



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:19 PM UTC

PDB ID : 7DXH / pdb\_00007dxh  
EMDB ID : EMD-30909  
Title : Cryo-EM structure of PSII intermediate Psb28-PSII complex  
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:

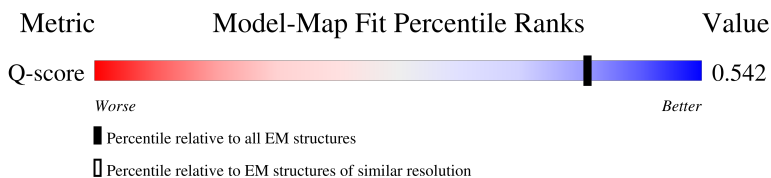
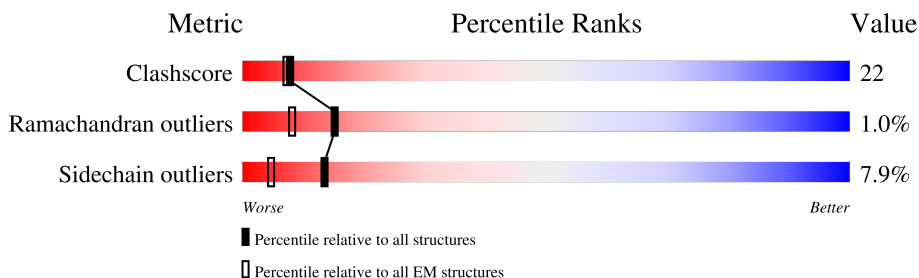
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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) : 2.49

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 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    |                  |
| 2   | B     | 56     |                  |
| 3   | a     | 360    |                  |
| 4   | b     | 505    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | d     | 342    |                  |
| 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     | 451    |                  |
| 15  | k     | 46     |                  |
| 16  | z     | 62     |                  |
| 17  | y     | 30     |                  |
| 18  | 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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 21  | CLA  | a     | 402 | X         | -        | -       | -                |
| 21  | CLA  | b     | 601 | X         | -        | -       | -                |
| 21  | CLA  | b     | 602 | X         | -        | -       | -                |
| 21  | CLA  | b     | 603 | X         | -        | -       | -                |
| 21  | CLA  | b     | 604 | X         | -        | -       | -                |
| 21  | CLA  | b     | 605 | X         | -        | X       | -                |
| 21  | CLA  | b     | 606 | X         | -        | -       | -                |
| 21  | CLA  | b     | 609 | X         | -        | -       | -                |
| 21  | CLA  | b     | 611 | X         | -        | -       | -                |
| 21  | CLA  | b     | 612 | X         | -        | -       | -                |
| 21  | CLA  | b     | 613 | X         | -        | -       | -                |
| 21  | CLA  | b     | 614 | X         | -        | -       | -                |
| 21  | CLA  | b     | 615 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 21  | CLA  | c     | 503 | X         | -        | X       | -                |
| 21  | CLA  | c     | 504 | X         | -        | -       | -                |
| 21  | CLA  | c     | 507 | -         | -        | X       | -                |
| 21  | CLA  | c     | 508 | X         | -        | -       | -                |
| 21  | CLA  | c     | 509 | X         | -        | -       | -                |
| 21  | CLA  | c     | 510 | X         | -        | X       | -                |
| 21  | CLA  | c     | 511 | X         | -        | -       | -                |
| 21  | CLA  | d     | 402 | X         | -        | -       | -                |
| 21  | CLA  | d     | 406 | X         | -        | -       | -                |
| 22  | BCR  | c     | 515 | -         | -        | X       | -                |
| 23  | CL   | a     | 405 | -         | -        | X       | -                |
| 31  | HTG  | h     | 102 | -         | -        | X       | -                |

## 2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 20054 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     | 48       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 349   | 227 | 63 | 59 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | a     | 297      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2304  | 1515 | 381 | 393 | 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     | 27       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 230   | 164 | 30 | 34 | 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 Photosystem II CP43 reaction center protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14  | c     | 403      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3130  | 2071 | 520 | 527 | 12 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 15  | k     | 34       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 264   | 186 | 36 | 42 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 16  | z     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 455   | 316 | 67 | 70 | 2 |         |       |

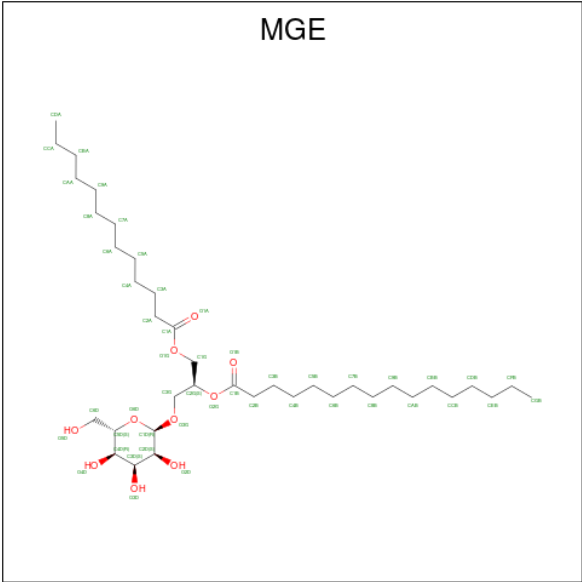
- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 17  | y     | 28       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 137   | 81 | 28 | 28 |         |       |

- Molecule 18 is a protein called unidentified transmembrane protein.

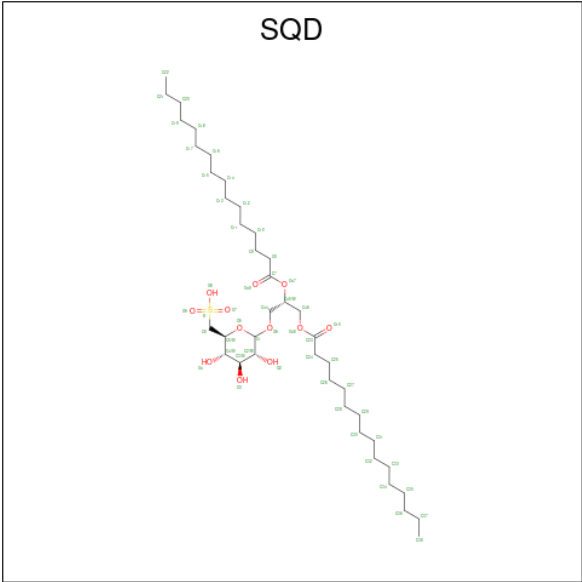
| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 18  | C     | 23       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 115   | 69 | 23 | 23 |         |       |

- Molecule 19 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>).



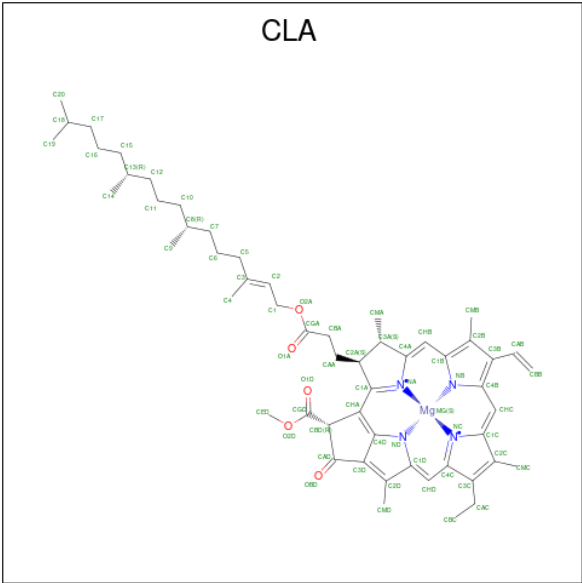
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 19  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 19  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 19  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 41    | 31 | 10 |         |
| 19  | d     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 19  | f     | 1        | Total | C  | O  | 0       |
|     |       |          | 47    | 37 | 10 |         |
| 19  | m     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 19  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |

- Molecule 20 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 20  | a     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 26    | 13 | 12 | 1 |         |
| 20  | 1     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 47    | 34 | 12 | 1 |         |

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 21  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 21  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |

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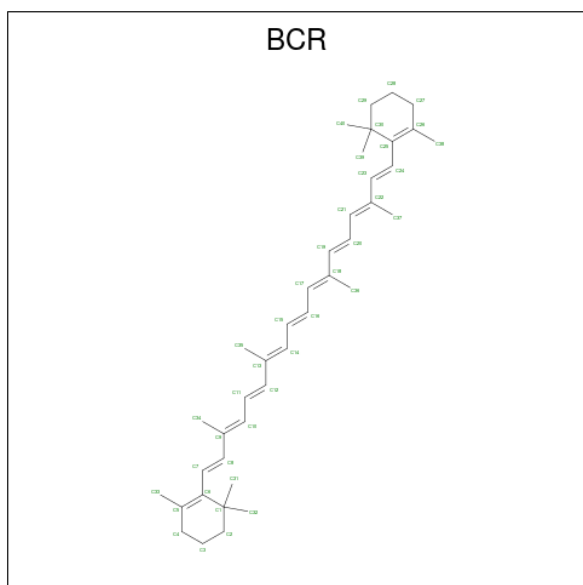
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 21  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | b     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | b     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | b     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | d     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | d     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | d     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 21  | h     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 21  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 21  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 21  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 21  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 21  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 21  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 21  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 63    | 53 | 1  | 4 | 5 |         |
| 21  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 21  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 21  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 21  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 21  | k     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).

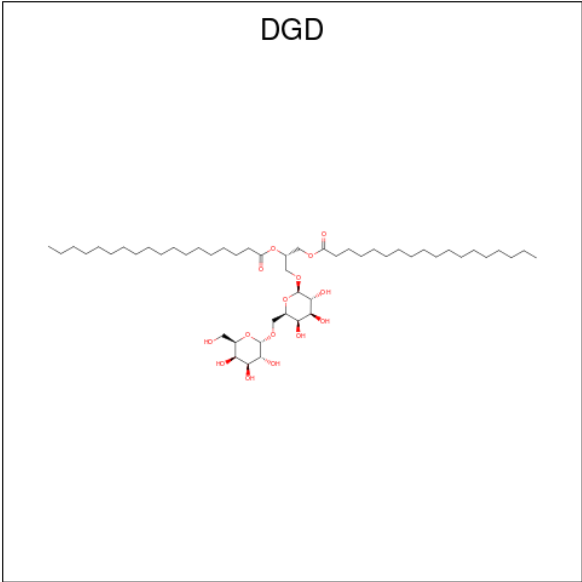


| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 22  | a     | 1        | Total C<br>40 40 | 0       |
| 22  | b     | 1        | Total C<br>40 40 | 0       |
| 22  | b     | 1        | Total C<br>40 40 | 0       |
| 22  | b     | 1        | Total C<br>40 40 | 0       |
| 22  | d     | 1        | Total C<br>40 40 | 0       |
| 22  | h     | 1        | Total C<br>40 40 | 0       |
| 22  | c     | 1        | Total C<br>40 40 | 0       |
| 22  | c     | 1        | Total C<br>40 40 | 0       |
| 22  | z     | 1        | Total C<br>40 40 | 0       |

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

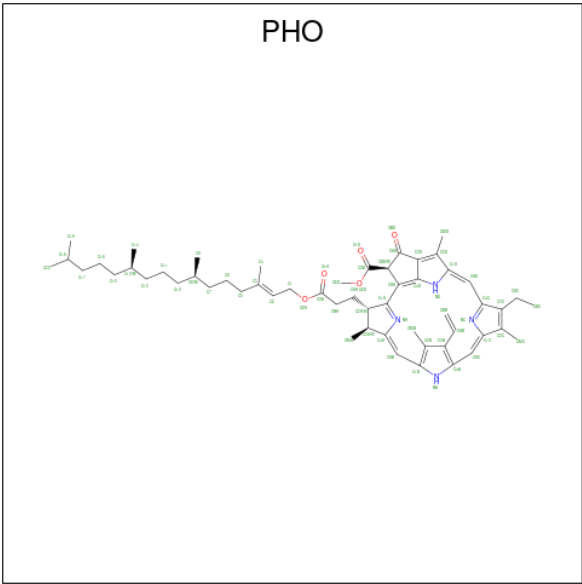
| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 23  | a     | 1        | Total Cl<br>1 1 | 0       |
| 23  | c     | 1        | Total Cl<br>1 1 | 0       |

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



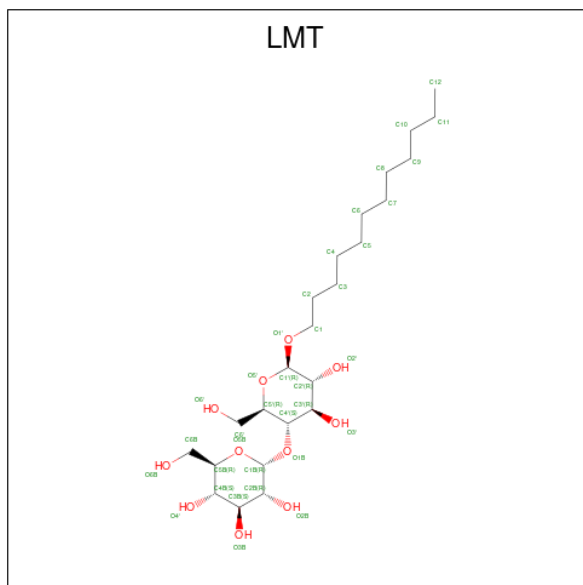
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 24  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 57    | 42 | 15 |         |
| 24  | h     | 1        | Total | C  | O  | 0       |
|     |       |          | 54    | 39 | 15 |         |
| 24  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 53    | 38 | 15 |         |
| 24  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 47    | 32 | 15 |         |

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 25  | d     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 25  | d     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |

- Molecule 26 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).

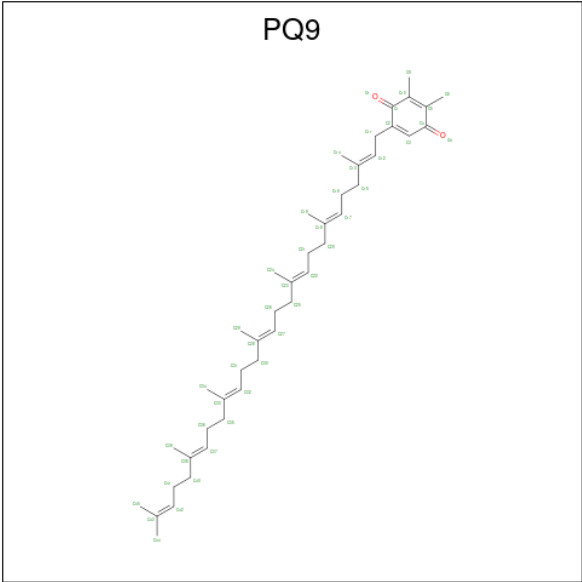


| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 26  | d     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 26  | m     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 26  | t     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

- Molecule 27 is FE (II) ION (CCD ID: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 27  | d     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 28 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:  $C_{43}H_{64}O_2$ ).

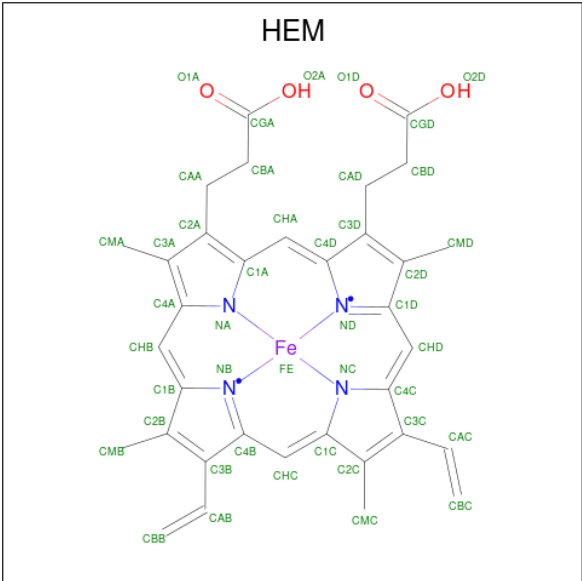


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 28  | d     | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 43 | 2 |         |

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

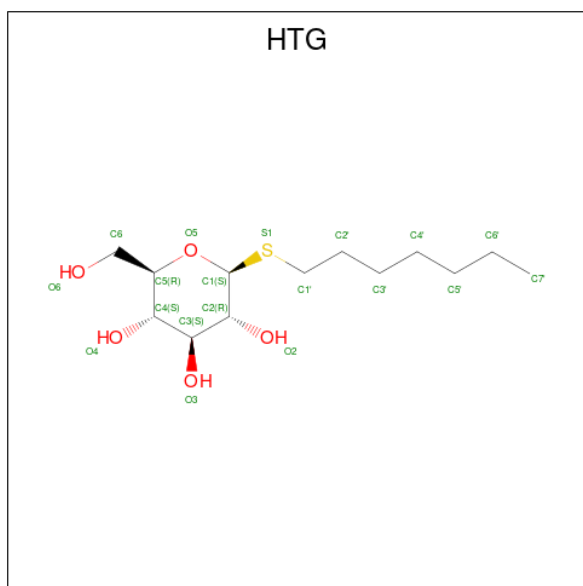
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 29  | d     | 2        | Total | C  | O | 0       |
|     |       |          | 53    | 47 | 6 |         |

- Molecule 30 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 30  | e     | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |

- Molecule 31 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula:  $C_{13}H_{26}O_5S$ ).

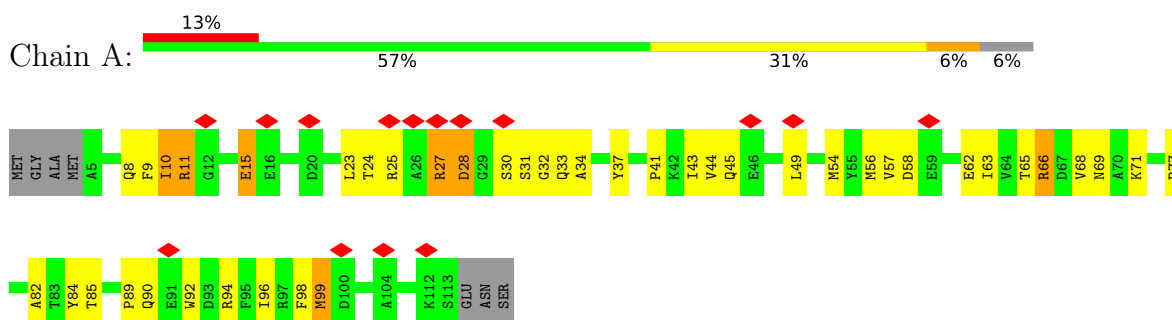


| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 31  | h     | 1        | Total | C  | O | S | 0       |
|     |       |          | 16    | 10 | 5 | 1 |         |

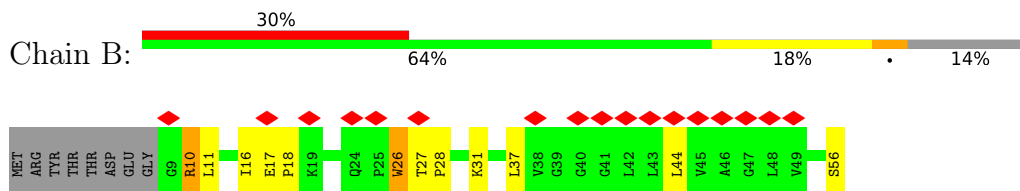
### 3 Residue-property plots

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.

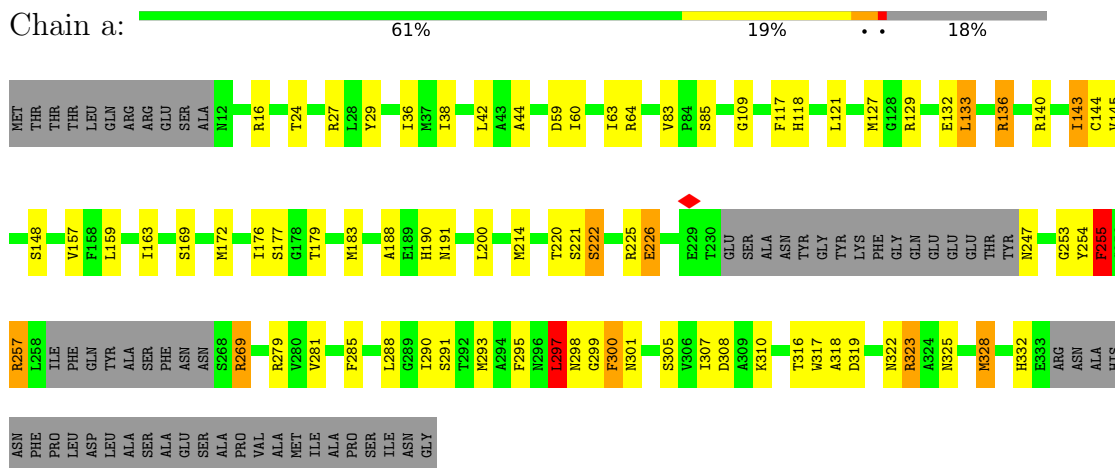
- Molecule 1: Photosystem II reaction center Psb28 protein



- Molecule 2: Tsl0063 protein

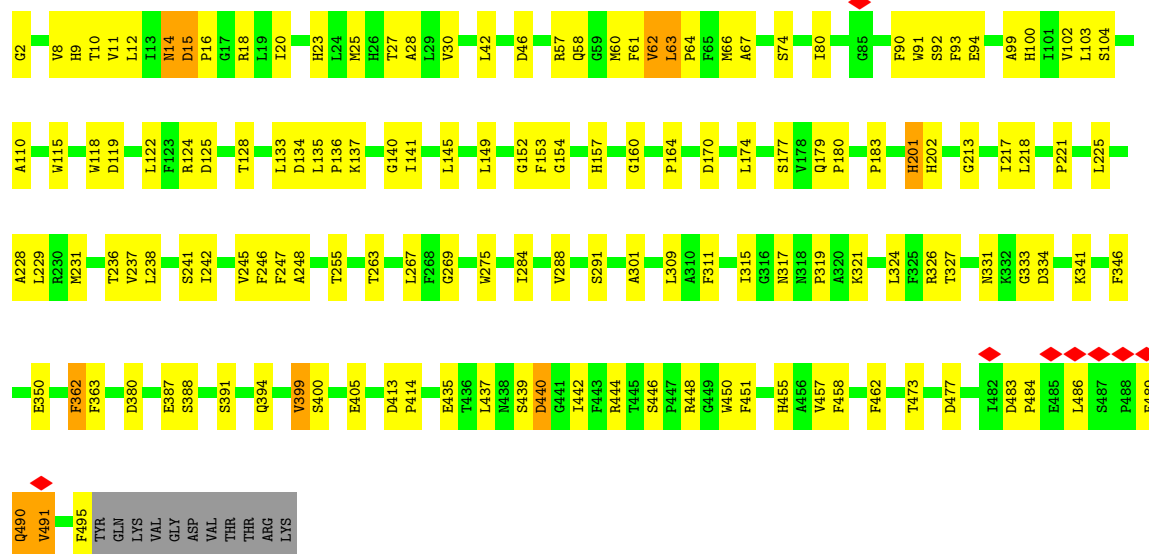


- Molecule 3: Photosystem II protein D1



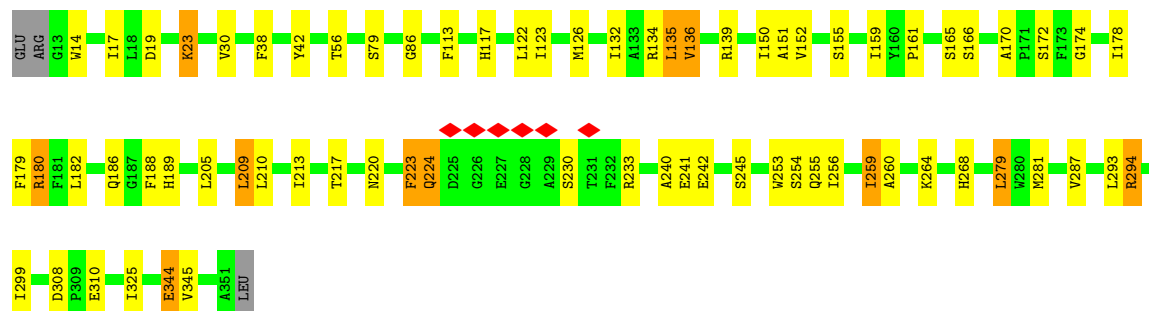
- Molecule 4: Photosystem II CP47 reaction center protein

Chain b: 



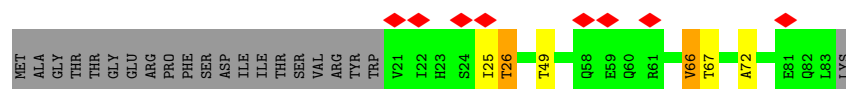
- Molecule 5: Photosystem II D2 protein

Chain d: 

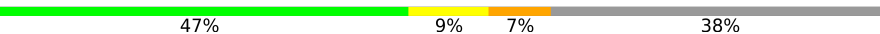


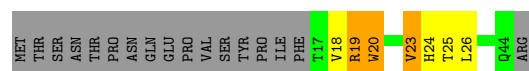
- Molecule 6: Cytochrome b559 subunit alpha

Chain e: 



- Molecule 7: Cytochrome b559 subunit beta

Chain f: 



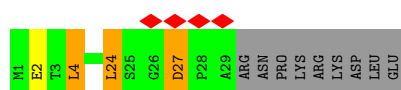
- Molecule 8: Photosystem II reaction center protein H

Chain h:  68% 23% • • 5%



• Molecule 9: Photosystem II reaction center protein I

Chain i:  11% 66% • 8% 24%



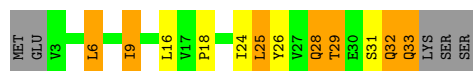
• Molecule 10: Photosystem II reaction center protein L

Chain l:  11% 59% 32% 8%



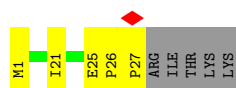
• Molecule 11: Photosystem II reaction center protein M

Chain m:  53% 14% 19% 14%



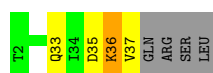
• Molecule 12: Photosystem II reaction center protein T

Chain t:  69% 16% 16%



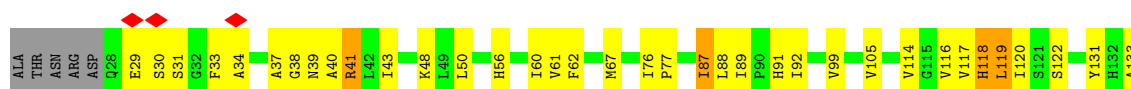
• Molecule 13: Photosystem II reaction center protein X

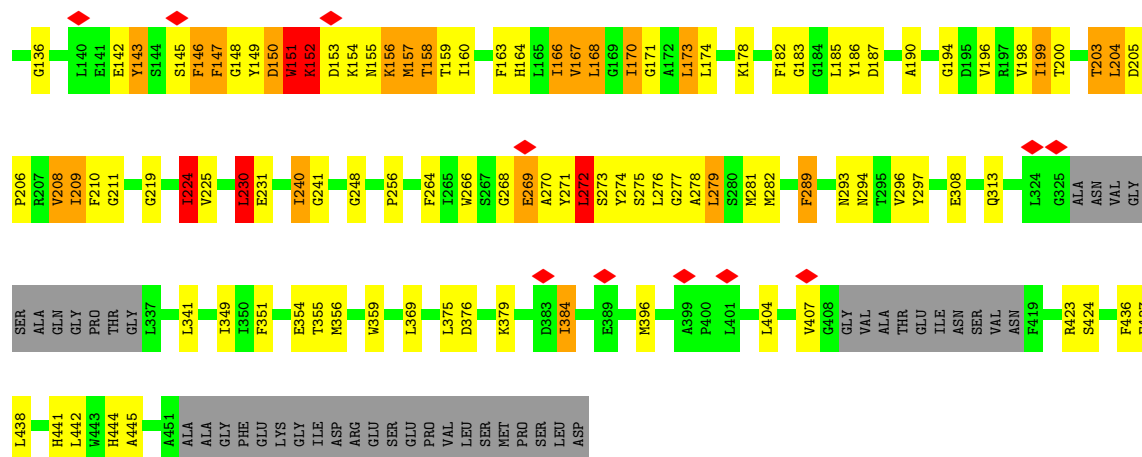
Chain x:  80% 8% • 10%



• Molecule 14: Photosystem II CP43 reaction center protein

Chain c:  58% 24% 6% • 11%

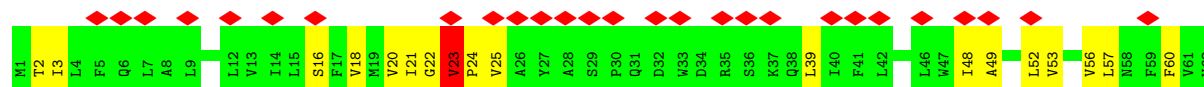




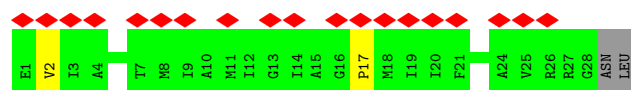
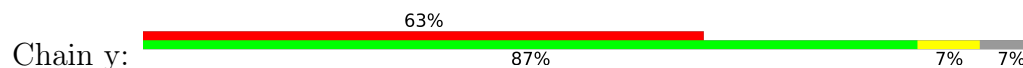
• Molecule 15: Photosystem II reaction center protein K



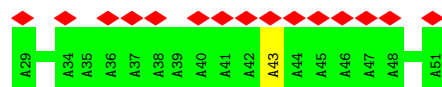
• Molecule 16: Photosystem II reaction center protein Z



• Molecule 17: Photosystem II reaction center protein Ycf12



• Molecule 18: unidentified transmembrane protein



## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE           | Depositor |
| Imposed symmetry                     | POINT, Not provided       |           |
| Number of particles used             | 194738                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF         | Depositor |
| CTF correction method                | NONE                      | 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                    | 0.261                     | Depositor |
| Minimum map value                    | -0.150                    | Depositor |
| Average map value                    | 0.000                     | Depositor |
| Map value standard deviation         | 0.007                     | Depositor |
| Recommended contour level            | 0.024                     | Depositor |
| Map size ( $\text{\AA}$ )            | 261.308, 261.308, 261.308 | wwPDB     |
| Map dimensions                       | 200, 200, 200             | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0          | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 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: MGE, PQ9, UNL, HEM, PHO, CLA, HTG, BCR, FE2, SQD, CL, DGD, LMT

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     | 0.48         | 0/892       | 0.76        | 0/1202          |
| 2   | B     | 0.27         | 0/355       | 0.72        | 1/484 (0.2%)    |
| 3   | a     | 0.36         | 0/2376      | 0.74        | 2/3239 (0.1%)   |
| 4   | b     | 0.36         | 0/4025      | 0.67        | 6/5486 (0.1%)   |
| 5   | d     | 0.40         | 0/2789      | 0.69        | 1/3803 (0.0%)   |
| 6   | e     | 0.27         | 0/523       | 0.60        | 0/714           |
| 7   | f     | 0.37         | 0/225       | 0.79        | 0/308           |
| 8   | h     | 0.36         | 0/506       | 0.70        | 0/690           |
| 9   | i     | 0.38         | 0/237       | 0.90        | 1/322 (0.3%)    |
| 10  | l     | 0.32         | 0/311       | 0.73        | 1/422 (0.2%)    |
| 11  | m     | 0.46         | 0/248       | 1.01        | 2/339 (0.6%)    |
| 12  | t     | 0.28         | 0/239       | 0.50        | 0/324           |
| 13  | x     | 0.26         | 0/264       | 0.60        | 0/358           |
| 14  | c     | 0.36         | 0/3237      | 0.79        | 7/4408 (0.2%)   |
| 15  | k     | 0.34         | 0/274       | 1.12        | 3/379 (0.8%)    |
| 16  | z     | 0.28         | 0/466       | 0.70        | 1/641 (0.2%)    |
| 17  | y     | 0.39         | 0/136       | 1.05        | 1/187 (0.5%)    |
| 18  | C     | 0.41         | 0/114       | 0.76        | 0/158           |
| All | All   | 0.37         | 0/17217     | 0.73        | 26/23464 (0.1%) |

There are no bond length outliers.

All (26) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 15  | k     | 25  | LEU  | CA-C-N | 8.36  | 130.29      | 119.84   |
| 15  | k     | 25  | LEU  | C-N-CA | 8.36  | 130.29      | 119.84   |
| 5   | d     | 242 | GLU  | N-CA-C | -8.28 | 104.05      | 114.56   |
| 11  | m     | 16  | LEU  | CA-C-N | 7.76  | 125.13      | 120.24   |
| 11  | m     | 16  | LEU  | C-N-CA | 7.76  | 125.13      | 120.24   |
| 3   | a     | 297 | LEU  | N-CA-C | -7.70 | 93.44       | 107.75   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 26  | TRP  | N-CA-C  | 6.80  | 118.62      | 110.19   |
| 17  | y     | 17  | PRO  | N-CA-CB | 6.71  | 110.64      | 103.52   |
| 10  | l     | 16  | SER  | N-CA-C  | -6.64 | 104.20      | 112.90   |
| 14  | c     | 76  | ILE  | CA-C-N  | 6.41  | 127.85      | 119.84   |
| 14  | c     | 76  | ILE  | C-N-CA  | 6.41  | 127.85      | 119.84   |
| 4   | b     | 15  | ASP  | CA-C-N  | 6.35  | 126.04      | 119.56   |
| 4   | b     | 15  | ASP  | C-N-CA  | 6.35  | 126.04      | 119.56   |
| 14  | c     | 155 | ASN  | N-CA-C  | -6.00 | 106.60      | 114.04   |
| 14  | c     | 224 | ILE  | N-CA-C  | -5.92 | 108.09      | 113.71   |
| 4   | b     | 435 | GLU  | CA-C-N  | 5.81  | 132.64      | 121.54   |
| 4   | b     | 435 | GLU  | C-N-CA  | 5.81  | 132.64      | 121.54   |
| 4   | b     | 350 | GLU  | N-CA-C  | -5.66 | 107.38      | 114.56   |
| 15  | k     | 28  | ILE  | CB-CA-C | -5.59 | 108.39      | 113.70   |
| 9   | i     | 4   | LEU  | N-CA-C  | -5.49 | 106.94      | 113.97   |
| 16  | z     | 3   | ILE  | N-CA-C  | -5.39 | 107.49      | 112.83   |
| 14  | c     | 158 | THR  | N-CA-C  | -5.27 | 106.54      | 112.87   |
| 3   | a     | 255 | PHE  | CB-CA-C | 5.24  | 120.85      | 110.42   |
| 4   | b     | 14  | ASN  | N-CA-C  | 5.22  | 119.28      | 113.02   |
| 14  | c     | 272 | LEU  | N-CA-C  | -5.17 | 105.73      | 111.36   |
| 14  | c     | 230 | LEU  | N-CA-C  | -5.15 | 107.13      | 113.41   |

There are no chirality outliers.

There are no planarity outliers.

## 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      | 83      | 0            |
| 2   | B     | 349   | 0        | 368      | 18      | 0            |
| 3   | a     | 2304  | 0        | 2235     | 119     | 0            |
| 4   | b     | 3886  | 0        | 3741     | 198     | 0            |
| 5   | d     | 2694  | 0        | 2588     | 94      | 0            |
| 6   | e     | 509   | 0        | 499      | 3       | 0            |
| 7   | f     | 219   | 0        | 228      | 6       | 0            |
| 8   | h     | 493   | 0        | 513      | 30      | 0            |
| 9   | i     | 231   | 0        | 243      | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | l     | 304   | 0        | 316      | 14      | 0            |
| 11  | m     | 244   | 0        | 256      | 15      | 0            |
| 12  | t     | 230   | 0        | 231      | 4       | 0            |
| 13  | x     | 261   | 0        | 291      | 2       | 0            |
| 14  | c     | 3130  | 0        | 3059     | 231     | 0            |
| 15  | k     | 264   | 0        | 269      | 25      | 0            |
| 16  | z     | 455   | 0        | 474      | 16      | 0            |
| 17  | y     | 137   | 0        | 72       | 0       | 0            |
| 18  | C     | 115   | 0        | 114      | 3       | 0            |
| 19  | B     | 48    | 0        | 72       | 8       | 0            |
| 19  | b     | 89    | 0        | 127      | 9       | 0            |
| 19  | c     | 48    | 0        | 69       | 0       | 0            |
| 19  | d     | 48    | 0        | 71       | 11      | 0            |
| 19  | f     | 47    | 0        | 67       | 0       | 0            |
| 19  | m     | 48    | 0        | 72       | 1       | 0            |
| 20  | a     | 26    | 0        | 16       | 0       | 0            |
| 20  | l     | 47    | 0        | 61       | 3       | 0            |
| 21  | a     | 181   | 0        | 185      | 13      | 0            |
| 21  | b     | 932   | 0        | 988      | 109     | 0            |
| 21  | c     | 613   | 0        | 573      | 128     | 0            |
| 21  | d     | 176   | 0        | 172      | 16      | 0            |
| 21  | h     | 41    | 0        | 29       | 0       | 0            |
| 21  | k     | 46    | 0        | 33       | 1       | 0            |
| 22  | a     | 40    | 0        | 56       | 2       | 0            |
| 22  | b     | 120   | 0        | 168      | 12      | 0            |
| 22  | c     | 80    | 0        | 112      | 49      | 0            |
| 22  | d     | 40    | 0        | 56       | 2       | 0            |
| 22  | h     | 40    | 0        | 56       | 2       | 0            |
| 22  | z     | 40    | 0        | 56       | 4       | 0            |
| 23  | a     | 1     | 0        | 0        | 2       | 0            |
| 23  | c     | 1     | 0        | 0        | 1       | 0            |
| 24  | a     | 57    | 0        | 72       | 5       | 0            |
| 24  | c     | 100   | 0        | 112      | 3       | 0            |
| 24  | h     | 54    | 0        | 66       | 3       | 0            |
| 25  | d     | 128   | 0        | 148      | 16      | 0            |
| 26  | d     | 35    | 0        | 46       | 1       | 0            |
| 26  | m     | 35    | 0        | 46       | 0       | 0            |
| 26  | t     | 35    | 0        | 46       | 2       | 0            |
| 27  | d     | 1     | 0        | 0        | 0       | 0            |
| 28  | d     | 45    | 0        | 64       | 6       | 0            |
| 29  | d     | 53    | 0        | 0        | 2       | 0            |
| 30  | e     | 43    | 0        | 30       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 31  | h     | 16    | 0        | 17       | 10      | 0            |
| All | All   | 20054 | 0        | 20022    | 901     | 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 22.

