



## Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 10:33 PM JST

PDB ID : 8Y15 / pdb\_00008y15  
EMDB ID : EMD-38825  
Title : Cryo-EM structure of Light-harvesting complex from *Spinacia oleracea*  
Authors : Seki, S.; Miyata, T.; Tanaka, H.; Namba, K.; Kurisu, G.; Fujii, R.  
Deposited on : 2024-01-23  
Resolution : 2.17 Å (reported)  
Based on initial model : 1RWT

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

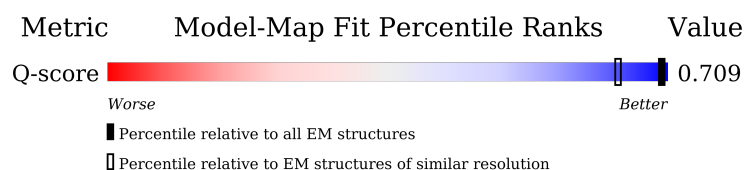
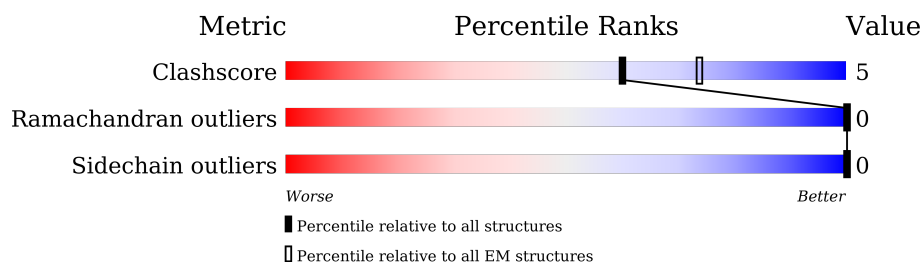
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

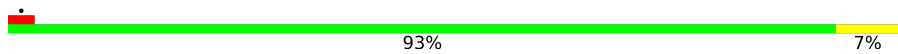
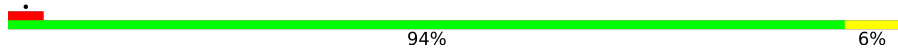
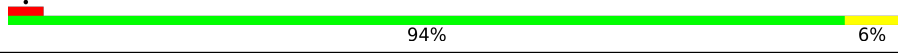
The reported resolution of this entry is 2.17 Å.

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                       | 2651 ( 1.67 - 2.67 )                                     |

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     | 216    |  |
| 1   | B     | 216    |  |
| 1   | C     | 216    |  |

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 crite-

ria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2   | CHL  | A     | 601  | X         | -        | -       | -                |
| 2   | CHL  | A     | 608  | X         | -        | -       | -                |
| 2   | CHL  | A     | 609  | X         | -        | -       | -                |
| 2   | CHL  | B     | 601  | X         | -        | -       | -                |
| 2   | CHL  | B     | 608  | X         | -        | -       | -                |
| 2   | CHL  | B     | 609  | X         | -        | -       | -                |
| 2   | CHL  | C     | 601  | X         | -        | -       | -                |
| 2   | CHL  | C     | 608  | X         | -        | -       | -                |
| 2   | CHL  | C     | 609  | X         | -        | -       | -                |
| 3   | CLA  | A     | 602  | X         | -        | -       | -                |
| 3   | CLA  | A     | 603  | X         | -        | -       | -                |
| 3   | CLA  | A     | 604  | X         | -        | -       | -                |
| 3   | CLA  | A     | 610  | X         | -        | -       | -                |
| 3   | CLA  | A     | 611  | X         | -        | -       | -                |
| 3   | CLA  | A     | 612  | X         | -        | -       | -                |
| 3   | CLA  | A     | 613  | X         | -        | -       | -                |
| 3   | CLA  | B     | 602  | X         | -        | -       | -                |
| 3   | CLA  | B     | 603  | X         | -        | -       | -                |
| 3   | CLA  | B     | 604  | X         | -        | -       | -                |
| 3   | CLA  | B     | 610  | X         | -        | -       | -                |
| 3   | CLA  | B     | 611  | X         | -        | -       | -                |
| 3   | CLA  | B     | 612  | X         | -        | -       | -                |
| 3   | CLA  | B     | 613  | X         | -        | -       | -                |
| 3   | CLA  | C     | 602  | X         | -        | -       | -                |
| 3   | CLA  | C     | 603  | X         | -        | -       | -                |
| 3   | CLA  | C     | 604  | X         | -        | -       | -                |
| 3   | CLA  | C     | 610  | X         | -        | -       | -                |
| 3   | CLA  | C     | 611  | X         | -        | -       | -                |
| 3   | CLA  | C     | 612  | X         | -        | -       | -                |
| 3   | CLA  | C     | 613  | X         | -        | -       | -                |
| 7   | XAT  | A     | 1004 | X         | -        | -       | -                |
| 7   | XAT  | B     | 1004 | X         | -        | -       | -                |
| 7   | XAT  | C     | 1004 | X         | -        | -       | -                |

2 Entry composition [i](#)

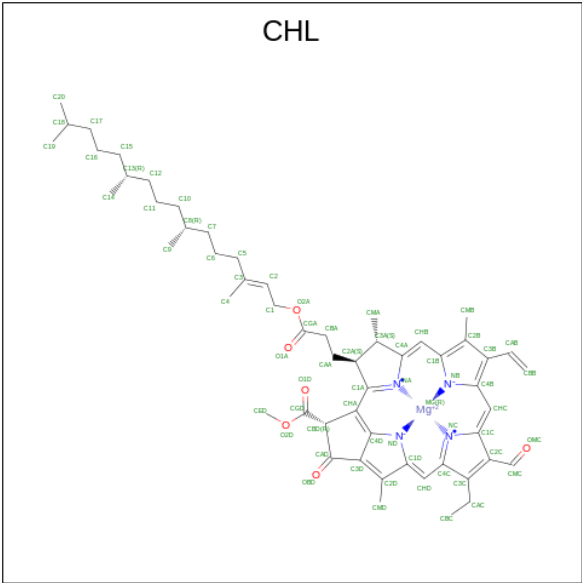
There are 8 unique types of molecules in this entry. The entry contains 8181 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1650  | 1072 | 268 | 303 | 7 |         |       |
| 1   | B     | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1650  | 1072 | 268 | 303 | 7 |         |       |
| 1   | C     | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1650  | 1072 | 268 | 303 | 7 |         |       |

- Molecule 2 is CHLOROPHYLL B (CCD ID: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



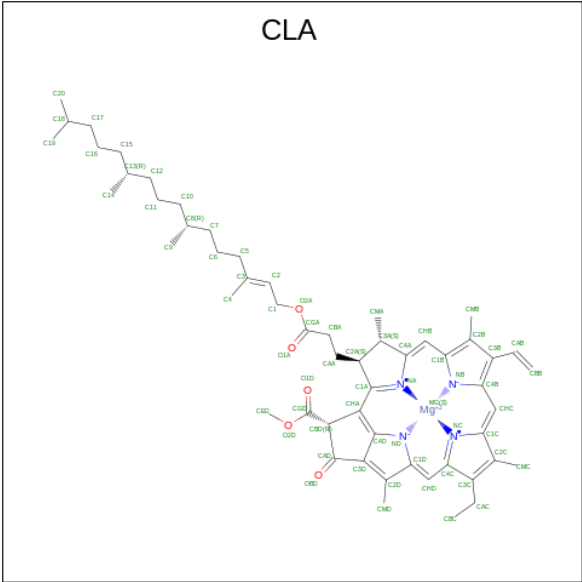
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 2   | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 2   | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 2   | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 2   | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 2   | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |
| 2   | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 2   | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 2   | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 2   | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 2   | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 2   | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |
| 2   | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 2   | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 2   | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 2   | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 2   | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 2   | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |
| 2   | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |

- Molecule 3 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



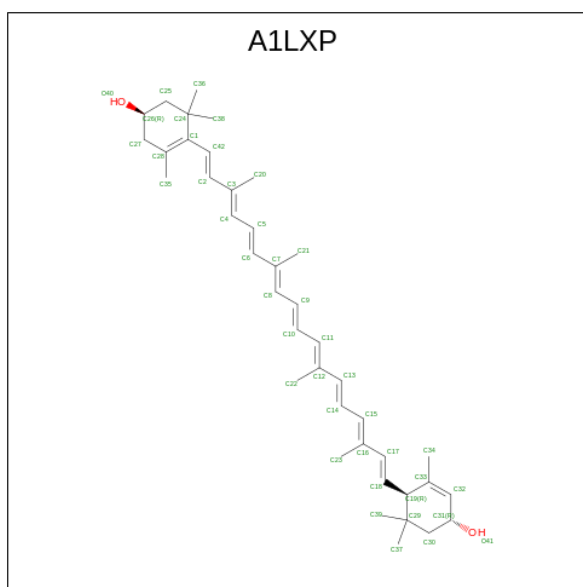
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 3   | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 3   | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 3   | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 3   | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 3   | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 3   | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 3   | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 3   | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 3   | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 3   | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |

- Molecule 4 is Lutein (CCD ID: A1LXP) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



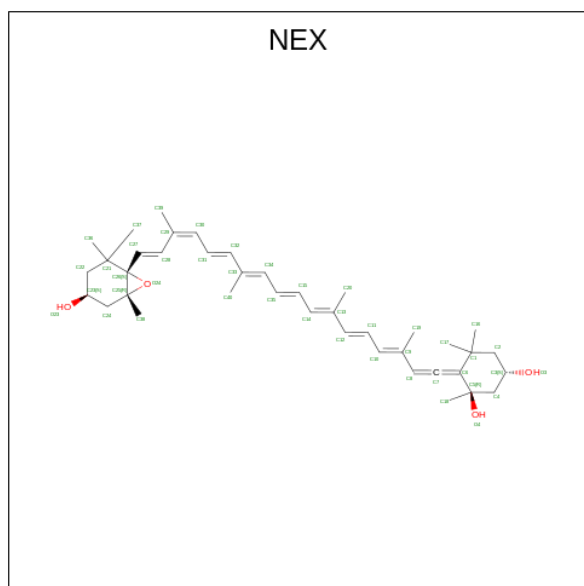
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 4   | A     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

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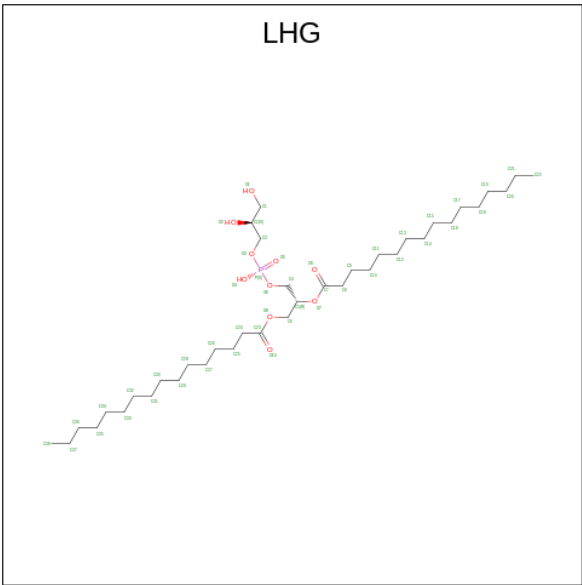
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 4   | A     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 4   | B     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 4   | B     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 4   | C     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 4   | C     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

- Molecule 5 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



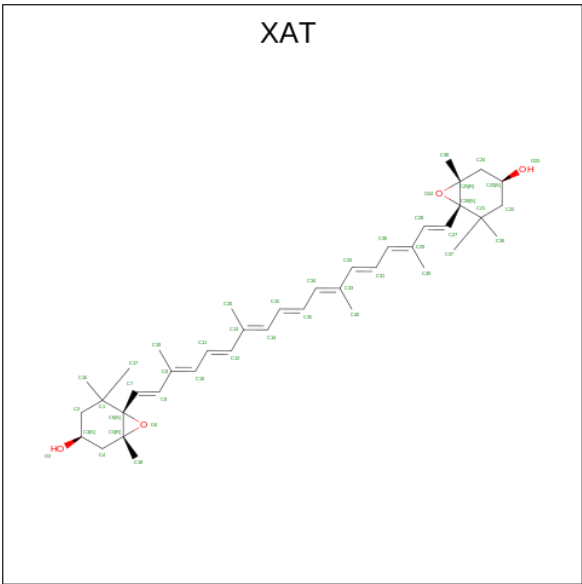
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 5   | A     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 5   | B     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 5   | C     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

- Molecule 6 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 6   | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 6   | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 6   | C     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |

- Molecule 7 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 7   | A     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 7   | B     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 7   | C     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

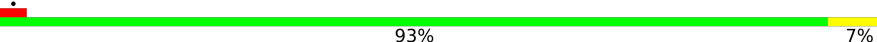
- Molecule 8 is water.

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 8   | A     | 45       | Total | O  | 0       |
|     |       |          | 45    | 45 |         |
| 8   | B     | 44       | Total | O  | 0       |
|     |       |          | 44    | 44 |         |
| 8   | C     | 43       | Total | O  | 0       |
|     |       |          | 43    | 43 |         |

### 3 Residue-property plots [i](#)

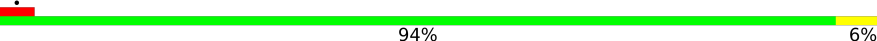
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

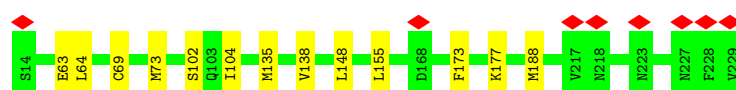
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain A:  93% 7%

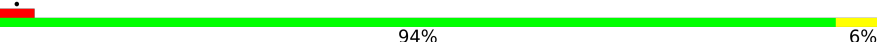


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain B:  94% 6%



- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain C:  94% 6%



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C3                               | Depositor |
| Number of particles used             | 479808                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | JEOL CRYO ARM 300                       | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 80                                      | Depositor |
| Minimum defocus (nm)                 | 700                                     | Depositor |
| Maximum defocus (nm)                 | 2200                                    | Depositor |
| Magnification                        | 60000                                   | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 2.880                                   | Depositor |
| Minimum map value                    | -1.503                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.069                                   | Depositor |
| Recommended contour level            | 0.4                                     | Depositor |
| Map size (Å)                         | 219.904, 219.904, 219.904               | wwPDB     |
| Map dimensions                       | 256, 256, 256                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.859, 0.859, 0.859                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CHL, LHG, A1LXP, NEX, CLA, XAT

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     | 0.12         | 0/1701      | 0.28        | 0/2316      |
| 1   | B     | 0.12         | 0/1701      | 0.26        | 0/2316      |
| 1   | C     | 0.12         | 0/1701      | 0.27        | 0/2316      |
| All | All   | 0.12         | 0/5103      | 0.27        | 0/6948      |

There are no bond length outliers.

There are no bond angle outliers.

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     | 1650  | 0        | 1582     | 10      | 0            |
| 1   | B     | 1650  | 0        | 1582     | 9       | 0            |
| 1   | C     | 1650  | 0        | 1582     | 10      | 0            |
| 2   | A     | 335   | 0        | 296      | 7       | 0            |
| 2   | B     | 335   | 0        | 296      | 8       | 0            |
| 2   | C     | 335   | 0        | 296      | 8       | 0            |
| 3   | A     | 477   | 0        | 489      | 11      | 0            |
| 3   | B     | 477   | 0        | 489      | 9       | 0            |
| 3   | C     | 477   | 0        | 489      | 10      | 0            |
| 4   | A     | 84    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | B     | 84    | 0        | 0        | 1       | 0            |
| 4   | C     | 84    | 0        | 0        | 1       | 0            |
| 5   | A     | 44    | 0        | 53       | 0       | 0            |
| 5   | B     | 44    | 0        | 53       | 0       | 0            |
| 5   | C     | 44    | 0        | 53       | 0       | 0            |
| 6   | A     | 49    | 0        | 74       | 2       | 0            |
| 6   | B     | 49    | 0        | 74       | 4       | 0            |
| 6   | C     | 49    | 0        | 74       | 6       | 0            |
| 7   | A     | 44    | 0        | 56       | 3       | 0            |
| 7   | B     | 44    | 0        | 56       | 2       | 0            |
| 7   | C     | 44    | 0        | 56       | 1       | 0            |
| 8   | A     | 45    | 0        | 0        | 0       | 0            |
| 8   | B     | 44    | 0        | 0        | 0       | 0            |
| 8   | C     | 43    | 0        | 0        | 0       | 0            |
| All | All   | 8181  | 0        | 7650     | 71      | 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 5.

All (71) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:185:ARG:HA    | 1:A:188:MET:HE3   | 1.76                     | 0.67              |
| 1:A:148:LEU:HG    | 2:A:608:CHL:HAB   | 1.83                     | 0.61              |
| 1:B:148:LEU:HG    | 2:B:608:CHL:HAB   | 1.83                     | 0.60              |
| 7:B:1004:XAT:H12  | 6:C:1005:LHG:H191 | 1.83                     | 0.59              |
| 7:A:1004:XAT:H363 | 6:B:1005:LHG:HC41 | 1.86                     | 0.56              |
| 2:A:606:CHL:HBD   | 2:A:606:CHL:HBA2  | 1.87                     | 0.56              |
| 2:B:606:CHL:HBD   | 2:B:606:CHL:HBA2  | 1.87                     | 0.56              |
| 1:C:148:LEU:HG    | 2:C:608:CHL:HAB   | 1.87                     | 0.56              |
| 1:C:185:ARG:HA    | 1:C:188:MET:HE3   | 1.88                     | 0.55              |
| 2:C:606:CHL:HBA2  | 2:C:606:CHL:HBD   | 1.87                     | 0.55              |
| 7:A:1004:XAT:H361 | 6:B:1005:LHG:HC92 | 1.89                     | 0.55              |
| 2:B:601:CHL:HED3  | 6:B:1005:LHG:H142 | 1.90                     | 0.54              |
| 3:C:610:CLA:H8    | 3:C:612:CLA:H102  | 1.90                     | 0.54              |
| 6:A:1005:LHG:HC41 | 7:C:1004:XAT:H363 | 1.89                     | 0.53              |
| 3:B:610:CLA:H8    | 3:B:612:CLA:H102  | 1.89                     | 0.53              |
| 7:B:1004:XAT:H363 | 6:C:1005:LHG:HC41 | 1.90                     | 0.53              |
| 1:C:64:LEU:HD13   | 3:C:603:CLA:HBA1  | 1.90                     | 0.53              |
| 1:A:69:CYS:SG     | 1:A:188:MET:HE2   | 2.50                     | 0.51              |
| 2:C:601:CHL:H202  | 6:C:1005:LHG:H221 | 1.93                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:B:64:LEU:HD13   | 3:B:603:CLA:HBA1   | 1.93                     | 0.50              |
| 3:C:603:CLA:HBB1  | 2:C:609:CHL:H161   | 1.94                     | 0.50              |
| 1:A:64:LEU:HD13   | 3:A:603:CLA:HBA1   | 1.93                     | 0.49              |
| 1:C:189:PHE:HZ    | 6:C:1005:LHG:H151  | 1.79                     | 0.48              |
| 3:A:610:CLA:H8    | 3:A:612:CLA:H102   | 1.94                     | 0.48              |
| 1:A:63:GLU:HA     | 1:A:155:LEU:HD11   | 1.96                     | 0.47              |
| 1:B:102:SER:HB3   | 2:B:607:CHL:HED2   | 1.97                     | 0.47              |
| 3:A:603:CLA:HBB1  | 2:A:609:CHL:H13    | 1.95                     | 0.47              |
| 2:C:601:CHL:HBA1  | 2:C:601:CHL:H3A    | 1.69                     | 0.46              |
| 1:B:63:GLU:HA     | 1:B:155:LEU:HD11   | 1.97                     | 0.46              |
| 2:B:601:CHL:HBA1  | 2:B:601:CHL:H3A    | 1.68                     | 0.46              |
| 6:C:1005:LHG:H301 | 6:C:1005:LHG:H341  | 1.97                     | 0.46              |
| 3:B:603:CLA:HBB1  | 2:B:609:CHL:H13    | 1.98                     | 0.46              |
| 3:B:604:CLA:HBD   | 3:B:604:CLA:HBA1   | 1.98                     | 0.46              |
| 3:A:602:CLA:H41   | 3:A:602:CLA:H61    | 1.67                     | 0.45              |
| 1:C:135:MET:HA    | 1:C:138:VAL:HG22   | 1.97                     | 0.45              |
| 1:A:135:MET:HA    | 1:A:138:VAL:HG22   | 1.98                     | 0.45              |
| 3:C:612:CLA:HMA3  | 3:C:612:CLA:H101   | 1.98                     | 0.45              |
| 3:A:603:CLA:HAB   | 4:A:1002:A1LXP:C10 | 2.47                     | 0.44              |
| 3:A:604:CLA:HBA1  | 3:A:604:CLA:HBD    | 1.99                     | 0.44              |
| 3:B:613:CLA:H51   | 3:B:613:CLA:C3C    | 2.47                     | 0.44              |
| 1:C:102:SER:HB3   | 2:C:607:CHL:HED2   | 1.99                     | 0.44              |
| 1:B:135:MET:HA    | 1:B:138:VAL:HG22   | 1.99                     | 0.44              |
| 7:A:1004:XAT:H10  | 6:B:1005:LHG:H211  | 1.99                     | 0.44              |
| 1:B:73:MET:SD     | 3:B:610:CLA:HAB    | 2.58                     | 0.44              |
| 3:A:613:CLA:H51   | 3:A:613:CLA:C3C    | 2.47                     | 0.44              |
| 3:C:613:CLA:C3C   | 3:C:613:CLA:H51    | 2.48                     | 0.43              |
| 3:A:603:CLA:C4B   | 2:A:609:CHL:H111   | 2.48                     | 0.43              |
| 3:C:604:CLA:HBD   | 3:C:604:CLA:HBA1   | 2.00                     | 0.43              |
| 3:C:610:CLA:H41   | 3:C:612:CLA:H92    | 2.00                     | 0.43              |
| 1:C:63:GLU:HA     | 1:C:155:LEU:HD11   | 1.99                     | 0.43              |
| 3:A:603:CLA:HBB1  | 2:A:609:CHL:H161   | 2.00                     | 0.43              |
| 3:B:603:CLA:HAB   | 4:B:1002:A1LXP:C10 | 2.48                     | 0.43              |
| 1:B:69:CYS:SG     | 1:B:188:MET:HE2    | 2.59                     | 0.43              |
| 3:B:603:CLA:C4B   | 2:B:609:CHL:H111   | 2.49                     | 0.43              |
| 3:C:603:CLA:HAB   | 4:C:1002:A1LXP:C10 | 2.49                     | 0.43              |
| 3:B:610:CLA:H41   | 3:B:612:CLA:H92    | 2.01                     | 0.42              |
| 1:A:173:PHE:CZ    | 1:A:177:LYS:HE3    | 2.54                     | 0.42              |
| 2:C:601:CHL:H162  | 6:C:1005:LHG:H221  | 2.01                     | 0.42              |
| 3:C:603:CLA:C4B   | 2:C:609:CHL:H111   | 2.49                     | 0.42              |
| 1:A:102:SER:HB3   | 2:A:607:CHL:HED2   | 2.00                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:610:CLA:H41  | 3:A:612:CLA:H92   | 2.02                     | 0.42              |
| 1:C:73:MET:SD    | 3:C:610:CLA:HAB   | 2.60                     | 0.42              |
| 2:A:601:CHL:HMA3 | 6:A:1005:LHG:H121 | 2.02                     | 0.41              |
| 1:C:173:PHE:CZ   | 1:C:177:LYS:HE3   | 2.55                     | 0.41              |
| 1:B:173:PHE:CZ   | 1:B:177:LYS:HE3   | 2.55                     | 0.41              |
| 1:A:203:LYS:HD2  | 1:A:207:GLU:HG2   | 2.01                     | 0.41              |
| 2:B:601:CHL:H62  | 2:B:601:CHL:H41   | 1.81                     | 0.41              |
| 1:C:104:ILE:HD12 | 1:C:104:ILE:HA    | 1.90                     | 0.41              |
| 1:A:24:TYR:HB3   | 1:A:44:TYR:HB3    | 2.03                     | 0.41              |
| 1:B:104:ILE:HD12 | 1:B:104:ILE:HA    | 1.90                     | 0.40              |
| 3:A:613:CLA:H2   | 3:A:613:CLA:H61   | 1.82                     | 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     | 214/216 (99%) | 211 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 1   | B     | 214/216 (99%) | 212 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | C     | 214/216 (99%) | 212 (99%) | 2 (1%)  | 0        | 100         | 100 |
| All | All   | 642/648 (99%) | 635 (99%) | 7 (1%)  | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | A     | 167/167 (100%) | 167 (100%) | 0        | 100         | 100 |
| 1   | B     | 167/167 (100%) | 167 (100%) | 0        | 100         | 100 |
| 1   | C     | 167/167 (100%) | 167 (100%) | 0        | 100         | 100 |
| All | All   | 501/501 (100%) | 501 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 183 | ASN  |
| 1   | B     | 183 | ASN  |
| 1   | B     | 208 | ASN  |
| 1   | C     | 183 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

57 ligands are modelled in this entry.

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

| Mol | Type  | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|-------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |       |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | CLA   | B     | 611  | 6    | 69,73,73     | 1.72 | 9 (13%)  | 83,113,113  | 1.23 | 8 (9%)   |
| 4   | A1LXP | B     | 1001 | -    | 42,43,43     | 0.38 | 1 (2%)   | 51,60,60    | 0.42 | 0        |
| 2   | CHL   | B     | 608  | 8    | 65,69,74     | 1.05 | 5 (7%)   | 74,108,114  | 1.82 | 10 (13%) |
| 2   | CHL   | B     | 607  | 8    | 50,54,74     | 1.19 | 5 (10%)  | 56,90,114   | 2.18 | 11 (19%) |
| 7   | XAT   | B     | 1004 | -    | 39,47,47     | 0.09 | 0        | 54,74,74    | 2.51 | 1 (1%)   |
| 2   | CHL   | B     | 601  | 1    | 70,74,74     | 1.02 | 5 (7%)   | 80,114,114  | 1.80 | 10 (12%) |
| 2   | CHL   | A     | 607  | 8    | 50,54,74     | 1.20 | 5 (10%)  | 56,90,114   | 2.16 | 9 (16%)  |
| 2   | CHL   | A     | 606  | 8    | 55,59,74     | 1.12 | 5 (9%)   | 62,96,114   | 2.05 | 12 (19%) |
| 3   | CLA   | A     | 604  | 8    | 59,63,73     | 1.87 | 9 (15%)  | 71,101,113  | 1.29 | 8 (11%)  |
| 4   | A1LXP | A     | 1002 | -    | 42,43,43     | 0.37 | 0        | 51,60,60    | 0.45 | 0        |
| 3   | CLA   | B     | 604  | 8    | 59,63,73     | 1.86 | 8 (13%)  | 71,101,113  | 1.29 | 8 (11%)  |
| 2   | CHL   | A     | 608  | 8    | 65,69,74     | 1.04 | 4 (6%)   | 74,108,114  | 1.82 | 10 (13%) |
| 3   | CLA   | B     | 612  | 1    | 69,73,73     | 1.69 | 9 (13%)  | 83,113,113  | 1.18 | 9 (10%)  |
| 5   | NEX   | B     | 1003 | -    | 38,46,46     | 2.32 | 4 (10%)  | 50,70,70    | 0.61 | 1 (2%)   |
| 4   | A1LXP | A     | 1001 | -    | 42,43,43     | 0.37 | 0        | 51,60,60    | 0.41 | 0        |
| 4   | A1LXP | B     | 1002 | -    | 42,43,43     | 0.37 | 0        | 51,60,60    | 0.44 | 0        |
| 4   | A1LXP | C     | 1001 | -    | 42,43,43     | 0.38 | 1 (2%)   | 51,60,60    | 0.42 | 0        |
| 3   | CLA   | A     | 602  | 1    | 69,73,73     | 1.69 | 9 (13%)  | 83,113,113  | 1.09 | 8 (9%)   |
| 3   | CLA   | C     | 602  | 1    | 69,73,73     | 1.69 | 9 (13%)  | 83,113,113  | 1.10 | 9 (10%)  |
| 2   | CHL   | C     | 608  | 8    | 65,69,74     | 1.04 | 4 (6%)   | 74,108,114  | 1.84 | 10 (13%) |
| 3   | CLA   | C     | 614  | 1    | 46,50,73     | 2.08 | 9 (19%)  | 55,85,113   | 1.41 | 8 (14%)  |
| 3   | CLA   | C     | 603  | 1    | 59,63,73     | 1.82 | 9 (15%)  | 71,101,113  | 1.28 | 9 (12%)  |
| 2   | CHL   | C     | 607  | 8    | 50,54,74     | 1.19 | 5 (10%)  | 56,90,114   | 2.16 | 10 (17%) |
| 3   | CLA   | C     | 604  | 8    | 59,63,73     | 1.86 | 8 (13%)  | 71,101,113  | 1.30 | 8 (11%)  |
| 5   | NEX   | A     | 1003 | -    | 38,46,46     | 2.43 | 4 (10%)  | 50,70,70    | 0.62 | 1 (2%)   |
| 7   | XAT   | C     | 1004 | -    | 39,47,47     | 0.09 | 0        | 54,74,74    | 2.53 | 1 (1%)   |
| 2   | CHL   | B     | 609  | 1    | 70,74,74     | 1.01 | 4 (5%)   | 80,114,114  | 1.71 | 10 (12%) |
| 2   | CHL   | C     | 606  | 8    | 55,59,74     | 1.12 | 5 (9%)   | 62,96,114   | 2.06 | 11 (17%) |
| 2   | CHL   | A     | 605  | 1    | 49,53,74     | 1.22 | 4 (8%)   | 53,88,114   | 2.17 | 11 (20%) |
| 2   | CHL   | C     | 605  | 1    | 49,53,74     | 1.22 | 4 (8%)   | 53,88,114   | 2.16 | 11 (20%) |
| 3   | CLA   | A     | 612  | 1    | 69,73,73     | 1.68 | 9 (13%)  | 83,113,113  | 1.18 | 9 (10%)  |
| 3   | CLA   | B     | 614  | 1    | 46,50,73     | 2.08 | 9 (19%)  | 55,85,113   | 1.40 | 8 (14%)  |
| 3   | CLA   | B     | 610  | 1    | 69,73,73     | 1.71 | 9 (13%)  | 83,113,113  | 1.12 | 9 (10%)  |
| 2   | CHL   | C     | 601  | 1    | 70,74,74     | 1.02 | 4 (5%)   | 80,114,114  | 1.78 | 10 (12%) |
| 3   | CLA   | B     | 603  | 1    | 59,63,73     | 1.83 | 9 (15%)  | 71,101,113  | 1.29 | 9 (12%)  |

| Mol | Type  | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|-------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |       |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | CHL   | A     | 609  | 1    | 70,74,74     | 1.01 | 4 (5%)   | 80,114,114  | 1.70 | 10 (12%) |
| 3   | CLA   | B     | 613  | 1    | 69,73,73     | 1.68 | 8 (11%)  | 83,113,113  | 1.11 | 9 (10%)  |
| 4   | A1LXP | C     | 1002 | -    | 42,43,43     | 0.36 | 0        | 51,60,60    | 0.45 | 0        |
| 3   | CLA   | C     | 612  | 1    | 69,73,73     | 1.69 | 8 (11%)  | 83,113,113  | 1.18 | 9 (10%)  |
| 5   | NEX   | C     | 1003 | -    | 38,46,46     | 2.43 | 4 (10%)  | 50,70,70    | 0.60 | 1 (2%)   |
| 6   | LHG   | B     | 1005 | 3    | 48,48,48     | 0.24 | 0        | 51,54,54    | 0.27 | 0        |
| 2   | CHL   | C     | 609  | 1    | 70,74,74     | 1.01 | 5 (7%)   | 80,114,114  | 1.71 | 10 (12%) |
| 2   | CHL   | B     | 606  | 8    | 55,59,74     | 1.12 | 5 (9%)   | 62,96,114   | 2.07 | 12 (19%) |
| 3   | CLA   | A     | 613  | 1    | 69,73,73     | 1.69 | 9 (13%)  | 83,113,113  | 1.11 | 8 (9%)   |
| 3   | CLA   | A     | 611  | 6    | 69,73,73     | 1.72 | 9 (13%)  | 83,113,113  | 1.24 | 8 (9%)   |
| 3   | CLA   | A     | 610  | 1    | 69,73,73     | 1.70 | 9 (13%)  | 83,113,113  | 1.13 | 9 (10%)  |
| 3   | CLA   | A     | 614  | 1    | 46,50,73     | 2.09 | 9 (19%)  | 55,85,113   | 1.40 | 8 (14%)  |
| 6   | LHG   | A     | 1005 | 3    | 48,48,48     | 0.24 | 0        | 51,54,54    | 0.27 | 0        |
| 2   | CHL   | B     | 605  | 1    | 49,53,74     | 1.23 | 4 (8%)   | 53,88,114   | 2.15 | 10 (18%) |
| 3   | CLA   | C     | 611  | 6    | 69,73,73     | 1.72 | 9 (13%)  | 83,113,113  | 1.23 | 8 (9%)   |
| 3   | CLA   | B     | 602  | 1    | 69,73,73     | 1.70 | 9 (13%)  | 83,113,113  | 1.09 | 8 (9%)   |
| 3   | CLA   | A     | 603  | 1    | 59,63,73     | 1.82 | 9 (15%)  | 71,101,113  | 1.29 | 9 (12%)  |
| 6   | LHG   | C     | 1005 | 3    | 48,48,48     | 0.24 | 0        | 51,54,54    | 0.26 | 0        |
| 3   | CLA   | C     | 610  | 1    | 69,73,73     | 1.71 | 9 (13%)  | 83,113,113  | 1.12 | 9 (10%)  |
| 3   | CLA   | C     | 613  | 1    | 69,73,73     | 1.69 | 8 (11%)  | 83,113,113  | 1.11 | 8 (9%)   |
| 7   | XAT   | A     | 1004 | -    | 39,47,47     | 0.09 | 0        | 54,74,74    | 2.53 | 1 (1%)   |
| 2   | CHL   | A     | 601  | 1    | 70,74,74     | 1.01 | 4 (5%)   | 80,114,114  | 1.82 | 9 (11%)  |

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   |
|-----|-------|-------|------|------|-----------|---------------|---------|
| 3   | CLA   | B     | 611  | 6    | 1/1/15/20 | 14/39/115/115 | -       |
| 4   | A1LXP | B     | 1001 | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 2   | CHL   | B     | 608  | 8    | 1/1/14/21 | 7/35/111/117  | -       |
| 2   | CHL   | B     | 607  | 8    | -         | 6/17/93/117   | -       |
| 7   | XAT   | B     | 1004 | -    | 2/2/12/26 | 0/31/93/93    | 0/4/4/4 |
| 2   | CHL   | B     | 601  | 1    | 1/1/15/21 | 12/41/117/117 | -       |
| 2   | CHL   | A     | 607  | 8    | -         | 5/17/93/117   | -       |
| 3   | CLA   | A     | 604  | 8    | 1/1/13/20 | 7/27/103/115  | -       |

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| Mol | Type  | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|-------|-------|------|------|-----------|---------------|---------|
| 2   | CHL   | A     | 606  | 8    | -         | 5/23/99/117   | -       |
| 4   | A1LXP | A     | 1002 | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 3   | CLA   | B     | 604  | 8    | 1/1/13/20 | 7/27/103/115  | -       |
| 2   | CHL   | A     | 608  | 8    | 1/1/14/21 | 8/35/111/117  | -       |
| 3   | CLA   | B     | 612  | 1    | 1/1/15/20 | 9/39/115/115  | -       |
| 5   | NEX   | B     | 1003 | -    | -         | 2/27/83/83    | 0/3/3/3 |
| 4   | A1LXP | A     | 1001 | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 4   | A1LXP | B     | 1002 | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 4   | A1LXP | C     | 1001 | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 3   | CLA   | A     | 602  | 1    | 1/1/15/20 | 7/39/115/115  | -       |
| 3   | CLA   | C     | 602  | 1    | 1/1/15/20 | 6/39/115/115  | -       |
| 2   | CHL   | C     | 608  | 8    | 1/1/14/21 | 10/35/111/117 | -       |
| 3   | CLA   | C     | 614  | 1    | -         | 3/12/88/115   | -       |
| 3   | CLA   | C     | 603  | 1    | 1/1/13/20 | 5/27/103/115  | -       |
| 3   | CLA   | C     | 604  | 8    | 1/1/13/20 | 7/27/103/115  | -       |
| 2   | CHL   | C     | 607  | 8    | -         | 5/17/93/117   | -       |
| 7   | XAT   | C     | 1004 | -    | 2/2/12/26 | 0/31/93/93    | 0/4/4/4 |
| 5   | NEX   | A     | 1003 | -    | -         | 2/27/83/83    | 0/3/3/3 |
| 2   | CHL   | B     | 609  | 1    | 1/1/15/21 | 6/41/117/117  | -       |
| 2   | CHL   | A     | 605  | 1    | -         | 4/15/92/117   | -       |
| 2   | CHL   | C     | 606  | 8    | -         | 7/23/99/117   | -       |
| 2   | CHL   | C     | 605  | 1    | -         | 4/15/92/117   | -       |
| 3   | CLA   | A     | 612  | 1    | 1/1/15/20 | 9/39/115/115  | -       |
| 3   | CLA   | B     | 614  | 1    | -         | 3/12/88/115   | -       |
| 3   | CLA   | B     | 610  | 1    | 1/1/15/20 | 2/39/115/115  | -       |
| 2   | CHL   | C     | 601  | 1    | 1/1/15/21 | 12/41/117/117 | -       |
| 3   | CLA   | B     | 603  | 1    | 1/1/13/20 | 5/27/103/115  | -       |
| 2   | CHL   | A     | 609  | 1    | 1/1/15/21 | 8/41/117/117  | -       |
| 3   | CLA   | B     | 613  | 1    | 1/1/15/20 | 6/39/115/115  | -       |
| 4   | A1LXP | C     | 1002 | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 3   | CLA   | C     | 612  | 1    | 1/1/15/20 | 9/39/115/115  | -       |
| 5   | NEX   | C     | 1003 | -    | -         | 2/27/83/83    | 0/3/3/3 |
| 6   | LHG   | B     | 1005 | 3    | -         | 11/53/53/53   | -       |
| 2   | CHL   | C     | 609  | 1    | 1/1/15/21 | 9/41/117/117  | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 2   | CHL  | B     | 606  | 8    | -         | 7/23/99/117   | -       |
| 3   | CLA  | A     | 613  | 1    | 1/1/15/20 | 6/39/115/115  | -       |
| 3   | CLA  | A     | 611  | 6    | 1/1/15/20 | 14/39/115/115 | -       |
| 3   | CLA  | A     | 610  | 1    | 1/1/15/20 | 2/39/115/115  | -       |
| 3   | CLA  | A     | 614  | 1    | -         | 3/12/88/115   | -       |
| 6   | LHG  | A     | 1005 | 3    | -         | 7/53/53/53    | -       |
| 2   | CHL  | B     | 605  | 1    | -         | 4/15/92/117   | -       |
| 3   | CLA  | C     | 611  | 6    | 1/1/15/20 | 14/39/115/115 | -       |
| 3   | CLA  | B     | 602  | 1    | 1/1/15/20 | 11/39/115/115 | -       |
| 3   | CLA  | A     | 603  | 1    | 1/1/13/20 | 5/27/103/115  | -       |
| 6   | LHG  | C     | 1005 | 3    | -         | 11/53/53/53   | -       |
| 3   | CLA  | C     | 610  | 1    | 1/1/15/20 | 2/39/115/115  | -       |
| 3   | CLA  | C     | 613  | 1    | 1/1/15/20 | 6/39/115/115  | -       |
| 7   | XAT  | A     | 1004 | -    | 2/2/12/26 | 0/31/93/93    | 0/4/4/4 |
| 2   | CHL  | A     | 601  | 1    | 1/1/15/21 | 13/41/117/117 | -       |

