



## Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 10:18 PM UTC

PDB ID : 8IWX / pdb\_00008iwx  
EMDB ID : EMD-35782  
Title : Cryo-EM structure of unprotonated LHCII in detergent solution at high pH value  
Authors : Ruan, M.X.; Ding, W.  
Deposited on : 2023-03-31  
Resolution : 2.59 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

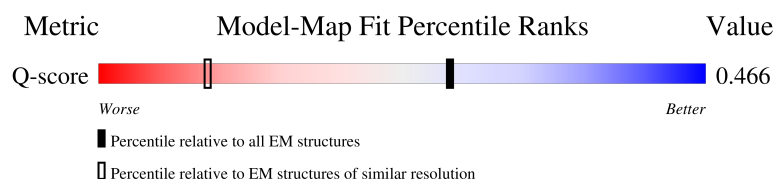
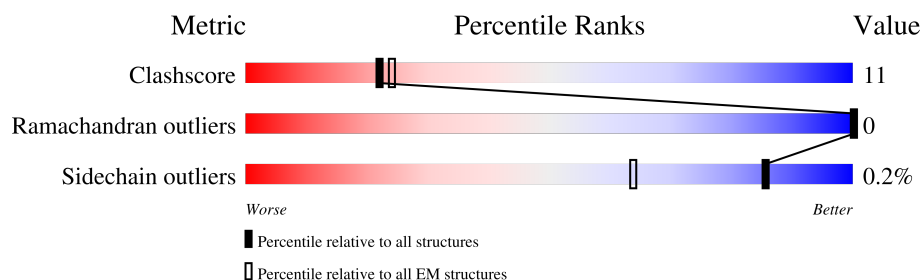
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.59 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                       | 7741 ( 2.09 - 3.09 )                                     |

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   | G     | 218    | 85% 15%          |
| 1   | N     | 218    | 87% 13%          |
| 1   | Y     | 218    | 86% 13%          |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | CHL  | G     | 601 | X         | -        | -       | -                |
| 2   | CHL  | G     | 605 | X         | -        | -       | -                |
| 2   | CHL  | G     | 606 | X         | -        | -       | -                |
| 2   | CHL  | G     | 607 | X         | -        | -       | -                |
| 2   | CHL  | G     | 608 | X         | -        | -       | -                |
| 2   | CHL  | G     | 609 | X         | -        | -       | -                |
| 2   | CHL  | N     | 601 | X         | -        | -       | -                |
| 2   | CHL  | N     | 605 | X         | -        | -       | -                |
| 2   | CHL  | N     | 606 | X         | -        | -       | -                |
| 2   | CHL  | N     | 607 | X         | -        | -       | -                |
| 2   | CHL  | N     | 608 | X         | -        | -       | -                |
| 2   | CHL  | N     | 609 | X         | -        | -       | -                |
| 2   | CHL  | Y     | 601 | X         | -        | -       | -                |
| 2   | CHL  | Y     | 605 | X         | -        | -       | -                |
| 2   | CHL  | Y     | 606 | X         | -        | -       | -                |
| 2   | CHL  | Y     | 607 | X         | -        | -       | -                |
| 2   | CHL  | Y     | 608 | X         | -        | -       | -                |
| 2   | CHL  | Y     | 609 | X         | -        | -       | -                |
| 3   | CLA  | G     | 602 | X         | -        | -       | -                |
| 3   | CLA  | G     | 603 | X         | -        | -       | -                |
| 3   | CLA  | G     | 604 | X         | -        | -       | -                |
| 3   | CLA  | G     | 610 | X         | -        | -       | -                |
| 3   | CLA  | G     | 612 | X         | -        | -       | -                |
| 3   | CLA  | G     | 613 | X         | -        | -       | -                |
| 3   | CLA  | G     | 614 | X         | -        | -       | -                |
| 3   | CLA  | N     | 602 | X         | -        | -       | -                |
| 3   | CLA  | N     | 603 | X         | -        | -       | -                |
| 3   | CLA  | N     | 604 | X         | -        | -       | -                |
| 3   | CLA  | N     | 610 | X         | -        | -       | -                |
| 3   | CLA  | N     | 611 | X         | -        | -       | -                |
| 3   | CLA  | N     | 612 | X         | -        | -       | -                |
| 3   | CLA  | N     | 613 | X         | -        | -       | -                |
| 3   | CLA  | N     | 614 | X         | -        | -       | -                |
| 3   | CLA  | Y     | 602 | X         | -        | -       | -                |
| 3   | CLA  | Y     | 603 | X         | -        | -       | -                |
| 3   | CLA  | Y     | 604 | X         | -        | -       | -                |
| 3   | CLA  | Y     | 610 | X         | -        | -       | -                |
| 3   | CLA  | Y     | 611 | X         | -        | -       | -                |
| 3   | CLA  | Y     | 612 | X         | -        | -       | -                |
| 3   | CLA  | Y     | 613 | X         | -        | -       | -                |
| 3   | CLA  | Y     | 614 | X         | -        | -       | -                |

2 Entry composition [i](#)

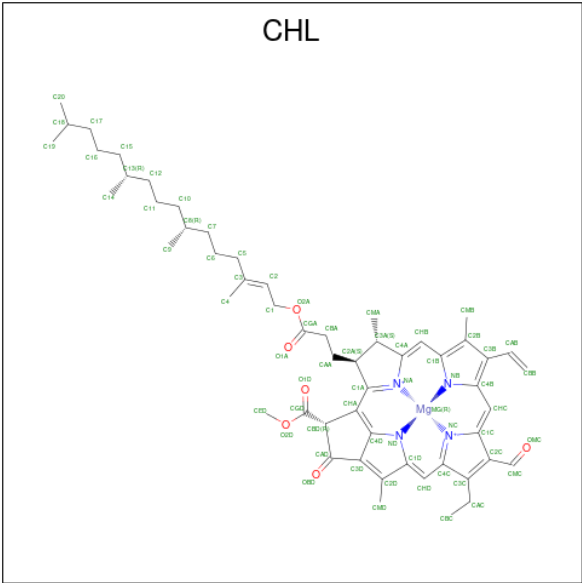
There are 7 unique types of molecules in this entry. The entry contains 8238 atoms, of which 0 are hydrogens and 0 are deuteriums.

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   | N     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1661  | 1079 | 270 | 305 | 7 |         |       |
| 1   | G     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1661  | 1079 | 270 | 305 | 7 |         |       |
| 1   | Y     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1661  | 1079 | 270 | 305 | 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).



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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 2   | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 2   | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 2   | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 2   | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 2   | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |
| 2   | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 2   | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 2   | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 2   | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 2   | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 2   | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |
| 2   | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 2   | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 2   | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 2   | Y     | 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).

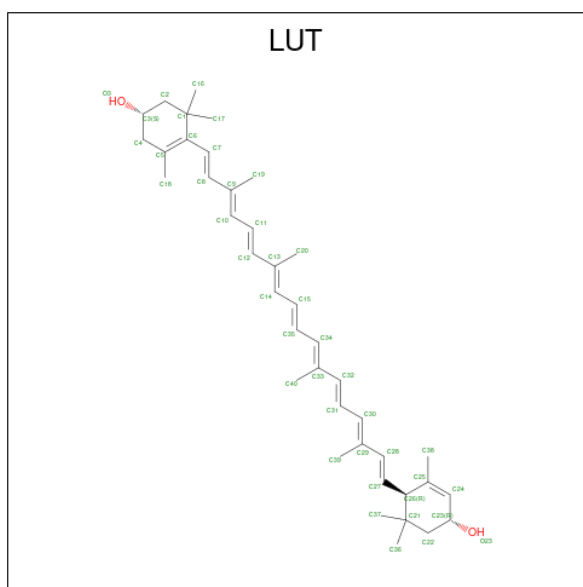


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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 3   | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 3   | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 62    | 52 | 1  | 4 | 5 |         |
| 3   | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 3   | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |

- Molecule 4 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



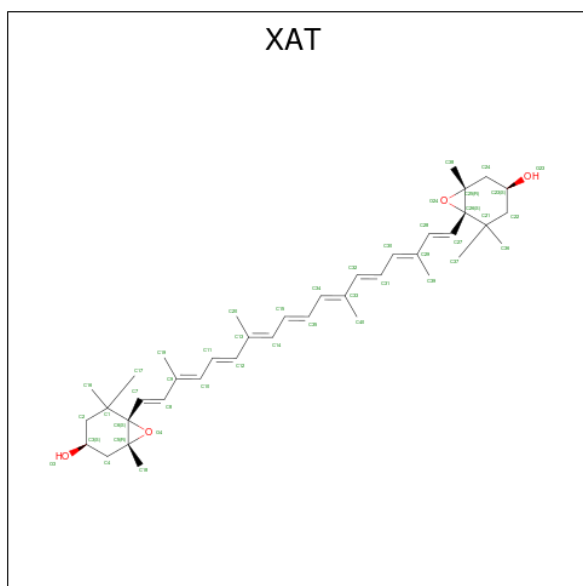
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 4   | N     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

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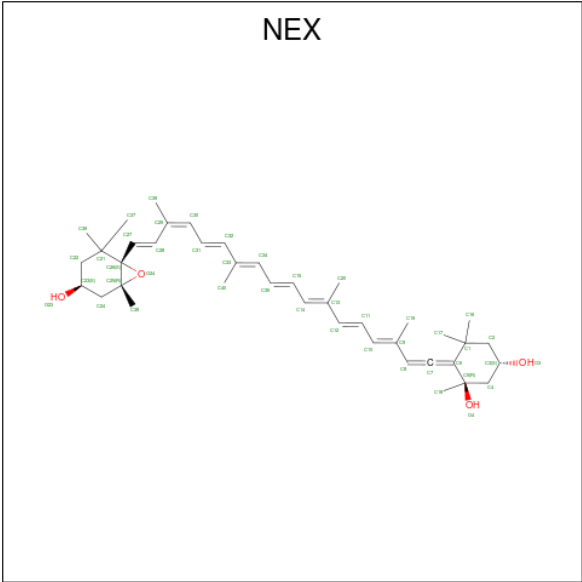
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 4   | N     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 4   | G     | 1        | Total | C  | O | 0       |
|     |       |          | 42 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

- Molecule 5 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>).



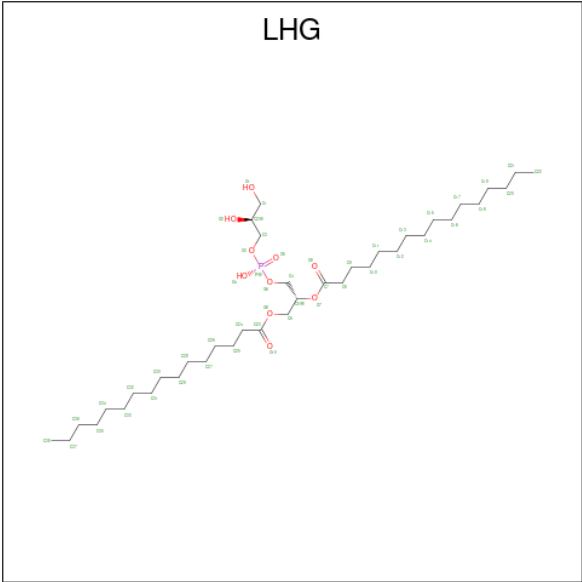
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 5   | N     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 5   | N     | 1        | Total | C  | O | 0       |
|     |       |          | 44 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

- Molecule 6 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 |
|-----|-------|----------|-------|----|---|---------|
| 6   | N     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 6   | G     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 6   | Y     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

- Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



| Mol | Chain | Residues | Atoms       |         |         |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|
| 7   | N     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 7   | G     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 7   | Y     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |

### 3 Residue-property plots

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

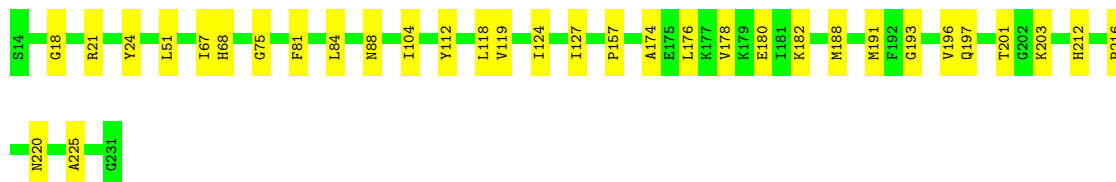
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain N:  87% 13%



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

Chain G:  85% 15%



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

Chain Y:  86% 13%



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 653924                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                                      | Depositor |
| Minimum defocus (nm)                 | 1800                                    | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | 22500                                   | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.467                                   | Depositor |
| Minimum map value                    | -0.199                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.020                                   | Depositor |
| Recommended contour level            | 0.05                                    | Depositor |
| Map size (Å)                         | 214.00002, 214.00002, 214.00002         | wwPDB     |
| Map dimensions                       | 200, 200, 200                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.07, 1.07, 1.07                        | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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   | G     | 0.28         | 0/1713  | 0.55        | 0/2333  |
| 1   | N     | 0.30         | 0/1713  | 0.56        | 0/2333  |
| 1   | Y     | 0.29         | 0/1713  | 0.55        | 0/2333  |
| All | All   | 0.29         | 0/5139  | 0.55        | 0/6999  |

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 [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | G     | 1661  | 0        | 1592     | 28      | 0            |
| 1   | N     | 1661  | 0        | 1591     | 23      | 0            |
| 1   | Y     | 1661  | 0        | 1591     | 27      | 0            |
| 2   | G     | 363   | 0        | 350      | 21      | 0            |
| 2   | N     | 363   | 0        | 350      | 21      | 0            |
| 2   | Y     | 363   | 0        | 350      | 22      | 0            |
| 3   | G     | 501   | 0        | 534      | 22      | 0            |
| 3   | N     | 501   | 0        | 534      | 15      | 0            |
| 3   | Y     | 501   | 0        | 534      | 29      | 0            |
| 4   | G     | 84    | 0        | 112      | 10      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | N     | 84    | 0        | 112      | 9       | 0            |
| 4   | Y     | 84    | 0        | 112      | 13      | 0            |
| 5   | G     | 44    | 0        | 56       | 9       | 0            |
| 5   | N     | 88    | 0        | 112      | 11      | 0            |
| 6   | G     | 44    | 0        | 56       | 1       | 0            |
| 6   | N     | 44    | 0        | 56       | 0       | 0            |
| 6   | Y     | 44    | 0        | 56       | 2       | 0            |
| 7   | G     | 49    | 0        | 74       | 3       | 0            |
| 7   | N     | 49    | 0        | 74       | 3       | 0            |
| 7   | Y     | 49    | 0        | 74       | 8       | 0            |
| All | All   | 8238  | 0        | 8320     | 190     | 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 11.

All (190) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:602:CLA:HAB  | 4:N:616:LUT:H32  | 1.55                     | 0.87              |
| 1:Y:191:MET:HE2  | 4:Y:616:LUT:H10  | 1.62                     | 0.81              |
| 3:Y:602:CLA:HAB  | 4:Y:616:LUT:H32  | 1.64                     | 0.80              |
| 2:G:601:CHL:HAC1 | 7:G:618:LHG:HC12 | 1.64                     | 0.77              |
| 5:N:617:XAT:H242 | 2:Y:601:CHL:HMC  | 1.68                     | 0.74              |
| 2:N:601:CHL:HMC  | 5:N:620:XAT:H242 | 1.73                     | 0.70              |
| 1:G:212:HIS:HD1  | 3:G:613:CLA:HAA2 | 1.58                     | 0.68              |
| 3:N:610:CLA:H52  | 4:N:615:LUT:H30  | 1.76                     | 0.66              |
| 1:G:112:TYR:HB2  | 1:G:119:VAL:HG22 | 1.79                     | 0.63              |
| 3:Y:613:CLA:H8   | 3:Y:614:CLA:HMD3 | 1.78                     | 0.63              |
| 1:N:112:TYR:HB2  | 1:N:119:VAL:HG22 | 1.80                     | 0.61              |
| 3:G:602:CLA:H52  | 4:G:616:LUT:H28  | 1.82                     | 0.61              |
| 2:N:609:CHL:HMC  | 2:Y:601:CHL:H72  | 1.83                     | 0.60              |
| 1:N:102:SER:HB2  | 2:N:607:CHL:HED2 | 1.81                     | 0.60              |
| 3:Y:610:CLA:H52  | 4:Y:615:LUT:H30  | 1.83                     | 0.60              |
| 1:G:84:LEU:O     | 1:G:88:ASN:ND2   | 2.34                     | 0.60              |
| 1:G:201:THR:HG22 | 1:G:203:LYS:HG3  | 1.82                     | 0.60              |
| 7:N:619:LHG:HC91 | 7:N:619:LHG:H282 | 1.85                     | 0.59              |
| 3:G:610:CLA:H52  | 4:G:615:LUT:H30  | 1.86                     | 0.58              |
| 1:Y:112:TYR:HB2  | 1:Y:119:VAL:HG22 | 1.85                     | 0.58              |
| 1:Y:161:PHE:HD1  | 2:Y:608:CHL:H61  | 1.67                     | 0.58              |
| 1:G:24:TYR:HD2   | 2:G:601:CHL:HAA2 | 1.68                     | 0.58              |
| 1:Y:197:GLN:O    | 1:Y:201:THR:OG1  | 2.22                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:112:TYR:HD2  | 1:N:118:LEU:HD23 | 1.69                     | 0.57              |
| 1:G:178:VAL:O    | 1:G:182:LYS:HG3  | 2.04                     | 0.57              |
| 2:Y:608:CHL:HAA2 | 2:Y:608:CHL:H171 | 1.86                     | 0.57              |
| 2:G:607:CHL:H18  | 2:G:609:CHL:H52  | 1.86                     | 0.57              |
| 7:G:618:LHG:H281 | 7:G:618:LHG:HC91 | 1.87                     | 0.56              |
| 1:Y:112:TYR:HB3  | 1:Y:118:LEU:HB3  | 1.86                     | 0.56              |
| 3:Y:611:CLA:H121 | 3:Y:612:CLA:HBB1 | 1.87                     | 0.56              |
| 2:N:601:CHL:H72  | 2:G:609:CHL:HMC  | 1.86                     | 0.56              |
| 3:Y:602:CLA:H52  | 4:Y:616:LUT:H28  | 1.88                     | 0.55              |
| 2:G:601:CHL:H8   | 5:G:619:XAT:H14  | 1.88                     | 0.55              |
| 2:G:601:CHL:HMC  | 5:G:619:XAT:H242 | 1.87                     | 0.55              |
| 2:N:606:CHL:HBC2 | 2:N:607:CHL:HHD  | 1.89                     | 0.55              |
| 1:N:70:ARG:NH1   | 2:N:608:CHL:OBD  | 2.40                     | 0.54              |
| 1:G:157:PRO:HB3  | 2:G:608:CHL:HBC2 | 1.90                     | 0.54              |
| 1:G:51:LEU:HD13  | 3:G:602:CLA:H42  | 1.89                     | 0.53              |
| 1:G:75:GLY:HA2   | 4:G:616:LUT:H181 | 1.89                     | 0.53              |
| 3:G:604:CLA:O2A  | 6:G:617:NEX:H241 | 2.08                     | 0.53              |
| 1:Y:51:LEU:HD13  | 3:Y:602:CLA:H42  | 1.90                     | 0.53              |
| 2:G:608:CHL:HHC  | 2:G:608:CHL:HBB1 | 1.91                     | 0.52              |
| 3:Y:613:CLA:H151 | 3:Y:614:CLA:HBA2 | 1.92                     | 0.52              |
| 3:G:610:CLA:HBB1 | 4:G:615:LUT:H32  | 1.91                     | 0.52              |
| 1:Y:41:PRO:HG2   | 1:Y:177:LYS:HD2  | 1.91                     | 0.52              |
| 2:Y:606:CHL:HMB1 | 2:Y:609:CHL:HMC  | 1.92                     | 0.52              |
| 2:N:607:CHL:H18  | 2:N:609:CHL:H52  | 1.92                     | 0.51              |
| 1:N:115:ASN:HD22 | 1:N:118:LEU:HD13 | 1.75                     | 0.51              |
| 3:N:613:CLA:H141 | 3:N:614:CLA:H2   | 1.91                     | 0.51              |
| 1:Y:139:GLU:OE1  | 1:Y:142:ARG:NH2  | 2.43                     | 0.51              |
| 2:G:607:CHL:H12  | 2:G:607:CHL:HMA2 | 1.93                     | 0.51              |
| 2:N:608:CHL:H3A  | 2:N:608:CHL:H151 | 1.92                     | 0.51              |
| 2:N:601:CHL:HHB  | 2:G:609:CHL:HMB2 | 1.93                     | 0.50              |
| 1:G:188:MET:HE1  | 3:G:602:CLA:HBB1 | 1.91                     | 0.50              |
| 1:Y:73:MET:HE1   | 3:Y:610:CLA:HHC  | 1.93                     | 0.50              |
| 1:Y:75:GLY:HA2   | 4:Y:616:LUT:H181 | 1.94                     | 0.49              |
| 1:N:157:PRO:HB3  | 2:N:608:CHL:HBC2 | 1.94                     | 0.49              |
| 1:G:104:ILE:HG21 | 1:G:124:ILE:HD13 | 1.94                     | 0.49              |
| 3:G:610:CLA:CBB  | 4:G:615:LUT:H32  | 2.43                     | 0.49              |
| 3:N:610:CLA:CBB  | 4:N:615:LUT:H32  | 2.42                     | 0.49              |
| 2:Y:608:CHL:H11  | 3:Y:610:CLA:HMD2 | 1.95                     | 0.49              |
| 1:N:134:LEU:HD21 | 2:N:606:CHL:H43  | 1.94                     | 0.49              |
| 2:N:609:CHL:HMB2 | 2:Y:601:CHL:HHB  | 1.95                     | 0.48              |
| 1:Y:134:LEU:HD23 | 6:Y:617:NEX:C14  | 2.43                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:112:TYR:HB3  | 1:N:118:LEU:HB3  | 1.95                     | 0.48              |
| 1:N:176:LEU:HD23 | 1:N:179:LYS:HD2  | 1.95                     | 0.48              |
| 5:N:617:XAT:H12  | 2:Y:601:CHL:H111 | 1.95                     | 0.48              |
| 2:Y:606:CHL:HBC2 | 2:Y:607:CHL:HHD  | 1.95                     | 0.48              |
| 3:Y:611:CLA:H102 | 3:Y:611:CLA:H62  | 1.35                     | 0.48              |
| 3:Y:603:CLA:H102 | 2:Y:609:CHL:H143 | 1.96                     | 0.48              |
| 3:Y:610:CLA:H2   | 4:Y:615:LUT:H28  | 1.96                     | 0.48              |
| 3:Y:603:CLA:HBB1 | 2:Y:609:CHL:H122 | 1.95                     | 0.47              |
| 1:G:191:MET:HE2  | 4:G:616:LUT:H10  | 1.96                     | 0.47              |
| 1:Y:212:HIS:ND1  | 3:Y:613:CLA:HAA2 | 2.30                     | 0.47              |
| 1:Y:180:GLU:HB2  | 3:Y:610:CLA:C1B  | 2.45                     | 0.47              |
| 1:G:216:PRO:O    | 1:G:220:ASN:ND2  | 2.47                     | 0.47              |
| 2:G:606:CHL:HBC2 | 2:G:607:CHL:HHD  | 1.97                     | 0.47              |
| 1:G:112:TYR:HB3  | 1:G:118:LEU:HB3  | 1.96                     | 0.47              |
| 2:Y:609:CHL:HBB1 | 2:Y:609:CHL:HHC  | 1.97                     | 0.47              |
| 1:Y:182:LYS:HB3  | 3:Y:611:CLA:HMD2 | 1.96                     | 0.47              |
| 7:Y:618:LHG:H172 | 7:Y:618:LHG:H201 | 1.54                     | 0.47              |
| 1:G:196:VAL:HG11 | 3:G:613:CLA:HAC2 | 1.97                     | 0.46              |
| 2:N:601:CHL:HBA1 | 2:N:601:CHL:H3A  | 1.64                     | 0.46              |
| 3:N:611:CLA:H91  | 3:N:611:CLA:H112 | 1.60                     | 0.46              |
| 1:G:176:LEU:HB3  | 3:G:610:CLA:HHB  | 1.96                     | 0.46              |
| 1:G:212:HIS:CD2  | 3:G:614:CLA:NB   | 2.84                     | 0.46              |
| 1:N:18:GLY:O     | 1:N:21:ARG:NH1   | 2.39                     | 0.46              |
| 3:N:613:CLA:H2   | 3:N:613:CLA:H61  | 1.49                     | 0.46              |
| 3:N:613:CLA:H93  | 7:N:619:LHG:H131 | 1.97                     | 0.46              |
| 2:N:609:CHL:CMB  | 2:Y:601:CHL:HHB  | 2.46                     | 0.46              |
| 3:N:611:CLA:H101 | 3:N:611:CLA:H62  | 1.40                     | 0.46              |
| 1:G:180:GLU:HG3  | 3:G:610:CLA:C4B  | 2.45                     | 0.46              |
| 1:N:181:ILE:HG21 | 1:N:185:ARG:HH21 | 1.80                     | 0.46              |
| 5:N:617:XAT:H35  | 5:N:617:XAT:H401 | 1.76                     | 0.46              |
| 1:Y:134:LEU:HD23 | 6:Y:617:NEX:C15  | 2.45                     | 0.46              |
| 3:Y:610:CLA:H61  | 4:Y:615:LUT:H371 | 1.97                     | 0.46              |
| 5:N:620:XAT:H401 | 5:N:620:XAT:H35  | 1.73                     | 0.45              |
| 1:G:68:HIS:HB3   | 1:G:188:MET:SD   | 2.55                     | 0.45              |
| 2:N:608:CHL:H11  | 3:N:610:CLA:HMD2 | 1.99                     | 0.45              |
| 1:G:81:PHE:HD2   | 3:G:604:CLA:HHD  | 1.81                     | 0.45              |
| 1:Y:167:ALA:HB1  | 1:Y:173:PHE:CD2  | 2.51                     | 0.45              |
| 2:G:601:CHL:H111 | 5:G:619:XAT:H12  | 1.98                     | 0.45              |
| 1:N:175:GLU:O    | 1:N:179:LYS:HG3  | 2.16                     | 0.45              |
| 1:G:18:GLY:O     | 1:G:21:ARG:NH1   | 2.42                     | 0.45              |
| 4:Y:616:LUT:H11  | 4:Y:616:LUT:H191 | 1.86                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:G:619:XAT:H35  | 5:G:619:XAT:H401 | 1.78                     | 0.45              |
| 3:N:610:CLA:H2   | 4:N:615:LUT:H28  | 1.99                     | 0.45              |
| 1:G:193:GLY:O    | 1:G:197:GLN:HG3  | 2.17                     | 0.45              |
| 3:Y:611:CLA:HMA3 | 7:Y:618:LHG:HC32 | 1.99                     | 0.45              |
| 4:G:616:LUT:H15  | 4:G:616:LUT:H201 | 1.77                     | 0.45              |
| 2:N:606:CHL:HBA2 | 2:N:606:CHL:H12  | 1.84                     | 0.45              |
| 1:N:182:LYS:HB3  | 3:N:611:CLA:HMD1 | 1.99                     | 0.44              |
| 2:Y:607:CHL:H92  | 2:Y:609:CHL:H18  | 1.99                     | 0.44              |
| 1:N:161:PHE:HA   | 2:N:608:CHL:H72  | 1.99                     | 0.44              |
| 1:Y:115:ASN:HB3  | 1:Y:118:LEU:HB2  | 1.99                     | 0.44              |
| 2:Y:607:CHL:H12  | 2:Y:607:CHL:HMA2 | 1.99                     | 0.44              |
| 3:Y:611:CLA:H71  | 3:Y:612:CLA:ND   | 2.33                     | 0.44              |
| 3:N:604:CLA:H61  | 3:N:604:CLA:H101 | 1.81                     | 0.44              |
| 1:G:118:LEU:HG   | 3:G:604:CLA:H102 | 2.00                     | 0.44              |
| 3:N:603:CLA:H72  | 3:N:603:CLA:H112 | 1.80                     | 0.44              |
| 3:G:611:CLA:H143 | 3:G:611:CLA:H111 | 1.83                     | 0.44              |
| 1:Y:185:ARG:HB3  | 7:Y:618:LHG:H252 | 2.00                     | 0.44              |
| 1:N:59:ALA:HA    | 1:N:62:ARG:CZ    | 2.48                     | 0.44              |
| 1:Y:70:ARG:HG2   | 3:Y:610:CLA:C3C  | 2.48                     | 0.44              |
| 4:N:616:LUT:H35  | 4:N:616:LUT:H401 | 1.83                     | 0.44              |
| 1:G:127:ILE:HG12 | 2:G:605:CHL:HAC1 | 2.00                     | 0.43              |
| 3:G:611:CLA:HBB1 | 5:G:619:XAT:H221 | 1.99                     | 0.43              |
| 1:Y:52:SER:HB3   | 1:Y:58:PHE:HD1   | 1.81                     | 0.43              |
| 1:N:178:VAL:HG12 | 1:N:182:LYS:HE2  | 1.99                     | 0.43              |
| 3:Y:613:CLA:H112 | 7:Y:618:LHG:H342 | 1.99                     | 0.43              |
| 2:Y:608:CHL:H151 | 2:Y:608:CHL:H3A  | 2.00                     | 0.43              |
| 1:N:56:GLU:O     | 1:N:60:LYS:HG2   | 2.19                     | 0.43              |
| 5:N:617:XAT:H10  | 2:Y:601:CHL:H13  | 2.00                     | 0.43              |
| 5:G:619:XAT:H15  | 5:G:619:XAT:H201 | 1.71                     | 0.43              |
| 1:Y:110:LEU:HB3  | 1:Y:121:ALA:HB3  | 2.00                     | 0.43              |
| 2:Y:608:CHL:H201 | 3:Y:610:CLA:H141 | 2.00                     | 0.43              |
| 2:N:609:CHL:HHC  | 2:Y:601:CHL:H52  | 2.01                     | 0.43              |
| 7:N:619:LHG:H282 | 7:N:619:LHG:H312 | 1.80                     | 0.43              |
| 3:G:613:CLA:H61  | 3:G:613:CLA:H2   | 1.66                     | 0.43              |
| 1:Y:112:TYR:HE2  | 3:Y:604:CLA:H143 | 1.84                     | 0.43              |
| 4:Y:615:LUT:H31  | 4:Y:615:LUT:H391 | 1.92                     | 0.43              |
| 3:Y:603:CLA:HBB2 | 2:Y:609:CHL:H202 | 2.00                     | 0.43              |
| 1:N:139:GLU:HG3  | 1:N:142:ARG:HH21 | 1.83                     | 0.43              |
| 2:G:601:CHL:H51  | 5:G:619:XAT:H401 | 2.00                     | 0.43              |
| 4:N:615:LUT:H35  | 4:N:615:LUT:H401 | 1.82                     | 0.43              |
| 1:Y:118:LEU:HD21 | 3:Y:604:CLA:H161 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:Y:618:LHG:H332 | 7:Y:618:LHG:H301 | 1.41                     | 0.43              |
| 5:N:617:XAT:H31  | 5:N:617:XAT:H391 | 1.86                     | 0.42              |
| 2:G:607:CHL:H143 | 2:G:607:CHL:H111 | 1.80                     | 0.42              |
| 3:Y:611:CLA:H142 | 3:Y:611:CLA:H111 | 1.55                     | 0.42              |
| 4:Y:616:LUT:H201 | 4:Y:616:LUT:H15  | 1.80                     | 0.42              |
| 1:N:174:ALA:O    | 1:N:178:VAL:HG23 | 2.19                     | 0.42              |
| 2:G:601:CHL:C3C  | 5:G:619:XAT:H362 | 2.50                     | 0.42              |
| 3:Y:603:CLA:H61  | 3:Y:603:CLA:H2   | 1.79                     | 0.42              |
| 1:G:174:ALA:O    | 1:G:178:VAL:HG23 | 2.20                     | 0.42              |
| 1:G:225:ALA:HB3  | 1:Y:105:PHE:HE2  | 1.85                     | 0.42              |
| 2:G:601:CHL:H141 | 2:G:601:CHL:H162 | 1.73                     | 0.42              |
| 4:Y:615:LUT:H11  | 4:Y:615:LUT:H191 | 1.87                     | 0.42              |
| 7:Y:618:LHG:H332 | 7:Y:618:LHG:HC91 | 2.02                     | 0.42              |
| 2:G:607:CHL:H93  | 2:G:607:CHL:H61  | 1.83                     | 0.42              |
| 4:G:616:LUT:H35  | 4:G:616:LUT:H401 | 1.90                     | 0.42              |
| 2:G:601:CHL:HMA1 | 5:G:619:XAT:H403 | 2.01                     | 0.41              |
| 1:N:75:GLY:HA2   | 4:N:616:LUT:H181 | 2.02                     | 0.41              |
| 2:G:601:CHL:H161 | 2:G:601:CHL:H202 | 1.82                     | 0.41              |
| 2:G:601:CHL:H13  | 7:G:618:LHG:H211 | 2.02                     | 0.41              |
| 5:N:620:XAT:H201 | 5:N:620:XAT:H15  | 1.67                     | 0.41              |
| 3:Y:610:CLA:CBB  | 4:Y:615:LUT:H32  | 2.51                     | 0.41              |
| 1:N:191:MET:HE2  | 4:N:616:LUT:H10  | 2.03                     | 0.41              |
| 1:Y:180:GLU:HB2  | 3:Y:610:CLA:C2B  | 2.51                     | 0.41              |
| 2:N:608:CHL:H162 | 2:N:608:CHL:H122 | 1.70                     | 0.41              |
| 4:N:616:LUT:H11  | 4:N:616:LUT:H191 | 1.87                     | 0.41              |
| 3:G:602:CLA:H93  | 3:G:602:CLA:H111 | 1.92                     | 0.41              |
| 1:N:185:ARG:HH11 | 3:N:602:CLA:C1D  | 2.34                     | 0.41              |
| 5:N:617:XAT:H28  | 7:Y:618:LHG:H362 | 2.02                     | 0.41              |
| 5:N:617:XAT:H14  | 2:Y:601:CHL:H8   | 2.02                     | 0.41              |
| 1:G:67:ILE:HD13  | 1:G:67:ILE:HA    | 1.91                     | 0.41              |
| 1:Y:17:TYR:HE2   | 1:Y:174:ALA:HB1  | 1.86                     | 0.41              |
| 2:Y:601:CHL:HBA1 | 2:Y:601:CHL:H3A  | 1.71                     | 0.41              |
| 1:N:85:LEU:HD23  | 1:N:85:LEU:HA    | 1.91                     | 0.40              |
| 3:G:610:CLA:H2   | 4:G:615:LUT:H28  | 2.02                     | 0.40              |
| 7:Y:618:LHG:H271 | 7:Y:618:LHG:HC62 | 2.02                     | 0.40              |
| 2:N:607:CHL:H12  | 2:N:607:CHL:HMA2 | 2.01                     | 0.40              |
| 5:N:617:XAT:H15  | 5:N:617:XAT:H201 | 1.71                     | 0.40              |
| 1:G:112:TYR:HD2  | 1:G:118:LEU:HD23 | 1.85                     | 0.40              |
| 3:G:602:CLA:H161 | 3:G:602:CLA:H141 | 1.84                     | 0.40              |
| 1:Y:17:TYR:CE2   | 1:Y:174:ALA:HB1  | 2.56                     | 0.40              |
| 3:N:603:CLA:H91  | 2:N:609:CHL:H143 | 2.03                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:G:610:CLA:H61 | 4:G:615:LUT:H371 | 2.03                     | 0.40              |
| 3:G:613:CLA:H2A | 3:G:613:CLA:HED3 | 2.02                     | 0.40              |
| 4:Y:616:LUT:H31 | 4:Y:616:LUT:H391 | 1.93                     | 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   | G     | 216/218 (99%) | 210 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | N     | 216/218 (99%) | 211 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | Y     | 216/218 (99%) | 209 (97%) | 7 (3%)  | 0        | 100         | 100 |
| All | All   | 648/654 (99%) | 630 (97%) | 18 (3%) | 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   | G     | 168/168 (100%) | 168 (100%) | 0        | 100         | 100 |
| 1   | N     | 168/168 (100%) | 168 (100%) | 0        | 100         | 100 |
| 1   | Y     | 168/168 (100%) | 167 (99%)  | 1 (1%)   | 78          | 91  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |    |
|-----|-------|----------------|------------|----------|-------------|----|
| All | All   | 504/504 (100%) | 503 (100%) | 1 (0%)   | 85          | 95 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Y     | 182 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 115 | ASN  |
| 1   | G     | 183 | ASN  |
| 1   | Y     | 131 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

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 |
| 4   | LUT  | Y     | 616 | -    | 42,43,43     | 0.77 | 0        | 51,60,60    | 1.82 | 10 (19%) |
| 4   | LUT  | N     | 615 | -    | 42,43,43     | 0.72 | 0        | 51,60,60    | 1.75 | 10 (19%) |
| 4   | LUT  | N     | 616 | -    | 42,43,43     | 0.76 | 0        | 51,60,60    | 1.67 | 10 (19%) |
| 3   | CLA  | N     | 602 | 1    | 69,73,73     | 1.19 | 6 (8%)   | 82,113,113  | 1.24 | 8 (9%)   |
| 3   | CLA  | G     | 614 | -    | 53,57,73     | 1.36 | 7 (13%)  | 61,93,113   | 1.22 | 5 (8%)   |
| 2   | CHL  | G     | 601 | -    | 60,74,74     | 2.21 | 11 (18%) | 58,114,114  | 1.54 | 14 (24%) |
| 3   | CLA  | G     | 611 | 7    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.14 | 6 (7%)   |
| 3   | CLA  | Y     | 602 | 1    | 69,73,73     | 1.17 | 6 (8%)   | 82,113,113  | 1.18 | 6 (7%)   |
| 3   | CLA  | G     | 603 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.22 | 5 (6%)   |
| 4   | LUT  | G     | 615 | -    | 42,43,43     | 0.72 | 0        | 51,60,60    | 1.71 | 11 (21%) |
| 4   | LUT  | G     | 616 | -    | 42,43,43     | 0.72 | 0        | 51,60,60    | 1.69 | 11 (21%) |
| 3   | CLA  | N     | 614 | -    | 53,57,73     | 1.35 | 7 (13%)  | 61,93,113   | 1.27 | 4 (6%)   |
| 5   | XAT  | G     | 619 | -    | 41,47,47     | 0.96 | 2 (4%)   | 54,74,74    | 2.56 | 19 (35%) |
| 2   | CHL  | G     | 608 | -    | 60,74,74     | 2.33 | 11 (18%) | 58,114,114  | 1.44 | 10 (17%) |
| 2   | CHL  | N     | 607 | -    | 60,74,74     | 2.26 | 11 (18%) | 58,114,114  | 1.64 | 12 (20%) |
| 2   | CHL  | Y     | 606 | -    | 45,59,74     | 2.65 | 9 (20%)  | 40,96,114   | 1.79 | 14 (35%) |
| 3   | CLA  | Y     | 603 | -    | 69,73,73     | 1.16 | 6 (8%)   | 82,113,113  | 1.30 | 7 (8%)   |
| 5   | XAT  | N     | 620 | -    | 41,47,47     | 0.93 | 2 (4%)   | 54,74,74    | 2.59 | 19 (35%) |
| 7   | LHG  | G     | 618 | 3    | 48,48,48     | 0.94 | 2 (4%)   | 51,54,54    | 1.07 | 3 (5%)   |
| 3   | CLA  | G     | 602 | 1    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.13 | 6 (7%)   |
| 3   | CLA  | N     | 604 | -    | 66,70,73     | 1.21 | 6 (9%)   | 78,109,113  | 1.21 | 6 (7%)   |
| 6   | NEX  | Y     | 617 | -    | 40,46,46     | 1.20 | 6 (15%)  | 50,70,70    | 1.51 | 10 (20%) |
| 3   | CLA  | N     | 603 | -    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.24 | 6 (7%)   |
| 6   | NEX  | N     | 618 | -    | 40,46,46     | 1.20 | 6 (15%)  | 50,70,70    | 1.50 | 10 (20%) |
| 3   | CLA  | Y     | 612 | 1    | 69,73,73     | 1.15 | 7 (10%)  | 82,113,113  | 1.10 | 5 (6%)   |
| 3   | CLA  | G     | 613 | 1    | 69,73,73     | 1.16 | 6 (8%)   | 82,113,113  | 1.28 | 6 (7%)   |
| 5   | XAT  | N     | 617 | -    | 41,47,47     | 0.96 | 2 (4%)   | 54,74,74    | 2.54 | 20 (37%) |
| 3   | CLA  | N     | 612 | -    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.17 | 5 (6%)   |
| 2   | CHL  | N     | 605 | -    | 42,56,74     | 2.72 | 9 (21%)  | 36,92,114   | 1.68 | 12 (33%) |
| 3   | CLA  | Y     | 613 | 1    | 69,73,73     | 1.16 | 6 (8%)   | 82,113,113  | 1.19 | 4 (4%)   |
| 3   | CLA  | Y     | 604 | -    | 66,70,73     | 1.20 | 6 (9%)   | 78,109,113  | 1.35 | 9 (11%)  |
| 2   | CHL  | Y     | 608 | -    | 60,74,74     | 2.28 | 10 (16%) | 58,114,114  | 1.48 | 10 (17%) |
| 3   | CLA  | N     | 613 | 1    | 69,73,73     | 1.18 | 6 (8%)   | 82,113,113  | 1.26 | 6 (7%)   |
| 7   | LHG  | Y     | 618 | 3    | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.08 | 3 (5%)   |
| 2   | CHL  | N     | 609 | 1    | 60,74,74     | 2.27 | 12 (20%) | 58,114,114  | 1.83 | 16 (27%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | CLA  | Y     | 610 | 1    | 69,73,73     | 1.16 | 7 (10%)  | 82,113,113  | 1.11 | 6 (7%)   |
| 7   | LHG  | N     | 619 | 3    | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.05 | 2 (3%)   |
| 3   | CLA  | N     | 610 | 1    | 69,73,73     | 1.15 | 7 (10%)  | 82,113,113  | 1.12 | 8 (9%)   |
| 2   | CHL  | G     | 607 | -    | 60,74,74     | 2.25 | 11 (18%) | 58,114,114  | 1.68 | 12 (20%) |
| 3   | CLA  | G     | 604 | -    | 66,70,73     | 1.20 | 7 (10%)  | 78,109,113  | 1.25 | 9 (11%)  |
| 2   | CHL  | G     | 609 | 1    | 60,74,74     | 2.29 | 12 (20%) | 58,114,114  | 1.87 | 14 (24%) |
| 2   | CHL  | N     | 606 | -    | 45,59,74     | 2.64 | 9 (20%)  | 40,96,114   | 1.84 | 15 (37%) |
| 4   | LUT  | Y     | 615 | -    | 42,43,43     | 0.77 | 0        | 51,60,60    | 1.65 | 11 (21%) |
| 6   | NEX  | G     | 617 | -    | 40,46,46     | 1.19 | 6 (15%)  | 50,70,70    | 1.50 | 10 (20%) |
| 2   | CHL  | G     | 606 | -    | 45,59,74     | 2.58 | 9 (20%)  | 40,96,114   | 1.87 | 15 (37%) |
| 2   | CHL  | Y     | 609 | 1    | 60,74,74     | 2.28 | 11 (18%) | 58,114,114  | 1.51 | 13 (22%) |
| 2   | CHL  | N     | 601 | 1    | 60,74,74     | 2.27 | 9 (15%)  | 58,114,114  | 1.50 | 14 (24%) |
| 3   | CLA  | G     | 610 | 1    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.20 | 11 (13%) |
| 3   | CLA  | G     | 612 | 1    | 69,73,73     | 1.16 | 7 (10%)  | 82,113,113  | 1.24 | 7 (8%)   |
| 2   | CHL  | G     | 605 | -    | 42,56,74     | 2.73 | 9 (21%)  | 36,92,114   | 1.67 | 9 (25%)  |
| 3   | CLA  | Y     | 614 | -    | 53,57,73     | 1.34 | 7 (13%)  | 61,93,113   | 1.18 | 5 (8%)   |
| 2   | CHL  | Y     | 607 | -    | 60,74,74     | 2.24 | 10 (16%) | 58,114,114  | 1.63 | 13 (22%) |
| 2   | CHL  | Y     | 601 | 1    | 60,74,74     | 2.28 | 10 (16%) | 58,114,114  | 1.50 | 12 (20%) |
| 3   | CLA  | Y     | 611 | 7    | 69,73,73     | 1.13 | 9 (13%)  | 82,113,113  | 1.14 | 4 (4%)   |
| 2   | CHL  | N     | 608 | -    | 60,74,74     | 2.30 | 10 (16%) | 58,114,114  | 1.39 | 11 (18%) |
| 3   | CLA  | N     | 611 | 7    | 69,73,73     | 1.14 | 9 (13%)  | 82,113,113  | 1.15 | 4 (4%)   |
| 2   | CHL  | Y     | 605 | -    | 42,56,74     | 2.70 | 10 (23%) | 36,92,114   | 1.67 | 12 (33%) |

