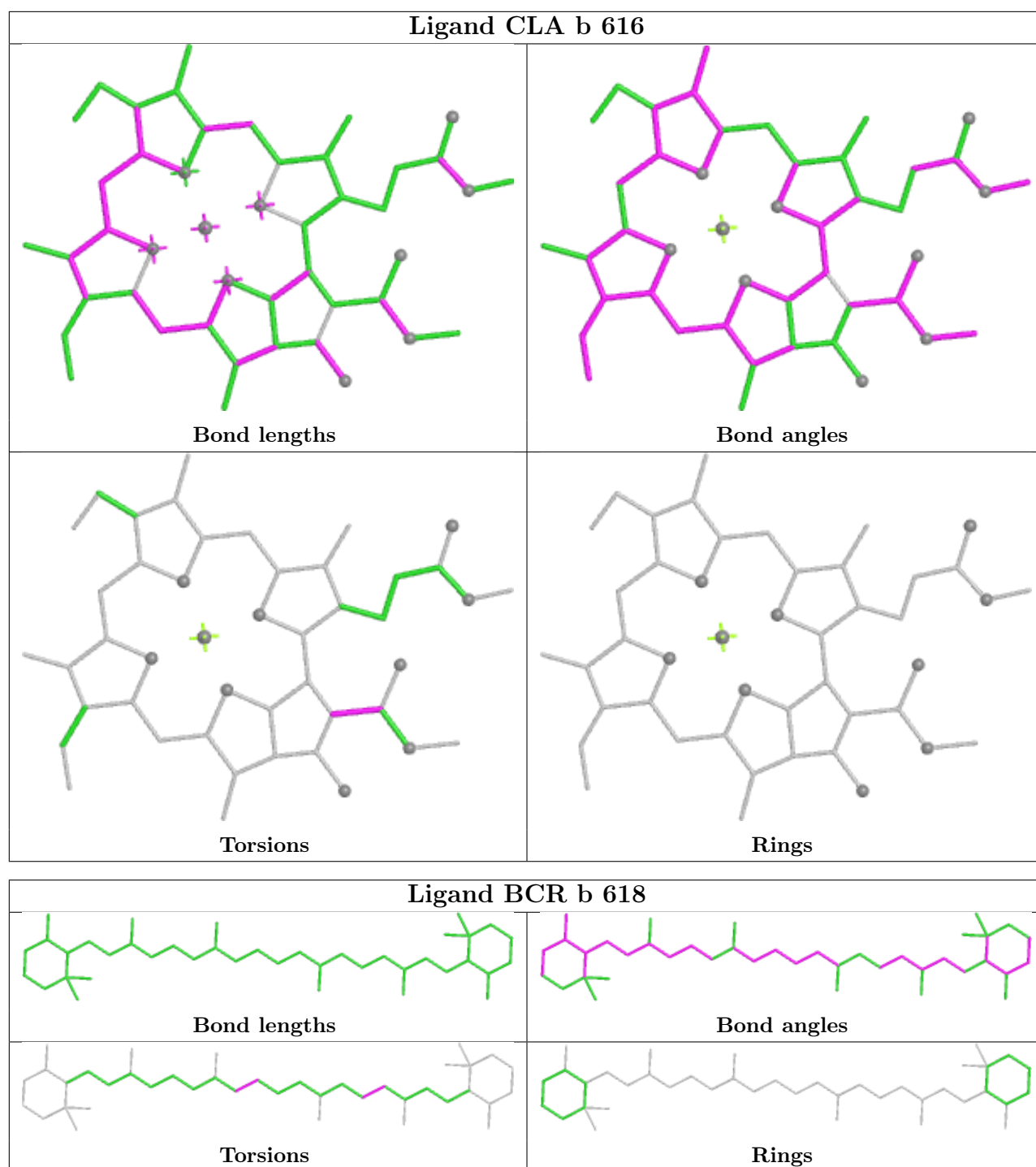


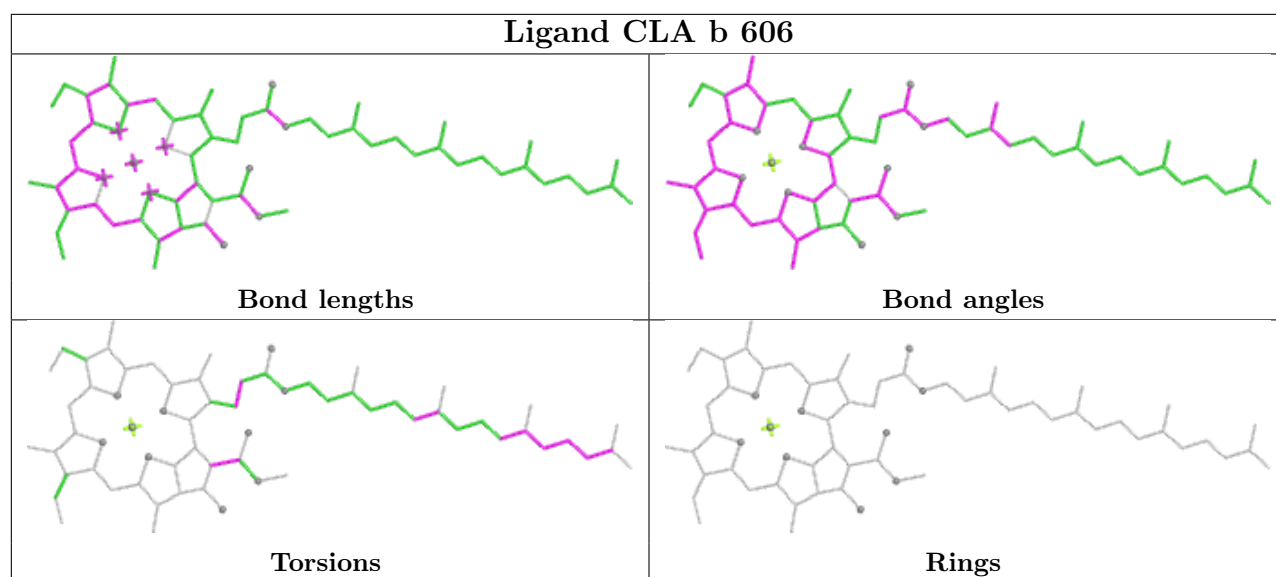