All (306) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 5   | A     | 1003 | NEX  | C40-C33 | -13.13 | 1.23        | 1.50     |
| 5   | B     | 1003 | NEX  | C40-C33 | -12.79 | 1.24        | 1.50     |
| 5   | C     | 1003 | NEX  | C40-C33 | -12.60 | 1.24        | 1.50     |
| 3   | A     | 614  | CLA  | C4B-NB  | 8.76   | 1.48        | 1.37     |
| 3   | B     | 603  | CLA  | C4B-NB  | 8.75   | 1.48        | 1.37     |
| 3   | A     | 603  | CLA  | C4B-NB  | 8.65   | 1.48        | 1.37     |
| 3   | C     | 614  | CLA  | C4B-NB  | 8.64   | 1.48        | 1.37     |
| 3   | B     | 614  | CLA  | C4B-NB  | 8.63   | 1.48        | 1.37     |
| 3   | C     | 603  | CLA  | C4B-NB  | 8.62   | 1.48        | 1.37     |
| 3   | B     | 602  | CLA  | C4B-NB  | 8.61   | 1.48        | 1.37     |
| 3   | C     | 612  | CLA  | C4B-NB  | 8.57   | 1.48        | 1.37     |
| 3   | A     | 602  | CLA  | C4B-NB  | 8.53   | 1.48        | 1.37     |
| 3   | B     | 612  | CLA  | C4B-NB  | 8.53   | 1.48        | 1.37     |
| 3   | A     | 604  | CLA  | C4B-NB  | 8.51   | 1.48        | 1.37     |
| 3   | C     | 610  | CLA  | C4B-NB  | 8.51   | 1.48        | 1.37     |
| 3   | B     | 610  | CLA  | C4B-NB  | 8.48   | 1.48        | 1.37     |
| 3   | A     | 610  | CLA  | C4B-NB  | 8.47   | 1.48        | 1.37     |
| 3   | B     | 613  | CLA  | C4B-NB  | 8.46   | 1.48        | 1.37     |
| 3   | C     | 602  | CLA  | C4B-NB  | 8.46   | 1.48        | 1.37     |
| 3   | A     | 612  | CLA  | C4B-NB  | 8.46   | 1.48        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | A     | 613  | CLA  | C4B-NB  | 8.45  | 1.48        | 1.37     |
| 3   | B     | 604  | CLA  | C4B-NB  | 8.43  | 1.48        | 1.37     |
| 3   | C     | 604  | CLA  | C4B-NB  | 8.43  | 1.48        | 1.37     |
| 3   | C     | 613  | CLA  | C4B-NB  | 8.43  | 1.48        | 1.37     |
| 3   | C     | 611  | CLA  | C4B-NB  | 8.37  | 1.48        | 1.37     |
| 3   | B     | 611  | CLA  | C4B-NB  | 8.37  | 1.48        | 1.37     |
| 3   | A     | 611  | CLA  | C4B-NB  | 8.35  | 1.48        | 1.37     |
| 2   | B     | 605  | CHL  | C4B-NB  | 6.14  | 1.45        | 1.37     |
| 2   | C     | 605  | CHL  | C4B-NB  | 6.10  | 1.45        | 1.37     |
| 2   | A     | 605  | CHL  | C4B-NB  | 6.09  | 1.45        | 1.37     |
| 2   | B     | 601  | CHL  | C4B-NB  | 6.01  | 1.45        | 1.37     |
| 2   | C     | 601  | CHL  | C4B-NB  | 5.94  | 1.45        | 1.37     |
| 2   | A     | 601  | CHL  | C4B-NB  | 5.92  | 1.45        | 1.37     |
| 2   | B     | 608  | CHL  | C4B-NB  | 5.89  | 1.45        | 1.37     |
| 2   | C     | 609  | CHL  | C4B-NB  | 5.89  | 1.45        | 1.37     |
| 2   | A     | 609  | CHL  | C4B-NB  | 5.84  | 1.45        | 1.37     |
| 2   | C     | 608  | CHL  | C4B-NB  | 5.83  | 1.45        | 1.37     |
| 2   | B     | 609  | CHL  | C4B-NB  | 5.82  | 1.44        | 1.37     |
| 2   | A     | 608  | CHL  | C4B-NB  | 5.80  | 1.44        | 1.37     |
| 2   | B     | 607  | CHL  | C4B-NB  | 5.78  | 1.44        | 1.37     |
| 2   | A     | 606  | CHL  | C4B-NB  | 5.73  | 1.44        | 1.37     |
| 2   | A     | 607  | CHL  | C4B-NB  | 5.73  | 1.44        | 1.37     |
| 2   | C     | 606  | CHL  | C4B-NB  | 5.72  | 1.44        | 1.37     |
| 2   | C     | 607  | CHL  | C4B-NB  | 5.72  | 1.44        | 1.37     |
| 2   | B     | 606  | CHL  | C4B-NB  | 5.66  | 1.44        | 1.37     |
| 3   | C     | 611  | CLA  | MG-NB   | -5.09 | 1.95        | 2.05     |
| 3   | A     | 604  | CLA  | MG-NB   | -5.09 | 1.95        | 2.05     |
| 3   | C     | 604  | CLA  | MG-NB   | -5.07 | 1.95        | 2.05     |
| 3   | B     | 611  | CLA  | MG-NB   | -5.04 | 1.95        | 2.05     |
| 3   | C     | 610  | CLA  | MG-NB   | -5.03 | 1.95        | 2.05     |
| 3   | B     | 604  | CLA  | MG-NB   | -5.03 | 1.95        | 2.05     |
| 3   | A     | 604  | CLA  | MG-ND   | -5.02 | 1.95        | 2.05     |
| 3   | C     | 613  | CLA  | MG-NB   | -5.02 | 1.95        | 2.05     |
| 3   | B     | 602  | CLA  | MG-NB   | -5.01 | 1.95        | 2.05     |
| 5   | C     | 1003 | NEX  | C28-C27 | 5.01  | 1.43        | 1.32     |
| 3   | B     | 610  | CLA  | MG-NB   | -5.01 | 1.95        | 2.05     |
| 3   | A     | 602  | CLA  | MG-NB   | -5.01 | 1.95        | 2.05     |
| 3   | A     | 610  | CLA  | MG-NB   | -5.00 | 1.95        | 2.05     |
| 3   | C     | 602  | CLA  | MG-NB   | -5.00 | 1.95        | 2.05     |
| 3   | B     | 613  | CLA  | MG-NB   | -4.99 | 1.95        | 2.05     |
| 3   | B     | 604  | CLA  | MG-ND   | -4.99 | 1.95        | 2.05     |
| 3   | C     | 604  | CLA  | MG-ND   | -4.98 | 1.95        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | A     | 613  | CLA  | MG-NB   | -4.98 | 1.95        | 2.05     |
| 3   | B     | 611  | CLA  | MG-ND   | -4.96 | 1.96        | 2.05     |
| 3   | A     | 611  | CLA  | MG-NB   | -4.95 | 1.96        | 2.05     |
| 3   | C     | 611  | CLA  | MG-ND   | -4.92 | 1.96        | 2.05     |
| 3   | A     | 611  | CLA  | MG-ND   | -4.91 | 1.96        | 2.05     |
| 3   | C     | 610  | CLA  | MG-ND   | -4.90 | 1.96        | 2.05     |
| 3   | B     | 610  | CLA  | MG-ND   | -4.89 | 1.96        | 2.05     |
| 3   | C     | 602  | CLA  | MG-ND   | -4.87 | 1.96        | 2.05     |
| 3   | A     | 610  | CLA  | MG-ND   | -4.86 | 1.96        | 2.05     |
| 3   | A     | 602  | CLA  | MG-ND   | -4.85 | 1.96        | 2.05     |
| 3   | B     | 602  | CLA  | MG-ND   | -4.85 | 1.96        | 2.05     |
| 3   | A     | 614  | CLA  | MG-NB   | -4.84 | 1.96        | 2.05     |
| 3   | C     | 614  | CLA  | MG-NB   | -4.83 | 1.96        | 2.05     |
| 3   | C     | 613  | CLA  | MG-ND   | -4.82 | 1.96        | 2.05     |
| 3   | B     | 614  | CLA  | MG-NB   | -4.81 | 1.96        | 2.05     |
| 3   | A     | 613  | CLA  | MG-ND   | -4.81 | 1.96        | 2.05     |
| 3   | B     | 613  | CLA  | MG-ND   | -4.79 | 1.96        | 2.05     |
| 3   | B     | 612  | CLA  | MG-NB   | -4.76 | 1.96        | 2.05     |
| 3   | C     | 612  | CLA  | MG-NB   | -4.75 | 1.96        | 2.05     |
| 3   | A     | 612  | CLA  | MG-NB   | -4.74 | 1.96        | 2.05     |
| 3   | A     | 612  | CLA  | MG-ND   | -4.71 | 1.96        | 2.05     |
| 3   | B     | 612  | CLA  | MG-ND   | -4.69 | 1.96        | 2.05     |
| 3   | C     | 612  | CLA  | MG-ND   | -4.68 | 1.96        | 2.05     |
| 3   | B     | 603  | CLA  | MG-NB   | -4.65 | 1.96        | 2.05     |
| 3   | C     | 603  | CLA  | MG-NB   | -4.63 | 1.96        | 2.05     |
| 3   | B     | 614  | CLA  | MG-ND   | -4.59 | 1.96        | 2.05     |
| 3   | A     | 614  | CLA  | MG-ND   | -4.58 | 1.96        | 2.05     |
| 3   | A     | 603  | CLA  | MG-NB   | -4.58 | 1.96        | 2.05     |
| 3   | C     | 614  | CLA  | MG-ND   | -4.57 | 1.96        | 2.05     |
| 3   | B     | 603  | CLA  | MG-ND   | -4.52 | 1.96        | 2.05     |
| 3   | A     | 603  | CLA  | MG-ND   | -4.51 | 1.96        | 2.05     |
| 3   | C     | 603  | CLA  | MG-ND   | -4.51 | 1.96        | 2.05     |
| 5   | A     | 1003 | NEX  | C34-C33 | -4.40 | 1.29        | 1.35     |
| 5   | C     | 1003 | NEX  | C34-C33 | -4.35 | 1.30        | 1.35     |
| 3   | A     | 611  | CLA  | MG-NA   | -4.28 | 1.96        | 2.06     |
| 3   | C     | 603  | CLA  | C1D-ND  | 4.28  | 1.43        | 1.37     |
| 3   | B     | 611  | CLA  | MG-NA   | -4.27 | 1.96        | 2.06     |
| 3   | C     | 614  | CLA  | C1D-ND  | 4.25  | 1.43        | 1.37     |
| 3   | A     | 614  | CLA  | C1D-ND  | 4.23  | 1.43        | 1.37     |
| 3   | C     | 611  | CLA  | MG-NA   | -4.22 | 1.96        | 2.06     |
| 3   | B     | 614  | CLA  | C1D-ND  | 4.21  | 1.43        | 1.37     |
| 3   | A     | 603  | CLA  | C1D-ND  | 4.21  | 1.43        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | B     | 612  | CLA  | C1D-ND  | 4.20  | 1.42        | 1.37     |
| 3   | B     | 603  | CLA  | C1D-ND  | 4.20  | 1.42        | 1.37     |
| 3   | C     | 604  | CLA  | MG-NA   | -4.17 | 1.96        | 2.06     |
| 3   | A     | 612  | CLA  | C1D-ND  | 4.16  | 1.42        | 1.37     |
| 3   | B     | 604  | CLA  | MG-NA   | -4.16 | 1.96        | 2.06     |
| 3   | C     | 612  | CLA  | C1D-ND  | 4.14  | 1.42        | 1.37     |
| 3   | A     | 604  | CLA  | MG-NA   | -4.12 | 1.96        | 2.06     |
| 3   | C     | 610  | CLA  | MG-NA   | -4.09 | 1.96        | 2.06     |
| 3   | A     | 610  | CLA  | MG-NA   | -4.08 | 1.96        | 2.06     |
| 3   | B     | 610  | CLA  | MG-NA   | -4.03 | 1.96        | 2.06     |
| 3   | A     | 613  | CLA  | C1D-ND  | 4.03  | 1.42        | 1.37     |
| 5   | A     | 1003 | NEX  | C28-C27 | 4.03  | 1.41        | 1.32     |
| 3   | A     | 604  | CLA  | C1D-ND  | 3.98  | 1.42        | 1.37     |
| 3   | C     | 604  | CLA  | C1D-ND  | 3.97  | 1.42        | 1.37     |
| 3   | A     | 611  | CLA  | C1D-ND  | 3.97  | 1.42        | 1.37     |
| 3   | B     | 611  | CLA  | C1D-ND  | 3.96  | 1.42        | 1.37     |
| 3   | B     | 604  | CLA  | C1D-ND  | 3.93  | 1.42        | 1.37     |
| 3   | B     | 613  | CLA  | C1D-ND  | 3.93  | 1.42        | 1.37     |
| 3   | C     | 613  | CLA  | C1D-ND  | 3.93  | 1.42        | 1.37     |
| 3   | C     | 611  | CLA  | C1D-ND  | 3.90  | 1.42        | 1.37     |
| 3   | B     | 610  | CLA  | C1D-ND  | 3.89  | 1.42        | 1.37     |
| 3   | C     | 613  | CLA  | MG-NA   | -3.86 | 1.97        | 2.06     |
| 3   | B     | 602  | CLA  | MG-NA   | -3.84 | 1.97        | 2.06     |
| 3   | A     | 610  | CLA  | C1D-ND  | 3.83  | 1.42        | 1.37     |
| 3   | A     | 602  | CLA  | C1D-ND  | 3.82  | 1.42        | 1.37     |
| 3   | C     | 602  | CLA  | C1D-ND  | 3.81  | 1.42        | 1.37     |
| 3   | B     | 613  | CLA  | MG-NA   | -3.81 | 1.97        | 2.06     |
| 3   | A     | 613  | CLA  | MG-NA   | -3.79 | 1.97        | 2.06     |
| 3   | C     | 602  | CLA  | MG-NA   | -3.79 | 1.97        | 2.06     |
| 3   | A     | 602  | CLA  | MG-NA   | -3.77 | 1.97        | 2.06     |
| 3   | B     | 602  | CLA  | C1D-ND  | 3.75  | 1.42        | 1.37     |
| 3   | C     | 610  | CLA  | C1D-ND  | 3.71  | 1.42        | 1.37     |
| 3   | A     | 614  | CLA  | MG-NA   | -3.68 | 1.97        | 2.06     |
| 3   | B     | 611  | CLA  | MG-NC   | -3.67 | 1.97        | 2.06     |
| 3   | B     | 614  | CLA  | MG-NA   | -3.67 | 1.97        | 2.06     |
| 3   | C     | 614  | CLA  | MG-NA   | -3.63 | 1.97        | 2.06     |
| 3   | A     | 611  | CLA  | MG-NC   | -3.62 | 1.97        | 2.06     |
| 3   | C     | 604  | CLA  | MG-NC   | -3.61 | 1.97        | 2.06     |
| 3   | C     | 611  | CLA  | MG-NC   | -3.61 | 1.97        | 2.06     |
| 3   | A     | 604  | CLA  | MG-NC   | -3.60 | 1.97        | 2.06     |
| 5   | B     | 1003 | NEX  | C28-C27 | 3.60  | 1.40        | 1.32     |
| 3   | B     | 604  | CLA  | MG-NC   | -3.59 | 1.97        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | B     | 612  | CLA  | MG-NA   | -3.57 | 1.97        | 2.06     |
| 3   | A     | 612  | CLA  | MG-NA   | -3.56 | 1.97        | 2.06     |
| 3   | A     | 610  | CLA  | MG-NC   | -3.54 | 1.97        | 2.06     |
| 3   | C     | 612  | CLA  | MG-NA   | -3.53 | 1.97        | 2.06     |
| 3   | C     | 610  | CLA  | MG-NC   | -3.51 | 1.97        | 2.06     |
| 3   | B     | 610  | CLA  | MG-NC   | -3.50 | 1.98        | 2.06     |
| 3   | B     | 614  | CLA  | C1B-NB  | 3.49  | 1.42        | 1.37     |
| 3   | B     | 614  | CLA  | MG-NC   | -3.48 | 1.98        | 2.06     |
| 3   | A     | 614  | CLA  | MG-NC   | -3.47 | 1.98        | 2.06     |
| 3   | C     | 614  | CLA  | MG-NC   | -3.46 | 1.98        | 2.06     |
| 3   | A     | 603  | CLA  | C1B-NB  | 3.46  | 1.42        | 1.37     |
| 3   | C     | 603  | CLA  | MG-NA   | -3.44 | 1.98        | 2.06     |
| 3   | B     | 603  | CLA  | C1B-NB  | 3.43  | 1.42        | 1.37     |
| 3   | B     | 603  | CLA  | MG-NA   | -3.42 | 1.98        | 2.06     |
| 3   | A     | 611  | CLA  | C1B-NB  | 3.42  | 1.42        | 1.37     |
| 3   | C     | 611  | CLA  | C1B-NB  | 3.42  | 1.42        | 1.37     |
| 3   | C     | 603  | CLA  | C1B-NB  | 3.42  | 1.42        | 1.37     |
| 3   | C     | 614  | CLA  | C1B-NB  | 3.41  | 1.42        | 1.37     |
| 3   | B     | 611  | CLA  | C1B-NB  | 3.38  | 1.41        | 1.37     |
| 3   | A     | 614  | CLA  | C1B-NB  | 3.38  | 1.41        | 1.37     |
| 3   | C     | 610  | CLA  | C1B-NB  | 3.37  | 1.41        | 1.37     |
| 3   | A     | 603  | CLA  | MG-NA   | -3.37 | 1.98        | 2.06     |
| 3   | A     | 613  | CLA  | C1B-NB  | 3.35  | 1.41        | 1.37     |
| 3   | B     | 603  | CLA  | MG-NC   | -3.35 | 1.98        | 2.06     |
| 3   | B     | 610  | CLA  | C1B-NB  | 3.35  | 1.41        | 1.37     |
| 3   | A     | 603  | CLA  | MG-NC   | -3.34 | 1.98        | 2.06     |
| 3   | C     | 613  | CLA  | C1B-NB  | 3.33  | 1.41        | 1.37     |
| 3   | C     | 604  | CLA  | C1B-NB  | 3.33  | 1.41        | 1.37     |
| 3   | A     | 604  | CLA  | C1B-NB  | 3.33  | 1.41        | 1.37     |
| 3   | A     | 610  | CLA  | C1B-NB  | 3.32  | 1.41        | 1.37     |
| 3   | C     | 612  | CLA  | C1B-NB  | 3.32  | 1.41        | 1.37     |
| 3   | A     | 602  | CLA  | C1B-NB  | 3.32  | 1.41        | 1.37     |
| 3   | C     | 602  | CLA  | C1B-NB  | 3.32  | 1.41        | 1.37     |
| 3   | B     | 613  | CLA  | MG-NC   | -3.32 | 1.98        | 2.06     |
| 3   | C     | 602  | CLA  | MG-NC   | -3.32 | 1.98        | 2.06     |
| 3   | A     | 613  | CLA  | MG-NC   | -3.31 | 1.98        | 2.06     |
| 3   | B     | 612  | CLA  | C1B-NB  | 3.30  | 1.41        | 1.37     |
| 3   | A     | 602  | CLA  | MG-NC   | -3.30 | 1.98        | 2.06     |
| 5   | C     | 1003 | NEX  | C39-C29 | -3.29 | 1.44        | 1.50     |
| 3   | C     | 613  | CLA  | MG-NC   | -3.29 | 1.98        | 2.06     |
| 3   | A     | 612  | CLA  | C1B-NB  | 3.27  | 1.41        | 1.37     |
| 3   | B     | 602  | CLA  | MG-NC   | -3.27 | 1.98        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | C     | 603  | CLA  | MG-NC   | -3.26 | 1.98        | 2.06     |
| 3   | B     | 604  | CLA  | C1B-NB  | 3.26  | 1.41        | 1.37     |
| 3   | B     | 612  | CLA  | MG-NC   | -3.23 | 1.98        | 2.06     |
| 3   | C     | 612  | CLA  | MG-NC   | -3.23 | 1.98        | 2.06     |
| 3   | B     | 613  | CLA  | C1B-NB  | 3.23  | 1.41        | 1.37     |
| 3   | A     | 612  | CLA  | MG-NC   | -3.22 | 1.98        | 2.06     |
| 3   | B     | 602  | CLA  | C1B-NB  | 3.22  | 1.41        | 1.37     |
| 5   | B     | 1003 | NEX  | C34-C33 | -3.10 | 1.31        | 1.35     |
| 5   | B     | 1003 | NEX  | C39-C29 | -2.90 | 1.44        | 1.50     |
| 5   | A     | 1003 | NEX  | C39-C29 | -2.82 | 1.45        | 1.50     |
| 3   | B     | 602  | CLA  | C1C-C2C | 2.39  | 1.49        | 1.44     |
| 3   | C     | 610  | CLA  | C1D-C2D | -2.34 | 1.40        | 1.45     |
| 3   | A     | 610  | CLA  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 3   | B     | 610  | CLA  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 3   | B     | 604  | CLA  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 3   | C     | 611  | CLA  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 3   | C     | 612  | CLA  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 3   | A     | 611  | CLA  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 3   | B     | 611  | CLA  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 3   | C     | 602  | CLA  | C1C-C2C | 2.32  | 1.49        | 1.44     |
| 3   | B     | 612  | CLA  | C1D-C2D | -2.32 | 1.40        | 1.45     |
| 3   | A     | 612  | CLA  | C1D-C2D | -2.32 | 1.40        | 1.45     |
| 3   | C     | 604  | CLA  | C1D-C2D | -2.31 | 1.40        | 1.45     |
| 2   | A     | 607  | CHL  | C1B-NB  | -2.31 | 1.34        | 1.37     |
| 3   | C     | 602  | CLA  | C1D-C2D | -2.31 | 1.40        | 1.45     |
| 3   | A     | 613  | CLA  | C1D-C2D | -2.31 | 1.40        | 1.45     |
| 3   | A     | 602  | CLA  | C1D-C2D | -2.31 | 1.40        | 1.45     |
| 3   | C     | 603  | CLA  | C1D-C2D | -2.31 | 1.40        | 1.45     |
| 3   | C     | 614  | CLA  | C1D-C2D | -2.31 | 1.40        | 1.45     |
| 3   | A     | 604  | CLA  | C1D-C2D | -2.30 | 1.40        | 1.45     |
| 2   | C     | 607  | CHL  | C1B-NB  | -2.30 | 1.35        | 1.37     |
| 3   | B     | 602  | CLA  | C1D-C2D | -2.29 | 1.40        | 1.45     |
| 3   | A     | 614  | CLA  | C1D-C2D | -2.29 | 1.40        | 1.45     |
| 3   | B     | 614  | CLA  | C1D-C2D | -2.28 | 1.40        | 1.45     |
| 3   | B     | 603  | CLA  | C1D-C2D | -2.27 | 1.40        | 1.45     |
| 2   | C     | 607  | CHL  | C1D-C2D | -2.27 | 1.40        | 1.45     |
| 2   | A     | 607  | CHL  | C1D-C2D | -2.27 | 1.40        | 1.45     |
| 3   | C     | 613  | CLA  | C1D-C2D | -2.27 | 1.40        | 1.45     |
| 3   | B     | 613  | CLA  | C1D-C2D | -2.26 | 1.40        | 1.45     |
| 3   | A     | 603  | CLA  | C1D-C2D | -2.26 | 1.40        | 1.45     |
| 2   | B     | 606  | CHL  | C1D-C2D | -2.24 | 1.40        | 1.45     |
| 2   | B     | 607  | CHL  | C1D-C2D | -2.24 | 1.40        | 1.45     |

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| Mol | Chain | Res  | Type  | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|-------|---------|-------|-------------|----------|
| 2   | A     | 608  | CHL   | C1D-C2D | -2.23 | 1.40        | 1.45     |
| 2   | C     | 606  | CHL   | C1D-C2D | -2.22 | 1.41        | 1.45     |
| 3   | A     | 602  | CLA   | C1C-C2C | 2.21  | 1.48        | 1.44     |
| 2   | A     | 605  | CHL   | C1D-C2D | -2.20 | 1.41        | 1.45     |
| 2   | A     | 606  | CHL   | C1D-C2D | -2.20 | 1.41        | 1.45     |
| 2   | A     | 601  | CHL   | C1D-C2D | -2.20 | 1.41        | 1.45     |
| 2   | C     | 601  | CHL   | C1D-C2D | -2.20 | 1.41        | 1.45     |
| 2   | B     | 607  | CHL   | C1B-NB  | -2.19 | 1.35        | 1.37     |
| 2   | C     | 608  | CHL   | C1D-C2D | -2.19 | 1.41        | 1.45     |
| 2   | B     | 601  | CHL   | C1D-C2D | -2.19 | 1.41        | 1.45     |
| 2   | C     | 605  | CHL   | C1D-C2D | -2.18 | 1.41        | 1.45     |
| 2   | B     | 605  | CHL   | C1D-C2D | -2.17 | 1.41        | 1.45     |
| 2   | A     | 601  | CHL   | C1B-C2B | 2.17  | 1.48        | 1.43     |
| 3   | C     | 610  | CLA   | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 2   | B     | 609  | CHL   | C1D-C2D | -2.17 | 1.41        | 1.45     |
| 2   | B     | 608  | CHL   | C1D-C2D | -2.16 | 1.41        | 1.45     |
| 2   | B     | 606  | CHL   | C1B-C2B | 2.14  | 1.48        | 1.43     |
| 2   | A     | 609  | CHL   | C1D-C2D | -2.14 | 1.41        | 1.45     |
| 2   | C     | 609  | CHL   | C1D-C2D | -2.13 | 1.41        | 1.45     |
| 2   | B     | 606  | CHL   | C1B-NB  | -2.13 | 1.35        | 1.37     |
| 2   | A     | 606  | CHL   | C1B-C2B | 2.12  | 1.48        | 1.43     |
| 2   | C     | 608  | CHL   | C1B-NB  | -2.12 | 1.35        | 1.37     |
| 3   | A     | 614  | CLA   | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 2   | C     | 606  | CHL   | C1B-C2B | 2.10  | 1.48        | 1.43     |
| 3   | B     | 614  | CLA   | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 3   | B     | 610  | CLA   | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 3   | C     | 614  | CLA   | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 2   | B     | 609  | CHL   | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 2   | C     | 601  | CHL   | C1B-NB  | -2.08 | 1.35        | 1.37     |
| 2   | C     | 606  | CHL   | C1B-NB  | -2.07 | 1.35        | 1.37     |
| 2   | B     | 601  | CHL   | C1B-C2B | 2.07  | 1.48        | 1.43     |
| 2   | A     | 606  | CHL   | C1B-NB  | -2.06 | 1.35        | 1.37     |
| 4   | B     | 1001 | A1LXP | C30-C31 | -2.06 | 1.49        | 1.53     |
| 2   | B     | 607  | CHL   | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 2   | C     | 608  | CHL   | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 2   | B     | 608  | CHL   | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 2   | A     | 607  | CHL   | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 2   | C     | 605  | CHL   | C1B-C2B | 2.05  | 1.48        | 1.43     |
| 3   | C     | 603  | CLA   | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 4   | C     | 1001 | A1LXP | C30-C31 | -2.05 | 1.49        | 1.53     |
| 2   | B     | 601  | CHL   | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 2   | C     | 607  | CHL   | C3D-C4D | -2.05 | 1.39        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | A     | 605 | CHL  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 2   | C     | 609 | CHL  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 2   | C     | 607 | CHL  | C1B-C2B | 2.04  | 1.48        | 1.43     |
| 2   | C     | 609 | CHL  | C1B-NB  | -2.04 | 1.35        | 1.37     |
| 2   | A     | 609 | CHL  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 2   | A     | 608 | CHL  | C1B-NB  | -2.04 | 1.35        | 1.37     |
| 2   | B     | 605 | CHL  | C1B-C2B | 2.04  | 1.48        | 1.43     |
| 2   | A     | 605 | CHL  | C1B-C2B | 2.04  | 1.48        | 1.43     |
| 3   | C     | 611 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 2   | C     | 605 | CHL  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 2   | C     | 601 | CHL  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 2   | A     | 609 | CHL  | C1B-C2B | 2.04  | 1.48        | 1.43     |
| 2   | B     | 601 | CHL  | C1B-NB  | -2.04 | 1.35        | 1.37     |
| 2   | B     | 605 | CHL  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 2   | A     | 607 | CHL  | C1B-C2B | 2.03  | 1.48        | 1.43     |
| 2   | B     | 608 | CHL  | C1B-NB  | -2.03 | 1.35        | 1.37     |
| 2   | C     | 606 | CHL  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 3   | B     | 612 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 2   | C     | 609 | CHL  | C1B-C2B | 2.02  | 1.48        | 1.43     |
| 3   | A     | 612 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 2   | A     | 608 | CHL  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 3   | A     | 603 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 2   | B     | 607 | CHL  | C1B-C2B | 2.02  | 1.48        | 1.43     |
| 3   | B     | 611 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 3   | A     | 604 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 3   | A     | 610 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 3   | B     | 603 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 2   | A     | 606 | CHL  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 3   | A     | 611 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 2   | B     | 609 | CHL  | C1B-NB  | -2.01 | 1.35        | 1.37     |
| 3   | A     | 613 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 2   | A     | 601 | CHL  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 2   | B     | 606 | CHL  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 2   | B     | 608 | CHL  | C1B-C2B | 2.00  | 1.48        | 1.43     |