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   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 4   | LUT  | Y     | 616 | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 4   | LUT  | N     | 615 | -    | -         | 5/29/67/67    | 0/2/2/2 |
| 4   | LUT  | N     | 616 | -    | -         | 1/29/67/67    | 0/2/2/2 |
| 3   | CLA  | N     | 602 | 1    | 1/1/15/20 | 7/39/115/115  | -       |
| 3   | CLA  | G     | 614 | -    | 1/1/11/20 | 10/20/96/115  | -       |
| 2   | CHL  | G     | 601 | -    | 3/3/20/26 | 13/39/137/137 | -       |
| 3   | CLA  | Y     | 602 | 1    | 1/1/15/20 | 9/39/115/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 3   | CLA  | G     | 611 | 7    | -         | 13/39/115/115 | -       |
| 3   | CLA  | G     | 603 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 4   | LUT  | G     | 615 | -    | -         | 4/29/67/67    | 0/2/2/2 |
| 4   | LUT  | G     | 616 | -    | -         | 3/29/67/67    | 0/2/2/2 |
| 3   | CLA  | N     | 614 | -    | 1/1/11/20 | 10/20/96/115  | -       |
| 5   | XAT  | G     | 619 | -    | -         | 7/31/93/93    | 0/4/4/4 |
| 2   | CHL  | G     | 608 | -    | 3/3/20/26 | 13/39/137/137 | -       |
| 2   | CHL  | N     | 607 | -    | 3/3/20/26 | 16/39/137/137 | -       |
| 2   | CHL  | Y     | 606 | -    | 3/3/17/26 | 7/21/119/137  | -       |
| 3   | CLA  | Y     | 603 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 5   | XAT  | N     | 620 | -    | -         | 7/31/93/93    | 0/4/4/4 |
| 7   | LHG  | G     | 618 | 3    | -         | 28/53/53/53   | -       |
| 3   | CLA  | G     | 602 | 1    | 1/1/15/20 | 14/39/115/115 | -       |
| 3   | CLA  | N     | 604 | -    | 1/1/14/20 | 11/36/112/115 | -       |
| 6   | NEX  | Y     | 617 | -    | -         | 9/27/83/83    | 0/3/3/3 |
| 3   | CLA  | N     | 603 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 6   | NEX  | N     | 618 | -    | -         | 9/27/83/83    | 0/3/3/3 |
| 3   | CLA  | Y     | 612 | 1    | 1/1/15/20 | 16/39/115/115 | -       |
| 3   | CLA  | G     | 613 | 1    | 1/1/15/20 | 10/39/115/115 | -       |
| 5   | XAT  | N     | 617 | -    | -         | 7/31/93/93    | 0/4/4/4 |
| 3   | CLA  | N     | 612 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 2   | CHL  | N     | 605 | -    | 3/3/16/26 | 7/18/116/137  | -       |
| 3   | CLA  | Y     | 613 | 1    | 1/1/15/20 | 8/39/115/115  | -       |
| 3   | CLA  | Y     | 604 | -    | 1/1/14/20 | 12/36/112/115 | -       |
| 2   | CHL  | Y     | 608 | -    | 3/3/20/26 | 13/39/137/137 | -       |
| 3   | CLA  | N     | 613 | 1    | 1/1/15/20 | 12/39/115/115 | -       |
| 7   | LHG  | Y     | 618 | 3    | -         | 35/53/53/53   | -       |
| 2   | CHL  | N     | 609 | 1    | 3/3/20/26 | 13/39/137/137 | -       |
| 3   | CLA  | Y     | 610 | 1    | 1/1/15/20 | 4/39/115/115  | -       |
| 7   | LHG  | N     | 619 | 3    | -         | 27/53/53/53   | -       |
| 3   | CLA  | N     | 610 | 1    | 1/1/15/20 | 6/39/115/115  | -       |
| 2   | CHL  | G     | 607 | -    | 3/3/20/26 | 13/39/137/137 | -       |
| 3   | CLA  | G     | 604 | -    | 1/1/14/20 | 12/36/112/115 | -       |
| 2   | CHL  | G     | 609 | 1    | 3/3/20/26 | 15/39/137/137 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 2   | CHL  | N     | 606 | -    | 3/3/17/26 | 9/21/119/137  | -       |
| 4   | LUT  | Y     | 615 | -    | -         | 4/29/67/67    | 0/2/2/2 |
| 6   | NEX  | G     | 617 | -    | -         | 9/27/83/83    | 0/3/3/3 |
| 2   | CHL  | G     | 606 | -    | 3/3/17/26 | 7/21/119/137  | -       |
| 2   | CHL  | Y     | 609 | 1    | 3/3/20/26 | 9/39/137/137  | -       |
| 2   | CHL  | N     | 601 | 1    | 3/3/20/26 | 10/39/137/137 | -       |
| 3   | CLA  | G     | 610 | 1    | 1/1/15/20 | 5/39/115/115  | -       |
| 3   | CLA  | G     | 612 | 1    | 1/1/15/20 | 18/39/115/115 | -       |
| 2   | CHL  | G     | 605 | -    | 3/3/16/26 | 8/18/116/137  | -       |
| 3   | CLA  | Y     | 614 | -    | 1/1/11/20 | 9/20/96/115   | -       |
| 2   | CHL  | Y     | 607 | -    | 3/3/20/26 | 13/39/137/137 | -       |
| 2   | CHL  | Y     | 601 | 1    | 3/3/20/26 | 8/39/137/137  | -       |
| 3   | CLA  | Y     | 611 | 7    | 1/1/15/20 | 15/39/115/115 | -       |
| 2   | CHL  | N     | 608 | -    | 3/3/20/26 | 12/39/137/137 | -       |
| 3   | CLA  | N     | 611 | 7    | 1/1/15/20 | 15/39/115/115 | -       |
| 2   | CHL  | Y     | 605 | -    | 3/3/16/26 | 8/18/116/137  | -       |

All (379) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | N     | 608 | CHL  | C3B-C4B | 10.03 | 1.51        | 1.41     |
| 2   | G     | 608 | CHL  | C3B-C4B | 10.02 | 1.51        | 1.41     |
| 2   | Y     | 608 | CHL  | C3B-C4B | 9.71  | 1.50        | 1.41     |
| 2   | Y     | 606 | CHL  | C3B-C4B | 9.21  | 1.50        | 1.41     |
| 2   | Y     | 609 | CHL  | C3B-C4B | 9.19  | 1.50        | 1.41     |
| 2   | Y     | 601 | CHL  | C3B-C4B | 9.13  | 1.50        | 1.41     |
| 2   | N     | 601 | CHL  | C3B-C4B | 9.01  | 1.50        | 1.41     |
| 2   | N     | 605 | CHL  | C3B-C4B | 8.93  | 1.50        | 1.41     |
| 2   | N     | 606 | CHL  | C3B-C4B | 8.92  | 1.50        | 1.41     |
| 2   | N     | 609 | CHL  | C3B-C4B | 8.88  | 1.50        | 1.41     |
| 2   | G     | 609 | CHL  | C3B-C4B | 8.82  | 1.50        | 1.41     |
| 2   | N     | 607 | CHL  | C3B-C4B | 8.81  | 1.50        | 1.41     |
| 2   | G     | 605 | CHL  | C3B-C4B | 8.78  | 1.49        | 1.41     |
| 2   | Y     | 605 | CHL  | C1B-C2B | 8.69  | 1.49        | 1.39     |
| 2   | Y     | 605 | CHL  | C3B-C4B | 8.62  | 1.49        | 1.41     |
| 2   | G     | 607 | CHL  | C3B-C4B | 8.57  | 1.49        | 1.41     |
| 2   | G     | 605 | CHL  | C1B-C2B | 8.57  | 1.49        | 1.39     |
| 2   | N     | 605 | CHL  | C1B-C2B | 8.54  | 1.49        | 1.39     |
| 2   | G     | 607 | CHL  | C1B-C2B | 8.53  | 1.49        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | Y     | 607 | CHL  | C1B-C2B | 8.49 | 1.49        | 1.39     |
| 2   | Y     | 607 | CHL  | C3B-C4B | 8.48 | 1.49        | 1.41     |
| 2   | N     | 606 | CHL  | C1B-C2B | 8.45 | 1.49        | 1.39     |
| 2   | G     | 606 | CHL  | C3B-C4B | 8.42 | 1.49        | 1.41     |
| 2   | N     | 601 | CHL  | C1B-C2B | 8.40 | 1.49        | 1.39     |
| 2   | Y     | 601 | CHL  | C1B-C2B | 8.35 | 1.49        | 1.39     |
| 2   | G     | 606 | CHL  | C1B-C2B | 8.28 | 1.49        | 1.39     |
| 2   | N     | 607 | CHL  | C1B-C2B | 8.20 | 1.48        | 1.39     |
| 2   | Y     | 609 | CHL  | C1B-C2B | 8.16 | 1.48        | 1.39     |
| 2   | Y     | 606 | CHL  | C1B-C2B | 8.16 | 1.48        | 1.39     |
| 2   | G     | 605 | CHL  | C1D-C2D | 8.10 | 1.48        | 1.39     |
| 2   | G     | 609 | CHL  | C1B-C2B | 8.09 | 1.48        | 1.39     |
| 2   | N     | 609 | CHL  | C1D-C2D | 8.07 | 1.48        | 1.39     |
| 2   | G     | 608 | CHL  | C1D-C2D | 8.06 | 1.48        | 1.39     |
| 2   | Y     | 609 | CHL  | C1D-C2D | 8.06 | 1.48        | 1.39     |
| 2   | G     | 601 | CHL  | C3B-C4B | 8.04 | 1.49        | 1.41     |
| 2   | Y     | 601 | CHL  | C1D-C2D | 8.01 | 1.48        | 1.39     |
| 2   | G     | 609 | CHL  | C1D-C2D | 8.00 | 1.48        | 1.39     |
| 2   | N     | 605 | CHL  | C1D-C2D | 7.99 | 1.48        | 1.39     |
| 2   | G     | 601 | CHL  | C1B-C2B | 7.98 | 1.48        | 1.39     |
| 2   | N     | 608 | CHL  | C1B-C2B | 7.98 | 1.48        | 1.39     |
| 2   | G     | 608 | CHL  | C1B-C2B | 7.96 | 1.48        | 1.39     |
| 2   | Y     | 605 | CHL  | C1D-C2D | 7.95 | 1.48        | 1.39     |
| 2   | N     | 606 | CHL  | C1D-C2D | 7.89 | 1.48        | 1.39     |
| 2   | N     | 608 | CHL  | C1D-C2D | 7.86 | 1.48        | 1.39     |
| 2   | N     | 601 | CHL  | C1D-C2D | 7.83 | 1.48        | 1.39     |
| 2   | Y     | 606 | CHL  | C1D-C2D | 7.81 | 1.48        | 1.39     |
| 2   | Y     | 608 | CHL  | C1B-C2B | 7.77 | 1.48        | 1.39     |
| 2   | Y     | 608 | CHL  | C1D-C2D | 7.74 | 1.48        | 1.39     |
| 2   | N     | 607 | CHL  | C1D-C2D | 7.72 | 1.48        | 1.39     |
| 2   | G     | 606 | CHL  | C1D-C2D | 7.69 | 1.48        | 1.39     |
| 2   | Y     | 607 | CHL  | C1D-C2D | 7.65 | 1.48        | 1.39     |
| 2   | G     | 607 | CHL  | C1D-C2D | 7.54 | 1.48        | 1.39     |
| 2   | G     | 601 | CHL  | C1D-C2D | 7.46 | 1.48        | 1.39     |
| 2   | N     | 609 | CHL  | C1B-C2B | 7.11 | 1.47        | 1.39     |
| 2   | N     | 609 | CHL  | C2C-C3C | 4.65 | 1.40        | 1.36     |
| 2   | G     | 609 | CHL  | C2C-C3C | 4.60 | 1.40        | 1.36     |
| 2   | Y     | 606 | CHL  | C3D-C4D | 4.60 | 1.48        | 1.41     |
| 2   | G     | 606 | CHL  | C3D-C4D | 4.58 | 1.48        | 1.41     |
| 2   | N     | 606 | CHL  | C2C-C3C | 4.54 | 1.40        | 1.36     |
| 2   | N     | 606 | CHL  | C3D-C4D | 4.51 | 1.48        | 1.41     |
| 2   | Y     | 606 | CHL  | C2C-C3C | 4.51 | 1.40        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | G     | 607 | CHL  | C3D-C4D | 4.50 | 1.48        | 1.41     |
| 2   | Y     | 607 | CHL  | C3D-C4D | 4.48 | 1.48        | 1.41     |
| 2   | Y     | 608 | CHL  | C3D-C4D | 4.46 | 1.48        | 1.41     |
| 2   | N     | 607 | CHL  | C3D-C4D | 4.44 | 1.48        | 1.41     |
| 2   | N     | 605 | CHL  | C3D-C4D | 4.40 | 1.48        | 1.41     |
| 2   | Y     | 609 | CHL  | C3D-C4D | 4.38 | 1.48        | 1.41     |
| 2   | N     | 608 | CHL  | C3D-C4D | 4.35 | 1.48        | 1.41     |
| 2   | G     | 605 | CHL  | C3D-C4D | 4.35 | 1.48        | 1.41     |
| 7   | G     | 618 | LHG  | O8-C23  | 4.34 | 1.46        | 1.33     |
| 2   | Y     | 605 | CHL  | C3D-C4D | 4.28 | 1.48        | 1.41     |
| 2   | G     | 606 | CHL  | C2C-C3C | 4.27 | 1.40        | 1.36     |
| 2   | N     | 609 | CHL  | C3D-C4D | 4.23 | 1.48        | 1.41     |
| 2   | G     | 609 | CHL  | C3D-C4D | 4.19 | 1.47        | 1.41     |
| 2   | G     | 605 | CHL  | C2C-C3C | 4.19 | 1.40        | 1.36     |
| 7   | Y     | 618 | LHG  | O8-C23  | 4.14 | 1.45        | 1.33     |
| 7   | N     | 619 | LHG  | O8-C23  | 4.14 | 1.45        | 1.33     |
| 2   | N     | 601 | CHL  | C3D-C4D | 4.14 | 1.47        | 1.41     |
| 2   | N     | 607 | CHL  | C2C-C3C | 4.08 | 1.40        | 1.36     |
| 2   | G     | 608 | CHL  | C3D-C4D | 4.04 | 1.47        | 1.41     |
| 7   | N     | 619 | LHG  | O7-C7   | 3.95 | 1.45        | 1.34     |
| 7   | Y     | 618 | LHG  | O7-C7   | 3.94 | 1.45        | 1.34     |
| 3   | N     | 602 | CLA  | C1D-ND  | 3.94 | 1.43        | 1.37     |
| 2   | Y     | 601 | CHL  | C3D-C4D | 3.91 | 1.47        | 1.41     |
| 2   | N     | 605 | CHL  | C2C-C3C | 3.91 | 1.40        | 1.36     |
| 3   | N     | 613 | CLA  | C1D-ND  | 3.90 | 1.43        | 1.37     |
| 7   | G     | 618 | LHG  | O7-C7   | 3.88 | 1.45        | 1.34     |
| 2   | G     | 607 | CHL  | C2C-C3C | 3.86 | 1.40        | 1.36     |
| 2   | Y     | 607 | CHL  | C2C-C3C | 3.82 | 1.40        | 1.36     |
| 2   | G     | 601 | CHL  | C3D-C4D | 3.81 | 1.47        | 1.41     |
| 3   | N     | 603 | CLA  | C1D-ND  | 3.76 | 1.42        | 1.37     |
| 2   | Y     | 605 | CHL  | C2C-C3C | 3.74 | 1.40        | 1.36     |
| 3   | G     | 614 | CLA  | C1D-ND  | 3.70 | 1.42        | 1.37     |
| 3   | N     | 614 | CLA  | C1D-ND  | 3.69 | 1.42        | 1.37     |
| 3   | Y     | 614 | CLA  | C1D-ND  | 3.65 | 1.42        | 1.37     |
| 3   | Y     | 610 | CLA  | C1D-ND  | 3.65 | 1.42        | 1.37     |
| 3   | G     | 611 | CLA  | C1D-ND  | 3.64 | 1.42        | 1.37     |
| 3   | G     | 610 | CLA  | C1D-ND  | 3.62 | 1.42        | 1.37     |
| 2   | G     | 601 | CHL  | C2C-C3C | 3.60 | 1.39        | 1.36     |
| 3   | G     | 603 | CLA  | C1D-ND  | 3.59 | 1.42        | 1.37     |
| 2   | G     | 608 | CHL  | C2C-C3C | 3.57 | 1.39        | 1.36     |
| 3   | Y     | 602 | CLA  | C1D-ND  | 3.56 | 1.42        | 1.37     |
| 3   | N     | 604 | CLA  | C1D-ND  | 3.54 | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | Y     | 601 | CHL  | C2C-C3C | 3.54  | 1.39        | 1.36     |
| 3   | N     | 610 | CLA  | C1D-ND  | 3.51  | 1.42        | 1.37     |
| 3   | G     | 602 | CLA  | C1D-ND  | 3.51  | 1.42        | 1.37     |
| 3   | G     | 614 | CLA  | C4B-NB  | 3.50  | 1.42        | 1.37     |
| 3   | Y     | 613 | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 3   | N     | 612 | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 3   | Y     | 603 | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 3   | G     | 611 | CLA  | C4B-NB  | 3.45  | 1.42        | 1.37     |
| 3   | G     | 613 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 3   | G     | 602 | CLA  | C4B-NB  | 3.43  | 1.42        | 1.37     |
| 3   | Y     | 614 | CLA  | C4B-NB  | 3.42  | 1.42        | 1.37     |
| 2   | N     | 601 | CHL  | C2C-C3C | 3.42  | 1.39        | 1.36     |
| 3   | G     | 612 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 2   | Y     | 609 | CHL  | C2C-C3C | 3.39  | 1.39        | 1.36     |
| 3   | G     | 604 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 3   | N     | 614 | CLA  | C4B-NB  | 3.39  | 1.42        | 1.37     |
| 3   | N     | 612 | CLA  | C4B-NB  | 3.32  | 1.42        | 1.37     |
| 3   | G     | 610 | CLA  | C4B-NB  | 3.28  | 1.42        | 1.37     |
| 2   | N     | 608 | CHL  | C2C-C3C | 3.27  | 1.39        | 1.36     |
| 3   | Y     | 612 | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 3   | N     | 603 | CLA  | C4B-NB  | 3.26  | 1.42        | 1.37     |
| 3   | G     | 603 | CLA  | C4B-NB  | 3.25  | 1.42        | 1.37     |
| 2   | N     | 609 | CHL  | CMB-C2B | -3.24 | 1.45        | 1.51     |
| 3   | G     | 613 | CLA  | C4B-NB  | 3.23  | 1.42        | 1.37     |
| 2   | Y     | 608 | CHL  | C2C-C3C | 3.22  | 1.39        | 1.36     |
| 3   | Y     | 604 | CLA  | C1D-ND  | 3.22  | 1.42        | 1.37     |
| 2   | G     | 601 | CHL  | C1A-CHA | -3.20 | 1.36        | 1.40     |
| 3   | G     | 604 | CLA  | C4B-NB  | 3.19  | 1.42        | 1.37     |
| 3   | N     | 613 | CLA  | C4B-NB  | 3.18  | 1.42        | 1.37     |
| 3   | Y     | 613 | CLA  | C4B-NB  | 3.18  | 1.42        | 1.37     |
| 3   | N     | 604 | CLA  | C4B-NB  | 3.17  | 1.42        | 1.37     |
| 2   | G     | 608 | CHL  | CMD-C2D | -3.12 | 1.45        | 1.51     |
| 3   | Y     | 603 | CLA  | C4B-NB  | 3.09  | 1.41        | 1.37     |
| 3   | Y     | 612 | CLA  | C4B-NB  | 3.08  | 1.41        | 1.37     |
| 3   | Y     | 604 | CLA  | C4B-NB  | 3.08  | 1.41        | 1.37     |
| 5   | G     | 619 | XAT  | O4-C5   | -3.03 | 1.42        | 1.46     |
| 3   | Y     | 610 | CLA  | C4B-NB  | 3.03  | 1.41        | 1.37     |
| 3   | N     | 602 | CLA  | C4B-NB  | 3.02  | 1.41        | 1.37     |
| 3   | G     | 612 | CLA  | C4B-NB  | 2.99  | 1.41        | 1.37     |
| 2   | G     | 601 | CHL  | CMD-C2D | -2.98 | 1.45        | 1.51     |
| 5   | N     | 617 | XAT  | O4-C5   | -2.97 | 1.42        | 1.46     |
| 2   | G     | 609 | CHL  | CMB-C2B | -2.96 | 1.45        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | Y     | 609 | CHL  | CMB-C2B | -2.95 | 1.45        | 1.51     |
| 2   | G     | 601 | CHL  | CAC-C3C | -2.93 | 1.46        | 1.51     |
| 2   | N     | 601 | CHL  | CMD-C2D | -2.89 | 1.45        | 1.51     |
| 2   | G     | 606 | CHL  | CMB-C2B | -2.87 | 1.45        | 1.51     |
| 2   | Y     | 601 | CHL  | CMD-C2D | -2.87 | 1.45        | 1.51     |
| 3   | N     | 610 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 3   | Y     | 613 | CLA  | C1B-C2B | 2.83  | 1.49        | 1.43     |
| 3   | Y     | 602 | CLA  | C4B-NB  | 2.83  | 1.41        | 1.37     |
| 3   | N     | 611 | CLA  | C4B-NB  | 2.79  | 1.41        | 1.37     |
| 3   | N     | 611 | CLA  | C1D-ND  | 2.78  | 1.41        | 1.37     |
| 3   | Y     | 611 | CLA  | C4B-NB  | 2.76  | 1.41        | 1.37     |
| 5   | N     | 620 | XAT  | O4-C5   | -2.76 | 1.42        | 1.46     |
| 3   | N     | 613 | CLA  | C1B-C2B | 2.73  | 1.49        | 1.43     |
| 2   | G     | 607 | CHL  | CMD-C2D | -2.73 | 1.46        | 1.51     |
| 2   | Y     | 608 | CHL  | CAC-C3C | -2.72 | 1.46        | 1.51     |
| 3   | G     | 613 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 3   | Y     | 611 | CLA  | C1D-ND  | 2.70  | 1.41        | 1.37     |
| 3   | Y     | 614 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 2   | Y     | 608 | CHL  | CMB-C2B | -2.69 | 1.46        | 1.51     |
| 2   | Y     | 607 | CHL  | CMD-C2D | -2.67 | 1.46        | 1.51     |
| 2   | G     | 608 | CHL  | CMB-C2B | -2.66 | 1.46        | 1.51     |
| 3   | N     | 603 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 3   | N     | 614 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 3   | Y     | 603 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 3   | G     | 610 | CLA  | C3B-C4B | 2.62  | 1.50        | 1.42     |
| 3   | G     | 611 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 2   | G     | 601 | CHL  | CMB-C2B | -2.61 | 1.46        | 1.51     |
| 5   | N     | 617 | XAT  | O24-C25 | -2.61 | 1.42        | 1.46     |
| 3   | N     | 612 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 2   | Y     | 608 | CHL  | CMD-C2D | -2.60 | 1.46        | 1.51     |
| 2   | G     | 606 | CHL  | CMD-C2D | -2.59 | 1.46        | 1.51     |
| 2   | Y     | 606 | CHL  | CMB-C2B | -2.59 | 1.46        | 1.51     |
| 5   | G     | 619 | XAT  | O24-C25 | -2.59 | 1.42        | 1.46     |
| 2   | N     | 608 | CHL  | CMB-C2B | -2.59 | 1.46        | 1.51     |
| 3   | N     | 610 | CLA  | C3B-C4B | 2.59  | 1.50        | 1.42     |
| 3   | G     | 602 | CLA  | C3B-C4B | 2.59  | 1.50        | 1.42     |
| 2   | Y     | 601 | CHL  | C1A-CHA | -2.59 | 1.37        | 1.40     |
| 2   | G     | 605 | CHL  | CMD-C2D | -2.58 | 1.46        | 1.51     |
| 2   | N     | 608 | CHL  | CMD-C2D | -2.58 | 1.46        | 1.51     |
| 3   | N     | 604 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 2   | N     | 607 | CHL  | CMD-C2D | -2.56 | 1.46        | 1.51     |
| 2   | N     | 605 | CHL  | CMB-C2B | -2.56 | 1.46        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | N     | 605 | CHL  | CMD-C2D | -2.55 | 1.46        | 1.51     |
| 2   | Y     | 605 | CHL  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 2   | N     | 609 | CHL  | MG-NB   | -2.55 | 2.00        | 2.05     |
| 3   | Y     | 611 | CLA  | CMD-C2D | -2.55 | 1.45        | 1.50     |
| 3   | Y     | 610 | CLA  | C3B-C4B | 2.54  | 1.50        | 1.42     |
| 3   | G     | 614 | CLA  | C3B-C4B | 2.54  | 1.50        | 1.42     |
| 2   | Y     | 609 | CHL  | CHC-C4B | -2.54 | 1.35        | 1.39     |
| 3   | Y     | 604 | CLA  | CMB-C2B | -2.53 | 1.45        | 1.50     |
| 2   | G     | 607 | CHL  | CMB-C2B | -2.53 | 1.46        | 1.51     |
| 2   | Y     | 607 | CHL  | CMB-C2B | -2.53 | 1.46        | 1.51     |
| 5   | N     | 620 | XAT  | O24-C25 | -2.53 | 1.43        | 1.46     |
| 3   | N     | 610 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 3   | N     | 614 | CLA  | C3B-C4B | 2.52  | 1.50        | 1.42     |
| 3   | Y     | 604 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 2   | Y     | 606 | CHL  | CMD-C2D | -2.52 | 1.46        | 1.51     |
| 3   | G     | 603 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 2   | Y     | 601 | CHL  | CAC-C3C | -2.51 | 1.47        | 1.51     |
| 3   | G     | 602 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 3   | G     | 611 | CLA  | C3B-C4B | 2.51  | 1.50        | 1.42     |
| 2   | N     | 606 | CHL  | CMD-C2D | -2.50 | 1.46        | 1.51     |
| 3   | N     | 602 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 2   | N     | 601 | CHL  | C1A-CHA | -2.50 | 1.37        | 1.40     |
| 2   | N     | 606 | CHL  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 2   | G     | 609 | CHL  | CMD-C2D | -2.48 | 1.46        | 1.51     |
| 3   | N     | 612 | CLA  | C3B-C4B | 2.48  | 1.50        | 1.42     |
| 2   | Y     | 605 | CHL  | CMD-C2D | -2.48 | 1.46        | 1.51     |
| 3   | G     | 603 | CLA  | C3B-C4B | 2.48  | 1.50        | 1.42     |
| 2   | Y     | 601 | CHL  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 2   | N     | 601 | CHL  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 2   | G     | 605 | CHL  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 2   | N     | 607 | CHL  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 2   | Y     | 609 | CHL  | CMD-C2D | -2.47 | 1.46        | 1.51     |
| 3   | G     | 614 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 3   | Y     | 611 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 2   | N     | 609 | CHL  | CMD-C2D | -2.46 | 1.46        | 1.51     |
| 2   | G     | 608 | CHL  | CAC-C3C | -2.45 | 1.47        | 1.51     |
| 2   | G     | 609 | CHL  | MG-NB   | -2.45 | 2.00        | 2.05     |
| 3   | N     | 611 | CLA  | CMD-C2D | -2.44 | 1.45        | 1.50     |
| 3   | N     | 611 | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 6   | G     | 617 | NEX  | C32-C33 | -2.42 | 1.40        | 1.46     |
| 3   | Y     | 612 | CLA  | C1B-C2B | 2.42  | 1.48        | 1.43     |
| 2   | Y     | 609 | CHL  | CAC-C3C | -2.42 | 1.47        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | N     | 618 | NEX  | C32-C33 | -2.42 | 1.40        | 1.46     |
| 3   | Y     | 602 | CLA  | C3B-C4B | 2.42  | 1.49        | 1.42     |
| 6   | N     | 618 | NEX  | C28-C29 | -2.41 | 1.40        | 1.46     |
| 3   | G     | 612 | CLA  | CMB-C2B | -2.40 | 1.45        | 1.50     |
| 2   | Y     | 605 | CHL  | CAC-C3C | -2.40 | 1.47        | 1.51     |
| 6   | Y     | 617 | NEX  | C28-C29 | -2.39 | 1.40        | 1.46     |
| 6   | G     | 617 | NEX  | C28-C29 | -2.39 | 1.40        | 1.46     |
| 6   | Y     | 617 | NEX  | C32-C33 | -2.39 | 1.40        | 1.46     |
| 3   | N     | 603 | CLA  | C3B-C4B | 2.39  | 1.49        | 1.42     |
| 3   | N     | 602 | CLA  | C3B-C4B | 2.39  | 1.49        | 1.42     |
| 2   | N     | 601 | CHL  | CAC-C3C | -2.38 | 1.47        | 1.51     |
| 3   | Y     | 602 | CLA  | C1B-C2B | 2.38  | 1.48        | 1.43     |
| 2   | Y     | 609 | CHL  | C1A-CHA | -2.38 | 1.37        | 1.40     |
| 2   | N     | 606 | CHL  | CAC-C3C | -2.37 | 1.47        | 1.51     |
| 2   | N     | 607 | CHL  | CAC-C3C | -2.37 | 1.47        | 1.51     |
| 2   | G     | 605 | CHL  | CAC-C3C | -2.37 | 1.47        | 1.51     |
| 3   | Y     | 603 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 3   | Y     | 610 | CLA  | C1B-C2B | 2.36  | 1.48        | 1.43     |
| 2   | N     | 609 | CHL  | CBD-CGD | -2.35 | 1.49        | 1.52     |
| 2   | N     | 608 | CHL  | CAC-C3C | -2.35 | 1.47        | 1.51     |
| 2   | Y     | 607 | CHL  | CAC-C3C | -2.35 | 1.47        | 1.51     |
| 6   | Y     | 617 | NEX  | C12-C13 | -2.35 | 1.40        | 1.46     |
| 2   | G     | 607 | CHL  | CAC-C3C | -2.35 | 1.47        | 1.51     |
| 3   | G     | 604 | CLA  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 2   | G     | 601 | CHL  | CBD-CGD | -2.34 | 1.49        | 1.52     |
| 3   | G     | 610 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.38     |
| 3   | G     | 614 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.38     |
| 2   | G     | 608 | CHL  | C3B-C2B | -2.34 | 1.37        | 1.40     |
| 3   | Y     | 612 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 6   | N     | 618 | NEX  | C12-C13 | -2.33 | 1.41        | 1.46     |
| 3   | N     | 613 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 2   | G     | 609 | CHL  | CBD-CGD | -2.33 | 1.49        | 1.52     |
| 3   | G     | 604 | CLA  | CMB-C2B | -2.32 | 1.46        | 1.50     |
| 6   | G     | 617 | NEX  | C12-C13 | -2.32 | 1.41        | 1.46     |
| 3   | Y     | 614 | CLA  | CMD-C2D | -2.32 | 1.46        | 1.50     |
| 2   | N     | 607 | CHL  | CBD-CGD | -2.31 | 1.49        | 1.52     |
| 3   | Y     | 604 | CLA  | CMD-C2D | -2.31 | 1.46        | 1.50     |
| 2   | N     | 605 | CHL  | CAC-C3C | -2.31 | 1.47        | 1.51     |
| 2   | N     | 608 | CHL  | C3B-C2B | -2.29 | 1.37        | 1.40     |
| 3   | G     | 610 | CLA  | C1B-C2B | 2.29  | 1.48        | 1.43     |
| 2   | N     | 609 | CHL  | C1A-CHA | -2.29 | 1.37        | 1.40     |
| 2   | G     | 607 | CHL  | CBD-CGD | -2.28 | 1.49        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | N     | 609 | CHL  | MG-ND   | -2.28 | 2.01        | 2.05     |
| 3   | Y     | 612 | CLA  | CMB-C2B | -2.27 | 1.46        | 1.50     |
| 3   | G     | 613 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 3   | G     | 604 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 2   | G     | 609 | CHL  | MG-ND   | -2.27 | 2.01        | 2.05     |
| 3   | G     | 612 | CLA  | MG-NA   | 2.26  | 2.11        | 2.06     |
| 2   | Y     | 606 | CHL  | CAC-C3C | -2.26 | 1.47        | 1.51     |
| 2   | G     | 606 | CHL  | CAC-C3C | -2.26 | 1.47        | 1.51     |
| 3   | G     | 612 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 2   | G     | 601 | CHL  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 2   | G     | 606 | CHL  | CHC-C4B | -2.25 | 1.36        | 1.39     |
| 3   | G     | 602 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 3   | Y     | 614 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 3   | N     | 604 | CLA  | CMB-C2B | -2.24 | 1.46        | 1.50     |
| 2   | G     | 609 | CHL  | CAC-C3C | -2.23 | 1.47        | 1.51     |
| 3   | Y     | 612 | CLA  | CMC-C2C | -2.23 | 1.46        | 1.50     |
| 3   | Y     | 611 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 2   | N     | 609 | CHL  | CAC-C3C | -2.23 | 1.47        | 1.51     |
| 3   | Y     | 613 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 3   | N     | 604 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 3   | N     | 611 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 2   | Y     | 608 | CHL  | CHC-C4B | -2.22 | 1.36        | 1.39     |
| 3   | G     | 614 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 6   | Y     | 617 | NEX  | C14-C13 | 2.20  | 1.40        | 1.35     |
| 3   | Y     | 604 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 3   | N     | 603 | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |
| 2   | Y     | 608 | CHL  | C3B-C2B | -2.19 | 1.37        | 1.40     |
| 2   | N     | 607 | CHL  | CHC-C1C | 2.19  | 1.43        | 1.39     |
| 3   | G     | 604 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 2   | Y     | 606 | CHL  | CBD-CGD | -2.18 | 1.49        | 1.52     |
| 6   | N     | 618 | NEX  | C14-C13 | 2.17  | 1.40        | 1.35     |
| 6   | N     | 618 | NEX  | C30-C29 | 2.17  | 1.40        | 1.35     |
| 3   | Y     | 603 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 3   | N     | 611 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 6   | G     | 617 | NEX  | C30-C29 | 2.17  | 1.40        | 1.35     |
| 3   | Y     | 611 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 3   | N     | 614 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 3   | G     | 612 | CLA  | C1B-C2B | 2.16  | 1.48        | 1.43     |
| 3   | G     | 613 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 3   | G     | 603 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 6   | Y     | 617 | NEX  | C30-C29 | 2.16  | 1.40        | 1.35     |
| 3   | N     | 602 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | N     | 613 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 6   | Y     | 617 | NEX  | C34-C33 | 2.15  | 1.40        | 1.35     |
| 3   | N     | 611 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 3   | N     | 610 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 3   | Y     | 602 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 3   | Y     | 612 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 2   | Y     | 607 | CHL  | CBD-CGD | -2.14 | 1.49        | 1.52     |
| 3   | G     | 603 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 3   | Y     | 613 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 6   | G     | 617 | NEX  | C14-C13 | 2.14  | 1.40        | 1.35     |
| 2   | G     | 605 | CHL  | CHC-C1C | 2.13  | 1.43        | 1.39     |
| 2   | N     | 605 | CHL  | CHC-C1C | 2.13  | 1.43        | 1.39     |
| 6   | N     | 618 | NEX  | C34-C33 | 2.13  | 1.40        | 1.35     |
| 3   | Y     | 613 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 6   | G     | 617 | NEX  | C34-C33 | 2.12  | 1.40        | 1.35     |
| 3   | N     | 612 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 3   | N     | 610 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 3   | N     | 610 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 2   | N     | 607 | CHL  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 3   | N     | 614 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 3   | N     | 603 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 2   | G     | 607 | CHL  | CHC-C1C | 2.11  | 1.43        | 1.39     |
| 2   | N     | 606 | CHL  | CBD-CGD | -2.11 | 1.49        | 1.52     |
| 3   | N     | 611 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 3   | G     | 604 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 3   | G     | 610 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 2   | Y     | 609 | CHL  | C3B-C2B | -2.10 | 1.37        | 1.40     |
| 2   | Y     | 605 | CHL  | C1A-CHA | -2.10 | 1.37        | 1.40     |
| 3   | G     | 610 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 3   | Y     | 610 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 3   | Y     | 602 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 3   | Y     | 603 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 3   | N     | 604 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 3   | N     | 612 | CLA  | CHC-C1C | 2.08  | 1.42        | 1.38     |
| 3   | Y     | 614 | CLA  | CHC-C1C | 2.08  | 1.42        | 1.38     |
| 3   | N     | 612 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 3   | N     | 613 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 2   | G     | 608 | CHL  | C1A-CHA | -2.08 | 1.37        | 1.40     |
| 3   | G     | 614 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 3   | Y     | 610 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 3   | G     | 611 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 3   | G     | 611 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | Y     | 607 | CHL  | CHC-C1C | 2.06  | 1.43        | 1.39     |
| 3   | G     | 603 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 3   | Y     | 611 | CLA  | C3B-C4B | 2.06  | 1.48        | 1.42     |
| 2   | G     | 609 | CHL  | C1A-CHA | -2.06 | 1.37        | 1.40     |
| 3   | Y     | 611 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 2   | Y     | 601 | CHL  | CHC-C4B | -2.05 | 1.36        | 1.39     |
| 2   | G     | 608 | CHL  | CHC-C1C | 2.05  | 1.43        | 1.39     |
| 3   | G     | 611 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 3   | Y     | 614 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 3   | N     | 602 | CLA  | C1D-C2D | 2.04  | 1.49        | 1.45     |
| 3   | G     | 610 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 3   | Y     | 610 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 3   | G     | 611 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 3   | G     | 612 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 3   | N     | 603 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 3   | N     | 611 | CLA  | MG-ND   | -2.03 | 2.01        | 2.05     |
| 2   | G     | 607 | CHL  | MG-NB   | -2.02 | 2.01        | 2.05     |
| 2   | Y     | 605 | CHL  | CHC-C1C | 2.02  | 1.43        | 1.39     |
| 3   | G     | 613 | CLA  | CHC-C1C | 2.02  | 1.42        | 1.38     |
| 3   | N     | 614 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 3   | Y     | 611 | CLA  | MG-ND   | -2.02 | 2.01        | 2.05     |
| 2   | N     | 608 | CHL  | CHC-C1C | 2.01  | 1.43        | 1.39     |
| 3   | G     | 602 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 3   | G     | 602 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |

All (535) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | G     | 609 | CHL  | C1B-CHB-C4A | -6.53 | 117.12      | 121.32   |
| 3   | G     | 613 | CLA  | C4A-NA-C1A  | 6.32  | 109.56      | 106.68   |
| 5   | G     | 619 | XAT  | O24-C25-C24 | 6.11  | 119.22      | 113.49   |
| 3   | Y     | 613 | CLA  | C4A-NA-C1A  | 6.07  | 109.45      | 106.68   |
| 5   | N     | 620 | XAT  | C15-C14-C13 | -5.92 | 118.98      | 127.28   |
| 5   | N     | 620 | XAT  | O24-C25-C24 | 5.85  | 118.97      | 113.49   |
| 5   | N     | 617 | XAT  | C15-C14-C13 | -5.64 | 119.37      | 127.28   |
| 5   | N     | 617 | XAT  | O24-C25-C24 | 5.58  | 118.72      | 113.49   |
| 3   | Y     | 603 | CLA  | C4A-NA-C1A  | 5.51  | 109.19      | 106.68   |
| 5   | G     | 619 | XAT  | C15-C14-C13 | -5.49 | 119.57      | 127.28   |
| 5   | N     | 620 | XAT  | O4-C5-C4    | 5.49  | 118.63      | 113.49   |
| 5   | N     | 617 | XAT  | O4-C5-C4    | 5.45  | 118.60      | 113.49   |
| 5   | N     | 620 | XAT  | O24-C25-C38 | 5.43  | 121.11      | 115.05   |
| 3   | N     | 613 | CLA  | C4A-NA-C1A  | 5.35  | 109.12      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | G     | 607 | CHL  | C1B-CHB-C4A | -5.32 | 117.90      | 121.32   |
| 5   | G     | 619 | XAT  | O4-C5-C4    | 5.30  | 118.46      | 113.49   |
| 3   | N     | 603 | CLA  | C4A-NA-C1A  | 5.29  | 109.09      | 106.68   |
| 5   | N     | 617 | XAT  | O24-C25-C38 | 5.21  | 120.87      | 115.05   |
| 2   | G     | 608 | CHL  | C1B-CHB-C4A | 5.16  | 124.64      | 121.32   |
| 5   | G     | 619 | XAT  | O24-C25-C38 | 4.98  | 120.62      | 115.05   |
| 2   | N     | 609 | CHL  | O2D-CGD-CBD | 4.98  | 116.42      | 110.95   |
| 3   | Y     | 611 | CLA  | C4A-NA-C1A  | 4.98  | 108.95      | 106.68   |
| 5   | G     | 619 | XAT  | O4-C5-C18   | 4.98  | 120.61      | 115.05   |
| 3   | Y     | 604 | CLA  | C4A-NA-C1A  | 4.97  | 108.95      | 106.68   |
| 3   | G     | 611 | CLA  | C4A-NA-C1A  | 4.95  | 108.94      | 106.68   |
| 3   | G     | 604 | CLA  | C4A-NA-C1A  | 4.93  | 108.93      | 106.68   |
| 3   | N     | 611 | CLA  | C4A-NA-C1A  | 4.91  | 108.92      | 106.68   |
| 2   | N     | 609 | CHL  | C1B-CHB-C4A | -4.86 | 118.20      | 121.32   |
| 3   | G     | 603 | CLA  | C4A-NA-C1A  | 4.82  | 108.88      | 106.68   |
| 3   | N     | 612 | CLA  | C4A-NA-C1A  | 4.81  | 108.87      | 106.68   |
| 5   | N     | 620 | XAT  | C35-C34-C33 | -4.77 | 120.59      | 127.28   |
| 3   | N     | 614 | CLA  | C4A-NA-C1A  | 4.76  | 108.85      | 106.68   |
| 2   | Y     | 608 | CHL  | C1B-CHB-C4A | 4.73  | 124.36      | 121.32   |
| 3   | N     | 602 | CLA  | C4A-NA-C1A  | 4.71  | 108.83      | 106.68   |
| 2   | G     | 606 | CHL  | O2D-CGD-CBD | 4.70  | 116.11      | 110.95   |
| 5   | N     | 617 | XAT  | O4-C5-C18   | 4.64  | 120.24      | 115.05   |
| 5   | N     | 617 | XAT  | C35-C34-C33 | -4.63 | 120.79      | 127.28   |
| 5   | G     | 619 | XAT  | C11-C10-C9  | -4.55 | 120.90      | 127.28   |
| 5   | N     | 620 | XAT  | C18-C5-C6   | -4.52 | 114.86      | 122.30   |
| 3   | N     | 604 | CLA  | C4A-NA-C1A  | 4.51  | 108.74      | 106.68   |
| 5   | N     | 620 | XAT  | C11-C10-C9  | -4.50 | 120.97      | 127.28   |
| 5   | N     | 620 | XAT  | O4-C5-C18   | 4.49  | 120.07      | 115.05   |
| 5   | G     | 619 | XAT  | C18-C5-C6   | -4.47 | 114.94      | 122.30   |
| 2   | G     | 609 | CHL  | O2D-CGD-CBD | 4.39  | 115.77      | 110.95   |
| 2   | N     | 607 | CHL  | C1B-CHB-C4A | -4.37 | 118.51      | 121.32   |
| 4   | Y     | 616 | LUT  | C15-C14-C13 | -4.32 | 121.21      | 127.28   |
| 5   | G     | 619 | XAT  | C35-C34-C33 | -4.28 | 121.28      | 127.28   |
| 5   | N     | 617 | XAT  | C18-C5-C6   | -4.27 | 115.27      | 122.30   |
| 4   | G     | 616 | LUT  | C15-C14-C13 | -4.27 | 121.29      | 127.28   |
| 2   | G     | 607 | CHL  | C4D-CHA-CBD | -4.25 | 104.69      | 108.97   |
| 4   | Y     | 616 | LUT  | C31-C30-C29 | -4.23 | 121.35      | 127.28   |
| 5   | N     | 620 | XAT  | C38-C25-C26 | -4.19 | 115.40      | 122.30   |
| 5   | G     | 619 | XAT  | C38-C25-C26 | -4.19 | 115.40      | 122.30   |
| 4   | N     | 615 | LUT  | C7-C8-C9    | -4.18 | 120.06      | 126.23   |
| 5   | N     | 617 | XAT  | C38-C25-C26 | -4.17 | 115.43      | 122.30   |
| 2   | G     | 609 | CHL  | C4D-ND-C1D  | 4.17  | 108.38      | 105.22   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | N     | 617 | XAT  | C11-C10-C9  | -4.13 | 121.49      | 127.28   |
| 2   | G     | 606 | CHL  | C4D-CHA-CBD | -4.12 | 104.81      | 108.97   |
| 2   | Y     | 607 | CHL  | C1B-CHB-C4A | -4.10 | 118.68      | 121.32   |
| 2   | N     | 607 | CHL  | C4D-CHA-CBD | -4.08 | 104.85      | 108.97   |
| 2   | Y     | 601 | CHL  | C1B-CHB-C4A | 4.07  | 123.94      | 121.32   |
| 2   | N     | 606 | CHL  | C4D-CHA-CBD | -4.05 | 104.88      | 108.97   |
| 3   | N     | 610 | CLA  | C4A-NA-C1A  | 4.03  | 108.52      | 106.68   |
| 4   | G     | 615 | LUT  | C21-C26-C27 | -4.03 | 108.19      | 112.83   |
| 4   | G     | 616 | LUT  | C31-C30-C29 | -4.02 | 121.64      | 127.28   |
| 4   | N     | 615 | LUT  | C35-C34-C33 | -4.02 | 121.65      | 127.28   |
| 2   | Y     | 607 | CHL  | C4D-CHA-CBD | -3.99 | 104.94      | 108.97   |
| 3   | G     | 602 | CLA  | C4A-NA-C1A  | 3.98  | 108.50      | 106.68   |
| 4   | N     | 615 | LUT  | C15-C14-C13 | -3.97 | 121.71      | 127.28   |
| 4   | N     | 616 | LUT  | C21-C26-C27 | -3.96 | 108.28      | 112.83   |
| 2   | Y     | 606 | CHL  | C4D-CHA-CBD | -3.95 | 104.98      | 108.97   |
| 4   | Y     | 616 | LUT  | C21-C26-C27 | -3.95 | 108.29      | 112.83   |
| 2   | N     | 606 | CHL  | O2D-CGD-CBD | 3.94  | 115.27      | 110.95   |
| 2   | N     | 609 | CHL  | C4D-ND-C1D  | 3.92  | 108.19      | 105.22   |
| 4   | G     | 615 | LUT  | C35-C34-C33 | -3.91 | 121.80      | 127.28   |
| 2   | N     | 609 | CHL  | CMB-C2B-C3B | 3.91  | 132.49      | 124.68   |
| 6   | G     | 617 | NEX  | C35-C15-C14 | 3.89  | 131.47      | 123.52   |
| 3   | G     | 614 | CLA  | C4A-NA-C1A  | 3.88  | 108.45      | 106.68   |
| 6   | N     | 618 | NEX  | C35-C15-C14 | 3.87  | 131.44      | 123.52   |
| 6   | Y     | 617 | NEX  | C35-C15-C14 | 3.87  | 131.44      | 123.52   |
| 3   | Y     | 604 | CLA  | C4-C3-C5    | 3.87  | 121.94      | 115.23   |
| 4   | N     | 615 | LUT  | C11-C10-C9  | -3.80 | 121.94      | 127.28   |
| 3   | Y     | 602 | CLA  | C4A-NA-C1A  | 3.80  | 108.41      | 106.68   |
| 4   | N     | 615 | LUT  | C21-C26-C27 | -3.80 | 108.46      | 112.83   |
| 4   | Y     | 615 | LUT  | C11-C10-C9  | -3.78 | 121.97      | 127.28   |
| 5   | N     | 620 | XAT  | C26-C27-C28 | -3.75 | 118.06      | 125.99   |
| 4   | Y     | 616 | LUT  | C27-C28-C29 | -3.74 | 118.28      | 126.32   |
| 7   | Y     | 618 | LHG  | O7-C7-C8    | 3.71  | 119.51      | 111.48   |
| 3   | G     | 610 | CLA  | CAC-C3C-C4C | 3.69  | 129.59      | 124.79   |
| 5   | G     | 619 | XAT  | C26-C27-C28 | -3.67 | 118.22      | 125.99   |
| 7   | G     | 618 | LHG  | O8-C23-C24  | 3.67  | 123.03      | 111.83   |
| 2   | N     | 607 | CHL  | O2D-CGD-CBD | 3.62  | 114.92      | 110.95   |
| 2   | Y     | 608 | CHL  | C4D-CHA-CBD | -3.56 | 105.38      | 108.97   |
| 2   | G     | 601 | CHL  | O2D-CGD-CBD | 3.55  | 114.84      | 110.95   |
| 3   | Y     | 612 | CLA  | C4A-NA-C1A  | 3.53  | 108.29      | 106.68   |
| 5   | G     | 619 | XAT  | C17-C1-C2   | -3.51 | 102.80      | 108.97   |
| 5   | N     | 620 | XAT  | C11-C12-C13 | -3.50 | 116.76      | 126.36   |
| 5   | N     | 617 | XAT  | C26-C27-C28 | -3.49 | 118.62      | 125.99   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | N     | 617 | XAT  | C17-C1-C2   | -3.47 | 102.87      | 108.97   |
| 6   | G     | 617 | NEX  | C15-C35-C34 | 3.46  | 130.61      | 123.52   |
| 6   | Y     | 617 | NEX  | C15-C35-C34 | 3.46  | 130.60      | 123.52   |
| 6   | N     | 618 | NEX  | C15-C35-C34 | 3.46  | 130.60      | 123.52   |
| 4   | G     | 616 | LUT  | C7-C8-C9    | -3.44 | 121.14      | 126.23   |
| 6   | Y     | 617 | NEX  | C39-C29-C30 | -3.44 | 117.24      | 122.82   |
| 2   | Y     | 605 | CHL  | O2D-CGD-CBD | 3.44  | 114.72      | 110.95   |
| 6   | N     | 618 | NEX  | C39-C29-C30 | -3.43 | 117.26      | 122.82   |
| 2   | G     | 601 | CHL  | C1B-CHB-C4A | 3.41  | 123.52      | 121.32   |
| 4   | N     | 616 | LUT  | C35-C34-C33 | -3.40 | 122.50      | 127.28   |
| 6   | G     | 617 | NEX  | C39-C29-C30 | -3.40 | 117.31      | 122.82   |
| 5   | N     | 617 | XAT  | C31-C30-C29 | -3.39 | 122.53      | 127.28   |
| 4   | Y     | 616 | LUT  | C35-C34-C33 | -3.38 | 122.54      | 127.28   |
| 3   | Y     | 614 | CLA  | C4A-NA-C1A  | 3.37  | 108.22      | 106.68   |
| 4   | N     | 616 | LUT  | C15-C14-C13 | -3.37 | 122.55      | 127.28   |
| 4   | N     | 616 | LUT  | C31-C30-C29 | -3.36 | 122.56      | 127.28   |
| 5   | N     | 617 | XAT  | C11-C12-C13 | -3.36 | 117.14      | 126.36   |
| 2   | Y     | 606 | CHL  | O2D-CGD-CBD | 3.36  | 114.63      | 110.95   |
| 4   | Y     | 616 | LUT  | C7-C8-C9    | -3.35 | 121.28      | 126.23   |
| 4   | Y     | 615 | LUT  | C15-C14-C13 | -3.35 | 122.58      | 127.28   |
| 4   | G     | 615 | LUT  | C11-C10-C9  | -3.35 | 122.58      | 127.28   |
| 2   | Y     | 609 | CHL  | C1C-CHC-C4B | 3.34  | 128.01      | 116.07   |
| 4   | G     | 616 | LUT  | C27-C28-C29 | -3.33 | 119.16      | 126.32   |
| 4   | G     | 616 | LUT  | C21-C26-C27 | -3.33 | 109.00      | 112.83   |
| 2   | G     | 608 | CHL  | C1C-CHC-C4B | 3.32  | 127.94      | 116.07   |
| 2   | G     | 609 | CHL  | C3D-C4D-CHA | 3.32  | 113.58      | 108.54   |
| 2   | Y     | 606 | CHL  | CMB-C2B-C3B | 3.32  | 131.31      | 124.68   |
| 4   | G     | 615 | LUT  | C15-C14-C13 | -3.31 | 122.63      | 127.28   |
| 2   | N     | 608 | CHL  | C4D-CHA-CBD | -3.29 | 105.65      | 108.97   |
| 2   | G     | 601 | CHL  | OMC-CMC-C2C | -3.29 | 119.41      | 125.12   |
| 5   | G     | 619 | XAT  | C11-C12-C13 | -3.28 | 117.37      | 126.36   |
| 5   | N     | 620 | XAT  | C18-C5-C4   | 3.27  | 117.91      | 114.24   |
| 2   | Y     | 607 | CHL  | O2D-CGD-CBD | 3.27  | 114.53      | 110.95   |
| 4   | Y     | 616 | LUT  | C11-C10-C9  | -3.26 | 122.71      | 127.28   |
| 3   | G     | 604 | CLA  | CMB-C2B-C1B | -3.25 | 120.47      | 125.42   |
| 4   | G     | 615 | LUT  | C7-C8-C9    | -3.25 | 121.42      | 126.23   |
| 4   | N     | 616 | LUT  | C11-C10-C9  | -3.25 | 122.72      | 127.28   |
| 2   | Y     | 607 | CHL  | C4D-ND-C1D  | 3.25  | 107.68      | 105.22   |
| 5   | G     | 619 | XAT  | C31-C30-C29 | -3.24 | 122.74      | 127.28   |
| 2   | G     | 607 | CHL  | C4D-ND-C1D  | 3.23  | 107.67      | 105.22   |
| 3   | Y     | 604 | CLA  | O2D-CGD-O1D | -3.22 | 117.58      | 123.85   |
| 2   | N     | 609 | CHL  | C3D-C4D-CHA | 3.22  | 113.44      | 108.54   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | Y     | 609 | CHL  | O2D-CGD-CBD | 3.22  | 114.48      | 110.95   |
| 5   | N     | 620 | XAT  | C17-C1-C2   | -3.21 | 103.33      | 108.97   |
| 2   | G     | 605 | CHL  | C4D-CHA-CBD | -3.21 | 105.73      | 108.97   |
| 3   | Y     | 604 | CLA  | CMB-C2B-C1B | -3.21 | 120.53      | 125.42   |
| 2   | G     | 609 | CHL  | C4D-CHA-CBD | -3.19 | 105.75      | 108.97   |
| 2   | N     | 607 | CHL  | C4D-ND-C1D  | 3.19  | 107.64      | 105.22   |
| 2   | N     | 608 | CHL  | C1B-CHB-C4A | 3.19  | 123.37      | 121.32   |
| 2   | G     | 607 | CHL  | C3D-C4D-CHA | 3.19  | 113.39      | 108.54   |
| 4   | Y     | 615 | LUT  | C21-C26-C27 | -3.17 | 109.19      | 112.83   |
| 2   | Y     | 605 | CHL  | O2D-CGD-O1D | -3.16 | 117.69      | 123.85   |
| 3   | G     | 611 | CLA  | O2D-CGD-O1D | -3.15 | 117.71      | 123.85   |
| 2   | N     | 609 | CHL  | C4D-CHA-CBD | -3.15 | 105.79      | 108.97   |
| 2   | G     | 609 | CHL  | CMB-C2B-C3B | 3.15  | 130.98      | 124.68   |
| 2   | N     | 607 | CHL  | C3D-C4D-CHA | 3.15  | 113.33      | 108.54   |
| 2   | N     | 606 | CHL  | CMB-C2B-C3B | 3.15  | 130.97      | 124.68   |
| 3   | N     | 610 | CLA  | O2D-CGD-O1D | -3.14 | 117.74      | 123.85   |
| 3   | Y     | 610 | CLA  | C4A-NA-C1A  | 3.14  | 108.11      | 106.68   |
| 4   | Y     | 615 | LUT  | C7-C8-C9    | -3.14 | 121.60      | 126.23   |
| 2   | G     | 606 | CHL  | O2D-CGD-O1D | -3.12 | 117.77      | 123.85   |
| 3   | G     | 612 | CLA  | CAA-C2A-C3A | -3.12 | 104.57      | 113.00   |
| 2   | Y     | 609 | CHL  | CHA-C1A-C2A | -3.12 | 125.99      | 133.31   |
| 3   | N     | 602 | CLA  | O2D-CGD-O1D | -3.11 | 117.79      | 123.85   |
| 2   | N     | 605 | CHL  | O2D-CGD-CBD | 3.09  | 114.34      | 110.95   |
| 4   | Y     | 615 | LUT  | C35-C34-C33 | -3.09 | 122.95      | 127.28   |
| 2   | N     | 605 | CHL  | O2D-CGD-O1D | -3.08 | 117.86      | 123.85   |
| 2   | N     | 607 | CHL  | CMB-C2B-C3B | 3.07  | 130.81      | 124.68   |
| 2   | Y     | 609 | CHL  | C1B-CHB-C4A | 3.06  | 123.29      | 121.32   |
| 2   | Y     | 607 | CHL  | C3D-C4D-CHA | 3.06  | 113.19      | 108.54   |
| 3   | Y     | 603 | CLA  | CAA-C2A-C3A | -3.06 | 104.73      | 113.00   |
| 6   | G     | 617 | NEX  | C32-C33-C34 | 3.04  | 123.79      | 119.01   |
| 3   | Y     | 610 | CLA  | C3B-C4B-NB  | -3.04 | 107.82      | 110.53   |
| 5   | G     | 619 | XAT  | C18-C5-C4   | 3.03  | 117.64      | 114.24   |
| 6   | N     | 618 | NEX  | C32-C33-C34 | 3.03  | 123.77      | 119.01   |
| 6   | Y     | 617 | NEX  | C32-C33-C34 | 3.02  | 123.76      | 119.01   |
| 2   | N     | 608 | CHL  | C1C-CHC-C4B | 3.01  | 126.84      | 116.07   |
| 2   | Y     | 608 | CHL  | C1C-CHC-C4B | 3.01  | 126.83      | 116.07   |
| 5   | N     | 617 | XAT  | C18-C5-C4   | 3.01  | 117.62      | 114.24   |
| 3   | G     | 602 | CLA  | O2D-CGD-O1D | -3.00 | 118.01      | 123.85   |
| 7   | N     | 619 | LHG  | O7-C7-C8    | 3.00  | 117.97      | 111.48   |
| 3   | G     | 610 | CLA  | C4A-NA-C1A  | 3.00  | 108.05      | 106.68   |
| 2   | G     | 606 | CHL  | C1B-CHB-C4A | 2.99  | 123.25      | 121.32   |
| 3   | Y     | 603 | CLA  | O2D-CGD-O1D | -2.99 | 118.02      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | G     | 617 | NEX  | C12-C13-C14 | 2.99  | 123.71      | 119.01   |
| 2   | N     | 609 | CHL  | O2D-CGD-O1D | -2.98 | 118.04      | 123.85   |
| 2   | G     | 605 | CHL  | O2D-CGD-CBD | 2.98  | 114.22      | 110.95   |
| 2   | Y     | 606 | CHL  | C3D-C4D-CHA | 2.98  | 113.07      | 108.54   |
| 2   | G     | 605 | CHL  | O2D-CGD-O1D | -2.97 | 118.06      | 123.85   |
| 3   | G     | 612 | CLA  | C4A-NA-C1A  | 2.97  | 108.03      | 106.68   |
| 6   | Y     | 617 | NEX  | C12-C13-C14 | 2.97  | 123.68      | 119.01   |
| 4   | N     | 615 | LUT  | C27-C28-C29 | -2.97 | 119.94      | 126.32   |
| 6   | N     | 618 | NEX  | C12-C13-C14 | 2.97  | 123.67      | 119.01   |
| 3   | N     | 604 | CLA  | O2D-CGD-O1D | -2.97 | 118.08      | 123.85   |
| 5   | N     | 620 | XAT  | C6-C7-C8    | -2.95 | 119.75      | 125.99   |
| 3   | N     | 613 | CLA  | CMB-C2B-C1B | -2.95 | 120.92      | 125.42   |
| 6   | G     | 617 | NEX  | C40-C33-C34 | -2.95 | 118.04      | 122.82   |
| 2   | G     | 606 | CHL  | C3D-C4D-CHA | 2.95  | 113.02      | 108.54   |
| 2   | G     | 601 | CHL  | C1C-CHC-C4B | 2.94  | 126.58      | 116.07   |
| 2   | G     | 601 | CHL  | C3C-C4C-NC  | -2.94 | 107.47      | 114.65   |
| 6   | N     | 618 | NEX  | C40-C33-C34 | -2.94 | 118.06      | 122.82   |
| 2   | Y     | 609 | CHL  | OBD-CAD-CBD | -2.94 | 121.51      | 125.82   |
| 6   | Y     | 617 | NEX  | C40-C33-C34 | -2.93 | 118.06      | 122.82   |
| 2   | Y     | 601 | CHL  | O2D-CGD-O1D | -2.93 | 118.14      | 123.85   |
| 3   | G     | 612 | CLA  | O2D-CGD-O1D | -2.93 | 118.14      | 123.85   |
| 3   | N     | 614 | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 2   | Y     | 605 | CHL  | C1C-CHC-C4B | 2.92  | 126.53      | 116.07   |
| 3   | N     | 603 | CLA  | CAA-C2A-C3A | -2.92 | 105.12      | 113.00   |
| 6   | Y     | 617 | NEX  | C20-C13-C14 | -2.92 | 118.09      | 122.82   |
| 6   | G     | 617 | NEX  | C20-C13-C14 | -2.91 | 118.10      | 122.82   |
| 6   | N     | 618 | NEX  | C20-C13-C14 | -2.91 | 118.10      | 122.82   |
| 2   | G     | 609 | CHL  | C1C-CHC-C4B | 2.91  | 126.48      | 116.07   |
| 2   | G     | 609 | CHL  | O2D-CGD-O1D | -2.91 | 118.19      | 123.85   |
| 2   | Y     | 607 | CHL  | CMB-C2B-C3B | 2.91  | 130.49      | 124.68   |
| 2   | N     | 601 | CHL  | CMB-C2B-C3B | 2.90  | 130.49      | 124.68   |
| 2   | G     | 601 | CHL  | CMB-C2B-C3B | 2.90  | 130.47      | 124.68   |
| 3   | Y     | 614 | CLA  | O2D-CGD-O1D | -2.90 | 118.21      | 123.85   |
| 2   | N     | 605 | CHL  | C1C-CHC-C4B | 2.89  | 126.41      | 116.07   |
| 2   | N     | 605 | CHL  | C4D-CHA-CBD | -2.88 | 106.06      | 108.97   |
| 3   | G     | 610 | CLA  | O2D-CGD-O1D | -2.88 | 118.24      | 123.85   |
| 3   | N     | 603 | CLA  | O2D-CGD-O1D | -2.88 | 118.24      | 123.85   |
| 4   | N     | 616 | LUT  | C7-C8-C9    | -2.88 | 121.98      | 126.23   |
| 2   | G     | 607 | CHL  | CMB-C2B-C3B | 2.88  | 130.43      | 124.68   |
| 3   | N     | 612 | CLA  | O2D-CGD-O1D | -2.87 | 118.26      | 123.85   |
| 5   | N     | 620 | XAT  | C7-C8-C9    | -2.87 | 121.08      | 125.53   |
| 2   | G     | 607 | CHL  | O2D-CGD-CBD | 2.86  | 114.09      | 110.95   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | Y     | 603 | CLA  | CHB-C4A-NA  | 2.86  | 128.53      | 124.40   |
| 2   | Y     | 606 | CHL  | C1C-CHC-C4B | 2.86  | 126.32      | 116.07   |
| 3   | G     | 614 | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 3   | G     | 602 | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 2   | G     | 601 | CHL  | O2D-CGD-O1D | -2.85 | 118.31      | 123.85   |
| 2   | Y     | 601 | CHL  | CMB-C2B-C3B | 2.84  | 130.36      | 124.68   |
| 2   | G     | 609 | CHL  | OMC-CMC-C2C | -2.84 | 120.19      | 125.12   |
| 3   | Y     | 602 | CLA  | O2D-CGD-O1D | -2.84 | 118.33      | 123.85   |
| 6   | N     | 618 | NEX  | C28-C29-C30 | 2.83  | 123.47      | 119.01   |
| 6   | Y     | 617 | NEX  | C28-C29-C30 | 2.83  | 123.47      | 119.01   |
| 2   | N     | 606 | CHL  | C1C-CHC-C4B | 2.83  | 126.19      | 116.07   |
| 3   | G     | 614 | CLA  | C3B-C4B-NB  | -2.83 | 108.01      | 110.53   |
| 4   | N     | 616 | LUT  | C27-C28-C29 | -2.82 | 120.25      | 126.32   |
| 2   | N     | 607 | CHL  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 2   | N     | 606 | CHL  | C1B-CHB-C4A | 2.82  | 123.14      | 121.32   |
| 2   | Y     | 609 | CHL  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 2   | N     | 609 | CHL  | C1C-CHC-C4B | 2.82  | 126.16      | 116.07   |
| 2   | Y     | 601 | CHL  | OMC-CMC-C2C | -2.81 | 120.23      | 125.12   |
| 2   | N     | 606 | CHL  | C3D-C4D-CHA | 2.81  | 112.81      | 108.54   |
| 6   | G     | 617 | NEX  | C28-C29-C30 | 2.81  | 123.43      | 119.01   |
| 2   | G     | 605 | CHL  | C3C-C4C-NC  | -2.81 | 107.79      | 114.65   |
| 3   | Y     | 610 | CLA  | O2D-CGD-O1D | -2.80 | 118.39      | 123.85   |
| 2   | N     | 601 | CHL  | CHA-C1A-C2A | -2.80 | 126.73      | 133.31   |
| 2   | N     | 606 | CHL  | O2D-CGD-O1D | -2.80 | 118.40      | 123.85   |
| 3   | G     | 610 | CLA  | C3B-C4B-NB  | -2.79 | 108.03      | 110.53   |
| 2   | N     | 601 | CHL  | C1C-CHC-C4B | 2.79  | 126.04      | 116.07   |
| 4   | G     | 616 | LUT  | C11-C10-C9  | -2.78 | 123.37      | 127.28   |
| 2   | N     | 607 | CHL  | C1C-CHC-C4B | 2.78  | 126.01      | 116.07   |
| 3   | N     | 613 | CLA  | O2A-CGA-O1A | -2.76 | 116.72      | 123.63   |
| 2   | G     | 607 | CHL  | C1C-CHC-C4B | 2.76  | 125.95      | 116.07   |
| 2   | G     | 608 | CHL  | CHA-C1A-C2A | -2.76 | 126.83      | 133.31   |
| 7   | G     | 618 | LHG  | O7-C7-C8    | 2.76  | 117.45      | 111.48   |
| 2   | N     | 605 | CHL  | CMB-C2B-C3B | 2.75  | 130.19      | 124.68   |
| 2   | Y     | 608 | CHL  | O2D-CGD-O1D | -2.75 | 118.50      | 123.85   |
| 2   | G     | 608 | CHL  | O2D-CGD-O1D | -2.74 | 118.52      | 123.85   |
| 3   | G     | 613 | CLA  | O2D-CGD-O1D | -2.74 | 118.52      | 123.85   |
| 2   | Y     | 601 | CHL  | CHA-C1A-C2A | -2.73 | 126.89      | 133.31   |
| 3   | G     | 603 | CLA  | O2D-CGD-O1D | -2.73 | 118.53      | 123.85   |
| 2   | G     | 606 | CHL  | CMB-C2B-C3B | 2.73  | 130.13      | 124.68   |
| 2   | G     | 607 | CHL  | OMC-CMC-C2C | -2.73 | 120.39      | 125.12   |
| 2   | Y     | 607 | CHL  | C1C-CHC-C4B | 2.72  | 125.82      | 116.07   |
| 2   | N     | 601 | CHL  | C1-C2-C3    | -2.72 | 121.73      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | G     | 605 | CHL  | CMB-C2B-C3B | 2.71  | 130.10      | 124.68   |
| 3   | N     | 603 | CLA  | CHB-C4A-NA  | 2.71  | 128.31      | 124.40   |
| 3   | N     | 611 | CLA  | O2D-CGD-O1D | -2.71 | 118.58      | 123.85   |
| 2   | Y     | 601 | CHL  | C1C-CHC-C4B | 2.70  | 125.74      | 116.07   |
| 3   | G     | 603 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 4   | G     | 615 | LUT  | C27-C28-C29 | -2.70 | 120.52      | 126.32   |
| 2   | N     | 605 | CHL  | C3C-C4C-NC  | -2.69 | 108.08      | 114.65   |
| 3   | Y     | 613 | CLA  | O2D-CGD-O1D | -2.69 | 118.61      | 123.85   |
| 2   | Y     | 607 | CHL  | OMC-CMC-C2C | -2.69 | 120.46      | 125.12   |
| 2   | N     | 609 | CHL  | OBD-CAD-CBD | -2.68 | 121.89      | 125.82   |
| 2   | G     | 609 | CHL  | C3C-C4C-NC  | -2.68 | 108.11      | 114.65   |
| 2   | N     | 609 | CHL  | C3C-C4C-NC  | -2.67 | 108.12      | 114.65   |
| 2   | Y     | 606 | CHL  | C1-C2-C3    | -2.67 | 122.45      | 126.76   |
| 2   | Y     | 607 | CHL  | O2D-CGD-O1D | -2.67 | 118.66      | 123.85   |
| 7   | Y     | 618 | LHG  | O8-C23-C24  | 2.67  | 119.96      | 111.83   |
| 3   | N     | 604 | CLA  | CMB-C2B-C1B | -2.66 | 121.37      | 125.42   |
| 2   | N     | 609 | CHL  | OMC-CMC-C2C | -2.66 | 120.50      | 125.12   |
| 2   | Y     | 601 | CHL  | O1D-CGD-CBD | 2.65  | 128.75      | 124.72   |
| 2   | Y     | 605 | CHL  | C3C-C4C-NC  | -2.65 | 108.17      | 114.65   |
| 5   | N     | 617 | XAT  | C15-C35-C34 | -2.65 | 118.10      | 123.52   |
| 2   | Y     | 608 | CHL  | O2D-CGD-CBD | 2.65  | 113.85      | 110.95   |
| 3   | N     | 613 | CLA  | O2D-CGD-O1D | -2.65 | 118.70      | 123.85   |
| 3   | Y     | 602 | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 3   | N     | 611 | CLA  | CHB-C4A-NA  | 2.64  | 128.21      | 124.40   |
| 4   | G     | 615 | LUT  | C30-C31-C32 | -2.64 | 115.56      | 123.20   |
| 5   | N     | 620 | XAT  | C31-C30-C29 | -2.64 | 123.58      | 127.28   |
| 2   | G     | 605 | CHL  | C3D-C4D-CHA | 2.63  | 112.54      | 108.54   |
| 3   | N     | 604 | CLA  | C1-C2-C3    | -2.63 | 121.89      | 126.20   |
| 5   | N     | 617 | XAT  | C27-C28-C29 | -2.63 | 121.46      | 125.53   |
| 2   | G     | 605 | CHL  | C4C-CHD-C1D | 2.62  | 125.45      | 116.07   |
| 4   | Y     | 616 | LUT  | C35-C15-C14 | -2.62 | 118.16      | 123.52   |
| 2   | N     | 601 | CHL  | O2D-CGD-O1D | -2.62 | 118.75      | 123.85   |
| 3   | Y     | 611 | CLA  | CHB-C4A-NA  | 2.62  | 128.18      | 124.40   |
| 2   | Y     | 608 | CHL  | C3D-C4D-CHA | 2.62  | 112.52      | 108.54   |
| 2   | G     | 609 | CHL  | OBD-CAD-CBD | -2.61 | 121.99      | 125.82   |
| 2   | G     | 605 | CHL  | C4D-ND-C1D  | 2.61  | 107.20      | 105.22   |
| 3   | Y     | 604 | CLA  | C5-C3-C2    | -2.61 | 115.32      | 121.17   |
| 3   | Y     | 612 | CLA  | CAA-C2A-C3A | -2.61 | 105.96      | 113.00   |
| 2   | N     | 608 | CHL  | O2D-CGD-O1D | -2.60 | 118.78      | 123.85   |
| 2   | G     | 606 | CHL  | C1C-CHC-C4B | 2.60  | 125.36      | 116.07   |
| 2   | Y     | 608 | CHL  | CMB-C2B-C3B | 2.60  | 129.87      | 124.68   |
| 3   | G     | 603 | CLA  | CHB-C4A-NA  | 2.60  | 128.15      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | G     | 619 | XAT  | C15-C35-C34 | -2.60 | 118.21      | 123.52   |
| 3   | Y     | 614 | CLA  | CHB-C4A-NA  | 2.59  | 128.14      | 124.40   |
| 4   | G     | 615 | LUT  | C18-C5-C6   | -2.59 | 121.65      | 124.48   |
| 2   | G     | 605 | CHL  | C1C-CHC-C4B | 2.59  | 125.33      | 116.07   |
| 2   | G     | 608 | CHL  | C4D-CHA-CBD | -2.59 | 106.36      | 108.97   |
| 2   | N     | 606 | CHL  | C1-C2-C3    | -2.59 | 122.58      | 126.76   |
| 5   | G     | 619 | XAT  | C7-C8-C9    | -2.58 | 121.52      | 125.53   |
| 3   | N     | 610 | CLA  | CHB-C4A-NA  | 2.58  | 128.12      | 124.40   |
| 2   | Y     | 605 | CHL  | C4D-CHA-CBD | -2.57 | 106.38      | 108.97   |
| 2   | G     | 608 | CHL  | C3C-C4C-NC  | -2.56 | 108.39      | 114.65   |
| 7   | N     | 619 | LHG  | O8-C23-C24  | 2.56  | 119.65      | 111.83   |
| 2   | Y     | 609 | CHL  | C3D-C4D-CHA | 2.56  | 112.43      | 108.54   |
| 3   | G     | 613 | CLA  | CHB-C4A-NA  | 2.56  | 128.09      | 124.40   |
| 2   | Y     | 606 | CHL  | CBA-CAA-C2A | -2.55 | 106.27      | 113.78   |
| 4   | G     | 616 | LUT  | C16-C1-C6   | -2.55 | 106.25      | 110.24   |
| 3   | Y     | 611 | CLA  | O2D-CGD-O1D | -2.55 | 118.89      | 123.85   |
| 6   | Y     | 617 | NEX  | C19-C9-C10  | -2.55 | 118.69      | 122.82   |
| 2   | Y     | 606 | CHL  | O2D-CGD-O1D | -2.55 | 118.89      | 123.85   |
| 2   | N     | 605 | CHL  | C3D-C4D-CHA | 2.53  | 112.39      | 108.54   |
| 6   | N     | 618 | NEX  | C19-C9-C10  | -2.53 | 118.71      | 122.82   |
| 2   | N     | 601 | CHL  | OMC-CMC-C2C | -2.53 | 120.72      | 125.12   |
| 3   | N     | 613 | CLA  | CMB-C2B-C3B | 2.53  | 132.50      | 126.55   |
| 2   | Y     | 609 | CHL  | C3C-C4C-NC  | -2.53 | 108.46      | 114.65   |
| 2   | Y     | 608 | CHL  | C3C-C4C-NC  | -2.53 | 108.47      | 114.65   |
| 3   | N     | 612 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 2   | Y     | 605 | CHL  | C3D-C4D-CHA | 2.53  | 112.38      | 108.54   |
| 2   | G     | 601 | CHL  | C4C-CHD-C1D | 2.53  | 125.11      | 116.07   |
| 3   | Y     | 610 | CLA  | CHB-C4A-NA  | 2.53  | 128.04      | 124.40   |
| 2   | N     | 609 | CHL  | CMD-C2D-C3D | 2.52  | 129.72      | 124.68   |
| 2   | N     | 605 | CHL  | C4C-CHD-C1D | 2.52  | 125.09      | 116.07   |
| 3   | N     | 614 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 6   | G     | 617 | NEX  | C19-C9-C10  | -2.52 | 118.73      | 122.82   |
| 2   | N     | 608 | CHL  | O2D-CGD-CBD | 2.52  | 113.71      | 110.95   |
| 2   | Y     | 609 | CHL  | C4D-CHA-CBD | -2.51 | 106.44      | 108.97   |
| 3   | G     | 604 | CLA  | O2D-CGD-O1D | -2.50 | 118.97      | 123.85   |
| 3   | G     | 612 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 2   | N     | 601 | CHL  | C4D-CHA-CBD | -2.50 | 106.45      | 108.97   |
| 3   | Y     | 612 | CLA  | O2D-CGD-O1D | -2.50 | 118.99      | 123.85   |
| 3   | N     | 602 | CLA  | CHB-C4A-NA  | 2.50  | 128.00      | 124.40   |
| 4   | G     | 615 | LUT  | C35-C15-C14 | -2.49 | 118.42      | 123.52   |
| 2   | Y     | 605 | CHL  | CMB-C2B-C3B | 2.49  | 129.66      | 124.68   |
| 2   | Y     | 607 | CHL  | CAA-C2A-C3A | -2.49 | 106.27      | 113.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | Y     | 602 | CLA  | CHB-C4A-NA  | 2.48  | 127.99      | 124.40   |
| 2   | N     | 608 | CHL  | OMC-CMC-C2C | -2.48 | 120.81      | 125.12   |
| 2   | N     | 608 | CHL  | C3D-C4D-CHA | 2.48  | 112.31      | 108.54   |
| 2   | Y     | 601 | CHL  | C1-C2-C3    | -2.48 | 122.13      | 126.20   |
| 2   | N     | 608 | CHL  | CHA-C1A-C2A | -2.48 | 127.49      | 133.31   |
| 2   | G     | 609 | CHL  | CMD-C2D-C3D | 2.48  | 129.63      | 124.68   |
| 4   | N     | 615 | LUT  | C30-C31-C32 | -2.47 | 116.04      | 123.20   |
| 2   | G     | 606 | CHL  | C4D-ND-C1D  | 2.47  | 107.09      | 105.22   |
| 2   | Y     | 605 | CHL  | C4C-CHD-C1D | 2.47  | 124.89      | 116.07   |
| 3   | G     | 612 | CLA  | CMB-C2B-C1B | -2.46 | 121.67      | 125.42   |
| 3   | G     | 604 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 3   | G     | 610 | CLA  | CHB-C4A-NA  | 2.45  | 127.94      | 124.40   |
| 4   | Y     | 615 | LUT  | C18-C5-C6   | -2.45 | 121.81      | 124.48   |
| 6   | Y     | 617 | NEX  | C27-C28-C29 | -2.45 | 121.73      | 125.53   |
| 3   | Y     | 603 | CLA  | C1-C2-C3    | -2.45 | 122.19      | 126.20   |
| 5   | N     | 617 | XAT  | C7-C8-C9    | -2.44 | 121.74      | 125.53   |
| 3   | Y     | 611 | CLA  | C3B-C4B-NB  | -2.44 | 108.36      | 110.53   |
| 3   | N     | 611 | CLA  | C3B-C4B-NB  | -2.43 | 108.36      | 110.53   |
| 2   | Y     | 609 | CHL  | C16-C15-C13 | -2.43 | 107.88      | 115.97   |
| 2   | G     | 609 | CHL  | O2A-CGA-O1A | -2.43 | 117.54      | 123.63   |
| 6   | G     | 617 | NEX  | C27-C28-C29 | -2.43 | 121.76      | 125.53   |
| 2   | N     | 607 | CHL  | CMD-C2D-C3D | 2.42  | 129.53      | 124.68   |
| 2   | G     | 607 | CHL  | O2D-CGD-O1D | -2.42 | 119.13      | 123.85   |
| 5   | N     | 617 | XAT  | C6-C7-C8    | -2.42 | 120.88      | 125.99   |
| 3   | G     | 604 | CLA  | CMB-C2B-C3B | 2.42  | 132.24      | 126.55   |
| 6   | N     | 618 | NEX  | C27-C28-C29 | -2.42 | 121.78      | 125.53   |
| 2   | N     | 608 | CHL  | CMB-C2B-C3B | 2.41  | 129.50      | 124.68   |
| 2   | N     | 601 | CHL  | O1D-CGD-CBD | 2.41  | 128.38      | 124.72   |
| 2   | Y     | 601 | CHL  | C3C-C4C-NC  | -2.41 | 108.76      | 114.65   |
| 3   | Y     | 613 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 2   | Y     | 601 | CHL  | C4D-ND-C1D  | 2.40  | 107.04      | 105.22   |
| 3   | Y     | 604 | CLA  | C1-C2-C3    | -2.40 | 122.27      | 126.20   |
| 2   | N     | 609 | CHL  | CHA-C1A-C2A | -2.39 | 127.68      | 133.31   |
| 5   | G     | 619 | XAT  | C6-C7-C8    | -2.39 | 120.93      | 125.99   |
| 2   | Y     | 609 | CHL  | CMB-C2B-C3B | 2.39  | 129.46      | 124.68   |
| 2   | N     | 606 | CHL  | C3C-C4C-NC  | -2.39 | 108.81      | 114.65   |
| 2   | Y     | 607 | CHL  | C3C-C4C-NC  | -2.39 | 108.81      | 114.65   |
| 3   | G     | 611 | CLA  | C3B-C4B-NB  | -2.38 | 108.41      | 110.53   |
| 4   | N     | 615 | LUT  | C35-C15-C14 | -2.38 | 118.66      | 123.52   |
| 3   | G     | 613 | CLA  | O2A-CGA-O1A | -2.38 | 117.68      | 123.63   |
| 2   | N     | 608 | CHL  | C3C-C4C-NC  | -2.37 | 108.85      | 114.65   |
| 2   | Y     | 606 | CHL  | C3C-C4C-NC  | -2.37 | 108.85      | 114.65   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | N     | 601 | CHL  | C3D-C4D-CHA | 2.37  | 112.14      | 108.54   |
| 3   | G     | 610 | CLA  | C1-C2-C3    | -2.37 | 122.31      | 126.20   |
| 3   | Y     | 604 | CLA  | CHB-C4A-NA  | 2.37  | 127.81      | 124.40   |
| 2   | N     | 601 | CHL  | C1B-CHB-C4A | 2.36  | 122.84      | 121.32   |
| 4   | Y     | 615 | LUT  | C27-C28-C29 | -2.36 | 121.25      | 126.32   |
| 3   | N     | 614 | CLA  | C3B-C4B-NB  | -2.36 | 108.42      | 110.53   |
| 3   | N     | 612 | CLA  | C3B-C4B-NB  | -2.36 | 108.42      | 110.53   |
| 2   | G     | 606 | CHL  | C1C-C2C-CMC | -2.35 | 122.56      | 126.80   |
| 3   | N     | 603 | CLA  | C3B-C4B-NB  | -2.35 | 108.43      | 110.53   |
| 5   | N     | 620 | XAT  | C15-C35-C34 | -2.35 | 118.71      | 123.52   |
| 2   | G     | 601 | CHL  | O2A-CGA-O1A | -2.35 | 117.75      | 123.63   |
| 2   | G     | 606 | CHL  | CMD-C2D-C3D | 2.35  | 129.38      | 124.68   |
| 3   | G     | 611 | CLA  | O2D-CGD-CBD | 2.35  | 115.33      | 111.23   |
| 3   | G     | 602 | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 2   | N     | 605 | CHL  | C4D-ND-C1D  | 2.34  | 107.00      | 105.22   |
| 2   | G     | 601 | CHL  | C4D-ND-C1D  | 2.34  | 106.99      | 105.22   |
| 2   | N     | 601 | CHL  | C3C-C4C-NC  | -2.33 | 108.94      | 114.65   |
| 2   | Y     | 608 | CHL  | C4C-CHD-C1D | 2.33  | 124.41      | 116.07   |
| 2   | G     | 601 | CHL  | CHA-C1A-C2A | -2.33 | 127.84      | 133.31   |
| 2   | N     | 607 | CHL  | C3C-C4C-NC  | -2.32 | 108.98      | 114.65   |
| 3   | N     | 610 | CLA  | O2A-CGA-O1A | -2.32 | 117.83      | 123.63   |
| 2   | Y     | 606 | CHL  | C4D-ND-C1D  | 2.32  | 106.98      | 105.22   |
| 2   | N     | 608 | CHL  | C4C-CHD-C1D | 2.32  | 124.35      | 116.07   |
| 2   | G     | 607 | CHL  | C3C-C4C-NC  | -2.31 | 109.00      | 114.65   |
| 3   | Y     | 604 | CLA  | CMB-C2B-C3B | 2.31  | 131.99      | 126.55   |
| 3   | N     | 613 | CLA  | CHB-C4A-NA  | 2.31  | 127.73      | 124.40   |
| 7   | G     | 618 | LHG  | O8-C23-O10  | -2.31 | 117.85      | 123.63   |
| 3   | N     | 602 | CLA  | O2D-CGD-CBD | 2.31  | 115.26      | 111.23   |
| 2   | G     | 607 | CHL  | CAA-C2A-C3A | -2.31 | 106.77      | 113.00   |
| 3   | G     | 610 | CLA  | CMC-C2C-C1C | 2.31  | 128.64      | 125.03   |
| 3   | N     | 612 | CLA  | CAA-C2A-C3A | -2.31 | 106.77      | 113.00   |
| 4   | N     | 616 | LUT  | C26-C27-C28 | -2.30 | 121.00      | 124.58   |
| 2   | Y     | 601 | CHL  | C4D-CHA-CBD | -2.30 | 106.65      | 108.97   |
| 5   | G     | 619 | XAT  | C27-C28-C29 | -2.29 | 121.97      | 125.53   |
| 2   | N     | 607 | CHL  | CAA-C2A-C3A | -2.29 | 106.81      | 113.00   |
| 2   | N     | 606 | CHL  | CHA-C1A-C2A | -2.29 | 127.93      | 133.31   |
| 2   | G     | 601 | CHL  | C3D-C4D-CHA | 2.29  | 112.02      | 108.54   |
| 2   | N     | 606 | CHL  | C1C-C2C-CMC | -2.29 | 122.68      | 126.80   |
| 3   | Y     | 602 | CLA  | CMB-C2B-C3B | 2.29  | 131.93      | 126.55   |
| 2   | Y     | 605 | CHL  | O2A-CGA-O1A | -2.29 | 117.91      | 123.63   |
| 3   | Y     | 604 | CLA  | O2D-CGD-CBD | 2.28  | 115.22      | 111.23   |
| 3   | Y     | 612 | CLA  | C3B-C4B-NB  | -2.28 | 108.50      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | G     | 613 | CLA  | CMB-C2B-C1B | -2.28 | 121.95      | 125.42   |
| 2   | G     | 601 | CHL  | C4D-CHA-CBD | -2.28 | 106.67      | 108.97   |
| 2   | Y     | 601 | CHL  | C3D-C4D-CHA | 2.28  | 112.00      | 108.54   |
| 4   | Y     | 615 | LUT  | C8-C7-C6    | -2.27 | 120.92      | 127.00   |
| 2   | G     | 601 | CHL  | C1-C2-C3    | -2.27 | 122.48      | 126.20   |
| 3   | N     | 604 | CLA  | CHB-C4A-NA  | 2.26  | 127.67      | 124.40   |
| 2   | N     | 607 | CHL  | OMC-CMC-C2C | -2.26 | 121.19      | 125.12   |
| 5   | N     | 620 | XAT  | C27-C28-C29 | -2.26 | 122.02      | 125.53   |
| 3   | G     | 614 | CLA  | CHB-C1B-NB  | 2.26  | 127.44      | 124.05   |
| 3   | N     | 602 | CLA  | C3B-C4B-NB  | -2.26 | 108.51      | 110.53   |
| 4   | Y     | 616 | LUT  | C1-C2-C3    | 2.25  | 118.53      | 113.59   |
| 4   | N     | 616 | LUT  | C16-C1-C6   | -2.25 | 106.72      | 110.24   |
| 4   | Y     | 616 | LUT  | C38-C25-C24 | -2.24 | 118.05      | 123.36   |
| 2   | G     | 607 | CHL  | CMD-C2D-C3D | 2.24  | 129.17      | 124.68   |
| 2   | G     | 608 | CHL  | C4C-CHD-C1D | 2.24  | 124.09      | 116.07   |
| 2   | Y     | 607 | CHL  | CMD-C2D-C3D | 2.24  | 129.16      | 124.68   |
| 3   | N     | 610 | CLA  | C1-C2-C3    | -2.24 | 122.52      | 126.20   |
| 2   | G     | 606 | CHL  | C3C-C4C-NC  | -2.24 | 109.18      | 114.65   |
| 2   | G     | 608 | CHL  | O1D-CGD-CBD | 2.23  | 128.11      | 124.72   |
| 3   | Y     | 602 | CLA  | CMB-C2B-C1B | -2.23 | 122.02      | 125.42   |
| 2   | Y     | 606 | CHL  | O2A-CGA-O1A | -2.23 | 118.05      | 123.63   |
| 2   | N     | 609 | CHL  | O2A-CGA-O1A | -2.23 | 118.06      | 123.63   |
| 4   | G     | 616 | LUT  | C38-C25-C24 | -2.23 | 118.09      | 123.36   |
| 2   | G     | 609 | CHL  | CHA-C1A-C2A | -2.22 | 128.10      | 133.31   |
| 4   | N     | 615 | LUT  | C26-C27-C28 | -2.21 | 121.14      | 124.58   |
| 3   | G     | 612 | CLA  | CMB-C2B-C3B | 2.20  | 131.74      | 126.55   |
| 2   | G     | 608 | CHL  | O2D-CGD-CBD | 2.20  | 113.37      | 110.95   |
| 3   | G     | 611 | CLA  | CHB-C4A-NA  | 2.20  | 127.58      | 124.40   |
| 2   | Y     | 609 | CHL  | O2A-CGA-O1A | -2.20 | 118.13      | 123.63   |
| 2   | G     | 606 | CHL  | C4C-CHD-C1D | 2.20  | 123.93      | 116.07   |
| 2   | N     | 609 | CHL  | C1C-C2C-CMC | -2.20 | 122.84      | 126.80   |
| 3   | G     | 610 | CLA  | CAC-C3C-C2C | -2.20 | 123.53      | 127.56   |
| 3   | Y     | 603 | CLA  | C3B-C4B-NB  | -2.19 | 108.58      | 110.53   |
| 7   | Y     | 618 | LHG  | C5-O7-C7    | -2.19 | 112.57      | 117.80   |
| 4   | G     | 615 | LUT  | C38-C25-C24 | -2.18 | 118.19      | 123.36   |
| 2   | Y     | 608 | CHL  | CHA-C1A-C2A | -2.18 | 128.18      | 133.31   |
| 3   | N     | 602 | CLA  | CMB-C2B-C1B | -2.18 | 122.10      | 125.42   |
| 5   | N     | 620 | XAT  | O3-C3-C2    | -2.16 | 105.32      | 109.75   |
| 5   | N     | 617 | XAT  | C24-C23-C22 | -2.16 | 106.74      | 110.79   |
| 3   | G     | 610 | CLA  | O2A-CGA-O1A | -2.16 | 118.22      | 123.63   |
| 2   | G     | 606 | CHL  | O2A-CGA-O1A | -2.16 | 118.22      | 123.63   |
| 3   | Y     | 614 | CLA  | O2A-CGA-O1A | -2.16 | 118.22      | 123.63   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | N     | 605 | CHL  | O2A-CGA-O1A | -2.16 | 118.23      | 123.63   |
| 2   | G     | 608 | CHL  | CMB-C2B-C3B | 2.15  | 128.99      | 124.68   |
| 2   | Y     | 606 | CHL  | CHA-C1A-C2A | -2.15 | 128.26      | 133.31   |
| 3   | Y     | 610 | CLA  | CHB-C1B-NB  | 2.14  | 127.27      | 124.05   |
| 4   | G     | 616 | LUT  | C15-C35-C34 | -2.14 | 119.13      | 123.52   |
| 2   | Y     | 606 | CHL  | C4C-CHD-C1D | 2.14  | 123.73      | 116.07   |
| 4   | G     | 616 | LUT  | C35-C34-C33 | -2.14 | 124.28      | 127.28   |
| 2   | N     | 609 | CHL  | C1A-CHA-C4D | 2.13  | 122.54      | 118.98   |
| 3   | G     | 612 | CLA  | CHB-C1B-C2B | -2.13 | 121.24      | 127.43   |
| 4   | Y     | 615 | LUT  | C31-C30-C29 | -2.13 | 124.29      | 127.28   |
| 2   | N     | 601 | CHL  | C4D-ND-C1D  | 2.13  | 106.83      | 105.22   |
| 3   | Y     | 613 | CLA  | O2A-CGA-O1A | -2.13 | 118.31      | 123.63   |
| 2   | Y     | 605 | CHL  | C4D-ND-C1D  | 2.12  | 106.83      | 105.22   |
| 5   | G     | 619 | XAT  | O3-C3-C2    | -2.12 | 105.40      | 109.75   |
| 4   | G     | 615 | LUT  | C8-C7-C6    | -2.12 | 121.34      | 127.00   |
| 4   | Y     | 615 | LUT  | C30-C31-C32 | -2.12 | 117.06      | 123.20   |
| 3   | G     | 602 | CLA  | O2D-CGD-CBD | 2.12  | 114.93      | 111.23   |
| 2   | N     | 606 | CHL  | O2A-CGA-O1A | -2.11 | 118.35      | 123.63   |
| 4   | Y     | 615 | LUT  | C35-C15-C14 | -2.11 | 119.20      | 123.52   |
| 3   | N     | 604 | CLA  | CMB-C2B-C3B | 2.11  | 131.50      | 126.55   |
| 3   | N     | 602 | CLA  | CMB-C2B-C3B | 2.11  | 131.50      | 126.55   |
| 2   | Y     | 609 | CHL  | CMD-C2D-C3D | 2.10  | 128.89      | 124.68   |
| 2   | N     | 601 | CHL  | C16-C15-C13 | -2.10 | 108.97      | 115.97   |
| 2   | N     | 601 | CHL  | C7-C6-C5    | -2.10 | 107.67      | 113.26   |
| 3   | Y     | 612 | CLA  | CHB-C4A-NA  | 2.10  | 127.43      | 124.40   |
| 3   | G     | 604 | CLA  | CHB-C1B-NB  | 2.10  | 127.19      | 124.05   |
| 2   | N     | 606 | CHL  | CBA-CAA-C2A | -2.09 | 107.62      | 113.78   |
| 4   | N     | 616 | LUT  | C35-C15-C14 | -2.09 | 119.24      | 123.52   |
| 3   | G     | 611 | CLA  | CHB-C1B-NB  | 2.09  | 127.18      | 124.05   |
| 2   | N     | 606 | CHL  | C4C-CHD-C1D | 2.09  | 123.53      | 116.07   |
| 2   | Y     | 605 | CHL  | CHA-C1A-C2A | -2.08 | 128.41      | 133.31   |
| 3   | G     | 604 | CLA  | C3B-C4B-NB  | -2.08 | 108.67      | 110.53   |
| 2   | Y     | 605 | CHL  | CMD-C2D-C3D | 2.08  | 128.84      | 124.68   |
| 3   | G     | 604 | CLA  | C1-C2-C3    | -2.08 | 122.80      | 126.20   |
| 2   | Y     | 606 | CHL  | C1C-C2C-CMC | -2.07 | 123.07      | 126.80   |
| 2   | N     | 605 | CHL  | CHA-C1A-C2A | -2.07 | 128.45      | 133.31   |
| 3   | G     | 610 | CLA  | CHB-C1B-NB  | 2.07  | 127.15      | 124.05   |
| 3   | G     | 602 | CLA  | C1-C2-C3    | -2.07 | 122.81      | 126.20   |
| 3   | Y     | 610 | CLA  | O2A-CGA-O1A | -2.07 | 118.46      | 123.63   |
| 3   | Y     | 614 | CLA  | C3B-C4B-NB  | -2.06 | 108.69      | 110.53   |
| 3   | G     | 614 | CLA  | CHB-C4A-NA  | 2.06  | 127.37      | 124.40   |
| 3   | N     | 603 | CLA  | O2A-CGA-O1A | -2.05 | 118.49      | 123.63   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | Y     | 603 | CLA  | O2A-CGA-O1A | -2.05 | 118.50      | 123.63   |
| 3   | G     | 610 | CLA  | CHB-C1B-C2B | -2.04 | 121.50      | 127.43   |
| 3   | N     | 602 | CLA  | C1-C2-C3    | -2.04 | 122.86      | 126.20   |
| 3   | G     | 613 | CLA  | CMB-C2B-C3B | 2.04  | 131.34      | 126.55   |
| 2   | G     | 606 | CHL  | C1-C2-C3    | -2.04 | 123.47      | 126.76   |
| 4   | N     | 615 | LUT  | C16-C1-C6   | -2.04 | 107.05      | 110.24   |
| 2   | N     | 605 | CHL  | O1D-CGD-CBD | 2.03  | 127.80      | 124.72   |
| 3   | G     | 603 | CLA  | CHA-C1A-NA  | -2.03 | 121.80      | 126.39   |
| 2   | Y     | 607 | CHL  | CMA-C3A-C4A | -2.02 | 110.25      | 114.61   |
| 3   | N     | 610 | CLA  | CAC-C3C-C4C | 2.02  | 127.42      | 124.79   |
| 4   | G     | 616 | LUT  | C10-C11-C12 | -2.02 | 117.34      | 123.20   |
| 2   | G     | 606 | CHL  | CHA-C1A-C2A | -2.02 | 128.56      | 133.31   |
| 2   | N     | 606 | CHL  | C4D-ND-C1D  | 2.01  | 106.75      | 105.22   |
| 5   | N     | 617 | XAT  | C31-C32-C33 | -2.01 | 120.84      | 126.36   |
| 3   | N     | 610 | CLA  | CMC-C2C-C1C | 2.01  | 128.17      | 125.03   |
| 3   | G     | 604 | CLA  | O2A-CGA-O1A | -2.01 | 118.61      | 123.63   |
| 3   | N     | 610 | CLA  | C3B-C4B-NB  | -2.00 | 108.74      | 110.53   |

