



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 06:33 PM JST

PDB ID : 8HQ8  
Title : Bry-LHCII homotrimer of Bryopsis corticulans  
Authors : Li, Z.H.; Shen, J.R.; Wang, W.D.  
Deposited on : 2022-12-13  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

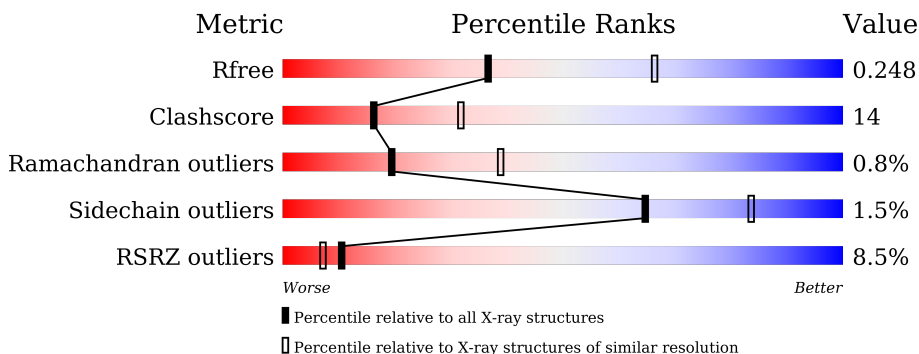
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 3163 (2.60-2.60)                                      |
| Clashscore            | 141614                      | 3518 (2.60-2.60)                                      |
| Ramachandran outliers | 138981                      | 3455 (2.60-2.60)                                      |
| Sidechain outliers    | 138945                      | 3455 (2.60-2.60)                                      |
| RSRZ outliers         | 127900                      | 3104 (2.60-2.60)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 249    |                  |
| 1   | B     | 249    |                  |
| 1   | C     | 249    |                  |
| 1   | D     | 249    |                  |
| 1   | E     | 249    |                  |
| 1   | F     | 249    |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 10  | BET  | B     | 321 | -         | -        | -       | X                |
| 11  | LMG  | F     | 319 | -         | -        | -       | X                |
| 3   | NEX  | A     | 303 | -         | -        | -       | X                |
| 3   | NEX  | D     | 303 | -         | -        | -       | X                |
| 4   | LMU  | A     | 304 | -         | -        | -       | X                |
| 4   | LMU  | B     | 305 | -         | -        | -       | X                |
| 5   | CHL  | A     | 305 | X         | -        | -       | -                |
| 5   | CHL  | A     | 306 | X         | -        | -       | -                |
| 5   | CHL  | A     | 309 | X         | -        | -       | -                |
| 5   | CHL  | A     | 310 | X         | -        | -       | -                |
| 5   | CHL  | A     | 311 | X         | -        | -       | -                |
| 5   | CHL  | A     | 312 | X         | -        | -       | -                |
| 5   | CHL  | A     | 313 | X         | -        | -       | -                |
| 5   | CHL  | A     | 318 | X         | -        | -       | -                |
| 5   | CHL  | B     | 306 | X         | -        | -       | -                |
| 5   | CHL  | B     | 307 | X         | -        | -       | -                |
| 5   | CHL  | B     | 310 | X         | -        | -       | -                |
| 5   | CHL  | B     | 311 | X         | -        | -       | -                |
| 5   | CHL  | B     | 312 | X         | -        | -       | -                |
| 5   | CHL  | B     | 313 | X         | -        | -       | -                |
| 5   | CHL  | B     | 314 | X         | -        | -       | -                |
| 5   | CHL  | B     | 319 | X         | -        | -       | -                |
| 5   | CHL  | C     | 305 | X         | -        | -       | -                |
| 5   | CHL  | C     | 306 | X         | -        | -       | -                |
| 5   | CHL  | C     | 309 | X         | -        | -       | -                |
| 5   | CHL  | C     | 310 | X         | -        | -       | -                |
| 5   | CHL  | C     | 311 | X         | -        | -       | -                |
| 5   | CHL  | C     | 312 | X         | -        | -       | -                |
| 5   | CHL  | C     | 313 | X         | -        | -       | -                |
| 5   | CHL  | C     | 318 | X         | -        | -       | -                |
| 5   | CHL  | D     | 305 | X         | -        | -       | -                |
| 5   | CHL  | D     | 306 | X         | -        | -       | -                |
| 5   | CHL  | D     | 309 | X         | -        | -       | -                |
| 5   | CHL  | D     | 310 | X         | -        | -       | -                |
| 5   | CHL  | D     | 311 | X         | -        | -       | -                |
| 5   | CHL  | D     | 312 | X         | -        | -       | -                |
| 5   | CHL  | D     | 313 | X         | -        | -       | -                |
| 5   | CHL  | D     | 318 | X         | -        | -       | -                |
| 5   | CHL  | E     | 304 | X         | -        | -       | -                |
| 5   | CHL  | E     | 305 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 5   | CHL  | E     | 308 | X         | -        | -       | -                |
| 5   | CHL  | E     | 309 | X         | -        | -       | -                |
| 5   | CHL  | E     | 310 | X         | -        | -       | -                |
| 5   | CHL  | E     | 311 | X         | -        | -       | -                |
| 5   | CHL  | E     | 312 | X         | -        | -       | -                |
| 5   | CHL  | E     | 317 | X         | -        | -       | -                |
| 5   | CHL  | F     | 304 | X         | -        | -       | -                |
| 5   | CHL  | F     | 305 | X         | -        | -       | -                |
| 5   | CHL  | F     | 308 | X         | -        | -       | -                |
| 5   | CHL  | F     | 309 | X         | -        | -       | -                |
| 5   | CHL  | F     | 310 | X         | -        | -       | -                |
| 5   | CHL  | F     | 311 | X         | -        | -       | -                |
| 5   | CHL  | F     | 312 | X         | -        | -       | -                |
| 5   | CHL  | F     | 317 | X         | -        | -       | -                |
| 6   | CLA  | A     | 307 | X         | -        | -       | -                |
| 6   | CLA  | A     | 308 | X         | -        | -       | -                |
| 6   | CLA  | A     | 314 | X         | -        | -       | -                |
| 6   | CLA  | A     | 315 | X         | -        | -       | -                |
| 6   | CLA  | A     | 316 | X         | -        | -       | -                |
| 6   | CLA  | A     | 317 | X         | -        | -       | -                |
| 6   | CLA  | B     | 308 | X         | -        | -       | -                |
| 6   | CLA  | B     | 309 | X         | -        | -       | -                |
| 6   | CLA  | B     | 315 | X         | -        | -       | -                |
| 6   | CLA  | B     | 316 | X         | -        | -       | -                |
| 6   | CLA  | B     | 317 | X         | -        | -       | -                |
| 6   | CLA  | B     | 318 | X         | -        | -       | -                |
| 6   | CLA  | C     | 307 | X         | -        | -       | -                |
| 6   | CLA  | C     | 308 | X         | -        | -       | -                |
| 6   | CLA  | C     | 314 | X         | -        | -       | -                |
| 6   | CLA  | C     | 315 | X         | -        | -       | -                |
| 6   | CLA  | C     | 316 | X         | -        | -       | -                |
| 6   | CLA  | C     | 317 | X         | -        | -       | -                |
| 6   | CLA  | D     | 307 | X         | -        | -       | -                |
| 6   | CLA  | D     | 308 | X         | -        | -       | -                |
| 6   | CLA  | D     | 314 | X         | -        | -       | -                |
| 6   | CLA  | D     | 315 | X         | -        | -       | -                |
| 6   | CLA  | D     | 316 | X         | -        | -       | -                |
| 6   | CLA  | D     | 317 | X         | -        | -       | -                |
| 6   | CLA  | E     | 306 | X         | -        | -       | -                |
| 6   | CLA  | E     | 307 | X         | -        | -       | -                |
| 6   | CLA  | E     | 313 | X         | -        | -       | -                |
| 6   | CLA  | E     | 314 | X         | -        | -       | -                |

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| <b>Mol</b> | <b>Type</b> | <b>Chain</b> | <b>Res</b> | <b>Chirality</b> | <b>Geometry</b> | <b>Clashes</b> | <b>Electron density</b> |
|------------|-------------|--------------|------------|------------------|-----------------|----------------|-------------------------|
| 6          | CLA         | E            | 315        | X                | -               | -              | -                       |
| 6          | CLA         | E            | 316        | X                | -               | -              | -                       |
| 6          | CLA         | F            | 306        | X                | -               | -              | -                       |
| 6          | CLA         | F            | 307        | X                | -               | -              | -                       |
| 6          | CLA         | F            | 313        | X                | -               | -              | -                       |
| 6          | CLA         | F            | 314        | X                | -               | -              | -                       |
| 6          | CLA         | F            | 315        | X                | -               | -              | -                       |
| 6          | CLA         | F            | 316        | X                | -               | -              | -                       |

## 2 Entry composition [i](#)

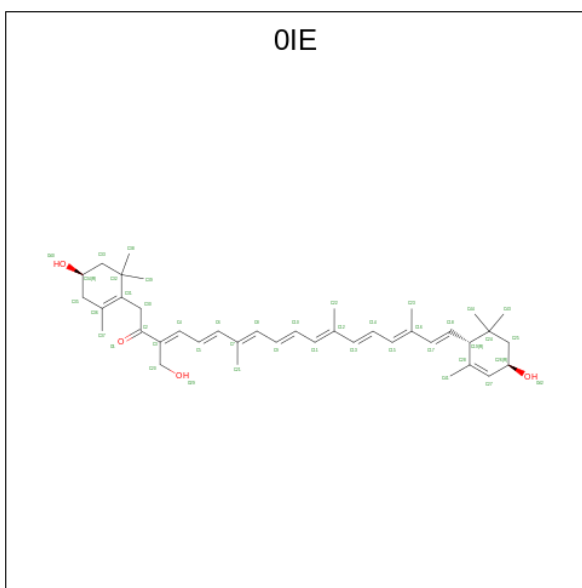
There are 12 unique types of molecules in this entry. The entry contains 16480 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1.

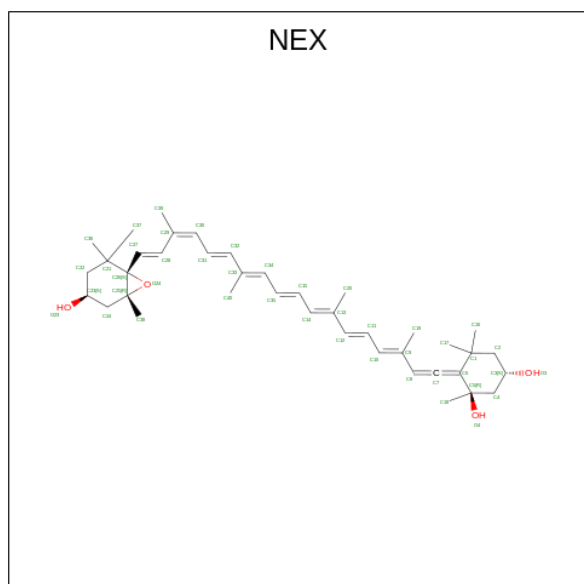
| Mol | Chain | Residues | Atoms         |           |          |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|---------|-------|
|     |       |          | Total         | C         | N        | O        | S       |         |         |       |
| 1   | A     | 223      | Total<br>1672 | C<br>1083 | N<br>265 | O<br>314 | S<br>10 | 0       | 0       | 0     |
| 1   | B     | 223      | Total<br>1669 | C<br>1083 | N<br>266 | O<br>310 | S<br>10 | 0       | 0       | 0     |
| 1   | C     | 222      | Total<br>1659 | C<br>1075 | N<br>264 | O<br>310 | S<br>10 | 0       | 0       | 0     |
| 1   | D     | 223      | Total<br>1682 | C<br>1090 | N<br>267 | O<br>315 | S<br>10 | 0       | 0       | 0     |
| 1   | E     | 223      | Total<br>1684 | C<br>1095 | N<br>267 | O<br>312 | S<br>10 | 0       | 0       | 0     |
| 1   | F     | 223      | Total<br>1685 | C<br>1094 | N<br>267 | O<br>314 | S<br>10 | 0       | 0       | 0     |

- Molecule 2 is Siphonaxanthin (three-letter code: OIE) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



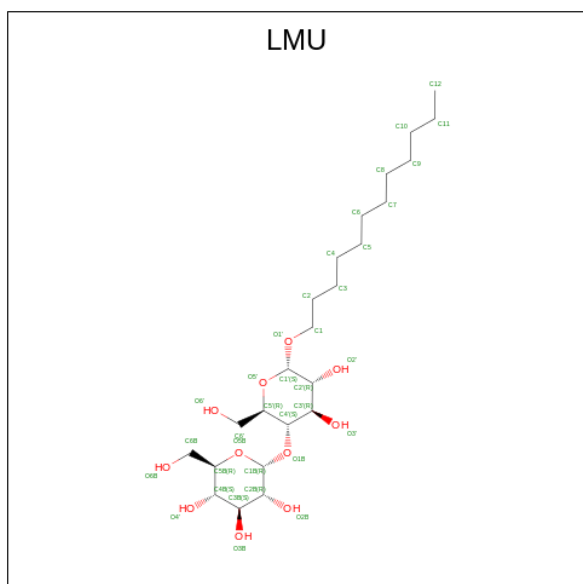
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 2   | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 40 | 4 |         |         |
| 2   | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 40 | 4 |         |         |
| 2   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 40 | 4 |         |         |
| 2   | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 40 | 4 |         |         |
| 2   | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 40 | 4 |         |         |
| 2   | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 40 | 4 |         |         |
| 2   | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 40 | 4 |         |         |
| 2   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 40 | 4 |         |         |
| 2   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 40 | 4 |         |         |
| 2   | F     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 40 | 4 |         |         |
| 2   | F     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 40 | 4 |         |         |

- Molecule 3 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-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: 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                | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 3   | A     | 1        | Total C O<br>44 40 4 | 0       | 0       |
| 3   | B     | 1        | Total C O<br>44 40 4 | 0       | 0       |
| 3   | C     | 1        | Total C O<br>44 40 4 | 0       | 0       |
| 3   | D     | 1        | Total C O<br>44 40 4 | 0       | 0       |
| 3   | E     | 1        | Total C O<br>44 40 4 | 0       | 0       |
| 3   | F     | 1        | Total C O<br>44 40 4 | 0       | 0       |

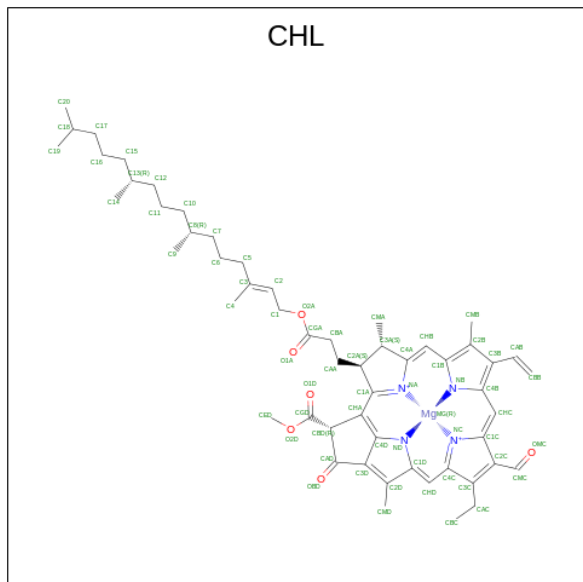
- Molecule 4 is DODECYL-ALPHA-D-MALTOSE (three-letter code: LMU) (formula:  $C_{24}H_{46}O_{11}$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms                 | ZeroOcc | AltConf |
|-----|-------|----------|-----------------------|---------|---------|
| 4   | A     | 1        | Total C O<br>35 24 11 | 0       | 0       |
| 4   | B     | 1        | Total C O<br>33 23 10 | 0       | 0       |
| 4   | B     | 1        | Total C O<br>35 24 11 | 0       | 0       |
| 4   | D     | 1        | Total C O<br>35 24 11 | 0       | 0       |
| 4   | E     | 1        | Total C O<br>35 24 11 | 0       | 0       |



- Molecule 5 is CHLOROPHYLL B (three-letter code: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |   |
|-----|-------|----------|-------|----|----|---|---------|---------|---|
| 5   | A     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 66    | 55 | 1  | 4 | 6       |         |   |
| 5   | A     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 64    | 53 | 1  | 4 | 6       |         |   |
| 5   | A     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |   |
| 5   | A     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 51    | 40 | 1  | 4 | 6       |         |   |
| 5   | A     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 61    | 50 | 1  | 4 | 6       |         |   |
| 5   | A     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 56    | 45 | 1  | 4 | 6       |         |   |
| 5   | A     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 66    | 55 | 1  | 4 | 6       |         |   |
| 5   | A     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 42    | 33 | 1  | 4 | 4       |         |   |
| 5   | B     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 66    | 55 | 1  | 4 | 6       |         |   |
| 5   | B     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 65    | 54 | 1  | 4 | 6       |         |   |
| 5   | B     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |   |
| 5   | B     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 51    | 40 | 1  | 4 | 6       |         |   |

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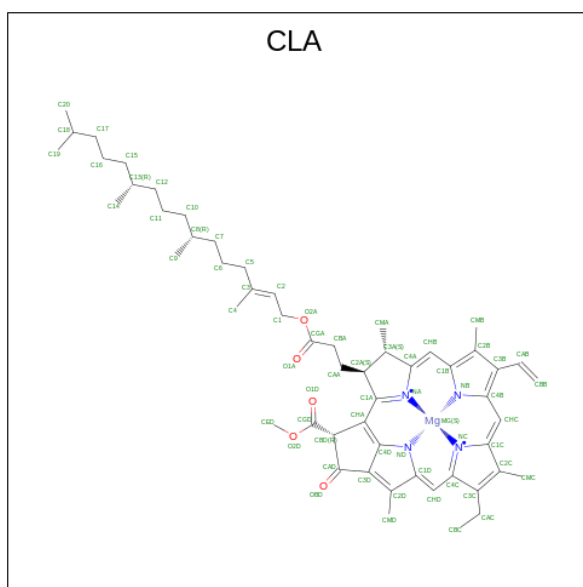
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |   |
|-----|-------|----------|-------|----|----|---|---------|---------|---|
| 5   | B     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 62    | 51 | 1  | 4 | 6       |         |   |
| 5   | B     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 57    | 46 | 1  | 4 | 6       |         |   |
| 5   | B     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 66    | 55 | 1  | 4 | 6       |         |   |
| 5   | B     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 47    | 36 | 1  | 4 | 6       |         |   |
| 5   | C     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 66    | 55 | 1  | 4 | 6       |         |   |
| 5   | C     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 66    | 55 | 1  | 4 | 6       |         |   |
| 5   | C     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 42    | 33 | 1  | 4 | 4       |         |   |
| 5   | C     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 44    | 35 | 1  | 4 | 4       |         |   |
| 5   | C     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 61    | 50 | 1  | 4 | 6       |         |   |
| 5   | C     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 56    | 45 | 1  | 4 | 6       |         |   |
| 5   | C     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 66    | 55 | 1  | 4 | 6       |         |   |
| 5   | C     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 44    | 35 | 1  | 4 | 4       |         |   |
| 5   | D     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 66    | 55 | 1  | 4 | 6       |         |   |
| 5   | D     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 65    | 54 | 1  | 4 | 6       |         |   |
| 5   | D     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 42    | 33 | 1  | 4 | 4       |         |   |
| 5   | D     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 45    | 35 | 1  | 4 | 5       |         |   |
| 5   | D     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 62    | 51 | 1  | 4 | 6       |         |   |
| 5   | D     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 57    | 46 | 1  | 4 | 6       |         |   |
| 5   | D     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 66    | 55 | 1  | 4 | 6       |         |   |
| 5   | D     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 46    | 35 | 1  | 4 | 6       |         |   |
| 5   | E     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 66    | 55 | 1  | 4 | 6       |         |   |

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| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |   |
|-----|-------|----------|-------|----|----|---|---------|---------|---|
| 5   | E     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 64    | 53 | 1  | 4 | 6       |         |   |
| 5   | E     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 41    | 32 | 1  | 4 | 4       |         |   |
| 5   | E     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |   |
| 5   | E     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 61    | 50 | 1  | 4 | 6       |         |   |
| 5   | E     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 56    | 45 | 1  | 4 | 6       |         |   |
| 5   | E     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 66    | 55 | 1  | 4 | 6       |         |   |
| 5   | E     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 41    | 32 | 1  | 4 | 4       |         |   |
| 5   | F     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 66    | 55 | 1  | 4 | 6       |         |   |
| 5   | F     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 66    | 55 | 1  | 4 | 6       |         |   |
| 5   | F     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 42    | 33 | 1  | 4 | 4       |         |   |
| 5   | F     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 42    | 33 | 1  | 4 | 4       |         |   |
| 5   | F     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 61    | 50 | 1  | 4 | 6       |         |   |
| 5   | F     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 56    | 45 | 1  | 4 | 6       |         |   |
| 5   | F     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 66    | 55 | 1  | 4 | 6       |         |   |
| 5   | F     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 46    | 35 | 1  | 4 | 6       |         |   |

- Molecule 6 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |   |
|-----|-------|----------|-------|----|----|---|---------|---------|---|
| 6   | A     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 65    | 55 | 1  | 4 | 5       |         |   |
| 6   | A     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 50    | 40 | 1  | 4 | 5       |         |   |
| 6   | A     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 55    | 45 | 1  | 4 | 5       |         |   |
| 6   | A     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 63    | 53 | 1  | 4 | 5       |         |   |
| 6   | A     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 45    | 35 | 1  | 4 | 5       |         |   |
| 6   | A     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 55    | 45 | 1  | 4 | 5       |         |   |
| 6   | B     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 65    | 55 | 1  | 4 | 5       |         |   |
| 6   | B     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 46    | 36 | 1  | 4 | 5       |         |   |
| 6   | B     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 58    | 48 | 1  | 4 | 5       |         |   |
| 6   | B     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 65    | 55 | 1  | 4 | 5       |         |   |
| 6   | B     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 45    | 35 | 1  | 4 | 5       |         |   |
| 6   | B     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 65    | 55 | 1  | 4 | 5       |         |   |
| 6   | C     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 65    | 55 | 1  | 4 | 5       |         |   |
| 6   | C     | 1        | Total | C  | Mg | N | O       | 0       | 0 |
|     |       |          | 46    | 36 | 1  | 4 | 5       |         |   |

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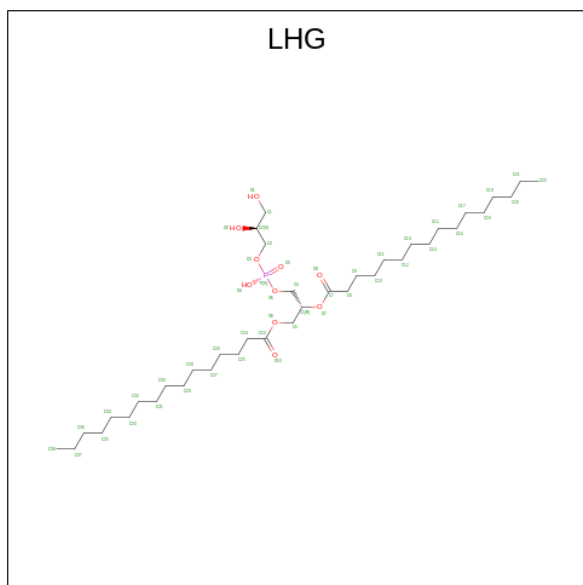
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 6   | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 53    | 43 | 1  | 4 | 5 |         |         |
| 6   | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 6   | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 6   | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |         |
| 6   | D     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 6   | D     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 6   | D     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |         |
| 6   | D     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 6   | D     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 6   | D     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 6   | E     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 6   | E     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 6   | E     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 6   | E     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 63    | 53 | 1  | 4 | 5 |         |         |
| 6   | E     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 6   | E     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 6   | F     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 6   | F     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 6   | F     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |         |
| 6   | F     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 6   | F     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
|     |       |          | Total | C  | Mg | N | O |         |         |
| 6   | F     | 1        | 56    | 46 | 1  | 4 | 5 | 0       | 0       |

- Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).

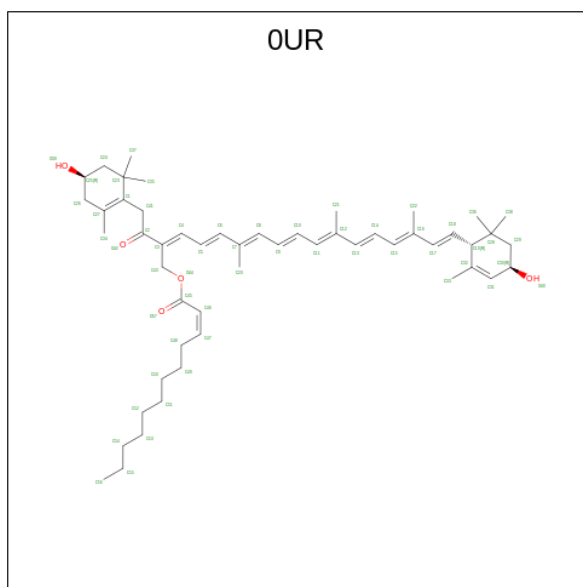


| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
|     |       |          | Total | C  | O  | P |         |         |
| 7   | A     | 1        | 47    | 36 | 10 | 1 | 0       | 0       |
| 7   | B     | 1        | 46    | 35 | 10 | 1 | 0       | 0       |
| 7   | B     | 1        | 31    | 20 | 10 | 1 | 0       | 0       |
| 7   | C     | 1        | 25    | 14 | 10 | 1 | 0       | 0       |
| 7   | C     | 1        | 45    | 34 | 10 | 1 | 0       | 0       |
| 7   | D     | 1        | 46    | 35 | 10 | 1 | 0       | 0       |
| 7   | E     | 1        | 41    | 30 | 10 | 1 | 0       | 0       |
| 7   | F     | 1        | 45    | 34 | 10 | 1 | 0       | 0       |

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

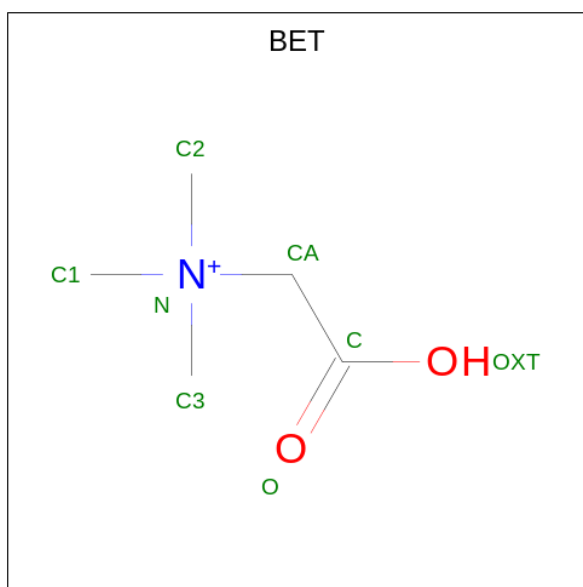
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 8   | A     | 2        | Total Mg<br>2 2 | 0       | 0       |
| 8   | D     | 1        | Total Mg<br>1 1 | 0       | 0       |

- Molecule 9 is Siphonein (three-letter code: 0UR) (formula: C<sub>52</sub>H<sub>76</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



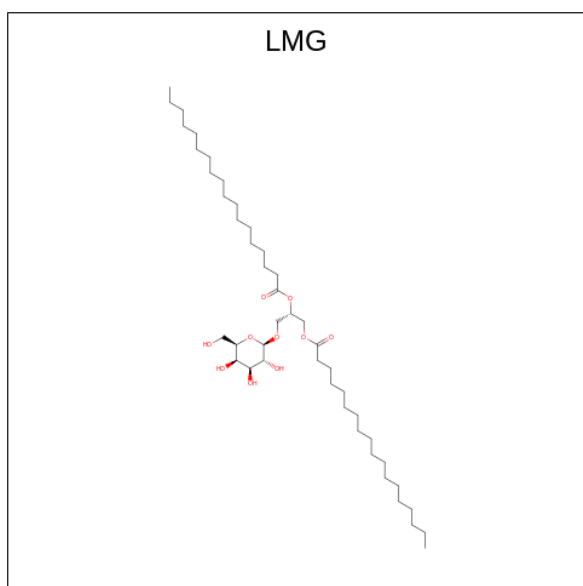
| Mol | Chain | Residues | Atoms                | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 9   | A     | 1        | Total C O<br>52 47 5 | 0       | 0       |
| 9   | B     | 1        | Total C O<br>50 45 5 | 0       | 0       |
| 9   | B     | 1        | Total C O<br>52 47 5 | 0       | 0       |
| 9   | C     | 1        | Total C O<br>52 47 5 | 0       | 0       |
| 9   | D     | 1        | Total C O<br>52 47 5 | 0       | 0       |
| 9   | E     | 1        | Total C O<br>52 47 5 | 0       | 0       |
| 9   | F     | 1        | Total C O<br>52 47 5 | 0       | 0       |

- Molecule 10 is TRIMETHYL GLYCINE (three-letter code: BET) (formula: C<sub>5</sub>H<sub>12</sub>NO<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
|     |       |          | Total | C | N | O |         |         |
| 10  | B     | 1        | 8     | 5 | 1 | 2 | 0       | 0       |
| 10  | B     | 1        | 8     | 5 | 1 | 2 | 0       | 0       |
| 10  | C     | 1        | 8     | 5 | 1 | 2 | 0       | 0       |

- Molecule 11 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).





| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 11  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 30    | 20 | 10 |         |         |
| 11  | F     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 30    | 20 | 10 |         |         |

- Molecule 12 is water.

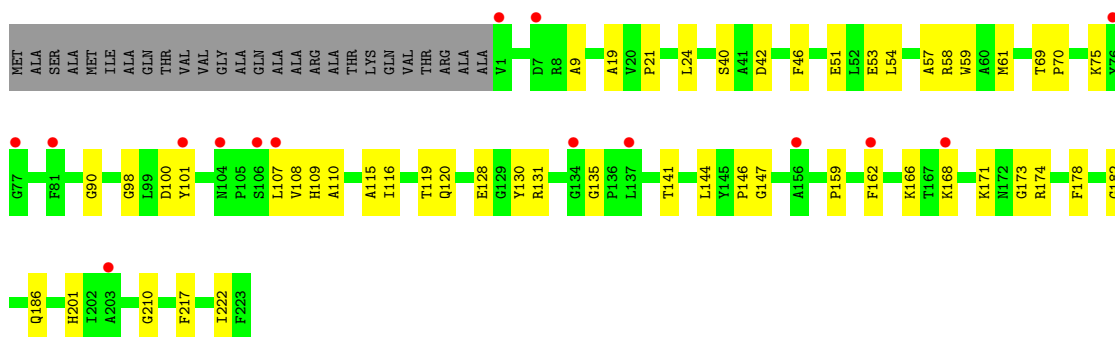
| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 12  | A     | 8        | Total | O | 0       | 0       |
|     |       |          | 8     | 8 |         |         |
| 12  | B     | 7        | Total | O | 0       | 0       |
|     |       |          | 7     | 7 |         |         |
| 12  | C     | 8        | Total | O | 0       | 0       |
|     |       |          | 8     | 8 |         |         |
| 12  | D     | 4        | Total | O | 0       | 0       |
|     |       |          | 4     | 4 |         |         |
| 12  | E     | 6        | Total | O | 0       | 0       |
|     |       |          | 6     | 6 |         |         |
| 12  | F     | 8        | Total | O | 0       | 0       |
|     |       |          | 8     | 8 |         |         |

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

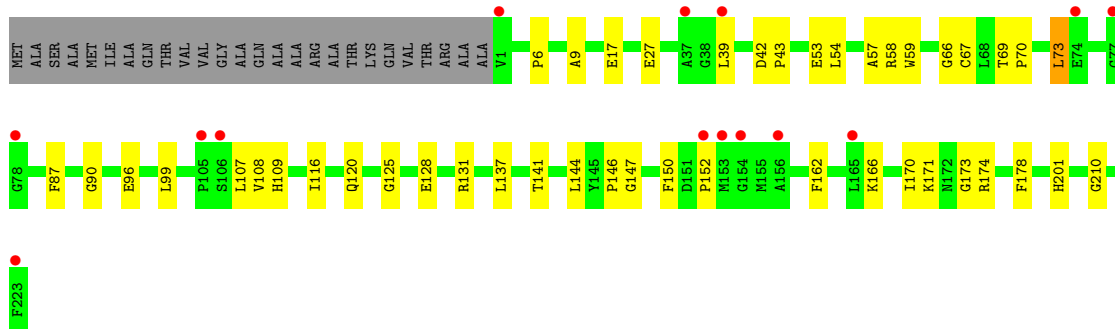
- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1

Chain A: 



- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1

Chain B: 



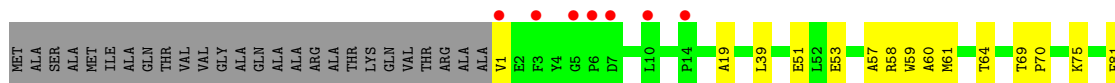
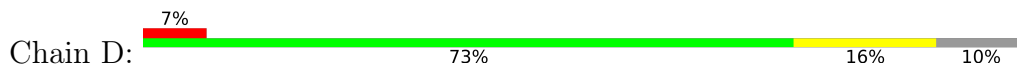
- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1

Chain C: 

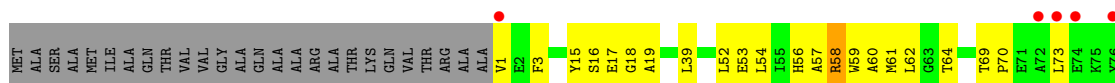




- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1



- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1



- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 109.72Å 91.61Å 169.22Å<br>90.00° 103.52° 90.00°             | Depositor        |
| Resolution (Å)  | 39.90 – 2.60<br>47.58 – 2.45                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 66.2 (39.90-2.60)<br>56.8 (47.58-2.45)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.06  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.20 (at 2.45Å)   | Xtrriage         |
| Refinement program  | PHENIX (1.18_3861: ???)                                     | Depositor        |
| R, $R_{free}$   | 0.207 , 0.249<br>0.214 , 0.248                              | Depositor<br>DCC |
| $R_{free}$ test set   | 2000 reflections (2.93%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 75.7  | Xtrriage         |
| Anisotropy  | 0.099   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 70.9   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtrriage         |
| Estimated twinning fraction   | No twinning to report.                                      | Xtrriage         |
| $F_o, F_c$ correlation  | 0.91  | EDS              |
| Total number of atoms   | 16480   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 83.0  | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0UR, LMU, CLA, LMG, LHG, CHL, MG, NEX, BET, OIE

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

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | A     | 0.30         | 0/1725  | 0.47        | 0/2350  |
| 1   | B     | 0.29         | 0/1722  | 0.47        | 0/2345  |
| 1   | C     | 0.30         | 0/1712  | 0.45        | 0/2332  |
| 1   | D     | 0.29         | 0/1735  | 0.46        | 0/2361  |
| 1   | E     | 0.28         | 0/1737  | 0.45        | 0/2364  |
| 1   | F     | 0.31         | 0/1738  | 0.49        | 0/2366  |
| All | All   | 0.30         | 0/10369 | 0.46        | 0/14118 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1672  | 0        | 1547     | 47      | 0            |
| 1   | B     | 1669  | 0        | 1552     | 43      | 0            |
| 1   | C     | 1659  | 0        | 1523     | 44      | 0            |
| 1   | D     | 1682  | 0        | 1572     | 35      | 0            |
| 1   | E     | 1684  | 0        | 1581     | 52      | 0            |
| 1   | F     | 1685  | 0        | 1579     | 40      | 0            |
| 2   | A     | 88    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | B     | 44    | 0        | 0        | 1       | 0            |
| 2   | C     | 88    | 0        | 0        | 3       | 0            |
| 2   | D     | 88    | 0        | 0        | 0       | 0            |
| 2   | E     | 88    | 0        | 0        | 1       | 0            |
| 2   | F     | 88    | 0        | 0        | 0       | 0            |
| 3   | A     | 44    | 0        | 56       | 3       | 0            |
| 3   | B     | 44    | 0        | 54       | 4       | 0            |
| 3   | C     | 44    | 0        | 55       | 4       | 0            |
| 3   | D     | 44    | 0        | 55       | 4       | 0            |
| 3   | E     | 44    | 0        | 55       | 3       | 0            |
| 3   | F     | 44    | 0        | 53       | 2       | 0            |
| 4   | A     | 35    | 0        | 46       | 4       | 0            |
| 4   | B     | 68    | 0        | 85       | 3       | 0            |
| 4   | D     | 35    | 0        | 46       | 3       | 0            |
| 4   | E     | 35    | 0        | 46       | 3       | 0            |
| 5   | A     | 449   | 0        | 397      | 26      | 0            |
| 5   | B     | 457   | 0        | 407      | 35      | 0            |
| 5   | C     | 445   | 0        | 403      | 36      | 0            |
| 5   | D     | 449   | 0        | 402      | 35      | 0            |
| 5   | E     | 438   | 0        | 384      | 33      | 0            |
| 5   | F     | 445   | 0        | 397      | 34      | 0            |
| 6   | A     | 333   | 0        | 305      | 21      | 0            |
| 6   | B     | 344   | 0        | 337      | 23      | 0            |
| 6   | C     | 330   | 0        | 306      | 29      | 0            |
| 6   | D     | 344   | 0        | 337      | 21      | 0            |
| 6   | E     | 333   | 0        | 305      | 21      | 0            |
| 6   | F     | 325   | 0        | 293      | 25      | 0            |
| 7   | A     | 47    | 0        | 67       | 3       | 0            |
| 7   | B     | 77    | 0        | 97       | 13      | 0            |
| 7   | C     | 70    | 0        | 83       | 4       | 0            |
| 7   | D     | 46    | 0        | 65       | 5       | 0            |
| 7   | E     | 41    | 0        | 52       | 7       | 0            |
| 7   | F     | 45    | 0        | 63       | 8       | 0            |
| 8   | A     | 2     | 0        | 0        | 0       | 0            |
| 8   | D     | 1     | 0        | 0        | 0       | 0            |
| 9   | A     | 52    | 0        | 0        | 0       | 0            |
| 9   | B     | 102   | 0        | 0        | 5       | 0            |
| 9   | C     | 52    | 0        | 0        | 3       | 0            |
| 9   | D     | 52    | 0        | 0        | 0       | 0            |
| 9   | E     | 52    | 0        | 0        | 3       | 0            |
| 9   | F     | 52    | 0        | 0        | 2       | 0            |
| 10  | B     | 16    | 0        | 22       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | C     | 8     | 0        | 11       | 0       | 0            |
| 11  | B     | 30    | 0        | 30       | 0       | 0            |
| 11  | F     | 30    | 0        | 30       | 1       | 0            |
| 12  | A     | 8     | 0        | 0        | 0       | 0            |
| 12  | B     | 7     | 0        | 0        | 1       | 0            |
| 12  | C     | 8     | 0        | 0        | 1       | 0            |
| 12  | D     | 4     | 0        | 0        | 1       | 0            |
| 12  | E     | 6     | 0        | 0        | 0       | 0            |
| 12  | F     | 8     | 0        | 0        | 2       | 0            |
| All | All   | 16480 | 0        | 14698    | 449     | 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 14.