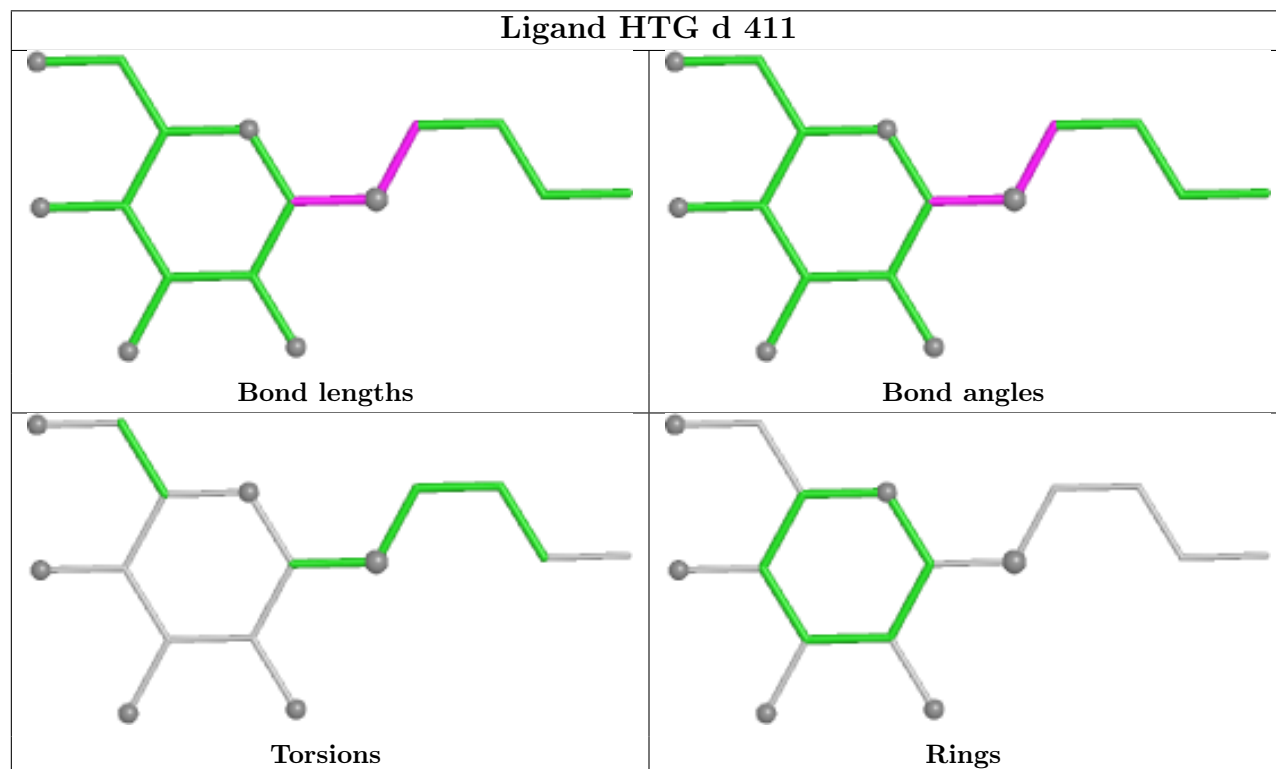
## Ligand CLA b 602