All (395) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 7   | A     | 1004 | XAT  | O24-C25-C24 | -18.28 | 99.65       | 113.38   |
| 7   | C     | 1004 | XAT  | O24-C25-C24 | -18.28 | 99.65       | 113.38   |
| 7   | B     | 1004 | XAT  | O24-C25-C24 | -18.17 | 99.73       | 113.38   |
| 2   | A     | 601  | CHL  | C4A-NA-C1A  | 11.46  | 111.86      | 106.71   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 607 | CHL  | C4A-NA-C1A | 11.41 | 111.83      | 106.71   |
| 2   | A     | 607 | CHL  | C4A-NA-C1A | 11.39 | 111.83      | 106.71   |
| 2   | C     | 607 | CHL  | C4A-NA-C1A | 11.32 | 111.80      | 106.71   |
| 2   | B     | 606 | CHL  | C4A-NA-C1A | 11.31 | 111.79      | 106.71   |
| 2   | C     | 606 | CHL  | C4A-NA-C1A | 11.28 | 111.78      | 106.71   |
| 2   | A     | 606 | CHL  | C4A-NA-C1A | 11.21 | 111.75      | 106.71   |
| 2   | B     | 601 | CHL  | C4A-NA-C1A | 11.09 | 111.69      | 106.71   |
| 2   | C     | 601 | CHL  | C4A-NA-C1A | 11.00 | 111.65      | 106.71   |
| 2   | C     | 608 | CHL  | C4A-NA-C1A | 10.93 | 111.62      | 106.71   |
| 2   | A     | 605 | CHL  | C4A-NA-C1A | 10.82 | 111.57      | 106.71   |
| 2   | B     | 608 | CHL  | C4A-NA-C1A | 10.76 | 111.54      | 106.71   |
| 2   | C     | 605 | CHL  | C4A-NA-C1A | 10.69 | 111.51      | 106.71   |
| 2   | B     | 605 | CHL  | C4A-NA-C1A | 10.62 | 111.48      | 106.71   |
| 2   | A     | 608 | CHL  | C4A-NA-C1A | 10.61 | 111.48      | 106.71   |
| 2   | B     | 609 | CHL  | C4A-NA-C1A | 10.27 | 111.32      | 106.71   |
| 2   | C     | 609 | CHL  | C4A-NA-C1A | 10.19 | 111.29      | 106.71   |
| 2   | A     | 609 | CHL  | C4A-NA-C1A | 10.12 | 111.25      | 106.71   |
| 3   | C     | 611 | CLA  | C4A-NA-C1A | -6.34 | 103.86      | 106.71   |
| 3   | A     | 611 | CLA  | C4A-NA-C1A | -6.33 | 103.86      | 106.71   |
| 3   | B     | 611 | CLA  | C4A-NA-C1A | -6.24 | 103.90      | 106.71   |
| 3   | C     | 604 | CLA  | C4A-NA-C1A | -5.99 | 104.02      | 106.71   |
| 3   | A     | 604 | CLA  | C4A-NA-C1A | -5.91 | 104.05      | 106.71   |
| 3   | B     | 604 | CLA  | C4A-NA-C1A | -5.80 | 104.10      | 106.71   |
| 3   | A     | 603 | CLA  | C4A-NA-C1A | -5.59 | 104.19      | 106.71   |
| 3   | B     | 603 | CLA  | C4A-NA-C1A | -5.59 | 104.19      | 106.71   |
| 3   | C     | 603 | CLA  | C4A-NA-C1A | -5.37 | 104.29      | 106.71   |
| 3   | A     | 612 | CLA  | C4A-NA-C1A | -5.28 | 104.33      | 106.71   |
| 3   | B     | 612 | CLA  | C4A-NA-C1A | -5.23 | 104.35      | 106.71   |
| 3   | B     | 614 | CLA  | C4A-NA-C1A | -5.21 | 104.36      | 106.71   |
| 3   | C     | 612 | CLA  | C4A-NA-C1A | -5.21 | 104.36      | 106.71   |
| 3   | A     | 614 | CLA  | C4A-NA-C1A | -5.18 | 104.38      | 106.71   |
| 3   | C     | 614 | CLA  | C4A-NA-C1A | -5.16 | 104.39      | 106.71   |
| 3   | A     | 610 | CLA  | C4A-NA-C1A | -4.82 | 104.54      | 106.71   |
| 3   | B     | 610 | CLA  | C4A-NA-C1A | -4.69 | 104.60      | 106.71   |
| 3   | C     | 610 | CLA  | C4A-NA-C1A | -4.68 | 104.60      | 106.71   |
| 2   | C     | 605 | CHL  | C3B-C4B-NB | -4.63 | 106.22      | 110.52   |
| 2   | B     | 605 | CHL  | C3B-C4B-NB | -4.62 | 106.23      | 110.52   |
| 2   | C     | 601 | CHL  | C3B-C4B-NB | -4.61 | 106.24      | 110.52   |
| 2   | A     | 605 | CHL  | C3B-C4B-NB | -4.60 | 106.25      | 110.52   |
| 2   | B     | 601 | CHL  | C3B-C4B-NB | -4.58 | 106.27      | 110.52   |
| 2   | B     | 607 | CHL  | C3B-C4B-NB | -4.50 | 106.34      | 110.52   |
| 2   | C     | 607 | CHL  | C3B-C4B-NB | -4.48 | 106.36      | 110.52   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 609 | CHL  | C3B-C4B-NB | -4.46 | 106.38      | 110.52   |
| 2   | A     | 601 | CHL  | C3B-C4B-NB | -4.43 | 106.41      | 110.52   |
| 2   | C     | 609 | CHL  | C3B-C4B-NB | -4.43 | 106.41      | 110.52   |
| 2   | A     | 607 | CHL  | C3B-C4B-NB | -4.42 | 106.41      | 110.52   |
| 2   | B     | 608 | CHL  | C3B-C4B-NB | -4.41 | 106.42      | 110.52   |
| 2   | A     | 609 | CHL  | CHD-C1D-ND | -4.40 | 120.41      | 124.45   |
| 2   | C     | 609 | CHL  | CHD-C1D-ND | -4.39 | 120.42      | 124.45   |
| 2   | B     | 606 | CHL  | C3B-C4B-NB | -4.39 | 106.44      | 110.52   |
| 3   | C     | 602 | CLA  | C4A-NA-C1A | -4.39 | 104.73      | 106.71   |
| 2   | A     | 608 | CHL  | C3B-C4B-NB | -4.39 | 106.44      | 110.52   |
| 2   | A     | 606 | CHL  | C3B-C4B-NB | -4.39 | 106.45      | 110.52   |
| 2   | B     | 609 | CHL  | CHD-C1D-ND | -4.38 | 120.43      | 124.45   |
| 2   | B     | 608 | CHL  | CHD-C1D-ND | -4.38 | 120.43      | 124.45   |
| 3   | B     | 602 | CLA  | C4A-NA-C1A | -4.37 | 104.74      | 106.71   |
| 2   | A     | 609 | CHL  | C3B-C4B-NB | -4.36 | 106.47      | 110.52   |
| 2   | C     | 608 | CHL  | C3B-C4B-NB | -4.36 | 106.47      | 110.52   |
| 2   | A     | 608 | CHL  | CHD-C1D-ND | -4.35 | 120.45      | 124.45   |
| 2   | C     | 606 | CHL  | C3B-C4B-NB | -4.33 | 106.50      | 110.52   |
| 2   | C     | 608 | CHL  | CHD-C1D-ND | -4.33 | 120.48      | 124.45   |
| 3   | A     | 602 | CLA  | C4A-NA-C1A | -4.26 | 104.79      | 106.71   |
| 2   | B     | 606 | CHL  | CHD-C1D-ND | -4.24 | 120.56      | 124.45   |
| 2   | B     | 605 | CHL  | CHD-C1D-ND | -4.23 | 120.57      | 124.45   |
| 2   | C     | 606 | CHL  | CHD-C1D-ND | -4.22 | 120.58      | 124.45   |
| 2   | A     | 605 | CHL  | CHD-C1D-ND | -4.22 | 120.58      | 124.45   |
| 3   | A     | 613 | CLA  | C4A-NA-C1A | -4.21 | 104.81      | 106.71   |
| 2   | A     | 606 | CHL  | CHD-C1D-ND | -4.20 | 120.59      | 124.45   |
| 2   | B     | 601 | CHL  | CHD-C1D-ND | -4.19 | 120.60      | 124.45   |
| 2   | C     | 601 | CHL  | CHD-C1D-ND | -4.19 | 120.61      | 124.45   |
| 2   | A     | 601 | CHL  | CHD-C1D-ND | -4.19 | 120.61      | 124.45   |
| 2   | C     | 605 | CHL  | CHD-C1D-ND | -4.17 | 120.62      | 124.45   |
| 2   | B     | 607 | CHL  | CHD-C1D-ND | -4.17 | 120.62      | 124.45   |
| 2   | C     | 607 | CHL  | CHD-C1D-ND | -4.16 | 120.63      | 124.45   |
| 2   | A     | 607 | CHL  | CHD-C1D-ND | -4.14 | 120.65      | 124.45   |
| 3   | C     | 613 | CLA  | C4A-NA-C1A | -4.14 | 104.85      | 106.71   |
| 3   | B     | 613 | CLA  | C4A-NA-C1A | -4.13 | 104.85      | 106.71   |
| 2   | B     | 606 | CHL  | C2B-C1B-NB | -4.00 | 107.55      | 110.23   |
| 2   | C     | 606 | CHL  | C2B-C1B-NB | -3.90 | 107.62      | 110.23   |
| 2   | A     | 601 | CHL  | C2B-C1B-NB | -3.87 | 107.64      | 110.23   |
| 3   | A     | 610 | CLA  | CHD-C1D-ND | -3.87 | 120.90      | 124.45   |
| 3   | C     | 614 | CLA  | CHD-C1D-ND | -3.80 | 120.96      | 124.45   |
| 2   | C     | 605 | CHL  | C2B-C1B-NB | -3.76 | 107.71      | 110.23   |
| 2   | A     | 606 | CHL  | C2B-C1B-NB | -3.75 | 107.72      | 110.23   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | B     | 610 | CLA  | CHD-C1D-ND | -3.74 | 121.02      | 124.45   |
| 3   | C     | 610 | CLA  | CHD-C1D-ND | -3.73 | 121.02      | 124.45   |
| 3   | C     | 602 | CLA  | CHD-C1D-ND | -3.71 | 121.04      | 124.45   |
| 3   | A     | 614 | CLA  | CHD-C1D-ND | -3.70 | 121.06      | 124.45   |
| 3   | A     | 611 | CLA  | CHD-C1D-ND | -3.69 | 121.06      | 124.45   |
| 2   | B     | 605 | CHL  | C2B-C1B-NB | -3.69 | 107.76      | 110.23   |
| 2   | B     | 601 | CHL  | C2B-C1B-NB | -3.69 | 107.76      | 110.23   |
| 3   | B     | 614 | CLA  | CHD-C1D-ND | -3.68 | 121.07      | 124.45   |
| 2   | A     | 605 | CHL  | C2B-C1B-NB | -3.67 | 107.77      | 110.23   |
| 3   | B     | 604 | CLA  | CHD-C1D-ND | -3.67 | 121.08      | 124.45   |
| 3   | A     | 613 | CLA  | CHD-C1D-ND | -3.66 | 121.09      | 124.45   |
| 3   | C     | 604 | CLA  | CHD-C1D-ND | -3.65 | 121.10      | 124.45   |
| 3   | B     | 603 | CLA  | CHD-C1D-ND | -3.65 | 121.10      | 124.45   |
| 3   | C     | 603 | CLA  | CHD-C1D-ND | -3.64 | 121.11      | 124.45   |
| 3   | B     | 602 | CLA  | CHD-C1D-ND | -3.64 | 121.11      | 124.45   |
| 3   | A     | 604 | CLA  | CHD-C1D-ND | -3.64 | 121.11      | 124.45   |
| 2   | B     | 609 | CHL  | C2B-C1B-NB | -3.63 | 107.80      | 110.23   |
| 3   | A     | 602 | CLA  | CHD-C1D-ND | -3.62 | 121.12      | 124.45   |
| 2   | B     | 606 | CHL  | CHC-C1C-NC | 3.62  | 129.69      | 124.20   |
| 2   | A     | 605 | CHL  | CHC-C1C-NC | 3.62  | 129.69      | 124.20   |
| 3   | B     | 613 | CLA  | CHD-C1D-ND | -3.60 | 121.14      | 124.45   |
| 2   | C     | 606 | CHL  | CHC-C1C-NC | 3.60  | 129.67      | 124.20   |
| 2   | A     | 606 | CHL  | CHC-C1C-NC | 3.60  | 129.67      | 124.20   |
| 2   | C     | 605 | CHL  | CHC-C1C-NC | 3.60  | 129.66      | 124.20   |
| 2   | B     | 605 | CHL  | CHC-C1C-NC | 3.60  | 129.66      | 124.20   |
| 3   | C     | 613 | CLA  | CHD-C1D-ND | -3.59 | 121.15      | 124.45   |
| 3   | B     | 611 | CLA  | CHD-C1D-ND | -3.58 | 121.16      | 124.45   |
| 2   | C     | 607 | CHL  | CHC-C1C-NC | 3.57  | 129.62      | 124.20   |
| 2   | A     | 609 | CHL  | C2B-C1B-NB | -3.57 | 107.84      | 110.23   |
| 3   | A     | 603 | CLA  | CHD-C1D-ND | -3.57 | 121.17      | 124.45   |
| 3   | A     | 612 | CLA  | CHD-C1D-ND | -3.57 | 121.17      | 124.45   |
| 3   | B     | 612 | CLA  | CHD-C1D-ND | -3.57 | 121.18      | 124.45   |
| 2   | C     | 608 | CHL  | CHC-C1C-NC | 3.56  | 129.61      | 124.20   |
| 3   | C     | 611 | CLA  | CHD-C1D-ND | -3.55 | 121.19      | 124.45   |
| 2   | C     | 609 | CHL  | C2B-C1B-NB | -3.55 | 107.85      | 110.23   |
| 2   | B     | 607 | CHL  | CHC-C1C-NC | 3.55  | 129.59      | 124.20   |
| 2   | C     | 609 | CHL  | CHC-C1C-NC | 3.55  | 129.59      | 124.20   |
| 2   | C     | 601 | CHL  | C2B-C1B-NB | -3.54 | 107.86      | 110.23   |
| 2   | A     | 601 | CHL  | CHC-C1C-NC | 3.53  | 129.56      | 124.20   |
| 2   | B     | 601 | CHL  | CHC-C1C-NC | 3.53  | 129.55      | 124.20   |
| 2   | B     | 607 | CHL  | C2B-C1B-NB | -3.52 | 107.88      | 110.23   |
| 3   | C     | 612 | CLA  | CHD-C1D-ND | -3.51 | 121.22      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 608 | CHL  | CHC-C1C-NC  | 3.49  | 129.50      | 124.20   |
| 2   | B     | 608 | CHL  | CHC-C1C-NC  | 3.47  | 129.47      | 124.20   |
| 2   | B     | 609 | CHL  | CHC-C1C-NC  | 3.47  | 129.46      | 124.20   |
| 2   | A     | 607 | CHL  | C2B-C1B-NB  | -3.47 | 107.91      | 110.23   |
| 2   | C     | 601 | CHL  | CHC-C1C-NC  | 3.46  | 129.46      | 124.20   |
| 2   | C     | 607 | CHL  | C2B-C1B-NB  | -3.45 | 107.92      | 110.23   |
| 2   | A     | 608 | CHL  | C2B-C1B-NB  | -3.44 | 107.93      | 110.23   |
| 2   | B     | 608 | CHL  | C2B-C1B-NB  | -3.42 | 107.94      | 110.23   |
| 2   | A     | 609 | CHL  | CHC-C1C-NC  | 3.41  | 129.38      | 124.20   |
| 2   | C     | 608 | CHL  | C2B-C1B-NB  | -3.40 | 107.95      | 110.23   |
| 2   | A     | 607 | CHL  | CHC-C1C-NC  | 3.39  | 129.34      | 124.20   |
| 2   | B     | 607 | CHL  | C4D-CHA-C1A | 3.30  | 125.27      | 121.25   |
| 2   | B     | 607 | CHL  | CHB-C4A-NA  | 3.24  | 128.99      | 124.51   |
| 3   | B     | 611 | CLA  | CHB-C1B-NB  | -3.23 | 120.83      | 124.26   |
| 2   | A     | 607 | CHL  | C4D-CHA-C1A | 3.23  | 125.17      | 121.25   |
| 2   | C     | 607 | CHL  | C4D-CHA-C1A | 3.22  | 125.17      | 121.25   |
| 3   | A     | 613 | CLA  | CHB-C1B-NB  | -3.22 | 120.85      | 124.26   |
| 2   | A     | 607 | CHL  | CHB-C4A-NA  | 3.22  | 128.96      | 124.51   |
| 3   | B     | 613 | CLA  | CHB-C1B-NB  | -3.20 | 120.87      | 124.26   |
| 3   | C     | 613 | CLA  | CHB-C1B-NB  | -3.20 | 120.87      | 124.26   |
| 2   | C     | 607 | CHL  | CHB-C4A-NA  | 3.20  | 128.93      | 124.51   |
| 3   | A     | 611 | CLA  | CHB-C1B-NB  | -3.19 | 120.88      | 124.26   |
| 3   | C     | 612 | CLA  | CHB-C1B-NB  | -3.19 | 120.88      | 124.26   |
| 3   | C     | 610 | CLA  | CHB-C1B-NB  | -3.19 | 120.88      | 124.26   |
| 3   | C     | 603 | CLA  | CHB-C1B-NB  | -3.19 | 120.89      | 124.26   |
| 3   | C     | 603 | CLA  | C1D-ND-C4D  | -3.18 | 104.07      | 106.33   |
| 2   | B     | 605 | CHL  | C4D-CHA-C1A | 3.18  | 125.12      | 121.25   |
| 2   | A     | 605 | CHL  | C4D-CHA-C1A | 3.17  | 125.11      | 121.25   |
| 3   | B     | 612 | CLA  | CHB-C1B-NB  | -3.17 | 120.90      | 124.26   |
| 3   | B     | 602 | CLA  | CHB-C1B-NB  | -3.17 | 120.90      | 124.26   |
| 2   | B     | 601 | CHL  | CHB-C4A-NA  | 3.16  | 128.89      | 124.51   |
| 3   | C     | 611 | CLA  | CHB-C1B-NB  | -3.16 | 120.91      | 124.26   |
| 3   | B     | 610 | CLA  | CHB-C1B-NB  | -3.16 | 120.91      | 124.26   |
| 3   | A     | 602 | CLA  | CHB-C1B-NB  | -3.15 | 120.92      | 124.26   |
| 2   | C     | 601 | CHL  | CHB-C4A-NA  | 3.15  | 128.87      | 124.51   |
| 3   | C     | 602 | CLA  | CHB-C1B-NB  | -3.15 | 120.92      | 124.26   |
| 3   | A     | 612 | CLA  | CHB-C1B-NB  | -3.15 | 120.92      | 124.26   |
| 3   | A     | 603 | CLA  | CHB-C1B-NB  | -3.15 | 120.93      | 124.26   |
| 2   | C     | 605 | CHL  | C4D-CHA-C1A | 3.14  | 125.07      | 121.25   |
| 3   | A     | 614 | CLA  | CHB-C1B-NB  | -3.14 | 120.94      | 124.26   |
| 3   | B     | 603 | CLA  | CHB-C1B-NB  | -3.14 | 120.94      | 124.26   |
| 2   | C     | 608 | CHL  | C4D-CHA-C1A | 3.13  | 125.06      | 121.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | B     | 614  | CLA  | CHB-C1B-NB  | -3.13 | 120.94      | 124.26   |
| 2   | A     | 606  | CHL  | C4D-CHA-C1A | 3.13  | 125.06      | 121.25   |
| 3   | B     | 612  | CLA  | C1D-ND-C4D  | -3.13 | 104.11      | 106.33   |
| 3   | C     | 614  | CLA  | CHB-C1B-NB  | -3.13 | 120.95      | 124.26   |
| 3   | A     | 610  | CLA  | CHB-C1B-NB  | -3.12 | 120.95      | 124.26   |
| 3   | C     | 614  | CLA  | C1D-ND-C4D  | -3.12 | 104.12      | 106.33   |
| 2   | C     | 606  | CHL  | C4D-CHA-C1A | 3.11  | 125.03      | 121.25   |
| 2   | B     | 606  | CHL  | C4D-CHA-C1A | 3.11  | 125.03      | 121.25   |
| 3   | B     | 604  | CLA  | CHB-C1B-NB  | -3.11 | 120.97      | 124.26   |
| 2   | B     | 601  | CHL  | C4D-CHA-C1A | 3.10  | 125.02      | 121.25   |
| 2   | A     | 601  | CHL  | CHB-C4A-NA  | 3.10  | 128.79      | 124.51   |
| 3   | A     | 612  | CLA  | C1D-ND-C4D  | -3.09 | 104.14      | 106.33   |
| 3   | A     | 603  | CLA  | C1D-ND-C4D  | -3.08 | 104.14      | 106.33   |
| 3   | B     | 603  | CLA  | C1D-ND-C4D  | -3.08 | 104.14      | 106.33   |
| 3   | A     | 614  | CLA  | C1D-ND-C4D  | -3.08 | 104.15      | 106.33   |
| 3   | C     | 612  | CLA  | C1D-ND-C4D  | -3.08 | 104.15      | 106.33   |
| 2   | B     | 608  | CHL  | C4D-CHA-C1A | 3.07  | 124.99      | 121.25   |
| 2   | A     | 608  | CHL  | C4D-CHA-C1A | 3.07  | 124.99      | 121.25   |
| 2   | B     | 606  | CHL  | C2A-C1A-CHA | 3.07  | 129.23      | 123.86   |
| 2   | C     | 608  | CHL  | CHB-C4A-NA  | 3.05  | 128.74      | 124.51   |
| 2   | A     | 601  | CHL  | C4D-CHA-C1A | 3.05  | 124.96      | 121.25   |
| 2   | C     | 601  | CHL  | C4D-CHA-C1A | 3.05  | 124.96      | 121.25   |
| 2   | B     | 608  | CHL  | CHB-C4A-NA  | 3.04  | 128.72      | 124.51   |
| 3   | B     | 614  | CLA  | C1D-ND-C4D  | -3.04 | 104.17      | 106.33   |
| 3   | C     | 604  | CLA  | CHB-C1B-NB  | -3.04 | 121.04      | 124.26   |
| 2   | A     | 606  | CHL  | C2A-C1A-CHA | 3.04  | 129.17      | 123.86   |
| 2   | C     | 606  | CHL  | C2A-C1A-CHA | 3.04  | 129.17      | 123.86   |
| 2   | A     | 608  | CHL  | CHB-C4A-NA  | 3.02  | 128.69      | 124.51   |
| 2   | C     | 606  | CHL  | CHB-C4A-NA  | 3.00  | 128.67      | 124.51   |
| 2   | A     | 606  | CHL  | CHB-C4A-NA  | 3.00  | 128.67      | 124.51   |
| 3   | A     | 604  | CLA  | CHB-C1B-NB  | -2.99 | 121.09      | 124.26   |
| 5   | A     | 1003 | NEX  | O24-C25-C24 | 2.99  | 115.63      | 113.38   |
| 2   | A     | 609  | CHL  | CHB-C4A-NA  | 2.98  | 128.64      | 124.51   |
| 2   | B     | 606  | CHL  | CHB-C4A-NA  | 2.98  | 128.63      | 124.51   |
| 3   | A     | 613  | CLA  | C1D-ND-C4D  | -2.98 | 104.22      | 106.33   |
| 5   | B     | 1003 | NEX  | O24-C25-C24 | 2.95  | 115.59      | 113.38   |
| 2   | C     | 609  | CHL  | CHB-C4A-NA  | 2.93  | 128.56      | 124.51   |
| 2   | B     | 609  | CHL  | CHB-C4A-NA  | 2.93  | 128.56      | 124.51   |
| 2   | A     | 609  | CHL  | C4D-CHA-C1A | 2.92  | 124.81      | 121.25   |
| 2   | A     | 605  | CHL  | CHB-C4A-NA  | 2.91  | 128.54      | 124.51   |
| 3   | B     | 613  | CLA  | C1D-ND-C4D  | -2.90 | 104.28      | 106.33   |
| 2   | C     | 609  | CHL  | C4D-CHA-C1A | 2.89  | 124.77      | 121.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | C     | 1003 | NEX  | O24-C25-C24 | 2.89  | 115.55      | 113.38   |
| 2   | B     | 609  | CHL  | C4D-CHA-C1A | 2.88  | 124.76      | 121.25   |
| 2   | B     | 605  | CHL  | C2A-C1A-CHA | 2.88  | 128.89      | 123.86   |
| 3   | C     | 613  | CLA  | C1D-ND-C4D  | -2.88 | 104.29      | 106.33   |
| 2   | B     | 607  | CHL  | C2A-C1A-CHA | 2.88  | 128.89      | 123.86   |
| 2   | B     | 605  | CHL  | CHB-C4A-NA  | 2.87  | 128.49      | 124.51   |
| 2   | C     | 605  | CHL  | CHB-C4A-NA  | 2.86  | 128.47      | 124.51   |
| 2   | A     | 605  | CHL  | C2A-C1A-CHA | 2.86  | 128.87      | 123.86   |
| 2   | C     | 607  | CHL  | C2A-C1A-CHA | 2.86  | 128.86      | 123.86   |
| 3   | C     | 602  | CLA  | C1D-ND-C4D  | -2.86 | 104.31      | 106.33   |
| 2   | C     | 605  | CHL  | C2A-C1A-CHA | 2.85  | 128.84      | 123.86   |
| 2   | A     | 609  | CHL  | C2A-C1A-CHA | 2.84  | 128.83      | 123.86   |
| 2   | A     | 607  | CHL  | C2A-C1A-CHA | 2.83  | 128.81      | 123.86   |
| 3   | C     | 612  | CLA  | C2C-C1C-NC  | 2.81  | 112.60      | 109.97   |
| 3   | A     | 602  | CLA  | C1D-ND-C4D  | -2.81 | 104.34      | 106.33   |
| 2   | A     | 608  | CHL  | C2A-C1A-CHA | 2.81  | 128.76      | 123.86   |
| 2   | C     | 609  | CHL  | C2A-C1A-CHA | 2.79  | 128.74      | 123.86   |
| 3   | B     | 610  | CLA  | C1D-ND-C4D  | -2.79 | 104.35      | 106.33   |
| 3   | B     | 602  | CLA  | C1D-ND-C4D  | -2.78 | 104.36      | 106.33   |
| 2   | C     | 608  | CHL  | C2A-C1A-CHA | 2.77  | 128.70      | 123.86   |
| 3   | C     | 610  | CLA  | C1D-ND-C4D  | -2.77 | 104.37      | 106.33   |
| 3   | A     | 610  | CLA  | C1D-ND-C4D  | -2.77 | 104.37      | 106.33   |
| 3   | A     | 612  | CLA  | C2C-C1C-NC  | 2.77  | 112.56      | 109.97   |
| 2   | B     | 609  | CHL  | C2A-C1A-CHA | 2.76  | 128.69      | 123.86   |
| 2   | C     | 601  | CHL  | C2A-C1A-CHA | 2.76  | 128.68      | 123.86   |
| 3   | B     | 612  | CLA  | C2C-C1C-NC  | 2.75  | 112.55      | 109.97   |
| 2   | A     | 601  | CHL  | C2A-C1A-CHA | 2.75  | 128.66      | 123.86   |
| 2   | B     | 608  | CHL  | C2A-C1A-CHA | 2.74  | 128.64      | 123.86   |
| 2   | B     | 601  | CHL  | C2A-C1A-CHA | 2.73  | 128.63      | 123.86   |
| 3   | B     | 613  | CLA  | C2C-C1C-NC  | 2.72  | 112.52      | 109.97   |
| 3   | C     | 613  | CLA  | C2C-C1C-NC  | 2.70  | 112.50      | 109.97   |
| 3   | C     | 604  | CLA  | C1D-ND-C4D  | -2.66 | 104.45      | 106.33   |
| 3   | B     | 604  | CLA  | C1D-ND-C4D  | -2.64 | 104.46      | 106.33   |
| 3   | A     | 611  | CLA  | C1D-ND-C4D  | -2.64 | 104.46      | 106.33   |
| 3   | A     | 604  | CLA  | C1D-ND-C4D  | -2.64 | 104.46      | 106.33   |
| 3   | A     | 613  | CLA  | C2C-C1C-NC  | 2.64  | 112.44      | 109.97   |
| 3   | A     | 612  | CLA  | CHC-C1C-C2C | -2.61 | 119.48      | 126.73   |
| 3   | C     | 611  | CLA  | C1D-ND-C4D  | -2.60 | 104.49      | 106.33   |
| 3   | C     | 603  | CLA  | C2C-C1C-NC  | 2.60  | 112.41      | 109.97   |
| 3   | A     | 603  | CLA  | C2C-C1C-NC  | 2.59  | 112.40      | 109.97   |
| 3   | B     | 603  | CLA  | C2C-C1C-NC  | 2.59  | 112.40      | 109.97   |
| 3   | B     | 611  | CLA  | C1D-ND-C4D  | -2.58 | 104.50      | 106.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | C     | 612 | CLA  | CHC-C1C-C2C | -2.58 | 119.56      | 126.73   |
| 3   | B     | 603 | CLA  | CHC-C1C-C2C | -2.58 | 119.57      | 126.73   |
| 3   | A     | 603 | CLA  | C1-C2-C3    | -2.58 | 121.59      | 126.04   |
| 3   | B     | 613 | CLA  | CHC-C1C-C2C | -2.57 | 119.58      | 126.73   |
| 3   | C     | 613 | CLA  | CHC-C1C-C2C | -2.57 | 119.59      | 126.73   |
| 3   | A     | 603 | CLA  | CHC-C1C-C2C | -2.57 | 119.60      | 126.73   |
| 3   | C     | 603 | CLA  | CHC-C1C-C2C | -2.57 | 119.60      | 126.73   |
| 3   | B     | 612 | CLA  | CHC-C1C-C2C | -2.56 | 119.61      | 126.73   |
| 3   | A     | 613 | CLA  | CHC-C1C-C2C | -2.56 | 119.61      | 126.73   |
| 3   | A     | 612 | CLA  | C1-C2-C3    | -2.56 | 121.61      | 126.04   |
| 3   | B     | 603 | CLA  | C1-C2-C3    | -2.56 | 121.62      | 126.04   |
| 3   | C     | 612 | CLA  | C1-C2-C3    | -2.54 | 121.65      | 126.04   |
| 3   | B     | 603 | CLA  | CHC-C1C-NC  | 2.51  | 128.01      | 124.20   |
| 3   | B     | 612 | CLA  | C1-C2-C3    | -2.51 | 121.71      | 126.04   |
| 3   | A     | 602 | CLA  | C2C-C1C-NC  | 2.51  | 112.32      | 109.97   |
| 3   | A     | 611 | CLA  | CHC-C1C-C2C | -2.49 | 119.82      | 126.73   |
| 3   | A     | 603 | CLA  | CHC-C1C-NC  | 2.49  | 127.98      | 124.20   |
| 3   | C     | 603 | CLA  | CHC-C1C-NC  | 2.48  | 127.97      | 124.20   |
| 3   | A     | 610 | CLA  | C2C-C1C-NC  | 2.48  | 112.30      | 109.97   |
| 3   | A     | 612 | CLA  | CHC-C1C-NC  | 2.47  | 127.95      | 124.20   |
| 3   | C     | 604 | CLA  | CHC-C1C-NC  | 2.47  | 127.95      | 124.20   |
| 3   | A     | 610 | CLA  | CHC-C1C-C2C | -2.47 | 119.88      | 126.73   |
| 3   | C     | 614 | CLA  | CHC-C1C-C2C | -2.46 | 119.89      | 126.73   |
| 3   | B     | 610 | CLA  | C2C-C1C-NC  | 2.46  | 112.28      | 109.97   |
| 3   | A     | 614 | CLA  | CHC-C1C-C2C | -2.46 | 119.90      | 126.73   |
| 3   | C     | 604 | CLA  | CHC-C1C-C2C | -2.46 | 119.90      | 126.73   |
| 3   | C     | 611 | CLA  | CHC-C1C-C2C | -2.46 | 119.90      | 126.73   |
| 3   | B     | 604 | CLA  | CHC-C1C-C2C | -2.46 | 119.91      | 126.73   |
| 3   | B     | 614 | CLA  | CHC-C1C-C2C | -2.46 | 119.91      | 126.73   |
| 3   | A     | 611 | CLA  | C2C-C1C-NC  | 2.45  | 112.27      | 109.97   |
| 3   | C     | 603 | CLA  | C1-C2-C3    | -2.45 | 121.80      | 126.04   |
| 3   | B     | 611 | CLA  | CHC-C1C-C2C | -2.45 | 119.92      | 126.73   |
| 3   | A     | 613 | CLA  | CHC-C1C-NC  | 2.45  | 127.92      | 124.20   |
| 3   | C     | 611 | CLA  | C2C-C1C-NC  | 2.45  | 112.26      | 109.97   |
| 3   | A     | 604 | CLA  | CHC-C1C-C2C | -2.44 | 119.95      | 126.73   |
| 3   | B     | 611 | CLA  | CHA-C1A-NA  | -2.44 | 120.81      | 126.40   |
| 3   | A     | 611 | CLA  | CHA-C1A-NA  | -2.44 | 120.81      | 126.40   |
| 3   | B     | 610 | CLA  | CHC-C1C-C2C | -2.44 | 119.96      | 126.73   |
| 3   | C     | 611 | CLA  | CHA-C1A-NA  | -2.44 | 120.82      | 126.40   |
| 3   | B     | 604 | CLA  | CHC-C1C-NC  | 2.43  | 127.89      | 124.20   |
| 3   | C     | 613 | CLA  | CHC-C1C-NC  | 2.43  | 127.89      | 124.20   |
| 3   | B     | 614 | CLA  | C2C-C1C-NC  | 2.43  | 112.25      | 109.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | A     | 611 | CLA  | CHC-C1C-NC  | 2.42  | 127.88      | 124.20   |
| 3   | B     | 613 | CLA  | CHC-C1C-NC  | 2.42  | 127.88      | 124.20   |
| 3   | C     | 610 | CLA  | CHC-C1C-C2C | -2.42 | 120.01      | 126.73   |
| 3   | A     | 602 | CLA  | CHC-C1C-C2C | -2.41 | 120.02      | 126.73   |
| 3   | B     | 611 | CLA  | C2C-C1C-NC  | 2.41  | 112.23      | 109.97   |
| 3   | C     | 614 | CLA  | C2C-C1C-NC  | 2.41  | 112.23      | 109.97   |
| 3   | A     | 614 | CLA  | C2C-C1C-NC  | 2.41  | 112.23      | 109.97   |
| 3   | A     | 604 | CLA  | CHC-C1C-NC  | 2.40  | 127.84      | 124.20   |
| 3   | B     | 612 | CLA  | CHC-C1C-NC  | 2.40  | 127.84      | 124.20   |
| 3   | C     | 612 | CLA  | CHC-C1C-NC  | 2.39  | 127.84      | 124.20   |
| 3   | C     | 614 | CLA  | CHC-C1C-NC  | 2.39  | 127.83      | 124.20   |
| 3   | A     | 614 | CLA  | CHC-C1C-NC  | 2.39  | 127.83      | 124.20   |
| 3   | B     | 604 | CLA  | CHA-C1A-NA  | -2.39 | 120.93      | 126.40   |
| 3   | C     | 604 | CLA  | CHA-C1A-NA  | -2.38 | 120.95      | 126.40   |
| 3   | B     | 611 | CLA  | CHC-C1C-NC  | 2.38  | 127.81      | 124.20   |
| 3   | A     | 610 | CLA  | CHC-C1C-NC  | 2.38  | 127.81      | 124.20   |
| 3   | C     | 610 | CLA  | CHC-C1C-NC  | 2.38  | 127.81      | 124.20   |
| 3   | C     | 611 | CLA  | CHC-C1C-NC  | 2.37  | 127.80      | 124.20   |
| 3   | B     | 614 | CLA  | CHC-C1C-NC  | 2.37  | 127.80      | 124.20   |
| 3   | A     | 604 | CLA  | CHA-C1A-NA  | -2.37 | 120.97      | 126.40   |
| 3   | A     | 604 | CLA  | C2C-C1C-NC  | 2.35  | 112.17      | 109.97   |
| 3   | C     | 610 | CLA  | C2C-C1C-NC  | 2.35  | 112.17      | 109.97   |
| 3   | C     | 602 | CLA  | CHC-C1C-C2C | -2.34 | 120.22      | 126.73   |
| 3   | B     | 604 | CLA  | C2C-C1C-NC  | 2.34  | 112.17      | 109.97   |
| 3   | B     | 602 | CLA  | CHC-C1C-C2C | -2.34 | 120.24      | 126.73   |
| 3   | B     | 610 | CLA  | CHC-C1C-NC  | 2.33  | 127.74      | 124.20   |
| 3   | C     | 604 | CLA  | C2C-C1C-NC  | 2.30  | 112.12      | 109.97   |
| 3   | B     | 602 | CLA  | C2C-C1C-NC  | 2.29  | 112.11      | 109.97   |
| 3   | C     | 602 | CLA  | C2C-C1C-NC  | 2.29  | 112.11      | 109.97   |
| 3   | C     | 602 | CLA  | C1-C2-C3    | -2.25 | 122.15      | 126.04   |
| 3   | C     | 602 | CLA  | CHC-C1C-NC  | 2.25  | 127.61      | 124.20   |
| 3   | A     | 602 | CLA  | CHC-C1C-NC  | 2.24  | 127.61      | 124.20   |
| 3   | B     | 602 | CLA  | CHC-C1C-NC  | 2.24  | 127.60      | 124.20   |
| 3   | C     | 610 | CLA  | C1-C2-C3    | -2.23 | 122.18      | 126.04   |
| 3   | B     | 602 | CLA  | CHA-C1A-NA  | -2.23 | 121.30      | 126.40   |
| 3   | A     | 602 | CLA  | CHA-C1A-NA  | -2.21 | 121.33      | 126.40   |
| 2   | C     | 606 | CHL  | CHA-C1A-NA  | -2.21 | 121.34      | 126.40   |
| 2   | A     | 606 | CHL  | CHA-C1A-NA  | -2.21 | 121.34      | 126.40   |
| 3   | A     | 612 | CLA  | CHA-C1A-NA  | -2.20 | 121.35      | 126.40   |
| 3   | C     | 614 | CLA  | CHA-C1A-NA  | -2.20 | 121.35      | 126.40   |
| 2   | B     | 606 | CHL  | CHA-C1A-NA  | -2.20 | 121.35      | 126.40   |
| 3   | B     | 612 | CLA  | CHA-C1A-NA  | -2.19 | 121.38      | 126.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | C     | 612 | CLA  | CHA-C1A-NA  | -2.19 | 121.38      | 126.40   |
| 3   | B     | 613 | CLA  | CHA-C1A-NA  | -2.19 | 121.38      | 126.40   |
| 2   | B     | 607 | CHL  | CHA-C1A-NA  | -2.19 | 121.39      | 126.40   |
| 3   | A     | 614 | CLA  | CHA-C1A-NA  | -2.19 | 121.39      | 126.40   |
| 3   | C     | 602 | CLA  | CHA-C1A-NA  | -2.18 | 121.39      | 126.40   |
| 3   | B     | 614 | CLA  | CHA-C1A-NA  | -2.18 | 121.40      | 126.40   |
| 2   | C     | 607 | CHL  | CHA-C1A-NA  | -2.18 | 121.42      | 126.40   |
| 3   | C     | 610 | CLA  | CHA-C1A-NA  | -2.18 | 121.42      | 126.40   |
| 2   | A     | 607 | CHL  | CHA-C1A-NA  | -2.17 | 121.42      | 126.40   |
| 3   | A     | 613 | CLA  | CHA-C1A-NA  | -2.16 | 121.45      | 126.40   |
| 3   | C     | 613 | CLA  | CHA-C1A-NA  | -2.16 | 121.46      | 126.40   |
| 3   | A     | 610 | CLA  | CHA-C1A-NA  | -2.15 | 121.47      | 126.40   |
| 3   | B     | 610 | CLA  | CHA-C1A-NA  | -2.15 | 121.48      | 126.40   |
| 3   | A     | 610 | CLA  | C1-C2-C3    | -2.12 | 122.37      | 126.04   |
| 3   | A     | 603 | CLA  | CHA-C1A-NA  | -2.11 | 121.56      | 126.40   |
| 3   | B     | 603 | CLA  | CHA-C1A-NA  | -2.11 | 121.58      | 126.40   |
| 3   | C     | 603 | CLA  | CHA-C1A-NA  | -2.10 | 121.59      | 126.40   |
| 2   | B     | 608 | CHL  | CHD-C1D-C2D | 2.10  | 129.88      | 125.48   |
| 2   | C     | 609 | CHL  | CHD-C1D-C2D | 2.09  | 129.86      | 125.48   |
| 2   | A     | 608 | CHL  | CHD-C1D-C2D | 2.09  | 129.86      | 125.48   |
| 2   | B     | 606 | CHL  | C1-C2-C3    | -2.09 | 123.38      | 126.75   |
| 2   | B     | 609 | CHL  | CHD-C1D-C2D | 2.09  | 129.86      | 125.48   |
| 2   | C     | 608 | CHL  | CHD-C1D-C2D | 2.08  | 129.85      | 125.48   |
| 2   | A     | 609 | CHL  | CHD-C1D-C2D | 2.08  | 129.84      | 125.48   |
| 3   | B     | 610 | CLA  | C1-C2-C3    | -2.07 | 122.47      | 126.04   |
| 2   | A     | 606 | CHL  | C1-C2-C3    | -2.07 | 123.41      | 126.75   |
| 2   | B     | 605 | CHL  | CHA-C1A-NA  | -2.06 | 121.67      | 126.40   |
| 2   | B     | 601 | CHL  | CHA-C1A-NA  | -2.06 | 121.68      | 126.40   |
| 2   | C     | 601 | CHL  | CHA-C1A-NA  | -2.05 | 121.69      | 126.40   |
| 2   | A     | 609 | CHL  | CHA-C1A-NA  | -2.05 | 121.70      | 126.40   |
| 2   | A     | 608 | CHL  | CHA-C1A-NA  | -2.04 | 121.72      | 126.40   |
| 2   | C     | 606 | CHL  | C1-C2-C3    | -2.04 | 123.45      | 126.75   |
| 2   | A     | 605 | CHL  | CHA-C1A-NA  | -2.04 | 121.72      | 126.40   |
| 2   | C     | 608 | CHL  | CHA-C1A-NA  | -2.04 | 121.73      | 126.40   |
| 2   | A     | 606 | CHL  | CHC-C1C-C2C | -2.04 | 118.71      | 126.11   |
| 2   | B     | 605 | CHL  | CHD-C1D-C2D | 2.04  | 129.76      | 125.48   |
| 2   | B     | 606 | CHL  | CHD-C1D-C2D | 2.04  | 129.75      | 125.48   |
| 2   | A     | 606 | CHL  | CHD-C1D-C2D | 2.03  | 129.75      | 125.48   |
| 2   | A     | 601 | CHL  | CHA-C1A-NA  | -2.03 | 121.75      | 126.40   |
| 2   | C     | 605 | CHL  | CHA-C1A-NA  | -2.03 | 121.75      | 126.40   |
| 2   | B     | 608 | CHL  | CHA-C1A-NA  | -2.03 | 121.76      | 126.40   |
| 2   | C     | 606 | CHL  | CHD-C1D-C2D | 2.03  | 129.73      | 125.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 605 | CHL  | CHD-C1D-C2D | 2.03  | 129.73      | 125.48   |
| 2   | A     | 605 | CHL  | C4B-CHC-C1C | -2.02 | 121.54      | 126.34   |
| 2   | C     | 605 | CHL  | CHD-C1D-C2D | 2.02  | 129.72      | 125.48   |
| 2   | C     | 609 | CHL  | CHA-C1A-NA  | -2.02 | 121.77      | 126.40   |
| 2   | C     | 607 | CHL  | C4B-CHC-C1C | -2.01 | 121.56      | 126.34   |
| 2   | B     | 601 | CHL  | CHD-C1D-C2D | 2.01  | 129.70      | 125.48   |
| 2   | C     | 605 | CHL  | C4B-CHC-C1C | -2.01 | 121.57      | 126.34   |
| 2   | B     | 609 | CHL  | CHA-C1A-NA  | -2.01 | 121.80      | 126.40   |
| 2   | B     | 607 | CHL  | CHD-C1D-C2D | 2.01  | 129.69      | 125.48   |
| 2   | C     | 601 | CHL  | CHD-C1D-C2D | 2.01  | 129.69      | 125.48   |
| 3   | B     | 613 | CLA  | C1-C2-C3    | -2.00 | 122.58      | 126.04   |
| 2   | B     | 606 | CHL  | CHC-C1C-C2C | -2.00 | 118.85      | 126.11   |
| 2   | B     | 607 | CHL  | C4B-CHC-C1C | -2.00 | 121.59      | 126.34   |

All (36) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 2   | A     | 601 | CHL  | C8   |
| 2   | A     | 608 | CHL  | C8   |
| 2   | A     | 609 | CHL  | C8   |
| 2   | B     | 601 | CHL  | C8   |
| 2   | B     | 608 | CHL  | C8   |
| 2   | B     | 609 | CHL  | C8   |
| 2   | C     | 601 | CHL  | C8   |
| 2   | C     | 608 | CHL  | C8   |
| 2   | C     | 609 | CHL  | C8   |
| 3   | A     | 602 | CLA  | C8   |
| 3   | A     | 603 | CLA  | C8   |
| 3   | A     | 604 | CLA  | C8   |
| 3   | A     | 610 | CLA  | C8   |
| 3   | A     | 611 | CLA  | C8   |
| 3   | A     | 612 | CLA  | C8   |
| 3   | A     | 613 | CLA  | C8   |
| 3   | B     | 602 | CLA  | C8   |
| 3   | B     | 603 | CLA  | C8   |
| 3   | B     | 604 | CLA  | C8   |
| 3   | B     | 610 | CLA  | C8   |
| 3   | B     | 611 | CLA  | C8   |
| 3   | B     | 612 | CLA  | C8   |
| 3   | B     | 613 | CLA  | C8   |
| 3   | C     | 602 | CLA  | C8   |
| 3   | C     | 603 | CLA  | C8   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 3   | C     | 604  | CLA  | C8   |
| 3   | C     | 610  | CLA  | C8   |
| 3   | C     | 611  | CLA  | C8   |
| 3   | C     | 612  | CLA  | C8   |
| 3   | C     | 613  | CLA  | C8   |
| 7   | A     | 1004 | XAT  | C26  |
| 7   | A     | 1004 | XAT  | C25  |
| 7   | B     | 1004 | XAT  | C26  |
| 7   | B     | 1004 | XAT  | C25  |
| 7   | C     | 1004 | XAT  | C26  |
| 7   | C     | 1004 | XAT  | C25  |

All (341) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 2   | A     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 2   | A     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 2   | A     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 2   | A     | 605 | CHL  | C1C-C2C-CMC-OMC |
| 2   | A     | 605 | CHL  | C3C-C2C-CMC-OMC |
| 2   | A     | 606 | CHL  | C1A-C2A-CAA-CBA |
| 2   | A     | 609 | CHL  | C6-C7-C8-C9     |
| 2   | B     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 2   | B     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 2   | B     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 2   | B     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 2   | B     | 605 | CHL  | C1C-C2C-CMC-OMC |
| 2   | B     | 605 | CHL  | C3C-C2C-CMC-OMC |
| 2   | B     | 606 | CHL  | C1A-C2A-CAA-CBA |
| 2   | B     | 606 | CHL  | C1C-C2C-CMC-OMC |
| 2   | B     | 607 | CHL  | C3C-C2C-CMC-OMC |
| 2   | B     | 609 | CHL  | C6-C7-C8-C9     |
| 2   | C     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 2   | C     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 2   | C     | 601 | CHL  | C4B-C3B-CAB-CBB |
| 2   | C     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 2   | C     | 605 | CHL  | C1C-C2C-CMC-OMC |
| 2   | C     | 605 | CHL  | C3C-C2C-CMC-OMC |
| 2   | C     | 606 | CHL  | C1A-C2A-CAA-CBA |
| 2   | C     | 606 | CHL  | C1C-C2C-CMC-OMC |
| 2   | C     | 607 | CHL  | C1C-C2C-CMC-OMC |