All (449) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:83:GLU:H     | 1:E:92:GLN:HE21  | 1.12                     | 0.94              |
| 6:F:313:CLA:H43  | 6:F:315:CLA:HBA1 | 1.50                     | 0.89              |
| 3:D:303:NEX:H42  | 4:D:304:LMU:H6'2 | 1.56                     | 0.88              |
| 5:D:311:CHL:H62  | 5:D:313:CHL:H193 | 1.61                     | 0.81              |
| 1:B:150:PHE:HD1  | 5:B:313:CHL:H2   | 1.47                     | 0.79              |
| 1:B:42:ASP:OD2   | 7:B:324:LHG:O3   | 2.02                     | 0.78              |
| 1:D:135:GLY:HA2  | 4:D:304:LMU:H3B  | 1.68                     | 0.75              |
| 1:E:150:PHE:HA   | 5:E:311:CHL:H51  | 1.67                     | 0.75              |
| 6:F:306:CLA:HAC2 | 5:F:310:CHL:H142 | 1.69                     | 0.75              |
| 1:F:57:ALA:HB1   | 1:F:173:GLY:HA3  | 1.69                     | 0.74              |
| 1:C:131:ARG:NH2  | 5:C:313:CHL:O1D  | 2.20                     | 0.74              |
| 1:A:42:ASP:OD2   | 7:B:324:LHG:HC41 | 1.87                     | 0.74              |
| 1:C:119:THR:HG21 | 5:C:310:CHL:HED2 | 1.71                     | 0.73              |
| 1:B:57:ALA:HB1   | 1:B:173:GLY:HA3  | 1.71                     | 0.73              |
| 5:F:305:CHL:CHB  | 5:F:305:CHL:H11  | 2.19                     | 0.73              |
| 5:D:311:CHL:H93  | 5:D:313:CHL:H152 | 1.71                     | 0.72              |
| 1:A:57:ALA:HB1   | 1:A:173:GLY:HA3  | 1.71                     | 0.72              |
| 1:C:111:GLN:HG3  | 5:C:309:CHL:HAB  | 1.69                     | 0.72              |
| 1:C:125:GLY:HA2  | 5:C:313:CHL:HAB  | 1.72                     | 0.72              |
| 5:B:311:CHL:HAB  | 5:B:312:CHL:HMC  | 1.70                     | 0.71              |
| 6:D:314:CLA:HMB1 | 6:D:314:CLA:HBB1 | 1.72                     | 0.71              |
| 1:C:198:TRP:HE1  | 5:C:318:CHL:CMC  | 2.04                     | 0.71              |
| 1:E:171:LYS:NZ   | 7:E:318:LHG:O4   | 2.24                     | 0.71              |
| 1:D:57:ALA:HB1   | 1:D:173:GLY:HA3  | 1.72                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:A:314:CLA:HBB1 | 6:A:314:CLA:HMB1 | 1.73                     | 0.70              |
| 1:E:131:ARG:NH2  | 5:E:312:CHL:O1D  | 2.24                     | 0.70              |
| 1:E:16:SER:O     | 1:E:18:GLY:N     | 2.24                     | 0.70              |
| 1:F:26:GLY:O     | 1:F:28:PHE:N     | 2.24                     | 0.69              |
| 1:E:57:ALA:HB1   | 1:E:173:GLY:HA3  | 1.73                     | 0.69              |
| 1:B:152:PRO:HD2  | 9:B:325:OUR:O40  | 1.93                     | 0.69              |
| 5:E:312:CHL:HHC  | 5:E:312:CHL:HBB1 | 1.75                     | 0.69              |
| 1:E:58:ARG:NH1   | 1:E:169:GLU:OE2  | 2.27                     | 0.68              |
| 6:C:307:CLA:HBB1 | 5:C:313:CHL:H172 | 1.76                     | 0.68              |
| 6:A:307:CLA:H91  | 5:A:313:CHL:H121 | 1.75                     | 0.67              |
| 1:D:131:ARG:NH2  | 5:D:313:CHL:O1D  | 2.27                     | 0.66              |
| 1:C:58:ARG:NH1   | 5:C:312:CHL:OBD  | 2.27                     | 0.66              |
| 1:A:90:GLY:HA2   | 5:A:310:CHL:HAC2 | 1.78                     | 0.66              |
| 1:A:201:HIS:CG   | 6:A:317:CLA:HAA2 | 2.31                     | 0.66              |
| 1:F:92:GLN:HG3   | 1:F:99:LEU:HG    | 1.78                     | 0.66              |
| 1:B:120:GLN:NE2  | 5:B:314:CHL:OMC  | 2.26                     | 0.66              |
| 1:B:131:ARG:NH2  | 5:B:314:CHL:O1D  | 2.28                     | 0.66              |
| 1:C:137:LEU:HD13 | 5:C:312:CHL:HAB  | 1.77                     | 0.66              |
| 1:A:100:ASP:OD1  | 1:A:109:HIS:ND1  | 2.25                     | 0.65              |
| 1:F:132:CYS:SG   | 12:F:406:HOH:O   | 2.53                     | 0.65              |
| 1:E:100:ASP:OD1  | 1:E:109:HIS:ND1  | 2.25                     | 0.65              |
| 6:F:313:CLA:HBB1 | 6:F:313:CLA:HMB1 | 1.77                     | 0.65              |
| 1:A:147:GLY:HA3  | 6:A:314:CLA:HED1 | 1.78                     | 0.65              |
| 6:C:307:CLA:CBB  | 5:C:313:CHL:H172 | 2.27                     | 0.64              |
| 5:B:306:CHL:HMD3 | 7:B:320:LHG:HC62 | 1.80                     | 0.64              |
| 6:D:317:CLA:H2   | 5:D:318:CHL:HMD1 | 1.80                     | 0.64              |
| 1:B:150:PHE:CD1  | 5:B:313:CHL:H2   | 2.30                     | 0.64              |
| 1:B:120:GLN:NE2  | 5:B:312:CHL:OMC  | 2.30                     | 0.63              |
| 1:B:43:PRO:HB2   | 1:F:6:PRO:HB3    | 1.80                     | 0.63              |
| 1:F:201:HIS:CG   | 6:F:316:CLA:HAA2 | 2.33                     | 0.63              |
| 1:E:168:LYS:O    | 1:E:172:ASN:ND2  | 2.26                     | 0.63              |
| 2:A:302:OIE:C25  | 6:A:315:CLA:HBB1 | 2.28                     | 0.62              |
| 6:F:316:CLA:H93  | 7:F:318:LHG:H142 | 1.80                     | 0.62              |
| 5:A:305:CHL:H52  | 5:C:313:CHL:HBB1 | 1.82                     | 0.61              |
| 1:E:90:GLY:HA2   | 5:E:309:CHL:HAC2 | 1.81                     | 0.61              |
| 6:B:318:CLA:HMB2 | 5:B:319:CHL:HHD  | 1.81                     | 0.61              |
| 5:D:311:CHL:H71  | 5:D:313:CHL:H171 | 1.82                     | 0.61              |
| 1:B:66:GLY:O     | 12:B:401:HOH:O   | 2.16                     | 0.61              |
| 5:D:310:CHL:HAB  | 5:D:311:CHL:HMC  | 1.82                     | 0.61              |
| 5:E:317:CHL:HHC  | 5:E:317:CHL:HBB1 | 1.82                     | 0.61              |
| 6:A:308:CLA:HBA1 | 6:A:308:CLA:HBD  | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:131:ARG:NH2  | 5:F:312:CHL:O1D  | 2.35                     | 0.60              |
| 5:D:306:CHL:H141 | 5:E:312:CHL:H42  | 1.83                     | 0.60              |
| 1:A:131:ARG:NH2  | 5:A:313:CHL:O1D  | 2.34                     | 0.60              |
| 1:F:147:GLY:HA3  | 6:F:313:CLA:HED1 | 1.84                     | 0.60              |
| 6:C:314:CLA:HAB  | 9:C:321:OUR:C13  | 2.31                     | 0.60              |
| 1:B:147:GLY:HA3  | 6:B:315:CLA:HED1 | 1.84                     | 0.59              |
| 1:B:152:PRO:HD2  | 9:B:325:OUR:C30  | 2.32                     | 0.59              |
| 1:D:147:GLY:HA3  | 6:D:314:CLA:HED1 | 1.85                     | 0.59              |
| 1:E:1:VAL:HG22   | 1:E:3:PHE:H      | 1.67                     | 0.59              |
| 1:F:178:PHE:CD1  | 5:F:305:CHL:H191 | 2.38                     | 0.59              |
| 5:E:312:CHL:H202 | 6:F:306:CLA:H141 | 1.85                     | 0.59              |
| 1:E:39:LEU:HD12  | 5:E:305:CHL:H11  | 1.85                     | 0.59              |
| 6:E:316:CLA:HAB  | 5:E:317:CHL:HHD  | 1.84                     | 0.59              |
| 1:D:132:CYS:SG   | 12:D:404:HOH:O   | 2.57                     | 0.58              |
| 1:B:90:GLY:HA2   | 5:B:311:CHL:HAC2 | 1.84                     | 0.58              |
| 6:F:313:CLA:O1D  | 6:F:313:CLA:H2A  | 2.02                     | 0.58              |
| 1:C:92:GLN:NE2   | 6:C:308:CLA:O1D  | 2.37                     | 0.58              |
| 5:D:310:CHL:CAB  | 5:D:311:CHL:HMC  | 2.35                     | 0.57              |
| 1:E:83:GLU:N     | 1:E:92:GLN:HE21  | 1.93                     | 0.57              |
| 1:D:59:TRP:CD1   | 5:D:313:CHL:HMD3 | 2.40                     | 0.57              |
| 1:D:201:HIS:CG   | 6:D:317:CLA:HAA2 | 2.39                     | 0.57              |
| 1:C:201:HIS:ND1  | 1:C:208:ASN:O    | 2.34                     | 0.57              |
| 1:C:115:ALA:HB3  | 5:C:309:CHL:HMC  | 1.86                     | 0.57              |
| 1:E:201:HIS:ND1  | 1:E:208:ASN:O    | 2.29                     | 0.57              |
| 5:A:311:CHL:H62  | 5:A:313:CHL:H193 | 1.87                     | 0.56              |
| 1:B:201:HIS:CG   | 6:B:318:CLA:HAA2 | 2.40                     | 0.56              |
| 6:D:307:CLA:H51  | 5:F:305:CHL:H91  | 1.86                     | 0.56              |
| 1:B:42:ASP:OD2   | 7:B:324:LHG:C3   | 2.53                     | 0.56              |
| 6:E:315:CLA:HED2 | 6:E:315:CLA:H2A  | 1.88                     | 0.56              |
| 1:B:137:LEU:HD13 | 5:B:313:CHL:HAB  | 1.87                     | 0.56              |
| 5:F:312:CHL:HHC  | 5:F:312:CHL:HBB1 | 1.88                     | 0.56              |
| 1:C:201:HIS:CG   | 6:C:317:CLA:HAA2 | 2.39                     | 0.56              |
| 5:C:305:CHL:HBB1 | 5:C:305:CHL:HHC  | 1.87                     | 0.56              |
| 6:E:307:CLA:HMB1 | 6:E:307:CLA:HBB1 | 1.88                     | 0.56              |
| 1:B:9:ALA:HA     | 10:B:322:BET:H23 | 1.88                     | 0.55              |
| 6:B:315:CLA:HHD  | 6:B:315:CLA:HBC2 | 1.88                     | 0.55              |
| 6:B:316:CLA:NC   | 7:B:320:LHG:HC42 | 2.21                     | 0.55              |
| 6:C:308:CLA:HBB1 | 6:C:308:CLA:HMB1 | 1.89                     | 0.55              |
| 7:F:318:LHG:HC62 | 7:F:318:LHG:H281 | 1.89                     | 0.55              |
| 5:D:305:CHL:HMA3 | 7:D:319:LHG:H122 | 1.90                     | 0.55              |
| 6:F:306:CLA:HMC3 | 5:F:310:CHL:H93  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:51:GLU:HA    | 1:D:144:LEU:HD11 | 1.89                     | 0.54              |
| 1:A:168:LYS:HD3  | 6:A:316:CLA:HAA2 | 1.90                     | 0.54              |
| 6:C:317:CLA:H91  | 7:C:319:LHG:H322 | 1.88                     | 0.54              |
| 1:E:182:GLY:O    | 1:E:186:GLN:HB2  | 2.07                     | 0.54              |
| 1:C:111:GLN:CG   | 5:C:309:CHL:HAB  | 2.36                     | 0.54              |
| 1:A:116:ILE:CD1  | 5:A:310:CHL:HMD3 | 2.38                     | 0.54              |
| 1:E:201:HIS:CG   | 6:E:316:CLA:HAA2 | 2.42                     | 0.54              |
| 1:D:120:GLN:NE2  | 5:D:313:CHL:OMC  | 2.32                     | 0.53              |
| 1:F:9:ALA:HB1    | 5:F:304:CHL:HBC1 | 1.89                     | 0.53              |
| 6:F:314:CLA:C4C  | 7:F:318:LHG:HC61 | 2.38                     | 0.53              |
| 1:A:9:ALA:HB1    | 5:A:305:CHL:HBC1 | 1.91                     | 0.53              |
| 1:A:59:TRP:CD1   | 5:A:313:CHL:HMD3 | 2.43                     | 0.53              |
| 1:C:198:TRP:NE1  | 5:C:318:CHL:OMC  | 2.35                     | 0.53              |
| 5:F:310:CHL:H71  | 5:F:310:CHL:HMB2 | 1.90                     | 0.53              |
| 1:F:53:GLU:OE2   | 1:F:174:ARG:NE   | 2.38                     | 0.53              |
| 1:B:58:ARG:NH1   | 5:B:313:CHL:OBD  | 2.34                     | 0.53              |
| 6:B:315:CLA:H2A  | 6:B:315:CLA:O1D  | 2.08                     | 0.53              |
| 1:E:15:TYR:OH    | 4:E:319:LMU:H1B  | 2.08                     | 0.53              |
| 1:C:125:GLY:CA   | 5:C:313:CHL:HAB  | 2.38                     | 0.53              |
| 1:B:125:GLY:HA2  | 5:B:314:CHL:HAB  | 1.90                     | 0.53              |
| 1:E:101:TYR:CE2  | 6:E:307:CLA:H2   | 2.44                     | 0.53              |
| 1:F:32:TYR:OH    | 7:F:318:LHG:O5   | 2.18                     | 0.53              |
| 1:B:6:PRO:HB3    | 1:F:43:PRO:HB2   | 1.91                     | 0.52              |
| 1:D:120:GLN:NE2  | 5:D:311:CHL:OMC  | 2.42                     | 0.52              |
| 1:D:168:LYS:O    | 1:D:172:ASN:ND2  | 2.31                     | 0.52              |
| 1:E:150:PHE:HD1  | 5:E:311:CHL:H2   | 1.74                     | 0.52              |
| 1:A:42:ASP:OD2   | 7:B:324:LHG:O4   | 2.28                     | 0.52              |
| 1:B:67:CYS:SG    | 2:B:301:OIE:C39  | 2.98                     | 0.52              |
| 1:D:58:ARG:NH1   | 5:D:312:CHL:OBD  | 2.35                     | 0.52              |
| 1:B:53:GLU:OE2   | 1:B:174:ARG:NE   | 2.40                     | 0.52              |
| 6:A:307:CLA:H51  | 5:B:307:CHL:H91  | 1.92                     | 0.52              |
| 1:E:128:GLU:HG3  | 5:E:312:CHL:NB   | 2.24                     | 0.52              |
| 1:D:115:ALA:HB3  | 5:D:309:CHL:HMC  | 1.90                     | 0.51              |
| 5:D:310:CHL:HAA2 | 5:D:310:CHL:HBD  | 1.93                     | 0.51              |
| 1:E:54:LEU:O     | 1:E:58:ARG:HG2   | 2.11                     | 0.51              |
| 6:F:306:CLA:O1A  | 6:F:306:CLA:H2A  | 2.01                     | 0.51              |
| 1:A:58:ARG:NH1   | 5:A:312:CHL:OBD  | 2.43                     | 0.51              |
| 1:B:152:PRO:CD   | 9:B:325:OUR:O40  | 2.58                     | 0.51              |
| 6:C:317:CLA:H101 | 7:C:319:LHG:H142 | 1.91                     | 0.51              |
| 1:F:92:GLN:HE22  | 6:F:307:CLA:HED2 | 1.76                     | 0.51              |
| 1:E:162:PHE:CZ   | 6:E:313:CLA:HED3 | 2.46                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:213:TYR:O    | 1:E:216:LYS:HG2  | 2.10                     | 0.51              |
| 1:C:57:ALA:HB1   | 1:C:173:GLY:HA3  | 1.93                     | 0.51              |
| 1:A:58:ARG:HA    | 1:A:61:MET:HE3   | 1.93                     | 0.50              |
| 1:B:54:LEU:HD23  | 1:B:144:LEU:HD13 | 1.92                     | 0.50              |
| 6:D:317:CLA:H92  | 7:D:319:LHG:H151 | 1.93                     | 0.50              |
| 1:E:52:LEU:O     | 1:E:56:HIS:ND1   | 2.43                     | 0.50              |
| 1:A:53:GLU:OE2   | 1:A:174:ARG:NE   | 2.44                     | 0.50              |
| 1:A:146:PRO:HG3  | 5:A:312:CHL:HMD2 | 1.93                     | 0.50              |
| 1:F:54:LEU:HD23  | 1:F:144:LEU:HD13 | 1.93                     | 0.50              |
| 1:F:178:PHE:HE1  | 5:F:305:CHL:H201 | 1.76                     | 0.50              |
| 6:E:307:CLA:HBD  | 6:E:307:CLA:HBA1 | 1.93                     | 0.50              |
| 6:F:306:CLA:HMA2 | 6:F:306:CLA:H2   | 1.94                     | 0.50              |
| 1:A:128:GLU:HG3  | 5:A:313:CHL:NB   | 2.26                     | 0.49              |
| 1:C:92:GLN:HE22  | 6:C:308:CLA:HED3 | 1.76                     | 0.49              |
| 3:D:303:NEX:H42  | 4:D:304:LMU:C6B  | 2.37                     | 0.49              |
| 1:A:210:GLY:HA2  | 6:A:317:CLA:OBD  | 2.13                     | 0.49              |
| 6:B:308:CLA:O1A  | 6:B:308:CLA:H2A  | 2.12                     | 0.49              |
| 1:C:90:GLY:HA2   | 5:C:310:CHL:HAC2 | 1.94                     | 0.49              |
| 6:C:307:CLA:CAD  | 5:C:313:CHL:H2   | 2.41                     | 0.49              |
| 1:D:116:ILE:HG12 | 5:D:309:CHL:HAC1 | 1.92                     | 0.49              |
| 5:D:305:CHL:HAC1 | 7:D:319:LHG:HC2  | 1.93                     | 0.49              |
| 5:E:304:CHL:HED3 | 7:E:318:LHG:H141 | 1.95                     | 0.49              |
| 6:F:316:CLA:HHB  | 5:F:317:CHL:HHD  | 1.94                     | 0.49              |
| 1:F:66:GLY:O     | 12:F:401:HOH:O   | 2.19                     | 0.49              |
| 6:D:317:CLA:H122 | 7:D:319:LHG:H322 | 1.95                     | 0.49              |
| 5:D:311:CHL:O1A  | 1:F:217:PHE:HB2  | 2.13                     | 0.49              |
| 1:F:89:ALA:O     | 1:F:92:GLN:HG2   | 2.13                     | 0.49              |
| 6:B:318:CLA:H111 | 7:B:320:LHG:H312 | 1.93                     | 0.49              |
| 1:C:152:PRO:HD2  | 9:C:321:OUR:C30  | 2.43                     | 0.49              |
| 1:A:159:PRO:HD2  | 1:D:1:VAL:HB     | 1.94                     | 0.49              |
| 1:A:21:PRO:HD2   | 1:A:24:LEU:HD12  | 1.95                     | 0.48              |
| 1:B:116:ILE:HG12 | 5:B:310:CHL:HAC1 | 1.94                     | 0.48              |
| 1:D:53:GLU:OE2   | 1:D:174:ARG:NE   | 2.45                     | 0.48              |
| 1:C:201:HIS:CD2  | 6:C:317:CLA:HAA2 | 2.49                     | 0.48              |
| 1:E:152:PRO:HD2  | 9:E:320:OUR:C30  | 2.43                     | 0.48              |
| 5:E:305:CHL:H102 | 6:E:306:CLA:HMB3 | 1.95                     | 0.48              |
| 1:A:69:THR:HB    | 1:A:70:PRO:HD3   | 1.95                     | 0.48              |
| 5:F:309:CHL:CAB  | 5:F:310:CHL:HMC  | 2.43                     | 0.48              |
| 1:A:19:ALA:HB2   | 1:C:132:CYS:HB3  | 1.95                     | 0.48              |
| 5:B:314:CHL:H141 | 5:B:314:CHL:H161 | 1.57                     | 0.48              |
| 1:E:201:HIS:CD2  | 6:E:316:CLA:HAA2 | 2.49                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:201:HIS:CD2  | 6:A:317:CLA:HAA2 | 2.48                     | 0.48              |
| 7:F:318:LHG:H272 | 7:F:318:LHG:H242 | 1.49                     | 0.48              |
| 1:B:152:PRO:HD2  | 9:B:325:OUR:C31  | 2.44                     | 0.48              |
| 1:E:131:ARG:HG3  | 5:E:311:CHL:HMD3 | 1.94                     | 0.48              |
| 5:B:312:CHL:H142 | 5:B:314:CHL:H102 | 1.95                     | 0.48              |
| 1:B:107:LEU:O    | 1:B:109:HIS:N    | 2.47                     | 0.48              |
| 5:E:308:CHL:HHC  | 5:E:308:CHL:HBB1 | 1.94                     | 0.48              |
| 5:E:304:CHL:HBA1 | 5:E:304:CHL:H3A  | 1.63                     | 0.47              |
| 1:F:59:TRP:CD1   | 5:F:312:CHL:HMD3 | 2.49                     | 0.47              |
| 5:E:308:CHL:HHD  | 5:E:309:CHL:OBD  | 2.14                     | 0.47              |
| 1:A:130:TYR:CE1  | 4:A:304:LMU:H6D  | 2.49                     | 0.47              |
| 5:E:305:CHL:H71  | 6:E:306:CLA:HMA1 | 1.97                     | 0.47              |
| 5:F:311:CHL:HHC  | 5:F:311:CHL:HMC  | 1.60                     | 0.47              |
| 1:D:39:LEU:HD11  | 6:E:306:CLA:H12  | 1.97                     | 0.47              |
| 1:D:201:HIS:CD2  | 6:D:317:CLA:HAA2 | 2.49                     | 0.47              |
| 1:F:100:ASP:CG   | 1:F:105:PRO:HA   | 2.35                     | 0.47              |
| 5:F:311:CHL:CAD  | 6:F:313:CLA:HMD3 | 2.44                     | 0.47              |
| 4:B:304:LMU:H1B  | 4:B:304:LMU:H6'2 | 1.59                     | 0.47              |
| 7:B:324:LHG:H272 | 7:B:324:LHG:H241 | 1.50                     | 0.47              |
| 1:D:19:ALA:HB2   | 1:E:132:CYS:HB3  | 1.97                     | 0.47              |
| 4:E:319:LMU:O2'  | 3:F:303:NEX:H193 | 2.15                     | 0.47              |
| 1:F:182:GLY:O    | 1:F:186:GLN:HB2  | 2.15                     | 0.47              |
| 5:A:306:CHL:H121 | 5:A:306:CHL:H8   | 1.51                     | 0.47              |
| 5:D:311:CHL:HAB  | 5:D:311:CHL:H151 | 1.97                     | 0.47              |
| 1:E:58:ARG:NH2   | 1:E:144:LEU:O    | 2.47                     | 0.47              |
| 3:B:303:NEX:H15  | 3:B:303:NEX:H201 | 1.65                     | 0.47              |
| 1:C:107:LEU:HD23 | 5:C:309:CHL:HED2 | 1.97                     | 0.47              |
| 1:D:210:GLY:HA2  | 6:D:317:CLA:OBD  | 2.15                     | 0.47              |
| 1:F:9:ALA:HB1    | 5:F:304:CHL:CBC  | 2.44                     | 0.47              |
| 6:F:307:CLA:HMB1 | 6:F:307:CLA:HBB1 | 1.97                     | 0.47              |
| 5:B:307:CHL:H72  | 5:B:307:CHL:H111 | 1.62                     | 0.47              |
| 1:F:137:LEU:HD13 | 5:F:311:CHL:HAB  | 1.96                     | 0.47              |
| 1:F:146:PRO:HD2  | 6:F:313:CLA:OBD  | 2.15                     | 0.47              |
| 6:F:313:CLA:H72  | 9:F:320:OUR:C15  | 2.45                     | 0.47              |
| 1:B:171:LYS:NZ   | 7:B:320:LHG:O4   | 2.44                     | 0.46              |
| 6:C:307:CLA:H91  | 5:C:313:CHL:H143 | 1.97                     | 0.46              |
| 4:A:304:LMU:H91  | 4:A:304:LMU:H62  | 1.45                     | 0.46              |
| 1:C:182:GLY:O    | 1:C:186:GLN:HB2  | 2.14                     | 0.46              |
| 3:C:303:NEX:O24  | 5:C:310:CHL:HAA2 | 2.16                     | 0.46              |
| 1:E:120:GLN:OE1  | 5:E:310:CHL:HMC  | 2.16                     | 0.46              |
| 1:F:107:LEU:O    | 1:F:109:HIS:N    | 2.48                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:B:314:CHL:H91  | 5:B:314:CHL:H112 | 1.62                     | 0.46              |
| 6:B:318:CLA:H2   | 5:B:319:CHL:HMD1 | 1.98                     | 0.46              |
| 6:C:315:CLA:H151 | 6:C:316:CLA:HBB1 | 1.97                     | 0.46              |
| 5:A:306:CHL:H92  | 5:A:306:CHL:H61  | 1.52                     | 0.46              |
| 5:B:306:CHL:HBA1 | 5:B:306:CHL:H3A  | 1.59                     | 0.46              |
| 5:C:309:CHL:HHD  | 5:C:310:CHL:OBD  | 2.16                     | 0.46              |
| 1:F:178:PHE:HD1  | 5:F:305:CHL:H191 | 1.76                     | 0.46              |
| 1:C:89:ALA:O     | 1:C:92:GLN:HG2   | 2.16                     | 0.46              |
| 6:F:306:CLA:CAC  | 5:F:310:CHL:H142 | 2.41                     | 0.46              |
| 5:A:305:CHL:H61  | 5:A:305:CHL:H41  | 1.35                     | 0.46              |
| 6:A:307:CLA:H202 | 6:A:307:CLA:H161 | 1.80                     | 0.46              |
| 1:E:19:ALA:HB2   | 1:F:132:CYS:HB3  | 1.97                     | 0.46              |
| 6:E:314:CLA:C4C  | 7:E:318:LHG:HC61 | 2.46                     | 0.46              |
| 1:D:128:GLU:HG3  | 5:D:313:CHL:NB   | 2.31                     | 0.46              |
| 1:B:58:ARG:HB3   | 6:B:315:CLA:HAC2 | 1.97                     | 0.46              |
| 3:D:303:NEX:H32  | 5:D:312:CHL:HMA1 | 1.97                     | 0.46              |
| 5:D:313:CHL:CMB  | 5:F:304:CHL:HHB  | 2.46                     | 0.46              |
| 6:D:315:CLA:HBD  | 6:D:316:CLA:OBD  | 2.16                     | 0.46              |
| 5:D:313:CHL:HMB2 | 5:F:304:CHL:HHB  | 1.98                     | 0.45              |
| 6:A:307:CLA:H12  | 1:B:39:LEU:HD11  | 1.98                     | 0.45              |
| 1:B:162:PHE:CZ   | 1:B:166:LYS:HE3  | 2.51                     | 0.45              |
| 5:C:306:CHL:H43  | 5:C:306:CHL:HMB2 | 1.98                     | 0.45              |
| 1:A:51:GLU:HA    | 1:A:144:LEU:HD11 | 1.99                     | 0.45              |
| 3:A:303:NEX:H401 | 3:A:303:NEX:H35  | 1.58                     | 0.45              |
| 1:D:61:MET:SD    | 6:D:314:CLA:HHC  | 2.56                     | 0.45              |
| 6:D:307:CLA:H91  | 5:D:313:CHL:H121 | 1.99                     | 0.45              |
| 5:A:306:CHL:H101 | 6:C:307:CLA:H72  | 1.97                     | 0.45              |
| 5:F:304:CHL:H111 | 7:F:318:LHG:H211 | 1.98                     | 0.45              |
| 5:C:305:CHL:H41  | 5:C:305:CHL:H61  | 1.58                     | 0.45              |
| 1:C:107:LEU:O    | 1:C:109:HIS:N    | 2.50                     | 0.45              |
| 5:C:305:CHL:O1A  | 5:C:305:CHL:H3A  | 2.16                     | 0.45              |
| 6:C:315:CLA:H162 | 6:C:315:CLA:H141 | 1.69                     | 0.45              |
| 1:E:59:TRP:NE1   | 5:E:311:CHL:HED2 | 2.31                     | 0.45              |
| 7:E:318:LHG:HC62 | 7:E:318:LHG:H272 | 1.99                     | 0.45              |
| 1:F:186:GLN:HB2  | 1:F:186:GLN:HE21 | 1.65                     | 0.45              |
| 1:F:201:HIS:CD2  | 6:F:316:CLA:HAA2 | 2.51                     | 0.45              |
| 5:F:305:CHL:H93  | 6:F:306:CLA:HMA1 | 1.99                     | 0.45              |
| 4:B:305:LMU:H32  | 4:B:305:LMU:H61  | 1.48                     | 0.45              |
| 3:C:303:NEX:H191 | 3:C:303:NEX:H11  | 1.73                     | 0.45              |
| 6:C:314:CLA:HMB1 | 6:C:314:CLA:HBB1 | 1.99                     | 0.45              |
| 3:F:303:NEX:H392 | 5:F:309:CHL:HMB2 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:B:313:CHL:HAA1 | 6:B:315:CLA:HBC1 | 1.99                     | 0.45              |
| 1:C:209:ASN:HB2  | 5:C:318:CHL:HED1 | 1.97                     | 0.45              |
| 1:D:81:PHE:CE2   | 1:D:102:LEU:HD23 | 2.52                     | 0.45              |
| 1:C:210:GLY:HA2  | 6:C:317:CLA:OBD  | 2.16                     | 0.45              |
| 5:F:304:CHL:H143 | 5:F:304:CHL:H161 | 1.67                     | 0.45              |
| 1:A:178:PHE:HE2  | 6:A:317:CLA:HAB  | 1.82                     | 0.44              |
| 1:C:61:MET:HE3   | 1:C:173:GLY:N    | 2.32                     | 0.44              |
| 5:D:306:CHL:H172 | 5:D:306:CHL:H13  | 1.44                     | 0.44              |
| 7:F:318:LHG:H182 | 7:F:318:LHG:H151 | 1.72                     | 0.44              |
| 3:B:303:NEX:H362 | 6:B:309:CLA:HAB  | 1.99                     | 0.44              |
| 5:B:312:CHL:H101 | 5:B:314:CHL:H152 | 2.00                     | 0.44              |
| 6:C:317:CLA:H2   | 6:C:317:CLA:H61  | 1.66                     | 0.44              |
| 1:D:60:ALA:O     | 1:D:64:THR:HG23  | 2.17                     | 0.44              |
| 1:D:146:PRO:HG3  | 5:D:312:CHL:HMD2 | 1.98                     | 0.44              |
| 5:E:305:CHL:H41  | 6:E:306:CLA:HBA1 | 1.99                     | 0.44              |
| 1:F:69:THR:HB    | 1:F:70:PRO:HD3   | 1.98                     | 0.44              |
| 1:A:116:ILE:HD13 | 5:A:310:CHL:HMD3 | 1.99                     | 0.44              |
| 1:A:130:TYR:HE1  | 4:A:304:LMU:H6D  | 1.82                     | 0.44              |
| 1:B:178:PHE:HD1  | 5:B:307:CHL:H191 | 1.83                     | 0.44              |
| 1:C:132:CYS:SG   | 12:C:405:HOH:O   | 2.62                     | 0.44              |
| 1:E:107:LEU:O    | 1:E:109:HIS:N    | 2.51                     | 0.44              |
| 1:C:162:PHE:CZ   | 6:C:314:CLA:HED3 | 2.52                     | 0.44              |
| 1:D:92:GLN:HG3   | 1:D:99:LEU:HD13  | 1.99                     | 0.44              |
| 6:A:314:CLA:H43  | 6:A:316:CLA:HBA1 | 1.99                     | 0.44              |
| 7:F:318:LHG:H223 | 7:F:318:LHG:H191 | 1.75                     | 0.44              |
| 1:C:181:PHE:HD1  | 6:C:307:CLA:HBB2 | 1.83                     | 0.44              |
| 5:D:313:CHL:HBB1 | 5:F:304:CHL:H52  | 2.00                     | 0.44              |
| 6:E:314:CLA:HBD  | 6:E:315:CLA:OBD  | 2.18                     | 0.44              |
| 5:E:304:CHL:H202 | 5:E:304:CHL:H161 | 1.64                     | 0.44              |
| 3:D:303:NEX:H191 | 3:D:303:NEX:H11  | 1.70                     | 0.44              |
| 1:E:61:MET:SD    | 6:E:313:CLA:HHC  | 2.58                     | 0.44              |
| 6:B:317:CLA:HMC1 | 9:B:325:OUR:C46  | 2.48                     | 0.43              |
| 2:C:301:OIE:C7   | 6:C:307:CLA:HMC2 | 2.48                     | 0.43              |
| 5:C:312:CHL:HHC  | 5:C:312:CHL:HMC  | 1.53                     | 0.43              |
| 6:B:308:CLA:H12  | 1:C:39:LEU:HD11  | 2.00                     | 0.43              |
| 5:B:319:CHL:HHC  | 5:B:319:CHL:HMC  | 1.77                     | 0.43              |
| 4:E:319:LMU:H101 | 4:E:319:LMU:H71  | 1.67                     | 0.43              |
| 1:A:171:LYS:NZ   | 7:A:319:LHG:O4   | 2.52                     | 0.43              |
| 1:C:9:ALA:HB1    | 5:C:305:CHL:HBC1 | 2.01                     | 0.43              |
| 1:A:135:GLY:HA2  | 4:A:304:LMU:H12  | 2.00                     | 0.43              |
| 5:B:307:CHL:H41  | 6:B:308:CLA:HBA1 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:B:324:LHG:H261 | 7:B:324:LHG:H292 | 1.35                     | 0.43              |
| 1:C:128:GLU:HG3  | 5:C:313:CHL:NB   | 2.33                     | 0.43              |
| 1:F:115:ALA:HB3  | 5:F:308:CHL:HMC  | 1.99                     | 0.43              |
| 1:A:101:TYR:CE2  | 6:A:308:CLA:H2   | 2.54                     | 0.43              |
| 5:A:306:CHL:H111 | 6:C:307:CLA:H121 | 2.01                     | 0.43              |
| 1:D:69:THR:HB    | 1:D:70:PRO:HD3   | 2.01                     | 0.43              |
| 1:E:178:PHE:HZ   | 7:E:318:LHG:H142 | 1.83                     | 0.43              |
| 1:F:53:GLU:HB2   | 5:F:305:CHL:C1B  | 2.49                     | 0.43              |
| 1:A:178:PHE:CE2  | 6:A:317:CLA:HAB  | 2.54                     | 0.43              |
| 3:C:303:NEX:H31  | 3:C:303:NEX:H28  | 1.93                     | 0.43              |
| 1:E:179:ALA:HB1  | 9:E:320:OUR:O42  | 2.18                     | 0.43              |
| 5:B:311:CHL:HAC2 | 5:B:311:CHL:HMC  | 1.58                     | 0.43              |
| 1:D:61:MET:SD    | 6:D:314:CLA:HAB  | 2.59                     | 0.43              |
| 1:D:181:PHE:HD2  | 6:D:317:CLA:HMC1 | 1.83                     | 0.43              |
| 1:E:116:ILE:HG12 | 5:E:308:CHL:HAC1 | 2.01                     | 0.43              |
| 1:A:162:PHE:CZ   | 1:A:166:LYS:HE3  | 2.54                     | 0.43              |
| 1:A:182:GLY:O    | 1:A:186:GLN:HB2  | 2.18                     | 0.43              |
| 5:C:306:CHL:H93  | 6:C:307:CLA:HMA1 | 2.00                     | 0.43              |
| 5:D:305:CHL:H41  | 5:D:305:CHL:H61  | 1.47                     | 0.43              |
| 3:A:303:NEX:H241 | 6:A:308:CLA:C2   | 2.48                     | 0.42              |
| 5:B:312:CHL:HMC  | 5:B:312:CHL:HHC  | 1.63                     | 0.42              |
| 1:C:152:PRO:HD2  | 9:C:321:OUR:O40  | 2.18                     | 0.42              |
| 1:D:210:GLY:HA2  | 6:D:317:CLA:CAD  | 2.49                     | 0.42              |
| 5:E:310:CHL:H62  | 5:E:312:CHL:H192 | 2.01                     | 0.42              |
| 3:A:303:NEX:H201 | 3:A:303:NEX:H15  | 1.62                     | 0.42              |
| 1:B:128:GLU:HG3  | 5:B:314:CHL:NB   | 2.34                     | 0.42              |
| 1:C:186:GLN:HE21 | 1:C:197:CYS:HB3  | 1.84                     | 0.42              |
| 5:C:306:CHL:C9   | 6:C:307:CLA:HMA1 | 2.49                     | 0.42              |
| 6:D:316:CLA:O1A  | 6:D:316:CLA:H2A  | 2.18                     | 0.42              |
| 6:D:317:CLA:H143 | 6:D:317:CLA:H161 | 1.89                     | 0.42              |
| 1:E:150:PHE:CE1  | 5:E:311:CHL:H92  | 2.55                     | 0.42              |
| 1:F:162:PHE:CZ   | 1:F:166:LYS:HE3  | 2.53                     | 0.42              |
| 6:B:318:CLA:HMB1 | 7:B:320:LHG:H341 | 2.00                     | 0.42              |
| 2:C:302:OIE:C15  | 7:C:319:LHG:H111 | 2.50                     | 0.42              |
| 6:A:307:CLA:HBB1 | 5:A:313:CHL:H161 | 2.01                     | 0.42              |
| 5:B:314:CHL:HMC  | 5:B:314:CHL:HHC  | 1.75                     | 0.42              |
| 1:C:158:ASP:HB3  | 1:C:161:THR:OG1  | 2.19                     | 0.42              |
| 1:E:59:TRP:HE1   | 5:E:311:CHL:HED2 | 1.84                     | 0.42              |
| 5:B:311:CHL:CAB  | 5:B:312:CHL:HMC  | 2.45                     | 0.42              |
| 3:E:303:NEX:H35  | 3:E:303:NEX:H401 | 1.42                     | 0.42              |
| 1:B:59:TRP:CD1   | 5:B:314:CHL:HMD3 | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2:GLU:O       | 1:C:9:ALA:N       | 2.50                     | 0.42              |
| 1:D:90:GLY:HA2    | 5:D:310:CHL:HAC2  | 2.02                     | 0.42              |
| 1:E:53:GLU:OE2    | 1:E:174:ARG:NE    | 2.46                     | 0.42              |
| 1:A:9:ALA:HB1     | 5:A:305:CHL:CBC   | 2.49                     | 0.42              |
| 5:A:310:CHL:HBB2  | 5:A:311:CHL:CBB   | 2.49                     | 0.42              |
| 3:B:303:NEX:H191  | 3:B:303:NEX:H11   | 1.73                     | 0.42              |
| 3:C:303:NEX:H15   | 3:C:303:NEX:H201  | 1.57                     | 0.42              |
| 5:D:306:CHL:H122  | 5:D:306:CHL:H8    | 1.55                     | 0.42              |
| 7:A:319:LHG:H341  | 7:A:319:LHG:H312  | 1.91                     | 0.42              |
| 6:B:308:CLA:H51   | 5:C:306:CHL:H91   | 2.01                     | 0.42              |
| 5:B:312:CHL:H151  | 5:B:312:CHL:HAB   | 2.01                     | 0.42              |
| 6:C:307:CLA:HMC3  | 5:C:311:CHL:H91   | 2.01                     | 0.42              |
| 1:E:210:GLY:HA2   | 6:E:316:CLA:CAD   | 2.50                     | 0.42              |
| 6:E:314:CLA:H112  | 6:E:314:CLA:H142  | 1.76                     | 0.42              |
| 1:F:81:PHE:CD2    | 6:F:307:CLA:HED3  | 2.55                     | 0.42              |
| 1:A:54:LEU:HD23   | 1:A:144:LEU:HB3   | 2.02                     | 0.42              |
| 1:B:69:THR:HB     | 1:B:70:PRO:HD3    | 2.01                     | 0.42              |
| 1:B:210:GLY:HA2   | 6:B:318:CLA:OBD   | 2.20                     | 0.42              |
| 5:C:313:CHL:H91   | 5:C:313:CHL:H112  | 1.77                     | 0.42              |
| 11:F:319:LMG:HC92 | 11:F:319:LMG:H291 | 1.70                     | 0.42              |
| 1:A:217:PHE:HB2   | 5:C:311:CHL:O1A   | 2.20                     | 0.42              |
| 5:B:312:CHL:H122  | 5:B:312:CHL:H8    | 1.83                     | 0.42              |
| 1:C:69:THR:HB     | 1:C:70:PRO:HD3    | 2.02                     | 0.42              |
| 1:D:39:LEU:HD12   | 5:D:306:CHL:H11   | 2.02                     | 0.42              |
| 1:D:178:PHE:HE1   | 5:D:306:CHL:H191  | 1.85                     | 0.42              |
| 5:D:313:CHL:CHC   | 5:F:304:CHL:H52   | 2.50                     | 0.42              |
| 6:B:316:CLA:H112  | 6:B:316:CLA:H151  | 1.82                     | 0.41              |
| 1:E:62:LEU:HB3    | 6:E:307:CLA:HAB   | 2.02                     | 0.41              |
| 1:E:189:GLN:HG3   | 1:E:213:TYR:HB2   | 2.02                     | 0.41              |
| 1:F:152:PRO:HD2   | 9:F:320:OUR:C30   | 2.50                     | 0.41              |
| 6:F:316:CLA:H2    | 6:F:316:CLA:H61   | 1.74                     | 0.41              |
| 1:A:128:GLU:OE2   | 1:A:131:ARG:NH1   | 2.53                     | 0.41              |
| 5:A:305:CHL:H202  | 5:A:305:CHL:H161  | 1.67                     | 0.41              |
| 5:A:305:CHL:H3A   | 5:A:305:CHL:HBA1  | 1.56                     | 0.41              |
| 1:B:147:GLY:HA3   | 6:B:315:CLA:CED   | 2.50                     | 0.41              |
| 1:D:107:LEU:O     | 1:D:109:HIS:N     | 2.53                     | 0.41              |
| 1:E:60:ALA:O      | 1:E:64:THR:HG23   | 2.21                     | 0.41              |
| 1:F:168:LYS:HD3   | 6:F:315:CLA:HAA2  | 2.03                     | 0.41              |
| 1:A:42:ASP:OD2    | 7:B:324:LHG:C4    | 2.61                     | 0.41              |
| 1:A:98:GLY:HA3    | 1:A:110:ALA:O     | 2.19                     | 0.41              |
| 1:A:115:ALA:O     | 1:A:119:THR:OG1   | 2.30                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:302:OIE:C8   | 5:C:305:CHL:H91  | 2.50                     | 0.41              |
| 6:D:315:CLA:H112 | 6:D:315:CLA:H151 | 1.79                     | 0.41              |
| 3:E:303:NEX:H11  | 3:E:303:NEX:H191 | 1.68                     | 0.41              |
| 6:E:313:CLA:H72  | 9:E:320:OUR:C15  | 2.50                     | 0.41              |
| 1:A:120:GLN:HE22 | 5:A:311:CHL:CMC  | 2.32                     | 0.41              |
| 1:B:137:LEU:CD1  | 5:B:313:CHL:HAB  | 2.51                     | 0.41              |
| 5:E:305:CHL:H161 | 5:E:305:CHL:H141 | 1.81                     | 0.41              |
| 5:E:317:CHL:HAB  | 5:E:317:CHL:HMB1 | 1.93                     | 0.41              |
| 1:A:101:TYR:HB3  | 1:A:107:LEU:HB3  | 2.03                     | 0.41              |
| 3:B:303:NEX:H12  | 4:B:304:LMU:H82  | 2.03                     | 0.41              |
| 6:B:318:CLA:H111 | 6:B:318:CLA:H91  | 1.69                     | 0.41              |
| 1:D:168:LYS:HD3  | 6:D:316:CLA:HAA2 | 2.02                     | 0.41              |
| 1:E:69:THR:HB    | 1:E:70:PRO:HD3   | 2.02                     | 0.41              |
| 1:E:87:PHE:O     | 5:E:310:CHL:HED3 | 2.19                     | 0.41              |
| 5:E:304:CHL:HAC1 | 7:E:318:LHG:HC32 | 2.02                     | 0.41              |
| 1:A:75:LYS:HB2   | 1:A:75:LYS:HE3   | 1.66                     | 0.41              |
| 1:B:73:LEU:HD12  | 1:B:73:LEU:HA    | 1.90                     | 0.41              |
| 7:B:324:LHG:H262 | 1:F:21:PRO:HA    | 2.01                     | 0.41              |
| 1:C:197:CYS:HB3  | 6:C:317:CLA:O1D  | 2.20                     | 0.41              |
| 1:C:168:LYS:HD3  | 6:C:316:CLA:HAA2 | 2.03                     | 0.41              |
| 5:A:318:CHL:HMA2 | 1:C:114:LEU:HD13 | 2.03                     | 0.41              |
| 1:B:87:PHE:O     | 5:B:312:CHL:HED3 | 2.21                     | 0.41              |
| 1:E:58:ARG:HG2   | 1:E:58:ARG:H     | 1.67                     | 0.41              |
| 1:A:120:GLN:OE1  | 5:A:311:CHL:HMC  | 2.21                     | 0.41              |
| 6:A:315:CLA:HBD  | 6:A:316:CLA:OBD  | 2.21                     | 0.41              |
| 1:B:170:ILE:HD12 | 1:B:170:ILE:HA   | 1.89                     | 0.41              |
| 1:C:189:GLN:HG3  | 1:C:213:TYR:HB2  | 2.03                     | 0.41              |
| 5:C:311:CHL:H91  | 5:C:311:CHL:H112 | 1.77                     | 0.41              |
| 6:D:317:CLA:H61  | 6:D:317:CLA:H101 | 1.86                     | 0.41              |
| 1:E:52:LEU:HD23  | 5:E:312:CHL:OBD  | 2.21                     | 0.41              |
| 1:E:120:GLN:HE21 | 5:E:312:CHL:CMC  | 2.34                     | 0.41              |
| 5:F:312:CHL:HMB1 | 5:F:312:CHL:HAB  | 1.82                     | 0.41              |
| 5:F:317:CHL:HMC  | 5:F:317:CHL:HHC  | 1.85                     | 0.41              |
| 6:A:315:CLA:H142 | 6:A:315:CLA:H112 | 1.75                     | 0.41              |
| 5:D:311:CHL:H61  | 5:D:311:CHL:H2   | 1.80                     | 0.41              |
| 3:E:303:NEX:C31  | 5:E:309:CHL:H3A  | 2.51                     | 0.41              |
| 6:F:306:CLA:HBB1 | 5:F:312:CHL:H162 | 2.03                     | 0.41              |
| 1:A:107:LEU:O    | 1:A:109:HIS:N    | 2.54                     | 0.40              |
| 1:E:218:PHE:N    | 2:E:302:OIE:O40  | 2.51                     | 0.40              |
| 1:A:40:SER:HB3   | 1:A:46:PHE:CD1   | 2.56                     | 0.40              |
| 5:A:306:CHL:H62  | 5:A:306:CHL:H41  | 1.86                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:A:314:CLA:O1D  | 6:A:314:CLA:H2A  | 2.20                     | 0.40              |
| 6:C:315:CLA:H151 | 6:C:316:CLA:CBB  | 2.51                     | 0.40              |
| 6:D:315:CLA:HAC1 | 7:D:319:LHG:H301 | 2.02                     | 0.40              |
| 1:E:210:GLY:HA2  | 6:E:316:CLA:OBD  | 2.21                     | 0.40              |
| 1:F:81:PHE:HB2   | 1:F:84:ALA:HB2   | 2.04                     | 0.40              |
| 1:B:146:PRO:HD2  | 6:B:315:CLA:OBD  | 2.21                     | 0.40              |
| 7:A:319:LHG:H272 | 7:A:319:LHG:H242 | 1.77                     | 0.40              |
| 1:B:27:GLU:CD    | 1:F:27:GLU:HB2   | 2.41                     | 0.40              |
| 1:C:168:LYS:NZ   | 6:C:316:CLA:O1A  | 2.44                     | 0.40              |
| 5:D:310:CHL:HAA2 | 5:D:310:CHL:CBD  | 2.52                     | 0.40              |
| 5:F:310:CHL:H41  | 5:F:310:CHL:H62  | 1.83                     | 0.40              |
| 6:B:308:CLA:H162 | 6:B:308:CLA:H122 | 1.60                     | 0.40              |
| 1:C:178:PHE:CD2  | 7:C:319:LHG:H291 | 2.56                     | 0.40              |
| 1:E:217:PHE:CE1  | 5:F:310:CHL:H2   | 2.56                     | 0.40              |
| 6:E:316:CLA:HBB2 | 7:E:318:LHG:H311 | 2.03                     | 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|---------|----------|-------------|----|
| 1   | A     | 221/249 (89%)   | 213 (96%)  | 7 (3%)  | 1 (0%)   | 29          | 52 |
| 1   | B     | 221/249 (89%)   | 213 (96%)  | 6 (3%)  | 2 (1%)   | 17          | 35 |
| 1   | C     | 220/249 (88%)   | 212 (96%)  | 7 (3%)  | 1 (0%)   | 29          | 52 |
| 1   | D     | 221/249 (89%)   | 214 (97%)  | 6 (3%)  | 1 (0%)   | 29          | 52 |
| 1   | E     | 221/249 (89%)   | 211 (96%)  | 7 (3%)  | 3 (1%)   | 11          | 22 |
| 1   | F     | 221/249 (89%)   | 214 (97%)  | 5 (2%)  | 2 (1%)   | 17          | 35 |
| All | All   | 1325/1494 (89%) | 1277 (96%) | 38 (3%) | 10 (1%)  | 19          | 39 |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 17  | GLU  |
| 1   | F     | 27  | GLU  |
| 1   | B     | 17  | GLU  |
| 1   | C     | 108 | VAL  |
| 1   | E     | 92  | GLN  |
| 1   | E     | 108 | VAL  |
| 1   | A     | 108 | VAL  |
| 1   | B     | 108 | VAL  |
| 1   | F     | 108 | VAL  |
| 1   | D     | 108 | VAL  |