All (77) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 2   | N     | 601 | CHL  | NA   |
| 2   | N     | 601 | CHL  | NC   |
| 2   | N     | 601 | CHL  | ND   |
| 2   | N     | 605 | CHL  | NA   |
| 2   | N     | 605 | CHL  | NC   |
| 2   | N     | 605 | CHL  | ND   |
| 2   | N     | 606 | CHL  | NA   |
| 2   | N     | 606 | CHL  | NC   |
| 2   | N     | 606 | CHL  | ND   |
| 2   | N     | 607 | CHL  | NA   |
| 2   | N     | 607 | CHL  | NC   |
| 2   | N     | 607 | CHL  | ND   |
| 2   | N     | 608 | CHL  | NA   |
| 2   | N     | 608 | CHL  | NC   |
| 2   | N     | 608 | CHL  | ND   |
| 2   | N     | 609 | CHL  | NA   |
| 2   | N     | 609 | CHL  | NC   |
| 2   | N     | 609 | CHL  | ND   |
| 2   | G     | 601 | CHL  | NA   |
| 2   | G     | 601 | CHL  | NC   |
| 2   | G     | 601 | CHL  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 2   | G     | 605 | CHL  | NA   |
| 2   | G     | 605 | CHL  | NC   |
| 2   | G     | 605 | CHL  | ND   |
| 2   | G     | 606 | CHL  | NA   |
| 2   | G     | 606 | CHL  | NC   |
| 2   | G     | 606 | CHL  | ND   |
| 2   | G     | 607 | CHL  | NA   |
| 2   | G     | 607 | CHL  | NC   |
| 2   | G     | 607 | CHL  | ND   |
| 2   | G     | 608 | CHL  | NA   |
| 2   | G     | 608 | CHL  | NC   |
| 2   | G     | 608 | CHL  | ND   |
| 2   | G     | 609 | CHL  | NA   |
| 2   | G     | 609 | CHL  | NC   |
| 2   | G     | 609 | CHL  | ND   |
| 2   | Y     | 601 | CHL  | NA   |
| 2   | Y     | 601 | CHL  | NC   |
| 2   | Y     | 601 | CHL  | ND   |
| 2   | Y     | 605 | CHL  | NA   |
| 2   | Y     | 605 | CHL  | NC   |
| 2   | Y     | 605 | CHL  | ND   |
| 2   | Y     | 606 | CHL  | NA   |
| 2   | Y     | 606 | CHL  | NC   |
| 2   | Y     | 606 | CHL  | ND   |
| 2   | Y     | 607 | CHL  | NA   |
| 2   | Y     | 607 | CHL  | NC   |
| 2   | Y     | 607 | CHL  | ND   |
| 2   | Y     | 608 | CHL  | NA   |
| 2   | Y     | 608 | CHL  | NC   |
| 2   | Y     | 608 | CHL  | ND   |
| 2   | Y     | 609 | CHL  | NA   |
| 2   | Y     | 609 | CHL  | NC   |
| 2   | Y     | 609 | CHL  | ND   |
| 3   | N     | 602 | CLA  | ND   |
| 3   | N     | 603 | CLA  | ND   |
| 3   | N     | 604 | CLA  | ND   |
| 3   | N     | 610 | CLA  | ND   |
| 3   | N     | 611 | CLA  | ND   |
| 3   | N     | 612 | CLA  | ND   |
| 3   | N     | 613 | CLA  | ND   |
| 3   | N     | 614 | CLA  | ND   |
| 3   | G     | 602 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 3   | G     | 603 | CLA  | ND   |
| 3   | G     | 604 | CLA  | ND   |
| 3   | G     | 610 | CLA  | ND   |
| 3   | G     | 612 | CLA  | ND   |
| 3   | G     | 613 | CLA  | ND   |
| 3   | G     | 614 | CLA  | ND   |
| 3   | Y     | 602 | CLA  | ND   |
| 3   | Y     | 603 | CLA  | ND   |
| 3   | Y     | 604 | CLA  | ND   |
| 3   | Y     | 610 | CLA  | ND   |
| 3   | Y     | 611 | CLA  | ND   |
| 3   | Y     | 612 | CLA  | ND   |
| 3   | Y     | 613 | CLA  | ND   |
| 3   | Y     | 614 | CLA  | ND   |

All (634) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | N     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 2   | N     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 2   | N     | 606 | CHL  | C1A-C2A-CAA-CBA |
| 2   | N     | 606 | CHL  | C3C-C2C-CMC-OMC |
| 2   | N     | 607 | CHL  | C1C-C2C-CMC-OMC |
| 2   | N     | 607 | CHL  | C3C-C2C-CMC-OMC |
| 2   | N     | 607 | CHL  | CHA-CBD-CGD-O1D |
| 2   | N     | 607 | CHL  | CHA-CBD-CGD-O2D |
| 2   | N     | 608 | CHL  | C1C-C2C-CMC-OMC |
| 2   | N     | 608 | CHL  | C3C-C2C-CMC-OMC |
| 2   | N     | 609 | CHL  | C1C-C2C-CMC-OMC |
| 2   | N     | 609 | CHL  | C3C-C2C-CMC-OMC |
| 2   | N     | 609 | CHL  | C4C-C3C-CAC-CBC |
| 2   | G     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 2   | G     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 2   | G     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 2   | G     | 605 | CHL  | C1A-C2A-CAA-CBA |
| 2   | G     | 605 | CHL  | CHA-CBD-CGD-O1D |
| 2   | G     | 606 | CHL  | C1A-C2A-CAA-CBA |
| 2   | G     | 607 | CHL  | C1C-C2C-CMC-OMC |
| 2   | G     | 607 | CHL  | C3C-C2C-CMC-OMC |
| 2   | G     | 608 | CHL  | C1C-C2C-CMC-OMC |
| 2   | G     | 608 | CHL  | C3C-C2C-CMC-OMC |
| 2   | G     | 608 | CHL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | G     | 609 | CHL  | C1C-C2C-CMC-OMC |
| 2   | G     | 609 | CHL  | C3C-C2C-CMC-OMC |
| 2   | G     | 609 | CHL  | C4C-C3C-CAC-CBC |
| 2   | Y     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 2   | Y     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 2   | Y     | 605 | CHL  | C1C-C2C-CMC-OMC |
| 2   | Y     | 605 | CHL  | CBD-CGD-O2D-CED |
| 2   | Y     | 606 | CHL  | C1A-C2A-CAA-CBA |
| 2   | Y     | 606 | CHL  | CBA-CGA-O2A-C1  |
| 2   | Y     | 606 | CHL  | C1C-C2C-CMC-OMC |
| 2   | Y     | 606 | CHL  | C3C-C2C-CMC-OMC |
| 2   | Y     | 607 | CHL  | C1C-C2C-CMC-OMC |
| 2   | Y     | 607 | CHL  | C3C-C2C-CMC-OMC |
| 2   | Y     | 608 | CHL  | C1C-C2C-CMC-OMC |
| 2   | Y     | 608 | CHL  | C3C-C2C-CMC-OMC |
| 2   | Y     | 609 | CHL  | C1C-C2C-CMC-OMC |
| 2   | Y     | 609 | CHL  | C3C-C2C-CMC-OMC |
| 3   | N     | 602 | CLA  | CHA-CBD-CGD-O1D |
| 3   | N     | 602 | CLA  | CHA-CBD-CGD-O2D |
| 3   | N     | 610 | CLA  | C2B-C3B-CAB-CBB |
| 3   | N     | 610 | CLA  | C4B-C3B-CAB-CBB |
| 3   | N     | 611 | CLA  | C2B-C3B-CAB-CBB |
| 3   | N     | 611 | CLA  | C4B-C3B-CAB-CBB |
| 3   | G     | 602 | CLA  | C2B-C3B-CAB-CBB |
| 3   | G     | 602 | CLA  | C4B-C3B-CAB-CBB |
| 3   | G     | 602 | CLA  | CHA-CBD-CGD-O1D |
| 3   | G     | 602 | CLA  | CHA-CBD-CGD-O2D |
| 3   | G     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 3   | G     | 613 | CLA  | CBD-CGD-O2D-CED |
| 3   | G     | 614 | CLA  | CBD-CGD-O2D-CED |
| 3   | Y     | 602 | CLA  | CBD-CGD-O2D-CED |
| 3   | Y     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 3   | Y     | 604 | CLA  | CHA-CBD-CGD-O1D |
| 3   | Y     | 604 | CLA  | CHA-CBD-CGD-O2D |
| 3   | Y     | 611 | CLA  | C2B-C3B-CAB-CBB |
| 3   | Y     | 611 | CLA  | C4B-C3B-CAB-CBB |
| 3   | Y     | 611 | CLA  | C11-C12-C13-C14 |
| 3   | Y     | 614 | CLA  | C2B-C3B-CAB-CBB |
| 3   | Y     | 614 | CLA  | C4B-C3B-CAB-CBB |
| 4   | G     | 615 | LUT  | C27-C28-C29-C30 |
| 5   | N     | 617 | XAT  | O4-C6-C7-C8     |
| 5   | N     | 617 | XAT  | C7-C8-C9-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | N     | 617 | XAT  | C7-C8-C9-C19    |
| 5   | N     | 620 | XAT  | O4-C6-C7-C8     |
| 5   | N     | 620 | XAT  | C7-C8-C9-C10    |
| 5   | N     | 620 | XAT  | C31-C32-C33-C34 |
| 5   | G     | 619 | XAT  | O4-C6-C7-C8     |
| 5   | G     | 619 | XAT  | C7-C8-C9-C10    |
| 5   | G     | 619 | XAT  | C7-C8-C9-C19    |
| 5   | G     | 619 | XAT  | O24-C26-C27-C28 |
| 5   | G     | 619 | XAT  | C31-C32-C33-C34 |
| 6   | N     | 618 | NEX  | C11-C10-C9-C8   |
| 6   | N     | 618 | NEX  | C11-C10-C9-C19  |
| 6   | N     | 618 | NEX  | C10-C11-C12-C13 |
| 6   | G     | 617 | NEX  | C11-C10-C9-C8   |
| 6   | G     | 617 | NEX  | C11-C10-C9-C19  |
| 6   | G     | 617 | NEX  | C10-C11-C12-C13 |
| 6   | Y     | 617 | NEX  | C11-C10-C9-C8   |
| 6   | Y     | 617 | NEX  | C11-C10-C9-C19  |
| 6   | Y     | 617 | NEX  | C10-C11-C12-C13 |
| 7   | G     | 618 | LHG  | C3-O3-P-O5      |
| 7   | G     | 618 | LHG  | C4-O6-P-O3      |
| 7   | G     | 618 | LHG  | C4-O6-P-O4      |
| 7   | Y     | 618 | LHG  | O1-C1-C2-C3     |
| 7   | Y     | 618 | LHG  | C2-C3-O3-P      |
| 7   | Y     | 618 | LHG  | C3-O3-P-O4      |
| 7   | Y     | 618 | LHG  | C3-O3-P-O6      |
| 7   | Y     | 618 | LHG  | C4-O6-P-O4      |
| 3   | Y     | 604 | CLA  | O1D-CGD-O2D-CED |
| 2   | N     | 605 | CHL  | CBD-CGD-O2D-CED |
| 3   | N     | 610 | CLA  | CBD-CGD-O2D-CED |
| 3   | Y     | 603 | CLA  | CBD-CGD-O2D-CED |
| 3   | Y     | 604 | CLA  | CBD-CGD-O2D-CED |
| 3   | Y     | 613 | CLA  | CBD-CGD-O2D-CED |
| 3   | Y     | 614 | CLA  | CBD-CGD-O2D-CED |
| 2   | N     | 606 | CHL  | O1A-CGA-O2A-C1  |
| 2   | Y     | 606 | CHL  | O1A-CGA-O2A-C1  |
| 2   | N     | 606 | CHL  | CBA-CGA-O2A-C1  |
| 2   | G     | 601 | CHL  | CBD-CGD-O2D-CED |
| 3   | G     | 603 | CLA  | CBD-CGD-O2D-CED |
| 2   | N     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 2   | G     | 606 | CHL  | O1A-CGA-O2A-C1  |
| 2   | G     | 607 | CHL  | O1A-CGA-O2A-C1  |
| 2   | Y     | 607 | CHL  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | Y     | 614 | CLA  | O1A-CGA-O2A-C1  |
| 7   | N     | 619 | LHG  | O10-C23-O8-C6   |
| 7   | G     | 618 | LHG  | O10-C23-O8-C6   |
| 7   | Y     | 618 | LHG  | O10-C23-O8-C6   |
| 3   | G     | 614 | CLA  | O1D-CGD-O2D-CED |
| 3   | Y     | 602 | CLA  | O1D-CGD-O2D-CED |
| 3   | G     | 613 | CLA  | O1D-CGD-O2D-CED |
| 3   | Y     | 611 | CLA  | C3-C5-C6-C7     |
| 2   | G     | 608 | CHL  | O1D-CGD-O2D-CED |
| 2   | G     | 606 | CHL  | CBA-CGA-O2A-C1  |
| 2   | G     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 7   | G     | 618 | LHG  | C24-C23-O8-C6   |
| 7   | Y     | 618 | LHG  | C24-C23-O8-C6   |
| 2   | N     | 607 | CHL  | CBD-CGD-O2D-CED |
| 3   | N     | 613 | CLA  | CBD-CGD-O2D-CED |
| 3   | N     | 614 | CLA  | CBD-CGD-O2D-CED |
| 3   | G     | 612 | CLA  | CBD-CGD-O2D-CED |
| 3   | Y     | 612 | CLA  | CBD-CGD-O2D-CED |
| 2   | Y     | 605 | CHL  | O1D-CGD-O2D-CED |
| 3   | Y     | 613 | CLA  | O1D-CGD-O2D-CED |
| 2   | G     | 607 | CHL  | C2A-CAA-CBA-CGA |
| 2   | G     | 607 | CHL  | C3-C5-C6-C7     |
| 3   | G     | 604 | CLA  | C3-C5-C6-C7     |
| 3   | Y     | 612 | CLA  | C3-C5-C6-C7     |
| 2   | N     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 2   | Y     | 607 | CHL  | CBA-CGA-O2A-C1  |
| 3   | Y     | 614 | CLA  | CBA-CGA-O2A-C1  |
| 7   | N     | 619 | LHG  | C24-C23-O8-C6   |
| 4   | G     | 616 | LUT  | C29-C30-C31-C32 |
| 2   | N     | 605 | CHL  | O1D-CGD-O2D-CED |
| 3   | N     | 610 | CLA  | O1D-CGD-O2D-CED |
| 2   | G     | 601 | CHL  | C3-C5-C6-C7     |
| 2   | Y     | 601 | CHL  | CBD-CGD-O2D-CED |
| 3   | N     | 604 | CLA  | CBD-CGD-O2D-CED |
| 3   | N     | 614 | CLA  | CBA-CGA-O2A-C1  |
| 3   | Y     | 603 | CLA  | O1D-CGD-O2D-CED |
| 3   | N     | 614 | CLA  | O1A-CGA-O2A-C1  |
| 2   | Y     | 607 | CHL  | C3-C5-C6-C7     |
| 3   | N     | 604 | CLA  | C3-C5-C6-C7     |
| 3   | N     | 611 | CLA  | C3-C5-C6-C7     |
| 3   | G     | 612 | CLA  | C3-C5-C6-C7     |
| 2   | N     | 606 | CHL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | G     | 610 | CLA  | CBD-CGD-O2D-CED |
| 3   | Y     | 610 | CLA  | CBD-CGD-O2D-CED |
| 2   | N     | 607 | CHL  | C2A-CAA-CBA-CGA |
| 3   | Y     | 614 | CLA  | O1D-CGD-O2D-CED |
| 3   | G     | 614 | CLA  | CBA-CGA-O2A-C1  |
| 3   | G     | 614 | CLA  | O1A-CGA-O2A-C1  |
| 3   | G     | 603 | CLA  | O1D-CGD-O2D-CED |
| 3   | N     | 603 | CLA  | CBD-CGD-O2D-CED |
| 7   | Y     | 618 | LHG  | C15-C16-C17-C18 |
| 2   | G     | 601 | CHL  | O1D-CGD-O2D-CED |
| 2   | G     | 608 | CHL  | C11-C12-C13-C14 |
| 2   | Y     | 608 | CHL  | C11-C12-C13-C14 |
| 2   | Y     | 609 | CHL  | C6-C7-C8-C9     |
| 2   | Y     | 609 | CHL  | C11-C12-C13-C14 |
| 3   | N     | 611 | CLA  | C11-C10-C8-C9   |
| 3   | G     | 612 | CLA  | O1D-CGD-O2D-CED |
| 7   | Y     | 618 | LHG  | C33-C34-C35-C36 |
| 3   | N     | 613 | CLA  | O1D-CGD-O2D-CED |
| 3   | N     | 614 | CLA  | O1D-CGD-O2D-CED |
| 4   | N     | 615 | LUT  | C27-C28-C29-C39 |
| 4   | G     | 615 | LUT  | C27-C28-C29-C39 |
| 4   | Y     | 615 | LUT  | C27-C28-C29-C39 |
| 5   | N     | 620 | XAT  | C7-C8-C9-C19    |
| 5   | N     | 620 | XAT  | C31-C32-C33-C40 |
| 5   | G     | 619 | XAT  | C31-C32-C33-C40 |
| 7   | Y     | 618 | LHG  | C17-C18-C19-C20 |
| 2   | Y     | 607 | CHL  | C2A-CAA-CBA-CGA |
| 7   | N     | 619 | LHG  | C28-C29-C30-C31 |
| 3   | Y     | 612 | CLA  | O1D-CGD-O2D-CED |
| 2   | G     | 601 | CHL  | C15-C16-C17-C18 |
| 3   | Y     | 613 | CLA  | C13-C15-C16-C17 |
| 7   | Y     | 618 | LHG  | O1-C1-C2-O2     |
| 2   | Y     | 601 | CHL  | C15-C16-C17-C18 |
| 3   | Y     | 611 | CLA  | C10-C11-C12-C13 |
| 2   | N     | 601 | CHL  | CBD-CGD-O2D-CED |
| 2   | N     | 608 | CHL  | C12-C13-C15-C16 |
| 2   | G     | 608 | CHL  | C12-C13-C15-C16 |
| 3   | N     | 611 | CLA  | C6-C7-C8-C10    |
| 3   | Y     | 611 | CLA  | C6-C7-C8-C10    |
| 3   | Y     | 612 | CLA  | CBA-CGA-O2A-C1  |
| 3   | G     | 613 | CLA  | C3-C5-C6-C7     |
| 3   | N     | 611 | CLA  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | Y     | 611 | CLA  | C15-C16-C17-C18 |
| 3   | G     | 602 | CLA  | C10-C11-C12-C13 |
| 2   | N     | 607 | CHL  | O1D-CGD-O2D-CED |
| 3   | N     | 612 | CLA  | C3-C5-C6-C7     |
| 3   | N     | 603 | CLA  | C13-C15-C16-C17 |
| 3   | G     | 603 | CLA  | C5-C6-C7-C8     |
| 7   | Y     | 618 | LHG  | C23-C24-C25-C26 |
| 2   | G     | 607 | CHL  | C5-C6-C7-C8     |
| 3   | N     | 604 | CLA  | O1D-CGD-O2D-CED |
| 2   | Y     | 607 | CHL  | C5-C6-C7-C8     |
| 3   | Y     | 611 | CLA  | C5-C6-C7-C8     |
| 3   | N     | 612 | CLA  | CBA-CGA-O2A-C1  |
| 3   | G     | 612 | CLA  | CBA-CGA-O2A-C1  |
| 3   | G     | 612 | CLA  | C8-C10-C11-C12  |
| 3   | Y     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 3   | N     | 611 | CLA  | C5-C6-C7-C8     |
| 3   | N     | 611 | CLA  | C8-C10-C11-C12  |
| 3   | G     | 611 | CLA  | C3-C5-C6-C7     |
| 3   | G     | 603 | CLA  | C15-C16-C17-C18 |
| 3   | Y     | 611 | CLA  | C8-C10-C11-C12  |
| 3   | G     | 603 | CLA  | C10-C11-C12-C13 |
| 6   | N     | 618 | NEX  | C20-C13-C14-C15 |
| 6   | N     | 618 | NEX  | C39-C29-C30-C31 |
| 6   | G     | 617 | NEX  | C20-C13-C14-C15 |
| 6   | G     | 617 | NEX  | C39-C29-C30-C31 |
| 6   | Y     | 617 | NEX  | C20-C13-C14-C15 |
| 6   | Y     | 617 | NEX  | C39-C29-C30-C31 |
| 7   | N     | 619 | LHG  | C23-C24-C25-C26 |
| 2   | Y     | 601 | CHL  | O1D-CGD-O2D-CED |
| 2   | N     | 601 | CHL  | C15-C16-C17-C18 |
| 3   | N     | 611 | CLA  | C13-C15-C16-C17 |
| 3   | G     | 604 | CLA  | C13-C15-C16-C17 |
| 4   | N     | 615 | LUT  | C27-C28-C29-C30 |
| 3   | G     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 3   | Y     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 2   | Y     | 608 | CHL  | C2A-CAA-CBA-CGA |
| 3   | Y     | 603 | CLA  | C2A-CAA-CBA-CGA |
| 2   | N     | 606 | CHL  | O1D-CGD-O2D-CED |
| 3   | Y     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 6   | N     | 618 | NEX  | C12-C13-C14-C15 |
| 6   | N     | 618 | NEX  | C28-C29-C30-C31 |
| 6   | G     | 617 | NEX  | C12-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | G     | 617 | NEX  | C28-C29-C30-C31 |
| 6   | Y     | 617 | NEX  | C12-C13-C14-C15 |
| 6   | Y     | 617 | NEX  | C28-C29-C30-C31 |
| 3   | G     | 610 | CLA  | O1D-CGD-O2D-CED |
| 3   | Y     | 610 | CLA  | O1D-CGD-O2D-CED |
| 2   | N     | 605 | CHL  | CBA-CGA-O2A-C1  |
| 3   | N     | 613 | CLA  | C3-C5-C6-C7     |
| 3   | Y     | 613 | CLA  | C3-C5-C6-C7     |
| 3   | Y     | 604 | CLA  | C2-C1-O2A-CGA   |
| 2   | N     | 608 | CHL  | CBD-CGD-O2D-CED |
| 7   | N     | 619 | LHG  | C25-C26-C27-C28 |
| 3   | N     | 612 | CLA  | O1A-CGA-O2A-C1  |
| 3   | N     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 3   | G     | 611 | CLA  | CBA-CGA-O2A-C1  |
| 7   | Y     | 618 | LHG  | C32-C33-C34-C35 |
| 3   | G     | 610 | CLA  | C4B-C3B-CAB-CBB |
| 3   | Y     | 610 | CLA  | C4B-C3B-CAB-CBB |
| 2   | N     | 608 | CHL  | C2A-CAA-CBA-CGA |
| 2   | G     | 601 | CHL  | C2A-CAA-CBA-CGA |
| 2   | Y     | 608 | CHL  | C11-C12-C13-C15 |
| 2   | N     | 605 | CHL  | C3A-C2A-CAA-CBA |
| 2   | N     | 606 | CHL  | C3A-C2A-CAA-CBA |
| 2   | G     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 2   | G     | 605 | CHL  | C3A-C2A-CAA-CBA |
| 2   | G     | 606 | CHL  | C3A-C2A-CAA-CBA |
| 2   | Y     | 606 | CHL  | C3A-C2A-CAA-CBA |
| 3   | N     | 603 | CLA  | C3A-C2A-CAA-CBA |
| 3   | G     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 3   | Y     | 603 | CLA  | C3A-C2A-CAA-CBA |
| 7   | Y     | 618 | LHG  | C30-C31-C32-C33 |
| 3   | Y     | 603 | CLA  | C10-C11-C12-C13 |
| 7   | N     | 619 | LHG  | C15-C16-C17-C18 |
| 7   | G     | 618 | LHG  | C9-C10-C11-C12  |
| 7   | G     | 618 | LHG  | C23-C24-C25-C26 |
| 7   | Y     | 618 | LHG  | C24-C25-C26-C27 |
| 3   | N     | 603 | CLA  | C2B-C3B-CAB-CBB |
| 3   | N     | 612 | CLA  | C2B-C3B-CAB-CBB |
| 3   | G     | 603 | CLA  | C2B-C3B-CAB-CBB |
| 3   | G     | 610 | CLA  | C2B-C3B-CAB-CBB |
| 4   | G     | 615 | LUT  | C1-C6-C7-C8     |
| 7   | N     | 619 | LHG  | C32-C33-C34-C35 |
| 3   | N     | 612 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | N     | 605 | CHL  | O1A-CGA-O2A-C1  |
| 3   | N     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 3   | G     | 611 | CLA  | O1A-CGA-O2A-C1  |
| 2   | G     | 608 | CHL  | C6-C7-C8-C9     |
| 2   | Y     | 609 | CHL  | C11-C10-C8-C9   |
| 3   | G     | 613 | CLA  | C13-C15-C16-C17 |
| 7   | G     | 618 | LHG  | C32-C33-C34-C35 |
| 7   | G     | 618 | LHG  | C14-C15-C16-C17 |
| 7   | N     | 619 | LHG  | C8-C7-O7-C5     |
| 7   | G     | 618 | LHG  | C8-C7-O7-C5     |
| 7   | Y     | 618 | LHG  | C8-C7-O7-C5     |
| 3   | N     | 604 | CLA  | C13-C15-C16-C17 |
| 7   | N     | 619 | LHG  | O9-C7-O7-C5     |
| 7   | G     | 618 | LHG  | O9-C7-O7-C5     |
| 7   | G     | 618 | LHG  | C29-C30-C31-C32 |
| 5   | N     | 617 | XAT  | C11-C12-C13-C20 |
| 7   | Y     | 618 | LHG  | C14-C15-C16-C17 |
| 2   | N     | 609 | CHL  | C4-C3-C5-C6     |
| 3   | G     | 603 | CLA  | C3-C5-C6-C7     |
| 3   | N     | 611 | CLA  | C15-C16-C17-C18 |
| 3   | N     | 603 | CLA  | O1D-CGD-O2D-CED |
| 7   | Y     | 618 | LHG  | C13-C14-C15-C16 |
| 3   | G     | 612 | CLA  | C16-C17-C18-C20 |
| 2   | N     | 601 | CHL  | C13-C15-C16-C17 |
| 3   | G     | 612 | CLA  | C15-C16-C17-C18 |
| 2   | N     | 609 | CHL  | C2-C3-C5-C6     |
| 7   | Y     | 618 | LHG  | O9-C7-O7-C5     |
| 2   | G     | 606 | CHL  | CBD-CGD-O2D-CED |
| 3   | N     | 612 | CLA  | C10-C11-C12-C13 |
| 3   | Y     | 612 | CLA  | C10-C11-C12-C13 |
| 7   | N     | 619 | LHG  | C14-C15-C16-C17 |
| 7   | G     | 618 | LHG  | C25-C26-C27-C28 |
| 7   | Y     | 618 | LHG  | C11-C10-C9-C8   |
| 3   | N     | 603 | CLA  | C1A-C2A-CAA-CBA |
| 3   | N     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 3   | Y     | 602 | CLA  | C1A-C2A-CAA-CBA |
| 3   | Y     | 603 | CLA  | C1A-C2A-CAA-CBA |
| 3   | Y     | 614 | CLA  | C1A-C2A-CAA-CBA |
| 3   | Y     | 602 | CLA  | C15-C16-C17-C18 |
| 3   | N     | 612 | CLA  | C8-C10-C11-C12  |
| 2   | N     | 607 | CHL  | C12-C13-C15-C16 |
| 2   | G     | 607 | CHL  | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | Y     | 607 | CHL  | C12-C13-C15-C16 |
| 3   | N     | 602 | CLA  | C6-C7-C8-C10    |
| 3   | N     | 603 | CLA  | C6-C7-C8-C10    |
| 3   | G     | 603 | CLA  | C11-C10-C8-C7   |
| 3   | G     | 612 | CLA  | C11-C10-C8-C7   |
| 3   | G     | 612 | CLA  | C11-C12-C13-C15 |
| 3   | G     | 613 | CLA  | C12-C13-C15-C16 |
| 3   | Y     | 603 | CLA  | C6-C7-C8-C10    |
| 3   | Y     | 612 | CLA  | C11-C12-C13-C15 |
| 2   | N     | 607 | CHL  | C15-C16-C17-C18 |
| 3   | G     | 611 | CLA  | C8-C10-C11-C12  |
| 3   | Y     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 2   | N     | 607 | CHL  | C14-C13-C15-C16 |
| 2   | N     | 608 | CHL  | C14-C13-C15-C16 |
| 2   | Y     | 607 | CHL  | C11-C10-C8-C9   |
| 2   | Y     | 607 | CHL  | C14-C13-C15-C16 |
| 3   | N     | 603 | CLA  | C6-C7-C8-C9     |
| 3   | G     | 603 | CLA  | C11-C10-C8-C9   |
| 3   | G     | 611 | CLA  | C14-C13-C15-C16 |
| 3   | G     | 612 | CLA  | C11-C10-C8-C9   |
| 3   | G     | 612 | CLA  | C11-C12-C13-C14 |
| 3   | Y     | 611 | CLA  | C6-C7-C8-C9     |
| 3   | Y     | 611 | CLA  | C11-C10-C8-C9   |
| 3   | G     | 612 | CLA  | C16-C17-C18-C19 |
| 7   | G     | 618 | LHG  | C28-C29-C30-C31 |
| 7   | G     | 618 | LHG  | C33-C34-C35-C36 |
| 2   | N     | 609 | CHL  | CHA-CBD-CGD-O1D |
| 2   | N     | 609 | CHL  | CHA-CBD-CGD-O2D |
| 2   | G     | 605 | CHL  | CHA-CBD-CGD-O2D |
| 2   | G     | 608 | CHL  | C5-C6-C7-C8     |
| 3   | G     | 602 | CLA  | C15-C16-C17-C18 |
| 2   | G     | 605 | CHL  | C2A-CAA-CBA-CGA |
| 7   | G     | 618 | LHG  | C10-C11-C12-C13 |
| 2   | Y     | 605 | CHL  | C3C-C2C-CMC-OMC |
| 7   | Y     | 618 | LHG  | C35-C36-C37-C38 |
| 3   | Y     | 604 | CLA  | C3-C5-C6-C7     |
| 7   | Y     | 618 | LHG  | C11-C12-C13-C14 |
| 7   | N     | 619 | LHG  | C24-C25-C26-C27 |
| 7   | G     | 618 | LHG  | C27-C28-C29-C30 |
| 2   | N     | 606 | CHL  | C1C-C2C-CMC-OMC |
| 2   | G     | 609 | CHL  | C4-C3-C5-C6     |
| 3   | Y     | 612 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | N     | 608 | CHL  | C11-C10-C8-C9   |
| 2   | G     | 607 | CHL  | C14-C13-C15-C16 |
| 2   | G     | 609 | CHL  | C14-C13-C15-C16 |
| 3   | N     | 602 | CLA  | C6-C7-C8-C9     |
| 3   | N     | 604 | CLA  | C11-C12-C13-C14 |
| 3   | N     | 611 | CLA  | C6-C7-C8-C9     |
| 3   | N     | 613 | CLA  | C6-C7-C8-C9     |
| 3   | G     | 611 | CLA  | C11-C10-C8-C9   |
| 3   | G     | 612 | CLA  | C14-C13-C15-C16 |
| 3   | G     | 613 | CLA  | C14-C13-C15-C16 |
| 3   | Y     | 603 | CLA  | C6-C7-C8-C9     |
| 3   | Y     | 612 | CLA  | C11-C12-C13-C14 |
| 3   | N     | 603 | CLA  | C4B-C3B-CAB-CBB |
| 3   | N     | 612 | CLA  | C4B-C3B-CAB-CBB |
| 3   | G     | 603 | CLA  | C4B-C3B-CAB-CBB |
| 3   | G     | 614 | CLA  | C4B-C3B-CAB-CBB |
| 2   | N     | 607 | CHL  | C11-C10-C8-C7   |
| 2   | G     | 607 | CHL  | C11-C10-C8-C7   |
| 2   | G     | 609 | CHL  | C12-C13-C15-C16 |
| 2   | Y     | 607 | CHL  | C11-C10-C8-C7   |
| 3   | N     | 603 | CLA  | C11-C12-C13-C15 |
| 3   | N     | 603 | CLA  | C12-C13-C15-C16 |
| 3   | N     | 604 | CLA  | C11-C12-C13-C15 |
| 3   | N     | 613 | CLA  | C6-C7-C8-C10    |
| 3   | G     | 611 | CLA  | C11-C10-C8-C7   |
| 3   | Y     | 611 | CLA  | C11-C10-C8-C7   |
| 3   | Y     | 603 | CLA  | C8-C10-C11-C12  |
| 7   | Y     | 618 | LHG  | C31-C32-C33-C34 |
| 2   | N     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 3   | Y     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 7   | G     | 618 | LHG  | C26-C27-C28-C29 |
| 4   | Y     | 616 | LUT  | C29-C30-C31-C32 |
| 3   | Y     | 612 | CLA  | C8-C10-C11-C12  |
| 4   | Y     | 615 | LUT  | C27-C28-C29-C30 |
| 2   | N     | 605 | CHL  | C1A-C2A-CAA-CBA |
| 2   | N     | 609 | CHL  | C1A-C2A-CAA-CBA |
| 7   | G     | 618 | LHG  | C15-C16-C17-C18 |
| 7   | Y     | 618 | LHG  | O6-C4-C5-O7     |
| 4   | G     | 615 | LUT  | C5-C6-C7-C8     |
| 4   | Y     | 615 | LUT  | C1-C6-C7-C8     |
| 3   | N     | 602 | CLA  | C10-C11-C12-C13 |
| 7   | N     | 619 | LHG  | O7-C5-C6-O8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | G     | 609 | CHL  | C2-C3-C5-C6     |
| 3   | Y     | 612 | CLA  | C2-C3-C5-C6     |
| 7   | N     | 619 | LHG  | C27-C28-C29-C30 |
| 3   | Y     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 2   | N     | 607 | CHL  | C11-C10-C8-C9   |
| 2   | G     | 607 | CHL  | C11-C10-C8-C9   |
| 3   | N     | 612 | CLA  | O1D-CGD-O2D-CED |
| 3   | N     | 614 | CLA  | O2A-C1-C2-C3    |
| 3   | G     | 614 | CLA  | O2A-C1-C2-C3    |
| 2   | N     | 608 | CHL  | O1D-CGD-O2D-CED |
| 7   | Y     | 618 | LHG  | C34-C35-C36-C37 |
| 2   | N     | 601 | CHL  | O1D-CGD-O2D-CED |
| 3   | G     | 611 | CLA  | C13-C15-C16-C17 |
| 7   | N     | 619 | LHG  | O1-C1-C2-O2     |
| 7   | G     | 618 | LHG  | O1-C1-C2-O2     |
| 2   | Y     | 608 | CHL  | C3-C5-C6-C7     |
| 5   | N     | 620 | XAT  | C9-C10-C11-C12  |
| 2   | N     | 607 | CHL  | C10-C11-C12-C13 |
| 2   | N     | 609 | CHL  | CBA-CGA-O2A-C1  |
| 7   | G     | 618 | LHG  | O6-C4-C5-C6     |
| 7   | Y     | 618 | LHG  | O6-C4-C5-C6     |
| 2   | N     | 608 | CHL  | C11-C10-C8-C7   |
| 3   | N     | 611 | CLA  | C12-C13-C15-C16 |
| 3   | G     | 611 | CLA  | C12-C13-C15-C16 |
| 3   | Y     | 602 | CLA  | C11-C12-C13-C15 |
| 5   | N     | 617 | XAT  | C11-C12-C13-C14 |
| 3   | Y     | 603 | CLA  | O1A-CGA-O2A-C1  |
| 3   | G     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 2   | G     | 609 | CHL  | CBA-CGA-O2A-C1  |
| 4   | N     | 616 | LUT  | C29-C30-C31-C32 |
| 3   | N     | 613 | CLA  | C16-C17-C18-C20 |
| 7   | N     | 619 | LHG  | C4-C5-C6-O8     |
| 7   | G     | 618 | LHG  | C4-C5-C6-O8     |
| 7   | N     | 619 | LHG  | C29-C30-C31-C32 |
| 3   | G     | 612 | CLA  | C10-C11-C12-C13 |
| 7   | G     | 618 | LHG  | O7-C5-C6-O8     |
| 7   | Y     | 618 | LHG  | O7-C5-C6-O8     |
| 3   | G     | 603 | CLA  | C14-C13-C15-C16 |
| 7   | N     | 619 | LHG  | C30-C31-C32-C33 |
| 3   | G     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 3   | G     | 603 | CLA  | C13-C15-C16-C17 |
| 2   | G     | 606 | CHL  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | Y     | 605 | CHL  | CBA-CGA-O2A-C1  |
| 3   | G     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 3   | N     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 3   | N     | 614 | CLA  | C4B-C3B-CAB-CBB |
| 3   | G     | 602 | CLA  | C1A-C2A-CAA-CBA |
| 3   | G     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 3   | G     | 611 | CLA  | C4B-C3B-CAB-CBB |
| 3   | Y     | 603 | CLA  | C4B-C3B-CAB-CBB |
| 3   | Y     | 611 | CLA  | C4-C3-C5-C6     |
| 2   | Y     | 609 | CHL  | C16-C17-C18-C20 |
| 3   | G     | 604 | CLA  | C2A-CAA-CBA-CGA |
| 2   | N     | 601 | CHL  | C11-C10-C8-C7   |
| 2   | Y     | 608 | CHL  | C6-C7-C8-C10    |
| 3   | N     | 611 | CLA  | C11-C10-C8-C7   |
| 3   | N     | 613 | CLA  | C12-C13-C15-C16 |
| 3   | G     | 604 | CLA  | C12-C13-C15-C16 |
| 3   | Y     | 613 | CLA  | C12-C13-C15-C16 |
| 7   | G     | 618 | LHG  | C30-C31-C32-C33 |
| 7   | G     | 618 | LHG  | O6-C4-C5-O7     |
| 3   | N     | 603 | CLA  | C14-C13-C15-C16 |
| 3   | N     | 611 | CLA  | C14-C13-C15-C16 |
| 3   | Y     | 602 | CLA  | C11-C12-C13-C14 |
| 5   | N     | 617 | XAT  | C9-C10-C11-C12  |
| 3   | N     | 614 | CLA  | C1-C2-C3-C4     |
| 3   | G     | 614 | CLA  | C1-C2-C3-C4     |
| 3   | Y     | 614 | CLA  | C1-C2-C3-C4     |
| 2   | Y     | 605 | CHL  | O1A-CGA-O2A-C1  |
| 3   | Y     | 612 | CLA  | C5-C6-C7-C8     |
| 7   | Y     | 618 | LHG  | C4-C5-C6-O8     |
| 2   | N     | 609 | CHL  | C2C-C3C-CAC-CBC |
| 3   | N     | 614 | CLA  | CAD-CBD-CGD-O2D |
| 3   | G     | 614 | CLA  | CAD-CBD-CGD-O2D |
| 3   | G     | 603 | CLA  | C8-C10-C11-C12  |
| 7   | N     | 619 | LHG  | C13-C14-C15-C16 |
| 2   | G     | 609 | CHL  | CHA-CBD-CGD-O1D |
| 2   | G     | 609 | CHL  | CHA-CBD-CGD-O2D |
| 3   | N     | 614 | CLA  | CAD-CBD-CGD-O1D |
| 3   | G     | 614 | CLA  | CAD-CBD-CGD-O1D |
| 7   | N     | 619 | LHG  | C3-O3-P-O5      |
| 7   | N     | 619 | LHG  | C4-O6-P-O4      |
| 7   | Y     | 618 | LHG  | C4-O6-P-O3      |
| 3   | N     | 614 | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | G     | 614 | CLA  | C2B-C3B-CAB-CBB |
| 3   | Y     | 603 | CLA  | C2B-C3B-CAB-CBB |
| 3   | Y     | 610 | CLA  | C2B-C3B-CAB-CBB |
| 7   | Y     | 618 | LHG  | C4-C5-O7-C7     |
| 7   | Y     | 618 | LHG  | C12-C13-C14-C15 |
| 5   | G     | 619 | XAT  | C9-C10-C11-C12  |
| 2   | Y     | 601 | CHL  | C13-C15-C16-C17 |
| 7   | N     | 619 | LHG  | O6-C4-C5-C6     |
| 2   | N     | 609 | CHL  | C14-C13-C15-C16 |
| 2   | G     | 608 | CHL  | C14-C13-C15-C16 |
| 3   | N     | 603 | CLA  | C11-C12-C13-C14 |
| 2   | N     | 609 | CHL  | C12-C13-C15-C16 |
| 3   | G     | 602 | CLA  | C6-C7-C8-C10    |
| 3   | G     | 603 | CLA  | C12-C13-C15-C16 |
| 7   | N     | 619 | LHG  | O6-C4-C5-O7     |
| 3   | Y     | 603 | CLA  | C5-C6-C7-C8     |
| 6   | G     | 617 | NEX  | C33-C34-C35-C15 |
| 2   | G     | 608 | CHL  | C2A-CAA-CBA-CGA |
| 6   | N     | 618 | NEX  | C33-C34-C35-C15 |
| 6   | Y     | 617 | NEX  | C33-C34-C35-C15 |
| 3   | N     | 612 | CLA  | C4-C3-C5-C6     |
| 3   | G     | 602 | CLA  | C8-C10-C11-C12  |
| 3   | Y     | 611 | CLA  | C2-C3-C5-C6     |
| 2   | G     | 609 | CHL  | C2C-C3C-CAC-CBC |
| 3   | N     | 613 | CLA  | C16-C17-C18-C19 |
| 3   | N     | 613 | CLA  | C14-C13-C15-C16 |
| 3   | G     | 602 | CLA  | C6-C7-C8-C9     |
| 3   | G     | 604 | CLA  | C14-C13-C15-C16 |
| 2   | G     | 601 | CHL  | C13-C15-C16-C17 |
| 2   | G     | 601 | CHL  | CBA-CGA-O2A-C1  |
| 2   | Y     | 608 | CHL  | C4-C3-C5-C6     |
| 3   | G     | 604 | CLA  | C4-C3-C5-C6     |
| 3   | N     | 612 | CLA  | C11-C10-C8-C7   |
| 3   | G     | 602 | CLA  | C11-C12-C13-C15 |
| 2   | N     | 609 | CHL  | O1A-CGA-O2A-C1  |
| 2   | Y     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 2   | Y     | 605 | CHL  | C3A-C2A-CAA-CBA |
| 3   | G     | 612 | CLA  | C4-C3-C5-C6     |
| 3   | N     | 610 | CLA  | C5-C6-C7-C8     |
| 2   | G     | 609 | CHL  | C2-C1-O2A-CGA   |
| 3   | N     | 612 | CLA  | C2-C3-C5-C6     |
| 2   | G     | 607 | CHL  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | Y     | 607 | CHL  | C6-C7-C8-C9     |
| 3   | N     | 612 | CLA  | C11-C10-C8-C9   |
| 3   | Y     | 604 | CLA  | C11-C12-C13-C14 |
| 7   | N     | 619 | LHG  | C4-C5-O7-C7     |
| 2   | G     | 607 | CHL  | C15-C16-C17-C18 |
| 2   | G     | 608 | CHL  | C1A-C2A-CAA-CBA |
| 2   | G     | 609 | CHL  | C1A-C2A-CAA-CBA |
| 2   | Y     | 609 | CHL  | C1A-C2A-CAA-CBA |
| 2   | N     | 608 | CHL  | C16-C17-C18-C20 |
| 3   | Y     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 2   | G     | 608 | CHL  | C16-C17-C18-C19 |
| 4   | N     | 615 | LUT  | C1-C6-C7-C8     |
| 4   | G     | 616 | LUT  | C1-C6-C7-C8     |
| 4   | Y     | 615 | LUT  | C5-C6-C7-C8     |
| 4   | Y     | 616 | LUT  | C1-C6-C7-C8     |
| 2   | G     | 609 | CHL  | C16-C17-C18-C19 |
| 2   | Y     | 608 | CHL  | C2-C3-C5-C6     |
| 3   | G     | 612 | CLA  | C2-C3-C5-C6     |
| 3   | N     | 603 | CLA  | C10-C11-C12-C13 |
| 3   | N     | 612 | CLA  | C11-C12-C13-C15 |
| 3   | Y     | 603 | CLA  | C12-C13-C15-C16 |
| 3   | Y     | 612 | CLA  | C16-C17-C18-C20 |
| 3   | N     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 3   | G     | 613 | CLA  | C15-C16-C17-C18 |
| 6   | N     | 618 | NEX  | C30-C31-C32-C33 |
| 6   | G     | 617 | NEX  | C30-C31-C32-C33 |
| 6   | Y     | 617 | NEX  | C30-C31-C32-C33 |
| 3   | G     | 604 | CLA  | C2-C3-C5-C6     |
| 3   | N     | 612 | CLA  | C5-C6-C7-C8     |
| 3   | Y     | 612 | CLA  | C16-C17-C18-C19 |
| 3   | Y     | 614 | CLA  | O2A-C1-C2-C3    |
| 2   | G     | 601 | CHL  | O1A-CGA-O2A-C1  |
| 3   | G     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 3   | G     | 602 | CLA  | C13-C15-C16-C17 |
| 7   | Y     | 618 | LHG  | C27-C28-C29-C30 |
| 3   | N     | 603 | CLA  | O1A-CGA-O2A-C1  |
| 2   | G     | 605 | CHL  | O1D-CGD-O2D-CED |
| 3   | N     | 611 | CLA  | C4-C3-C5-C6     |
| 2   | N     | 601 | CHL  | C11-C10-C8-C9   |
| 2   | Y     | 608 | CHL  | C6-C7-C8-C9     |
| 3   | N     | 613 | CLA  | C11-C12-C13-C14 |
| 3   | Y     | 612 | CLA  | C11-C10-C8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | Y     | 613 | CLA  | C14-C13-C15-C16 |
| 7   | N     | 619 | LHG  | C34-C35-C36-C37 |
| 2   | Y     | 601 | CHL  | C2-C1-O2A-CGA   |
| 3   | N     | 604 | CLA  | C2-C1-O2A-CGA   |
| 3   | G     | 603 | CLA  | C16-C17-C18-C20 |
| 7   | N     | 619 | LHG  | C6-C5-O7-C7     |
| 7   | G     | 618 | LHG  | C4-C5-O7-C7     |
| 7   | G     | 618 | LHG  | C6-C5-O7-C7     |
| 3   | Y     | 613 | CLA  | C15-C16-C17-C18 |
| 2   | Y     | 608 | CHL  | C16-C17-C18-C19 |
| 5   | N     | 620 | XAT  | O24-C26-C27-C28 |
| 2   | G     | 605 | CHL  | CBA-CGA-O2A-C1  |
| 3   | G     | 603 | CLA  | C16-C17-C18-C19 |
| 2   | N     | 607 | CHL  | C5-C6-C7-C8     |
| 2   | G     | 609 | CHL  | O1A-CGA-O2A-C1  |
| 3   | G     | 612 | CLA  | C5-C6-C7-C8     |
| 2   | Y     | 609 | CHL  | C6-C7-C8-C10    |
| 3   | Y     | 612 | CLA  | C11-C10-C8-C7   |
| 4   | N     | 615 | LUT  | C5-C6-C7-C8     |
| 4   | G     | 616 | LUT  | C5-C6-C7-C8     |
| 2   | G     | 601 | CHL  | C2-C1-O2A-CGA   |
| 2   | G     | 606 | CHL  | C1C-C2C-CMC-OMC |
| 2   | Y     | 608 | CHL  | CAA-CBA-CGA-O2A |
| 3   | N     | 604 | CLA  | C4-C3-C5-C6     |
| 2   | N     | 608 | CHL  | CAA-CBA-CGA-O2A |
| 3   | Y     | 602 | CLA  | C13-C15-C16-C17 |
| 3   | G     | 602 | CLA  | C11-C12-C13-C14 |
| 3   | Y     | 603 | CLA  | CAA-CBA-CGA-O2A |
| 4   | N     | 615 | LUT  | C29-C30-C31-C32 |
| 3   | N     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 7   | Y     | 618 | LHG  | O8-C23-C24-C25  |
| 3   | N     | 603 | CLA  | C2A-CAA-CBA-CGA |
| 2   | N     | 606 | CHL  | C2-C1-O2A-CGA   |
| 3   | G     | 604 | CLA  | C2-C1-O2A-CGA   |
| 2   | G     | 608 | CHL  | C6-C7-C8-C10    |
| 3   | N     | 602 | CLA  | C11-C12-C13-C15 |
| 3   | N     | 613 | CLA  | C11-C12-C13-C15 |
| 3   | Y     | 611 | CLA  | C11-C12-C13-C15 |
| 7   | Y     | 618 | LHG  | C6-C5-O7-C7     |
| 7   | G     | 618 | LHG  | O8-C23-C24-C25  |
| 3   | G     | 611 | CLA  | C16-C17-C18-C20 |
| 3   | G     | 613 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | G     | 605 | CHL  | O1A-CGA-O2A-C1  |
| 2   | Y     | 609 | CHL  | C14-C13-C15-C16 |
| 3   | N     | 612 | CLA  | C11-C12-C13-C14 |
| 5   | N     | 617 | XAT  | C31-C32-C33-C34 |
| 3   | G     | 613 | CLA  | CBA-CGA-O2A-C1  |
| 2   | N     | 608 | CHL  | CAA-CBA-CGA-O1A |
| 3   | N     | 613 | CLA  | C13-C15-C16-C17 |
| 7   | N     | 619 | LHG  | C9-C10-C11-C12  |
| 2   | N     | 605 | CHL  | CAD-CBD-CGD-O2D |
| 2   | Y     | 606 | CHL  | CAD-CBD-CGD-O2D |
| 7   | Y     | 618 | LHG  | O10-C23-C24-C25 |
| 3   | G     | 611 | CLA  | C10-C11-C12-C13 |
| 3   | G     | 611 | CLA  | C2-C1-O2A-CGA   |
| 2   | Y     | 608 | CHL  | CAA-CBA-CGA-O1A |
| 3   | Y     | 603 | CLA  | CAA-CBA-CGA-O1A |
| 2   | N     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 2   | Y     | 605 | CHL  | C1A-C2A-CAA-CBA |
| 2   | Y     | 607 | CHL  | C15-C16-C17-C18 |
| 3   | N     | 603 | CLA  | CAA-CBA-CGA-O2A |
| 3   | Y     | 604 | CLA  | CAA-CBA-CGA-O2A |
| 7   | N     | 619 | LHG  | O8-C23-C24-C25  |
| 3   | Y     | 602 | CLA  | C8-C10-C11-C12  |