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| Mol | Chain | Res  | Type  | Atoms           |
|-----|-------|------|-------|-----------------|
| 2   | C     | 607  | CHL   | C3C-C2C-CMC-OMC |
| 2   | C     | 608  | CHL   | C1C-C2C-CMC-OMC |
| 2   | C     | 608  | CHL   | C3C-C2C-CMC-OMC |
| 2   | C     | 609  | CHL   | C3C-C2C-CMC-OMC |
| 2   | C     | 609  | CHL   | C6-C7-C8-C9     |
| 3   | A     | 603  | CLA   | C2B-C3B-CAB-CBB |
| 3   | A     | 603  | CLA   | C4B-C3B-CAB-CBB |
| 3   | A     | 604  | CLA   | C1A-C2A-CAA-CBA |
| 3   | A     | 611  | CLA   | C1A-C2A-CAA-CBA |
| 3   | A     | 611  | CLA   | C2B-C3B-CAB-CBB |
| 3   | A     | 611  | CLA   | C4B-C3B-CAB-CBB |
| 3   | A     | 612  | CLA   | C2B-C3B-CAB-CBB |
| 3   | A     | 612  | CLA   | C4B-C3B-CAB-CBB |
| 3   | A     | 614  | CLA   | C2B-C3B-CAB-CBB |
| 3   | A     | 614  | CLA   | C4B-C3B-CAB-CBB |
| 3   | B     | 603  | CLA   | C2B-C3B-CAB-CBB |
| 3   | B     | 603  | CLA   | C4B-C3B-CAB-CBB |
| 3   | B     | 604  | CLA   | C1A-C2A-CAA-CBA |
| 3   | B     | 611  | CLA   | C1A-C2A-CAA-CBA |
| 3   | B     | 612  | CLA   | C2B-C3B-CAB-CBB |
| 3   | B     | 612  | CLA   | C4B-C3B-CAB-CBB |
| 3   | B     | 614  | CLA   | C2B-C3B-CAB-CBB |
| 3   | B     | 614  | CLA   | C4B-C3B-CAB-CBB |
| 3   | C     | 603  | CLA   | C2B-C3B-CAB-CBB |
| 3   | C     | 603  | CLA   | C4B-C3B-CAB-CBB |
| 3   | C     | 604  | CLA   | C1A-C2A-CAA-CBA |
| 3   | C     | 611  | CLA   | C1A-C2A-CAA-CBA |
| 3   | C     | 611  | CLA   | C2B-C3B-CAB-CBB |
| 3   | C     | 611  | CLA   | C4B-C3B-CAB-CBB |
| 3   | C     | 612  | CLA   | C2B-C3B-CAB-CBB |
| 3   | C     | 612  | CLA   | C4B-C3B-CAB-CBB |
| 3   | C     | 614  | CLA   | C2B-C3B-CAB-CBB |
| 3   | C     | 614  | CLA   | C4B-C3B-CAB-CBB |
| 4   | A     | 1001 | A1LXP | C24-C1-C42-C2   |
| 4   | C     | 1001 | A1LXP | C24-C1-C42-C2   |
| 6   | A     | 1005 | LHG   | C3-O3-P-O6      |
| 6   | B     | 1005 | LHG   | C3-O3-P-O4      |
| 6   | B     | 1005 | LHG   | C4-O6-P-O5      |
| 6   | C     | 1005 | LHG   | C3-O3-P-O4      |
| 2   | A     | 608  | CHL   | C2A-CAA-CBA-CGA |
| 2   | B     | 608  | CHL   | C2A-CAA-CBA-CGA |
| 2   | C     | 608  | CHL   | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res  | Type  | Atoms           |
|-----|-------|------|-------|-----------------|
| 2   | A     | 601  | CHL   | C11-C10-C8-C9   |
| 2   | C     | 601  | CHL   | C11-C10-C8-C9   |
| 2   | B     | 601  | CHL   | C5-C6-C7-C8     |
| 6   | B     | 1005 | LHG   | C3-O3-P-O6      |
| 6   | B     | 1005 | LHG   | C4-O6-P-O3      |
| 6   | C     | 1005 | LHG   | C3-O3-P-O6      |
| 3   | A     | 602  | CLA   | C4-C3-C5-C6     |
| 2   | C     | 608  | CHL   | C5-C6-C7-C8     |
| 2   | A     | 601  | CHL   | C11-C12-C13-C14 |
| 2   | C     | 601  | CHL   | C11-C12-C13-C14 |
| 3   | B     | 602  | CLA   | C14-C13-C15-C16 |
| 2   | A     | 608  | CHL   | C5-C6-C7-C8     |
| 2   | B     | 608  | CHL   | C5-C6-C7-C8     |
| 2   | A     | 607  | CHL   | C4B-C3B-CAB-CBB |
| 2   | B     | 601  | CHL   | C4B-C3B-CAB-CBB |
| 2   | B     | 607  | CHL   | C4B-C3B-CAB-CBB |
| 2   | C     | 607  | CHL   | C4B-C3B-CAB-CBB |
| 3   | B     | 604  | CLA   | C4B-C3B-CAB-CBB |
| 3   | B     | 611  | CLA   | C4B-C3B-CAB-CBB |
| 3   | A     | 603  | CLA   | C3A-C2A-CAA-CBA |
| 3   | B     | 603  | CLA   | C3A-C2A-CAA-CBA |
| 3   | C     | 603  | CLA   | C3A-C2A-CAA-CBA |
| 6   | B     | 1005 | LHG   | C23-C24-C25-C26 |
| 2   | A     | 609  | CHL   | C2-C3-C5-C6     |
| 3   | A     | 613  | CLA   | C2-C3-C5-C6     |
| 2   | A     | 601  | CHL   | C2B-C3B-CAB-CBB |
| 2   | A     | 607  | CHL   | C2B-C3B-CAB-CBB |
| 2   | B     | 601  | CHL   | C2B-C3B-CAB-CBB |
| 2   | B     | 607  | CHL   | C2B-C3B-CAB-CBB |
| 2   | C     | 601  | CHL   | C2B-C3B-CAB-CBB |
| 2   | C     | 607  | CHL   | C2B-C3B-CAB-CBB |
| 3   | A     | 613  | CLA   | C2B-C3B-CAB-CBB |
| 3   | B     | 604  | CLA   | C2B-C3B-CAB-CBB |
| 3   | B     | 611  | CLA   | C2B-C3B-CAB-CBB |
| 3   | B     | 613  | CLA   | C2B-C3B-CAB-CBB |
| 4   | B     | 1001 | A1LXP | C24-C1-C42-C2   |
| 3   | B     | 613  | CLA   | C4-C3-C5-C6     |
| 3   | A     | 602  | CLA   | C2-C3-C5-C6     |
| 3   | B     | 602  | CLA   | C12-C13-C15-C16 |
| 3   | B     | 613  | CLA   | C2-C3-C5-C6     |
| 3   | C     | 602  | CLA   | C11-C12-C13-C15 |
| 3   | C     | 613  | CLA   | C2-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 6   | A     | 1005 | LHG  | C23-C24-C25-C26 |
| 6   | C     | 1005 | LHG  | C23-C24-C25-C26 |
| 3   | C     | 611  | CLA  | C5-C6-C7-C8     |
| 2   | A     | 609  | CHL  | C4-C3-C5-C6     |
| 3   | A     | 613  | CLA  | C4-C3-C5-C6     |
| 3   | C     | 613  | CLA  | C4-C3-C5-C6     |
| 3   | A     | 603  | CLA  | C1A-C2A-CAA-CBA |
| 3   | B     | 603  | CLA  | C1A-C2A-CAA-CBA |
| 3   | C     | 603  | CLA  | C1A-C2A-CAA-CBA |
| 3   | A     | 611  | CLA  | C5-C6-C7-C8     |
| 2   | B     | 609  | CHL  | C4-C3-C5-C6     |
| 3   | B     | 611  | CLA  | C5-C6-C7-C8     |
| 2   | B     | 607  | CHL  | C2A-CAA-CBA-CGA |
| 2   | C     | 601  | CHL  | C2-C1-O2A-CGA   |
| 2   | C     | 601  | CHL  | C6-C7-C8-C10    |
| 3   | B     | 602  | CLA  | C11-C10-C8-C9   |
| 3   | C     | 602  | CLA  | C11-C12-C13-C14 |
| 6   | C     | 1005 | LHG  | C31-C32-C33-C34 |
| 2   | A     | 601  | CHL  | C4B-C3B-CAB-CBB |
| 2   | A     | 605  | CHL  | C4B-C3B-CAB-CBB |
| 2   | B     | 605  | CHL  | C4B-C3B-CAB-CBB |
| 2   | B     | 608  | CHL  | C4B-C3B-CAB-CBB |
| 2   | C     | 605  | CHL  | C4B-C3B-CAB-CBB |
| 3   | A     | 604  | CLA  | C4B-C3B-CAB-CBB |
| 3   | A     | 610  | CLA  | C4B-C3B-CAB-CBB |
| 3   | A     | 613  | CLA  | C4B-C3B-CAB-CBB |
| 3   | B     | 610  | CLA  | C4B-C3B-CAB-CBB |
| 3   | B     | 613  | CLA  | C4B-C3B-CAB-CBB |
| 3   | C     | 604  | CLA  | C4B-C3B-CAB-CBB |
| 3   | C     | 613  | CLA  | C4B-C3B-CAB-CBB |
| 3   | B     | 602  | CLA  | C4-C3-C5-C6     |
| 2   | B     | 609  | CHL  | C2-C3-C5-C6     |
| 2   | C     | 609  | CHL  | C8-C10-C11-C12  |
| 2   | B     | 609  | CHL  | C8-C10-C11-C12  |
| 2   | B     | 606  | CHL  | C3C-C2C-CMC-OMC |
| 2   | C     | 606  | CHL  | C3C-C2C-CMC-OMC |
| 2   | A     | 605  | CHL  | C2B-C3B-CAB-CBB |
| 2   | B     | 605  | CHL  | C2B-C3B-CAB-CBB |
| 2   | C     | 605  | CHL  | C2B-C3B-CAB-CBB |
| 3   | A     | 604  | CLA  | C2B-C3B-CAB-CBB |
| 3   | C     | 604  | CLA  | C2B-C3B-CAB-CBB |
| 3   | C     | 613  | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type  | Atoms           |
|-----|-------|------|-------|-----------------|
| 2   | C     | 607  | CHL   | C2A-CAA-CBA-CGA |
| 4   | A     | 1001 | A1LXP | C28-C1-C42-C2   |
| 4   | A     | 1002 | A1LXP | C24-C1-C42-C2   |
| 4   | B     | 1002 | A1LXP | C24-C1-C42-C2   |
| 4   | B     | 1002 | A1LXP | C28-C1-C42-C2   |
| 4   | C     | 1001 | A1LXP | C28-C1-C42-C2   |
| 4   | C     | 1002 | A1LXP | C24-C1-C42-C2   |
| 4   | C     | 1002 | A1LXP | C28-C1-C42-C2   |
| 2   | A     | 609  | CHL   | C6-C7-C8-C10    |
| 2   | B     | 609  | CHL   | C6-C7-C8-C10    |
| 2   | C     | 609  | CHL   | C6-C7-C8-C10    |
| 3   | B     | 602  | CLA   | C11-C10-C8-C7   |
| 2   | A     | 609  | CHL   | C8-C10-C11-C12  |
| 3   | A     | 612  | CLA   | CAD-CBD-CGD-O2D |
| 3   | B     | 603  | CLA   | CAD-CBD-CGD-O2D |
| 3   | C     | 604  | CLA   | C4-C3-C5-C6     |
| 3   | A     | 602  | CLA   | CHA-CBD-CGD-O1D |
| 3   | A     | 602  | CLA   | CHA-CBD-CGD-O2D |
| 3   | B     | 602  | CLA   | CHA-CBD-CGD-O1D |
| 3   | B     | 602  | CLA   | CHA-CBD-CGD-O2D |
| 3   | C     | 602  | CLA   | CHA-CBD-CGD-O1D |
| 3   | C     | 602  | CLA   | CHA-CBD-CGD-O2D |
| 3   | A     | 604  | CLA   | C4-C3-C5-C6     |
| 3   | A     | 612  | CLA   | C4-C3-C5-C6     |
| 3   | B     | 604  | CLA   | C4-C3-C5-C6     |
| 3   | A     | 612  | CLA   | C11-C10-C8-C9   |
| 3   | B     | 602  | CLA   | C2-C3-C5-C6     |
| 6   | A     | 1005 | LHG   | C3-O3-P-O4      |
| 6   | B     | 1005 | LHG   | C4-O6-P-O4      |
| 3   | A     | 614  | CLA   | CAD-CBD-CGD-O1D |
| 3   | B     | 614  | CLA   | CAD-CBD-CGD-O1D |
| 3   | C     | 614  | CLA   | CAD-CBD-CGD-O1D |
| 6   | B     | 1005 | LHG   | C25-C26-C27-C28 |
| 2   | A     | 606  | CHL   | C3A-C2A-CAA-CBA |
| 2   | B     | 606  | CHL   | C3A-C2A-CAA-CBA |
| 2   | A     | 607  | CHL   | C2A-CAA-CBA-CGA |
| 2   | B     | 607  | CHL   | C1C-C2C-CMC-OMC |
| 2   | C     | 601  | CHL   | C1C-C2C-CMC-OMC |
| 2   | C     | 609  | CHL   | C1C-C2C-CMC-OMC |
| 3   | C     | 612  | CLA   | C4-C3-C5-C6     |
| 3   | A     | 604  | CLA   | C2-C3-C5-C6     |
| 3   | C     | 604  | CLA   | C2-C3-C5-C6     |

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| Mol | Chain | Res  | Type  | Atoms           |
|-----|-------|------|-------|-----------------|
| 2   | A     | 608  | CHL   | C2B-C3B-CAB-CBB |
| 2   | B     | 608  | CHL   | C2B-C3B-CAB-CBB |
| 2   | C     | 608  | CHL   | C2B-C3B-CAB-CBB |
| 3   | A     | 602  | CLA   | C2B-C3B-CAB-CBB |
| 3   | A     | 610  | CLA   | C2B-C3B-CAB-CBB |
| 3   | B     | 602  | CLA   | C2B-C3B-CAB-CBB |
| 3   | B     | 610  | CLA   | C2B-C3B-CAB-CBB |
| 3   | C     | 610  | CLA   | C2B-C3B-CAB-CBB |
| 3   | B     | 612  | CLA   | C4-C3-C5-C6     |
| 3   | A     | 612  | CLA   | C2-C3-C5-C6     |
| 3   | A     | 611  | CLA   | C13-C15-C16-C17 |
| 2   | C     | 606  | CHL   | C2A-CAA-CBA-CGA |
| 4   | A     | 1002 | A1LXP | C28-C1-C42-C2   |
| 4   | B     | 1001 | A1LXP | C28-C1-C42-C2   |
| 3   | B     | 604  | CLA   | C2-C3-C5-C6     |
| 6   | C     | 1005 | LHG   | C4-O6-P-O3      |
| 3   | C     | 611  | CLA   | C12-C13-C15-C16 |
| 3   | B     | 612  | CLA   | C11-C10-C8-C9   |
| 3   | B     | 611  | CLA   | C13-C15-C16-C17 |
| 3   | B     | 602  | CLA   | C3-C5-C6-C7     |
| 3   | A     | 602  | CLA   | C3-C5-C6-C7     |
| 3   | C     | 611  | CLA   | C13-C15-C16-C17 |
| 2   | A     | 608  | CHL   | C4B-C3B-CAB-CBB |
| 2   | A     | 609  | CHL   | C4B-C3B-CAB-CBB |
| 2   | C     | 608  | CHL   | C4B-C3B-CAB-CBB |
| 2   | C     | 609  | CHL   | C4B-C3B-CAB-CBB |
| 3   | C     | 610  | CLA   | C4B-C3B-CAB-CBB |
| 6   | C     | 1005 | LHG   | C12-C13-C14-C15 |
| 2   | C     | 609  | CHL   | C2-C3-C5-C6     |
| 6   | B     | 1005 | LHG   | C16-C17-C18-C19 |
| 2   | A     | 606  | CHL   | C2A-CAA-CBA-CGA |
| 2   | B     | 606  | CHL   | C2A-CAA-CBA-CGA |
| 2   | C     | 606  | CHL   | C3A-C2A-CAA-CBA |
| 2   | C     | 609  | CHL   | C4-C3-C5-C6     |
| 3   | B     | 611  | CLA   | C3-C5-C6-C7     |
| 3   | A     | 611  | CLA   | C11-C10-C8-C9   |
| 3   | A     | 613  | CLA   | C6-C7-C8-C9     |
| 3   | B     | 611  | CLA   | C11-C10-C8-C9   |
| 3   | C     | 613  | CLA   | C6-C7-C8-C9     |
| 5   | A     | 1003 | NEX   | C39-C29-C30-C31 |
| 5   | B     | 1003 | NEX   | C39-C29-C30-C31 |
| 5   | C     | 1003 | NEX   | C39-C29-C30-C31 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | B     | 611  | CLA  | C4-C3-C5-C6     |
| 3   | A     | 611  | CLA  | C12-C13-C15-C16 |
| 3   | B     | 611  | CLA  | C12-C13-C15-C16 |
| 2   | B     | 609  | CHL  | C3C-C2C-CMC-OMC |
| 6   | A     | 1005 | LHG  | C4-O6-P-O3      |
| 2   | A     | 609  | CHL  | C2B-C3B-CAB-CBB |
| 2   | C     | 609  | CHL  | C2B-C3B-CAB-CBB |
| 3   | C     | 602  | CLA  | C2B-C3B-CAB-CBB |
| 5   | A     | 1003 | NEX  | C28-C29-C30-C31 |
| 5   | B     | 1003 | NEX  | C28-C29-C30-C31 |
| 5   | C     | 1003 | NEX  | C28-C29-C30-C31 |
| 6   | C     | 1005 | LHG  | C25-C26-C27-C28 |
| 2   | A     | 601  | CHL  | C2-C1-O2A-CGA   |
| 2   | B     | 601  | CHL  | C2-C1-O2A-CGA   |
| 3   | C     | 612  | CLA  | C2-C3-C5-C6     |
| 3   | B     | 613  | CLA  | C6-C7-C8-C9     |
| 3   | C     | 611  | CLA  | C11-C10-C8-C9   |
| 3   | C     | 612  | CLA  | C11-C10-C8-C9   |
| 3   | A     | 611  | CLA  | C3-C5-C6-C7     |
| 3   | A     | 611  | CLA  | C4-C3-C5-C6     |
| 3   | B     | 612  | CLA  | C2-C3-C5-C6     |
| 3   | C     | 611  | CLA  | C3-C5-C6-C7     |
| 3   | A     | 602  | CLA  | C4B-C3B-CAB-CBB |
| 3   | B     | 602  | CLA  | C4B-C3B-CAB-CBB |
| 3   | C     | 602  | CLA  | C4B-C3B-CAB-CBB |
| 3   | B     | 604  | CLA  | CAA-CBA-CGA-O2A |
| 2   | B     | 601  | CHL  | C4-C3-C5-C6     |
| 3   | A     | 612  | CLA  | C11-C10-C8-C7   |
| 3   | A     | 611  | CLA  | CAA-CBA-CGA-O2A |
| 3   | C     | 611  | CLA  | CAA-CBA-CGA-O2A |
| 3   | C     | 611  | CLA  | C14-C13-C15-C16 |
| 6   | C     | 1005 | LHG  | O8-C23-C24-C25  |
| 3   | A     | 603  | CLA  | CAD-CBD-CGD-O2D |
| 3   | B     | 612  | CLA  | CAD-CBD-CGD-O2D |
| 3   | C     | 612  | CLA  | CAD-CBD-CGD-O2D |
| 6   | B     | 1005 | LHG  | C11-C10-C9-C8   |
| 3   | C     | 611  | CLA  | C4-C3-C5-C6     |
| 3   | A     | 611  | CLA  | C2-C3-C5-C6     |
| 3   | B     | 611  | CLA  | C2-C3-C5-C6     |
| 3   | B     | 611  | CLA  | CAA-CBA-CGA-O2A |
| 3   | C     | 604  | CLA  | CAA-CBA-CGA-O2A |
| 6   | B     | 1005 | LHG  | O8-C23-C24-C25  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | A     | 608  | CHL  | O2A-C1-C2-C3    |
| 2   | B     | 608  | CHL  | O2A-C1-C2-C3    |
| 2   | C     | 608  | CHL  | O2A-C1-C2-C3    |
| 3   | C     | 612  | CLA  | CAA-CBA-CGA-O2A |
| 2   | A     | 601  | CHL  | CHA-CBD-CGD-O1D |
| 2   | A     | 601  | CHL  | CHA-CBD-CGD-O2D |
| 2   | B     | 601  | CHL  | CHA-CBD-CGD-O1D |
| 2   | B     | 601  | CHL  | CHA-CBD-CGD-O2D |
| 2   | C     | 601  | CHL  | CHA-CBD-CGD-O1D |
| 2   | C     | 601  | CHL  | CHA-CBD-CGD-O2D |
| 3   | C     | 603  | CLA  | CHA-CBD-CGD-O2D |
| 3   | B     | 612  | CLA  | CAA-CBA-CGA-O2A |
| 6   | A     | 1005 | LHG  | O8-C23-C24-C25  |
| 2   | A     | 607  | CHL  | CAA-CBA-CGA-O2A |
| 2   | C     | 606  | CHL  | CAA-CBA-CGA-O2A |
| 3   | A     | 612  | CLA  | CAA-CBA-CGA-O2A |
| 2   | B     | 606  | CHL  | CAA-CBA-CGA-O2A |
| 3   | A     | 604  | CLA  | CAA-CBA-CGA-O2A |
| 2   | A     | 601  | CHL  | C11-C10-C8-C7   |
| 2   | C     | 608  | CHL  | C6-C7-C8-C10    |
| 3   | C     | 611  | CLA  | C2-C3-C5-C6     |
| 2   | A     | 606  | CHL  | CAA-CBA-CGA-O2A |
| 3   | A     | 611  | CLA  | CAA-CBA-CGA-O1A |
| 3   | B     | 611  | CLA  | CAA-CBA-CGA-O1A |
| 3   | C     | 611  | CLA  | CAA-CBA-CGA-O1A |
| 2   | A     | 606  | CHL  | CAA-CBA-CGA-O1A |
| 3   | A     | 612  | CLA  | CAA-CBA-CGA-O1A |
| 6   | C     | 1005 | LHG  | C4-O6-P-O4      |
| 3   | B     | 612  | CLA  | CAA-CBA-CGA-O1A |
| 3   | C     | 612  | CLA  | CAA-CBA-CGA-O1A |
| 2   | C     | 606  | CHL  | CAA-CBA-CGA-O1A |
| 6   | A     | 1005 | LHG  | O10-C23-C24-C25 |
| 6   | B     | 1005 | LHG  | O10-C23-C24-C25 |
| 6   | C     | 1005 | LHG  | O10-C23-C24-C25 |
| 3   | C     | 613  | CLA  | C2A-CAA-CBA-CGA |
| 2   | B     | 606  | CHL  | CAA-CBA-CGA-O1A |
| 6   | A     | 1005 | LHG  | C25-C26-C27-C28 |
| 2   | A     | 607  | CHL  | CAA-CBA-CGA-O1A |
| 2   | B     | 601  | CHL  | CAD-CBD-CGD-O1D |
| 3   | A     | 604  | CLA  | CAD-CBD-CGD-O1D |
| 3   | B     | 604  | CLA  | CAD-CBD-CGD-O1D |
| 3   | C     | 604  | CLA  | CAD-CBD-CGD-O1D |

*Continued on next page...*

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | A     | 611  | CLA  | C14-C13-C15-C16 |
| 3   | B     | 611  | CLA  | C14-C13-C15-C16 |
| 2   | C     | 608  | CHL  | CAA-CBA-CGA-O2A |
| 6   | C     | 1005 | LHG  | C15-C16-C17-C18 |
| 3   | A     | 613  | CLA  | C2A-CAA-CBA-CGA |
| 2   | B     | 608  | CHL  | CAA-CBA-CGA-O2A |
| 2   | A     | 601  | CHL  | C6-C7-C8-C10    |
| 2   | A     | 608  | CHL  | C6-C7-C8-C10    |
| 3   | A     | 611  | CLA  | C3A-C2A-CAA-CBA |
| 3   | B     | 611  | CLA  | C3A-C2A-CAA-CBA |
| 3   | B     | 612  | CLA  | C11-C10-C8-C7   |
| 3   | C     | 611  | CLA  | C3A-C2A-CAA-CBA |
| 3   | C     | 612  | CLA  | C11-C10-C8-C7   |
| 2   | C     | 608  | CHL  | CAA-CBA-CGA-O1A |
| 2   | A     | 608  | CHL  | CAA-CBA-CGA-O2A |
| 2   | B     | 607  | CHL  | CAA-CBA-CGA-O2A |
| 2   | A     | 608  | CHL  | CAA-CBA-CGA-O1A |
| 2   | B     | 608  | CHL  | CAA-CBA-CGA-O1A |
| 3   | B     | 613  | CLA  | C2A-CAA-CBA-CGA |
| 2   | A     | 609  | CHL  | C15-C16-C17-C18 |

There are no ring outliers.

40 monomers are involved in 54 short contacts:

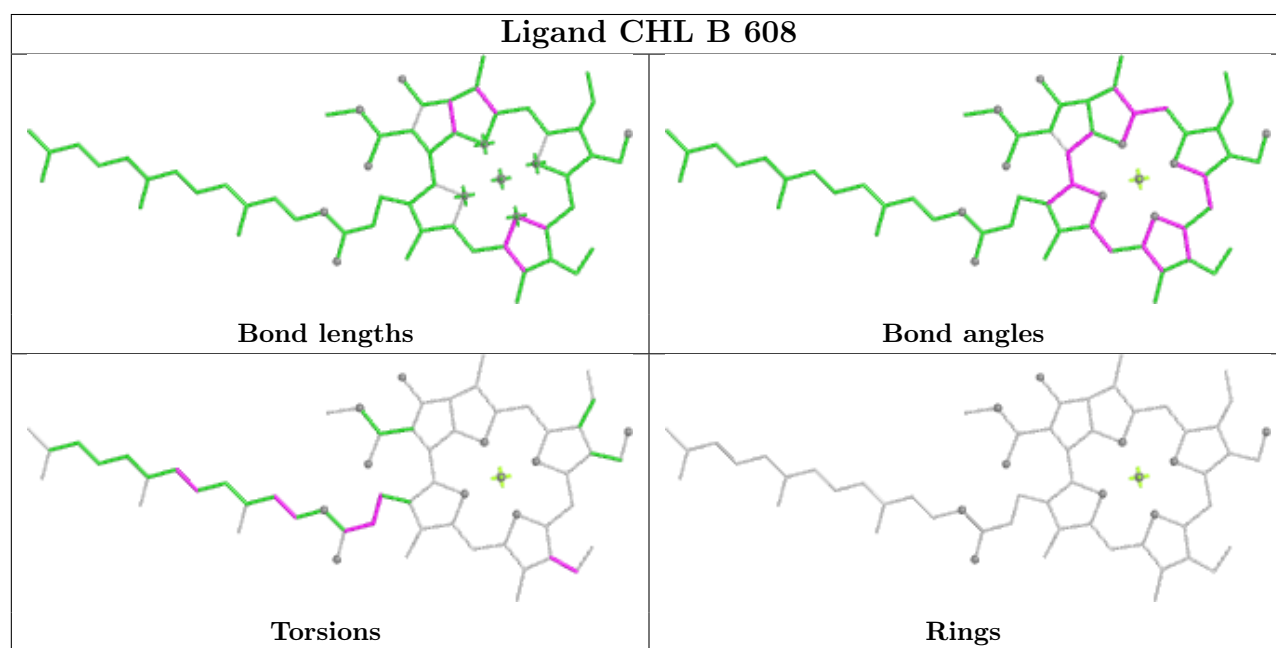
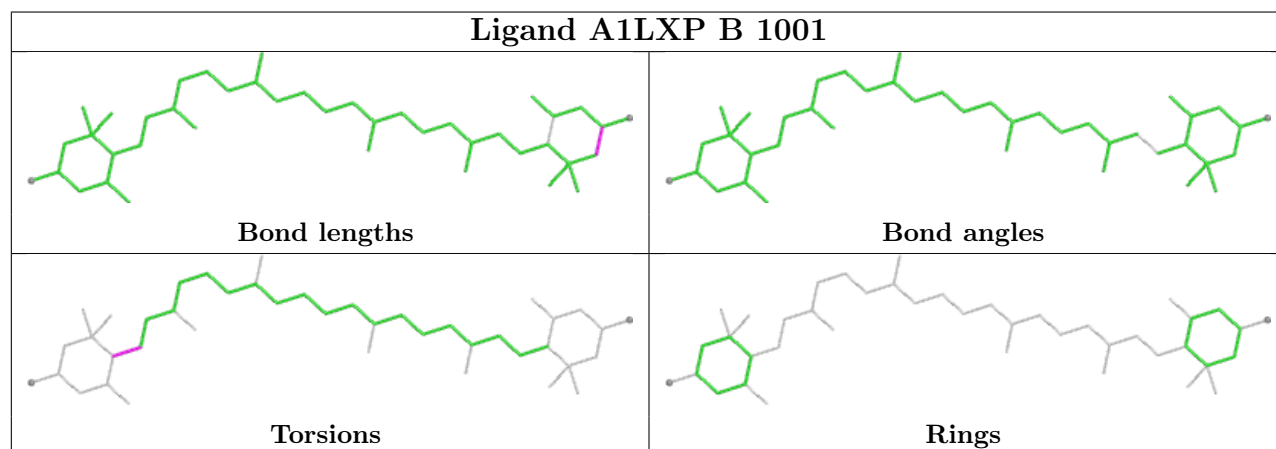
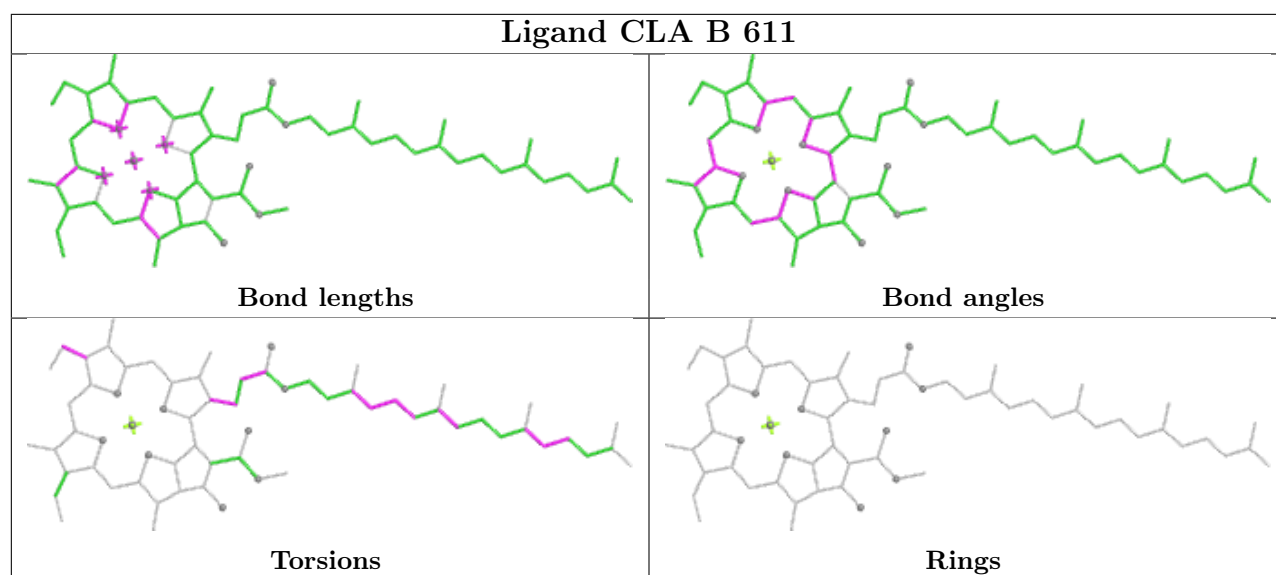
| Mol | Chain | Res  | Type  | Clashes | Symm-Clashes |
|-----|-------|------|-------|---------|--------------|
| 2   | B     | 608  | CHL   | 1       | 0            |
| 2   | B     | 607  | CHL   | 1       | 0            |
| 7   | B     | 1004 | XAT   | 2       | 0            |
| 2   | B     | 601  | CHL   | 3       | 0            |
| 2   | A     | 607  | CHL   | 1       | 0            |
| 2   | A     | 606  | CHL   | 1       | 0            |
| 3   | A     | 604  | CLA   | 1       | 0            |
| 4   | A     | 1002 | A1LXP | 1       | 0            |
| 3   | B     | 604  | CLA   | 1       | 0            |
| 2   | A     | 608  | CHL   | 1       | 0            |
| 3   | B     | 612  | CLA   | 2       | 0            |
| 4   | B     | 1002 | A1LXP | 1       | 0            |
| 3   | A     | 602  | CLA   | 1       | 0            |
| 2   | C     | 608  | CHL   | 1       | 0            |
| 3   | C     | 603  | CLA   | 4       | 0            |
| 2   | C     | 607  | CHL   | 1       | 0            |
| 3   | C     | 604  | CLA   | 1       | 0            |

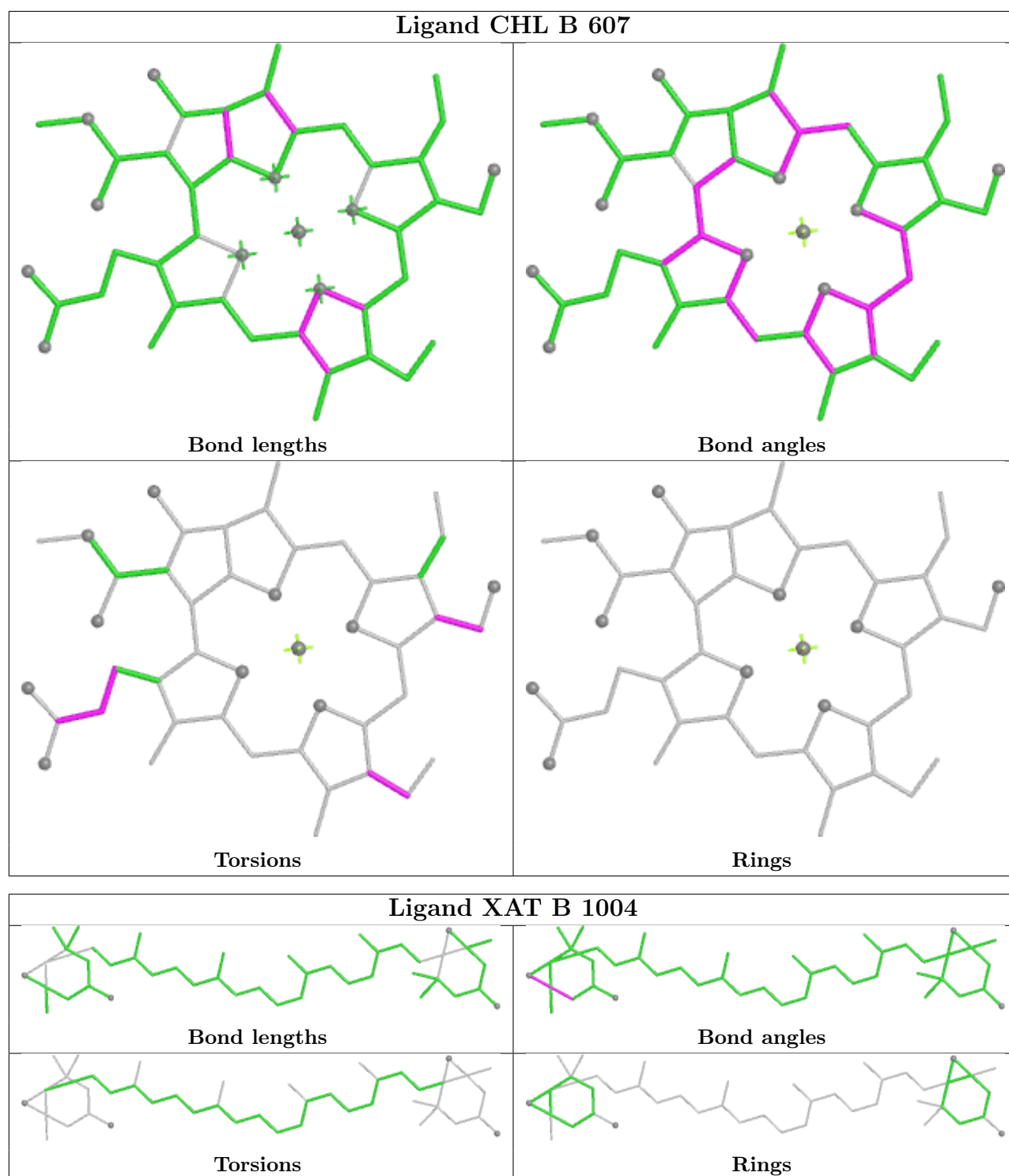
*Continued on next page...*

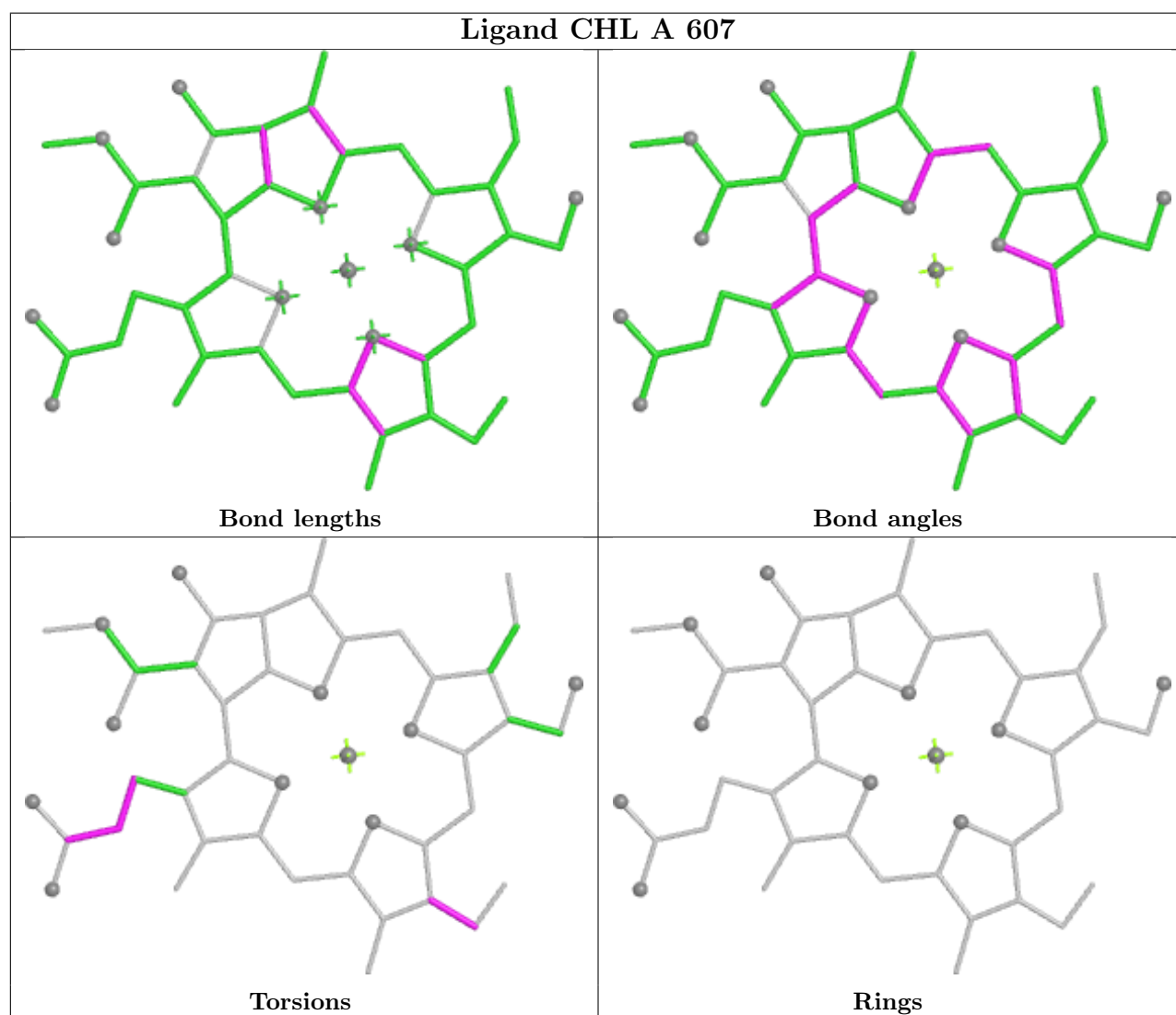
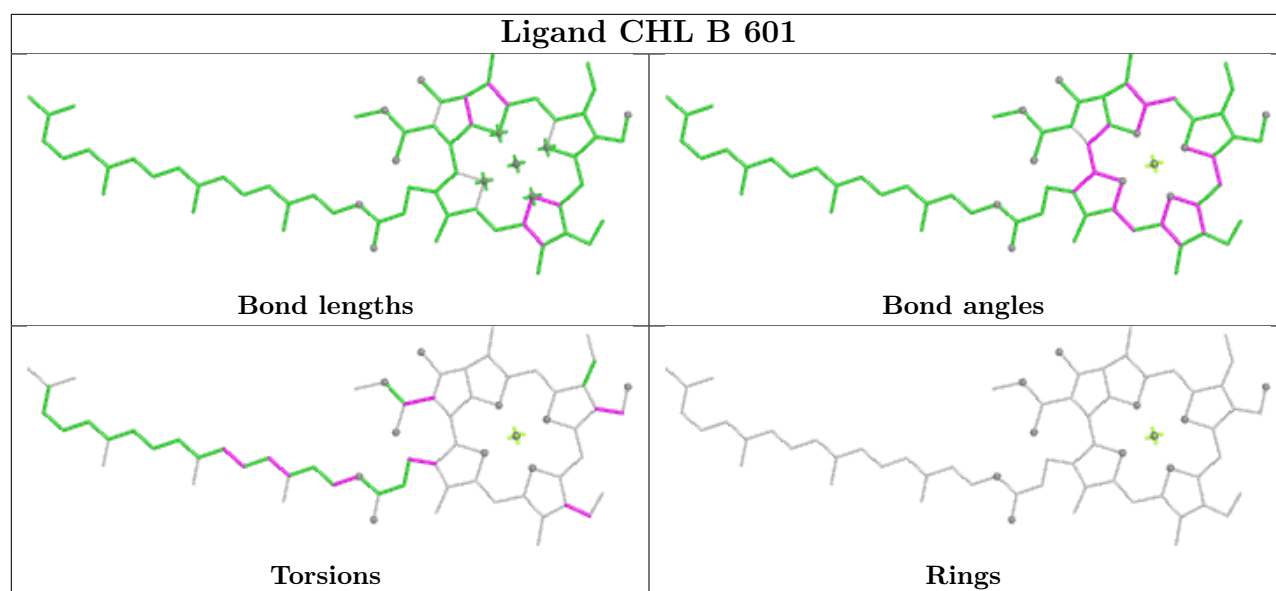
*Continued from previous page...*

| Mol | Chain | Res  | Type  | Clashes | Symm-Clashes |
|-----|-------|------|-------|---------|--------------|
| 7   | C     | 1004 | XAT   | 1       | 0            |
| 2   | B     | 609  | CHL   | 2       | 0            |
| 2   | C     | 606  | CHL   | 1       | 0            |
| 3   | A     | 612  | CLA   | 2       | 0            |
| 3   | B     | 610  | CLA   | 3       | 0            |
| 2   | C     | 601  | CHL   | 3       | 0            |
| 3   | B     | 603  | CLA   | 4       | 0            |
| 2   | A     | 609  | CHL   | 3       | 0            |
| 3   | B     | 613  | CLA   | 1       | 0            |
| 4   | C     | 1002 | A1LXP | 1       | 0            |
| 3   | C     | 612  | CLA   | 3       | 0            |
| 6   | B     | 1005 | LHG   | 4       | 0            |
| 2   | C     | 609  | CHL   | 2       | 0            |
| 2   | B     | 606  | CHL   | 1       | 0            |
| 3   | A     | 613  | CLA   | 2       | 0            |
| 3   | A     | 610  | CLA   | 2       | 0            |
| 6   | A     | 1005 | LHG   | 2       | 0            |
| 3   | A     | 603  | CLA   | 5       | 0            |
| 6   | C     | 1005 | LHG   | 6       | 0            |
| 3   | C     | 610  | CLA   | 3       | 0            |
| 3   | C     | 613  | CLA   | 1       | 0            |
| 7   | A     | 1004 | XAT   | 3       | 0            |
| 2   | A     | 601  | CHL   | 1       | 0            |