All (901) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:a:293:MET:HE1   | 3:a:298:ASN:CB    | 1.23                     | 1.64              |
| 14:c:157:MET:HE1  | 14:c:271:TYR:CD2  | 1.46                     | 1.49              |
| 3:a:269:ARG:CD    | 5:d:240:ALA:HB2   | 1.46                     | 1.45              |
| 21:b:606:CLA:H201 | 19:b:620:MGE:C6A  | 1.51                     | 1.40              |
| 14:c:157:MET:HE1  | 14:c:271:TYR:CE2  | 1.54                     | 1.40              |
| 3:a:269:ARG:HD2   | 5:d:240:ALA:CB    | 1.58                     | 1.33              |
| 3:a:293:MET:CE    | 3:a:298:ASN:CB    | 2.06                     | 1.32              |
| 3:a:293:MET:CE    | 3:a:298:ASN:HB3   | 1.60                     | 1.31              |
| 14:c:39:ASN:OD1   | 21:c:510:CLA:CBB  | 1.81                     | 1.27              |
| 1:A:66:ARG:O      | 3:a:255:PHE:CE2   | 1.89                     | 1.26              |
| 14:c:205:ASP:O    | 14:c:209:ILE:HG12 | 1.16                     | 1.26              |
| 11:m:25:LEU:O     | 11:m:29:THR:CG2   | 1.85                     | 1.25              |
| 11:m:25:LEU:O     | 11:m:29:THR:HG22  | 1.36                     | 1.20              |
| 3:a:293:MET:SD    | 3:a:298:ASN:HA    | 1.80                     | 1.18              |
| 1:A:33:GLN:HB2    | 1:A:84:TYR:O      | 1.39                     | 1.18              |
| 4:b:236:THR:CG2   | 4:b:473:THR:HG21  | 1.74                     | 1.18              |
| 1:A:31:SER:HB2    | 4:b:486:LEU:CD2   | 1.74                     | 1.17              |
| 3:a:190:HIS:HB3   | 3:a:293:MET:CE    | 1.73                     | 1.17              |
| 21:c:509:CLA:H91  | 22:c:515:BCR:H363 | 1.26                     | 1.16              |
| 14:c:157:MET:CE   | 14:c:271:TYR:CE2  | 2.29                     | 1.15              |
| 14:c:205:ASP:O    | 14:c:209:ILE:CG1  | 1.94                     | 1.15              |
| 14:c:296:VAL:HG11 | 21:c:503:CLA:HAA2 | 1.25                     | 1.15              |
| 3:a:190:HIS:HB3   | 3:a:293:MET:HE2   | 1.14                     | 1.14              |
| 14:c:152:LYS:HE2  | 14:c:152:LYS:HA   | 1.25                     | 1.13              |
| 1:A:33:GLN:HB3    | 1:A:85:THR:HA     | 1.31                     | 1.13              |
| 21:b:605:CLA:H71  | 22:b:618:BCR:H342 | 1.19                     | 1.13              |
| 14:c:438:LEU:HD11 | 21:c:507:CLA:HAB  | 1.29                     | 1.12              |
| 4:b:100:HIS:ND1   | 21:b:605:CLA:H42  | 1.65                     | 1.11              |
| 4:b:388:SER:O     | 4:b:394:GLN:OE1   | 1.66                     | 1.11              |
| 10:l:28:ALA:O     | 10:l:32:SER:OG    | 1.66                     | 1.11              |
| 1:A:31:SER:HB2    | 4:b:486:LEU:HD23  | 1.12                     | 1.11              |
| 14:c:442:LEU:HD21 | 21:c:507:CLA:HMB1 | 1.32                     | 1.11              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:k:22:VAL:HA    | 15:k:25:LEU:CD1   | 1.81                     | 1.10              |
| 14:c:296:VAL:HG11 | 21:c:503:CLA:CAA  | 1.81                     | 1.10              |
| 21:a:402:CLA:HMC2 | 21:d:406:CLA:HAC2 | 1.19                     | 1.09              |
| 21:c:509:CLA:C9   | 22:c:515:BCR:H363 | 1.81                     | 1.09              |
| 4:b:80:ILE:HD11   | 4:b:93:PHE:HZ     | 1.10                     | 1.08              |
| 4:b:100:HIS:ND1   | 21:b:605:CLA:C4   | 2.17                     | 1.07              |
| 1:A:33:GLN:CB     | 1:A:84:TYR:O      | 2.02                     | 1.07              |
| 1:A:41:PRO:HG2    | 1:A:44:VAL:HG23   | 1.34                     | 1.07              |
| 4:b:236:THR:HG22  | 4:b:473:THR:HG21  | 1.15                     | 1.07              |
| 1:A:66:ARG:O      | 3:a:255:PHE:CZ    | 2.08                     | 1.06              |
| 15:k:22:VAL:CA    | 15:k:25:LEU:HD12  | 1.85                     | 1.06              |
| 3:a:293:MET:HE1   | 3:a:298:ASN:HB3   | 1.20                     | 1.06              |
| 16:z:52:LEU:O     | 16:z:56:VAL:HG23  | 1.53                     | 1.06              |
| 5:d:178:ILE:HD11  | 25:d:403:PHO:C20  | 1.86                     | 1.05              |
| 3:a:190:HIS:CD2   | 3:a:293:MET:HE3   | 1.90                     | 1.05              |
| 5:d:178:ILE:HD11  | 25:d:403:PHO:H201 | 1.07                     | 1.04              |
| 14:c:157:MET:CE   | 14:c:271:TYR:CD2  | 2.41                     | 1.04              |
| 1:A:24:THR:HG23   | 4:b:491:VAL:O     | 1.57                     | 1.02              |
| 9:i:24:LEU:O      | 9:i:27:ASP:OD1    | 1.77                     | 1.02              |
| 14:c:436:PHE:HB3  | 21:c:511:CLA:C9   | 1.87                     | 1.02              |
| 4:b:80:ILE:HD11   | 4:b:93:PHE:CZ     | 1.93                     | 1.02              |
| 14:c:376:ASP:OD2  | 14:c:379:LYS:HG3  | 1.59                     | 1.01              |
| 14:c:436:PHE:HB3  | 21:c:511:CLA:H93  | 1.40                     | 1.01              |
| 1:A:10:ILE:HD11   | 1:A:43:ILE:CD1    | 1.92                     | 0.99              |
| 14:c:296:VAL:HG21 | 21:c:503:CLA:HMA2 | 1.40                     | 0.99              |
| 21:b:607:CLA:HBB1 | 5:d:126:MET:HE2   | 1.41                     | 0.99              |
| 19:b:619:MGE:O1B  | 11:m:6:LEU:HD11   | 1.63                     | 0.99              |
| 14:c:152:LYS:HZ3  | 14:c:154:LYS:HE3  | 1.26                     | 0.99              |
| 14:c:39:ASN:OD1   | 21:c:510:CLA:HBB1 | 1.64                     | 0.98              |
| 3:a:269:ARG:CD    | 5:d:240:ALA:CB    | 2.30                     | 0.97              |
| 14:c:438:LEU:HD11 | 21:c:507:CLA:CAB  | 1.94                     | 0.97              |
| 5:d:178:ILE:CD1   | 25:d:403:PHO:H201 | 1.94                     | 0.97              |
| 4:b:62:VAL:CG1    | 21:b:604:CLA:HED3 | 1.94                     | 0.97              |
| 5:d:209:LEU:O     | 5:d:213:ILE:HG13  | 1.64                     | 0.97              |
| 21:b:606:CLA:C20  | 19:b:620:MGE:C6A  | 2.43                     | 0.96              |
| 14:c:159:THR:HG22 | 14:c:163:PHE:CE2  | 2.01                     | 0.96              |
| 14:c:205:ASP:OD1  | 14:c:206:PRO:HD2  | 1.65                     | 0.96              |
| 14:c:204:LEU:HD22 | 14:c:204:LEU:H    | 1.31                     | 0.95              |
| 21:b:605:CLA:C7   | 22:b:618:BCR:H342 | 1.97                     | 0.94              |
| 21:b:605:CLA:H71  | 22:b:618:BCR:C34  | 1.98                     | 0.93              |
| 14:c:274:TYR:CE1  | 21:c:507:CLA:HED2 | 2.04                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:a:318:ALA:O     | 3:a:322:ASN:ND2   | 2.01                     | 0.92              |
| 15:k:25:LEU:CB    | 15:k:26:PRO:CD    | 2.48                     | 0.92              |
| 1:A:85:THR:OG1    | 4:b:486:LEU:HD11  | 1.69                     | 0.92              |
| 4:b:141:ILE:HD11  | 8:h:14:LEU:CD2    | 2.00                     | 0.92              |
| 3:a:293:MET:CE    | 3:a:298:ASN:HB2   | 1.85                     | 0.91              |
| 22:c:515:BCR:H403 | 22:c:515:BCR:H371 | 1.53                     | 0.91              |
| 4:b:62:VAL:HG13   | 21:b:604:CLA:HED3 | 1.51                     | 0.91              |
| 14:c:272:LEU:HB2  | 21:c:510:CLA:CHD  | 2.01                     | 0.90              |
| 22:c:515:BCR:H403 | 22:c:515:BCR:C37  | 2.01                     | 0.90              |
| 14:c:240:ILE:CD1  | 22:c:515:BCR:H392 | 2.02                     | 0.90              |
| 14:c:442:LEU:HD11 | 21:c:507:CLA:HMB3 | 1.54                     | 0.90              |
| 3:a:16:ARG:HG2    | 3:a:16:ARG:HH11   | 1.34                     | 0.89              |
| 14:c:152:LYS:NZ   | 14:c:154:LYS:HE3  | 1.87                     | 0.89              |
| 14:c:296:VAL:CG1  | 21:c:503:CLA:CAA  | 2.51                     | 0.88              |
| 21:c:507:CLA:HAA2 | 21:c:507:CLA:C1   | 2.02                     | 0.88              |
| 22:c:515:BCR:H272 | 22:c:515:BCR:H402 | 1.56                     | 0.88              |
| 3:a:293:MET:SD    | 3:a:298:ASN:CA    | 2.61                     | 0.88              |
| 4:b:236:THR:CG2   | 4:b:473:THR:CG2   | 2.51                     | 0.88              |
| 3:a:293:MET:HE1   | 3:a:298:ASN:HB2   | 0.89                     | 0.87              |
| 3:a:332:HIS:HD2   | 23:a:405:CL:CL    | 1.93                     | 0.87              |
| 14:c:264:PHE:HD1  | 22:c:515:BCR:H322 | 1.37                     | 0.87              |
| 3:a:269:ARG:HA    | 3:a:269:ARG:NE    | 1.87                     | 0.87              |
| 14:c:157:MET:SD   | 14:c:271:TYR:CE2  | 2.68                     | 0.87              |
| 21:a:402:CLA:CMC  | 21:d:406:CLA:HAC2 | 2.04                     | 0.86              |
| 1:A:66:ARG:O      | 3:a:255:PHE:HE2   | 1.50                     | 0.86              |
| 14:c:438:LEU:CD1  | 21:c:507:CLA:HAB  | 2.04                     | 0.86              |
| 15:k:28:ILE:HB    | 15:k:29:PRO:HD3   | 1.58                     | 0.86              |
| 5:d:14:TRP:CB     | 31:h:102:HTG:H61  | 2.05                     | 0.86              |
| 4:b:30:VAL:HG12   | 21:b:604:CLA:HHD  | 1.58                     | 0.86              |
| 14:c:152:LYS:NZ   | 14:c:154:LYS:CE   | 2.39                     | 0.86              |
| 4:b:80:ILE:CD1    | 4:b:93:PHE:HZ     | 1.87                     | 0.86              |
| 14:c:61:VAL:HG13  | 14:c:118:HIS:HD2  | 1.38                     | 0.86              |
| 1:A:31:SER:CB     | 4:b:486:LEU:HD23  | 2.03                     | 0.86              |
| 4:b:91:TRP:CZ2    | 21:b:605:CLA:H18  | 2.11                     | 0.86              |
| 4:b:236:THR:HG22  | 4:b:473:THR:CG2   | 2.05                     | 0.86              |
| 3:a:190:HIS:HD2   | 3:a:293:MET:HE3   | 1.39                     | 0.86              |
| 21:c:511:CLA:H201 | 15:k:33:LEU:HD22  | 1.57                     | 0.86              |
| 16:z:23:VAL:H     | 16:z:24:PRO:CD    | 1.90                     | 0.85              |
| 4:b:346:PHE:CE2   | 4:b:399:VAL:HG23  | 2.12                     | 0.85              |
| 14:c:442:LEU:HD21 | 21:c:507:CLA:CMB  | 2.07                     | 0.85              |
| 21:c:503:CLA:HMB3 | 22:c:515:BCR:C40  | 2.07                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:c:507:CLA:CHB  | 21:c:507:CLA:H42  | 2.06                     | 0.85              |
| 14:c:33:PHE:HB3   | 14:c:37:ALA:O     | 1.77                     | 0.85              |
| 1:A:57:VAL:HG22   | 1:A:62:GLU:OE2    | 1.77                     | 0.84              |
| 14:c:296:VAL:CG1  | 21:c:503:CLA:HAA2 | 2.06                     | 0.84              |
| 1:A:31:SER:CB     | 4:b:486:LEU:CD2   | 2.55                     | 0.84              |
| 4:b:90:PHE:CE2    | 21:b:605:CLA:H162 | 2.13                     | 0.83              |
| 1:A:10:ILE:HD11   | 1:A:43:ILE:HD11   | 1.61                     | 0.83              |
| 4:b:346:PHE:CD2   | 4:b:399:VAL:HG23  | 2.13                     | 0.82              |
| 14:c:240:ILE:CD1  | 22:c:515:BCR:C39  | 2.58                     | 0.82              |
| 3:a:190:HIS:CB    | 3:a:293:MET:CE    | 2.57                     | 0.82              |
| 14:c:159:THR:CG2  | 14:c:163:PHE:CE2  | 2.62                     | 0.82              |
| 5:d:30:VAL:HG22   | 5:d:38:PHE:CE2    | 2.14                     | 0.82              |
| 14:c:436:PHE:CB   | 21:c:511:CLA:H93  | 2.09                     | 0.82              |
| 14:c:274:TYR:HE1  | 21:c:507:CLA:CED  | 1.94                     | 0.81              |
| 2:B:44:LEU:HB2    | 18:C:43:ALA:CB    | 2.10                     | 0.81              |
| 4:b:125:ASP:OD2   | 4:b:128:THR:OG1   | 1.99                     | 0.80              |
| 22:c:515:BCR:H371 | 22:c:515:BCR:C25  | 2.11                     | 0.80              |
| 8:h:12:ARG:HD3    | 8:h:12:ARG:C      | 2.06                     | 0.80              |
| 14:c:436:PHE:CB   | 21:c:511:CLA:C9   | 2.58                     | 0.80              |
| 21:c:503:CLA:H161 | 22:c:515:BCR:C12  | 2.11                     | 0.80              |
| 1:A:41:PRO:HD2    | 1:A:44:VAL:HG21   | 1.64                     | 0.80              |
| 3:a:332:HIS:CD2   | 23:a:405:CL:CL    | 2.71                     | 0.80              |
| 3:a:60:ILE:HD11   | 3:a:83:VAL:HG13   | 1.62                     | 0.79              |
| 21:c:503:CLA:HMB3 | 22:c:515:BCR:H401 | 1.64                     | 0.79              |
| 1:A:33:GLN:CB     | 1:A:85:THR:HA     | 2.11                     | 0.79              |
| 9:i:4:LEU:O       | 9:i:4:LEU:HD23    | 1.83                     | 0.79              |
| 3:a:293:MET:HE3   | 3:a:298:ASN:HB3   | 1.63                     | 0.79              |
| 2:B:44:LEU:HB2    | 18:C:43:ALA:HB1   | 1.64                     | 0.79              |
| 21:b:607:CLA:HBB1 | 5:d:126:MET:CE    | 2.12                     | 0.79              |
| 14:c:438:LEU:HD21 | 21:c:507:CLA:HBB2 | 1.65                     | 0.78              |
| 21:b:606:CLA:H92  | 19:b:619:MGE:H8B1 | 1.65                     | 0.78              |
| 8:h:12:ARG:HD3    | 8:h:12:ARG:O      | 1.83                     | 0.78              |
| 4:b:247:PHE:CE2   | 21:b:602:CLA:H41  | 2.18                     | 0.78              |
| 3:a:279:ARG:CG    | 25:d:401:PHO:HAC1 | 2.14                     | 0.77              |
| 4:b:141:ILE:HD11  | 8:h:14:LEU:HD22   | 1.64                     | 0.77              |
| 1:A:41:PRO:HG2    | 1:A:44:VAL:CG2    | 2.14                     | 0.77              |
| 1:A:33:GLN:HB2    | 1:A:84:TYR:C      | 2.10                     | 0.76              |
| 14:c:159:THR:HG22 | 14:c:163:PHE:CD2  | 2.20                     | 0.76              |
| 14:c:436:PHE:HB3  | 21:c:511:CLA:H92  | 1.67                     | 0.76              |
| 14:c:240:ILE:HD12 | 22:c:515:BCR:C39  | 2.16                     | 0.76              |
| 1:A:33:GLN:CA     | 1:A:84:TYR:O      | 2.34                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:c:274:TYR:CE1  | 21:c:507:CLA:CED  | 2.69                     | 0.76              |
| 4:b:16:PRO:O      | 4:b:20:ILE:HG12   | 1.84                     | 0.76              |
| 21:c:503:CLA:H121 | 22:c:515:BCR:H14C | 1.68                     | 0.75              |
| 4:b:388:SER:HB2   | 4:b:391:SER:HB2   | 1.68                     | 0.75              |
| 1:A:33:GLN:HB3    | 1:A:85:THR:CA     | 2.13                     | 0.75              |
| 3:a:317:TRP:CZ3   | 5:d:180:ARG:HD2   | 2.22                     | 0.75              |
| 14:c:272:LEU:N    | 21:c:510:CLA:HMD3 | 2.01                     | 0.75              |
| 4:b:141:ILE:HD11  | 8:h:14:LEU:HD23   | 1.69                     | 0.75              |
| 4:b:100:HIS:CE1   | 21:b:605:CLA:C4   | 2.70                     | 0.74              |
| 4:b:102:VAL:HG23  | 21:b:605:CLA:H102 | 1.67                     | 0.74              |
| 21:c:503:CLA:CMB  | 22:c:515:BCR:H401 | 2.18                     | 0.74              |
| 14:c:277:GLY:O    | 21:c:507:CLA:HMC1 | 1.87                     | 0.74              |
| 4:b:236:THR:HG23  | 4:b:473:THR:HG21  | 1.70                     | 0.74              |
| 11:m:29:THR:O     | 11:m:33:GLN:HG3   | 1.88                     | 0.74              |
| 14:c:39:ASN:OD1   | 21:c:510:CLA:HBB2 | 1.86                     | 0.74              |
| 14:c:43:ILE:O     | 14:c:151:TRP:HZ2  | 1.71                     | 0.74              |
| 14:c:270:ALA:O    | 14:c:274:TYR:CD1  | 2.41                     | 0.74              |
| 14:c:204:LEU:HD22 | 14:c:204:LEU:N    | 2.01                     | 0.74              |
| 4:b:380:ASP:OD2   | 5:d:344:GLU:OE2   | 2.05                     | 0.73              |
| 14:c:166:ILE:HD11 | 14:c:248:GLY:C    | 2.13                     | 0.73              |
| 14:c:166:ILE:HD13 | 14:c:166:ILE:N    | 2.02                     | 0.73              |
| 15:k:22:VAL:HA    | 15:k:25:LEU:HD12  | 0.88                     | 0.73              |
| 21:c:503:CLA:CMB  | 22:c:515:BCR:C40  | 2.66                     | 0.73              |
| 4:b:62:VAL:HG11   | 21:b:604:CLA:HED3 | 1.71                     | 0.73              |
| 4:b:236:THR:HG23  | 4:b:473:THR:CG2   | 2.18                     | 0.73              |
| 15:k:25:LEU:HB3   | 15:k:26:PRO:CD    | 2.18                     | 0.73              |
| 3:a:297:LEU:HD21  | 14:c:404:LEU:HG   | 1.69                     | 0.72              |
| 14:c:271:TYR:C    | 21:c:510:CLA:HMD3 | 2.13                     | 0.72              |
| 15:k:25:LEU:CB    | 15:k:26:PRO:HD2   | 2.18                     | 0.72              |
| 22:c:515:BCR:H371 | 22:c:515:BCR:C40  | 2.18                     | 0.72              |
| 4:b:346:PHE:CE2   | 4:b:399:VAL:CG2   | 2.72                     | 0.72              |
| 5:d:14:TRP:HB2    | 31:h:102:HTG:H61  | 1.71                     | 0.72              |
| 21:c:507:CLA:HAA2 | 21:c:507:CLA:H11  | 1.70                     | 0.72              |
| 1:A:27:ARG:NH1    | 1:A:27:ARG:HG2    | 2.04                     | 0.72              |
| 3:a:307:ILE:HG22  | 3:a:308:ASP:N     | 2.04                     | 0.72              |
| 6:e:66:VAL:HG11   | 6:e:72:ALA:HB1    | 1.71                     | 0.72              |
| 1:A:27:ARG:HG2    | 1:A:27:ARG:HH11   | 1.54                     | 0.72              |
| 14:c:376:ASP:OD1  | 14:c:379:LYS:HB2  | 1.89                     | 0.72              |
| 5:d:259:ILE:CD1   | 19:d:410:MGE:H5A1 | 2.19                     | 0.72              |
| 4:b:141:ILE:CD1   | 8:h:14:LEU:HD22   | 2.20                     | 0.71              |
| 4:b:118:TRP:CZ2   | 10:l:4:ASN:HA     | 2.25                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:k:25:LEU:HB2   | 15:k:26:PRO:HD2   | 1.71                     | 0.71              |
| 13:x:33:GLN:OE1   | 13:x:36:LYS:NZ    | 2.23                     | 0.71              |
| 14:c:240:ILE:HD12 | 22:c:515:BCR:H392 | 1.70                     | 0.71              |
| 5:d:209:LEU:HD23  | 5:d:209:LEU:C     | 2.14                     | 0.71              |
| 14:c:38:GLY:O     | 14:c:41:ARG:HG3   | 1.91                     | 0.71              |
| 4:b:149:LEU:HD13  | 21:b:603:CLA:H203 | 1.73                     | 0.71              |
| 14:c:39:ASN:CG    | 21:c:510:CLA:CBB  | 2.63                     | 0.71              |
| 4:b:319:PRO:HB3   | 4:b:446:SER:OG    | 1.89                     | 0.71              |
| 22:c:515:BCR:H402 | 22:c:515:BCR:C27  | 2.21                     | 0.71              |
| 1:A:10:ILE:HD11   | 1:A:43:ILE:HD13   | 1.72                     | 0.70              |
| 5:d:17:ILE:HD13   | 13:x:36:LYS:HD3   | 1.73                     | 0.70              |
| 3:a:200:LEU:HD13  | 3:a:285:PHE:CD2   | 2.26                     | 0.70              |
| 5:d:132:ILE:O     | 5:d:136:VAL:HG23  | 1.92                     | 0.70              |
| 4:b:100:HIS:ND1   | 21:b:605:CLA:H43  | 2.06                     | 0.70              |
| 11:m:29:THR:O     | 11:m:33:GLN:HA    | 1.91                     | 0.70              |
| 5:d:152:VAL:HG21  | 5:d:279:LEU:HD13  | 1.74                     | 0.69              |
| 1:A:63:ILE:HD11   | 1:A:94:ARG:HG3    | 1.73                     | 0.69              |
| 3:a:118:HIS:HD2   | 21:a:403:CLA:HMA3 | 1.56                     | 0.69              |
| 14:c:296:VAL:HG11 | 21:c:503:CLA:C2A  | 2.22                     | 0.69              |
| 14:c:67:MET:HB3   | 14:c:88:LEU:CD1   | 2.23                     | 0.69              |
| 21:c:507:CLA:H42  | 21:c:507:CLA:C1B  | 2.22                     | 0.69              |
| 16:z:20:VAL:HG12  | 16:z:21:ILE:HG23  | 1.75                     | 0.69              |
| 4:b:100:HIS:CE1   | 21:b:605:CLA:H42  | 2.28                     | 0.69              |
| 3:a:190:HIS:CG    | 3:a:293:MET:HE3   | 2.28                     | 0.68              |
| 4:b:238:LEU:HD22  | 21:b:611:CLA:CHD  | 2.22                     | 0.68              |
| 14:c:166:ILE:O    | 14:c:170:ILE:HG12 | 1.92                     | 0.68              |
| 3:a:200:LEU:HD23  | 24:a:406:DGD:HBW2 | 1.75                     | 0.68              |
| 21:c:509:CLA:C9   | 22:c:515:BCR:C36  | 2.69                     | 0.68              |
| 1:A:11:ARG:HG3    | 1:A:11:ARG:HH11   | 1.59                     | 0.68              |
| 14:c:60:ILE:HG22  | 21:c:505:CLA:HHD  | 1.76                     | 0.68              |
| 14:c:62:PHE:CE1   | 14:c:119:LEU:HD11 | 2.28                     | 0.68              |
| 4:b:450:TRP:CD1   | 21:b:606:CLA:H3A  | 2.29                     | 0.68              |
| 14:c:33:PHE:CE2   | 14:c:40:ALA:O     | 2.47                     | 0.68              |
| 1:A:23:LEU:HD21   | 1:A:96:ILE:HD11   | 1.74                     | 0.68              |
| 15:k:13:GLU:OE2   | 15:k:13:GLU:HA    | 1.93                     | 0.67              |
| 5:d:205:LEU:HD13  | 25:d:401:PHO:HAB  | 1.77                     | 0.67              |
| 5:d:30:VAL:HG22   | 5:d:38:PHE:HE2    | 1.55                     | 0.67              |
| 3:a:307:ILE:CG2   | 3:a:308:ASP:N     | 2.58                     | 0.67              |
| 4:b:100:HIS:CE1   | 21:b:605:CLA:H43  | 2.29                     | 0.67              |
| 4:b:462:PHE:CZ    | 21:b:612:CLA:HMB3 | 2.30                     | 0.67              |
| 21:c:503:CLA:H102 | 22:c:515:BCR:H362 | 1.77                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:a:16:ARG:HG2    | 3:a:16:ARG:NH1    | 2.08                     | 0.66              |
| 14:c:48:LYS:HD2   | 14:c:133:ALA:O    | 1.94                     | 0.66              |
| 14:c:61:VAL:HG13  | 14:c:118:HIS:CD2  | 2.27                     | 0.66              |
| 4:b:122:LEU:HD21  | 21:b:614:CLA:HBC2 | 1.77                     | 0.66              |
| 4:b:231:MET:HE2   | 21:b:609:CLA:HMC2 | 1.77                     | 0.66              |
| 5:d:259:ILE:CD1   | 19:d:410:MGE:H7A1 | 2.25                     | 0.66              |
| 21:c:507:CLA:HHB  | 21:c:507:CLA:H12  | 1.76                     | 0.66              |
| 21:c:503:CLA:H161 | 22:c:515:BCR:H12C | 1.77                     | 0.66              |
| 3:a:200:LEU:HD13  | 3:a:285:PHE:HD2   | 1.60                     | 0.66              |
| 14:c:152:LYS:O    | 14:c:154:LYS:N    | 2.29                     | 0.66              |
| 25:d:403:PHO:CBB  | 21:d:406:CLA:H12  | 2.26                     | 0.66              |
| 3:a:200:LEU:CD2   | 24:a:406:DGD:HBN1 | 2.26                     | 0.66              |
| 3:a:279:ARG:CG    | 25:d:401:PHO:CAC  | 2.73                     | 0.66              |
| 4:b:125:ASP:CG    | 4:b:128:THR:OG1   | 2.39                     | 0.66              |
| 15:k:25:LEU:HB3   | 15:k:26:PRO:HD3   | 1.77                     | 0.66              |
| 3:a:63:ILE:HG22   | 3:a:64:ARG:H      | 1.61                     | 0.66              |
| 5:d:14:TRP:HB3    | 31:h:102:HTG:H61  | 1.75                     | 0.65              |
| 22:c:515:BCR:H403 | 22:c:515:BCR:H373 | 1.78                     | 0.65              |
| 4:b:164:PRO:HG3   | 21:b:605:CLA:O1D  | 1.96                     | 0.65              |
| 5:d:14:TRP:HB3    | 31:h:102:HTG:C6   | 2.26                     | 0.65              |
| 3:a:293:MET:SD    | 3:a:298:ASN:CB    | 2.85                     | 0.65              |
| 14:c:281:MET:HE3  | 21:c:507:CLA:HBC3 | 1.78                     | 0.65              |
| 3:a:200:LEU:CD2   | 24:a:406:DGD:HBW2 | 2.27                     | 0.65              |
| 4:b:388:SER:CB    | 4:b:391:SER:HB2   | 2.27                     | 0.65              |
| 14:c:264:PHE:CD1  | 22:c:515:BCR:H322 | 2.28                     | 0.64              |
| 14:c:41:ARG:NH1   | 21:k:501:CLA:HMD3 | 2.11                     | 0.64              |
| 21:c:505:CLA:H18  | 21:c:511:CLA:HBB2 | 1.79                     | 0.64              |
| 4:b:46:ASP:H      | 4:b:58:GLN:HE22   | 1.45                     | 0.64              |
| 14:c:204:LEU:H    | 14:c:204:LEU:CD2  | 2.07                     | 0.64              |
| 14:c:203:THR:HG23 | 14:c:231:GLU:O    | 1.97                     | 0.64              |
| 5:d:19:ASP:OD1    | 5:d:23:LYS:NZ     | 2.29                     | 0.63              |
| 5:d:259:ILE:HD13  | 19:d:410:MGE:C6A  | 2.29                     | 0.63              |
| 14:c:157:MET:CE   | 14:c:271:TYR:HE2  | 2.08                     | 0.63              |
| 15:k:25:LEU:HB2   | 15:k:26:PRO:CD    | 2.24                     | 0.63              |
| 1:A:31:SER:CB     | 4:b:486:LEU:HD22  | 2.27                     | 0.63              |
| 5:d:14:TRP:CB     | 31:h:102:HTG:C6   | 2.76                     | 0.63              |
| 3:a:188:ALA:HB2   | 3:a:328:MET:HB2   | 1.81                     | 0.63              |
| 1:A:24:THR:HG22   | 4:b:490:GLN:OE1   | 1.97                     | 0.63              |
| 21:b:614:CLA:H2   | 21:b:615:CLA:HBB2 | 1.81                     | 0.63              |
| 14:c:152:LYS:HE2  | 14:c:152:LYS:CA   | 2.16                     | 0.63              |
| 14:c:203:THR:CG2  | 14:c:231:GLU:O    | 2.46                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:d:259:ILE:HD13  | 19:d:410:MGE:H5A1 | 1.81                     | 0.62              |
| 3:a:226:GLU:O     | 3:a:226:GLU:HG3   | 1.98                     | 0.62              |
| 14:c:152:LYS:HZ1  | 14:c:154:LYS:CE   | 2.11                     | 0.62              |
| 3:a:63:ILE:HG22   | 3:a:64:ARG:N      | 2.13                     | 0.62              |
| 11:m:6:LEU:HA     | 11:m:9:ILE:HG13   | 1.81                     | 0.62              |
| 2:B:10:ARG:HD3    | 19:B:101:MGE:H4D  | 1.80                     | 0.62              |
| 21:a:402:CLA:HMC2 | 21:d:406:CLA:CAC  | 2.12                     | 0.62              |
| 4:b:231:MET:HE2   | 21:b:609:CLA:CMC  | 2.29                     | 0.62              |
| 14:c:157:MET:SD   | 14:c:271:TYR:HE2  | 2.19                     | 0.62              |
| 4:b:153:PHE:HB2   | 21:b:605:CLA:HHC  | 1.82                     | 0.62              |
| 14:c:156:LYS:O    | 14:c:156:LYS:HG3  | 1.97                     | 0.62              |
| 21:b:606:CLA:H191 | 19:b:620:MGE:C6A  | 2.30                     | 0.62              |
| 3:a:118:HIS:CD2   | 21:a:403:CLA:HMA3 | 2.34                     | 0.62              |
| 4:b:149:LEU:HB2   | 21:b:603:CLA:H171 | 1.80                     | 0.61              |
| 21:c:503:CLA:H143 | 22:c:515:BCR:H12C | 1.80                     | 0.61              |
| 4:b:319:PRO:HB3   | 4:b:446:SER:HG    | 1.64                     | 0.61              |
| 5:d:186:GLN:HB2   | 21:d:406:CLA:HBC1 | 1.82                     | 0.61              |
| 11:m:28:GLN:O     | 11:m:28:GLN:HG2   | 1.99                     | 0.61              |
| 1:A:11:ARG:HH11   | 1:A:11:ARG:CG     | 2.12                     | 0.61              |
| 1:A:41:PRO:CG     | 1:A:44:VAL:HG23   | 2.22                     | 0.61              |
| 14:c:296:VAL:CG1  | 21:c:503:CLA:HAA1 | 2.30                     | 0.61              |
| 16:z:21:ILE:O     | 16:z:21:ILE:HG13  | 2.00                     | 0.61              |
| 4:b:122:LEU:CD2   | 21:b:614:CLA:HBC2 | 2.31                     | 0.61              |
| 1:A:66:ARG:CG     | 1:A:66:ARG:HH21   | 2.13                     | 0.61              |
| 1:A:27:ARG:HH11   | 1:A:27:ARG:CG     | 2.14                     | 0.60              |
| 1:A:28:ASP:OD1    | 1:A:28:ASP:N      | 2.34                     | 0.60              |
| 5:d:259:ILE:HD13  | 19:d:410:MGE:C5A  | 2.32                     | 0.60              |
| 15:k:25:LEU:O     | 15:k:28:ILE:HG12  | 2.01                     | 0.60              |
| 5:d:217:THR:HG21  | 5:d:253:TRP:HE1   | 1.67                     | 0.60              |
| 14:c:43:ILE:CD1   | 14:c:269:GLU:OE1  | 2.50                     | 0.60              |
| 14:c:62:PHE:HD2   | 15:k:29:PRO:HG3   | 1.65                     | 0.60              |
| 14:c:168:LEU:HD22 | 21:c:509:CLA:CED  | 2.32                     | 0.60              |
| 3:a:226:GLU:OE2   | 5:d:264:LYS:HB2   | 2.02                     | 0.60              |
| 4:b:64:PRO:HB3    | 4:b:267:LEU:HB3   | 1.83                     | 0.60              |
| 14:c:67:MET:HB3   | 14:c:88:LEU:HD12  | 1.82                     | 0.60              |
| 5:d:259:ILE:HD12  | 19:d:410:MGE:H7A1 | 1.82                     | 0.60              |
| 14:c:436:PHE:CB   | 21:c:511:CLA:H92  | 2.29                     | 0.60              |
| 5:d:259:ILE:HD11  | 19:d:410:MGE:H5A1 | 1.83                     | 0.60              |
| 16:z:23:VAL:H     | 16:z:24:PRO:HD3   | 1.66                     | 0.60              |
| 3:a:293:MET:HE1   | 3:a:298:ASN:CA    | 2.22                     | 0.59              |
| 3:a:143:ILE:HD12  | 5:d:220:ASN:ND2   | 2.18                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:a:214:MET:SD    | 25:d:403:PHO:HED3 | 2.42                     | 0.59              |
| 21:c:507:CLA:CHB  | 21:c:507:CLA:H12  | 2.32                     | 0.59              |
| 3:a:200:LEU:CD1   | 3:a:285:PHE:HD2   | 2.15                     | 0.59              |
| 3:a:269:ARG:HG3   | 5:d:240:ALA:HB1   | 1.83                     | 0.59              |
| 4:b:102:VAL:HG23  | 21:b:605:CLA:C10  | 2.32                     | 0.59              |
| 21:b:613:CLA:OBD  | 10:l:10:VAL:HG21  | 2.01                     | 0.59              |
| 3:a:316:THR:HG23  | 3:a:318:ALA:H     | 1.66                     | 0.59              |
| 4:b:149:LEU:HD13  | 21:b:603:CLA:C20  | 2.32                     | 0.59              |
| 21:b:603:CLA:H43  | 21:b:604:CLA:H2   | 1.83                     | 0.59              |
| 19:B:101:MGE:H8B2 | 10:l:19:LEU:HD22  | 1.85                     | 0.59              |
| 5:d:174:GLY:O     | 5:d:178:ILE:HD12  | 2.02                     | 0.59              |
| 11:m:32:GLN:O     | 11:m:32:GLN:HG2   | 2.02                     | 0.59              |
| 14:c:384:ILE:HG22 | 14:c:384:ILE:O    | 2.02                     | 0.59              |
| 3:a:38:ILE:O      | 3:a:42:LEU:HG     | 2.03                     | 0.59              |
| 4:b:91:TRP:CH2    | 21:b:605:CLA:H161 | 2.38                     | 0.59              |
| 4:b:451:PHE:HZ    | 21:b:603:CLA:O2D  | 1.84                     | 0.59              |
| 4:b:201:HIS:O     | 4:b:201:HIS:ND1   | 2.35                     | 0.59              |
| 14:c:269:GLU:CB   | 21:c:510:CLA:HBC1 | 2.33                     | 0.59              |
| 8:h:25:TRP:CG     | 31:h:102:HTG:H1   | 2.38                     | 0.59              |
| 14:c:159:THR:O    | 14:c:163:PHE:CD2  | 2.56                     | 0.58              |
| 3:a:200:LEU:CD1   | 3:a:285:PHE:CD2   | 2.86                     | 0.58              |
| 1:A:41:PRO:HD2    | 1:A:44:VAL:CG2    | 2.34                     | 0.58              |
| 1:A:56:MET:HB3    | 1:A:98:PHE:CE2    | 2.39                     | 0.58              |
| 2:B:10:ARG:NE     | 19:B:101:MGE:O3D  | 2.36                     | 0.58              |
| 14:c:444:HIS:CE1  | 21:c:511:CLA:H11  | 2.38                     | 0.58              |
| 1:A:56:MET:HB3    | 1:A:98:PHE:CZ     | 2.38                     | 0.58              |
| 14:c:203:THR:O    | 14:c:209:ILE:HD11 | 2.04                     | 0.58              |
| 14:c:444:HIS:HE1  | 21:c:511:CLA:H11  | 1.68                     | 0.58              |
| 14:c:296:VAL:HG11 | 21:c:503:CLA:H2A  | 1.86                     | 0.58              |
| 22:c:515:BCR:H10C | 22:c:515:BCR:H352 | 1.85                     | 0.58              |
| 4:b:122:LEU:HD12  | 8:h:8:GLY:HA2     | 1.86                     | 0.58              |
| 4:b:100:HIS:HE1   | 21:b:605:CLA:H11  | 1.68                     | 0.58              |
| 8:h:7:LEU:HG      | 8:h:11:LEU:CD1    | 2.33                     | 0.58              |
| 1:A:57:VAL:CG2    | 1:A:62:GLU:OE2    | 2.48                     | 0.58              |
| 3:a:269:ARG:HD2   | 5:d:240:ALA:HB2   | 0.65                     | 0.58              |
| 4:b:23:HIS:ND1    | 21:b:614:CLA:OBD  | 2.37                     | 0.58              |
| 14:c:199:ILE:O    | 14:c:199:ILE:HG22 | 2.04                     | 0.58              |
| 21:c:511:CLA:C20  | 15:k:33:LEU:HD22  | 2.33                     | 0.58              |
| 14:c:203:THR:CG2  | 14:c:231:GLU:C    | 2.76                     | 0.57              |
| 1:A:63:ILE:CG2    | 1:A:84:TYR:CE2    | 2.87                     | 0.57              |
| 14:c:159:THR:CG2  | 14:c:163:PHE:HE2  | 2.15                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:b:242:ILE:HG13  | 21:b:611:CLA:HED1 | 1.86                     | 0.57              |
| 25:d:403:PHO:HBC2 | 25:d:403:PHO:HHD  | 1.86                     | 0.57              |
| 21:c:510:CLA:HBB1 | 21:c:510:CLA:HMB1 | 1.86                     | 0.57              |
| 14:c:159:THR:HG22 | 14:c:163:PHE:HE2  | 1.63                     | 0.57              |
| 14:c:296:VAL:CG1  | 21:c:503:CLA:H2A  | 2.34                     | 0.57              |
| 3:a:319:ASP:O     | 3:a:323:ARG:HB2   | 2.05                     | 0.57              |
| 14:c:276:LEU:HD23 | 21:c:510:CLA:HED1 | 1.87                     | 0.57              |
| 14:c:146:PHE:CD1  | 14:c:146:PHE:N    | 2.72                     | 0.57              |
| 21:c:508:CLA:HBB1 | 21:c:508:CLA:HMB1 | 1.86                     | 0.57              |
| 5:d:126:MET:SD    | 5:d:150:ILE:HD12  | 2.45                     | 0.56              |
| 5:d:79:SER:HA     | 5:d:172:SER:HB3   | 1.85                     | 0.56              |
| 8:h:12:ARG:H      | 8:h:13:PRO:CD     | 2.18                     | 0.56              |
| 14:c:156:LYS:O    | 14:c:160:ILE:HG13 | 2.04                     | 0.56              |
| 14:c:274:TYR:CD1  | 14:c:274:TYR:N    | 2.73                     | 0.56              |
| 21:c:509:CLA:H91  | 22:c:515:BCR:C36  | 2.18                     | 0.56              |
| 4:b:380:ASP:CG    | 5:d:344:GLU:OE2   | 2.48                     | 0.56              |
| 21:a:407:CLA:HMC1 | 21:d:406:CLA:H2   | 1.87                     | 0.56              |
| 4:b:103:LEU:HD22  | 21:b:605:CLA:H41  | 1.86                     | 0.56              |
| 4:b:213:GLY:O     | 4:b:217:ILE:HG13  | 2.06                     | 0.56              |
| 4:b:451:PHE:CZ    | 21:b:603:CLA:CED  | 2.88                     | 0.56              |
| 5:d:294:ARG:H     | 5:d:294:ARG:HD2   | 1.71                     | 0.56              |
| 21:c:503:CLA:HBB2 | 22:c:515:BCR:H361 | 1.86                     | 0.56              |
| 21:c:513:CLA:HBB1 | 22:z:101:BCR:H23C | 1.88                     | 0.56              |
| 15:k:25:LEU:CB    | 15:k:26:PRO:HD3   | 2.29                     | 0.56              |
| 16:z:23:VAL:H     | 16:z:24:PRO:HD2   | 1.69                     | 0.56              |
| 4:b:100:HIS:HE1   | 21:b:605:CLA:C1   | 2.18                     | 0.56              |
| 14:c:185:LEU:HD11 | 21:c:503:CLA:HED2 | 1.87                     | 0.55              |
| 1:A:94:ARG:HH12   | 1:A:98:PHE:HB2    | 1.71                     | 0.55              |
| 4:b:247:PHE:HE1   | 21:b:601:CLA:H102 | 1.71                     | 0.55              |
| 14:c:438:LEU:HD21 | 21:c:507:CLA:CBB  | 2.35                     | 0.55              |
| 14:c:114:VAL:HG21 | 21:c:505:CLA:HMA3 | 1.89                     | 0.55              |
| 14:c:205:ASP:O    | 14:c:209:ILE:HG13 | 2.02                     | 0.55              |
| 3:a:221:SER:HB2   | 5:d:139:ARG:O     | 2.07                     | 0.55              |
| 3:a:222:SER:O     | 3:a:222:SER:OG    | 2.23                     | 0.55              |
| 3:a:293:MET:SD    | 3:a:298:ASN:HB3   | 2.44                     | 0.55              |
| 1:A:44:VAL:HG13   | 1:A:77:PRO:HB2    | 1.89                     | 0.55              |
| 14:c:274:TYR:N    | 14:c:274:TYR:HD1  | 2.03                     | 0.55              |
| 4:b:311:PHE:O     | 4:b:317:ASN:ND2   | 2.40                     | 0.55              |
| 14:c:43:ILE:O     | 14:c:151:TRP:CZ2  | 2.57                     | 0.55              |
| 3:a:317:TRP:HZ3   | 5:d:180:ARG:HD2   | 1.72                     | 0.54              |
| 14:c:271:TYR:C    | 21:c:510:CLA:CMD  | 2.79                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:a:60:ILE:HG23   | 3:a:169:SER:HB2   | 1.88                     | 0.54              |
| 4:b:18:ARG:HD2    | 10:l:4:ASN:OD1    | 2.08                     | 0.54              |
| 8:h:12:ARG:H      | 8:h:13:PRO:HD2    | 1.72                     | 0.54              |
| 3:a:60:ILE:HD11   | 3:a:83:VAL:CG1    | 2.36                     | 0.54              |
| 3:a:157:VAL:HG22  | 3:a:290:ILE:CD1   | 2.37                     | 0.54              |
| 11:m:29:THR:O     | 11:m:33:GLN:CA    | 2.54                     | 0.54              |
| 14:c:351:PHE:CE2  | 14:c:375:LEU:HD12 | 2.42                     | 0.54              |
| 4:b:326:ARG:HG2   | 5:d:299:ILE:HD11  | 1.89                     | 0.54              |
| 5:d:264:LYS:O     | 5:d:268:HIS:ND1   | 2.40                     | 0.54              |
| 3:a:190:HIS:CD2   | 3:a:293:MET:CE    | 2.80                     | 0.54              |
| 30:e:101:HEM:HMD2 | 7:f:23:VAL:HG11   | 1.88                     | 0.54              |
| 8:h:41:PHE:CZ     | 8:h:45:ILE:HD11   | 2.41                     | 0.54              |
| 14:c:203:THR:HG22 | 14:c:231:GLU:HB3  | 1.90                     | 0.54              |
| 4:b:67:ALA:HB2    | 4:b:80:ILE:CD1    | 2.38                     | 0.54              |
| 4:b:269:GLY:O     | 4:b:448:ARG:NH1   | 2.41                     | 0.54              |
| 14:c:62:PHE:CD1   | 14:c:119:LEU:HD11 | 2.42                     | 0.54              |
| 14:c:282:MET:HE3  | 21:c:505:CLA:H91  | 1.88                     | 0.54              |
| 2:B:37:LEU:CG     | 4:b:218:LEU:HD11  | 2.34                     | 0.54              |
| 3:a:269:ARG:CG    | 5:d:240:ALA:CB    | 2.86                     | 0.54              |
| 19:d:410:MGE:H9A2 | 12:t:21:ILE:HD11  | 1.90                     | 0.54              |
| 21:c:503:CLA:C2B  | 22:c:515:BCR:H401 | 2.38                     | 0.54              |
| 3:a:44:ALA:HB2    | 3:a:118:HIS:HB2   | 1.89                     | 0.54              |
| 4:b:362:PHE:HE1   | 5:d:189:HIS:CE1   | 2.26                     | 0.54              |
| 5:d:14:TRP:HB2    | 31:h:102:HTG:C6   | 2.38                     | 0.54              |
| 29:d:412:UNL:C36  | 8:h:35:MET:HE2    | 2.38                     | 0.54              |
| 14:c:89:ILE:HA    | 14:c:92:ILE:HD12  | 1.90                     | 0.54              |
| 14:c:209:ILE:C    | 14:c:211:GLY:H    | 2.16                     | 0.54              |
| 4:b:164:PRO:HD3   | 21:b:605:CLA:O1D  | 2.08                     | 0.53              |
| 28:d:408:PQ9:H193 | 19:d:410:MGE:H7B1 | 1.90                     | 0.53              |
| 20:l:101:SQD:H301 | 20:l:101:SQD:H192 | 1.89                     | 0.53              |
| 21:c:507:CLA:H42  | 21:c:507:CLA:HBB  | 1.88                     | 0.53              |
| 21:b:612:CLA:HBB1 | 21:b:612:CLA:HMB1 | 1.91                     | 0.53              |
| 5:d:56:THR:HB     | 6:e:49:THR:HG23   | 1.89                     | 0.53              |
| 14:c:209:ILE:C    | 14:c:211:GLY:N    | 2.66                     | 0.53              |
| 1:A:68:VAL:HG12   | 3:a:254:TYR:CE1   | 2.43                     | 0.53              |
| 3:a:307:ILE:CG2   | 3:a:308:ASP:H     | 2.20                     | 0.53              |
| 4:b:100:HIS:CE1   | 21:b:605:CLA:H11  | 2.43                     | 0.53              |
| 5:d:174:GLY:O     | 5:d:178:ILE:CD1   | 2.56                     | 0.53              |
| 14:c:67:MET:HB3   | 14:c:88:LEU:HD11  | 1.90                     | 0.53              |
| 1:A:94:ARG:NH1    | 1:A:98:PHE:HB2    | 2.23                     | 0.53              |
| 3:a:133:LEU:O     | 3:a:133:LEU:HD22  | 2.07                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:b:57:ARG:NH1    | 4:b:334:ASP:OD1   | 2.41                     | 0.53              |
| 4:b:255:THR:HG21  | 21:b:601:CLA:HED1 | 1.91                     | 0.53              |
| 10:l:15:THR:HG23  | 12:t:25:GLU:OE1   | 2.09                     | 0.53              |
| 3:a:36:ILE:HG23   | 21:a:403:CLA:HBB1 | 1.90                     | 0.53              |
| 14:c:190:ALA:HB3  | 14:c:194:GLY:HA2  | 1.90                     | 0.53              |
| 14:c:269:GLU:HB2  | 21:c:510:CLA:HBC1 | 1.90                     | 0.53              |
| 14:c:341:LEU:HD12 | 14:c:349:ILE:HG22 | 1.89                     | 0.53              |
| 1:A:63:ILE:HG23   | 1:A:84:TYR:CE2    | 2.44                     | 0.53              |
| 14:c:266:TRP:NE1  | 14:c:271:TYR:OH   | 2.42                     | 0.53              |
| 14:c:293:ASN:HD21 | 14:c:296:VAL:H    | 1.55                     | 0.53              |
| 4:b:15:ASP:OD1    | 4:b:18:ARG:HB2    | 2.09                     | 0.52              |
| 21:c:509:CLA:H92  | 22:c:515:BCR:H363 | 1.84                     | 0.52              |
| 4:b:9:HIS:HB3     | 21:b:611:CLA:HAB  | 1.90                     | 0.52              |
| 11:m:25:LEU:O     | 11:m:29:THR:HG23  | 1.97                     | 0.52              |
| 14:c:171:GLY:HA3  | 21:c:512:CLA:H41  | 1.91                     | 0.52              |
| 3:a:24:THR:O      | 5:d:255:GLN:NE2   | 2.43                     | 0.52              |
| 4:b:99:ALA:HA     | 21:b:605:CLA:H121 | 1.92                     | 0.52              |
| 8:h:12:ARG:N      | 8:h:13:PRO:CD     | 2.72                     | 0.52              |
| 4:b:284:ILE:O     | 4:b:288:VAL:HG23  | 2.09                     | 0.52              |
| 19:b:619:MGE:O1B  | 11:m:6:LEU:CD1    | 2.49                     | 0.52              |
| 5:d:14:TRP:HB3    | 31:h:102:HTG:O6   | 2.09                     | 0.52              |
| 5:d:86:GLY:HA2    | 5:d:166:SER:HB3   | 1.91                     | 0.52              |
| 1:A:23:LEU:HD12   | 1:A:24:THR:H      | 1.74                     | 0.52              |
| 1:A:68:VAL:HG12   | 1:A:68:VAL:O      | 2.09                     | 0.52              |
| 4:b:12:LEU:HD11   | 21:b:613:CLA:HMA1 | 1.91                     | 0.52              |
| 5:d:209:LEU:O     | 5:d:209:LEU:HD23  | 2.09                     | 0.52              |
| 15:k:15:TYR:N     | 15:k:15:TYR:CD1   | 2.77                     | 0.52              |
| 3:a:140:ARG:O     | 5:d:220:ASN:ND2   | 2.42                     | 0.52              |
| 4:b:27:THR:HG22   | 21:b:611:CLA:H42  | 1.91                     | 0.52              |
| 4:b:217:ILE:HG22  | 4:b:217:ILE:O     | 2.09                     | 0.52              |
| 4:b:247:PHE:HE2   | 21:b:602:CLA:H41  | 1.74                     | 0.52              |
| 21:b:609:CLA:H203 | 21:b:609:CLA:H152 | 1.92                     | 0.52              |
| 14:c:209:ILE:O    | 14:c:211:GLY:N    | 2.43                     | 0.52              |
| 1:A:30:SER:HA     | 1:A:89:PRO:HG3    | 1.92                     | 0.52              |
| 3:a:163:ILE:HG12  | 24:c:516:DGD:HB21 | 1.92                     | 0.52              |
| 4:b:122:LEU:HD11  | 8:h:11:LEU:HB2    | 1.91                     | 0.52              |
| 8:h:51:SER:O      | 8:h:51:SER:OG     | 2.22                     | 0.52              |
| 2:B:10:ARG:HA     | 4:b:2:GLY:O       | 2.10                     | 0.51              |
| 3:a:288:LEU:HA    | 3:a:291:SER:HB2   | 1.91                     | 0.51              |
| 21:b:606:CLA:H172 | 5:d:281:MET:HE2   | 1.92                     | 0.51              |
| 4:b:245:VAL:HG13  | 21:b:611:CLA:C20  | 2.40                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:26:TRP:CD1    | 2:B:26:TRP:N      | 2.75                     | 0.51              |
| 3:a:190:HIS:CG    | 3:a:293:MET:CE    | 2.92                     | 0.51              |
| 4:b:67:ALA:HB2    | 4:b:80:ILE:HD13   | 1.91                     | 0.51              |
| 14:c:264:PHE:HD1  | 22:c:515:BCR:C32  | 2.17                     | 0.51              |
| 3:a:301:ASN:HD21  | 14:c:407:VAL:HG12 | 1.74                     | 0.51              |
| 1:A:41:PRO:CG     | 1:A:44:VAL:CG2    | 2.85                     | 0.51              |
| 4:b:458:PHE:HB3   | 21:b:603:CLA:HBC2 | 1.93                     | 0.51              |
| 21:c:504:CLA:CGA  | 21:c:505:CLA:H42  | 2.41                     | 0.51              |
| 1:A:41:PRO:CD     | 1:A:44:VAL:HG21   | 2.39                     | 0.51              |
| 3:a:183:MET:HA    | 21:a:402:CLA:HMD2 | 1.92                     | 0.51              |
| 4:b:16:PRO:HB3    | 4:b:133:LEU:HD21  | 1.93                     | 0.51              |
| 4:b:327:THR:HG21  | 19:b:619:MGE:H2B2 | 1.92                     | 0.51              |
| 21:b:607:CLA:HMB2 | 5:d:126:MET:HE3   | 1.92                     | 0.51              |
| 11:m:24:ILE:O     | 11:m:28:GLN:HB3   | 2.10                     | 0.51              |
| 4:b:149:LEU:HD22  | 21:b:603:CLA:H152 | 1.92                     | 0.51              |
| 4:b:455:HIS:HE1   | 21:b:606:CLA:CBB  | 2.24                     | 0.51              |
| 4:b:455:HIS:HE1   | 21:b:606:CLA:HBB2 | 1.75                     | 0.51              |
| 14:c:152:LYS:HA   | 14:c:152:LYS:CE   | 2.07                     | 0.51              |
| 4:b:9:HIS:CD2     | 21:b:610:CLA:H12  | 2.46                     | 0.51              |
| 4:b:362:PHE:O     | 5:d:188:PHE:HD2   | 1.94                     | 0.50              |
| 14:c:270:ALA:HB1  | 14:c:274:TYR:CE1  | 2.46                     | 0.50              |
| 15:k:20:PRO:O     | 15:k:24:VAL:HG22  | 2.10                     | 0.50              |
| 14:c:438:LEU:CG   | 21:c:507:CLA:HAB  | 2.41                     | 0.50              |
| 4:b:61:PHE:CE2    | 21:b:603:CLA:HMA1 | 2.47                     | 0.50              |
| 4:b:237:VAL:HG13  | 21:b:609:CLA:C1D  | 2.41                     | 0.50              |
| 14:c:143:TYR:CZ   | 21:c:513:CLA:HED1 | 2.47                     | 0.50              |
| 14:c:205:ASP:OD1  | 14:c:206:PRO:CD   | 2.48                     | 0.50              |
| 4:b:103:LEU:HD22  | 21:b:605:CLA:H51  | 1.94                     | 0.50              |
| 5:d:223:PHE:CE1   | 5:d:245:SER:HB3   | 2.46                     | 0.50              |
| 14:c:146:PHE:HA   | 14:c:156:LYS:HE3  | 1.93                     | 0.50              |
| 1:A:33:GLN:HA     | 1:A:84:TYR:O      | 2.08                     | 0.50              |
| 3:a:16:ARG:NH1    | 3:a:16:ARG:CG     | 2.73                     | 0.50              |
| 4:b:248:ALA:HA    | 21:b:602:CLA:H42  | 1.92                     | 0.50              |
| 14:c:152:LYS:HZ1  | 14:c:154:LYS:HE2  | 1.76                     | 0.50              |
| 3:a:63:ILE:CG2    | 3:a:64:ARG:H      | 2.24                     | 0.50              |
| 21:b:614:CLA:H2   | 21:b:615:CLA:CBB  | 2.41                     | 0.50              |
| 3:a:257:ARG:CG    | 3:a:257:ARG:HH11  | 2.25                     | 0.50              |
| 4:b:9:HIS:ND1     | 21:b:611:CLA:CBB  | 2.75                     | 0.50              |
| 4:b:324:LEU:HA    | 5:d:293:LEU:HD22  | 1.94                     | 0.50              |
| 2:B:44:LEU:HB2    | 18:C:43:ALA:HB3   | 1.92                     | 0.50              |
| 14:c:269:GLU:CA   | 21:c:510:CLA:HBC1 | 2.41                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:c:166:ILE:CD1  | 14:c:248:GLY:HA3  | 2.42                     | 0.49              |
| 14:c:275:SER:O    | 14:c:279:LEU:HG   | 2.13                     | 0.49              |
| 2:B:10:ARG:CZ     | 19:B:101:MGE:O3D  | 2.60                     | 0.49              |
| 3:a:269:ARG:HD3   | 5:d:240:ALA:HB2   | 1.75                     | 0.49              |
| 4:b:346:PHE:CZ    | 4:b:399:VAL:CG2   | 2.95                     | 0.49              |
| 4:b:462:PHE:CE2   | 21:b:612:CLA:HMB3 | 2.48                     | 0.49              |
| 14:c:224:ILE:HD12 | 22:c:515:BCR:H272 | 1.95                     | 0.49              |
| 1:A:85:THR:OG1    | 4:b:486:LEU:CD1   | 2.54                     | 0.49              |
| 3:a:191:ASN:OD1   | 3:a:325:ASN:ND2   | 2.44                     | 0.49              |
| 14:c:297:TYR:O    | 14:c:423:ARG:NH2  | 2.40                     | 0.49              |
| 21:c:503:CLA:C10  | 22:c:515:BCR:H362 | 2.41                     | 0.49              |
| 3:a:295:PHE:O     | 14:c:424:SER:OG   | 2.30                     | 0.49              |
| 3:a:297:LEU:C     | 3:a:297:LEU:CD2   | 2.85                     | 0.49              |
| 19:d:410:MGE:H5D  | 10:l:15:THR:OG1   | 2.12                     | 0.49              |
| 1:A:98:PHE:CD1    | 1:A:98:PHE:C      | 2.90                     | 0.49              |
| 14:c:183:GLY:HA2  | 14:c:198:VAL:HG22 | 1.95                     | 0.49              |
| 14:c:356:MET:O    | 14:c:359:TRP:HD1  | 1.94                     | 0.49              |
| 21:c:503:CLA:CMB  | 22:c:515:BCR:H403 | 2.40                     | 0.49              |
| 7:f:18:VAL:C      | 7:f:20:TRP:H      | 2.21                     | 0.49              |
| 14:c:33:PHE:CB    | 14:c:37:ALA:O     | 2.58                     | 0.49              |
| 14:c:62:PHE:CD2   | 15:k:29:PRO:HG3   | 2.46                     | 0.49              |
| 2:B:10:ARG:HD3    | 19:B:101:MGE:H3D  | 1.94                     | 0.49              |
| 3:a:29:TYR:HE2    | 3:a:132:GLU:HG2   | 1.78                     | 0.49              |
| 14:c:437:PHE:CE1  | 21:c:511:CLA:H8   | 2.48                     | 0.49              |
| 5:d:134:ARG:HG3   | 5:d:134:ARG:O     | 2.12                     | 0.48              |
| 14:c:39:ASN:HB3   | 21:c:510:CLA:CAB  | 2.43                     | 0.48              |
| 14:c:148:GLY:O    | 14:c:156:LYS:HG2  | 2.13                     | 0.48              |
| 14:c:240:ILE:HD13 | 22:c:515:BCR:C39  | 2.41                     | 0.48              |
| 14:c:39:ASN:CB    | 21:c:510:CLA:CBB  | 2.91                     | 0.48              |
| 21:a:402:CLA:C2C  | 21:d:406:CLA:HMC3 | 2.43                     | 0.48              |
| 6:e:25:ILE:HG13   | 6:e:26:THR:HG22   | 1.95                     | 0.48              |
| 14:c:173:LEU:HD12 | 14:c:241:GLY:HA3  | 1.96                     | 0.48              |
| 3:a:127:MET:HE3   | 3:a:144:CYS:SG    | 2.53                     | 0.48              |
| 1:A:69:ASN:CB     | 3:a:253:GLY:HA2   | 2.44                     | 0.48              |
| 4:b:90:PHE:HE2    | 21:b:605:CLA:H162 | 1.73                     | 0.48              |
| 4:b:291:SER:OG    | 4:b:301:ALA:HB1   | 2.14                     | 0.48              |
| 4:b:331:ASN:HB3   | 4:b:437:LEU:CD1   | 2.43                     | 0.48              |
| 1:A:23:LEU:HD12   | 1:A:33:GLN:O      | 2.14                     | 0.48              |
| 1:A:69:ASN:HB3    | 3:a:253:GLY:HA2   | 1.95                     | 0.48              |
| 3:a:214:MET:CE    | 25:d:403:PHO:CED  | 2.91                     | 0.48              |
| 4:b:118:TRP:CE2   | 10:l:4:ASN:HB2    | 2.49                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:b:229:LEU:O     | 4:b:236:THR:HG21  | 2.13                     | 0.48              |
| 4:b:451:PHE:CZ    | 21:b:603:CLA:HED1 | 2.48                     | 0.48              |
| 3:a:60:ILE:CG2    | 3:a:169:SER:HB2   | 2.44                     | 0.48              |
| 4:b:9:HIS:ND1     | 21:b:611:CLA:CAB  | 2.77                     | 0.48              |
| 14:c:62:PHE:CD1   | 14:c:119:LEU:CD1  | 2.96                     | 0.48              |
| 14:c:166:ILE:HD11 | 14:c:248:GLY:CA   | 2.44                     | 0.48              |
| 1:A:49:LEU:O      | 5:d:233:ARG:NH2   | 2.44                     | 0.48              |
| 3:a:29:TYR:O      | 3:a:129:ARG:NH1   | 2.40                     | 0.48              |
| 3:a:183:MET:SD    | 21:d:402:CLA:HAC1 | 2.53                     | 0.48              |
| 4:b:321:LYS:NZ    | 4:b:363:PHE:O     | 2.46                     | 0.48              |
| 5:d:134:ARG:HE    | 5:d:134:ARG:HA    | 1.79                     | 0.48              |
| 14:c:272:LEU:HA   | 21:c:510:CLA:C2D  | 2.44                     | 0.48              |
| 1:A:66:ARG:HH21   | 1:A:66:ARG:HG2    | 1.79                     | 0.48              |
| 14:c:157:MET:C    | 14:c:159:THR:N    | 2.70                     | 0.48              |
| 4:b:118:TRP:CZ2   | 10:l:4:ASN:CA     | 2.96                     | 0.48              |
| 14:c:87:ILE:CD1   | 21:c:506:CLA:CHB  | 2.92                     | 0.48              |
| 14:c:277:GLY:O    | 21:c:507:CLA:CMC  | 2.61                     | 0.47              |
| 1:A:11:ARG:CG     | 1:A:11:ARG:NH1    | 2.73                     | 0.47              |
| 22:a:404:BCR:H11C | 22:a:404:BCR:H341 | 1.64                     | 0.47              |
| 4:b:331:ASN:O     | 4:b:439:SER:OG    | 2.30                     | 0.47              |
| 5:d:210:LEU:HD21  | 28:d:408:PQ9:H17  | 1.97                     | 0.47              |
| 3:a:63:ILE:CG2    | 3:a:64:ARG:N      | 2.78                     | 0.47              |
| 3:a:200:LEU:HD21  | 24:a:406:DGD:HBN1 | 1.94                     | 0.47              |
| 1:A:99:MET:HG3    | 4:b:495:PHE:CZ    | 2.50                     | 0.47              |
| 25:d:403:PHO:NC   | 25:d:403:PHO:ND   | 2.63                     | 0.47              |
| 14:c:279:LEU:CD1  | 21:c:511:CLA:CMB  | 2.92                     | 0.47              |
| 21:c:508:CLA:C2D  | 21:c:509:CLA:H172 | 2.44                     | 0.47              |
| 3:a:27:ARG:NH1    | 5:d:254:SER:O     | 2.41                     | 0.47              |
| 4:b:154:GLY:HA3   | 4:b:202:HIS:HB2   | 1.97                     | 0.47              |
| 20:l:101:SQD:H132 | 20:l:101:SQD:H252 | 1.96                     | 0.47              |
| 14:c:61:VAL:HG12  | 14:c:118:HIS:O    | 2.15                     | 0.47              |
| 14:c:278:ALA:CA   | 21:c:507:CLA:HAC1 | 2.44                     | 0.47              |
| 21:c:503:CLA:H172 | 21:c:509:CLA:HMB2 | 1.97                     | 0.47              |
| 3:a:85:SER:HA     | 3:a:109:GLY:HA3   | 1.97                     | 0.47              |
| 25:d:403:PHO:CBB  | 21:d:406:CLA:C1   | 2.93                     | 0.47              |
| 25:d:403:PHO:CAB  | 21:d:406:CLA:H11  | 2.45                     | 0.47              |
| 14:c:147:PHE:CD1  | 21:c:512:CLA:HMC3 | 2.50                     | 0.47              |
| 14:c:158:THR:HG21 | 14:c:256:PRO:HD3  | 1.97                     | 0.47              |
| 14:c:187:ASP:HB3  | 14:c:230:LEU:CD1  | 2.45                     | 0.47              |
| 4:b:30:VAL:HB     | 21:b:604:CLA:HAC2 | 1.96                     | 0.47              |
| 4:b:103:LEU:HB2   | 21:b:605:CLA:H62  | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:d:408:PQ9:H391 | 28:d:408:PQ9:H411 | 1.64                     | 0.47              |
| 10:l:4:ASN:ND2    | 10:l:6:ASN:HB2    | 2.30                     | 0.47              |
| 14:c:272:LEU:CA   | 21:c:510:CLA:HMD3 | 2.44                     | 0.47              |
| 14:c:351:PHE:CE2  | 14:c:375:LEU:CD1  | 2.98                     | 0.47              |
| 1:A:56:MET:SD     | 1:A:63:ILE:HG22   | 2.55                     | 0.47              |
| 21:a:407:CLA:HAB  | 21:d:406:CLA:H72  | 1.97                     | 0.47              |
| 14:c:119:LEU:O    | 14:c:122:SER:OG   | 2.25                     | 0.46              |
| 14:c:272:LEU:HA   | 21:c:510:CLA:CMD  | 2.45                     | 0.46              |
| 4:b:122:LEU:CD2   | 21:b:614:CLA:CBC  | 2.93                     | 0.46              |
| 4:b:145:LEU:HD22  | 21:b:603:CLA:H192 | 1.96                     | 0.46              |
| 5:d:209:LEU:C     | 5:d:209:LEU:CD2   | 2.86                     | 0.46              |
| 14:c:39:ASN:HB3   | 21:c:510:CLA:CBB  | 2.45                     | 0.46              |
| 14:c:170:ILE:HD13 | 14:c:170:ILE:HA   | 1.76                     | 0.46              |
| 4:b:103:LEU:CD2   | 21:b:605:CLA:H41  | 2.45                     | 0.46              |
| 4:b:134:ASP:CG    | 8:h:17:GLU:O      | 2.58                     | 0.46              |
| 4:b:346:PHE:CZ    | 4:b:399:VAL:HG21  | 2.50                     | 0.46              |
| 14:c:166:ILE:HD11 | 14:c:248:GLY:HA3  | 1.98                     | 0.46              |
| 21:c:504:CLA:HMB2 | 21:c:506:CLA:HHC  | 1.97                     | 0.46              |
| 22:c:515:BCR:H371 | 22:c:515:BCR:C30  | 2.46                     | 0.46              |
| 16:z:23:VAL:HG21  | 16:z:39:LEU:HD13  | 1.97                     | 0.46              |
| 1:A:33:GLN:CB     | 1:A:84:TYR:C      | 2.77                     | 0.46              |
| 1:A:68:VAL:HG22   | 1:A:82:ALA:HB2    | 1.98                     | 0.46              |
| 4:b:62:VAL:CG1    | 4:b:66:MET:HE2    | 2.46                     | 0.46              |
| 4:b:160:GLY:HA3   | 4:b:180:PRO:HB3   | 1.97                     | 0.46              |
| 21:d:406:CLA:H61  | 21:d:406:CLA:H41  | 1.64                     | 0.46              |
| 19:B:101:MGE:H6B1 | 10:l:23:LEU:HD22  | 1.98                     | 0.46              |
| 4:b:62:VAL:HG12   | 4:b:66:MET:HE2    | 1.98                     | 0.46              |
| 21:b:605:CLA:H2   | 22:b:618:BCR:H321 | 1.98                     | 0.46              |
| 8:h:50:ASN:HB3    | 8:h:52:THR:CG2    | 2.46                     | 0.46              |
| 14:c:294:ASN:ND2  | 14:c:308:GLU:OE1  | 2.47                     | 0.46              |
| 1:A:32:GLY:N      | 4:b:486:LEU:HD22  | 2.31                     | 0.46              |
| 4:b:11:VAL:HG11   | 21:b:613:CLA:HED2 | 1.97                     | 0.46              |
| 4:b:341:LYS:HA    | 4:b:405:GLU:HB3   | 1.98                     | 0.46              |
| 4:b:462:PHE:HZ    | 21:b:612:CLA:HMB3 | 1.77                     | 0.46              |
| 5:d:308:ASP:OD1   | 5:d:308:ASP:N     | 2.47                     | 0.46              |
| 14:c:149:TYR:C    | 14:c:149:TYR:CD1  | 2.93                     | 0.46              |
| 4:b:177:SER:OG    | 4:b:179:GLN:NE2   | 2.46                     | 0.46              |
| 4:b:164:PRO:CD    | 21:b:605:CLA:O1D  | 2.64                     | 0.46              |
| 14:c:205:ASP:HB3  | 14:c:208:VAL:HB   | 1.97                     | 0.46              |
| 21:c:507:CLA:H43  | 21:c:507:CLA:O2A  | 2.15                     | 0.46              |
| 16:z:49:ALA:O     | 16:z:53:VAL:HG23  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:b:201:HIS:ND1   | 4:b:201:HIS:C     | 2.73                     | 0.46              |
| 5:d:122:LEU:HD23  | 25:d:403:PHO:H42  | 1.98                     | 0.46              |
| 8:h:7:LEU:HG      | 8:h:11:LEU:HD11   | 1.96                     | 0.46              |
| 14:c:178:LYS:HA   | 14:c:182:PHE:HB2  | 1.98                     | 0.46              |
| 15:k:25:LEU:N     | 15:k:26:PRO:HD2   | 2.29                     | 0.46              |
| 4:b:25:MET:HG2    | 22:b:616:BCR:H23C | 1.97                     | 0.45              |
| 21:b:602:CLA:HAB  | 21:b:604:CLA:H171 | 1.98                     | 0.45              |
| 21:b:609:CLA:H203 | 21:b:609:CLA:C15  | 2.46                     | 0.45              |
| 8:h:25:TRP:CD1    | 31:h:102:HTG:H1   | 2.50                     | 0.45              |
| 14:c:296:VAL:HG21 | 21:c:503:CLA:CMA  | 2.28                     | 0.45              |
| 16:z:48:ILE:O     | 16:z:52:LEU:HG    | 2.16                     | 0.45              |
| 5:d:224:GLN:NE2   | 5:d:230:SER:O     | 2.50                     | 0.45              |
| 11:m:26:TYR:HA    | 11:m:29:THR:HG23  | 1.96                     | 0.45              |
| 14:c:149:TYR:CD2  | 21:c:512:CLA:HBC1 | 2.52                     | 0.45              |
| 14:c:187:ASP:HB3  | 14:c:230:LEU:HD12 | 1.98                     | 0.45              |
| 14:c:225:VAL:HG13 | 14:c:289:PHE:HA   | 1.97                     | 0.45              |
| 21:c:503:CLA:H202 | 22:c:515:BCR:C10  | 2.46                     | 0.45              |
| 3:a:200:LEU:HD13  | 3:a:285:PHE:CE2   | 2.51                     | 0.45              |
| 3:a:269:ARG:CG    | 5:d:240:ALA:HB1   | 2.47                     | 0.45              |
| 4:b:8:VAL:HG23    | 4:b:9:HIS:HD2     | 1.80                     | 0.45              |
| 4:b:413:ASP:HA    | 4:b:414:PRO:HD3   | 1.78                     | 0.45              |
| 4:b:451:PHE:CE1   | 21:b:603:CLA:HED1 | 2.51                     | 0.45              |
| 5:d:135:LEU:HD23  | 5:d:135:LEU:HA    | 1.85                     | 0.45              |
| 5:d:253:TRP:HB2   | 5:d:260:ALA:HB2   | 1.99                     | 0.45              |
| 8:h:41:PHE:CE2    | 8:h:45:ILE:HD11   | 2.52                     | 0.45              |
| 12:t:1:MET:N      | 26:t:301:LMT:O6'  | 2.48                     | 0.45              |
| 14:c:131:TYR:O    | 14:c:136:GLY:N    | 2.49                     | 0.45              |
| 21:c:505:CLA:H18  | 21:c:511:CLA:CBB  | 2.45                     | 0.45              |
| 4:b:457:VAL:HG11  | 19:b:619:MGE:H133 | 1.98                     | 0.45              |
| 8:h:35:MET:HG2    | 22:h:103:BCR:H312 | 1.99                     | 0.45              |
| 14:c:116:VAL:HG21 | 22:z:101:BCR:HC31 | 1.98                     | 0.45              |
| 16:z:18:VAL:O     | 16:z:22:GLY:HA3   | 2.16                     | 0.45              |
| 14:c:33:PHE:HD2   | 14:c:41:ARG:HG2   | 1.81                     | 0.45              |
| 14:c:160:ILE:HG22 | 14:c:164:HIS:CE1  | 2.51                     | 0.45              |
| 4:b:153:PHE:O     | 4:b:157:HIS:HB3   | 2.17                     | 0.45              |
| 4:b:275:TRP:CE2   | 4:b:315:ILE:HD13  | 2.51                     | 0.45              |
| 14:c:39:ASN:CG    | 21:c:510:CLA:HBB2 | 2.39                     | 0.45              |
| 14:c:203:THR:HG22 | 14:c:231:GLU:C    | 2.40                     | 0.45              |
| 4:b:102:VAL:CG2   | 21:b:605:CLA:H122 | 2.46                     | 0.45              |
| 4:b:237:VAL:HG22  | 21:b:609:CLA:HBC2 | 1.98                     | 0.45              |
| 21:b:605:CLA:H2   | 22:b:618:BCR:C32  | 2.47                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:b:614:CLA:HBB1 | 21:b:614:CLA:HMB3 | 1.98                     | 0.45              |
| 9:i:27:ASP:OD1    | 9:i:27:ASP:N      | 2.49                     | 0.45              |
| 3:a:27:ARG:NH1    | 3:a:27:ARG:O      | 2.49                     | 0.45              |
| 5:d:241:GLU:OE2   | 5:d:268:HIS:NE2   | 2.50                     | 0.45              |
| 1:A:66:ARG:CG     | 1:A:66:ARG:NH2    | 2.73                     | 0.45              |
| 5:d:279:LEU:HD22  | 21:d:406:CLA:HMA2 | 1.99                     | 0.45              |
| 14:c:87:ILE:HD13  | 21:c:506:CLA:CHB  | 2.46                     | 0.45              |
| 14:c:219:GLY:HA2  | 24:c:516:DGD:HD2  | 1.97                     | 0.45              |
| 16:z:18:VAL:O     | 16:z:22:GLY:N     | 2.50                     | 0.45              |
| 2:B:16:ILE:HD12   | 4:b:14:ASN:OD1    | 2.17                     | 0.45              |
| 4:b:119:ASP:OD2   | 4:b:124:ARG:NH2   | 2.50                     | 0.45              |
| 4:b:149:LEU:HD22  | 21:b:603:CLA:C17  | 2.47                     | 0.45              |
| 4:b:225:LEU:HA    | 4:b:228:ALA:HB3   | 1.98                     | 0.45              |
| 4:b:446:SER:OG    | 4:b:448:ARG:HB3   | 2.17                     | 0.45              |
| 14:c:88:LEU:O     | 14:c:91:HIS:N     | 2.49                     | 0.45              |
| 14:c:240:ILE:HD11 | 22:c:515:BCR:H392 | 1.95                     | 0.45              |
| 16:z:23:VAL:N     | 16:z:24:PRO:HD3   | 2.30                     | 0.45              |
| 21:b:606:CLA:H2   | 19:b:619:MGE:H6A1 | 1.99                     | 0.44              |
| 5:d:178:ILE:CD1   | 25:d:403:PHO:C20  | 2.70                     | 0.44              |
| 4:b:28:ALA:O      | 4:b:104:SER:OG    | 2.29                     | 0.44              |
| 4:b:67:ALA:CB     | 4:b:80:ILE:HD13   | 2.47                     | 0.44              |
| 10:l:4:ASN:HD22   | 10:l:4:ASN:C      | 2.23                     | 0.44              |
| 1:A:65:THR:CG2    | 1:A:84:TYR:HB2    | 2.47                     | 0.44              |
| 4:b:241:SER:O     | 4:b:245:VAL:HG23  | 2.16                     | 0.44              |
| 22:c:515:BCR:H10C | 22:c:515:BCR:C35  | 2.47                     | 0.44              |
| 16:z:16:SER:O     | 16:z:16:SER:OG    | 2.33                     | 0.44              |
| 2:B:56:SER:HB3    | 4:b:183:PRO:HG2   | 2.00                     | 0.44              |
| 24:h:104:DGD:HB21 | 24:h:104:DGD:HB51 | 1.89                     | 0.44              |
| 14:c:269:GLU:O    | 21:c:510:CLA:HBC1 | 2.18                     | 0.44              |
| 1:A:11:ARG:NH1    | 1:A:11:ARG:HB2    | 2.33                     | 0.44              |
| 3:a:129:ARG:NH2   | 5:d:256:ILE:O     | 2.48                     | 0.44              |
| 4:b:152:GLY:C     | 21:b:605:CLA:HMC1 | 2.43                     | 0.44              |
| 8:h:12:ARG:HB3    | 8:h:13:PRO:HD3    | 2.00                     | 0.44              |
| 14:c:272:LEU:HD21 | 14:c:444:HIS:ND1  | 2.33                     | 0.44              |
| 8:h:52:THR:O      | 8:h:52:THR:OG1    | 2.25                     | 0.44              |
| 14:c:230:LEU:HD23 | 14:c:230:LEU:HA   | 1.72                     | 0.44              |
| 1:A:9:PHE:CE2     | 1:A:15:GLU:HG2    | 2.52                     | 0.44              |
| 2:B:26:TRP:HE3    | 2:B:31:LYS:HG2    | 1.82                     | 0.44              |
| 4:b:42:LEU:HD13   | 4:b:94:GLU:HG3    | 1.99                     | 0.44              |
| 4:b:489:GLU:O     | 4:b:489:GLU:HG2   | 2.18                     | 0.44              |
| 29:d:412:UNL:C36  | 8:h:35:MET:CE     | 2.96                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:f:20:TRP:O      | 7:f:20:TRP:CG     | 2.70                     | 0.44              |
| 14:c:33:PHE:CE2   | 14:c:41:ARG:HA    | 2.52                     | 0.44              |
| 14:c:157:MET:C    | 14:c:159:THR:H    | 2.26                     | 0.44              |
| 21:c:504:CLA:HBD  | 21:c:505:CLA:H43  | 1.99                     | 0.44              |
| 1:A:9:PHE:HE2     | 1:A:15:GLU:HG2    | 1.83                     | 0.44              |
| 14:c:146:PHE:C    | 14:c:148:GLY:H    | 2.26                     | 0.44              |
| 15:k:28:ILE:N     | 15:k:29:PRO:CD    | 2.80                     | 0.44              |
| 1:A:15:GLU:OE2    | 1:A:15:GLU:HA     | 2.13                     | 0.44              |
| 1:A:23:LEU:HD21   | 1:A:96:ILE:CD1    | 2.45                     | 0.44              |
| 2:B:17:GLU:OE1    | 4:b:484:PRO:HB2   | 2.17                     | 0.44              |
| 2:B:27:THR:HB     | 2:B:28:PRO:CD     | 2.48                     | 0.44              |
| 14:c:114:VAL:HG21 | 21:c:505:CLA:CMA  | 2.47                     | 0.44              |
| 21:c:503:CLA:H203 | 22:c:515:BCR:C13  | 2.48                     | 0.44              |
| 15:k:18:PHE:HB3   | 15:k:21:LEU:HD23  | 1.99                     | 0.44              |
| 4:b:455:HIS:CE1   | 21:b:606:CLA:CBB  | 3.00                     | 0.43              |
| 22:d:409:BCR:H11C | 22:d:409:BCR:H341 | 1.87                     | 0.43              |
| 3:a:328:MET:HG2   | 5:d:325:ILE:CG1   | 2.48                     | 0.43              |
| 3:a:157:VAL:CG1   | 3:a:172:MET:HB2   | 2.48                     | 0.43              |
| 8:h:38:PHE:HD1    | 22:h:103:BCR:H12C | 1.82                     | 0.43              |
| 9:i:24:LEU:N      | 9:i:24:LEU:CD1    | 2.81                     | 0.43              |
| 5:d:179:PHE:HA    | 5:d:182:LEU:HD12  | 2.01                     | 0.43              |
| 5:d:161:PRO:HG3   | 5:d:170:ALA:HB2   | 2.01                     | 0.43              |
| 3:a:157:VAL:HG12  | 3:a:172:MET:HB2   | 2.01                     | 0.43              |
| 4:b:60:MET:HB3    | 4:b:63:LEU:HB2    | 2.00                     | 0.43              |
| 4:b:102:VAL:HG21  | 21:b:605:CLA:H122 | 2.00                     | 0.43              |
| 14:c:50:LEU:HD11  | 21:c:513:CLA:HAB  | 2.00                     | 0.43              |
| 3:a:145:VAL:O     | 3:a:148:SER:OG    | 2.35                     | 0.43              |
| 8:h:7:LEU:HG      | 8:h:11:LEU:HD12   | 2.00                     | 0.43              |
| 14:c:313:GLN:HB2  | 14:c:396:MET:HG3  | 2.01                     | 0.43              |
| 14:c:375:LEU:HD23 | 14:c:375:LEU:HA   | 1.86                     | 0.43              |
| 3:a:29:TYR:CE2    | 3:a:132:GLU:HG2   | 2.54                     | 0.43              |
| 4:b:18:ARG:NH1    | 4:b:115:TRP:O     | 2.52                     | 0.43              |
| 4:b:135:LEU:HB2   | 4:b:136:PRO:HD3   | 2.00                     | 0.43              |
| 26:d:404:LMT:H2O2 | 26:t:301:LMT:H3O2 | 1.63                     | 0.43              |
| 15:k:13:GLU:HB3   | 15:k:14:ALA:H     | 1.59                     | 0.43              |
| 1:A:11:ARG:NH1    | 1:A:11:ARG:CB     | 2.82                     | 0.43              |
| 3:a:143:ILE:HD12  | 5:d:220:ASN:HD22  | 1.83                     | 0.43              |
| 4:b:137:LYS:O     | 4:b:140:GLY:N     | 2.51                     | 0.43              |
| 4:b:145:LEU:HD11  | 21:b:614:CLA:CMB  | 2.49                     | 0.43              |
| 4:b:164:PRO:CG    | 21:b:605:CLA:O1D  | 2.64                     | 0.43              |
| 4:b:247:PHE:CD2   | 21:b:602:CLA:H41  | 2.54                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:c:88:LEU:HD23  | 14:c:88:LEU:HA    | 1.87                     | 0.43              |
| 14:c:224:ILE:CD1  | 22:c:515:BCR:H272 | 2.49                     | 0.43              |
| 1:A:11:ARG:CB     | 1:A:11:ARG:CZ     | 2.97                     | 0.43              |
| 2:B:37:LEU:HG     | 4:b:218:LEU:HD11  | 2.00                     | 0.43              |
| 4:b:74:SER:HA     | 4:b:92:SER:HB2    | 2.01                     | 0.43              |
| 21:d:406:CLA:H93  | 21:d:406:CLA:H62  | 1.82                     | 0.43              |
| 14:c:56:HIS:NE2   | 21:c:511:CLA:NC   | 2.67                     | 0.43              |
| 14:c:354:GLU:HB2  | 23:c:501:CL:CL    | 2.55                     | 0.43              |
| 21:c:503:CLA:HBB1 | 22:c:515:BCR:H373 | 2.00                     | 0.43              |
| 15:k:28:ILE:CB    | 15:k:29:PRO:HD3   | 2.37                     | 0.43              |
| 4:b:170:ASP:OD1   | 4:b:174:LEU:N     | 2.47                     | 0.42              |
| 21:d:406:CLA:H11  | 21:d:406:CLA:H52  | 1.85                     | 0.42              |
| 21:c:505:CLA:CMB  | 21:c:505:CLA:HBB1 | 2.49                     | 0.42              |
| 2:B:10:ARG:HD3    | 19:B:101:MGE:C3D  | 2.49                     | 0.42              |
| 22:a:404:BCR:H24C | 22:a:404:BCR:H371 | 1.66                     | 0.42              |
| 5:d:259:ILE:HD13  | 19:d:410:MGE:H6A2 | 2.00                     | 0.42              |
| 7:f:19:ARG:HD3    | 7:f:19:ARG:HA     | 1.37                     | 0.42              |
| 3:a:117:PHE:HB3   | 21:a:403:CLA:HMA2 | 2.00                     | 0.42              |
| 3:a:200:LEU:HD23  | 24:a:406:DGD:HBN1 | 2.01                     | 0.42              |
| 4:b:315:ILE:HG13  | 4:b:321:LYS:HG3   | 2.00                     | 0.42              |
| 22:b:617:BCR:H371 | 22:b:617:BCR:H24C | 1.83                     | 0.42              |
| 14:c:146:PHE:C    | 14:c:148:GLY:N    | 2.75                     | 0.42              |
| 14:c:186:TYR:HA   | 14:c:196:VAL:HA   | 2.00                     | 0.42              |
| 14:c:277:GLY:C    | 21:c:507:CLA:HMC1 | 2.45                     | 0.42              |
| 1:A:8:GLN:OE1     | 1:A:11:ARG:HA     | 2.20                     | 0.42              |
| 4:b:440:ASP:OD2   | 4:b:444:ARG:NH1   | 2.28                     | 0.42              |
| 21:b:613:CLA:H41  | 21:b:613:CLA:H62  | 1.35                     | 0.42              |
| 5:d:174:GLY:O     | 5:d:178:ILE:HG13  | 2.18                     | 0.42              |
| 14:c:119:LEU:HD13 | 14:c:119:LEU:HA   | 1.82                     | 0.42              |
| 22:z:101:BCR:H392 | 22:z:101:BCR:H371 | 2.02                     | 0.42              |
| 1:A:57:VAL:HG12   | 1:A:58:ASP:N      | 2.34                     | 0.42              |
| 3:a:300:PHE:CE1   | 14:c:404:LEU:HB2  | 2.54                     | 0.42              |
| 21:a:402:CLA:HBB1 | 21:a:402:CLA:HMB1 | 2.02                     | 0.42              |
| 4:b:27:THR:CG2    | 21:b:611:CLA:H42  | 2.50                     | 0.42              |
| 21:b:612:CLA:OBD  | 21:b:613:CLA:HHC  | 2.18                     | 0.42              |
| 5:d:123:ILE:HD11  | 24:h:104:DGD:HAE2 | 2.00                     | 0.42              |
| 21:c:511:CLA:H161 | 21:c:511:CLA:H121 | 1.76                     | 0.42              |
| 2:B:17:GLU:HA     | 2:B:18:PRO:HD3    | 1.90                     | 0.42              |
| 28:d:408:PQ9:H241 | 28:d:408:PQ9:H262 | 1.86                     | 0.42              |
| 20:l:101:SQD:H162 | 19:m:102:MGE:H9B2 | 2.01                     | 0.42              |
| 1:A:31:SER:OG     | 4:b:486:LEU:HD22  | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:66:ARG:O      | 3:a:255:PHE:HZ    | 1.87                     | 0.42              |
| 8:h:25:TRP:CD1    | 31:h:102:HTG:H5   | 2.55                     | 0.42              |
| 14:c:224:ILE:CG2  | 14:c:289:PHE:HE2  | 2.33                     | 0.42              |
| 14:c:369:LEU:HD21 | 14:c:384:ILE:HD11 | 2.01                     | 0.42              |
| 21:b:614:CLA:H92  | 21:b:614:CLA:H61  | 1.81                     | 0.42              |
| 22:b:618:BCR:H11C | 22:b:618:BCR:H341 | 1.90                     | 0.42              |
| 21:c:508:CLA:HBB2 | 21:c:509:CLA:CED  | 2.49                     | 0.42              |
| 1:A:54:MET:HB2    | 1:A:68:VAL:HG21   | 2.01                     | 0.42              |
| 3:a:301:ASN:HD21  | 14:c:407:VAL:CG1  | 2.32                     | 0.42              |
| 3:a:323:ARG:HA    | 3:a:323:ARG:HD3   | 1.58                     | 0.42              |
| 4:b:346:PHE:CE2   | 4:b:399:VAL:HG21  | 2.52                     | 0.42              |
| 4:b:442:ILE:HD12  | 5:d:299:ILE:HG12  | 2.02                     | 0.42              |
| 3:a:59:ASP:OD1    | 3:a:59:ASP:N      | 2.40                     | 0.42              |
| 4:b:10:THR:HG23   | 21:b:610:CLA:HAA2 | 2.01                     | 0.42              |
| 4:b:388:SER:OG    | 4:b:391:SER:HB2   | 2.19                     | 0.42              |
| 22:b:616:BCR:H15C | 22:b:616:BCR:H351 | 1.85                     | 0.42              |
| 5:d:42:TYR:CE1    | 7:f:25:THR:O      | 2.73                     | 0.42              |
| 14:c:117:VAL:HG22 | 22:z:101:BCR:H10C | 2.02                     | 0.42              |
| 14:c:437:PHE:CZ   | 21:c:511:CLA:HMA1 | 2.54                     | 0.42              |
| 21:c:503:CLA:H203 | 22:c:515:BCR:C12  | 2.50                     | 0.42              |
| 16:z:23:VAL:N     | 16:z:24:PRO:CD    | 2.61                     | 0.42              |
| 16:z:57:LEU:HA    | 16:z:60:PHE:HB2   | 2.00                     | 0.42              |
| 14:c:279:LEU:HD23 | 14:c:279:LEU:HA   | 1.81                     | 0.41              |
| 21:c:503:CLA:H102 | 22:c:515:BCR:C36  | 2.46                     | 0.41              |
| 1:A:23:LEU:HD13   | 1:A:34:ALA:HB2    | 2.01                     | 0.41              |
| 4:b:174:LEU:HD21  | 4:b:309:LEU:HB2   | 2.02                     | 0.41              |
| 8:h:50:ASN:HB3    | 8:h:52:THR:HG22   | 2.01                     | 0.41              |
| 21:c:503:CLA:HMB1 | 22:c:515:BCR:H403 | 2.01                     | 0.41              |
| 4:b:221:PRO:HA    | 21:b:608:CLA:HED3 | 2.03                     | 0.41              |
| 4:b:333:GLY:O     | 4:b:440:ASP:O     | 2.38                     | 0.41              |
| 28:d:408:PQ9:H211 | 28:d:408:PQ9:H191 | 1.87                     | 0.41              |
| 14:c:33:PHE:HE2   | 14:c:41:ARG:HA    | 1.86                     | 0.41              |
| 14:c:224:ILE:HG22 | 14:c:289:PHE:CE2  | 2.55                     | 0.41              |
| 22:c:515:BCR:C37  | 22:c:515:BCR:C25  | 2.92                     | 0.41              |
| 1:A:25:ARG:C      | 4:b:490:GLN:HG2   | 2.44                     | 0.41              |
| 5:d:113:PHE:O     | 5:d:117:HIS:ND1   | 2.53                     | 0.41              |
| 3:a:257:ARG:CG    | 3:a:257:ARG:NH1   | 2.82                     | 0.41              |
| 4:b:263:THR:O     | 4:b:448:ARG:NH2   | 2.49                     | 0.41              |
| 25:d:401:PHO:NC   | 25:d:401:PHO:ND   | 2.69                     | 0.41              |
| 12:t:26:PRO:HA    | 12:t:27:PRO:HD3   | 1.92                     | 0.41              |
| 14:c:43:ILE:HD12  | 14:c:269:GLU:OE1  | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:c:174:LEU:HD23 | 14:c:174:LEU:HA   | 1.87                     | 0.41              |
| 14:c:224:ILE:CG2  | 14:c:289:PHE:CE2  | 3.03                     | 0.41              |
| 15:k:25:LEU:H     | 15:k:26:PRO:HD2   | 1.86                     | 0.41              |
| 1:A:41:PRO:CD     | 1:A:44:VAL:CG2    | 2.98                     | 0.41              |
| 4:b:380:ASP:OD1   | 5:d:344:GLU:OE2   | 2.38                     | 0.41              |
| 22:b:618:BCR:H20C | 22:b:618:BCR:H361 | 1.81                     | 0.41              |
| 5:d:151:ALA:O     | 5:d:155:SER:OG    | 2.37                     | 0.41              |
| 14:c:152:LYS:CA   | 14:c:152:LYS:CE   | 2.86                     | 0.41              |
| 21:c:508:CLA:CBB  | 21:c:509:CLA:HED1 | 2.50                     | 0.41              |
| 22:c:514:BCR:H371 | 22:c:514:BCR:H24C | 1.83                     | 0.41              |
| 22:c:515:BCR:H361 | 22:c:515:BCR:H20C | 1.61                     | 0.41              |
| 4:b:110:ALA:HB2   | 22:b:618:BCR:H17C | 2.03                     | 0.41              |
| 4:b:236:THR:HG23  | 4:b:473:THR:HG23  | 1.99                     | 0.41              |
| 14:c:160:ILE:HA   | 14:c:163:PHE:HB2  | 2.03                     | 0.41              |
| 19:B:101:MGE:H241 | 10:l:26:VAL:HG21  | 2.03                     | 0.41              |
| 21:a:402:CLA:HAB  | 5:d:182:LEU:HD22  | 2.03                     | 0.41              |
| 22:b:618:BCR:H15C | 22:b:618:BCR:H351 | 1.90                     | 0.41              |
| 5:d:224:GLN:H     | 5:d:224:GLN:HG2   | 1.73                     | 0.41              |
| 11:m:25:LEU:O     | 11:m:29:THR:HG21  | 2.03                     | 0.41              |
| 14:c:199:ILE:HD12 | 14:c:199:ILE:HA   | 1.83                     | 0.41              |
| 14:c:240:ILE:HD13 | 22:c:515:BCR:H391 | 2.03                     | 0.41              |
| 14:c:271:TYR:O    | 21:c:510:CLA:HMD1 | 2.21                     | 0.41              |
| 21:c:505:CLA:HBB1 | 21:c:505:CLA:HMB1 | 2.03                     | 0.41              |
| 14:c:376:ASP:CG   | 14:c:379:LYS:HG3  | 2.41                     | 0.41              |
| 14:c:441:HIS:HE1  | 21:c:507:CLA:NB   | 2.19                     | 0.41              |
| 3:a:176:ILE:O     | 3:a:179:THR:OG1   | 2.39                     | 0.40              |
| 7:f:18:VAL:HG23   | 7:f:20:TRP:HB3    | 2.04                     | 0.40              |
| 14:c:167:VAL:HG11 | 21:c:512:CLA:HAA1 | 2.03                     | 0.40              |
| 14:c:279:LEU:HD11 | 21:c:511:CLA:CMB  | 2.51                     | 0.40              |
| 14:c:296:VAL:CG1  | 21:c:503:CLA:C2A  | 2.93                     | 0.40              |
| 1:A:37:TYR:OH     | 1:A:71:LYS:NZ     | 2.49                     | 0.40              |
| 1:A:89:PRO:HA     | 1:A:92:TRP:HB3    | 2.02                     | 0.40              |
| 4:b:451:PHE:CZ    | 21:b:603:CLA:O2D  | 2.68                     | 0.40              |
| 5:d:159:ILE:HG21  | 5:d:287:VAL:HG22  | 2.03                     | 0.40              |
| 21:d:402:CLA:H42  | 28:d:408:PQ9:H22  | 2.03                     | 0.40              |
| 8:h:61:SER:HA     | 24:h:104:DGD:HE2  | 2.03                     | 0.40              |
| 14:c:294:ASN:H    | 24:c:516:DGD:HE4  | 1.87                     | 0.40              |
| 3:a:143:ILE:HD11  | 5:d:217:THR:HG22  | 2.02                     | 0.40              |
| 4:b:99:ALA:CB     | 21:b:605:CLA:H121 | 2.52                     | 0.40              |
| 16:z:2:THR:O      | 16:z:2:THR:OG1    | 2.35                     | 0.40              |
| 3:a:136:ARG:HH11  | 3:a:136:ARG:HG2   | 1.86                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:b:238:LEU:HD13  | 21:b:611:CLA:C2D  | 2.51                     | 0.40              |
| 14:c:87:ILE:HG21  | 21:c:506:CLA:HHB  | 2.03                     | 0.40              |
| 14:c:150:ASP:O    | 14:c:152:LYS:N    | 2.54                     | 0.40              |
| 14:c:185:LEU:CD1  | 21:c:503:CLA:HED2 | 2.51                     | 0.40              |
| 14:c:273:SER:OG   | 14:c:445:ALA:HB2  | 2.20                     | 0.40              |
| 3:a:27:ARG:HA     | 3:a:27:ARG:HD2    | 1.93                     | 0.40              |
| 22:d:409:BCR:H361 | 22:d:409:BCR:H20C | 1.85                     | 0.40              |
| 10:l:24:ILE:HG13  | 11:m:18:PRO:HB2   | 2.04                     | 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%) | 95 (89%)  | 11 (10%) | 1 (1%)   | 14          | 41  |
| 2   | B     | 46/56 (82%)   | 44 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 3   | a     | 291/360 (81%) | 279 (96%) | 10 (3%)  | 2 (1%)   | 18          | 47  |
| 4   | b     | 492/505 (97%) | 470 (96%) | 21 (4%)  | 1 (0%)   | 43          | 70  |
| 5   | d     | 329/342 (96%) | 315 (96%) | 14 (4%)  | 0        | 100         | 100 |
| 6   | e     | 61/84 (73%)   | 56 (92%)  | 5 (8%)   | 0        | 100         | 100 |
| 7   | f     | 26/45 (58%)   | 22 (85%)  | 4 (15%)  | 0        | 100         | 100 |
| 8   | h     | 60/65 (92%)   | 54 (90%)  | 5 (8%)   | 1 (2%)   | 7           | 27  |
| 9   | i     | 27/38 (71%)   | 25 (93%)  | 2 (7%)   | 0        | 100         | 100 |
| 10  | l     | 35/37 (95%)   | 31 (89%)  | 2 (6%)   | 2 (6%)   | 1           | 7   |
| 11  | m     | 29/36 (81%)   | 28 (97%)  | 1 (3%)   | 0        | 100         | 100 |
| 12  | t     | 25/32 (78%)   | 24 (96%)  | 1 (4%)   | 0        | 100         | 100 |
| 13  | x     | 34/40 (85%)   | 32 (94%)  | 2 (6%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 14  | c     | 397/451 (88%)   | 355 (89%)  | 32 (8%)  | 10 (2%)  | 4           | 19  |
| 15  | k     | 32/46 (70%)     | 26 (81%)   | 4 (12%)  | 2 (6%)   | 1           | 6   |
| 16  | z     | 60/62 (97%)     | 48 (80%)   | 10 (17%) | 2 (3%)   | 3           | 14  |
| 17  | y     | 26/30 (87%)     | 20 (77%)   | 5 (19%)  | 1 (4%)   | 2           | 13  |
| 18  | C     | 21/23 (91%)     | 18 (86%)   | 3 (14%)  | 0        | 100         | 100 |
| All | All   | 2098/2368 (89%) | 1942 (93%) | 134 (6%) | 22 (1%)  | 15          | 38  |

All (22) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | l     | 7   | ARG  |
| 14  | c     | 151 | TRP  |
| 14  | c     | 153 | ASP  |
| 14  | c     | 210 | PHE  |
| 16  | z     | 23  | VAL  |
| 17  | y     | 2   | VAL  |
| 14  | c     | 152 | LYS  |
| 14  | c     | 209 | ILE  |
| 14  | c     | 268 | GLY  |
| 16  | z     | 25  | VAL  |
| 14  | c     | 30  | SER  |
| 14  | c     | 34  | ALA  |
| 14  | c     | 147 | PHE  |
| 15  | k     | 26  | PRO  |
| 1   | A     | 45  | GLN  |
| 3   | a     | 299 | GLY  |
| 10  | l     | 5   | PRO  |
| 14  | c     | 77  | PRO  |
| 15  | k     | 25  | LEU  |
| 3   | a     | 255 | PHE  |
| 4   | b     | 491 | VAL  |
| 8   | h     | 12  | ARG  |

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | A     | 92/97 (95%)     | 84 (91%)   | 8 (9%)   | 9           | 30  |
| 2   | B     | 34/42 (81%)     | 32 (94%)   | 2 (6%)   | 18          | 44  |
| 3   | a     | 236/290 (81%)   | 215 (91%)  | 21 (9%)  | 9           | 29  |
| 4   | b     | 392/403 (97%)   | 380 (97%)  | 12 (3%)  | 35          | 60  |
| 5   | d     | 272/277 (98%)   | 258 (95%)  | 14 (5%)  | 21          | 48  |
| 6   | e     | 55/73 (75%)     | 52 (94%)   | 3 (6%)   | 19          | 46  |
| 7   | f     | 22/39 (56%)     | 17 (77%)   | 5 (23%)  | 1           | 4   |
| 8   | h     | 53/54 (98%)     | 48 (91%)   | 5 (9%)   | 8           | 28  |
| 9   | i     | 26/35 (74%)     | 23 (88%)   | 3 (12%)  | 5           | 20  |
| 10  | l     | 35/35 (100%)    | 30 (86%)   | 5 (14%)  | 3           | 13  |
| 11  | m     | 28/33 (85%)     | 20 (71%)   | 8 (29%)  | 0           | 1   |
| 12  | t     | 24/29 (83%)     | 24 (100%)  | 0        | 100         | 100 |
| 13  | x     | 29/33 (88%)     | 26 (90%)   | 3 (10%)  | 7           | 24  |
| 14  | c     | 312/352 (89%)   | 275 (88%)  | 37 (12%) | 5           | 19  |
| 15  | k     | 27/37 (73%)     | 21 (78%)   | 6 (22%)  | 1           | 4   |
| 16  | z     | 45/52 (86%)     | 44 (98%)   | 1 (2%)   | 45          | 67  |
| All | All   | 1682/1881 (89%) | 1549 (92%) | 133 (8%) | 13          | 34  |