There are no ring outliers.

51 monomers are involved in 151 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | Y     | 616 | LUT  | 7       | 0            |
| 4   | N     | 615 | LUT  | 4       | 0            |
| 4   | N     | 616 | LUT  | 5       | 0            |
| 3   | N     | 602 | CLA  | 2       | 0            |
| 3   | G     | 614 | CLA  | 1       | 0            |
| 2   | G     | 601 | CHL  | 11      | 0            |
| 3   | G     | 611 | CLA  | 2       | 0            |
| 3   | Y     | 602 | CLA  | 3       | 0            |
| 4   | G     | 615 | LUT  | 5       | 0            |
| 4   | G     | 616 | LUT  | 5       | 0            |
| 3   | N     | 614 | CLA  | 1       | 0            |
| 5   | G     | 619 | XAT  | 9       | 0            |
| 2   | G     | 608 | CHL  | 2       | 0            |
| 2   | N     | 607 | CHL  | 4       | 0            |
| 2   | Y     | 606 | CHL  | 2       | 0            |

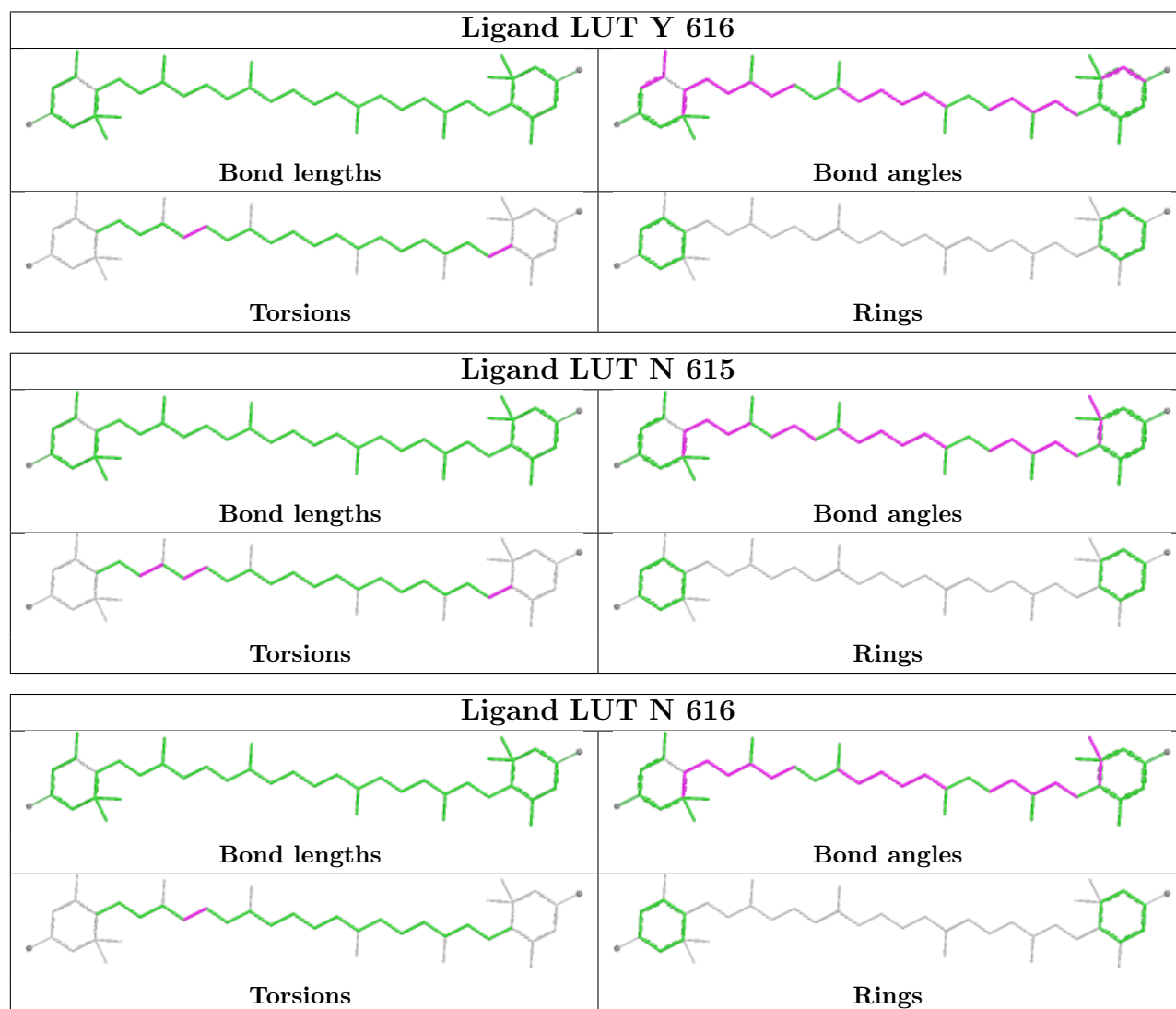
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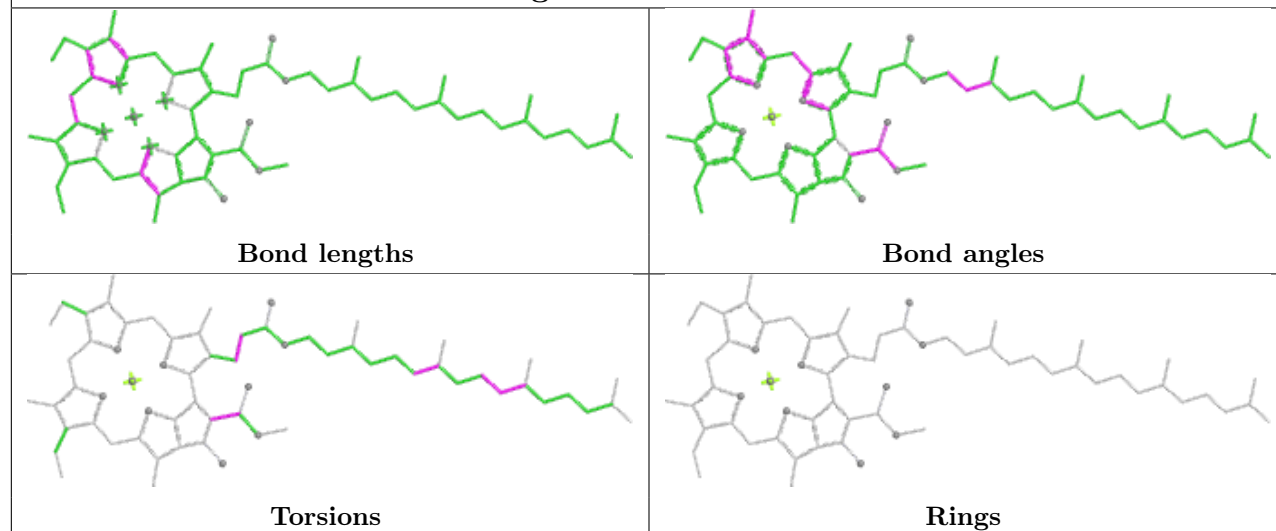
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | Y     | 603 | CLA  | 4       | 0            |
| 5   | N     | 620 | XAT  | 3       | 0            |
| 7   | G     | 618 | LHG  | 3       | 0            |
| 3   | G     | 602 | CLA  | 5       | 0            |
| 3   | N     | 604 | CLA  | 1       | 0            |
| 6   | Y     | 617 | NEX  | 2       | 0            |
| 3   | N     | 603 | CLA  | 2       | 0            |
| 3   | Y     | 612 | CLA  | 2       | 0            |
| 3   | G     | 613 | CLA  | 4       | 0            |
| 5   | N     | 617 | XAT  | 8       | 0            |
| 3   | Y     | 613 | CLA  | 4       | 0            |
| 3   | Y     | 604 | CLA  | 2       | 0            |
| 2   | Y     | 608 | CHL  | 5       | 0            |
| 3   | N     | 613 | CLA  | 3       | 0            |
| 7   | Y     | 618 | LHG  | 8       | 0            |
| 2   | N     | 609 | CHL  | 6       | 0            |
| 3   | Y     | 610 | CLA  | 10      | 0            |
| 7   | N     | 619 | LHG  | 3       | 0            |
| 3   | N     | 610 | CLA  | 4       | 0            |
| 2   | G     | 607 | CHL  | 5       | 0            |
| 3   | G     | 604 | CLA  | 3       | 0            |
| 2   | G     | 609 | CHL  | 3       | 0            |
| 2   | N     | 606 | CHL  | 3       | 0            |
| 4   | Y     | 615 | LUT  | 6       | 0            |
| 6   | G     | 617 | NEX  | 1       | 0            |
| 2   | G     | 606 | CHL  | 1       | 0            |
| 2   | Y     | 609 | CHL  | 6       | 0            |
| 2   | N     | 601 | CHL  | 4       | 0            |
| 3   | G     | 610 | CLA  | 7       | 0            |
| 2   | G     | 605 | CHL  | 1       | 0            |
| 3   | Y     | 614 | CLA  | 2       | 0            |
| 2   | Y     | 607 | CHL  | 3       | 0            |
| 2   | Y     | 601 | CHL  | 9       | 0            |
| 3   | Y     | 611 | CLA  | 6       | 0            |
| 2   | N     | 608 | CHL  | 6       | 0            |
| 3   | N     | 611 | CLA  | 3       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

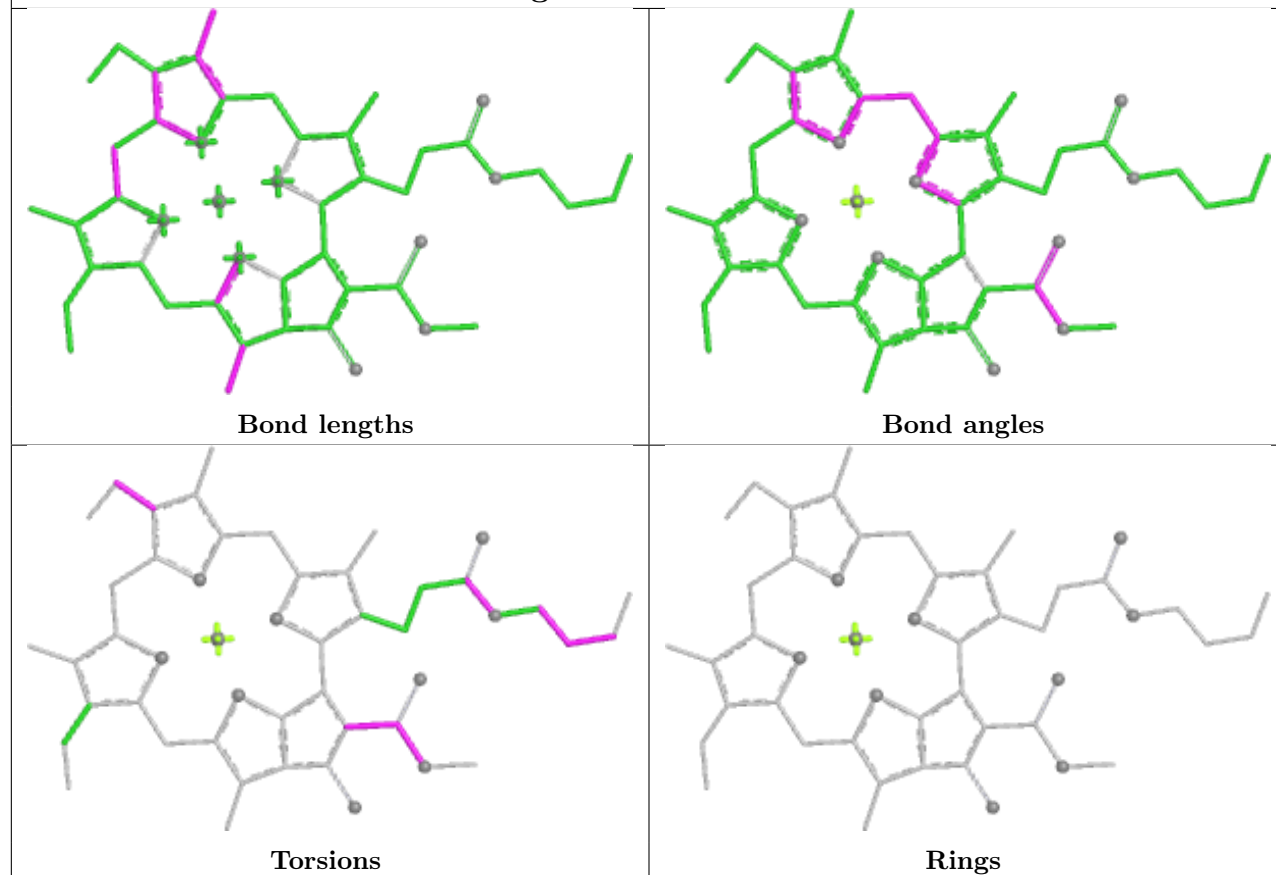
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

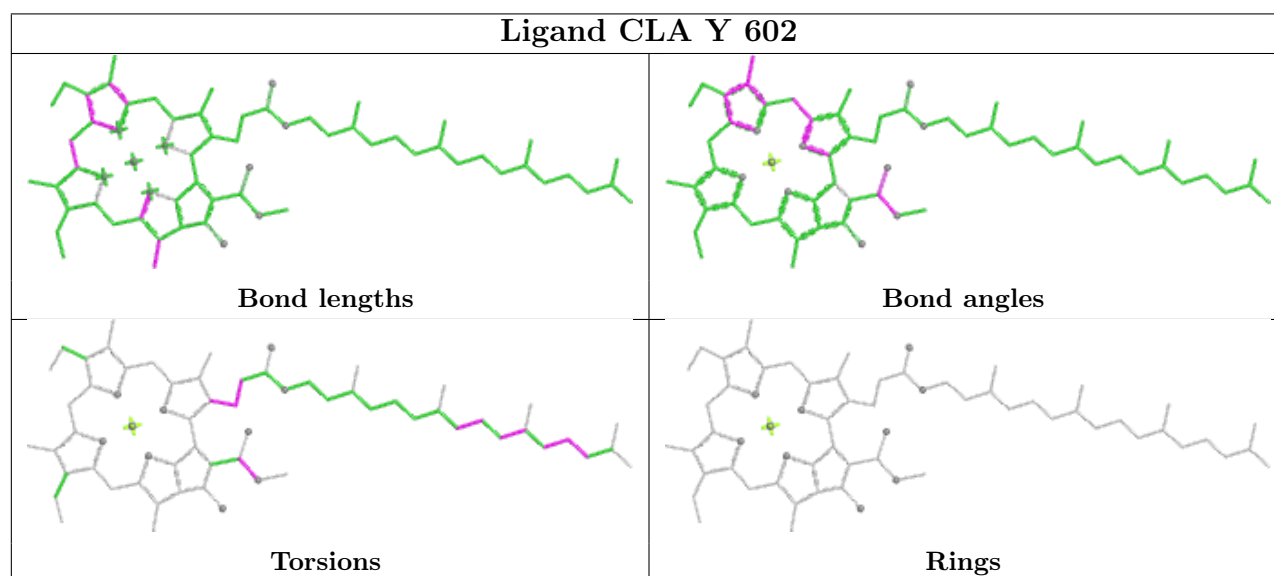
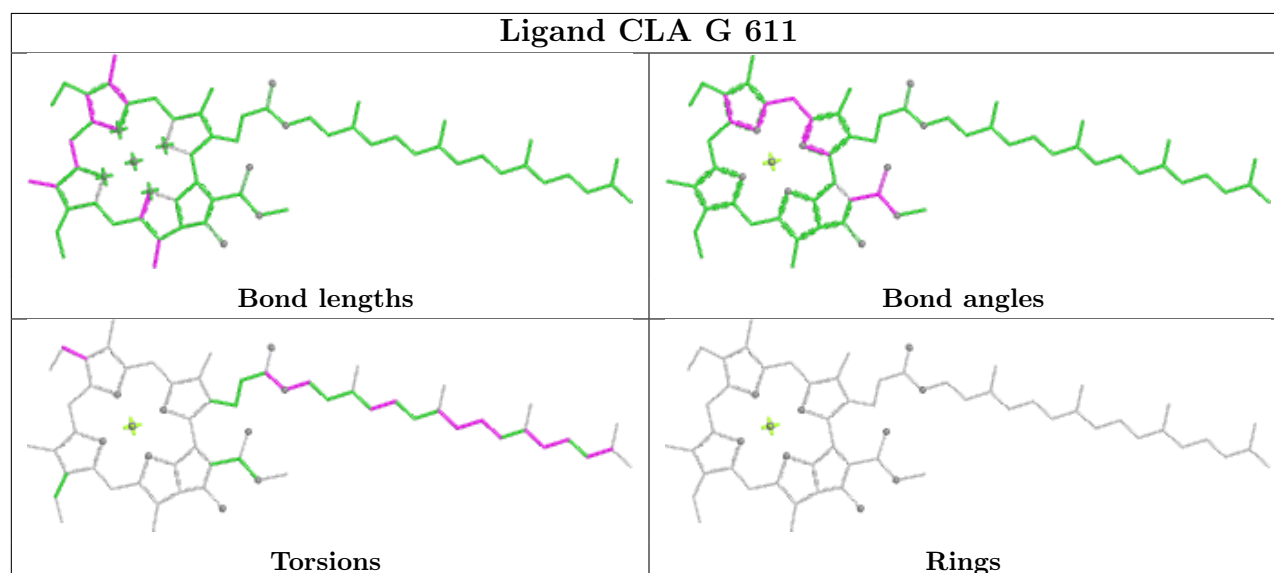
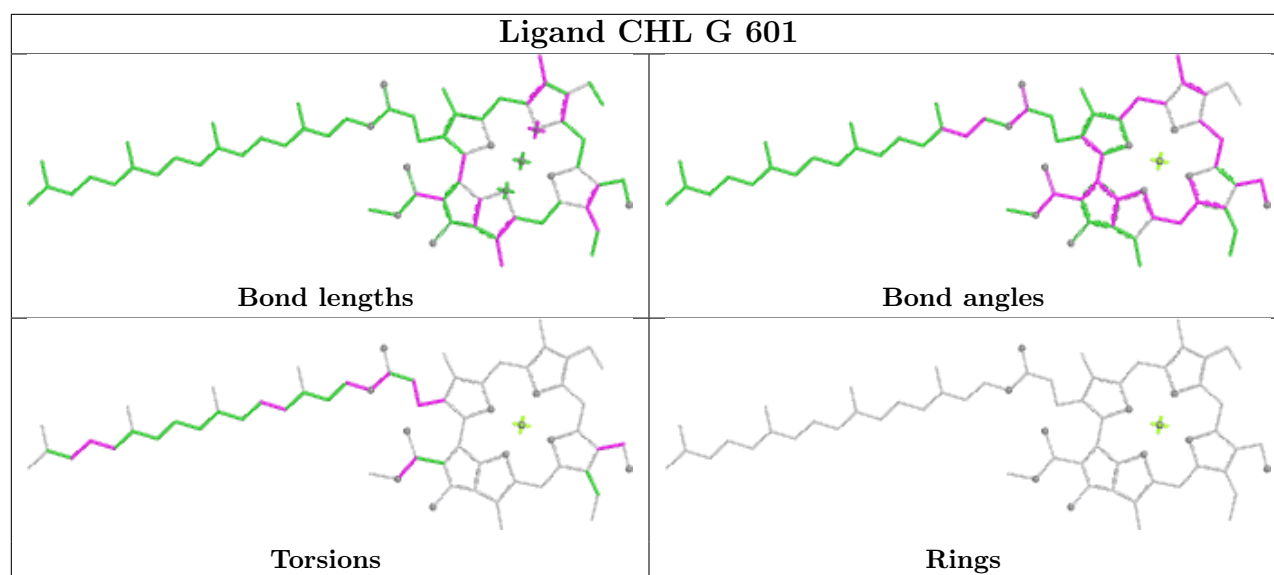


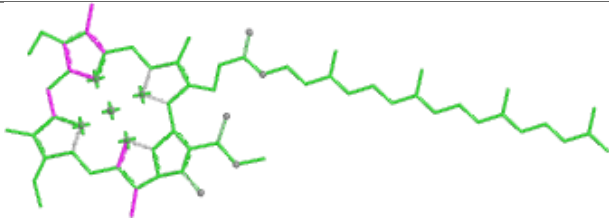
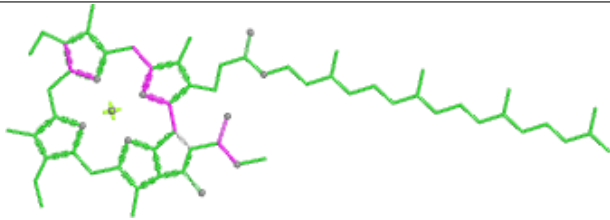
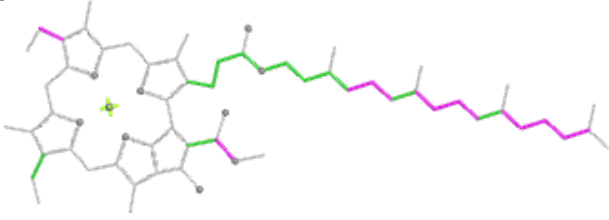
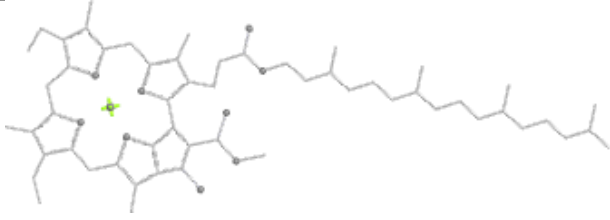
## Ligand CLA N 602

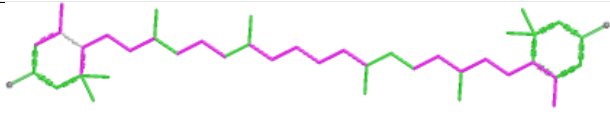
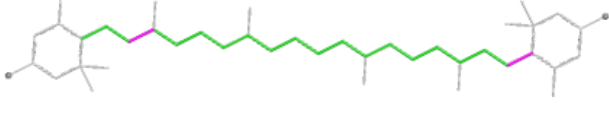
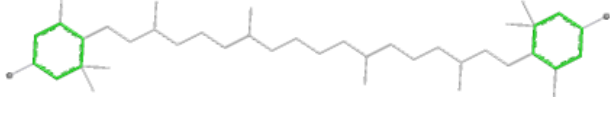


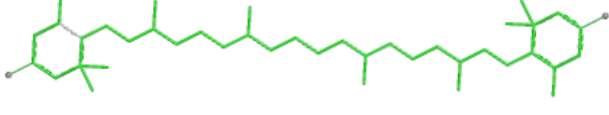
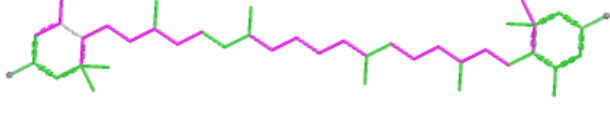
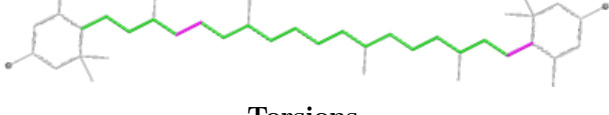
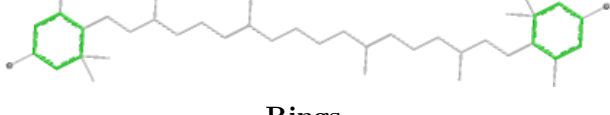
## Ligand CLA G 614

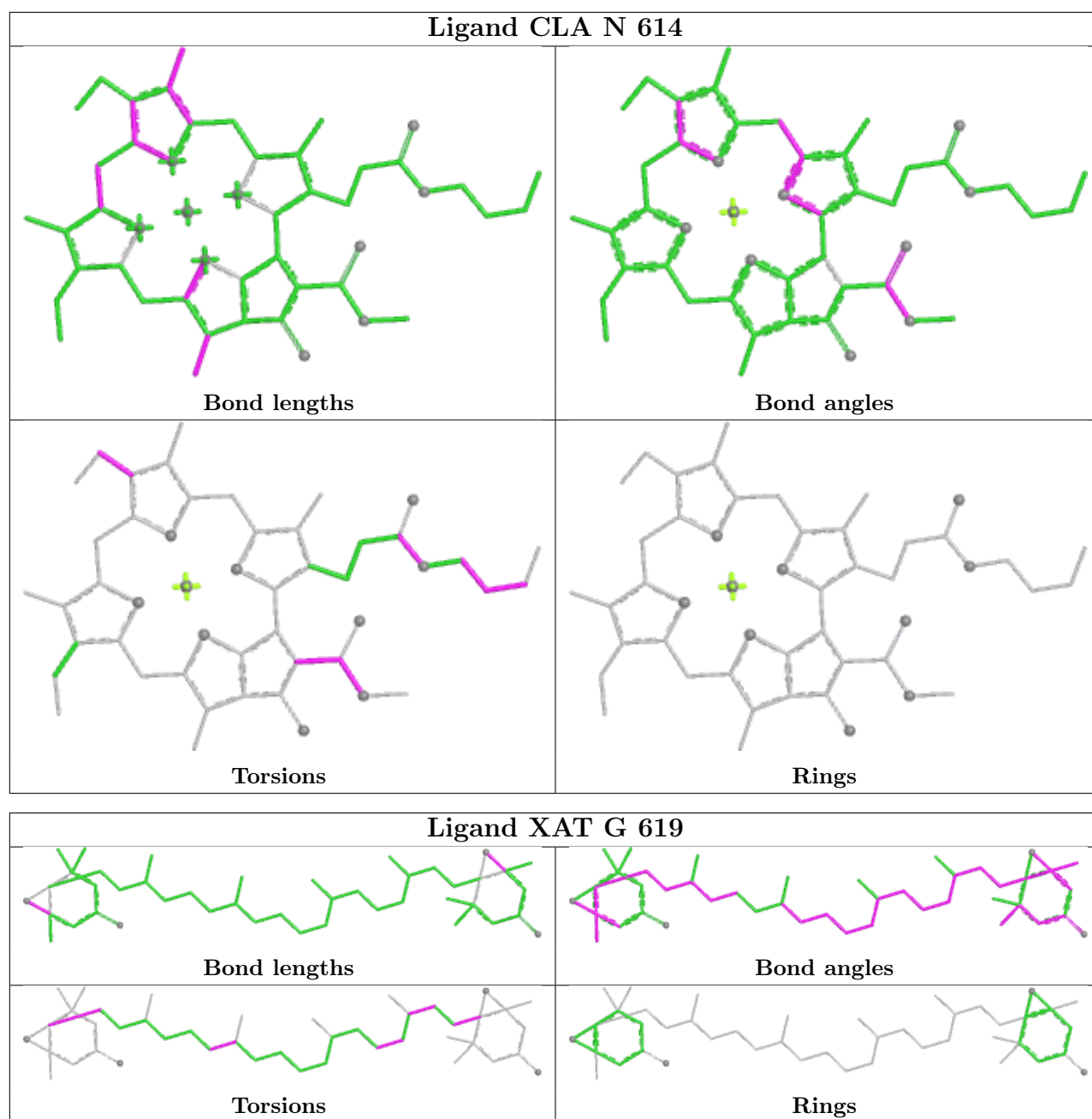


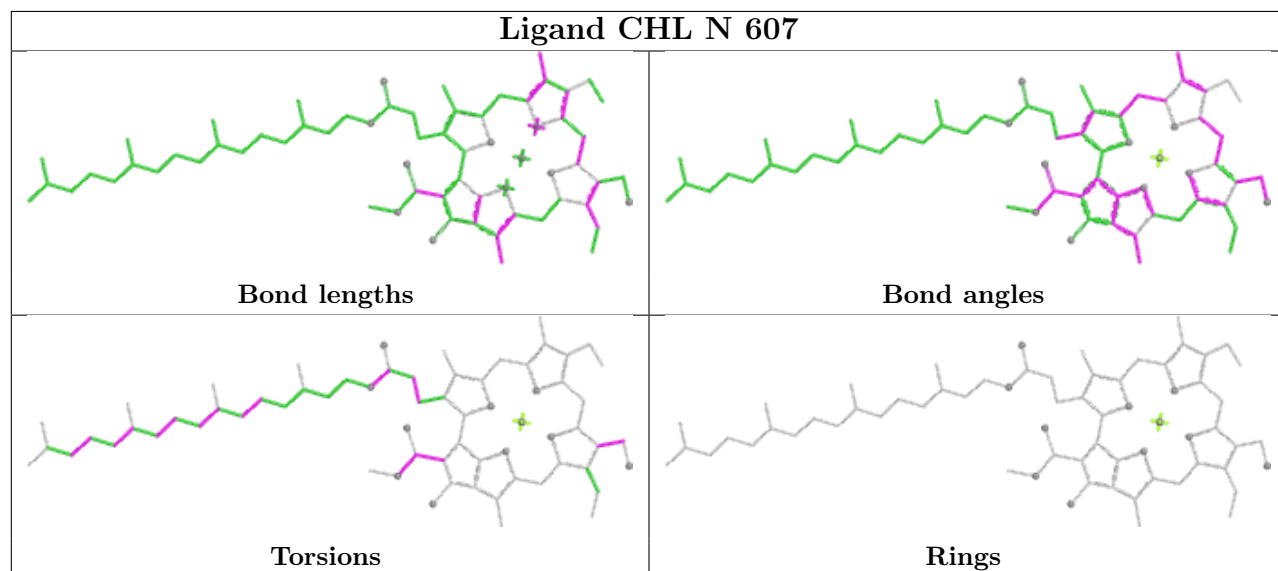
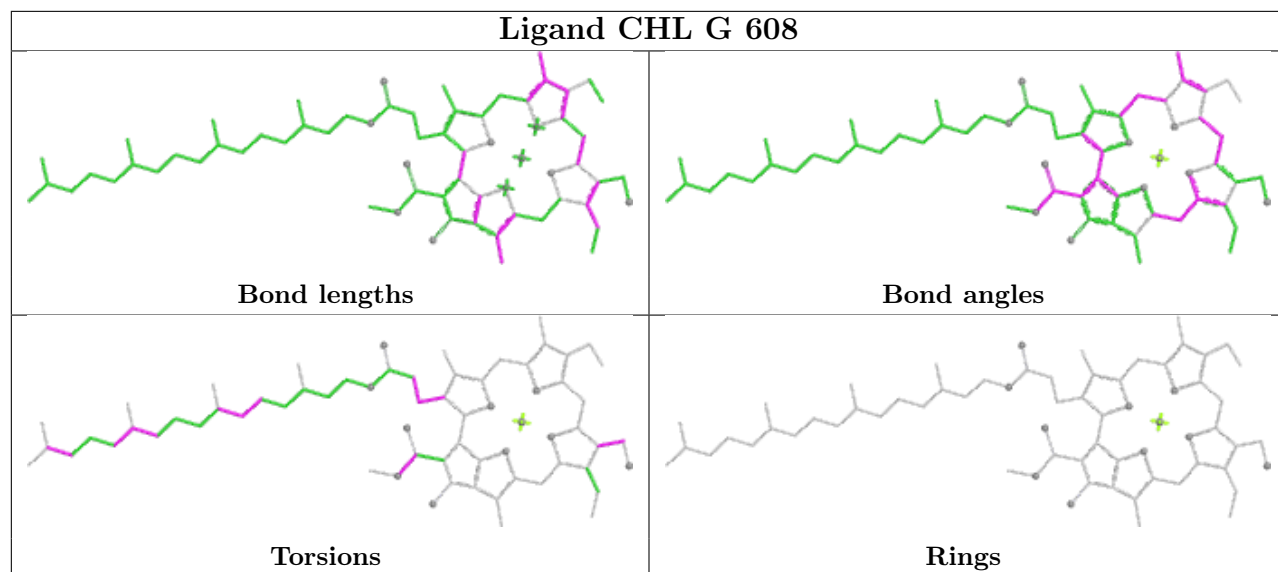


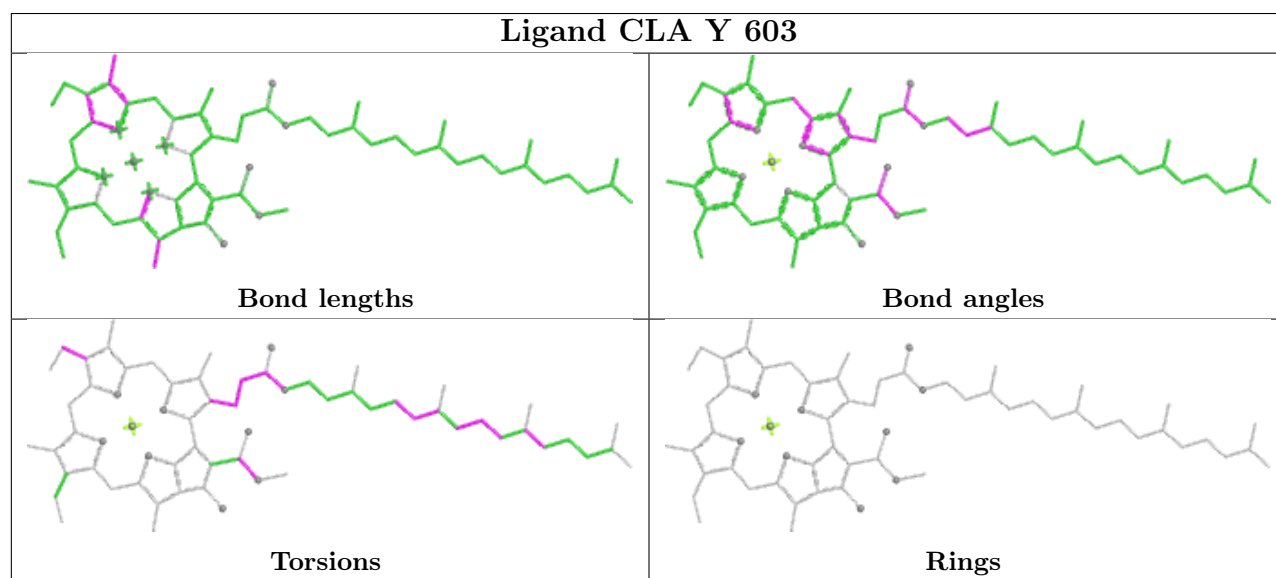
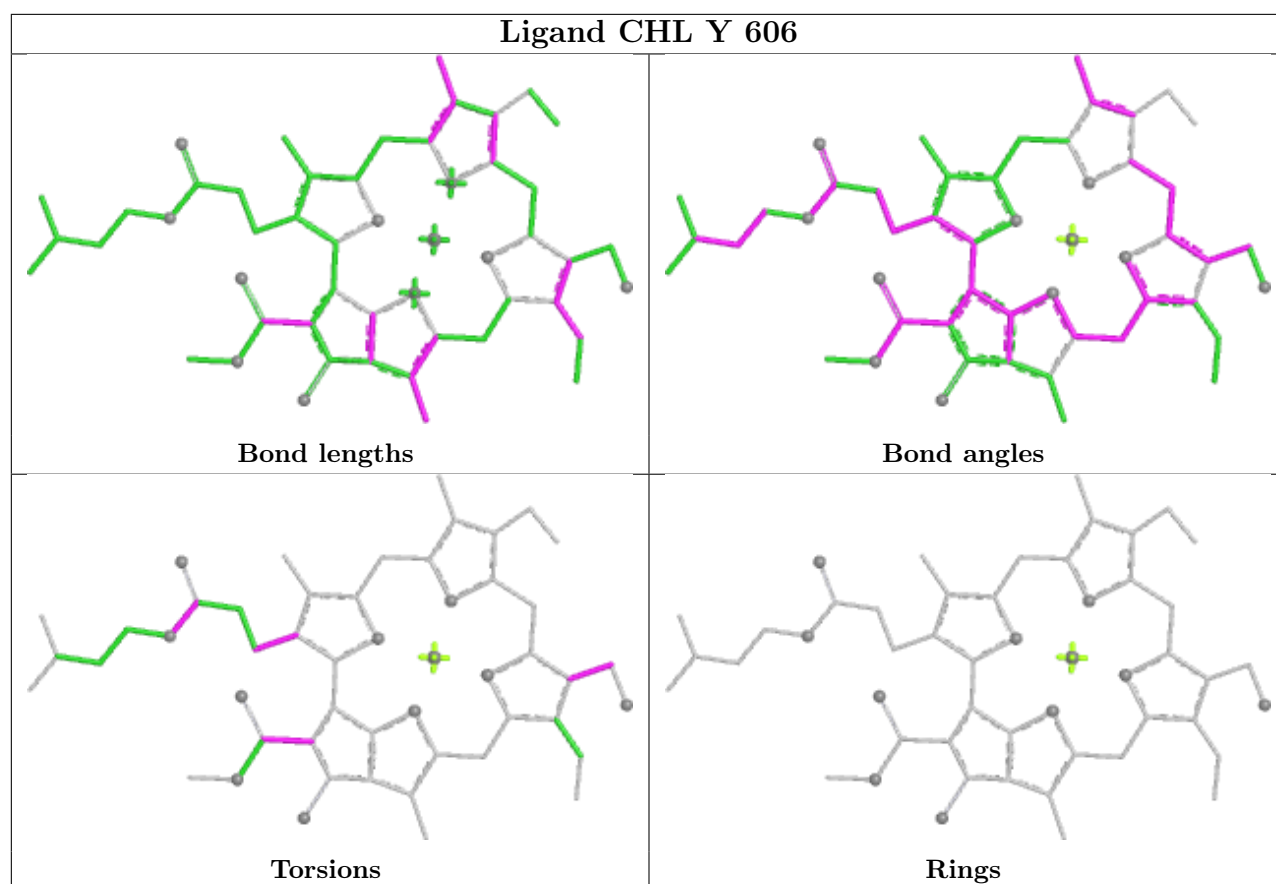
| Ligand CLA G 603                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