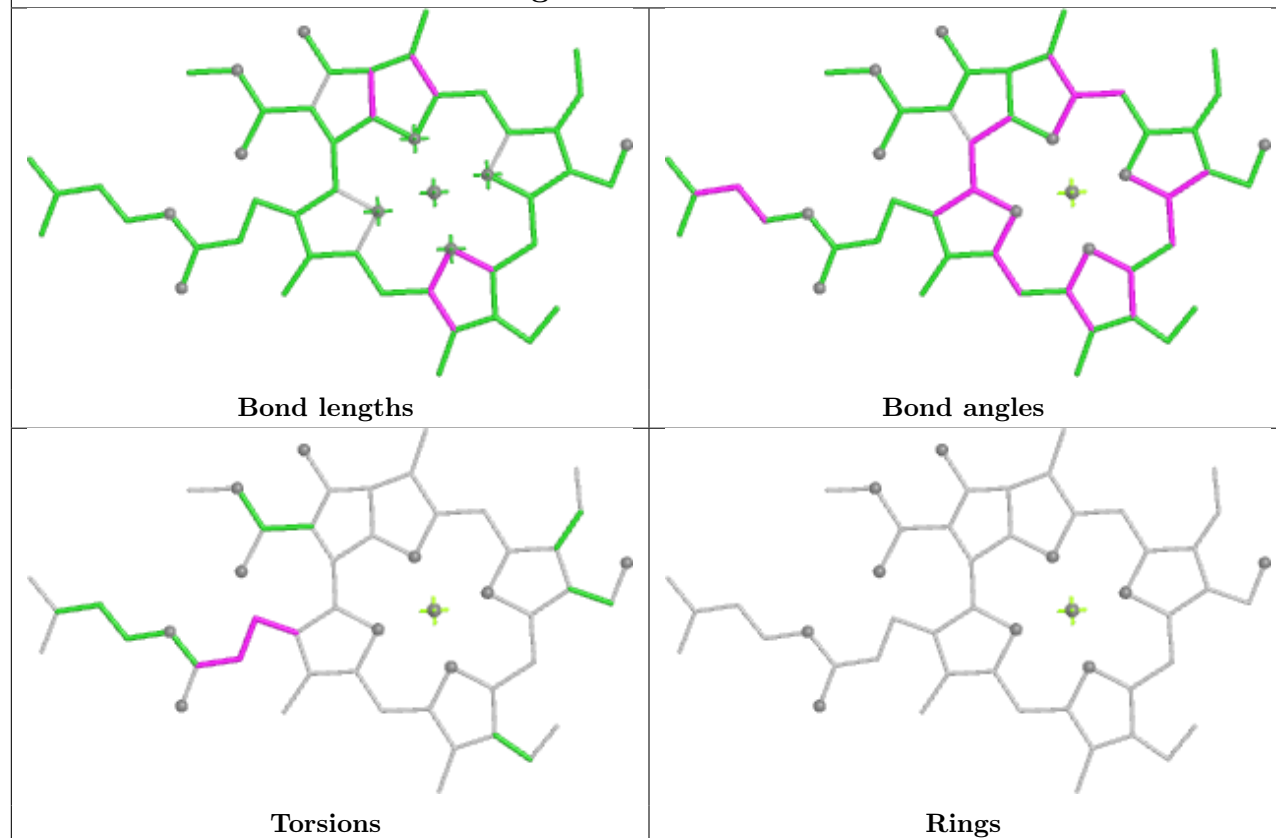
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



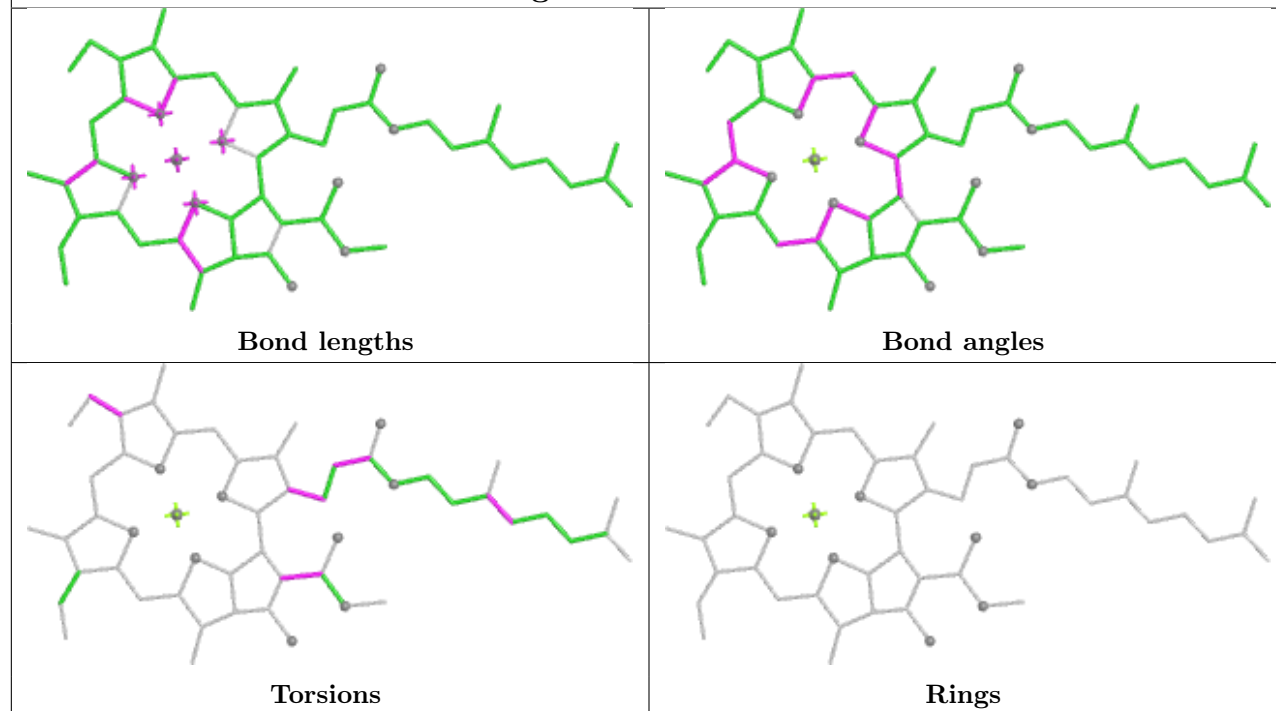


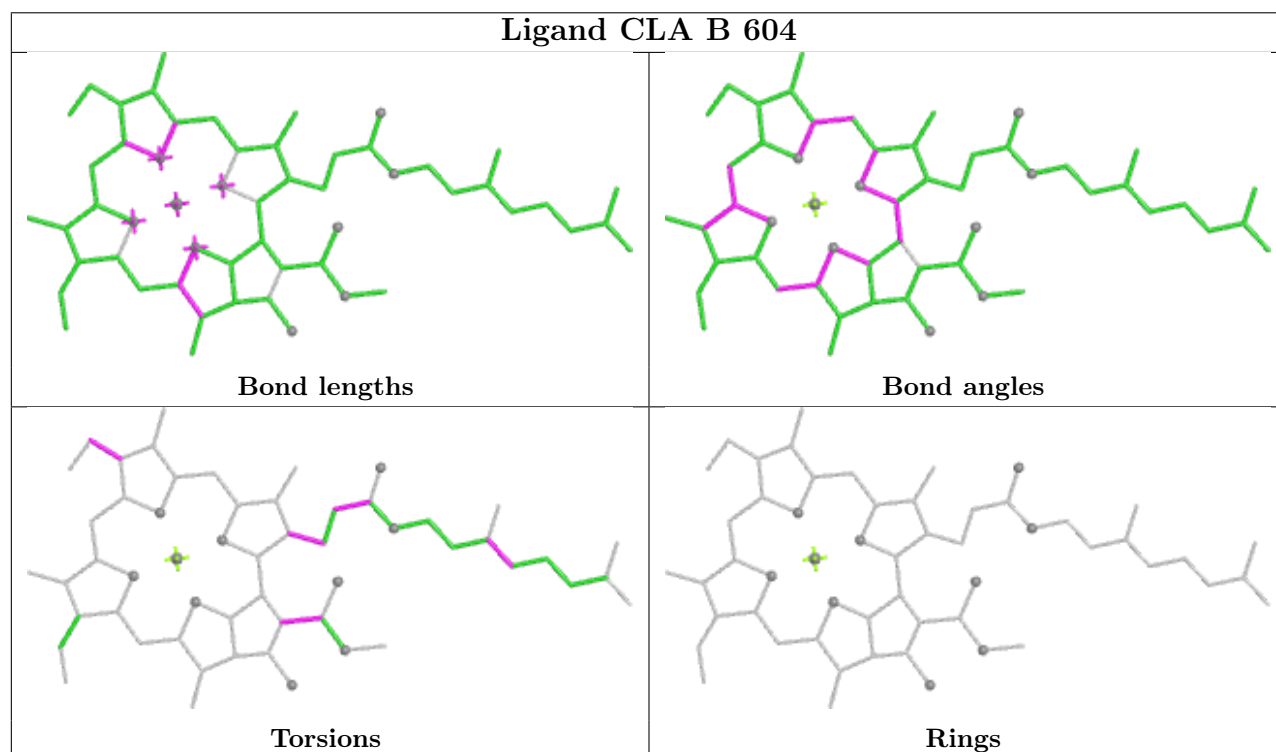
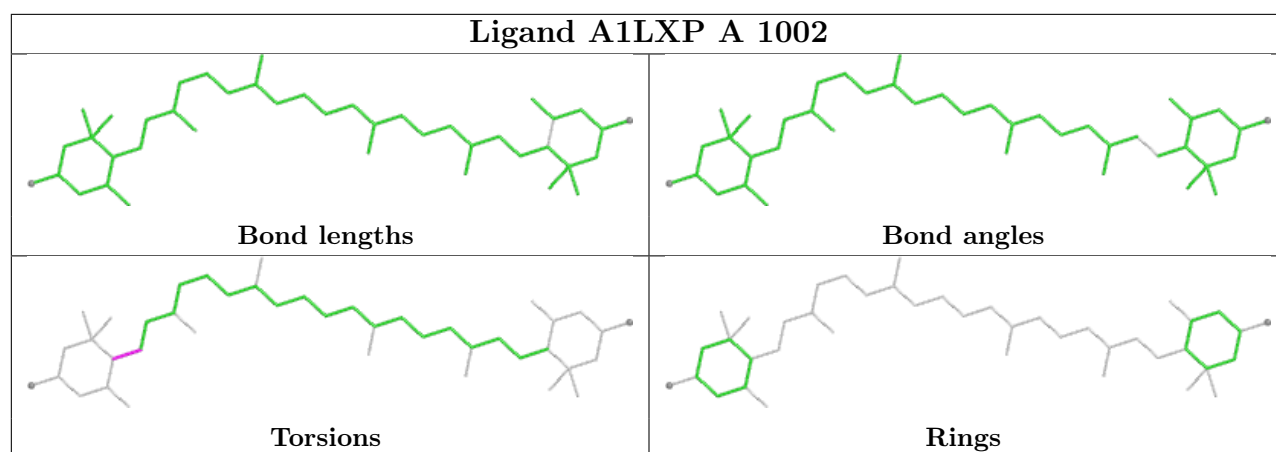


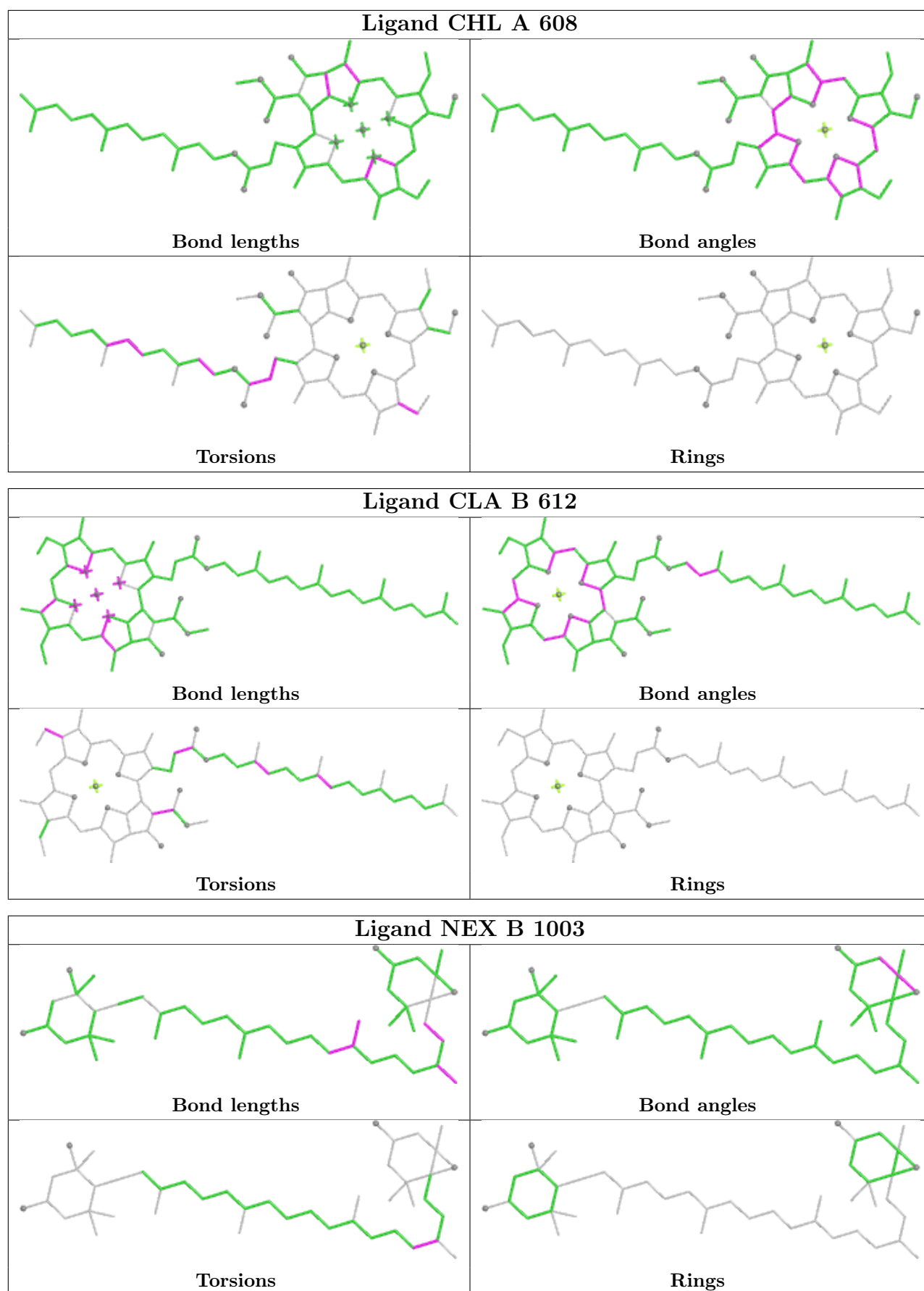
## Ligand CHL A 606

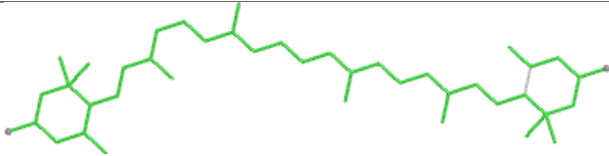
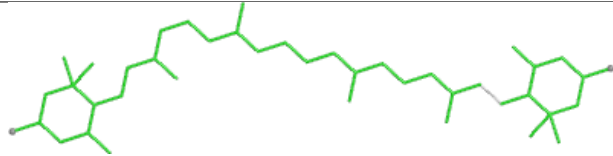
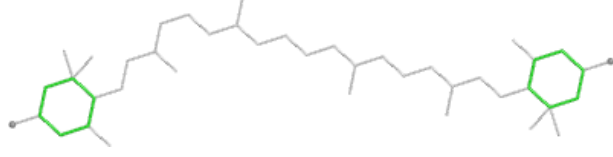
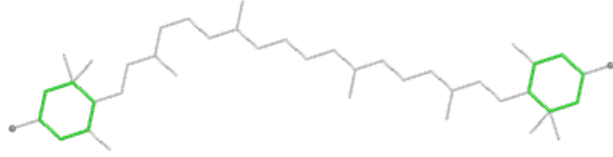
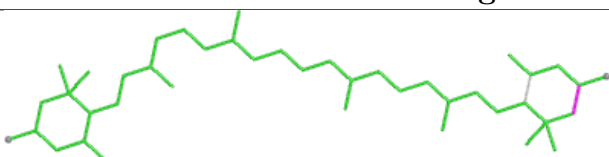
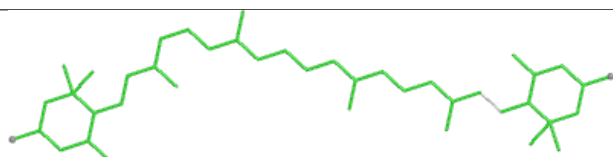
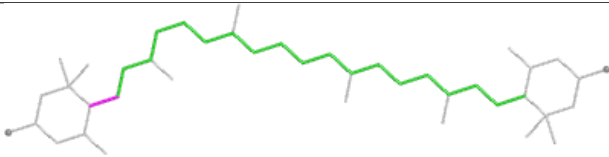
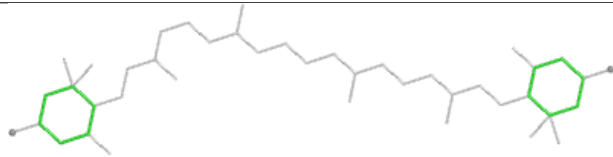


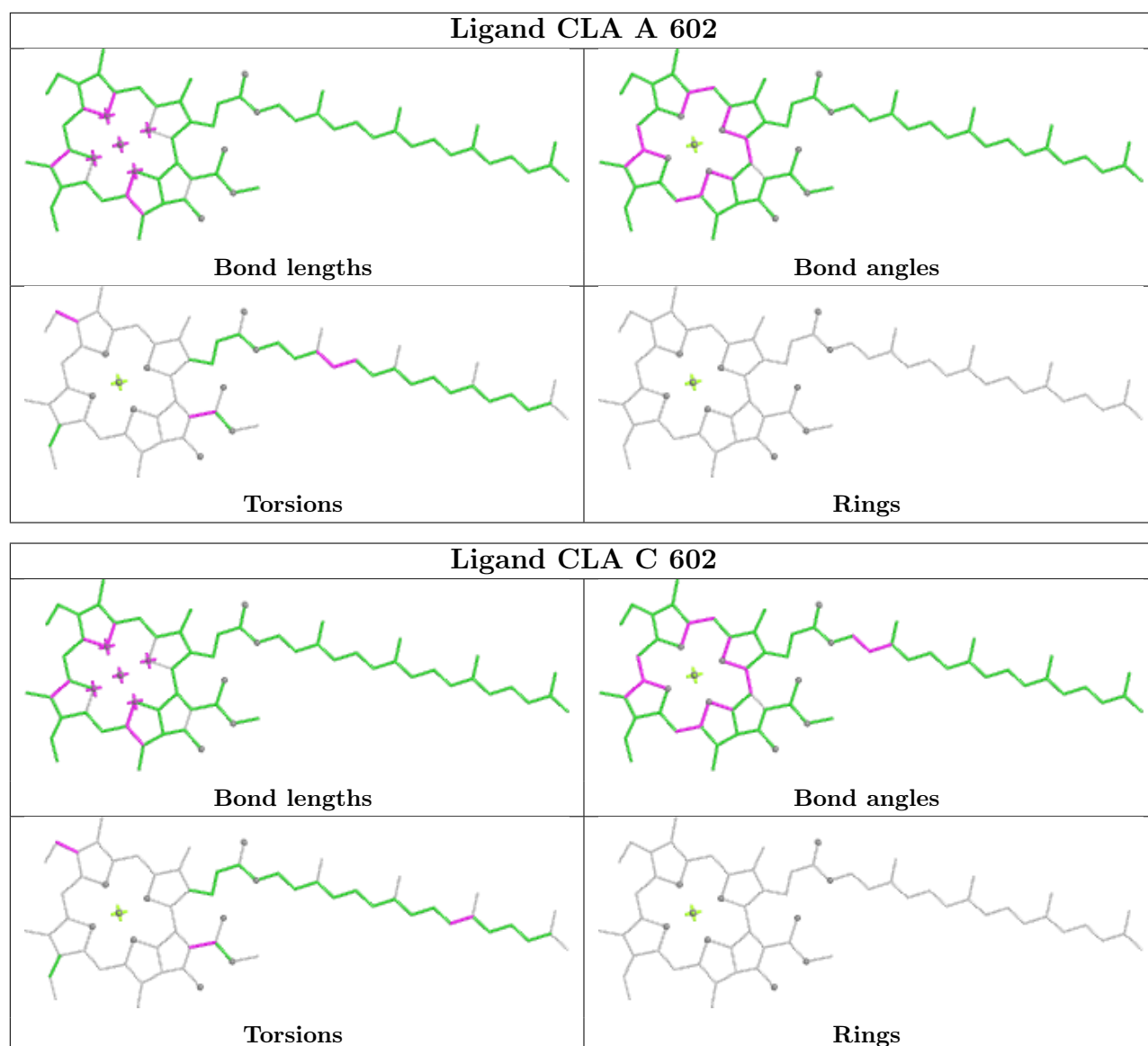
## Ligand CLA A 604

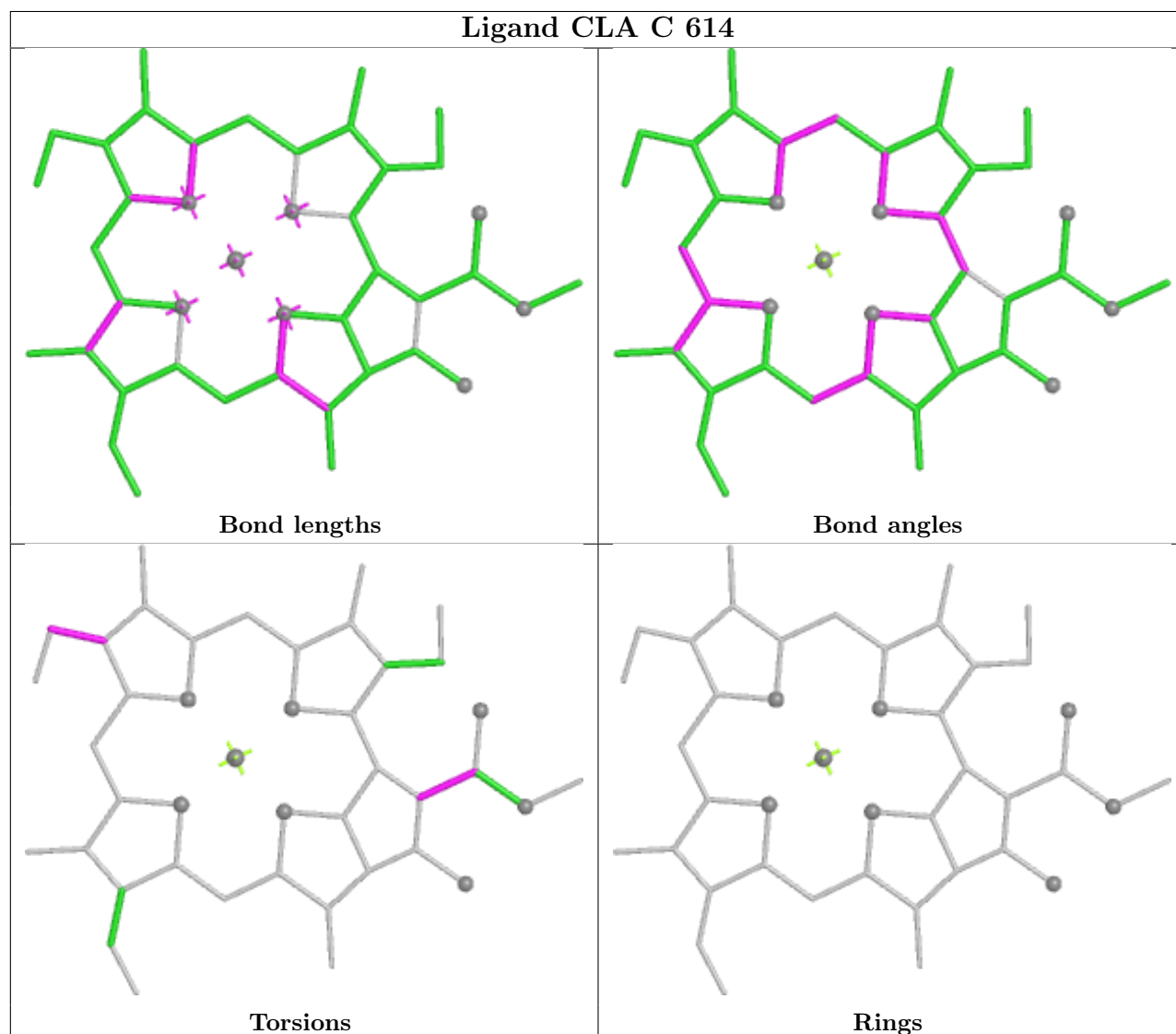
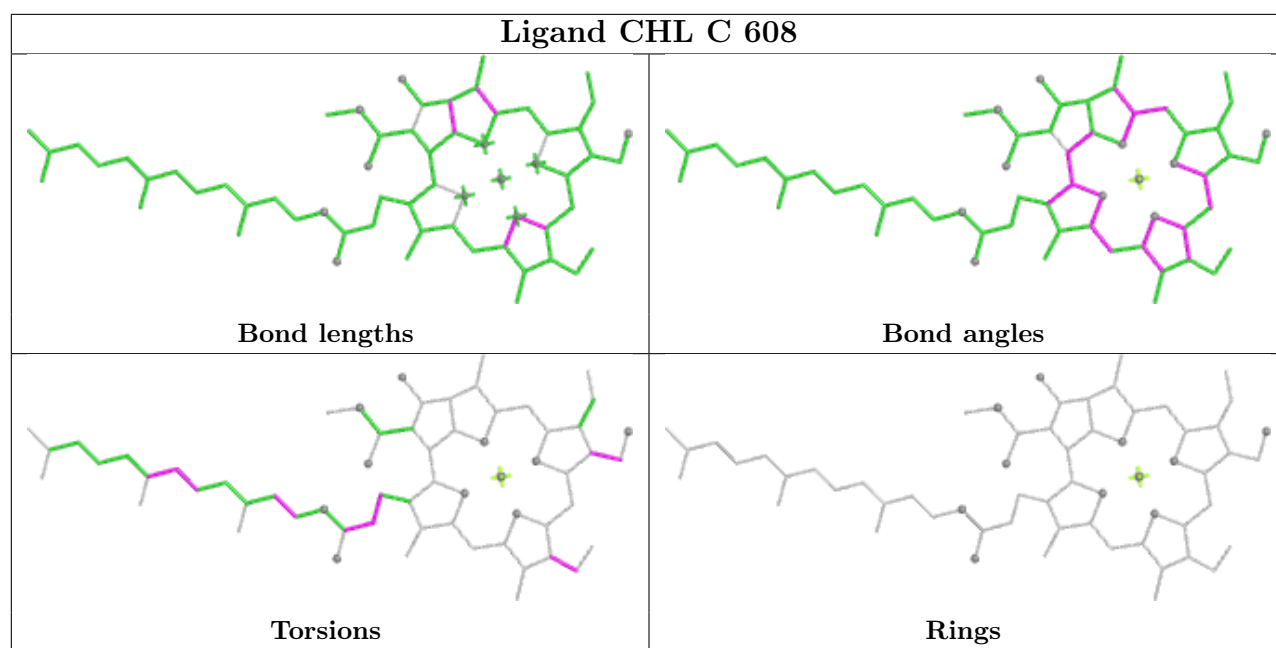


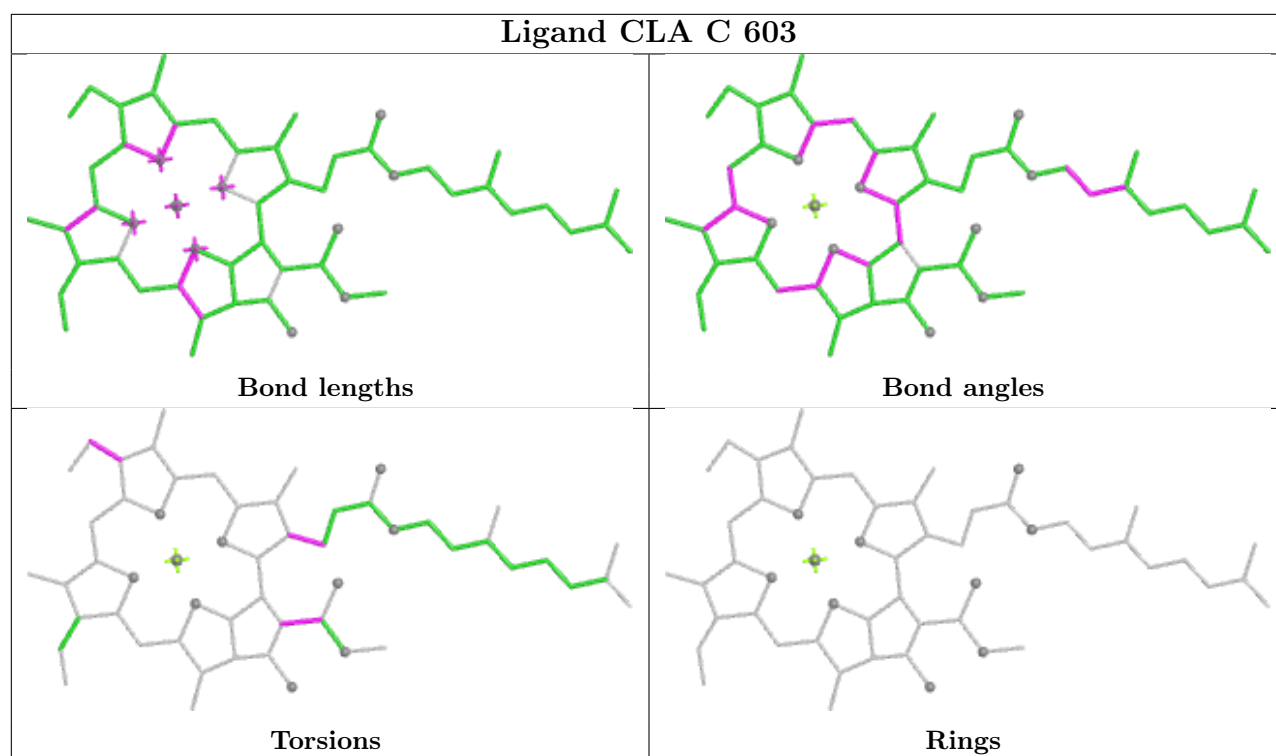


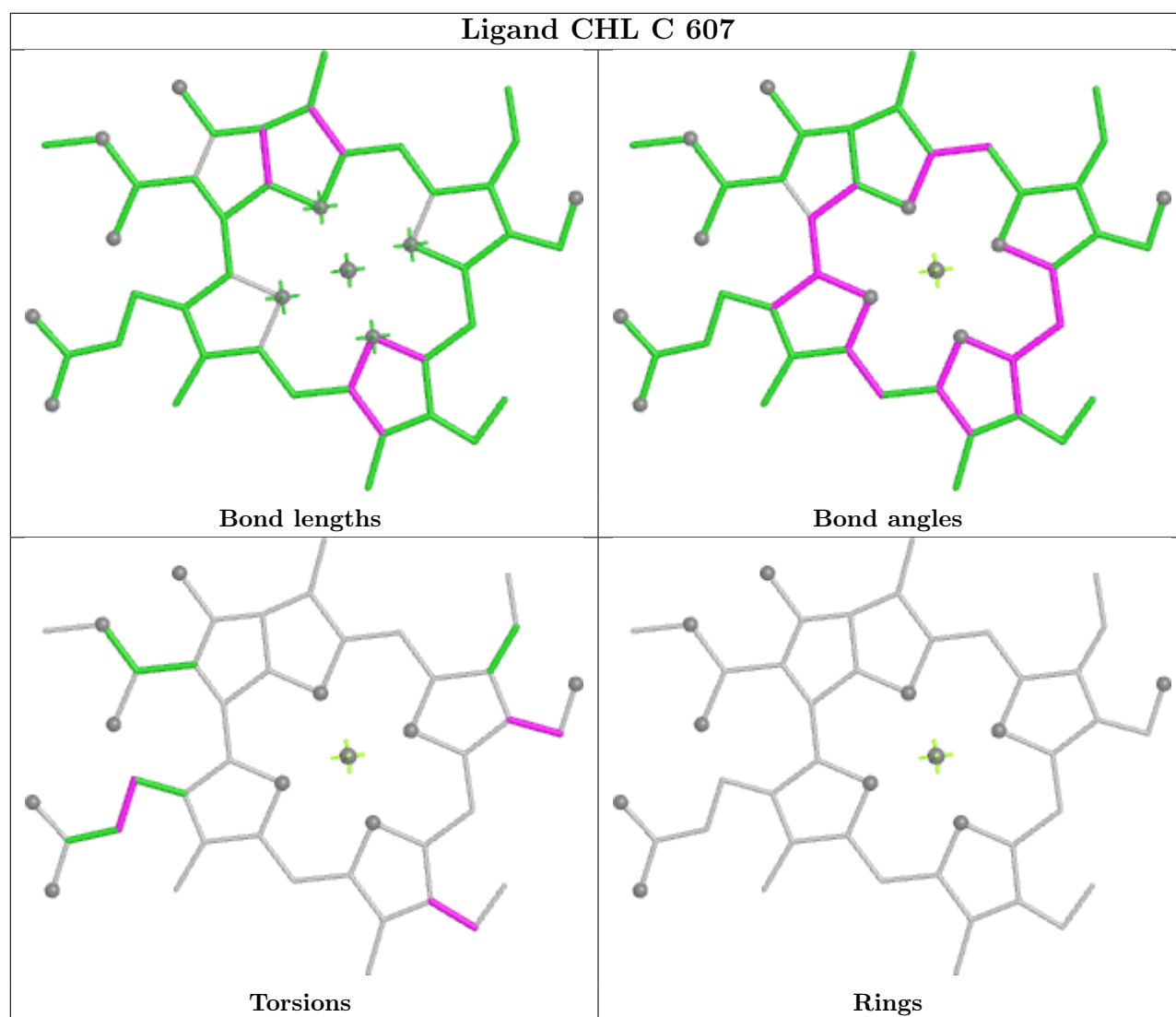


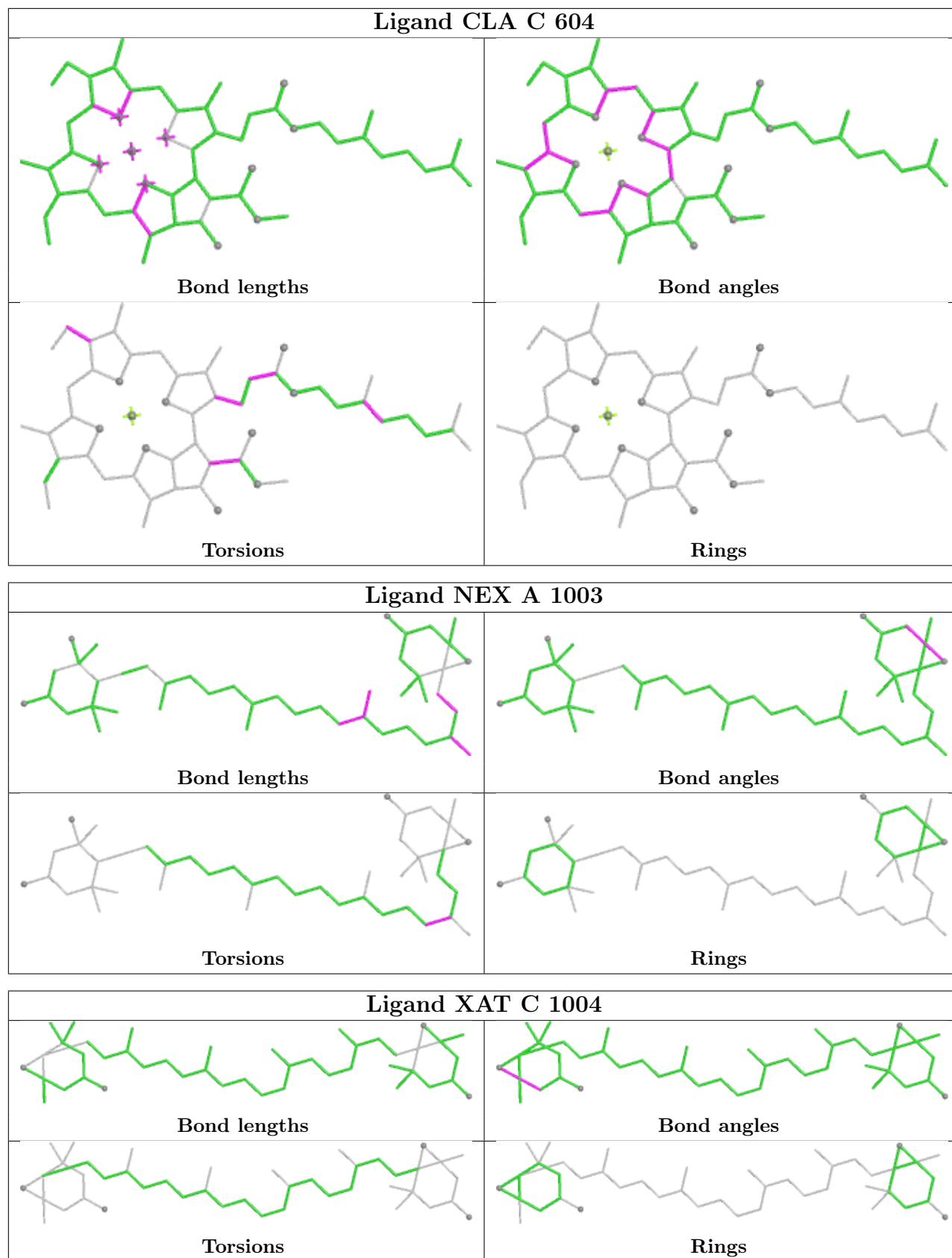
| Ligand A1LXP A 1001                                                                                     |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand A1LXP B 1002                                                                                     |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand A1LXP C 1001                                                                                     |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