All (133) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | ILE  |
| 1   | A     | 11  | ARG  |
| 1   | A     | 15  | GLU  |
| 1   | A     | 27  | ARG  |
| 1   | A     | 28  | ASP  |
| 1   | A     | 66  | ARG  |
| 1   | A     | 90  | GLN  |
| 1   | A     | 99  | MET  |
| 2   | B     | 10  | ARG  |
| 2   | B     | 11  | LEU  |
| 3   | a     | 121 | LEU  |
| 3   | a     | 133 | LEU  |
| 3   | a     | 136 | ARG  |
| 3   | a     | 143 | ILE  |
| 3   | a     | 159 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | a     | 177 | SER  |
| 3   | a     | 220 | THR  |
| 3   | a     | 222 | SER  |
| 3   | a     | 225 | ARG  |
| 3   | a     | 226 | GLU  |
| 3   | a     | 247 | ASN  |
| 3   | a     | 255 | PHE  |
| 3   | a     | 257 | ARG  |
| 3   | a     | 269 | ARG  |
| 3   | a     | 281 | VAL  |
| 3   | a     | 297 | LEU  |
| 3   | a     | 300 | PHE  |
| 3   | a     | 305 | SER  |
| 3   | a     | 310 | LYS  |
| 3   | a     | 323 | ARG  |
| 3   | a     | 328 | MET  |
| 4   | b     | 62  | VAL  |
| 4   | b     | 63  | LEU  |
| 4   | b     | 201 | HIS  |
| 4   | b     | 246 | PHE  |
| 4   | b     | 362 | PHE  |
| 4   | b     | 387 | GLU  |
| 4   | b     | 399 | VAL  |
| 4   | b     | 400 | SER  |
| 4   | b     | 440 | ASP  |
| 4   | b     | 477 | ASP  |
| 4   | b     | 483 | ASP  |
| 4   | b     | 490 | GLN  |
| 5   | d     | 23  | LYS  |
| 5   | d     | 135 | LEU  |
| 5   | d     | 136 | VAL  |
| 5   | d     | 165 | SER  |
| 5   | d     | 180 | ARG  |
| 5   | d     | 209 | LEU  |
| 5   | d     | 223 | PHE  |
| 5   | d     | 224 | GLN  |
| 5   | d     | 259 | ILE  |
| 5   | d     | 279 | LEU  |
| 5   | d     | 294 | ARG  |
| 5   | d     | 310 | GLU  |
| 5   | d     | 344 | GLU  |
| 5   | d     | 345 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | e     | 26  | THR  |
| 6   | e     | 66  | VAL  |
| 6   | e     | 67  | THR  |
| 7   | f     | 19  | ARG  |
| 7   | f     | 20  | TRP  |
| 7   | f     | 23  | VAL  |
| 7   | f     | 24  | HIS  |
| 7   | f     | 26  | LEU  |
| 8   | h     | 10  | ILE  |
| 8   | h     | 12  | ARG  |
| 8   | h     | 43  | LEU  |
| 8   | h     | 51  | SER  |
| 8   | h     | 52  | THR  |
| 9   | i     | 2   | GLU  |
| 9   | i     | 24  | LEU  |
| 9   | i     | 27  | ASP  |
| 10  | l     | 1   | MET  |
| 10  | l     | 4   | ASN  |
| 10  | l     | 7   | ARG  |
| 10  | l     | 32  | SER  |
| 10  | l     | 33  | SER  |
| 11  | m     | 6   | LEU  |
| 11  | m     | 9   | ILE  |
| 11  | m     | 25  | LEU  |
| 11  | m     | 28  | GLN  |
| 11  | m     | 29  | THR  |
| 11  | m     | 31  | SER  |
| 11  | m     | 32  | GLN  |
| 11  | m     | 33  | GLN  |
| 13  | x     | 35  | ASP  |
| 13  | x     | 36  | LYS  |
| 13  | x     | 37  | VAL  |
| 14  | c     | 29  | GLU  |
| 14  | c     | 31  | SER  |
| 14  | c     | 41  | ARG  |
| 14  | c     | 87  | ILE  |
| 14  | c     | 99  | VAL  |
| 14  | c     | 105 | VAL  |
| 14  | c     | 118 | HIS  |
| 14  | c     | 119 | LEU  |
| 14  | c     | 120 | ILE  |
| 14  | c     | 142 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | c     | 143 | TYR  |
| 14  | c     | 145 | SER  |
| 14  | c     | 146 | PHE  |
| 14  | c     | 150 | ASP  |
| 14  | c     | 151 | TRP  |
| 14  | c     | 152 | LYS  |
| 14  | c     | 156 | LYS  |
| 14  | c     | 157 | MET  |
| 14  | c     | 166 | ILE  |
| 14  | c     | 167 | VAL  |
| 14  | c     | 168 | LEU  |
| 14  | c     | 170 | ILE  |
| 14  | c     | 173 | LEU  |
| 14  | c     | 199 | ILE  |
| 14  | c     | 200 | THR  |
| 14  | c     | 203 | THR  |
| 14  | c     | 204 | LEU  |
| 14  | c     | 208 | VAL  |
| 14  | c     | 224 | ILE  |
| 14  | c     | 230 | LEU  |
| 14  | c     | 240 | ILE  |
| 14  | c     | 269 | GLU  |
| 14  | c     | 272 | LEU  |
| 14  | c     | 279 | LEU  |
| 14  | c     | 289 | PHE  |
| 14  | c     | 355 | THR  |
| 14  | c     | 384 | ILE  |
| 15  | k     | 13  | GLU  |
| 15  | k     | 15  | TYR  |
| 15  | k     | 24  | VAL  |
| 15  | k     | 25  | LEU  |
| 15  | k     | 27  | VAL  |
| 15  | k     | 39  | TRP  |
| 16  | z     | 23  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 48  | ASN  |
| 1   | A     | 90  | GLN  |
| 2   | B     | 22  | GLN  |
| 2   | B     | 24  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | a     | 113 | GLN  |
| 3   | a     | 118 | HIS  |
| 3   | a     | 165 | GLN  |
| 3   | a     | 181 | ASN  |
| 3   | a     | 190 | HIS  |
| 3   | a     | 195 | HIS  |
| 3   | a     | 198 | HIS  |
| 3   | a     | 215 | HIS  |
| 3   | a     | 247 | ASN  |
| 3   | a     | 303 | ASN  |
| 3   | a     | 304 | HIS  |
| 3   | a     | 332 | HIS  |
| 4   | b     | 58  | GLN  |
| 4   | b     | 179 | GLN  |
| 4   | b     | 274 | GLN  |
| 4   | b     | 285 | ASN  |
| 4   | b     | 338 | GLN  |
| 4   | b     | 374 | ASN  |
| 4   | b     | 394 | GLN  |
| 4   | b     | 409 | GLN  |
| 4   | b     | 438 | ASN  |
| 4   | b     | 455 | HIS  |
| 5   | d     | 129 | GLN  |
| 5   | d     | 332 | GLN  |
| 6   | e     | 82  | GLN  |
| 7   | f     | 41  | GLN  |
| 14  | c     | 118 | HIS  |
| 14  | c     | 228 | ASN  |
| 14  | c     | 293 | ASN  |
| 14  | c     | 311 | GLN  |
| 14  | c     | 378 | ASN  |
| 14  | c     | 441 | HIS  |
| 16  | z     | 38  | GLN  |

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 69 ligands modelled in this entry, 3 are monoatomic and 2 are unknown - leaving 64 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 | $\# Z  > 2$ |
| 24  | DGD  | c     | 517 | -    | 48,48,67     | 1.02 | 2 (4%)      | 62,62,81    | 1.11 | 5 (8%)      |
| 19  | MGE  | f     | 101 | -    | 47,47,48     | 0.99 | 2 (4%)      | 55,55,56    | 1.33 | 7 (12%)     |
| 21  | CLA  | b     | 601 | -    | 69,73,73     | 2.14 | 18 (26%)    | 82,113,113  | 2.17 | 28 (34%)    |
| 25  | PHO  | d     | 401 | -    | 58,69,69     | 2.26 | 12 (20%)    | 55,99,99    | 2.75 | 14 (25%)    |
| 31  | HTG  | h     | 102 | -    | 16,16,19     | 1.08 | 2 (12%)     | 20,21,24    | 1.50 | 2 (10%)     |
| 21  | CLA  | c     | 507 | -    | 55,59,73     | 2.20 | 18 (32%)    | 64,96,113   | 3.66 | 31 (48%)    |
| 21  | CLA  | c     | 511 | -    | 69,73,73     | 2.14 | 19 (27%)    | 82,113,113  | 2.07 | 28 (34%)    |
| 21  | CLA  | c     | 513 | -    | 54,58,73     | 2.26 | 16 (29%)    | 64,95,113   | 3.85 | 35 (54%)    |
| 21  | CLA  | c     | 506 | -    | 50,54,73     | 2.28 | 18 (36%)    | 59,90,113   | 4.59 | 28 (47%)    |
| 22  | BCR  | d     | 409 | -    | 41,41,41     | 0.66 | 0           | 56,56,56    | 1.74 | 10 (17%)    |
| 21  | CLA  | h     | 101 | -    | 45,49,73     | 2.38 | 16 (35%)    | 54,84,113   | 4.46 | 28 (51%)    |
| 26  | LMT  | t     | 301 | -    | 36,36,36     | 0.49 | 0           | 47,47,47    | 0.90 | 1 (2%)      |
| 21  | CLA  | b     | 604 | -    | 69,73,73     | 1.96 | 18 (26%)    | 82,113,113  | 2.43 | 28 (34%)    |
| 22  | BCR  | a     | 404 | -    | 41,41,41     | 0.70 | 0           | 56,56,56    | 2.31 | 17 (30%)    |
| 24  | DGD  | c     | 516 | -    | 54,54,67     | 0.99 | 2 (3%)      | 68,68,81    | 1.46 | 14 (20%)    |
| 28  | PQ9  | d     | 408 | -    | 45,45,45     | 0.72 | 1 (2%)      | 56,57,57    | 1.50 | 14 (25%)    |
| 24  | DGD  | h     | 104 | -    | 55,55,67     | 0.93 | 2 (3%)      | 69,69,81    | 1.07 | 5 (7%)      |
| 21  | CLA  | b     | 606 | -    | 69,73,73     | 2.31 | 18 (26%)    | 82,113,113  | 2.04 | 27 (32%)    |
| 21  | CLA  | b     | 603 | -    | 69,73,73     | 2.12 | 18 (26%)    | 82,113,113  | 2.46 | 28 (34%)    |
| 22  | BCR  | h     | 103 | -    | 41,41,41     | 0.73 | 0           | 56,56,56    | 1.95 | 16 (28%)    |
| 21  | CLA  | b     | 608 | -    | 69,73,73     | 2.37 | 22 (31%)    | 82,113,113  | 1.98 | 25 (30%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 19  | MGE  | B     | 101 | -    | 48,48,48     | 0.95 | 2 (4%)   | 56,56,56    | 1.29 | 6 (10%)  |
| 21  | CLA  | d     | 402 | -    | 69,73,73     | 1.99 | 21 (30%) | 82,113,113  | 2.20 | 24 (29%) |
| 26  | LMT  | d     | 404 | -    | 36,36,36     | 0.45 | 0        | 47,47,47    | 0.83 | 1 (2%)   |
| 22  | BCR  | b     | 616 | -    | 41,41,41     | 0.66 | 0        | 56,56,56    | 1.92 | 20 (35%) |
| 19  | MGE  | m     | 102 | -    | 48,48,48     | 1.00 | 3 (6%)   | 56,56,56    | 1.14 | 3 (5%)   |
| 22  | BCR  | c     | 515 | -    | 41,41,41     | 0.84 | 1 (2%)   | 56,56,56    | 2.61 | 21 (37%) |
| 25  | PHO  | d     | 403 | -    | 58,69,69     | 2.61 | 12 (20%) | 55,99,99    | 3.10 | 18 (32%) |
| 21  | CLA  | b     | 609 | -    | 69,73,73     | 2.16 | 18 (26%) | 82,113,113  | 2.44 | 26 (31%) |
| 21  | CLA  | c     | 504 | -    | 69,73,73     | 2.20 | 18 (26%) | 82,113,113  | 2.57 | 28 (34%) |
| 22  | BCR  | b     | 618 | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 2.06 | 17 (30%) |
| 24  | DGD  | a     | 406 | -    | 58,58,67     | 0.92 | 2 (3%)   | 72,72,81    | 1.00 | 4 (5%)   |
| 21  | CLA  | c     | 510 | -    | 50,54,73     | 2.73 | 21 (42%) | 59,90,113   | 2.79 | 30 (50%) |
| 19  | MGE  | b     | 619 | -    | 48,48,48     | 0.99 | 2 (4%)   | 56,56,56    | 1.18 | 5 (8%)   |
| 19  | MGE  | b     | 620 | -    | 41,41,48     | 1.04 | 2 (4%)   | 49,49,56    | 1.20 | 6 (12%)  |
| 21  | CLA  | c     | 505 | -    | 69,73,73     | 2.48 | 19 (27%) | 82,113,113  | 2.26 | 28 (34%) |
| 21  | CLA  | c     | 508 | -    | 50,54,73     | 2.60 | 18 (36%) | 59,90,113   | 2.93 | 29 (49%) |
| 21  | CLA  | b     | 605 | -    | 69,73,73     | 2.32 | 20 (28%) | 82,113,113  | 2.42 | 30 (36%) |
| 19  | MGE  | c     | 502 | -    | 48,48,48     | 0.97 | 2 (4%)   | 56,56,56    | 1.09 | 4 (7%)   |
| 21  | CLA  | d     | 407 | -    | 54,58,73     | 2.17 | 15 (27%) | 64,95,113   | 4.11 | 34 (53%) |
| 21  | CLA  | c     | 503 | -    | 69,73,73     | 2.08 | 19 (27%) | 82,113,113  | 2.68 | 29 (35%) |
| 21  | CLA  | k     | 501 | -    | 50,54,73     | 2.24 | 16 (32%) | 59,90,113   | 4.62 | 34 (57%) |
| 22  | BCR  | c     | 514 | -    | 41,41,41     | 0.62 | 0        | 56,56,56    | 2.03 | 13 (23%) |
| 20  | SQD  | a     | 401 | -    | 24,26,54     | 1.63 | 3 (12%)  | 34,37,65    | 4.21 | 7 (20%)  |
| 21  | CLA  | b     | 610 | -    | 69,73,73     | 2.06 | 16 (23%) | 82,113,113  | 2.29 | 29 (35%) |
| 21  | CLA  | b     | 614 | -    | 69,73,73     | 2.05 | 17 (24%) | 82,113,113  | 2.39 | 28 (34%) |
| 22  | BCR  | b     | 617 | -    | 41,41,41     | 0.66 | 0        | 56,56,56    | 1.88 | 16 (28%) |
| 30  | HEM  | e     | 101 | -    | 50,50,50     | 1.56 | 8 (16%)  | 67,82,82    | 1.60 | 12 (17%) |
| 21  | CLA  | a     | 403 | -    | 55,59,73     | 2.17 | 19 (34%) | 64,96,113   | 2.77 | 33 (51%) |
| 22  | BCR  | z     | 101 | -    | 41,41,41     | 0.69 | 0        | 56,56,56    | 2.08 | 16 (28%) |
| 21  | CLA  | b     | 613 | -    | 56,60,73     | 2.10 | 17 (30%) | 65,97,113   | 3.09 | 36 (55%) |
| 21  | CLA  | a     | 407 | -    | 69,73,73     | 1.79 | 18 (26%) | 82,113,113  | 2.38 | 36 (43%) |
| 21  | CLA  | a     | 402 | -    | 69,73,73     | 1.91 | 16 (23%) | 82,113,113  | 2.28 | 29 (35%) |
| 21  | CLA  | b     | 615 | -    | 50,54,73     | 2.52 | 19 (38%) | 59,90,113   | 2.69 | 27 (45%) |
| 19  | MGE  | d     | 410 | -    | 48,48,48     | 0.95 | 2 (4%)   | 56,56,56    | 1.29 | 5 (8%)   |
| 21  | CLA  | d     | 406 | -    | 65,69,73     | 1.91 | 12 (18%) | 77,108,113  | 3.86 | 39 (50%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 20  | SQD  | l     | 101 | -    | 45,47,54     | 1.25 | 3 (6%)   | 55,58,65    | 3.38 | 9 (16%)  |
| 26  | LMT  | m     | 101 | -    | 36,36,36     | 0.47 | 0        | 47,47,47    | 0.96 | 3 (6%)   |
| 21  | CLA  | c     | 512 | -    | 55,59,73     | 2.19 | 16 (29%) | 64,96,113   | 4.15 | 32 (50%) |
| 21  | CLA  | c     | 509 | -    | 67,71,73     | 2.40 | 21 (31%) | 79,110,113  | 2.49 | 30 (37%) |
| 21  | CLA  | b     | 611 | -    | 69,73,73     | 2.20 | 18 (26%) | 82,113,113  | 2.50 | 28 (34%) |
| 21  | CLA  | b     | 602 | -    | 69,73,73     | 2.06 | 19 (27%) | 82,113,113  | 2.45 | 30 (36%) |
| 21  | CLA  | b     | 612 | -    | 58,62,73     | 2.11 | 18 (31%) | 68,99,113   | 2.47 | 25 (36%) |
| 21  | CLA  | b     | 607 | -    | 69,73,73     | 2.10 | 18 (26%) | 82,113,113  | 2.10 | 25 (30%) |

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   |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 24  | DGD  | c     | 517 | -    | -         | 9/36/76/95   | 0/2/2/2 |
| 21  | CLA  | b     | 601 | -    | 1/1/15/20 | 2/39/115/115 | -       |
| 19  | MGE  | f     | 101 | -    | -         | 3/42/62/63   | 0/1/1/1 |
| 25  | PHO  | d     | 401 | -    | -         | 1/37/103/103 | 0/5/6/6 |
| 31  | HTG  | h     | 102 | -    | -         | 0/7/27/30    | 0/1/1/1 |
| 21  | CLA  | c     | 507 | -    | -         | 13/23/99/115 | -       |
| 21  | CLA  | c     | 511 | -    | 1/1/15/20 | 6/39/115/115 | -       |
| 21  | CLA  | c     | 513 | -    | -         | 9/21/97/115  | -       |
| 21  | CLA  | c     | 506 | -    | -         | 6/17/93/115  | -       |
| 22  | BCR  | d     | 409 | -    | -         | 8/29/63/63   | 0/2/2/2 |
| 21  | CLA  | h     | 101 | -    | -         | 6/10/86/115  | -       |
| 26  | LMT  | t     | 301 | -    | -         | 7/21/61/61   | 0/2/2/2 |
| 21  | CLA  | b     | 604 | -    | 1/1/15/20 | 3/39/115/115 | -       |
| 22  | BCR  | a     | 404 | -    | -         | 10/29/63/63  | 0/2/2/2 |
| 24  | DGD  | c     | 516 | -    | -         | 12/42/82/95  | 0/2/2/2 |
| 28  | PQ9  | d     | 408 | -    | -         | 7/41/61/61   | 0/1/1/1 |
| 24  | DGD  | h     | 104 | -    | -         | 13/43/83/95  | 0/2/2/2 |
| 21  | CLA  | b     | 606 | -    | 1/1/15/20 | 2/39/115/115 | -       |
| 21  | CLA  | b     | 603 | -    | 1/1/15/20 | 5/39/115/115 | -       |
| 22  | BCR  | h     | 103 | -    | -         | 7/29/63/63   | 0/2/2/2 |
| 21  | CLA  | b     | 608 | -    | -         | 2/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 21  | CLA  | d     | 402 | -    | 1/1/15/20 | 3/39/115/115  | -       |
| 19  | MGE  | B     | 101 | -    | -         | 16/43/63/63   | 0/1/1/1 |
| 26  | LMT  | d     | 404 | -    | -         | 4/21/61/61    | 0/2/2/2 |
| 22  | BCR  | b     | 616 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 19  | MGE  | m     | 102 | -    | -         | 10/43/63/63   | 0/1/1/1 |
| 22  | BCR  | c     | 515 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 25  | PHO  | d     | 403 | -    | -         | 2/37/103/103  | 0/5/6/6 |
| 21  | CLA  | b     | 609 | -    | 1/1/15/20 | 3/39/115/115  | -       |
| 21  | CLA  | c     | 504 | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 22  | BCR  | b     | 618 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 24  | DGD  | a     | 406 | -    | -         | 19/46/86/95   | 0/2/2/2 |
| 21  | CLA  | c     | 510 | -    | 1/1/11/20 | 2/17/93/115   | -       |
| 19  | MGE  | b     | 619 | -    | -         | 11/43/63/63   | 0/1/1/1 |
| 19  | MGE  | b     | 620 | -    | -         | 6/36/56/63    | 0/1/1/1 |
| 21  | CLA  | c     | 505 | -    | -         | 1/39/115/115  | -       |
| 21  | CLA  | c     | 508 | -    | 1/1/11/20 | 1/17/93/115   | -       |
| 21  | CLA  | b     | 605 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 19  | MGE  | c     | 502 | -    | -         | 12/43/63/63   | 0/1/1/1 |
| 21  | CLA  | d     | 407 | -    | -         | 6/21/97/115   | -       |
| 21  | CLA  | c     | 503 | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 21  | CLA  | k     | 501 | -    | -         | 7/17/93/115   | -       |
| 22  | BCR  | c     | 514 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 20  | SQD  | a     | 401 | -    | -         | 5/19/39/69    | 0/1/1/1 |
| 21  | CLA  | b     | 614 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 21  | CLA  | b     | 610 | -    | -         | 5/39/115/115  | -       |
| 22  | BCR  | b     | 617 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 30  | HEM  | e     | 101 | -    | -         | 7/14/54/54    | -       |
| 21  | CLA  | a     | 403 | -    | -         | 1/23/99/115   | -       |
| 22  | BCR  | z     | 101 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 21  | CLA  | b     | 613 | -    | 1/1/12/20 | 7/24/100/115  | -       |
| 21  | CLA  | a     | 407 | -    | -         | 8/39/115/115  | -       |
| 21  | CLA  | a     | 402 | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 21  | CLA  | b     | 615 | -    | 1/1/11/20 | 1/17/93/115   | -       |
| 19  | MGE  | d     | 410 | -    | -         | 13/43/63/63   | 0/1/1/1 |
| 21  | CLA  | d     | 406 | -    | 1/1/14/20 | 10/35/111/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 20  | SQD  | l     | 101 | -    | -         | 8/42/62/69   | 0/1/1/1 |
| 26  | LMT  | m     | 101 | -    | -         | 2/21/61/61   | 0/2/2/2 |
| 21  | CLA  | c     | 512 | -    | -         | 8/23/99/115  | -       |
| 21  | CLA  | c     | 509 | -    | 1/1/14/20 | 8/37/113/115 | -       |
| 21  | CLA  | b     | 611 | -    | 1/1/15/20 | 6/39/115/115 | -       |
| 21  | CLA  | b     | 602 | -    | 1/1/15/20 | 4/39/115/115 | -       |
| 21  | CLA  | b     | 612 | -    | 1/1/12/20 | 0/26/102/115 | -       |
| 21  | CLA  | b     | 607 | -    | -         | 1/39/115/115 | -       |

All (675) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | b     | 611 | CLA  | MG-NA   | 10.39 | 2.31        | 2.06     |
| 21  | b     | 605 | CLA  | MG-NA   | 10.30 | 2.30        | 2.06     |
| 21  | c     | 505 | CLA  | MG-NA   | 9.83  | 2.29        | 2.06     |
| 25  | d     | 403 | PHO  | C1B-C2B | 9.14  | 1.49        | 1.39     |
| 25  | d     | 403 | PHO  | C1D-C2D | 8.79  | 1.49        | 1.39     |
| 21  | c     | 505 | CLA  | MG-NC   | 8.62  | 2.26        | 2.06     |
| 21  | b     | 614 | CLA  | MG-NA   | 8.39  | 2.26        | 2.06     |
| 21  | b     | 610 | CLA  | MG-NA   | 8.37  | 2.26        | 2.06     |
| 21  | b     | 603 | CLA  | MG-NA   | 8.24  | 2.25        | 2.06     |
| 21  | c     | 508 | CLA  | MG-ND   | -8.19 | 1.89        | 2.05     |
| 21  | c     | 503 | CLA  | MG-NA   | 8.13  | 2.25        | 2.06     |
| 21  | c     | 506 | CLA  | C1D-ND  | 8.08  | 1.48        | 1.37     |
| 21  | c     | 510 | CLA  | MG-NA   | 7.80  | 2.24        | 2.06     |
| 21  | b     | 607 | CLA  | MG-NA   | 7.70  | 2.24        | 2.06     |
| 21  | d     | 406 | CLA  | C1D-ND  | 7.68  | 1.47        | 1.37     |
| 21  | d     | 407 | CLA  | C1D-ND  | 7.65  | 1.47        | 1.37     |
| 21  | h     | 101 | CLA  | C1D-ND  | 7.63  | 1.47        | 1.37     |
| 21  | c     | 512 | CLA  | C1D-ND  | 7.57  | 1.47        | 1.37     |
| 21  | k     | 501 | CLA  | C1D-ND  | 7.52  | 1.47        | 1.37     |
| 25  | d     | 401 | PHO  | C1B-C2B | 7.39  | 1.47        | 1.39     |
| 21  | c     | 504 | CLA  | MG-ND   | -7.39 | 1.91        | 2.05     |
| 21  | c     | 504 | CLA  | MG-NA   | 7.38  | 2.23        | 2.06     |
| 21  | c     | 510 | CLA  | MG-ND   | -7.34 | 1.91        | 2.05     |
| 21  | c     | 513 | CLA  | C1D-ND  | 7.33  | 1.47        | 1.37     |
| 21  | c     | 507 | CLA  | C1D-ND  | 7.24  | 1.47        | 1.37     |
| 21  | b     | 606 | CLA  | MG-NA   | 7.13  | 2.23        | 2.06     |
| 25  | d     | 403 | PHO  | C3B-C4B | 6.94  | 1.48        | 1.41     |
| 21  | c     | 510 | CLA  | OBD-CAD | 6.90  | 1.34        | 1.22     |
| 21  | b     | 608 | CLA  | MG-NC   | 6.78  | 2.22        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | d     | 401 | PHO  | C1D-C2D | 6.63  | 1.46        | 1.39     |
| 21  | c     | 509 | CLA  | MG-NA   | 6.57  | 2.21        | 2.06     |
| 21  | c     | 509 | CLA  | MG-NC   | 6.53  | 2.21        | 2.06     |
| 21  | c     | 511 | CLA  | MG-NC   | 6.47  | 2.21        | 2.06     |
| 21  | b     | 608 | CLA  | CHC-C1C | 6.37  | 1.51        | 1.38     |
| 21  | d     | 402 | CLA  | MG-NA   | 6.33  | 2.21        | 2.06     |
| 21  | c     | 508 | CLA  | MG-NB   | 6.32  | 2.18        | 2.05     |
| 21  | a     | 402 | CLA  | MG-NA   | 6.32  | 2.21        | 2.06     |
| 21  | b     | 601 | CLA  | MG-NC   | 6.17  | 2.20        | 2.06     |
| 21  | c     | 509 | CLA  | MG-ND   | 6.11  | 2.17        | 2.05     |
| 21  | b     | 609 | CLA  | MG-NA   | 6.10  | 2.20        | 2.06     |
| 21  | b     | 606 | CLA  | C3C-C2C | 5.98  | 1.49        | 1.36     |
| 21  | b     | 612 | CLA  | MG-NA   | 5.97  | 2.20        | 2.06     |
| 21  | b     | 606 | CLA  | CHC-C1C | 5.94  | 1.50        | 1.38     |
| 21  | b     | 615 | CLA  | CHC-C1C | 5.89  | 1.50        | 1.38     |
| 21  | b     | 601 | CLA  | C3C-C2C | 5.86  | 1.49        | 1.36     |
| 21  | b     | 615 | CLA  | MG-NA   | 5.83  | 2.20        | 2.06     |
| 25  | d     | 403 | PHO  | C4D-CHA | 5.76  | 1.48        | 1.39     |
| 21  | b     | 602 | CLA  | MG-NA   | 5.70  | 2.19        | 2.06     |
| 21  | b     | 606 | CLA  | MG-NC   | 5.66  | 2.19        | 2.06     |
| 21  | b     | 608 | CLA  | O2D-CGD | 5.60  | 1.47        | 1.33     |
| 21  | b     | 609 | CLA  | C3C-C2C | 5.55  | 1.48        | 1.36     |
| 21  | b     | 604 | CLA  | C1D-ND  | -5.52 | 1.30        | 1.37     |
| 21  | c     | 509 | CLA  | C3C-C2C | 5.46  | 1.48        | 1.36     |
| 21  | b     | 611 | CLA  | C3C-C2C | 5.45  | 1.48        | 1.36     |
| 21  | b     | 613 | CLA  | MG-NA   | 5.43  | 2.19        | 2.06     |
| 21  | c     | 505 | CLA  | C3C-C2C | 5.43  | 1.48        | 1.36     |
| 21  | c     | 508 | CLA  | O2D-CGD | 5.40  | 1.46        | 1.33     |
| 21  | b     | 605 | CLA  | MG-NC   | 5.33  | 2.18        | 2.06     |
| 21  | d     | 402 | CLA  | CHC-C1C | 5.32  | 1.49        | 1.38     |
| 21  | b     | 608 | CLA  | C3C-C2C | 5.32  | 1.48        | 1.36     |
| 21  | b     | 602 | CLA  | CHC-C1C | 5.30  | 1.49        | 1.38     |
| 30  | e     | 101 | HEM  | FE-NB   | 5.23  | 2.11        | 1.94     |
| 21  | b     | 603 | CLA  | CHC-C1C | 5.22  | 1.48        | 1.38     |
| 25  | d     | 401 | PHO  | C4D-CHA | 5.20  | 1.47        | 1.39     |
| 21  | h     | 101 | CLA  | O2D-CGD | 5.19  | 1.46        | 1.33     |
| 21  | b     | 602 | CLA  | C3C-C2C | 5.19  | 1.48        | 1.36     |
| 21  | c     | 513 | CLA  | O2D-CGD | 5.10  | 1.45        | 1.33     |
| 21  | b     | 609 | CLA  | O2D-CGD | 5.09  | 1.45        | 1.33     |
| 21  | b     | 610 | CLA  | CHD-C1D | 5.07  | 1.48        | 1.38     |
| 21  | b     | 608 | CLA  | CHD-C1D | 5.07  | 1.48        | 1.38     |
| 21  | b     | 604 | CLA  | MG-NA   | 5.06  | 2.18        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | a     | 403 | CLA  | MG-NA   | 5.05  | 2.18        | 2.06     |
| 21  | b     | 601 | CLA  | OBD-CAD | 5.05  | 1.31        | 1.22     |
| 21  | b     | 601 | CLA  | CHC-C1C | 5.04  | 1.48        | 1.38     |
| 25  | d     | 403 | PHO  | C3D-C4D | -5.02 | 1.34        | 1.41     |
| 21  | b     | 612 | CLA  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 21  | b     | 602 | CLA  | C1D-ND  | -5.02 | 1.31        | 1.37     |
| 21  | c     | 512 | CLA  | O2D-CGD | 5.02  | 1.45        | 1.33     |
| 21  | c     | 511 | CLA  | O2D-CGD | 5.01  | 1.45        | 1.33     |
| 21  | b     | 603 | CLA  | C3C-C2C | 5.00  | 1.47        | 1.36     |
| 21  | c     | 507 | CLA  | O2D-CGD | 5.00  | 1.45        | 1.33     |
| 21  | k     | 501 | CLA  | O2D-CGD | 5.00  | 1.45        | 1.33     |
| 21  | c     | 504 | CLA  | O2D-CGD | 5.00  | 1.45        | 1.33     |
| 21  | c     | 508 | CLA  | MG-NA   | 4.99  | 2.18        | 2.06     |
| 20  | a     | 401 | SQD  | O47-C7  | 4.98  | 1.46        | 1.35     |
| 21  | b     | 604 | CLA  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 21  | b     | 604 | CLA  | CHC-C1C | 4.94  | 1.48        | 1.38     |
| 21  | c     | 506 | CLA  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 21  | b     | 614 | CLA  | C3C-C2C | 4.92  | 1.47        | 1.36     |
| 21  | c     | 505 | CLA  | CHC-C1C | 4.92  | 1.48        | 1.38     |
| 21  | a     | 403 | CLA  | CHC-C1C | 4.88  | 1.48        | 1.38     |
| 25  | d     | 403 | PHO  | C3D-C2D | 4.87  | 1.48        | 1.39     |
| 21  | a     | 402 | CLA  | OBD-CAD | 4.86  | 1.30        | 1.22     |
| 21  | c     | 510 | CLA  | O2D-CGD | 4.86  | 1.45        | 1.33     |
| 21  | c     | 509 | CLA  | CHC-C1C | 4.85  | 1.48        | 1.38     |
| 21  | b     | 610 | CLA  | CHB-C1B | 4.85  | 1.50        | 1.39     |
| 21  | b     | 601 | CLA  | C1D-ND  | -4.85 | 1.31        | 1.37     |
| 21  | b     | 612 | CLA  | CHC-C1C | 4.84  | 1.48        | 1.38     |
| 21  | d     | 406 | CLA  | O2D-CGD | 4.83  | 1.45        | 1.33     |
| 21  | d     | 406 | CLA  | C3D-C4D | -4.82 | 1.33        | 1.44     |
| 25  | d     | 401 | PHO  | C3D-C2D | 4.82  | 1.47        | 1.39     |
| 20  | l     | 101 | SQD  | O8-S    | 4.80  | 1.65        | 1.47     |
| 21  | b     | 604 | CLA  | C3C-C2C | 4.79  | 1.47        | 1.36     |
| 21  | c     | 508 | CLA  | C3C-C2C | 4.77  | 1.47        | 1.36     |
| 21  | c     | 511 | CLA  | C3C-C2C | 4.75  | 1.47        | 1.36     |
| 21  | b     | 609 | CLA  | CHD-C1D | 4.75  | 1.47        | 1.38     |
| 21  | d     | 402 | CLA  | C3C-C2C | 4.75  | 1.47        | 1.36     |
| 21  | b     | 615 | CLA  | C3C-C2C | 4.73  | 1.47        | 1.36     |
| 20  | a     | 401 | SQD  | O8-S    | 4.72  | 1.65        | 1.47     |
| 21  | d     | 407 | CLA  | O2D-CGD | 4.72  | 1.44        | 1.33     |
| 25  | d     | 401 | PHO  | O2D-CGD | 4.72  | 1.44        | 1.33     |
| 21  | b     | 613 | CLA  | CHD-C1D | 4.71  | 1.47        | 1.38     |
| 21  | b     | 615 | CLA  | O2D-CGD | 4.71  | 1.44        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | b     | 601 | CLA  | CHD-C4C | 4.70  | 1.49        | 1.39     |
| 21  | b     | 615 | CLA  | C1D-ND  | -4.69 | 1.31        | 1.37     |
| 21  | a     | 403 | CLA  | CHB-C1B | 4.68  | 1.49        | 1.39     |
| 21  | k     | 501 | CLA  | O2A-CGA | 4.67  | 1.47        | 1.33     |
| 21  | c     | 504 | CLA  | OBD-CAD | 4.66  | 1.30        | 1.22     |
| 21  | h     | 101 | CLA  | C3D-C4D | -4.66 | 1.33        | 1.44     |
| 21  | a     | 402 | CLA  | C3C-C2C | 4.66  | 1.46        | 1.36     |
| 21  | b     | 605 | CLA  | C3C-C2C | 4.65  | 1.46        | 1.36     |
| 21  | k     | 501 | CLA  | C3D-C4D | -4.64 | 1.33        | 1.44     |
| 21  | c     | 506 | CLA  | C3D-C4D | -4.64 | 1.33        | 1.44     |
| 25  | d     | 401 | PHO  | C3B-C4B | 4.62  | 1.46        | 1.41     |
| 21  | c     | 505 | CLA  | CHB-C1B | 4.61  | 1.49        | 1.39     |
| 21  | b     | 609 | CLA  | MG-ND   | -4.60 | 1.96        | 2.05     |
| 21  | c     | 505 | CLA  | CHD-C1D | 4.59  | 1.47        | 1.38     |
| 21  | c     | 513 | CLA  | C3C-C2C | 4.59  | 1.46        | 1.36     |
| 21  | d     | 407 | CLA  | C3D-C4D | -4.58 | 1.33        | 1.44     |
| 21  | c     | 512 | CLA  | C3D-C4D | -4.57 | 1.33        | 1.44     |
| 21  | b     | 614 | CLA  | O2D-CGD | 4.57  | 1.44        | 1.33     |
| 21  | b     | 614 | CLA  | OBD-CAD | 4.55  | 1.30        | 1.22     |
| 21  | b     | 602 | CLA  | O2D-CGD | 4.54  | 1.44        | 1.33     |
| 21  | a     | 403 | CLA  | C3C-C2C | 4.54  | 1.46        | 1.36     |
| 21  | c     | 503 | CLA  | CHB-C1B | 4.53  | 1.49        | 1.39     |
| 21  | b     | 606 | CLA  | CHD-C1D | 4.51  | 1.47        | 1.38     |
| 21  | a     | 407 | CLA  | CHC-C1C | 4.50  | 1.47        | 1.38     |
| 21  | b     | 614 | CLA  | CHD-C4C | 4.48  | 1.49        | 1.39     |
| 21  | b     | 607 | CLA  | C4B-NB  | -4.47 | 1.32        | 1.37     |
| 21  | b     | 605 | CLA  | CHD-C1D | 4.46  | 1.47        | 1.38     |
| 21  | b     | 610 | CLA  | O2D-CGD | 4.45  | 1.44        | 1.33     |
| 21  | c     | 511 | CLA  | MG-NA   | 4.45  | 2.16        | 2.06     |
| 21  | h     | 101 | CLA  | C3C-C2C | 4.44  | 1.46        | 1.36     |
| 21  | c     | 512 | CLA  | C3C-C2C | 4.43  | 1.46        | 1.36     |
| 21  | c     | 504 | CLA  | CHB-C1B | 4.43  | 1.49        | 1.39     |
| 21  | c     | 503 | CLA  | CHD-C1D | 4.43  | 1.47        | 1.38     |
| 21  | c     | 513 | CLA  | C3D-C4D | -4.43 | 1.34        | 1.44     |
| 21  | c     | 510 | CLA  | CHD-C1D | 4.42  | 1.47        | 1.38     |
| 21  | b     | 613 | CLA  | O2A-CGA | 4.42  | 1.46        | 1.33     |
| 19  | b     | 619 | MGE  | O2G-C1B | 4.41  | 1.46        | 1.34     |
| 21  | c     | 504 | CLA  | CHD-C1D | 4.40  | 1.47        | 1.38     |
| 21  | b     | 608 | CLA  | MG-NB   | 4.40  | 2.14        | 2.05     |
| 21  | c     | 507 | CLA  | C3D-C4D | -4.39 | 1.34        | 1.44     |
| 21  | b     | 605 | CLA  | O2D-CGD | 4.36  | 1.44        | 1.33     |
| 21  | b     | 610 | CLA  | CHC-C1C | 4.34  | 1.47        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | b     | 603 | CLA  | MG-ND   | -4.34 | 1.97        | 2.05     |
| 21  | c     | 513 | CLA  | O2A-CGA | 4.33  | 1.46        | 1.33     |
| 21  | b     | 615 | CLA  | CHD-C1D | 4.32  | 1.46        | 1.38     |
| 21  | b     | 612 | CLA  | C3C-C2C | 4.30  | 1.46        | 1.36     |
| 21  | c     | 507 | CLA  | C3C-C2C | 4.29  | 1.46        | 1.36     |
| 21  | c     | 511 | CLA  | CHC-C1C | 4.29  | 1.47        | 1.38     |
| 21  | b     | 607 | CLA  | CHC-C1C | 4.28  | 1.47        | 1.38     |
| 20  | l     | 101 | SQD  | O47-C7  | 4.27  | 1.46        | 1.34     |
| 21  | c     | 503 | CLA  | C3C-C2C | 4.27  | 1.46        | 1.36     |
| 21  | c     | 512 | CLA  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 21  | b     | 601 | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 21  | c     | 505 | CLA  | O2D-CGD | 4.26  | 1.43        | 1.33     |
| 21  | b     | 613 | CLA  | CHB-C1B | 4.25  | 1.49        | 1.39     |
| 21  | d     | 402 | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 25  | d     | 403 | PHO  | C3B-C2B | 4.25  | 1.46        | 1.40     |
| 19  | b     | 619 | MGE  | O1G-C1A | 4.24  | 1.45        | 1.33     |
| 19  | m     | 102 | MGE  | O1G-C1A | 4.24  | 1.45        | 1.33     |
| 21  | a     | 407 | CLA  | C3C-C2C | 4.24  | 1.45        | 1.36     |
| 21  | a     | 402 | CLA  | C4B-NB  | -4.24 | 1.32        | 1.37     |
| 21  | b     | 612 | CLA  | O2A-CGA | 4.23  | 1.45        | 1.33     |
| 25  | d     | 403 | PHO  | O2D-CGD | 4.22  | 1.43        | 1.33     |
| 19  | b     | 620 | MGE  | O2G-C1B | 4.22  | 1.46        | 1.34     |
| 21  | b     | 607 | CLA  | C3C-C2C | 4.22  | 1.45        | 1.36     |
| 21  | c     | 507 | CLA  | O2A-CGA | 4.21  | 1.45        | 1.33     |
| 21  | d     | 407 | CLA  | O2A-CGA | 4.20  | 1.45        | 1.33     |
| 21  | c     | 509 | CLA  | CHC-C4B | 4.20  | 1.48        | 1.39     |
| 19  | c     | 502 | MGE  | O2G-C1B | 4.20  | 1.46        | 1.34     |
| 21  | b     | 611 | CLA  | CHC-C1C | 4.19  | 1.46        | 1.38     |
| 21  | c     | 509 | CLA  | CHB-C1B | 4.19  | 1.48        | 1.39     |
| 20  | l     | 101 | SQD  | O48-C23 | 4.18  | 1.45        | 1.33     |
| 21  | c     | 506 | CLA  | O2A-CGA | 4.18  | 1.46        | 1.33     |
| 19  | m     | 102 | MGE  | O2G-C1B | 4.18  | 1.46        | 1.34     |
| 21  | d     | 407 | CLA  | C3C-C2C | 4.17  | 1.45        | 1.36     |
| 21  | c     | 510 | CLA  | C3C-C2C | 4.17  | 1.45        | 1.36     |
| 21  | k     | 501 | CLA  | C3C-C2C | 4.17  | 1.45        | 1.36     |
| 21  | c     | 508 | CLA  | CHD-C4C | 4.17  | 1.48        | 1.39     |
| 21  | b     | 607 | CLA  | OBD-CAD | 4.17  | 1.29        | 1.22     |
| 19  | f     | 101 | MGE  | O1G-C1A | 4.16  | 1.45        | 1.33     |
| 30  | e     | 101 | HEM  | FE-NC   | 4.16  | 2.08        | 1.95     |
| 21  | a     | 407 | CLA  | MG-NA   | 4.15  | 2.16        | 2.06     |
| 19  | f     | 101 | MGE  | O2G-C1B | 4.15  | 1.46        | 1.34     |
| 24  | c     | 516 | DGD  | O2G-C1B | 4.14  | 1.46        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | c     | 502 | MGE  | O1G-C1A | 4.14  | 1.45        | 1.33     |
| 24  | h     | 104 | DGD  | O1G-C1A | 4.13  | 1.45        | 1.33     |
| 24  | c     | 517 | DGD  | O2G-C1B | 4.13  | 1.45        | 1.34     |
| 25  | d     | 401 | PHO  | C3B-C2B | 4.13  | 1.46        | 1.40     |
| 19  | d     | 410 | MGE  | O1G-C1A | 4.13  | 1.45        | 1.33     |
| 21  | b     | 615 | CLA  | O2A-CGA | 4.12  | 1.45        | 1.33     |
| 21  | b     | 611 | CLA  | C1B-C2B | 4.11  | 1.52        | 1.43     |
| 24  | a     | 406 | DGD  | O1G-C1A | 4.11  | 1.45        | 1.33     |
| 19  | B     | 101 | MGE  | O2G-C1B | 4.10  | 1.45        | 1.34     |
| 25  | d     | 403 | PHO  | C3A-C2A | -4.09 | 1.51        | 1.54     |
| 24  | c     | 516 | DGD  | O1G-C1A | 4.08  | 1.45        | 1.33     |
| 24  | c     | 517 | DGD  | O1G-C1A | 4.08  | 1.45        | 1.33     |
| 21  | c     | 503 | CLA  | CHC-C1C | 4.06  | 1.46        | 1.38     |
| 21  | b     | 605 | CLA  | CHC-C1C | 4.06  | 1.46        | 1.38     |
| 19  | b     | 620 | MGE  | O1G-C1A | 4.06  | 1.45        | 1.33     |
| 21  | c     | 511 | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 21  | b     | 606 | CLA  | O2D-CGD | 4.05  | 1.43        | 1.33     |
| 21  | c     | 511 | CLA  | CHB-C1B | 4.04  | 1.48        | 1.39     |
| 21  | c     | 506 | CLA  | C3C-C2C | 4.03  | 1.45        | 1.36     |
| 21  | b     | 605 | CLA  | CHB-C1B | 4.03  | 1.48        | 1.39     |
| 21  | b     | 603 | CLA  | O2D-CGD | 4.02  | 1.43        | 1.33     |
| 21  | b     | 609 | CLA  | CHC-C1C | 4.02  | 1.46        | 1.38     |
| 21  | b     | 609 | CLA  | C4C-C3C | 4.01  | 1.51        | 1.45     |
| 24  | a     | 406 | DGD  | O2G-C1B | 4.00  | 1.45        | 1.34     |
| 21  | b     | 601 | CLA  | CHB-C1B | 3.99  | 1.48        | 1.39     |
| 21  | b     | 615 | CLA  | MG-ND   | 3.99  | 2.13        | 2.05     |
| 21  | d     | 402 | CLA  | CHD-C4C | 3.99  | 1.48        | 1.39     |
| 21  | d     | 406 | CLA  | O2A-CGA | 3.98  | 1.45        | 1.33     |
| 21  | b     | 603 | CLA  | CHD-C1D | 3.98  | 1.46        | 1.38     |
| 21  | b     | 608 | CLA  | MG-NA   | 3.98  | 2.15        | 2.06     |
| 21  | b     | 609 | CLA  | OBD-CAD | 3.98  | 1.29        | 1.22     |
| 21  | c     | 509 | CLA  | CHD-C1D | 3.97  | 1.46        | 1.38     |
| 21  | b     | 615 | CLA  | CHB-C1B | 3.97  | 1.48        | 1.39     |
| 21  | c     | 511 | CLA  | O2A-CGA | 3.96  | 1.44        | 1.33     |
| 24  | h     | 104 | DGD  | O2G-C1B | 3.96  | 1.45        | 1.34     |
| 21  | b     | 613 | CLA  | O2D-CGD | 3.95  | 1.42        | 1.33     |
| 21  | d     | 406 | CLA  | C3C-C2C | 3.95  | 1.45        | 1.36     |
| 19  | B     | 101 | MGE  | O1G-C1A | 3.94  | 1.44        | 1.33     |
| 21  | b     | 610 | CLA  | C3C-C2C | 3.94  | 1.45        | 1.36     |
| 21  | b     | 613 | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 21  | c     | 509 | CLA  | CHD-C4C | 3.93  | 1.48        | 1.39     |
| 21  | b     | 606 | CLA  | MG-NB   | 3.93  | 2.13        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | a     | 402 | CLA  | MG-NB   | -3.93 | 1.98        | 2.05     |
| 21  | b     | 611 | CLA  | O2D-CGD | 3.92  | 1.42        | 1.33     |
| 21  | b     | 615 | CLA  | CHC-C4B | 3.92  | 1.48        | 1.39     |
| 19  | d     | 410 | MGE  | O2G-C1B | 3.92  | 1.45        | 1.34     |
| 21  | c     | 511 | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 21  | b     | 607 | CLA  | CHB-C1B | 3.91  | 1.48        | 1.39     |
| 21  | c     | 508 | CLA  | O2A-CGA | 3.88  | 1.45        | 1.33     |
| 21  | c     | 505 | CLA  | CHC-C4B | 3.86  | 1.48        | 1.39     |
| 21  | b     | 613 | CLA  | CHC-C4B | 3.84  | 1.48        | 1.39     |
| 21  | b     | 605 | CLA  | CHD-C4C | 3.84  | 1.47        | 1.39     |
| 21  | c     | 503 | CLA  | O2A-CGA | 3.83  | 1.44        | 1.33     |
| 21  | c     | 509 | CLA  | C4B-NB  | -3.83 | 1.32        | 1.37     |
| 21  | b     | 614 | CLA  | CHC-C1C | 3.83  | 1.46        | 1.38     |
| 21  | b     | 609 | CLA  | CHD-C4C | 3.83  | 1.47        | 1.39     |
| 21  | a     | 402 | CLA  | O2D-CGD | 3.82  | 1.42        | 1.33     |
| 21  | a     | 403 | CLA  | C1D-ND  | -3.82 | 1.32        | 1.37     |
| 21  | c     | 513 | CLA  | CHC-C1C | 3.82  | 1.46        | 1.38     |
| 21  | c     | 503 | CLA  | O2D-CGD | 3.81  | 1.42        | 1.33     |
| 21  | b     | 606 | CLA  | C3D-C2D | 3.81  | 1.49        | 1.39     |
| 21  | c     | 510 | CLA  | CHC-C1C | 3.81  | 1.46        | 1.38     |
| 21  | b     | 603 | CLA  | CHB-C1B | 3.78  | 1.47        | 1.39     |
| 21  | c     | 504 | CLA  | CHC-C1C | 3.78  | 1.46        | 1.38     |
| 21  | c     | 505 | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 21  | b     | 608 | CLA  | CHB-C1B | 3.77  | 1.47        | 1.39     |
| 21  | b     | 607 | CLA  | CHD-C1D | 3.77  | 1.45        | 1.38     |
| 21  | b     | 607 | CLA  | CHD-C4C | 3.76  | 1.47        | 1.39     |
| 21  | b     | 602 | CLA  | CHD-C1D | 3.74  | 1.45        | 1.38     |
| 21  | b     | 606 | CLA  | MG-ND   | 3.72  | 2.13        | 2.05     |
| 21  | b     | 606 | CLA  | C1D-ND  | -3.70 | 1.33        | 1.37     |
| 21  | a     | 403 | CLA  | O2A-CGA | 3.69  | 1.44        | 1.33     |
| 21  | a     | 403 | CLA  | CHD-C1D | 3.69  | 1.45        | 1.38     |
| 21  | c     | 507 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 25  | d     | 401 | PHO  | OBD-CAD | 3.68  | 1.27        | 1.22     |
| 21  | h     | 101 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 21  | b     | 613 | CLA  | CHC-C1C | 3.68  | 1.45        | 1.38     |
| 21  | b     | 614 | CLA  | C3D-C2D | 3.67  | 1.49        | 1.39     |
| 21  | b     | 609 | CLA  | CHC-C4B | 3.66  | 1.47        | 1.39     |
| 21  | b     | 608 | CLA  | O2A-CGA | 3.66  | 1.44        | 1.33     |
| 21  | k     | 501 | CLA  | CHC-C1C | 3.66  | 1.45        | 1.38     |
| 21  | c     | 511 | CLA  | CHC-C4B | 3.66  | 1.47        | 1.39     |
| 21  | b     | 606 | CLA  | CHB-C1B | 3.65  | 1.47        | 1.39     |
| 21  | b     | 605 | CLA  | CHC-C4B | 3.65  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | b     | 607 | CLA  | CHC-C4B | 3.64  | 1.47        | 1.39     |
| 21  | b     | 602 | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 21  | b     | 603 | CLA  | MG-NC   | 3.62  | 2.14        | 2.06     |
| 21  | b     | 612 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 25  | d     | 401 | PHO  | C4B-NB  | -3.60 | 1.32        | 1.38     |
| 21  | c     | 509 | CLA  | O2A-CGA | 3.60  | 1.43        | 1.33     |
| 21  | b     | 610 | CLA  | CHD-C4C | 3.59  | 1.47        | 1.39     |
| 21  | c     | 507 | CLA  | CHC-C1C | 3.59  | 1.45        | 1.38     |
| 21  | c     | 510 | CLA  | CHB-C1B | 3.58  | 1.47        | 1.39     |
| 21  | c     | 510 | CLA  | O2A-CGA | 3.58  | 1.44        | 1.33     |
| 21  | b     | 610 | CLA  | O2A-CGA | 3.57  | 1.43        | 1.33     |
| 21  | c     | 503 | CLA  | CHD-C4C | 3.57  | 1.47        | 1.39     |
| 25  | d     | 403 | PHO  | O2A-CGA | 3.56  | 1.43        | 1.33     |
| 21  | b     | 611 | CLA  | CHD-C1D | 3.55  | 1.45        | 1.38     |
| 21  | c     | 511 | CLA  | MG-ND   | -3.55 | 1.98        | 2.05     |
| 21  | h     | 101 | CLA  | CHC-C1C | 3.54  | 1.45        | 1.38     |
| 21  | c     | 513 | CLA  | CHD-C4C | 3.53  | 1.47        | 1.39     |
| 21  | a     | 407 | CLA  | O2D-CGD | 3.53  | 1.41        | 1.33     |
| 21  | b     | 604 | CLA  | C1B-NB  | -3.52 | 1.33        | 1.37     |
| 21  | b     | 602 | CLA  | C1B-NB  | -3.52 | 1.33        | 1.37     |
| 21  | c     | 512 | CLA  | CHC-C1C | 3.52  | 1.45        | 1.38     |
| 21  | c     | 508 | CLA  | CHD-C1D | 3.52  | 1.45        | 1.38     |
| 21  | c     | 509 | CLA  | O2D-CGD | 3.52  | 1.41        | 1.33     |
| 21  | b     | 606 | CLA  | C1B-C2B | 3.51  | 1.51        | 1.43     |
| 21  | k     | 501 | CLA  | OBD-CAD | 3.50  | 1.28        | 1.22     |
| 21  | c     | 513 | CLA  | OBD-CAD | 3.50  | 1.28        | 1.22     |
| 21  | b     | 612 | CLA  | CHC-C4B | 3.50  | 1.47        | 1.39     |
| 21  | b     | 613 | CLA  | C3C-C2C | 3.50  | 1.44        | 1.36     |
| 21  | b     | 607 | CLA  | C1B-NB  | -3.49 | 1.33        | 1.37     |
| 21  | a     | 403 | CLA  | CHD-C4C | 3.49  | 1.47        | 1.39     |
| 21  | b     | 609 | CLA  | CHB-C1B | 3.49  | 1.47        | 1.39     |
| 31  | h     | 102 | HTG  | C1'-S1  | -3.49 | 1.76        | 1.81     |
| 21  | a     | 403 | CLA  | O2D-CGD | 3.48  | 1.41        | 1.33     |
| 21  | c     | 508 | CLA  | CHC-C1C | 3.48  | 1.45        | 1.38     |
| 21  | b     | 611 | CLA  | CHB-C1B | 3.47  | 1.47        | 1.39     |
| 21  | c     | 503 | CLA  | CHC-C4B | 3.47  | 1.47        | 1.39     |
| 21  | a     | 403 | CLA  | MG-NB   | -3.47 | 1.98        | 2.05     |
| 21  | c     | 513 | CLA  | CHD-C1D | 3.46  | 1.45        | 1.38     |
| 21  | c     | 512 | CLA  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 21  | b     | 608 | CLA  | C3B-C4B | 3.45  | 1.52        | 1.42     |
| 21  | c     | 509 | CLA  | C3D-C2D | 3.44  | 1.48        | 1.39     |
| 21  | c     | 511 | CLA  | OBD-CAD | 3.44  | 1.28        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | c     | 504 | CLA  | C3C-C2C | 3.44  | 1.44        | 1.36     |
| 21  | c     | 510 | CLA  | MG-NC   | 3.43  | 2.14        | 2.06     |
| 21  | d     | 407 | CLA  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 21  | c     | 503 | CLA  | C4C-C3C | 3.43  | 1.50        | 1.45     |
| 21  | b     | 607 | CLA  | O2D-CGD | 3.43  | 1.41        | 1.33     |
| 21  | a     | 403 | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 21  | b     | 608 | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 21  | c     | 508 | CLA  | CHB-C1B | 3.40  | 1.47        | 1.39     |
| 21  | c     | 506 | CLA  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 21  | a     | 407 | CLA  | C3D-C2D | 3.39  | 1.48        | 1.39     |
| 21  | h     | 101 | CLA  | CHD-C1D | 3.39  | 1.45        | 1.38     |
| 21  | b     | 609 | CLA  | MG-NC   | 3.38  | 2.14        | 2.06     |
| 21  | b     | 608 | CLA  | C1B-C2B | 3.38  | 1.51        | 1.43     |
| 21  | c     | 504 | CLA  | O2A-CGA | 3.37  | 1.43        | 1.33     |
| 21  | b     | 601 | CLA  | O2A-CGA | 3.37  | 1.43        | 1.33     |
| 21  | b     | 602 | CLA  | C4B-NB  | -3.35 | 1.33        | 1.37     |
| 21  | d     | 406 | CLA  | CHC-C1C | 3.35  | 1.45        | 1.38     |
| 30  | e     | 101 | HEM  | C1B-NB  | -3.35 | 1.34        | 1.40     |
| 21  | a     | 402 | CLA  | CHD-C4C | 3.33  | 1.46        | 1.39     |
| 21  | c     | 509 | CLA  | OBD-CAD | 3.32  | 1.28        | 1.22     |
| 21  | d     | 407 | CLA  | CHC-C1C | 3.32  | 1.45        | 1.38     |
| 21  | b     | 601 | CLA  | C1B-C2B | 3.31  | 1.50        | 1.43     |
| 21  | b     | 605 | CLA  | C4D-CHA | 3.31  | 1.49        | 1.38     |
| 21  | a     | 407 | CLA  | C4D-CHA | 3.30  | 1.49        | 1.38     |
| 21  | a     | 407 | CLA  | CHB-C1B | 3.30  | 1.46        | 1.39     |
| 21  | b     | 606 | CLA  | CHC-C4B | 3.29  | 1.46        | 1.39     |
| 21  | c     | 509 | CLA  | C4D-CHA | 3.29  | 1.49        | 1.38     |
| 21  | b     | 608 | CLA  | CHC-C4B | 3.28  | 1.46        | 1.39     |
| 21  | b     | 609 | CLA  | C1B-NB  | -3.28 | 1.33        | 1.37     |
| 21  | b     | 612 | CLA  | CHD-C1D | 3.28  | 1.44        | 1.38     |
| 21  | h     | 101 | CLA  | CHD-C4C | 3.26  | 1.46        | 1.39     |
| 21  | b     | 611 | CLA  | CHC-C4B | 3.24  | 1.46        | 1.39     |
| 21  | c     | 513 | CLA  | C3D-C2D | 3.23  | 1.47        | 1.39     |
| 21  | c     | 505 | CLA  | O2A-CGA | 3.23  | 1.42        | 1.33     |
| 21  | b     | 602 | CLA  | CHD-C4C | 3.23  | 1.46        | 1.39     |
| 21  | b     | 608 | CLA  | CHD-C4C | 3.22  | 1.46        | 1.39     |
| 21  | b     | 602 | CLA  | CHB-C1B | 3.22  | 1.46        | 1.39     |
| 30  | e     | 101 | HEM  | C4D-ND  | -3.21 | 1.34        | 1.40     |
| 21  | b     | 613 | CLA  | MG-ND   | -3.21 | 1.99        | 2.05     |
| 21  | d     | 402 | CLA  | CHB-C1B | 3.20  | 1.46        | 1.39     |
| 21  | b     | 615 | CLA  | C3D-C2D | 3.19  | 1.47        | 1.39     |
| 21  | b     | 606 | CLA  | C1B-NB  | -3.19 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | d     | 402 | CLA  | C1D-ND  | -3.18 | 1.33        | 1.37     |
| 21  | c     | 506 | CLA  | CHC-C1C | 3.18  | 1.44        | 1.38     |
| 21  | a     | 407 | CLA  | CHD-C4C | 3.17  | 1.46        | 1.39     |
| 21  | b     | 603 | CLA  | CHD-C4C | 3.17  | 1.46        | 1.39     |
| 21  | d     | 406 | CLA  | OBD-CAD | 3.17  | 1.27        | 1.22     |
| 21  | b     | 611 | CLA  | O2A-CGA | 3.17  | 1.42        | 1.33     |
| 21  | c     | 507 | CLA  | C3D-C2D | 3.17  | 1.47        | 1.39     |
| 21  | b     | 615 | CLA  | C4B-NB  | -3.17 | 1.33        | 1.37     |
| 21  | c     | 504 | CLA  | CHC-C4B | 3.15  | 1.46        | 1.39     |
| 21  | b     | 608 | CLA  | C4B-NB  | -3.15 | 1.33        | 1.37     |
| 21  | b     | 615 | CLA  | OBD-CAD | 3.15  | 1.27        | 1.22     |
| 21  | c     | 505 | CLA  | C4D-CHA | 3.14  | 1.49        | 1.38     |
| 21  | d     | 402 | CLA  | O2A-CGA | 3.13  | 1.42        | 1.33     |
| 21  | c     | 504 | CLA  | CHD-C4C | 3.12  | 1.46        | 1.39     |
| 21  | c     | 510 | CLA  | C3D-C2D | 3.12  | 1.47        | 1.39     |
| 21  | c     | 503 | CLA  | OBD-CAD | 3.11  | 1.27        | 1.22     |
| 21  | b     | 607 | CLA  | C1D-ND  | -3.11 | 1.33        | 1.37     |
| 21  | b     | 614 | CLA  | CHB-C1B | 3.11  | 1.46        | 1.39     |
| 21  | c     | 510 | CLA  | CHC-C4B | 3.10  | 1.46        | 1.39     |
| 21  | b     | 610 | CLA  | C3D-C2D | 3.10  | 1.47        | 1.39     |
| 21  | b     | 608 | CLA  | C3D-C2D | 3.10  | 1.47        | 1.39     |
| 21  | a     | 407 | CLA  | C1D-ND  | -3.10 | 1.33        | 1.37     |
| 21  | c     | 505 | CLA  | C3D-C2D | 3.08  | 1.47        | 1.39     |
| 21  | b     | 604 | CLA  | C3B-C4B | 3.07  | 1.51        | 1.42     |
| 21  | c     | 512 | CLA  | CHD-C1D | 3.06  | 1.44        | 1.38     |
| 21  | a     | 407 | CLA  | CHC-C4B | 3.05  | 1.46        | 1.39     |
| 21  | b     | 606 | CLA  | CHD-C4C | 3.05  | 1.46        | 1.39     |
| 21  | b     | 610 | CLA  | C4D-CHA | 3.04  | 1.48        | 1.38     |
| 21  | c     | 513 | CLA  | C1D-C2D | 3.04  | 1.51        | 1.45     |
| 25  | d     | 401 | PHO  | CMA-C3A | 3.04  | 1.58        | 1.53     |
| 21  | b     | 607 | CLA  | C3B-C4B | 3.03  | 1.51        | 1.42     |
| 21  | b     | 614 | CLA  | CHD-C1D | 3.02  | 1.44        | 1.38     |
| 21  | c     | 507 | CLA  | CHD-C4C | 3.01  | 1.46        | 1.39     |
| 21  | c     | 513 | CLA  | C1B-NB  | -3.01 | 1.33        | 1.37     |
| 21  | d     | 407 | CLA  | CHD-C1D | 3.01  | 1.44        | 1.38     |
| 21  | b     | 611 | CLA  | C3D-C2D | 3.01  | 1.47        | 1.39     |
| 21  | b     | 611 | CLA  | C4B-NB  | -2.99 | 1.33        | 1.37     |
| 21  | c     | 503 | CLA  | C4D-CHA | 2.99  | 1.48        | 1.38     |
| 21  | b     | 602 | CLA  | C4D-CHA | 2.98  | 1.48        | 1.38     |
| 21  | d     | 402 | CLA  | OBD-CAD | 2.98  | 1.27        | 1.22     |
| 21  | c     | 507 | CLA  | CHD-C1D | 2.98  | 1.44        | 1.38     |
| 21  | b     | 615 | CLA  | CHD-C4C | 2.98  | 1.46        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | b     | 614 | CLA  | C1B-C2B | 2.96  | 1.50        | 1.43     |
| 21  | b     | 606 | CLA  | C4D-CHA | 2.96  | 1.48        | 1.38     |
| 21  | a     | 402 | CLA  | C4D-CHA | 2.96  | 1.48        | 1.38     |
| 21  | b     | 605 | CLA  | C3D-C2D | 2.96  | 1.47        | 1.39     |
| 21  | b     | 603 | CLA  | C4B-NB  | -2.95 | 1.34        | 1.37     |
| 21  | b     | 614 | CLA  | C4D-CHA | 2.95  | 1.48        | 1.38     |
| 21  | b     | 607 | CLA  | C4D-CHA | 2.94  | 1.48        | 1.38     |
| 21  | b     | 602 | CLA  | C3D-C2D | 2.94  | 1.47        | 1.39     |
| 21  | a     | 407 | CLA  | CHD-C1D | 2.93  | 1.44        | 1.38     |
| 21  | c     | 511 | CLA  | C4D-CHA | 2.93  | 1.48        | 1.38     |
| 21  | b     | 611 | CLA  | MG-NC   | -2.93 | 1.99        | 2.06     |
| 21  | c     | 509 | CLA  | C1D-ND  | -2.93 | 1.34        | 1.37     |
| 21  | b     | 608 | CLA  | C1D-ND  | -2.92 | 1.34        | 1.37     |
| 21  | c     | 506 | CLA  | CHB-C4A | -2.91 | 1.30        | 1.37     |
| 21  | b     | 604 | CLA  | O2A-CGA | 2.91  | 1.41        | 1.33     |
| 21  | d     | 402 | CLA  | CHC-C4B | 2.91  | 1.45        | 1.39     |
| 21  | c     | 508 | CLA  | CHC-C4B | 2.91  | 1.45        | 1.39     |
| 21  | b     | 612 | CLA  | CHD-C4C | 2.90  | 1.45        | 1.39     |
| 25  | d     | 401 | PHO  | CBD-CGD | -2.90 | 1.48        | 1.52     |
| 21  | b     | 608 | CLA  | C4D-CHA | 2.89  | 1.48        | 1.38     |
| 21  | c     | 505 | CLA  | C4C-C3C | 2.89  | 1.50        | 1.45     |
| 21  | c     | 504 | CLA  | C4D-CHA | 2.89  | 1.48        | 1.38     |
| 21  | a     | 402 | CLA  | CHB-C1B | 2.89  | 1.45        | 1.39     |
| 21  | b     | 612 | CLA  | C3B-C4B | 2.89  | 1.51        | 1.42     |
| 21  | d     | 402 | CLA  | MG-ND   | -2.88 | 2.00        | 2.05     |
| 21  | a     | 407 | CLA  | O2A-CGA | 2.88  | 1.41        | 1.33     |
| 21  | b     | 601 | CLA  | C1B-NB  | -2.88 | 1.34        | 1.37     |
| 21  | b     | 606 | CLA  | C3B-C4B | 2.88  | 1.51        | 1.42     |
| 21  | a     | 402 | CLA  | O2A-CGA | 2.87  | 1.41        | 1.33     |
| 21  | a     | 402 | CLA  | CHC-C1C | 2.87  | 1.44        | 1.38     |
| 21  | b     | 615 | CLA  | C1C-C2C | 2.87  | 1.50        | 1.44     |
| 21  | b     | 604 | CLA  | CHB-C1B | 2.86  | 1.45        | 1.39     |
| 21  | b     | 611 | CLA  | C1B-NB  | -2.85 | 1.34        | 1.37     |
| 25  | d     | 401 | PHO  | C3D-C4D | -2.85 | 1.37        | 1.41     |
| 21  | c     | 510 | CLA  | CHD-C4C | 2.85  | 1.45        | 1.39     |
| 21  | b     | 612 | CLA  | C3D-C2D | 2.85  | 1.46        | 1.39     |
| 21  | b     | 601 | CLA  | CHC-C4B | 2.85  | 1.45        | 1.39     |
| 21  | d     | 407 | CLA  | CHD-C4C | 2.85  | 1.45        | 1.39     |
| 21  | h     | 101 | CLA  | CHB-C4A | -2.84 | 1.30        | 1.37     |
| 21  | b     | 615 | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 21  | b     | 601 | CLA  | MG-NB   | 2.83  | 2.11        | 2.05     |
| 21  | b     | 612 | CLA  | C1D-ND  | -2.83 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | c     | 506 | CLA  | CHD-C4C | 2.83  | 1.45        | 1.39     |
| 22  | c     | 515 | BCR  | C30-C25 | -2.82 | 1.50        | 1.53     |
| 21  | c     | 504 | CLA  | CBD-CAD | -2.82 | 1.44        | 1.56     |
| 21  | b     | 603 | CLA  | C3D-C2D | 2.81  | 1.46        | 1.39     |
| 21  | c     | 512 | CLA  | CHD-C4C | 2.80  | 1.45        | 1.39     |
| 21  | b     | 604 | CLA  | CHD-C1D | 2.79  | 1.43        | 1.38     |
| 21  | b     | 601 | CLA  | C3B-C4B | 2.78  | 1.50        | 1.42     |
| 25  | d     | 403 | PHO  | OBD-CAD | 2.76  | 1.25        | 1.22     |
| 21  | b     | 604 | CLA  | OBD-CAD | 2.75  | 1.27        | 1.22     |
| 21  | b     | 612 | CLA  | C4D-CHA | 2.74  | 1.47        | 1.38     |
| 21  | b     | 608 | CLA  | C4C-C3C | 2.74  | 1.49        | 1.45     |
| 21  | c     | 511 | CLA  | C1B-NB  | -2.74 | 1.34        | 1.37     |
| 21  | b     | 605 | CLA  | O2A-CGA | 2.74  | 1.41        | 1.33     |
| 21  | c     | 508 | CLA  | C1C-C2C | 2.74  | 1.50        | 1.44     |
| 21  | c     | 511 | CLA  | C3D-C2D | 2.73  | 1.46        | 1.39     |
| 21  | b     | 602 | CLA  | O2A-CGA | 2.73  | 1.41        | 1.33     |
| 21  | b     | 601 | CLA  | C4C-C3C | 2.73  | 1.49        | 1.45     |
| 21  | c     | 507 | CLA  | C1D-C2D | 2.72  | 1.50        | 1.45     |
| 21  | a     | 402 | CLA  | CHD-C1D | 2.72  | 1.43        | 1.38     |
| 21  | c     | 513 | CLA  | CHB-C4A | -2.70 | 1.30        | 1.37     |
| 21  | b     | 609 | CLA  | C4D-CHA | 2.70  | 1.47        | 1.38     |
| 21  | c     | 511 | CLA  | MG-NB   | -2.70 | 2.00        | 2.05     |
| 21  | b     | 604 | CLA  | CHD-C4C | 2.69  | 1.45        | 1.39     |
| 21  | c     | 506 | CLA  | CHD-C1D | 2.69  | 1.43        | 1.38     |
| 21  | b     | 614 | CLA  | MG-NC   | 2.69  | 2.12        | 2.06     |
| 21  | c     | 509 | CLA  | C1C-C2C | 2.69  | 1.50        | 1.44     |
| 21  | d     | 407 | CLA  | CHB-C4A | -2.68 | 1.31        | 1.37     |
| 21  | b     | 605 | CLA  | OBD-CAD | 2.68  | 1.27        | 1.22     |
| 21  | d     | 402 | CLA  | C1-C2   | 2.67  | 1.56        | 1.49     |
| 21  | c     | 512 | CLA  | C3D-C2D | 2.67  | 1.46        | 1.39     |
| 21  | c     | 510 | CLA  | MG-NB   | -2.67 | 2.00        | 2.05     |
| 21  | b     | 606 | CLA  | O2A-CGA | 2.67  | 1.41        | 1.33     |
| 21  | c     | 512 | CLA  | CHB-C4A | -2.66 | 1.31        | 1.37     |
| 21  | b     | 615 | CLA  | C1C-NC  | -2.66 | 1.33        | 1.37     |
| 21  | k     | 501 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 21  | h     | 101 | CLA  | C3D-C2D | 2.66  | 1.46        | 1.39     |
| 20  | a     | 401 | SQD  | O48-C23 | 2.64  | 1.46        | 1.33     |
| 21  | c     | 510 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 21  | b     | 607 | CLA  | O2A-CGA | 2.64  | 1.41        | 1.33     |
| 21  | d     | 406 | CLA  | CHC-C4B | 2.64  | 1.45        | 1.39     |
| 21  | b     | 603 | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 21  | b     | 605 | CLA  | C3B-C4B | 2.63  | 1.50        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | b     | 614 | CLA  | O2A-CGA | 2.63  | 1.41        | 1.33     |
| 21  | c     | 513 | CLA  | CHC-C4B | 2.63  | 1.45        | 1.39     |
| 21  | b     | 605 | CLA  | MG-NB   | 2.63  | 2.11        | 2.05     |
| 21  | h     | 101 | CLA  | C1D-C2D | 2.62  | 1.50        | 1.45     |
| 21  | b     | 614 | CLA  | CHC-C4B | 2.62  | 1.45        | 1.39     |
| 21  | h     | 101 | CLA  | C3A-C2A | -2.62 | 1.52        | 1.54     |
| 21  | b     | 603 | CLA  | C3B-C4B | 2.62  | 1.50        | 1.42     |
| 21  | b     | 613 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 21  | c     | 507 | CLA  | CHC-C4B | 2.61  | 1.45        | 1.39     |
| 21  | c     | 503 | CLA  | MG-NB   | -2.61 | 2.00        | 2.05     |
| 21  | c     | 512 | CLA  | CHC-C4B | 2.60  | 1.45        | 1.39     |
| 21  | b     | 604 | CLA  | CHC-C4B | 2.60  | 1.45        | 1.39     |
| 21  | b     | 614 | CLA  | C1D-ND  | -2.60 | 1.34        | 1.37     |
| 21  | d     | 402 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 21  | a     | 402 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 21  | d     | 406 | CLA  | CHB-C4A | -2.59 | 1.31        | 1.37     |
| 21  | d     | 406 | CLA  | CHB-C1B | 2.59  | 1.45        | 1.39     |
| 21  | a     | 407 | CLA  | OBD-CAD | 2.59  | 1.26        | 1.22     |
| 21  | b     | 607 | CLA  | C3D-C2D | 2.59  | 1.46        | 1.39     |
| 21  | b     | 612 | CLA  | C4C-C3C | 2.58  | 1.49        | 1.45     |
| 21  | a     | 407 | CLA  | C4C-C3C | 2.58  | 1.49        | 1.45     |
| 21  | c     | 505 | CLA  | MG-ND   | 2.58  | 2.10        | 2.05     |
| 21  | b     | 605 | CLA  | C1C-NC  | -2.57 | 1.33        | 1.37     |
| 21  | c     | 506 | CLA  | C1D-C2D | 2.56  | 1.50        | 1.45     |
| 21  | a     | 402 | CLA  | CHC-C4B | 2.56  | 1.45        | 1.39     |
| 21  | c     | 507 | CLA  | CHB-C4A | -2.56 | 1.31        | 1.37     |
| 21  | b     | 602 | CLA  | MG-ND   | 2.56  | 2.10        | 2.05     |
| 21  | b     | 608 | CLA  | C1B-NB  | -2.55 | 1.34        | 1.37     |
| 21  | a     | 407 | CLA  | MG-ND   | -2.55 | 2.00        | 2.05     |
| 21  | c     | 509 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 21  | c     | 508 | CLA  | OBD-CAD | 2.55  | 1.26        | 1.22     |
| 21  | k     | 501 | CLA  | CHD-C1D | 2.54  | 1.43        | 1.38     |
| 21  | b     | 610 | CLA  | C1B-NB  | -2.54 | 1.34        | 1.37     |
| 21  | a     | 403 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 28  | d     | 408 | PQ9  | C10-C5  | 2.54  | 1.47        | 1.35     |
| 21  | c     | 510 | CLA  | C1C-NC  | -2.53 | 1.33        | 1.37     |
| 21  | b     | 605 | CLA  | MG-ND   | 2.53  | 2.10        | 2.05     |
| 21  | b     | 601 | CLA  | C3D-C2D | 2.53  | 1.45        | 1.39     |
| 21  | d     | 407 | CLA  | CHC-C4B | 2.52  | 1.45        | 1.39     |
| 21  | b     | 601 | CLA  | C4D-CHA | 2.52  | 1.47        | 1.38     |
| 30  | e     | 101 | HEM  | FE-ND   | -2.52 | 1.87        | 1.94     |
| 21  | c     | 508 | CLA  | C3D-C2D | 2.52  | 1.45        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | b     | 611 | CLA  | OBD-CAD | 2.51  | 1.26        | 1.22     |
| 21  | c     | 512 | CLA  | CHB-C1B | 2.51  | 1.45        | 1.39     |
| 21  | b     | 609 | CLA  | C3D-C2D | 2.51  | 1.45        | 1.39     |
| 21  | d     | 402 | CLA  | C1B-NB  | -2.51 | 1.34        | 1.37     |
| 21  | c     | 512 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 21  | a     | 407 | CLA  | C4B-NB  | -2.50 | 1.34        | 1.37     |
| 21  | c     | 505 | CLA  | C1D-ND  | -2.48 | 1.34        | 1.37     |
| 21  | k     | 501 | CLA  | CHD-C4C | 2.48  | 1.44        | 1.39     |
| 21  | c     | 508 | CLA  | C1C-NC  | -2.48 | 1.34        | 1.37     |
| 21  | b     | 604 | CLA  | C4D-CHA | 2.48  | 1.46        | 1.38     |
| 21  | b     | 611 | CLA  | C3B-C4B | 2.48  | 1.49        | 1.42     |
| 21  | c     | 504 | CLA  | C1C-NC  | -2.48 | 1.34        | 1.37     |
| 21  | b     | 610 | CLA  | C3B-C4B | 2.47  | 1.49        | 1.42     |
| 21  | b     | 609 | CLA  | O2A-CGA | 2.47  | 1.40        | 1.33     |
| 21  | b     | 602 | CLA  | CHC-C4B | 2.46  | 1.44        | 1.39     |
| 21  | c     | 504 | CLA  | C3D-C2D | 2.46  | 1.45        | 1.39     |
| 21  | c     | 511 | CLA  | CBD-CAD | -2.46 | 1.45        | 1.56     |
| 21  | k     | 501 | CLA  | CHB-C4A | -2.46 | 1.31        | 1.37     |
| 21  | b     | 602 | CLA  | C3B-C4B | 2.45  | 1.49        | 1.42     |
| 21  | b     | 610 | CLA  | C1D-ND  | -2.45 | 1.34        | 1.37     |
| 21  | b     | 602 | CLA  | C1B-C2B | 2.45  | 1.48        | 1.43     |
| 21  | b     | 603 | CLA  | MG-NB   | 2.45  | 2.10        | 2.05     |
| 21  | c     | 510 | CLA  | C1B-C2B | 2.45  | 1.48        | 1.43     |
| 21  | c     | 503 | CLA  | MG-NC   | 2.44  | 2.12        | 2.06     |
| 21  | c     | 504 | CLA  | C4C-C3C | 2.43  | 1.49        | 1.45     |
| 21  | d     | 407 | CLA  | C1D-C2D | 2.43  | 1.50        | 1.45     |
| 21  | d     | 402 | CLA  | O2D-CGD | 2.43  | 1.39        | 1.33     |
| 21  | c     | 506 | CLA  | CHC-C4B | 2.43  | 1.44        | 1.39     |
| 21  | b     | 603 | CLA  | C1C-NC  | -2.43 | 1.34        | 1.37     |
| 21  | b     | 604 | CLA  | C4B-NB  | -2.41 | 1.34        | 1.37     |
| 21  | h     | 101 | CLA  | CHC-C4B | 2.41  | 1.44        | 1.39     |
| 21  | d     | 407 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 21  | c     | 508 | CLA  | C4D-CHA | 2.40  | 1.46        | 1.38     |
| 21  | d     | 407 | CLA  | CHB-C1B | 2.40  | 1.44        | 1.39     |
| 21  | c     | 513 | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 21  | b     | 609 | CLA  | C4B-NB  | -2.40 | 1.34        | 1.37     |
| 25  | d     | 403 | PHO  | CBD-CGD | -2.40 | 1.49        | 1.52     |
| 21  | a     | 403 | CLA  | C4D-CHA | 2.39  | 1.46        | 1.38     |
| 21  | c     | 503 | CLA  | C1B-C2B | 2.38  | 1.48        | 1.43     |
| 21  | c     | 507 | CLA  | CHB-C1B | 2.38  | 1.44        | 1.39     |
| 21  | b     | 605 | CLA  | C1C-C2C | 2.38  | 1.49        | 1.44     |
| 21  | b     | 614 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | b     | 611 | CLA  | C4D-CHA | 2.38  | 1.46        | 1.38     |
| 21  | c     | 503 | CLA  | C3D-C2D | 2.37  | 1.45        | 1.39     |
| 21  | b     | 604 | CLA  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 21  | c     | 505 | CLA  | C1B-NB  | -2.35 | 1.34        | 1.37     |
| 21  | c     | 509 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 21  | c     | 507 | CLA  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 21  | c     | 506 | CLA  | CHB-C1B | 2.34  | 1.44        | 1.39     |
| 21  | b     | 612 | CLA  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 21  | b     | 614 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 21  | d     | 407 | CLA  | C3D-C2D | 2.34  | 1.45        | 1.39     |
| 21  | b     | 611 | CLA  | CHD-C4C | 2.33  | 1.44        | 1.39     |
| 21  | b     | 613 | CLA  | C4D-CHA | 2.33  | 1.46        | 1.38     |
| 21  | b     | 604 | CLA  | MG-NB   | 2.32  | 2.10        | 2.05     |
| 30  | e     | 101 | HEM  | C1C-C2C | -2.31 | 1.40        | 1.45     |
| 21  | c     | 509 | CLA  | C1C-NC  | -2.31 | 1.34        | 1.37     |
| 21  | c     | 510 | CLA  | C3D-C4D | -2.29 | 1.39        | 1.44     |
| 21  | c     | 506 | CLA  | C3D-C2D | 2.29  | 1.45        | 1.39     |
| 21  | c     | 510 | CLA  | C4C-C3C | 2.29  | 1.48        | 1.45     |
| 21  | d     | 406 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 21  | b     | 612 | CLA  | C3D-C4D | -2.28 | 1.39        | 1.44     |
| 21  | d     | 402 | CLA  | C4D-CHA | 2.28  | 1.46        | 1.38     |
| 21  | b     | 615 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 21  | a     | 402 | CLA  | C3D-C2D | 2.27  | 1.45        | 1.39     |
| 21  | a     | 403 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 21  | k     | 501 | CLA  | CHB-C1B | 2.26  | 1.44        | 1.39     |
| 21  | h     | 101 | CLA  | CHB-C1B | 2.25  | 1.44        | 1.39     |
| 21  | k     | 501 | CLA  | C1C-C2C | 2.25  | 1.49        | 1.44     |
| 21  | a     | 403 | CLA  | CBD-CAD | -2.24 | 1.46        | 1.56     |
| 21  | c     | 504 | CLA  | C3D-C4D | -2.24 | 1.39        | 1.44     |
| 30  | e     | 101 | HEM  | C1D-ND  | -2.24 | 1.34        | 1.38     |
| 21  | b     | 613 | CLA  | C4B-NB  | -2.23 | 1.34        | 1.37     |
| 21  | c     | 508 | CLA  | C1B-C2B | 2.22  | 1.48        | 1.43     |
| 21  | k     | 501 | CLA  | CHC-C4B | 2.22  | 1.44        | 1.39     |
| 21  | d     | 406 | CLA  | C1B-C2B | 2.21  | 1.48        | 1.43     |
| 21  | b     | 613 | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 21  | a     | 403 | CLA  | CHC-C4B | 2.20  | 1.44        | 1.39     |
| 21  | c     | 513 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 21  | b     | 603 | CLA  | O2A-CGA | 2.20  | 1.39        | 1.33     |
| 21  | c     | 503 | CLA  | C3B-C2B | 2.20  | 1.48        | 1.41     |
| 21  | b     | 601 | CLA  | CBD-CAD | -2.20 | 1.46        | 1.56     |
| 21  | b     | 602 | CLA  | MG-NC   | -2.20 | 2.01        | 2.06     |
| 21  | b     | 607 | CLA  | C1B-C2B | 2.19  | 1.48        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | c     | 507 | CLA  | MG-ND   | 2.19  | 2.10        | 2.05     |
| 21  | a     | 403 | CLA  | MG-ND   | 2.19  | 2.10        | 2.05     |
| 21  | c     | 505 | CLA  | OBD-CAD | 2.18  | 1.26        | 1.22     |
| 21  | c     | 512 | CLA  | C1D-C2D | 2.18  | 1.49        | 1.45     |
| 21  | a     | 407 | CLA  | CBD-CAD | -2.17 | 1.46        | 1.56     |
| 21  | b     | 608 | CLA  | MG-ND   | 2.17  | 2.10        | 2.05     |
| 21  | c     | 507 | CLA  | C4C-C3C | 2.17  | 1.48        | 1.45     |
| 21  | c     | 509 | CLA  | C1A-CHA | 2.17  | 1.52        | 1.43     |
| 21  | d     | 402 | CLA  | C4B-NB  | -2.17 | 1.35        | 1.37     |
| 21  | c     | 510 | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 21  | b     | 611 | CLA  | C1D-ND  | -2.16 | 1.35        | 1.37     |
| 21  | b     | 613 | CLA  | OBD-CAD | 2.15  | 1.26        | 1.22     |
| 21  | c     | 506 | CLA  | C1B-C2B | 2.15  | 1.48        | 1.43     |
| 21  | b     | 612 | CLA  | C1-C2   | 2.15  | 1.55        | 1.49     |
| 21  | b     | 608 | CLA  | O2D-CED | -2.14 | 1.40        | 1.45     |
| 21  | b     | 605 | CLA  | C4C-C3C | 2.14  | 1.48        | 1.45     |
| 21  | d     | 402 | CLA  | CMD-C2D | 2.13  | 1.55        | 1.50     |
| 21  | k     | 501 | CLA  | C3D-C2D | 2.12  | 1.44        | 1.39     |
| 21  | d     | 402 | CLA  | C4C-C3C | 2.12  | 1.48        | 1.45     |
| 21  | c     | 506 | CLA  | C3B-C4B | 2.12  | 1.48        | 1.42     |
| 21  | b     | 612 | CLA  | C1B-NB  | -2.12 | 1.35        | 1.37     |
| 21  | b     | 603 | CLA  | C1B-C2B | 2.12  | 1.48        | 1.43     |
| 21  | k     | 501 | CLA  | C1D-C2D | 2.11  | 1.49        | 1.45     |
| 21  | a     | 403 | CLA  | C3D-C2D | 2.11  | 1.44        | 1.39     |
| 21  | b     | 607 | CLA  | CAA-C2A | 2.11  | 1.57        | 1.54     |
| 21  | c     | 505 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 21  | c     | 503 | CLA  | C1C-NC  | -2.10 | 1.34        | 1.37     |
| 21  | b     | 613 | CLA  | C3D-C2D | 2.10  | 1.44        | 1.39     |
| 31  | h     | 102 | HTG  | C1-S1   | -2.10 | 1.77        | 1.80     |
| 21  | c     | 505 | CLA  | C1B-C2B | 2.09  | 1.48        | 1.43     |
| 21  | a     | 403 | CLA  | C4C-C3C | 2.09  | 1.48        | 1.45     |
| 21  | h     | 101 | CLA  | C1B-NB  | -2.09 | 1.35        | 1.37     |
| 21  | b     | 605 | CLA  | C3B-C2B | 2.08  | 1.48        | 1.41     |
| 21  | c     | 507 | CLA  | C3B-C4B | 2.08  | 1.48        | 1.42     |
| 21  | c     | 511 | CLA  | C1B-C2B | 2.08  | 1.48        | 1.43     |
| 30  | e     | 101 | HEM  | C3C-C4C | -2.07 | 1.42        | 1.46     |
| 21  | h     | 101 | CLA  | C4B-NB  | -2.07 | 1.35        | 1.37     |
| 21  | b     | 610 | CLA  | MG-NC   | 2.07  | 2.11        | 2.06     |
| 21  | d     | 402 | CLA  | C3D-C2D | 2.06  | 1.44        | 1.39     |
| 21  | d     | 402 | CLA  | C3B-C4B | 2.06  | 1.48        | 1.42     |
| 21  | b     | 610 | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 21  | b     | 610 | CLA  | C1B-C2B | 2.06  | 1.48        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | b     | 609 | CLA  | C3B-C4B | 2.05  | 1.48        | 1.42     |
| 21  | c     | 506 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 21  | b     | 604 | CLA  | C1C-NC  | -2.05 | 1.34        | 1.37     |
| 21  | c     | 506 | CLA  | MG-NC   | 2.05  | 2.11        | 2.06     |
| 21  | a     | 402 | CLA  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 21  | c     | 511 | CLA  | C4C-C3C | 2.04  | 1.48        | 1.45     |
| 21  | c     | 510 | CLA  | C3B-C4B | 2.04  | 1.48        | 1.42     |
| 21  | a     | 407 | CLA  | C1B-C2B | 2.04  | 1.47        | 1.43     |
| 21  | c     | 512 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 21  | c     | 504 | CLA  | C3B-C2B | 2.03  | 1.48        | 1.41     |
| 21  | b     | 615 | CLA  | MG-NC   | 2.03  | 2.11        | 2.06     |
| 19  | m     | 102 | MGE  | O3G-C1D | 2.03  | 1.43        | 1.40     |
| 21  | b     | 603 | CLA  | CHC-C4B | 2.02  | 1.44        | 1.39     |
| 21  | c     | 508 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 21  | c     | 503 | CLA  | CHB-C4A | -2.01 | 1.32        | 1.37     |
| 21  | b     | 613 | CLA  | C1-C2   | 2.00  | 1.54        | 1.49     |