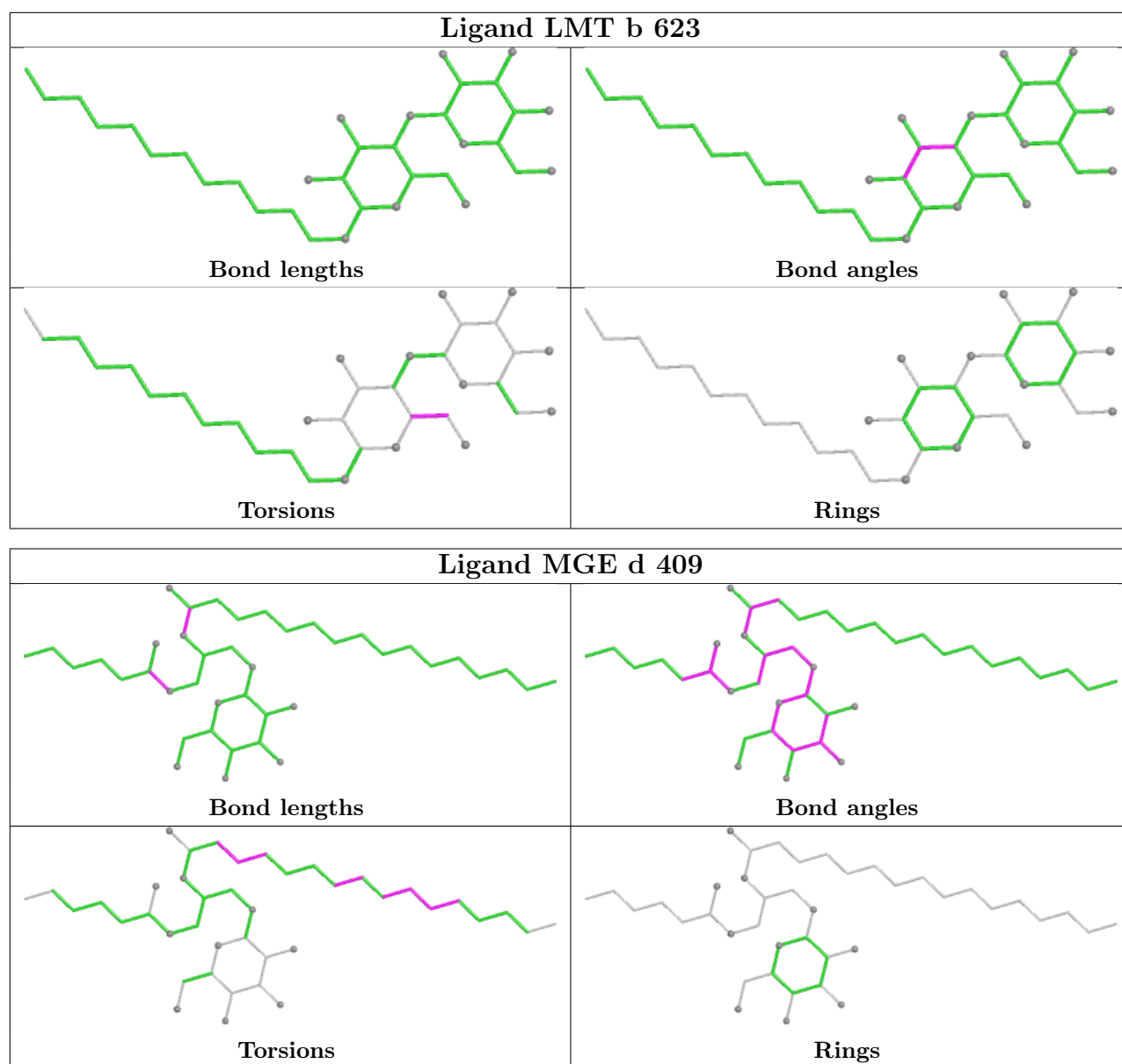


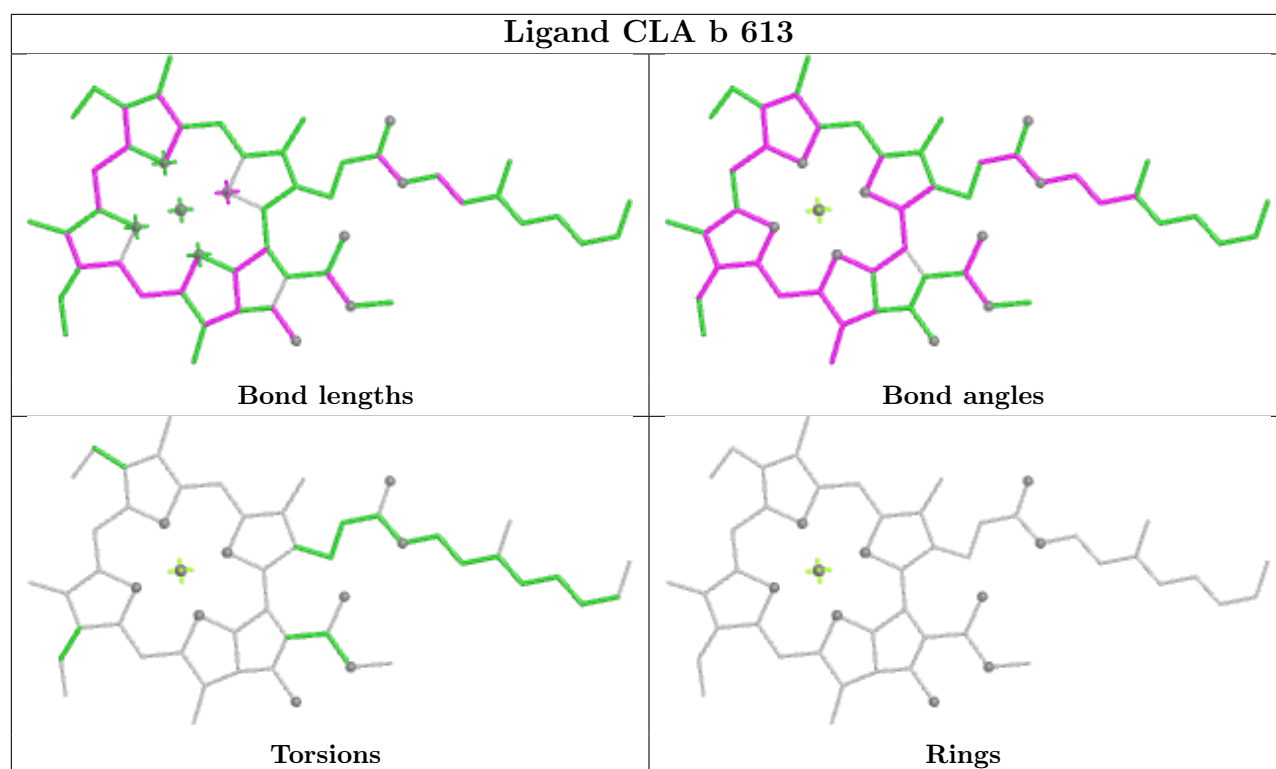


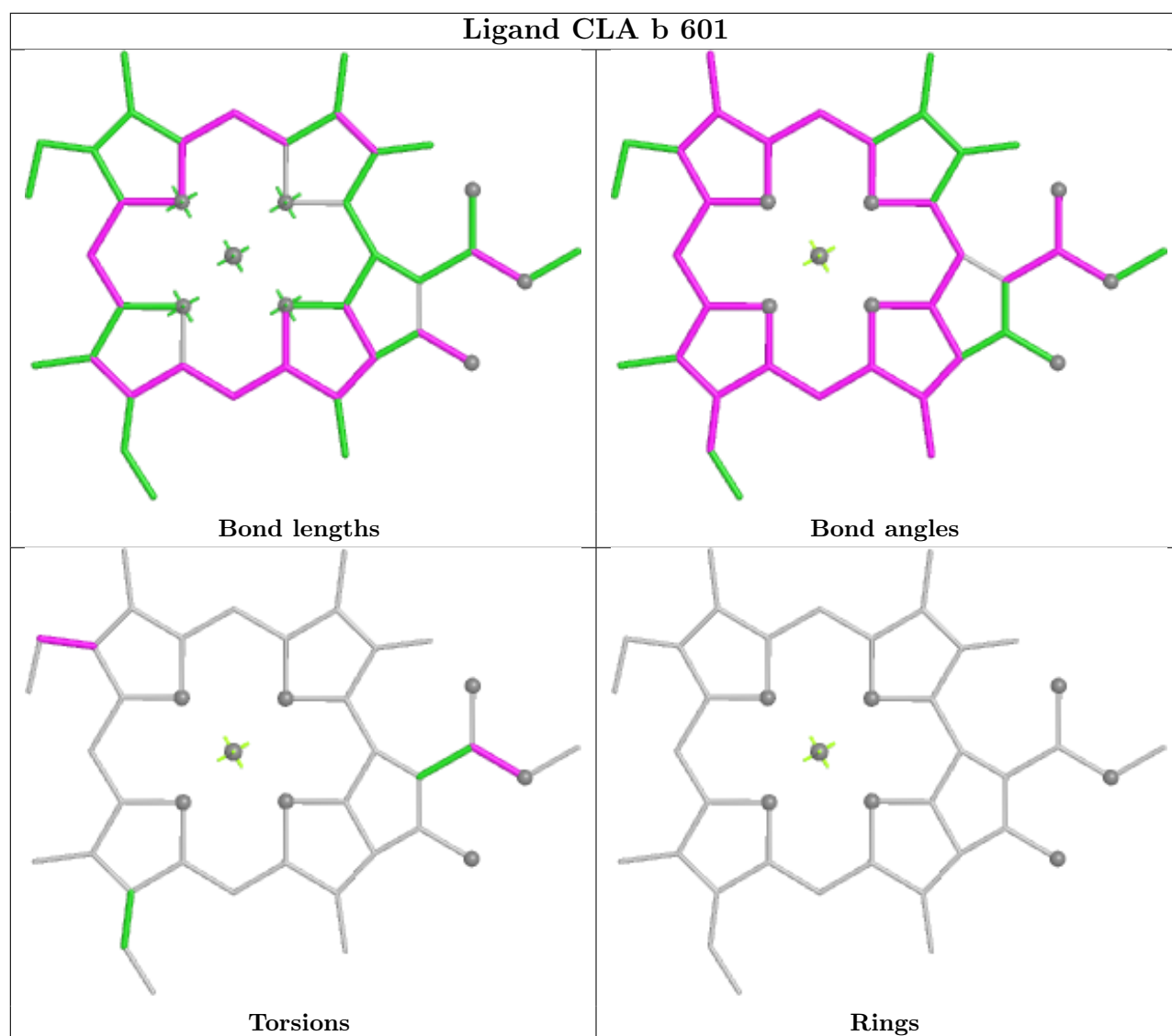












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

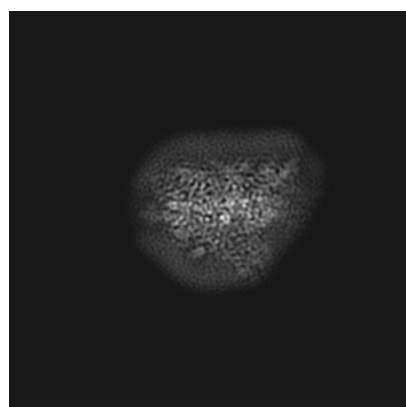
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30902. These allow visual inspection of the internal detail of the map and identification of artifacts.

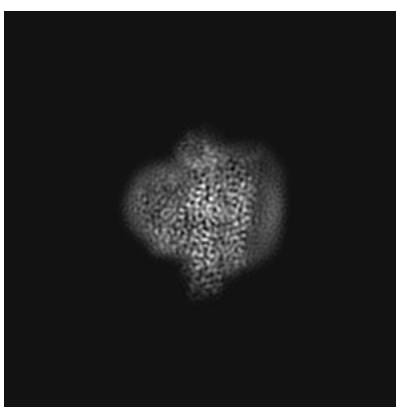
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