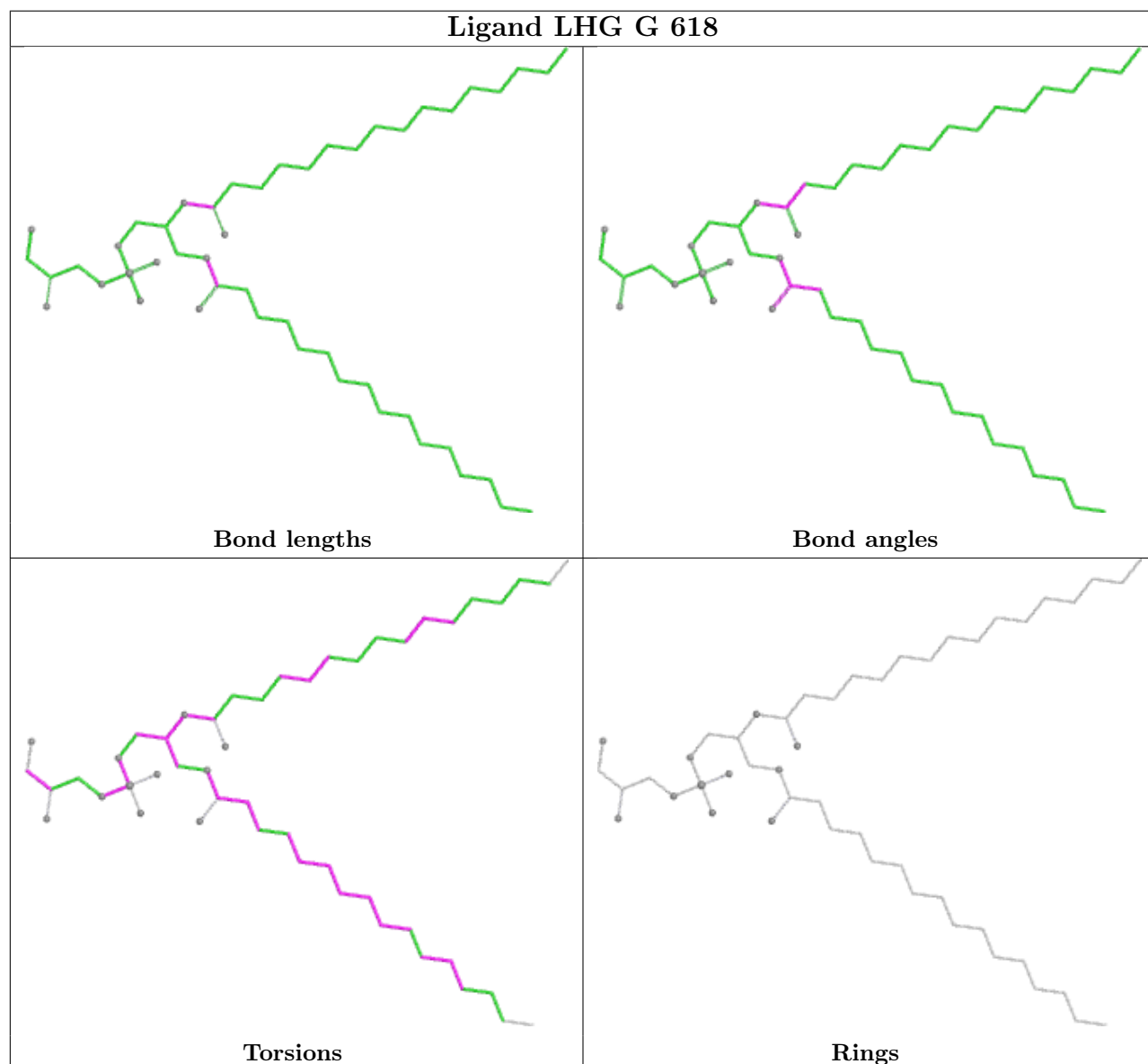
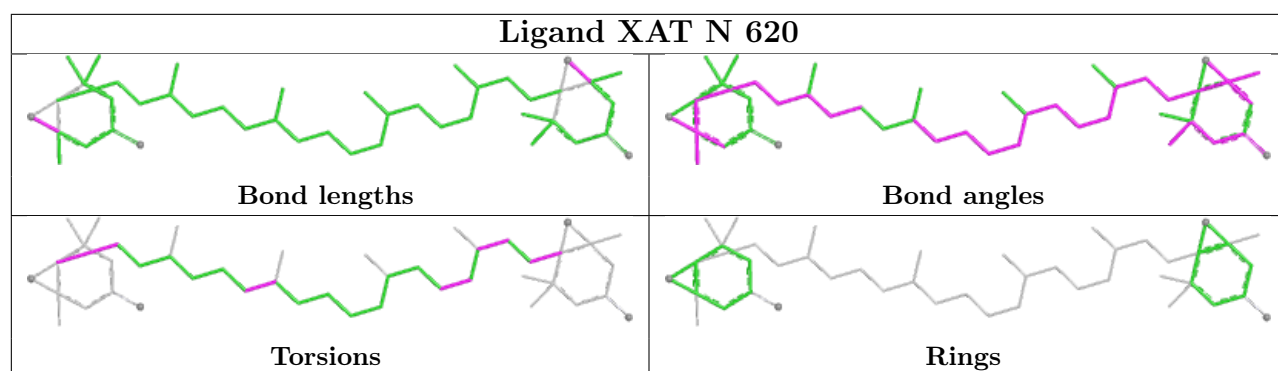
| Ligand LUT G 615                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

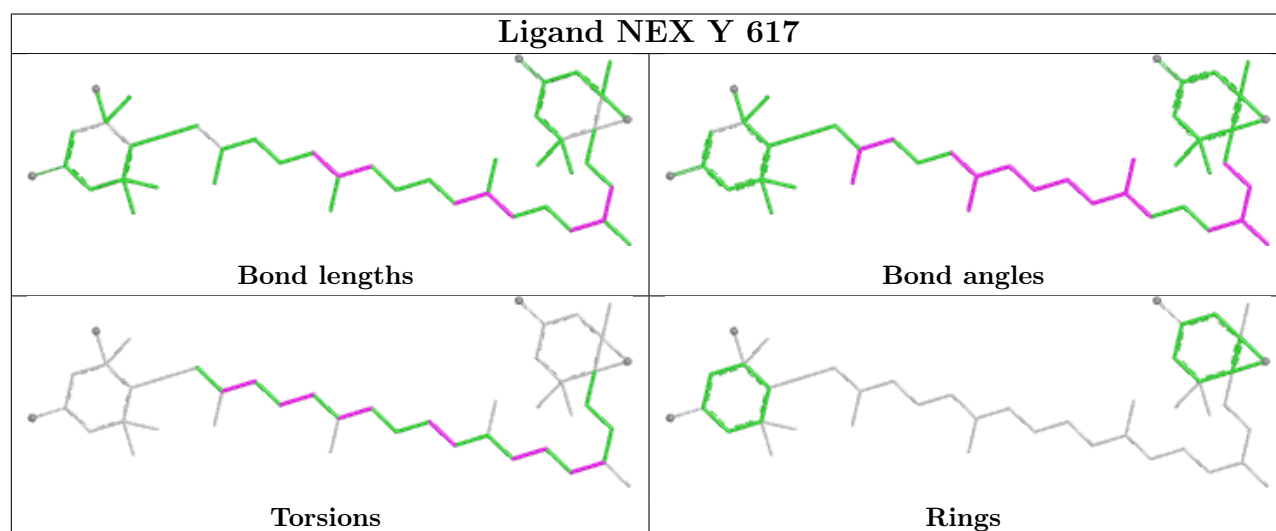
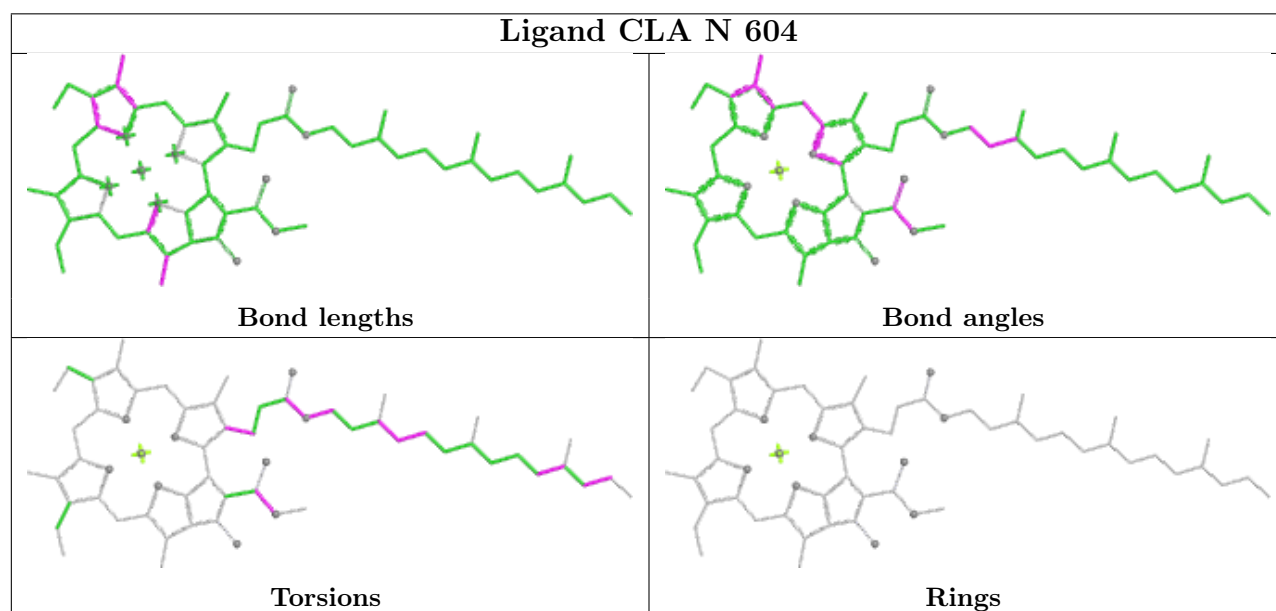
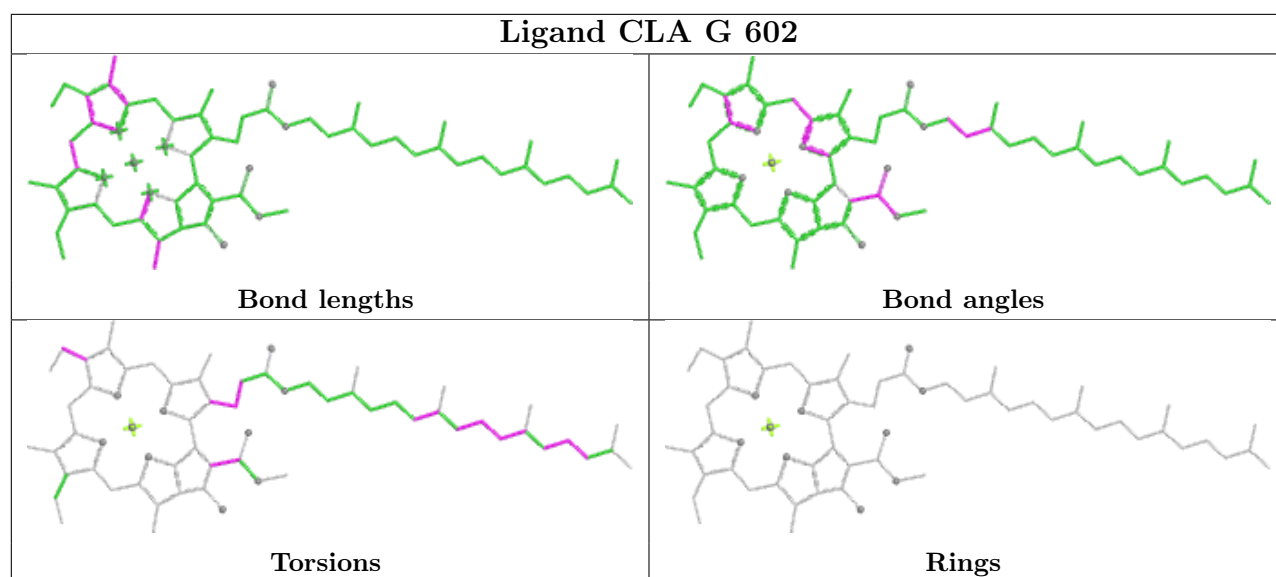
| Ligand LUT G 616                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

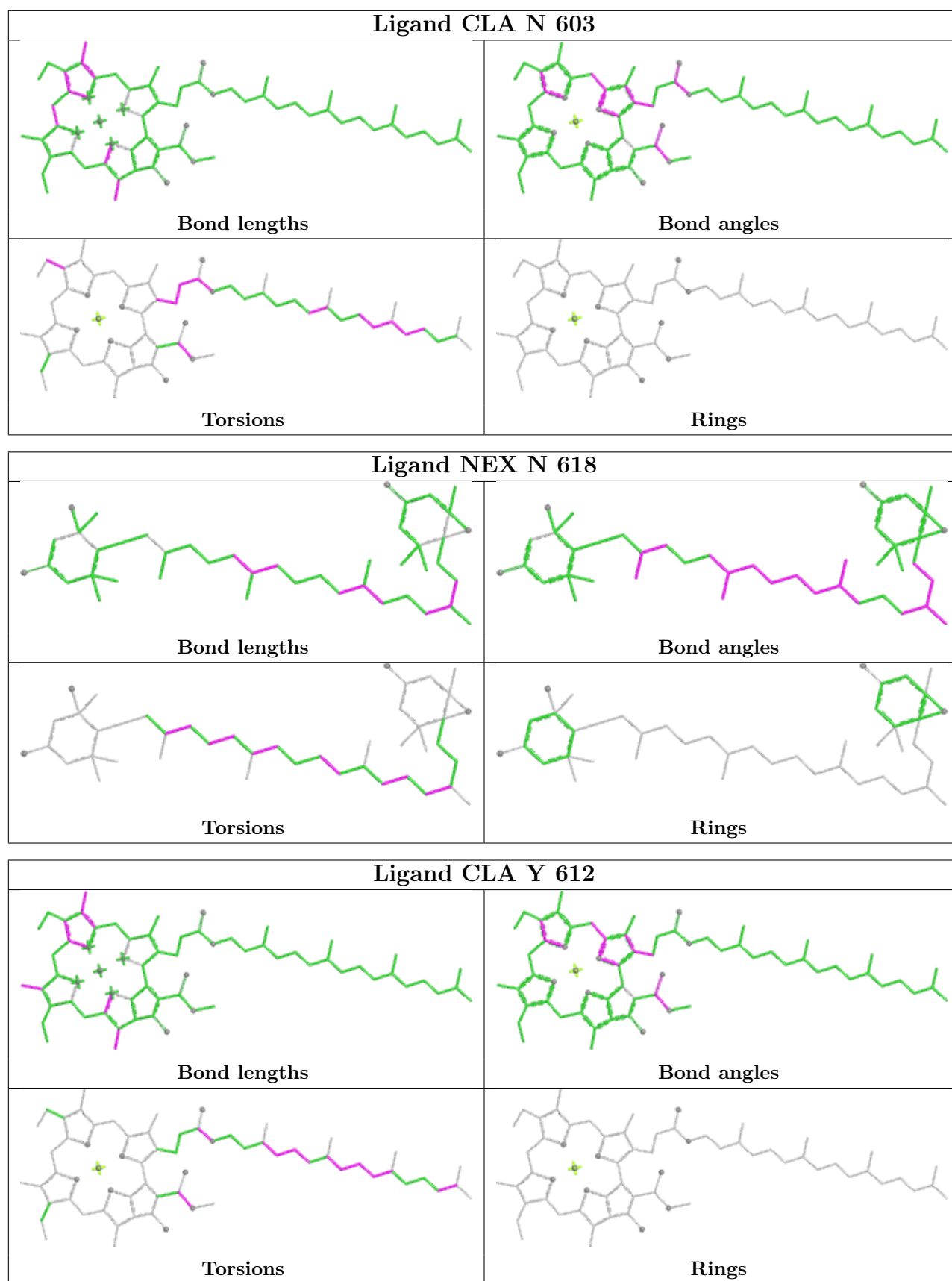


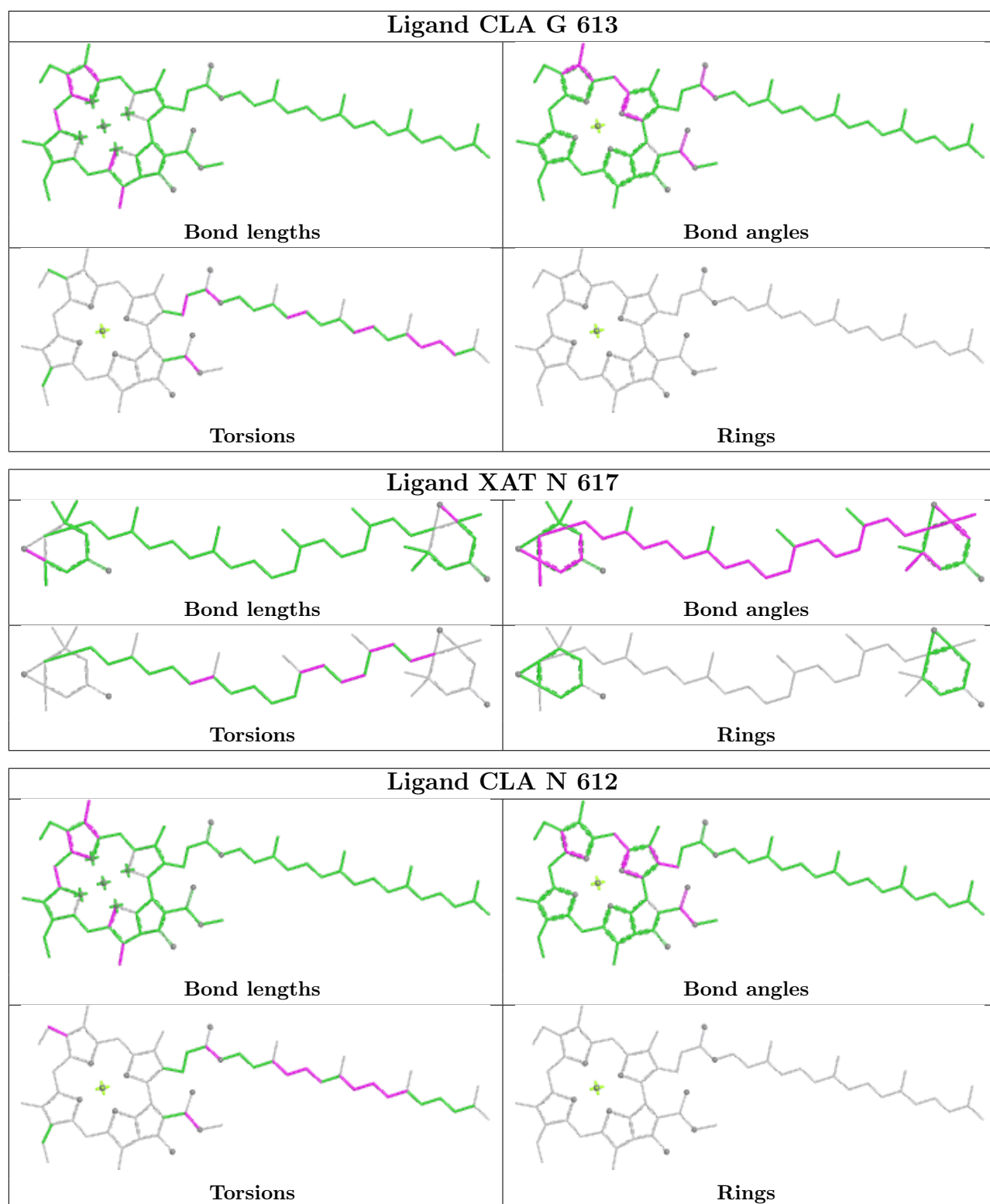




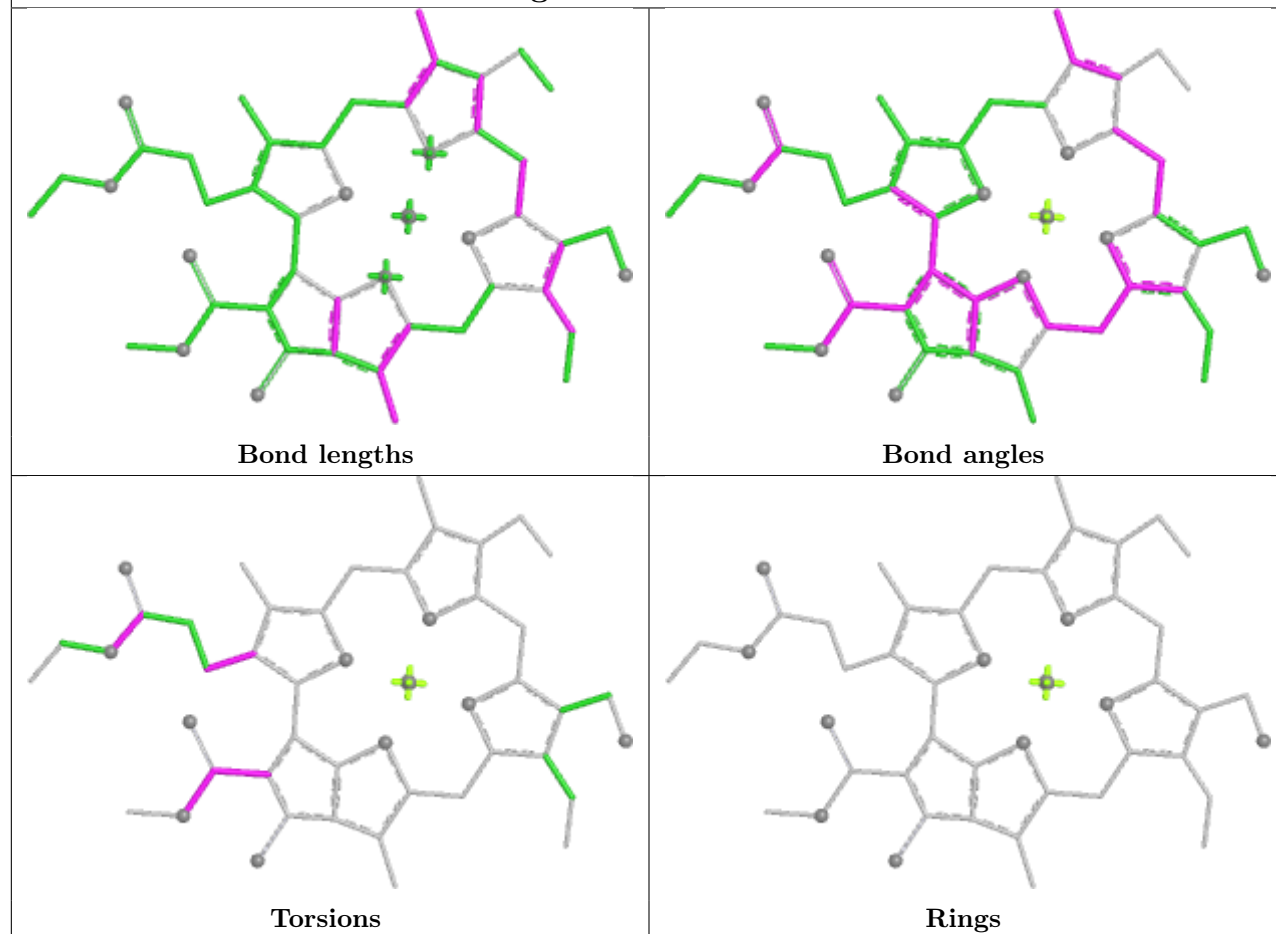




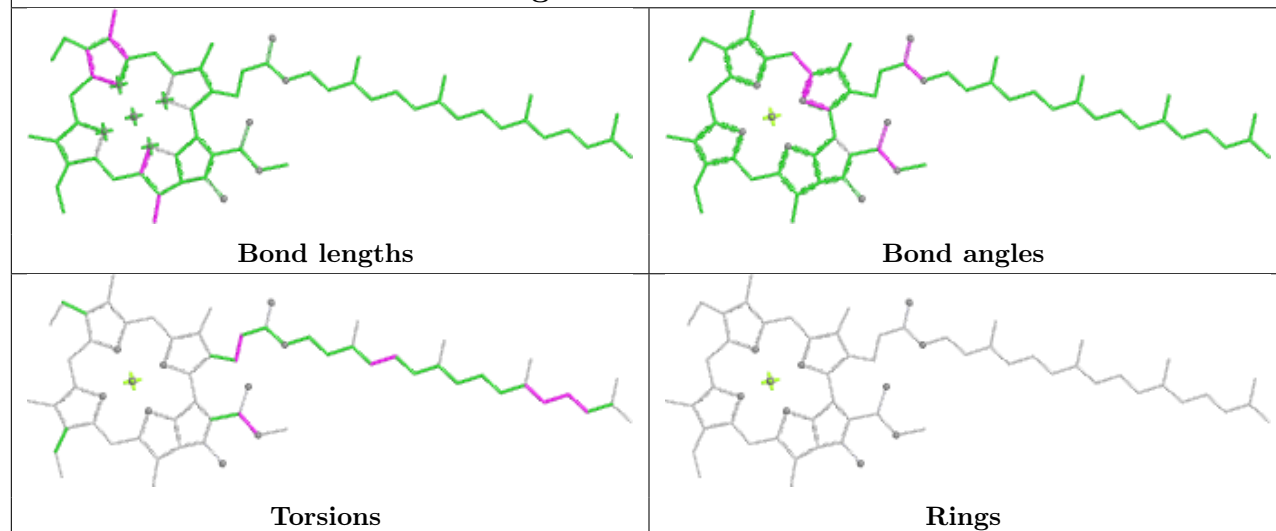


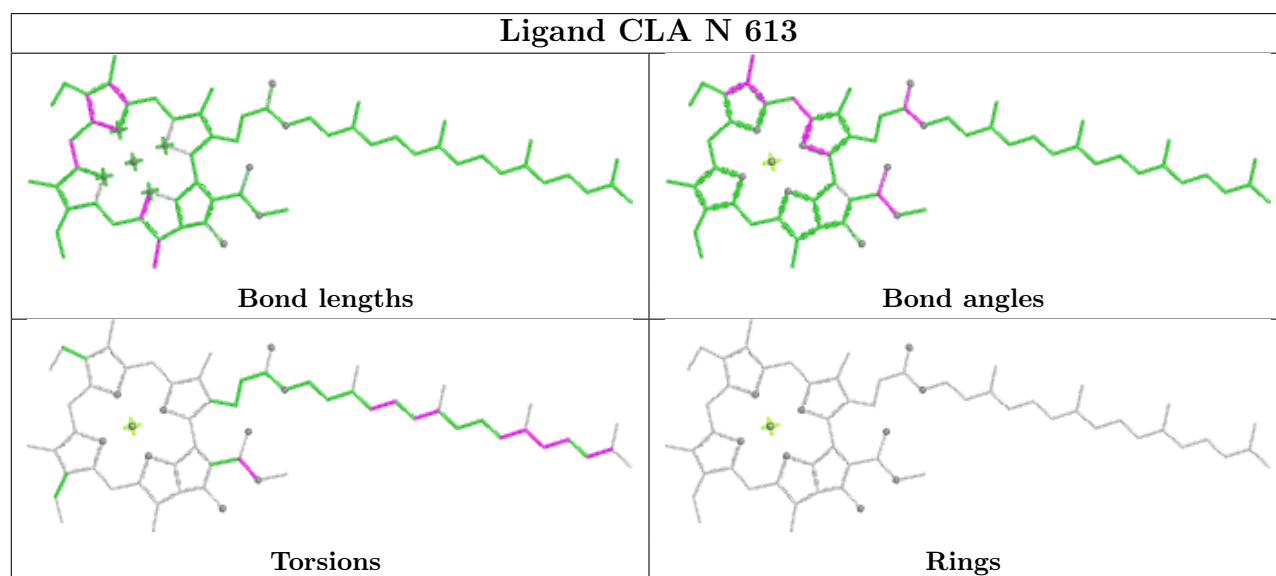
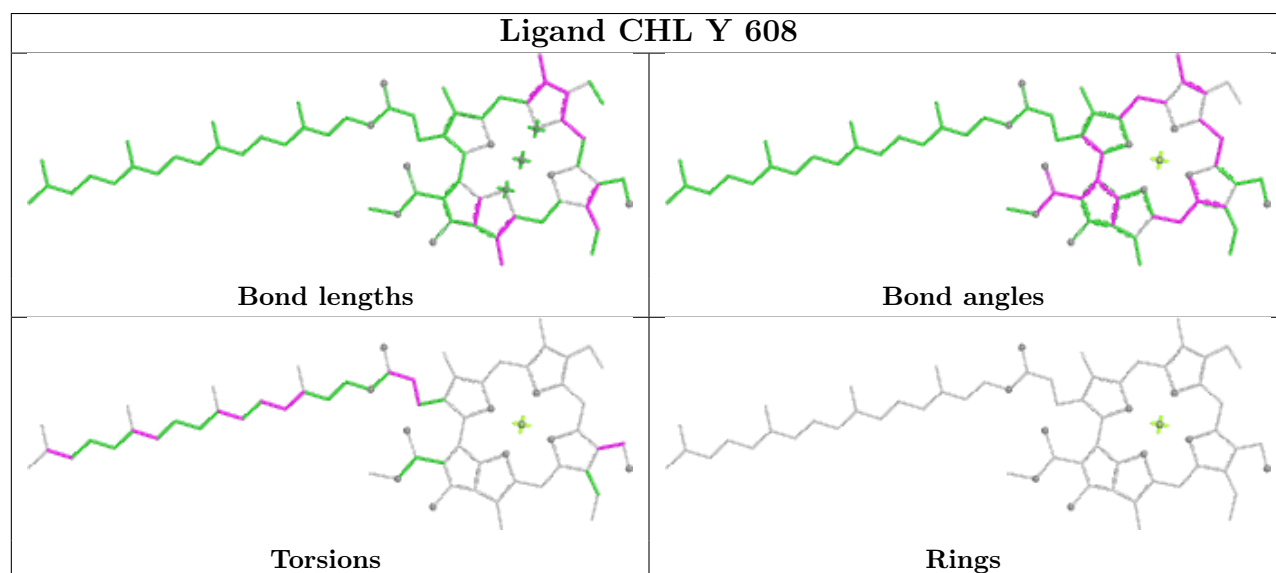
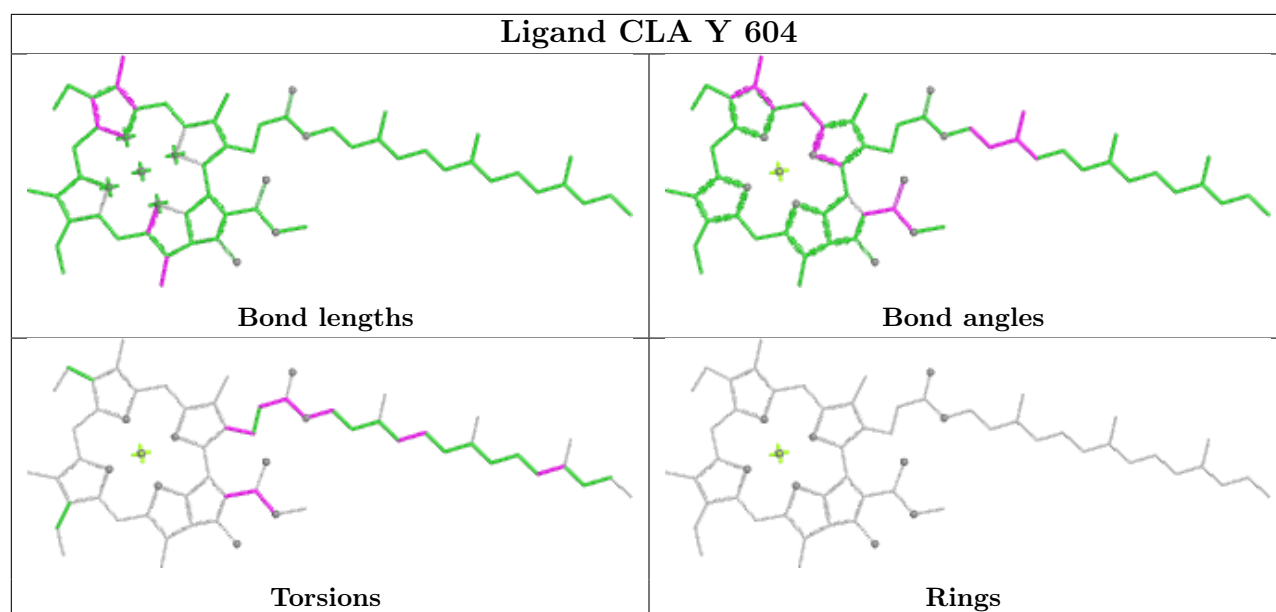


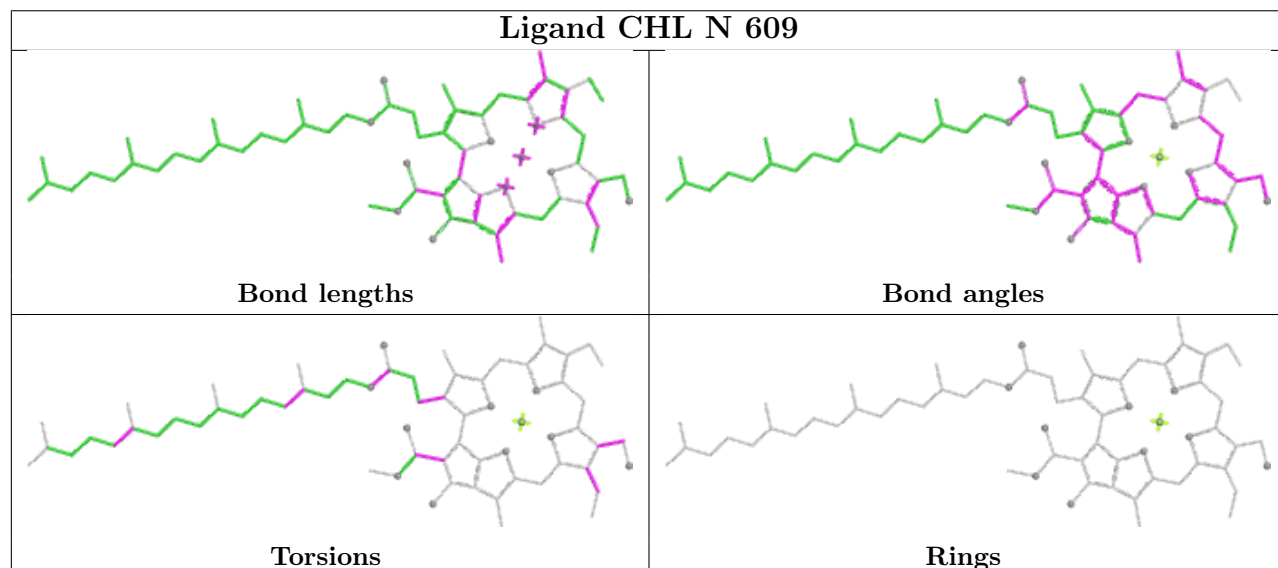
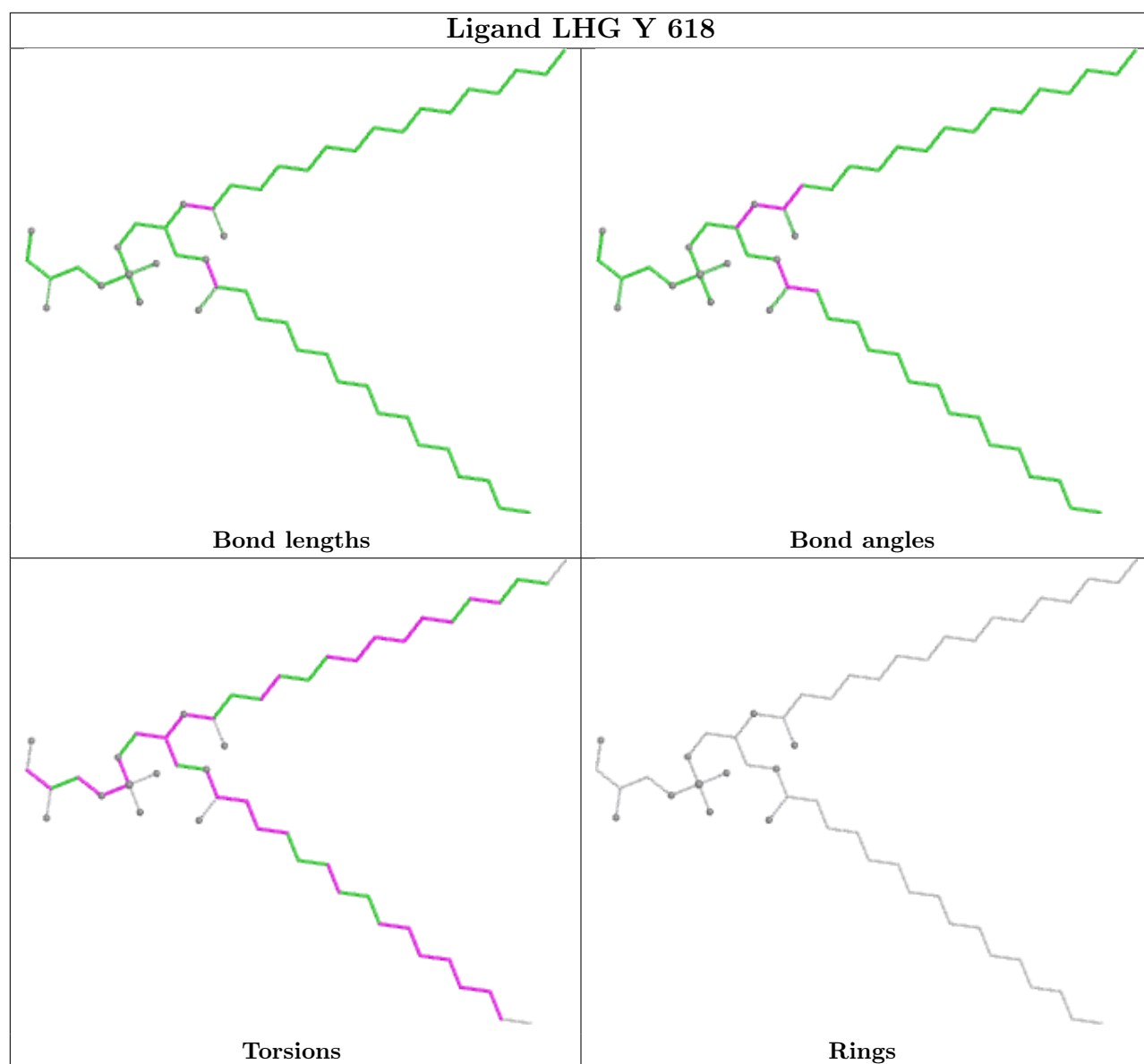
## Ligand CHL N 605

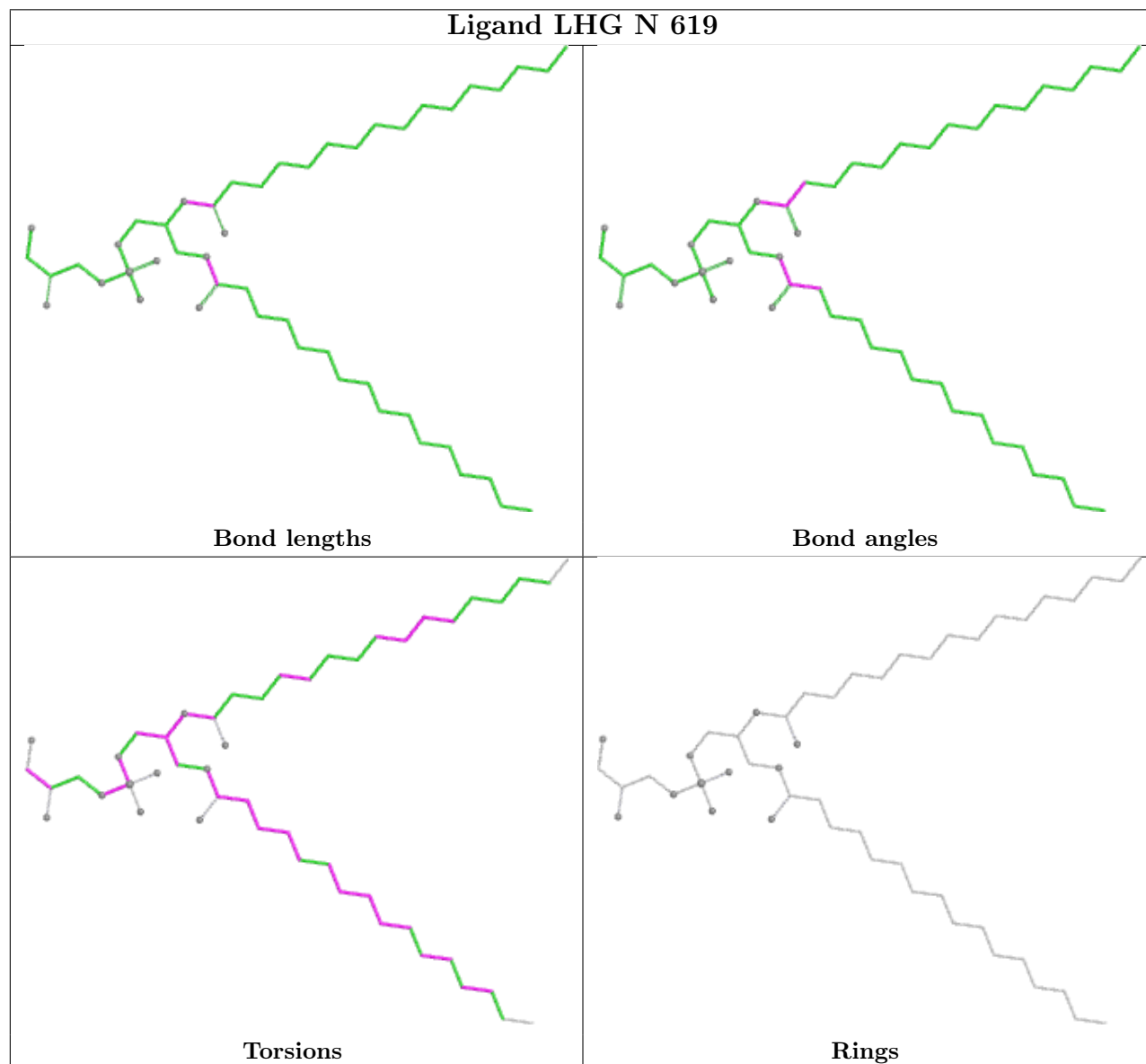
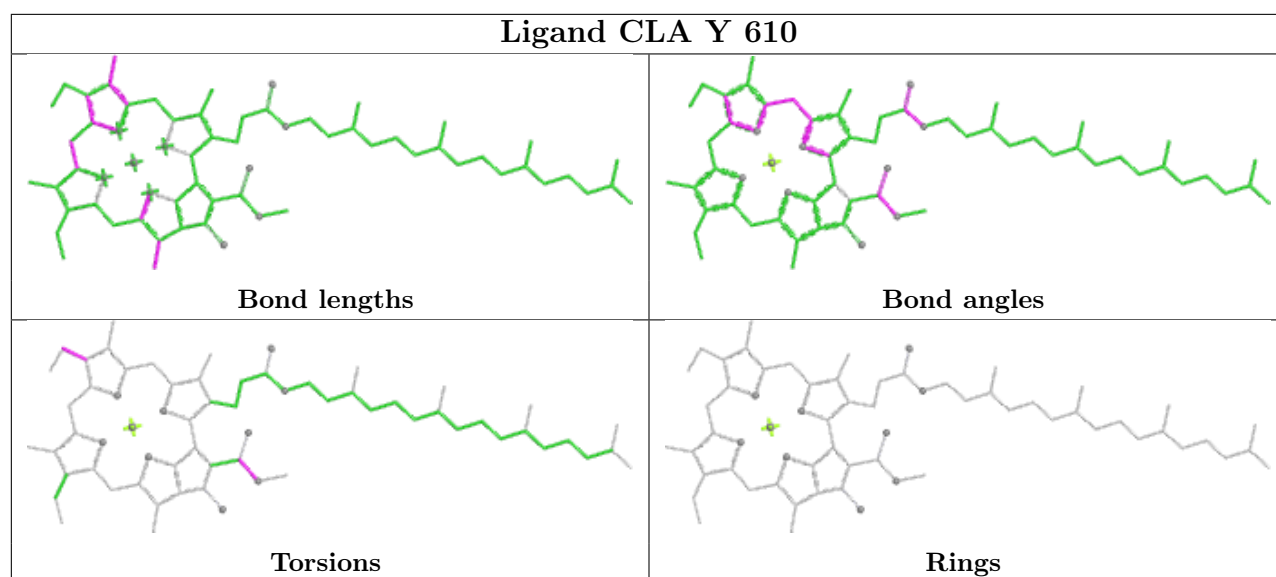