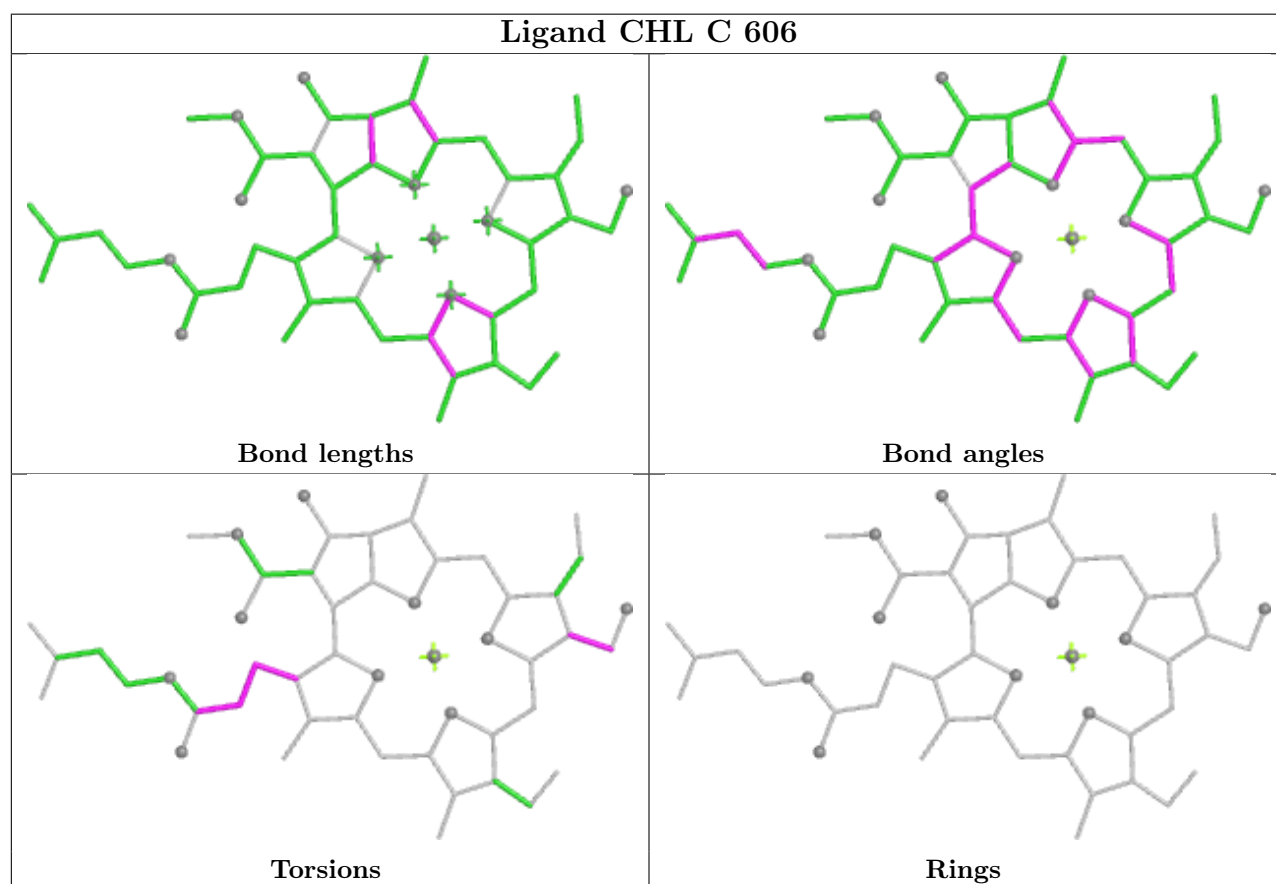
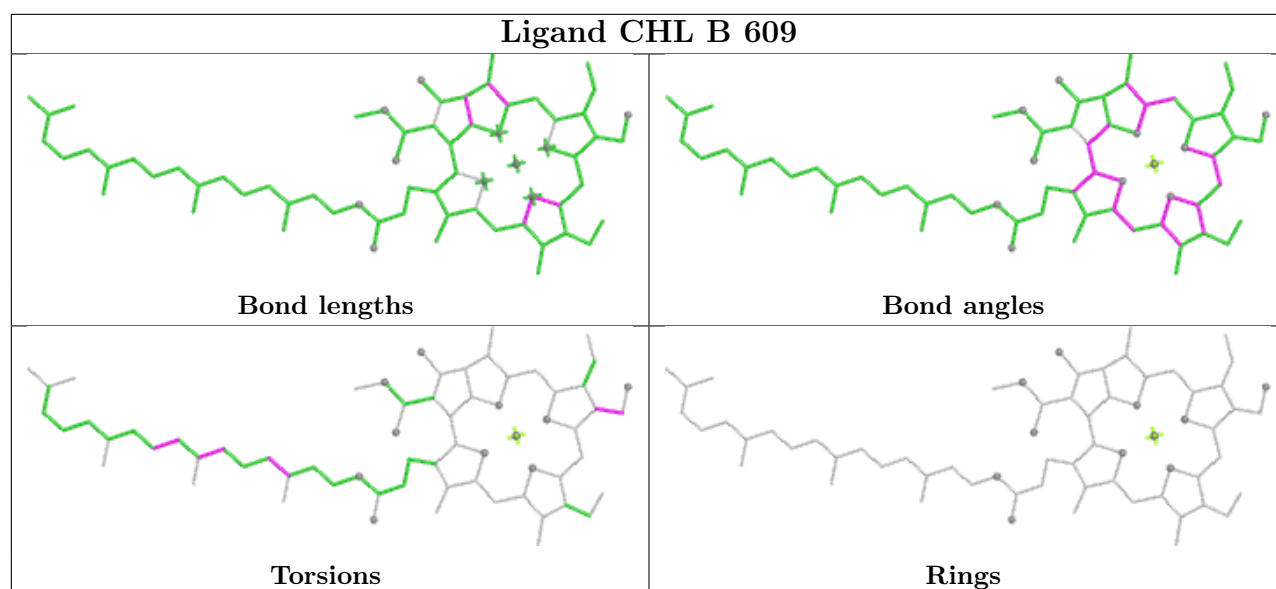


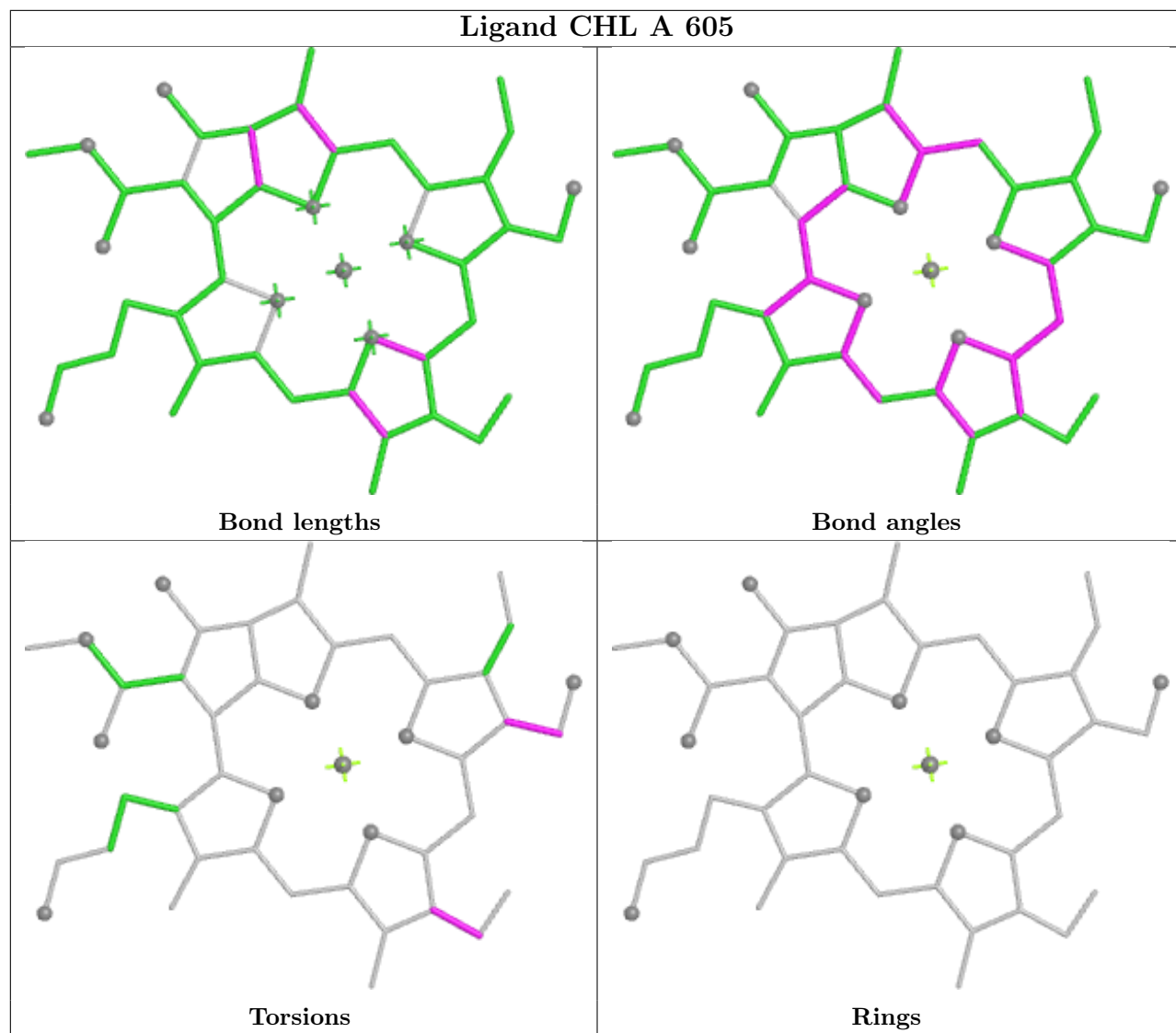


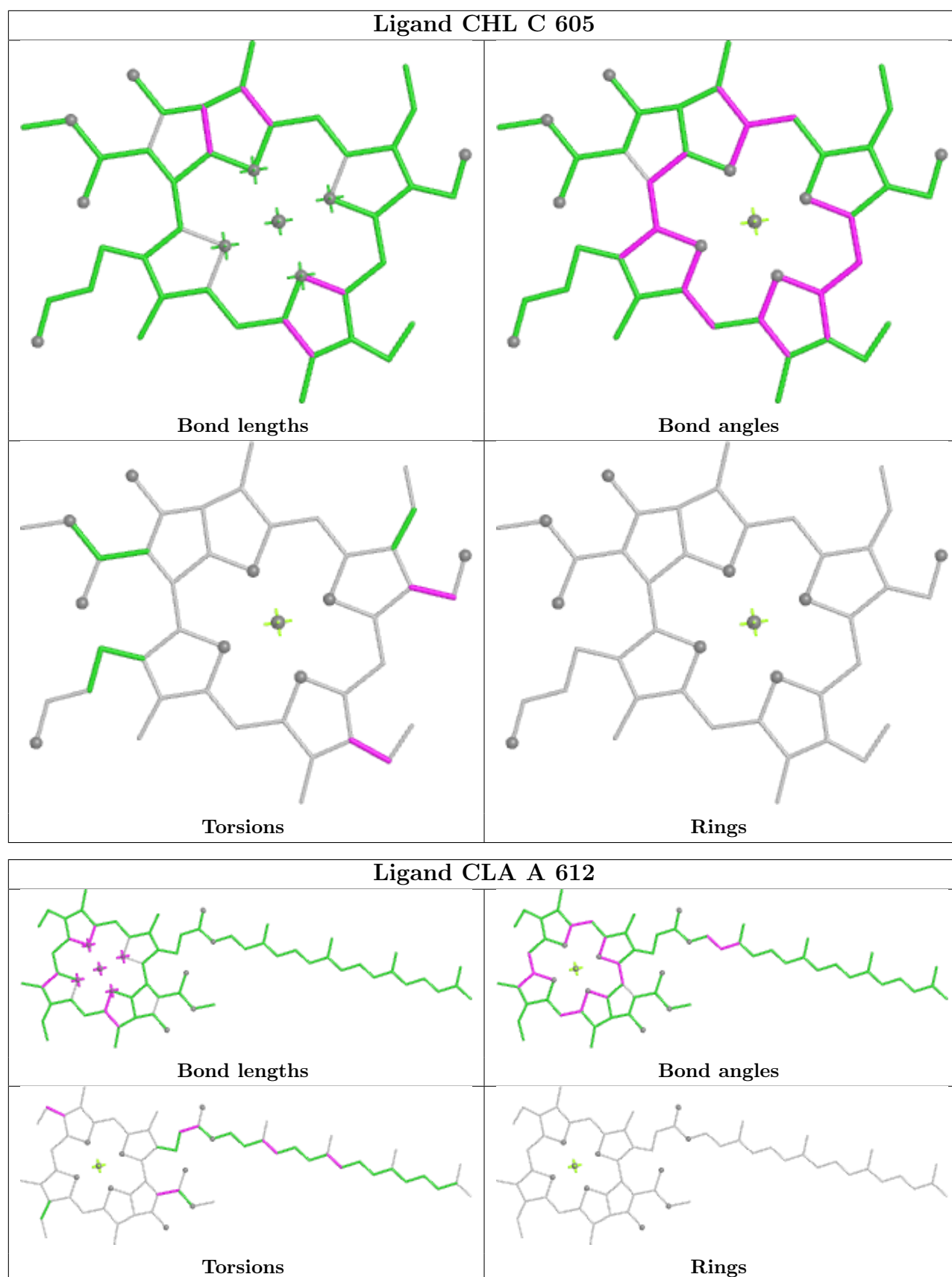


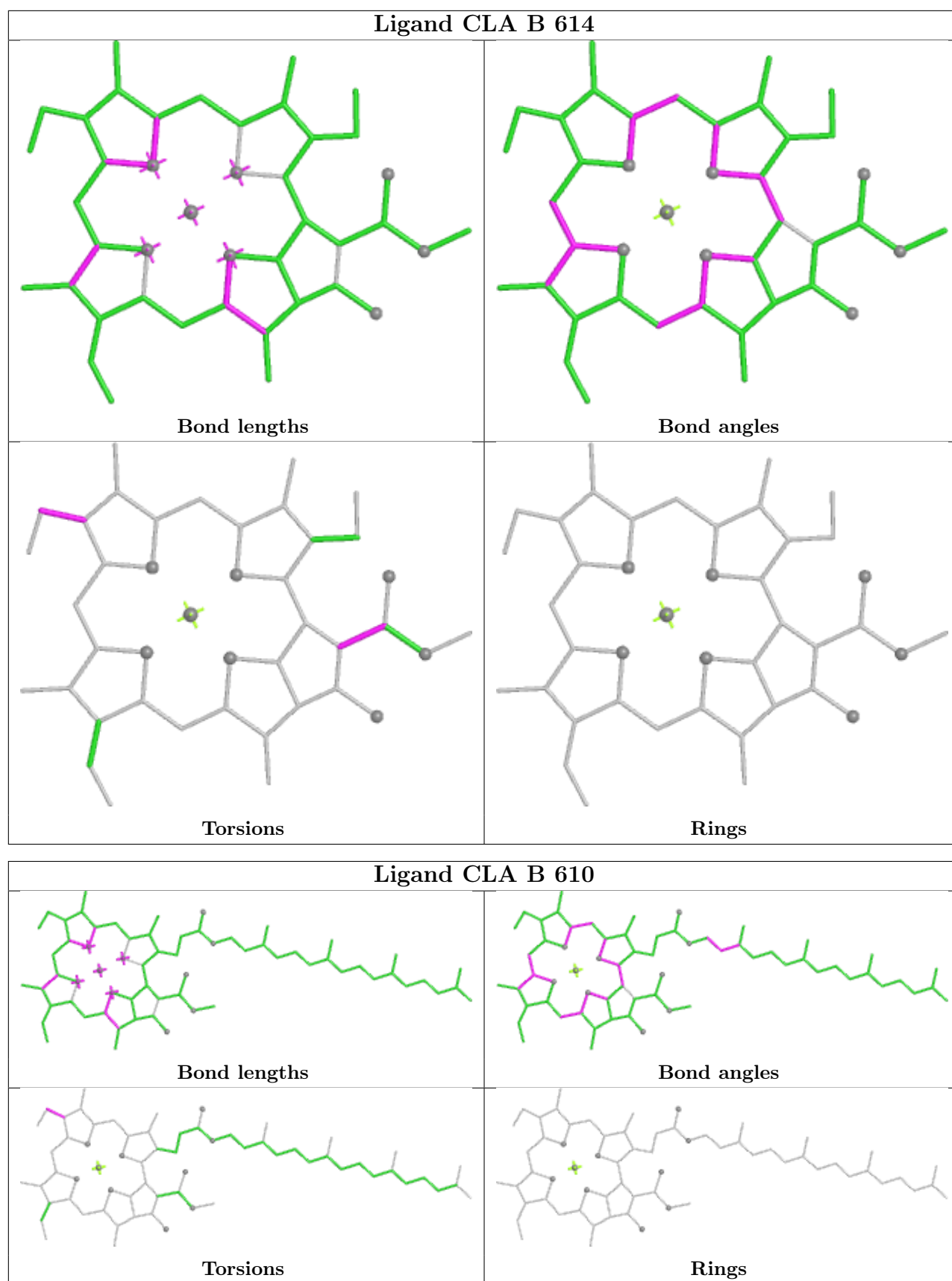


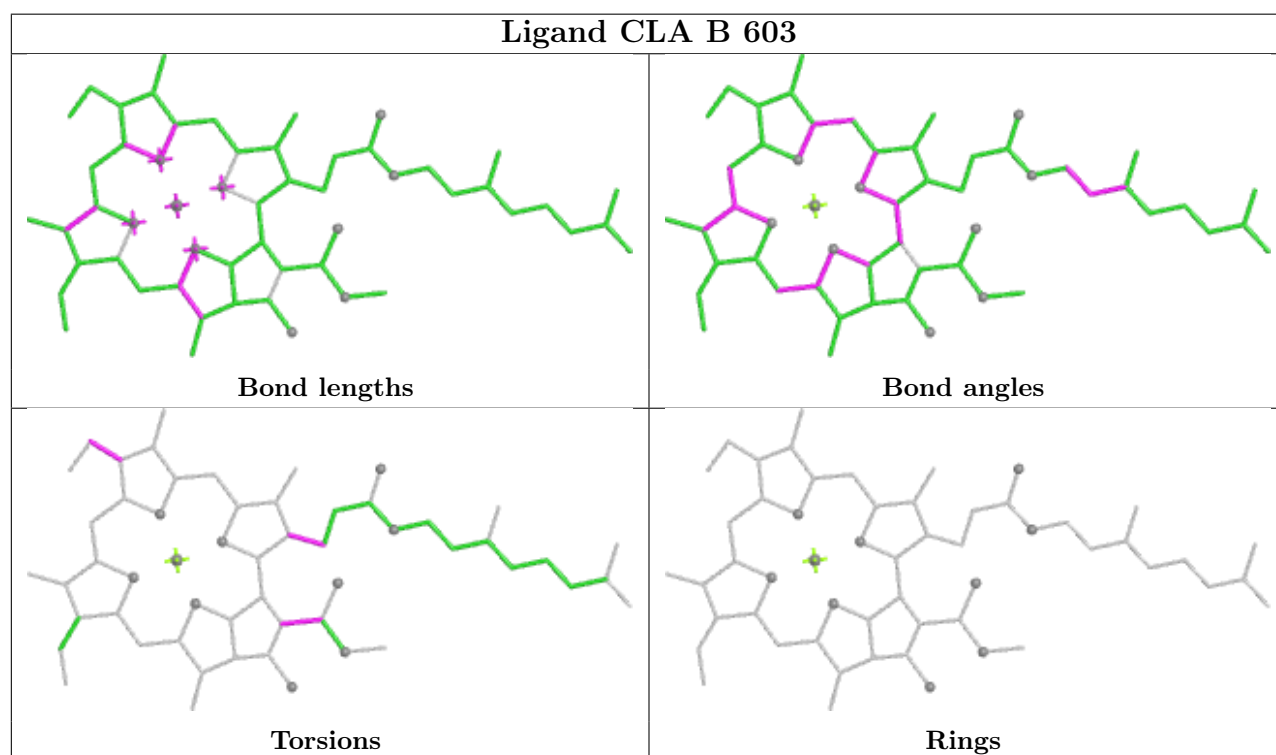
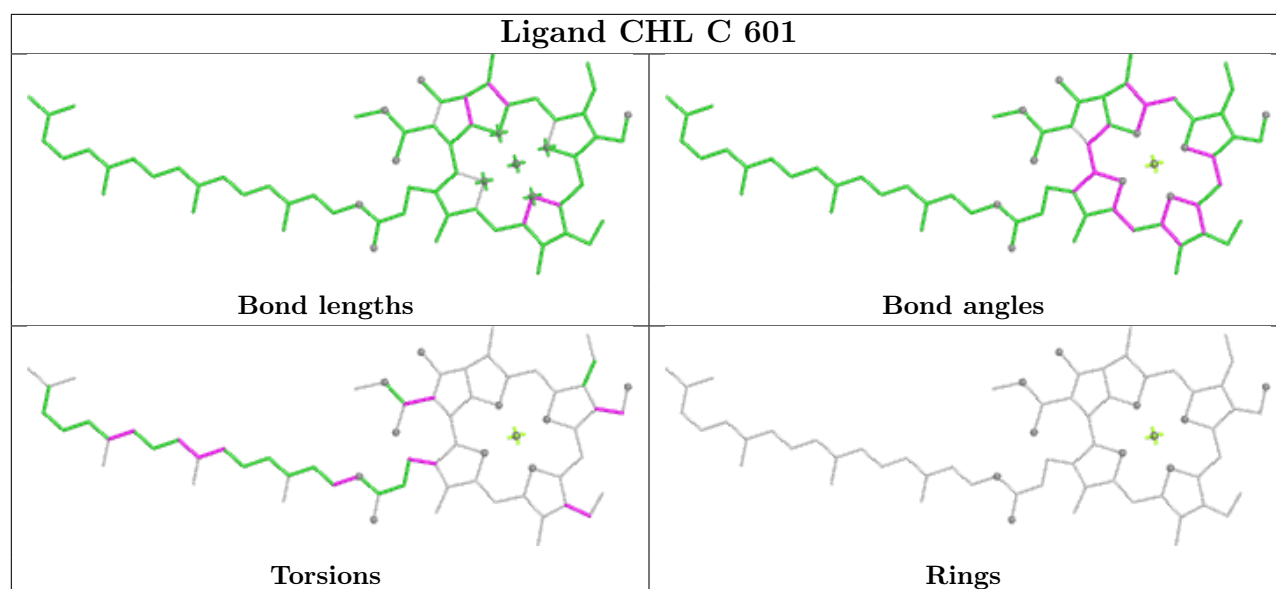


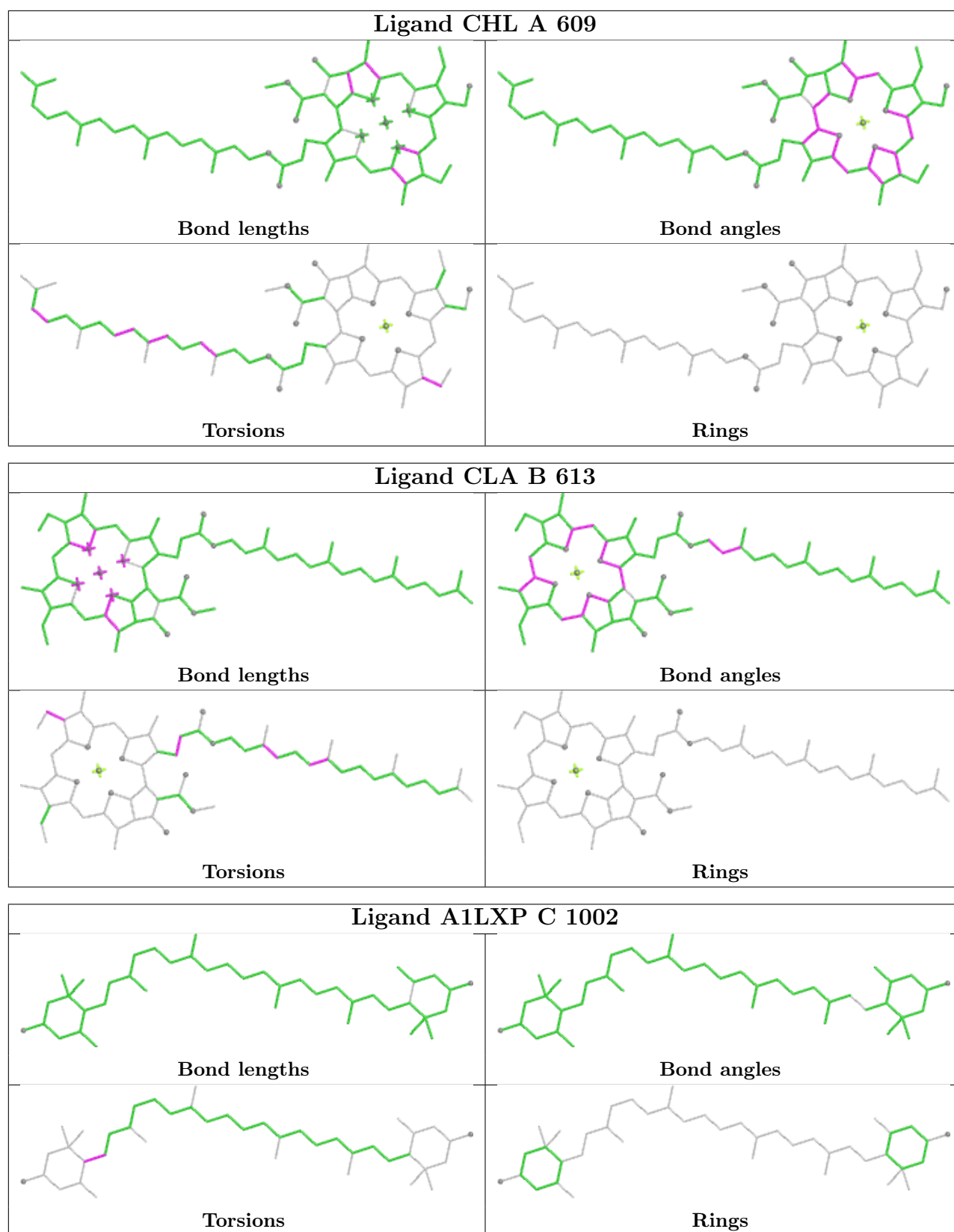


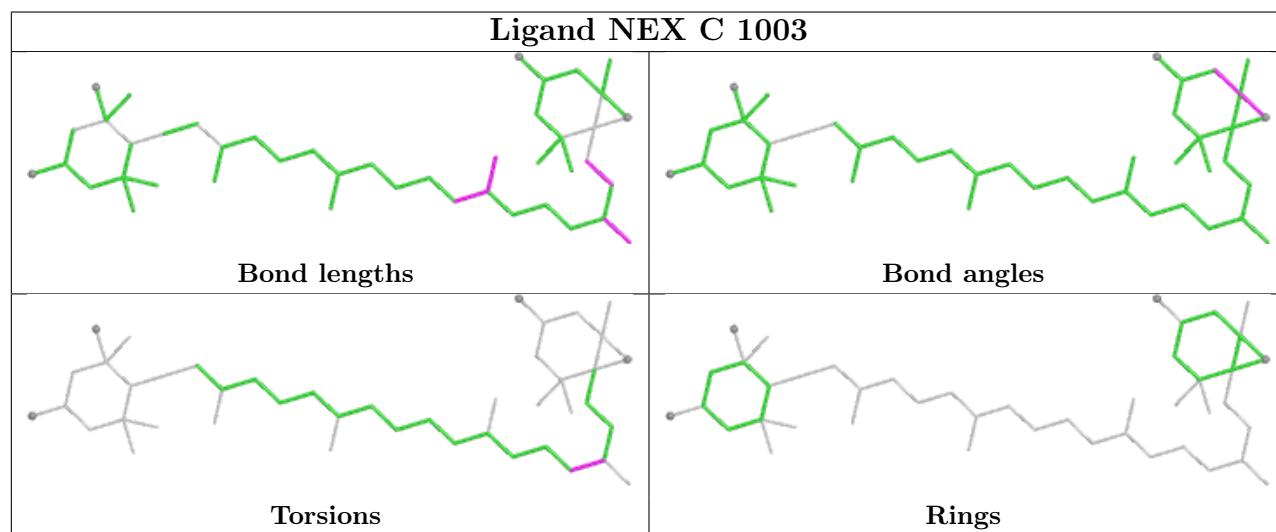
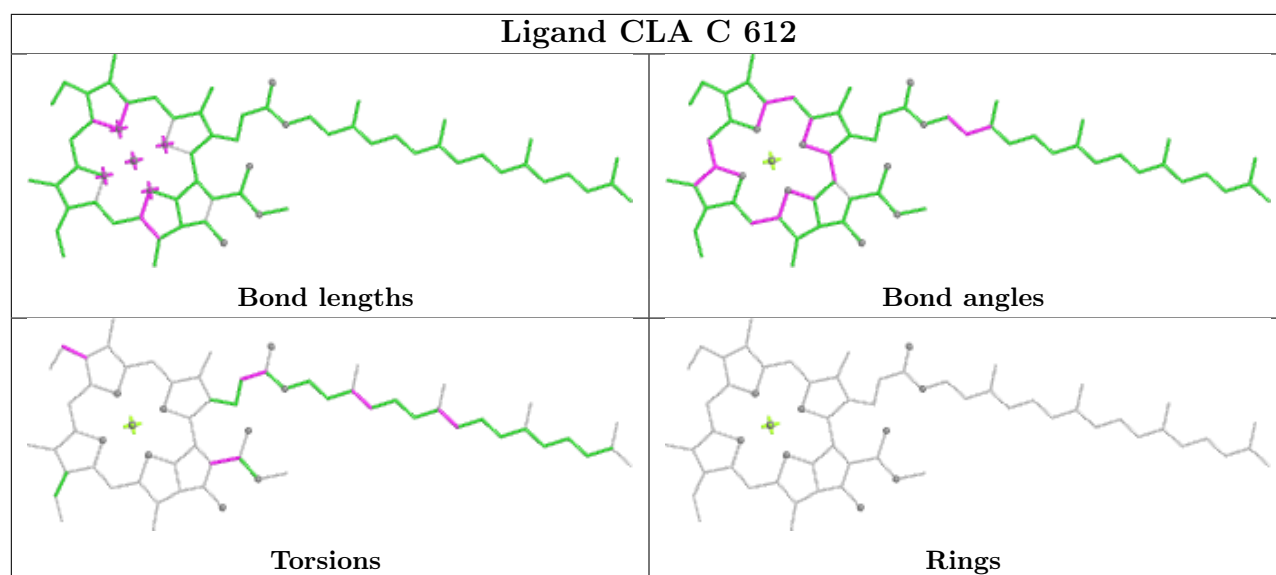


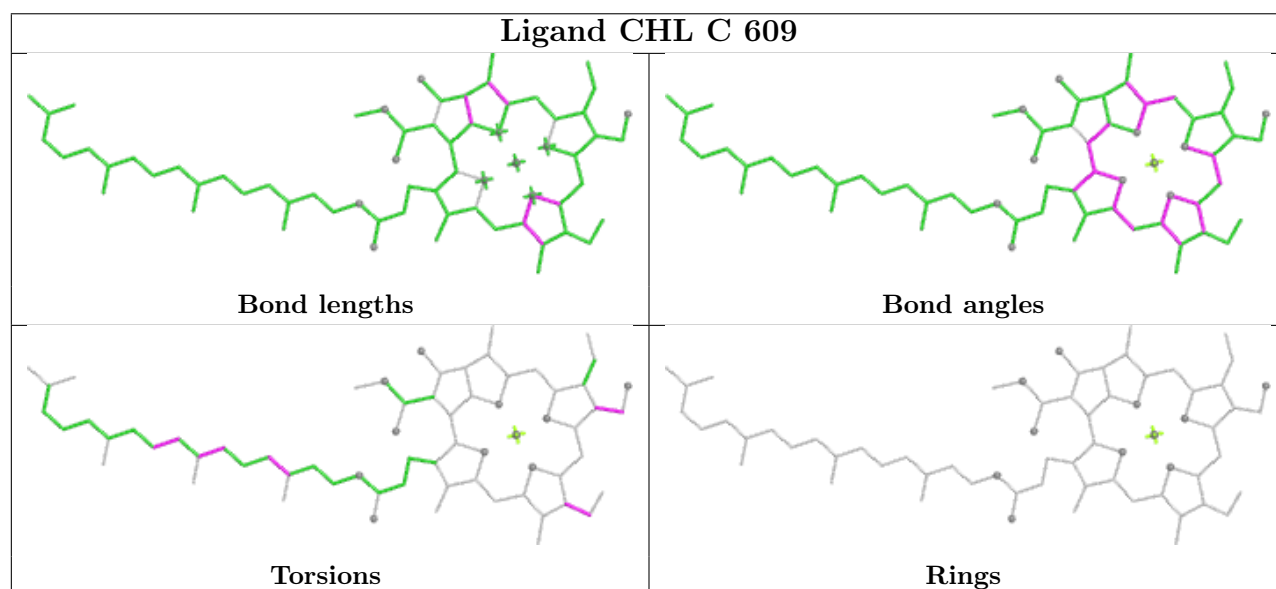
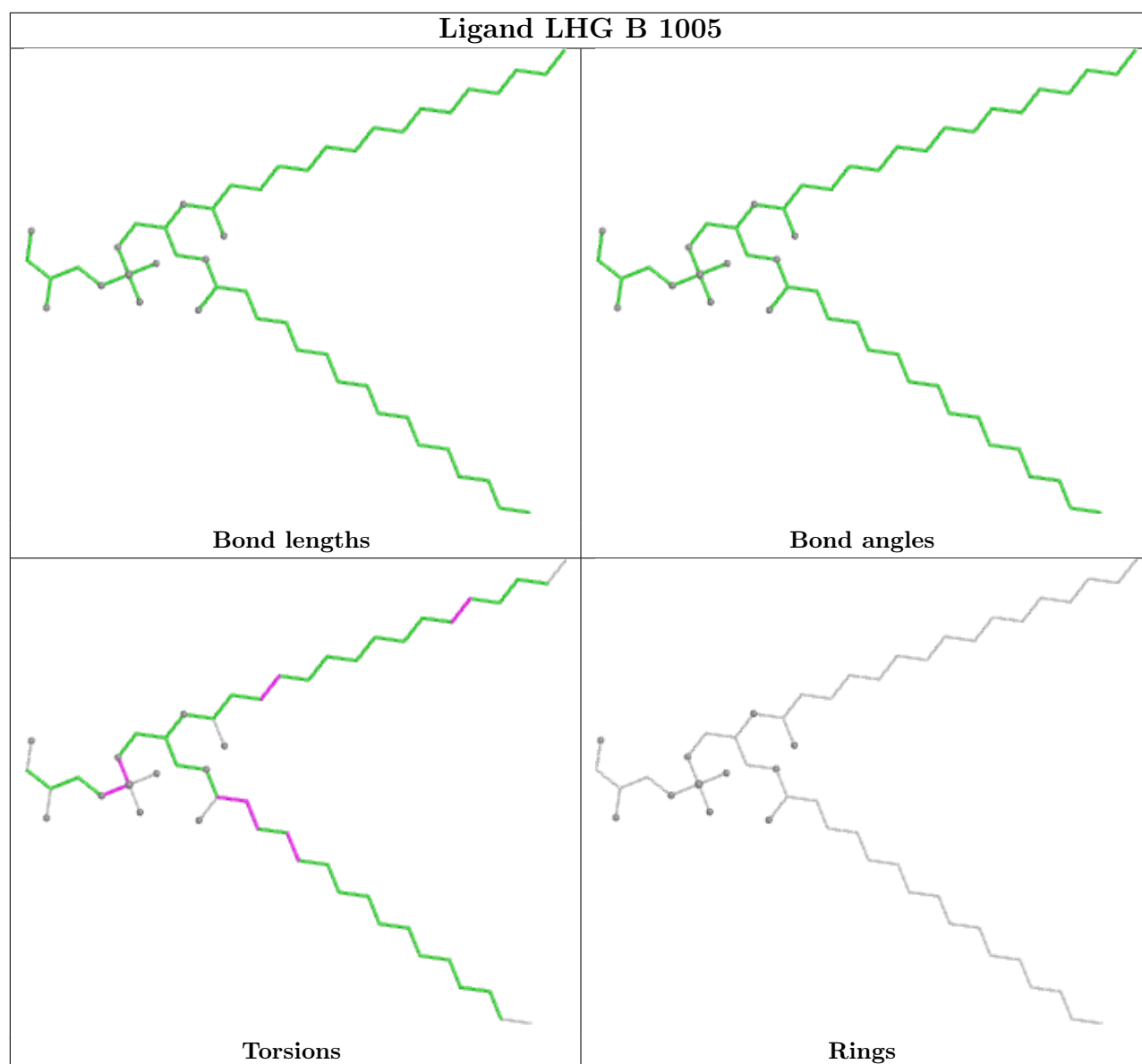