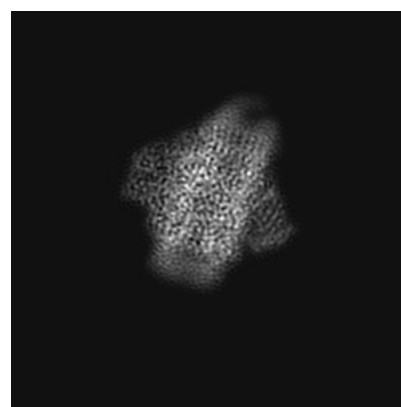
#### 6.1.1 Primary map



X



Y

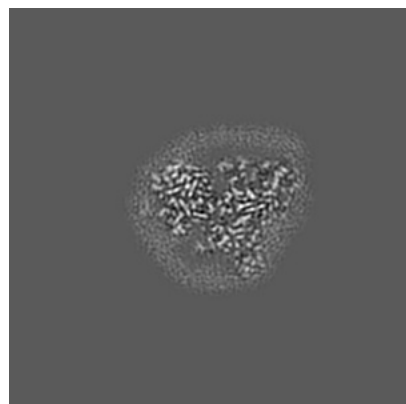


Z

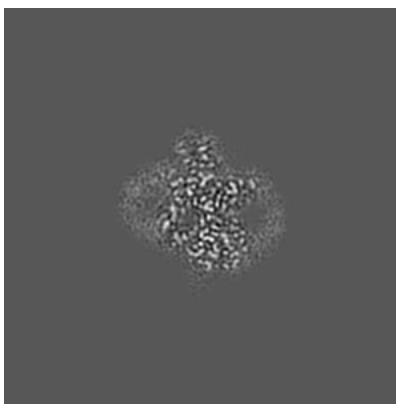
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

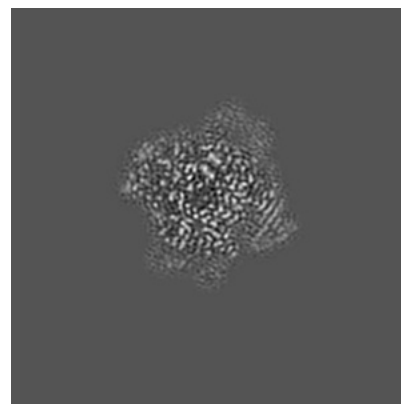
#### 6.2.1 Primary map



X Index: 100



Y Index: 100

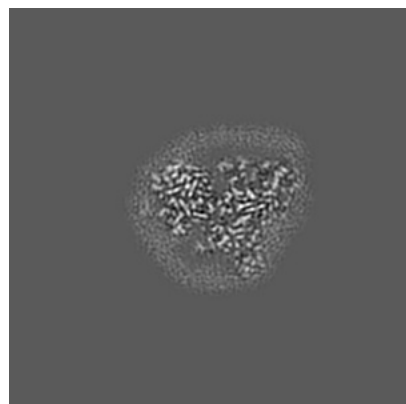


Z Index: 100

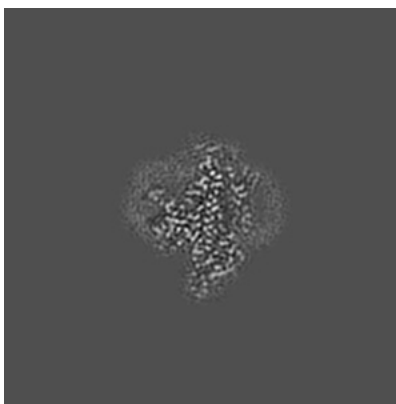
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