All (1296) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 21  | k     | 501 | CLA  | C1D-ND-C4D  | -18.32 | 93.46       | 106.31   |
| 21  | c     | 506 | CLA  | C1D-ND-C4D  | -17.50 | 94.03       | 106.31   |
| 21  | d     | 407 | CLA  | C1D-ND-C4D  | -16.83 | 94.50       | 106.31   |
| 21  | d     | 406 | CLA  | C1D-ND-C4D  | -16.76 | 94.55       | 106.31   |
| 21  | c     | 512 | CLA  | C1D-ND-C4D  | -15.60 | 95.36       | 106.31   |
| 21  | h     | 101 | CLA  | C1D-ND-C4D  | -15.49 | 95.45       | 106.31   |
| 20  | l     | 101 | SQD  | O9-S-C6     | -15.37 | 83.80       | 106.76   |
| 20  | a     | 401 | SQD  | O9-S-C6     | -14.80 | 84.65       | 106.76   |
| 21  | b     | 605 | CLA  | C4A-NA-C1A  | 11.67  | 112.00      | 106.68   |
| 20  | l     | 101 | SQD  | O8-S-O9     | -11.60 | 82.39       | 111.40   |
| 20  | a     | 401 | SQD  | O8-S-O9     | -11.59 | 82.41       | 111.40   |
| 21  | c     | 505 | CLA  | C4A-NA-C1A  | 10.56  | 111.50      | 106.68   |
| 21  | c     | 513 | CLA  | C2B-C1B-NB  | 10.40  | 121.11      | 110.33   |
| 21  | c     | 506 | CLA  | C4A-NA-C1A  | -10.30 | 101.98      | 106.68   |
| 21  | c     | 503 | CLA  | C4A-NA-C1A  | 9.97   | 111.23      | 106.68   |
| 21  | c     | 507 | CLA  | C4A-NA-C1A  | -9.78  | 102.22      | 106.68   |
| 21  | b     | 603 | CLA  | C4A-NA-C1A  | 9.73   | 111.12      | 106.68   |
| 20  | a     | 401 | SQD  | O9-S-O7     | -9.65  | 82.43       | 113.82   |
| 20  | l     | 101 | SQD  | O9-S-O7     | -9.54  | 82.80       | 113.82   |
| 25  | d     | 403 | PHO  | C2D-C1D-ND  | 9.51   | 116.31      | 109.43   |
| 25  | d     | 403 | PHO  | O2D-CGD-CBD | 9.36   | 121.23      | 110.95   |
| 21  | d     | 406 | CLA  | C2C-C1C-NC  | 9.30   | 119.75      | 109.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | c     | 512 | CLA  | C4A-NA-C1A  | -9.14 | 102.51      | 106.68   |
| 21  | h     | 101 | CLA  | C4D-CHA-C1A | -9.14 | 110.35      | 121.24   |
| 21  | c     | 506 | CLA  | C2B-C1B-NB  | 9.11  | 119.77      | 110.33   |
| 21  | c     | 513 | CLA  | C1D-ND-C4D  | -9.10 | 99.93       | 106.31   |
| 21  | h     | 101 | CLA  | C2B-C1B-NB  | 8.98  | 119.64      | 110.33   |
| 21  | c     | 506 | CLA  | C2C-C1C-NC  | 8.98  | 119.41      | 109.98   |
| 25  | d     | 401 | PHO  | C3B-C4B-NB  | 8.93  | 113.29      | 107.46   |
| 25  | d     | 401 | PHO  | C2D-C1D-ND  | 8.84  | 115.82      | 109.43   |
| 21  | c     | 507 | CLA  | C2B-C1B-NB  | 8.80  | 119.45      | 110.33   |
| 21  | d     | 407 | CLA  | C2C-C1C-NC  | 8.79  | 119.21      | 109.98   |
| 21  | k     | 501 | CLA  | C2B-C1B-NB  | 8.76  | 119.41      | 110.33   |
| 21  | k     | 501 | CLA  | CMD-C2D-C1D | 8.74  | 140.12      | 124.73   |
| 21  | b     | 609 | CLA  | C4A-NA-C1A  | 8.73  | 110.66      | 106.68   |
| 21  | c     | 513 | CLA  | C1D-CHD-C4C | -8.71 | 107.51      | 126.02   |
| 22  | c     | 515 | BCR  | C11-C10-C9  | -8.60 | 115.22      | 127.28   |
| 21  | c     | 507 | CLA  | C1D-ND-C4D  | -8.59 | 100.28      | 106.31   |
| 25  | d     | 403 | PHO  | C3B-C4B-NB  | 8.58  | 113.06      | 107.46   |
| 21  | h     | 101 | CLA  | CMD-C2D-C1D | 8.53  | 139.75      | 124.73   |
| 21  | c     | 506 | CLA  | CMD-C2D-C1D | 8.52  | 139.74      | 124.73   |
| 21  | c     | 512 | CLA  | C2C-C1C-NC  | 8.50  | 118.91      | 109.98   |
| 21  | b     | 613 | CLA  | C4A-NA-C1A  | 8.45  | 110.54      | 106.68   |
| 21  | c     | 507 | CLA  | C2C-C1C-NC  | 8.45  | 118.86      | 109.98   |
| 21  | b     | 611 | CLA  | CAC-C3C-C4C | 8.39  | 135.71      | 124.79   |
| 21  | d     | 406 | CLA  | CHD-C4C-C3C | -8.37 | 112.56      | 124.77   |
| 21  | d     | 407 | CLA  | CMD-C2D-C1D | 8.28  | 139.31      | 124.73   |
| 21  | k     | 501 | CLA  | C4D-CHA-C1A | -8.24 | 111.41      | 121.24   |
| 21  | d     | 406 | CLA  | C2B-C1B-NB  | 8.21  | 118.84      | 110.33   |
| 25  | d     | 401 | PHO  | O2D-CGD-CBD | 8.19  | 119.95      | 110.95   |
| 21  | k     | 501 | CLA  | C3B-C4B-NB  | 8.18  | 117.83      | 110.53   |
| 21  | c     | 513 | CLA  | CMD-C2D-C1D | 8.14  | 139.06      | 124.73   |
| 21  | d     | 407 | CLA  | C2B-C1B-NB  | 8.05  | 118.68      | 110.33   |
| 21  | c     | 509 | CLA  | C4A-NA-C1A  | 8.05  | 110.35      | 106.68   |
| 21  | c     | 507 | CLA  | CMD-C2D-C1D | 8.03  | 138.88      | 124.73   |
| 22  | c     | 515 | BCR  | C16-C17-C18 | -8.03 | 116.01      | 127.28   |
| 21  | k     | 501 | CLA  | C2C-C1C-NC  | 8.02  | 118.41      | 109.98   |
| 21  | b     | 610 | CLA  | C4A-NA-C1A  | 7.95  | 110.31      | 106.68   |
| 21  | c     | 504 | CLA  | C1D-ND-C4D  | -7.86 | 100.80      | 106.31   |
| 20  | a     | 401 | SQD  | O7-S-C6     | 7.86  | 118.49      | 106.76   |
| 20  | l     | 101 | SQD  | O7-S-C6     | 7.79  | 118.39      | 106.76   |
| 21  | b     | 611 | CLA  | C4A-NA-C1A  | 7.79  | 110.23      | 106.68   |
| 21  | h     | 101 | CLA  | C2C-C1C-NC  | 7.75  | 118.13      | 109.98   |
| 21  | d     | 406 | CLA  | C3C-C4C-NC  | 7.73  | 120.34      | 110.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | k     | 501 | CLA  | C3D-C4D-ND  | 7.73  | 122.55      | 109.99   |
| 21  | d     | 406 | CLA  | CMD-C2D-C1D | 7.67  | 138.24      | 124.73   |
| 21  | c     | 513 | CLA  | C4A-NA-C1A  | -7.64 | 103.19      | 106.68   |
| 21  | c     | 512 | CLA  | C2B-C1B-NB  | 7.56  | 118.17      | 110.33   |
| 21  | c     | 506 | CLA  | C3D-C4D-ND  | 7.49  | 122.17      | 109.99   |
| 21  | k     | 501 | CLA  | C2D-C1D-ND  | 7.45  | 117.50      | 110.13   |
| 21  | c     | 512 | CLA  | C4B-CHC-C1C | -7.45 | 108.72      | 126.25   |
| 21  | c     | 512 | CLA  | C4D-CHA-C1A | -7.40 | 112.42      | 121.24   |
| 21  | d     | 407 | CLA  | C3D-C4D-ND  | 7.38  | 121.99      | 109.99   |
| 21  | c     | 513 | CLA  | C3B-C2B-C1B | -7.35 | 98.51       | 107.17   |
| 21  | c     | 506 | CLA  | C4D-CHA-C1A | -7.33 | 112.50      | 121.24   |
| 21  | c     | 513 | CLA  | C2C-C1C-NC  | 7.29  | 117.64      | 109.98   |
| 21  | c     | 510 | CLA  | C4A-NA-C1A  | 7.27  | 109.99      | 106.68   |
| 21  | c     | 508 | CLA  | CHD-C4C-C3C | -7.21 | 114.26      | 124.77   |
| 25  | d     | 403 | PHO  | C4D-ND-C1D  | -7.19 | 100.26      | 108.87   |
| 25  | d     | 403 | PHO  | C2B-C1B-NB  | 7.18  | 114.62      | 109.43   |
| 21  | h     | 101 | CLA  | C3D-C4D-ND  | 7.15  | 121.61      | 109.99   |
| 21  | c     | 512 | CLA  | CMD-C2D-C1D | 7.14  | 137.29      | 124.73   |
| 21  | b     | 613 | CLA  | C4D-CHA-C1A | -7.02 | 112.87      | 121.24   |
| 21  | b     | 614 | CLA  | C4A-NA-C1A  | 7.00  | 109.87      | 106.68   |
| 21  | c     | 504 | CLA  | C2D-C1D-ND  | 7.00  | 117.05      | 110.13   |
| 21  | k     | 501 | CLA  | C3C-C4C-NC  | 6.98  | 119.38      | 110.43   |
| 21  | a     | 403 | CLA  | C2C-C1C-NC  | 6.98  | 117.31      | 109.98   |
| 21  | d     | 407 | CLA  | C3B-C4B-NB  | 6.98  | 116.76      | 110.53   |
| 21  | b     | 604 | CLA  | CAC-C3C-C4C | 6.98  | 133.87      | 124.79   |
| 21  | a     | 402 | CLA  | CAC-C3C-C4C | 6.94  | 133.82      | 124.79   |
| 21  | c     | 512 | CLA  | C3D-C4D-ND  | 6.93  | 121.26      | 109.99   |
| 21  | b     | 613 | CLA  | C2D-C1D-ND  | 6.89  | 116.94      | 110.13   |
| 21  | b     | 615 | CLA  | CHD-C4C-C3C | -6.84 | 114.81      | 124.77   |
| 21  | b     | 613 | CLA  | C1D-ND-C4D  | -6.82 | 101.53      | 106.31   |
| 21  | c     | 506 | CLA  | C3C-C4C-NC  | 6.77  | 119.10      | 110.43   |
| 21  | c     | 513 | CLA  | C4D-CHA-C1A | -6.75 | 113.19      | 121.24   |
| 21  | c     | 512 | CLA  | C3B-C4B-NB  | 6.72  | 116.53      | 110.53   |
| 21  | c     | 506 | CLA  | C3B-C4B-NB  | 6.69  | 116.50      | 110.53   |
| 21  | h     | 101 | CLA  | C4A-NA-C1A  | -6.69 | 103.63      | 106.68   |
| 21  | h     | 101 | CLA  | C3B-C2B-C1B | -6.67 | 99.31       | 107.17   |
| 21  | c     | 504 | CLA  | C4A-NA-C1A  | 6.66  | 109.72      | 106.68   |
| 21  | c     | 513 | CLA  | CHD-C1D-ND  | -6.64 | 115.46      | 124.80   |
| 21  | c     | 506 | CLA  | C2D-C1D-ND  | 6.62  | 116.68      | 110.13   |
| 21  | c     | 507 | CLA  | C4D-CHA-C1A | -6.60 | 113.37      | 121.24   |
| 21  | b     | 609 | CLA  | C2D-C1D-ND  | 6.56  | 116.62      | 110.13   |
| 21  | c     | 508 | CLA  | C4D-CHA-C1A | -6.54 | 113.44      | 121.24   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20  | a     | 401 | SQD  | O8-S-C6     | 6.51  | 118.55      | 105.97   |
| 22  | c     | 515 | BCR  | C7-C8-C9    | -6.50 | 116.62      | 126.23   |
| 21  | d     | 406 | CLA  | C2D-C1D-ND  | 6.49  | 116.55      | 110.13   |
| 21  | h     | 101 | CLA  | CHD-C1D-ND  | -6.47 | 115.70      | 124.80   |
| 21  | a     | 407 | CLA  | C2C-C1C-NC  | 6.46  | 116.76      | 109.98   |
| 20  | l     | 101 | SQD  | O8-S-C6     | 6.44  | 118.40      | 105.97   |
| 21  | b     | 612 | CLA  | C4A-NA-C1A  | 6.43  | 109.61      | 106.68   |
| 21  | d     | 407 | CLA  | C2D-C1D-ND  | 6.43  | 116.49      | 110.13   |
| 21  | b     | 604 | CLA  | C2C-C1C-NC  | 6.40  | 116.70      | 109.98   |
| 21  | b     | 613 | CLA  | O2D-CGD-CBD | 6.38  | 122.39      | 111.23   |
| 21  | c     | 509 | CLA  | O2D-CGD-CBD | 6.37  | 122.37      | 111.23   |
| 21  | c     | 507 | CLA  | C3C-C4C-NC  | 6.35  | 118.57      | 110.43   |
| 21  | b     | 602 | CLA  | C2C-C1C-NC  | 6.35  | 116.65      | 109.98   |
| 21  | b     | 615 | CLA  | O2D-CGD-CBD | 6.31  | 122.27      | 111.23   |
| 21  | c     | 507 | CLA  | C3B-C2B-C1B | -6.29 | 99.76       | 107.17   |
| 22  | h     | 103 | BCR  | C7-C8-C9    | -6.28 | 116.95      | 126.23   |
| 21  | d     | 406 | CLA  | C3B-C4B-NB  | 6.24  | 116.10      | 110.53   |
| 21  | d     | 406 | CLA  | O2D-CGD-CBD | 6.24  | 122.14      | 111.23   |
| 21  | d     | 406 | CLA  | C3D-C4D-ND  | 6.22  | 120.10      | 109.99   |
| 25  | d     | 403 | PHO  | C3D-C4D-ND  | 6.21  | 115.67      | 107.71   |
| 21  | c     | 503 | CLA  | C1D-ND-C4D  | -6.21 | 101.96      | 106.31   |
| 21  | d     | 407 | CLA  | C3C-C4C-NC  | 6.16  | 118.33      | 110.43   |
| 21  | d     | 407 | CLA  | C4D-CHA-C1A | -6.14 | 113.92      | 121.24   |
| 21  | a     | 407 | CLA  | CAC-C3C-C4C | 6.12  | 132.75      | 124.79   |
| 22  | a     | 404 | BCR  | C11-C10-C9  | -6.09 | 118.74      | 127.28   |
| 21  | k     | 501 | CLA  | CHD-C4C-C3C | -6.08 | 115.90      | 124.77   |
| 21  | c     | 507 | CLA  | C3B-C4B-NB  | 6.07  | 115.95      | 110.53   |
| 21  | d     | 406 | CLA  | C4D-CHA-C1A | -6.02 | 114.06      | 121.24   |
| 21  | c     | 506 | CLA  | C3B-C2B-C1B | -6.01 | 100.08      | 107.17   |
| 21  | b     | 611 | CLA  | CHD-C4C-C3C | -6.01 | 116.00      | 124.77   |
| 21  | k     | 501 | CLA  | C3B-C2B-C1B | -6.01 | 100.08      | 107.17   |
| 21  | a     | 403 | CLA  | CHD-C4C-C3C | -5.99 | 116.04      | 124.77   |
| 21  | h     | 101 | CLA  | C3C-C4C-NC  | 5.98  | 118.09      | 110.43   |
| 21  | c     | 509 | CLA  | CHD-C4C-C3C | -5.96 | 116.08      | 124.77   |
| 21  | c     | 512 | CLA  | C2D-C1D-ND  | 5.96  | 116.02      | 110.13   |
| 21  | d     | 407 | CLA  | C4A-NA-C1A  | -5.95 | 103.96      | 106.68   |
| 22  | b     | 616 | BCR  | C28-C27-C26 | -5.95 | 103.45      | 114.06   |
| 22  | a     | 404 | BCR  | C7-C8-C9    | -5.95 | 117.44      | 126.23   |
| 21  | k     | 501 | CLA  | C4A-NA-C1A  | -5.89 | 103.99      | 106.68   |
| 21  | a     | 402 | CLA  | C2D-C1D-ND  | 5.88  | 115.95      | 110.13   |
| 21  | d     | 402 | CLA  | CHD-C4C-C3C | -5.85 | 116.24      | 124.77   |
| 21  | c     | 506 | CLA  | O2D-CGD-CBD | 5.84  | 121.44      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | z     | 101 | BCR  | C16-C17-C18 | -5.80 | 119.14      | 127.28   |
| 21  | b     | 603 | CLA  | C2C-C1C-NC  | 5.78  | 116.06      | 109.98   |
| 21  | c     | 513 | CLA  | CMA-C3A-C4A | -5.77 | 96.27       | 111.77   |
| 21  | a     | 403 | CLA  | CAC-C3C-C4C | 5.77  | 132.29      | 124.79   |
| 21  | c     | 503 | CLA  | C2D-C1D-ND  | 5.76  | 115.82      | 110.13   |
| 25  | d     | 401 | PHO  | C2B-C1B-NB  | 5.75  | 113.58      | 109.43   |
| 21  | c     | 512 | CLA  | C3C-C4C-NC  | 5.70  | 117.73      | 110.43   |
| 21  | b     | 602 | CLA  | CHD-C4C-C3C | -5.64 | 116.55      | 124.77   |
| 21  | c     | 510 | CLA  | C4D-CHA-C1A | -5.64 | 114.52      | 121.24   |
| 21  | d     | 406 | CLA  | C1C-C2C-C3C | -5.63 | 101.05      | 106.98   |
| 21  | c     | 504 | CLA  | C2B-C1B-NB  | 5.63  | 116.17      | 110.33   |
| 21  | b     | 612 | CLA  | C2C-C1C-NC  | 5.62  | 115.88      | 109.98   |
| 21  | h     | 101 | CLA  | CHB-C1B-NB  | -5.60 | 115.65      | 124.05   |
| 21  | c     | 506 | CLA  | CHD-C4C-C3C | -5.57 | 116.66      | 124.77   |
| 21  | d     | 407 | CLA  | C3B-C2B-C1B | -5.54 | 100.64      | 107.17   |
| 21  | c     | 513 | CLA  | C3C-C4C-NC  | 5.54  | 117.53      | 110.43   |
| 21  | c     | 512 | CLA  | C3B-C2B-C1B | -5.53 | 100.65      | 107.17   |
| 21  | b     | 609 | CLA  | C2B-C1B-NB  | 5.53  | 116.06      | 110.33   |
| 21  | h     | 101 | CLA  | C2D-C1D-ND  | 5.51  | 115.58      | 110.13   |
| 21  | b     | 611 | CLA  | C4D-CHA-C1A | -5.51 | 114.67      | 121.24   |
| 21  | c     | 504 | CLA  | CHD-C4C-C3C | -5.50 | 116.75      | 124.77   |
| 21  | c     | 512 | CLA  | C1C-C2C-C3C | -5.46 | 101.24      | 106.98   |
| 21  | c     | 510 | CLA  | C2B-C1B-NB  | 5.46  | 115.99      | 110.33   |
| 22  | c     | 514 | BCR  | C7-C8-C9    | -5.45 | 118.17      | 126.23   |
| 21  | b     | 612 | CLA  | CAC-C3C-C4C | 5.45  | 131.88      | 124.79   |
| 21  | b     | 615 | CLA  | C4A-NA-C1A  | 5.44  | 109.16      | 106.68   |
| 21  | c     | 506 | CLA  | C3D-C2D-C1D | -5.43 | 98.42       | 105.83   |
| 21  | c     | 504 | CLA  | O2D-CGD-CBD | 5.41  | 120.69      | 111.23   |
| 22  | c     | 514 | BCR  | C28-C27-C26 | -5.38 | 104.46      | 114.06   |
| 21  | k     | 501 | CLA  | C3D-C2D-C1D | -5.37 | 98.50       | 105.83   |
| 21  | c     | 508 | CLA  | C2D-C1D-ND  | 5.36  | 115.44      | 110.13   |
| 21  | b     | 609 | CLA  | C1D-ND-C4D  | -5.34 | 102.56      | 106.31   |
| 21  | b     | 612 | CLA  | C1-C2-C3    | -5.31 | 117.50      | 126.20   |
| 21  | h     | 101 | CLA  | C3B-C4B-NB  | 5.31  | 115.27      | 110.53   |
| 21  | b     | 602 | CLA  | C2B-C1B-NB  | 5.30  | 115.82      | 110.33   |
| 31  | h     | 102 | HTG  | C1'-S1-C1   | 5.30  | 111.89      | 100.45   |
| 21  | c     | 503 | CLA  | C1C-C2C-C3C | -5.29 | 101.41      | 106.98   |
| 21  | d     | 406 | CLA  | C3D-C2D-C1D | -5.29 | 98.62       | 105.83   |
| 21  | b     | 608 | CLA  | CAC-C3C-C4C | 5.26  | 131.64      | 124.79   |
| 21  | b     | 614 | CLA  | C2B-C1B-NB  | 5.26  | 115.78      | 110.33   |
| 21  | h     | 101 | CLA  | C1D-CHD-C4C | -5.26 | 114.85      | 126.02   |
| 22  | d     | 409 | BCR  | C24-C23-C22 | -5.25 | 118.46      | 126.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | d     | 402 | CLA  | C2C-C1C-NC  | 5.24  | 115.48      | 109.98   |
| 21  | c     | 509 | CLA  | O2D-CGD-O1D | -5.23 | 113.66      | 123.85   |
| 21  | d     | 406 | CLA  | C3B-C2B-C1B | -5.21 | 101.03      | 107.17   |
| 21  | a     | 402 | CLA  | C3B-C2B-C1B | -5.21 | 101.03      | 107.17   |
| 21  | d     | 407 | CLA  | C3D-C2D-C1D | -5.20 | 98.74       | 105.83   |
| 21  | k     | 501 | CLA  | CHD-C1D-ND  | -5.19 | 117.50      | 124.80   |
| 21  | b     | 614 | CLA  | C1C-C2C-C3C | -5.17 | 101.54      | 106.98   |
| 22  | a     | 404 | BCR  | C20-C21-C22 | -5.16 | 120.04      | 127.28   |
| 21  | c     | 504 | CLA  | C3B-C2B-C1B | -5.15 | 101.10      | 107.17   |
| 21  | c     | 511 | CLA  | C2D-C1D-ND  | 5.15  | 115.22      | 110.13   |
| 21  | b     | 602 | CLA  | C1C-C2C-C3C | -5.14 | 101.57      | 106.98   |
| 21  | c     | 508 | CLA  | CHD-C4C-NC  | 5.14  | 132.20      | 124.23   |
| 21  | c     | 508 | CLA  | C2B-C1B-NB  | 5.14  | 115.65      | 110.33   |
| 21  | b     | 608 | CLA  | C2C-C1C-NC  | 5.13  | 115.38      | 109.98   |
| 21  | b     | 614 | CLA  | C2C-C1C-NC  | 5.10  | 115.34      | 109.98   |
| 22  | a     | 404 | BCR  | C24-C23-C22 | -5.09 | 118.70      | 126.23   |
| 21  | c     | 506 | CLA  | CHD-C1D-ND  | -5.07 | 117.67      | 124.80   |
| 21  | d     | 407 | CLA  | CHD-C4C-C3C | -5.05 | 117.40      | 124.77   |
| 21  | d     | 407 | CLA  | C1C-C2C-C3C | -5.04 | 101.68      | 106.98   |
| 21  | b     | 602 | CLA  | O2D-CGD-O1D | -5.04 | 114.04      | 123.85   |
| 21  | d     | 407 | CLA  | CHD-C1D-ND  | -5.04 | 117.71      | 124.80   |
| 21  | c     | 508 | CLA  | C3B-C2B-C1B | -5.03 | 101.24      | 107.17   |
| 22  | b     | 618 | BCR  | C7-C8-C9    | -5.01 | 118.82      | 126.23   |
| 21  | b     | 607 | CLA  | O2D-CGD-CBD | 5.00  | 119.97      | 111.23   |
| 21  | b     | 603 | CLA  | C1C-C2C-C3C | -4.97 | 101.75      | 106.98   |
| 21  | b     | 607 | CLA  | C2C-C1C-NC  | 4.97  | 115.20      | 109.98   |
| 21  | b     | 611 | CLA  | C3C-C4C-NC  | 4.96  | 116.79      | 110.43   |
| 21  | h     | 101 | CLA  | C3D-C2D-C1D | -4.95 | 99.07       | 105.83   |
| 21  | c     | 503 | CLA  | C4D-CHA-C1A | -4.95 | 115.34      | 121.24   |
| 21  | b     | 612 | CLA  | C2D-C1D-ND  | 4.95  | 115.02      | 110.13   |
| 21  | d     | 402 | CLA  | C2D-C1D-ND  | 4.95  | 115.02      | 110.13   |
| 21  | a     | 402 | CLA  | C3D-C2D-C1D | -4.95 | 99.08       | 105.83   |
| 21  | c     | 509 | CLA  | C2C-C1C-NC  | 4.95  | 115.18      | 109.98   |
| 19  | d     | 410 | MGE  | O2G-C1B-C2B | 4.94  | 122.18      | 111.48   |
| 21  | b     | 615 | CLA  | C3B-C2B-C1B | -4.94 | 101.34      | 107.17   |
| 21  | c     | 506 | CLA  | C1C-C2C-C3C | -4.94 | 101.79      | 106.98   |
| 21  | b     | 602 | CLA  | CHD-C1D-ND  | -4.92 | 117.88      | 124.80   |
| 21  | c     | 508 | CLA  | CMD-C2D-C1D | 4.92  | 133.39      | 124.73   |
| 21  | d     | 406 | CLA  | C1D-CHD-C4C | -4.91 | 115.58      | 126.02   |
| 21  | a     | 407 | CLA  | C1C-C2C-C3C | -4.89 | 101.83      | 106.98   |
| 21  | c     | 503 | CLA  | C2C-C1C-NC  | 4.89  | 115.12      | 109.98   |
| 21  | c     | 512 | CLA  | O2D-CGD-CBD | 4.88  | 119.77      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | b     | 601 | CLA  | C2D-C1D-ND  | 4.88  | 114.96      | 110.13   |
| 21  | b     | 613 | CLA  | C1-C2-C3    | -4.87 | 118.21      | 126.20   |
| 21  | c     | 503 | CLA  | C3B-C2B-C1B | -4.87 | 101.43      | 107.17   |
| 21  | b     | 602 | CLA  | C4-C3-C5    | 4.87  | 123.67      | 115.23   |
| 21  | b     | 614 | CLA  | C3B-C2B-C1B | -4.87 | 101.43      | 107.17   |
| 21  | b     | 606 | CLA  | CHD-C4C-C3C | -4.86 | 117.69      | 124.77   |
| 21  | b     | 612 | CLA  | CHD-C4C-C3C | -4.85 | 117.70      | 124.77   |
| 21  | b     | 607 | CLA  | C1C-C2C-C3C | -4.85 | 101.88      | 106.98   |
| 21  | b     | 613 | CLA  | O2D-CGD-O1D | -4.85 | 114.41      | 123.85   |
| 21  | b     | 602 | CLA  | C2D-C1D-ND  | 4.84  | 114.92      | 110.13   |
| 21  | c     | 506 | CLA  | C1D-CHD-C4C | -4.84 | 115.73      | 126.02   |
| 21  | c     | 508 | CLA  | C1D-ND-C4D  | -4.83 | 102.92      | 106.31   |
| 25  | d     | 403 | PHO  | O2D-CGD-O1D | -4.83 | 114.45      | 123.85   |
| 21  | b     | 604 | CLA  | CHD-C4C-C3C | -4.83 | 117.74      | 124.77   |
| 21  | c     | 512 | CLA  | C3D-C2D-C1D | -4.82 | 99.25       | 105.83   |
| 21  | b     | 609 | CLA  | C2C-C1C-NC  | 4.82  | 115.05      | 109.98   |
| 21  | d     | 407 | CLA  | O2D-CGD-CBD | 4.81  | 119.64      | 111.23   |
| 21  | b     | 611 | CLA  | C4C-C3C-C2C | -4.80 | 99.91       | 106.89   |
| 22  | a     | 404 | BCR  | C11-C12-C13 | -4.79 | 113.22      | 126.36   |
| 21  | b     | 601 | CLA  | O2D-CGD-CBD | 4.79  | 119.60      | 111.23   |
| 21  | b     | 615 | CLA  | C2B-C1B-NB  | 4.79  | 115.29      | 110.33   |
| 22  | c     | 515 | BCR  | C33-C5-C6   | -4.79 | 119.26      | 124.48   |
| 25  | d     | 401 | PHO  | O2D-CGD-O1D | -4.79 | 114.53      | 123.85   |
| 21  | k     | 501 | CLA  | O2D-CGD-CBD | 4.78  | 119.59      | 111.23   |
| 21  | c     | 503 | CLA  | O2D-CGD-CBD | 4.77  | 119.58      | 111.23   |
| 21  | c     | 510 | CLA  | CHD-C4C-C3C | -4.77 | 117.82      | 124.77   |
| 21  | c     | 507 | CLA  | C1D-CHD-C4C | -4.76 | 115.90      | 126.02   |
| 21  | b     | 603 | CLA  | CAC-C3C-C4C | 4.76  | 130.98      | 124.79   |
| 21  | b     | 604 | CLA  | C4-C3-C5    | 4.76  | 123.49      | 115.23   |
| 21  | c     | 503 | CLA  | C2B-C1B-NB  | 4.76  | 115.26      | 110.33   |
| 21  | c     | 503 | CLA  | O2D-CGD-O1D | -4.74 | 114.61      | 123.85   |
| 21  | b     | 604 | CLA  | C2D-C1D-ND  | 4.72  | 114.80      | 110.13   |
| 21  | b     | 612 | CLA  | C3D-C2D-C1D | -4.71 | 99.40       | 105.83   |
| 21  | b     | 615 | CLA  | C2D-C1D-ND  | 4.71  | 114.79      | 110.13   |
| 21  | a     | 407 | CLA  | C3D-C2D-C1D | -4.70 | 99.41       | 105.83   |
| 30  | e     | 101 | HEM  | CHC-C4B-NB  | 4.70  | 129.48      | 124.42   |
| 21  | k     | 501 | CLA  | C1D-CHD-C4C | -4.68 | 116.07      | 126.02   |
| 21  | c     | 509 | CLA  | C3B-C2B-C1B | -4.68 | 101.66      | 107.17   |
| 21  | c     | 510 | CLA  | C2C-C1C-NC  | 4.66  | 114.88      | 109.98   |
| 21  | b     | 602 | CLA  | C3B-C2B-C1B | -4.66 | 101.68      | 107.17   |
| 21  | b     | 614 | CLA  | CHC-C4B-NB  | 4.65  | 131.03      | 124.05   |
| 21  | c     | 513 | CLA  | O2D-CGD-CBD | 4.65  | 119.36      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | b     | 608 | CLA  | O2D-CGD-CBD | 4.65  | 119.36      | 111.23   |
| 21  | b     | 603 | CLA  | C2D-C1D-ND  | 4.64  | 114.72      | 110.13   |
| 22  | b     | 618 | BCR  | C27-C26-C25 | -4.64 | 116.44      | 122.70   |
| 21  | b     | 609 | CLA  | C1C-C2C-C3C | -4.64 | 102.10      | 106.98   |
| 21  | c     | 507 | CLA  | CHD-C4C-C3C | -4.63 | 118.02      | 124.77   |
| 21  | b     | 601 | CLA  | C3B-C2B-C1B | -4.63 | 101.71      | 107.17   |
| 22  | b     | 618 | BCR  | C24-C23-C22 | -4.62 | 119.40      | 126.23   |
| 21  | b     | 606 | CLA  | CAC-C3C-C4C | 4.62  | 130.80      | 124.79   |
| 21  | c     | 507 | CLA  | O2D-CGD-CBD | 4.62  | 119.30      | 111.23   |
| 21  | b     | 605 | CLA  | CHD-C4C-C3C | -4.61 | 118.05      | 124.77   |
| 21  | b     | 605 | CLA  | C2D-C1D-ND  | 4.61  | 114.69      | 110.13   |
| 21  | c     | 505 | CLA  | C3D-C2D-C1D | -4.60 | 99.55       | 105.83   |
| 21  | c     | 511 | CLA  | C4A-NA-C1A  | 4.60  | 108.78      | 106.68   |
| 21  | b     | 611 | CLA  | C2C-C1C-NC  | 4.60  | 114.81      | 109.98   |
| 21  | a     | 402 | CLA  | C2C-C1C-NC  | 4.59  | 114.81      | 109.98   |
| 21  | b     | 611 | CLA  | C2D-C1D-ND  | 4.59  | 114.67      | 110.13   |
| 21  | c     | 513 | CLA  | CHB-C1B-NB  | -4.59 | 117.17      | 124.05   |
| 21  | b     | 607 | CLA  | CHD-C4C-C3C | -4.59 | 118.08      | 124.77   |
| 21  | a     | 403 | CLA  | C2D-C1D-ND  | 4.58  | 114.66      | 110.13   |
| 21  | b     | 603 | CLA  | CHD-C4C-C3C | -4.58 | 118.09      | 124.77   |
| 21  | a     | 407 | CLA  | CHD-C4C-C3C | -4.58 | 118.09      | 124.77   |
| 21  | b     | 604 | CLA  | O2D-CGD-CBD | 4.58  | 119.23      | 111.23   |
| 25  | d     | 401 | PHO  | C4D-ND-C1D  | -4.56 | 103.41      | 108.87   |
| 21  | b     | 614 | CLA  | C1D-CHD-C4C | -4.55 | 116.35      | 126.02   |
| 21  | d     | 402 | CLA  | C1D-CHD-C4C | -4.54 | 116.36      | 126.02   |
| 21  | a     | 403 | CLA  | CHC-C4B-NB  | 4.54  | 130.86      | 124.05   |
| 21  | b     | 609 | CLA  | C3B-C2B-C1B | -4.54 | 101.82      | 107.17   |
| 21  | c     | 510 | CLA  | CHC-C4B-NB  | 4.54  | 130.86      | 124.05   |
| 21  | b     | 610 | CLA  | C1C-C2C-C3C | -4.53 | 102.21      | 106.98   |
| 24  | h     | 104 | DGD  | O2G-C1B-C2B | 4.53  | 121.27      | 111.48   |
| 21  | c     | 512 | CLA  | CHD-C4C-C3C | -4.52 | 118.19      | 124.77   |
| 21  | c     | 510 | CLA  | C3B-C2B-C1B | -4.51 | 101.85      | 107.17   |
| 22  | z     | 101 | BCR  | C7-C8-C9    | -4.50 | 119.58      | 126.23   |
| 21  | c     | 504 | CLA  | C1D-CHD-C4C | -4.49 | 116.47      | 126.02   |
| 22  | z     | 101 | BCR  | C24-C23-C22 | 4.49  | 132.88      | 126.23   |
| 21  | c     | 513 | CLA  | C3B-C4B-NB  | 4.48  | 114.53      | 110.53   |
| 21  | b     | 610 | CLA  | C2C-C1C-NC  | 4.46  | 114.67      | 109.98   |
| 21  | b     | 606 | CLA  | C3D-C2D-C1D | -4.46 | 99.74       | 105.83   |
| 22  | c     | 514 | BCR  | C15-C14-C13 | -4.46 | 121.03      | 127.28   |
| 21  | a     | 402 | CLA  | CHD-C4C-C3C | -4.45 | 118.28      | 124.77   |
| 20  | a     | 401 | SQD  | O47-C7-C8   | 4.45  | 119.03      | 111.09   |
| 21  | c     | 503 | CLA  | CHD-C4C-C3C | -4.45 | 118.28      | 124.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | d     | 402 | CLA  | C3B-C2B-C1B | -4.45 | 101.93      | 107.17   |
| 21  | c     | 503 | CLA  | CMD-C2D-C1D | 4.44  | 132.54      | 124.73   |
| 21  | c     | 507 | CLA  | C3D-C2D-C1D | -4.44 | 99.77       | 105.83   |
| 21  | k     | 501 | CLA  | C1C-C2C-C3C | -4.44 | 102.31      | 106.98   |
| 22  | d     | 409 | BCR  | C16-C17-C18 | -4.43 | 121.06      | 127.28   |
| 21  | h     | 101 | CLA  | C1C-C2C-C3C | -4.43 | 102.32      | 106.98   |
| 21  | a     | 403 | CLA  | C4-C3-C5    | 4.42  | 121.33      | 116.13   |
| 21  | b     | 603 | CLA  | C3D-C2D-C1D | -4.41 | 99.81       | 105.83   |
| 21  | c     | 513 | CLA  | C3D-C4D-ND  | 4.40  | 117.15      | 109.99   |
| 21  | k     | 501 | CLA  | C4B-CHC-C1C | -4.40 | 115.89      | 126.25   |
| 21  | b     | 606 | CLA  | C4A-NA-C1A  | 4.40  | 108.69      | 106.68   |
| 22  | c     | 514 | BCR  | C24-C23-C22 | -4.39 | 119.73      | 126.23   |
| 21  | b     | 601 | CLA  | O2D-CGD-O1D | -4.39 | 115.30      | 123.85   |
| 21  | c     | 511 | CLA  | C4D-CHA-C1A | -4.38 | 116.02      | 121.24   |
| 21  | c     | 507 | CLA  | C1C-C2C-C3C | -4.37 | 102.38      | 106.98   |
| 22  | c     | 515 | BCR  | C30-C25-C26 | -4.37 | 116.67      | 122.64   |
| 21  | b     | 604 | CLA  | CMD-C2D-C1D | 4.36  | 132.41      | 124.73   |
| 22  | z     | 101 | BCR  | C16-C15-C14 | -4.36 | 114.61      | 123.52   |
| 30  | e     | 101 | HEM  | CHD-C1D-ND  | 4.35  | 129.10      | 124.42   |
| 21  | c     | 511 | CLA  | C1D-ND-C4D  | -4.35 | 103.26      | 106.31   |
| 21  | b     | 607 | CLA  | C2D-C1D-ND  | 4.33  | 114.42      | 110.13   |
| 21  | h     | 101 | CLA  | O2D-CGD-CBD | 4.32  | 118.79      | 111.23   |
| 21  | b     | 610 | CLA  | C1-C2-C3    | -4.32 | 119.12      | 126.20   |
| 19  | B     | 101 | MGE  | O2G-C1B-C2B | 4.32  | 120.82      | 111.48   |
| 21  | c     | 509 | CLA  | C1C-C2C-C3C | -4.32 | 102.44      | 106.98   |
| 21  | b     | 614 | CLA  | C2D-C1D-ND  | 4.32  | 114.40      | 110.13   |
| 21  | b     | 613 | CLA  | CHD-C4C-C3C | -4.31 | 118.49      | 124.77   |
| 21  | a     | 407 | CLA  | C3C-C4C-NC  | 4.30  | 115.94      | 110.43   |
| 21  | c     | 503 | CLA  | CHD-C1D-ND  | -4.29 | 118.76      | 124.80   |
| 21  | a     | 403 | CLA  | O2D-CGD-CBD | 4.29  | 118.73      | 111.23   |
| 21  | c     | 503 | CLA  | CMB-C2B-C1B | 4.29  | 131.94      | 125.42   |
| 21  | b     | 610 | CLA  | CHD-C4C-C3C | -4.28 | 118.53      | 124.77   |
| 21  | b     | 604 | CLA  | C3C-C4C-NC  | 4.28  | 115.91      | 110.43   |
| 22  | z     | 101 | BCR  | C11-C10-C9  | -4.28 | 121.28      | 127.28   |
| 21  | b     | 614 | CLA  | O2D-CGD-CBD | 4.27  | 118.70      | 111.23   |
| 21  | c     | 512 | CLA  | CHD-C1D-ND  | -4.27 | 118.79      | 124.80   |
| 22  | b     | 617 | BCR  | C24-C23-C22 | -4.27 | 119.92      | 126.23   |
| 21  | d     | 402 | CLA  | CHC-C4B-NB  | 4.26  | 130.44      | 124.05   |
| 21  | c     | 508 | CLA  | CHD-C1D-ND  | -4.26 | 118.81      | 124.80   |
| 21  | c     | 513 | CLA  | C3D-C2D-C1D | -4.25 | 100.03      | 105.83   |
| 21  | b     | 605 | CLA  | C2B-C1B-NB  | 4.24  | 114.72      | 110.33   |
| 22  | c     | 514 | BCR  | C20-C21-C22 | -4.23 | 121.34      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | a     | 403 | CLA  | CHD-C1D-ND  | -4.23 | 118.85      | 124.80   |
| 21  | b     | 604 | CLA  | CHD-C1D-ND  | -4.23 | 118.85      | 124.80   |
| 21  | c     | 510 | CLA  | C2D-C1D-ND  | 4.23  | 114.31      | 110.13   |
| 22  | z     | 101 | BCR  | C37-C22-C23 | 4.22  | 124.54      | 118.09   |
| 21  | a     | 403 | CLA  | C1C-C2C-C3C | -4.22 | 102.54      | 106.98   |
| 21  | c     | 508 | CLA  | C3D-C2D-C1D | -4.22 | 100.08      | 105.83   |
| 21  | b     | 608 | CLA  | C4D-CHA-C1A | -4.21 | 116.23      | 121.24   |
| 22  | d     | 409 | BCR  | C7-C8-C9    | -4.20 | 120.02      | 126.23   |
| 21  | c     | 509 | CLA  | C2D-C1D-ND  | 4.20  | 114.28      | 110.13   |
| 22  | b     | 618 | BCR  | C11-C10-C9  | -4.20 | 121.39      | 127.28   |
| 21  | b     | 604 | CLA  | C1C-C2C-C3C | -4.19 | 102.57      | 106.98   |
| 21  | b     | 604 | CLA  | C3D-C2D-C1D | -4.19 | 100.12      | 105.83   |
| 21  | c     | 512 | CLA  | CHC-C1C-NC  | -4.18 | 118.01      | 124.31   |
| 21  | b     | 606 | CLA  | C2C-C1C-NC  | 4.18  | 114.37      | 109.98   |
| 21  | d     | 407 | CLA  | C1D-CHD-C4C | -4.18 | 117.14      | 126.02   |
| 21  | c     | 505 | CLA  | C2D-C1D-ND  | 4.16  | 114.25      | 110.13   |
| 21  | b     | 613 | CLA  | C2C-C1C-NC  | 4.15  | 114.35      | 109.98   |
| 24  | c     | 516 | DGD  | O2G-C1B-C2B | 4.15  | 120.46      | 111.48   |
| 21  | c     | 505 | CLA  | C1-C2-C3    | -4.14 | 119.42      | 126.20   |
| 21  | d     | 402 | CLA  | C3D-C2D-C1D | -4.14 | 100.18      | 105.83   |
| 21  | a     | 403 | CLA  | C2B-C1B-NB  | 4.13  | 114.61      | 110.33   |
| 21  | b     | 615 | CLA  | C3D-C2D-C1D | -4.13 | 100.19      | 105.83   |
| 21  | b     | 610 | CLA  | CHA-C4D-ND  | 4.13  | 141.06      | 132.55   |
| 21  | c     | 505 | CLA  | C3B-C2B-C1B | -4.12 | 102.31      | 107.17   |
| 22  | b     | 616 | BCR  | C15-C14-C13 | -4.10 | 121.52      | 127.28   |
| 22  | b     | 617 | BCR  | C15-C14-C13 | -4.10 | 121.53      | 127.28   |
| 21  | b     | 609 | CLA  | C3D-C2D-C1D | -4.09 | 100.25      | 105.83   |
| 21  | c     | 505 | CLA  | C2C-C1C-NC  | 4.09  | 114.28      | 109.98   |
| 21  | b     | 603 | CLA  | O2D-CGD-CBD | 4.09  | 118.37      | 111.23   |
| 21  | b     | 606 | CLA  | C1D-ND-C4D  | 4.08  | 109.18      | 106.31   |
| 22  | c     | 514 | BCR  | C21-C20-C19 | -4.07 | 111.40      | 123.20   |
| 21  | b     | 601 | CLA  | C1C-C2C-C3C | -4.07 | 102.70      | 106.98   |
| 21  | b     | 614 | CLA  | CHD-C4C-C3C | -4.06 | 118.85      | 124.77   |
| 21  | b     | 610 | CLA  | C4D-CHA-C1A | -4.06 | 116.40      | 121.24   |
| 25  | d     | 401 | PHO  | C3D-C4D-ND  | 4.05  | 112.91      | 107.71   |
| 21  | b     | 614 | CLA  | O2D-CGD-O1D | -4.05 | 115.96      | 123.85   |
| 21  | b     | 604 | CLA  | CMC-C2C-C1C | 4.04  | 131.35      | 125.03   |
| 21  | a     | 402 | CLA  | C1C-C2C-C3C | -4.04 | 102.73      | 106.98   |
| 21  | c     | 509 | CLA  | C3D-C2D-C1D | -4.04 | 100.32      | 105.83   |
| 21  | c     | 512 | CLA  | C1D-CHD-C4C | -4.04 | 117.44      | 126.02   |
| 21  | b     | 602 | CLA  | C3D-C2D-C1D | -4.04 | 100.32      | 105.83   |
| 21  | c     | 504 | CLA  | C2C-C1C-NC  | 4.03  | 114.22      | 109.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | a     | 403 | CLA  | C3B-C4B-NB  | 4.03  | 114.13      | 110.53   |
| 22  | a     | 404 | BCR  | C1-C6-C5    | -4.03 | 117.13      | 122.64   |
| 21  | b     | 603 | CLA  | O2D-CGD-O1D | -4.02 | 116.02      | 123.85   |
| 22  | c     | 514 | BCR  | C16-C17-C18 | -4.02 | 121.64      | 127.28   |
| 21  | b     | 613 | CLA  | C3D-C2D-C1D | -4.01 | 100.36      | 105.83   |
| 21  | b     | 601 | CLA  | C2C-C1C-NC  | 4.01  | 114.19      | 109.98   |
| 21  | c     | 504 | CLA  | C4D-CHA-C1A | -4.01 | 116.46      | 121.24   |
| 21  | b     | 611 | CLA  | C1-C2-C3    | -4.01 | 119.63      | 126.20   |
| 21  | b     | 605 | CLA  | C3D-C2D-C1D | -4.01 | 100.36      | 105.83   |
| 21  | b     | 605 | CLA  | C2C-C1C-NC  | 4.00  | 114.19      | 109.98   |
| 21  | b     | 615 | CLA  | C2C-C1C-NC  | 4.00  | 114.19      | 109.98   |
| 21  | b     | 610 | CLA  | C2D-C1D-ND  | 4.00  | 114.09      | 110.13   |
| 22  | c     | 514 | BCR  | C10-C11-C12 | -4.00 | 111.62      | 123.20   |
| 21  | b     | 601 | CLA  | C3D-C2D-C1D | -3.99 | 100.39      | 105.83   |
| 21  | c     | 510 | CLA  | C1C-C2C-C3C | -3.99 | 102.78      | 106.98   |
| 21  | b     | 610 | CLA  | C2B-C1B-NB  | 3.99  | 114.46      | 110.33   |
| 21  | b     | 604 | CLA  | C4D-CHA-C1A | -3.99 | 116.49      | 121.24   |
| 21  | c     | 505 | CLA  | C1C-C2C-C3C | -3.99 | 102.79      | 106.98   |
| 21  | b     | 612 | CLA  | C2B-C1B-NB  | 3.98  | 114.46      | 110.33   |
| 19  | m     | 102 | MGE  | O2G-C1B-C2B | 3.98  | 120.08      | 111.48   |
| 21  | b     | 607 | CLA  | O2D-CGD-O1D | -3.97 | 116.11      | 123.85   |
| 21  | c     | 512 | CLA  | CHC-C4B-NB  | -3.97 | 118.09      | 124.05   |
| 21  | c     | 507 | CLA  | CHD-C1D-ND  | -3.97 | 119.22      | 124.80   |
| 21  | b     | 610 | CLA  | C4B-C3B-C2B | -3.97 | 102.37      | 107.30   |
| 22  | a     | 404 | BCR  | C15-C14-C13 | -3.97 | 121.72      | 127.28   |
| 21  | b     | 605 | CLA  | C1C-C2C-C3C | -3.96 | 102.81      | 106.98   |
| 21  | c     | 508 | CLA  | CHB-C4A-NA  | 3.95  | 130.10      | 124.40   |
| 21  | b     | 607 | CLA  | C3D-C2D-C1D | -3.95 | 100.44      | 105.83   |
| 24  | a     | 406 | DGD  | O2G-C1B-C2B | 3.95  | 120.02      | 111.48   |
| 25  | d     | 401 | PHO  | CMB-C2B-C3B | 3.94  | 132.55      | 124.68   |
| 21  | b     | 615 | CLA  | CAC-C3C-C4C | 3.93  | 129.91      | 124.79   |
| 21  | b     | 615 | CLA  | C3C-C4C-NC  | 3.93  | 115.47      | 110.43   |
| 21  | b     | 614 | CLA  | C3D-C2D-C1D | -3.93 | 100.47      | 105.83   |
| 21  | b     | 608 | CLA  | C3B-C2B-C1B | -3.91 | 102.56      | 107.17   |
| 21  | c     | 513 | CLA  | C1C-C2C-C3C | -3.91 | 102.87      | 106.98   |
| 21  | c     | 510 | CLA  | C1D-ND-C4D  | -3.90 | 103.57      | 106.31   |
| 21  | b     | 610 | CLA  | C3B-C4B-NB  | 3.90  | 114.01      | 110.53   |
| 21  | c     | 505 | CLA  | CHA-C4D-ND  | 3.89  | 140.58      | 132.55   |
| 21  | b     | 610 | CLA  | O2D-CGD-CBD | 3.89  | 118.03      | 111.23   |
| 21  | d     | 402 | CLA  | C2B-C1B-NB  | 3.89  | 114.36      | 110.33   |
| 21  | d     | 402 | CLA  | C1C-C2C-C3C | -3.88 | 102.90      | 106.98   |
| 22  | h     | 103 | BCR  | C11-C10-C9  | -3.88 | 121.84      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | c     | 509 | CLA  | CHC-C4B-NB  | 3.87  | 129.86      | 124.05   |
| 21  | b     | 602 | CLA  | CHC-C4B-NB  | 3.86  | 129.85      | 124.05   |
| 21  | b     | 611 | CLA  | C3D-C2D-C1D | -3.86 | 100.57      | 105.83   |
| 22  | b     | 618 | BCR  | C16-C17-C18 | -3.85 | 121.88      | 127.28   |
| 19  | f     | 101 | MGE  | C1D-O6D-C5D | 3.85  | 121.23      | 113.72   |
| 21  | b     | 612 | CLA  | CMD-C2D-C1D | 3.84  | 131.49      | 124.73   |
| 21  | b     | 611 | CLA  | O2D-CGD-O1D | -3.84 | 116.38      | 123.85   |
| 21  | a     | 403 | CLA  | C1-C2-C3    | -3.83 | 119.92      | 126.20   |
| 22  | c     | 515 | BCR  | C16-C15-C14 | -3.83 | 115.68      | 123.52   |
| 21  | b     | 606 | CLA  | CHA-C4D-ND  | 3.83  | 140.44      | 132.55   |
| 21  | b     | 601 | CLA  | C2B-C1B-NB  | 3.83  | 114.29      | 110.33   |
| 19  | c     | 502 | MGE  | O2G-C1B-C2B | 3.82  | 119.75      | 111.48   |
| 21  | b     | 607 | CLA  | C2B-C1B-NB  | 3.81  | 114.28      | 110.33   |
| 21  | c     | 506 | CLA  | CHB-C1B-NB  | -3.81 | 118.33      | 124.05   |
| 21  | c     | 511 | CLA  | C2C-C1C-NC  | 3.81  | 113.98      | 109.98   |
| 21  | c     | 508 | CLA  | CMB-C2B-C1B | 3.81  | 131.22      | 125.42   |
| 21  | b     | 609 | CLA  | C4D-CHA-C1A | -3.81 | 116.70      | 121.24   |
| 19  | b     | 620 | MGE  | O2G-C1B-C2B | 3.80  | 119.71      | 111.48   |
| 21  | c     | 511 | CLA  | C1C-C2C-C3C | -3.80 | 102.98      | 106.98   |
| 22  | c     | 514 | BCR  | C15-C16-C17 | -3.80 | 115.74      | 123.52   |
| 21  | d     | 402 | CLA  | CHD-C4C-NC  | 3.80  | 130.13      | 124.23   |
| 22  | h     | 103 | BCR  | C8-C9-C10   | 3.79  | 124.97      | 119.01   |
| 21  | b     | 603 | CLA  | C6-C5-C3    | -3.78 | 104.25      | 113.47   |
| 20  | l     | 101 | SQD  | O47-C7-C8   | 3.78  | 119.67      | 111.48   |
| 22  | d     | 409 | BCR  | C11-C10-C9  | -3.78 | 121.98      | 127.28   |
| 21  | b     | 602 | CLA  | CHD-C4C-NC  | 3.78  | 130.09      | 124.23   |
| 21  | a     | 407 | CLA  | C4D-CHA-C1A | -3.77 | 116.74      | 121.24   |
| 21  | h     | 101 | CLA  | CHD-C4C-C3C | -3.77 | 119.27      | 124.77   |
| 21  | b     | 613 | CLA  | O2A-CGA-O1A | -3.77 | 114.19      | 123.63   |
| 21  | c     | 508 | CLA  | CHA-C4D-ND  | 3.77  | 140.32      | 132.55   |
| 21  | b     | 601 | CLA  | CHD-C4C-C3C | -3.76 | 119.29      | 124.77   |
| 21  | d     | 402 | CLA  | C4D-CHA-C1A | -3.76 | 116.76      | 121.24   |
| 21  | b     | 614 | CLA  | CAC-C3C-C4C | 3.76  | 129.68      | 124.79   |
| 21  | c     | 510 | CLA  | C3B-C4B-NB  | 3.75  | 113.88      | 110.53   |
| 21  | a     | 407 | CLA  | C4-C3-C5    | 3.75  | 121.74      | 115.23   |
| 21  | b     | 609 | CLA  | CHD-C4C-C3C | -3.75 | 119.31      | 124.77   |
| 19  | f     | 101 | MGE  | C4D-C3D-C2D | 3.75  | 117.41      | 110.83   |
| 22  | c     | 515 | BCR  | C27-C26-C25 | -3.75 | 117.64      | 122.70   |
| 21  | b     | 613 | CLA  | CMD-C2D-C1D | 3.75  | 131.33      | 124.73   |
| 21  | c     | 511 | CLA  | O2D-CGD-CBD | 3.74  | 117.77      | 111.23   |
| 21  | a     | 402 | CLA  | C1D-ND-C4D  | -3.74 | 103.69      | 106.31   |
| 21  | b     | 609 | CLA  | O2D-CGD-CBD | 3.73  | 117.76      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | b     | 604 | CLA  | CHC-C4B-NB  | 3.71  | 129.61      | 124.05   |
| 21  | c     | 509 | CLA  | C4-C3-C5    | 3.70  | 121.66      | 115.23   |
| 21  | b     | 610 | CLA  | CBC-CAC-C3C | -3.70 | 102.38      | 112.42   |
| 21  | c     | 509 | CLA  | CHD-C1D-ND  | -3.70 | 119.59      | 124.80   |
| 21  | b     | 603 | CLA  | CMC-C2C-C1C | 3.70  | 130.81      | 125.03   |
| 21  | b     | 607 | CLA  | C4B-C3B-C2B | -3.70 | 102.70      | 107.30   |
| 21  | b     | 605 | CLA  | C3B-C2B-C1B | -3.70 | 102.81      | 107.17   |
| 21  | c     | 508 | CLA  | CMC-C2C-C1C | 3.69  | 130.80      | 125.03   |
| 21  | c     | 504 | CLA  | C3D-C2D-C1D | -3.69 | 100.80      | 105.83   |
| 21  | c     | 507 | CLA  | C1-C2-C3    | -3.69 | 120.16      | 126.20   |
| 30  | e     | 101 | HEM  | C1B-NB-C4B  | 3.69  | 109.57      | 105.21   |
| 21  | b     | 603 | CLA  | C3C-C4C-NC  | 3.68  | 115.15      | 110.43   |
| 21  | b     | 605 | CLA  | CHD-C1D-ND  | -3.68 | 119.63      | 124.80   |
| 21  | c     | 508 | CLA  | C1C-C2C-C3C | -3.68 | 103.11      | 106.98   |
| 21  | a     | 402 | CLA  | CMB-C2B-C1B | 3.68  | 131.02      | 125.42   |
| 21  | c     | 505 | CLA  | CHD-C4C-C3C | -3.68 | 119.41      | 124.77   |
| 21  | c     | 504 | CLA  | O2D-CGD-O1D | -3.68 | 116.69      | 123.85   |
| 21  | c     | 507 | CLA  | C4C-C3C-C2C | -3.68 | 101.54      | 106.89   |
| 21  | b     | 601 | CLA  | CHD-C1D-ND  | -3.68 | 119.63      | 124.80   |
| 21  | b     | 603 | CLA  | CHC-C4B-NB  | 3.67  | 129.55      | 124.05   |
| 21  | c     | 503 | CLA  | C3D-C2D-C1D | -3.67 | 100.83      | 105.83   |
| 21  | k     | 501 | CLA  | C4C-C3C-C2C | -3.67 | 101.55      | 106.89   |
| 21  | b     | 613 | CLA  | C2B-C1B-NB  | 3.66  | 114.12      | 110.33   |
| 21  | c     | 509 | CLA  | CMB-C2B-C1B | 3.66  | 130.99      | 125.42   |
| 21  | b     | 615 | CLA  | O1D-CGD-CBD | -3.65 | 117.31      | 124.52   |
| 21  | b     | 607 | CLA  | C3B-C2B-C1B | -3.65 | 102.87      | 107.17   |
| 22  | a     | 404 | BCR  | C21-C20-C19 | 3.64  | 133.75      | 123.20   |
| 21  | b     | 601 | CLA  | CHA-C4D-ND  | 3.64  | 140.06      | 132.55   |
| 21  | b     | 602 | CLA  | CHA-C4D-ND  | 3.64  | 140.06      | 132.55   |
| 21  | b     | 608 | CLA  | C1-C2-C3    | -3.64 | 120.24      | 126.20   |
| 21  | c     | 511 | CLA  | C3D-C2D-C1D | -3.63 | 100.87      | 105.83   |
| 21  | a     | 407 | CLA  | O2D-CGD-CBD | 3.63  | 117.58      | 111.23   |
| 21  | b     | 613 | CLA  | C1C-C2C-C3C | -3.61 | 103.18      | 106.98   |
| 21  | c     | 513 | CLA  | CAC-C3C-C4C | 3.60  | 129.48      | 124.79   |
| 21  | c     | 504 | CLA  | C1-C2-C3    | -3.60 | 120.30      | 126.20   |
| 19  | d     | 410 | MGE  | C2G-O2G-C1B | -3.60 | 109.18      | 117.80   |
| 21  | c     | 511 | CLA  | CHC-C4B-NB  | 3.59  | 129.44      | 124.05   |
| 21  | k     | 501 | CLA  | C1-O2A-CGA  | 3.59  | 127.58      | 116.07   |
| 21  | c     | 510 | CLA  | CMD-C2D-C1D | 3.59  | 131.05      | 124.73   |
| 21  | c     | 510 | CLA  | O2D-CGD-CBD | 3.59  | 117.50      | 111.23   |
| 21  | b     | 603 | CLA  | CHA-C4D-ND  | 3.59  | 139.95      | 132.55   |
| 21  | c     | 504 | CLA  | CHD-C4C-NC  | 3.58  | 129.79      | 124.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | b     | 611 | CLA  | C3B-C2B-C1B | -3.58 | 102.95      | 107.17   |
| 21  | c     | 513 | CLA  | C4C-C3C-C2C | -3.58 | 101.69      | 106.89   |
| 21  | c     | 509 | CLA  | CHD-C4C-NC  | 3.57  | 129.77      | 124.23   |
| 21  | b     | 614 | CLA  | CMC-C2C-C1C | 3.57  | 130.61      | 125.03   |
| 21  | c     | 508 | CLA  | C1D-CHD-C4C | -3.57 | 118.44      | 126.02   |
| 21  | c     | 503 | CLA  | C3B-C4B-NB  | 3.57  | 113.71      | 110.53   |
| 22  | b     | 618 | BCR  | C20-C21-C22 | -3.56 | 122.29      | 127.28   |
| 21  | a     | 407 | CLA  | CMD-C2D-C1D | 3.55  | 130.99      | 124.73   |
| 21  | c     | 511 | CLA  | CHD-C4C-C3C | -3.55 | 119.59      | 124.77   |
| 21  | b     | 605 | CLA  | O2D-CGD-CBD | 3.55  | 117.44      | 111.23   |
| 19  | b     | 619 | MGE  | O1G-C1A-C2A | 3.55  | 122.66      | 111.83   |
| 21  | c     | 503 | CLA  | CHD-C4C-NC  | 3.55  | 129.73      | 124.23   |
| 21  | c     | 505 | CLA  | CHC-C4B-NB  | 3.55  | 129.37      | 124.05   |
| 21  | b     | 610 | CLA  | O2D-CGD-O1D | -3.55 | 116.95      | 123.85   |
| 21  | b     | 602 | CLA  | CAC-C3C-C4C | 3.54  | 129.40      | 124.79   |
| 21  | b     | 615 | CLA  | CHD-C4C-NC  | 3.54  | 129.72      | 124.23   |
| 19  | f     | 101 | MGE  | O2G-C1B-C2B | 3.54  | 119.14      | 111.48   |
| 21  | b     | 608 | CLA  | CHD-C4C-C3C | -3.54 | 119.62      | 124.77   |
| 21  | c     | 507 | CLA  | C3D-C4D-ND  | 3.53  | 115.73      | 109.99   |
| 25  | d     | 403 | PHO  | C4-C3-C5    | 3.53  | 121.36      | 115.23   |
| 21  | c     | 511 | CLA  | C4-C3-C5    | 3.53  | 121.36      | 115.23   |
| 21  | d     | 402 | CLA  | CBC-CAC-C3C | -3.53 | 102.85      | 112.42   |
| 21  | b     | 603 | CLA  | C2B-C1B-NB  | 3.53  | 113.98      | 110.33   |
| 22  | h     | 103 | BCR  | C16-C17-C18 | -3.52 | 122.34      | 127.28   |
| 24  | c     | 517 | DGD  | O2G-C1B-C2B | 3.51  | 119.08      | 111.48   |
| 21  | b     | 607 | CLA  | C4D-CHA-C1A | -3.51 | 117.06      | 121.24   |
| 21  | c     | 508 | CLA  | CHB-C1B-NB  | -3.51 | 118.79      | 124.05   |
| 21  | b     | 610 | CLA  | C1D-CHD-C4C | -3.50 | 118.57      | 126.02   |
| 21  | a     | 407 | CLA  | CHA-C4D-ND  | 3.50  | 139.77      | 132.55   |
| 21  | b     | 602 | CLA  | CMC-C2C-C1C | 3.50  | 130.50      | 125.03   |
| 21  | c     | 511 | CLA  | C3B-C2B-C1B | -3.49 | 103.06      | 107.17   |
| 22  | b     | 618 | BCR  | C38-C26-C27 | 3.49  | 121.03      | 113.60   |
| 21  | b     | 601 | CLA  | CMB-C2B-C3B | 3.49  | 134.75      | 126.55   |
| 21  | b     | 603 | CLA  | C3B-C2B-C1B | -3.49 | 103.06      | 107.17   |
| 21  | b     | 610 | CLA  | C3D-C2D-C1D | -3.49 | 101.07      | 105.83   |
| 21  | d     | 406 | CLA  | C4C-C3C-C2C | -3.48 | 101.82      | 106.89   |
| 21  | d     | 406 | CLA  | C4A-NA-C1A  | -3.48 | 105.09      | 106.68   |
| 21  | b     | 602 | CLA  | C3B-C4B-NB  | 3.48  | 113.63      | 110.53   |
| 21  | b     | 615 | CLA  | CHD-C1D-ND  | -3.47 | 119.91      | 124.80   |
| 21  | c     | 508 | CLA  | CHC-C4B-NB  | 3.47  | 129.26      | 124.05   |
| 21  | c     | 513 | CLA  | CHC-C1C-C2C | -3.47 | 117.08      | 126.95   |
| 22  | b     | 617 | BCR  | C3-C4-C5    | -3.47 | 107.87      | 114.06   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | c     | 507 | CLA  | CHC-C1C-C2C | -3.47 | 117.09      | 126.95   |
| 21  | b     | 607 | CLA  | CHA-C4D-ND  | 3.47  | 139.70      | 132.55   |
| 21  | c     | 510 | CLA  | C4D-C3D-CAD | 3.46  | 111.87      | 108.11   |
| 21  | h     | 101 | CLA  | C4C-C3C-C2C | -3.46 | 101.85      | 106.89   |
| 21  | b     | 601 | CLA  | C1-C2-C3    | -3.46 | 120.53      | 126.20   |
| 21  | b     | 602 | CLA  | C4D-CHA-C1A | -3.45 | 117.12      | 121.24   |
| 21  | b     | 601 | CLA  | C1D-CHD-C4C | -3.45 | 118.69      | 126.02   |
| 21  | d     | 406 | CLA  | O2D-CGD-O1D | -3.45 | 117.14      | 123.85   |
| 21  | c     | 506 | CLA  | CHC-C1C-C2C | -3.45 | 117.15      | 126.95   |
| 21  | c     | 511 | CLA  | CHA-C4D-ND  | 3.44  | 139.65      | 132.55   |
| 21  | a     | 407 | CLA  | C2A-C1A-CHA | -3.44 | 117.90      | 123.87   |
| 21  | c     | 504 | CLA  | C1C-C2C-C3C | -3.43 | 103.37      | 106.98   |
| 21  | a     | 407 | CLA  | CMB-C2B-C1B | 3.42  | 130.63      | 125.42   |
| 22  | b     | 617 | BCR  | C11-C10-C9  | -3.42 | 122.48      | 127.28   |
| 22  | a     | 404 | BCR  | C4-C5-C6    | -3.42 | 118.08      | 122.70   |
| 21  | c     | 507 | CLA  | CAC-C3C-C4C | 3.41  | 129.23      | 124.79   |
| 21  | b     | 614 | CLA  | CHA-C4D-ND  | 3.41  | 139.59      | 132.55   |
| 21  | a     | 407 | CLA  | C3B-C2B-C1B | -3.41 | 103.15      | 107.17   |
| 22  | c     | 515 | BCR  | C20-C21-C22 | -3.41 | 122.50      | 127.28   |
| 21  | a     | 403 | CLA  | C4D-CHA-C1A | -3.41 | 117.18      | 121.24   |
| 21  | b     | 608 | CLA  | C3C-C4C-NC  | 3.41  | 114.79      | 110.43   |
| 21  | b     | 613 | CLA  | CMB-C2B-C1B | 3.41  | 130.60      | 125.42   |
| 21  | a     | 402 | CLA  | C7-C6-C5    | -3.40 | 104.20      | 113.26   |
| 21  | k     | 501 | CLA  | CMC-C2C-C1C | 3.40  | 130.34      | 125.03   |
| 22  | b     | 617 | BCR  | C20-C21-C22 | -3.40 | 122.51      | 127.28   |
| 22  | b     | 618 | BCR  | C15-C14-C13 | -3.40 | 122.52      | 127.28   |
| 21  | c     | 510 | CLA  | CHA-C4D-ND  | 3.40  | 139.56      | 132.55   |
| 21  | a     | 403 | CLA  | C3B-C2B-C1B | -3.39 | 103.17      | 107.17   |
| 21  | c     | 506 | CLA  | C4C-C3C-C2C | -3.39 | 101.96      | 106.89   |
| 22  | d     | 409 | BCR  | C20-C21-C22 | -3.38 | 122.53      | 127.28   |
| 21  | a     | 402 | CLA  | C1D-CHD-C4C | -3.38 | 118.83      | 126.02   |
| 21  | a     | 403 | CLA  | C3C-C4C-NC  | 3.38  | 114.76      | 110.43   |
| 24  | c     | 516 | DGD  | C1D-C2D-C3D | 3.38  | 117.12      | 110.01   |
| 22  | z     | 101 | BCR  | C30-C25-C26 | -3.37 | 118.03      | 122.64   |
| 21  | a     | 407 | CLA  | C1-O2A-CGA  | 3.37  | 124.82      | 116.65   |
| 21  | c     | 508 | CLA  | C2C-C1C-NC  | 3.37  | 113.52      | 109.98   |
| 21  | b     | 608 | CLA  | C4C-C3C-C2C | -3.36 | 102.00      | 106.89   |
| 21  | b     | 612 | CLA  | C1C-C2C-C3C | -3.36 | 103.44      | 106.98   |
| 22  | b     | 616 | BCR  | C16-C17-C18 | -3.36 | 122.57      | 127.28   |
| 22  | b     | 616 | BCR  | C27-C26-C25 | -3.36 | 118.17      | 122.70   |
| 22  | a     | 404 | BCR  | C16-C17-C18 | -3.36 | 122.57      | 127.28   |
| 21  | c     | 505 | CLA  | C2B-C1B-NB  | 3.35  | 113.80      | 110.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | c     | 505 | CLA  | C1D-CHD-C4C | -3.34 | 118.92      | 126.02   |
| 21  | b     | 613 | CLA  | C4-C3-C2    | -3.33 | 115.08      | 123.63   |
| 21  | b     | 605 | CLA  | C4D-CHA-C1A | -3.32 | 117.28      | 121.24   |
| 22  | h     | 103 | BCR  | C24-C23-C22 | -3.32 | 121.33      | 126.23   |
| 21  | c     | 510 | CLA  | CMB-C2B-C1B | 3.31  | 130.46      | 125.42   |
| 21  | b     | 605 | CLA  | O2D-CGD-O1D | -3.31 | 117.40      | 123.85   |
| 24  | c     | 517 | DGD  | O6D-C5D-C6D | 3.31  | 113.25      | 106.69   |
| 21  | a     | 402 | CLA  | C2B-C1B-NB  | 3.31  | 113.75      | 110.33   |
| 21  | b     | 613 | CLA  | C3B-C4B-NB  | 3.30  | 113.48      | 110.53   |
| 21  | b     | 608 | CLA  | C2D-C1D-ND  | 3.29  | 113.39      | 110.13   |
| 21  | b     | 603 | CLA  | C4D-CHA-C1A | -3.29 | 117.32      | 121.24   |
| 21  | b     | 615 | CLA  | C4C-C3C-C2C | -3.29 | 102.10      | 106.89   |
| 22  | d     | 409 | BCR  | C16-C15-C14 | -3.29 | 116.78      | 123.52   |
| 21  | a     | 407 | CLA  | C1D-ND-C4D  | 3.29  | 108.62      | 106.31   |
| 21  | b     | 611 | CLA  | CHC-C4B-NB  | 3.29  | 128.98      | 124.05   |
| 21  | b     | 604 | CLA  | C3B-C2B-C1B | -3.29 | 103.29      | 107.17   |
| 21  | h     | 101 | CLA  | CHC-C1C-C2C | -3.29 | 117.61      | 126.95   |
| 21  | b     | 603 | CLA  | CMD-C2D-C1D | 3.29  | 130.51      | 124.73   |
| 22  | b     | 617 | BCR  | C8-C7-C6    | -3.28 | 118.24      | 127.00   |
| 21  | b     | 606 | CLA  | C4-C3-C5    | 3.27  | 120.91      | 115.23   |
| 21  | b     | 614 | CLA  | CMD-C2D-C3D | 3.27  | 135.20      | 127.69   |
| 22  | a     | 404 | BCR  | C36-C18-C19 | 3.27  | 123.09      | 118.09   |
| 21  | b     | 605 | CLA  | CMD-C2D-C1D | 3.27  | 130.49      | 124.73   |
| 21  | c     | 509 | CLA  | C2B-C1B-NB  | 3.27  | 113.71      | 110.33   |
| 19  | m     | 102 | MGE  | C1D-O6D-C5D | 3.26  | 120.09      | 113.72   |
| 21  | d     | 407 | CLA  | C4C-C3C-C2C | -3.26 | 102.14      | 106.89   |
| 21  | b     | 607 | CLA  | O2A-CGA-O1A | -3.26 | 115.47      | 123.63   |
| 28  | d     | 408 | PQ9  | C39-C38-C40 | 3.25  | 120.87      | 115.23   |
| 21  | b     | 612 | CLA  | C4B-C3B-C2B | -3.24 | 103.27      | 107.30   |
| 21  | c     | 513 | CLA  | CMB-C2B-C1B | 3.24  | 130.35      | 125.42   |
| 21  | c     | 512 | CLA  | CMB-C2B-C1B | 3.24  | 130.35      | 125.42   |
| 22  | b     | 617 | BCR  | C4-C5-C6    | -3.23 | 118.34      | 122.70   |
| 21  | d     | 406 | CLA  | O2A-CGA-CBA | 3.23  | 121.68      | 111.83   |
| 22  | c     | 515 | BCR  | C20-C19-C18 | -3.23 | 117.51      | 126.36   |
| 22  | c     | 515 | BCR  | C38-C26-C27 | 3.23  | 120.47      | 113.60   |
| 21  | c     | 507 | CLA  | C4-C3-C5    | 3.22  | 119.92      | 116.13   |
| 22  | b     | 617 | BCR  | C16-C17-C18 | -3.22 | 122.76      | 127.28   |
| 21  | c     | 513 | CLA  | CHD-C1D-C2D | 3.22  | 132.18      | 125.49   |