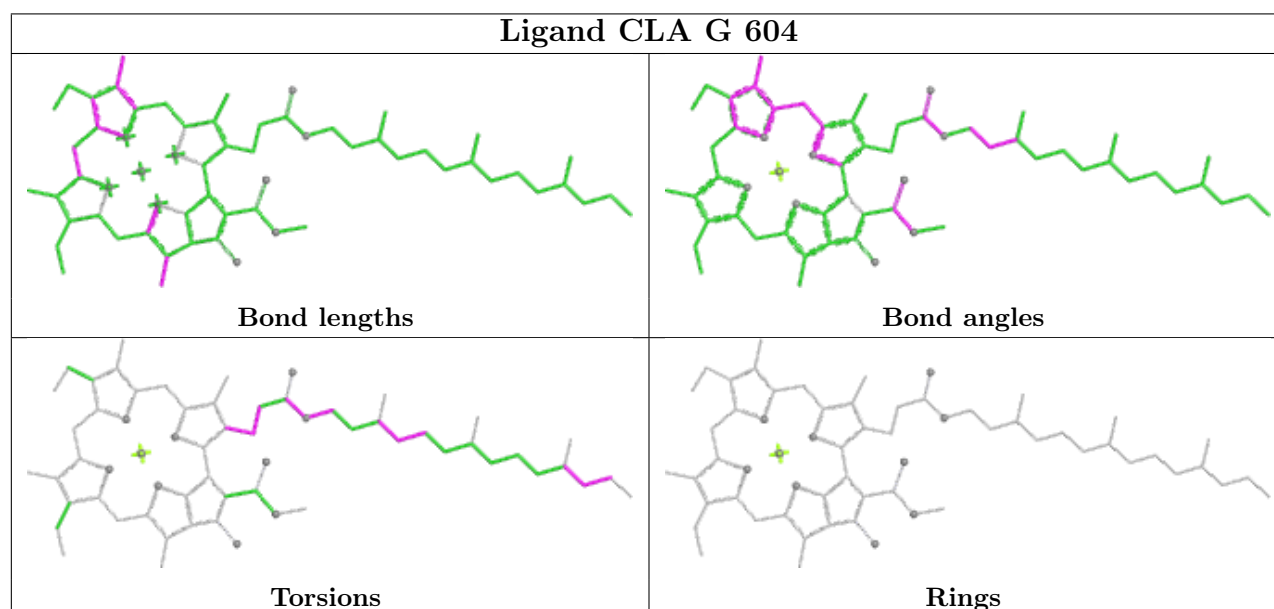
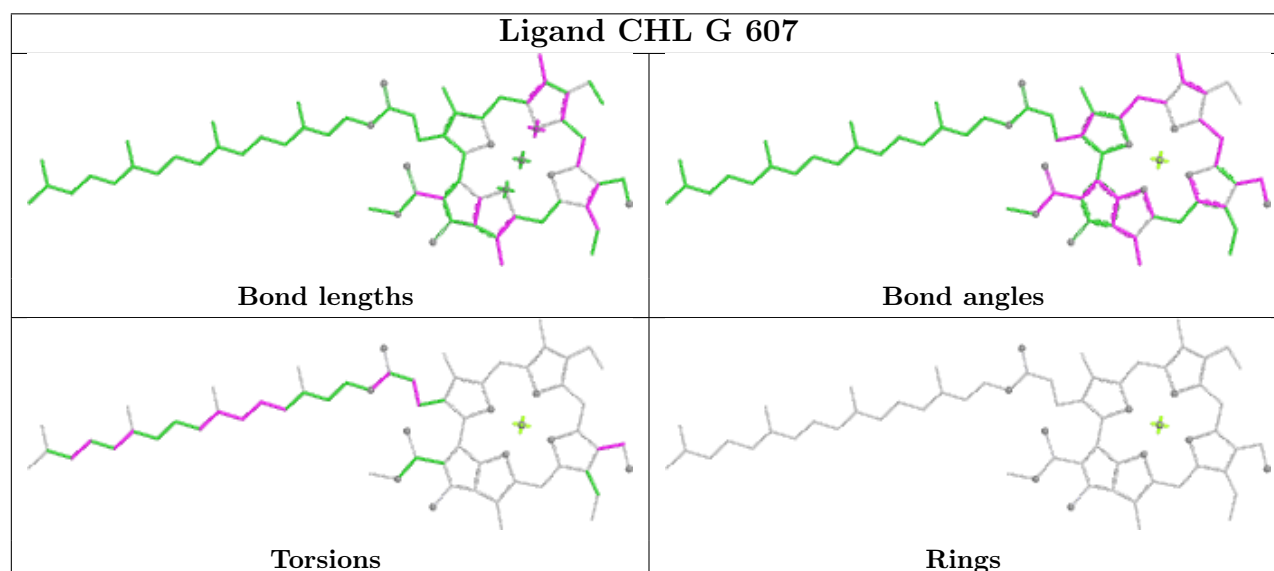
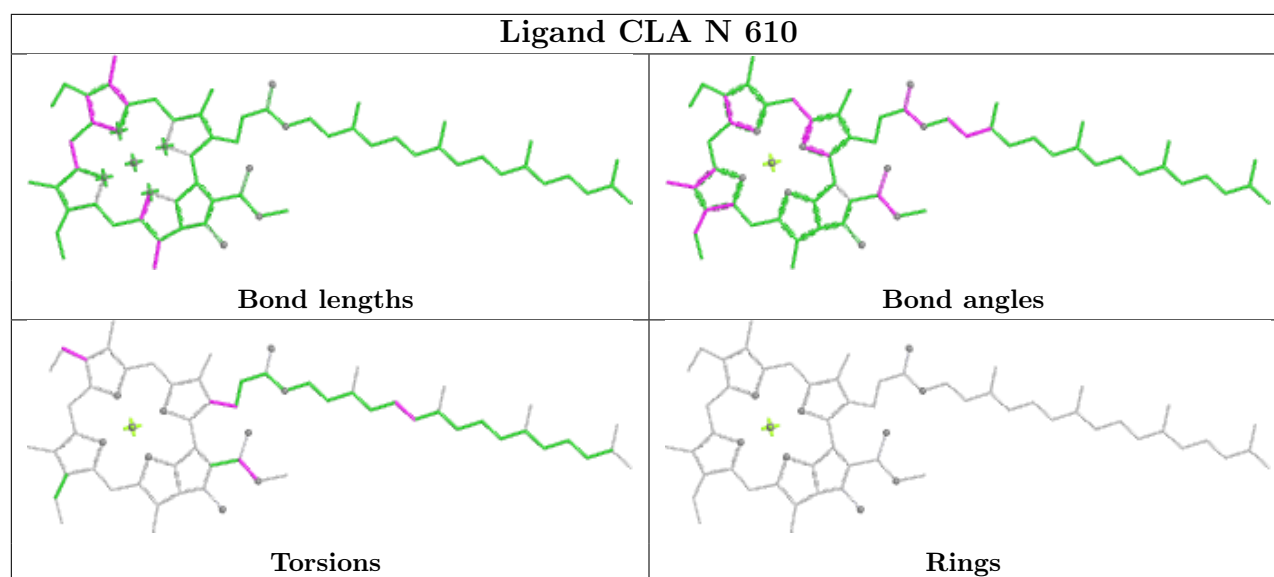
## Ligand CLA Y 613

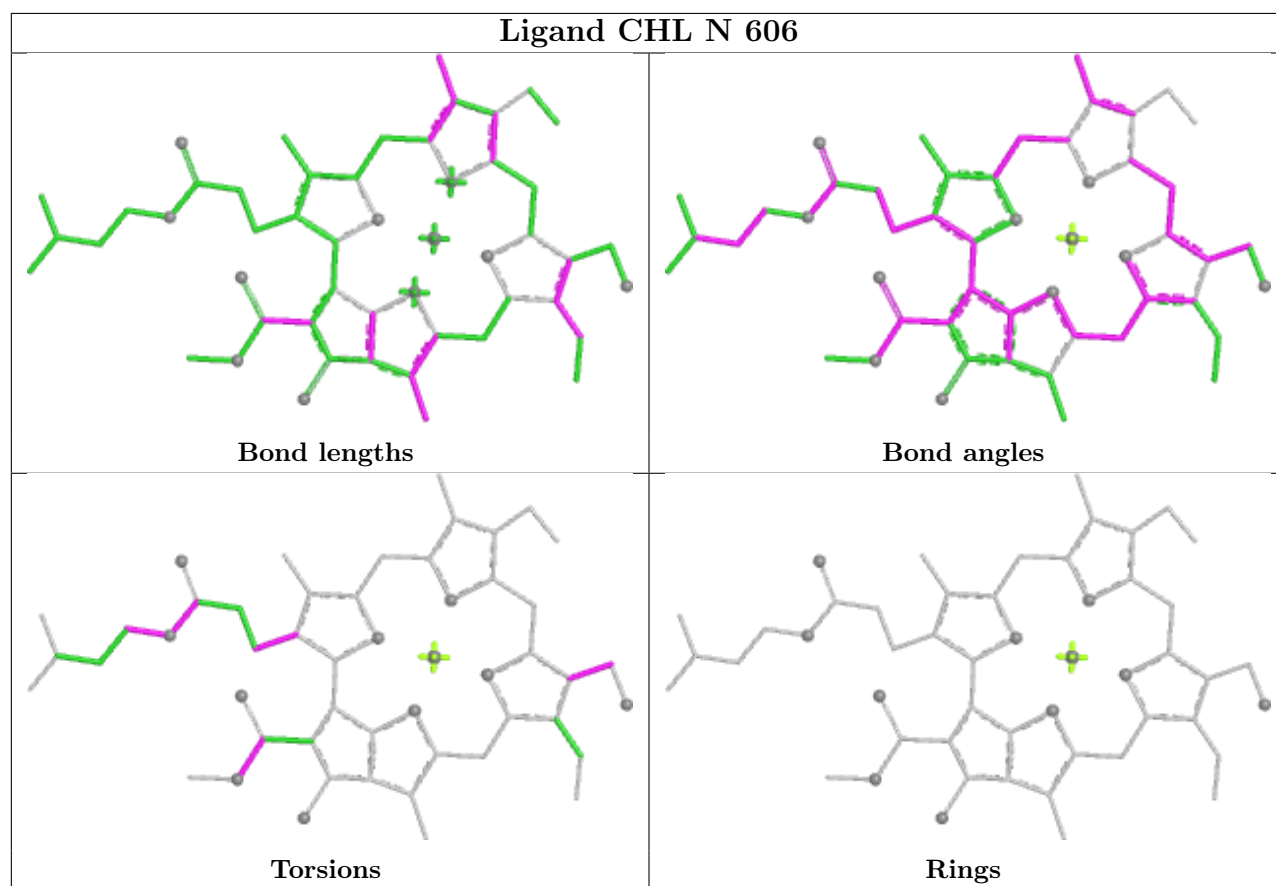
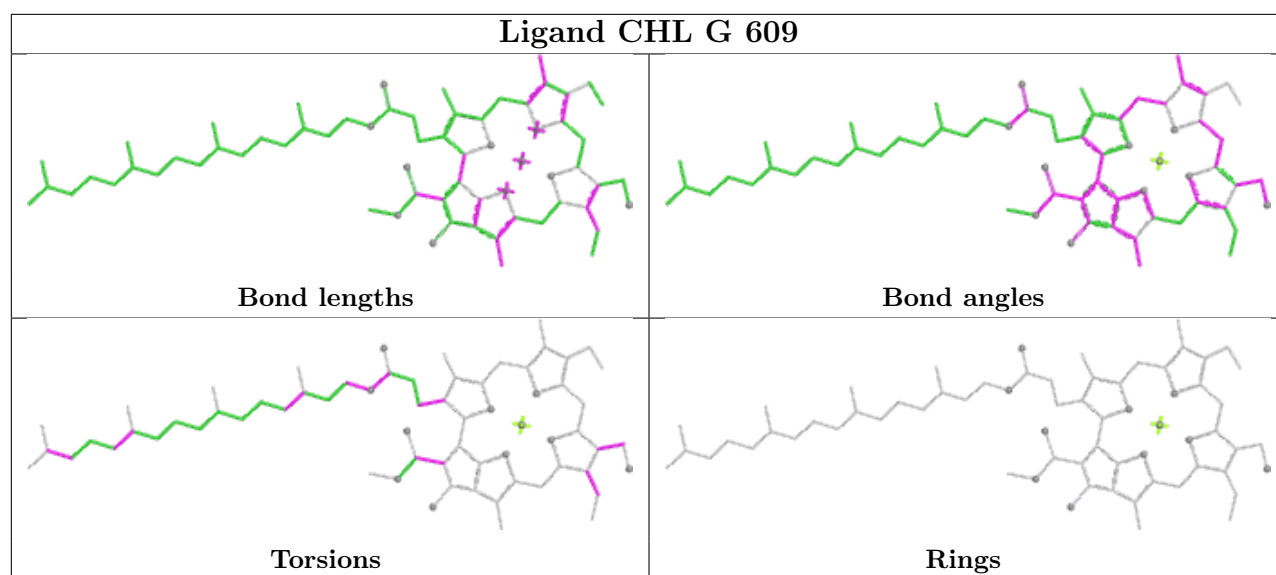


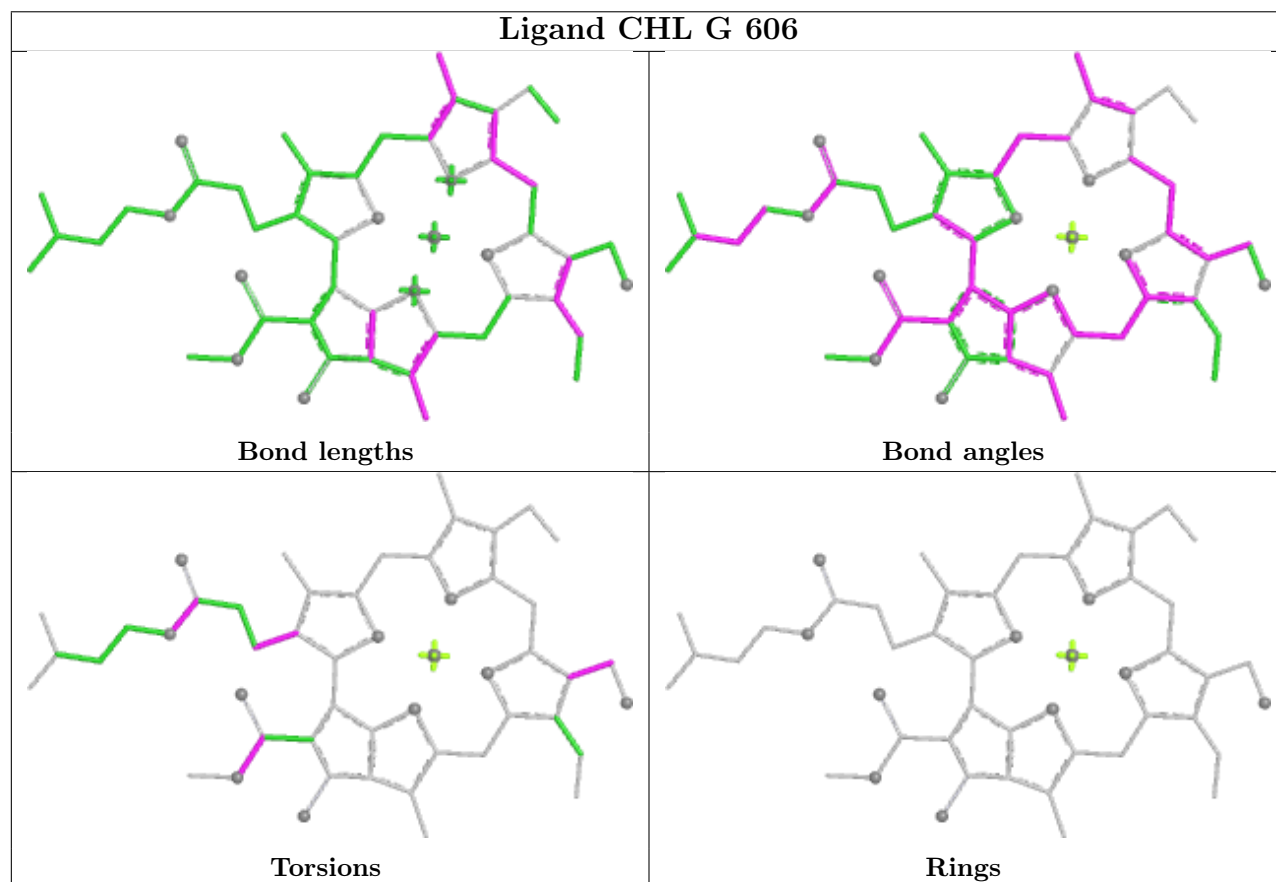
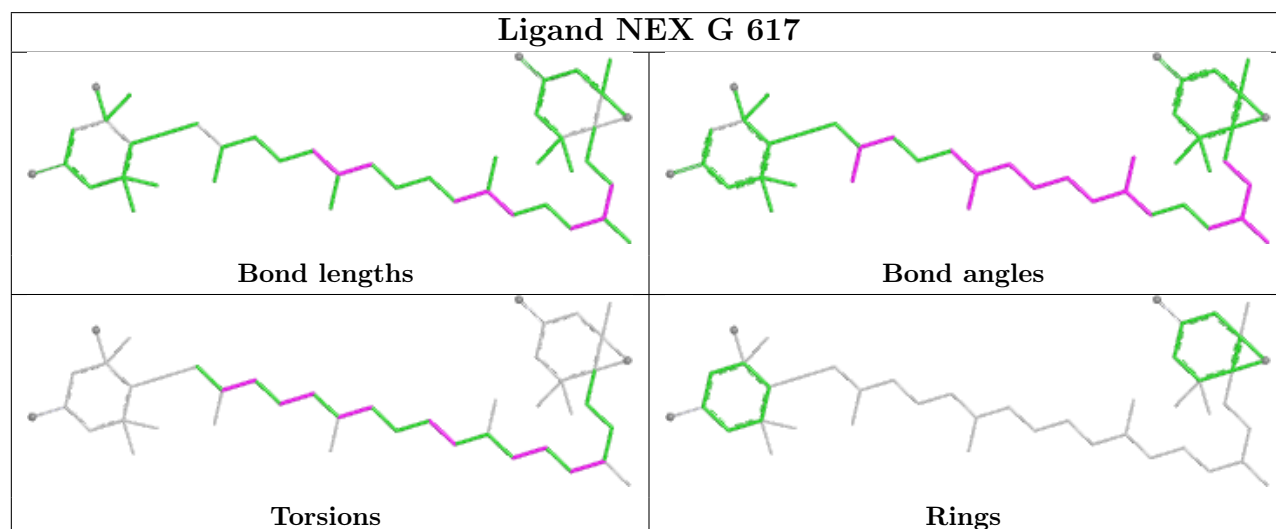
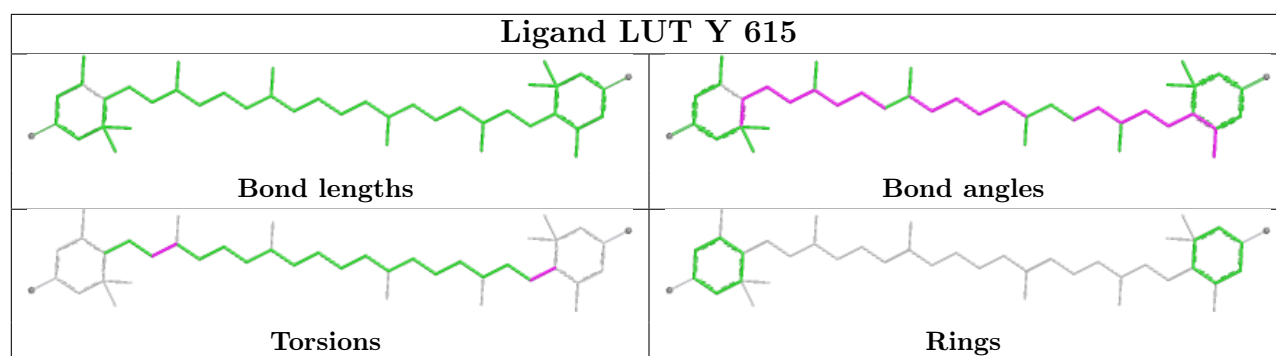


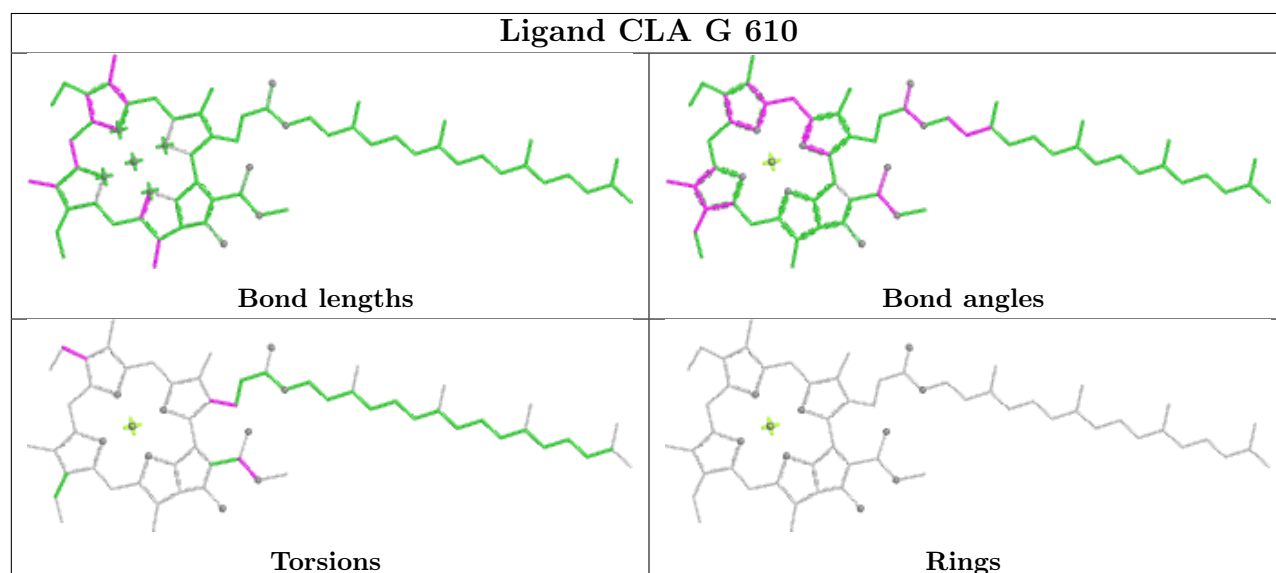
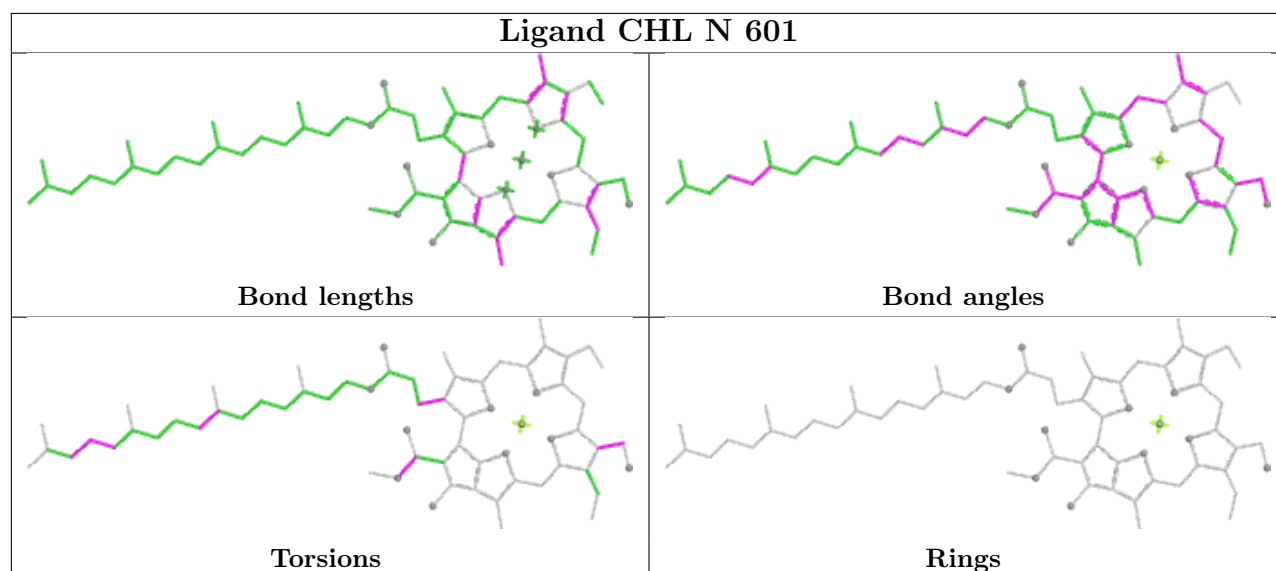
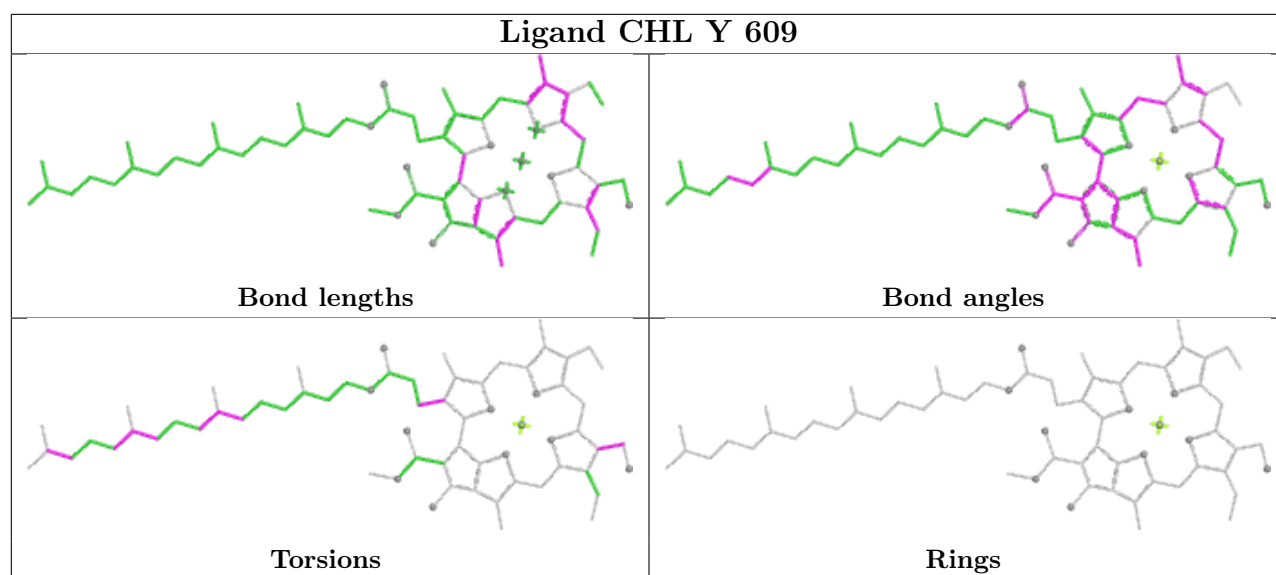


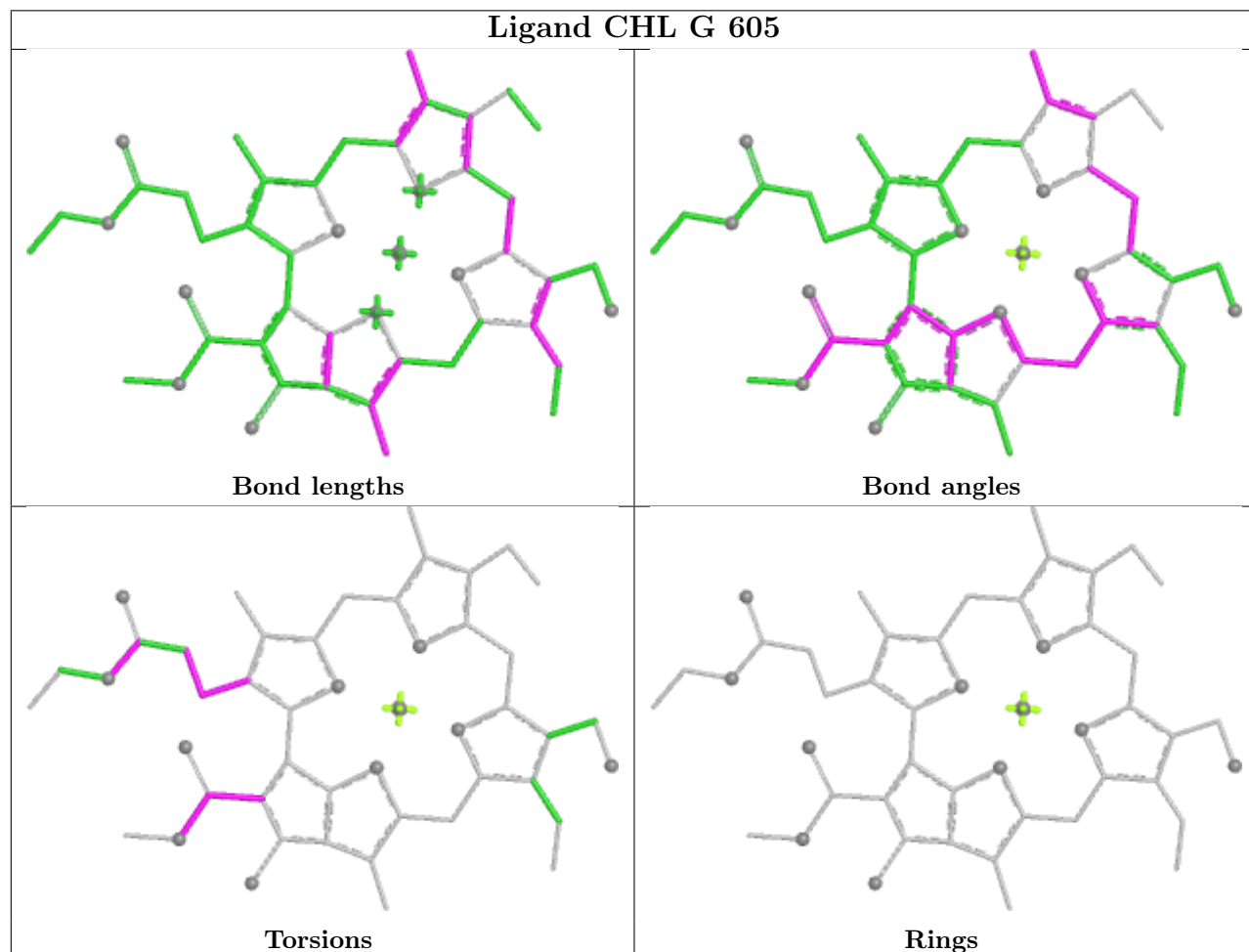
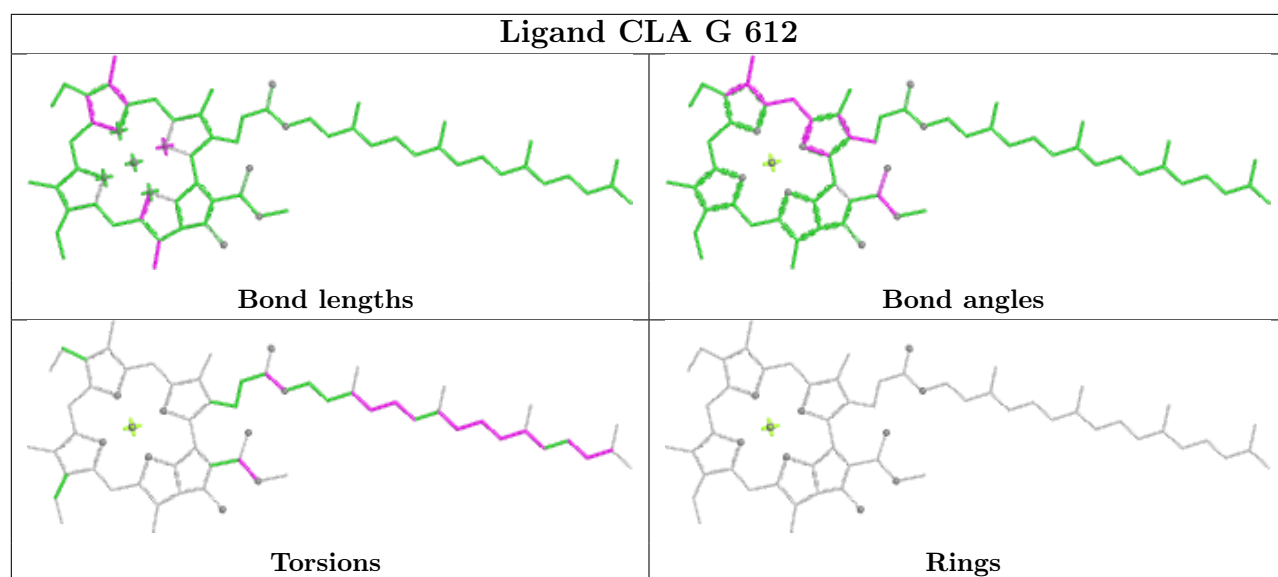




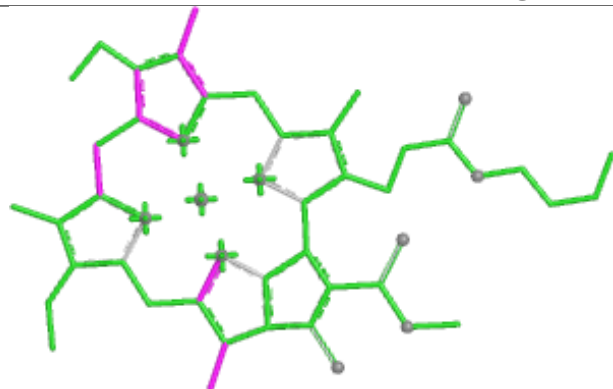




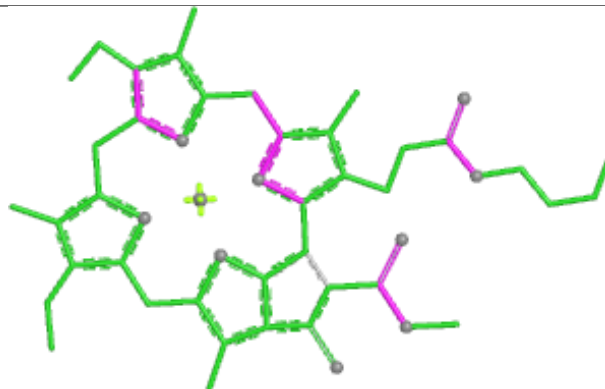




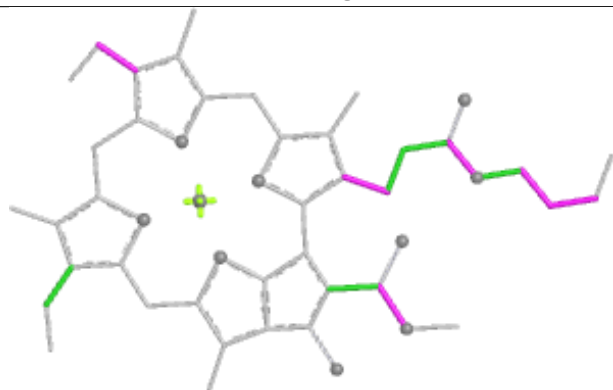
## Ligand CLA Y 614



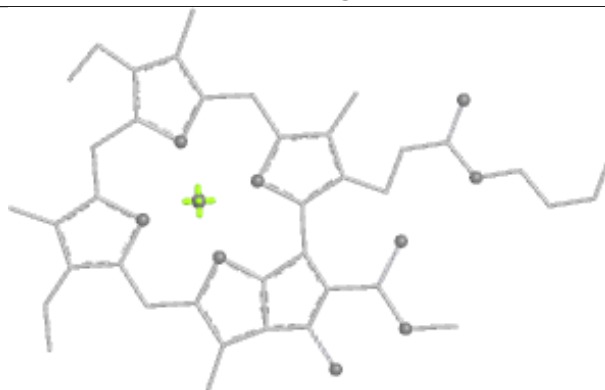
Bond lengths



Bond angles

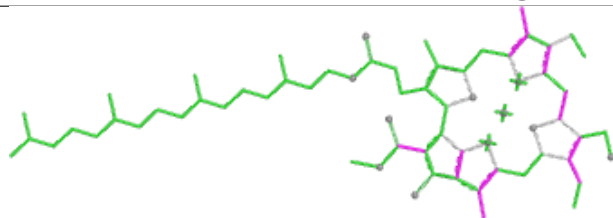


Torsions

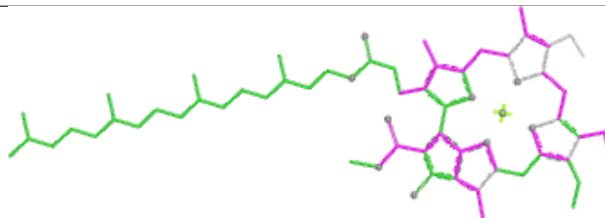


Rings

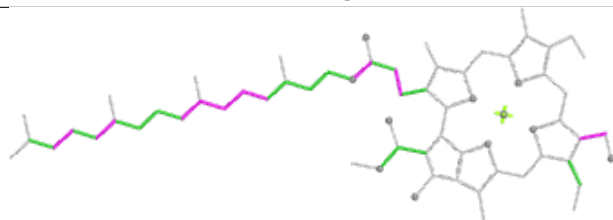
## Ligand CHL Y 607



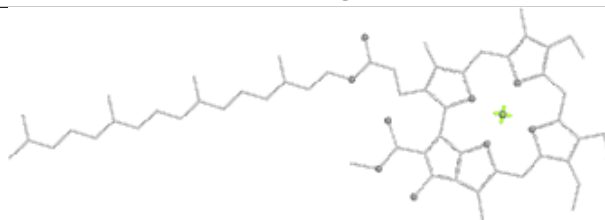
Bond lengths



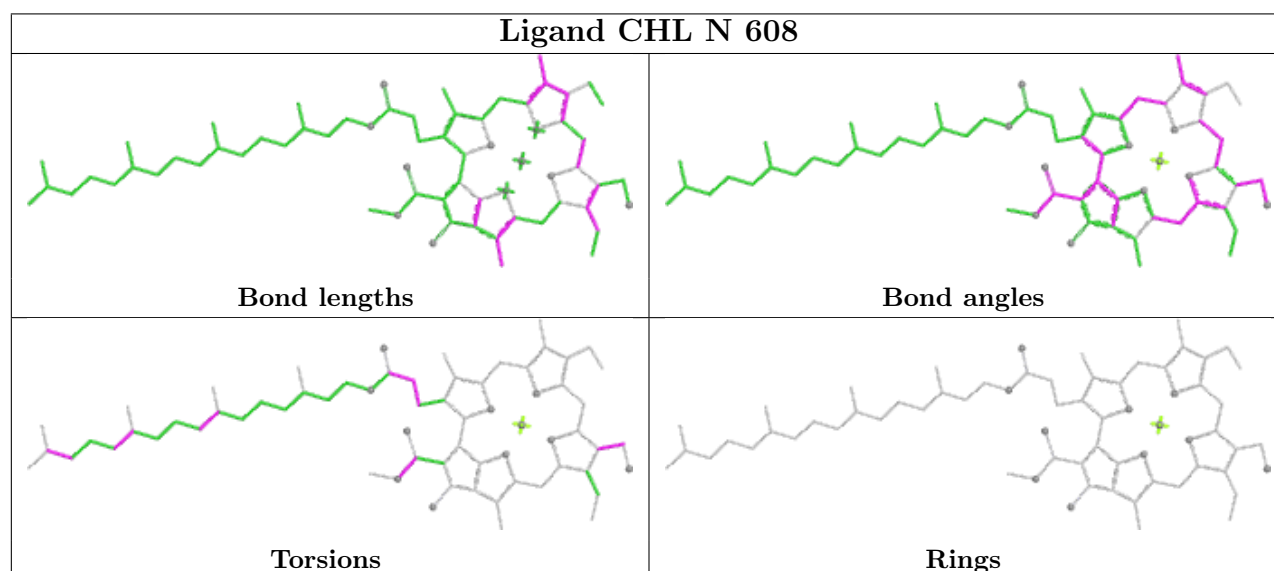
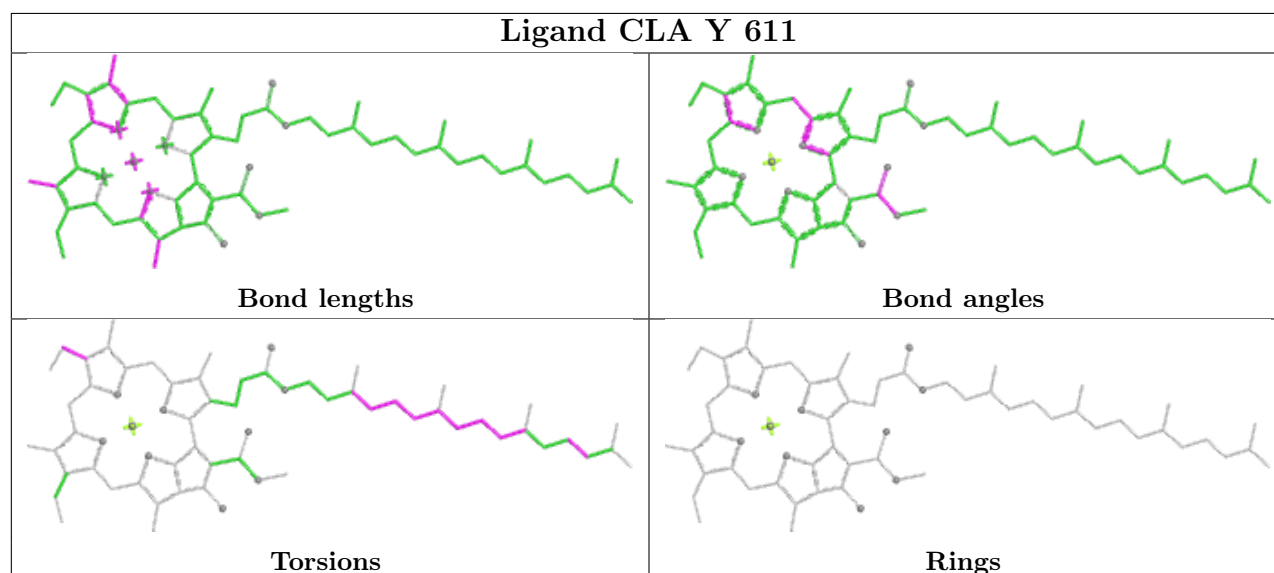
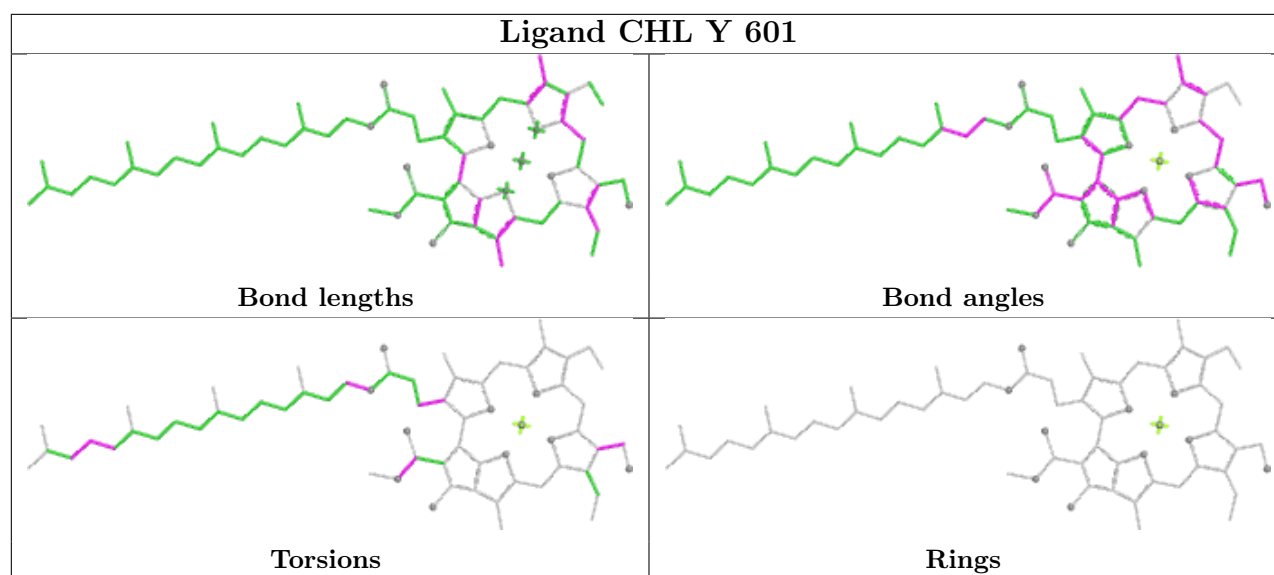
Bond angles

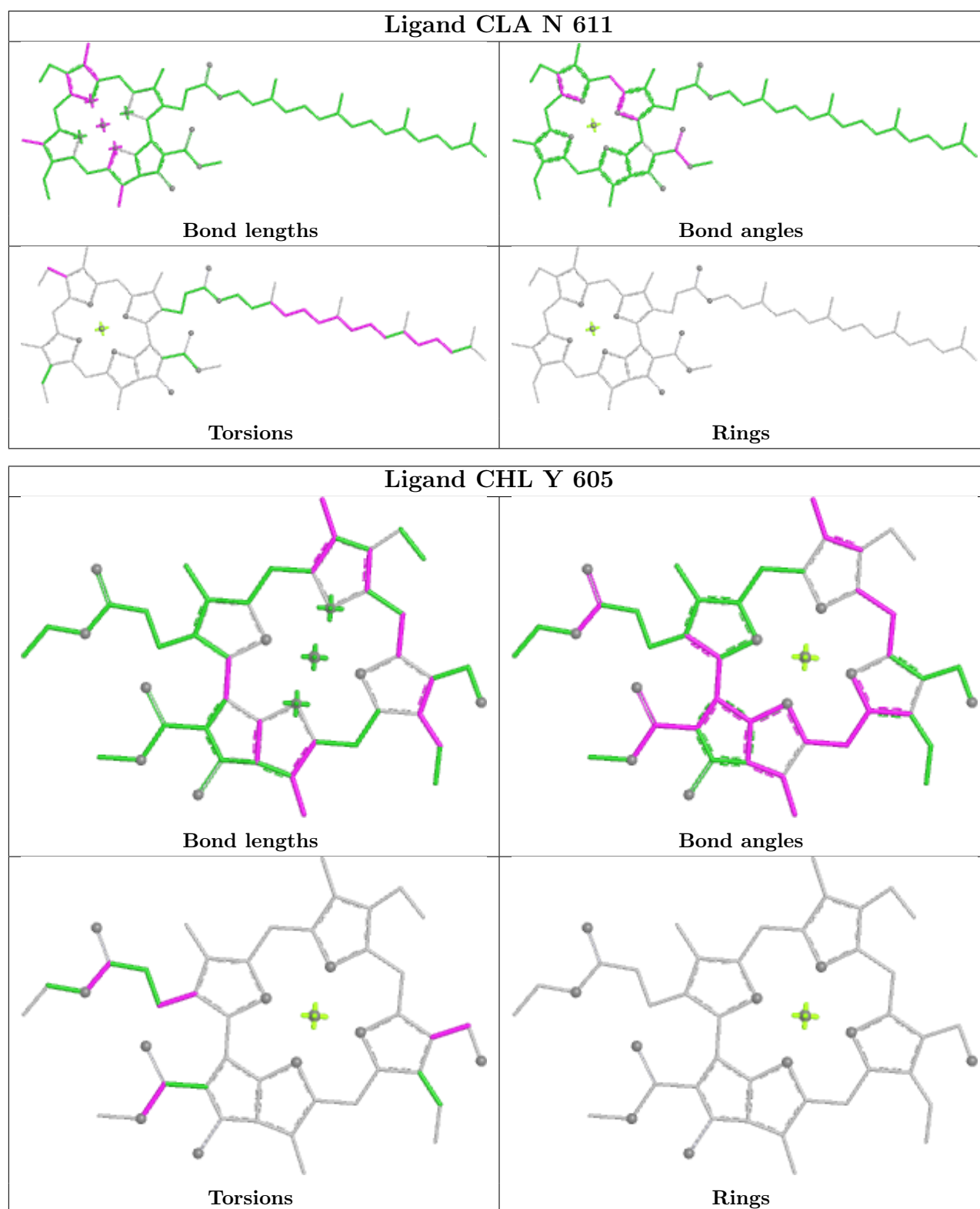


Torsions



Rings





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

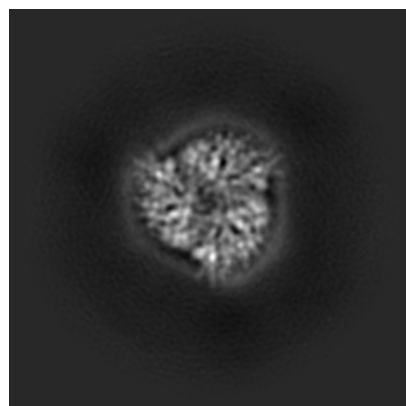
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35782. These allow visual inspection of the internal detail of the map and identification of artifacts.