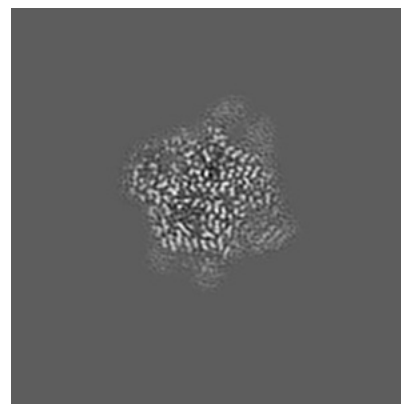
### 6.3.1 Primary map



X Index: 100



Y Index: 110

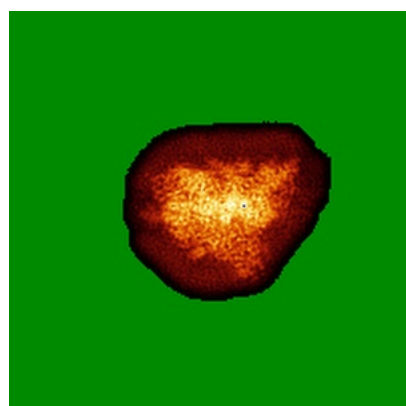


Z Index: 103

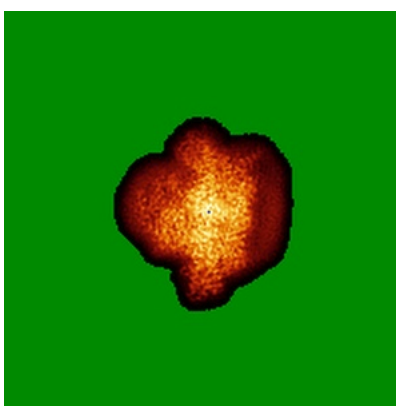
The images above show the largest variance slices of the map in three orthogonal directions.

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

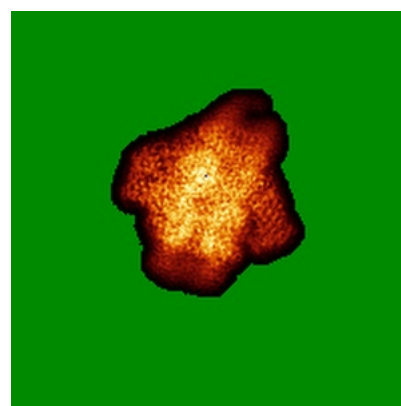
### 6.4.1 Primary map



X



Y

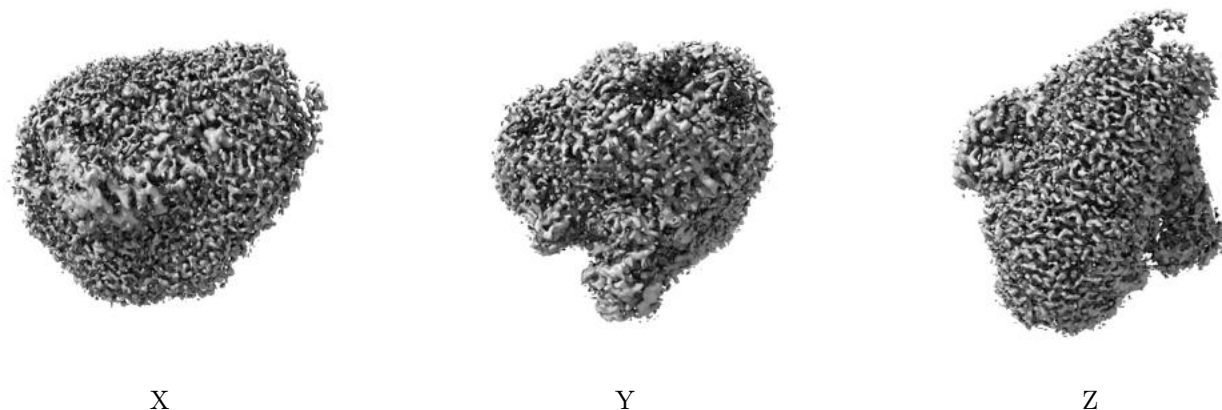


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

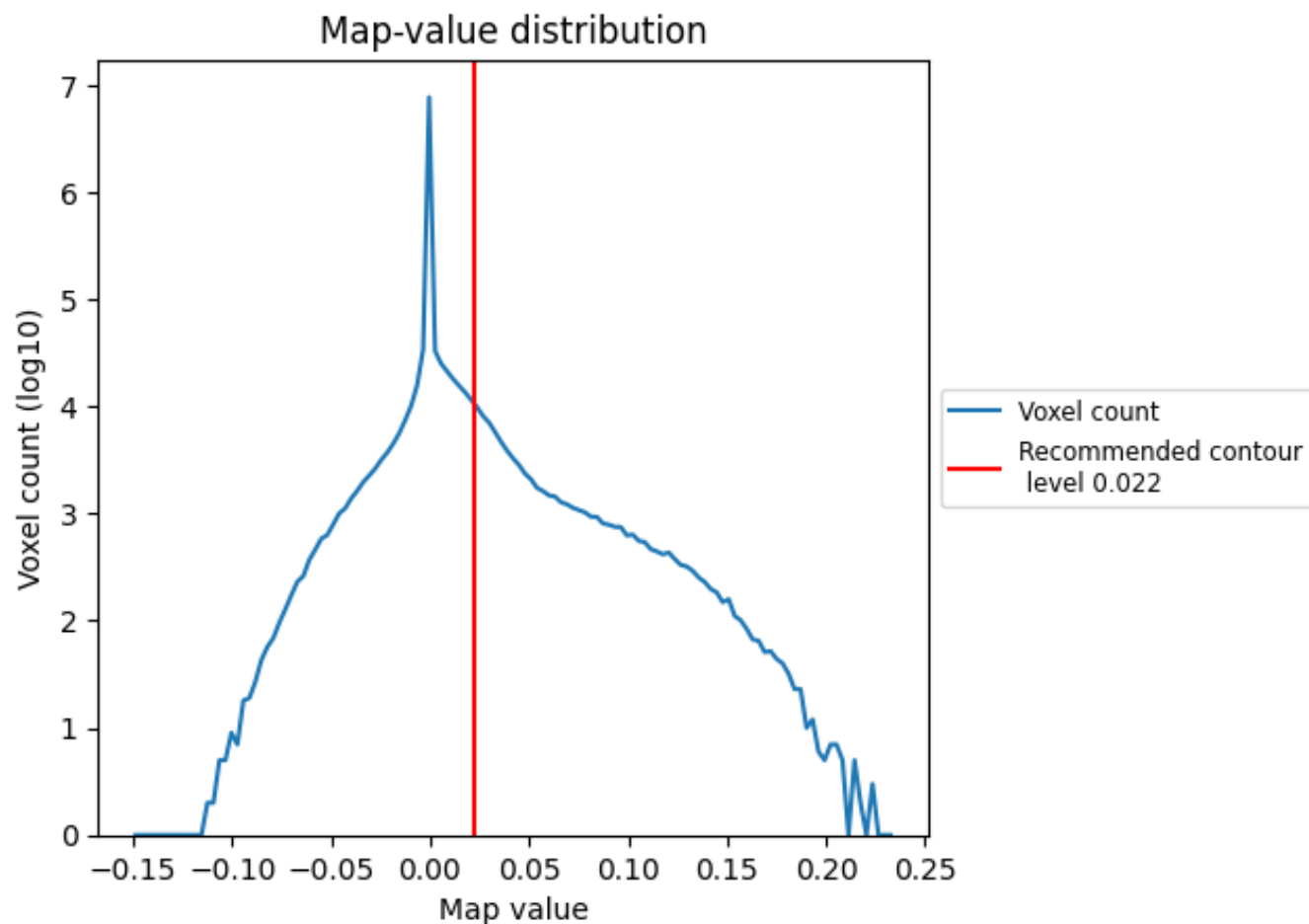
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