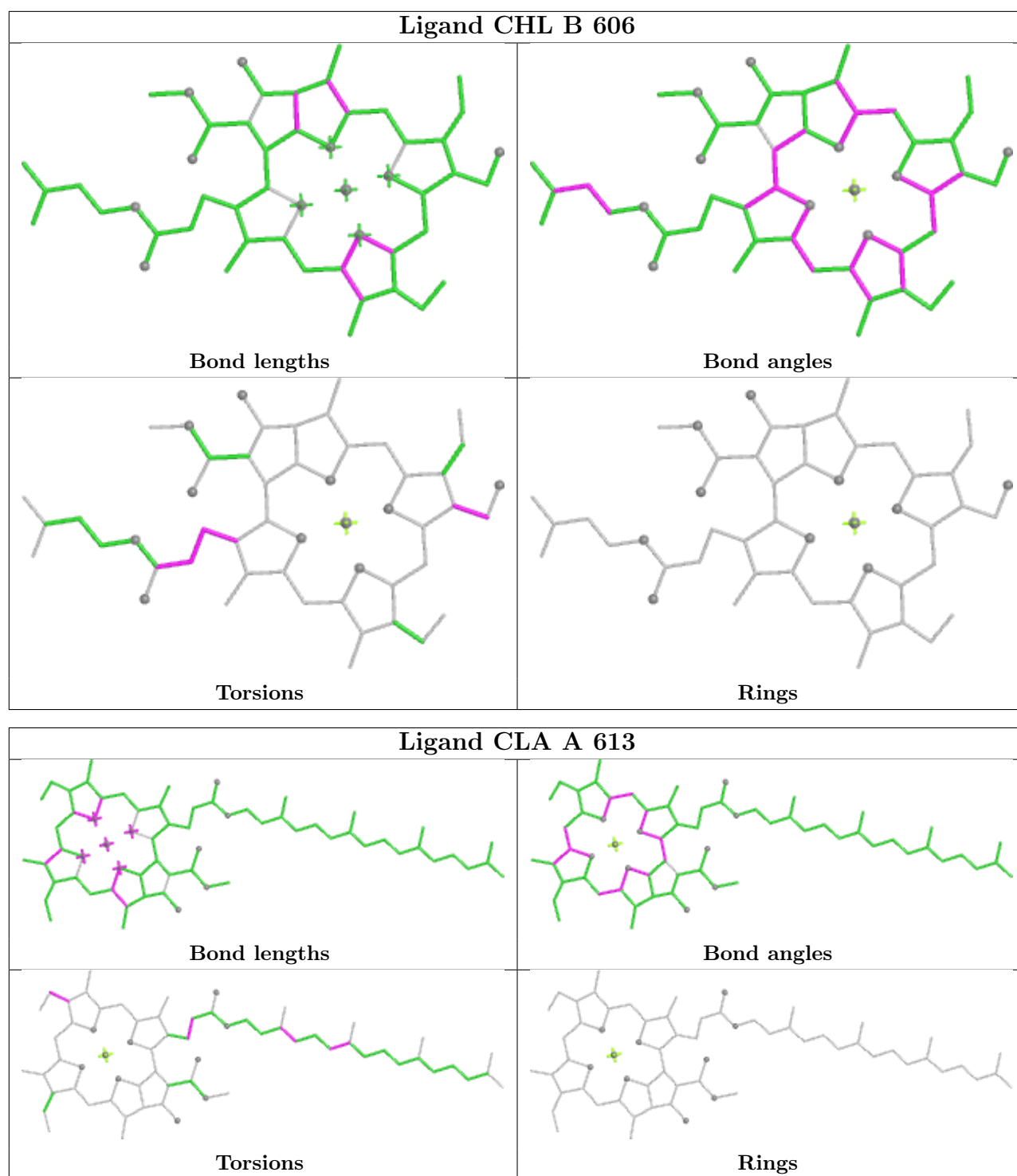


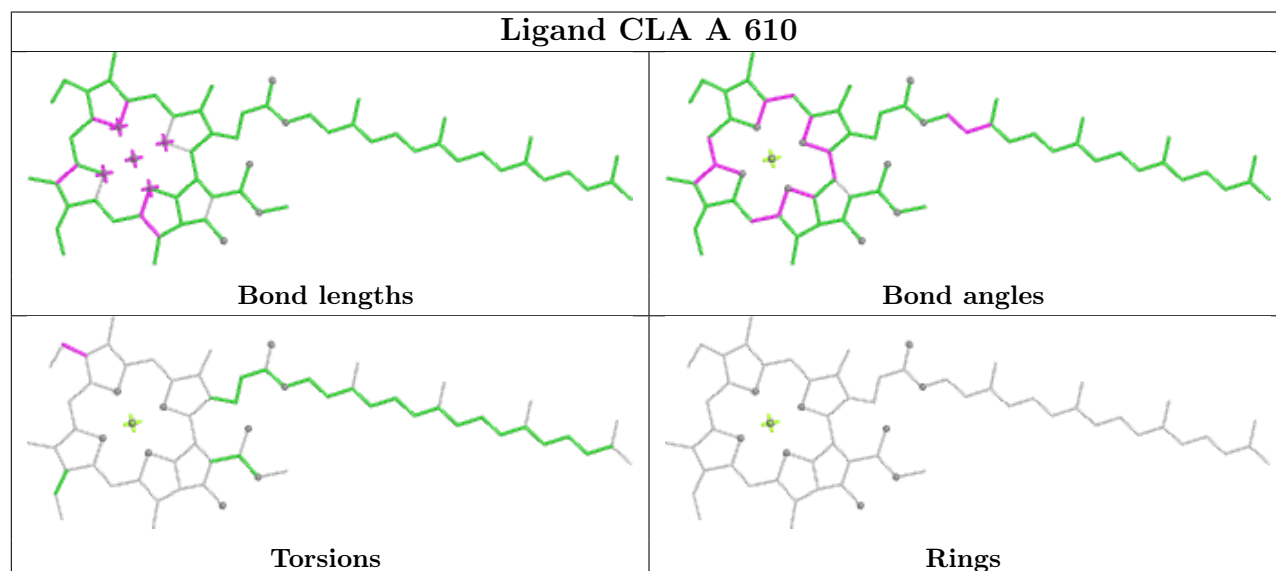
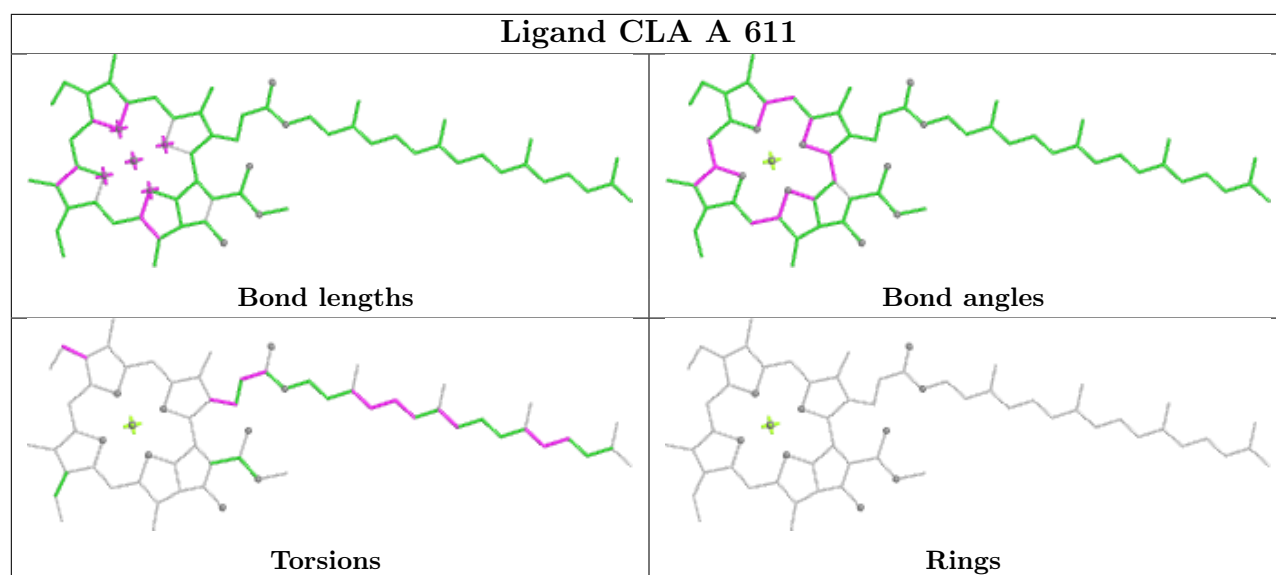


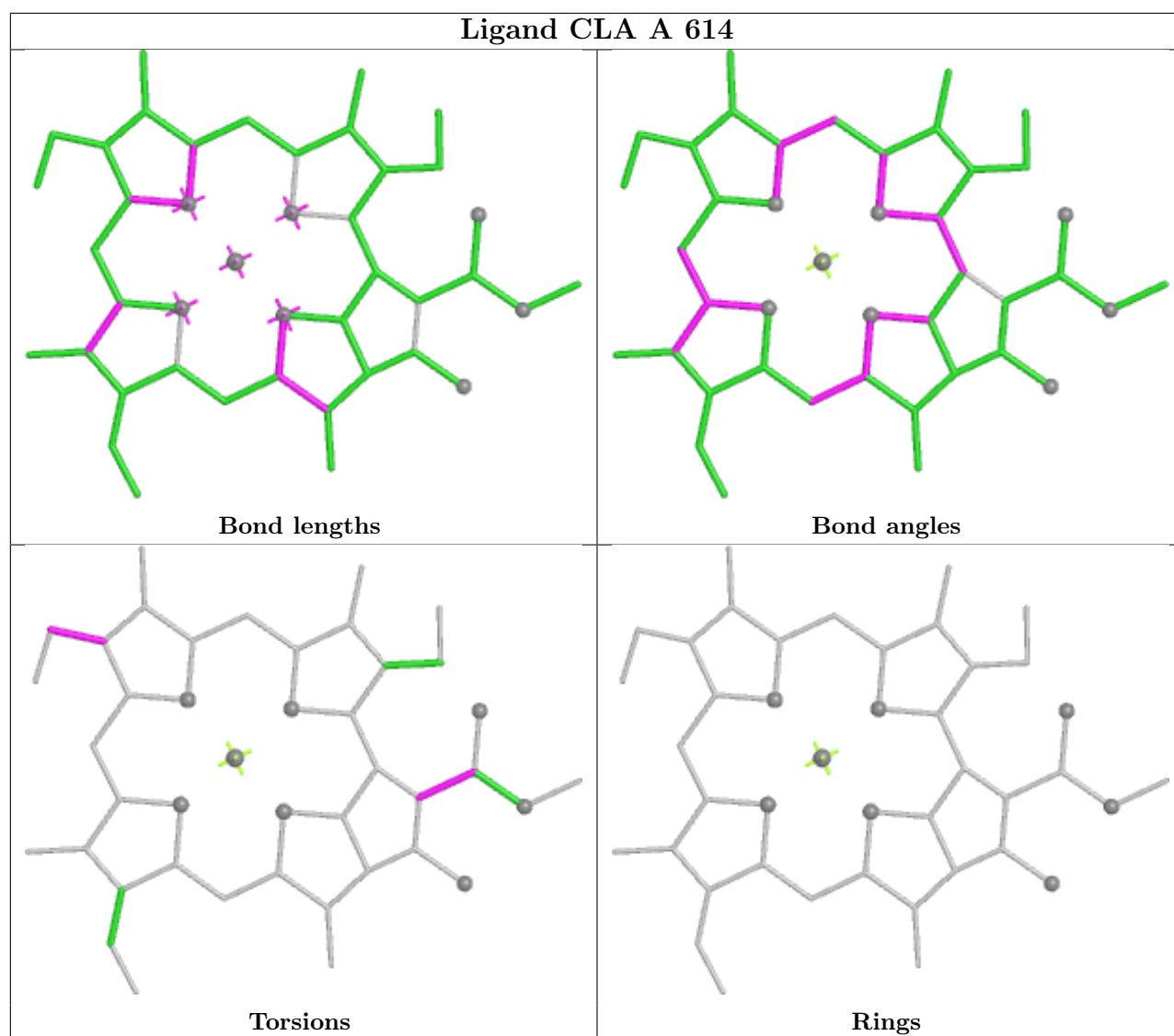


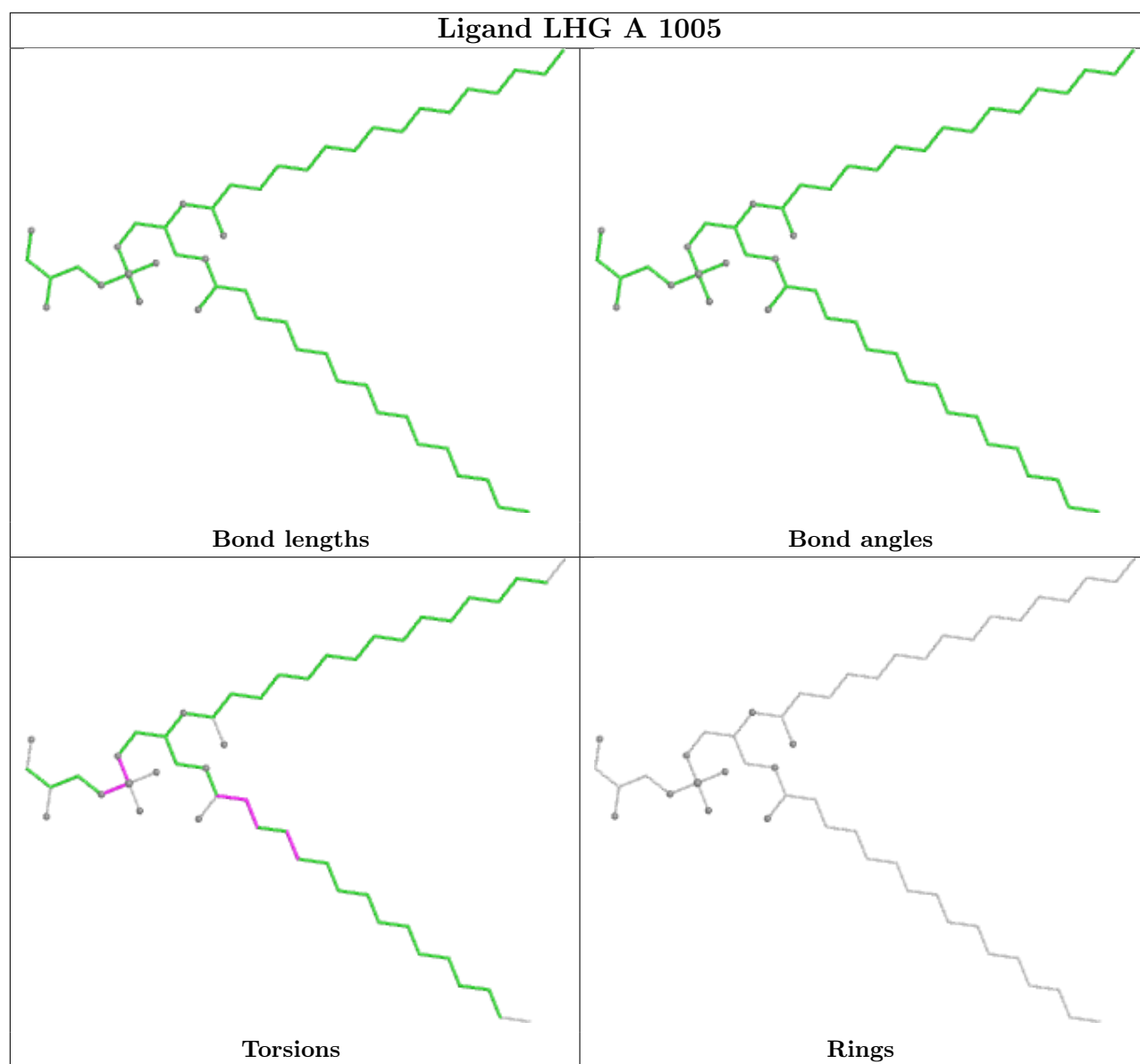


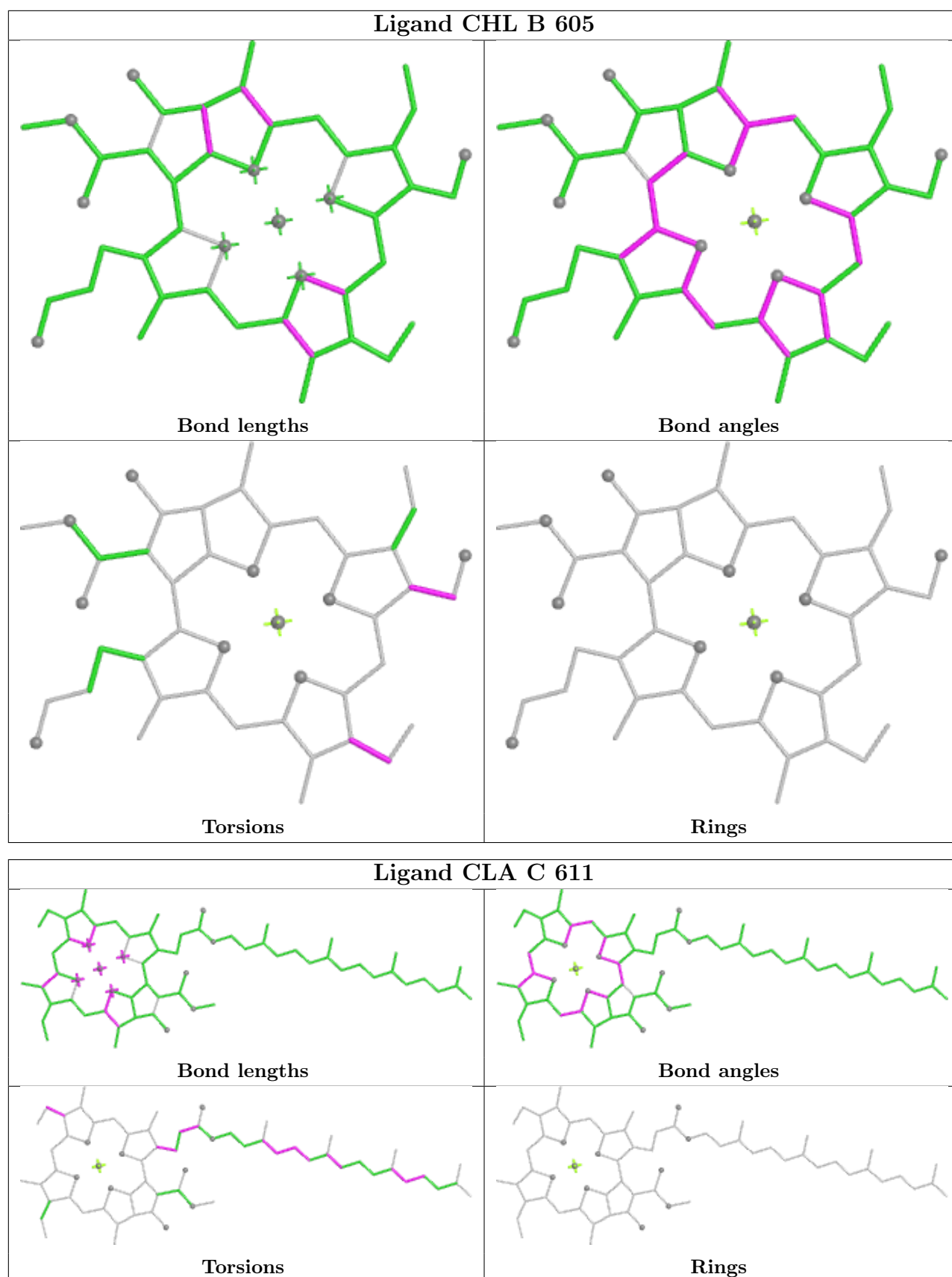


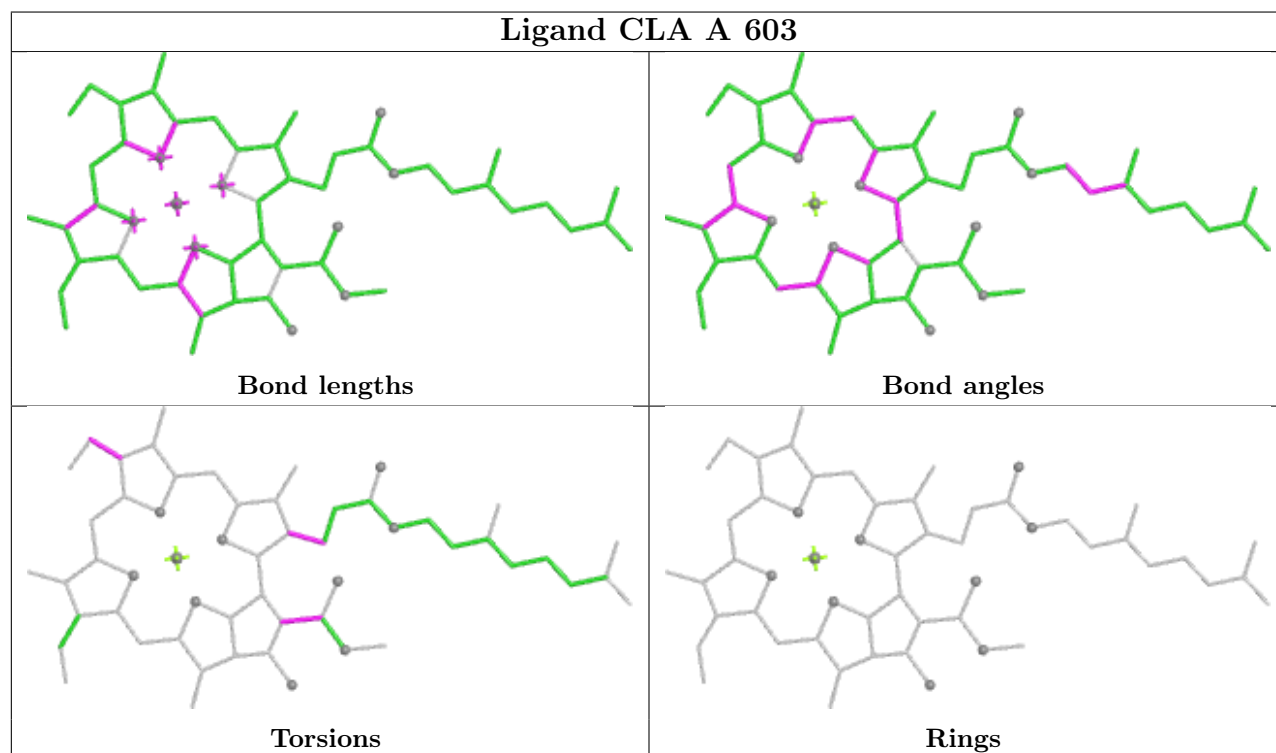
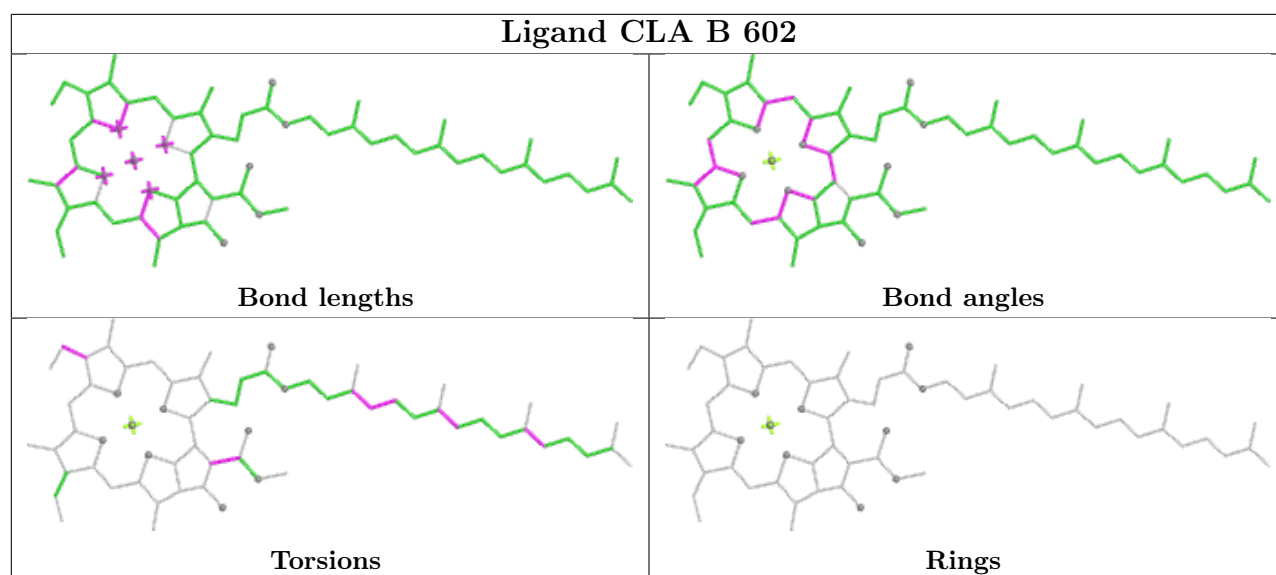


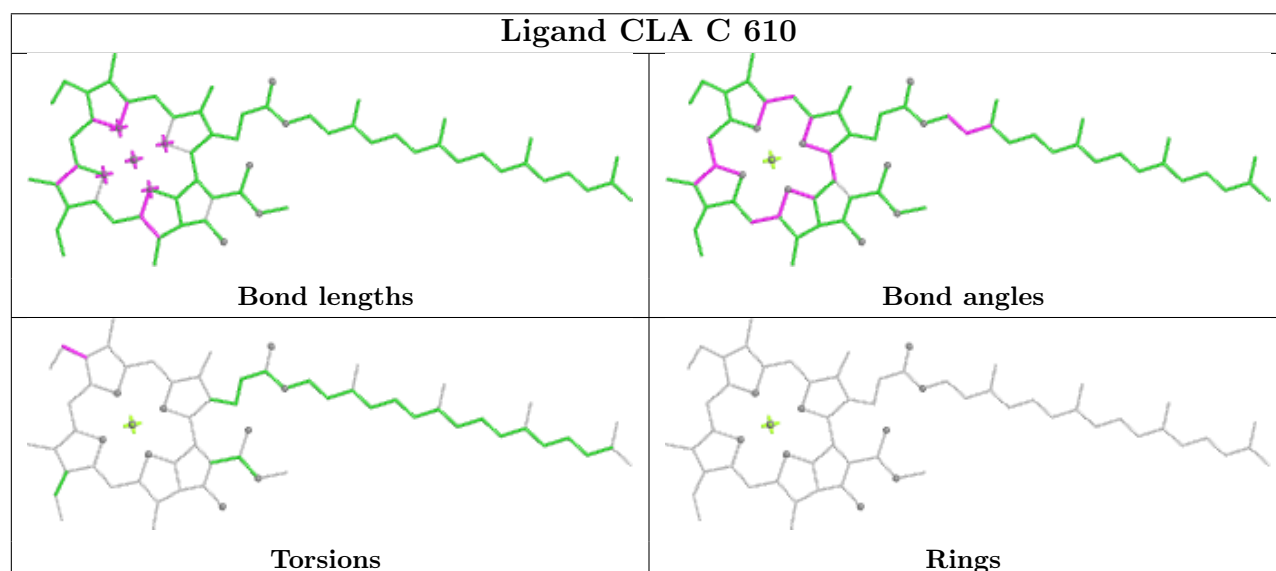
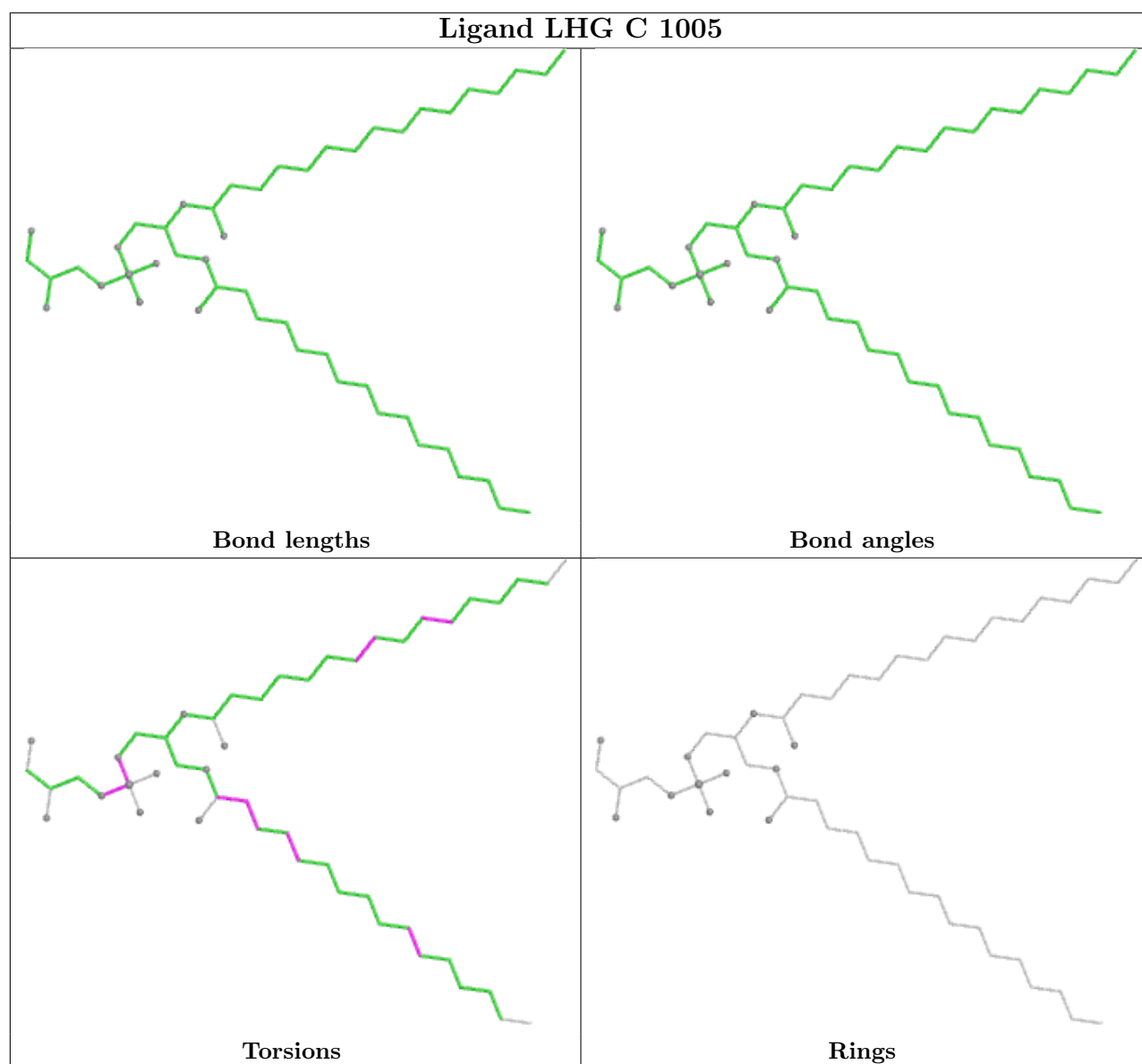


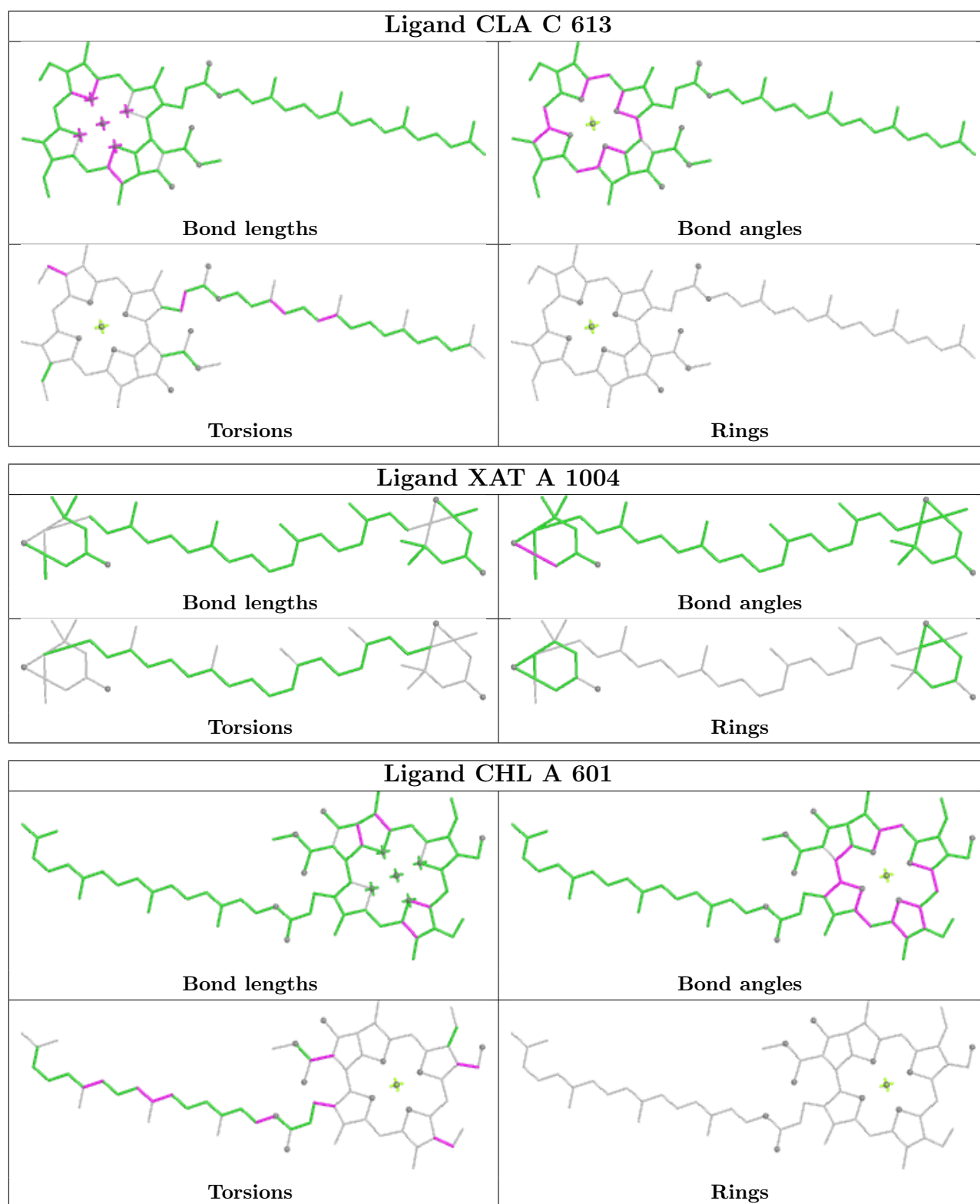












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

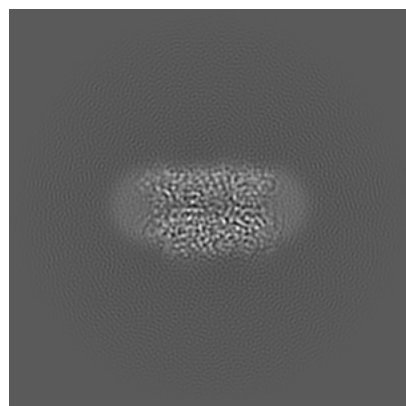
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38825. These allow visual inspection of the internal detail of the map and identification of artifacts.