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A     | 160/184 (87%)  | 158 (99%) | 2 (1%)   | 69          | 86 |
| 1   | B     | 159/184 (86%)  | 155 (98%) | 4 (2%)   | 47          | 73 |
| 1   | C     | 156/184 (85%)  | 155 (99%) | 1 (1%)   | 86          | 95 |
| 1   | D     | 163/184 (89%)  | 161 (99%) | 2 (1%)   | 71          | 87 |
| 1   | E     | 162/184 (88%)  | 160 (99%) | 2 (1%)   | 71          | 87 |
| 1   | F     | 163/184 (89%)  | 160 (98%) | 3 (2%)   | 59          | 80 |
| All | All   | 963/1104 (87%) | 949 (98%) | 14 (2%)  | 65          | 83 |

All (14) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 141 | THR  |
| 1   | A     | 222 | ILE  |
| 1   | B     | 73  | LEU  |
| 1   | B     | 96  | GLU  |
| 1   | B     | 99  | LEU  |
| 1   | B     | 141 | THR  |
| 1   | C     | 141 | THR  |
| 1   | D     | 75  | LYS  |
| 1   | D     | 160 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 58  | ARG  |
| 1   | E     | 73  | LEU  |
| 1   | F     | 7   | ASP  |
| 1   | F     | 99  | LEU  |
| 1   | F     | 141 | THR  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 186 | GLN  |
| 1   | E     | 92  | GLN  |
| 1   | F     | 49  | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 129 ligands modelled in this entry, 3 are monoatomic - leaving 126 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | LMU  | B     | 304 | -    | 34,34,36     | 0.39 | 0           | 42,44,47    | 1.07 | 3 (7%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | NEX  | A     | 303 | -    | 38,46,46     | 0.96 | 2 (5%)   | 50,70,70    | 4.90 | 19 (38%) |
| 5   | CHL  | C     | 309 | 1    | 42,50,74     | 3.27 | 17 (40%) | 44,85,114   | 3.37 | 24 (54%) |
| 5   | CHL  | B     | 310 | 1    | 43,51,74     | 3.21 | 17 (39%) | 45,86,114   | 3.54 | 22 (48%) |
| 5   | CHL  | A     | 312 | 12   | 56,64,74     | 2.82 | 19 (33%) | 61,102,114  | 2.98 | 28 (45%) |
| 9   | OUR  | E     | 320 | -    | 50,53,58     | 0.99 | 1 (2%)   | 58,72,77    | 2.05 | 19 (32%) |
| 6   | CLA  | D     | 314 | 1    | 58,66,73     | 1.56 | 11 (18%) | 67,104,113  | 1.54 | 12 (17%) |
| 5   | CHL  | C     | 305 | 1    | 66,74,74     | 2.57 | 20 (30%) | 73,114,114  | 2.74 | 26 (35%) |
| 5   | CHL  | D     | 312 | 12   | 57,65,74     | 2.74 | 19 (33%) | 62,103,114  | 2.67 | 28 (45%) |
| 9   | OUR  | B     | 325 | -    | 50,53,58     | 1.01 | 2 (4%)   | 58,72,77    | 2.09 | 18 (31%) |
| 6   | CLA  | F     | 307 | 12   | 46,54,73     | 1.74 | 5 (10%)  | 53,90,113   | 1.60 | 7 (13%)  |
| 6   | CLA  | D     | 317 | 1    | 65,73,73     | 1.50 | 7 (10%)  | 76,113,113  | 1.36 | 8 (10%)  |
| 5   | CHL  | B     | 313 | 12   | 57,65,74     | 2.73 | 19 (33%) | 62,103,114  | 3.39 | 26 (41%) |
| 5   | CHL  | C     | 313 | 1    | 66,74,74     | 2.49 | 18 (27%) | 73,114,114  | 2.45 | 25 (34%) |
| 6   | CLA  | C     | 314 | 1    | 53,61,73     | 1.66 | 5 (9%)   | 61,98,113   | 1.56 | 10 (16%) |
| 5   | CHL  | D     | 309 | 1    | 42,50,74     | 3.31 | 18 (42%) | 44,85,114   | 5.62 | 27 (61%) |
| 9   | OUR  | B     | 302 | -    | 48,51,58     | 1.14 | 3 (6%)   | 56,70,77    | 2.80 | 19 (33%) |
| 5   | CHL  | C     | 318 | -    | 44,52,74     | 3.23 | 18 (40%) | 46,87,114   | 3.82 | 23 (50%) |
| 5   | CHL  | C     | 311 | 12   | 61,69,74     | 3.18 | 19 (31%) | 67,108,114  | 2.76 | 27 (40%) |
| 5   | CHL  | B     | 312 | 12   | 62,70,74     | 2.89 | 18 (29%) | 68,109,114  | 2.76 | 28 (41%) |
| 6   | CLA  | D     | 307 | -    | 65,73,73     | 1.47 | 5 (7%)   | 76,113,113  | 1.44 | 7 (9%)   |
| 5   | CHL  | E     | 311 | 12   | 56,64,74     | 2.82 | 19 (33%) | 61,102,114  | 2.85 | 27 (44%) |
| 5   | CHL  | D     | 313 | 1    | 66,74,74     | 2.60 | 16 (24%) | 73,114,114  | 2.45 | 26 (35%) |
| 5   | CHL  | E     | 305 | 1    | 64,72,74     | 2.42 | 18 (28%) | 70,111,114  | 2.33 | 27 (38%) |
| 5   | CHL  | B     | 306 | 1    | 66,74,74     | 2.75 | 18 (27%) | 73,114,114  | 3.60 | 28 (38%) |
| 6   | CLA  | A     | 314 | 1    | 55,63,73     | 1.58 | 12 (21%) | 64,101,113  | 1.68 | 14 (21%) |
| 6   | CLA  | F     | 306 | -    | 65,73,73     | 1.51 | 5 (7%)   | 76,113,113  | 1.41 | 7 (9%)   |
| 5   | CHL  | A     | 318 | -    | 42,50,74     | 3.39 | 19 (45%) | 44,85,114   | 3.03 | 24 (54%) |
| 6   | CLA  | A     | 308 | 12   | 50,58,73     | 1.72 | 5 (10%)  | 58,95,113   | 1.58 | 8 (13%)  |
| 6   | CLA  | B     | 316 | 7    | 65,73,73     | 1.53 | 5 (7%)   | 76,113,113  | 1.42 | 9 (11%)  |
| 9   | OUR  | C     | 321 | -    | 50,53,58     | 0.97 | 1 (2%)   | 58,72,77    | 1.98 | 16 (27%) |
| 6   | CLA  | E     | 306 | -    | 65,73,73     | 1.53 | 5 (7%)   | 76,113,113  | 1.39 | 10 (13%) |
| 7   | LHG  | E     | 318 | 6    | 40,40,48     | 0.67 | 1 (2%)   | 43,46,54    | 1.30 | 6 (13%)  |
| 3   | NEX  | C     | 303 | -    | 38,46,46     | 0.96 | 1 (2%)   | 50,70,70    | 6.57 | 19 (38%) |
| 5   | CHL  | F     | 311 | 12   | 56,64,74     | 2.60 | 20 (35%) | 61,102,114  | 3.72 | 27 (44%) |
| 9   | OUR  | A     | 322 | -    | 50,53,58     | 1.01 | 2 (4%)   | 58,72,77    | 2.10 | 21 (36%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 7   | LHG  | F     | 318 | 6    | 44,44,48     | 0.67 | 1 (2%)   | 47,50,54    | 1.33 | 8 (17%)  |
| 6   | CLA  | E     | 316 | 1    | 55,63,73     | 1.61 | 6 (10%)  | 63,100,113  | 1.47 | 7 (11%)  |
| 6   | CLA  | A     | 307 | -    | 65,73,73     | 1.49 | 5 (7%)   | 76,113,113  | 1.37 | 8 (10%)  |
| 6   | CLA  | A     | 317 | 1    | 55,63,73     | 1.67 | 6 (10%)  | 63,100,113  | 1.45 | 9 (14%)  |
| 9   | OUR  | D     | 321 | -    | 50,53,58     | 0.88 | 1 (2%)   | 58,72,77    | 1.92 | 14 (24%) |
| 5   | CHL  | A     | 309 | 1    | 43,51,74     | 3.24 | 17 (39%) | 45,86,114   | 3.71 | 24 (53%) |
| 7   | LHG  | B     | 324 | -    | 30,30,48     | 1.18 | 2 (6%)   | 33,36,54    | 1.40 | 4 (12%)  |
| 5   | CHL  | F     | 305 | 1    | 66,74,74     | 2.15 | 16 (24%) | 73,114,114  | 3.24 | 31 (42%) |
| 6   | CLA  | B     | 309 | 12   | 46,54,73     | 1.82 | 6 (13%)  | 53,90,113   | 1.57 | 7 (13%)  |
| 6   | CLA  | E     | 315 | 1    | 45,53,73     | 1.75 | 6 (13%)  | 52,89,113   | 1.57 | 6 (11%)  |
| 2   | OIE  | E     | 302 | -    | 42,45,45     | 1.49 | 5 (11%)  | 49,63,63    | 1.76 | 9 (18%)  |
| 5   | CHL  | E     | 312 | 1    | 66,74,74     | 2.50 | 18 (27%) | 73,114,114  | 3.00 | 29 (39%) |
| 5   | CHL  | B     | 319 | -    | 47,55,74     | 3.24 | 19 (40%) | 50,91,114   | 4.04 | 24 (48%) |
| 6   | CLA  | B     | 308 | -    | 65,73,73     | 1.50 | 6 (9%)   | 76,113,113  | 1.47 | 9 (11%)  |
| 5   | CHL  | D     | 306 | 1    | 65,73,74     | 2.29 | 16 (24%) | 71,112,114  | 2.83 | 30 (42%) |
| 6   | CLA  | F     | 316 | -    | 56,64,73     | 1.60 | 6 (10%)  | 65,102,113  | 1.48 | 7 (10%)  |
| 11  | LMG  | B     | 323 | -    | 30,30,55     | 1.05 | 0        | 38,38,63    | 1.12 | 5 (13%)  |
| 6   | CLA  | E     | 313 | 1    | 55,63,73     | 1.60 | 5 (9%)   | 64,101,113  | 1.46 | 8 (12%)  |
| 2   | OIE  | F     | 301 | -    | 42,45,45     | 1.44 | 6 (14%)  | 49,63,63    | 1.74 | 10 (20%) |
| 6   | CLA  | C     | 315 | 7    | 65,73,73     | 1.50 | 5 (7%)   | 76,113,113  | 1.39 | 9 (11%)  |
| 6   | CLA  | D     | 316 | 1    | 45,53,73     | 1.80 | 7 (15%)  | 52,89,113   | 1.62 | 7 (13%)  |
| 2   | OIE  | C     | 302 | -    | 42,45,45     | 1.45 | 6 (14%)  | 49,63,63    | 1.67 | 9 (18%)  |
| 11  | LMG  | F     | 319 | -    | 30,30,55     | 0.93 | 0        | 38,38,63    | 1.21 | 3 (7%)   |
| 2   | OIE  | B     | 301 | -    | 42,45,45     | 1.41 | 6 (14%)  | 49,63,63    | 1.70 | 9 (18%)  |
| 5   | CHL  | A     | 306 | 1    | 64,72,74     | 2.35 | 17 (26%) | 70,111,114  | 2.57 | 29 (41%) |
| 5   | CHL  | A     | 311 | 12   | 61,69,74     | 2.90 | 18 (29%) | 66,107,114  | 3.78 | 30 (45%) |
| 6   | CLA  | B     | 317 | 1    | 45,53,73     | 1.79 | 8 (17%)  | 52,89,113   | 1.59 | 7 (13%)  |
| 5   | CHL  | E     | 317 | -    | 40,49,74     | 3.39 | 17 (42%) | 42,83,114   | 5.25 | 22 (52%) |
| 6   | CLA  | D     | 315 | 7    | 65,73,73     | 1.51 | 6 (9%)   | 76,113,113  | 1.36 | 9 (11%)  |
| 5   | CHL  | A     | 313 | 1    | 66,74,74     | 2.47 | 18 (27%) | 73,114,114  | 2.30 | 23 (31%) |
| 3   | NEX  | E     | 303 | -    | 38,46,46     | 0.94 | 1 (2%)   | 50,70,70    | 6.17 | 19 (38%) |
| 6   | CLA  | F     | 315 | 1    | 45,53,73     | 1.78 | 6 (13%)  | 52,89,113   | 1.64 | 7 (13%)  |
| 3   | NEX  | F     | 303 | -    | 38,46,46     | 0.96 | 1 (2%)   | 50,70,70    | 6.25 | 22 (44%) |
| 5   | CHL  | F     | 312 | 1    | 66,74,74     | 2.27 | 18 (27%) | 73,114,114  | 2.31 | 27 (36%) |
| 5   | CHL  | D     | 318 | -    | 46,54,74     | 3.23 | 19 (41%) | 49,90,114   | 3.02 | 23 (46%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | OIE  | C     | 301 | -    | 42,45,45     | 1.47 | 6 (14%)  | 49,63,63    | 1.71 | 9 (18%)  |
| 7   | LHG  | B     | 320 | 6    | 45,45,48     | 0.67 | 1 (2%)   | 48,51,54    | 1.30 | 6 (12%)  |
| 3   | NEX  | B     | 303 | -    | 38,46,46     | 0.94 | 2 (5%)   | 50,70,70    | 5.77 | 22 (44%) |
| 7   | LHG  | C     | 304 | -    | 24,24,48     | 0.87 | 0        | 27,30,54    | 1.22 | 2 (7%)   |
| 6   | CLA  | E     | 314 | 7    | 63,71,73     | 1.57 | 5 (7%)   | 73,110,113  | 1.38 | 8 (10%)  |
| 6   | CLA  | F     | 313 | 1    | 58,66,73     | 1.52 | 12 (20%) | 67,104,113  | 1.71 | 12 (17%) |
| 5   | CHL  | D     | 305 | 1    | 66,74,74     | 2.97 | 19 (28%) | 73,114,114  | 2.66 | 26 (35%) |
| 6   | CLA  | E     | 307 | -    | 50,58,73     | 1.69 | 6 (12%)  | 58,95,113   | 1.65 | 9 (15%)  |
| 6   | CLA  | C     | 307 | -    | 65,73,73     | 1.48 | 6 (9%)   | 76,113,113  | 1.49 | 9 (11%)  |
| 5   | CHL  | B     | 311 | -    | 51,59,74     | 3.09 | 19 (37%) | 55,96,114   | 5.12 | 29 (52%) |
| 2   | OIE  | E     | 301 | -    | 42,45,45     | 1.46 | 5 (11%)  | 49,63,63    | 1.79 | 10 (20%) |
| 5   | CHL  | E     | 309 | -    | 43,51,74     | 3.29 | 17 (39%) | 45,86,114   | 5.92 | 24 (53%) |
| 5   | CHL  | F     | 309 | -    | 42,50,74     | 3.60 | 18 (42%) | 44,85,114   | 3.43 | 26 (59%) |
| 5   | CHL  | E     | 310 | -    | 61,69,74     | 3.03 | 18 (29%) | 66,107,114  | 2.85 | 26 (39%) |
| 5   | CHL  | F     | 317 | -    | 46,54,74     | 3.43 | 19 (41%) | 49,90,114   | 3.54 | 26 (53%) |
| 6   | CLA  | C     | 316 | 1    | 45,53,73     | 1.78 | 6 (13%)  | 52,89,113   | 1.59 | 6 (11%)  |
| 10  | BET  | B     | 322 | -    | 7,7,7        | 1.02 | 0        | 10,10,10    | 0.87 | 1 (10%)  |
| 5   | CHL  | D     | 311 | -    | 62,70,74     | 2.99 | 20 (32%) | 68,109,114  | 2.92 | 30 (44%) |
| 5   | CHL  | A     | 305 | 1    | 66,74,74     | 2.73 | 18 (27%) | 73,114,114  | 3.24 | 31 (42%) |
| 6   | CLA  | A     | 316 | 1    | 45,53,73     | 1.81 | 6 (13%)  | 52,89,113   | 1.62 | 7 (13%)  |
| 6   | CLA  | C     | 317 | -    | 56,64,73     | 1.57 | 11 (19%) | 65,102,113  | 1.53 | 10 (15%) |
| 5   | CHL  | C     | 306 | 1    | 66,74,74     | 2.38 | 18 (27%) | 73,114,114  | 2.73 | 30 (41%) |
| 5   | CHL  | C     | 310 | -    | 44,52,74     | 3.20 | 18 (40%) | 46,87,114   | 3.01 | 20 (43%) |
| 2   | OIE  | A     | 301 | -    | 42,45,45     | 1.50 | 10 (23%) | 49,63,63    | 2.07 | 13 (26%) |
| 6   | CLA  | B     | 315 | 1    | 58,66,73     | 1.57 | 12 (20%) | 67,104,113  | 1.75 | 13 (19%) |
| 7   | LHG  | D     | 319 | 6    | 45,45,48     | 0.69 | 1 (2%)   | 48,51,54    | 1.28 | 7 (14%)  |
| 4   | LMU  | D     | 304 | -    | 36,36,36     | 0.50 | 0        | 47,47,47    | 1.19 | 4 (8%)   |
| 5   | CHL  | C     | 312 | 12   | 56,64,74     | 3.04 | 19 (33%) | 61,102,114  | 2.70 | 26 (42%) |
| 5   | CHL  | B     | 307 | 1    | 65,73,74     | 2.22 | 18 (27%) | 71,112,114  | 2.96 | 27 (38%) |
| 3   | NEX  | D     | 303 | -    | 38,46,46     | 0.95 | 2 (5%)   | 50,70,70    | 5.96 | 20 (40%) |
| 6   | CLA  | B     | 318 | 1    | 65,73,73     | 1.47 | 6 (9%)   | 76,113,113  | 1.40 | 8 (10%)  |
| 6   | CLA  | F     | 314 | 7    | 55,63,73     | 1.68 | 5 (9%)   | 64,101,113  | 1.46 | 8 (12%)  |
| 5   | CHL  | A     | 310 | -    | 51,59,74     | 3.18 | 17 (33%) | 55,96,114   | 3.26 | 26 (47%) |
| 4   | LMU  | E     | 319 | -    | 36,36,36     | 0.38 | 0        | 47,47,47    | 0.91 | 1 (2%)   |
| 2   | OIE  | F     | 302 | -    | 42,45,45     | 1.43 | 6 (14%)  | 49,63,63    | 1.71 | 9 (18%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | CHL  | B     | 314 | 1    | 66,74,74     | 2.29 | 18 (27%) | 73,114,114  | 2.54 | 25 (34%) |
| 7   | LHG  | A     | 319 | 6    | 46,46,48     | 0.64 | 1 (2%)   | 49,52,54    | 1.22 | 3 (6%)   |
| 6   | CLA  | D     | 308 | 12   | 46,54,73     | 1.76 | 6 (13%)  | 53,90,113   | 1.58 | 7 (13%)  |
| 4   | LMU  | A     | 304 | -    | 36,36,36     | 0.40 | 0        | 47,47,47    | 0.91 | 1 (2%)   |
| 9   | OUR  | F     | 320 | -    | 50,53,58     | 1.09 | 3 (6%)   | 58,72,77    | 1.89 | 16 (27%) |
| 5   | CHL  | F     | 304 | 1    | 66,74,74     | 2.54 | 18 (27%) | 73,114,114  | 3.38 | 30 (41%) |
| 5   | CHL  | D     | 310 | 12   | 45,53,74     | 3.16 | 17 (37%) | 46,88,114   | 3.18 | 20 (43%) |
| 6   | CLA  | A     | 315 | 7    | 63,71,73     | 1.55 | 6 (9%)   | 73,110,113  | 1.41 | 8 (10%)  |
| 6   | CLA  | C     | 308 | 12   | 46,54,73     | 1.76 | 5 (10%)  | 53,90,113   | 1.57 | 6 (11%)  |
| 10  | BET  | C     | 320 | -    | 7,7,7        | 1.01 | 0        | 10,10,10    | 0.75 | 0        |
| 5   | CHL  | F     | 308 | 1    | 42,50,74     | 3.28 | 18 (42%) | 44,85,114   | 3.85 | 26 (59%) |
| 2   | OIE  | A     | 302 | -    | 42,45,45     | 1.53 | 7 (16%)  | 49,63,63    | 2.04 | 10 (20%) |
| 5   | CHL  | E     | 304 | 1    | 66,74,74     | 2.42 | 18 (27%) | 73,114,114  | 3.63 | 31 (42%) |
| 2   | OIE  | D     | 302 | -    | 42,45,45     | 1.43 | 6 (14%)  | 49,63,63    | 1.68 | 11 (22%) |
| 5   | CHL  | E     | 308 | 1    | 40,49,74     | 3.57 | 18 (45%) | 42,83,114   | 3.07 | 19 (45%) |
| 7   | LHG  | C     | 319 | 6    | 44,44,48     | 0.73 | 1 (2%)   | 47,50,54    | 1.30 | 7 (14%)  |
| 4   | LMU  | B     | 305 | -    | 36,36,36     | 0.38 | 0        | 47,47,47    | 1.09 | 5 (10%)  |
| 2   | OIE  | D     | 301 | -    | 42,45,45     | 1.43 | 5 (11%)  | 49,63,63    | 1.86 | 10 (20%) |
| 10  | BET  | B     | 321 | -    | 7,7,7        | 1.03 | 0        | 10,10,10    | 0.85 | 1 (10%)  |
| 5   | CHL  | F     | 310 | 12   | 61,69,74     | 2.82 | 21 (34%) | 67,108,114  | 3.09 | 25 (37%) |

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   | LMU  | B     | 304 | -    | -         | 9/20/56/61    | 1/2/2/2 |
| 3   | NEX  | A     | 303 | -    | -         | 5/27/83/83    | 0/3/3/3 |
| 5   | CHL  | C     | 309 | 1    | 3/3/15/26 | 4/10/108/137  | -       |
| 5   | CHL  | B     | 310 | 1    | 3/3/15/26 | 6/12/110/137  | -       |
| 5   | CHL  | A     | 312 | 12   | 3/3/18/26 | 7/27/125/137  | -       |
| 9   | OUR  | E     | 320 | -    | -         | 6/42/81/86    | 0/2/2/2 |
| 6   | CLA  | D     | 314 | 1    | 1/1/13/20 | 9/29/107/115  | -       |
| 5   | CHL  | C     | 305 | 1    | 3/3/20/26 | 24/39/137/137 | -       |
| 5   | CHL  | D     | 312 | 12   | 3/3/18/26 | 5/29/127/137  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 9   | OUR  | B     | 325 | -    | -         | 7/42/81/86    | 0/2/2/2 |
| 6   | CLA  | F     | 307 | 12   | 1/1/11/20 | 4/15/93/115   | -       |
| 6   | CLA  | D     | 317 | 1    | 1/1/15/20 | 8/37/115/115  | -       |
| 5   | CHL  | B     | 313 | 12   | 3/3/18/26 | 7/29/127/137  | -       |
| 5   | CHL  | C     | 313 | 1    | 3/3/20/26 | 11/39/137/137 | -       |
| 6   | CLA  | C     | 314 | 1    | 1/1/12/20 | 5/23/101/115  | -       |
| 5   | CHL  | D     | 309 | 1    | 3/3/15/26 | 4/10/108/137  | -       |
| 9   | OUR  | B     | 302 | -    | -         | 16/40/79/86   | 0/2/2/2 |
| 5   | CHL  | C     | 318 | -    | 3/3/15/26 | 4/13/111/137  | -       |
| 5   | CHL  | C     | 311 | 12   | 3/3/19/26 | 15/33/131/137 | -       |
| 5   | CHL  | B     | 312 | 12   | 3/3/19/26 | 9/35/133/137  | -       |
| 6   | CLA  | D     | 307 | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 5   | CHL  | E     | 311 | 12   | 3/3/18/26 | 8/27/125/137  | -       |
| 5   | CHL  | D     | 313 | 1    | 3/3/20/26 | 18/39/137/137 | -       |
| 5   | CHL  | E     | 305 | 1    | 3/3/19/26 | 12/37/135/137 | -       |
| 5   | CHL  | B     | 306 | 1    | 3/3/20/26 | 16/39/137/137 | -       |
| 6   | CLA  | A     | 314 | 1    | 1/1/13/20 | 6/25/103/115  | -       |
| 6   | CLA  | F     | 306 | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 5   | CHL  | A     | 318 | -    | 3/3/15/26 | 5/10/108/137  | -       |
| 6   | CLA  | A     | 308 | 12   | 1/1/12/20 | 6/19/97/115   | -       |
| 6   | CLA  | B     | 316 | 7    | 1/1/15/20 | 6/37/115/115  | -       |
| 9   | OUR  | C     | 321 | -    | -         | 7/42/81/86    | 0/2/2/2 |
| 6   | CLA  | E     | 306 | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 7   | LHG  | E     | 318 | 6    | -         | 15/45/45/53   | -       |
| 3   | NEX  | C     | 303 | -    | -         | 2/27/83/83    | 0/3/3/3 |
| 5   | CHL  | F     | 311 | 12   | 3/3/18/26 | 12/27/125/137 | -       |
| 9   | OUR  | A     | 322 | -    | -         | 8/42/81/86    | 0/2/2/2 |
| 7   | LHG  | F     | 318 | 6    | -         | 23/49/49/53   | -       |
| 6   | CLA  | E     | 316 | 1    | 1/1/12/20 | 7/25/103/115  | -       |
| 6   | CLA  | A     | 307 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 6   | CLA  | A     | 317 | 1    | 1/1/12/20 | 10/25/103/115 | -       |
| 9   | OUR  | D     | 321 | -    | -         | 7/42/81/86    | 0/2/2/2 |
| 5   | CHL  | A     | 309 | 1    | 3/3/15/26 | 6/12/110/137  | -       |
| 7   | LHG  | B     | 324 | -    | -         | 24/35/35/53   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 5   | CHL  | F     | 305 | 1    | 3/3/20/26 | 18/39/137/137 | -       |
| 6   | CLA  | B     | 309 | 12   | 1/1/11/20 | 4/15/93/115   | -       |
| 6   | CLA  | E     | 315 | 1    | 1/1/11/20 | 6/13/91/115   | -       |
| 5   | CHL  | E     | 312 | 1    | 3/3/20/26 | 9/39/137/137  | -       |
| 2   | OIE  | E     | 302 | -    | -         | 12/33/72/72   | 0/2/2/2 |
| 5   | CHL  | B     | 319 | -    | 3/3/16/26 | 5/17/115/137  | -       |
| 6   | CLA  | B     | 308 | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 5   | CHL  | D     | 306 | 1    | 3/3/19/26 | 18/38/136/137 | -       |
| 6   | CLA  | F     | 316 | -    | 1/1/13/20 | 6/27/105/115  | -       |
| 11  | LMG  | B     | 323 | -    | -         | 9/25/45/70    | 0/1/1/1 |
| 6   | CLA  | E     | 313 | 1    | 1/1/13/20 | 4/25/103/115  | -       |
| 2   | OIE  | F     | 301 | -    | -         | 12/33/72/72   | 0/2/2/2 |
| 6   | CLA  | C     | 315 | 7    | 1/1/15/20 | 15/37/115/115 | -       |
| 6   | CLA  | D     | 316 | 1    | 1/1/11/20 | 2/13/91/115   | -       |
| 2   | OIE  | C     | 302 | -    | -         | 14/33/72/72   | 0/2/2/2 |
| 11  | LMG  | F     | 319 | -    | -         | 11/25/45/70   | 0/1/1/1 |
| 2   | OIE  | B     | 301 | -    | -         | 11/33/72/72   | 0/2/2/2 |
| 5   | CHL  | A     | 306 | 1    | 3/3/19/26 | 15/37/135/137 | -       |
| 5   | CHL  | A     | 311 | 12   | 3/3/18/26 | 14/33/131/137 | -       |
| 6   | CLA  | B     | 317 | 1    | 1/1/11/20 | 2/13/91/115   | -       |
| 5   | CHL  | E     | 317 | -    | 3/3/14/26 | 3/10/104/137  | -       |
| 6   | CLA  | D     | 315 | 7    | 1/1/15/20 | 9/37/115/115  | -       |
| 5   | CHL  | A     | 313 | 1    | 3/3/20/26 | 14/39/137/137 | -       |
| 3   | NEX  | E     | 303 | -    | -         | 4/27/83/83    | 0/3/3/3 |
| 6   | CLA  | F     | 315 | 1    | 1/1/11/20 | 4/13/91/115   | -       |
| 3   | NEX  | F     | 303 | -    | -         | 3/27/83/83    | 0/3/3/3 |
| 5   | CHL  | F     | 312 | 1    | 3/3/20/26 | 16/39/137/137 | -       |
| 5   | CHL  | D     | 318 | -    | 3/3/16/26 | 4/15/113/137  | -       |
| 2   | OIE  | C     | 301 | -    | -         | 9/33/72/72    | 0/2/2/2 |
| 7   | LHG  | B     | 320 | 6    | -         | 24/50/50/53   | -       |
| 3   | NEX  | B     | 303 | -    | -         | 2/27/83/83    | 0/3/3/3 |
| 7   | LHG  | C     | 304 | -    | -         | 16/29/29/53   | -       |
| 6   | CLA  | E     | 314 | 7    | 1/1/14/20 | 9/35/113/115  | -       |
| 6   | CLA  | F     | 313 | 1    | 1/1/13/20 | 12/29/107/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 5   | CHL  | D     | 305 | 1    | 3/3/20/26 | 20/39/137/137 | -       |
| 6   | CLA  | E     | 307 | -    | 1/1/12/20 | 2/19/97/115   | -       |
| 6   | CLA  | C     | 307 | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 5   | CHL  | B     | 311 | -    | 3/3/17/26 | 5/21/119/137  | -       |
| 2   | OIE  | E     | 301 | -    | -         | 7/33/72/72    | 0/2/2/2 |
| 5   | CHL  | E     | 309 | -    | 3/3/15/26 | 4/12/110/137  | -       |
| 5   | CHL  | F     | 309 | -    | 3/3/15/26 | 5/10/108/137  | -       |
| 5   | CHL  | E     | 310 | -    | 3/3/18/26 | 14/33/131/137 | -       |
| 5   | CHL  | F     | 317 | -    | 3/3/16/26 | 5/15/113/137  | -       |
| 6   | CLA  | C     | 316 | 1    | 1/1/11/20 | 4/13/91/115   | -       |
| 10  | BET  | B     | 322 | -    | -         | 5/5/5/5       | -       |
| 5   | CHL  | D     | 311 | -    | 3/3/19/26 | 15/35/133/137 | -       |
| 5   | CHL  | A     | 305 | 1    | 3/3/20/26 | 21/39/137/137 | -       |
| 6   | CLA  | A     | 316 | 1    | 1/1/11/20 | 4/13/91/115   | -       |
| 6   | CLA  | C     | 317 | -    | 1/1/13/20 | 5/27/105/115  | -       |
| 5   | CHL  | C     | 306 | 1    | 3/3/20/26 | 16/39/137/137 | -       |
| 5   | CHL  | C     | 310 | -    | 3/3/15/26 | 7/13/111/137  | -       |
| 6   | CLA  | B     | 315 | 1    | 1/1/13/20 | 6/29/107/115  | -       |
| 2   | OIE  | A     | 301 | -    | -         | 10/33/72/72   | 0/2/2/2 |
| 7   | LHG  | D     | 319 | 6    | -         | 16/50/50/53   | -       |
| 4   | LMU  | D     | 304 | -    | -         | 14/21/61/61   | 0/2/2/2 |
| 5   | CHL  | C     | 312 | 12   | 3/3/18/26 | 11/27/125/137 | -       |
| 5   | CHL  | B     | 307 | 1    | 3/3/19/26 | 13/38/136/137 | -       |
| 3   | NEX  | D     | 303 | -    | -         | 6/27/83/83    | 0/3/3/3 |
| 6   | CLA  | B     | 318 | 1    | 1/1/15/20 | 16/37/115/115 | -       |
| 6   | CLA  | F     | 314 | 7    | 1/1/13/20 | 4/25/103/115  | -       |
| 5   | CHL  | A     | 310 | -    | 3/3/17/26 | 4/21/119/137  | -       |
| 4   | LMU  | E     | 319 | -    | -         | 15/21/61/61   | 0/2/2/2 |
| 2   | OIE  | F     | 302 | -    | -         | 12/33/72/72   | 0/2/2/2 |
| 5   | CHL  | B     | 314 | 1    | 3/3/20/26 | 19/39/137/137 | -       |
| 7   | LHG  | A     | 319 | 6    | -         | 18/51/51/53   | -       |
| 6   | CLA  | D     | 308 | 12   | 1/1/11/20 | 6/15/93/115   | -       |
| 4   | LMU  | A     | 304 | -    | -         | 14/21/61/61   | 0/2/2/2 |
| 9   | OUR  | F     | 320 | -    | -         | 7/42/81/86    | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 5   | CHL  | F     | 304 | 1    | 3/3/20/26 | 16/39/137/137 | -       |
| 5   | CHL  | D     | 310 | 12   | 3/3/15/26 | 2/13/112/137  | -       |
| 6   | CLA  | A     | 315 | 7    | 1/1/14/20 | 9/35/113/115  | -       |
| 6   | CLA  | C     | 308 | 12   | 1/1/11/20 | 7/15/93/115   | -       |
| 10  | BET  | C     | 320 | -    | -         | 5/5/5/5       | -       |
| 5   | CHL  | F     | 308 | 1    | 3/3/15/26 | 4/10/108/137  | -       |
| 5   | CHL  | E     | 304 | 1    | 3/3/20/26 | 17/39/137/137 | -       |
| 2   | OIE  | A     | 302 | -    | -         | 11/33/72/72   | 0/2/2/2 |
| 2   | OIE  | D     | 302 | -    | -         | 16/33/72/72   | 0/2/2/2 |
| 5   | CHL  | E     | 308 | 1    | 3/3/14/26 | 4/10/104/137  | -       |
| 7   | LHG  | C     | 319 | 6    | -         | 18/49/49/53   | -       |
| 4   | LMU  | B     | 305 | -    | -         | 14/21/61/61   | 0/2/2/2 |
| 2   | OIE  | D     | 301 | -    | -         | 14/33/72/72   | 0/2/2/2 |
| 10  | BET  | B     | 321 | -    | -         | 5/5/5/5       | -       |
| 5   | CHL  | F     | 310 | 12   | 3/3/19/26 | 17/33/131/137 | -       |