| 24  | c     | 516 | DGD  | C4D-C3D-C2D | 3.22  | 116.48      | 110.83   |
| 21  | h     | 101 | CLA  | CMB-C2B-C1B | 3.21  | 130.31      | 125.42   |
| 21  | b     | 609 | CLA  | C1D-CHD-C4C | -3.21 | 119.19      | 126.02   |
| 22  | z     | 101 | BCR  | C27-C26-C25 | -3.21 | 118.36      | 122.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | b     | 606 | CLA  | C2D-C1D-ND  | 3.21  | 113.30      | 110.13   |
| 21  | d     | 407 | CLA  | CMB-C2B-C1B | 3.20  | 130.29      | 125.42   |
| 21  | a     | 407 | CLA  | C2B-C1B-NB  | 3.20  | 113.64      | 110.33   |
| 25  | d     | 403 | PHO  | C1-C2-C3    | -3.19 | 120.96      | 126.20   |
| 21  | b     | 612 | CLA  | C4D-CHA-C1A | -3.19 | 117.43      | 121.24   |
| 21  | b     | 611 | CLA  | O2D-CGD-CBD | 3.18  | 116.80      | 111.23   |
| 21  | a     | 403 | CLA  | C1D-ND-C4D  | -3.18 | 104.08      | 106.31   |
| 21  | a     | 403 | CLA  | CMC-C2C-C1C | 3.18  | 130.01      | 125.03   |
| 21  | b     | 602 | CLA  | C5-C3-C2    | -3.18 | 114.03      | 121.17   |
| 21  | b     | 609 | CLA  | CAA-CBA-CGA | -3.18 | 104.19      | 113.21   |
| 21  | a     | 403 | CLA  | C4B-C3B-C2B | -3.17 | 103.36      | 107.30   |
| 25  | d     | 401 | PHO  | CBA-CAA-C2A | -3.17 | 104.44      | 113.78   |
| 21  | a     | 407 | CLA  | CBC-CAC-C3C | -3.17 | 103.84      | 112.42   |
| 21  | c     | 512 | CLA  | CMC-C2C-C1C | 3.17  | 129.98      | 125.03   |
| 21  | b     | 608 | CLA  | CHC-C4B-NB  | 3.16  | 128.79      | 124.05   |
| 20  | l     | 101 | SQD  | O48-C23-C24 | 3.16  | 121.46      | 111.83   |
| 21  | b     | 613 | CLA  | CHC-C4B-NB  | 3.15  | 128.78      | 124.05   |
| 21  | b     | 604 | CLA  | CHA-C4D-ND  | 3.15  | 139.06      | 132.55   |
| 21  | c     | 506 | CLA  | CAC-C3C-C4C | 3.15  | 128.89      | 124.79   |
| 24  | h     | 104 | DGD  | O1G-C1A-C2A | 3.15  | 121.44      | 111.83   |
| 21  | a     | 403 | CLA  | CHD-C4C-NC  | 3.15  | 129.11      | 124.23   |
| 22  | z     | 101 | BCR  | C15-C14-C13 | -3.14 | 122.87      | 127.28   |
| 21  | d     | 406 | CLA  | CHC-C1C-C2C | -3.14 | 118.02      | 126.95   |
| 21  | b     | 605 | CLA  | CMC-C2C-C3C | 3.14  | 134.64      | 126.15   |
| 21  | c     | 509 | CLA  | CHA-C4D-ND  | 3.14  | 139.02      | 132.55   |
| 21  | b     | 612 | CLA  | C1-O2A-CGA  | 3.13  | 124.24      | 116.65   |
| 21  | d     | 407 | CLA  | C4B-CHC-C1C | -3.13 | 118.89      | 126.25   |
| 21  | d     | 406 | CLA  | CAC-C3C-C4C | 3.12  | 128.85      | 124.79   |
| 21  | d     | 402 | CLA  | CHA-C4D-ND  | 3.12  | 138.98      | 132.55   |
| 21  | c     | 503 | CLA  | CHC-C4B-NB  | 3.11  | 128.72      | 124.05   |
| 22  | b     | 617 | BCR  | C1-C6-C5    | -3.11 | 118.39      | 122.64   |
| 21  | d     | 402 | CLA  | C1D-ND-C4D  | -3.11 | 104.13      | 106.31   |
| 21  | b     | 614 | CLA  | C4-C3-C5    | 3.11  | 120.62      | 115.23   |
| 21  | b     | 613 | CLA  | CHB-C4A-NA  | 3.11  | 128.88      | 124.40   |
| 21  | b     | 615 | CLA  | O2A-CGA-CBA | 3.11  | 123.87      | 112.14   |
| 21  | a     | 402 | CLA  | CMD-C2D-C1D | 3.10  | 130.19      | 124.73   |
| 21  | b     | 604 | CLA  | C4C-C3C-C2C | -3.10 | 102.38      | 106.89   |
| 21  | b     | 606 | CLA  | C2B-C1B-NB  | 3.10  | 113.54      | 110.33   |
| 21  | b     | 613 | CLA  | C3B-C2B-C1B | -3.09 | 103.52      | 107.17   |
| 22  | z     | 101 | BCR  | C28-C27-C26 | -3.09 | 108.54      | 114.06   |
| 21  | a     | 403 | CLA  | C1D-CHD-C4C | -3.09 | 119.45      | 126.02   |
| 30  | e     | 101 | HEM  | CHB-C1B-NB  | 3.09  | 128.19      | 124.37   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | c     | 507 | CLA  | CMB-C2B-C1B | 3.09  | 130.12      | 125.42   |
| 21  | b     | 608 | CLA  | O2D-CGD-O1D | -3.09 | 117.84      | 123.85   |
| 21  | b     | 606 | CLA  | C3B-C2B-C1B | -3.09 | 103.53      | 107.17   |
| 21  | b     | 604 | CLA  | C3A-C2A-C1A | -3.09 | 96.72       | 101.34   |
| 21  | d     | 406 | CLA  | C4B-C3B-C2B | -3.08 | 103.47      | 107.30   |
| 21  | c     | 511 | CLA  | C1D-CHD-C4C | -3.08 | 119.48      | 126.02   |
| 21  | k     | 501 | CLA  | C4B-C3B-C2B | -3.08 | 103.47      | 107.30   |
| 21  | b     | 612 | CLA  | O2D-CGD-O1D | -3.08 | 117.86      | 123.85   |
| 21  | c     | 510 | CLA  | C3C-C4C-NC  | 3.08  | 114.37      | 110.43   |
| 21  | c     | 505 | CLA  | OBD-CAD-C3D | -3.07 | 121.23      | 128.42   |
| 21  | b     | 605 | CLA  | O2A-CGA-O1A | -3.07 | 115.95      | 123.63   |
| 22  | b     | 617 | BCR  | C15-C16-C17 | -3.06 | 117.25      | 123.52   |
| 22  | d     | 409 | BCR  | C15-C14-C13 | -3.06 | 122.98      | 127.28   |
| 21  | b     | 613 | CLA  | CAC-C3C-C4C | 3.06  | 128.77      | 124.79   |
| 21  | b     | 602 | CLA  | O2D-CGD-CBD | 3.06  | 116.57      | 111.23   |
| 21  | c     | 512 | CLA  | C2A-C3A-C4A | -3.05 | 96.94       | 101.87   |
| 21  | b     | 613 | CLA  | C1D-CHD-C4C | -3.05 | 119.53      | 126.02   |
| 21  | b     | 610 | CLA  | CMC-C2C-C1C | 3.05  | 129.80      | 125.03   |
| 21  | b     | 606 | CLA  | C1C-C2C-C3C | -3.05 | 103.77      | 106.98   |
| 21  | b     | 604 | CLA  | CMB-C2B-C1B | 3.05  | 130.06      | 125.42   |
| 21  | b     | 613 | CLA  | C1-O2A-CGA  | 3.05  | 124.02      | 116.65   |
| 21  | a     | 407 | CLA  | C1-C2-C3    | -3.04 | 121.21      | 126.20   |
| 21  | b     | 609 | CLA  | CMB-C2B-C1B | 3.04  | 130.05      | 125.42   |
| 21  | b     | 611 | CLA  | C4-C3-C5    | 3.04  | 120.51      | 115.23   |
| 21  | h     | 101 | CLA  | CAC-C3C-C4C | 3.04  | 128.74      | 124.79   |
| 21  | d     | 406 | CLA  | CHB-C4A-NA  | 3.04  | 128.78      | 124.40   |
| 21  | b     | 607 | CLA  | CHD-C1D-ND  | -3.04 | 120.53      | 124.80   |
| 21  | b     | 608 | CLA  | C2B-C1B-NB  | 3.03  | 113.47      | 110.33   |
| 22  | a     | 404 | BCR  | C20-C19-C18 | 3.02  | 134.64      | 126.36   |
| 21  | b     | 613 | CLA  | CHA-C4D-ND  | 3.01  | 138.76      | 132.55   |
| 21  | a     | 402 | CLA  | CHD-C4C-NC  | 3.01  | 128.90      | 124.23   |
| 21  | b     | 601 | CLA  | CMD-C2D-C3D | 3.01  | 134.59      | 127.69   |
| 22  | z     | 101 | BCR  | C23-C22-C21 | -3.01 | 114.27      | 119.01   |
| 21  | a     | 403 | CLA  | C3D-C2D-C1D | -3.01 | 101.72      | 105.83   |
| 21  | b     | 603 | CLA  | O2A-CGA-O1A | -3.01 | 116.10      | 123.63   |
| 21  | b     | 605 | CLA  | CHD-C4C-NC  | 3.01  | 128.89      | 124.23   |
| 19  | b     | 619 | MGE  | O2G-C1B-C2B | 3.00  | 117.98      | 111.48   |
| 21  | b     | 606 | CLA  | CMD-C2D-C1D | 3.00  | 130.01      | 124.73   |
| 21  | c     | 511 | CLA  | C2B-C1B-NB  | 3.00  | 113.43      | 110.33   |
| 21  | b     | 612 | CLA  | C2A-C1A-CHA | -2.99 | 118.67      | 123.87   |
| 21  | b     | 601 | CLA  | C4-C3-C5    | 2.99  | 120.41      | 115.23   |
| 19  | B     | 101 | MGE  | O1G-C1A-C2A | 2.98  | 120.92      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | b     | 601 | CLA  | C4D-CHA-C1A | -2.98 | 117.69      | 121.24   |
| 21  | b     | 604 | CLA  | C2B-C1B-NB  | 2.98  | 113.41      | 110.33   |
| 21  | b     | 613 | CLA  | CHD-C4C-NC  | 2.97  | 128.84      | 124.23   |
| 21  | c     | 507 | CLA  | CAA-CBA-CGA | -2.97 | 104.77      | 113.21   |
| 21  | c     | 507 | CLA  | CHB-C1B-NB  | -2.97 | 119.59      | 124.05   |
| 24  | c     | 517 | DGD  | O1G-C1A-C2A | 2.97  | 120.89      | 111.83   |
| 21  | b     | 612 | CLA  | C3B-C2B-C1B | -2.97 | 103.67      | 107.17   |
| 21  | c     | 513 | CLA  | CMD-C2D-C3D | -2.97 | 120.88      | 127.69   |
| 20  | l     | 101 | SQD  | O8-S-O7     | 2.97  | 118.82      | 111.40   |
| 21  | b     | 604 | CLA  | CHC-C1C-NC  | -2.97 | 119.84      | 124.31   |
| 21  | a     | 402 | CLA  | C4D-CHA-C1A | -2.96 | 117.71      | 121.24   |
| 21  | c     | 507 | CLA  | C2A-C3A-C4A | -2.96 | 97.09       | 101.87   |
| 21  | c     | 504 | CLA  | CMB-C2B-C1B | 2.96  | 129.92      | 125.42   |
| 21  | b     | 614 | CLA  | CHD-C4C-NC  | 2.96  | 128.81      | 124.23   |
| 21  | a     | 402 | CLA  | CHC-C4B-NB  | 2.95  | 128.48      | 124.05   |
| 21  | c     | 504 | CLA  | CAC-C3C-C4C | 2.95  | 128.63      | 124.79   |
| 20  | a     | 401 | SQD  | O8-S-O7     | 2.95  | 118.77      | 111.40   |
| 21  | b     | 612 | CLA  | CHD-C1D-ND  | -2.95 | 120.66      | 124.80   |
| 21  | c     | 513 | CLA  | CMA-C3A-C2A | -2.94 | 102.60      | 113.98   |
| 21  | b     | 612 | CLA  | CHC-C4B-NB  | 2.94  | 128.46      | 124.05   |
| 25  | d     | 403 | PHO  | CMA-C3A-C4A | -2.94 | 108.28      | 114.61   |
| 21  | c     | 510 | CLA  | C3D-C2D-C1D | -2.94 | 101.82      | 105.83   |
| 21  | k     | 501 | CLA  | CHB-C4A-NA  | 2.94  | 128.64      | 124.40   |
| 21  | b     | 609 | CLA  | CHA-C4D-ND  | 2.94  | 138.61      | 132.55   |
| 21  | c     | 503 | CLA  | CBC-CAC-C3C | -2.94 | 104.46      | 112.42   |
| 21  | d     | 407 | CLA  | C4B-C3B-C2B | -2.93 | 103.65      | 107.30   |
| 21  | b     | 601 | CLA  | C2A-C3A-C4A | -2.93 | 97.13       | 101.87   |
| 21  | b     | 606 | CLA  | C4C-C3C-C2C | -2.93 | 102.62      | 106.89   |
| 21  | b     | 607 | CLA  | CAC-C3C-C4C | 2.93  | 128.61      | 124.79   |
| 21  | b     | 609 | CLA  | CHB-C4A-NA  | 2.93  | 128.63      | 124.40   |
| 19  | b     | 620 | MGE  | O1G-C1A-C2A | 2.93  | 120.76      | 111.83   |
| 21  | b     | 611 | CLA  | C3B-C4B-NB  | 2.92  | 113.14      | 110.53   |
| 22  | b     | 616 | BCR  | C21-C20-C19 | -2.92 | 114.74      | 123.20   |
| 22  | h     | 103 | BCR  | C32-C1-C6   | 2.92  | 114.82      | 110.24   |
| 21  | c     | 510 | CLA  | O2D-CGD-O1D | -2.91 | 118.18      | 123.85   |
| 22  | h     | 103 | BCR  | C1-C6-C7    | 2.91  | 123.55      | 115.65   |
| 21  | d     | 407 | CLA  | CHB-C4A-NA  | 2.91  | 128.60      | 124.40   |
| 21  | a     | 402 | CLA  | CAC-C3C-C2C | -2.90 | 122.22      | 127.56   |
| 21  | b     | 606 | CLA  | CHD-C4C-NC  | 2.90  | 128.73      | 124.23   |
| 21  | c     | 509 | CLA  | C3C-C4C-NC  | 2.90  | 114.15      | 110.43   |
| 21  | b     | 604 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 19  | c     | 502 | MGE  | O1G-C1A-C2A | 2.90  | 120.67      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | c     | 514 | BCR  | C29-C30-C25 | 2.90  | 114.65      | 110.44   |
| 21  | b     | 606 | CLA  | CHD-C1D-ND  | -2.90 | 120.73      | 124.80   |
| 21  | a     | 407 | CLA  | CHB-C1B-C2B | -2.89 | 119.02      | 127.43   |
| 19  | b     | 619 | MGE  | C1D-O6D-C5D | 2.89  | 119.37      | 113.72   |
| 22  | c     | 515 | BCR  | C8-C9-C10   | 2.89  | 123.56      | 119.01   |
| 21  | b     | 615 | CLA  | C1C-C2C-C3C | -2.89 | 103.94      | 106.98   |
| 19  | d     | 410 | MGE  | O1G-C1A-C2A | 2.89  | 120.65      | 111.83   |
| 21  | c     | 510 | CLA  | C1D-CHD-C4C | -2.89 | 119.88      | 126.02   |
| 21  | c     | 513 | CLA  | O2A-CGA-CBA | 2.89  | 120.64      | 111.83   |
| 21  | b     | 607 | CLA  | C3C-C4C-NC  | 2.89  | 114.13      | 110.43   |
| 30  | e     | 101 | HEM  | CHA-C4D-ND  | 2.89  | 127.94      | 124.37   |
| 21  | b     | 612 | CLA  | C3C-C4C-NC  | 2.88  | 114.12      | 110.43   |
| 22  | z     | 101 | BCR  | C33-C5-C6   | -2.88 | 121.34      | 124.48   |
| 21  | c     | 512 | CLA  | C4C-C3C-C2C | -2.88 | 102.70      | 106.89   |
| 28  | d     | 408 | PQ9  | C11-C12-C13 | -2.88 | 121.88      | 126.83   |
| 21  | c     | 504 | CLA  | CHA-C4D-ND  | 2.87  | 138.48      | 132.55   |
| 21  | b     | 605 | CLA  | C1-O2A-CGA  | 2.87  | 123.61      | 116.65   |
| 21  | b     | 615 | CLA  | O2D-CGD-O1D | -2.87 | 118.26      | 123.85   |
| 25  | d     | 401 | PHO  | CMC-C2C-C1C | 2.87  | 129.90      | 124.73   |
| 21  | b     | 607 | CLA  | C3B-C4B-NB  | 2.86  | 113.08      | 110.53   |
| 21  | b     | 612 | CLA  | C3B-C4B-NB  | 2.86  | 113.08      | 110.53   |
| 21  | c     | 508 | CLA  | C3B-C4B-NB  | 2.86  | 113.08      | 110.53   |
| 21  | b     | 604 | CLA  | C2A-C1A-CHA | -2.86 | 118.91      | 123.87   |
| 21  | d     | 407 | CLA  | CAC-C3C-C4C | 2.85  | 128.50      | 124.79   |
| 21  | b     | 601 | CLA  | CMA-C3A-C4A | -2.85 | 104.11      | 111.77   |
| 21  | a     | 403 | CLA  | CHC-C4B-C3B | -2.85 | 115.01      | 127.37   |
| 21  | h     | 101 | CLA  | CMD-C2D-C3D | -2.84 | 121.17      | 127.69   |
| 21  | c     | 506 | CLA  | CMB-C2B-C1B | 2.84  | 129.74      | 125.42   |
| 21  | c     | 508 | CLA  | CED-O2D-CGD | 2.84  | 122.36      | 115.92   |
| 21  | b     | 601 | CLA  | O2A-CGA-O1A | -2.84 | 116.53      | 123.63   |
| 21  | b     | 608 | CLA  | C1C-C2C-C3C | -2.84 | 104.00      | 106.98   |
| 25  | d     | 403 | PHO  | C4B-NB-C1B  | -2.84 | 104.68      | 108.82   |
| 21  | b     | 605 | CLA  | C3B-C4B-NB  | 2.83  | 113.06      | 110.53   |
| 22  | b     | 617 | BCR  | C33-C5-C4   | 2.82  | 119.62      | 113.60   |
| 21  | c     | 503 | CLA  | C3D-C4D-ND  | 2.82  | 114.58      | 109.99   |
| 28  | d     | 408 | PQ9  | C19-C18-C20 | 2.82  | 120.12      | 115.23   |
| 21  | c     | 513 | CLA  | C2A-C1A-CHA | -2.82 | 118.97      | 123.87   |
| 21  | a     | 407 | CLA  | C2D-C1D-ND  | 2.82  | 112.91      | 110.13   |
| 21  | c     | 509 | CLA  | CBC-CAC-C3C | -2.81 | 104.80      | 112.42   |
| 21  | c     | 508 | CLA  | O2D-CGD-CBD | 2.81  | 116.14      | 111.23   |
| 25  | d     | 401 | PHO  | CMA-C3A-C4A | -2.81 | 108.56      | 114.61   |
| 21  | c     | 510 | CLA  | CHC-C1C-NC  | -2.81 | 120.08      | 124.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | d     | 401 | PHO  | CAA-CBA-CGA | -2.81 | 105.24      | 113.21   |
| 21  | a     | 403 | CLA  | O2D-CGD-O1D | -2.80 | 118.39      | 123.85   |
| 21  | c     | 504 | CLA  | C3D-C4D-ND  | 2.80  | 114.54      | 109.99   |
| 21  | c     | 504 | CLA  | C3B-C4B-NB  | 2.80  | 113.03      | 110.53   |
| 21  | c     | 510 | CLA  | CED-O2D-CGD | 2.80  | 122.27      | 115.92   |
| 21  | b     | 602 | CLA  | C2A-C1A-CHA | -2.80 | 119.01      | 123.87   |
| 21  | b     | 614 | CLA  | C3B-C4B-NB  | 2.80  | 113.03      | 110.53   |
| 22  | a     | 404 | BCR  | C15-C16-C17 | -2.79 | 117.81      | 123.52   |
| 21  | c     | 507 | CLA  | CMD-C2D-C3D | -2.79 | 121.29      | 127.69   |
| 21  | c     | 510 | CLA  | CHC-C4B-C3B | -2.79 | 115.26      | 127.37   |
| 19  | f     | 101 | MGE  | O1G-C1A-C2A | 2.78  | 120.32      | 111.83   |
| 21  | b     | 609 | CLA  | CHD-C4C-NC  | 2.78  | 128.55      | 124.23   |
| 21  | b     | 602 | CLA  | C1D-CHD-C4C | -2.78 | 120.11      | 126.02   |
| 21  | a     | 407 | CLA  | C3B-C4B-NB  | 2.78  | 113.01      | 110.53   |
| 21  | k     | 501 | CLA  | C4D-C3D-CAD | 2.78  | 111.12      | 108.11   |
| 21  | b     | 609 | CLA  | O2A-CGA-O1A | -2.77 | 116.69      | 123.63   |
| 21  | c     | 506 | CLA  | O2D-CGD-O1D | -2.77 | 118.45      | 123.85   |
| 25  | d     | 403 | PHO  | O2A-CGA-O1A | -2.77 | 116.70      | 123.63   |
| 21  | b     | 606 | CLA  | O2D-CGD-O1D | -2.77 | 118.46      | 123.85   |
| 21  | k     | 501 | CLA  | CMD-C2D-C3D | -2.77 | 121.35      | 127.69   |
| 28  | d     | 408 | PQ9  | C11-C2-C1   | 2.77  | 119.19      | 116.91   |
| 21  | k     | 501 | CLA  | CMB-C2B-C1B | 2.76  | 129.63      | 125.42   |
| 21  | b     | 613 | CLA  | C4B-C3B-C2B | -2.76 | 103.87      | 107.30   |
| 21  | d     | 406 | CLA  | C2A-C1A-CHA | -2.76 | 119.08      | 123.87   |
| 21  | b     | 613 | CLA  | C4-C3-C5    | 2.75  | 120.01      | 115.23   |
| 21  | b     | 606 | CLA  | C4B-C3B-C2B | -2.75 | 103.88      | 107.30   |
| 21  | b     | 605 | CLA  | C1D-ND-C4D  | -2.75 | 104.38      | 106.31   |
| 21  | b     | 614 | CLA  | CMB-C2B-C3B | 2.75  | 133.02      | 126.55   |
| 21  | b     | 609 | CLA  | CMD-C2D-C1D | 2.75  | 129.57      | 124.73   |
| 22  | b     | 616 | BCR  | C33-C5-C6   | -2.75 | 121.49      | 124.48   |
| 21  | a     | 402 | CLA  | CHD-C1D-ND  | -2.74 | 120.94      | 124.80   |
| 21  | d     | 402 | CLA  | CMB-C2B-C1B | 2.74  | 129.59      | 125.42   |
| 21  | d     | 406 | CLA  | CMC-C2C-C1C | 2.74  | 129.32      | 125.03   |
| 30  | e     | 101 | HEM  | C3B-C4B-NB  | -2.74 | 107.50      | 109.47   |
| 21  | b     | 606 | CLA  | C4D-CHA-C1A | -2.74 | 117.98      | 121.24   |
| 21  | a     | 402 | CLA  | CHA-C4D-ND  | 2.74  | 138.19      | 132.55   |
| 21  | d     | 407 | CLA  | CHC-C4B-NB  | -2.74 | 119.94      | 124.05   |
| 21  | c     | 509 | CLA  | O2A-CGA-CBA | 2.74  | 120.18      | 111.83   |
| 21  | c     | 506 | CLA  | C4B-C3B-C2B | -2.73 | 103.90      | 107.30   |
| 21  | a     | 402 | CLA  | O2D-CGD-O1D | -2.73 | 118.53      | 123.85   |
| 21  | b     | 615 | CLA  | C2A-C1A-CHA | -2.73 | 119.13      | 123.87   |
| 21  | b     | 610 | CLA  | C14-C13-C15 | -2.73 | 101.54      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | b     | 608 | CLA  | CHD-C1D-ND  | -2.73 | 120.96      | 124.80   |
| 21  | a     | 402 | CLA  | O2A-CGA-O1A | -2.73 | 116.80      | 123.63   |
| 22  | c     | 515 | BCR  | C19-C18-C17 | 2.73  | 123.30      | 119.01   |
| 21  | b     | 608 | CLA  | C7-C6-C5    | -2.72 | 106.00      | 113.26   |
| 21  | c     | 512 | CLA  | C4B-C3B-C2B | -2.72 | 103.92      | 107.30   |
| 21  | c     | 508 | CLA  | C2A-C1A-CHA | -2.72 | 119.15      | 123.87   |
| 21  | b     | 611 | CLA  | O2A-CGA-CBA | 2.72  | 120.12      | 111.83   |
| 21  | b     | 606 | CLA  | O2D-CGD-CBD | 2.72  | 115.98      | 111.23   |
| 22  | z     | 101 | BCR  | C23-C24-C25 | 2.71  | 134.25      | 127.00   |
| 21  | c     | 510 | CLA  | CHB-C4A-NA  | 2.71  | 128.31      | 124.40   |
| 24  | c     | 516 | DGD  | C6D-C5D-C4D | -2.71 | 106.38      | 112.07   |
| 21  | k     | 501 | CLA  | CHC-C1C-NC  | -2.71 | 120.23      | 124.31   |
| 22  | c     | 515 | BCR  | C28-C27-C26 | -2.71 | 109.23      | 114.06   |
| 19  | B     | 101 | MGE  | C1D-O6D-C5D | 2.71  | 119.00      | 113.72   |
| 21  | b     | 615 | CLA  | CHA-C4D-ND  | 2.70  | 138.13      | 132.55   |
| 21  | c     | 512 | CLA  | O2A-CGA-CBA | 2.70  | 120.08      | 111.83   |
| 21  | c     | 506 | CLA  | C2A-C1A-CHA | -2.70 | 119.18      | 123.87   |
| 21  | c     | 506 | CLA  | CMC-C2C-C1C | 2.70  | 129.25      | 125.03   |
| 21  | a     | 407 | CLA  | C4C-C3C-C2C | -2.70 | 102.96      | 106.89   |
| 24  | c     | 516 | DGD  | O1G-C1A-C2A | 2.70  | 120.07      | 111.83   |
| 21  | a     | 407 | CLA  | CHC-C4B-NB  | 2.70  | 128.10      | 124.05   |
| 21  | b     | 613 | CLA  | CBC-CAC-C3C | -2.70 | 105.11      | 112.42   |
| 22  | b     | 617 | BCR  | C29-C30-C25 | 2.69  | 114.35      | 110.44   |
| 21  | c     | 507 | CLA  | CMC-C2C-C1C | 2.69  | 129.24      | 125.03   |
| 24  | c     | 516 | DGD  | C6E-C5E-C4E | 2.69  | 119.62      | 113.02   |
| 24  | h     | 104 | DGD  | C1E-O6E-C5E | 2.69  | 118.97      | 113.72   |
| 21  | b     | 603 | CLA  | CED-O2D-CGD | 2.69  | 122.01      | 115.92   |
| 21  | b     | 604 | CLA  | C4A-NA-C1A  | -2.68 | 105.45      | 106.68   |
| 21  | b     | 609 | CLA  | CHC-C4B-NB  | 2.68  | 128.07      | 124.05   |
| 21  | b     | 613 | CLA  | C4B-CHC-C1C | -2.68 | 119.94      | 126.25   |
| 21  | b     | 612 | CLA  | O2A-CGA-CBA | 2.68  | 120.00      | 111.83   |
| 21  | b     | 602 | CLA  | C4B-C3B-C2B | -2.68 | 103.97      | 107.30   |
| 22  | c     | 515 | BCR  | C36-C18-C17 | -2.68 | 118.48      | 122.82   |
| 21  | b     | 601 | CLA  | CHC-C4B-NB  | 2.68  | 128.06      | 124.05   |
| 21  | b     | 612 | CLA  | C4C-C3C-C2C | -2.67 | 103.00      | 106.89   |
| 19  | B     | 101 | MGE  | C2G-O2G-C1B | -2.67 | 111.40      | 117.80   |
| 21  | d     | 406 | CLA  | C4D-C3D-CAD | 2.67  | 111.01      | 108.11   |
| 19  | m     | 102 | MGE  | O1G-C1A-C2A | 2.67  | 119.98      | 111.83   |
| 21  | a     | 407 | CLA  | CBA-CAA-C2A | -2.67 | 105.85      | 113.79   |
| 21  | a     | 407 | CLA  | CHC-C1C-C2C | -2.66 | 119.38      | 126.95   |
| 21  | b     | 602 | CLA  | C7-C6-C5    | -2.66 | 106.17      | 113.26   |
| 21  | c     | 505 | CLA  | CBC-CAC-C3C | -2.65 | 105.22      | 112.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | b     | 613 | CLA  | O2A-CGA-CBA | 2.65  | 119.92      | 111.83   |
| 21  | b     | 608 | CLA  | CHA-C4D-ND  | 2.65  | 138.01      | 132.55   |
| 22  | c     | 515 | BCR  | C33-C5-C4   | 2.64  | 119.23      | 113.60   |
| 21  | d     | 406 | CLA  | CGD-CBD-CAD | -2.64 | 102.30      | 110.85   |
| 24  | a     | 406 | DGD  | C2G-O2G-C1B | -2.64 | 111.49      | 117.80   |
| 21  | k     | 501 | CLA  | CHB-C1B-C2B | -2.64 | 119.78      | 127.43   |
| 22  | c     | 514 | BCR  | C27-C26-C25 | -2.63 | 119.14      | 122.70   |
| 21  | b     | 614 | CLA  | CHC-C4B-C3B | -2.63 | 115.94      | 127.37   |
| 21  | b     | 608 | CLA  | C3D-C2D-C1D | -2.63 | 102.24      | 105.83   |
| 19  | b     | 620 | MGE  | C1D-O6D-C5D | 2.63  | 118.86      | 113.72   |
| 21  | b     | 613 | CLA  | CHD-C1D-ND  | -2.63 | 121.10      | 124.80   |
| 21  | b     | 607 | CLA  | C1D-CHD-C4C | -2.63 | 120.43      | 126.02   |
| 21  | b     | 603 | CLA  | C4C-C3C-C2C | -2.63 | 103.07      | 106.89   |
| 30  | e     | 101 | HEM  | CHD-C1D-C2D | -2.62 | 120.90      | 125.03   |
| 22  | b     | 618 | BCR  | C30-C25-C26 | -2.61 | 119.07      | 122.64   |
| 21  | a     | 403 | CLA  | CHA-C4D-ND  | 2.61  | 137.93      | 132.55   |
| 21  | d     | 407 | CLA  | CMC-C2C-C1C | 2.61  | 129.10      | 125.03   |
| 19  | f     | 101 | MGE  | O6D-C1D-C2D | 2.60  | 115.70      | 110.37   |
| 28  | d     | 408 | PQ9  | C6-C5-C4    | 2.59  | 120.59      | 115.28   |
| 19  | f     | 101 | MGE  | C3D-C4D-C5D | 2.59  | 114.94      | 110.23   |
| 21  | b     | 602 | CLA  | CMB-C2B-C3B | 2.59  | 132.65      | 126.55   |
| 21  | a     | 407 | CLA  | C3A-C2A-C1A | -2.59 | 97.45       | 101.34   |
| 22  | b     | 618 | BCR  | C29-C28-C27 | 2.59  | 116.98      | 111.28   |
| 21  | b     | 609 | CLA  | O2D-CGD-O1D | -2.59 | 118.80      | 123.85   |
| 22  | b     | 616 | BCR  | C11-C10-C9  | -2.59 | 123.64      | 127.28   |
| 21  | b     | 609 | CLA  | CHD-C1D-ND  | -2.58 | 121.17      | 124.80   |
| 21  | d     | 407 | CLA  | CHB-C1B-C2B | -2.58 | 119.93      | 127.43   |
| 21  | b     | 614 | CLA  | CMA-C3A-C4A | -2.58 | 104.84      | 111.77   |
| 21  | c     | 510 | CLA  | C4C-C3C-C2C | -2.58 | 103.14      | 106.89   |
| 21  | b     | 606 | CLA  | CBC-CAC-C3C | -2.58 | 105.43      | 112.42   |
| 21  | c     | 503 | CLA  | C4-C3-C5    | 2.58  | 119.70      | 115.23   |
| 21  | c     | 510 | CLA  | O1D-CGD-CBD | -2.57 | 119.44      | 124.52   |
| 21  | c     | 513 | CLA  | CAA-C2A-C3A | 2.57  | 119.95      | 113.00   |
| 21  | k     | 501 | CLA  | CHC-C4B-NB  | -2.57 | 120.19      | 124.05   |
| 21  | d     | 402 | CLA  | C4A-NA-C1A  | -2.57 | 105.51      | 106.68   |
| 21  | d     | 407 | CLA  | O2D-CGD-O1D | -2.57 | 118.85      | 123.85   |
| 21  | b     | 601 | CLA  | CHD-C4C-NC  | 2.57  | 128.21      | 124.23   |
| 19  | b     | 619 | MGE  | C3G-O3G-C1D | -2.57 | 108.30      | 113.80   |
| 22  | b     | 618 | BCR  | C33-C5-C6   | -2.56 | 121.69      | 124.48   |
| 22  | b     | 618 | BCR  | C4-C5-C6    | -2.56 | 119.24      | 122.70   |
| 21  | c     | 506 | CLA  | CMD-C2D-C3D | -2.56 | 121.82      | 127.69   |
| 21  | b     | 610 | CLA  | CHD-C4C-NC  | 2.56  | 128.20      | 124.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | c     | 512 | CLA  | CAC-C3C-C4C | 2.55  | 128.10      | 124.79   |
| 21  | h     | 101 | CLA  | CHA-C1A-NA  | -2.54 | 120.63      | 126.39   |
| 21  | c     | 509 | CLA  | CAC-C3C-C4C | 2.54  | 128.10      | 124.79   |
| 21  | b     | 615 | CLA  | C4D-CHA-C1A | -2.54 | 118.21      | 121.24   |
| 21  | d     | 402 | CLA  | C1-O2A-CGA  | 2.54  | 122.80      | 116.65   |
| 22  | c     | 515 | BCR  | C34-C9-C10  | -2.54 | 118.70      | 122.82   |
| 21  | c     | 508 | CLA  | O2A-CGA-O1A | -2.54 | 115.62      | 123.20   |
| 21  | b     | 615 | CLA  | CED-O2D-CGD | 2.54  | 121.67      | 115.92   |
| 21  | c     | 508 | CLA  | C4A-NA-C1A  | 2.54  | 107.84      | 106.68   |
| 21  | d     | 407 | CLA  | C2A-C1A-CHA | -2.54 | 119.47      | 123.87   |
| 21  | b     | 613 | CLA  | CED-O2D-CGD | 2.54  | 121.67      | 115.92   |
| 26  | m     | 101 | LMT  | C2'-C3'-C4' | 2.53  | 115.43      | 109.68   |
| 21  | b     | 615 | CLA  | CBC-CAC-C3C | -2.53 | 105.56      | 112.42   |
| 21  | d     | 406 | CLA  | CMB-C2B-C1B | 2.53  | 129.27      | 125.42   |
| 22  | b     | 618 | BCR  | C33-C5-C4   | 2.52  | 118.98      | 113.60   |
| 21  | d     | 407 | CLA  | CHC-C1C-C2C | -2.52 | 119.79      | 126.95   |
| 21  | b     | 612 | CLA  | CHD-C4C-NC  | 2.52  | 128.13      | 124.23   |
| 21  | b     | 605 | CLA  | CBC-CAC-C3C | -2.52 | 105.60      | 112.42   |
| 21  | b     | 610 | CLA  | CMD-C2D-C1D | 2.52  | 129.16      | 124.73   |
| 24  | c     | 517 | DGD  | O5D-C6D-C5D | -2.52 | 103.75      | 109.42   |
| 21  | b     | 614 | CLA  | O2A-CGA-O1A | -2.51 | 117.34      | 123.63   |
| 21  | b     | 602 | CLA  | CHC-C4B-C3B | -2.51 | 116.46      | 127.37   |
| 21  | b     | 603 | CLA  | C4B-C3B-C2B | -2.51 | 104.18      | 107.30   |
| 21  | b     | 608 | CLA  | C2A-C1A-CHA | -2.51 | 119.51      | 123.87   |
| 21  | c     | 505 | CLA  | C7-C6-C5    | -2.51 | 106.57      | 113.26   |
| 21  | d     | 407 | CLA  | CMD-C2D-C3D | -2.51 | 121.94      | 127.69   |
| 21  | c     | 512 | CLA  | CHB-C1B-NB  | -2.51 | 120.29      | 124.05   |
| 21  | a     | 403 | CLA  | C4C-C3C-C2C | -2.51 | 103.24      | 106.89   |
| 21  | d     | 406 | CLA  | CHB-C1B-C2B | -2.51 | 120.15      | 127.43   |
| 22  | b     | 616 | BCR  | C20-C21-C22 | -2.51 | 123.76      | 127.28   |
| 21  | b     | 603 | CLA  | C7-C6-C5    | -2.50 | 106.59      | 113.26   |
| 21  | b     | 601 | CLA  | O2A-CGA-CBA | 2.50  | 119.46      | 111.83   |
| 22  | b     | 618 | BCR  | C28-C27-C26 | -2.50 | 109.60      | 114.06   |
| 21  | c     | 504 | CLA  | O2A-CGA-O1A | -2.49 | 117.39      | 123.63   |
| 24  | c     | 516 | DGD  | C6D-O5D-C1E | -2.49 | 108.45      | 113.80   |
| 21  | k     | 501 | CLA  | CAC-C3C-C4C | 2.49  | 128.03      | 124.79   |
| 22  | h     | 103 | BCR  | C7-C6-C5    | -2.49 | 115.82      | 121.56   |
| 22  | h     | 103 | BCR  | C15-C14-C13 | -2.49 | 123.79      | 127.28   |
| 21  | b     | 606 | CLA  | CGD-CBD-CAD | -2.49 | 102.79      | 110.85   |
| 21  | c     | 504 | CLA  | C16-C17-C18 | -2.49 | 104.83      | 115.94   |
| 30  | e     | 101 | HEM  | C1A-CHA-C4D | -2.49 | 120.39      | 126.25   |
| 21  | d     | 402 | CLA  | C3C-C4C-NC  | 2.49  | 113.62      | 110.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | c     | 512 | CLA  | O2D-CGD-O1D | -2.49 | 119.01      | 123.85   |
| 21  | c     | 505 | CLA  | CHD-C1D-ND  | -2.49 | 121.30      | 124.80   |
| 22  | b     | 617 | BCR  | C39-C30-C25 | -2.48 | 106.36      | 110.24   |
| 21  | a     | 407 | CLA  | O2D-CGD-O1D | -2.48 | 119.02      | 123.85   |
| 21  | b     | 602 | CLA  | O2A-CGA-O1A | -2.48 | 117.44      | 123.63   |
| 21  | c     | 509 | CLA  | CMD-C2D-C1D | 2.47  | 129.09      | 124.73   |
| 21  | c     | 505 | CLA  | CED-O2D-CGD | 2.47  | 121.53      | 115.92   |
| 21  | c     | 503 | CLA  | O2A-CGA-O1A | -2.47 | 117.44      | 123.63   |
| 30  | e     | 101 | HEM  | CHD-C4C-NC  | 2.47  | 127.15      | 124.45   |
| 21  | a     | 403 | CLA  | CHC-C1C-C2C | -2.47 | 119.93      | 126.95   |
| 22  | b     | 616 | BCR  | C29-C30-C25 | 2.47  | 114.02      | 110.44   |
| 25  | d     | 403 | PHO  | C4D-CHA-CBD | 2.47  | 109.64      | 108.45   |
| 21  | b     | 606 | CLA  | C7-C6-C5    | -2.47 | 106.69      | 113.26   |
| 21  | d     | 406 | CLA  | CHD-C1D-ND  | -2.47 | 121.33      | 124.80   |
| 21  | c     | 509 | CLA  | C4C-C3C-C2C | -2.46 | 103.30      | 106.89   |
| 21  | b     | 611 | CLA  | C4B-CHC-C1C | -2.46 | 120.46      | 126.25   |
| 22  | h     | 103 | BCR  | C30-C25-C26 | -2.46 | 119.28      | 122.64   |
| 19  | b     | 619 | MGE  | O1G-C1A-O1A | -2.45 | 117.49      | 123.63   |
| 21  | b     | 609 | CLA  | C3B-C4B-NB  | 2.45  | 112.72      | 110.53   |
| 21  | c     | 507 | CLA  | C2A-C1A-CHA | -2.45 | 119.61      | 123.87   |
| 22  | h     | 103 | BCR  | C39-C30-C25 | -2.45 | 106.40      | 110.24   |
| 21  | c     | 511 | CLA  | C4B-C3B-C2B | -2.44 | 104.26      | 107.30   |
| 21  | b     | 612 | CLA  | CHA-C4D-ND  | 2.44  | 137.59      | 132.55   |
| 21  | b     | 601 | CLA  | C2A-C1A-CHA | -2.44 | 119.63      | 123.87   |
| 21  | d     | 406 | CLA  | C1-C2-C3    | -2.44 | 122.20      | 126.20   |
| 21  | c     | 503 | CLA  | C2A-C1A-CHA | -2.44 | 119.63      | 123.87   |
| 24  | a     | 406 | DGD  | O1G-C1A-C2A | 2.44  | 119.27      | 111.83   |
| 22  | h     | 103 | BCR  | C16-C15-C14 | -2.44 | 118.54      | 123.52   |
| 22  | h     | 103 | BCR  | C28-C27-C26 | -2.43 | 109.71      | 114.06   |
| 21  | k     | 501 | CLA  | O2D-CGD-O1D | -2.43 | 119.12      | 123.85   |
| 21  | b     | 607 | CLA  | CMD-C2D-C1D | 2.42  | 128.99      | 124.73   |
| 21  | b     | 606 | CLA  | CHC-C4B-NB  | 2.42  | 127.68      | 124.05   |
| 21  | c     | 508 | CLA  | C3C-C4C-NC  | 2.42  | 113.53      | 110.43   |
| 21  | b     | 605 | CLA  | CMB-C2B-C1B | 2.42  | 129.10      | 125.42   |
| 21  | b     | 611 | CLA  | CED-O2D-CGD | 2.42  | 121.40      | 115.92   |
| 21  | a     | 402 | CLA  | C1-C2-C3    | -2.42 | 122.24      | 126.20   |
| 25  | d     | 401 | PHO  | C7-C6-C5    | -2.41 | 106.83      | 113.26   |
| 21  | b     | 601 | CLA  | C16-C17-C18 | -2.41 | 105.16      | 115.94   |
| 28  | d     | 408 | PQ9  | C11-C2-C3   | -2.41 | 120.54      | 123.39   |
| 22  | a     | 404 | BCR  | C36-C18-C17 | -2.41 | 118.91      | 122.82   |
| 21  | c     | 511 | CLA  | C4C-C3C-C2C | -2.41 | 103.39      | 106.89   |
| 21  | c     | 512 | CLA  | C1-C2-C3    | -2.41 | 122.26      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | c     | 514 | BCR  | C34-C9-C8   | 2.40  | 121.76      | 118.09   |
| 25  | d     | 403 | PHO  | OBD-CAD-C3D | -2.40 | 124.16      | 127.89   |
| 21  | c     | 513 | CLA  | C2A-C3A-C4A | -2.39 | 98.00       | 101.87   |
| 26  | m     | 101 | LMT  | O1'-C1'-C2' | 2.39  | 111.90      | 108.27   |
| 22  | c     | 515 | BCR  | C38-C26-C25 | -2.38 | 121.88      | 124.48   |
| 21  | c     | 511 | CLA  | CAC-C3C-C4C | 2.38  | 127.89      | 124.79   |
| 22  | b     | 616 | BCR  | C7-C8-C9    | -2.38 | 122.71      | 126.23   |
| 21  | c     | 505 | CLA  | O2D-CGD-O1D | -2.38 | 119.21      | 123.85   |
| 21  | b     | 605 | CLA  | C4B-C3B-C2B | -2.38 | 104.35      | 107.30   |
| 21  | b     | 606 | CLA  | C3B-C4B-NB  | 2.38  | 112.65      | 110.53   |
| 21  | c     | 504 | CLA  | CHD-C1D-ND  | -2.38 | 121.46      | 124.80   |
| 21  | d     | 407 | CLA  | O2A-CGA-CBA | 2.37  | 119.08      | 111.83   |
| 21  | b     | 606 | CLA  | C3C-C4C-NC  | 2.37  | 113.47      | 110.43   |
| 24  | c     | 516 | DGD  | C4E-C3E-C2E | 2.37  | 114.99      | 110.83   |
| 22  | b     | 616 | BCR  | C1-C6-C5    | -2.37 | 119.40      | 122.64   |
| 21  | b     | 606 | CLA  | C1-C2-C3    | -2.37 | 122.31      | 126.20   |
| 21  | b     | 610 | CLA  | C7-C6-C5    | -2.37 | 106.95      | 113.26   |
| 22  | b     | 616 | BCR  | C15-C16-C17 | -2.37 | 118.67      | 123.52   |
| 28  | d     | 408 | PQ9  | C31-C32-C33 | -2.36 | 122.22      | 127.62   |
| 21  | b     | 611 | CLA  | CMB-C2B-C1B | 2.36  | 129.01      | 125.42   |
| 21  | d     | 406 | CLA  | C4B-CHC-C1C | -2.36 | 120.70      | 126.25   |
| 21  | a     | 407 | CLA  | O2A-CGA-CBA | 2.36  | 119.03      | 111.83   |
| 21  | c     | 511 | CLA  | C2A-C1A-CHA | -2.36 | 119.78      | 123.87   |
| 22  | c     | 515 | BCR  | C35-C13-C12 | 2.36  | 121.69      | 118.09   |
| 21  | c     | 504 | CLA  | C4C-C3C-C2C | -2.36 | 103.46      | 106.89   |
| 30  | e     | 101 | HEM  | C1C-CHC-C4B | -2.35 | 121.02      | 126.02   |
| 28  | d     | 408 | PQ9  | C29-C28-C27 | -2.35 | 117.59      | 123.63   |
| 24  | c     | 516 | DGD  | O6D-C5D-C4D | -2.35 | 105.47      | 109.70   |
| 22  | h     | 103 | BCR  | C34-C9-C10  | -2.35 | 119.02      | 122.82   |
| 21  | b     | 610 | CLA  | C3B-C2B-C1B | -2.34 | 104.41      | 107.17   |
| 21  | d     | 406 | CLA  | O2A-CGA-O1A | -2.34 | 117.77      | 123.63   |
| 22  | b     | 616 | BCR  | C23-C24-C25 | -2.34 | 120.75      | 127.00   |
| 21  | b     | 604 | CLA  | C4B-C3B-C2B | -2.34 | 104.40      | 107.30   |
| 19  | b     | 620 | MGE  | C3G-C2G-C1G | -2.34 | 106.34      | 111.78   |
| 21  | c     | 511 | CLA  | C4-C3-C2    | -2.34 | 117.63      | 123.63   |
| 21  | b     | 604 | CLA  | C14-C13-C12 | -2.33 | 102.96      | 111.27   |
| 21  | a     | 402 | CLA  | CMC-C2C-C3C | 2.33  | 132.46      | 126.15   |
| 19  | B     | 101 | MGE  | C4D-C3D-C2D | 2.33  | 114.92      | 110.83   |
| 21  | k     | 501 | CLA  | C2A-C1A-CHA | -2.33 | 119.82      | 123.87   |
| 21  | b     | 615 | CLA  | CHC-C4B-NB  | 2.33  | 127.54      | 124.05   |
| 21  | a     | 402 | CLA  | O2A-CGA-CBA | 2.32  | 118.92      | 111.83   |
| 21  | c     | 504 | CLA  | C3C-C4C-NC  | 2.32  | 113.41      | 110.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28  | d     | 408 | PQ9  | C14-C13-C15 | 2.32  | 119.26      | 115.23   |
| 21  | b     | 615 | CLA  | C1-O2A-CGA  | 2.32  | 123.50      | 116.07   |
| 21  | b     | 613 | CLA  | C2A-C1A-CHA | -2.32 | 119.84      | 123.87   |
| 22  | b     | 618 | BCR  | C16-C15-C14 | -2.32 | 118.77      | 123.52   |
| 21  | c     | 510 | CLA  | C4B-C3B-C2B | -2.32 | 104.42      | 107.30   |
| 21  | b     | 604 | CLA  | C1-C2-C3    | -2.32 | 122.40      | 126.20   |
| 21  | d     | 402 | CLA  | CHC-C4B-C3B | -2.32 | 117.30      | 127.37   |
| 21  | c     | 505 | CLA  | O2A-CGA-CBA | 2.32  | 118.91      | 111.83   |
| 21  | b     | 608 | CLA  | CBC-CAC-C3C | -2.32 | 106.14      | 112.42   |
| 21  | c     | 511 | CLA  | C1-C2-C3    | -2.32 | 122.40      | 126.20   |
| 21  | b     | 615 | CLA  | CMB-C2B-C3B | 2.31  | 131.98      | 126.55   |
| 21  | c     | 510 | CLA  | CHD-C4C-NC  | 2.31  | 127.81      | 124.23   |
| 21  | c     | 509 | CLA  | O2A-CGA-O1A | -2.31 | 117.86      | 123.63   |
| 21  | b     | 608 | CLA  | C4B-C3B-C2B | -2.31 | 104.44      | 107.30   |
| 21  | c     | 511 | CLA  | C3C-C4C-NC  | 2.30  | 113.38      | 110.43   |
| 21  | a     | 402 | CLA  | C3B-C4B-NB  | 2.30  | 112.58      | 110.53   |
| 21  | a     | 403 | CLA  | C4B-CHC-C1C | -2.30 | 120.84      | 126.25   |
| 24  | c     | 516 | DGD  | C1E-O6E-C5E | 2.30  | 118.21      | 113.72   |
| 22  | c     | 515 | BCR  | C30-C25-C24 | 2.30  | 121.88      | 115.65   |
| 22  | b     | 616 | BCR  | C10-C11-C12 | -2.30 | 116.55      | 123.20   |
| 21  | c     | 505 | CLA  | C4C-C3C-C2C | -2.30 | 103.55      | 106.89   |
| 21  | b     | 614 | CLA  | C1-O2A-CGA  | 2.30  | 122.21      | 116.65   |
| 21  | b     | 607 | CLA  | CHD-C4C-NC  | 2.29  | 127.79      | 124.23   |
| 21  | b     | 614 | CLA  | C11-C10-C8  | -2.29 | 108.34      | 115.97   |
| 21  | a     | 403 | CLA  | O2A-CGA-CBA | 2.29  | 118.83      | 111.83   |
| 21  | c     | 507 | CLA  | C4B-C3B-C2B | -2.29 | 104.45      | 107.30   |
| 21  | c     | 509 | CLA  | C4D-CHA-C1A | -2.29 | 118.51      | 121.24   |
| 21  | c     | 513 | CLA  | CHD-C4C-C3C | -2.28 | 121.45      | 124.77   |
| 21  | c     | 509 | CLA  | C1-O2A-CGA  | 2.27  | 122.15      | 116.65   |
| 21  | b     | 605 | CLA  | O2A-CGA-CBA | 2.27  | 118.75      | 111.83   |
| 21  | c     | 504 | CLA  | C6-C5-C3    | -2.27 | 107.94      | 113.47   |
| 21  | c     | 511 | CLA  | CHD-C1D-ND  | -2.27 | 121.61      | 124.80   |
| 22  | b     | 617 | BCR  | C33-C5-C6   | -2.27 | 122.01      | 124.48   |
| 21  | c     | 504 | CLA  | O2A-CGA-CBA | 2.27  | 118.74      | 111.83   |
| 21  | b     | 613 | CLA  | C3D-C4D-ND  | 2.26  | 113.67      | 109.99   |
| 21  | c     | 503 | CLA  | CHC-C4B-C3B | -2.26 | 117.55      | 127.37   |
| 21  | c     | 511 | CLA  | CMB-C2B-C1B | 2.26  | 128.87      | 125.42   |
| 21  | b     | 601 | CLA  | CED-O2D-CGD | 2.26  | 121.05      | 115.92   |
| 30  | e     | 101 | HEM  | C4D-ND-C1D  | 2.26  | 107.89      | 105.21   |
| 21  | b     | 611 | CLA  | C4B-C3B-C2B | -2.26 | 104.49      | 107.30   |
| 22  | a     | 404 | BCR  | C8-C9-C10   | 2.26  | 122.57      | 119.01   |
| 21  | b     | 610 | CLA  | CAC-C3C-C4C | 2.26  | 127.73      | 124.79   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | d     | 410 | MGE  | O1G-C1A-O1A | -2.26 | 117.97      | 123.63   |
| 24  | c     | 516 | DGD  | O6D-C1D-C2D | 2.26  | 115.01      | 110.37   |
| 21  | b     | 605 | CLA  | CHA-C4D-ND  | 2.26  | 137.21      | 132.55   |
| 22  | b     | 616 | BCR  | C24-C23-C22 | -2.26 | 122.89      | 126.23   |
| 21  | d     | 406 | CLA  | C4-C3-C5    | 2.26  | 119.14      | 115.23   |
| 22  | a     | 404 | BCR  | C33-C5-C4   | 2.25  | 118.40      | 113.60   |
| 21  | c     | 508 | CLA  | CHC-C4B-C3B | -2.25 | 117.60      | 127.37   |
| 21  | c     | 509 | CLA  | O1D-CGD-CBD | -2.25 | 120.08      | 124.52   |
| 24  | h     | 104 | DGD  | O1G-C1A-O1A | -2.25 | 118.01      | 123.63   |
| 21  | c     | 507 | CLA  | CHB-C1B-C2B | -2.24 | 120.91      | 127.43   |
| 24  | c     | 516 | DGD  | O5D-C1E-C2E | 2.24  | 111.68      | 108.27   |
| 21  | c     | 506 | CLA  | O1D-CGD-CBD | -2.24 | 120.10      | 124.52   |
| 21  | b     | 609 | CLA  | O2A-CGA-CBA | 2.24  | 118.66      | 111.83   |
| 25  | d     | 403 | PHO  | C3D-CAD-CBD | 2.24  | 110.55      | 107.61   |
| 24  | c     | 517 | DGD  | O1G-C1A-O1A | -2.24 | 118.03      | 123.63   |
| 21  | c     | 503 | CLA  | C7-C6-C5    | -2.24 | 107.31      | 113.26   |
| 21  | a     | 407 | CLA  | C4B-CHC-C1C | -2.23 | 120.99      | 126.25   |
| 21  | d     | 406 | CLA  | CHC-C4B-NB  | -2.23 | 120.70      | 124.05   |
| 22  | b     | 617 | BCR  | C30-C25-C26 | -2.23 | 119.59      | 122.64   |
| 21  | b     | 611 | CLA  | C2B-C1B-NB  | 2.23  | 112.64      | 110.33   |
| 24  | c     | 516 | DGD  | O2G-C1B-O1B | -2.23 | 118.49      | 123.70   |
| 28  | d     | 408 | PQ9  | C24-C23-C25 | 2.23  | 119.10      | 115.23   |
| 21  | a     | 407 | CLA  | CED-O2D-CGD | 2.23  | 120.97      | 115.92   |
| 22  | b     | 616 | BCR  | C8-C7-C6    | -2.23 | 121.05      | 127.00   |
| 21  | a     | 407 | CLA  | O2A-CGA-O1A | -2.23 | 118.06      | 123.63   |
| 21  | b     | 613 | CLA  | C4D-C3D-CAD | 2.23  | 110.52      | 108.11   |
| 21  | c     | 513 | CLA  | CHD-C4C-NC  | -2.23 | 120.78      | 124.23   |
| 21  | c     | 513 | CLA  | C1-C2-C3    | -2.22 | 123.17      | 126.76   |
| 21  | b     | 602 | CLA  | C3C-C4C-NC  | 2.22  | 113.28      | 110.43   |
| 21  | b     | 613 | CLA  | CHC-C4B-C3B | -2.22 | 117.74      | 127.37   |
| 21  | c     | 503 | CLA  | O2A-CGA-CBA | 2.22  | 118.60      | 111.83   |
| 21  | h     | 101 | CLA  | O2D-CGD-O1D | -2.22 | 119.53      | 123.85   |
| 21  | c     | 511 | CLA  | O2D-CGD-O1D | -2.22 | 119.53      | 123.85   |
| 21  | b     | 607 | CLA  | C6-C5-C3    | -2.21 | 108.08      | 113.47   |
| 21  | b     | 611 | CLA  | CMC-C2C-C1C | 2.21  | 128.49      | 125.03   |
| 21  | b     | 611 | CLA  | CHC-C4B-C3B | -2.21 | 117.80      | 127.37   |
| 22  | b     | 618 | BCR  | C1-C6-C5    | -2.20 | 119.62      | 122.64   |
| 21  | d     | 407 | CLA  | CHC-C1C-NC  | -2.20 | 121.00      | 124.31   |
| 21  | b     | 603 | CLA  | C3B-C4B-NB  | 2.20  | 112.49      | 110.53   |
| 22  | b     | 616 | BCR  | C38-C26-C27 | 2.19  | 118.28      | 113.60   |
| 21  | c     | 509 | CLA  | CHC-C4B-C3B | -2.19 | 117.85      | 127.37   |
| 21  | a     | 407 | CLA  | C1D-CHD-C4C | -2.19 | 121.36      | 126.02   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | b     | 610 | CLA  | CHD-C1D-ND  | -2.19 | 121.72      | 124.80   |
| 21  | d     | 402 | CLA  | CGD-CBD-CAD | -2.19 | 103.76      | 110.85   |
| 21  | c     | 507 | CLA  | O2A-CGA-CBA | 2.18  | 118.50      | 111.83   |
| 19  | c     | 502 | MGE  | C3G-C2G-C1G | -2.18 | 106.71      | 111.78   |
| 21  | k     | 501 | CLA  | CHB-C1B-NB  | -2.18 | 120.78      | 124.05   |
| 21  | d     | 402 | CLA  | C4C-C3C-C2C | -2.17 | 103.73      | 106.89   |
| 21  | c     | 509 | CLA  | C11-C12-C13 | -2.17 | 108.74      | 115.97   |
| 21  | a     | 403 | CLA  | O2A-CGA-O1A | -2.17 | 118.19      | 123.63   |
| 21  | b     | 603 | CLA  | CHC-C4B-C3B | -2.17 | 117.94      | 127.37   |
| 21  | c     | 508 | CLA  | O2D-CGD-O1D | -2.17 | 119.62      | 123.85   |
| 21  | c     | 503 | CLA  | C1-O2A-CGA  | 2.17  | 121.91      | 116.65   |
| 21  | b     | 602 | CLA  | C1-C2-C3    | -2.17 | 122.64      | 126.20   |
| 21  | d     | 402 | CLA  | O2D-CGD-O1D | -2.17 | 119.63      | 123.85   |
| 22  | z     | 101 | BCR  | C38-C26-C27 | 2.17  | 118.22      | 113.60   |
| 22  | d     | 409 | BCR  | C28-C27-C26 | -2.16 | 110.21      | 114.06   |
| 21  | b     | 609 | CLA  | C4D-C3D-CAD | 2.16  | 110.45      | 108.11   |
| 21  | a     | 407 | CLA  | OBD-CAD-C3D | -2.15 | 123.38      | 128.42   |
| 19  | f     | 101 | MGE  | C3G-O3G-C1D | -2.15 | 109.18      | 113.80   |
| 21  | h     | 101 | CLA  | CED-O2D-CGD | 2.15  | 120.80      | 115.92   |
| 22  | b     | 616 | BCR  | C34-C9-C8   | 2.15  | 121.38      | 118.09   |
| 21  | b     | 610 | CLA  | C2A-C1A-CHA | -2.15 | 120.13      | 123.87   |
| 21  | b     | 610 | CLA  | C17-C16-C15 | -2.15 | 103.64      | 113.28   |
| 26  | m     | 101 | LMT  | C1-O1'-C1'  | -2.15 | 110.01      | 113.68   |
| 21  | d     | 402 | CLA  | OBD-CAD-C3D | -2.15 | 123.39      | 128.42   |
| 22  | c     | 514 | BCR  | C33-C5-C6   | -2.15 | 122.14      | 124.48   |
| 21  | b     | 605 | CLA  | CHC-C1C-C2C | -2.15 | 120.85      | 126.95   |
| 24  | c     | 516 | DGD  | O4D-C4D-C5D | -2.15 | 104.04      | 109.32   |
| 21  | c     | 505 | CLA  | O2D-CGD-CBD | 2.14  | 114.97      | 111.23   |
| 19  | B     | 101 | MGE  | O1G-C1A-O1A | -2.14 | 118.27      | 123.63   |
| 25  | d     | 403 | PHO  | CMB-C2B-C3B | 2.14  | 128.96      | 124.68   |
| 21  | c     | 513 | CLA  | CED-O2D-CGD | 2.14  | 120.77      | 115.92   |
| 21  | a     | 407 | CLA  | C4B-C3B-C2B | -2.14 | 104.64      | 107.30   |
| 21  | c     | 505 | CLA  | CHD-C4C-NC  | 2.14  | 127.55      | 124.23   |
| 21  | d     | 407 | CLA  | C4D-C3D-CAD | 2.14  | 110.43      | 108.11   |
| 21  | b     | 610 | CLA  | C3C-C4C-NC  | 2.14  | 113.17      | 110.43   |
| 21  | b     | 601 | CLA  | C17-C16-C15 | -2.14 | 103.70      | 113.28   |
| 22  | b     | 616 | BCR  | C33-C5-C4   | 2.13  | 118.15      | 113.60   |
| 21  | c     | 505 | CLA  | C2A-C1A-CHA | -2.13 | 120.16      | 123.87   |
| 21  | c     | 513 | CLA  | O2D-CGD-O1D | -2.13 | 119.69      | 123.85   |
| 21  | b     | 614 | CLA  | CBB-CAB-C3B | -2.13 | 116.86      | 127.53   |
| 21  | b     | 608 | CLA  | CMB-C2B-C1B | 2.13  | 128.67      | 125.42   |
| 28  | d     | 408 | PQ9  | C29-C28-C30 | 2.13  | 118.93      | 115.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | c     | 503 | CLA  | C4B-C3B-C2B | -2.13 | 104.65      | 107.30   |
| 28  | d     | 408 | PQ9  | C21-C22-C23 | -2.13 | 122.75      | 127.62   |
| 21  | b     | 615 | CLA  | C3B-C4B-NB  | 2.13  | 112.43      | 110.53   |
| 21  | c     | 513 | CLA  | C5-C3-C4    | 2.13  | 119.49      | 114.59   |
| 21  | b     | 605 | CLA  | C4-C3-C5    | 2.12  | 118.91      | 115.23   |
| 21  | c     | 509 | CLA  | CHC-C1C-NC  | -2.12 | 121.12      | 124.31   |
| 21  | h     | 101 | CLA  | CGD-CBD-CAD | 2.12  | 117.71      | 110.85   |
| 28  | d     | 408 | PQ9  | C3-C4-C5    | 2.12  | 121.52      | 119.00   |
| 21  | b     | 605 | CLA  | C1-C2-C3    | -2.12 | 122.72      | 126.20   |
| 21  | c     | 505 | CLA  | O2A-CGA-O1A | -2.12 | 118.33      | 123.63   |
| 26  | d     | 404 | LMT  | C1'-O5'-C5' | 2.12  | 117.85      | 113.72   |
| 21  | a     | 407 | CLA  | CHB-C1B-NB  | 2.12  | 127.22      | 124.05   |
| 21  | b     | 604 | CLA  | CAC-C3C-C2C | -2.11 | 123.67      | 127.56   |
| 21  | c     | 503 | CLA  | CHA-C4D-ND  | 2.11  | 136.91      | 132.55   |
| 21  | d     | 402 | CLA  | CMD-C2D-C3D | 2.11  | 132.53      | 127.69   |
| 21  | b     | 607 | CLA  | C6-C7-C8    | -2.11 | 108.95      | 115.97   |
| 21  | b     | 609 | CLA  | C4B-C3B-C2B | -2.11 | 104.68      | 107.30   |
| 21  | h     | 101 | CLA  | CHB-C4A-NA  | -2.11 | 121.36      | 124.40   |
| 21  | b     | 603 | CLA  | C1D-CHD-C4C | -2.11 | 121.54      | 126.02   |
| 22  | z     | 101 | BCR  | C19-C18-C17 | 2.11  | 122.33      | 119.01   |
| 22  | b     | 616 | BCR  | C16-C15-C14 | -2.11 | 119.21      | 123.52   |
| 24  | a     | 406 | DGD  | C1E-O6E-C5E | 2.11  | 117.83      | 113.72   |
| 21  | a     | 402 | CLA  | C6-C5-C3    | -2.10 | 108.35      | 113.47   |
| 21  | b     | 611 | CLA  | CHA-C4D-ND  | 2.10  | 136.89      | 132.55   |
| 21  | c     | 510 | CLA  | CMC-C2C-C1C | 2.10  | 128.32      | 125.03   |
| 26  | t     | 301 | LMT  | C4B-C3B-C2B | 2.10  | 114.52      | 110.83   |
| 25  | d     | 403 | PHO  | CBA-CAA-C2A | -2.10 | 107.60      | 113.78   |
| 21  | c     | 512 | CLA  | C4-C3-C5    | 2.10  | 118.60      | 116.13   |
| 21  | b     | 614 | CLA  | CBC-CAC-C3C | -2.10 | 106.74      | 112.42   |
| 21  | c     | 511 | CLA  | CHC-C4B-C3B | -2.09 | 118.28      | 127.37   |
| 22  | h     | 103 | BCR  | C31-C1-C6   | -2.09 | 106.96      | 110.24   |
| 25  | d     | 403 | PHO  | C16-C15-C13 | -2.09 | 109.01      | 115.97   |
| 21  | a     | 402 | CLA  | O2D-CGD-CBD | 2.09  | 114.89      | 111.23   |
| 19  | c     | 502 | MGE  | O1G-C1A-O1A | -2.09 | 118.40      | 123.63   |
| 21  | b     | 610 | CLA  | C16-C15-C13 | 2.09  | 122.91      | 115.97   |
| 21  | c     | 511 | CLA  | C3D-C4D-ND  | 2.09  | 113.38      | 109.99   |
| 22  | z     | 101 | BCR  | C20-C19-C18 | -2.08 | 120.65      | 126.36   |
| 19  | b     | 620 | MGE  | O1G-C1A-O1A | -2.08 | 118.43      | 123.63   |
| 22  | d     | 409 | BCR  | C33-C5-C6   | -2.07 | 122.22      | 124.48   |
| 22  | c     | 515 | BCR  | C37-C22-C23 | 2.07  | 121.25      | 118.09   |
| 21  | d     | 406 | CLA  | CBC-CAC-C3C | -2.07 | 106.81      | 112.42   |
| 21  | b     | 611 | CLA  | CMD-C2D-C1D | 2.07  | 128.37      | 124.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | b     | 608 | CLA  | CBB-CAB-C3B | -2.07 | 117.20      | 127.53   |
| 21  | b     | 602 | CLA  | CHC-C1C-NC  | -2.07 | 121.20      | 124.31   |
| 21  | b     | 614 | CLA  | CHB-C1B-C2B | -2.07 | 121.43      | 127.43   |
| 21  | b     | 601 | CLA  | CHB-C1B-C2B | -2.07 | 121.43      | 127.43   |
| 21  | c     | 504 | CLA  | CHC-C4B-NB  | 2.07  | 127.15      | 124.05   |
| 20  | l     | 101 | SQD  | O48-C23-O10 | -2.06 | 118.47      | 123.63   |
| 28  | d     | 408 | PQ9  | C31-C30-C28 | -2.06 | 106.35      | 113.19   |
| 21  | b     | 611 | CLA  | C2A-C1A-CHA | -2.06 | 120.29      | 123.87   |
| 21  | b     | 603 | CLA  | O2A-CGA-CBA | 2.06  | 118.12      | 111.83   |
| 21  | b     | 615 | CLA  | CHC-C1C-NC  | -2.06 | 121.21      | 124.31   |
| 21  | b     | 605 | CLA  | C4C-C3C-C2C | -2.06 | 103.90      | 106.89   |
| 21  | k     | 501 | CLA  | CMA-C3A-C4A | -2.06 | 106.25      | 111.77   |
| 21  | b     | 612 | CLA  | CHC-C4B-C3B | -2.06 | 118.45      | 127.37   |
| 21  | b     | 605 | CLA  | C3C-C4C-NC  | 2.05  | 113.06      | 110.43   |
| 22  | a     | 404 | BCR  | C29-C28-C27 | -2.05 | 106.76      | 111.28   |
| 22  | b     | 618 | BCR  | C20-C19-C18 | -2.05 | 120.73      | 126.36   |
| 21  | c     | 510 | CLA  | CHB-C1B-NB  | -2.05 | 120.97      | 124.05   |
| 19  | d     | 410 | MGE  | C1D-O6D-C5D | 2.05  | 117.72      | 113.72   |
| 22  | h     | 103 | BCR  | C2-C1-C6    | 2.05  | 113.41      | 110.44   |
| 21  | a     | 403 | CLA  | OBD-CAD-C3D | -2.05 | 123.63      | 128.42   |
| 21  | d     | 406 | CLA  | CHB-C1B-NB  | -2.04 | 120.98      | 124.05   |
| 21  | a     | 403 | CLA  | C4A-NA-C1A  | 2.04  | 107.61      | 106.68   |
| 21  | b     | 605 | CLA  | C4B-CHC-C1C | -2.04 | 121.45      | 126.25   |
| 21  | a     | 403 | CLA  | C2A-C1A-CHA | -2.04 | 120.33      | 123.87   |
| 21  | b     | 607 | CLA  | C2A-C1A-CHA | -2.04 | 120.33      | 123.87   |
| 22  | b     | 617 | BCR  | C1-C6-C7    | 2.04  | 121.17      | 115.65   |
| 21  | c     | 509 | CLA  | C5-C3-C2    | -2.04 | 116.60      | 121.17   |
| 21  | a     | 403 | CLA  | C3A-C2A-C1A | 2.03  | 104.39      | 101.34   |
| 30  | e     | 101 | HEM  | C4C-CHD-C1D | -2.03 | 121.70      | 126.02   |
| 21  | b     | 602 | CLA  | CBB-CAB-C3B | -2.03 | 117.38      | 127.53   |
| 21  | b     | 607 | CLA  | C1-O2A-CGA  | 2.03  | 121.56      | 116.65   |
| 21  | c     | 513 | CLA  | C4B-CHC-C1C | -2.03 | 121.48      | 126.25   |
| 21  | c     | 512 | CLA  | CHB-C1B-C2B | -2.03 | 121.54      | 127.43   |
| 21  | d     | 407 | CLA  | C1-C2-C3    | -2.02 | 123.49      | 126.76   |
| 21  | b     | 611 | CLA  | C1D-ND-C4D  | -2.02 | 104.89      | 106.31   |
| 21  | b     | 608 | CLA  | C4-C3-C5    | 2.02  | 118.73      | 115.23   |
| 21  | a     | 402 | CLA  | C4C-C3C-C2C | -2.02 | 103.95      | 106.89   |
| 21  | b     | 610 | CLA  | CHC-C4B-NB  | 2.02  | 127.08      | 124.05   |
| 21  | c     | 505 | CLA  | CMD-C2D-C3D | 2.02  | 132.32      | 127.69   |
| 21  | a     | 402 | CLA  | CHC-C1C-C2C | -2.02 | 121.22      | 126.95   |
| 25  | d     | 401 | PHO  | CAA-C2A-C3A | -2.01 | 107.56      | 113.00   |
| 22  | c     | 515 | BCR  | C29-C30-C25 | -2.01 | 107.51      | 110.44   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | b     | 603 | CLA  | CBB-CAB-C3B | -2.01 | 117.47      | 127.53   |
| 21  | c     | 505 | CLA  | C3C-C4C-NC  | 2.01  | 113.00      | 110.43   |
| 21  | b     | 607 | CLA  | CMC-C2C-C1C | 2.01  | 128.18      | 125.03   |
| 21  | c     | 505 | CLA  | CBB-CAB-C3B | -2.01 | 117.48      | 127.53   |
| 21  | c     | 508 | CLA  | C4C-C3C-C2C | -2.01 | 103.97      | 106.89   |
| 21  | d     | 406 | CLA  | CMD-C2D-C3D | -2.01 | 123.08      | 127.69   |
| 21  | b     | 608 | CLA  | O2A-CGA-O1A | -2.01 | 118.61      | 123.63   |
| 21  | d     | 406 | CLA  | C6-C5-C3    | -2.01 | 108.58      | 113.47   |
| 22  | d     | 409 | BCR  | C35-C13-C12 | 2.01  | 121.15      | 118.09   |
| 31  | h     | 102 | HTG  | C1-O5-C5    | 2.00  | 116.16      | 112.56   |
| 19  | b     | 620 | MGE  | C3G-O3G-C1D | -2.00 | 109.50      | 113.80   |
| 24  | h     | 104 | DGD  | O2G-C1B-O1B | -2.00 | 119.02      | 123.70   |
| 21  | c     | 505 | CLA  | C11-C10-C8  | -2.00 | 109.31      | 115.97   |
| 21  | c     | 511 | CLA  | O2A-CGA-O1A | -2.00 | 118.62      | 123.63   |