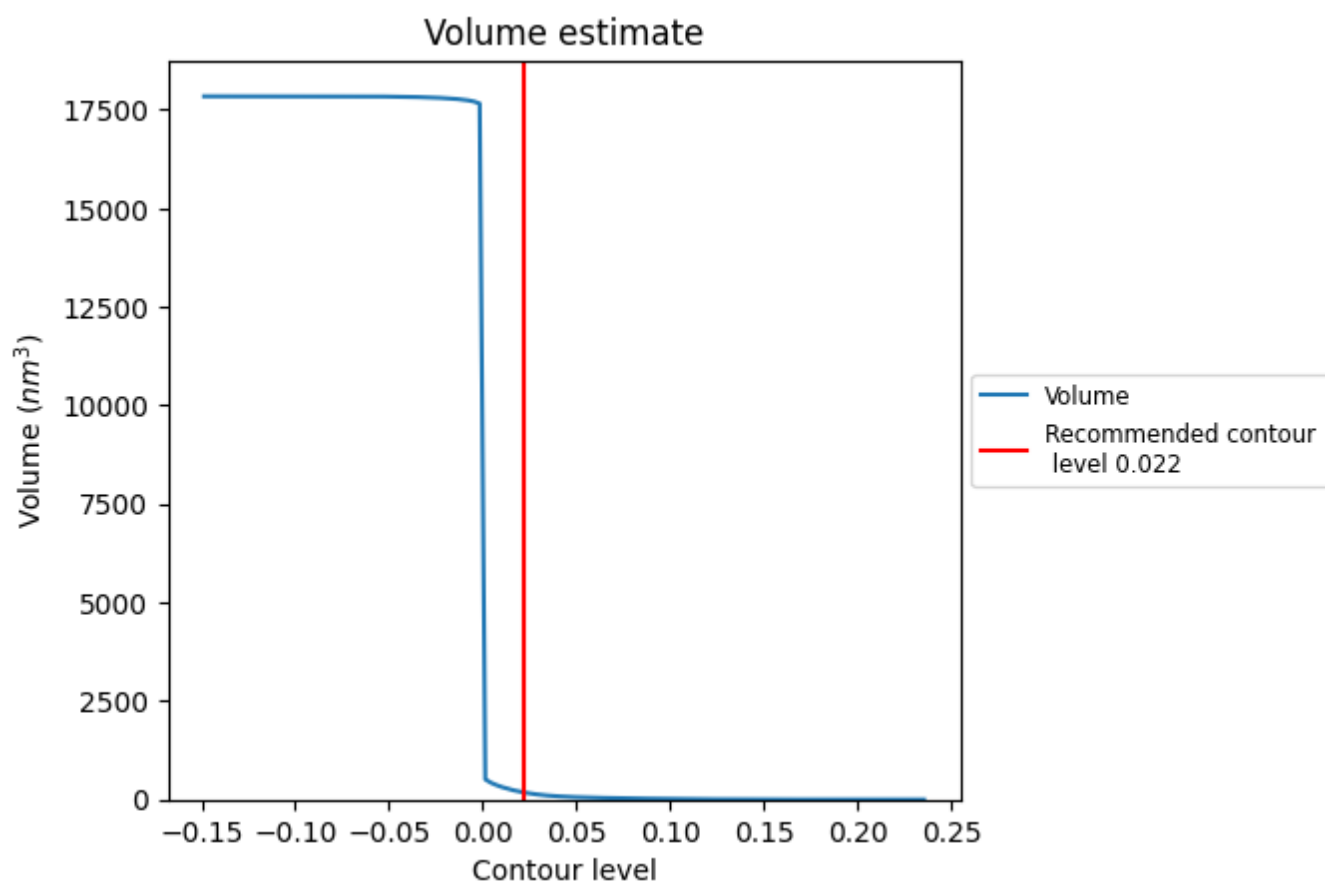
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