All (1204) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 5   | E     | 310 | CHL  | MG-ND | -13.99 | 1.78        | 2.05     |
| 5   | C     | 311 | CHL  | MG-ND | -13.00 | 1.80        | 2.05     |
| 5   | E     | 308 | CHL  | MG-NA | 12.97  | 2.37        | 2.06     |
| 5   | C     | 311 | CHL  | MG-NA | 12.90  | 2.36        | 2.06     |
| 5   | D     | 313 | CHL  | MG-NA | 12.84  | 2.36        | 2.06     |
| 5   | F     | 309 | CHL  | MG-NA | 12.49  | 2.35        | 2.06     |
| 5   | D     | 305 | CHL  | MG-NA | 12.35  | 2.35        | 2.06     |
| 5   | C     | 309 | CHL  | MG-NA | 12.24  | 2.35        | 2.06     |
| 5   | E     | 317 | CHL  | MG-NA | 12.19  | 2.35        | 2.06     |
| 5   | C     | 318 | CHL  | MG-NA | 12.06  | 2.34        | 2.06     |
| 5   | A     | 305 | CHL  | MG-NA | 11.91  | 2.34        | 2.06     |
| 5   | B     | 306 | CHL  | MG-NA | 11.91  | 2.34        | 2.06     |
| 5   | D     | 305 | CHL  | MG-ND | -11.66 | 1.82        | 2.05     |
| 5   | B     | 312 | CHL  | MG-NA | 11.61  | 2.33        | 2.06     |
| 5   | A     | 313 | CHL  | MG-NA | 11.61  | 2.33        | 2.06     |
| 5   | F     | 317 | CHL  | MG-NA | 11.56  | 2.33        | 2.06     |
| 5   | A     | 311 | CHL  | MG-ND | -11.55 | 1.82        | 2.05     |
| 5   | B     | 319 | CHL  | MG-NA | 11.41  | 2.33        | 2.06     |
| 5   | A     | 310 | CHL  | MG-ND | -11.36 | 1.83        | 2.05     |
| 5   | D     | 309 | CHL  | MG-NA | 11.28  | 2.33        | 2.06     |