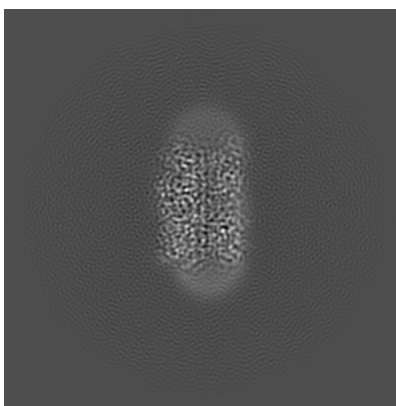
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

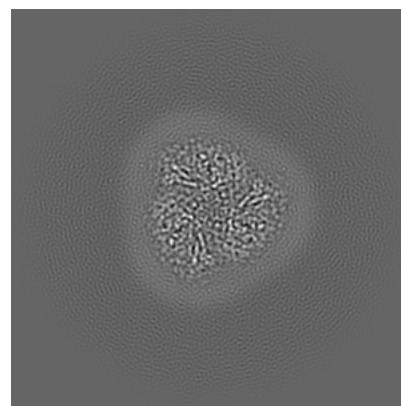
#### 6.1.1 Primary map



X

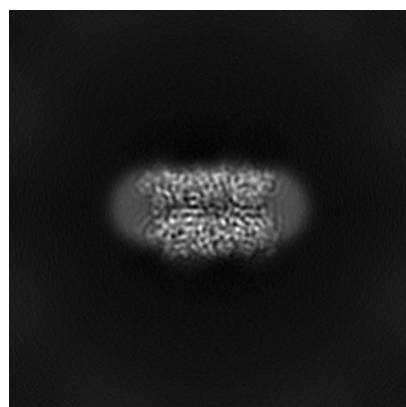


Y

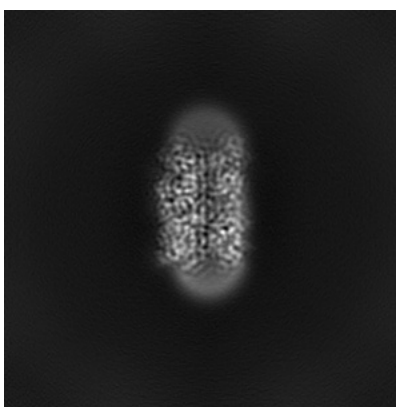


Z

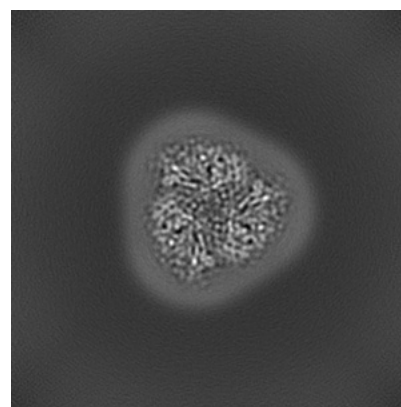
#### 6.1.2 Raw map



X



Y

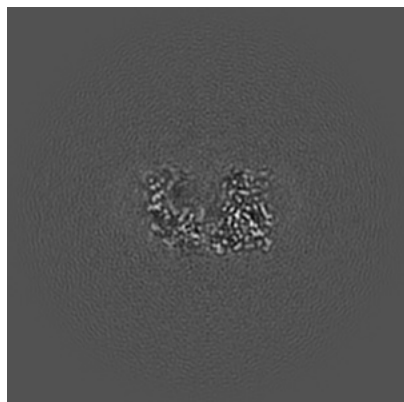


Z

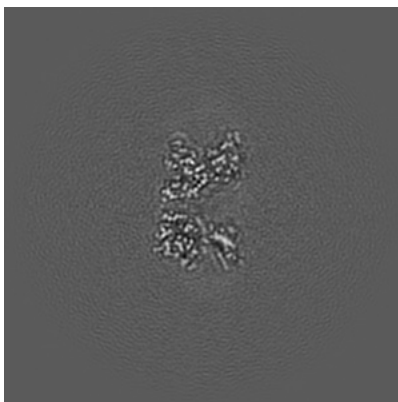
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

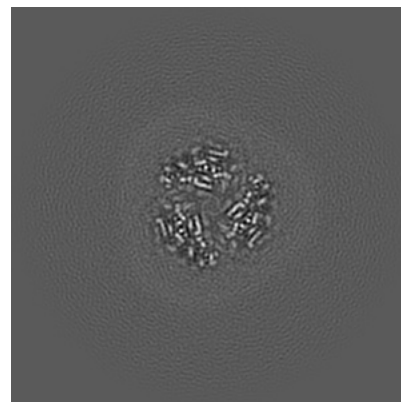
### 6.2.1 Primary map



X Index: 128

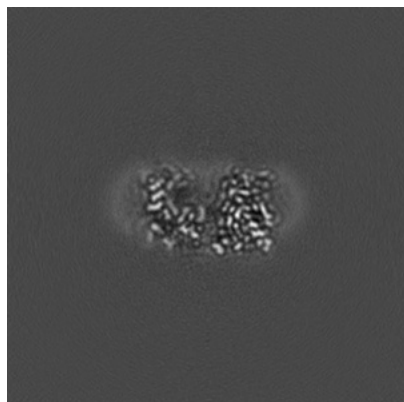


Y Index: 128

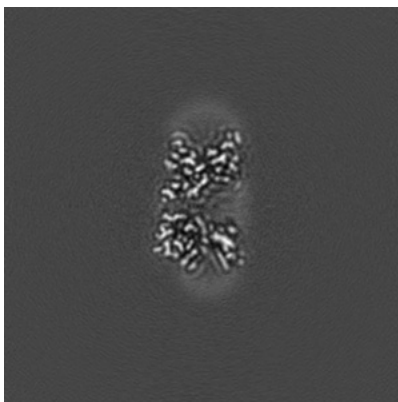


Z Index: 128

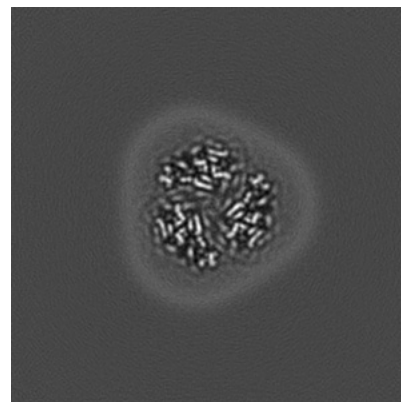
### 6.2.2 Raw map



X Index: 128



Y Index: 128

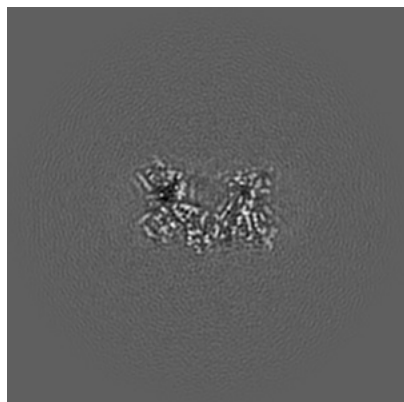


Z Index: 128

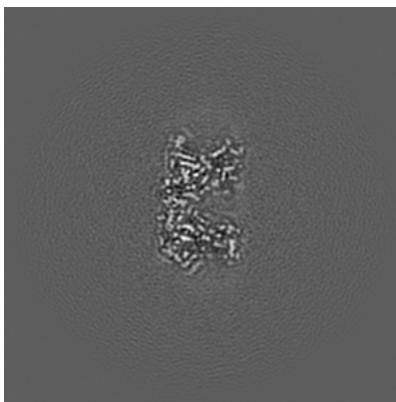
The images above show central slices of the map in three orthogonal directions.

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

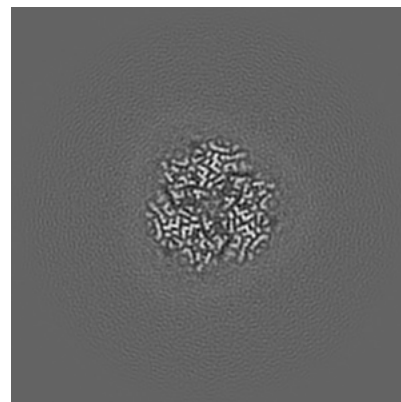
### 6.3.1 Primary map



X Index: 120

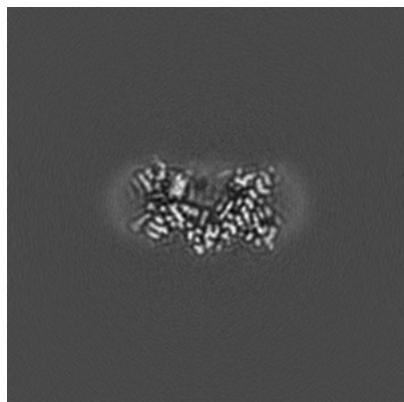


Y Index: 122

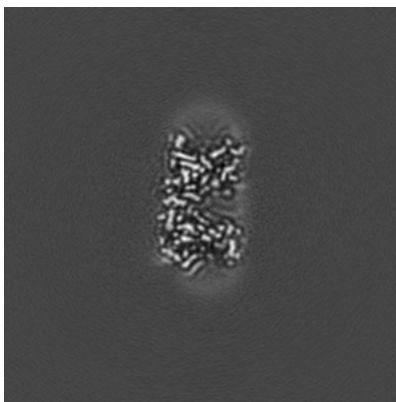


Z Index: 121

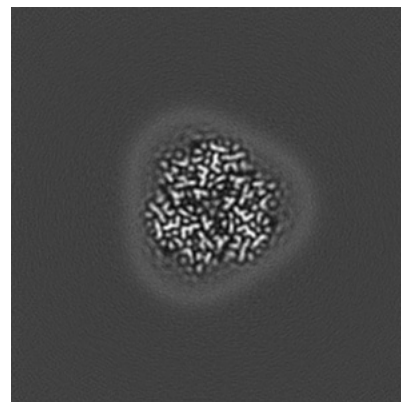
### 6.3.2 Raw map



X Index: 121



Y Index: 122

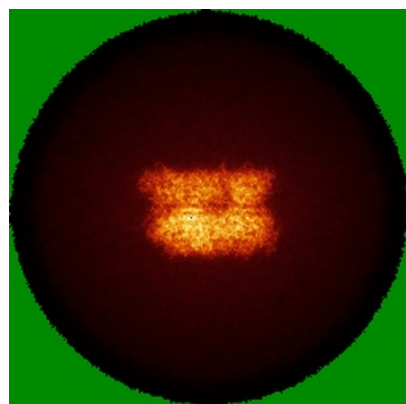


Z Index: 121

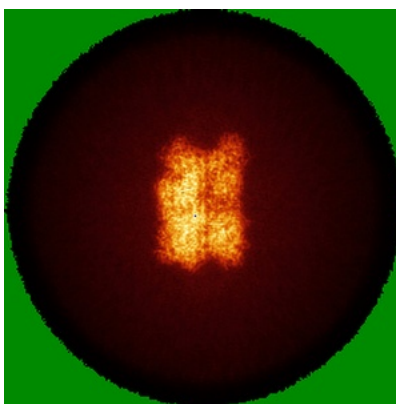
The images above show the largest variance slices of the map in three orthogonal directions.

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

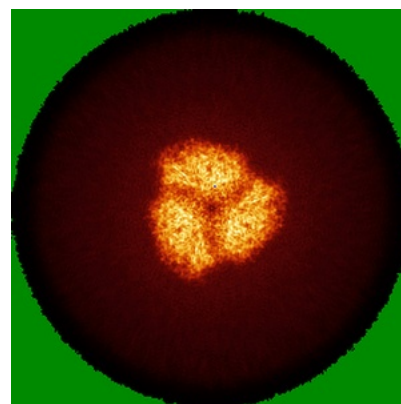
### 6.4.1 Primary map



X

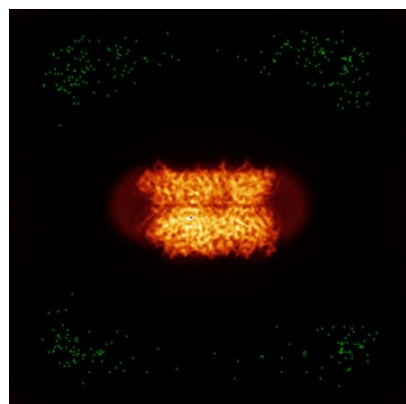


Y

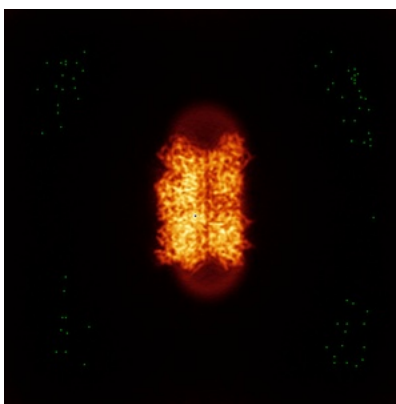


Z

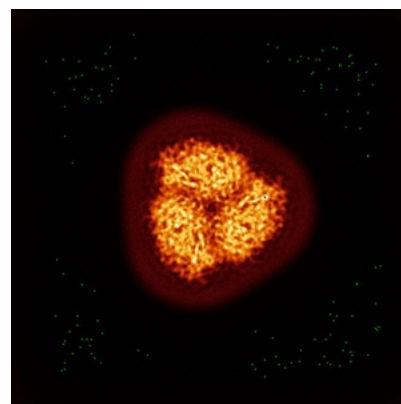
### 6.4.2 Raw map



X



Y

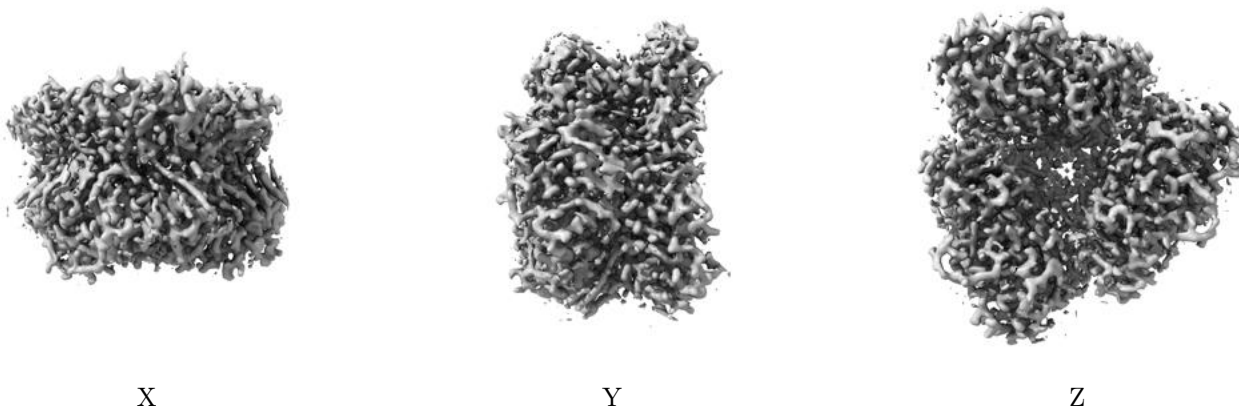


Z

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

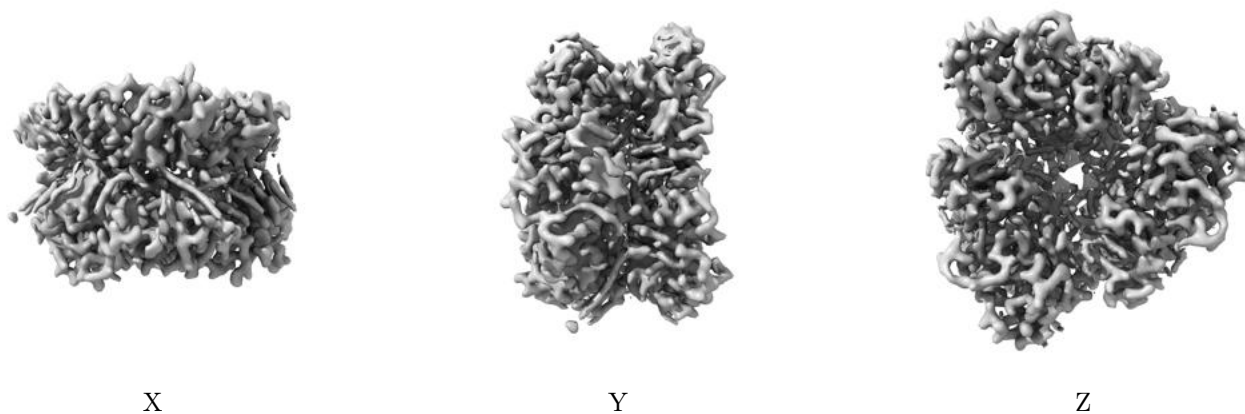
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

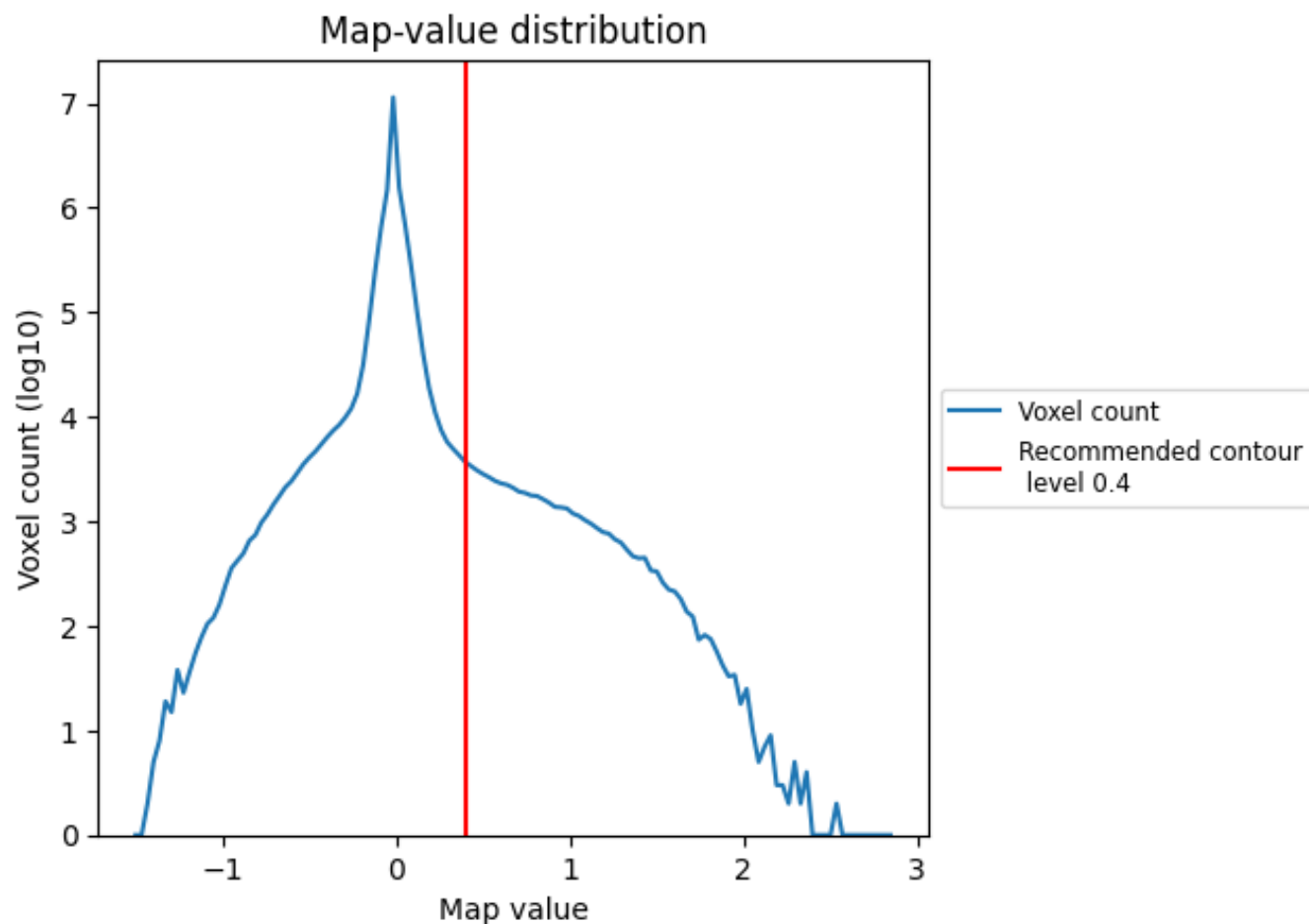
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

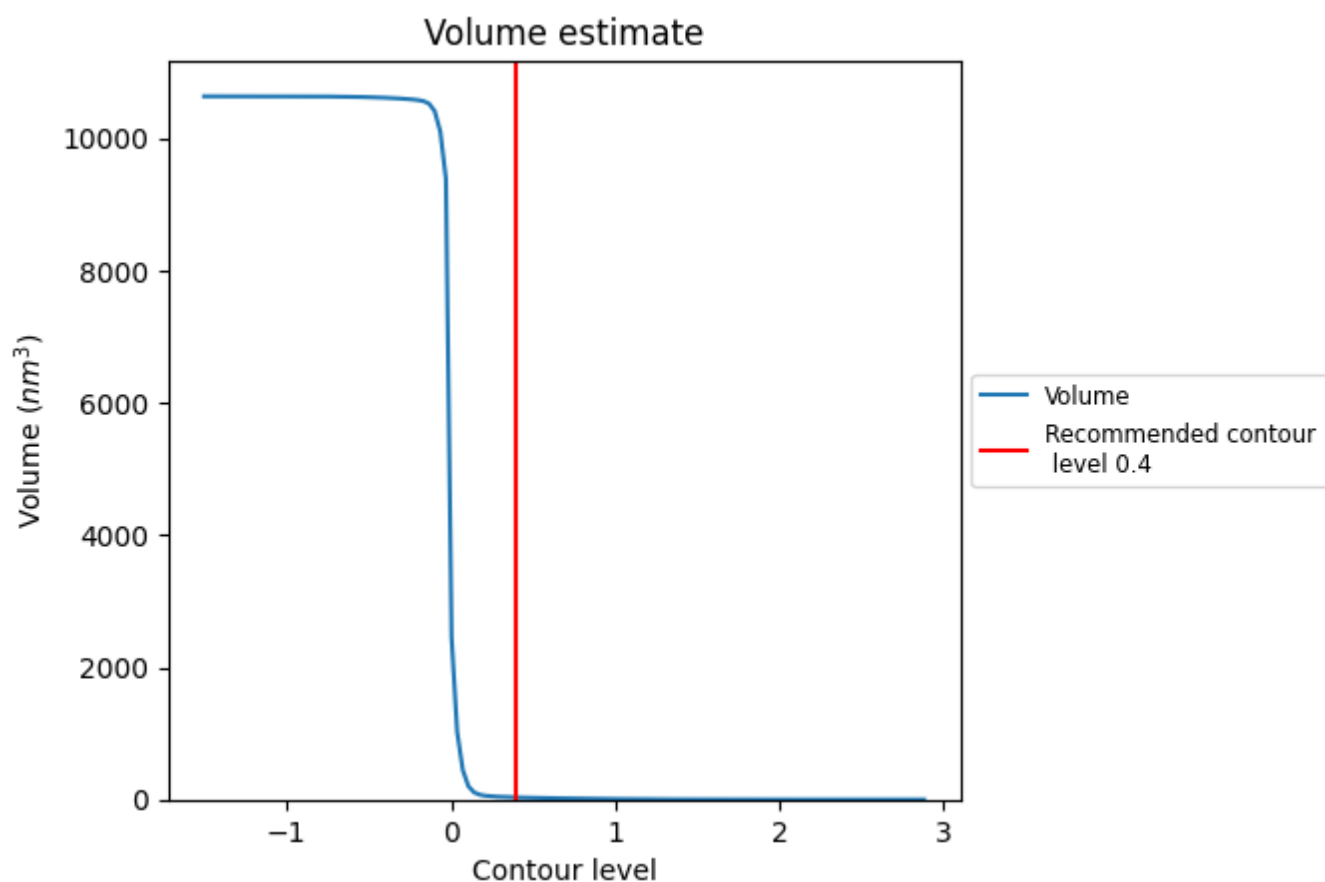
This section contains the results of statistical analysis of the map.

### 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.

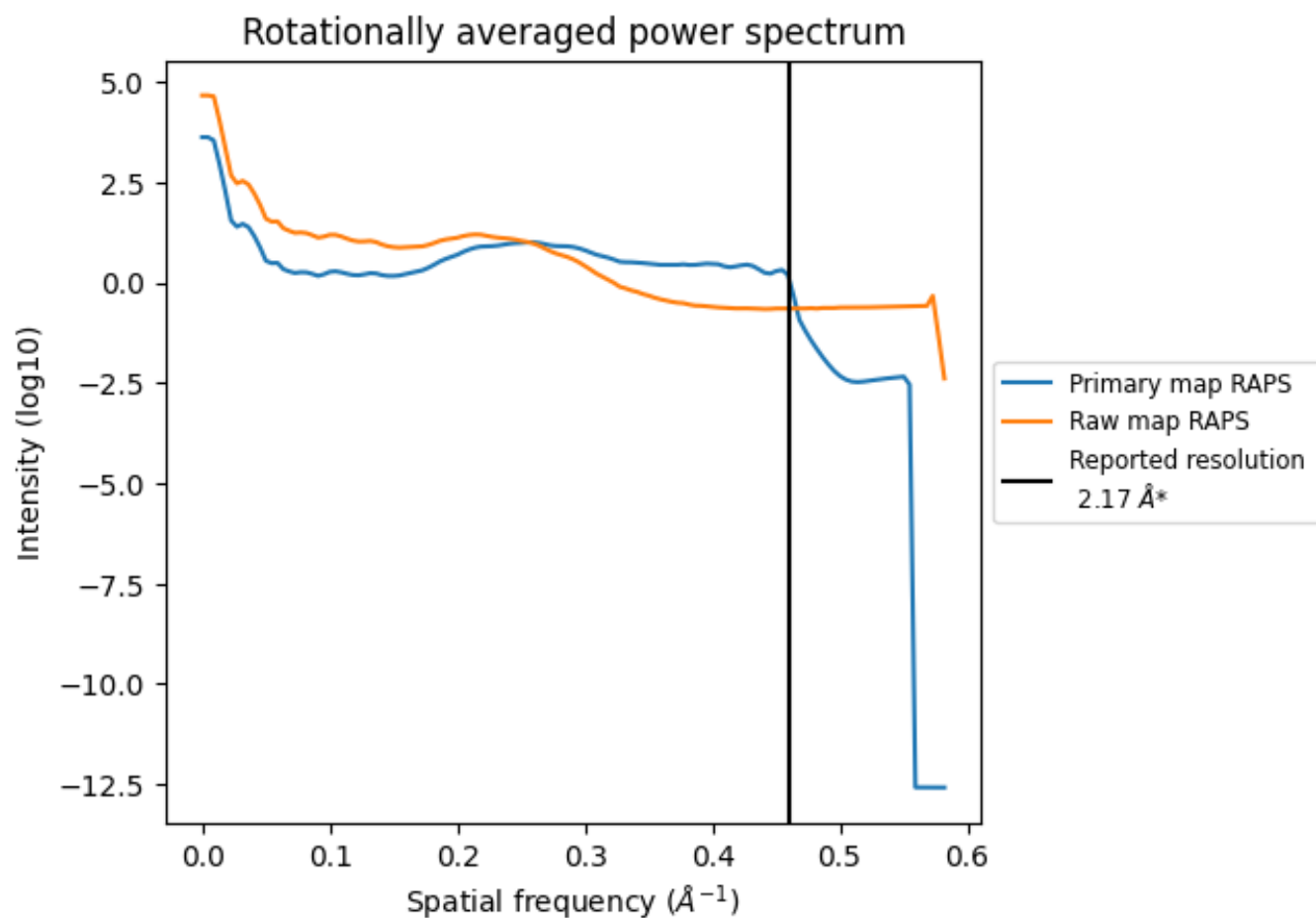
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 32 nm<sup>3</sup>; this corresponds to an approximate mass of 29 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 ⓘ

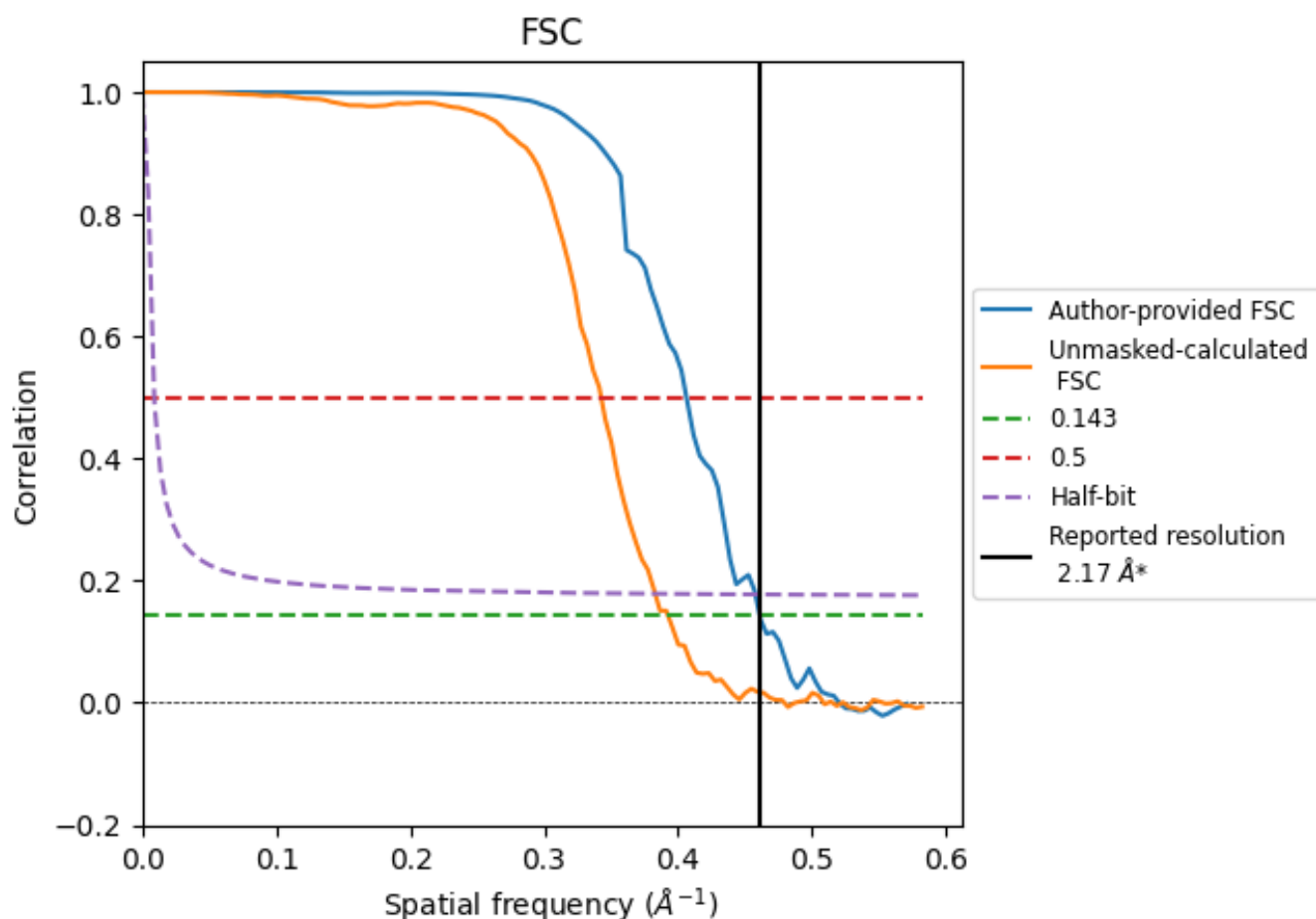


\*Reported resolution corresponds to spatial frequency of 0.461 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.461 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

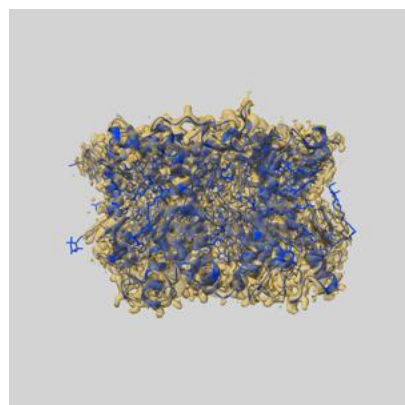
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.17                               | -    | -        |
| Author-provided FSC curve | 2.17                               | 2.46 | 2.19     |
| Unmasked-calculated*      | 2.55                               | 2.92 | 2.61     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.55 differs from the reported value 2.17 by more than 10 %

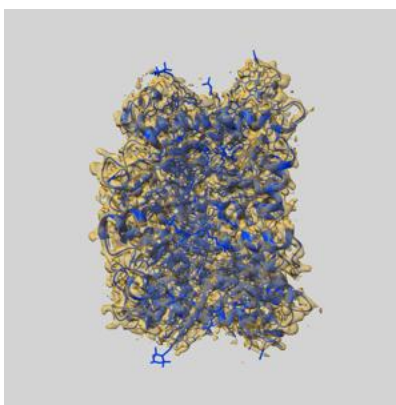
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38825 and PDB model 8Y15. Per-residue inclusion information can be found in section [3](#) on page [11](#).

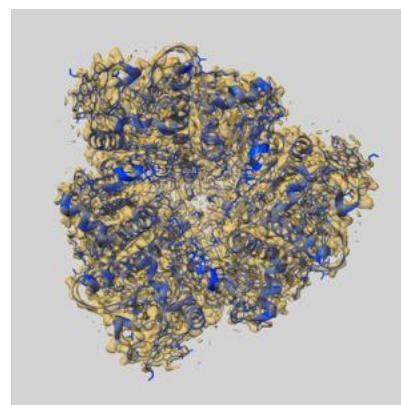
### 9.1 Map-model overlay [i](#)



X



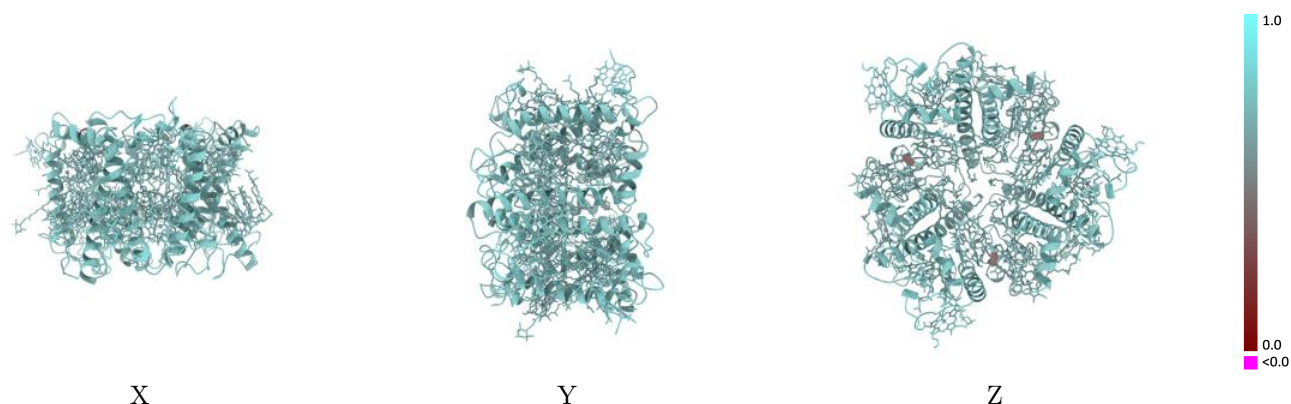
Y



Z

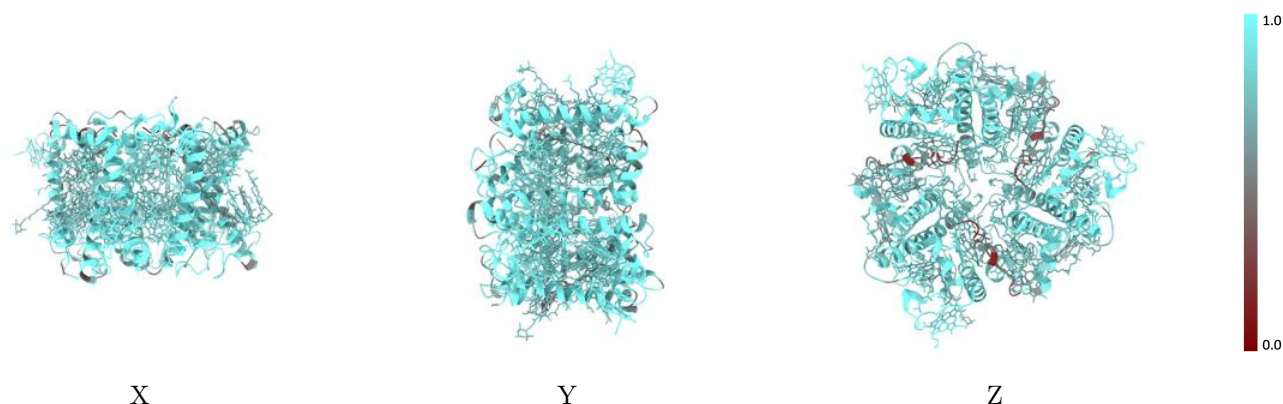
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



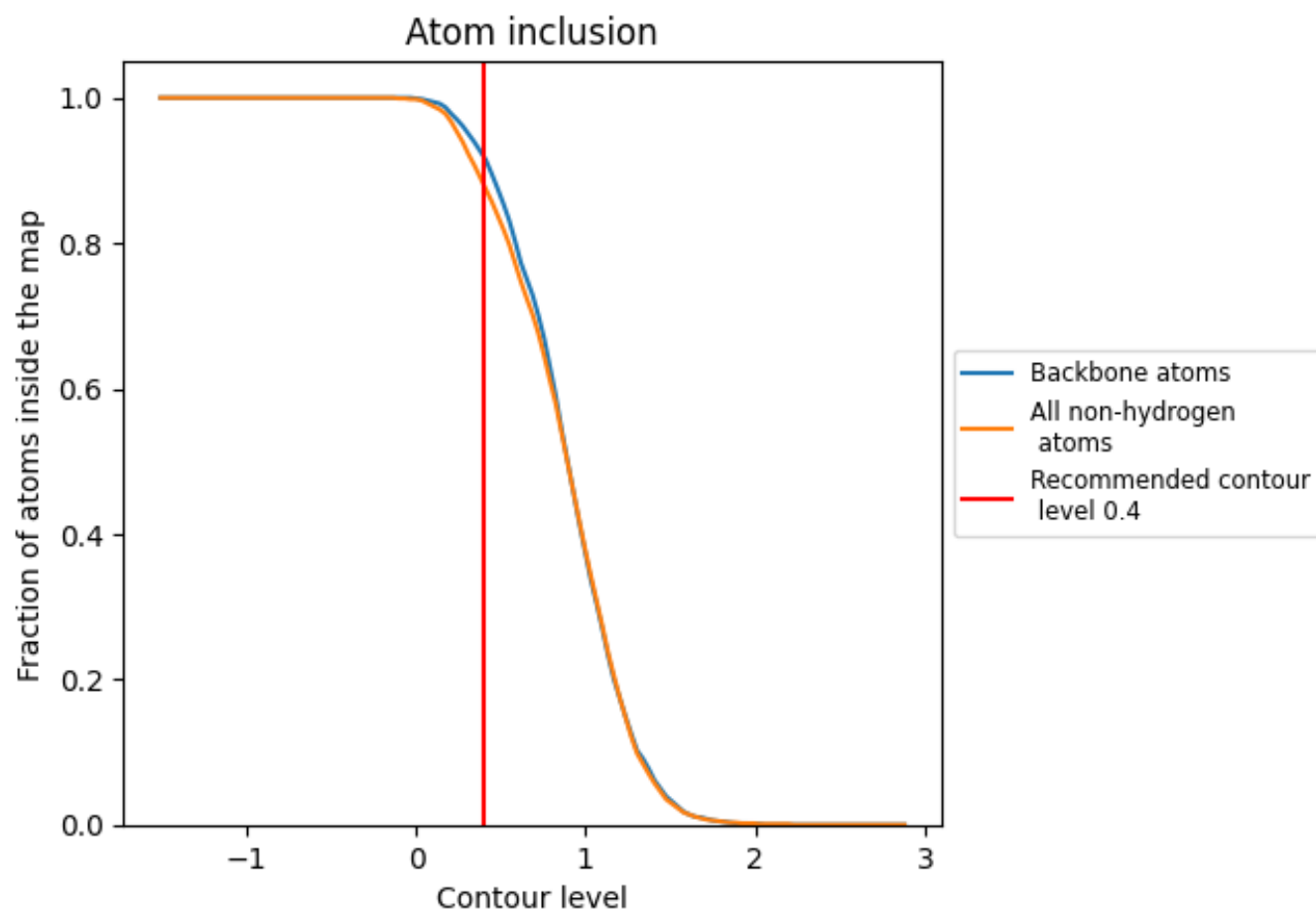
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.4) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.8810 | <div></div> 0.7090 |
| A     | <div></div> 0.8800 | <div></div> 0.7090 |
| B     | <div></div> 0.8780 | <div></div> 0.7090 |
| C     | <div></div> 0.8780 | <div></div> 0.7090 |