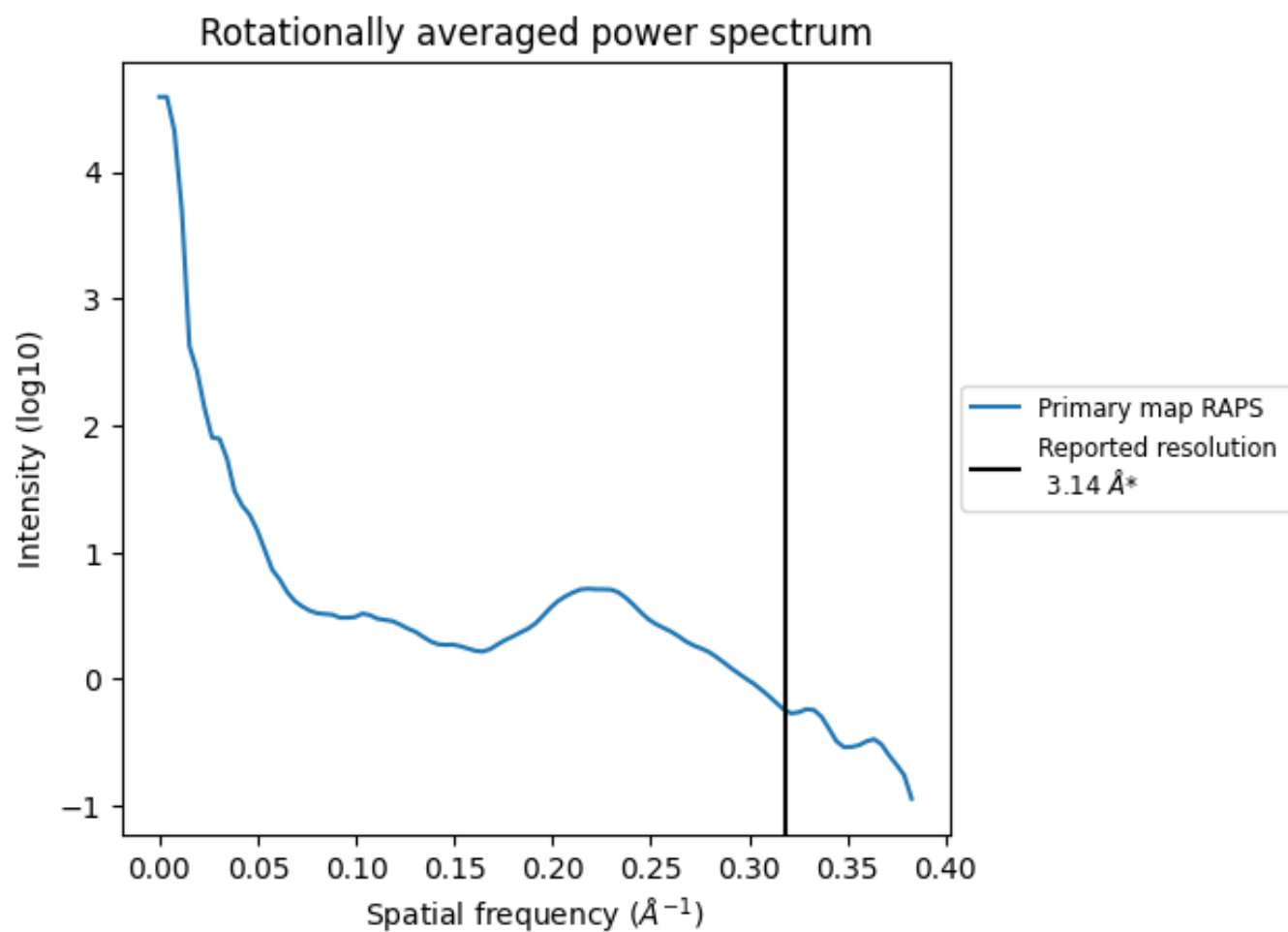
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 181 nm<sup>3</sup>; this corresponds to an approximate mass of 163 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.318 Å<sup>-1</sup>

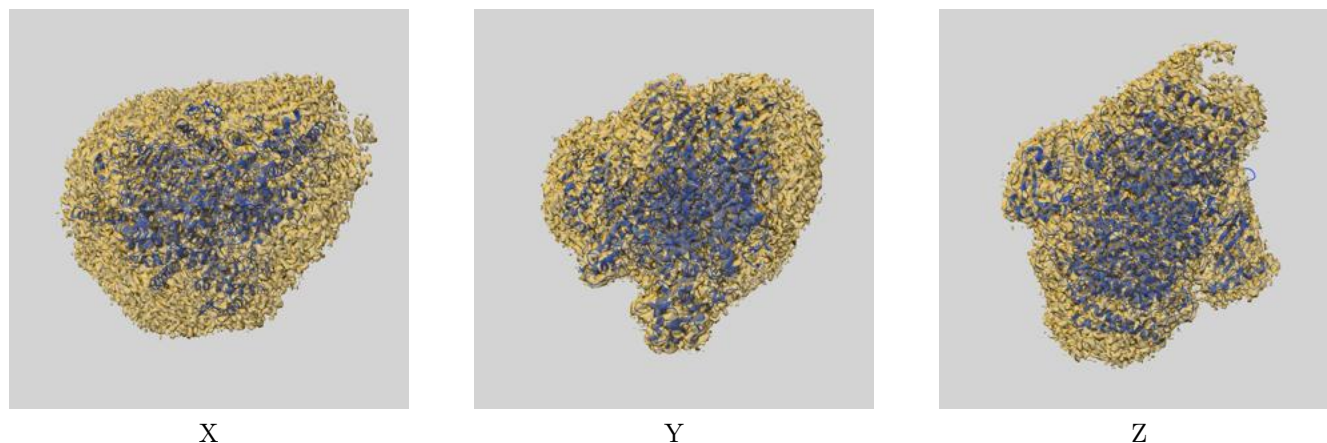
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

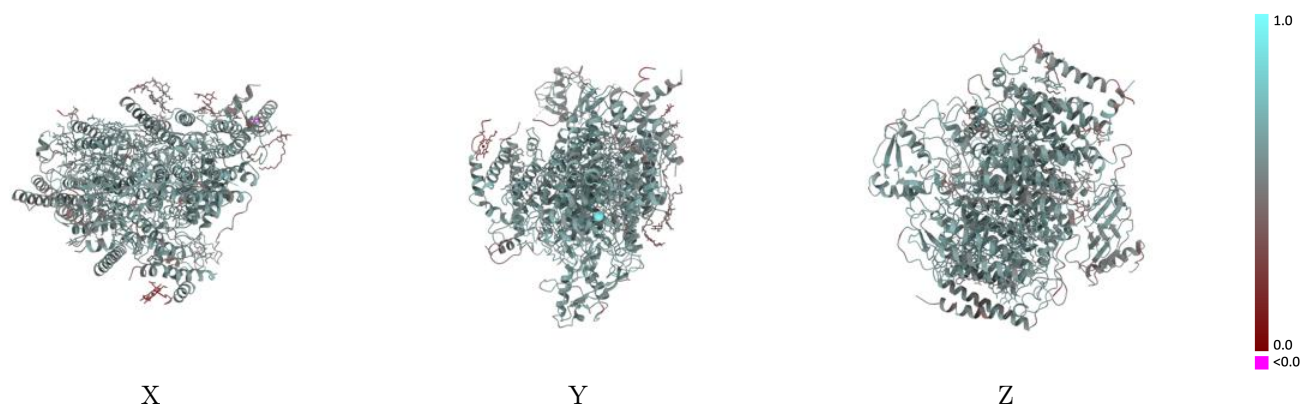
This section contains information regarding the fit between EMDB map EMD-30902 and PDB model 7DXA. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