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| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 5   | D     | 311 | CHL  | MG-ND | -11.12 | 1.83        | 2.05     |
| 5   | F     | 308 | CHL  | MG-NA | 11.08  | 2.32        | 2.06     |
| 5   | B     | 311 | CHL  | MG-NA | 11.05  | 2.32        | 2.06     |
| 5   | C     | 305 | CHL  | MG-NA | 10.98  | 2.32        | 2.06     |
| 5   | A     | 318 | CHL  | MG-NA | 10.91  | 2.32        | 2.06     |
| 5   | B     | 310 | CHL  | MG-NA | 10.60  | 2.31        | 2.06     |
| 5   | D     | 312 | CHL  | MG-NA | 10.59  | 2.31        | 2.06     |
| 5   | F     | 309 | CHL  | MG-ND | -10.43 | 1.85        | 2.05     |
| 5   | D     | 310 | CHL  | MG-NA | 10.42  | 2.31        | 2.06     |
| 5   | C     | 310 | CHL  | MG-NA | 10.27  | 2.30        | 2.06     |
| 5   | A     | 309 | CHL  | MG-NA | 10.20  | 2.30        | 2.06     |
| 5   | C     | 312 | CHL  | MG-NA | 10.02  | 2.30        | 2.06     |
| 5   | F     | 310 | CHL  | MG-ND | -9.98  | 1.86        | 2.05     |
| 5   | B     | 312 | CHL  | MG-ND | -9.90  | 1.86        | 2.05     |
| 5   | F     | 317 | CHL  | MG-ND | -9.82  | 1.86        | 2.05     |
| 5   | F     | 304 | CHL  | MG-NA | 9.68   | 2.29        | 2.06     |
| 5   | C     | 312 | CHL  | MG-ND | -9.58  | 1.86        | 2.05     |
| 5   | D     | 318 | CHL  | MG-NA | 9.57   | 2.29        | 2.06     |
| 5   | F     | 310 | CHL  | MG-NA | 9.53   | 2.28        | 2.06     |
| 5   | C     | 313 | CHL  | MG-NA | 9.41   | 2.28        | 2.06     |
| 5   | A     | 311 | CHL  | MG-NA | 9.38   | 2.28        | 2.06     |
| 5   | E     | 310 | CHL  | MG-NA | 9.21   | 2.28        | 2.06     |
| 5   | E     | 309 | CHL  | MG-NA | 9.20   | 2.28        | 2.06     |
| 5   | B     | 306 | CHL  | MG-ND | -9.08  | 1.87        | 2.05     |
| 5   | A     | 305 | CHL  | MG-ND | -8.95  | 1.88        | 2.05     |
| 5   | A     | 312 | CHL  | MG-NA | 8.95   | 2.27        | 2.06     |
| 5   | D     | 311 | CHL  | MG-NA | 8.78   | 2.27        | 2.06     |
| 5   | A     | 318 | CHL  | MG-ND | -8.76  | 1.88        | 2.05     |
| 5   | E     | 308 | CHL  | MG-ND | -8.67  | 1.88        | 2.05     |
| 5   | E     | 304 | CHL  | MG-NA | 8.64   | 2.26        | 2.06     |
| 5   | A     | 309 | CHL  | MG-ND | -8.51  | 1.88        | 2.05     |
| 5   | F     | 304 | CHL  | MG-ND | -8.48  | 1.89        | 2.05     |
| 5   | E     | 311 | CHL  | MG-ND | -8.46  | 1.89        | 2.05     |
| 5   | D     | 318 | CHL  | MG-ND | -8.45  | 1.89        | 2.05     |
| 5   | A     | 312 | CHL  | MG-ND | -8.43  | 1.89        | 2.05     |
| 5   | E     | 309 | CHL  | MG-ND | -8.41  | 1.89        | 2.05     |
| 5   | B     | 314 | CHL  | MG-NA | 8.26   | 2.25        | 2.06     |
| 5   | E     | 312 | CHL  | MG-ND | -8.11  | 1.89        | 2.05     |
| 5   | E     | 312 | CHL  | MG-NA | 8.11   | 2.25        | 2.06     |
| 5   | E     | 311 | CHL  | MG-NA | 8.10   | 2.25        | 2.06     |
| 5   | C     | 310 | CHL  | MG-ND | -8.06  | 1.89        | 2.05     |
| 5   | A     | 310 | CHL  | MG-NA | 7.99   | 2.25        | 2.06     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 6   | F     | 314 | CLA  | C4B-NB | 7.94  | 1.42        | 1.35     |
| 5   | B     | 310 | CHL  | MG-ND  | -7.90 | 1.90        | 2.05     |
| 6   | E     | 314 | CLA  | C4B-NB | 7.89  | 1.42        | 1.35     |
| 6   | B     | 309 | CLA  | C4B-NB | 7.88  | 1.42        | 1.35     |
| 5   | B     | 313 | CHL  | MG-NA  | 7.85  | 2.24        | 2.06     |
| 6   | E     | 306 | CLA  | C4B-NB | 7.72  | 1.42        | 1.35     |
| 6   | C     | 314 | CLA  | C4B-NB | 7.68  | 1.42        | 1.35     |
| 6   | C     | 315 | CLA  | C4B-NB | 7.62  | 1.42        | 1.35     |
| 5   | F     | 308 | CHL  | MG-ND  | -7.61 | 1.90        | 2.05     |
| 6   | A     | 315 | CLA  | C4B-NB | 7.61  | 1.42        | 1.35     |
| 6   | D     | 316 | CLA  | C4B-NB | 7.56  | 1.42        | 1.35     |
| 6   | B     | 316 | CLA  | C4B-NB | 7.54  | 1.41        | 1.35     |
| 5   | B     | 319 | CHL  | MG-ND  | -7.54 | 1.90        | 2.05     |
| 6   | E     | 316 | CLA  | C4B-NB | 7.54  | 1.41        | 1.35     |
| 6   | A     | 308 | CLA  | C4B-NB | 7.53  | 1.41        | 1.35     |
| 6   | D     | 315 | CLA  | C4B-NB | 7.51  | 1.41        | 1.35     |
| 6   | B     | 308 | CLA  | C4B-NB | 7.50  | 1.41        | 1.35     |
| 5   | E     | 317 | CHL  | MG-ND  | -7.49 | 1.90        | 2.05     |
| 6   | D     | 307 | CLA  | C4B-NB | 7.47  | 1.41        | 1.35     |
| 6   | A     | 317 | CLA  | C4B-NB | 7.47  | 1.41        | 1.35     |
| 6   | A     | 316 | CLA  | C4B-NB | 7.45  | 1.41        | 1.35     |
| 5   | D     | 309 | CHL  | MG-ND  | -7.43 | 1.91        | 2.05     |
| 6   | C     | 316 | CLA  | C4B-NB | 7.41  | 1.41        | 1.35     |
| 6   | B     | 317 | CLA  | C4B-NB | 7.40  | 1.41        | 1.35     |
| 6   | F     | 306 | CLA  | C4B-NB | 7.37  | 1.41        | 1.35     |
| 6   | C     | 307 | CLA  | C4B-NB | 7.36  | 1.41        | 1.35     |
| 6   | E     | 307 | CLA  | C4B-NB | 7.34  | 1.41        | 1.35     |
| 6   | A     | 307 | CLA  | C4B-NB | 7.34  | 1.41        | 1.35     |
| 6   | F     | 316 | CLA  | C4B-NB | 7.32  | 1.41        | 1.35     |
| 6   | C     | 308 | CLA  | C4B-NB | 7.29  | 1.41        | 1.35     |
| 6   | D     | 317 | CLA  | C4B-NB | 7.28  | 1.41        | 1.35     |
| 6   | B     | 318 | CLA  | C4B-NB | 7.26  | 1.41        | 1.35     |
| 6   | F     | 315 | CLA  | C4B-NB | 7.26  | 1.41        | 1.35     |
| 5   | A     | 306 | CHL  | MG-NA  | 7.26  | 2.23        | 2.06     |
| 6   | D     | 308 | CLA  | C4B-NB | 7.20  | 1.41        | 1.35     |
| 5   | E     | 309 | CHL  | MG-NC  | 7.19  | 2.23        | 2.06     |
| 5   | D     | 310 | CHL  | MG-ND  | -7.17 | 1.91        | 2.05     |
| 5   | B     | 313 | CHL  | MG-ND  | -7.15 | 1.91        | 2.05     |
| 6   | F     | 307 | CLA  | C4B-NB | 7.12  | 1.41        | 1.35     |
| 6   | E     | 313 | CLA  | C4B-NB | 7.09  | 1.41        | 1.35     |
| 6   | E     | 315 | CLA  | C4B-NB | 7.09  | 1.41        | 1.35     |
| 5   | D     | 306 | CHL  | MG-ND  | -6.98 | 1.91        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | E     | 305 | CHL  | MG-NA   | 6.94  | 2.22        | 2.06     |
| 5   | B     | 307 | CHL  | MG-NA   | 6.77  | 2.22        | 2.06     |
| 5   | B     | 311 | CHL  | MG-ND   | -6.72 | 1.92        | 2.05     |
| 5   | F     | 311 | CHL  | MG-NC   | 6.56  | 2.21        | 2.06     |
| 5   | C     | 318 | CHL  | MG-ND   | -6.53 | 1.92        | 2.05     |
| 5   | C     | 306 | CHL  | MG-NA   | 6.49  | 2.21        | 2.06     |
| 5   | C     | 312 | CHL  | MG-NC   | 6.44  | 2.21        | 2.06     |
| 5   | D     | 318 | CHL  | MG-NC   | 6.38  | 2.21        | 2.06     |
| 5   | F     | 311 | CHL  | MG-NA   | 6.28  | 2.21        | 2.06     |
| 5   | A     | 310 | CHL  | C3B-C2B | 6.27  | 1.49        | 1.40     |
| 5   | F     | 305 | CHL  | MG-NA   | 6.23  | 2.21        | 2.06     |
| 5   | B     | 311 | CHL  | C3B-C2B | 6.20  | 1.49        | 1.40     |
| 5   | D     | 311 | CHL  | C3B-C2B | 6.16  | 1.48        | 1.40     |
| 5   | C     | 306 | CHL  | C3B-C2B | 6.09  | 1.48        | 1.40     |
| 5   | A     | 310 | CHL  | MG-NC   | 6.06  | 2.20        | 2.06     |
| 5   | C     | 306 | CHL  | MG-ND   | -6.04 | 1.93        | 2.05     |
| 5   | F     | 312 | CHL  | MG-NA   | 6.03  | 2.20        | 2.06     |
| 5   | D     | 310 | CHL  | C3B-C2B | 5.99  | 1.48        | 1.40     |
| 5   | E     | 309 | CHL  | C3B-C2B | 5.99  | 1.48        | 1.40     |
| 5   | F     | 312 | CHL  | MG-NC   | 5.99  | 2.20        | 2.06     |
| 5   | B     | 313 | CHL  | MG-NC   | 5.96  | 2.20        | 2.06     |
| 6   | D     | 314 | CLA  | C4B-NB  | 5.95  | 1.40        | 1.35     |
| 5   | F     | 305 | CHL  | C3B-C2B | 5.95  | 1.48        | 1.40     |
| 5   | C     | 309 | CHL  | MG-ND   | -5.91 | 1.94        | 2.05     |
| 5   | A     | 311 | CHL  | C3B-C2B | 5.89  | 1.48        | 1.40     |
| 5   | E     | 308 | CHL  | C3B-C2B | 5.89  | 1.48        | 1.40     |
| 5   | B     | 311 | CHL  | C2C-C3C | 5.88  | 1.49        | 1.36     |
| 5   | A     | 312 | CHL  | C3B-C2B | 5.84  | 1.48        | 1.40     |
| 5   | B     | 319 | CHL  | C3B-C2B | 5.84  | 1.48        | 1.40     |
| 5   | A     | 309 | CHL  | C3B-C2B | 5.83  | 1.48        | 1.40     |
| 5   | C     | 318 | CHL  | C3B-C2B | 5.83  | 1.48        | 1.40     |
| 5   | E     | 305 | CHL  | C3B-C2B | 5.82  | 1.48        | 1.40     |
| 5   | E     | 304 | CHL  | MG-ND   | -5.81 | 1.94        | 2.05     |
| 5   | E     | 317 | CHL  | C3B-C2B | 5.81  | 1.48        | 1.40     |
| 5   | D     | 305 | CHL  | C3B-C2B | 5.80  | 1.48        | 1.40     |
| 5   | E     | 304 | CHL  | C3B-C2B | 5.79  | 1.48        | 1.40     |
| 5   | D     | 309 | CHL  | C2C-C3C | 5.78  | 1.49        | 1.36     |
| 5   | C     | 310 | CHL  | C3B-C2B | 5.77  | 1.48        | 1.40     |
| 5   | C     | 305 | CHL  | C3B-C2B | 5.77  | 1.48        | 1.40     |
| 5   | D     | 309 | CHL  | C3B-C2B | 5.77  | 1.48        | 1.40     |
| 5   | F     | 317 | CHL  | C3B-C2B | 5.77  | 1.48        | 1.40     |
| 5   | C     | 312 | CHL  | C3B-C2B | 5.76  | 1.48        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | B     | 314 | CHL  | C3B-C2B | 5.76  | 1.48        | 1.40     |
| 5   | D     | 306 | CHL  | MG-NA   | 5.76  | 2.19        | 2.06     |
| 5   | E     | 305 | CHL  | C2C-C3C | 5.75  | 1.49        | 1.36     |
| 5   | B     | 312 | CHL  | C2C-C3C | 5.73  | 1.49        | 1.36     |
| 5   | E     | 312 | CHL  | C3B-C2B | 5.73  | 1.48        | 1.40     |
| 5   | B     | 310 | CHL  | C2C-C3C | 5.73  | 1.49        | 1.36     |
| 5   | C     | 311 | CHL  | C3B-C2B | 5.72  | 1.48        | 1.40     |
| 5   | E     | 305 | CHL  | MG-ND   | -5.70 | 1.94        | 2.05     |
| 5   | D     | 318 | CHL  | C2C-C3C | 5.69  | 1.48        | 1.36     |
| 5   | B     | 313 | CHL  | C3B-C2B | 5.69  | 1.48        | 1.40     |
| 5   | B     | 312 | CHL  | C3B-C2B | 5.68  | 1.48        | 1.40     |
| 5   | F     | 308 | CHL  | C2C-C3C | 5.68  | 1.48        | 1.36     |
| 5   | C     | 313 | CHL  | C3B-C2B | 5.68  | 1.48        | 1.40     |
| 5   | A     | 306 | CHL  | C2C-C3C | 5.67  | 1.48        | 1.36     |
| 5   | A     | 305 | CHL  | C3B-C2B | 5.67  | 1.48        | 1.40     |
| 5   | B     | 310 | CHL  | C3B-C2B | 5.65  | 1.48        | 1.40     |
| 5   | A     | 318 | CHL  | C3B-C2B | 5.65  | 1.48        | 1.40     |
| 5   | C     | 309 | CHL  | C3B-C2B | 5.65  | 1.48        | 1.40     |
| 5   | A     | 309 | CHL  | C2C-C3C | 5.64  | 1.48        | 1.36     |
| 5   | F     | 310 | CHL  | C2C-C3C | 5.63  | 1.48        | 1.36     |
| 5   | D     | 318 | CHL  | C3B-C2B | 5.63  | 1.48        | 1.40     |
| 5   | E     | 310 | CHL  | C2C-C3C | 5.63  | 1.48        | 1.36     |
| 5   | D     | 305 | CHL  | C2C-C3C | 5.63  | 1.48        | 1.36     |
| 5   | E     | 308 | CHL  | C2C-C3C | 5.63  | 1.48        | 1.36     |
| 5   | F     | 311 | CHL  | C3B-C2B | 5.62  | 1.48        | 1.40     |
| 5   | E     | 317 | CHL  | C2C-C3C | 5.62  | 1.48        | 1.36     |
| 5   | E     | 311 | CHL  | C3B-C2B | 5.62  | 1.48        | 1.40     |
| 5   | E     | 309 | CHL  | C2C-C3C | 5.62  | 1.48        | 1.36     |
| 5   | F     | 309 | CHL  | C3B-C2B | 5.62  | 1.48        | 1.40     |
| 5   | A     | 318 | CHL  | C2C-C3C | 5.61  | 1.48        | 1.36     |
| 5   | D     | 310 | CHL  | C2C-C3C | 5.60  | 1.48        | 1.36     |
| 5   | D     | 313 | CHL  | C2C-C3C | 5.59  | 1.48        | 1.36     |
| 5   | D     | 312 | CHL  | C3B-C2B | 5.59  | 1.48        | 1.40     |
| 5   | D     | 311 | CHL  | C2C-C3C | 5.59  | 1.48        | 1.36     |
| 5   | E     | 311 | CHL  | MG-NC   | 5.58  | 2.19        | 2.06     |
| 5   | C     | 306 | CHL  | C2C-C3C | 5.57  | 1.48        | 1.36     |
| 5   | A     | 310 | CHL  | C2C-C3C | 5.57  | 1.48        | 1.36     |
| 5   | E     | 310 | CHL  | C3B-C2B | 5.55  | 1.48        | 1.40     |
| 5   | C     | 310 | CHL  | C2C-C3C | 5.55  | 1.48        | 1.36     |
| 5   | C     | 318 | CHL  | C2C-C3C | 5.55  | 1.48        | 1.36     |
| 5   | C     | 309 | CHL  | C2C-C3C | 5.54  | 1.48        | 1.36     |
| 5   | F     | 317 | CHL  | C2C-C3C | 5.54  | 1.48        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | C     | 311 | CHL  | C2C-C3C | 5.53  | 1.48        | 1.36     |
| 5   | F     | 312 | CHL  | C2C-C3C | 5.52  | 1.48        | 1.36     |
| 5   | A     | 311 | CHL  | C2C-C3C | 5.52  | 1.48        | 1.36     |
| 5   | E     | 311 | CHL  | C2C-C3C | 5.52  | 1.48        | 1.36     |
| 5   | B     | 306 | CHL  | C2C-C3C | 5.51  | 1.48        | 1.36     |
| 5   | F     | 317 | CHL  | MG-NC   | 5.50  | 2.19        | 2.06     |
| 5   | A     | 313 | CHL  | C3B-C2B | 5.50  | 1.48        | 1.40     |
| 5   | E     | 312 | CHL  | C2C-C3C | 5.50  | 1.48        | 1.36     |
| 5   | F     | 309 | CHL  | C2C-C3C | 5.49  | 1.48        | 1.36     |
| 5   | B     | 314 | CHL  | C2C-C3C | 5.49  | 1.48        | 1.36     |
| 5   | D     | 311 | CHL  | CHC-C1C | 5.48  | 1.49        | 1.35     |
| 5   | F     | 308 | CHL  | C3B-C2B | 5.48  | 1.48        | 1.40     |
| 5   | C     | 313 | CHL  | C2C-C3C | 5.47  | 1.48        | 1.36     |
| 5   | F     | 310 | CHL  | C3B-C2B | 5.47  | 1.48        | 1.40     |
| 5   | B     | 306 | CHL  | C3B-C2B | 5.47  | 1.48        | 1.40     |
| 5   | C     | 312 | CHL  | C2C-C3C | 5.45  | 1.48        | 1.36     |
| 5   | C     | 305 | CHL  | C2C-C3C | 5.45  | 1.48        | 1.36     |
| 5   | D     | 306 | CHL  | C3B-C2B | 5.44  | 1.47        | 1.40     |
| 5   | B     | 311 | CHL  | CHC-C1C | 5.44  | 1.48        | 1.35     |
| 5   | A     | 318 | CHL  | MG-NC   | 5.43  | 2.19        | 2.06     |
| 5   | B     | 312 | CHL  | CHC-C1C | 5.43  | 1.48        | 1.35     |
| 5   | F     | 304 | CHL  | C3B-C2B | 5.43  | 1.47        | 1.40     |
| 5   | C     | 312 | CHL  | CHD-C1D | 5.42  | 1.48        | 1.38     |
| 5   | B     | 319 | CHL  | C2C-C3C | 5.42  | 1.48        | 1.36     |
| 5   | D     | 311 | CHL  | O2D-CGD | 5.41  | 1.46        | 1.33     |
| 5   | B     | 313 | CHL  | C2C-C3C | 5.40  | 1.48        | 1.36     |
| 5   | A     | 306 | CHL  | C3B-C2B | 5.40  | 1.47        | 1.40     |
| 5   | A     | 310 | CHL  | CHC-C1C | 5.38  | 1.48        | 1.35     |
| 5   | C     | 310 | CHL  | MG-NC   | 5.37  | 2.19        | 2.06     |
| 5   | B     | 310 | CHL  | CHC-C1C | 5.37  | 1.48        | 1.35     |
| 5   | A     | 311 | CHL  | CHC-C1C | 5.37  | 1.48        | 1.35     |
| 5   | B     | 319 | CHL  | CHD-C1D | 5.37  | 1.48        | 1.38     |
| 5   | E     | 304 | CHL  | C2C-C3C | 5.37  | 1.48        | 1.36     |
| 5   | D     | 311 | CHL  | CHD-C1D | 5.36  | 1.48        | 1.38     |
| 6   | C     | 317 | CLA  | C4B-NB  | 5.36  | 1.40        | 1.35     |
| 6   | B     | 315 | CLA  | C4D-ND  | -5.36 | 1.30        | 1.37     |
| 5   | C     | 309 | CHL  | CHC-C1C | 5.36  | 1.48        | 1.35     |
| 5   | E     | 311 | CHL  | CHC-C1C | 5.36  | 1.48        | 1.35     |
| 5   | F     | 311 | CHL  | C2C-C3C | 5.36  | 1.48        | 1.36     |
| 5   | B     | 307 | CHL  | C3B-C2B | 5.35  | 1.47        | 1.40     |
| 5   | B     | 311 | CHL  | MG-NC   | 5.35  | 2.19        | 2.06     |
| 5   | E     | 305 | CHL  | CHC-C1C | 5.34  | 1.48        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 5   | E     | 305 | CHL  | O2D-CGD | 5.34 | 1.46        | 1.33     |
| 5   | C     | 313 | CHL  | CHC-C1C | 5.34 | 1.48        | 1.35     |
| 5   | C     | 312 | CHL  | CHC-C1C | 5.33 | 1.48        | 1.35     |
| 5   | A     | 305 | CHL  | C2C-C3C | 5.33 | 1.48        | 1.36     |
| 5   | A     | 313 | CHL  | CHC-C1C | 5.32 | 1.48        | 1.35     |
| 5   | A     | 312 | CHL  | C2C-C3C | 5.31 | 1.48        | 1.36     |
| 5   | A     | 313 | CHL  | C2C-C3C | 5.31 | 1.48        | 1.36     |
| 5   | D     | 306 | CHL  | C2C-C3C | 5.30 | 1.48        | 1.36     |
| 5   | A     | 312 | CHL  | CHD-C1D | 5.30 | 1.48        | 1.38     |
| 5   | C     | 306 | CHL  | CHC-C1C | 5.30 | 1.48        | 1.35     |
| 5   | D     | 310 | CHL  | O2D-CGD | 5.30 | 1.46        | 1.33     |
| 5   | E     | 309 | CHL  | CHC-C1C | 5.29 | 1.48        | 1.35     |
| 5   | B     | 311 | CHL  | CHD-C1D | 5.29 | 1.48        | 1.38     |
| 5   | C     | 311 | CHL  | CHC-C1C | 5.29 | 1.48        | 1.35     |
| 5   | F     | 317 | CHL  | CHD-C1D | 5.29 | 1.48        | 1.38     |
| 5   | A     | 306 | CHL  | O2D-CGD | 5.29 | 1.46        | 1.33     |
| 5   | D     | 306 | CHL  | CHC-C1C | 5.29 | 1.48        | 1.35     |
| 5   | E     | 311 | CHL  | O2D-CGD | 5.27 | 1.46        | 1.33     |
| 5   | B     | 310 | CHL  | CHD-C1D | 5.27 | 1.48        | 1.38     |
| 5   | D     | 309 | CHL  | CHC-C1C | 5.27 | 1.48        | 1.35     |
| 5   | F     | 304 | CHL  | C2C-C3C | 5.27 | 1.48        | 1.36     |
| 5   | D     | 310 | CHL  | CHD-C1D | 5.27 | 1.48        | 1.38     |
| 5   | B     | 314 | CHL  | CHC-C1C | 5.26 | 1.48        | 1.35     |
| 5   | D     | 318 | CHL  | CHD-C1D | 5.26 | 1.48        | 1.38     |
| 5   | E     | 308 | CHL  | CHC-C1C | 5.26 | 1.48        | 1.35     |
| 5   | F     | 312 | CHL  | C3B-C2B | 5.26 | 1.47        | 1.40     |
| 5   | F     | 305 | CHL  | C2C-C3C | 5.26 | 1.48        | 1.36     |
| 5   | B     | 313 | CHL  | CHC-C1C | 5.26 | 1.48        | 1.35     |
| 5   | F     | 309 | CHL  | O2D-CGD | 5.26 | 1.46        | 1.33     |
| 5   | D     | 312 | CHL  | MG-NC   | 5.25 | 2.18        | 2.06     |
| 5   | A     | 309 | CHL  | CHC-C1C | 5.25 | 1.48        | 1.35     |
| 5   | D     | 310 | CHL  | CHC-C1C | 5.25 | 1.48        | 1.35     |
| 5   | F     | 309 | CHL  | CHC-C1C | 5.24 | 1.48        | 1.35     |
| 5   | F     | 317 | CHL  | CHC-C1C | 5.24 | 1.48        | 1.35     |
| 5   | A     | 318 | CHL  | CHD-C1D | 5.24 | 1.48        | 1.38     |
| 5   | C     | 312 | CHL  | O2D-CGD | 5.23 | 1.46        | 1.33     |
| 5   | D     | 305 | CHL  | CHC-C1C | 5.23 | 1.48        | 1.35     |
| 5   | B     | 311 | CHL  | O2D-CGD | 5.23 | 1.46        | 1.33     |
| 5   | A     | 318 | CHL  | O2D-CGD | 5.23 | 1.45        | 1.33     |
| 5   | F     | 309 | CHL  | CHD-C1D | 5.22 | 1.48        | 1.38     |
| 5   | F     | 312 | CHL  | CHC-C1C | 5.22 | 1.48        | 1.35     |
| 5   | F     | 308 | CHL  | O2D-CGD | 5.22 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 5   | A     | 309 | CHL  | CHD-C1D | 5.22 | 1.48        | 1.38     |
| 5   | E     | 304 | CHL  | CHC-C1C | 5.22 | 1.48        | 1.35     |
| 5   | B     | 306 | CHL  | CHD-C1D | 5.22 | 1.48        | 1.38     |
| 5   | E     | 308 | CHL  | CHD-C1D | 5.21 | 1.48        | 1.38     |
| 5   | B     | 313 | CHL  | CHD-C1D | 5.21 | 1.48        | 1.38     |
| 5   | C     | 309 | CHL  | CHD-C1D | 5.21 | 1.48        | 1.38     |
| 5   | E     | 312 | CHL  | CHC-C1C | 5.21 | 1.48        | 1.35     |
| 5   | F     | 308 | CHL  | CHD-C1D | 5.21 | 1.48        | 1.38     |
| 5   | D     | 312 | CHL  | C2C-C3C | 5.21 | 1.47        | 1.36     |
| 5   | A     | 305 | CHL  | CHC-C1C | 5.20 | 1.48        | 1.35     |
| 5   | D     | 310 | CHL  | MG-NC   | 5.20 | 2.18        | 2.06     |
| 5   | F     | 310 | CHL  | CHC-C1C | 5.19 | 1.48        | 1.35     |
| 5   | D     | 312 | CHL  | CHD-C1D | 5.19 | 1.48        | 1.38     |
| 5   | C     | 313 | CHL  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 5   | E     | 309 | CHL  | CHD-C1D | 5.19 | 1.48        | 1.38     |
| 5   | D     | 318 | CHL  | CHC-C1C | 5.18 | 1.48        | 1.35     |
| 5   | F     | 308 | CHL  | CHC-C1C | 5.18 | 1.48        | 1.35     |
| 5   | B     | 312 | CHL  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 5   | A     | 309 | CHL  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 5   | D     | 309 | CHL  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 5   | E     | 310 | CHL  | CHC-C1C | 5.18 | 1.48        | 1.35     |
| 5   | F     | 311 | CHL  | CHC-C1C | 5.18 | 1.48        | 1.35     |
| 5   | B     | 319 | CHL  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 5   | F     | 311 | CHL  | CHD-C1D | 5.17 | 1.48        | 1.38     |
| 5   | B     | 306 | CHL  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 5   | F     | 312 | CHL  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 5   | C     | 313 | CHL  | CHD-C1D | 5.17 | 1.48        | 1.38     |
| 5   | B     | 306 | CHL  | CHC-C1C | 5.17 | 1.48        | 1.35     |
| 5   | A     | 306 | CHL  | CHC-C1C | 5.17 | 1.48        | 1.35     |
| 5   | D     | 305 | CHL  | O2D-CGD | 5.16 | 1.45        | 1.33     |
| 5   | F     | 310 | CHL  | CHD-C1D | 5.16 | 1.48        | 1.38     |
| 5   | C     | 310 | CHL  | CHC-C1C | 5.16 | 1.48        | 1.35     |
| 5   | A     | 305 | CHL  | O2D-CGD | 5.15 | 1.45        | 1.33     |
| 5   | D     | 313 | CHL  | CHC-C1C | 5.15 | 1.48        | 1.35     |
| 5   | E     | 310 | CHL  | O2D-CGD | 5.15 | 1.45        | 1.33     |
| 5   | F     | 311 | CHL  | O2D-CGD | 5.15 | 1.45        | 1.33     |
| 5   | A     | 312 | CHL  | O2D-CGD | 5.15 | 1.45        | 1.33     |
| 5   | B     | 313 | CHL  | O2D-CGD | 5.15 | 1.45        | 1.33     |
| 5   | D     | 309 | CHL  | CHD-C1D | 5.15 | 1.48        | 1.38     |
| 5   | A     | 311 | CHL  | CHD-C1D | 5.15 | 1.48        | 1.38     |
| 5   | E     | 304 | CHL  | O2D-CGD | 5.14 | 1.45        | 1.33     |
| 5   | D     | 305 | CHL  | CHD-C1D | 5.14 | 1.48        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 5   | A     | 312 | CHL  | CHC-C1C | 5.13 | 1.48        | 1.35     |
| 5   | F     | 304 | CHL  | O2D-CGD | 5.13 | 1.45        | 1.33     |
| 5   | D     | 313 | CHL  | O2D-CGD | 5.13 | 1.45        | 1.33     |
| 5   | F     | 304 | CHL  | CHC-C1C | 5.13 | 1.48        | 1.35     |
| 5   | C     | 309 | CHL  | O2D-CGD | 5.13 | 1.45        | 1.33     |
| 5   | E     | 308 | CHL  | O2D-CGD | 5.12 | 1.45        | 1.33     |
| 5   | E     | 305 | CHL  | CHD-C1D | 5.12 | 1.48        | 1.38     |
| 5   | F     | 317 | CHL  | O2D-CGD | 5.12 | 1.45        | 1.33     |
| 5   | A     | 310 | CHL  | CHD-C1D | 5.12 | 1.48        | 1.38     |
| 5   | B     | 319 | CHL  | CHC-C1C | 5.11 | 1.48        | 1.35     |
| 5   | C     | 318 | CHL  | CHD-C1D | 5.11 | 1.48        | 1.38     |
| 5   | D     | 313 | CHL  | C3B-C2B | 5.10 | 1.47        | 1.40     |
| 5   | C     | 305 | CHL  | CHC-C1C | 5.09 | 1.48        | 1.35     |
| 5   | B     | 312 | CHL  | CHD-C1D | 5.09 | 1.48        | 1.38     |
| 5   | D     | 312 | CHL  | O2D-CGD | 5.09 | 1.45        | 1.33     |
| 5   | E     | 317 | CHL  | CHC-C1C | 5.09 | 1.48        | 1.35     |
| 5   | E     | 304 | CHL  | CHD-C1D | 5.09 | 1.48        | 1.38     |
| 5   | D     | 318 | CHL  | O2D-CGD | 5.08 | 1.45        | 1.33     |
| 5   | A     | 318 | CHL  | CHC-C1C | 5.08 | 1.48        | 1.35     |
| 5   | C     | 318 | CHL  | CHC-C1C | 5.07 | 1.48        | 1.35     |
| 5   | C     | 310 | CHL  | CHD-C1D | 5.07 | 1.48        | 1.38     |
| 5   | C     | 305 | CHL  | O2D-CGD | 5.07 | 1.45        | 1.33     |
| 5   | C     | 305 | CHL  | CHD-C1D | 5.07 | 1.48        | 1.38     |
| 5   | B     | 310 | CHL  | O2D-CGD | 5.07 | 1.45        | 1.33     |
| 5   | C     | 311 | CHL  | CHD-C1D | 5.06 | 1.48        | 1.38     |
| 5   | B     | 307 | CHL  | C2C-C3C | 5.06 | 1.47        | 1.36     |
| 5   | B     | 307 | CHL  | CHC-C1C | 5.05 | 1.47        | 1.35     |
| 5   | A     | 311 | CHL  | O2D-CGD | 5.04 | 1.45        | 1.33     |
| 5   | E     | 309 | CHL  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 5   | E     | 312 | CHL  | CHD-C1D | 5.03 | 1.48        | 1.38     |
| 5   | B     | 307 | CHL  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 5   | E     | 311 | CHL  | CHD-C1D | 5.03 | 1.48        | 1.38     |
| 5   | D     | 306 | CHL  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 6   | A     | 314 | CLA  | C4B-NB  | 5.00 | 1.39        | 1.35     |
| 5   | D     | 311 | CHL  | C4B-NB  | 5.00 | 1.39        | 1.35     |
| 5   | F     | 305 | CHL  | CHC-C1C | 4.99 | 1.47        | 1.35     |
| 5   | F     | 304 | CHL  | CHD-C1D | 4.98 | 1.48        | 1.38     |
| 5   | E     | 312 | CHL  | O2D-CGD | 4.98 | 1.45        | 1.33     |
| 5   | E     | 317 | CHL  | CHD-C1D | 4.98 | 1.48        | 1.38     |
| 5   | D     | 312 | CHL  | CHC-C1C | 4.98 | 1.47        | 1.35     |
| 5   | B     | 319 | CHL  | MG-NC   | 4.97 | 2.18        | 2.06     |
| 5   | C     | 311 | CHL  | O2D-CGD | 4.97 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | C     | 306 | CHL  | O2D-CGD | 4.96  | 1.45        | 1.33     |
| 5   | A     | 305 | CHL  | CHD-C1D | 4.96  | 1.48        | 1.38     |
| 5   | E     | 310 | CHL  | CHD-C1D | 4.95  | 1.48        | 1.38     |
| 5   | F     | 312 | CHL  | CHD-C1D | 4.93  | 1.48        | 1.38     |
| 5   | F     | 305 | CHL  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 5   | B     | 307 | CHL  | CHD-C1D | 4.93  | 1.48        | 1.38     |
| 5   | D     | 313 | CHL  | MG-ND   | -4.92 | 1.96        | 2.05     |
| 5   | F     | 311 | CHL  | MG-ND   | -4.92 | 1.96        | 2.05     |
| 5   | C     | 306 | CHL  | CHD-C1D | 4.90  | 1.47        | 1.38     |
| 5   | D     | 311 | CHL  | MG-NC   | 4.89  | 2.17        | 2.06     |
| 5   | A     | 306 | CHL  | MG-ND   | -4.89 | 1.96        | 2.05     |
| 5   | B     | 314 | CHL  | O2D-CGD | 4.87  | 1.45        | 1.33     |
| 5   | C     | 305 | CHL  | MG-ND   | -4.86 | 1.96        | 2.05     |
| 5   | C     | 318 | CHL  | O2D-CGD | 4.85  | 1.45        | 1.33     |
| 5   | A     | 313 | CHL  | O2D-CGD | 4.82  | 1.45        | 1.33     |
| 5   | E     | 317 | CHL  | O2D-CGD | 4.81  | 1.44        | 1.33     |
| 5   | F     | 310 | CHL  | MG-NC   | 4.74  | 2.17        | 2.06     |
| 5   | F     | 310 | CHL  | O2D-CGD | 4.74  | 1.44        | 1.33     |
| 5   | A     | 306 | CHL  | CHD-C1D | 4.71  | 1.47        | 1.38     |
| 5   | F     | 305 | CHL  | CHD-C1D | 4.70  | 1.47        | 1.38     |
| 5   | A     | 312 | CHL  | MG-NC   | 4.69  | 2.17        | 2.06     |
| 5   | B     | 314 | CHL  | CHD-C1D | 4.67  | 1.47        | 1.38     |
| 5   | A     | 313 | CHL  | CHD-C1D | 4.65  | 1.47        | 1.38     |
| 5   | C     | 313 | CHL  | MG-NC   | 4.65  | 2.17        | 2.06     |
| 5   | D     | 318 | CHL  | O2A-CGA | 4.62  | 1.46        | 1.30     |
| 5   | D     | 306 | CHL  | CHD-C1D | 4.61  | 1.47        | 1.38     |
| 5   | D     | 313 | CHL  | CHD-C1D | 4.61  | 1.47        | 1.38     |
| 5   | F     | 309 | CHL  | MG-NC   | 4.60  | 2.17        | 2.06     |
| 5   | C     | 313 | CHL  | MG-ND   | -4.59 | 1.96        | 2.05     |
| 5   | F     | 317 | CHL  | O2A-CGA | 4.58  | 1.46        | 1.30     |
| 6   | B     | 315 | CLA  | C4B-NB  | 4.55  | 1.39        | 1.35     |
| 6   | D     | 314 | CLA  | C4D-ND  | -4.53 | 1.31        | 1.37     |
| 5   | C     | 306 | CHL  | MG-NC   | 4.52  | 2.17        | 2.06     |
| 5   | D     | 305 | CHL  | MG-NC   | 4.50  | 2.17        | 2.06     |
| 5   | D     | 313 | CHL  | O2A-CGA | 4.45  | 1.46        | 1.33     |
| 5   | E     | 310 | CHL  | O2A-CGA | 4.44  | 1.46        | 1.33     |
| 2   | A     | 302 | 0IE  | C15-C16 | 4.43  | 1.41        | 1.35     |
| 5   | C     | 313 | CHL  | O2A-CGA | 4.43  | 1.46        | 1.33     |
| 6   | F     | 313 | CLA  | C4D-ND  | -4.42 | 1.31        | 1.37     |
| 5   | C     | 318 | CHL  | MG-NC   | 4.40  | 2.16        | 2.06     |
| 5   | F     | 312 | CHL  | O2A-CGA | 4.39  | 1.46        | 1.33     |
| 5   | D     | 312 | CHL  | O2A-CGA | 4.39  | 1.46        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | E     | 312 | CHL  | O2A-CGA | 4.38  | 1.46        | 1.33     |
| 5   | E     | 311 | CHL  | O2A-CGA | 4.38  | 1.46        | 1.33     |
| 5   | A     | 311 | CHL  | MG-NC   | 4.36  | 2.16        | 2.06     |
| 6   | A     | 314 | CLA  | C4D-ND  | -4.36 | 1.31        | 1.37     |
| 2   | E     | 302 | 0IE  | C15-C16 | 4.35  | 1.41        | 1.35     |
| 5   | B     | 311 | CHL  | O2A-CGA | 4.32  | 1.46        | 1.33     |
| 2   | E     | 302 | 0IE  | C8-C7   | 4.32  | 1.41        | 1.35     |
| 5   | C     | 311 | CHL  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 5   | A     | 311 | CHL  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 5   | F     | 310 | CHL  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 5   | B     | 306 | CHL  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 7   | B     | 324 | LHG  | O8-C23  | 4.28  | 1.45        | 1.33     |
| 5   | B     | 314 | CHL  | O2A-CGA | 4.26  | 1.45        | 1.33     |
| 9   | B     | 302 | 0UR  | O44-C45 | 4.26  | 1.44        | 1.34     |
| 6   | F     | 313 | CLA  | C4B-NB  | 4.25  | 1.39        | 1.35     |
| 5   | A     | 305 | CHL  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 5   | C     | 312 | CHL  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 5   | D     | 311 | CHL  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 5   | B     | 319 | CHL  | CHD-C4C | 4.24  | 1.48        | 1.39     |
| 5   | D     | 312 | CHL  | CHD-C4C | 4.22  | 1.48        | 1.39     |
| 5   | C     | 312 | CHL  | CHD-C4C | 4.22  | 1.48        | 1.39     |
| 2   | C     | 301 | 0IE  | C15-C16 | 4.21  | 1.41        | 1.35     |
| 5   | F     | 311 | CHL  | O2A-CGA | 4.21  | 1.45        | 1.33     |
| 5   | B     | 312 | CHL  | O2A-CGA | 4.21  | 1.45        | 1.33     |
| 5   | E     | 304 | CHL  | O2A-CGA | 4.20  | 1.45        | 1.33     |
| 5   | D     | 306 | CHL  | O2A-CGA | 4.20  | 1.45        | 1.33     |
| 5   | A     | 313 | CHL  | O2A-CGA | 4.20  | 1.45        | 1.33     |
| 2   | E     | 301 | 0IE  | C11-C12 | 4.17  | 1.41        | 1.35     |
| 5   | D     | 312 | CHL  | MG-ND   | -4.17 | 1.97        | 2.05     |
| 5   | A     | 306 | CHL  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 5   | B     | 307 | CHL  | CHD-C4C | 4.17  | 1.48        | 1.39     |
| 5   | C     | 313 | CHL  | CHD-C4C | 4.16  | 1.48        | 1.39     |
| 5   | A     | 312 | CHL  | O2A-CGA | 4.16  | 1.45        | 1.33     |
| 5   | A     | 312 | CHL  | CHD-C4C | 4.15  | 1.48        | 1.39     |
| 6   | C     | 317 | CLA  | C4D-ND  | -4.15 | 1.32        | 1.37     |
| 5   | C     | 310 | CHL  | O2D-CGD | 4.15  | 1.43        | 1.33     |
| 5   | B     | 313 | CHL  | O2A-CGA | 4.14  | 1.45        | 1.33     |
| 5   | D     | 305 | CHL  | O2A-CGA | 4.14  | 1.45        | 1.33     |
| 2   | E     | 301 | 0IE  | C15-C16 | 4.13  | 1.41        | 1.35     |
| 5   | B     | 319 | CHL  | O2A-CGA | 4.13  | 1.46        | 1.33     |
| 5   | A     | 310 | CHL  | O2A-CGA | 4.13  | 1.45        | 1.33     |
| 6   | D     | 308 | CLA  | C1D-ND  | 4.13  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 6   | F     | 306 | CLA  | C1D-ND  | 4.13 | 1.42        | 1.37     |
| 6   | E     | 306 | CLA  | C1D-ND  | 4.13 | 1.42        | 1.37     |
| 5   | E     | 304 | CHL  | CHD-C4C | 4.12 | 1.48        | 1.39     |
| 2   | C     | 301 | 0IE  | C8-C7   | 4.12 | 1.41        | 1.35     |
| 5   | C     | 305 | CHL  | CHD-C4C | 4.12 | 1.48        | 1.39     |
| 6   | B     | 316 | CLA  | C1D-ND  | 4.11 | 1.42        | 1.37     |
| 5   | D     | 311 | CHL  | C1B-NB  | 4.11 | 1.38        | 1.35     |
| 2   | E     | 302 | 0IE  | C11-C12 | 4.11 | 1.41        | 1.35     |
| 2   | C     | 301 | 0IE  | C11-C12 | 4.10 | 1.41        | 1.35     |
| 5   | B     | 313 | CHL  | CHD-C4C | 4.10 | 1.48        | 1.39     |
| 6   | E     | 313 | CLA  | C1D-ND  | 4.10 | 1.42        | 1.37     |
| 6   | F     | 307 | CLA  | C1D-ND  | 4.09 | 1.42        | 1.37     |
| 5   | B     | 307 | CHL  | O2A-CGA | 4.09 | 1.45        | 1.33     |
| 5   | D     | 309 | CHL  | CHD-C4C | 4.08 | 1.48        | 1.39     |
| 5   | E     | 305 | CHL  | MG-NC   | 4.08 | 2.16        | 2.06     |
| 6   | C     | 307 | CLA  | C1D-ND  | 4.08 | 1.42        | 1.37     |
| 2   | D     | 302 | 0IE  | C15-C16 | 4.07 | 1.41        | 1.35     |
| 5   | F     | 311 | CHL  | CHD-C4C | 4.07 | 1.48        | 1.39     |
| 5   | E     | 308 | CHL  | CHD-C4C | 4.06 | 1.48        | 1.39     |
| 5   | C     | 306 | CHL  | O2A-CGA | 4.05 | 1.45        | 1.33     |
| 5   | B     | 313 | CHL  | OBD-CAD | 4.05 | 1.29        | 1.22     |
| 5   | A     | 318 | CHL  | CHD-C4C | 4.05 | 1.48        | 1.39     |
| 2   | C     | 302 | 0IE  | C15-C16 | 4.05 | 1.41        | 1.35     |
| 2   | E     | 301 | 0IE  | C8-C7   | 4.05 | 1.41        | 1.35     |
| 5   | B     | 311 | CHL  | CHD-C4C | 4.04 | 1.48        | 1.39     |
| 5   | E     | 311 | CHL  | CHD-C4C | 4.04 | 1.48        | 1.39     |
| 5   | A     | 309 | CHL  | CHD-C4C | 4.04 | 1.48        | 1.39     |
| 5   | F     | 308 | CHL  | CHD-C4C | 4.03 | 1.48        | 1.39     |
| 6   | A     | 308 | CLA  | C1D-ND  | 4.03 | 1.42        | 1.37     |
| 6   | A     | 316 | CLA  | C1D-ND  | 4.03 | 1.42        | 1.37     |
| 2   | F     | 301 | 0IE  | C8-C7   | 4.03 | 1.41        | 1.35     |
| 6   | D     | 317 | CLA  | C1D-ND  | 4.03 | 1.42        | 1.37     |
| 5   | C     | 309 | CHL  | CHD-C4C | 4.03 | 1.48        | 1.39     |
| 5   | D     | 318 | CHL  | CHD-C4C | 4.03 | 1.48        | 1.39     |
| 5   | E     | 305 | CHL  | CHD-C4C | 4.02 | 1.48        | 1.39     |
| 6   | B     | 309 | CLA  | C1D-ND  | 4.02 | 1.42        | 1.37     |
| 6   | E     | 314 | CLA  | C1D-ND  | 4.01 | 1.42        | 1.37     |
| 5   | A     | 306 | CHL  | OBD-CAD | 4.01 | 1.29        | 1.22     |
| 5   | D     | 311 | CHL  | CHD-C4C | 4.01 | 1.48        | 1.39     |
| 2   | F     | 302 | 0IE  | C11-C12 | 4.00 | 1.41        | 1.35     |
| 5   | A     | 306 | CHL  | CHD-C4C | 4.00 | 1.48        | 1.39     |
| 5   | A     | 305 | CHL  | CHD-C4C | 4.00 | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | C     | 302 | 0IE  | C11-C12 | 4.00 | 1.41        | 1.35     |
| 5   | E     | 312 | CHL  | MG-NC   | 3.99 | 2.15        | 2.06     |
| 5   | F     | 317 | CHL  | CHD-C4C | 3.98 | 1.48        | 1.39     |
| 7   | B     | 324 | LHG  | O7-C7   | 3.97 | 1.45        | 1.34     |
| 6   | A     | 317 | CLA  | C1D-ND  | 3.97 | 1.42        | 1.37     |
| 5   | D     | 310 | CHL  | CHD-C4C | 3.97 | 1.48        | 1.39     |
| 2   | D     | 301 | 0IE  | C15-C16 | 3.97 | 1.41        | 1.35     |
| 5   | E     | 309 | CHL  | CHD-C4C | 3.96 | 1.48        | 1.39     |
| 6   | E     | 307 | CLA  | C1D-ND  | 3.96 | 1.42        | 1.37     |
| 2   | F     | 301 | 0IE  | C11-C12 | 3.96 | 1.41        | 1.35     |
| 9   | B     | 325 | 0UR  | O44-C45 | 3.95 | 1.43        | 1.34     |
| 5   | B     | 314 | CHL  | CHD-C4C | 3.95 | 1.48        | 1.39     |
| 5   | A     | 313 | CHL  | CHD-C4C | 3.95 | 1.48        | 1.39     |
| 5   | C     | 306 | CHL  | CHD-C4C | 3.94 | 1.48        | 1.39     |
| 5   | F     | 309 | CHL  | CHD-C4C | 3.93 | 1.48        | 1.39     |
| 5   | B     | 306 | CHL  | CHD-C4C | 3.93 | 1.48        | 1.39     |
| 5   | B     | 310 | CHL  | CHD-C4C | 3.93 | 1.48        | 1.39     |
| 9   | E     | 320 | 0UR  | O44-C45 | 3.93 | 1.43        | 1.34     |
| 5   | D     | 313 | CHL  | CHD-C4C | 3.92 | 1.48        | 1.39     |
| 9   | A     | 322 | 0UR  | O44-C45 | 3.92 | 1.43        | 1.34     |
| 6   | D     | 316 | CLA  | C1D-ND  | 3.91 | 1.42        | 1.37     |
| 5   | F     | 308 | CHL  | MG-NC   | 3.91 | 2.15        | 2.06     |
| 2   | D     | 302 | 0IE  | C11-C12 | 3.91 | 1.41        | 1.35     |
| 5   | F     | 305 | CHL  | O2A-CGA | 3.89 | 1.44        | 1.33     |
| 5   | F     | 304 | CHL  | CHD-C4C | 3.89 | 1.48        | 1.39     |
| 5   | C     | 310 | CHL  | CHD-C4C | 3.88 | 1.48        | 1.39     |
| 6   | C     | 314 | CLA  | C1D-ND  | 3.88 | 1.42        | 1.37     |
| 9   | C     | 321 | 0UR  | O44-C45 | 3.88 | 1.43        | 1.34     |
| 5   | A     | 309 | CHL  | OBD-CAD | 3.88 | 1.29        | 1.22     |
| 6   | F     | 314 | CLA  | C1D-ND  | 3.88 | 1.42        | 1.37     |
| 6   | C     | 308 | CLA  | C1D-ND  | 3.88 | 1.42        | 1.37     |
| 5   | B     | 310 | CHL  | OBD-CAD | 3.87 | 1.29        | 1.22     |
| 2   | D     | 301 | 0IE  | C8-C7   | 3.87 | 1.40        | 1.35     |
| 5   | E     | 305 | CHL  | O2A-CGA | 3.86 | 1.44        | 1.33     |
| 5   | D     | 309 | CHL  | OBD-CAD | 3.86 | 1.29        | 1.22     |
| 9   | F     | 320 | 0UR  | O44-C45 | 3.85 | 1.43        | 1.34     |
| 5   | B     | 319 | CHL  | OBD-CAD | 3.85 | 1.29        | 1.22     |
| 5   | E     | 305 | CHL  | OBD-CAD | 3.84 | 1.29        | 1.22     |
| 2   | C     | 302 | 0IE  | C8-C7   | 3.84 | 1.40        | 1.35     |
| 5   | F     | 312 | CHL  | CHD-C4C | 3.83 | 1.48        | 1.39     |
| 5   | D     | 305 | CHL  | CHD-C4C | 3.83 | 1.48        | 1.39     |
| 6   | C     | 315 | CLA  | C1D-ND  | 3.82 | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 5   | E     | 308 | CHL  | OBD-CAD | 3.82 | 1.29        | 1.22     |
| 5   | E     | 311 | CHL  | OBD-CAD | 3.82 | 1.29        | 1.22     |
| 5   | C     | 318 | CHL  | CHD-C4C | 3.81 | 1.47        | 1.39     |
| 6   | B     | 318 | CLA  | C1D-ND  | 3.81 | 1.42        | 1.37     |
| 6   | B     | 308 | CLA  | C1D-ND  | 3.81 | 1.42        | 1.37     |
| 5   | F     | 310 | CHL  | CHD-C4C | 3.81 | 1.47        | 1.39     |
| 5   | E     | 312 | CHL  | CHD-C4C | 3.81 | 1.47        | 1.39     |
| 5   | F     | 305 | CHL  | CHD-C4C | 3.81 | 1.47        | 1.39     |
| 5   | C     | 305 | CHL  | OBD-CAD | 3.81 | 1.29        | 1.22     |
| 6   | F     | 316 | CLA  | C1D-ND  | 3.80 | 1.42        | 1.37     |
| 6   | F     | 315 | CLA  | C1D-ND  | 3.80 | 1.42        | 1.37     |
| 5   | A     | 305 | CHL  | OBD-CAD | 3.79 | 1.29        | 1.22     |
| 6   | A     | 307 | CLA  | C1D-ND  | 3.79 | 1.42        | 1.37     |
| 5   | F     | 312 | CHL  | OBD-CAD | 3.79 | 1.29        | 1.22     |
| 5   | A     | 310 | CHL  | CHD-C4C | 3.79 | 1.47        | 1.39     |
| 2   | D     | 301 | 0IE  | C11-C12 | 3.78 | 1.40        | 1.35     |
| 5   | D     | 318 | CHL  | OBD-CAD | 3.77 | 1.29        | 1.22     |
| 5   | D     | 306 | CHL  | OBD-CAD | 3.77 | 1.29        | 1.22     |
| 5   | F     | 317 | CHL  | OBD-CAD | 3.77 | 1.29        | 1.22     |
| 5   | B     | 307 | CHL  | OBD-CAD | 3.77 | 1.29        | 1.22     |
| 2   | F     | 302 | 0IE  | C8-C7   | 3.76 | 1.40        | 1.35     |
| 5   | C     | 306 | CHL  | C3D-C2D | 3.76 | 1.49        | 1.39     |
| 5   | A     | 318 | CHL  | OBD-CAD | 3.75 | 1.28        | 1.22     |
| 6   | B     | 317 | CLA  | C1D-ND  | 3.75 | 1.42        | 1.37     |
| 5   | B     | 307 | CHL  | C3D-C2D | 3.75 | 1.49        | 1.39     |
| 2   | B     | 301 | 0IE  | C11-C12 | 3.75 | 1.40        | 1.35     |
| 5   | C     | 318 | CHL  | OBD-CAD | 3.75 | 1.28        | 1.22     |
| 5   | F     | 309 | CHL  | OBD-CAD | 3.75 | 1.28        | 1.22     |
| 6   | A     | 315 | CLA  | C1D-ND  | 3.74 | 1.42        | 1.37     |
| 5   | E     | 304 | CHL  | OBD-CAD | 3.74 | 1.28        | 1.22     |
| 5   | E     | 310 | CHL  | OBD-CAD | 3.74 | 1.28        | 1.22     |
| 6   | D     | 315 | CLA  | C1D-ND  | 3.74 | 1.42        | 1.37     |
| 5   | E     | 317 | CHL  | OBD-CAD | 3.73 | 1.28        | 1.22     |
| 6   | E     | 315 | CLA  | C1D-ND  | 3.72 | 1.42        | 1.37     |
| 5   | A     | 312 | CHL  | OBD-CAD | 3.72 | 1.28        | 1.22     |
| 5   | E     | 310 | CHL  | CHD-C4C | 3.72 | 1.47        | 1.39     |
| 5   | C     | 312 | CHL  | OBD-CAD | 3.72 | 1.28        | 1.22     |
| 5   | C     | 309 | CHL  | C3D-C2D | 3.72 | 1.49        | 1.39     |
| 6   | C     | 316 | CLA  | C1D-ND  | 3.72 | 1.42        | 1.37     |
| 5   | E     | 317 | CHL  | CHD-C4C | 3.71 | 1.47        | 1.39     |
| 5   | F     | 305 | CHL  | OBD-CAD | 3.71 | 1.28        | 1.22     |
| 5   | E     | 309 | CHL  | OBD-CAD | 3.71 | 1.28        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | D     | 302 | 0IE  | C8-C7   | 3.71 | 1.40        | 1.35     |
| 5   | A     | 311 | CHL  | CHD-C4C | 3.70 | 1.47        | 1.39     |
| 5   | F     | 308 | CHL  | OBD-CAD | 3.70 | 1.28        | 1.22     |
| 2   | F     | 302 | 0IE  | C15-C16 | 3.70 | 1.40        | 1.35     |
| 5   | B     | 306 | CHL  | OBD-CAD | 3.70 | 1.28        | 1.22     |
| 5   | B     | 319 | CHL  | C3D-C2D | 3.70 | 1.49        | 1.39     |
| 5   | A     | 309 | CHL  | C3D-C2D | 3.69 | 1.49        | 1.39     |
| 5   | D     | 306 | CHL  | CHD-C4C | 3.69 | 1.47        | 1.39     |
| 5   | C     | 313 | CHL  | OBD-CAD | 3.69 | 1.28        | 1.22     |
| 5   | C     | 306 | CHL  | OBD-CAD | 3.68 | 1.28        | 1.22     |
| 5   | E     | 312 | CHL  | OBD-CAD | 3.67 | 1.28        | 1.22     |
| 5   | B     | 312 | CHL  | CHD-C4C | 3.66 | 1.47        | 1.39     |
| 5   | F     | 310 | CHL  | OBD-CAD | 3.66 | 1.28        | 1.22     |
| 2   | F     | 301 | 0IE  | C15-C16 | 3.66 | 1.40        | 1.35     |
| 5   | A     | 311 | CHL  | OBD-CAD | 3.65 | 1.28        | 1.22     |
| 5   | E     | 304 | CHL  | C3D-C2D | 3.65 | 1.49        | 1.39     |
| 5   | C     | 312 | CHL  | C3D-C2D | 3.65 | 1.49        | 1.39     |
| 5   | F     | 317 | CHL  | C3D-C2D | 3.65 | 1.49        | 1.39     |
| 5   | D     | 305 | CHL  | OBD-CAD | 3.64 | 1.28        | 1.22     |
| 2   | B     | 301 | 0IE  | C8-C7   | 3.64 | 1.40        | 1.35     |
| 5   | C     | 313 | CHL  | C3D-C2D | 3.64 | 1.49        | 1.39     |
| 6   | E     | 316 | CLA  | C1D-ND  | 3.63 | 1.42        | 1.37     |
| 5   | A     | 310 | CHL  | OBD-CAD | 3.63 | 1.28        | 1.22     |
| 5   | D     | 309 | CHL  | C3D-C2D | 3.62 | 1.49        | 1.39     |
| 5   | F     | 304 | CHL  | O2A-CGA | 3.61 | 1.43        | 1.33     |
| 5   | B     | 314 | CHL  | C3D-C2D | 3.61 | 1.49        | 1.39     |
| 5   | E     | 308 | CHL  | C3D-C2D | 3.61 | 1.49        | 1.39     |
| 5   | D     | 311 | CHL  | OBD-CAD | 3.61 | 1.28        | 1.22     |
| 5   | F     | 311 | CHL  | OBD-CAD | 3.60 | 1.28        | 1.22     |
| 5   | F     | 305 | CHL  | C3D-C2D | 3.60 | 1.49        | 1.39     |
| 5   | D     | 312 | CHL  | C3D-C2D | 3.59 | 1.48        | 1.39     |
| 5   | A     | 309 | CHL  | MG-NC   | 3.59 | 2.14        | 2.06     |
| 5   | F     | 311 | CHL  | C3D-C2D | 3.59 | 1.48        | 1.39     |
| 5   | C     | 309 | CHL  | OBD-CAD | 3.59 | 1.28        | 1.22     |
| 6   | D     | 307 | CLA  | C1D-ND  | 3.59 | 1.42        | 1.37     |
| 5   | B     | 311 | CHL  | OBD-CAD | 3.59 | 1.28        | 1.22     |
| 5   | A     | 311 | CHL  | C3D-C2D | 3.58 | 1.48        | 1.39     |
| 5   | C     | 311 | CHL  | OBD-CAD | 3.58 | 1.28        | 1.22     |
| 5   | B     | 311 | CHL  | C3D-C2D | 3.58 | 1.48        | 1.39     |
| 5   | C     | 305 | CHL  | C3D-C2D | 3.57 | 1.48        | 1.39     |
| 5   | C     | 311 | CHL  | CHD-C4C | 3.57 | 1.47        | 1.39     |
| 5   | A     | 312 | CHL  | C3D-C2D | 3.57 | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | B     | 314 | CHL  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 2   | A     | 301 | 0IE  | C17-C16 | -3.57 | 1.38        | 1.45     |
| 5   | A     | 318 | CHL  | C3D-C2D | 3.56  | 1.48        | 1.39     |
| 5   | E     | 312 | CHL  | C3D-C2D | 3.56  | 1.48        | 1.39     |
| 5   | D     | 311 | CHL  | C3D-C2D | 3.56  | 1.48        | 1.39     |
| 5   | C     | 318 | CHL  | C3D-C2D | 3.56  | 1.48        | 1.39     |