All (21) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 21  | a     | 402 | CLA  | ND   |
| 21  | b     | 601 | CLA  | ND   |
| 21  | b     | 602 | CLA  | ND   |
| 21  | b     | 603 | CLA  | ND   |
| 21  | b     | 604 | CLA  | ND   |
| 21  | b     | 605 | CLA  | ND   |
| 21  | b     | 606 | CLA  | ND   |
| 21  | b     | 609 | CLA  | ND   |
| 21  | b     | 611 | CLA  | ND   |
| 21  | b     | 612 | CLA  | ND   |
| 21  | b     | 613 | CLA  | ND   |
| 21  | b     | 614 | CLA  | ND   |
| 21  | b     | 615 | CLA  | ND   |
| 21  | d     | 402 | CLA  | ND   |
| 21  | d     | 406 | CLA  | C8   |
| 21  | c     | 503 | CLA  | ND   |
| 21  | c     | 504 | CLA  | ND   |
| 21  | c     | 508 | CLA  | ND   |
| 21  | c     | 509 | CLA  | ND   |
| 21  | c     | 510 | CLA  | ND   |
| 21  | c     | 511 | CLA  | ND   |

All (379) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | B     | 101 | MGE  | O2G-C2G-C3G-O3G |
| 19  | d     | 410 | MGE  | O6D-C1D-O3G-C3G |
| 19  | m     | 102 | MGE  | C2B-C1B-O2G-C2G |
| 20  | a     | 401 | SQD  | C5-C6-S-O8      |
| 20  | l     | 101 | SQD  | O47-C45-C46-O48 |
| 20  | l     | 101 | SQD  | C5-C6-S-O8      |
| 21  | a     | 407 | CLA  | C2B-C3B-CAB-CBB |
| 21  | a     | 407 | CLA  | C4B-C3B-CAB-CBB |
| 21  | b     | 604 | CLA  | C4-C3-C5-C6     |
| 21  | b     | 613 | CLA  | CAD-CBD-CGD-O1D |
| 21  | b     | 613 | CLA  | CAD-CBD-CGD-O2D |
| 21  | b     | 613 | CLA  | C3-C5-C6-C7     |
| 21  | d     | 407 | CLA  | C1A-C2A-CAA-CBA |
| 21  | h     | 101 | CLA  | CBD-CGD-O2D-CED |
| 21  | c     | 504 | CLA  | CAD-CBD-CGD-O1D |
| 21  | c     | 507 | CLA  | C1A-C2A-CAA-CBA |
| 21  | c     | 507 | CLA  | C2B-C3B-CAB-CBB |
| 21  | c     | 507 | CLA  | C4B-C3B-CAB-CBB |
| 21  | c     | 507 | CLA  | CBD-CGD-O2D-CED |
| 21  | c     | 509 | CLA  | CHA-CBD-CGD-O1D |
| 21  | c     | 510 | CLA  | CHA-CBD-CGD-O1D |
| 21  | c     | 512 | CLA  | C1A-C2A-CAA-CBA |
| 21  | c     | 512 | CLA  | C2B-C3B-CAB-CBB |
| 21  | c     | 512 | CLA  | C4B-C3B-CAB-CBB |
| 21  | c     | 512 | CLA  | C2-C3-C5-C6     |
| 21  | c     | 512 | CLA  | C4-C3-C5-C6     |
| 22  | a     | 404 | BCR  | C17-C18-C19-C20 |
| 22  | d     | 409 | BCR  | C21-C22-C23-C24 |
| 22  | d     | 409 | BCR  | C37-C22-C23-C24 |
| 22  | h     | 103 | BCR  | C7-C8-C9-C10    |
| 22  | h     | 103 | BCR  | C7-C8-C9-C34    |
| 22  | c     | 515 | BCR  | C23-C24-C25-C26 |
| 22  | z     | 101 | BCR  | C17-C18-C19-C20 |
| 22  | z     | 101 | BCR  | C36-C18-C19-C20 |
| 22  | z     | 101 | BCR  | C19-C20-C21-C22 |
| 22  | z     | 101 | BCR  | C21-C22-C23-C24 |
| 22  | z     | 101 | BCR  | C37-C22-C23-C24 |
| 24  | c     | 516 | DGD  | O2G-C2G-C3G-O3G |
| 30  | e     | 101 | HEM  | C2B-C3B-CAB-CBB |
| 30  | e     | 101 | HEM  | C4B-C3B-CAB-CBB |
| 30  | e     | 101 | HEM  | C2C-C3C-CAC-CBC |
| 30  | e     | 101 | HEM  | C4C-C3C-CAC-CBC |
| 30  | e     | 101 | HEM  | C3D-CAD-CBD-CGD |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | c     | 507 | CLA  | O1D-CGD-O2D-CED |
| 21  | c     | 513 | CLA  | CBD-CGD-O2D-CED |
| 21  | k     | 501 | CLA  | CBD-CGD-O2D-CED |
| 21  | c     | 507 | CLA  | O1A-CGA-O2A-C1  |
| 21  | h     | 101 | CLA  | O1D-CGD-O2D-CED |
| 21  | k     | 501 | CLA  | CBA-CGA-O2A-C1  |
| 21  | k     | 501 | CLA  | O1A-CGA-O2A-C1  |
| 21  | c     | 507 | CLA  | CBA-CGA-O2A-C1  |
| 21  | d     | 406 | CLA  | C4-C3-C5-C6     |
| 28  | d     | 408 | PQ9  | C39-C38-C40-C41 |
| 21  | b     | 604 | CLA  | C2-C3-C5-C6     |
| 28  | d     | 408 | PQ9  | C37-C38-C40-C41 |
| 21  | c     | 507 | CLA  | C2A-CAA-CBA-CGA |
| 21  | b     | 603 | CLA  | C3-C5-C6-C7     |
| 22  | c     | 515 | BCR  | C19-C20-C21-C22 |
| 19  | m     | 102 | MGE  | O1B-C1B-O2G-C2G |
| 24  | c     | 516 | DGD  | O6D-C5D-C6D-O5D |
| 21  | k     | 501 | CLA  | O1D-CGD-O2D-CED |
| 26  | d     | 404 | LMT  | O5'-C5'-C6'-O6' |
| 24  | a     | 406 | DGD  | O6E-C5E-C6E-O5E |
| 21  | b     | 613 | CLA  | C2-C3-C5-C6     |
| 28  | d     | 408 | PQ9  | C38-C40-C41-C42 |
| 26  | t     | 301 | LMT  | C4B-C5B-C6B-O6B |
| 26  | m     | 101 | LMT  | C4'-C5'-C6'-O6' |
| 24  | a     | 406 | DGD  | C2B-C1B-O2G-C2G |
| 21  | c     | 513 | CLA  | O1D-CGD-O2D-CED |
| 21  | d     | 407 | CLA  | CBA-CGA-O2A-C1  |
| 24  | c     | 516 | DGD  | C4D-C5D-C6D-O5D |
| 21  | b     | 613 | CLA  | C4-C3-C5-C6     |
| 21  | d     | 406 | CLA  | C2-C3-C5-C6     |
| 22  | a     | 404 | BCR  | C7-C8-C9-C34    |
| 22  | a     | 404 | BCR  | C11-C12-C13-C35 |
| 22  | a     | 404 | BCR  | C36-C18-C19-C20 |
| 22  | b     | 618 | BCR  | C37-C22-C23-C24 |
| 22  | c     | 514 | BCR  | C7-C8-C9-C34    |
| 26  | t     | 301 | LMT  | O5B-C5B-C6B-O6B |
| 22  | a     | 404 | BCR  | C11-C12-C13-C14 |
| 22  | c     | 514 | BCR  | C7-C8-C9-C10    |
| 21  | d     | 407 | CLA  | O1A-CGA-O2A-C1  |
| 26  | d     | 404 | LMT  | C4'-C5'-C6'-O6' |
| 21  | b     | 603 | CLA  | C13-C15-C16-C17 |
| 24  | c     | 516 | DGD  | C4E-C5E-C6E-O5E |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | b     | 605 | CLA  | C11-C12-C13-C15 |
| 24  | c     | 516 | DGD  | O6E-C5E-C6E-O5E |
| 26  | m     | 101 | LMT  | O5'-C5'-C6'-O6' |
| 24  | a     | 406 | DGD  | C1B-C2B-C3B-C4B |
| 21  | d     | 406 | CLA  | C8-C10-C11-C12  |
| 21  | d     | 406 | CLA  | C10-C11-C12-C13 |
| 22  | h     | 103 | BCR  | C9-C10-C11-C12  |
| 22  | c     | 514 | BCR  | C19-C20-C21-C22 |
| 21  | a     | 402 | CLA  | C15-C16-C17-C18 |
| 21  | b     | 602 | CLA  | C5-C6-C7-C8     |
| 25  | d     | 403 | PHO  | C2C-C3C-CAC-CBC |
| 24  | a     | 406 | DGD  | O1B-C1B-O2G-C2G |
| 19  | f     | 101 | MGE  | O6D-C5D-C6D-O5D |
| 21  | c     | 509 | CLA  | O1D-CGD-O2D-CED |
| 24  | a     | 406 | DGD  | C2E-C1E-O5D-C6D |
| 24  | c     | 517 | DGD  | C2D-C1D-O3G-C3G |
| 21  | b     | 605 | CLA  | C13-C15-C16-C17 |
| 22  | d     | 409 | BCR  | C7-C8-C9-C34    |
| 22  | c     | 514 | BCR  | C11-C12-C13-C35 |
| 22  | c     | 514 | BCR  | C11-C12-C13-C14 |
| 21  | b     | 614 | CLA  | C10-C11-C12-C13 |
| 21  | c     | 511 | CLA  | C8-C10-C11-C12  |
| 24  | a     | 406 | DGD  | O6E-C1E-O5D-C6D |
| 21  | b     | 605 | CLA  | C16-C17-C18-C19 |
| 19  | d     | 410 | MGE  | C7A-C8A-C9A-CAA |
| 19  | c     | 502 | MGE  | C3B-C4B-C5B-C6B |
| 26  | d     | 404 | LMT  | O1'-C1-C2-C3    |
| 19  | B     | 101 | MGE  | C8B-C9B-CAB-CBB |
| 24  | a     | 406 | DGD  | C5A-C6A-C7A-C8A |
| 21  | h     | 101 | CLA  | C4B-C3B-CAB-CBB |
| 21  | c     | 504 | CLA  | C16-C17-C18-C20 |
| 19  | B     | 101 | MGE  | C2B-C1B-O2G-C2G |
| 19  | d     | 410 | MGE  | C2B-C1B-O2G-C2G |
| 19  | b     | 619 | MGE  | C8A-C9A-CAA-CBA |
| 21  | b     | 605 | CLA  | C6-C7-C8-C10    |
| 26  | t     | 301 | LMT  | O1'-C1-C2-C3    |
| 19  | c     | 502 | MGE  | C1A-C2A-C3A-C4A |
| 21  | a     | 407 | CLA  | C13-C15-C16-C17 |
| 21  | d     | 407 | CLA  | C3A-C2A-CAA-CBA |
| 21  | c     | 506 | CLA  | C3A-C2A-CAA-CBA |
| 21  | c     | 507 | CLA  | C3A-C2A-CAA-CBA |
| 26  | t     | 301 | LMT  | C1-C2-C3-C4     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | a     | 404 | BCR  | C13-C14-C15-C16 |
| 21  | c     | 504 | CLA  | C16-C17-C18-C19 |
| 19  | m     | 102 | MGE  | C1A-C2A-C3A-C4A |
| 21  | b     | 610 | CLA  | O1D-CGD-O2D-CED |
| 21  | h     | 101 | CLA  | C2B-C3B-CAB-CBB |
| 21  | c     | 513 | CLA  | C2B-C3B-CAB-CBB |
| 22  | d     | 409 | BCR  | C1-C6-C7-C8     |
| 22  | d     | 409 | BCR  | C5-C6-C7-C8     |
| 22  | d     | 409 | BCR  | C23-C24-C25-C26 |
| 22  | d     | 409 | BCR  | C23-C24-C25-C30 |
| 22  | h     | 103 | BCR  | C1-C6-C7-C8     |
| 22  | h     | 103 | BCR  | C5-C6-C7-C8     |
| 22  | h     | 103 | BCR  | C23-C24-C25-C26 |
| 22  | h     | 103 | BCR  | C23-C24-C25-C30 |
| 22  | c     | 514 | BCR  | C1-C6-C7-C8     |
| 22  | c     | 515 | BCR  | C23-C24-C25-C30 |
| 19  | m     | 102 | MGE  | C7A-C8A-C9A-CAA |
| 19  | c     | 502 | MGE  | C4B-C5B-C6B-C7B |
| 21  | a     | 402 | CLA  | C2C-C3C-CAC-CBC |
| 21  | b     | 607 | CLA  | C13-C15-C16-C17 |
| 24  | a     | 406 | DGD  | CBB-CCB-CDB-CEB |
| 19  | B     | 101 | MGE  | O1B-C1B-O2G-C2G |
| 24  | h     | 104 | DGD  | C3B-C4B-C5B-C6B |
| 21  | b     | 605 | CLA  | C16-C17-C18-C20 |
| 19  | B     | 101 | MGE  | C5B-C6B-C7B-C8B |
| 24  | c     | 517 | DGD  | C8A-C9A-CAA-CBA |
| 21  | b     | 611 | CLA  | C13-C15-C16-C17 |
| 19  | d     | 410 | MGE  | O1B-C1B-O2G-C2G |
| 21  | d     | 402 | CLA  | C2C-C3C-CAC-CBC |
| 21  | d     | 406 | CLA  | C5-C6-C7-C8     |
| 26  | d     | 404 | LMT  | C5-C6-C7-C8     |
| 21  | b     | 602 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 620 | MGE  | O1G-C1G-C2G-O2G |
| 24  | c     | 517 | DGD  | O1G-C1G-C2G-O2G |
| 21  | c     | 503 | CLA  | O1D-CGD-O2D-CED |
| 21  | b     | 610 | CLA  | C13-C15-C16-C17 |
| 19  | b     | 619 | MGE  | C4A-C5A-C6A-C7A |
| 21  | b     | 601 | CLA  | C16-C17-C18-C19 |
| 24  | a     | 406 | DGD  | C4E-C5E-C6E-O5E |
| 24  | c     | 517 | DGD  | C4A-C5A-C6A-C7A |
| 21  | c     | 506 | CLA  | C1A-C2A-CAA-CBA |
| 21  | c     | 513 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | d     | 410 | MGE  | O6D-C5D-C6D-O5D |
| 21  | c     | 505 | CLA  | C6-C7-C8-C10    |
| 21  | c     | 509 | CLA  | C11-C10-C8-C7   |
| 19  | c     | 502 | MGE  | C7B-C8B-C9B-CAB |
| 21  | b     | 605 | CLA  | C2A-CAA-CBA-CGA |
| 19  | b     | 620 | MGE  | C1B-C2B-C3B-C4B |
| 19  | B     | 101 | MGE  | C1G-C2G-C3G-O3G |
| 24  | c     | 516 | DGD  | C1G-C2G-C3G-O3G |
| 21  | b     | 601 | CLA  | C16-C17-C18-C20 |
| 24  | h     | 104 | DGD  | O6E-C5E-C6E-O5E |
| 21  | b     | 613 | CLA  | O1D-CGD-O2D-CED |
| 22  | b     | 618 | BCR  | C21-C22-C23-C24 |
| 22  | d     | 409 | BCR  | C7-C8-C9-C10    |
| 20  | l     | 101 | SQD  | C24-C25-C26-C27 |
| 21  | c     | 507 | CLA  | O2A-C1-C2-C3    |
| 19  | d     | 410 | MGE  | C5B-C6B-C7B-C8B |
| 19  | m     | 102 | MGE  | C8A-C9A-CAA-CBA |
| 19  | b     | 619 | MGE  | O2G-C2G-C3G-O3G |
| 24  | a     | 406 | DGD  | O2G-C2G-C3G-O3G |
| 21  | c     | 506 | CLA  | CAA-CBA-CGA-O2A |
| 19  | b     | 619 | MGE  | CBB-CCB-CDB-CEB |
| 19  | c     | 502 | MGE  | C2A-C1A-O1G-C1G |
| 24  | h     | 104 | DGD  | C2B-C1B-O2G-C2G |
| 19  | b     | 620 | MGE  | C8B-C9B-CAB-CBB |
| 21  | b     | 611 | CLA  | C3-C5-C6-C7     |
| 21  | b     | 614 | CLA  | C16-C17-C18-C20 |
| 21  | b     | 610 | CLA  | C14-C13-C15-C16 |
| 21  | c     | 509 | CLA  | C11-C10-C8-C9   |
| 21  | b     | 608 | CLA  | C4B-C3B-CAB-CBB |
| 21  | c     | 513 | CLA  | C4B-C3B-CAB-CBB |
| 21  | k     | 501 | CLA  | C4B-C3B-CAB-CBB |
| 21  | a     | 407 | CLA  | C11-C10-C8-C7   |
| 21  | b     | 605 | CLA  | C12-C13-C15-C16 |
| 21  | b     | 610 | CLA  | C12-C13-C15-C16 |
| 21  | b     | 614 | CLA  | C5-C6-C7-C8     |
| 21  | c     | 512 | CLA  | C3A-C2A-CAA-CBA |
| 21  | c     | 511 | CLA  | C2-C3-C5-C6     |
| 24  | a     | 406 | DGD  | C4D-C5D-C6D-O5D |
| 19  | b     | 619 | MGE  | O1G-C1G-C2G-C3G |
| 19  | b     | 620 | MGE  | O1G-C1G-C2G-C3G |
| 20  | l     | 101 | SQD  | C44-C45-C46-O48 |
| 24  | a     | 406 | DGD  | C1G-C2G-C3G-O3G |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | c     | 517 | DGD  | O1G-C1G-C2G-C3G |
| 21  | c     | 511 | CLA  | C4-C3-C5-C6     |
| 21  | a     | 402 | CLA  | C4C-C3C-CAC-CBC |
| 22  | a     | 404 | BCR  | C23-C24-C25-C30 |
| 19  | d     | 410 | MGE  | C9B-CAB-CBB-CCB |
| 21  | b     | 614 | CLA  | O1D-CGD-O2D-CED |
| 21  | c     | 509 | CLA  | C5-C6-C7-C8     |
| 21  | d     | 402 | CLA  | C4C-C3C-CAC-CBC |
| 20  | l     | 101 | SQD  | C25-C26-C27-C28 |
| 24  | h     | 104 | DGD  | CAA-CBA-CCA-CDA |
| 21  | b     | 605 | CLA  | C11-C12-C13-C14 |
| 21  | b     | 609 | CLA  | C11-C12-C13-C14 |
| 24  | h     | 104 | DGD  | C9A-CAA-CBA-CCA |
| 24  | a     | 406 | DGD  | O6D-C1D-O3G-C3G |
| 21  | b     | 614 | CLA  | C16-C17-C18-C19 |
| 21  | a     | 402 | CLA  | C16-C17-C18-C20 |
| 19  | d     | 410 | MGE  | C2A-C3A-C4A-C5A |
| 24  | h     | 104 | DGD  | C6A-C7A-C8A-C9A |
| 21  | b     | 603 | CLA  | C6-C7-C8-C10    |
| 22  | a     | 404 | BCR  | C7-C8-C9-C10    |
| 19  | c     | 502 | MGE  | O1A-C1A-O1G-C1G |
| 19  | c     | 502 | MGE  | O6D-C1D-O3G-C3G |
| 24  | c     | 517 | DGD  | O6D-C1D-O3G-C3G |
| 19  | f     | 101 | MGE  | C5B-C6B-C7B-C8B |
| 19  | b     | 619 | MGE  | O1G-C1G-C2G-O2G |
| 19  | c     | 502 | MGE  | O1G-C1G-C2G-O2G |
| 21  | a     | 407 | CLA  | C6-C7-C8-C9     |
| 21  | a     | 407 | CLA  | C11-C10-C8-C9   |
| 19  | c     | 502 | MGE  | C8B-C9B-CAB-CBB |
| 19  | b     | 620 | MGE  | C2B-C3B-C4B-C5B |
| 19  | c     | 502 | MGE  | C3A-C4A-C5A-C6A |
| 21  | d     | 407 | CLA  | C4B-C3B-CAB-CBB |
| 21  | c     | 506 | CLA  | C4B-C3B-CAB-CBB |
| 24  | h     | 104 | DGD  | O1B-C1B-O2G-C2G |
| 21  | c     | 509 | CLA  | C11-C12-C13-C15 |
| 19  | B     | 101 | MGE  | C7A-C8A-C9A-CAA |
| 21  | b     | 603 | CLA  | C6-C7-C8-C9     |
| 21  | b     | 605 | CLA  | C14-C13-C15-C16 |
| 24  | a     | 406 | DGD  | O6D-C5D-C6D-O5D |
| 24  | h     | 104 | DGD  | C6B-C7B-C8B-C9B |
| 21  | a     | 403 | CLA  | O1D-CGD-O2D-CED |
| 21  | d     | 406 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | b     | 614 | CLA  | C13-C15-C16-C17 |
| 20  | a     | 401 | SQD  | O47-C45-C46-O48 |
| 19  | b     | 619 | MGE  | C1G-C2G-C3G-O3G |
| 19  | c     | 502 | MGE  | O1G-C1G-C2G-C3G |
| 24  | h     | 104 | DGD  | O1G-C1G-C2G-C3G |
| 21  | c     | 504 | CLA  | CAD-CBD-CGD-O2D |
| 21  | c     | 507 | CLA  | CAD-CBD-CGD-O2D |
| 21  | b     | 604 | CLA  | CAD-CBD-CGD-O1D |
| 21  | b     | 606 | CLA  | CAD-CBD-CGD-O1D |
| 21  | b     | 615 | CLA  | CHA-CBD-CGD-O1D |
| 21  | h     | 101 | CLA  | CHA-CBD-CGD-O1D |
| 21  | h     | 101 | CLA  | CHA-CBD-CGD-O2D |
| 21  | c     | 503 | CLA  | CHA-CBD-CGD-O1D |
| 21  | c     | 507 | CLA  | CAD-CBD-CGD-O1D |
| 21  | c     | 508 | CLA  | CAD-CBD-CGD-O1D |
| 21  | c     | 509 | CLA  | CHA-CBD-CGD-O2D |
| 22  | c     | 514 | BCR  | C15-C16-C17-C18 |
| 21  | k     | 501 | CLA  | C2B-C3B-CAB-CBB |
| 24  | c     | 516 | DGD  | C9A-CAA-CBA-CCA |
| 24  | a     | 406 | DGD  | C2A-C3A-C4A-C5A |
| 21  | b     | 605 | CLA  | C15-C16-C17-C18 |
| 22  | a     | 404 | BCR  | C18-C19-C20-C21 |
| 22  | c     | 515 | BCR  | C10-C11-C12-C13 |
| 24  | c     | 517 | DGD  | C1A-C2A-C3A-C4A |
| 21  | c     | 509 | CLA  | C11-C12-C13-C14 |
| 19  | B     | 101 | MGE  | C1A-C2A-C3A-C4A |
| 26  | t     | 301 | LMT  | C5-C6-C7-C8     |
| 19  | c     | 502 | MGE  | C5A-C6A-C7A-C8A |
| 19  | m     | 102 | MGE  | O1G-C1G-C2G-O2G |
| 24  | h     | 104 | DGD  | O1G-C1G-C2G-O2G |
| 21  | b     | 606 | CLA  | C3-C5-C6-C7     |
| 21  | d     | 406 | CLA  | CAA-CBA-CGA-O2A |
| 19  | B     | 101 | MGE  | C2G-C3G-O3G-C1D |
| 22  | b     | 618 | BCR  | C9-C10-C11-C12  |
| 21  | b     | 614 | CLA  | C14-C13-C15-C16 |
| 21  | d     | 406 | CLA  | C6-C7-C8-C9     |
| 21  | b     | 611 | CLA  | CBA-CGA-O2A-C1  |
| 19  | m     | 102 | MGE  | C2A-C3A-C4A-C5A |
| 28  | d     | 408 | PQ9  | C19-C18-C20-C21 |
| 21  | c     | 506 | CLA  | CAA-CBA-CGA-O1A |
| 21  | c     | 510 | CLA  | O1D-CGD-O2D-CED |
| 21  | b     | 611 | CLA  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | d     | 408 | PQ9  | C13-C15-C16-C17 |
| 21  | c     | 511 | CLA  | O1D-CGD-O2D-CED |
| 19  | B     | 101 | MGE  | C7B-C8B-C9B-CAB |
| 24  | c     | 516 | DGD  | C3B-C4B-C5B-C6B |
| 21  | d     | 407 | CLA  | C2B-C3B-CAB-CBB |
| 21  | c     | 506 | CLA  | C2B-C3B-CAB-CBB |
| 22  | a     | 404 | BCR  | C23-C24-C25-C26 |
| 22  | c     | 514 | BCR  | C5-C6-C7-C8     |
| 19  | m     | 102 | MGE  | C4B-C5B-C6B-C7B |
| 21  | d     | 406 | CLA  | C14-C13-C15-C16 |
| 26  | t     | 301 | LMT  | C7-C8-C9-C10    |
| 21  | a     | 407 | CLA  | C6-C7-C8-C10    |
| 21  | b     | 614 | CLA  | C12-C13-C15-C16 |
| 21  | b     | 609 | CLA  | C16-C17-C18-C20 |
| 19  | b     | 619 | MGE  | CAB-CBB-CCB-CDB |
| 19  | B     | 101 | MGE  | C4A-C5A-C6A-C7A |
| 21  | d     | 402 | CLA  | C15-C16-C17-C18 |
| 24  | h     | 104 | DGD  | C4B-C5B-C6B-C7B |
| 19  | d     | 410 | MGE  | C2D-C1D-O3G-C3G |
| 19  | f     | 101 | MGE  | C1A-C2A-C3A-C4A |
| 19  | d     | 410 | MGE  | O1G-C1G-C2G-C3G |
| 20  | a     | 401 | SQD  | C44-C45-C46-O48 |
| 21  | b     | 609 | CLA  | C2A-CAA-CBA-CGA |
| 28  | d     | 408 | PQ9  | C24-C23-C25-C26 |
| 28  | d     | 408 | PQ9  | C17-C18-C20-C21 |
| 19  | d     | 410 | MGE  | O2G-C1B-C2B-C3B |
| 25  | d     | 403 | PHO  | CHA-CBD-CGD-O2D |
| 30  | e     | 101 | HEM  | CAA-CBA-CGA-O2A |
| 19  | m     | 102 | MGE  | C5B-C6B-C7B-C8B |
| 21  | c     | 503 | CLA  | C13-C15-C16-C17 |
| 19  | B     | 101 | MGE  | C9B-CAB-CBB-CCB |
| 30  | e     | 101 | HEM  | CAA-CBA-CGA-O1A |
| 20  | l     | 101 | SQD  | C18-C19-C20-C21 |
| 24  | a     | 406 | DGD  | C1A-C2A-C3A-C4A |
| 21  | b     | 614 | CLA  | C3A-C2A-CAA-CBA |
| 26  | t     | 301 | LMT  | C4-C5-C6-C7     |
| 24  | h     | 104 | DGD  | O2G-C1B-C2B-C3B |
| 21  | c     | 513 | CLA  | CBA-CGA-O2A-C1  |
| 21  | c     | 513 | CLA  | O1A-CGA-O2A-C1  |
| 24  | c     | 517 | DGD  | C7A-C8A-C9A-CAA |
| 19  | B     | 101 | MGE  | C1B-C2B-C3B-C4B |
| 24  | c     | 516 | DGD  | O2G-C1B-C2B-C3B |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | d     | 410 | MGE  | C1B-C2B-C3B-C4B |
| 21  | b     | 608 | CLA  | C2B-C3B-CAB-CBB |
| 21  | b     | 613 | CLA  | C2-C1-O2A-CGA   |
| 21  | d     | 406 | CLA  | C12-C13-C15-C16 |
| 19  | d     | 410 | MGE  | C4B-C5B-C6B-C7B |
| 21  | c     | 512 | CLA  | CAA-CBA-CGA-O2A |
| 21  | b     | 602 | CLA  | C13-C15-C16-C17 |
| 24  | h     | 104 | DGD  | C2B-C3B-C4B-C5B |
| 24  | c     | 516 | DGD  | O1G-C1A-C2A-C3A |
| 19  | m     | 102 | MGE  | O1G-C1G-C2G-C3G |
| 21  | k     | 501 | CLA  | CAA-CBA-CGA-O2A |
| 19  | B     | 101 | MGE  | O1A-C1A-O1G-C1G |
| 21  | c     | 513 | CLA  | CAA-CBA-CGA-O2A |
| 21  | b     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 20  | a     | 401 | SQD  | C5-C6-S-O9      |
| 20  | l     | 101 | SQD  | C5-C6-S-O9      |
| 19  | b     | 620 | MGE  | C6B-C7B-C8B-C9B |
| 21  | c     | 507 | CLA  | C2-C1-O2A-CGA   |
| 21  | b     | 611 | CLA  | C11-C10-C8-C7   |
| 19  | B     | 101 | MGE  | C2A-C1A-O1G-C1G |
| 21  | c     | 511 | CLA  | C16-C17-C18-C20 |
| 24  | a     | 406 | DGD  | CCB-CDB-CEB-CFB |
| 21  | b     | 603 | CLA  | C16-C17-C18-C19 |
| 19  | B     | 101 | MGE  | O2G-C1B-C2B-C3B |
| 21  | c     | 513 | CLA  | CAA-CBA-CGA-O1A |
| 24  | c     | 516 | DGD  | O1B-C1B-C2B-C3B |
| 24  | a     | 406 | DGD  | C4A-C5A-C6A-C7A |
| 20  | l     | 101 | SQD  | C10-C11-C12-C13 |
| 21  | c     | 511 | CLA  | C16-C17-C18-C19 |
| 21  | c     | 512 | CLA  | CAA-CBA-CGA-O1A |
| 19  | b     | 619 | MGE  | C2G-C3G-O3G-C1D |
| 24  | c     | 517 | DGD  | C2G-C3G-O3G-C1D |
| 24  | c     | 516 | DGD  | O1A-C1A-C2A-C3A |
| 21  | b     | 611 | CLA  | CAD-CBD-CGD-O2D |
| 25  | d     | 401 | PHO  | CAD-CBD-CGD-O2D |
| 24  | a     | 406 | DGD  | O1G-C1A-C2A-C3A |
| 21  | a     | 407 | CLA  | C2C-C3C-CAC-CBC |
| 20  | a     | 401 | SQD  | O5-C1-O6-C44    |
| 21  | b     | 610 | CLA  | C16-C17-C18-C20 |
| 21  | c     | 503 | CLA  | CAA-CBA-CGA-O2A |
| 19  | b     | 619 | MGE  | C4B-C5B-C6B-C7B |
| 19  | b     | 619 | MGE  | C1A-C2A-C3A-C4A |

There are no ring outliers.

57 monomers are involved in 369 short contacts:

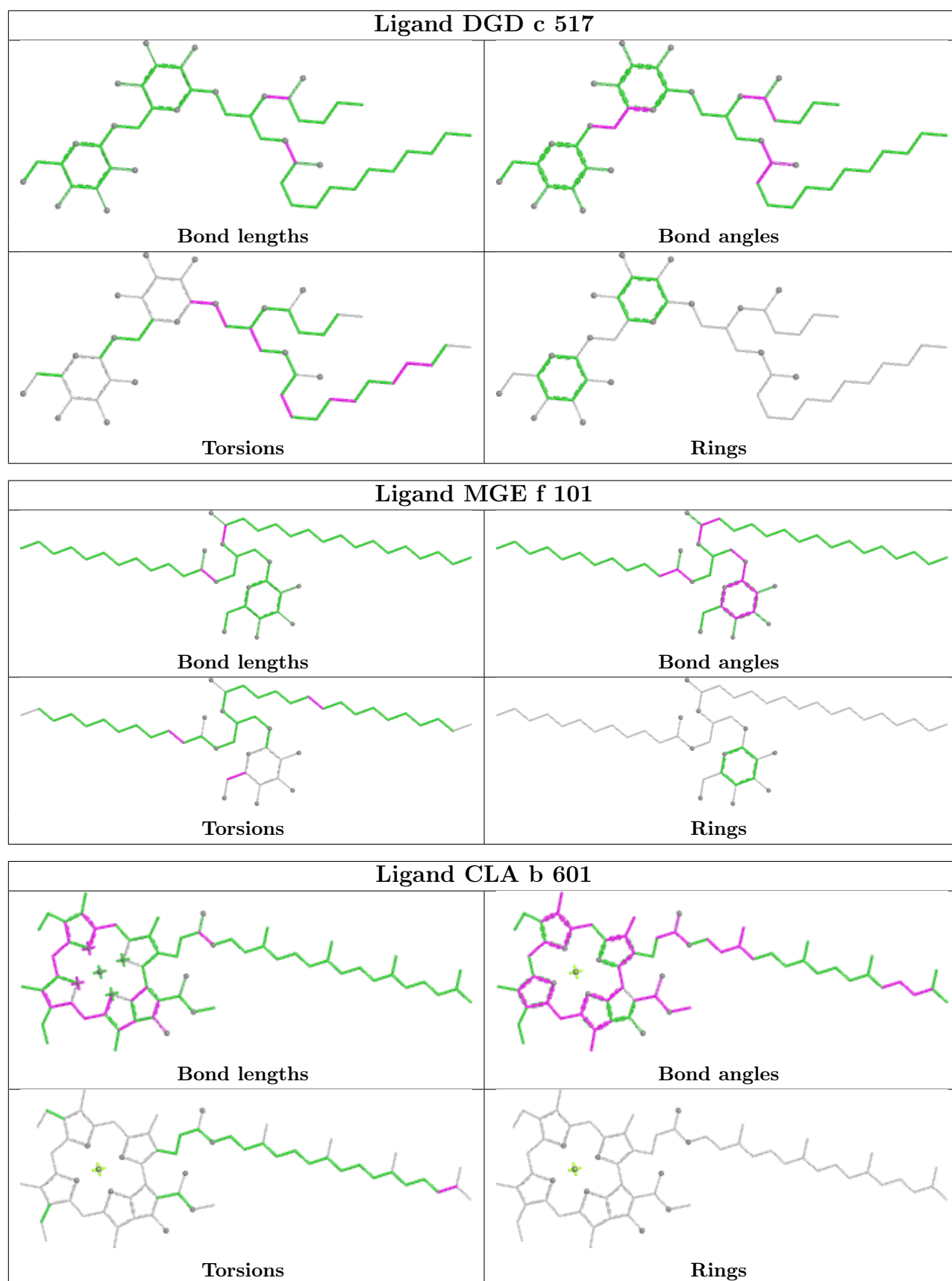
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 21  | b     | 601 | CLA  | 2       | 0            |
| 25  | d     | 401 | PHO  | 4       | 0            |
| 31  | h     | 102 | HTG  | 10      | 0            |
| 21  | c     | 507 | CLA  | 26      | 0            |
| 21  | c     | 511 | CLA  | 18      | 0            |
| 21  | c     | 513 | CLA  | 3       | 0            |
| 21  | c     | 506 | CLA  | 4       | 0            |
| 22  | d     | 409 | BCR  | 2       | 0            |
| 26  | t     | 301 | LMT  | 2       | 0            |
| 21  | b     | 604 | CLA  | 7       | 0            |
| 22  | a     | 404 | BCR  | 2       | 0            |
| 24  | c     | 516 | DGD  | 3       | 0            |
| 28  | d     | 408 | PQ9  | 6       | 0            |
| 24  | h     | 104 | DGD  | 3       | 0            |
| 21  | b     | 606 | CLA  | 10      | 0            |
| 21  | b     | 603 | CLA  | 14      | 0            |
| 22  | h     | 103 | BCR  | 2       | 0            |
| 21  | b     | 608 | CLA  | 1       | 0            |
| 19  | B     | 101 | MGE  | 8       | 0            |
| 21  | d     | 402 | CLA  | 2       | 0            |
| 26  | d     | 404 | LMT  | 1       | 0            |
| 22  | b     | 616 | BCR  | 2       | 0            |
| 19  | m     | 102 | MGE  | 1       | 0            |
| 22  | c     | 515 | BCR  | 48      | 0            |
| 25  | d     | 403 | PHO  | 12      | 0            |
| 21  | b     | 609 | CLA  | 6       | 0            |
| 21  | c     | 504 | CLA  | 3       | 0            |
| 22  | b     | 618 | BCR  | 9       | 0            |
| 24  | a     | 406 | DGD  | 5       | 0            |
| 21  | c     | 510 | CLA  | 22      | 0            |
| 19  | b     | 619 | MGE  | 6       | 0            |
| 19  | b     | 620 | MGE  | 3       | 0            |
| 21  | c     | 505 | CLA  | 10      | 0            |
| 21  | c     | 508 | CLA  | 4       | 0            |
| 21  | b     | 605 | CLA  | 34      | 0            |
| 21  | c     | 503 | CLA  | 33      | 0            |
| 21  | k     | 501 | CLA  | 1       | 0            |
| 22  | c     | 514 | BCR  | 1       | 0            |
| 21  | b     | 610 | CLA  | 2       | 0            |
| 21  | b     | 614 | CLA  | 9       | 0            |

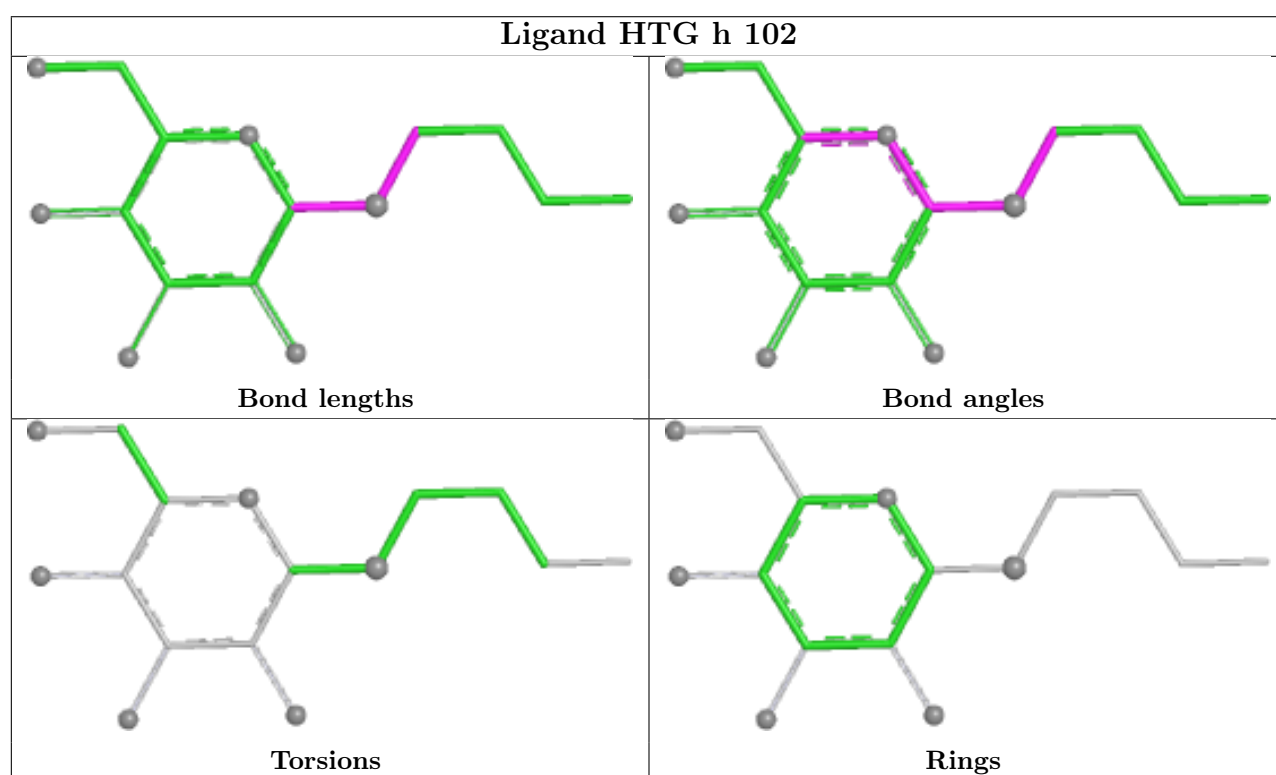
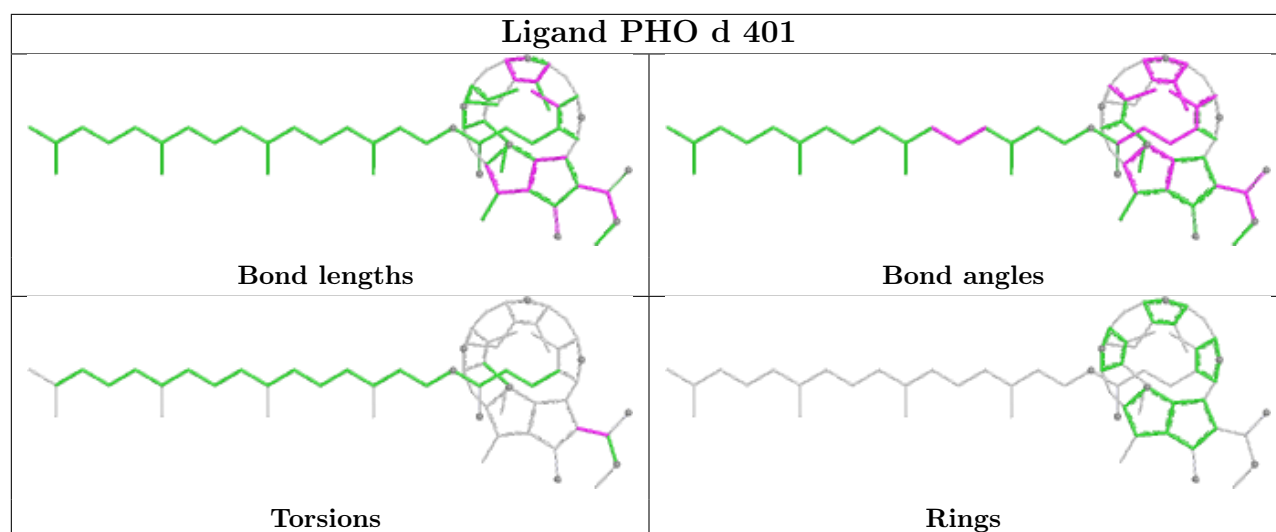
*Continued on next page...*

*Continued from previous page...*

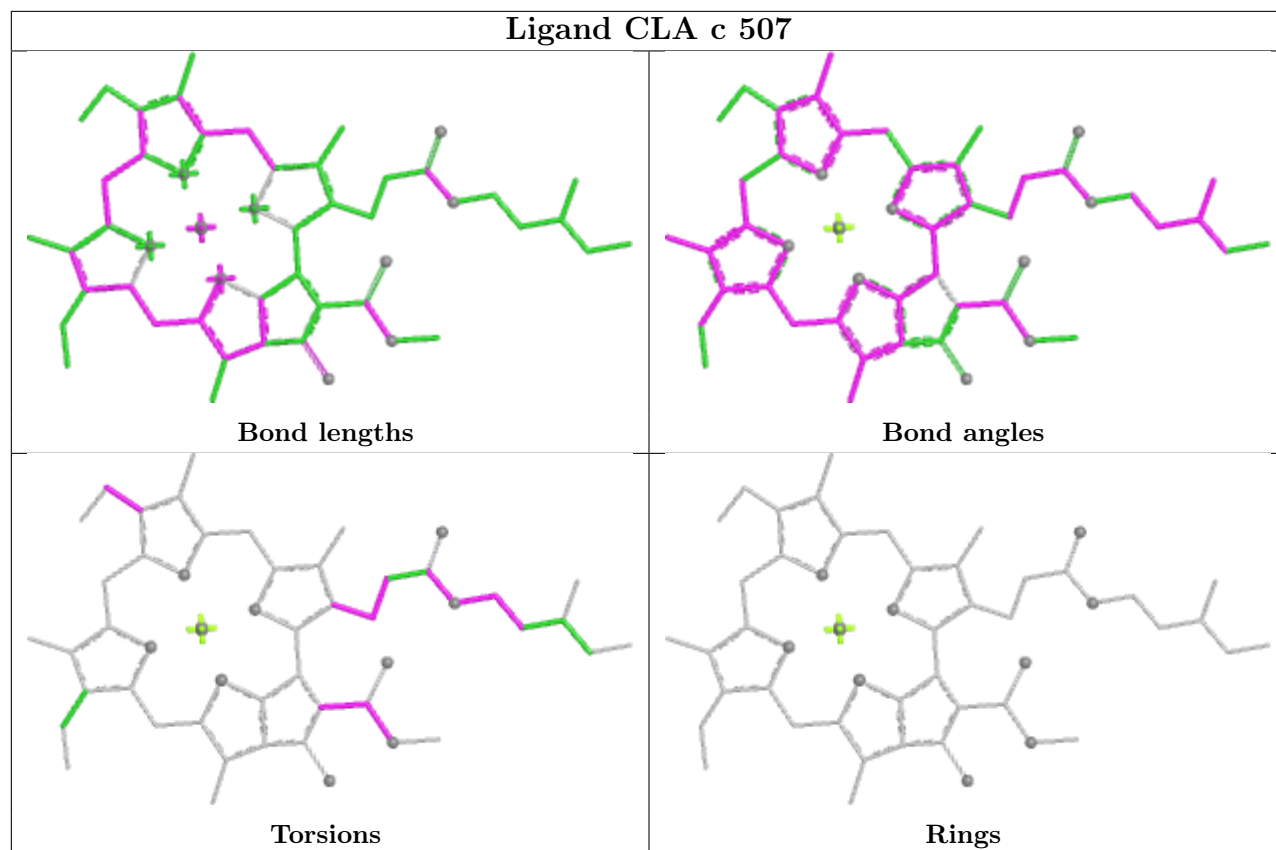
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | b     | 617 | BCR  | 1       | 0            |
| 30  | e     | 101 | HEM  | 1       | 0            |
| 21  | a     | 403 | CLA  | 4       | 0            |
| 22  | z     | 101 | BCR  | 4       | 0            |
| 21  | b     | 613 | CLA  | 5       | 0            |
| 21  | a     | 407 | CLA  | 2       | 0            |
| 21  | a     | 402 | CLA  | 7       | 0            |
| 21  | b     | 615 | CLA  | 2       | 0            |
| 19  | d     | 410 | MGE  | 11      | 0            |
| 21  | d     | 406 | CLA  | 14      | 0            |
| 20  | l     | 101 | SQD  | 3       | 0            |
| 21  | c     | 512 | CLA  | 4       | 0            |
| 21  | c     | 509 | CLA  | 10      | 0            |
| 21  | b     | 611 | CLA  | 9       | 0            |
| 21  | b     | 602 | CLA  | 5       | 0            |
| 21  | b     | 612 | CLA  | 5       | 0            |
| 21  | b     | 607 | CLA  | 3       | 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.