### 9.1 Map-model overlay [i](#)



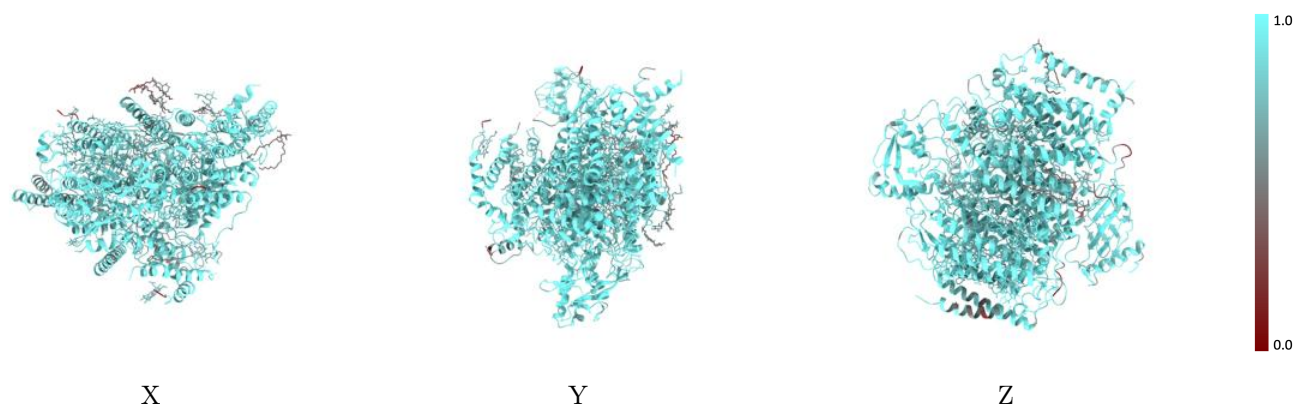
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



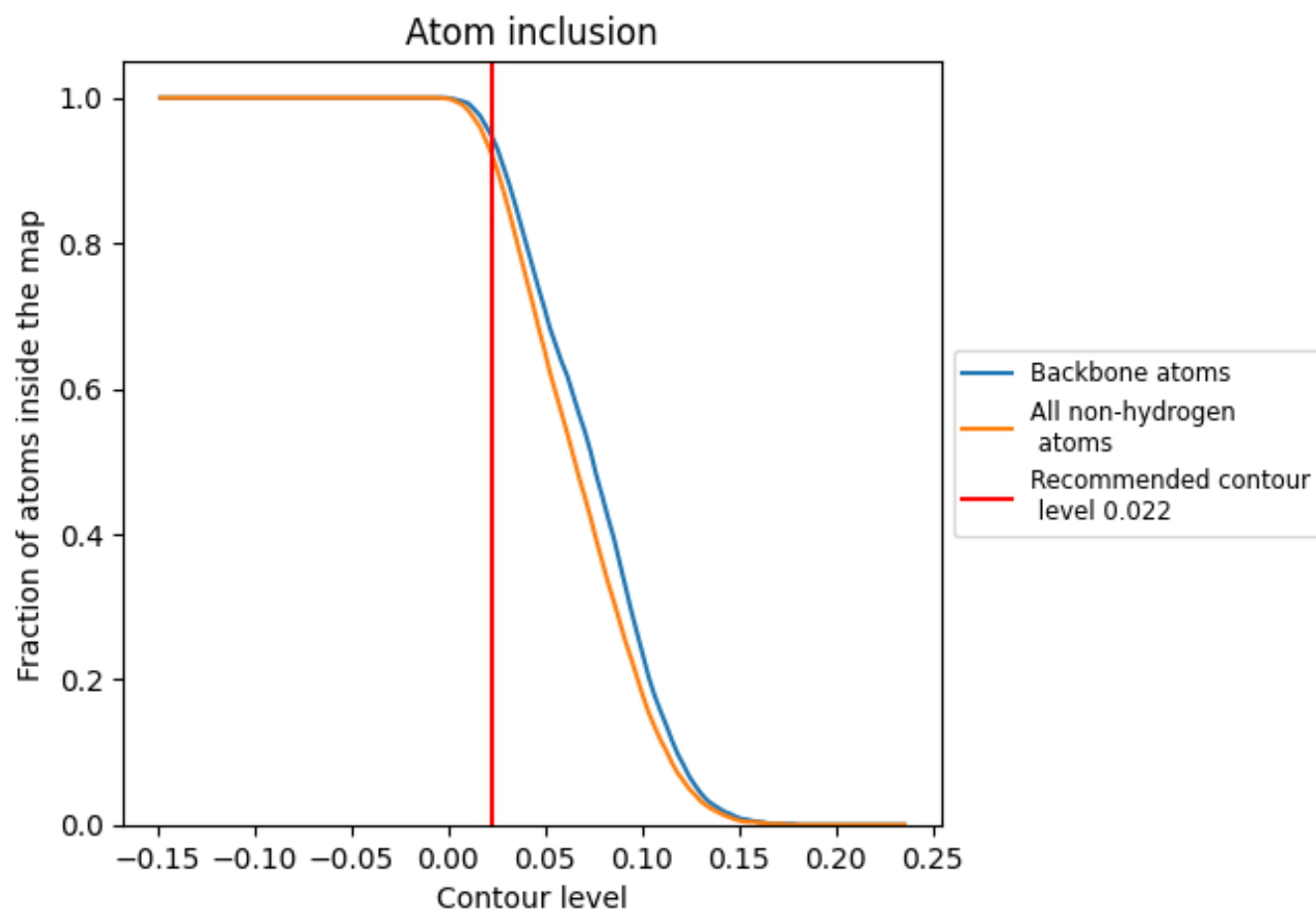
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.022) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.9240 | <div><div></div></div> 0.5680 |
| A     | <div><div></div></div> 0.9200 | <div><div></div></div> 0.5280 |
| B     | <div><div></div></div> 0.8660 | <div><div></div></div> 0.5290 |
| C     | <div><div></div></div> 0.7300 | <div><div></div></div> 0.4980 |
| a     | <div><div></div></div> 0.9400 | <div><div></div></div> 0.5640 |
| b     | <div><div></div></div> 0.9440 | <div><div></div></div> 0.5840 |
| d     | <div><div></div></div> 0.9500 | <div><div></div></div> 0.5940 |
| e     | <div><div></div></div> 0.8070 | <div><div></div></div> 0.4830 |
| f     | <div><div></div></div> 0.9540 | <div><div></div></div> 0.5290 |
| h     | <div><div></div></div> 0.9660 | <div><div></div></div> 0.5830 |
| i     | <div><div></div></div> 0.8440 | <div><div></div></div> 0.4770 |
| l     | <div><div></div></div> 0.8350 | <div><div></div></div> 0.5560 |
| m     | <div><div></div></div> 0.7870 | <div><div></div></div> 0.5070 |
| t     | <div><div></div></div> 0.7920 | <div><div></div></div> 0.5400 |
| x     | <div><div></div></div> 0.8810 | <div><div></div></div> 0.5480 |

1.0

0.0

<0.0