| 5   | B     | 310 | CHL  | C3D-C2D | 3.56  | 1.48        | 1.39     |
| 5   | A     | 305 | CHL  | C3D-C2D | 3.56  | 1.48        | 1.39     |
| 5   | A     | 310 | CHL  | O2D-CGD | 3.55  | 1.41        | 1.33     |
| 5   | E     | 305 | CHL  | C3D-C2D | 3.55  | 1.48        | 1.39     |
| 5   | B     | 313 | CHL  | C3D-C2D | 3.54  | 1.48        | 1.39     |
| 5   | E     | 309 | CHL  | C3D-C2D | 3.54  | 1.48        | 1.39     |
| 5   | D     | 310 | CHL  | C3D-C2D | 3.54  | 1.48        | 1.39     |
| 5   | D     | 318 | CHL  | C3D-C2D | 3.54  | 1.48        | 1.39     |
| 5   | F     | 312 | CHL  | C3D-C2D | 3.54  | 1.48        | 1.39     |
| 5   | A     | 310 | CHL  | C3D-C2D | 3.53  | 1.48        | 1.39     |
| 5   | A     | 306 | CHL  | C3D-C2D | 3.53  | 1.48        | 1.39     |
| 5   | D     | 313 | CHL  | C3D-C2D | 3.53  | 1.48        | 1.39     |
| 5   | E     | 317 | CHL  | C3D-C2D | 3.52  | 1.48        | 1.39     |
| 5   | D     | 312 | CHL  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 5   | E     | 311 | CHL  | C3D-C2D | 3.50  | 1.48        | 1.39     |
| 5   | D     | 306 | CHL  | C3D-C2D | 3.49  | 1.48        | 1.39     |
| 5   | F     | 308 | CHL  | C3D-C2D | 3.49  | 1.48        | 1.39     |
| 5   | F     | 304 | CHL  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 5   | D     | 305 | CHL  | C3D-C2D | 3.49  | 1.48        | 1.39     |
| 5   | B     | 312 | CHL  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 5   | C     | 310 | CHL  | C3D-C2D | 3.49  | 1.48        | 1.39     |
| 5   | F     | 305 | CHL  | C1D-ND  | -3.49 | 1.33        | 1.37     |
| 5   | E     | 310 | CHL  | MG-NC   | 3.48  | 2.14        | 2.06     |
| 5   | F     | 304 | CHL  | C3D-C2D | 3.48  | 1.48        | 1.39     |
| 2   | B     | 301 | 0IE  | C15-C16 | 3.47  | 1.40        | 1.35     |
| 5   | F     | 310 | CHL  | C3D-C2D | 3.46  | 1.48        | 1.39     |
| 5   | C     | 311 | CHL  | MG-NC   | 3.45  | 2.14        | 2.06     |
| 5   | F     | 309 | CHL  | C3D-C2D | 3.45  | 1.48        | 1.39     |
| 5   | A     | 313 | CHL  | C3D-C2D | 3.44  | 1.48        | 1.39     |
| 5   | B     | 306 | CHL  | C3D-C2D | 3.44  | 1.48        | 1.39     |
| 5   | A     | 313 | CHL  | MG-ND   | -3.41 | 1.99        | 2.05     |
| 3   | C     | 303 | NEX  | C7-C8   | -3.40 | 1.26        | 1.32     |
| 5   | A     | 313 | CHL  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 5   | C     | 311 | CHL  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 5   | B     | 312 | CHL  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 5   | E     | 310 | CHL  | C3D-C2D | 3.38  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | D     | 315 | CLA  | CHC-C1C | 3.36  | 1.43        | 1.35     |
| 3   | F     | 303 | NEX  | C7-C8   | -3.35 | 1.26        | 1.32     |
| 3   | A     | 303 | NEX  | C7-C8   | -3.34 | 1.26        | 1.32     |
| 2   | A     | 302 | 0IE  | C11-C12 | 3.33  | 1.40        | 1.35     |
| 5   | D     | 313 | CHL  | OBD-CAD | 3.33  | 1.28        | 1.22     |
| 6   | A     | 315 | CLA  | CHC-C1C | 3.32  | 1.43        | 1.35     |
| 6   | F     | 315 | CLA  | CHC-C1C | 3.31  | 1.43        | 1.35     |
| 2   | A     | 302 | 0IE  | C6-C7   | -3.30 | 1.38        | 1.45     |
| 5   | B     | 306 | CHL  | C4D-CHA | 3.30  | 1.50        | 1.38     |
| 5   | B     | 307 | CHL  | C1D-ND  | -3.29 | 1.33        | 1.37     |
| 6   | B     | 309 | CLA  | CHC-C1C | 3.29  | 1.43        | 1.35     |
| 5   | A     | 313 | CHL  | C1D-ND  | -3.28 | 1.33        | 1.37     |
| 6   | B     | 317 | CLA  | CHC-C1C | 3.27  | 1.43        | 1.35     |
| 6   | D     | 307 | CLA  | CHC-C1C | 3.26  | 1.43        | 1.35     |
| 5   | D     | 306 | CHL  | C1D-ND  | -3.26 | 1.33        | 1.37     |
| 6   | C     | 314 | CLA  | CHC-C1C | 3.25  | 1.43        | 1.35     |
| 6   | B     | 316 | CLA  | CHC-C1C | 3.25  | 1.43        | 1.35     |
| 5   | B     | 307 | CHL  | MG-ND   | -3.24 | 1.99        | 2.05     |
| 6   | A     | 316 | CLA  | CHC-C1C | 3.24  | 1.43        | 1.35     |
| 3   | D     | 303 | NEX  | C7-C8   | -3.23 | 1.26        | 1.32     |
| 6   | A     | 308 | CLA  | CHC-C1C | 3.23  | 1.43        | 1.35     |
| 5   | F     | 311 | CHL  | C1D-ND  | -3.22 | 1.33        | 1.37     |
| 6   | E     | 313 | CLA  | CHC-C1C | 3.21  | 1.43        | 1.35     |
| 5   | C     | 305 | CHL  | C1D-ND  | -3.21 | 1.33        | 1.37     |
| 6   | D     | 316 | CLA  | CHC-C1C | 3.20  | 1.43        | 1.35     |
| 6   | E     | 315 | CLA  | CHC-C1C | 3.20  | 1.43        | 1.35     |
| 6   | F     | 314 | CLA  | CHC-C1C | 3.19  | 1.43        | 1.35     |
| 3   | E     | 303 | NEX  | C7-C8   | -3.19 | 1.26        | 1.32     |
| 6   | F     | 306 | CLA  | CHC-C1C | 3.18  | 1.43        | 1.35     |
| 6   | C     | 315 | CLA  | CHC-C1C | 3.18  | 1.43        | 1.35     |
| 6   | E     | 307 | CLA  | CHC-C1C | 3.18  | 1.43        | 1.35     |
| 6   | A     | 314 | CLA  | MG-ND   | -3.18 | 1.99        | 2.05     |
| 6   | A     | 317 | CLA  | CHC-C1C | 3.17  | 1.43        | 1.35     |
| 6   | C     | 316 | CLA  | CHC-C1C | 3.16  | 1.43        | 1.35     |
| 5   | D     | 309 | CHL  | C1D-ND  | -3.16 | 1.33        | 1.37     |
| 5   | F     | 317 | CHL  | C4D-CHA | 3.16  | 1.49        | 1.38     |
| 3   | B     | 303 | NEX  | C7-C8   | -3.16 | 1.26        | 1.32     |
| 5   | E     | 308 | CHL  | C4D-CHA | 3.16  | 1.49        | 1.38     |
| 6   | A     | 307 | CLA  | CHC-C1C | 3.15  | 1.43        | 1.35     |
| 6   | C     | 308 | CLA  | CHC-C1C | 3.14  | 1.43        | 1.35     |
| 5   | C     | 311 | CHL  | C4D-CHA | 3.14  | 1.49        | 1.38     |
| 6   | E     | 314 | CLA  | CHC-C1C | 3.14  | 1.43        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | F     | 307 | CLA  | CHC-C1C | 3.13  | 1.43        | 1.35     |
| 5   | B     | 319 | CHL  | C4D-CHA | 3.13  | 1.49        | 1.38     |
| 5   | B     | 307 | CHL  | C4D-CHA | 3.13  | 1.49        | 1.38     |
| 5   | D     | 313 | CHL  | C1D-ND  | -3.13 | 1.33        | 1.37     |
| 2   | A     | 301 | 0IE  | C15-C16 | 3.12  | 1.39        | 1.35     |
| 5   | A     | 305 | CHL  | C4D-CHA | 3.12  | 1.49        | 1.38     |
| 6   | B     | 318 | CLA  | CHC-C1C | 3.11  | 1.42        | 1.35     |
| 6   | F     | 316 | CLA  | CHC-C1C | 3.11  | 1.42        | 1.35     |
| 6   | A     | 314 | CLA  | CMB-C2B | -3.09 | 1.45        | 1.51     |
| 6   | E     | 316 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 5   | A     | 306 | CHL  | C1D-ND  | -3.09 | 1.34        | 1.37     |
| 5   | C     | 309 | CHL  | C1D-ND  | -3.08 | 1.34        | 1.37     |
| 5   | D     | 305 | CHL  | C4D-CHA | 3.08  | 1.49        | 1.38     |
| 5   | C     | 318 | CHL  | C1D-ND  | -3.08 | 1.34        | 1.37     |
| 5   | C     | 318 | CHL  | C4D-CHA | 3.08  | 1.49        | 1.38     |
| 5   | E     | 305 | CHL  | C1D-ND  | -3.07 | 1.34        | 1.37     |
| 5   | A     | 311 | CHL  | C4D-CHA | 3.07  | 1.49        | 1.38     |
| 6   | D     | 308 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 6   | E     | 306 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 5   | C     | 305 | CHL  | C4D-CHA | 3.07  | 1.49        | 1.38     |
| 5   | E     | 310 | CHL  | C4D-CHA | 3.07  | 1.49        | 1.38     |
| 6   | D     | 317 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 5   | C     | 313 | CHL  | C4D-CHA | 3.06  | 1.49        | 1.38     |
| 6   | B     | 308 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 5   | D     | 318 | CHL  | C4D-CHA | 3.05  | 1.49        | 1.38     |
| 5   | B     | 312 | CHL  | C4D-CHA | 3.05  | 1.49        | 1.38     |
| 5   | B     | 313 | CHL  | C1D-ND  | -3.04 | 1.34        | 1.37     |
| 5   | E     | 308 | CHL  | C1D-ND  | -3.04 | 1.34        | 1.37     |
| 5   | A     | 318 | CHL  | C4D-CHA | 3.04  | 1.49        | 1.38     |
| 5   | B     | 310 | CHL  | C4D-CHA | 3.04  | 1.49        | 1.38     |
| 5   | F     | 308 | CHL  | C4D-CHA | 3.04  | 1.49        | 1.38     |
| 5   | B     | 314 | CHL  | MG-ND   | -3.03 | 1.99        | 2.05     |
| 5   | A     | 305 | CHL  | C1D-ND  | -3.03 | 1.34        | 1.37     |
| 5   | F     | 309 | CHL  | C1B-CHB | 3.03  | 1.49        | 1.41     |
| 5   | B     | 310 | CHL  | C1D-ND  | -3.03 | 1.34        | 1.37     |
| 5   | B     | 312 | CHL  | MG-NC   | 3.03  | 2.13        | 2.06     |
| 5   | D     | 312 | CHL  | C4D-CHA | 3.02  | 1.49        | 1.38     |
| 5   | C     | 309 | CHL  | C4D-CHA | 3.02  | 1.49        | 1.38     |
| 5   | D     | 310 | CHL  | C4D-CHA | 3.01  | 1.49        | 1.38     |
| 5   | E     | 317 | CHL  | C1D-ND  | -3.01 | 1.34        | 1.37     |
| 5   | E     | 317 | CHL  | C1B-CHB | 3.01  | 1.49        | 1.41     |
| 5   | D     | 310 | CHL  | C1B-CHB | 3.01  | 1.49        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | C     | 310 | CHL  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 5   | A     | 309 | CHL  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 6   | B     | 315 | CLA  | C3B-C2B | -3.00 | 1.36        | 1.40     |
| 5   | E     | 317 | CHL  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 6   | B     | 308 | CLA  | C4D-ND  | -3.00 | 1.33        | 1.37     |
| 5   | C     | 310 | CHL  | OBD-CAD | 3.00  | 1.27        | 1.22     |
| 5   | F     | 310 | CHL  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 5   | D     | 311 | CHL  | C4D-CHA | 2.99  | 1.49        | 1.38     |
| 5   | B     | 311 | CHL  | C1B-CHB | 2.99  | 1.49        | 1.41     |
| 5   | A     | 310 | CHL  | C4D-CHA | 2.98  | 1.49        | 1.38     |
| 5   | C     | 306 | CHL  | C1D-ND  | -2.98 | 1.34        | 1.37     |
| 5   | F     | 309 | CHL  | C4D-CHA | 2.98  | 1.49        | 1.38     |
| 6   | F     | 313 | CLA  | CMB-C2B | -2.98 | 1.45        | 1.51     |
| 5   | D     | 309 | CHL  | C4D-CHA | 2.97  | 1.49        | 1.38     |
| 6   | A     | 317 | CLA  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 6   | D     | 315 | CLA  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 5   | C     | 312 | CHL  | C4D-CHA | 2.97  | 1.48        | 1.38     |
| 5   | F     | 304 | CHL  | C4D-CHA | 2.97  | 1.48        | 1.38     |
| 6   | C     | 307 | CLA  | CHC-C1C | 2.96  | 1.42        | 1.35     |
| 5   | A     | 312 | CHL  | C4D-CHA | 2.94  | 1.48        | 1.38     |
| 5   | E     | 312 | CHL  | C4D-CHA | 2.94  | 1.48        | 1.38     |
| 6   | C     | 308 | CLA  | C4D-ND  | -2.94 | 1.33        | 1.37     |
| 6   | E     | 316 | CLA  | C4D-ND  | -2.94 | 1.33        | 1.37     |
| 5   | F     | 308 | CHL  | C1D-ND  | -2.93 | 1.34        | 1.37     |
| 5   | B     | 306 | CHL  | C1B-CHB | 2.93  | 1.49        | 1.41     |
| 5   | E     | 309 | CHL  | C1B-CHB | 2.93  | 1.49        | 1.41     |
| 6   | A     | 314 | CLA  | CMC-C2C | -2.93 | 1.44        | 1.50     |
| 5   | B     | 312 | CHL  | C1D-ND  | -2.93 | 1.34        | 1.37     |
| 5   | E     | 311 | CHL  | C1D-ND  | -2.93 | 1.34        | 1.37     |
| 5   | D     | 309 | CHL  | C1B-CHB | 2.92  | 1.49        | 1.41     |
| 5   | E     | 309 | CHL  | C4D-CHA | 2.92  | 1.48        | 1.38     |
| 5   | A     | 312 | CHL  | C1D-ND  | -2.92 | 1.34        | 1.37     |
| 5   | D     | 312 | CHL  | C1B-CHB | 2.92  | 1.49        | 1.41     |
| 5   | E     | 311 | CHL  | C4D-CHA | 2.92  | 1.48        | 1.38     |
| 6   | F     | 306 | CLA  | C4D-ND  | -2.92 | 1.33        | 1.37     |
| 5   | B     | 314 | CHL  | C4D-CHA | 2.91  | 1.48        | 1.38     |
| 5   | B     | 311 | CHL  | C4B-CHC | 2.91  | 1.49        | 1.41     |
| 5   | F     | 311 | CHL  | C4D-CHA | 2.91  | 1.48        | 1.38     |
| 6   | A     | 307 | CLA  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 5   | D     | 309 | CHL  | MG-NC   | 2.91  | 2.13        | 2.06     |
| 5   | B     | 313 | CHL  | C4D-CHA | 2.90  | 1.48        | 1.38     |
| 6   | C     | 317 | CLA  | CMB-C2B | -2.90 | 1.45        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | A     | 301 | 0IE  | C23-C16 | -2.90 | 1.44        | 1.50     |
| 5   | A     | 309 | CHL  | C1D-ND  | -2.90 | 1.34        | 1.37     |
| 6   | C     | 316 | CLA  | C4D-ND  | -2.90 | 1.33        | 1.37     |
| 5   | B     | 311 | CHL  | C4D-CHA | 2.90  | 1.48        | 1.38     |
| 6   | F     | 313 | CLA  | C3B-C2B | -2.90 | 1.36        | 1.40     |
| 6   | F     | 314 | CLA  | C4D-ND  | -2.88 | 1.33        | 1.37     |
| 5   | E     | 309 | CHL  | C4B-CHC | 2.88  | 1.49        | 1.41     |
| 5   | A     | 305 | CHL  | C1B-CHB | 2.88  | 1.49        | 1.41     |
| 2   | A     | 302 | 0IE  | C8-C7   | 2.88  | 1.39        | 1.35     |
| 5   | B     | 319 | CHL  | C1B-CHB | 2.88  | 1.49        | 1.41     |
| 5   | F     | 304 | CHL  | C1D-ND  | -2.88 | 1.34        | 1.37     |
| 5   | E     | 304 | CHL  | C4D-CHA | 2.88  | 1.48        | 1.38     |
| 6   | E     | 313 | CLA  | C4D-ND  | -2.88 | 1.33        | 1.37     |
| 5   | E     | 304 | CHL  | MG-NC   | 2.88  | 2.13        | 2.06     |
| 5   | C     | 313 | CHL  | C4B-CHC | 2.87  | 1.49        | 1.41     |
| 6   | E     | 307 | CLA  | C4D-ND  | -2.87 | 1.33        | 1.37     |
| 5   | A     | 310 | CHL  | C1B-CHB | 2.87  | 1.49        | 1.41     |
| 5   | D     | 313 | CHL  | C4D-CHA | 2.86  | 1.48        | 1.38     |
| 5   | D     | 305 | CHL  | C1B-CHB | 2.86  | 1.48        | 1.41     |
| 5   | E     | 317 | CHL  | MG-NC   | 2.86  | 2.13        | 2.06     |
| 2   | A     | 301 | 0IE  | C21-C7  | -2.86 | 1.45        | 1.50     |
| 5   | A     | 310 | CHL  | C4B-CHC | 2.86  | 1.48        | 1.41     |
| 5   | E     | 308 | CHL  | C1B-CHB | 2.86  | 1.48        | 1.41     |
| 5   | C     | 305 | CHL  | O2A-CGA | 2.86  | 1.41        | 1.33     |
| 5   | C     | 309 | CHL  | C1B-CHB | 2.86  | 1.48        | 1.41     |
| 5   | A     | 313 | CHL  | C4D-CHA | 2.86  | 1.48        | 1.38     |
| 2   | A     | 301 | 0IE  | C22-C12 | -2.85 | 1.45        | 1.50     |
| 5   | C     | 311 | CHL  | C1B-CHB | 2.85  | 1.48        | 1.41     |
| 5   | D     | 313 | CHL  | C1B-CHB | 2.85  | 1.48        | 1.41     |
| 5   | E     | 305 | CHL  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 6   | E     | 306 | CLA  | C4D-ND  | -2.84 | 1.33        | 1.37     |
| 6   | F     | 316 | CLA  | C4D-ND  | -2.84 | 1.33        | 1.37     |
| 6   | E     | 315 | CLA  | C4D-ND  | -2.84 | 1.33        | 1.37     |
| 6   | E     | 314 | CLA  | C4D-ND  | -2.84 | 1.33        | 1.37     |
| 5   | F     | 304 | CHL  | C1B-CHB | 2.84  | 1.48        | 1.41     |
| 5   | B     | 312 | CHL  | C1B-CHB | 2.83  | 1.48        | 1.41     |
| 5   | E     | 305 | CHL  | C4B-CHC | 2.83  | 1.48        | 1.41     |
| 5   | A     | 306 | CHL  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 5   | D     | 306 | CHL  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 5   | F     | 305 | CHL  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 5   | D     | 318 | CHL  | C4B-CHC | 2.82  | 1.48        | 1.41     |
| 6   | B     | 316 | CLA  | C4D-ND  | -2.82 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | C     | 310 | CHL  | C1B-CHB | 2.82  | 1.48        | 1.41     |
| 5   | A     | 306 | CHL  | C1B-CHB | 2.82  | 1.48        | 1.41     |
| 5   | E     | 311 | CHL  | C4B-CHC | 2.82  | 1.48        | 1.41     |
| 5   | C     | 305 | CHL  | C1B-CHB | 2.81  | 1.48        | 1.41     |
| 5   | B     | 310 | CHL  | C1B-CHB | 2.81  | 1.48        | 1.41     |
| 5   | F     | 308 | CHL  | C1B-CHB | 2.81  | 1.48        | 1.41     |
| 6   | C     | 317 | CLA  | C3B-C2B | -2.81 | 1.36        | 1.40     |
| 6   | D     | 317 | CLA  | C4D-ND  | -2.81 | 1.33        | 1.37     |
| 6   | B     | 315 | CLA  | CMB-C2B | -2.81 | 1.45        | 1.51     |
| 6   | D     | 316 | CLA  | C4D-ND  | -2.80 | 1.33        | 1.37     |
| 5   | C     | 318 | CHL  | C1B-CHB | 2.80  | 1.48        | 1.41     |
| 5   | F     | 317 | CHL  | C1B-CHB | 2.80  | 1.48        | 1.41     |
| 5   | F     | 312 | CHL  | C4B-CHC | 2.80  | 1.48        | 1.41     |
| 5   | E     | 317 | CHL  | C4B-CHC | 2.79  | 1.48        | 1.41     |
| 6   | B     | 318 | CLA  | C4D-ND  | -2.79 | 1.33        | 1.37     |
| 5   | B     | 312 | CHL  | C4B-CHC | 2.79  | 1.48        | 1.41     |
| 5   | C     | 306 | CHL  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 5   | C     | 312 | CHL  | C4B-CHC | 2.79  | 1.48        | 1.41     |
| 5   | B     | 310 | CHL  | MG-NC   | 2.79  | 2.12        | 2.06     |
| 5   | F     | 312 | CHL  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 5   | A     | 318 | CHL  | C1B-CHB | 2.79  | 1.48        | 1.41     |
| 5   | E     | 304 | CHL  | C1D-ND  | -2.79 | 1.34        | 1.37     |
| 5   | C     | 318 | CHL  | C4B-CHC | 2.79  | 1.48        | 1.41     |
| 6   | F     | 315 | CLA  | C4D-ND  | -2.78 | 1.33        | 1.37     |
| 5   | D     | 312 | CHL  | C1D-ND  | -2.78 | 1.34        | 1.37     |
| 5   | B     | 312 | CHL  | C2C-C1C | 2.78  | 1.50        | 1.44     |
| 5   | F     | 309 | CHL  | C2C-C1C | 2.78  | 1.50        | 1.44     |
| 5   | C     | 309 | CHL  | C4B-CHC | 2.78  | 1.48        | 1.41     |
| 5   | D     | 310 | CHL  | C4B-CHC | 2.78  | 1.48        | 1.41     |
| 5   | A     | 318 | CHL  | C4B-CHC | 2.78  | 1.48        | 1.41     |
| 5   | F     | 308 | CHL  | C4B-CHC | 2.77  | 1.48        | 1.41     |
| 5   | F     | 317 | CHL  | C4B-CHC | 2.77  | 1.48        | 1.41     |
| 5   | C     | 311 | CHL  | C1D-ND  | -2.77 | 1.34        | 1.37     |
| 5   | F     | 309 | CHL  | C4B-CHC | 2.77  | 1.48        | 1.41     |
| 5   | B     | 314 | CHL  | C1D-ND  | -2.77 | 1.34        | 1.37     |
| 5   | D     | 318 | CHL  | C1B-CHB | 2.76  | 1.48        | 1.41     |
| 6   | D     | 314 | CLA  | CMB-C2B | -2.76 | 1.45        | 1.51     |
| 6   | D     | 308 | CLA  | C4D-ND  | -2.75 | 1.33        | 1.37     |
| 6   | B     | 315 | CLA  | CMC-C2C | -2.75 | 1.45        | 1.50     |
| 6   | C     | 317 | CLA  | MG-ND   | -2.75 | 2.00        | 2.05     |
| 5   | F     | 317 | CHL  | C1D-ND  | -2.75 | 1.34        | 1.37     |
| 5   | C     | 312 | CHL  | C1B-CHB | 2.75  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | E     | 311 | CHL  | C1B-CHB | 2.74  | 1.48        | 1.41     |
| 5   | A     | 312 | CHL  | C1B-CHB | 2.74  | 1.48        | 1.41     |
| 6   | A     | 315 | CLA  | C4D-ND  | -2.74 | 1.33        | 1.37     |
| 5   | D     | 305 | CHL  | C1D-ND  | -2.74 | 1.34        | 1.37     |
| 5   | F     | 312 | CHL  | C1D-ND  | -2.73 | 1.34        | 1.37     |
| 5   | B     | 314 | CHL  | C1B-CHB | 2.73  | 1.48        | 1.41     |
| 6   | C     | 307 | CLA  | C4D-ND  | -2.73 | 1.33        | 1.37     |
| 6   | A     | 316 | CLA  | C4D-ND  | -2.73 | 1.33        | 1.37     |
| 9   | B     | 302 | OUR  | C19-C18 | 2.72  | 1.54        | 1.50     |
| 5   | B     | 313 | CHL  | C4B-CHC | 2.72  | 1.48        | 1.41     |
| 5   | D     | 305 | CHL  | C4B-CHC | 2.72  | 1.48        | 1.41     |
| 5   | E     | 309 | CHL  | C1D-ND  | -2.72 | 1.34        | 1.37     |
| 6   | A     | 314 | CLA  | C3B-C2B | -2.72 | 1.36        | 1.40     |
| 5   | B     | 319 | CHL  | C4B-CHC | 2.72  | 1.48        | 1.41     |
| 5   | C     | 311 | CHL  | C4B-CHC | 2.72  | 1.48        | 1.41     |
| 5   | C     | 310 | CHL  | C1D-ND  | -2.71 | 1.34        | 1.37     |
| 5   | C     | 310 | CHL  | C4B-CHC | 2.71  | 1.48        | 1.41     |
| 5   | A     | 318 | CHL  | C1D-ND  | -2.71 | 1.34        | 1.37     |
| 5   | C     | 313 | CHL  | C1B-CHB | 2.71  | 1.48        | 1.41     |
| 5   | C     | 306 | CHL  | C4B-CHC | 2.71  | 1.48        | 1.41     |
| 5   | E     | 304 | CHL  | C4B-CHC | 2.71  | 1.48        | 1.41     |
| 5   | B     | 314 | CHL  | MG-NC   | 2.71  | 2.12        | 2.06     |
| 5   | A     | 309 | CHL  | C1B-CHB | 2.71  | 1.48        | 1.41     |
| 5   | E     | 308 | CHL  | C4B-CHC | 2.71  | 1.48        | 1.41     |
| 5   | E     | 310 | CHL  | C1D-ND  | -2.71 | 1.34        | 1.37     |
| 6   | F     | 313 | CLA  | C1D-ND  | 2.71  | 1.41        | 1.37     |
| 5   | A     | 311 | CHL  | C4B-CHC | 2.71  | 1.48        | 1.41     |
| 5   | D     | 310 | CHL  | C1D-ND  | -2.70 | 1.34        | 1.37     |
| 5   | F     | 311 | CHL  | C1B-CHB | 2.70  | 1.48        | 1.41     |
| 6   | D     | 314 | CLA  | CMC-C2C | -2.70 | 1.45        | 1.50     |
| 5   | B     | 314 | CHL  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 2   | A     | 301 | OIE  | C13-C12 | -2.69 | 1.40        | 1.45     |
| 5   | D     | 311 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 5   | B     | 310 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 6   | B     | 317 | CLA  | C4D-ND  | -2.69 | 1.34        | 1.37     |
| 5   | E     | 312 | CHL  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 6   | B     | 309 | CLA  | C4D-ND  | -2.69 | 1.34        | 1.37     |
| 6   | A     | 308 | CLA  | C4D-ND  | -2.68 | 1.34        | 1.37     |
| 5   | C     | 313 | CHL  | C1D-ND  | -2.68 | 1.34        | 1.37     |
| 6   | D     | 314 | CLA  | CHC-C1C | 2.68  | 1.41        | 1.35     |
| 5   | E     | 312 | CHL  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 6   | C     | 314 | CLA  | C4D-ND  | -2.68 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | D     | 314 | CLA  | MG-ND   | -2.67 | 2.00        | 2.05     |
| 6   | F     | 316 | CLA  | CMB-C2B | -2.67 | 1.46        | 1.51     |
| 6   | B     | 315 | CLA  | CMD-C2D | -2.67 | 1.45        | 1.50     |
| 5   | B     | 313 | CHL  | C1B-CHB | 2.67  | 1.48        | 1.41     |
| 5   | A     | 313 | CHL  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 6   | F     | 307 | CLA  | C4D-ND  | -2.66 | 1.34        | 1.37     |
| 5   | C     | 312 | CHL  | C1D-ND  | -2.66 | 1.34        | 1.37     |
| 6   | C     | 317 | CLA  | CHC-C1C | 2.66  | 1.41        | 1.35     |
| 5   | E     | 304 | CHL  | C1B-CHB | 2.66  | 1.48        | 1.41     |
| 5   | F     | 311 | CHL  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 5   | F     | 309 | CHL  | C1D-ND  | -2.66 | 1.34        | 1.37     |
| 5   | B     | 306 | CHL  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 6   | C     | 315 | CLA  | C4D-ND  | -2.66 | 1.34        | 1.37     |
| 5   | F     | 310 | CHL  | C1C-NC  | -2.65 | 1.33        | 1.37     |
| 5   | A     | 309 | CHL  | C4B-CHC | 2.65  | 1.48        | 1.41     |
| 6   | B     | 316 | CLA  | CMB-C2B | -2.65 | 1.46        | 1.51     |
| 5   | D     | 309 | CHL  | C4B-CHC | 2.65  | 1.48        | 1.41     |
| 5   | C     | 305 | CHL  | C4B-CHC | 2.64  | 1.48        | 1.41     |
| 5   | B     | 319 | CHL  | C1D-ND  | -2.64 | 1.34        | 1.37     |
| 6   | D     | 308 | CLA  | CMB-C2B | -2.63 | 1.46        | 1.51     |
| 5   | A     | 306 | CHL  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 5   | C     | 309 | CHL  | C2C-C1C | 2.62  | 1.50        | 1.44     |
| 5   | F     | 310 | CHL  | C2C-C1C | 2.62  | 1.50        | 1.44     |
| 5   | B     | 310 | CHL  | C2C-C1C | 2.62  | 1.50        | 1.44     |
| 5   | D     | 311 | CHL  | C2C-C1C | 2.62  | 1.50        | 1.44     |
| 5   | F     | 305 | CHL  | MG-ND   | -2.62 | 2.00        | 2.05     |
| 5   | C     | 306 | CHL  | C1B-CHB | 2.61  | 1.48        | 1.41     |
| 5   | E     | 312 | CHL  | C1D-ND  | -2.61 | 1.34        | 1.37     |
| 6   | B     | 308 | CLA  | CMB-C2B | -2.61 | 1.46        | 1.51     |
| 5   | F     | 310 | CHL  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 5   | B     | 311 | CHL  | C1D-ND  | -2.61 | 1.34        | 1.37     |
| 6   | D     | 314 | CLA  | CMD-C2D | -2.61 | 1.45        | 1.50     |
| 5   | A     | 310 | CHL  | C2C-C1C | 2.60  | 1.50        | 1.44     |
| 5   | A     | 310 | CHL  | C1D-ND  | -2.60 | 1.34        | 1.37     |
| 5   | D     | 313 | CHL  | C4B-CHC | 2.60  | 1.48        | 1.41     |
| 6   | B     | 315 | CLA  | C3B-CAB | -2.59 | 1.42        | 1.47     |
| 5   | E     | 309 | CHL  | C2C-C1C | 2.59  | 1.50        | 1.44     |
| 5   | A     | 311 | CHL  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 6   | A     | 308 | CLA  | CMB-C2B | -2.59 | 1.46        | 1.51     |
| 6   | F     | 307 | CLA  | CMB-C2B | -2.58 | 1.46        | 1.51     |
| 5   | E     | 310 | CHL  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 5   | F     | 312 | CHL  | C1B-CHB | 2.57  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | A     | 305 | CHL  | C4B-CHC | 2.57  | 1.48        | 1.41     |
| 5   | E     | 308 | CHL  | C2C-C1C | 2.57  | 1.50        | 1.44     |
| 5   | A     | 312 | CHL  | C4B-CHC | 2.57  | 1.48        | 1.41     |
| 5   | A     | 311 | CHL  | C1D-ND  | -2.57 | 1.34        | 1.37     |
| 7   | C     | 319 | LHG  | O7-C5   | -2.56 | 1.40        | 1.46     |
| 5   | B     | 311 | CHL  | C2C-C1C | 2.56  | 1.50        | 1.44     |
| 5   | B     | 306 | CHL  | C1D-ND  | -2.56 | 1.34        | 1.37     |
| 6   | E     | 307 | CLA  | CMB-C2B | -2.56 | 1.46        | 1.51     |
| 5   | E     | 310 | CHL  | C4B-CHC | 2.56  | 1.48        | 1.41     |
| 5   | C     | 306 | CHL  | C2C-C1C | 2.56  | 1.50        | 1.44     |
| 6   | C     | 308 | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 5   | D     | 311 | CHL  | C1B-CHB | 2.55  | 1.48        | 1.41     |
| 5   | D     | 309 | CHL  | C2C-C1C | 2.55  | 1.50        | 1.44     |
| 5   | D     | 312 | CHL  | C4B-CHC | 2.54  | 1.48        | 1.41     |
| 5   | B     | 307 | CHL  | C4C-C3C | 2.54  | 1.49        | 1.45     |
| 5   | C     | 310 | CHL  | C2C-C1C | 2.53  | 1.49        | 1.44     |
| 6   | A     | 314 | CLA  | CMD-C2D | -2.53 | 1.45        | 1.50     |
| 5   | C     | 311 | CHL  | C2C-C1C | 2.53  | 1.49        | 1.44     |
| 5   | F     | 310 | CHL  | C1B-CHB | 2.53  | 1.48        | 1.41     |
| 2   | F     | 301 | 0IE  | C17-C16 | -2.52 | 1.40        | 1.45     |
| 5   | E     | 310 | CHL  | C2C-C1C | 2.52  | 1.49        | 1.44     |
| 5   | A     | 313 | CHL  | C1B-CHB | 2.52  | 1.48        | 1.41     |
| 5   | D     | 310 | CHL  | C2C-C1C | 2.52  | 1.49        | 1.44     |
| 5   | F     | 305 | CHL  | C1B-CHB | 2.52  | 1.48        | 1.41     |
| 6   | E     | 306 | CLA  | CMB-C2B | -2.52 | 1.46        | 1.51     |
| 5   | D     | 311 | CHL  | C1D-ND  | -2.51 | 1.34        | 1.37     |
| 2   | D     | 302 | 0IE  | C6-C7   | -2.51 | 1.40        | 1.45     |
| 5   | F     | 304 | CHL  | MG-NC   | 2.51  | 2.12        | 2.06     |
| 6   | A     | 307 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 5   | A     | 306 | CHL  | C2C-C1C | 2.51  | 1.49        | 1.44     |
| 5   | D     | 306 | CHL  | C2C-C1C | 2.51  | 1.49        | 1.44     |
| 6   | F     | 313 | CLA  | CMC-C2C | -2.51 | 1.45        | 1.50     |
| 6   | B     | 309 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 7   | B     | 320 | LHG  | O7-C5   | -2.51 | 1.40        | 1.46     |
| 5   | E     | 305 | CHL  | C1B-CHB | 2.51  | 1.48        | 1.41     |
| 5   | F     | 305 | CHL  | C4B-CHC | 2.50  | 1.47        | 1.41     |
| 5   | D     | 305 | CHL  | C2C-C1C | 2.49  | 1.49        | 1.44     |
| 5   | A     | 311 | CHL  | C2C-C1C | 2.49  | 1.49        | 1.44     |
| 5   | D     | 318 | CHL  | C2C-C1C | 2.49  | 1.49        | 1.44     |
| 6   | C     | 317 | CLA  | CMD-C2D | -2.49 | 1.45        | 1.50     |
| 5   | B     | 307 | CHL  | C1B-CHB | 2.49  | 1.47        | 1.41     |
| 5   | F     | 310 | CHL  | C1D-ND  | -2.49 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | B     | 318 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 5   | F     | 304 | CHL  | C4B-CHC | 2.48  | 1.47        | 1.41     |
| 6   | D     | 307 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 6   | C     | 317 | CLA  | C3B-CAB | -2.48 | 1.42        | 1.47     |
| 5   | D     | 318 | CHL  | C1D-ND  | -2.48 | 1.34        | 1.37     |
| 6   | F     | 306 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 6   | A     | 314 | CLA  | C3B-CAB | -2.47 | 1.42        | 1.47     |
| 5   | F     | 308 | CHL  | C2C-C1C | 2.47  | 1.49        | 1.44     |
| 5   | B     | 319 | CHL  | C4C-C3C | 2.47  | 1.49        | 1.45     |
| 6   | E     | 316 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 5   | C     | 318 | CHL  | C1C-NC  | -2.46 | 1.34        | 1.37     |
| 6   | F     | 313 | CLA  | CMD-C2D | -2.45 | 1.45        | 1.50     |
| 6   | D     | 315 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 6   | F     | 314 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 6   | D     | 307 | CLA  | C4D-ND  | -2.45 | 1.34        | 1.37     |
| 5   | D     | 306 | CHL  | C1B-CHB | 2.45  | 1.47        | 1.41     |
| 5   | D     | 312 | CHL  | C4C-C3C | 2.45  | 1.49        | 1.45     |
| 6   | F     | 313 | CLA  | CHC-C1C | 2.45  | 1.41        | 1.35     |
| 6   | F     | 313 | CLA  | C3B-CAB | -2.45 | 1.43        | 1.47     |
| 9   | D     | 321 | OUR  | O44-C45 | 2.45  | 1.40        | 1.34     |
| 2   | B     | 301 | OIE  | C13-C12 | -2.44 | 1.40        | 1.45     |
| 5   | A     | 318 | CHL  | C2C-C1C | 2.43  | 1.49        | 1.44     |
| 6   | A     | 315 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 5   | E     | 305 | CHL  | C2C-C1C | 2.43  | 1.49        | 1.44     |
| 6   | B     | 317 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 2   | A     | 301 | OIE  | C8-C7   | 2.43  | 1.39        | 1.35     |
| 5   | E     | 317 | CHL  | C2C-C1C | 2.42  | 1.49        | 1.44     |
| 5   | D     | 313 | CHL  | C2C-C1C | 2.42  | 1.49        | 1.44     |
| 5   | D     | 306 | CHL  | C4B-CHC | 2.42  | 1.47        | 1.41     |
| 6   | B     | 315 | CLA  | C4B-CHC | -2.42 | 1.34        | 1.41     |
| 5   | A     | 318 | CHL  | C1C-NC  | -2.41 | 1.34        | 1.37     |
| 5   | F     | 304 | CHL  | C2C-C1C | 2.40  | 1.49        | 1.44     |
| 6   | A     | 314 | CLA  | CHC-C1C | 2.40  | 1.41        | 1.35     |
| 6   | D     | 316 | CLA  | CMB-C2B | -2.40 | 1.46        | 1.51     |
| 6   | A     | 317 | CLA  | CMB-C2B | -2.40 | 1.46        | 1.51     |
| 5   | A     | 309 | CHL  | C2C-C1C | 2.40  | 1.49        | 1.44     |
| 5   | E     | 317 | CHL  | C1C-NC  | -2.40 | 1.34        | 1.37     |
| 2   | C     | 302 | OIE  | C17-C16 | -2.40 | 1.40        | 1.45     |
| 2   | F     | 302 | OIE  | C13-C12 | -2.39 | 1.40        | 1.45     |
| 2   | A     | 302 | OIE  | C17-C16 | -2.39 | 1.40        | 1.45     |
| 2   | B     | 301 | OIE  | C17-C16 | -2.39 | 1.40        | 1.45     |
| 6   | C     | 307 | CLA  | CMB-C2B | -2.38 | 1.46        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | C     | 314 | CLA  | CMB-C2B | -2.38 | 1.46        | 1.51     |
| 2   | A     | 302 | 0IE  | C13-C12 | -2.38 | 1.40        | 1.45     |
| 5   | B     | 306 | CHL  | C2C-C1C | 2.38  | 1.49        | 1.44     |
| 2   | F     | 302 | 0IE  | C6-C7   | -2.38 | 1.40        | 1.45     |
| 5   | B     | 307 | CHL  | C4B-CHC | 2.38  | 1.47        | 1.41     |
| 5   | C     | 312 | CHL  | C2C-C1C | 2.38  | 1.49        | 1.44     |
| 6   | E     | 315 | CLA  | CMB-C2B | -2.37 | 1.46        | 1.51     |
| 2   | F     | 302 | 0IE  | C17-C16 | -2.37 | 1.40        | 1.45     |
| 5   | F     | 317 | CHL  | C2C-C1C | 2.37  | 1.49        | 1.44     |
| 6   | F     | 315 | CLA  | CMB-C2B | -2.37 | 1.46        | 1.51     |
| 2   | E     | 302 | 0IE  | C6-C7   | -2.37 | 1.40        | 1.45     |
| 5   | B     | 319 | CHL  | C1C-NC  | -2.37 | 1.34        | 1.37     |
| 6   | E     | 314 | CLA  | CMB-C2B | -2.36 | 1.46        | 1.51     |
| 6   | D     | 317 | CLA  | CMB-C2B | -2.35 | 1.46        | 1.51     |
| 5   | A     | 313 | CHL  | C2C-C1C | 2.35  | 1.49        | 1.44     |
| 6   | A     | 316 | CLA  | CMB-C2B | -2.35 | 1.46        | 1.51     |
| 6   | C     | 317 | CLA  | C1D-ND  | 2.35  | 1.40        | 1.37     |
| 5   | B     | 319 | CHL  | C2C-C1C | 2.35  | 1.49        | 1.44     |
| 6   | C     | 317 | CLA  | CMC-C2C | -2.35 | 1.45        | 1.50     |
| 2   | C     | 302 | 0IE  | C13-C12 | -2.35 | 1.40        | 1.45     |
| 5   | C     | 318 | CHL  | C2C-C1C | 2.34  | 1.49        | 1.44     |
| 5   | F     | 317 | CHL  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 6   | F     | 313 | CLA  | C4B-CHC | -2.33 | 1.34        | 1.41     |
| 2   | D     | 301 | 0IE  | C13-C12 | -2.33 | 1.40        | 1.45     |
| 6   | C     | 316 | CLA  | CMB-C2B | -2.32 | 1.46        | 1.51     |
| 5   | F     | 312 | CHL  | C1C-NC  | -2.32 | 1.34        | 1.37     |
| 5   | E     | 311 | CHL  | C2C-C1C | 2.32  | 1.49        | 1.44     |
| 2   | B     | 301 | 0IE  | C6-C7   | -2.32 | 1.41        | 1.45     |
| 5   | E     | 308 | CHL  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 5   | D     | 309 | CHL  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 5   | E     | 304 | CHL  | C2C-C1C | 2.32  | 1.49        | 1.44     |
| 2   | D     | 302 | 0IE  | C17-C16 | -2.31 | 1.41        | 1.45     |
| 6   | E     | 313 | CLA  | CMB-C2B | -2.30 | 1.46        | 1.51     |
| 6   | D     | 314 | CLA  | C3B-C2B | -2.29 | 1.37        | 1.40     |
| 6   | C     | 315 | CLA  | CMB-C2B | -2.29 | 1.46        | 1.51     |
| 5   | C     | 305 | CHL  | O2A-C1  | -2.29 | 1.39        | 1.46     |
| 5   | A     | 312 | CHL  | C4C-C3C | 2.28  | 1.49        | 1.45     |
| 5   | A     | 311 | CHL  | C1C-NC  | -2.28 | 1.34        | 1.37     |
| 5   | B     | 313 | CHL  | C2C-C1C | 2.28  | 1.49        | 1.44     |
| 2   | D     | 302 | 0IE  | C13-C12 | -2.27 | 1.41        | 1.45     |
| 5   | E     | 309 | CHL  | C1C-NC  | -2.27 | 1.34        | 1.37     |
| 5   | F     | 311 | CHL  | C1C-NC  | -2.27 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | A     | 314 | CLA  | C4B-CHC | -2.27 | 1.34        | 1.41     |
| 5   | A     | 306 | CHL  | MG-NC   | 2.27  | 2.11        | 2.06     |
| 5   | B     | 314 | CHL  | C2C-C1C | 2.27  | 1.49        | 1.44     |
| 5   | C     | 313 | CHL  | C1C-NC  | -2.27 | 1.34        | 1.37     |
| 3   | D     | 303 | NEX  | O24-C25 | -2.27 | 1.43        | 1.46     |
| 6   | B     | 315 | CLA  | CHC-C1C | 2.26  | 1.40        | 1.35     |
| 2   | D     | 301 | OIE  | C17-C16 | -2.26 | 1.41        | 1.45     |
| 5   | C     | 305 | CHL  | C2A-C1A | -2.25 | 1.47        | 1.52     |
| 5   | D     | 310 | CHL  | C4C-C3C | 2.25  | 1.48        | 1.45     |
| 5   | B     | 306 | CHL  | MG-NC   | 2.25  | 2.11        | 2.06     |
| 5   | D     | 318 | CHL  | C4C-C3C | 2.25  | 1.48        | 1.45     |
| 5   | C     | 313 | CHL  | C2C-C1C | 2.25  | 1.49        | 1.44     |
| 5   | C     | 310 | CHL  | C1C-NC  | -2.24 | 1.34        | 1.37     |
| 5   | C     | 312 | CHL  | C4C-C3C | 2.24  | 1.48        | 1.45     |
| 5   | D     | 312 | CHL  | C1C-NC  | -2.23 | 1.34        | 1.37     |
| 5   | A     | 305 | CHL  | C2C-C1C | 2.23  | 1.49        | 1.44     |
| 5   | D     | 311 | CHL  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 2   | A     | 302 | OIE  | C22-C12 | -2.23 | 1.46        | 1.50     |
| 2   | A     | 301 | OIE  | C5-C6   | 2.22  | 1.40        | 1.34     |
| 5   | B     | 313 | CHL  | C1C-NC  | -2.22 | 1.34        | 1.37     |
| 5   | F     | 308 | CHL  | C1C-NC  | -2.22 | 1.34        | 1.37     |
| 5   | D     | 305 | CHL  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 6   | F     | 316 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 5   | A     | 312 | CHL  | C2C-C1C | 2.21  | 1.49        | 1.44     |
| 2   | C     | 302 | OIE  | C6-C7   | -2.21 | 1.41        | 1.45     |
| 2   | A     | 301 | OIE  | C10-C11 | -2.21 | 1.36        | 1.43     |
| 9   | A     | 322 | OUR  | C29-C28 | -2.21 | 1.51        | 1.54     |
| 6   | D     | 314 | CLA  | C1D-ND  | 2.21  | 1.40        | 1.37     |
| 5   | F     | 312 | CHL  | C2C-C1C | 2.20  | 1.49        | 1.44     |
| 2   | C     | 301 | OIE  | C13-C12 | -2.20 | 1.41        | 1.45     |
| 6   | D     | 317 | CLA  | CMC-C2C | -2.20 | 1.46        | 1.50     |
| 5   | E     | 311 | CHL  | C4C-C3C | 2.20  | 1.48        | 1.45     |
| 6   | F     | 313 | CLA  | C1B-NB  | -2.19 | 1.33        | 1.35     |
| 5   | A     | 318 | CHL  | C4C-C3C | 2.18  | 1.48        | 1.45     |
| 5   | E     | 312 | CHL  | C2C-C1C | 2.18  | 1.49        | 1.44     |
| 5   | A     | 309 | CHL  | C4C-C3C | 2.17  | 1.48        | 1.45     |
| 6   | C     | 317 | CLA  | C4B-CHC | -2.17 | 1.35        | 1.41     |
| 5   | D     | 318 | CHL  | C1C-NC  | -2.17 | 1.34        | 1.37     |
| 5   | F     | 311 | CHL  | C2C-C1C | 2.16  | 1.49        | 1.44     |
| 5   | C     | 312 | CHL  | C1C-NC  | -2.16 | 1.34        | 1.37     |
| 5   | F     | 310 | CHL  | C1D-C2D | 2.16  | 1.49        | 1.45     |
| 5   | F     | 304 | CHL  | C1C-NC  | -2.16 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9   | F     | 320 | 0UR  | C31-C32 | 2.16  | 1.35        | 1.33     |
| 5   | C     | 318 | CHL  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 5   | C     | 311 | CHL  | C1C-NC  | -2.15 | 1.34        | 1.37     |
| 5   | B     | 313 | CHL  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 5   | F     | 317 | CHL  | C1C-NC  | -2.15 | 1.34        | 1.37     |
| 5   | F     | 311 | CHL  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 3   | A     | 303 | NEX  | O24-C25 | -2.15 | 1.43        | 1.46     |
| 5   | F     | 305 | CHL  | C2C-C1C | 2.14  | 1.49        | 1.44     |
| 6   | A     | 314 | CLA  | C1D-ND  | 2.14  | 1.40        | 1.37     |
| 5   | F     | 309 | CHL  | C4C-C3C | 2.14  | 1.48        | 1.45     |
| 5   | B     | 312 | CHL  | C1C-NC  | -2.14 | 1.34        | 1.37     |
| 5   | D     | 312 | CHL  | C2C-C1C | 2.14  | 1.49        | 1.44     |
| 5   | C     | 309 | CHL  | C4C-C3C | 2.14  | 1.48        | 1.45     |
| 6   | A     | 317 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 2   | C     | 301 | 0IE  | C17-C16 | -2.13 | 1.41        | 1.45     |
| 2   | F     | 301 | 0IE  | C13-C12 | -2.13 | 1.41        | 1.45     |
| 7   | E     | 318 | LHG  | O7-C5   | -2.13 | 1.41        | 1.46     |
| 6   | D     | 314 | CLA  | C3B-CAB | -2.13 | 1.43        | 1.47     |
| 6   | B     | 315 | CLA  | CAC-C3C | -2.13 | 1.45        | 1.51     |
| 7   | F     | 318 | LHG  | O7-C5   | -2.13 | 1.41        | 1.46     |
| 6   | F     | 313 | CLA  | CAC-C3C | -2.12 | 1.45        | 1.51     |
| 6   | B     | 315 | CLA  | C1B-NB  | -2.12 | 1.33        | 1.35     |
| 5   | C     | 306 | CHL  | C4C-C3C | 2.12  | 1.48        | 1.45     |
| 2   | A     | 301 | 0IE  | C9-C8   | -2.12 | 1.36        | 1.43     |
| 5   | E     | 312 | CHL  | C1C-NC  | -2.11 | 1.34        | 1.37     |
| 6   | B     | 315 | CLA  | C1D-ND  | 2.11  | 1.40        | 1.37     |
| 5   | D     | 305 | CHL  | C1C-NC  | -2.11 | 1.34        | 1.37     |
| 6   | D     | 308 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 6   | D     | 316 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 6   | B     | 309 | CLA  | C1D-C2D | 2.11  | 1.49        | 1.45     |
| 6   | E     | 316 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 5   | C     | 311 | CHL  | C4C-C3C | 2.10  | 1.48        | 1.45     |
| 5   | B     | 310 | CHL  | C1C-NC  | -2.10 | 1.34        | 1.37     |
| 5   | A     | 312 | CHL  | C1C-NC  | -2.10 | 1.34        | 1.37     |
| 2   | C     | 301 | 0IE  | C6-C7   | -2.10 | 1.41        | 1.45     |
| 6   | B     | 317 | CLA  | C3B-CAB | -2.10 | 1.43        | 1.47     |
| 6   | D     | 314 | CLA  | C4B-CHC | -2.10 | 1.35        | 1.41     |
| 5   | E     | 304 | CHL  | C4C-C3C | 2.09  | 1.48        | 1.45     |
| 6   | A     | 314 | CLA  | CAC-C3C | -2.09 | 1.45        | 1.51     |
| 5   | F     | 308 | CHL  | C4C-C3C | 2.09  | 1.48        | 1.45     |
| 5   | A     | 313 | CHL  | C1C-NC  | -2.09 | 1.34        | 1.37     |
| 2   | E     | 301 | 0IE  | C17-C16 | -2.09 | 1.41        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | B     | 307 | CHL  | C1D-C2D | 2.09  | 1.49        | 1.45     |
| 5   | E     | 311 | CHL  | C1C-NC  | -2.08 | 1.34        | 1.37     |
| 5   | C     | 305 | CHL  | C4C-C3C | 2.08  | 1.48        | 1.45     |
| 2   | E     | 302 | 0IE  | C17-C16 | -2.08 | 1.41        | 1.45     |
| 5   | E     | 308 | CHL  | C1C-NC  | -2.08 | 1.34        | 1.37     |
| 5   | D     | 310 | CHL  | C1C-NC  | -2.07 | 1.34        | 1.37     |
| 5   | B     | 306 | CHL  | C4C-C3C | 2.07  | 1.48        | 1.45     |
| 6   | C     | 316 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 6   | D     | 316 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 6   | D     | 317 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 9   | F     | 320 | 0UR  | C19-C18 | 2.07  | 1.53        | 1.50     |
| 5   | C     | 310 | CHL  | C4C-C3C | 2.06  | 1.48        | 1.45     |
| 6   | A     | 315 | CLA  | C3B-C2B | -2.06 | 1.37        | 1.40     |
| 5   | A     | 313 | CHL  | C4C-C3C | 2.06  | 1.48        | 1.45     |
| 2   | E     | 301 | 0IE  | C13-C12 | -2.06 | 1.41        | 1.45     |
| 5   | B     | 307 | CHL  | C2C-C1C | 2.06  | 1.49        | 1.44     |
| 5   | F     | 309 | CHL  | C1C-NC  | -2.06 | 1.34        | 1.37     |
| 3   | B     | 303 | NEX  | O24-C25 | -2.06 | 1.43        | 1.46     |
| 5   | F     | 310 | CHL  | C4C-C3C | 2.05  | 1.48        | 1.45     |
| 7   | A     | 319 | LHG  | P-O6    | 2.05  | 1.67        | 1.59     |
| 6   | A     | 316 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 5   | A     | 305 | CHL  | C4C-C3C | 2.04  | 1.48        | 1.45     |
| 5   | C     | 309 | CHL  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 5   | F     | 311 | CHL  | C1D-C2D | 2.04  | 1.49        | 1.45     |
| 5   | E     | 310 | CHL  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 6   | B     | 308 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 6   | B     | 317 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 5   | B     | 314 | CHL  | C1C-NC  | -2.03 | 1.34        | 1.37     |
| 5   | F     | 310 | CHL  | CMC-C2C | 2.03  | 1.49        | 1.45     |
| 6   | E     | 315 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 9   | B     | 302 | 0UR  | O42-C2  | -2.03 | 1.19        | 1.23     |
| 6   | B     | 318 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 5   | E     | 308 | CHL  | MG-NC   | 2.03  | 2.11        | 2.06     |
| 6   | C     | 307 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 5   | C     | 305 | CHL  | C2C-C1C | 2.02  | 1.48        | 1.44     |
| 5   | B     | 311 | CHL  | C1C-NC  | -2.02 | 1.34        | 1.37     |
| 6   | E     | 307 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 9   | B     | 325 | 0UR  | C19-C18 | 2.02  | 1.53        | 1.50     |
| 5   | B     | 311 | CHL  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 5   | D     | 309 | CHL  | C1C-NC  | -2.02 | 1.34        | 1.37     |
| 6   | D     | 315 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 5   | C     | 305 | CHL  | C3A-C4A | -2.01 | 1.45        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | F     | 315 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 6   | B     | 317 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 5   | A     | 318 | CHL  | C3A-C2A | -2.01 | 1.52        | 1.54     |
| 5   | F     | 312 | CHL  | C1D-C2D | 2.01  | 1.49        | 1.45     |
| 2   | F     | 301 | OIE  | C6-C7   | -2.01 | 1.41        | 1.45     |
| 7   | D     | 319 | LHG  | P-O6    | 2.01  | 1.67        | 1.59     |
| 5   | A     | 305 | CHL  | C4D-ND  | 2.00  | 1.40        | 1.37     |
| 5   | E     | 305 | CHL  | C1C-NC  | -2.00 | 1.34        | 1.37     |