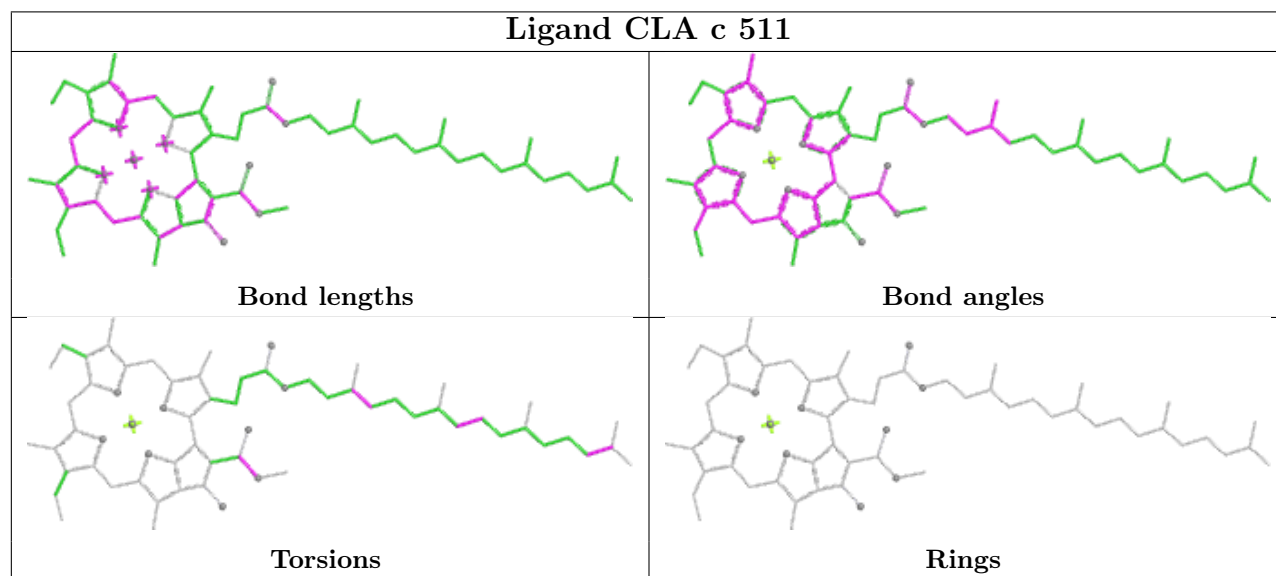




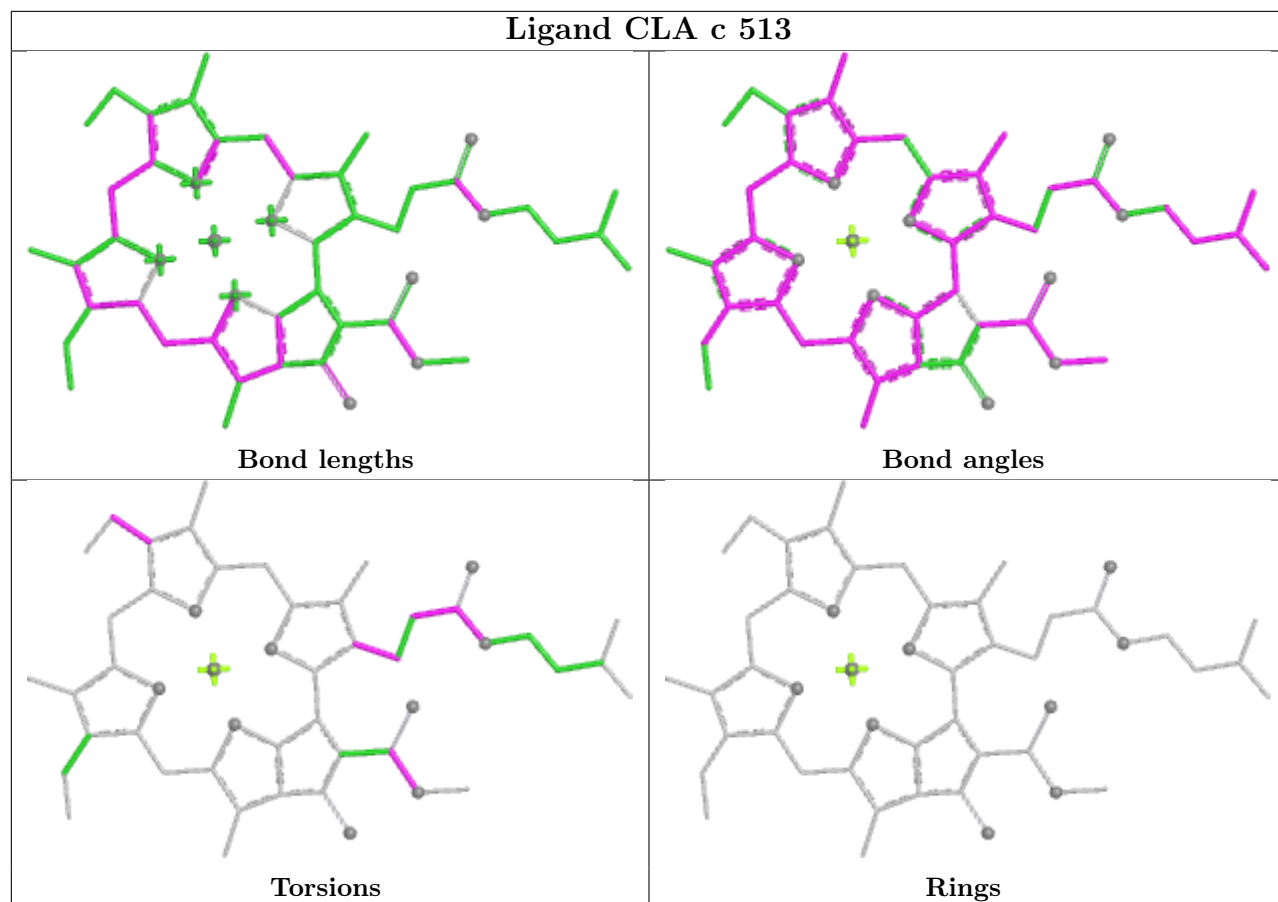
## Ligand CLA c 507



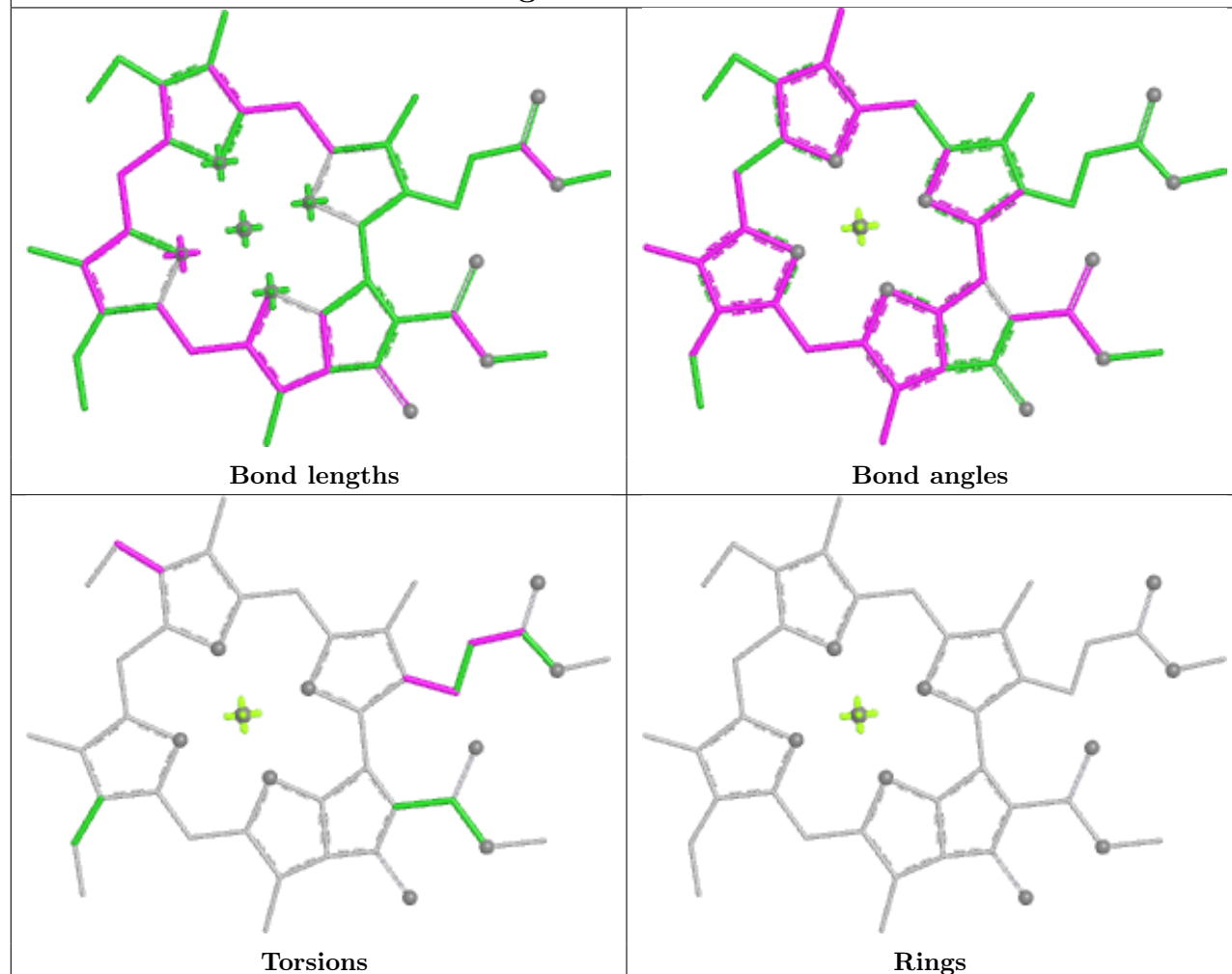
## Ligand CLA c 511



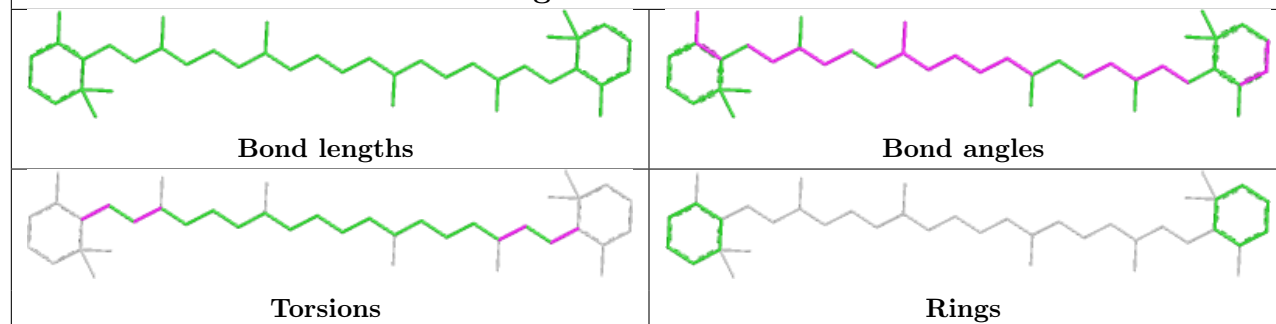
## Ligand CLA c 513



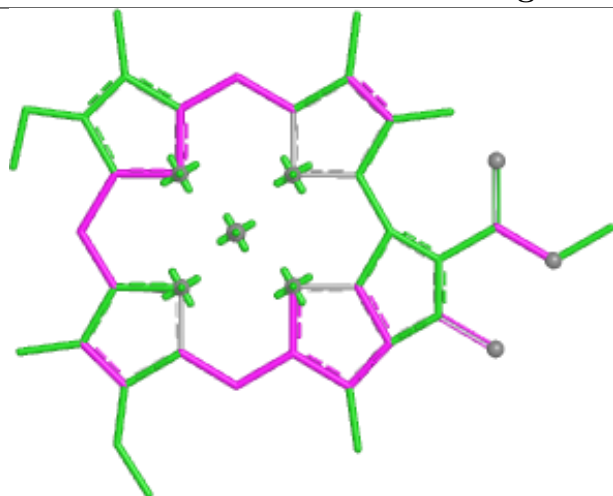
## Ligand CLA c 506



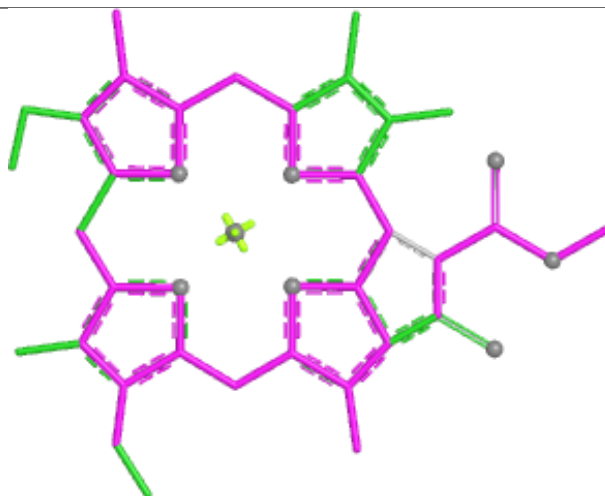
## Ligand BCR d 409



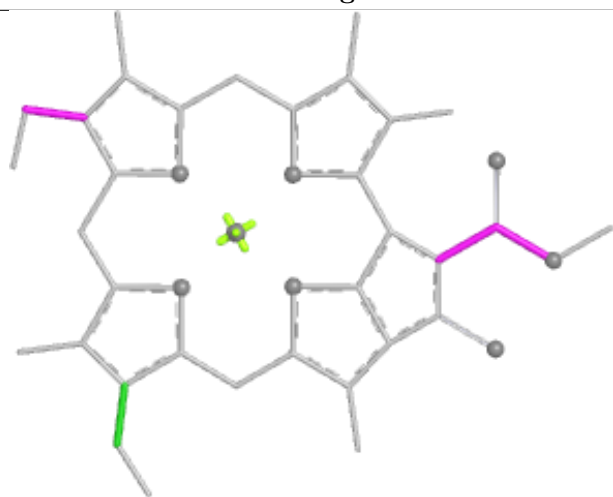
## Ligand CLA h 101



Bond lengths



Bond angles

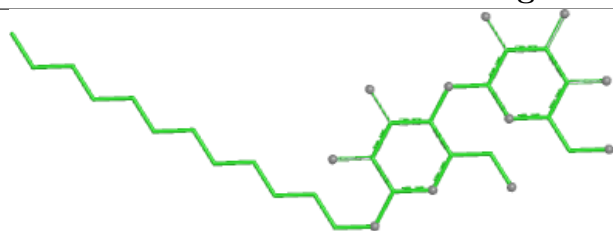


Torsions

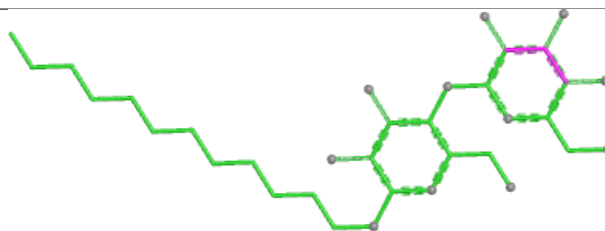


Rings

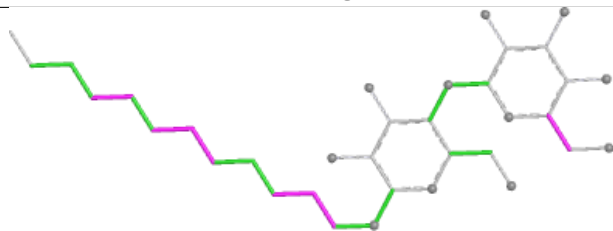
## Ligand LMT t 301



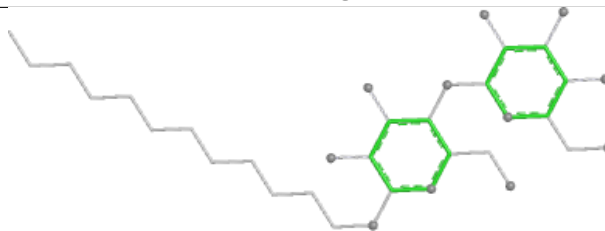
Bond lengths



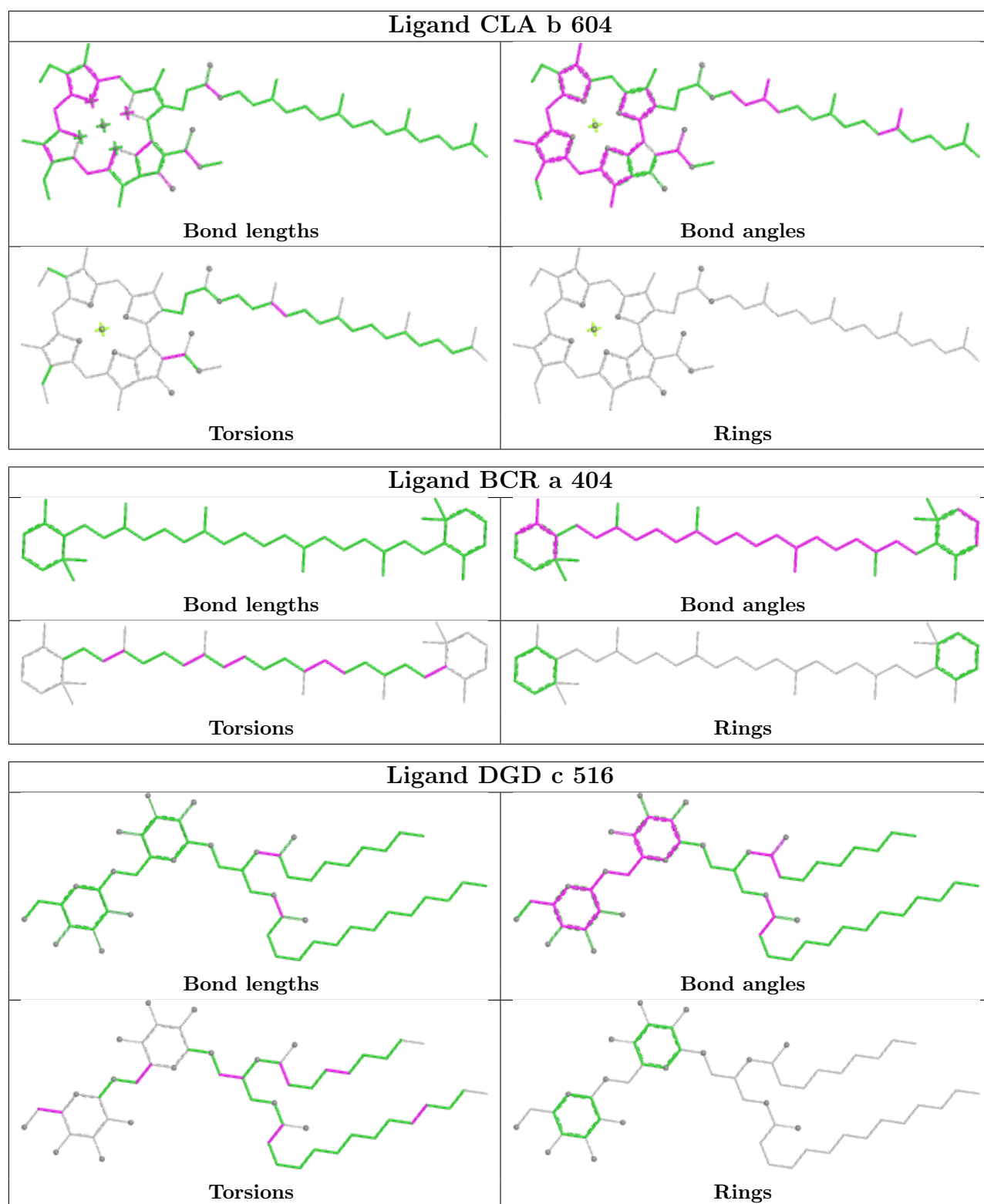
Bond angles

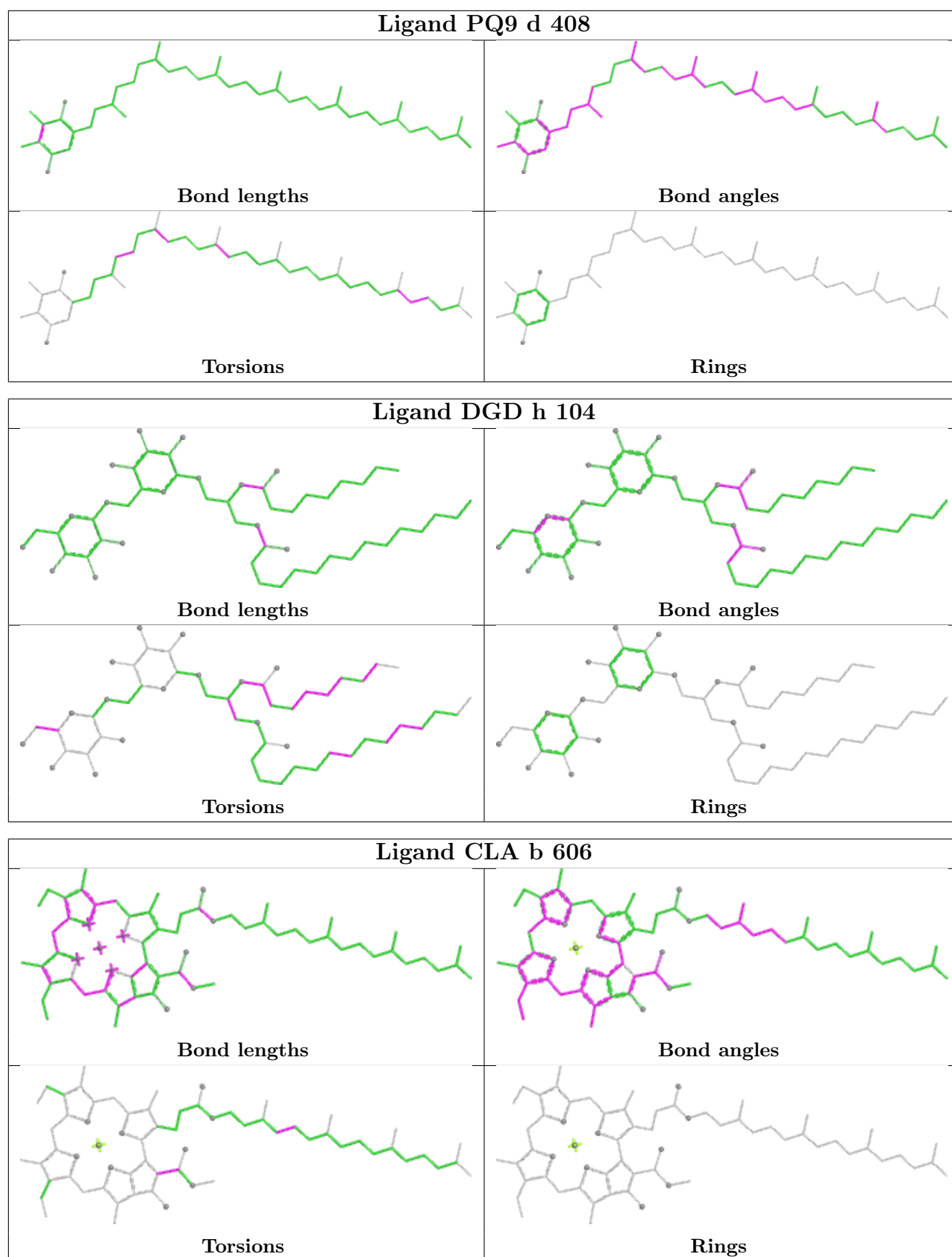


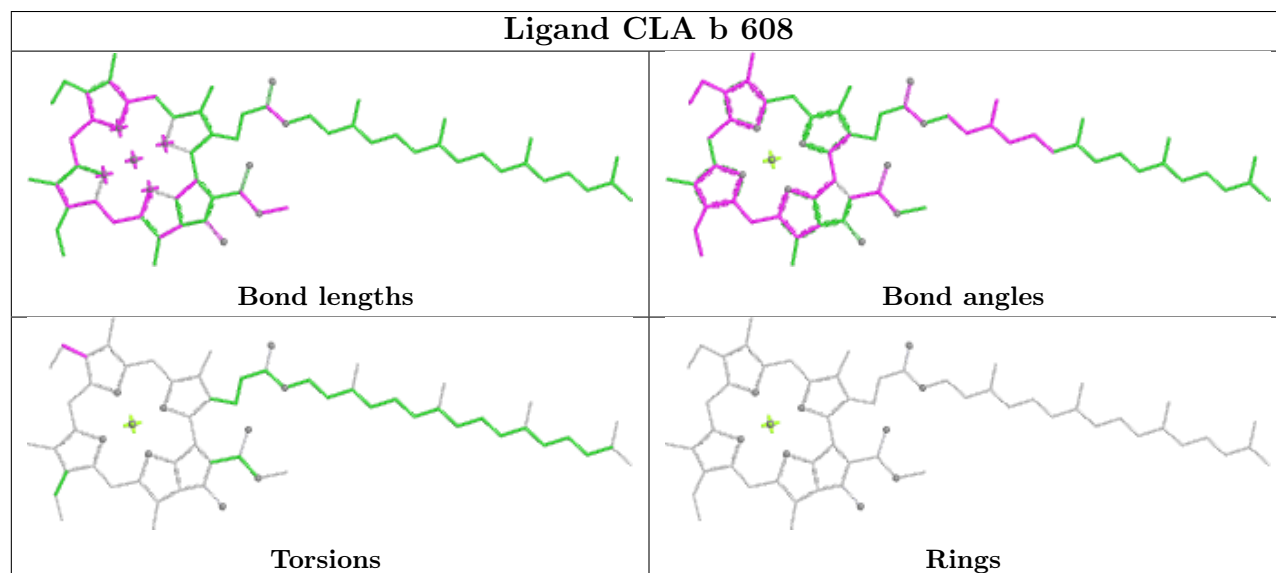
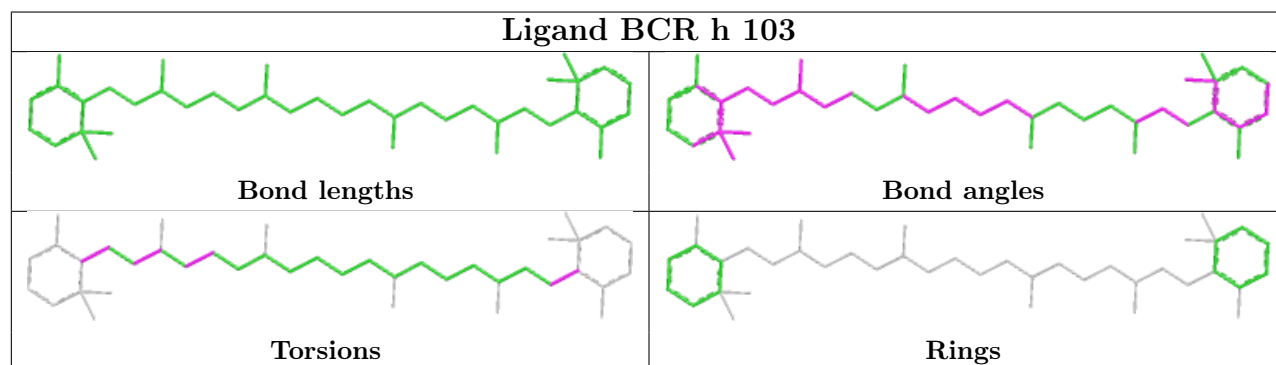
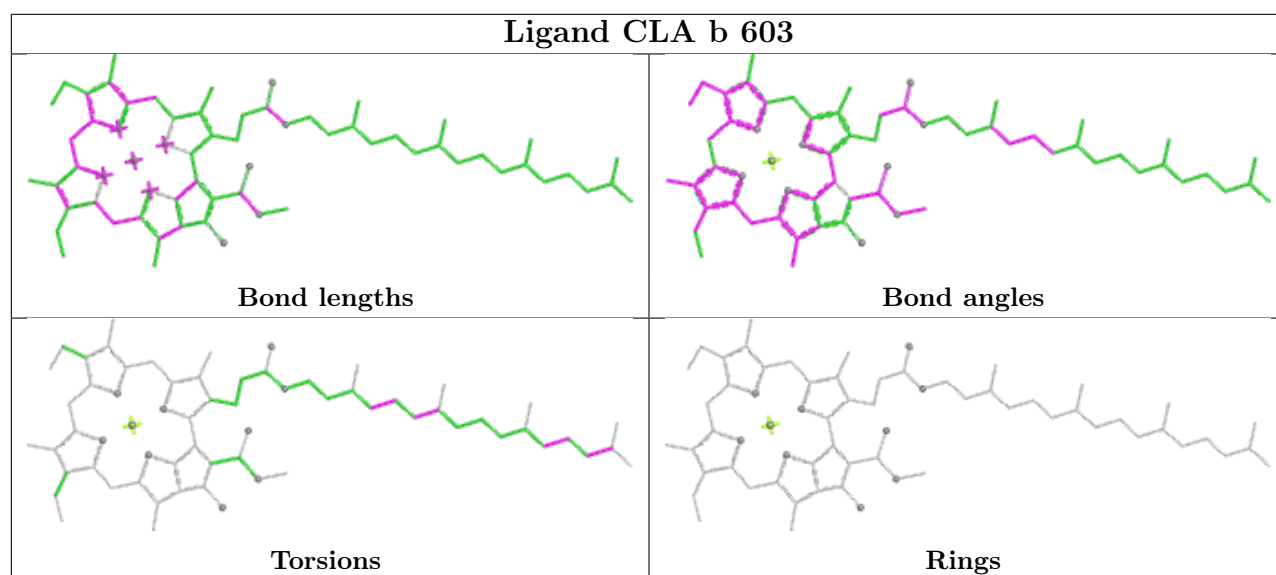
Torsions

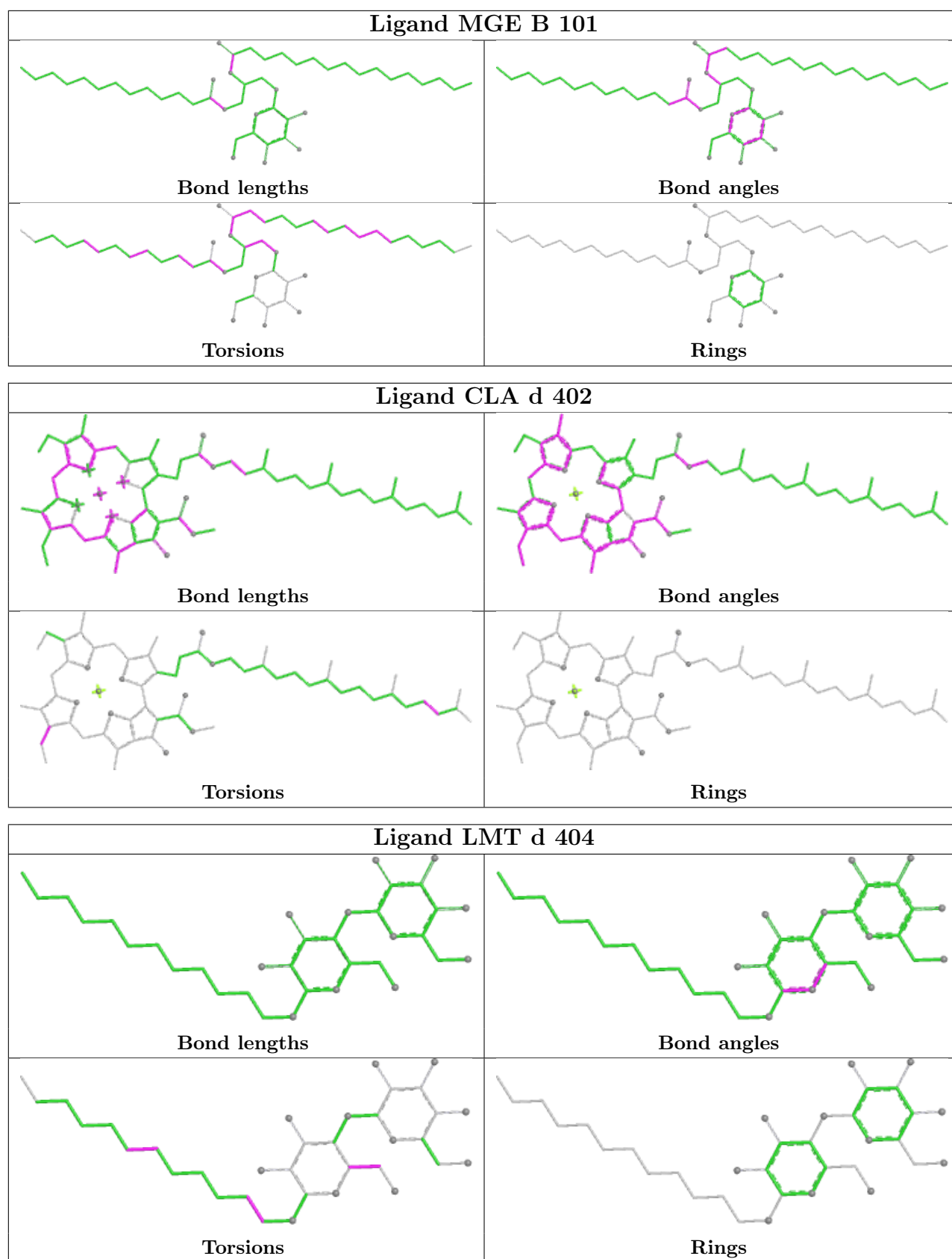


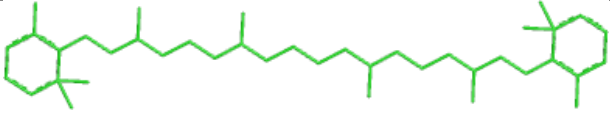
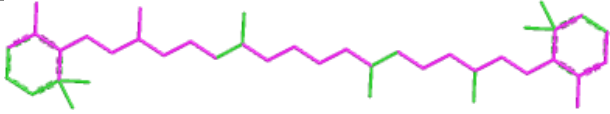
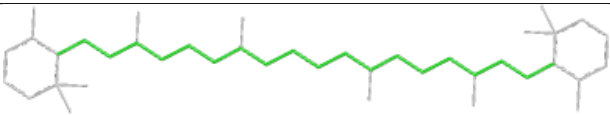
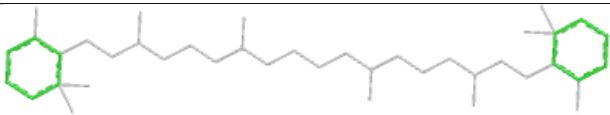
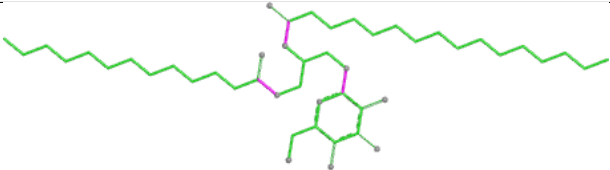
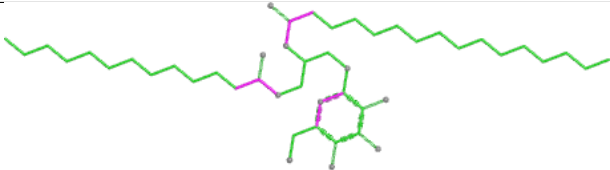
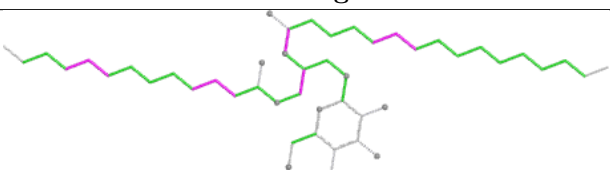
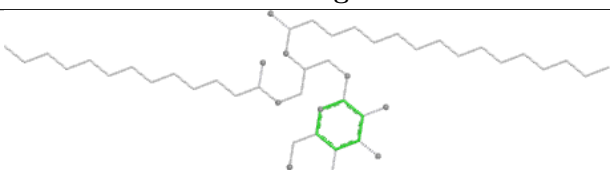
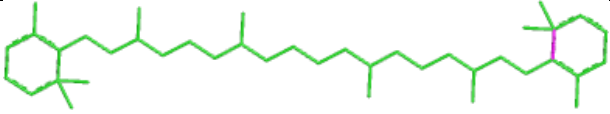
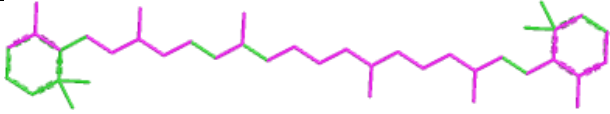
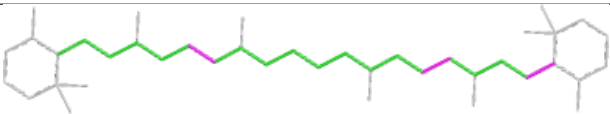
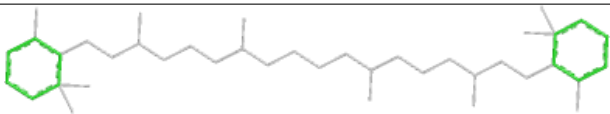
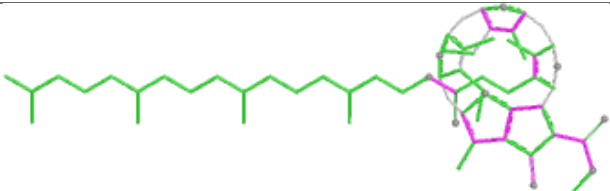
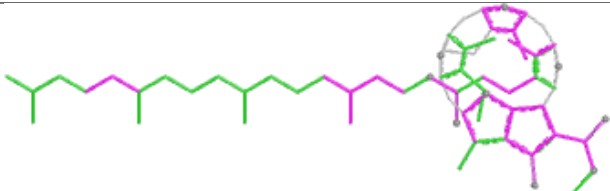
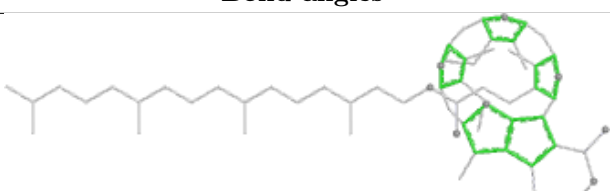
Rings

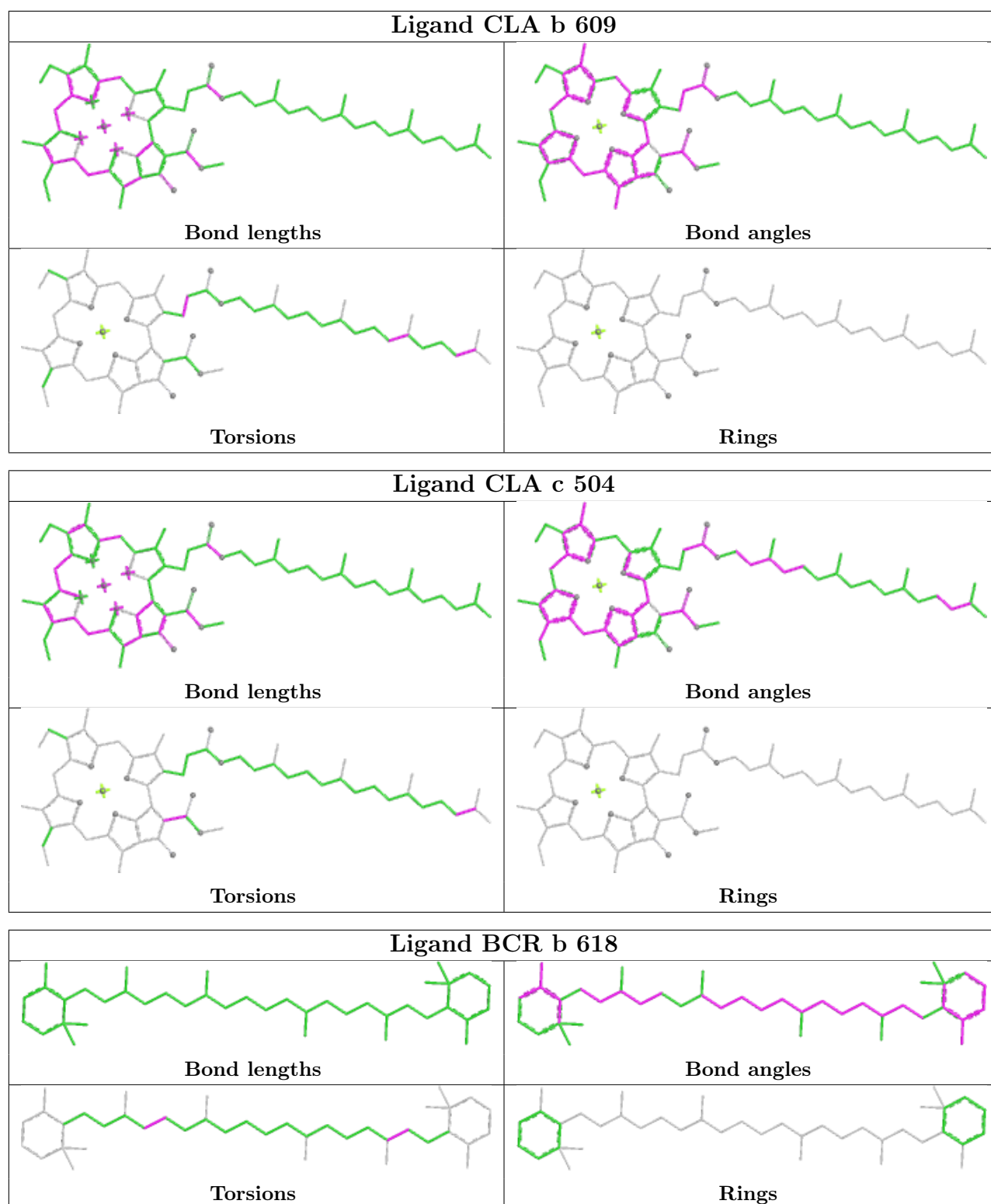


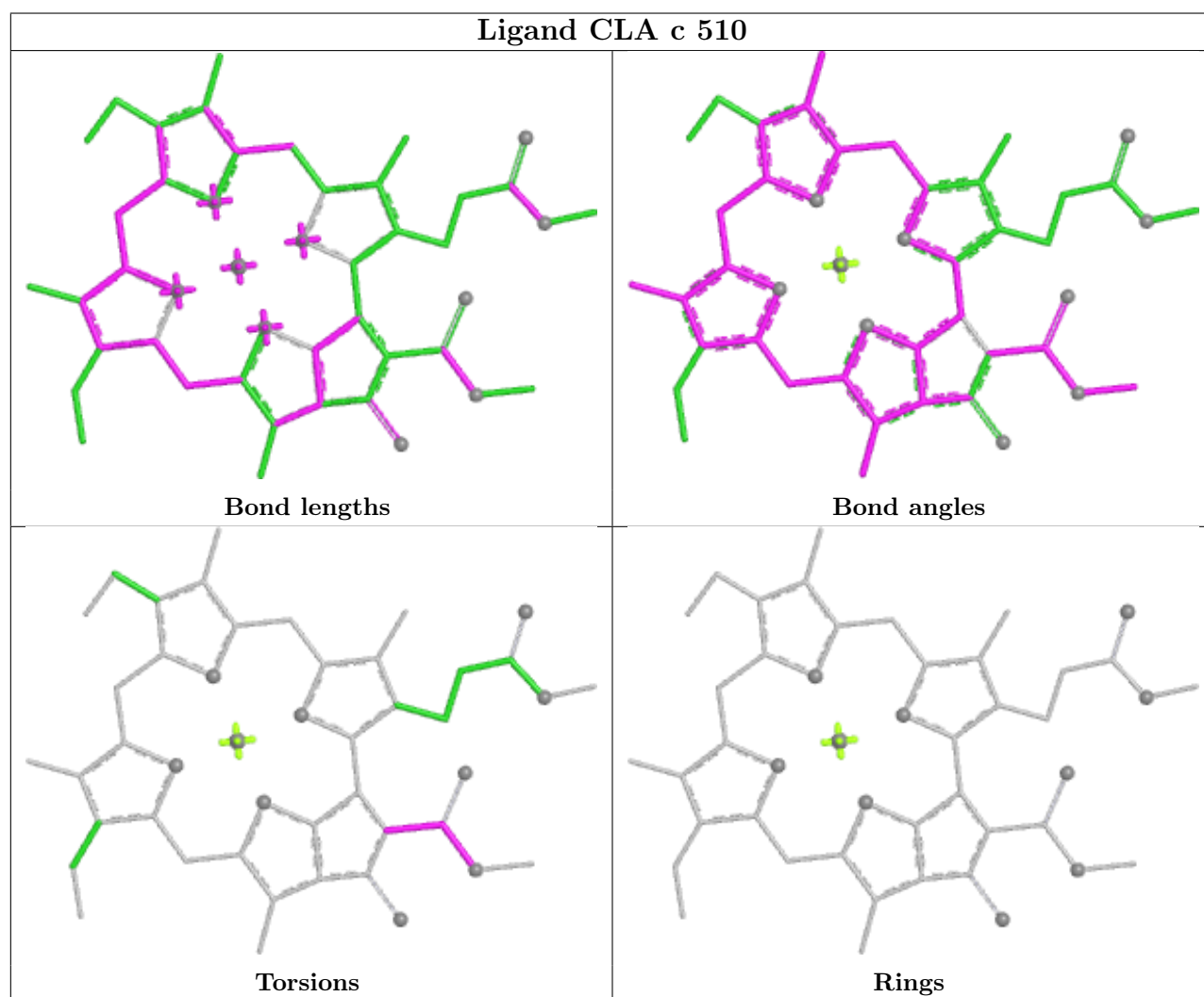
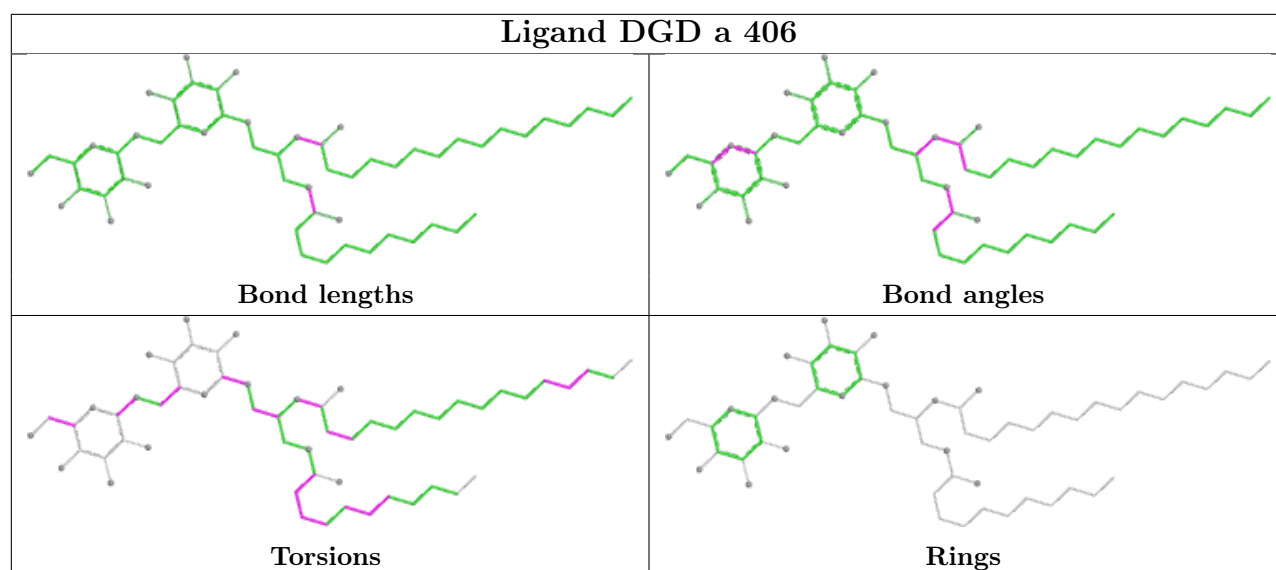


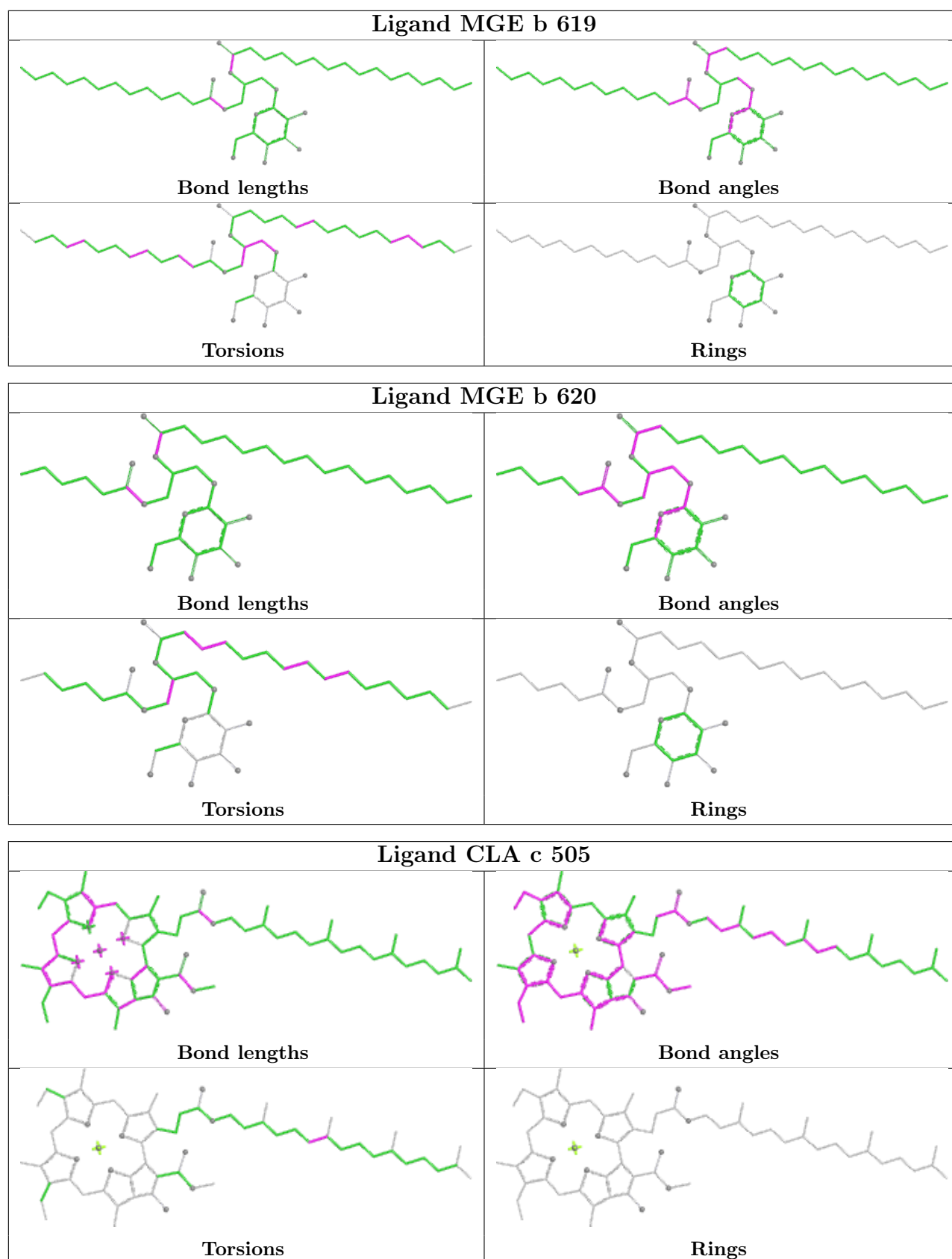




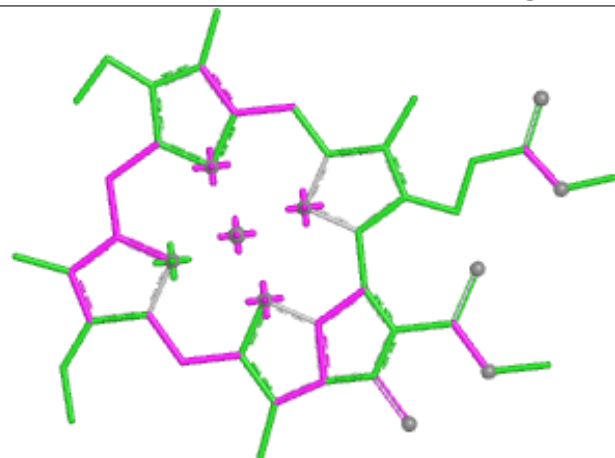
| Ligand BCR b 616                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand MGE m 102                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand BCR c 515                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand PHO d 403                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |



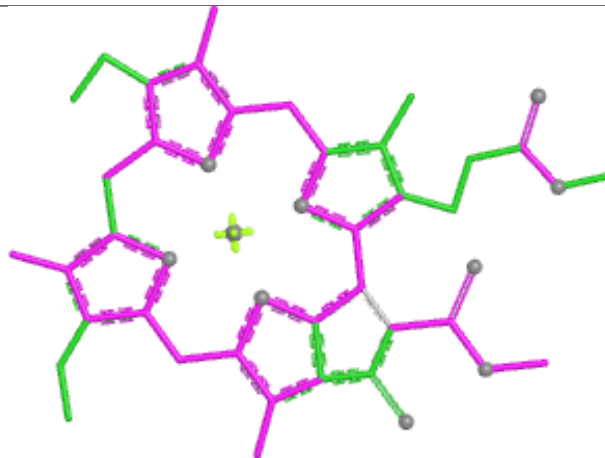




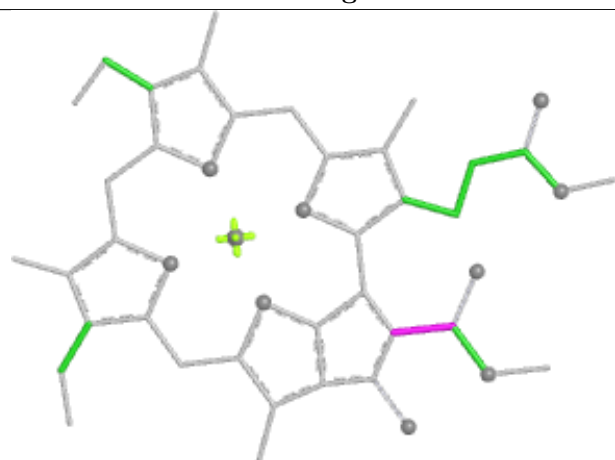
## Ligand CLA c 508



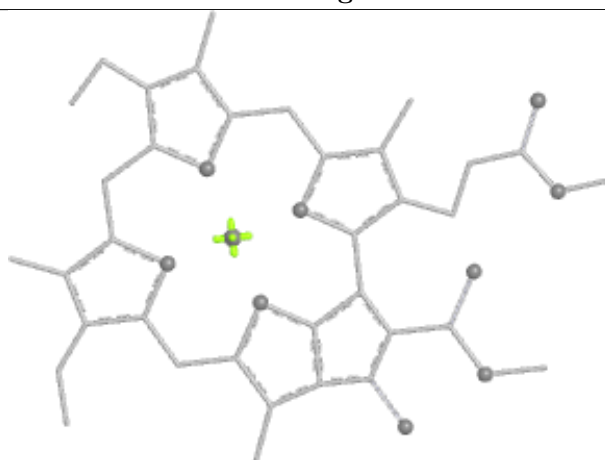
Bond lengths



Bond angles

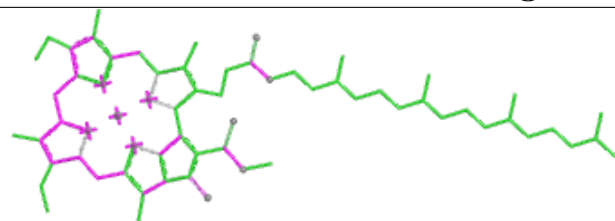


Torsions

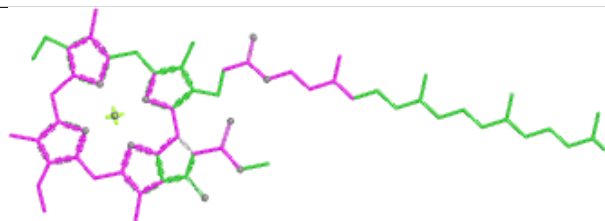


Rings

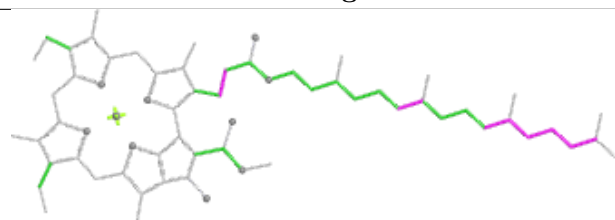
## Ligand CLA b 605



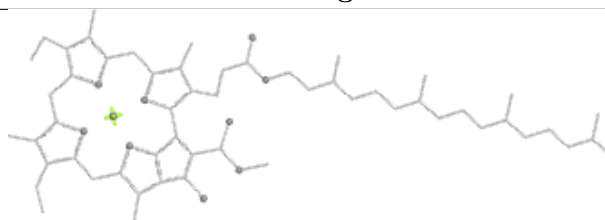
Bond lengths



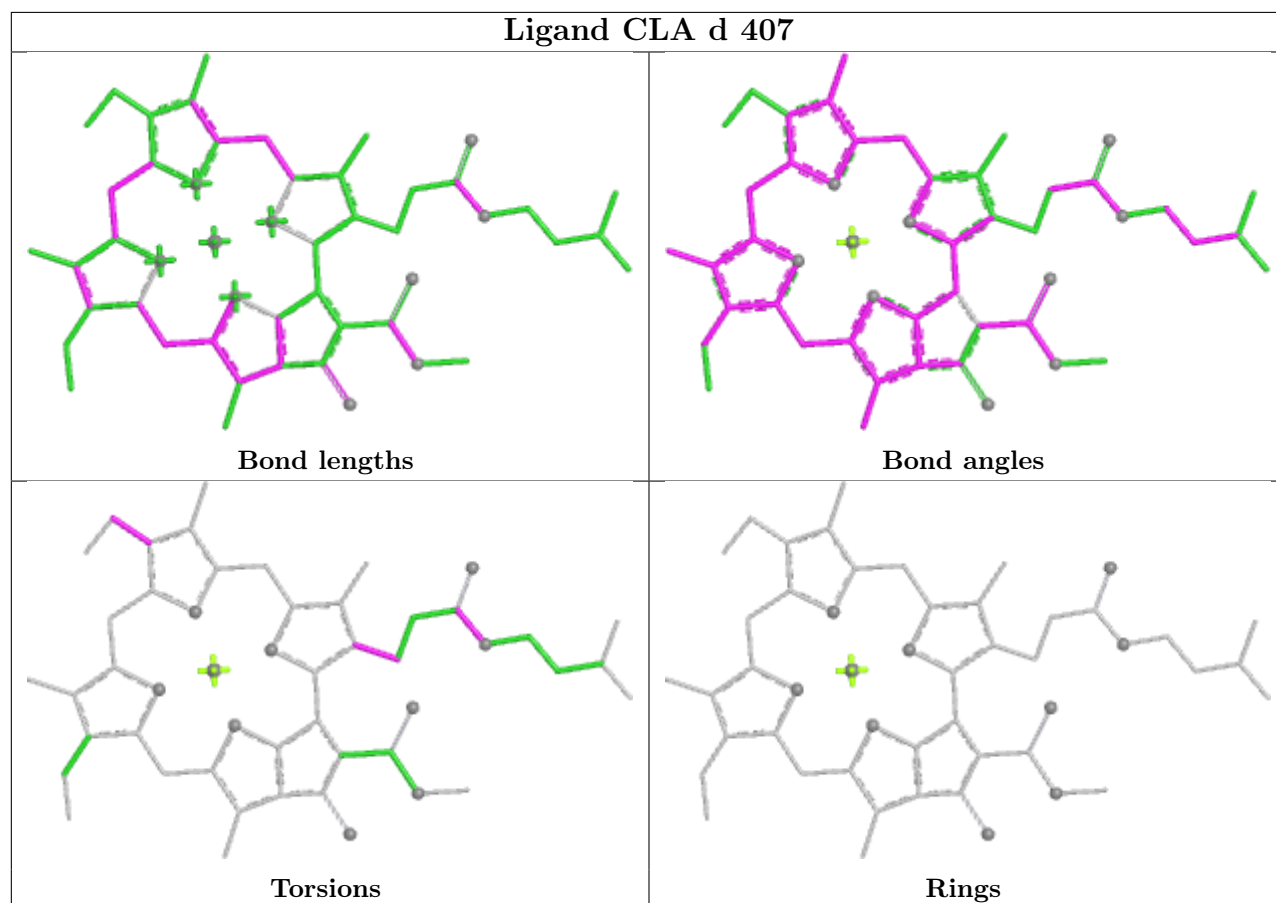
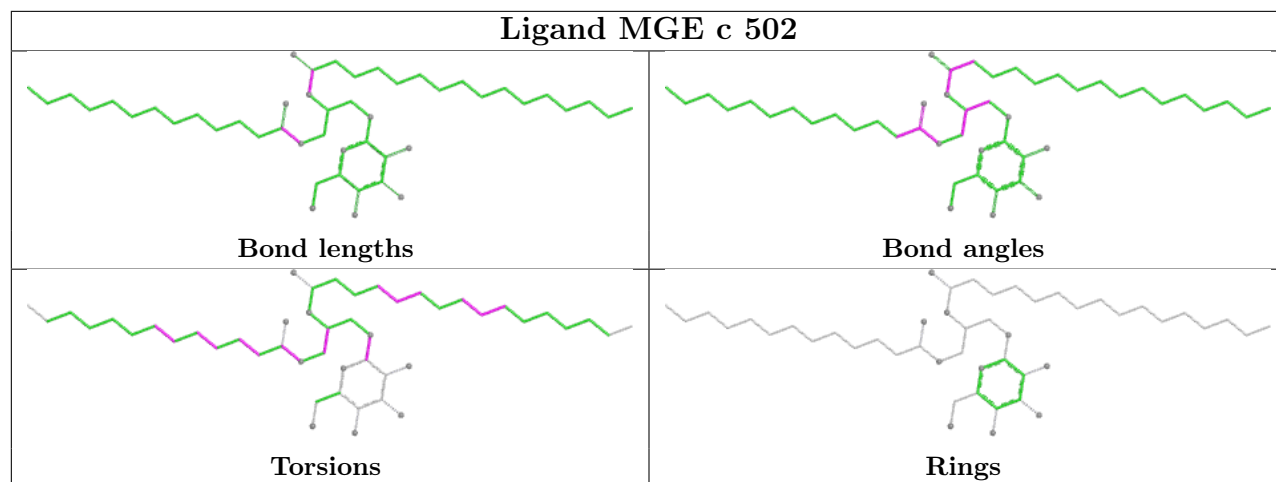
Bond angles



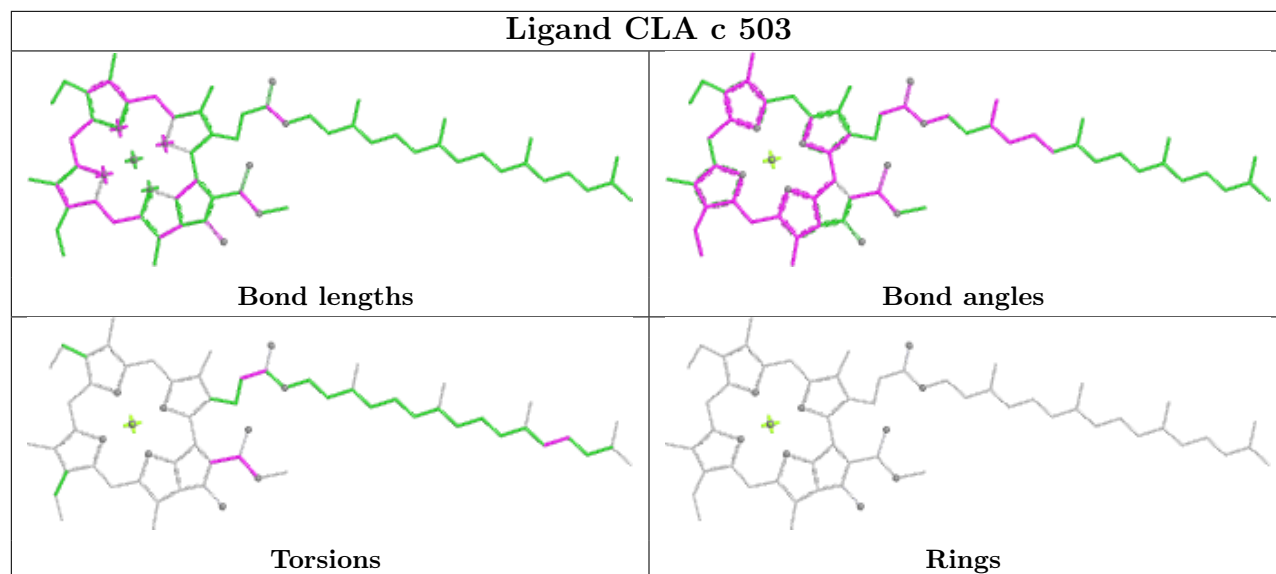
Torsions



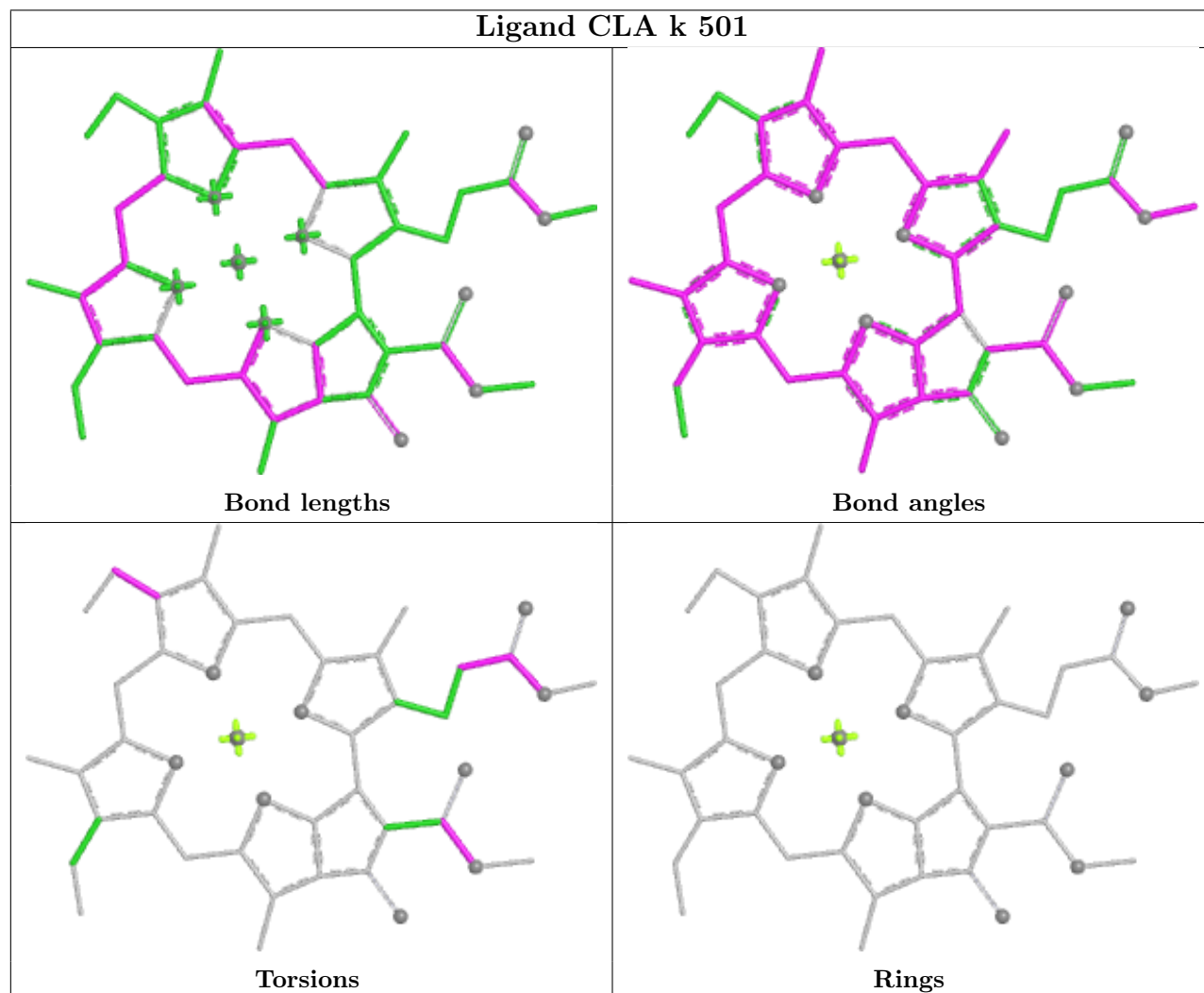
Rings

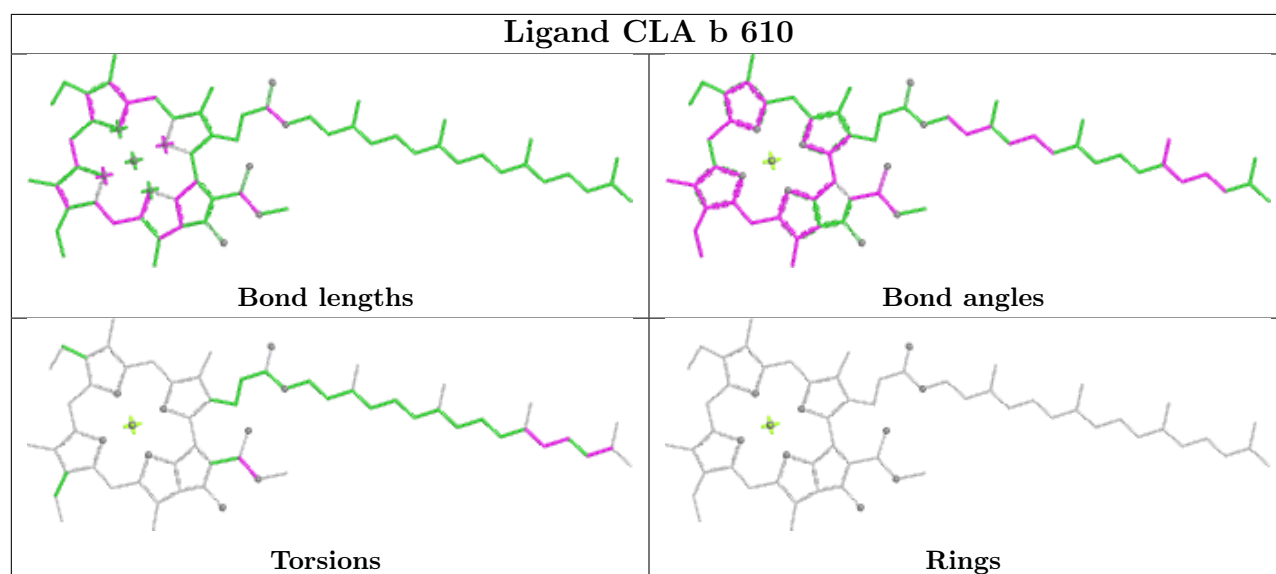
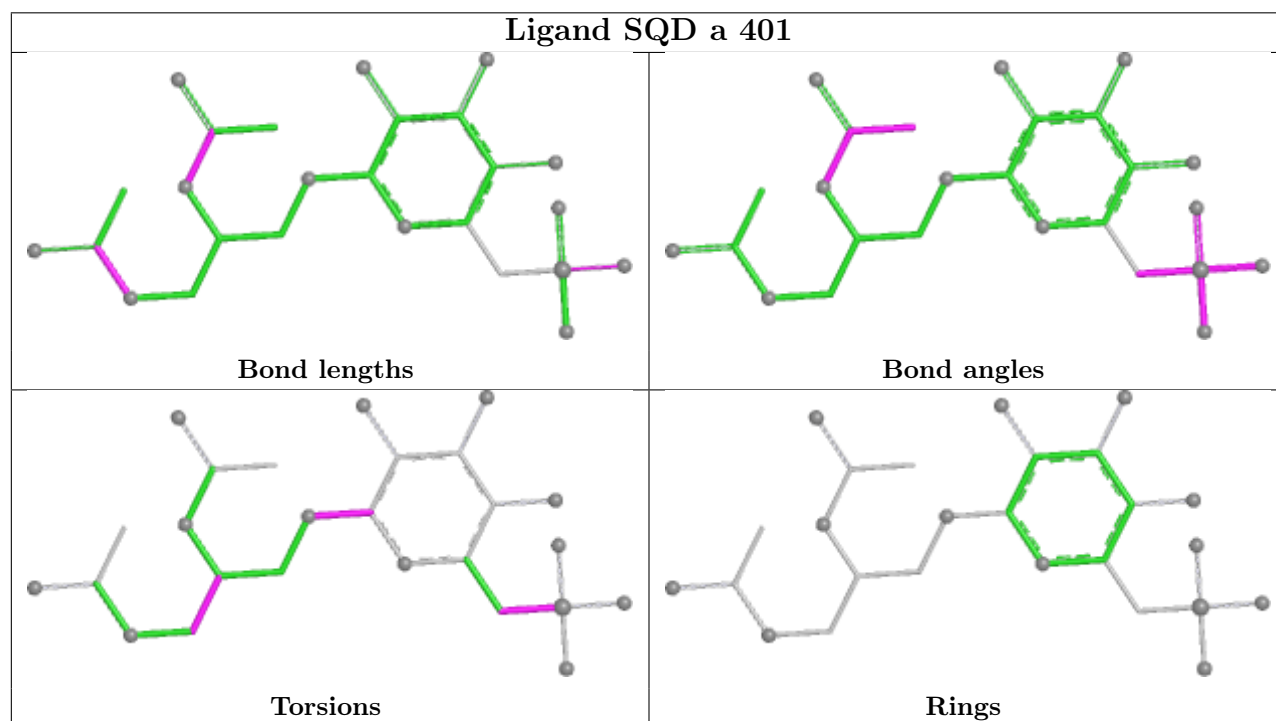
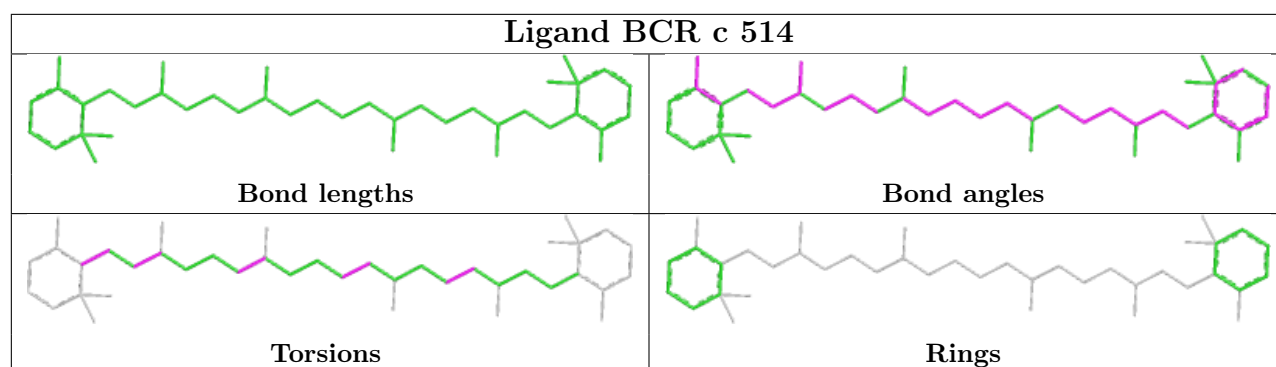