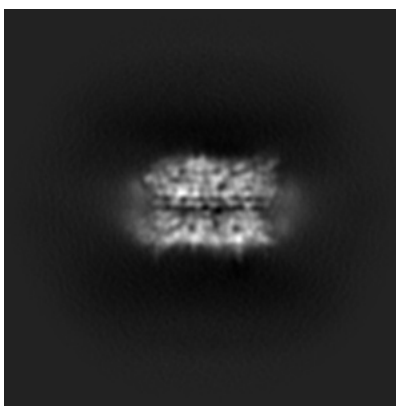
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

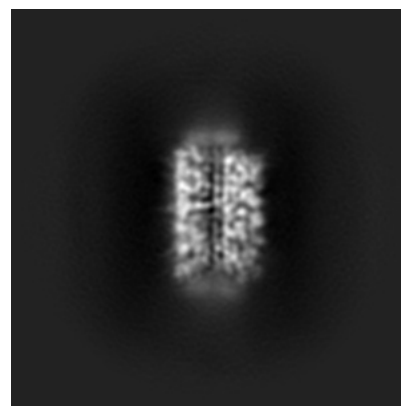
#### 6.1.1 Primary map



X

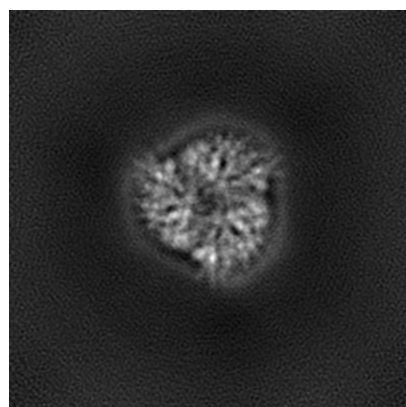


Y

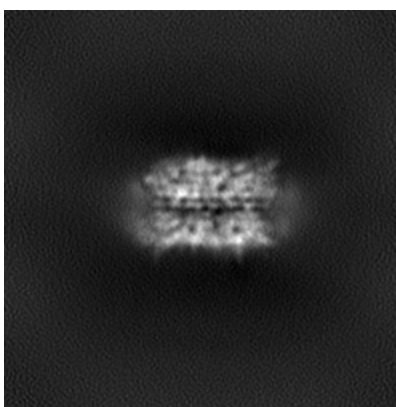


Z

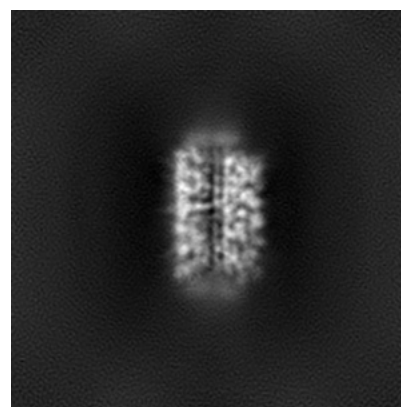
#### 6.1.2 Raw map



X



Y

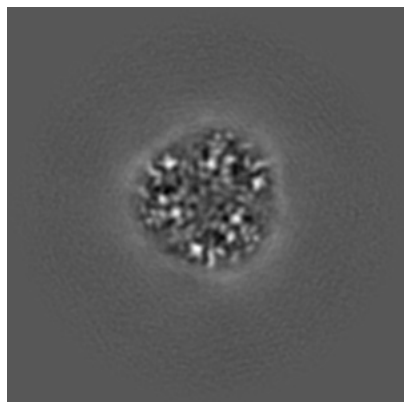


Z

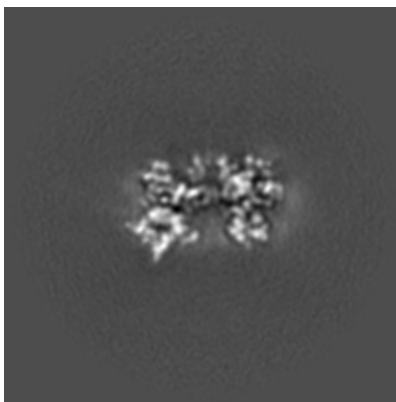
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

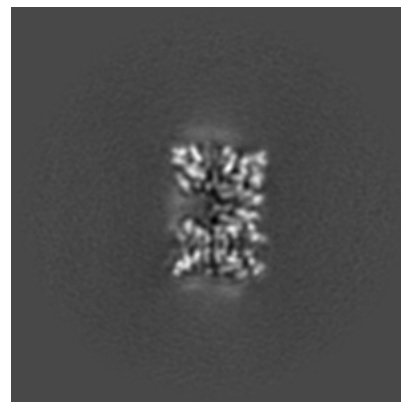
### 6.2.1 Primary map



X Index: 100

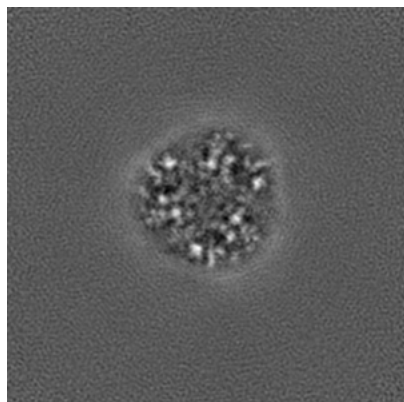


Y Index: 100

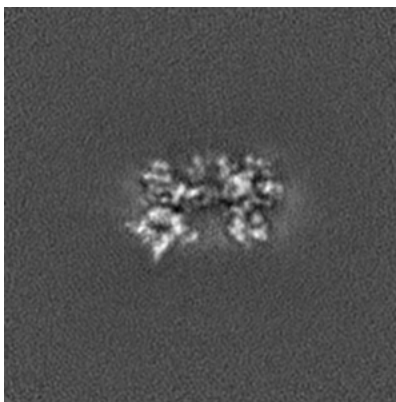


Z Index: 100

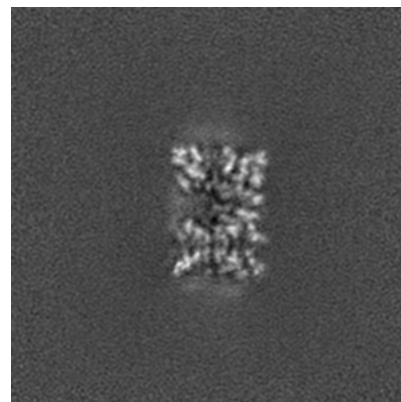
### 6.2.2 Raw map



X Index: 100



Y Index: 100

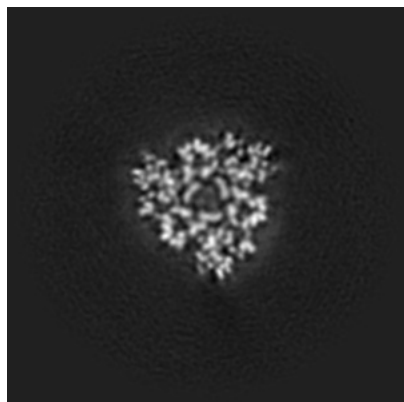


Z Index: 100

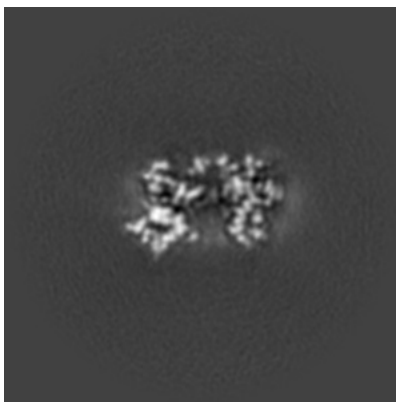
The images above show central slices of the map in three orthogonal directions.

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

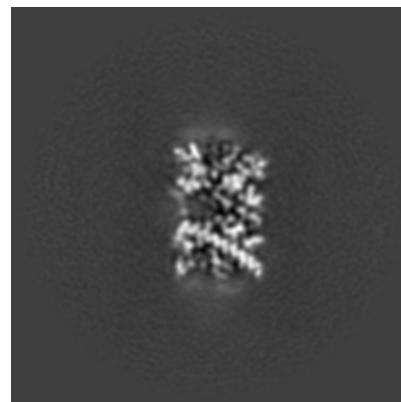
### 6.3.1 Primary map



X Index: 85

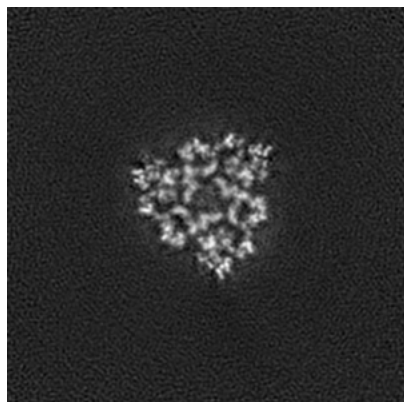


Y Index: 101

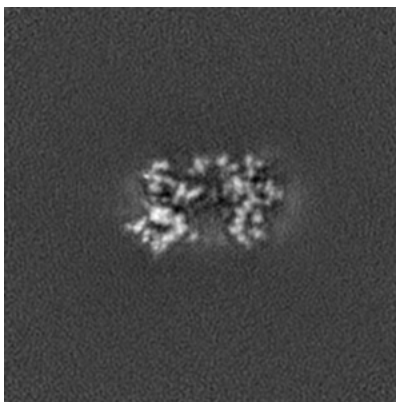


Z Index: 97

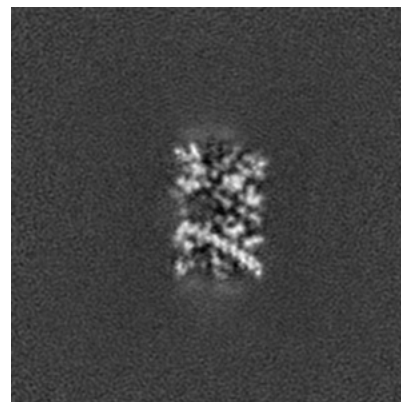
### 6.3.2 Raw map



X Index: 84



Y Index: 101

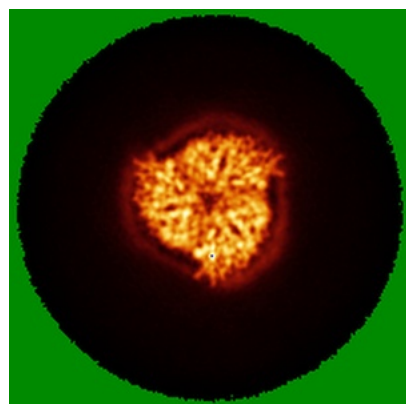


Z Index: 97

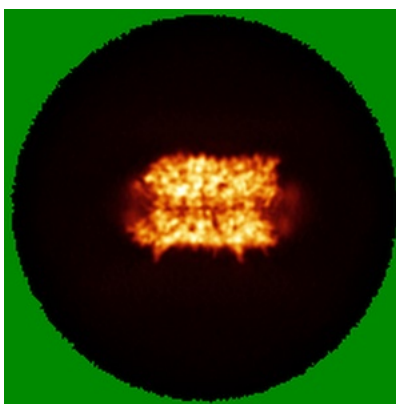
The images above show the largest variance slices of the map in three orthogonal directions.

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

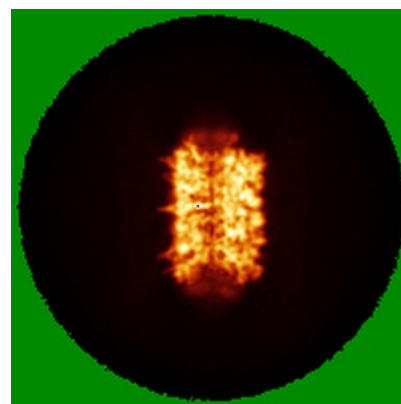
### 6.4.1 Primary map



X

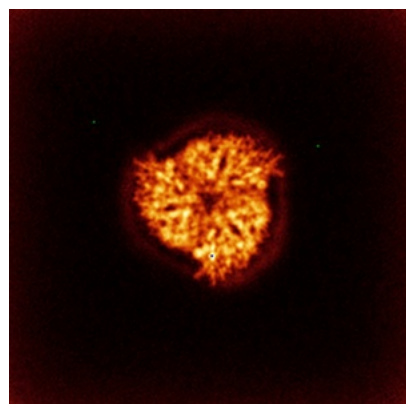


Y

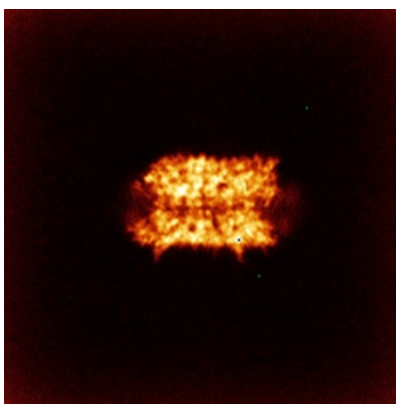


Z

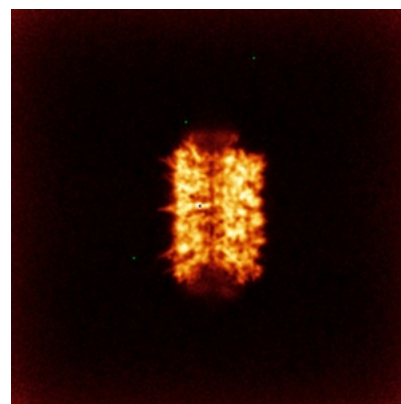
### 6.4.2 Raw map



X



Y

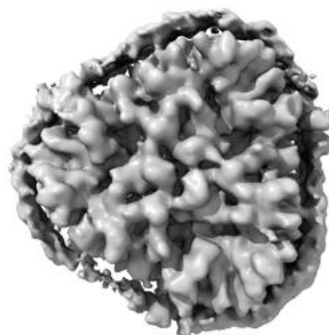


Z

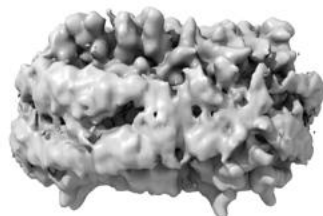
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



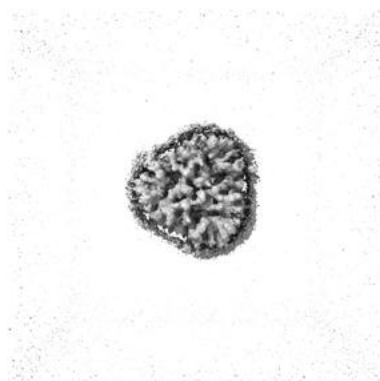
Y



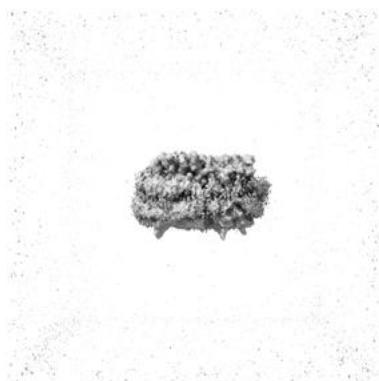
Z

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

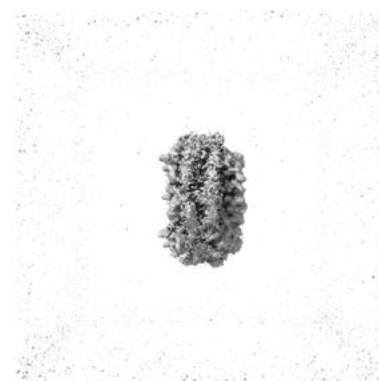
### 6.5.2 Raw map



X



Y



Z

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

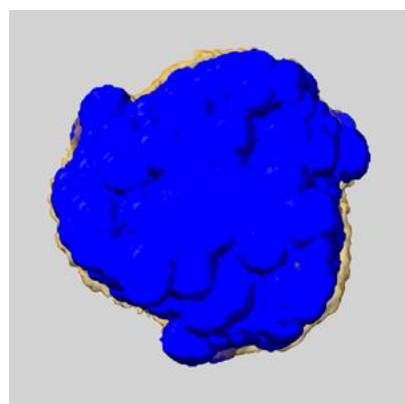
## 6.6 Mask visualisation [i](#)

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

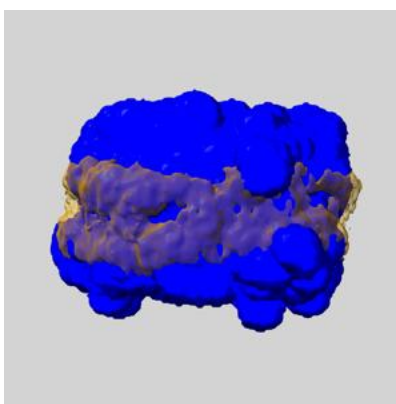
A mask typically either:

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

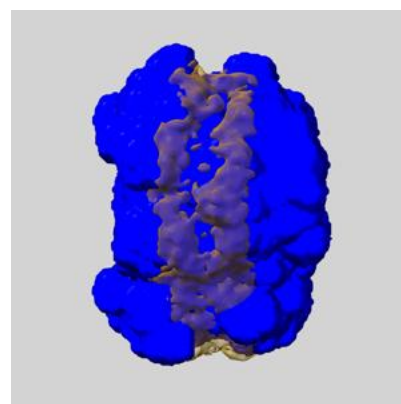
### 6.6.1 emd\_35782\_msk\_1.map [i](#)



X



Y

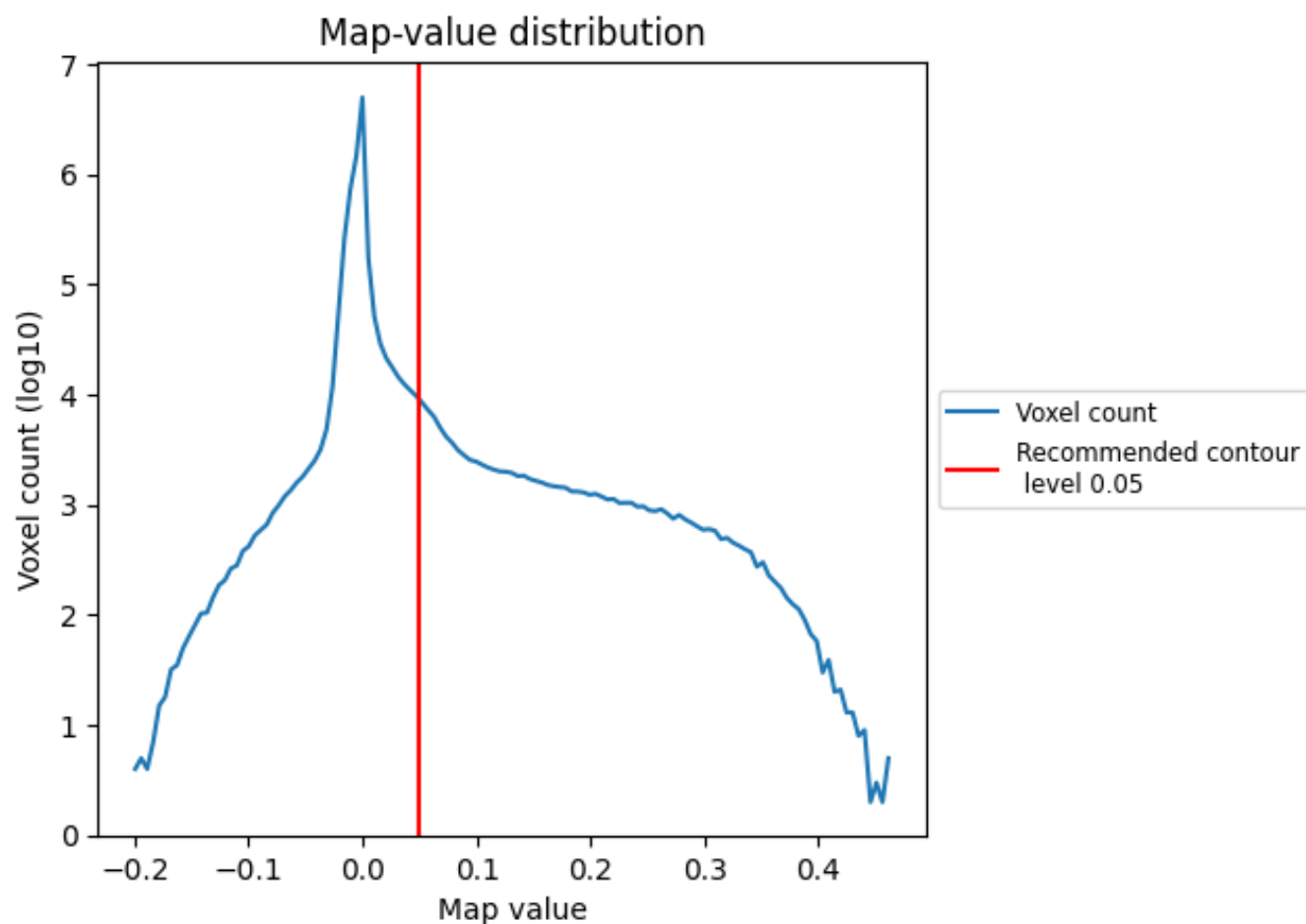


Z

## 7 Map analysis [i](#)

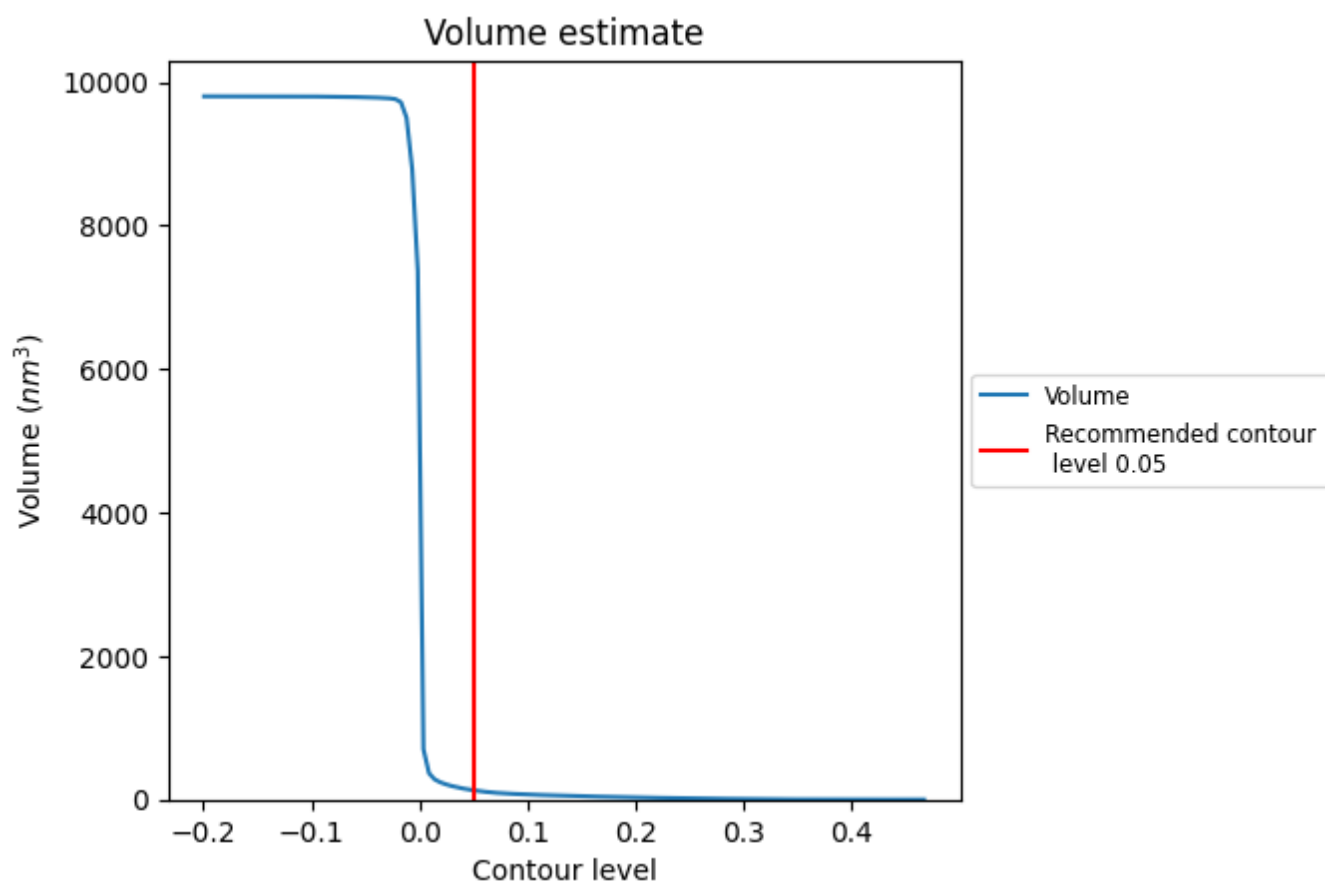
This section contains the results of statistical analysis of the map.

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



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

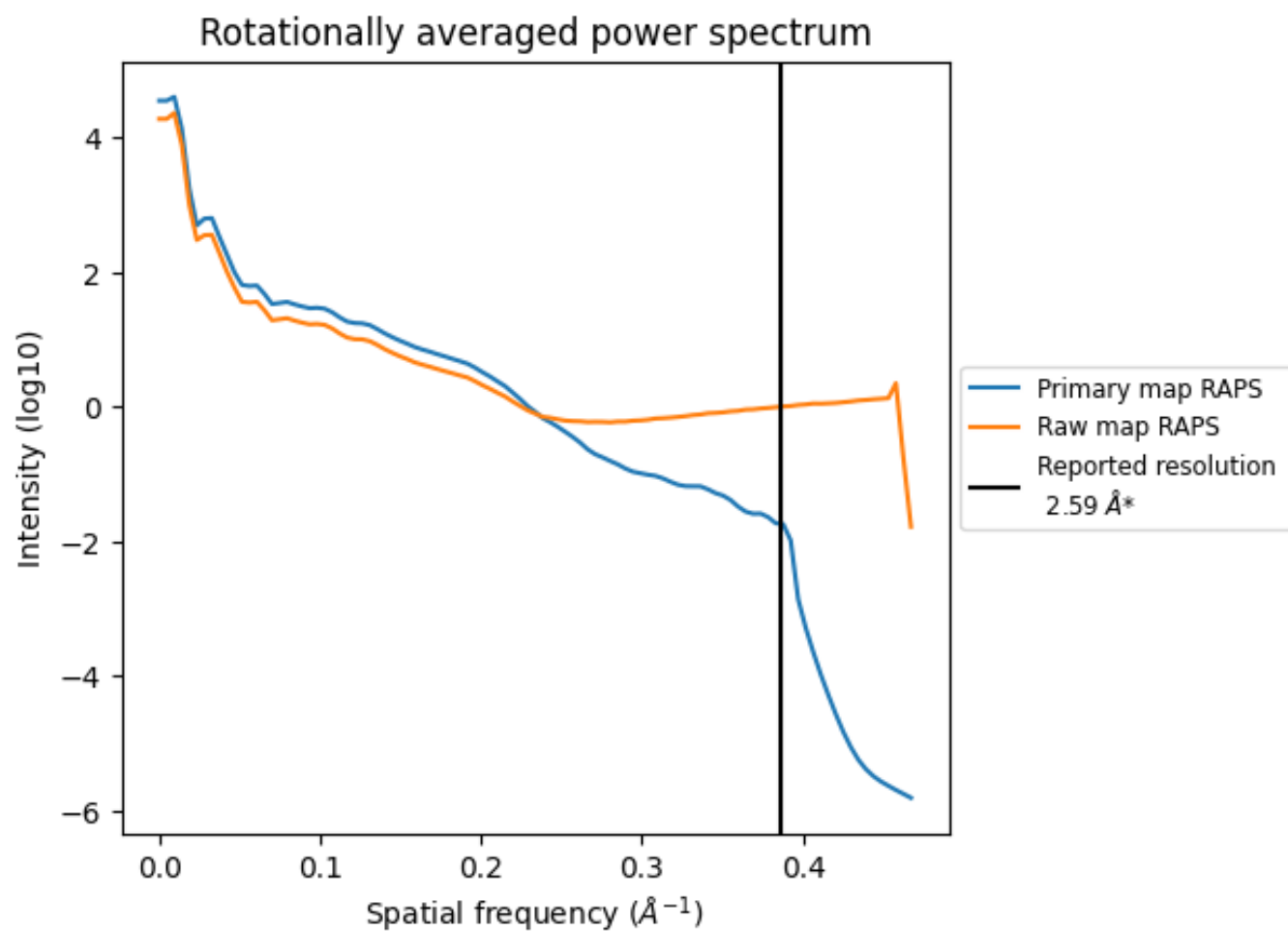
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 129 nm<sup>3</sup>; this corresponds to an approximate mass of 117 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 ⓘ

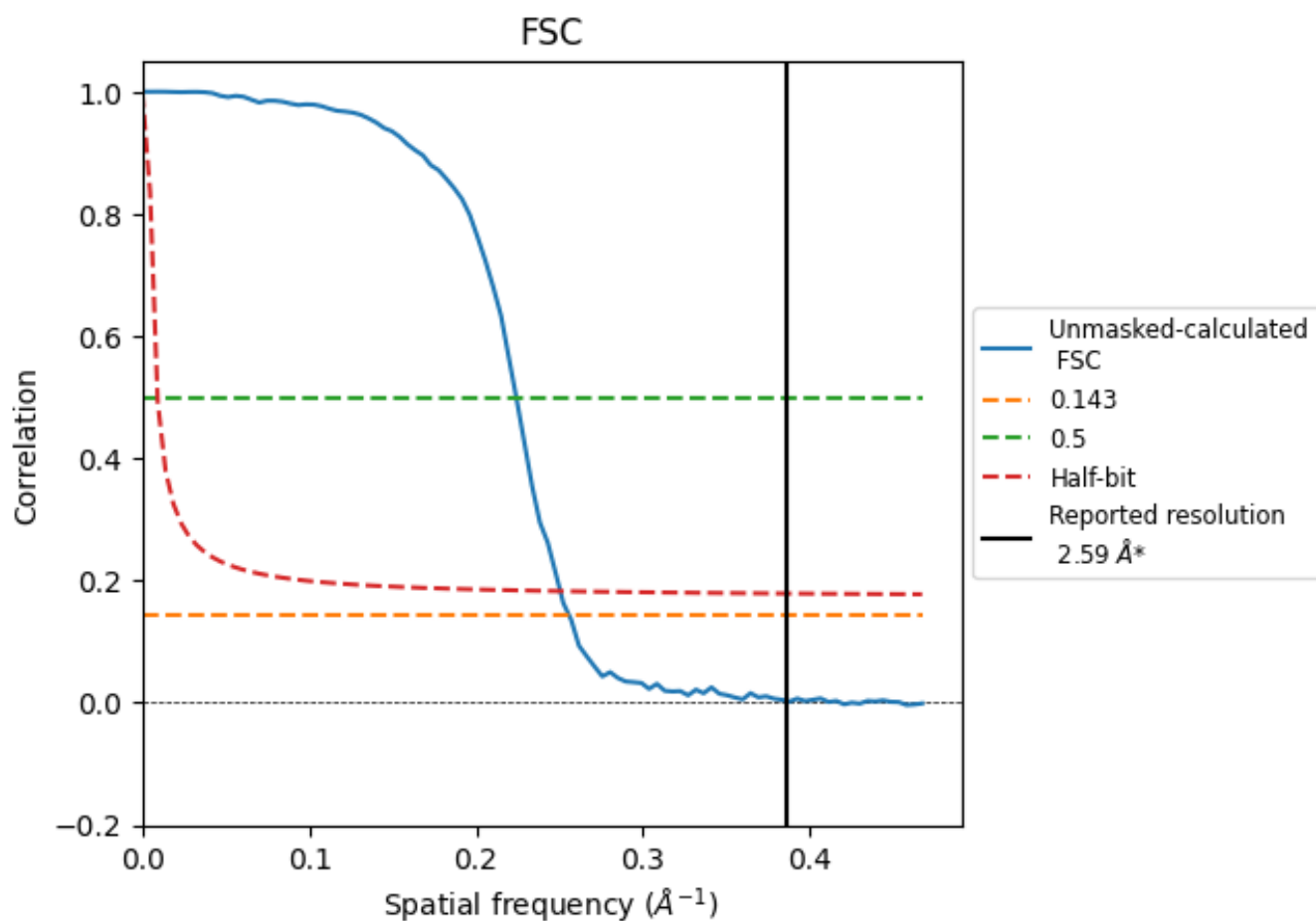


\*Reported resolution corresponds to spatial frequency of 0.386  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.386 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

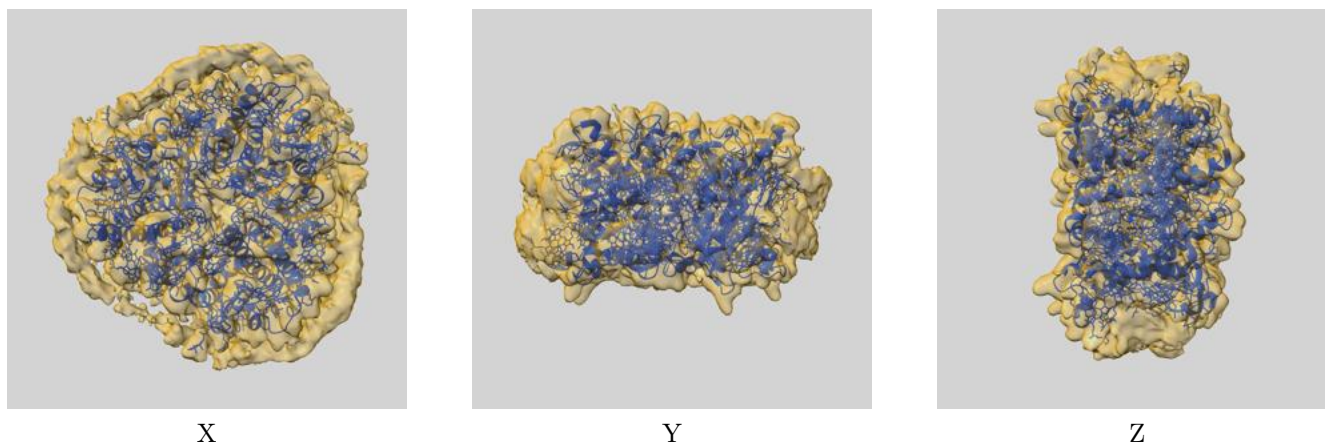
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.59                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.91                               | 4.46 | 3.99     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 2.59 by more than 10 %

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

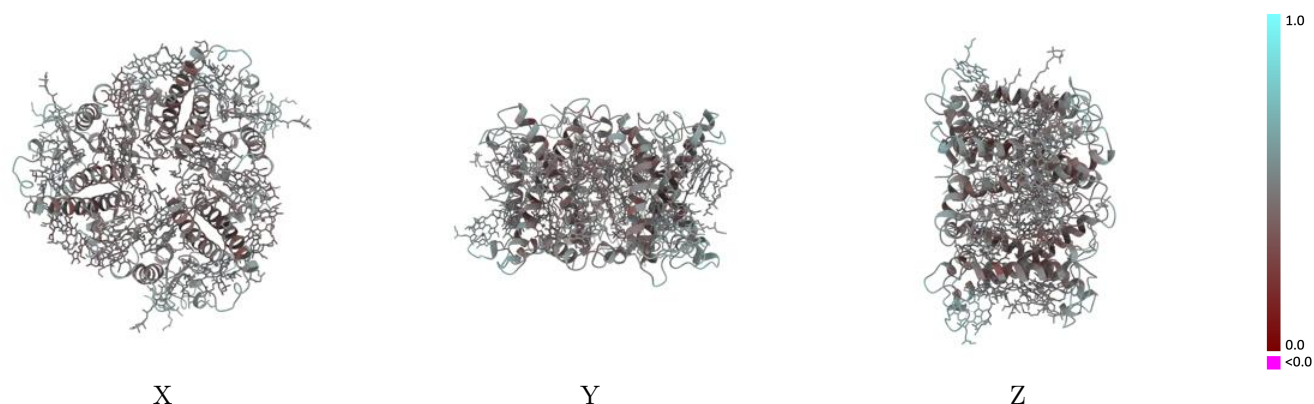
This section contains information regarding the fit between EMDB map EMD-35782 and PDB model 8IWX. Per-residue inclusion information can be found in section 3 on page 11.

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



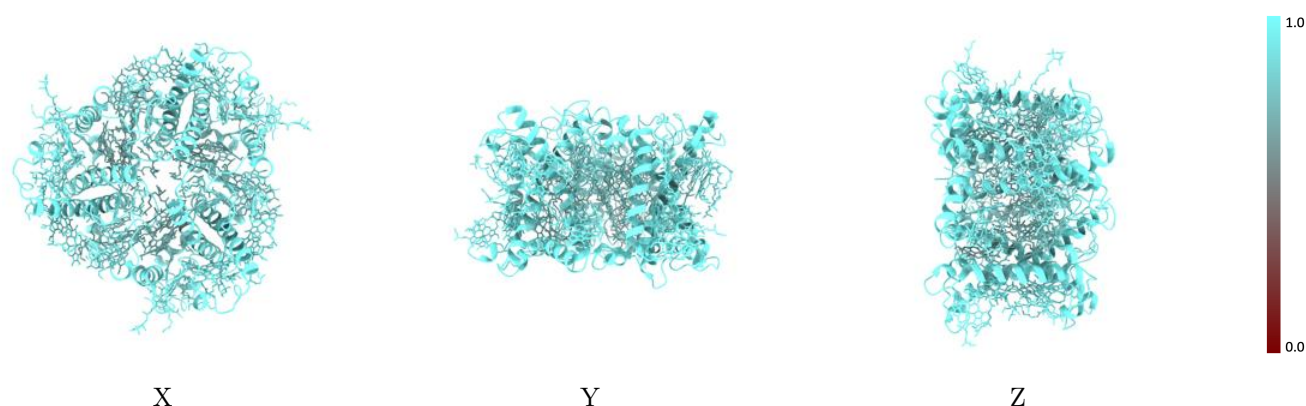
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



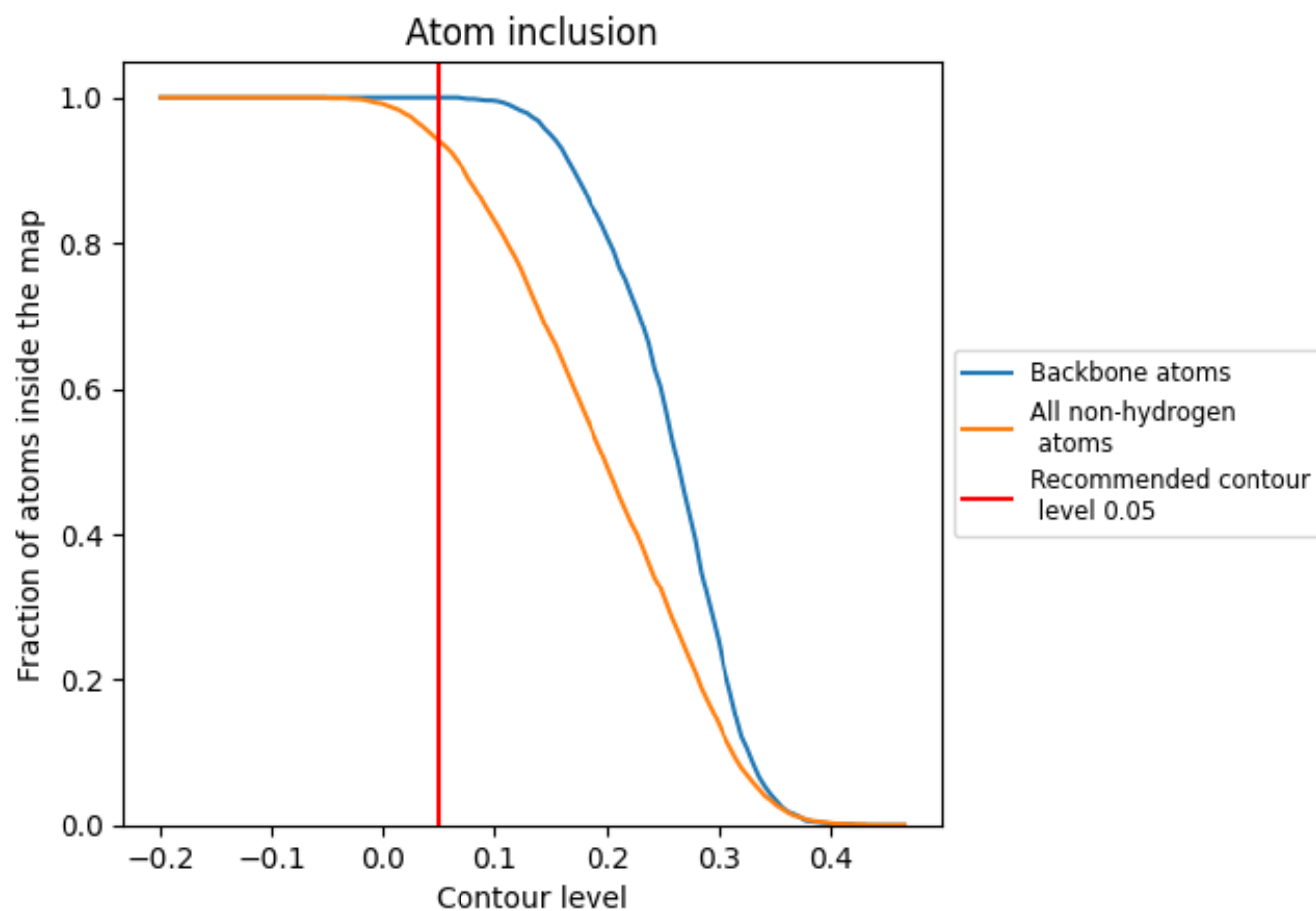
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.9400 | <div></div> 0.4660 |
| G     | <div></div> 0.9320 | <div></div> 0.4690 |
| N     | <div></div> 0.9430 | <div></div> 0.4640 |
| Y     | <div></div> 0.9450 | <div></div> 0.4660 |