All (1981) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 5   | B     | 311 | CHL  | O2A-C1-C2   | 26.61  | 178.56      | 108.64   |
| 3   | F     | 303 | NEX  | C15-C35-C34 | 26.60  | 177.96      | 123.47   |
| 3   | E     | 303 | NEX  | C35-C15-C14 | 25.85  | 176.43      | 123.47   |
| 3   | C     | 303 | NEX  | C15-C35-C34 | 24.82  | 174.32      | 123.47   |
| 5   | E     | 309 | CHL  | CMD-C2D-C1D | 24.02  | 167.04      | 124.71   |
| 3   | D     | 303 | NEX  | O24-C25-C24 | 23.90  | 131.34      | 113.38   |
| 5   | D     | 309 | CHL  | CMD-C2D-C1D | 23.16  | 165.53      | 124.71   |
| 3   | B     | 303 | NEX  | C15-C35-C34 | 22.24  | 169.03      | 123.47   |
| 3   | F     | 303 | NEX  | C35-C34-C33 | 21.78  | 158.39      | 127.31   |
| 3   | B     | 303 | NEX  | C35-C34-C33 | 21.67  | 158.24      | 127.31   |
| 5   | E     | 317 | CHL  | CMD-C2D-C1D | 20.99  | 161.71      | 124.71   |
| 3   | C     | 303 | NEX  | O24-C25-C24 | 20.61  | 128.87      | 113.38   |
| 3   | B     | 303 | NEX  | O24-C25-C24 | 20.18  | 128.54      | 113.38   |
| 3   | A     | 303 | NEX  | O24-C25-C24 | 19.68  | 128.16      | 113.38   |
| 5   | A     | 311 | CHL  | OBD-CAD-C3D | -18.98 | 82.85       | 128.52   |
| 3   | D     | 303 | NEX  | C35-C34-C33 | 18.43  | 153.61      | 127.31   |
| 5   | E     | 304 | CHL  | CMD-C2D-C1D | 17.86  | 156.18      | 124.71   |
| 5   | E     | 309 | CHL  | CMD-C2D-C3D | -16.99 | 88.53       | 127.61   |
| 5   | B     | 306 | CHL  | CMD-C2D-C1D | 16.96  | 154.61      | 124.71   |
| 5   | F     | 311 | CHL  | CMD-C2D-C1D | 16.49  | 153.78      | 124.71   |
| 5   | D     | 309 | CHL  | CMD-C2D-C3D | -16.31 | 90.10       | 127.61   |
| 3   | C     | 303 | NEX  | C27-C28-C29 | 16.07  | 150.46      | 125.53   |
| 3   | F     | 303 | NEX  | O24-C25-C24 | 15.49  | 125.02      | 113.38   |
| 3   | E     | 303 | NEX  | C20-C13-C12 | 15.30  | 142.18      | 118.08   |
| 3   | D     | 303 | NEX  | C12-C13-C14 | 14.73  | 141.55      | 118.94   |
| 5   | B     | 313 | CHL  | CMD-C2D-C1D | 14.72  | 150.65      | 124.71   |
| 5   | E     | 317 | CHL  | CMD-C2D-C3D | -14.38 | 94.53       | 127.61   |
| 3   | E     | 303 | NEX  | C12-C13-C14 | -14.14 | 97.24       | 118.94   |
| 5   | F     | 310 | CHL  | OBD-CAD-C3D | -14.04 | 94.73       | 128.52   |
| 5   | E     | 309 | CHL  | CAA-C2A-C1A | 13.85  | 142.81      | 112.14   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 3   | D     | 303 | NEX  | C15-C35-C34 | 13.80  | 151.74      | 123.47   |
| 5   | C     | 318 | CHL  | CMD-C2D-C1D | 13.62  | 148.72      | 124.71   |
| 3   | E     | 303 | NEX  | C15-C35-C34 | 13.57  | 151.27      | 123.47   |
| 3   | A     | 303 | NEX  | C20-C13-C12 | 13.48  | 139.31      | 118.08   |
| 3   | F     | 303 | NEX  | C27-C28-C29 | 12.99  | 145.69      | 125.53   |
| 5   | B     | 319 | CHL  | CMD-C2D-C1D | 12.97  | 147.56      | 124.71   |
| 5   | F     | 304 | CHL  | CMD-C2D-C1D | 12.90  | 147.45      | 124.71   |
| 5   | F     | 305 | CHL  | CMD-C2D-C1D | -12.81 | 102.14      | 124.71   |
| 5   | B     | 319 | CHL  | OBD-CAD-C3D | 12.75  | 159.19      | 128.52   |
| 3   | D     | 303 | NEX  | C20-C13-C12 | -12.31 | 98.68       | 118.08   |
| 5   | F     | 308 | CHL  | OBD-CAD-C3D | 12.26  | 158.03      | 128.52   |
| 3   | A     | 303 | NEX  | C12-C13-C14 | -12.15 | 100.29      | 118.94   |
| 5   | B     | 311 | CHL  | CMD-C2D-C1D | 12.11  | 146.05      | 124.71   |
| 5   | E     | 304 | CHL  | CMD-C2D-C3D | -11.98 | 100.05      | 127.61   |
| 5   | F     | 305 | CHL  | CMD-C2D-C3D | 11.69  | 154.51      | 127.61   |
| 5   | E     | 309 | CHL  | OBD-CAD-C3D | 11.62  | 156.47      | 128.52   |
| 5   | A     | 305 | CHL  | CMD-C2D-C1D | 11.37  | 144.74      | 124.71   |
| 5   | C     | 309 | CHL  | OBD-CAD-C3D | -11.30 | 101.33      | 128.52   |
| 5   | F     | 311 | CHL  | CMD-C2D-C3D | -11.27 | 101.69      | 127.61   |
| 5   | B     | 306 | CHL  | CMD-C2D-C3D | -11.26 | 101.72      | 127.61   |
| 3   | E     | 303 | NEX  | O24-C25-C38 | 11.25  | 128.53      | 115.06   |
| 3   | C     | 303 | NEX  | C26-C27-C28 | 11.04  | 149.34      | 125.99   |
| 5   | D     | 309 | CHL  | CAA-C2A-C1A | 11.02  | 139.02      | 111.81   |
| 5   | D     | 309 | CHL  | OBD-CAD-C3D | 10.92  | 154.80      | 128.52   |
| 5   | E     | 312 | CHL  | CMD-C2D-C1D | 10.84  | 143.82      | 124.71   |
| 5   | A     | 309 | CHL  | CMD-C2D-C1D | 10.79  | 143.73      | 124.71   |
| 3   | C     | 303 | NEX  | C20-C13-C12 | 10.69  | 134.91      | 118.08   |
| 5   | E     | 317 | CHL  | OBD-CAD-C3D | 10.64  | 154.12      | 128.52   |
| 5   | F     | 304 | CHL  | CAA-C2A-C1A | 10.34  | 145.86      | 111.97   |
| 3   | C     | 303 | NEX  | C30-C31-C32 | -10.02 | 91.95       | 123.22   |
| 5   | F     | 317 | CHL  | CMD-C2D-C1D | 9.92   | 142.19      | 124.71   |
| 5   | D     | 306 | CHL  | CMD-C2D-C1D | 9.88   | 142.12      | 124.71   |
| 5   | B     | 313 | CHL  | CMD-C2D-C3D | -9.87  | 104.92      | 127.61   |
| 5   | A     | 310 | CHL  | CHD-C1D-ND  | 9.85   | 133.51      | 124.45   |
| 5   | B     | 310 | CHL  | CMD-C2D-C1D | 9.62   | 141.67      | 124.71   |
| 3   | C     | 303 | NEX  | C35-C15-C14 | 9.60   | 143.15      | 123.47   |
| 3   | E     | 303 | NEX  | C35-C34-C33 | -9.57  | 113.65      | 127.31   |
| 9   | B     | 302 | OUR  | C5-C4-C3    | -9.55  | 115.53      | 127.00   |
| 5   | A     | 305 | CHL  | CAA-C2A-C1A | 9.51   | 143.12      | 111.97   |
| 5   | C     | 311 | CHL  | CHD-C1D-ND  | 9.50   | 133.18      | 124.45   |
| 5   | D     | 305 | CHL  | CHD-C1D-ND  | 9.49   | 133.18      | 124.45   |
| 5   | D     | 318 | CHL  | CHD-C1D-ND  | 9.28   | 132.98      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | B     | 314 | CHL  | CMD-C2D-C1D | 9.27  | 141.04      | 124.71   |
| 3   | A     | 303 | NEX  | C30-C31-C32 | -9.23 | 94.43       | 123.22   |
| 3   | C     | 303 | NEX  | C12-C13-C14 | -9.20 | 104.82      | 118.94   |
| 3   | C     | 303 | NEX  | C35-C34-C33 | 9.07  | 140.25      | 127.31   |
| 5   | B     | 307 | CHL  | CMD-C2D-C1D | -8.98 | 108.89      | 124.71   |
| 5   | E     | 310 | CHL  | CHD-C1D-ND  | 8.97  | 132.70      | 124.45   |
| 5   | B     | 311 | CHL  | OBD-CAD-C3D | 8.94  | 150.03      | 128.52   |
| 5   | E     | 309 | CHL  | CHD-C1D-ND  | 8.91  | 132.64      | 124.45   |
| 5   | C     | 318 | CHL  | CMD-C2D-C3D | -8.87 | 107.20      | 127.61   |
| 5   | C     | 305 | CHL  | C4A-NA-C1A  | 8.82  | 110.67      | 106.71   |
| 5   | F     | 317 | CHL  | CHD-C1D-ND  | 8.75  | 132.49      | 124.45   |
| 5   | F     | 309 | CHL  | CHD-C1D-ND  | 8.72  | 132.47      | 124.45   |
| 5   | C     | 306 | CHL  | CMD-C2D-C1D | -8.70 | 109.39      | 124.71   |
| 5   | C     | 305 | CHL  | CMD-C2D-C1D | 8.65  | 139.95      | 124.71   |
| 5   | F     | 311 | CHL  | OBD-CAD-C3D | 8.60  | 149.22      | 128.52   |
| 5   | C     | 312 | CHL  | CHD-C1D-ND  | 8.59  | 132.35      | 124.45   |
| 5   | B     | 307 | CHL  | CMD-C2D-C3D | 8.59  | 147.37      | 127.61   |
| 5   | B     | 311 | CHL  | CAA-C2A-C1A | 8.47  | 139.74      | 111.97   |
| 5   | D     | 311 | CHL  | OBD-CAD-C3D | -8.46 | 108.17      | 128.52   |
| 5   | B     | 307 | CHL  | OBD-CAD-C3D | 8.44  | 148.84      | 128.52   |
| 5   | B     | 319 | CHL  | CMD-C2D-C3D | -8.43 | 108.22      | 127.61   |
| 5   | A     | 311 | CHL  | CHD-C1D-ND  | 8.40  | 132.17      | 124.45   |
| 5   | E     | 304 | CHL  | CAA-C2A-C1A | 8.39  | 139.47      | 111.97   |
| 5   | A     | 305 | CHL  | C4A-NA-C1A  | 8.38  | 110.47      | 106.71   |
| 5   | F     | 304 | CHL  | OBD-CAD-C3D | 8.26  | 148.39      | 128.52   |
| 5   | C     | 306 | CHL  | CMD-C2D-C3D | 8.16  | 146.38      | 127.61   |
| 5   | B     | 306 | CHL  | CHD-C1D-ND  | 8.15  | 131.95      | 124.45   |
| 5   | F     | 304 | CHL  | CMD-C2D-C3D | -8.11 | 108.97      | 127.61   |
| 5   | B     | 306 | CHL  | C4A-NA-C1A  | 8.10  | 110.35      | 106.71   |
| 3   | C     | 303 | NEX  | C11-C12-C13 | -8.09 | 103.68      | 126.42   |
| 5   | D     | 311 | CHL  | CHD-C1D-ND  | 8.07  | 131.87      | 124.45   |
| 5   | A     | 312 | CHL  | CMD-C2D-C1D | -8.05 | 110.52      | 124.71   |
| 5   | A     | 310 | CHL  | CMD-C2D-C1D | 8.03  | 138.86      | 124.71   |
| 5   | D     | 310 | CHL  | C4A-NA-C1A  | 7.97  | 110.29      | 106.71   |
| 5   | F     | 308 | CHL  | CMD-C2D-C1D | 7.96  | 138.74      | 124.71   |
| 5   | B     | 319 | CHL  | CHD-C1D-ND  | 7.94  | 131.75      | 124.45   |
| 3   | E     | 303 | NEX  | C27-C28-C29 | -7.91 | 113.26      | 125.53   |
| 5   | F     | 310 | CHL  | CHD-C1D-ND  | 7.90  | 131.72      | 124.45   |
| 3   | E     | 303 | NEX  | O24-C25-C24 | 7.86  | 119.29      | 113.38   |
| 5   | B     | 312 | CHL  | CHD-C1D-ND  | 7.85  | 131.66      | 124.45   |
| 5   | A     | 318 | CHL  | CHD-C1D-ND  | 7.82  | 131.64      | 124.45   |
| 5   | D     | 310 | CHL  | CHD-C1D-ND  | 7.79  | 131.61      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | F     | 303 | NEX  | C30-C31-C32 | -7.78 | 98.94       | 123.22   |
| 5   | D     | 305 | CHL  | C4A-NA-C1A  | 7.77  | 110.20      | 106.71   |
| 3   | F     | 303 | NEX  | O24-C25-C38 | 7.75  | 124.35      | 115.06   |
| 5   | D     | 310 | CHL  | CMD-C2D-C1D | 7.75  | 138.36      | 124.71   |
| 5   | A     | 312 | CHL  | CMD-C2D-C3D | 7.72  | 145.38      | 127.61   |
| 5   | B     | 313 | CHL  | CHD-C1D-ND  | 7.71  | 131.54      | 124.45   |
| 6   | B     | 315 | CLA  | C4A-NA-C1A  | 7.68  | 110.16      | 106.71   |
| 5   | C     | 310 | CHL  | CHD-C1D-ND  | 7.67  | 131.51      | 124.45   |
| 5   | B     | 311 | CHL  | CMD-C2D-C3D | -7.66 | 110.00      | 127.61   |
| 5   | B     | 312 | CHL  | C4A-NA-C1A  | 7.65  | 110.15      | 106.71   |
| 5   | B     | 310 | CHL  | CAA-C2A-C1A | 7.64  | 129.06      | 112.14   |
| 5   | F     | 308 | CHL  | CAA-C2A-C1A | 7.63  | 130.66      | 111.81   |
| 5   | D     | 312 | CHL  | C4A-NA-C1A  | 7.62  | 110.13      | 106.71   |
| 5   | A     | 310 | CHL  | OBD-CAD-C3D | 7.60  | 146.82      | 128.52   |
| 6   | F     | 313 | CLA  | C4A-NA-C1A  | 7.53  | 110.09      | 106.71   |
| 5   | A     | 309 | CHL  | C4A-NA-C1A  | 7.52  | 110.09      | 106.71   |
| 5   | E     | 311 | CHL  | CHD-C1D-ND  | 7.51  | 131.35      | 124.45   |
| 5   | C     | 318 | CHL  | CHD-C1D-ND  | 7.47  | 131.32      | 124.45   |
| 5   | E     | 310 | CHL  | C4A-NA-C1A  | 7.47  | 110.06      | 106.71   |
| 5   | D     | 311 | CHL  | C4A-NA-C1A  | 7.42  | 110.04      | 106.71   |
| 5   | B     | 311 | CHL  | C4A-NA-C1A  | 7.30  | 109.99      | 106.71   |
| 5   | E     | 312 | CHL  | C4A-NA-C1A  | 7.30  | 109.99      | 106.71   |
| 5   | F     | 304 | CHL  | C4A-NA-C1A  | 7.28  | 109.98      | 106.71   |
| 5   | E     | 317 | CHL  | CHD-C1D-ND  | 7.26  | 131.12      | 124.45   |
| 6   | B     | 308 | CLA  | C4A-NA-C1A  | 7.22  | 109.95      | 106.71   |
| 9   | B     | 302 | OUR  | C5-C6-C7    | 7.21  | 146.67      | 126.42   |
| 5   | E     | 304 | CHL  | C4A-NA-C1A  | 7.20  | 109.94      | 106.71   |
| 5   | A     | 305 | CHL  | CHD-C1D-ND  | 7.19  | 131.06      | 124.45   |
| 5   | B     | 311 | CHL  | CHD-C1D-ND  | 7.18  | 131.05      | 124.45   |
| 5   | A     | 309 | CHL  | CAA-C2A-C1A | 7.18  | 128.03      | 112.14   |
| 6   | A     | 316 | CLA  | C4A-NA-C1A  | 7.14  | 109.92      | 106.71   |
| 5   | F     | 309 | CHL  | OBD-CAD-C3D | 7.14  | 145.70      | 128.52   |
| 5   | A     | 312 | CHL  | CHD-C1D-ND  | 7.13  | 131.01      | 124.45   |
| 5   | A     | 311 | CHL  | CMD-C2D-C3D | 7.12  | 143.98      | 127.61   |
| 5   | A     | 309 | CHL  | CHD-C1D-ND  | 7.11  | 130.99      | 124.45   |
| 3   | A     | 303 | NEX  | C27-C28-C29 | 7.10  | 136.54      | 125.53   |
| 5   | A     | 311 | CHL  | CMD-C2D-C1D | -7.09 | 112.22      | 124.71   |
| 5   | F     | 304 | CHL  | CHD-C1D-ND  | 7.08  | 130.96      | 124.45   |
| 5   | F     | 309 | CHL  | C4A-NA-C1A  | 7.08  | 109.89      | 106.71   |
| 5   | E     | 312 | CHL  | CHD-C1D-ND  | 7.08  | 130.96      | 124.45   |
| 5   | A     | 305 | CHL  | CMD-C2D-C3D | -7.08 | 111.34      | 127.61   |
| 5   | F     | 308 | CHL  | CHD-C1D-ND  | 7.06  | 130.94      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | E     | 303 | NEX  | C26-C27-C28 | 7.06  | 140.92      | 125.99   |
| 5   | E     | 310 | CHL  | CHB-C4A-NA  | 7.00  | 134.19      | 124.51   |
| 5   | C     | 310 | CHL  | CMD-C2D-C1D | 6.98  | 137.02      | 124.71   |
| 5   | C     | 313 | CHL  | CMD-C2D-C1D | 6.96  | 136.99      | 124.71   |
| 5   | E     | 308 | CHL  | CHD-C1D-ND  | 6.93  | 130.82      | 124.45   |
| 3   | A     | 303 | NEX  | C35-C34-C33 | -6.91 | 117.45      | 127.31   |
| 6   | C     | 307 | CLA  | C4A-NA-C1A  | 6.91  | 109.81      | 106.71   |
| 5   | E     | 309 | CHL  | C4A-NA-C1A  | 6.89  | 109.80      | 106.71   |
| 9   | A     | 322 | OUR  | C43-C3-C4   | -6.88 | 116.71      | 125.02   |
| 5   | B     | 306 | CHL  | OBD-CAD-C3D | 6.85  | 145.00      | 128.52   |
| 5   | A     | 311 | CHL  | C4A-NA-C1A  | 6.85  | 109.78      | 106.71   |
| 6   | D     | 316 | CLA  | C4A-NA-C1A  | 6.83  | 109.78      | 106.71   |
| 5   | E     | 312 | CHL  | OBD-CAD-C3D | 6.81  | 144.91      | 128.52   |
| 3   | A     | 303 | NEX  | C35-C15-C14 | 6.81  | 137.41      | 123.47   |
| 6   | E     | 316 | CLA  | C4A-NA-C1A  | 6.80  | 109.76      | 106.71   |
| 5   | B     | 310 | CHL  | CHD-C1D-ND  | 6.79  | 130.69      | 124.45   |
| 6   | C     | 316 | CLA  | C4A-NA-C1A  | 6.78  | 109.76      | 106.71   |
| 5   | C     | 311 | CHL  | C4A-NA-C1A  | 6.77  | 109.75      | 106.71   |
| 5   | A     | 309 | CHL  | CMD-C2D-C3D | -6.75 | 112.08      | 127.61   |
| 9   | B     | 325 | OUR  | C43-C3-C4   | -6.75 | 116.86      | 125.02   |
| 5   | B     | 319 | CHL  | C4A-NA-C1A  | 6.72  | 109.72      | 106.71   |
| 6   | F     | 306 | CLA  | C4A-NA-C1A  | 6.71  | 109.72      | 106.71   |
| 9   | B     | 302 | OUR  | C4-C5-C6    | 6.67  | 144.04      | 123.22   |
| 5   | E     | 308 | CHL  | C4A-NA-C1A  | 6.67  | 109.70      | 106.71   |
| 9   | D     | 321 | OUR  | C43-C3-C4   | -6.61 | 117.03      | 125.02   |
| 5   | D     | 309 | CHL  | CHD-C1D-ND  | 6.58  | 130.50      | 124.45   |
| 9   | B     | 302 | OUR  | C9-C8-C7    | -6.56 | 117.94      | 127.31   |
| 6   | E     | 315 | CLA  | C4A-NA-C1A  | 6.54  | 109.65      | 106.71   |
| 3   | E     | 303 | NEX  | C38-C25-C26 | -6.53 | 111.32      | 122.26   |
| 5   | E     | 312 | CHL  | CMD-C2D-C3D | -6.52 | 112.62      | 127.61   |
| 5   | F     | 311 | CHL  | CHD-C1D-ND  | 6.52  | 130.44      | 124.45   |
| 6   | F     | 316 | CLA  | C4A-NA-C1A  | 6.51  | 109.64      | 106.71   |
| 5   | D     | 313 | CHL  | CMD-C2D-C1D | 6.51  | 136.19      | 124.71   |
| 5   | C     | 310 | CHL  | C4A-NA-C1A  | 6.51  | 109.63      | 106.71   |
| 5   | C     | 318 | CHL  | C4A-NA-C1A  | 6.49  | 109.62      | 106.71   |
| 6   | F     | 307 | CLA  | C4A-NA-C1A  | 6.49  | 109.62      | 106.71   |
| 3   | D     | 303 | NEX  | C35-C15-C14 | -6.48 | 110.20      | 123.47   |
| 6   | B     | 316 | CLA  | C4A-NA-C1A  | 6.43  | 109.60      | 106.71   |
| 6   | C     | 317 | CLA  | C4A-NA-C1A  | 6.41  | 109.59      | 106.71   |
| 5   | D     | 311 | CHL  | CHB-C4A-NA  | 6.40  | 133.36      | 124.51   |
| 6   | B     | 317 | CLA  | C4A-NA-C1A  | 6.39  | 109.58      | 106.71   |
| 5   | E     | 311 | CHL  | C4A-NA-C1A  | 6.39  | 109.58      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | E     | 317 | CHL  | C4A-NA-C1A  | 6.38  | 109.57      | 106.71   |
| 5   | C     | 313 | CHL  | C4A-NA-C1A  | 6.36  | 109.56      | 106.71   |
| 6   | E     | 306 | CLA  | C4A-NA-C1A  | 6.36  | 109.56      | 106.71   |
| 5   | F     | 317 | CHL  | C1D-ND-C4D  | 6.33  | 110.83      | 106.33   |
| 3   | A     | 303 | NEX  | C11-C12-C13 | -6.33 | 108.62      | 126.42   |
| 5   | E     | 317 | CHL  | CBD-CHA-C1A | 6.33  | 135.96      | 128.50   |
| 6   | A     | 307 | CLA  | C4A-NA-C1A  | 6.32  | 109.55      | 106.71   |
| 6   | E     | 314 | CLA  | C4A-NA-C1A  | 6.31  | 109.54      | 106.71   |
| 6   | C     | 314 | CLA  | C4A-NA-C1A  | 6.31  | 109.54      | 106.71   |
| 5   | D     | 318 | CHL  | C1D-ND-C4D  | 6.28  | 110.80      | 106.33   |
| 6   | F     | 315 | CLA  | C4A-NA-C1A  | 6.27  | 109.53      | 106.71   |
| 5   | E     | 308 | CHL  | CBD-CHA-C1A | 6.26  | 135.88      | 128.50   |
| 6   | D     | 317 | CLA  | C4A-NA-C1A  | 6.24  | 109.51      | 106.71   |
| 5   | D     | 305 | CHL  | C1D-ND-C4D  | 6.22  | 110.76      | 106.33   |
| 2   | A     | 301 | OIE  | C20-C3-C4   | -6.22 | 116.83      | 124.83   |
| 6   | B     | 318 | CLA  | C4A-NA-C1A  | 6.20  | 109.49      | 106.71   |
| 5   | F     | 312 | CHL  | C4A-NA-C1A  | 6.20  | 109.49      | 106.71   |
| 5   | B     | 319 | CHL  | C1D-ND-C4D  | 6.19  | 110.73      | 106.33   |
| 5   | F     | 317 | CHL  | CMD-C2D-C3D | -6.14 | 113.48      | 127.61   |
| 6   | D     | 307 | CLA  | C4A-NA-C1A  | 6.13  | 109.46      | 106.71   |
| 5   | C     | 312 | CHL  | C4A-NA-C1A  | 6.12  | 109.46      | 106.71   |
| 5   | C     | 306 | CHL  | CHD-C1D-ND  | 6.09  | 130.05      | 124.45   |
| 3   | A     | 303 | NEX  | C38-C25-C26 | -6.09 | 112.06      | 122.26   |
| 5   | B     | 314 | CHL  | C4A-NA-C1A  | 6.09  | 109.44      | 106.71   |
| 9   | C     | 321 | OURL | C43-C3-C4   | -6.07 | 117.68      | 125.02   |
| 5   | A     | 311 | CHL  | CHB-C4A-NA  | 6.07  | 132.90      | 124.51   |
| 2   | A     | 301 | OIE  | C4-C3-C2    | 6.06  | 125.28      | 120.08   |
| 5   | D     | 318 | CHL  | C4A-NA-C1A  | 6.06  | 109.43      | 106.71   |
| 6   | A     | 317 | CLA  | C4A-NA-C1A  | 6.06  | 109.43      | 106.71   |
| 5   | C     | 313 | CHL  | CHD-C1D-ND  | 6.06  | 130.02      | 124.45   |
| 5   | D     | 312 | CHL  | CHD-C1D-ND  | 6.05  | 130.02      | 124.45   |
| 6   | A     | 315 | CLA  | C4A-NA-C1A  | 6.05  | 109.43      | 106.71   |
| 5   | B     | 306 | CHL  | C1D-ND-C4D  | 6.05  | 110.63      | 106.33   |
| 5   | A     | 305 | CHL  | OBD-CAD-C3D | 6.03  | 143.02      | 128.52   |
| 6   | C     | 308 | CLA  | C4A-NA-C1A  | 6.03  | 109.42      | 106.71   |
| 5   | F     | 308 | CHL  | C4A-NA-C1A  | 6.02  | 109.41      | 106.71   |
| 5   | F     | 317 | CHL  | C4A-NA-C1A  | 6.00  | 109.41      | 106.71   |
| 5   | E     | 311 | CHL  | CHB-C4A-NA  | 6.00  | 132.81      | 124.51   |
| 3   | C     | 303 | NEX  | C38-C25-C26 | -5.98 | 112.25      | 122.26   |
| 5   | A     | 306 | CHL  | C4A-NA-C1A  | 5.95  | 109.38      | 106.71   |
| 5   | D     | 306 | CHL  | CMD-C2D-C3D | -5.95 | 113.93      | 127.61   |
| 6   | F     | 314 | CLA  | C4A-NA-C1A  | 5.94  | 109.38      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | D     | 308 | CLA  | C4A-NA-C1A  | 5.94  | 109.38      | 106.71   |
| 3   | D     | 303 | NEX  | C38-C25-C26 | -5.93 | 112.32      | 122.26   |
| 9   | C     | 321 | OUR  | C29-C30-C31 | -5.91 | 105.01      | 111.74   |
| 3   | E     | 303 | NEX  | C31-C30-C29 | -5.91 | 118.88      | 127.31   |
| 5   | B     | 307 | CHL  | CHC-C1C-NC  | 5.89  | 133.15      | 124.20   |
| 5   | D     | 306 | CHL  | CHB-C4A-NA  | 5.89  | 132.65      | 124.51   |
| 5   | C     | 311 | CHL  | C2C-C3C-C4C | -5.88 | 102.30      | 106.49   |
| 3   | E     | 303 | NEX  | C30-C31-C32 | -5.88 | 104.86      | 123.22   |
| 5   | F     | 305 | CHL  | C1-O2A-CGA  | 5.87  | 131.86      | 116.44   |
| 3   | D     | 303 | NEX  | C27-C28-C29 | -5.87 | 116.42      | 125.53   |
| 6   | C     | 315 | CLA  | C4A-NA-C1A  | 5.86  | 109.34      | 106.71   |
| 2   | A     | 302 | OIE  | C10-C9-C8   | 5.86  | 135.47      | 123.47   |
| 5   | A     | 309 | CHL  | CHB-C4A-NA  | 5.85  | 132.60      | 124.51   |
| 5   | C     | 318 | CHL  | O2D-CGD-CBD | 5.85  | 121.66      | 111.27   |
| 6   | E     | 307 | CLA  | C4A-NA-C1A  | 5.84  | 109.33      | 106.71   |
| 6   | A     | 314 | CLA  | C4A-NA-C1A  | 5.83  | 109.33      | 106.71   |
| 5   | B     | 319 | CHL  | O2D-CGD-CBD | 5.82  | 121.61      | 111.27   |
| 3   | B     | 303 | NEX  | C26-C27-C28 | -5.81 | 113.70      | 125.99   |
| 5   | C     | 305 | CHL  | CHD-C1D-ND  | 5.81  | 129.79      | 124.45   |
| 5   | B     | 310 | CHL  | CMD-C2D-C3D | -5.80 | 114.26      | 127.61   |
| 5   | B     | 313 | CHL  | C4A-NA-C1A  | 5.79  | 109.31      | 106.71   |
| 3   | B     | 303 | NEX  | C38-C25-C26 | -5.78 | 112.58      | 122.26   |
| 6   | B     | 309 | CLA  | C4A-NA-C1A  | 5.77  | 109.30      | 106.71   |
| 9   | F     | 320 | OUR  | C43-C3-C4   | -5.76 | 118.05      | 125.02   |
| 3   | D     | 303 | NEX  | C15-C14-C13 | -5.75 | 119.10      | 127.31   |
| 5   | A     | 312 | CHL  | C4A-NA-C1A  | 5.75  | 109.29      | 106.71   |
| 3   | F     | 303 | NEX  | C38-C25-C26 | -5.74 | 112.64      | 122.26   |
| 5   | D     | 313 | CHL  | C4A-NA-C1A  | 5.74  | 109.28      | 106.71   |
| 5   | F     | 317 | CHL  | OBD-CAD-C3D | 5.73  | 142.32      | 128.52   |
| 6   | D     | 315 | CLA  | C4A-NA-C1A  | 5.69  | 109.27      | 106.71   |
| 5   | E     | 304 | CHL  | CHD-C1D-ND  | 5.69  | 129.68      | 124.45   |
| 5   | C     | 312 | CHL  | C1D-ND-C4D  | 5.68  | 110.37      | 106.33   |
| 3   | E     | 303 | NEX  | C11-C10-C9  | -5.66 | 119.23      | 127.31   |
| 5   | E     | 312 | CHL  | CHB-C4A-NA  | 5.66  | 132.34      | 124.51   |
| 5   | D     | 313 | CHL  | CHD-C1D-ND  | 5.66  | 129.65      | 124.45   |
| 5   | E     | 304 | CHL  | CHB-C4A-NA  | 5.65  | 132.32      | 124.51   |
| 5   | A     | 306 | CHL  | CHB-C4A-NA  | 5.65  | 132.32      | 124.51   |
| 5   | F     | 317 | CHL  | CAA-C2A-C1A | 5.64  | 130.46      | 111.97   |
| 5   | D     | 306 | CHL  | CHD-C1D-ND  | 5.64  | 129.63      | 124.45   |
| 5   | A     | 313 | CHL  | C1D-CHD-C4C | -5.64 | 113.90      | 126.06   |
| 5   | F     | 310 | CHL  | C4A-NA-C1A  | 5.63  | 109.24      | 106.71   |
| 6   | E     | 313 | CLA  | C4A-NA-C1A  | 5.63  | 109.24      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | A     | 308 | CLA  | C4A-NA-C1A  | 5.62  | 109.23      | 106.71   |
| 9   | B     | 302 | 0UR  | C48-C47-C46 | -5.61 | 119.47      | 125.84   |
| 5   | C     | 305 | CHL  | CHB-C4A-NA  | 5.61  | 132.26      | 124.51   |
| 5   | E     | 311 | CHL  | CMD-C2D-C3D | 5.60  | 140.50      | 127.61   |
| 5   | C     | 309 | CHL  | CHD-C1D-ND  | 5.60  | 129.60      | 124.45   |
| 5   | E     | 305 | CHL  | CHD-C1D-ND  | 5.60  | 129.60      | 124.45   |
| 5   | E     | 308 | CHL  | C1D-ND-C4D  | 5.59  | 110.31      | 106.33   |
| 5   | A     | 318 | CHL  | C1D-ND-C4D  | 5.59  | 110.31      | 106.33   |
| 5   | F     | 309 | CHL  | CAA-C2A-C1A | 5.59  | 125.61      | 111.81   |
| 5   | A     | 318 | CHL  | C4A-NA-C1A  | 5.57  | 109.21      | 106.71   |
| 5   | C     | 309 | CHL  | C4A-NA-C1A  | 5.57  | 109.21      | 106.71   |
| 5   | A     | 310 | CHL  | C4A-NA-C1A  | 5.54  | 109.20      | 106.71   |
| 5   | C     | 311 | CHL  | C1D-ND-C4D  | 5.54  | 110.27      | 106.33   |
| 5   | F     | 317 | CHL  | O2D-CGD-CBD | 5.54  | 121.11      | 111.27   |
| 5   | D     | 313 | CHL  | O2D-CGD-CBD | 5.53  | 121.10      | 111.27   |
| 2   | D     | 301 | 0IE  | C20-C3-C4   | -5.52 | 117.73      | 124.83   |
| 5   | F     | 310 | CHL  | O2D-CGD-CBD | 5.52  | 121.07      | 111.27   |
| 5   | A     | 309 | CHL  | C1D-ND-C4D  | 5.50  | 110.24      | 106.33   |
| 5   | C     | 318 | CHL  | C1D-ND-C4D  | 5.50  | 110.24      | 106.33   |
| 9   | E     | 320 | 0UR  | C29-C30-C31 | -5.47 | 105.51      | 111.74   |
| 5   | C     | 318 | CHL  | OBD-CAD-C3D | 5.46  | 141.66      | 128.52   |
| 5   | B     | 312 | CHL  | CMD-C2D-C1D | 5.45  | 134.32      | 124.71   |
| 5   | B     | 310 | CHL  | O2D-CGD-CBD | 5.44  | 120.94      | 111.27   |
| 5   | C     | 313 | CHL  | C1D-ND-C4D  | 5.44  | 110.20      | 106.33   |
| 5   | F     | 310 | CHL  | C1B-CHB-C4A | -5.44 | 119.34      | 130.12   |
| 5   | A     | 311 | CHL  | C2C-C3C-C4C | -5.44 | 102.61      | 106.49   |
| 5   | C     | 309 | CHL  | CAA-C2A-C1A | 5.41  | 125.17      | 111.81   |
| 5   | D     | 309 | CHL  | O2D-CGD-CBD | 5.41  | 120.88      | 111.27   |
| 5   | F     | 305 | CHL  | CHD-C4C-C3C | -5.40 | 116.90      | 124.84   |
| 5   | F     | 305 | CHL  | O2D-CGD-CBD | 5.40  | 120.86      | 111.27   |
| 5   | D     | 309 | CHL  | C4A-NA-C1A  | 5.39  | 109.13      | 106.71   |
| 2   | A     | 302 | 0IE  | C20-C3-C4   | -5.39 | 117.90      | 124.83   |
| 5   | B     | 310 | CHL  | CHB-C4A-NA  | 5.39  | 131.97      | 124.51   |
| 5   | E     | 310 | CHL  | C2C-C3C-C4C | -5.38 | 102.65      | 106.49   |
| 5   | D     | 310 | CHL  | C1D-ND-C4D  | 5.38  | 110.16      | 106.33   |
| 5   | B     | 306 | CHL  | C1D-CHD-C4C | -5.36 | 114.49      | 126.06   |
| 5   | E     | 317 | CHL  | O2D-CGD-CBD | 5.36  | 120.79      | 111.27   |
| 5   | B     | 314 | CHL  | CHD-C4C-C3C | -5.34 | 116.99      | 124.84   |
| 5   | B     | 310 | CHL  | C4A-NA-C1A  | 5.33  | 109.10      | 106.71   |
| 5   | E     | 309 | CHL  | C1D-ND-C4D  | 5.33  | 110.12      | 106.33   |
| 5   | A     | 313 | CHL  | C1B-CHB-C4A | -5.32 | 119.58      | 130.12   |
| 5   | D     | 311 | CHL  | C1D-ND-C4D  | 5.32  | 110.12      | 106.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | D     | 313 | CHL  | C1D-CHD-C4C | -5.32 | 114.58      | 126.06   |
| 5   | A     | 312 | CHL  | C1D-ND-C4D  | 5.31  | 110.10      | 106.33   |
| 5   | F     | 309 | CHL  | C1D-ND-C4D  | 5.30  | 110.10      | 106.33   |
| 5   | D     | 310 | CHL  | O2D-CGD-CBD | 5.30  | 120.68      | 111.27   |
| 5   | B     | 306 | CHL  | CHB-C4A-NA  | 5.28  | 131.81      | 124.51   |
| 5   | E     | 311 | CHL  | CMD-C2D-C1D | -5.27 | 115.42      | 124.71   |
| 3   | F     | 303 | NEX  | C38-C25-C24 | -5.27 | 108.35      | 114.28   |
| 3   | F     | 303 | NEX  | C15-C14-C13 | -5.27 | 119.79      | 127.31   |
| 5   | F     | 308 | CHL  | O2D-CGD-CBD | 5.27  | 120.62      | 111.27   |
| 3   | B     | 303 | NEX  | C11-C10-C9  | -5.26 | 119.80      | 127.31   |
| 5   | A     | 309 | CHL  | O2D-CGD-CBD | 5.24  | 120.58      | 111.27   |
| 5   | B     | 311 | CHL  | O2D-CGD-CBD | 5.24  | 120.57      | 111.27   |
| 5   | B     | 310 | CHL  | C1B-CHB-C4A | -5.23 | 119.76      | 130.12   |
| 5   | D     | 311 | CHL  | O2D-CGD-CBD | 5.23  | 120.56      | 111.27   |
| 5   | C     | 305 | CHL  | C1D-ND-C4D  | 5.22  | 110.04      | 106.33   |
| 5   | F     | 304 | CHL  | C1D-CHD-C4C | -5.22 | 114.80      | 126.06   |
| 5   | D     | 311 | CHL  | C1B-CHB-C4A | -5.22 | 119.78      | 130.12   |
| 3   | D     | 303 | NEX  | C11-C10-C9  | -5.22 | 119.86      | 127.31   |
| 5   | A     | 318 | CHL  | O2D-CGD-CBD | 5.21  | 120.53      | 111.27   |
| 5   | D     | 306 | CHL  | C1D-CHD-C4C | -5.21 | 114.82      | 126.06   |
| 5   | F     | 310 | CHL  | CHB-C4A-NA  | 5.19  | 131.69      | 124.51   |
| 5   | F     | 304 | CHL  | CHB-C4A-NA  | 5.19  | 131.69      | 124.51   |
| 5   | A     | 305 | CHL  | C1D-ND-C4D  | 5.19  | 110.02      | 106.33   |
| 5   | E     | 312 | CHL  | C1D-CHD-C4C | -5.19 | 114.87      | 126.06   |
| 3   | C     | 303 | NEX  | C15-C14-C13 | -5.18 | 119.91      | 127.31   |
| 5   | C     | 309 | CHL  | O2D-CGD-CBD | 5.17  | 120.46      | 111.27   |
| 6   | D     | 314 | CLA  | C4A-NA-C1A  | 5.17  | 109.03      | 106.71   |
| 5   | D     | 312 | CHL  | CMD-C2D-C3D | 5.17  | 139.51      | 127.61   |
| 5   | D     | 306 | CHL  | C1B-CHB-C4A | -5.16 | 119.89      | 130.12   |
| 5   | E     | 317 | CHL  | C1D-ND-C4D  | 5.16  | 110.00      | 106.33   |
| 9   | B     | 302 | OUR  | C6-C7-C8    | 5.16  | 126.86      | 118.94   |
| 3   | D     | 303 | NEX  | C11-C12-C13 | 5.16  | 140.91      | 126.42   |
| 5   | A     | 310 | CHL  | C1D-CHD-C4C | -5.16 | 114.94      | 126.06   |
| 5   | E     | 310 | CHL  | O2D-CGD-CBD | 5.15  | 120.43      | 111.27   |
| 5   | C     | 310 | CHL  | C1D-ND-C4D  | 5.15  | 110.00      | 106.33   |
| 5   | A     | 310 | CHL  | C1D-ND-C4D  | 5.15  | 109.99      | 106.33   |
| 5   | E     | 310 | CHL  | C1D-CHD-C4C | -5.15 | 114.96      | 126.06   |
| 5   | D     | 312 | CHL  | C1D-ND-C4D  | 5.14  | 109.99      | 106.33   |
| 5   | E     | 308 | CHL  | O2D-CGD-CBD | 5.13  | 120.38      | 111.27   |
| 5   | E     | 305 | CHL  | C1B-CHB-C4A | -5.13 | 119.96      | 130.12   |
| 5   | F     | 312 | CHL  | CHD-C1D-ND  | 5.13  | 129.17      | 124.45   |
| 5   | F     | 311 | CHL  | CHB-C4A-NA  | 5.13  | 131.60      | 124.51   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | F     | 311 | CHL  | C4A-NA-C1A  | 5.12  | 109.01      | 106.71   |
| 5   | D     | 312 | CHL  | C1B-CHB-C4A | -5.12 | 119.97      | 130.12   |
| 5   | E     | 311 | CHL  | C1B-CHB-C4A | -5.12 | 119.97      | 130.12   |
| 5   | B     | 314 | CHL  | C1D-CHD-C4C | -5.12 | 115.01      | 126.06   |
| 5   | C     | 311 | CHL  | C1B-CHB-C4A | -5.12 | 119.98      | 130.12   |
| 5   | F     | 312 | CHL  | C1D-CHD-C4C | -5.12 | 115.01      | 126.06   |
| 5   | B     | 311 | CHL  | C1D-ND-C4D  | 5.12  | 109.97      | 106.33   |
| 5   | D     | 309 | CHL  | C1D-ND-C4D  | 5.12  | 109.97      | 106.33   |
| 5   | A     | 306 | CHL  | CHD-C4C-C3C | -5.11 | 117.33      | 124.84   |
| 5   | A     | 311 | CHL  | C1B-CHB-C4A | -5.11 | 120.00      | 130.12   |
| 5   | A     | 305 | CHL  | CHB-C4A-NA  | 5.10  | 131.57      | 124.51   |
| 5   | F     | 309 | CHL  | CMD-C2D-C1D | 5.10  | 133.70      | 124.71   |
| 3   | C     | 303 | NEX  | C11-C10-C9  | -5.09 | 120.04      | 127.31   |
| 5   | F     | 309 | CHL  | C2C-C3C-C4C | -5.09 | 102.86      | 106.49   |
| 3   | A     | 303 | NEX  | C15-C35-C34 | 5.09  | 133.90      | 123.47   |
| 5   | F     | 308 | CHL  | C1D-ND-C4D  | 5.09  | 109.95      | 106.33   |
| 5   | C     | 309 | CHL  | C1B-CHB-C4A | -5.08 | 120.05      | 130.12   |
| 5   | B     | 313 | CHL  | C1D-ND-C4D  | 5.08  | 109.95      | 106.33   |
| 5   | E     | 312 | CHL  | C1D-ND-C4D  | 5.08  | 109.94      | 106.33   |
| 5   | A     | 311 | CHL  | C1D-ND-C4D  | 5.08  | 109.94      | 106.33   |