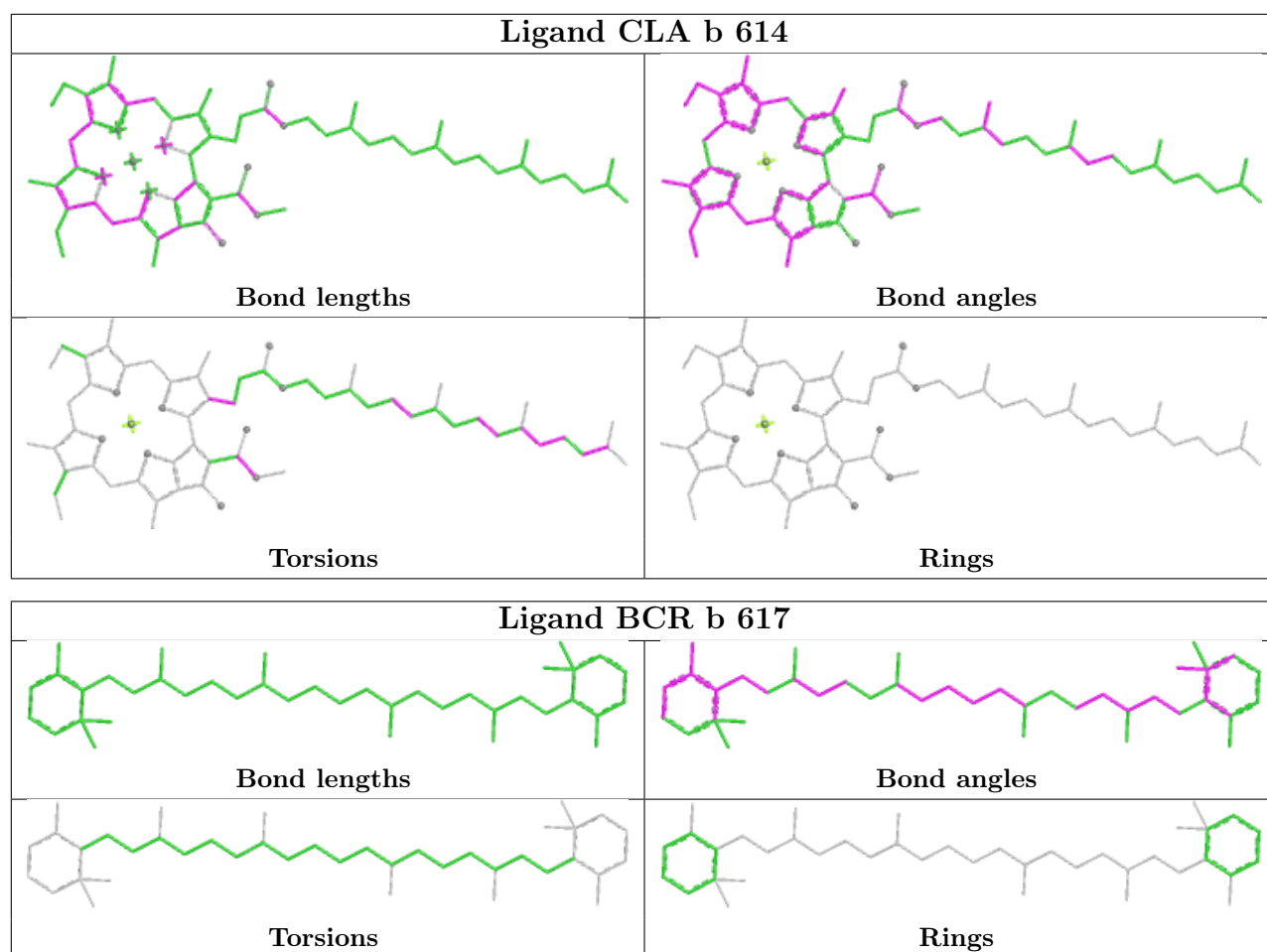
## Ligand CLA c 503

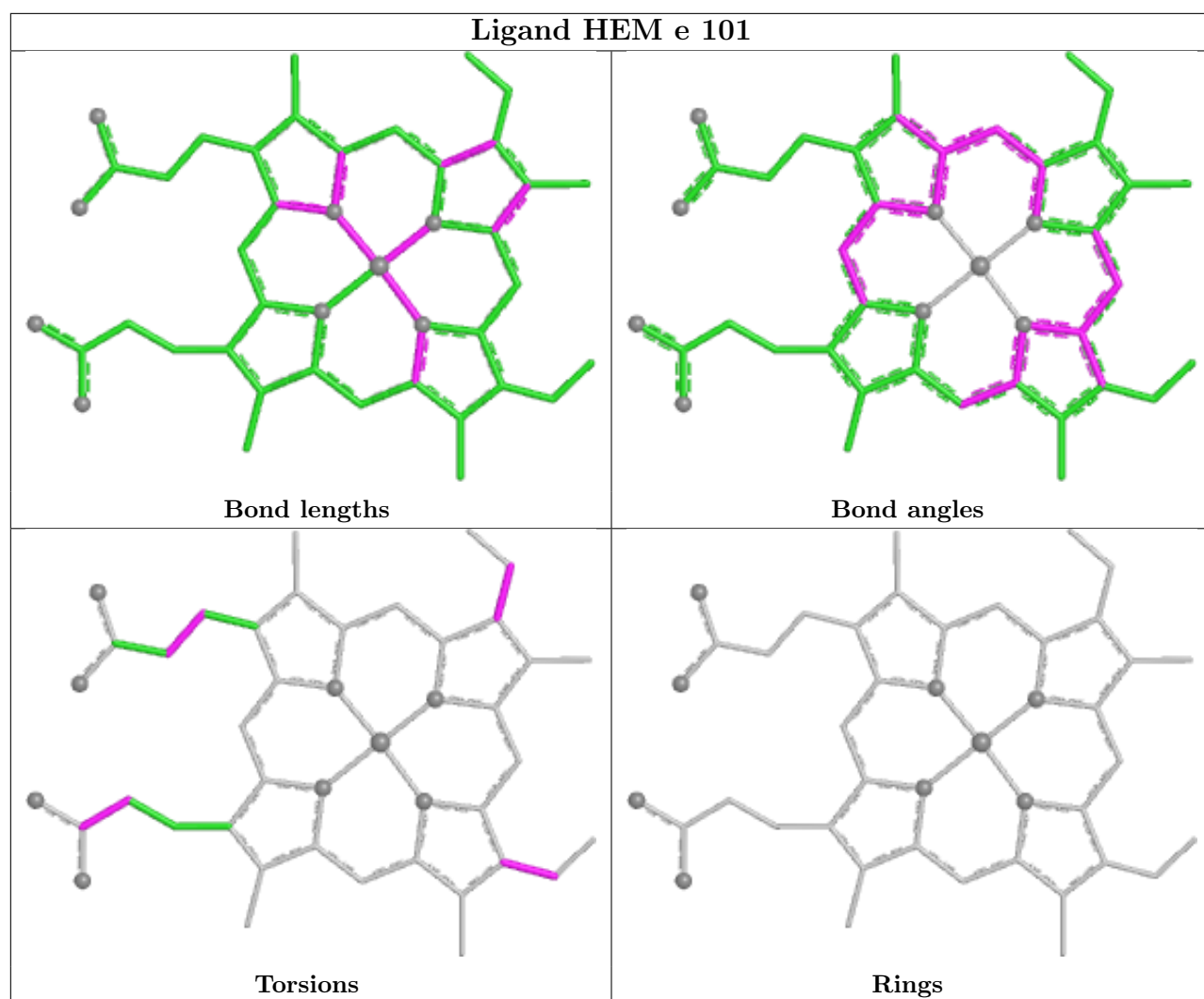


## Ligand CLA k 501

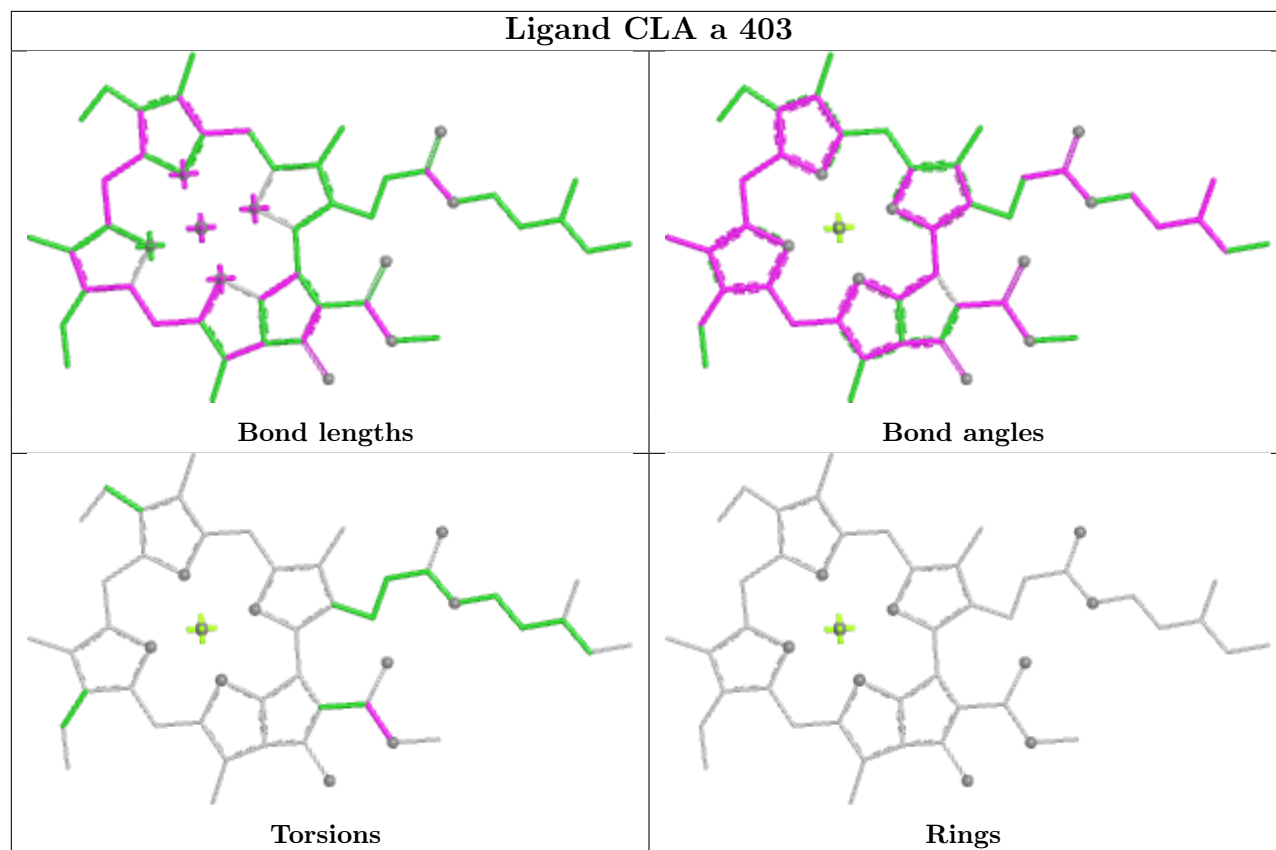




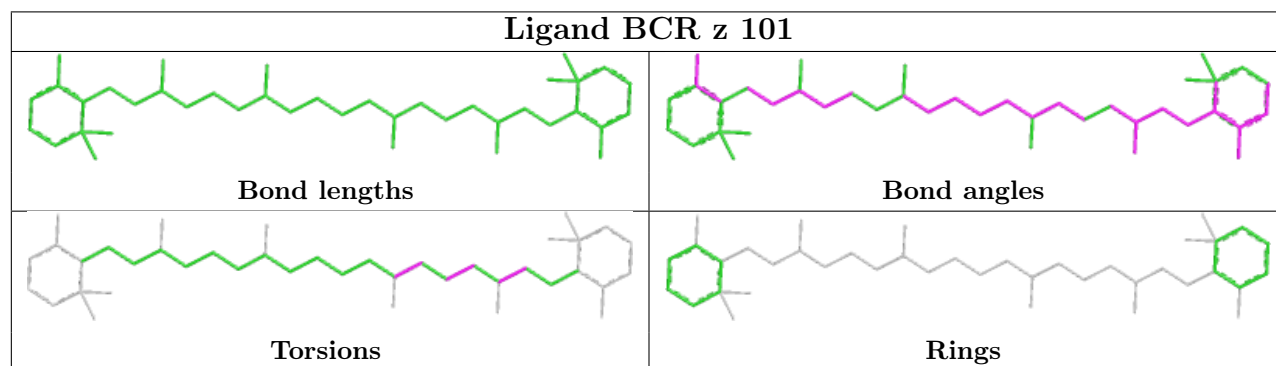




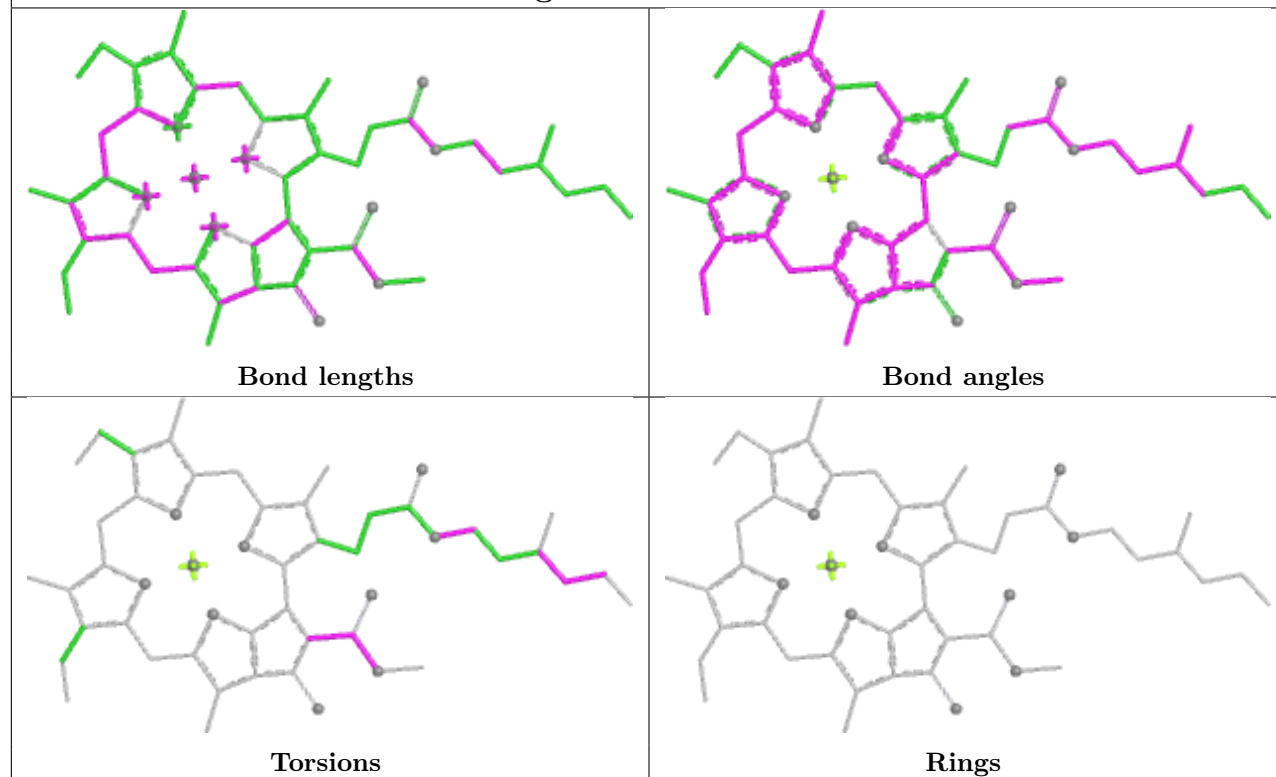
## Ligand CLA a 403



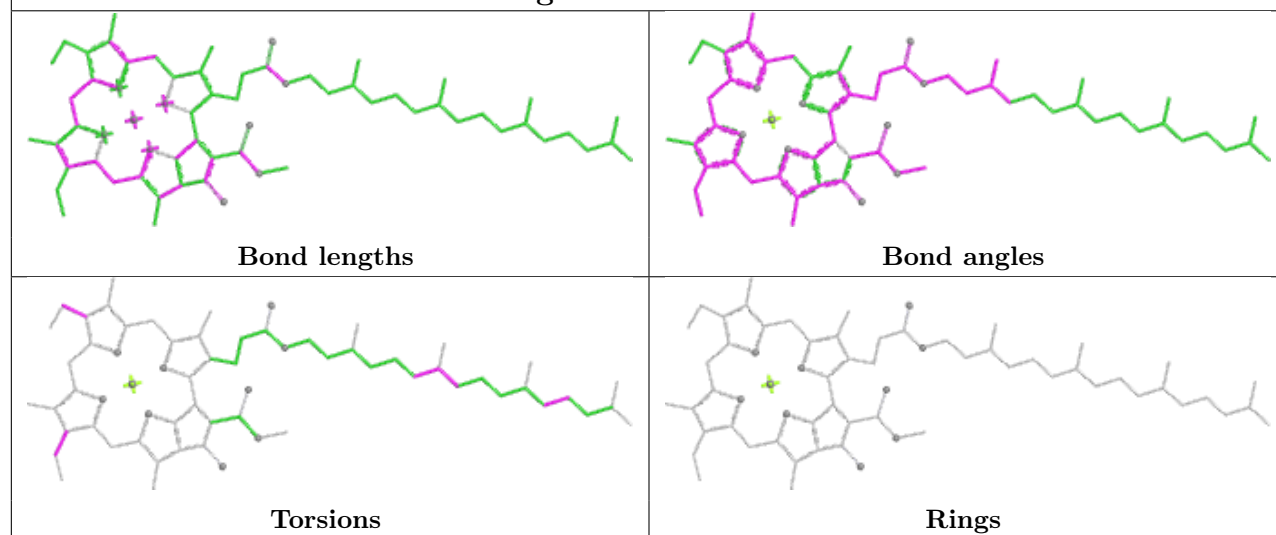
## Ligand BCR z 101



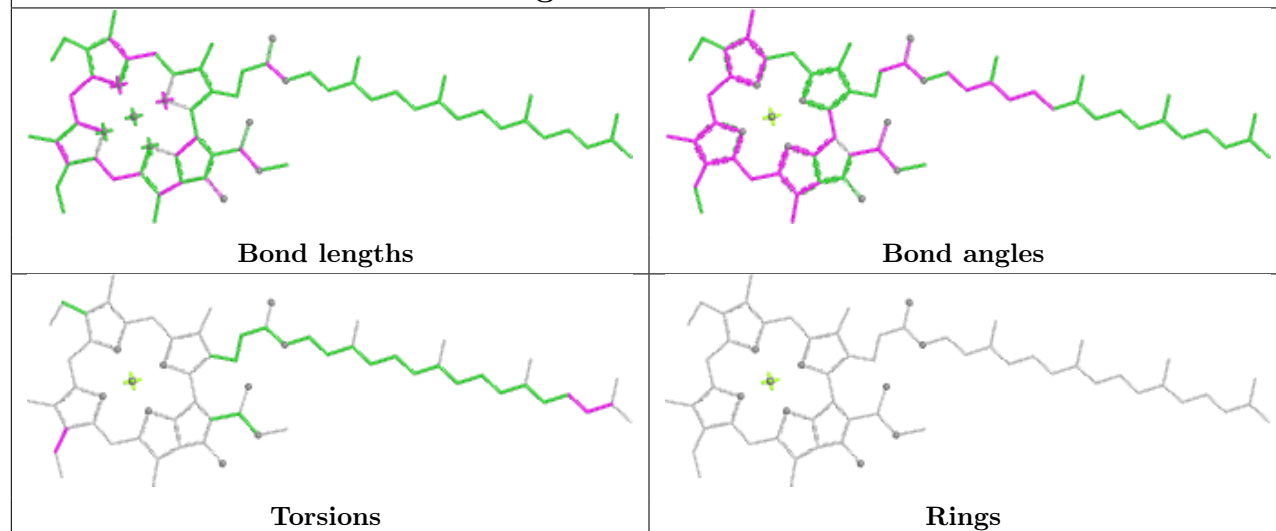
## Ligand CLA b 613



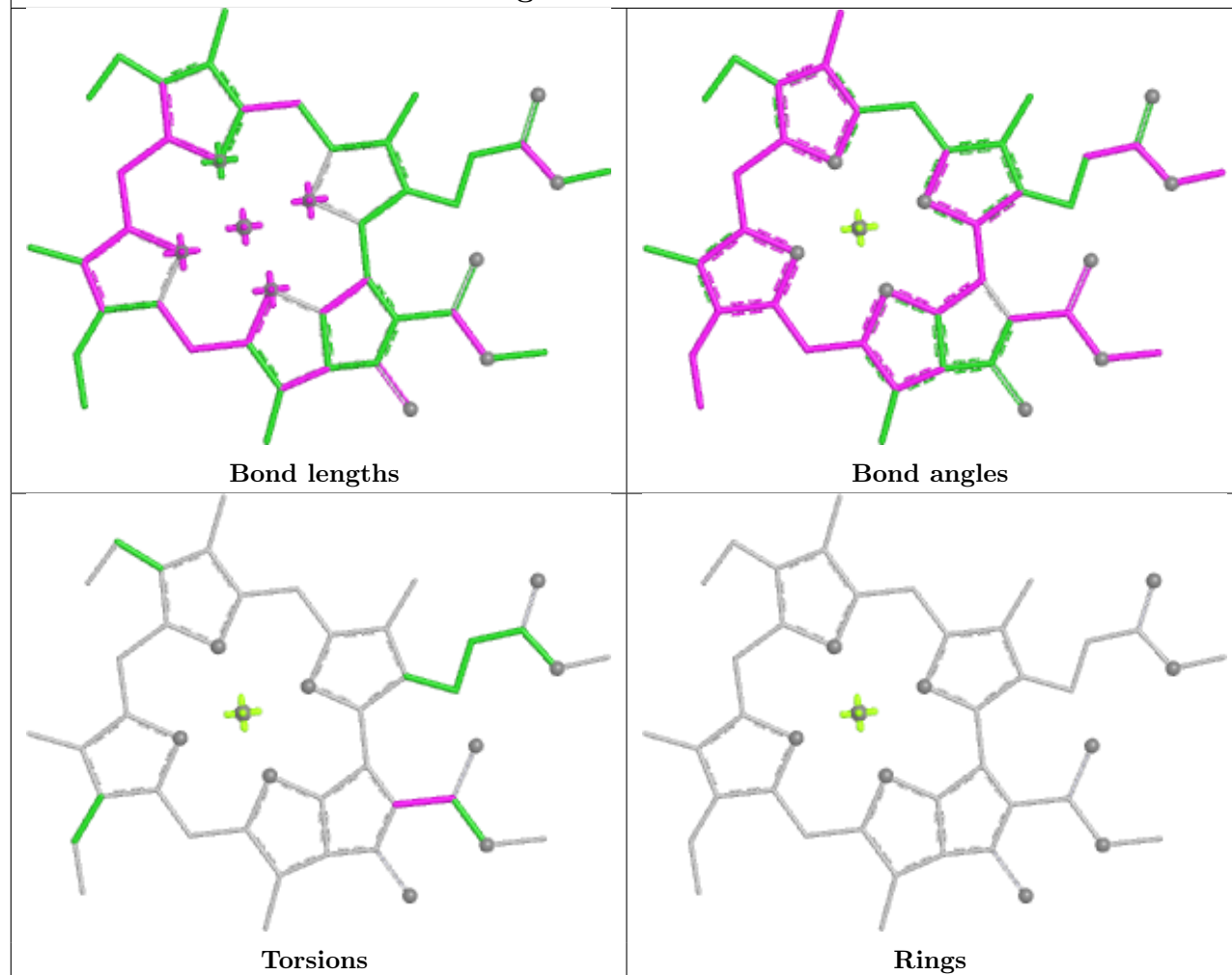
## Ligand CLA a 407

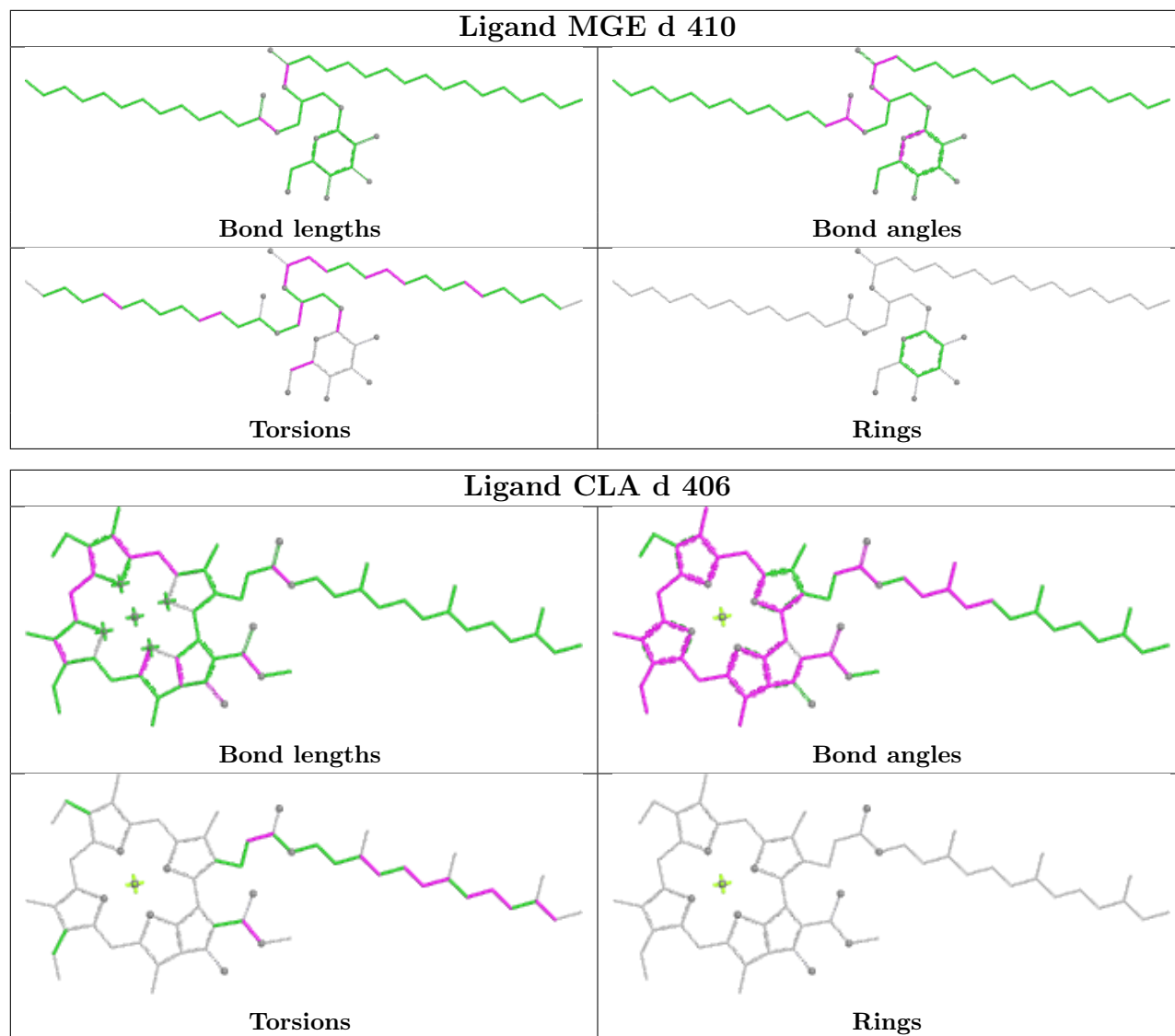


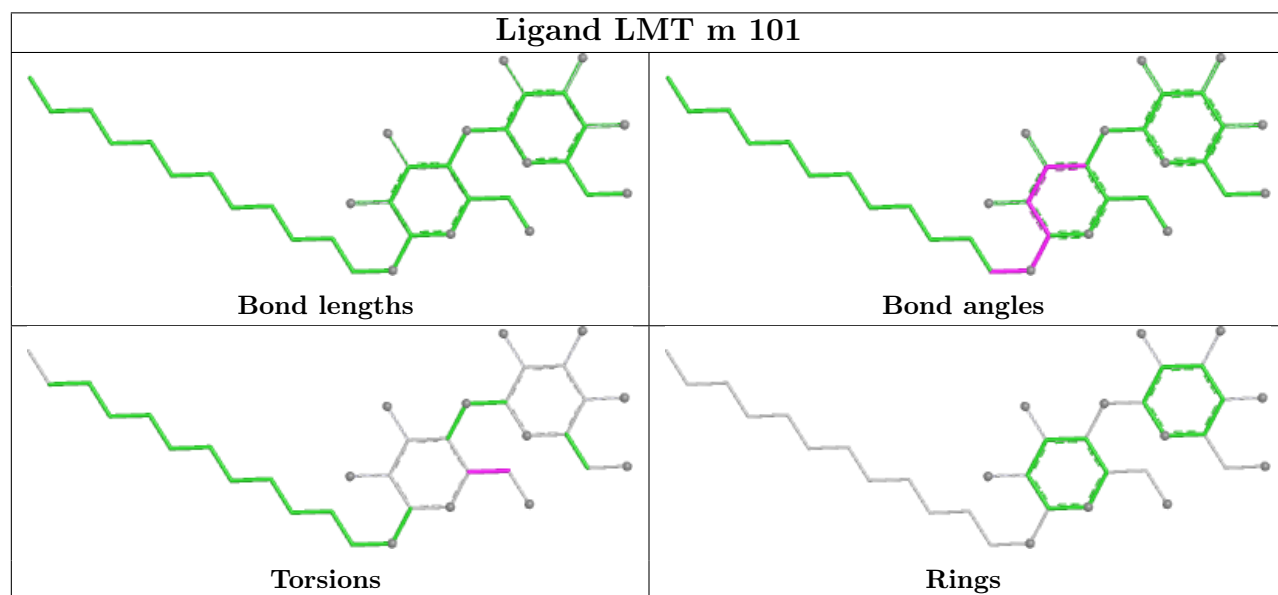
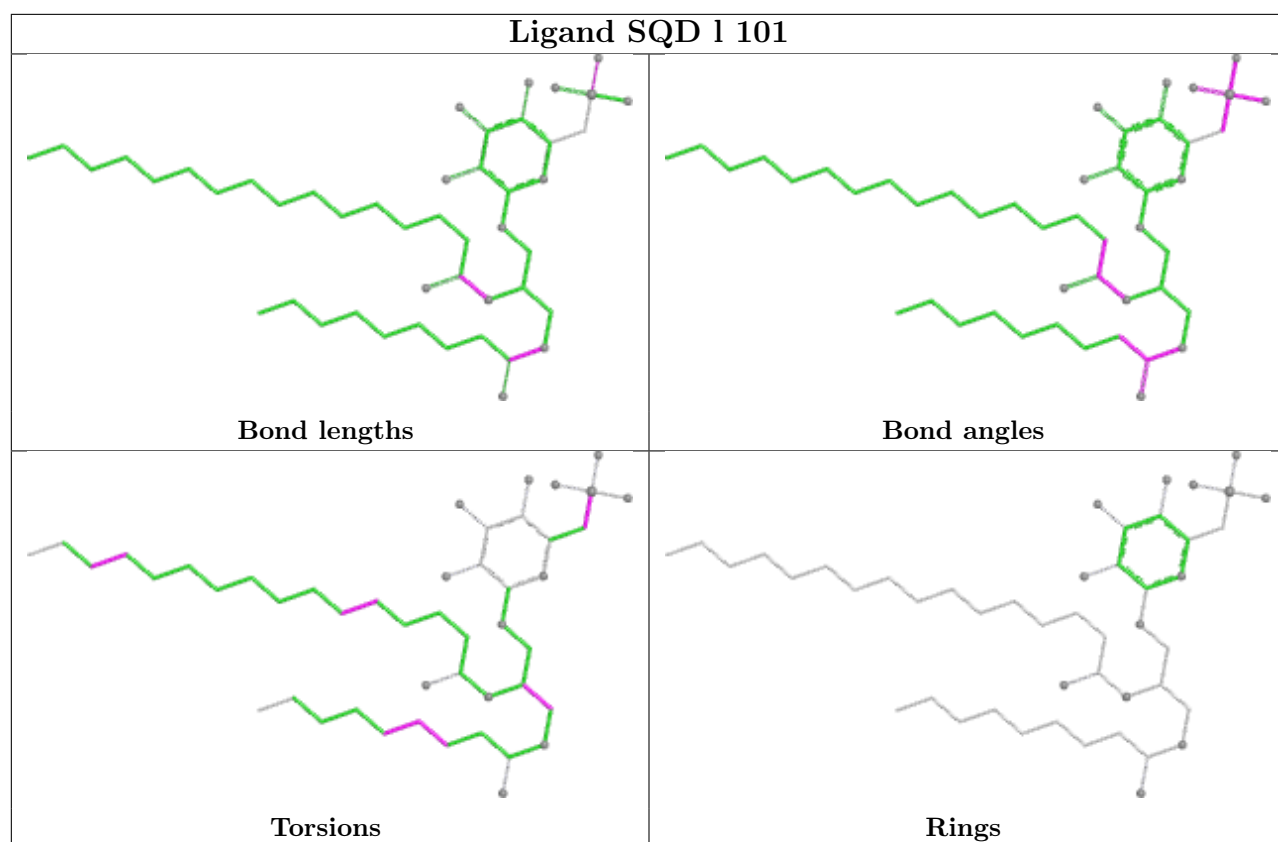
## Ligand CLA a 402



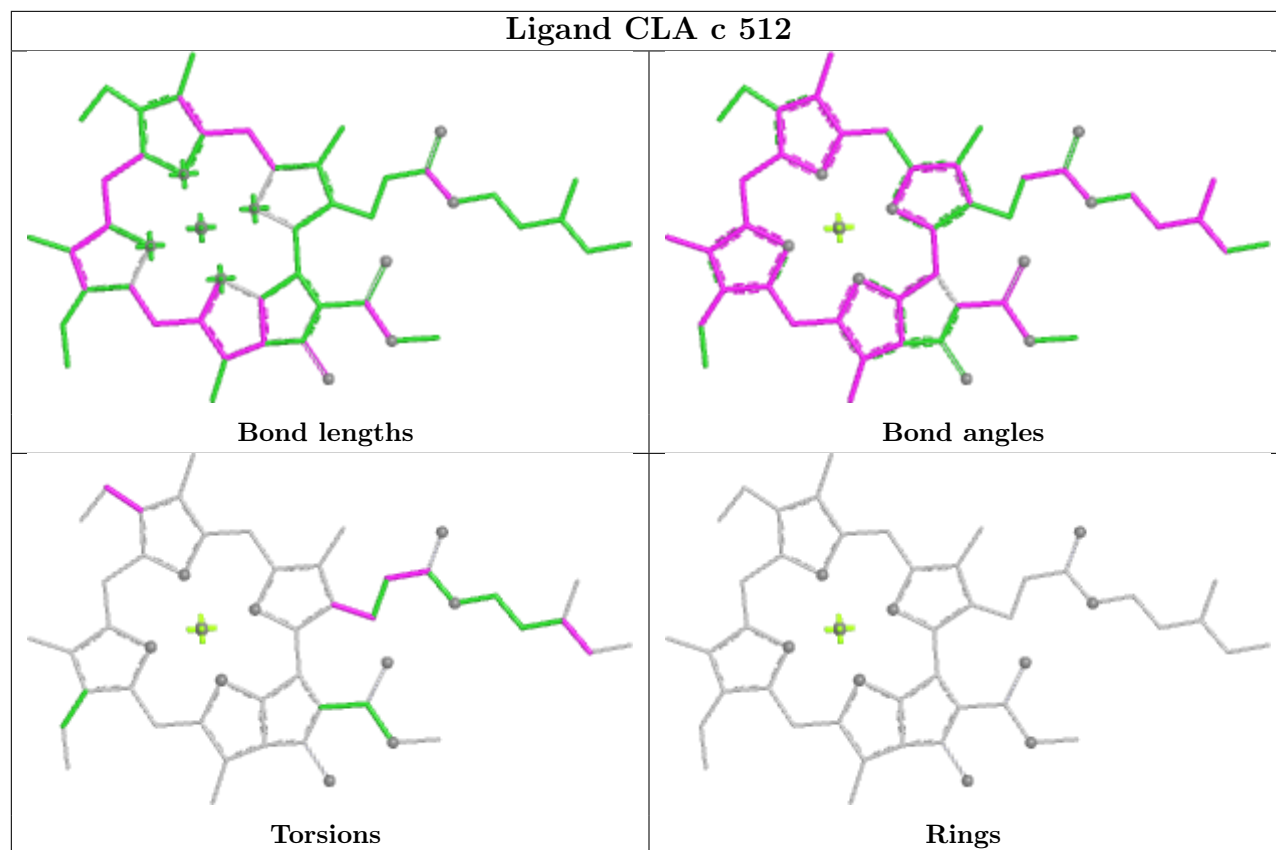
## Ligand CLA b 615



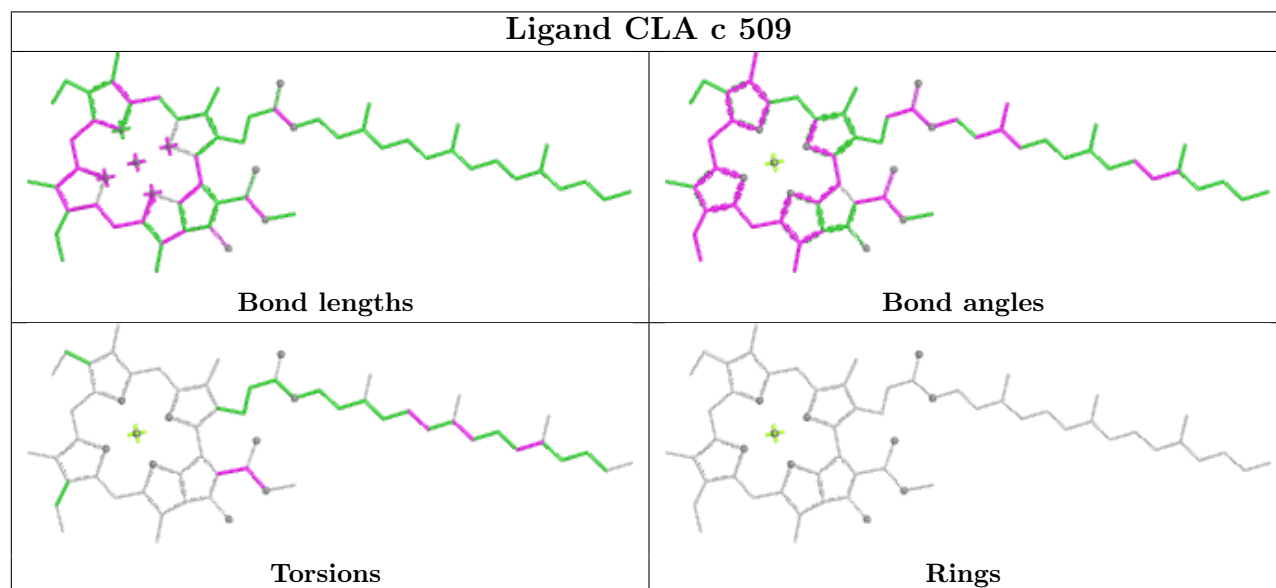


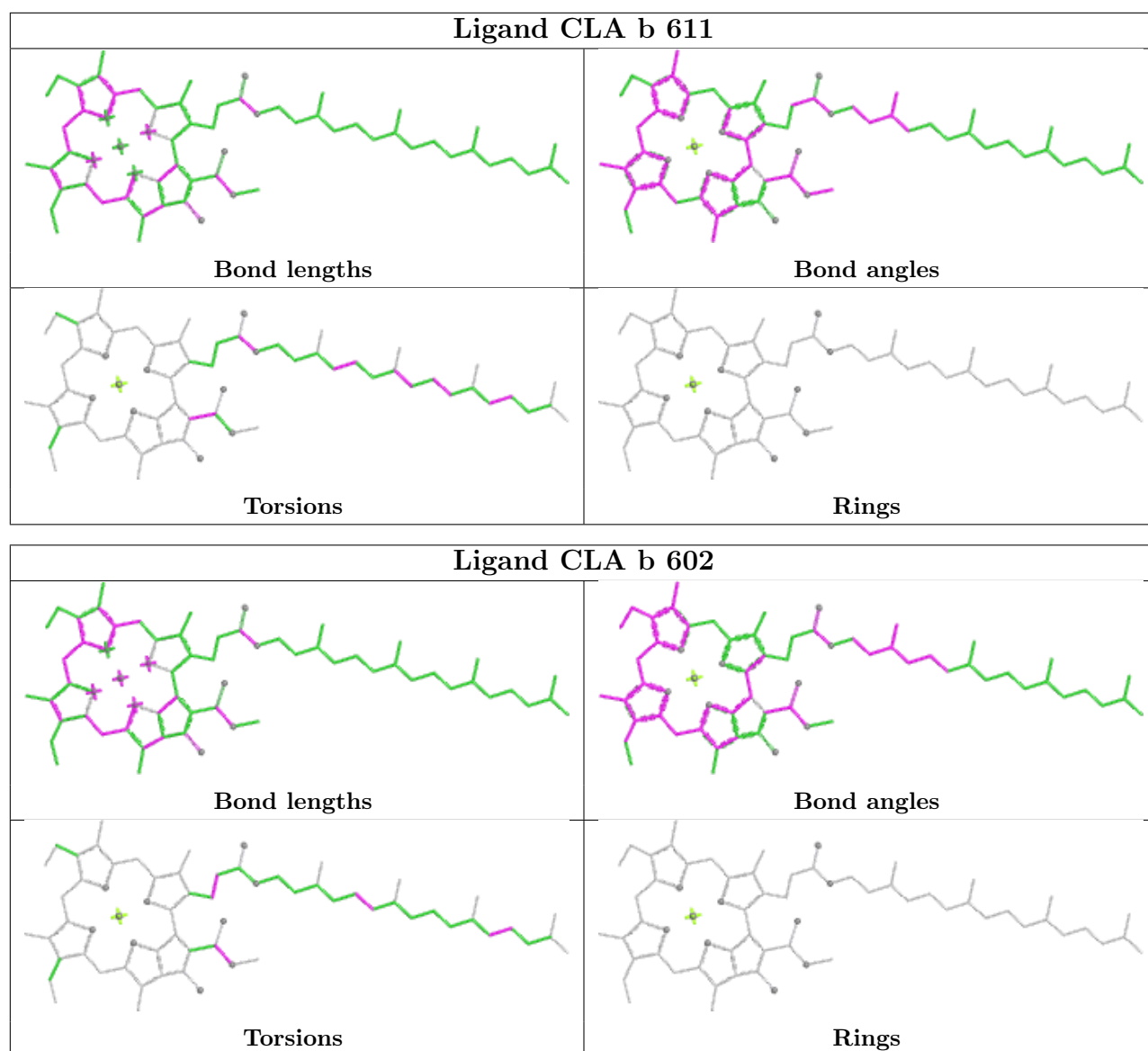


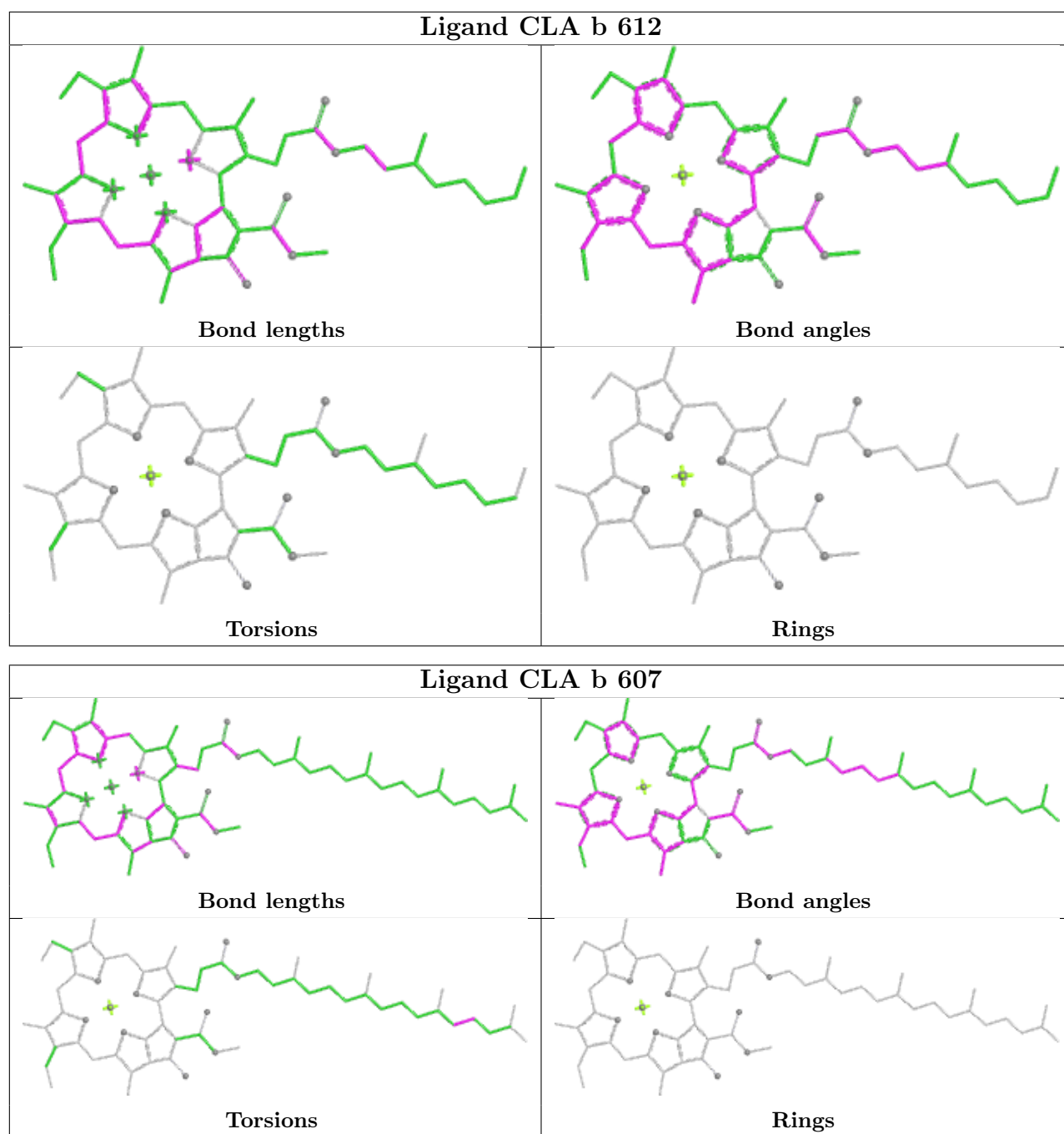
## Ligand CLA c 512



## Ligand CLA c 509







## 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.

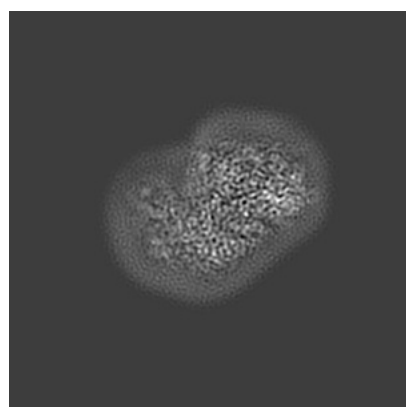
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30909. These allow visual inspection of the internal detail of the map and identification of artifacts.

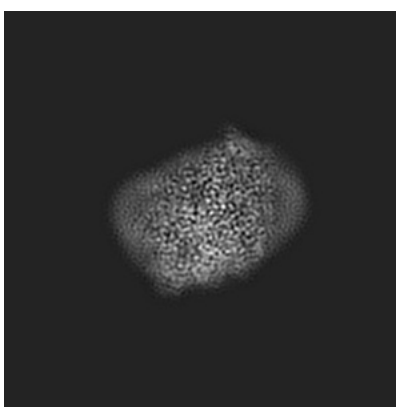
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

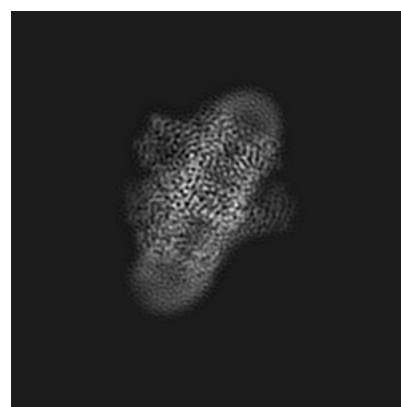
#### 6.1.1 Primary map



X



Y

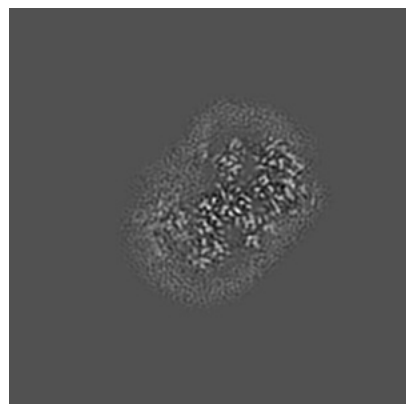


Z

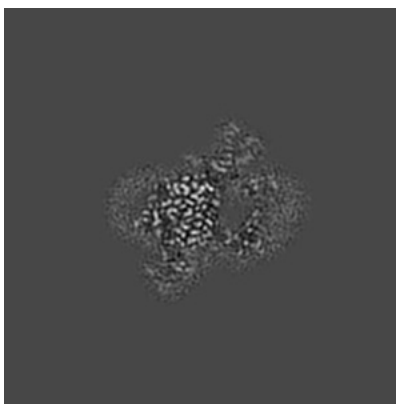
The images above show the map projected in three orthogonal directions.

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

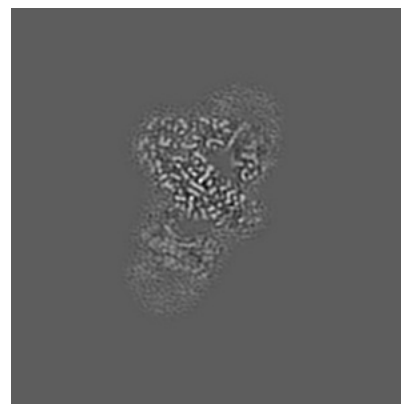
#### 6.2.1 Primary map



X Index: 100



Y Index: 100

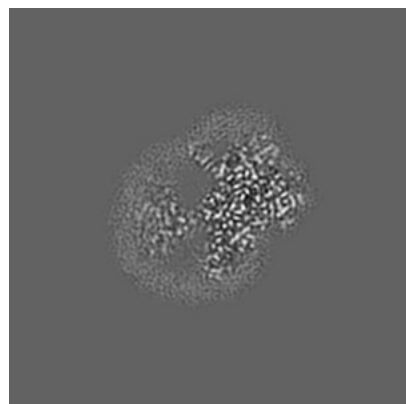


Z Index: 100

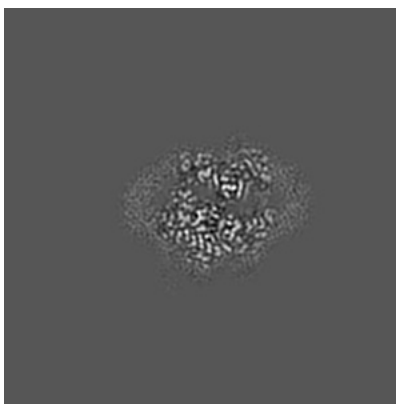
The images above show central slices of the map in three orthogonal directions.

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

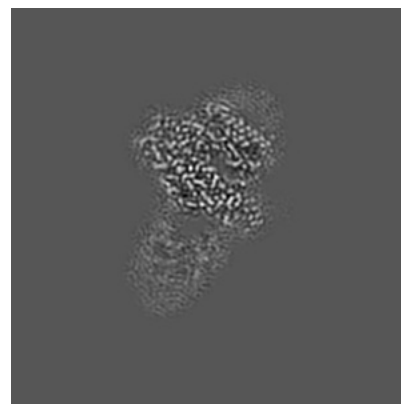
### 6.3.1 Primary map



X Index: 91



Y Index: 118

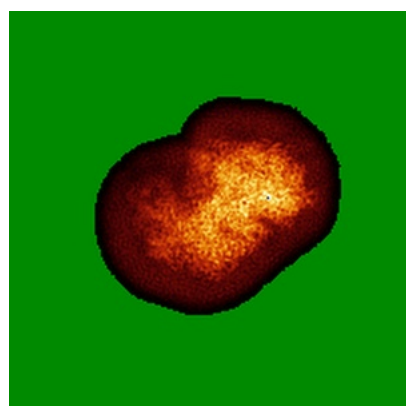


Z Index: 104

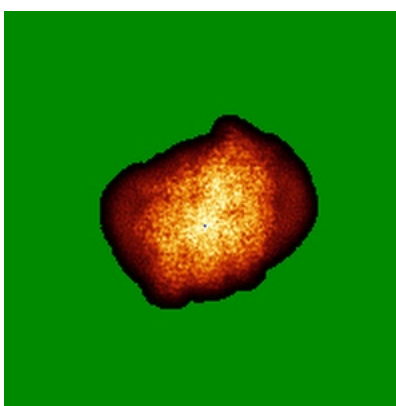
The images above show the largest variance slices of the map in three orthogonal directions.

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

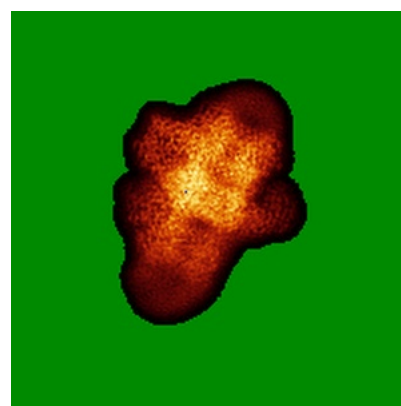
### 6.4.1 Primary map



X



Y

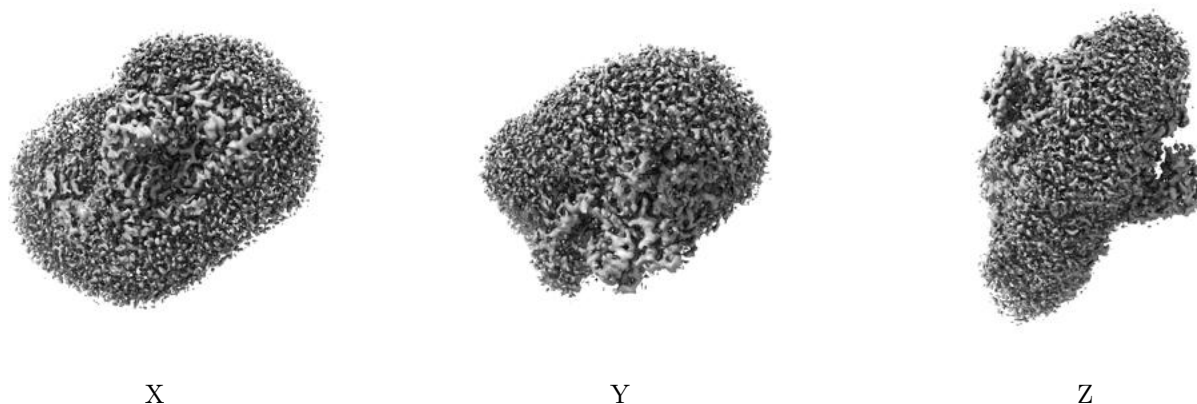


Z

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 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

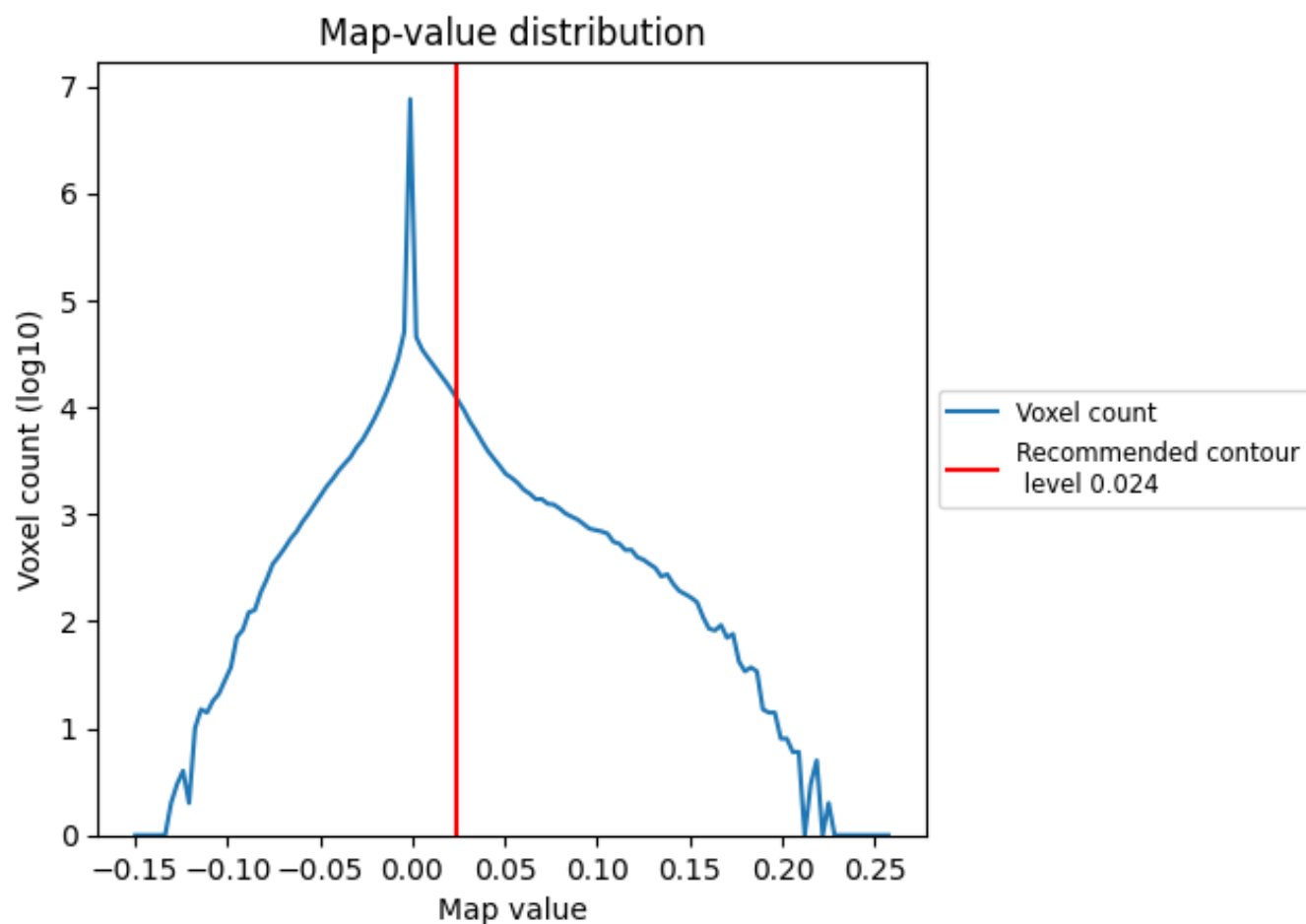
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

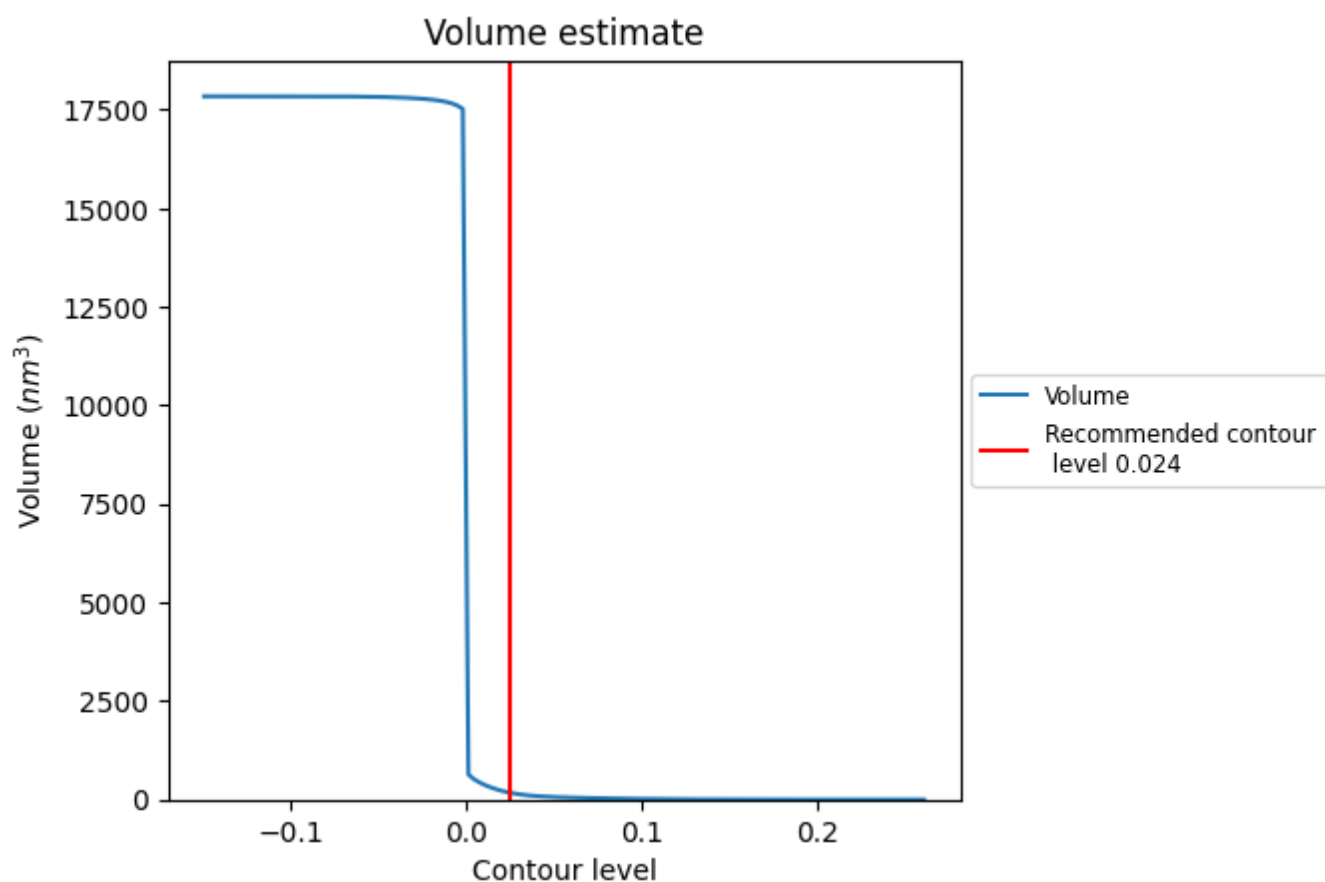
This section contains the results of statistical analysis of the map.

### 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.

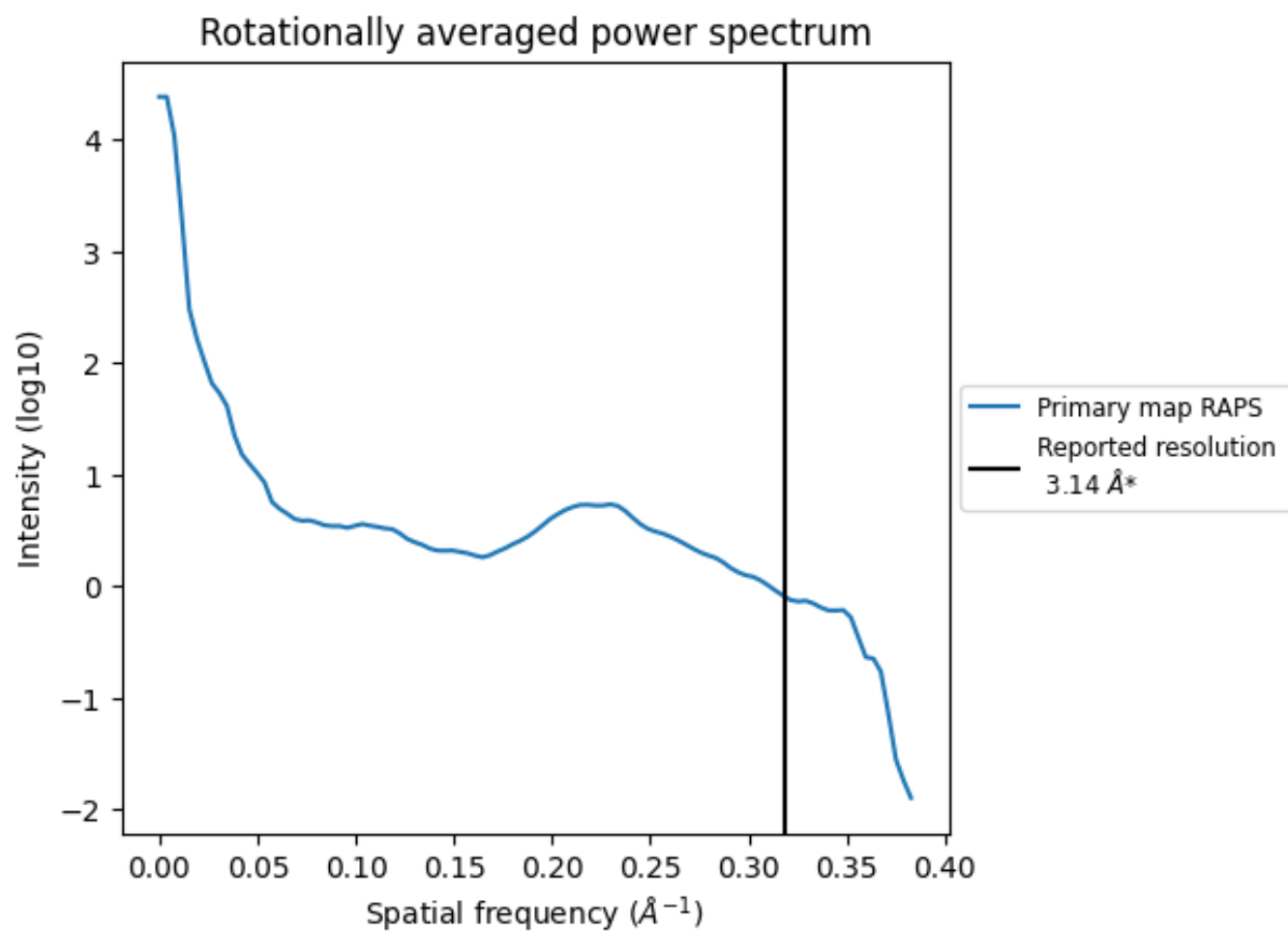
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 179  $\text{nm}^3$ ; this corresponds to an approximate mass of 162 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>

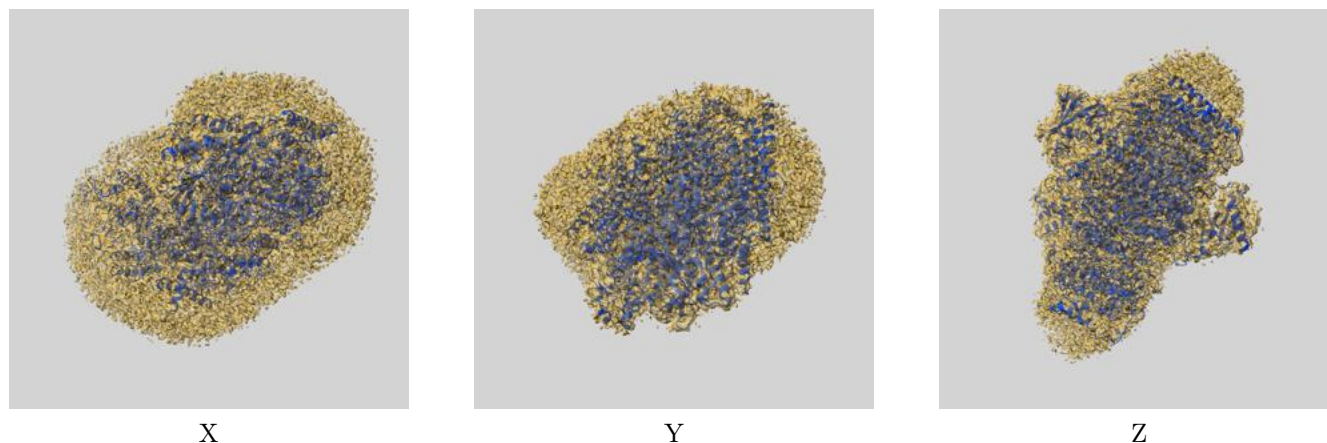
## 8 Fourier-Shell correlation ⓘ

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

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

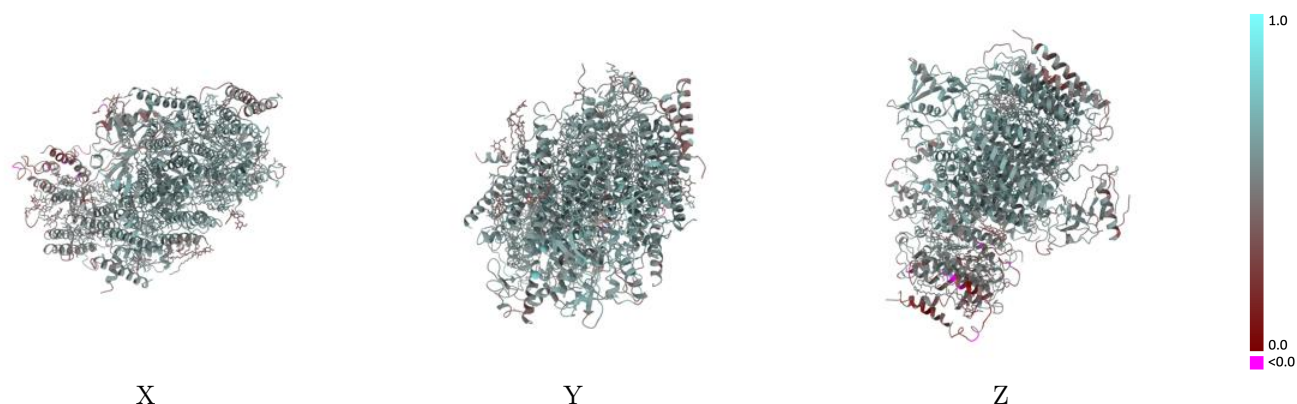
This section contains information regarding the fit between EMDB map EMD-30909 and PDB model 7DXH. Per-residue inclusion information can be found in section [3](#) on page [17](#).

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



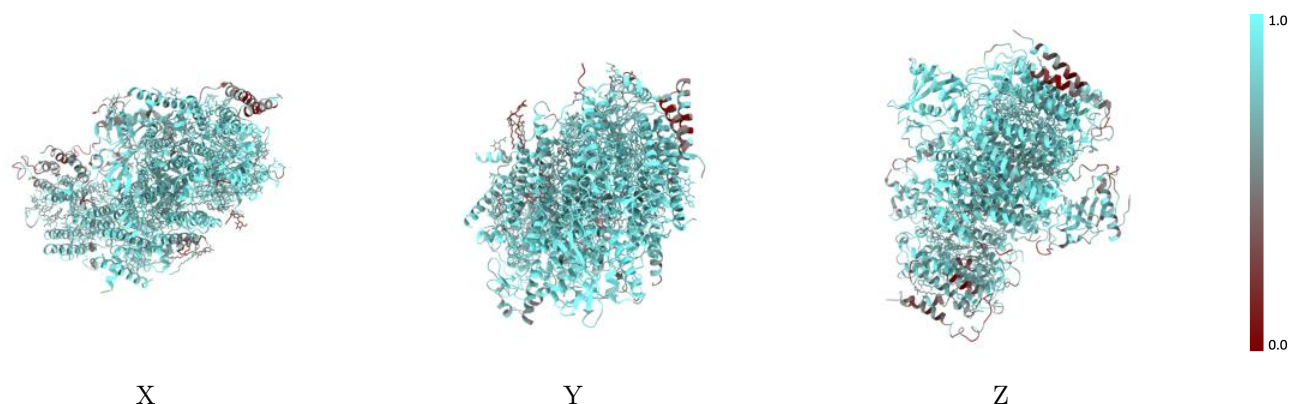
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



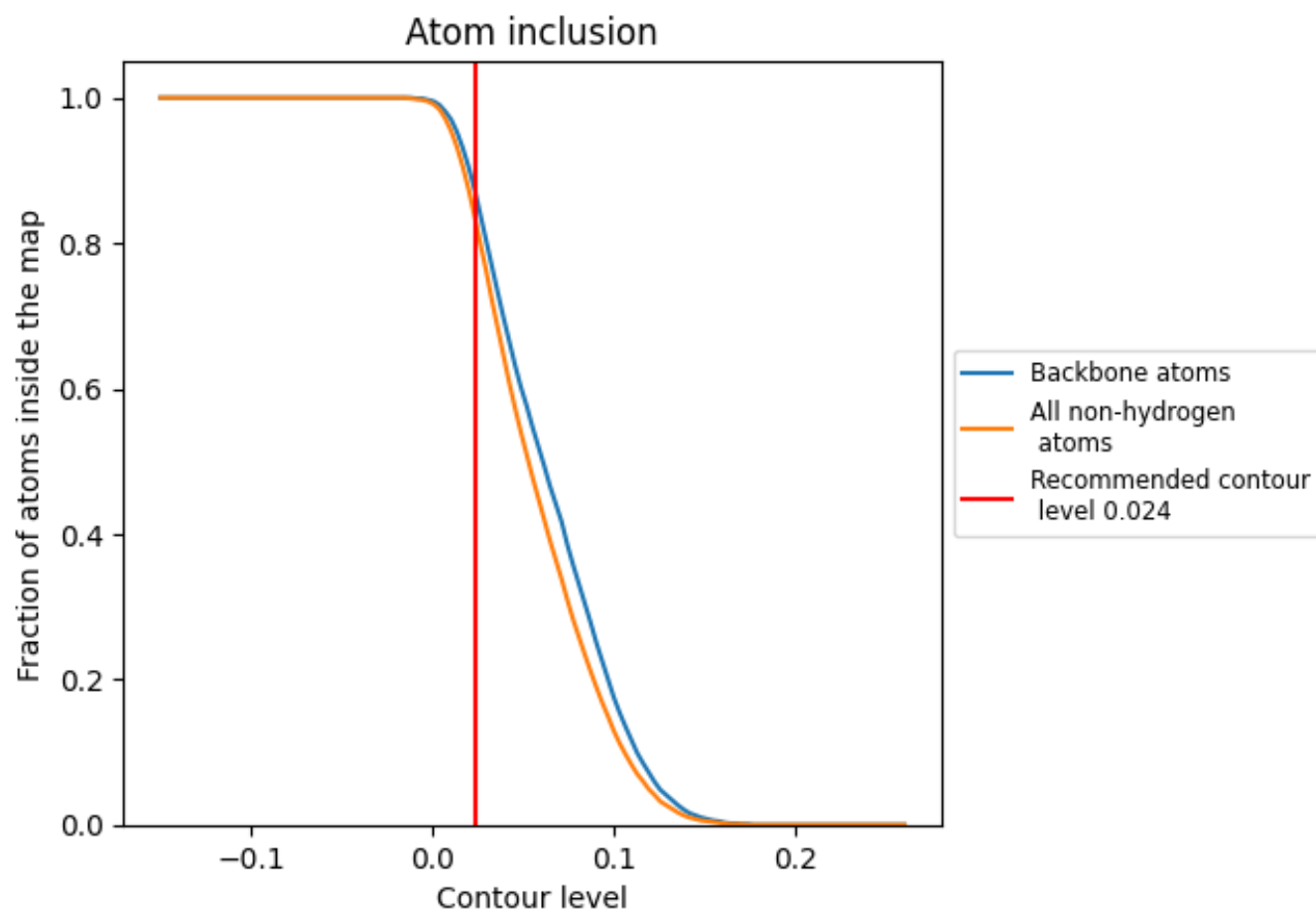
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.024).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (0.024) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.8310 | <div></div> 0.5420 |
| A     | <div></div> 0.6930 | <div></div> 0.4890 |
| B     | <div></div> 0.5420 | <div></div> 0.4840 |
| C     | <div></div> 0.4350 | <div></div> 0.4330 |
| a     | <div></div> 0.8940 | <div></div> 0.5730 |
| b     | <div></div> 0.8880 | <div></div> 0.5800 |
| c     | <div></div> 0.8260 | <div></div> 0.5060 |
| d     | <div></div> 0.9100 | <div></div> 0.5950 |
| e     | <div></div> 0.7530 | <div></div> 0.4920 |
| f     | <div></div> 0.8100 | <div></div> 0.5430 |
| h     | <div></div> 0.8920 | <div></div> 0.5710 |
| i     | <div></div> 0.8130 | <div></div> 0.5100 |
| k     | <div></div> 0.6910 | <div></div> 0.4490 |
| l     | <div></div> 0.7740 | <div></div> 0.5510 |
| m     | <div></div> 0.6660 | <div></div> 0.5040 |
| t     | <div></div> 0.7710 | <div></div> 0.5220 |
| x     | <div></div> 0.8310 | <div></div> 0.5580 |
| y     | <div></div> 0.3360 | <div></div> 0.2240 |
| z     | <div></div> 0.4530 | <div></div> 0.3120 |