| 5   | B     | 310 | CHL  | C1D-ND-C4D  | 5.07  | 109.94      | 106.33   |
| 9   | F     | 320 | OUR  | C29-C30-C31 | -5.07 | 105.97      | 111.74   |
| 5   | A     | 306 | CHL  | CHD-C1D-ND  | 5.07  | 129.12      | 124.45   |
| 5   | C     | 311 | CHL  | C1D-CHD-C4C | -5.07 | 115.12      | 126.06   |
| 5   | C     | 309 | CHL  | C1D-ND-C4D  | 5.06  | 109.93      | 106.33   |
| 5   | A     | 313 | CHL  | O2D-CGD-CBD | 5.06  | 120.26      | 111.27   |
| 9   | B     | 325 | OUR  | C29-C30-C31 | -5.06 | 105.98      | 111.74   |
| 5   | F     | 311 | CHL  | C1B-CHB-C4A | -5.04 | 120.13      | 130.12   |
| 2   | E     | 301 | OIE  | C20-C3-C4   | -5.04 | 118.34      | 124.83   |
| 5   | B     | 307 | CHL  | CHB-C4A-NA  | 5.04  | 131.48      | 124.51   |
| 3   | F     | 303 | NEX  | C11-C10-C9  | -5.04 | 120.12      | 127.31   |
| 5   | A     | 312 | CHL  | C1B-CHB-C4A | -5.04 | 120.14      | 130.12   |
| 9   | D     | 321 | OUR  | C29-C30-C31 | -5.03 | 106.02      | 111.74   |
| 5   | F     | 305 | CHL  | C1B-CHB-C4A | -5.03 | 120.17      | 130.12   |
| 5   | E     | 309 | CHL  | O2D-CGD-CBD | 5.00  | 120.16      | 111.27   |
| 5   | C     | 305 | CHL  | CMD-C2D-C3D | -4.99 | 116.13      | 127.61   |
| 3   | B     | 303 | NEX  | C38-C25-C24 | -4.99 | 108.66      | 114.28   |
| 5   | E     | 310 | CHL  | C1D-ND-C4D  | 4.99  | 109.88      | 106.33   |
| 5   | E     | 312 | CHL  | C1B-CHB-C4A | -4.99 | 120.24      | 130.12   |
| 5   | E     | 304 | CHL  | C1D-CHD-C4C | -4.98 | 115.31      | 126.06   |
| 5   | B     | 307 | CHL  | O2D-CGD-CBD | 4.98  | 120.12      | 111.27   |
| 5   | D     | 313 | CHL  | C1B-CHB-C4A | -4.98 | 120.25      | 130.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | D     | 306 | CHL  | C1-C2-C3    | -4.98 | 117.43      | 126.04   |
| 9   | E     | 320 | OUR  | C43-C3-C4   | -4.98 | 119.00      | 125.02   |
| 5   | E     | 304 | CHL  | OBD-CAD-C3D | 4.98  | 140.50      | 128.52   |
| 5   | D     | 305 | CHL  | CHB-C4A-NA  | 4.97  | 131.38      | 124.51   |
| 5   | C     | 318 | CHL  | C1B-CHB-C4A | -4.95 | 120.32      | 130.12   |
| 5   | A     | 312 | CHL  | CHB-C4A-NA  | 4.95  | 131.35      | 124.51   |
| 5   | F     | 311 | CHL  | O2D-CGD-CBD | 4.94  | 120.04      | 111.27   |
| 5   | A     | 305 | CHL  | C1D-CHD-C4C | -4.93 | 115.41      | 126.06   |
| 5   | D     | 318 | CHL  | O2D-CGD-CBD | 4.93  | 120.03      | 111.27   |
| 2   | A     | 302 | OIE  | C4-C3-C2    | 4.93  | 124.30      | 120.08   |
| 5   | B     | 312 | CHL  | O2D-CGD-CBD | 4.93  | 120.02      | 111.27   |
| 5   | D     | 313 | CHL  | CHD-C4C-C3C | -4.92 | 117.61      | 124.84   |
| 5   | F     | 312 | CHL  | CHB-C4A-NA  | 4.92  | 131.31      | 124.51   |
| 5   | E     | 310 | CHL  | C1B-CHB-C4A | -4.91 | 120.39      | 130.12   |
| 5   | B     | 314 | CHL  | CMD-C2D-C3D | -4.91 | 116.32      | 127.61   |
| 5   | B     | 314 | CHL  | CHD-C4C-NC  | 4.91  | 131.94      | 124.20   |
| 5   | F     | 312 | CHL  | CHD-C4C-C3C | -4.91 | 117.62      | 124.84   |
| 3   | B     | 303 | NEX  | C15-C14-C13 | -4.91 | 120.30      | 127.31   |
| 5   | A     | 318 | CHL  | C1B-CHB-C4A | -4.91 | 120.40      | 130.12   |
| 5   | B     | 314 | CHL  | C1B-CHB-C4A | -4.90 | 120.41      | 130.12   |
| 5   | C     | 311 | CHL  | O2D-CGD-CBD | 4.90  | 119.98      | 111.27   |
| 5   | F     | 308 | CHL  | C1B-CHB-C4A | -4.90 | 120.42      | 130.12   |
| 5   | A     | 306 | CHL  | C1D-CHD-C4C | -4.90 | 115.49      | 126.06   |
| 5   | F     | 309 | CHL  | O2D-CGD-CBD | 4.90  | 119.97      | 111.27   |
| 5   | B     | 319 | CHL  | C1B-CHB-C4A | -4.89 | 120.42      | 130.12   |
| 3   | F     | 303 | NEX  | C35-C15-C14 | 4.89  | 133.49      | 123.47   |
| 7   | B     | 324 | LHG  | O7-C7-C8    | 4.89  | 122.04      | 111.50   |
| 5   | C     | 310 | CHL  | C1B-CHB-C4A | -4.89 | 120.44      | 130.12   |
| 5   | B     | 310 | CHL  | C3A-C2A-C1A | -4.89 | 94.02       | 101.34   |
| 5   | F     | 312 | CHL  | C1B-CHB-C4A | -4.87 | 120.47      | 130.12   |
| 5   | A     | 313 | CHL  | CHD-C4C-C3C | -4.87 | 117.68      | 124.84   |
| 5   | B     | 312 | CHL  | C1D-ND-C4D  | 4.87  | 109.79      | 106.33   |
| 5   | B     | 312 | CHL  | C1B-CHB-C4A | -4.87 | 120.48      | 130.12   |
| 5   | E     | 317 | CHL  | C2C-C3C-C4C | -4.87 | 103.02      | 106.49   |
| 5   | F     | 305 | CHL  | CHB-C4A-NA  | 4.86  | 131.24      | 124.51   |
| 5   | C     | 313 | CHL  | C1D-CHD-C4C | -4.86 | 115.57      | 126.06   |
| 5   | D     | 318 | CHL  | C1B-CHB-C4A | -4.86 | 120.50      | 130.12   |
| 5   | D     | 305 | CHL  | C1D-CHD-C4C | -4.85 | 115.58      | 126.06   |
| 5   | C     | 312 | CHL  | O2D-CGD-CBD | 4.85  | 119.89      | 111.27   |
| 5   | E     | 317 | CHL  | C1D-CHD-C4C | -4.85 | 115.60      | 126.06   |
| 5   | B     | 313 | CHL  | C1B-CHB-C4A | -4.84 | 120.52      | 130.12   |
| 5   | E     | 304 | CHL  | C1B-CHB-C4A | -4.84 | 120.53      | 130.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | E     | 311 | CHL  | C1D-ND-C4D  | 4.83  | 109.77      | 106.33   |
| 5   | A     | 310 | CHL  | CMD-C2D-C3D | -4.83 | 116.50      | 127.61   |
| 3   | A     | 303 | NEX  | C15-C14-C13 | -4.82 | 120.43      | 127.31   |
| 5   | E     | 311 | CHL  | C1D-CHD-C4C | -4.81 | 115.67      | 126.06   |
| 5   | B     | 311 | CHL  | C1D-CHD-C4C | -4.81 | 115.68      | 126.06   |
| 5   | B     | 313 | CHL  | CHB-C4A-NA  | 4.81  | 131.16      | 124.51   |
| 5   | E     | 304 | CHL  | C1D-ND-C4D  | 4.81  | 109.75      | 106.33   |
| 5   | F     | 304 | CHL  | C1D-ND-C4D  | 4.81  | 109.75      | 106.33   |
| 5   | D     | 306 | CHL  | O2D-CGD-CBD | 4.81  | 119.81      | 111.27   |
| 5   | E     | 308 | CHL  | C1B-CHB-C4A | -4.81 | 120.60      | 130.12   |
| 5   | F     | 317 | CHL  | C1B-CHB-C4A | -4.80 | 120.61      | 130.12   |
| 3   | C     | 303 | NEX  | C31-C30-C29 | -4.80 | 120.47      | 127.31   |
| 5   | C     | 306 | CHL  | CHB-C4A-NA  | 4.80  | 131.14      | 124.51   |
| 2   | D     | 301 | OIE  | C4-C3-C2    | 4.79  | 124.19      | 120.08   |
| 5   | F     | 309 | CHL  | C1D-CHD-C4C | -4.79 | 115.72      | 126.06   |
| 5   | B     | 310 | CHL  | C1C-C2C-C3C | -4.79 | 103.31      | 107.11   |
| 5   | B     | 312 | CHL  | C2C-C3C-C4C | -4.79 | 103.08      | 106.49   |
| 5   | C     | 310 | CHL  | C1D-CHD-C4C | -4.78 | 115.74      | 126.06   |
| 5   | D     | 312 | CHL  | C1C-C2C-C3C | -4.78 | 103.32      | 107.11   |
| 5   | B     | 307 | CHL  | C4A-NA-C1A  | 4.78  | 108.85      | 106.71   |
| 5   | C     | 305 | CHL  | C1D-CHD-C4C | -4.78 | 115.76      | 126.06   |
| 5   | D     | 305 | CHL  | O2D-CGD-CBD | 4.77  | 119.75      | 111.27   |
| 5   | B     | 312 | CHL  | C1D-CHD-C4C | -4.77 | 115.77      | 126.06   |
| 5   | C     | 306 | CHL  | C1D-ND-C4D  | 4.77  | 109.72      | 106.33   |
| 5   | E     | 309 | CHL  | C1D-CHD-C4C | -4.76 | 115.78      | 126.06   |
| 5   | E     | 305 | CHL  | CHB-C4A-NA  | 4.75  | 131.08      | 124.51   |
| 5   | D     | 306 | CHL  | CHD-C4C-C3C | -4.75 | 117.86      | 124.84   |
| 5   | B     | 307 | CHL  | CHD-C4C-NC  | 4.75  | 131.68      | 124.20   |
| 3   | D     | 303 | NEX  | C38-C25-C24 | -4.75 | 108.94      | 114.28   |
| 5   | C     | 310 | CHL  | O2D-CGD-CBD | 4.73  | 119.68      | 111.27   |
| 5   | A     | 306 | CHL  | OBD-CAD-C3D | 4.73  | 139.91      | 128.52   |
| 5   | A     | 305 | CHL  | CHC-C1C-NC  | 4.73  | 131.38      | 124.20   |
| 5   | A     | 311 | CHL  | O2D-CGD-CBD | 4.73  | 119.67      | 111.27   |
| 5   | B     | 312 | CHL  | CHB-C4A-NA  | 4.73  | 131.05      | 124.51   |
| 5   | D     | 309 | CHL  | C1B-CHB-C4A | -4.72 | 120.76      | 130.12   |
| 5   | E     | 309 | CHL  | C1C-C2C-C3C | -4.72 | 103.37      | 107.11   |
| 5   | F     | 305 | CHL  | C1D-CHD-C4C | -4.71 | 115.89      | 126.06   |
| 5   | C     | 306 | CHL  | C1D-CHD-C4C | -4.71 | 115.91      | 126.06   |
| 9   | B     | 325 | OUI  | C5-C4-C3    | -4.70 | 121.36      | 127.00   |
| 5   | A     | 310 | CHL  | O2D-CGD-CBD | 4.69  | 119.61      | 111.27   |
| 5   | C     | 312 | CHL  | CHB-C4A-NA  | 4.69  | 131.00      | 124.51   |
| 2   | F     | 301 | OIE  | C20-C3-C4   | -4.68 | 118.81      | 124.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | D     | 318 | CHL  | C1D-CHD-C4C | -4.68 | 115.97      | 126.06   |
| 5   | C     | 313 | CHL  | O2D-CGD-CBD | 4.68  | 119.58      | 111.27   |
| 5   | C     | 311 | CHL  | CHB-C4A-NA  | 4.68  | 130.98      | 124.51   |
| 5   | A     | 309 | CHL  | C1B-CHB-C4A | -4.67 | 120.88      | 130.12   |
| 3   | B     | 303 | NEX  | C31-C30-C29 | -4.66 | 120.66      | 127.31   |
| 3   | B     | 303 | NEX  | C30-C31-C32 | -4.66 | 108.67      | 123.22   |
| 5   | A     | 318 | CHL  | C1D-CHD-C4C | -4.66 | 116.01      | 126.06   |
| 5   | D     | 311 | CHL  | C1D-CHD-C4C | -4.66 | 116.01      | 126.06   |
| 5   | F     | 310 | CHL  | C1D-CHD-C4C | -4.66 | 116.01      | 126.06   |
| 5   | C     | 305 | CHL  | O2D-CGD-CBD | 4.65  | 119.53      | 111.27   |
| 5   | C     | 306 | CHL  | C1B-CHB-C4A | -4.64 | 120.92      | 130.12   |
| 5   | E     | 305 | CHL  | O2D-CGD-CBD | 4.64  | 119.52      | 111.27   |
| 5   | A     | 305 | CHL  | O2D-CGD-CBD | 4.64  | 119.50      | 111.27   |
| 5   | D     | 310 | CHL  | C1D-CHD-C4C | -4.63 | 116.06      | 126.06   |
| 3   | A     | 303 | NEX  | C31-C30-C29 | -4.63 | 120.70      | 127.31   |
| 5   | A     | 306 | CHL  | O2D-CGD-CBD | 4.63  | 119.49      | 111.27   |
| 5   | B     | 310 | CHL  | C1D-CHD-C4C | -4.62 | 116.10      | 126.06   |
| 5   | B     | 312 | CHL  | OBD-CAD-C3D | -4.61 | 117.42      | 128.52   |
| 5   | F     | 305 | CHL  | CHD-C4C-NC  | 4.61  | 131.47      | 124.20   |
| 5   | D     | 312 | CHL  | CMD-C2D-C1D | -4.61 | 116.58      | 124.71   |
| 3   | E     | 303 | NEX  | C15-C14-C13 | -4.61 | 120.73      | 127.31   |
| 5   | A     | 306 | CHL  | C1C-C2C-C3C | -4.61 | 103.46      | 107.11   |
| 5   | E     | 312 | CHL  | O2D-CGD-CBD | 4.61  | 119.45      | 111.27   |
| 3   | C     | 303 | NEX  | C38-C25-C24 | -4.61 | 109.10      | 114.28   |
| 5   | E     | 311 | CHL  | OBD-CAD-C3D | -4.60 | 117.45      | 128.52   |
| 5   | C     | 306 | CHL  | O2D-CGD-CBD | 4.60  | 119.44      | 111.27   |
| 5   | D     | 311 | CHL  | C4D-CHA-C1A | -4.60 | 115.66      | 121.25   |
| 5   | B     | 307 | CHL  | C1D-CHD-C4C | -4.59 | 116.15      | 126.06   |
| 5   | C     | 312 | CHL  | C1B-CHB-C4A | -4.59 | 121.02      | 130.12   |
| 3   | A     | 303 | NEX  | O24-C25-C38 | 4.59  | 120.56      | 115.06   |
| 5   | F     | 305 | CHL  | O2A-C1-C2   | 4.59  | 120.69      | 108.64   |
| 5   | C     | 313 | CHL  | CHB-C4A-NA  | 4.59  | 130.86      | 124.51   |
| 5   | D     | 313 | CHL  | C1C-C2C-C3C | -4.59 | 103.47      | 107.11   |
| 6   | F     | 313 | CLA  | CMB-C2B-C1B | -4.59 | 121.41      | 128.46   |
| 5   | D     | 311 | CHL  | C2C-C3C-C4C | -4.58 | 103.22      | 106.49   |
| 5   | B     | 306 | CHL  | C1B-CHB-C4A | -4.58 | 121.04      | 130.12   |
| 5   | A     | 312 | CHL  | OBD-CAD-C3D | -4.58 | 117.50      | 128.52   |
| 5   | D     | 305 | CHL  | C1B-CHB-C4A | -4.58 | 121.05      | 130.12   |
| 3   | A     | 303 | NEX  | C38-C25-C24 | -4.58 | 109.13      | 114.28   |
| 5   | F     | 312 | CHL  | CHD-C4C-NC  | 4.57  | 131.41      | 124.20   |
| 5   | C     | 305 | CHL  | C1B-CHB-C4A | -4.57 | 121.07      | 130.12   |
| 5   | D     | 318 | CHL  | C4D-CHA-C1A | -4.57 | 115.69      | 121.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | F     | 308 | CHL  | C1D-CHD-C4C | -4.57 | 116.21      | 126.06   |
| 5   | A     | 309 | CHL  | C1D-CHD-C4C | -4.56 | 116.21      | 126.06   |
| 5   | D     | 305 | CHL  | C2C-C3C-C4C | -4.56 | 103.24      | 106.49   |
| 5   | F     | 310 | CHL  | C2C-C3C-C4C | -4.56 | 103.24      | 106.49   |
| 5   | B     | 314 | CHL  | CHB-C4A-NA  | 4.56  | 130.82      | 124.51   |
| 5   | A     | 313 | CHL  | C4A-NA-C1A  | 4.56  | 108.75      | 106.71   |
| 5   | E     | 309 | CHL  | C1B-CHB-C4A | -4.56 | 121.09      | 130.12   |
| 5   | E     | 311 | CHL  | C2C-C3C-C4C | -4.56 | 103.24      | 106.49   |
| 5   | F     | 310 | CHL  | C1D-ND-C4D  | 4.55  | 109.57      | 106.33   |
| 5   | D     | 313 | CHL  | C1D-ND-C4D  | 4.55  | 109.57      | 106.33   |
| 6   | E     | 307 | CLA  | CMB-C2B-C1B | -4.55 | 121.47      | 128.46   |
| 5   | A     | 311 | CHL  | C1D-CHD-C4C | -4.55 | 116.25      | 126.06   |
| 5   | D     | 312 | CHL  | C1D-CHD-C4C | -4.55 | 116.25      | 126.06   |
| 5   | A     | 310 | CHL  | C2C-C3C-C4C | -4.54 | 103.25      | 106.49   |
| 5   | F     | 308 | CHL  | CMD-C2D-C3D | -4.54 | 117.17      | 127.61   |
| 5   | C     | 310 | CHL  | C1C-C2C-C3C | -4.54 | 103.51      | 107.11   |
| 5   | B     | 311 | CHL  | C1C-C2C-C3C | -4.54 | 103.51      | 107.11   |
| 5   | A     | 306 | CHL  | C1B-CHB-C4A | -4.54 | 121.13      | 130.12   |
| 5   | C     | 312 | CHL  | CMD-C2D-C1D | 4.54  | 132.71      | 124.71   |
| 5   | E     | 310 | CHL  | CHC-C1C-NC  | 4.53  | 131.07      | 124.20   |
| 5   | E     | 305 | CHL  | C1D-CHD-C4C | -4.52 | 116.31      | 126.06   |
| 9   | A     | 322 | OUR  | O44-C45-C46 | 4.51  | 123.54      | 111.55   |
| 5   | B     | 313 | CHL  | C1D-CHD-C4C | -4.50 | 116.34      | 126.06   |
| 5   | E     | 308 | CHL  | CHB-C4A-NA  | 4.50  | 130.73      | 124.51   |
| 5   | D     | 310 | CHL  | C1B-CHB-C4A | -4.50 | 121.21      | 130.12   |
| 5   | F     | 311 | CHL  | C1D-CHD-C4C | -4.49 | 116.36      | 126.06   |
| 5   | E     | 310 | CHL  | C4D-CHA-C1A | -4.49 | 115.78      | 121.25   |
| 5   | C     | 313 | CHL  | C1B-CHB-C4A | -4.49 | 121.23      | 130.12   |
| 2   | F     | 301 | OIE  | C10-C9-C8   | 4.48  | 132.66      | 123.47   |
| 9   | E     | 320 | OUR  | C4-C3-C2    | -4.48 | 116.23      | 120.08   |
| 5   | D     | 310 | CHL  | CMD-C2D-C3D | -4.48 | 117.31      | 127.61   |
| 5   | F     | 311 | CHL  | C1D-ND-C4D  | 4.48  | 109.52      | 106.33   |
| 5   | F     | 305 | CHL  | C4A-NA-C1A  | 4.47  | 108.71      | 106.71   |
| 5   | F     | 311 | CHL  | C1C-C2C-C3C | -4.46 | 103.57      | 107.11   |
| 5   | A     | 312 | CHL  | C1D-CHD-C4C | -4.44 | 116.47      | 126.06   |
| 5   | F     | 308 | CHL  | C1C-C2C-C3C | -4.44 | 103.59      | 107.11   |
| 5   | C     | 318 | CHL  | C2C-C3C-C4C | -4.44 | 103.33      | 106.49   |
| 5   | A     | 311 | CHL  | C4D-CHA-C1A | -4.43 | 115.86      | 121.25   |
| 5   | D     | 310 | CHL  | C1C-C2C-C3C | -4.43 | 103.60      | 107.11   |
| 5   | B     | 311 | CHL  | C1B-CHB-C4A | -4.43 | 121.35      | 130.12   |
| 5   | D     | 306 | CHL  | CHC-C1C-NC  | 4.42  | 130.92      | 124.20   |
| 5   | E     | 308 | CHL  | C1D-CHD-C4C | -4.42 | 116.53      | 126.06   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | F     | 317 | CHL  | C1D-CHD-C4C | -4.42 | 116.53      | 126.06   |
| 9   | B     | 302 | OUR  | C43-C3-C4   | -4.42 | 119.68      | 125.02   |
| 5   | C     | 318 | CHL  | C1D-CHD-C4C | -4.42 | 116.53      | 126.06   |
| 5   | D     | 309 | CHL  | C1C-C2C-C3C | -4.41 | 103.61      | 107.11   |
| 5   | F     | 312 | CHL  | C1D-ND-C4D  | 4.41  | 109.47      | 106.33   |
| 5   | E     | 308 | CHL  | C2C-C3C-C4C | -4.41 | 103.34      | 106.49   |
| 5   | F     | 317 | CHL  | C2C-C3C-C4C | -4.40 | 103.36      | 106.49   |
| 5   | A     | 318 | CHL  | CMD-C2D-C1D | 4.38  | 132.43      | 124.71   |
| 5   | A     | 305 | CHL  | C4D-CHA-C1A | -4.38 | 115.92      | 121.25   |
| 3   | B     | 303 | NEX  | O24-C25-C38 | 4.38  | 120.30      | 115.06   |
| 5   | E     | 305 | CHL  | C1D-ND-C4D  | 4.37  | 109.44      | 106.33   |
| 5   | A     | 310 | CHL  | CHB-C4A-NA  | 4.37  | 130.56      | 124.51   |
| 5   | B     | 307 | CHL  | C1-C2-C3    | -4.37 | 118.49      | 126.04   |
| 5   | F     | 317 | CHL  | CHB-C4A-NA  | 4.37  | 130.55      | 124.51   |
| 5   | C     | 306 | CHL  | C1-C2-C3    | -4.37 | 118.49      | 126.04   |
| 5   | A     | 318 | CHL  | C1C-C2C-C3C | -4.36 | 103.65      | 107.11   |
| 5   | A     | 313 | CHL  | CHD-C4C-NC  | 4.36  | 131.08      | 124.20   |
| 5   | E     | 317 | CHL  | C1B-CHB-C4A | -4.36 | 121.49      | 130.12   |
| 5   | B     | 319 | CHL  | C1D-CHD-C4C | -4.35 | 116.66      | 126.06   |
| 5   | B     | 307 | CHL  | C1C-C2C-C3C | -4.35 | 103.66      | 107.11   |
| 9   | B     | 302 | OUR  | C29-C30-C31 | -4.35 | 106.79      | 111.74   |
| 6   | D     | 314 | CLA  | CMB-C2B-C1B | -4.35 | 121.78      | 128.46   |
| 2   | E     | 301 | OIE  | C23-C16-C15 | -4.34 | 116.84      | 122.92   |
| 6   | D     | 308 | CLA  | CMB-C2B-C1B | -4.33 | 121.81      | 128.46   |
| 5   | C     | 309 | CHL  | CHB-C4A-NA  | 4.33  | 130.50      | 124.51   |
| 6   | C     | 314 | CLA  | CMB-C2B-C1B | -4.32 | 121.82      | 128.46   |
| 6   | A     | 314 | CLA  | CMB-C2B-C1B | -4.32 | 121.82      | 128.46   |
| 6   | C     | 308 | CLA  | CMB-C2B-C1B | -4.32 | 121.82      | 128.46   |
| 5   | E     | 304 | CHL  | CHC-C1C-NC  | 4.32  | 130.76      | 124.20   |
| 2   | F     | 302 | OIE  | C20-C3-C4   | -4.32 | 119.28      | 124.83   |
| 5   | D     | 305 | CHL  | OBD-CAD-C3D | -4.31 | 118.15      | 128.52   |
| 5   | B     | 306 | CHL  | C4D-CHA-C1A | -4.31 | 116.01      | 121.25   |
| 5   | A     | 305 | CHL  | C1B-CHB-C4A | -4.30 | 121.60      | 130.12   |
| 5   | F     | 312 | CHL  | C1C-C2C-C3C | -4.30 | 103.70      | 107.11   |
| 2   | E     | 302 | OIE  | C23-C16-C15 | -4.30 | 116.90      | 122.92   |
| 5   | D     | 309 | CHL  | C1D-CHD-C4C | -4.30 | 116.78      | 126.06   |
| 5   | C     | 312 | CHL  | C1D-CHD-C4C | -4.30 | 116.79      | 126.06   |
| 3   | D     | 303 | NEX  | C31-C30-C29 | -4.30 | 121.18      | 127.31   |
| 2   | C     | 302 | OIE  | C20-C3-C4   | -4.29 | 119.31      | 124.83   |
| 2   | A     | 302 | OIE  | C6-C7-C8    | 4.29  | 125.53      | 118.94   |
| 9   | A     | 322 | OUR  | C10-C11-C12 | -4.29 | 121.19      | 127.31   |
| 5   | B     | 307 | CHL  | CHD-C4C-C3C | -4.29 | 118.54      | 124.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | F     | 304 | CHL  | C1B-CHB-C4A | -4.28 | 121.64      | 130.12   |
| 5   | D     | 318 | CHL  | C1C-C2C-C3C | -4.27 | 103.72      | 107.11   |
| 2   | F     | 302 | 0IE  | C9-C10-C11  | 4.27  | 132.23      | 123.47   |
| 2   | D     | 301 | 0IE  | C23-C16-C15 | -4.27 | 116.94      | 122.92   |
| 5   | D     | 310 | CHL  | CHB-C4A-NA  | 4.27  | 130.41      | 124.51   |
| 5   | C     | 310 | CHL  | CHB-C4A-NA  | 4.26  | 130.41      | 124.51   |
| 9   | B     | 325 | 0UR  | C34-C27-C1  | -4.26 | 118.90      | 124.49   |
| 6   | E     | 313 | CLA  | CMB-C2B-C1B | -4.26 | 121.92      | 128.46   |
| 5   | F     | 305 | CHL  | C1C-C2C-C3C | -4.26 | 103.73      | 107.11   |
| 2   | B     | 301 | 0IE  | C23-C16-C15 | -4.26 | 116.96      | 122.92   |
| 5   | F     | 308 | CHL  | CHB-C4A-NA  | 4.26  | 130.40      | 124.51   |
| 2   | B     | 301 | 0IE  | C20-C3-C4   | -4.26 | 119.36      | 124.83   |
| 5   | B     | 307 | CHL  | C1B-CHB-C4A | -4.25 | 121.69      | 130.12   |
| 5   | F     | 309 | CHL  | C1B-CHB-C4A | -4.25 | 121.70      | 130.12   |
| 5   | B     | 314 | CHL  | C1D-ND-C4D  | 4.25  | 109.35      | 106.33   |
| 9   | A     | 322 | 0UR  | C34-C27-C1  | -4.25 | 118.92      | 124.49   |
| 5   | D     | 309 | CHL  | CHB-C4A-NA  | 4.24  | 130.38      | 124.51   |
| 7   | E     | 318 | LHG  | O4-P-O5     | 4.24  | 133.19      | 112.24   |
| 5   | A     | 310 | CHL  | C1B-CHB-C4A | -4.24 | 121.72      | 130.12   |
| 5   | C     | 306 | CHL  | C4A-NA-C1A  | 4.24  | 108.61      | 106.71   |
| 5   | F     | 304 | CHL  | C1C-C2C-C3C | -4.23 | 103.75      | 107.11   |
| 5   | A     | 310 | CHL  | C4D-CHA-C1A | -4.22 | 116.11      | 121.25   |
| 5   | A     | 306 | CHL  | CHD-C4C-NC  | 4.21  | 130.84      | 124.20   |
| 5   | C     | 309 | CHL  | C2C-C3C-C4C | -4.21 | 103.49      | 106.49   |
| 5   | B     | 313 | CHL  | O2D-CGD-CBD | 4.21  | 118.75      | 111.27   |
| 5   | F     | 310 | CHL  | C1C-C2C-C3C | -4.21 | 103.78      | 107.11   |
| 5   | C     | 309 | CHL  | C1D-CHD-C4C | -4.20 | 116.99      | 126.06   |
| 9   | A     | 322 | 0UR  | C5-C4-C3    | -4.20 | 121.96      | 127.00   |
| 5   | D     | 312 | CHL  | CHB-C4A-NA  | 4.19  | 130.31      | 124.51   |
| 7   | C     | 304 | LHG  | O4-P-O5     | 4.18  | 132.92      | 112.24   |
| 6   | C     | 307 | CLA  | O2D-CGD-O1D | -4.18 | 115.66      | 123.84   |
| 5   | E     | 304 | CHL  | C1C-C2C-C3C | -4.18 | 103.80      | 107.11   |
| 7   | C     | 319 | LHG  | O4-P-O5     | 4.18  | 132.90      | 112.24   |
| 3   | C     | 303 | NEX  | O24-C25-C38 | 4.18  | 120.06      | 115.06   |
| 5   | D     | 318 | CHL  | CHB-C4A-NA  | 4.18  | 130.29      | 124.51   |
| 2   | F     | 301 | 0IE  | C23-C16-C15 | -4.18 | 117.07      | 122.92   |
| 7   | B     | 320 | LHG  | O4-P-O5     | 4.17  | 132.88      | 112.24   |
| 5   | B     | 314 | CHL  | O2D-CGD-CBD | 4.17  | 118.68      | 111.27   |
| 5   | C     | 318 | CHL  | C1C-C2C-C3C | -4.17 | 103.81      | 107.11   |
| 9   | E     | 320 | 0UR  | C34-C27-C1  | -4.16 | 119.02      | 124.49   |
| 9   | B     | 325 | 0UR  | O44-C45-C46 | 4.16  | 122.62      | 111.55   |
| 5   | B     | 313 | CHL  | C1C-C2C-C3C | -4.16 | 103.81      | 107.11   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 9   | B     | 302 | 0UR  | C20-C7-C8   | -4.15 | 117.11      | 122.92   |
| 5   | B     | 306 | CHL  | CHA-C4D-ND  | 4.15  | 141.17      | 132.50   |
| 5   | B     | 306 | CHL  | C1-C2-C3    | -4.13 | 118.89      | 126.04   |
| 5   | E     | 305 | CHL  | C1C-C2C-C3C | -4.13 | 103.83      | 107.11   |
| 5   | E     | 311 | CHL  | O2D-CGD-CBD | 4.13  | 118.60      | 111.27   |
| 5   | F     | 304 | CHL  | CHC-C1C-NC  | 4.12  | 130.46      | 124.20   |
| 2   | D     | 302 | 0IE  | C10-C9-C8   | 4.12  | 131.91      | 123.47   |
| 5   | C     | 305 | CHL  | C1C-C2C-C3C | -4.12 | 103.84      | 107.11   |
| 5   | F     | 312 | CHL  | O2D-CGD-CBD | 4.12  | 118.58      | 111.27   |
| 6   | F     | 315 | CLA  | CMB-C2B-C1B | -4.12 | 122.14      | 128.46   |
| 3   | F     | 303 | NEX  | C31-C30-C29 | -4.12 | 121.44      | 127.31   |
| 5   | C     | 311 | CHL  | CHA-C4D-ND  | 4.12  | 141.11      | 132.50   |
| 5   | C     | 306 | CHL  | C1C-C2C-C3C | -4.11 | 103.85      | 107.11   |
| 5   | E     | 312 | CHL  | C2C-C3C-C4C | -4.11 | 103.56      | 106.49   |
| 9   | D     | 321 | 0UR  | C34-C27-C1  | -4.11 | 119.10      | 124.49   |
| 5   | E     | 309 | CHL  | CHB-C4A-NA  | 4.11  | 130.19      | 124.51   |
| 5   | A     | 312 | CHL  | O2D-CGD-CBD | 4.11  | 118.57      | 111.27   |
| 5   | B     | 306 | CHL  | C2C-C3C-C4C | -4.11 | 103.56      | 106.49   |
| 5   | C     | 311 | CHL  | C3A-C2A-C1A | -4.10 | 95.19       | 101.34   |
| 5   | B     | 312 | CHL  | C4D-CHA-C1A | -4.10 | 116.26      | 121.25   |
| 5   | D     | 305 | CHL  | C1C-C2C-C3C | -4.10 | 103.86      | 107.11   |
| 5   | A     | 318 | CHL  | C2C-C3C-C4C | -4.10 | 103.57      | 106.49   |
| 2   | C     | 301 | 0IE  | C23-C16-C15 | -4.09 | 117.19      | 122.92   |
| 5   | B     | 314 | CHL  | C1C-C2C-C3C | -4.08 | 103.88      | 107.11   |
| 6   | A     | 308 | CLA  | CMB-C2B-C1B | -4.08 | 122.19      | 128.46   |
| 5   | A     | 313 | CHL  | CHD-C1D-ND  | 4.08  | 128.20      | 124.45   |
| 7   | D     | 319 | LHG  | O4-P-O5     | 4.08  | 132.41      | 112.24   |
| 5   | E     | 312 | CHL  | CHC-C1C-NC  | 4.08  | 130.39      | 124.20   |
| 5   | B     | 319 | CHL  | C1C-C2C-C3C | -4.08 | 103.88      | 107.11   |
| 2   | E     | 302 | 0IE  | C9-C10-C11  | 4.07  | 131.82      | 123.47   |
| 6   | F     | 313 | CLA  | CMB-C2B-C3B | 4.07  | 132.29      | 124.68   |
| 5   | D     | 305 | CHL  | CHA-C4D-ND  | 4.06  | 140.99      | 132.50   |
| 2   | F     | 302 | 0IE  | C23-C16-C15 | -4.05 | 117.25      | 122.92   |
| 5   | B     | 307 | CHL  | C1D-ND-C4D  | 4.05  | 109.21      | 106.33   |
| 5   | B     | 306 | CHL  | O2D-CGD-CBD | 4.05  | 118.47      | 111.27   |
| 7   | F     | 318 | LHG  | O4-P-O5     | 4.04  | 132.23      | 112.24   |
| 5   | A     | 309 | CHL  | CHC-C1C-NC  | 4.03  | 130.32      | 124.20   |
| 5   | E     | 304 | CHL  | O2D-CGD-CBD | 4.03  | 118.43      | 111.27   |
| 2   | A     | 302 | 0IE  | C23-C16-C15 | -4.02 | 117.29      | 122.92   |
| 5   | D     | 311 | CHL  | CHC-C1C-NC  | 4.02  | 130.31      | 124.20   |
| 5   | B     | 319 | CHL  | CHB-C4A-NA  | 4.01  | 130.06      | 124.51   |
| 6   | B     | 309 | CLA  | CMB-C2B-C1B | -4.01 | 122.30      | 128.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | D     | 312 | CHL  | O2D-CGD-CBD | 4.01  | 118.39      | 111.27   |
| 5   | C     | 312 | CHL  | C2C-C3C-C4C | -4.01 | 103.63      | 106.49   |
| 2   | C     | 302 | 0IE  | C23-C16-C15 | -4.00 | 117.31      | 122.92   |
| 5   | F     | 305 | CHL  | CHC-C1C-NC  | 4.00  | 130.27      | 124.20   |
| 5   | D     | 306 | CHL  | C2C-C3C-C4C | -4.00 | 103.64      | 106.49   |
| 6   | B     | 317 | CLA  | CMB-C2B-C1B | -4.00 | 122.32      | 128.46   |
| 6   | F     | 316 | CLA  | CMB-C2B-C1B | -4.00 | 122.32      | 128.46   |
| 5   | F     | 304 | CHL  | O2D-CGD-CBD | 4.00  | 118.37      | 111.27   |
| 2   | E     | 302 | 0IE  | C10-C9-C8   | 4.00  | 131.66      | 123.47   |
| 5   | B     | 306 | CHL  | CHC-C1C-NC  | 3.99  | 130.26      | 124.20   |
| 7   | A     | 319 | LHG  | O4-P-O5     | 3.99  | 131.95      | 112.24   |
| 5   | B     | 319 | CHL  | C2C-C3C-C4C | -3.99 | 103.65      | 106.49   |
| 6   | D     | 307 | CLA  | CMB-C2B-C1B | -3.99 | 122.34      | 128.46   |
| 5   | A     | 311 | CHL  | CHC-C1C-NC  | 3.98  | 130.25      | 124.20   |
| 5   | D     | 312 | CHL  | OBD-CAD-C3D | -3.98 | 118.94      | 128.52   |
| 2   | A     | 302 | 0IE  | C21-C7-C8   | -3.98 | 117.35      | 122.92   |
| 6   | D     | 315 | CLA  | CMB-C2B-C1B | -3.98 | 122.35      | 128.46   |
| 5   | D     | 318 | CHL  | C2C-C3C-C4C | -3.97 | 103.66      | 106.49   |
| 5   | A     | 310 | CHL  | C1C-C2C-C3C | -3.97 | 103.97      | 107.11   |
| 5   | E     | 317 | CHL  | CHD-C4C-C3C | -3.96 | 119.02      | 124.84   |
| 5   | B     | 312 | CHL  | C1C-C2C-C3C | -3.96 | 103.97      | 107.11   |
| 2   | D     | 302 | 0IE  | C23-C16-C15 | -3.95 | 117.38      | 122.92   |
| 3   | A     | 303 | NEX  | C11-C10-C9  | -3.95 | 121.67      | 127.31   |
| 6   | B     | 315 | CLA  | CMB-C2B-C1B | -3.94 | 122.40      | 128.46   |
| 5   | C     | 305 | CHL  | CHC-C1C-NC  | 3.94  | 130.19      | 124.20   |
| 6   | D     | 316 | CLA  | CMB-C2B-C1B | -3.93 | 122.42      | 128.46   |
| 5   | A     | 309 | CHL  | C2C-C3C-C4C | -3.93 | 103.69      | 106.49   |
| 2   | E     | 301 | 0IE  | C10-C9-C8   | 3.93  | 131.52      | 123.47   |
| 5   | F     | 317 | CHL  | C1C-C2C-C3C | -3.92 | 104.00      | 107.11   |
| 2   | C     | 301 | 0IE  | C20-C3-C4   | -3.92 | 119.78      | 124.83   |
| 5   | F     | 304 | CHL  | CHD-C4C-C3C | -3.92 | 119.07      | 124.84   |
| 5   | F     | 308 | CHL  | C2C-C3C-C4C | -3.92 | 103.69      | 106.49   |
| 5   | D     | 318 | CHL  | OBD-CAD-C3D | -3.92 | 119.08      | 128.52   |
| 5   | A     | 313 | CHL  | C1-C2-C3    | -3.92 | 119.27      | 126.04   |
| 5   | D     | 318 | CHL  | CHA-C4D-ND  | 3.92  | 140.69      | 132.50   |
| 5   | A     | 306 | CHL  | C1D-ND-C4D  | 3.91  | 109.12      | 106.33   |
| 6   | C     | 316 | CLA  | CMB-C2B-C1B | -3.91 | 122.45      | 128.46   |
| 5   | D     | 313 | CHL  | CHD-C4C-NC  | 3.91  | 130.37      | 124.20   |
| 5   | D     | 309 | CHL  | C2C-C3C-C4C | -3.91 | 103.70      | 106.49   |
| 5   | C     | 312 | CHL  | C1C-C2C-C3C | -3.91 | 104.01      | 107.11   |
| 5   | C     | 313 | CHL  | C1C-C2C-C3C | -3.90 | 104.02      | 107.11   |
| 2   | C     | 302 | 0IE  | C9-C10-C11  | 3.90  | 131.47      | 123.47   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | F     | 309 | CHL  | CHA-C4D-ND  | 3.90  | 140.66      | 132.50   |
| 5   | A     | 309 | CHL  | C1C-C2C-C3C | -3.90 | 104.02      | 107.11   |
| 5   | A     | 313 | CHL  | C1C-C2C-C3C | -3.90 | 104.02      | 107.11   |
| 2   | C     | 301 | 0IE  | C10-C9-C8   | 3.90  | 131.46      | 123.47   |
| 5   | C     | 312 | CHL  | C4D-CHA-C1A | -3.90 | 116.50      | 121.25   |
| 5   | C     | 318 | CHL  | CAA-C2A-C1A | 3.90  | 124.75      | 111.97   |
| 5   | A     | 313 | CHL  | CHC-C1C-NC  | 3.89  | 130.10      | 124.20   |
| 5   | A     | 318 | CHL  | CHB-C4A-NA  | 3.88  | 129.88      | 124.51   |
| 5   | A     | 305 | CHL  | C1C-C2C-C3C | -3.88 | 104.03      | 107.11   |
| 5   | B     | 319 | CHL  | CAA-C2A-C1A | -3.88 | 99.26       | 111.97   |
| 5   | E     | 317 | CHL  | CHB-C4A-NA  | 3.88  | 129.88      | 124.51   |
| 6   | F     | 307 | CLA  | CMB-C2B-C1B | -3.88 | 122.51      | 128.46   |
| 5   | E     | 305 | CHL  | CHD-C4C-C3C | -3.87 | 119.15      | 124.84   |
| 5   | E     | 305 | CHL  | C3A-C2A-C1A | -3.87 | 95.55       | 101.34   |
| 5   | C     | 305 | CHL  | CHD-C4C-C3C | -3.84 | 119.19      | 124.84   |
| 5   | C     | 306 | CHL  | CHD-C4C-C3C | -3.84 | 119.19      | 124.84   |
| 6   | F     | 314 | CLA  | CMB-C2B-C1B | -3.83 | 122.58      | 128.46   |
| 2   | C     | 301 | 0IE  | C9-C10-C11  | 3.83  | 131.31      | 123.47   |
| 5   | C     | 310 | CHL  | C2C-C3C-C4C | -3.82 | 103.77      | 106.49   |
| 5   | A     | 313 | CHL  | CHB-C4A-NA  | 3.82  | 129.79      | 124.51   |
| 5   | A     | 313 | CHL  | C1D-ND-C4D  | 3.82  | 109.05      | 106.33   |
| 5   | A     | 312 | CHL  | C2C-C3C-C4C | -3.82 | 103.77      | 106.49   |
| 6   | C     | 315 | CLA  | CMB-C2B-C1B | -3.81 | 122.61      | 128.46   |
| 5   | A     | 309 | CHL  | C3A-C2A-C1A | -3.80 | 95.64       | 101.34   |
| 5   | A     | 312 | CHL  | C1C-C2C-C3C | -3.80 | 104.10      | 107.11   |
| 5   | E     | 308 | CHL  | C1C-C2C-C3C | -3.80 | 104.10      | 107.11   |
| 5   | B     | 306 | CHL  | C1C-C2C-C3C | -3.80 | 104.10      | 107.11   |
| 5   | A     | 312 | CHL  | CHC-C1C-NC  | 3.79  | 129.96      | 124.20   |
| 5   | E     | 311 | CHL  | CHC-C1C-NC  | 3.79  | 129.96      | 124.20   |
| 5   | E     | 312 | CHL  | C1C-C2C-C3C | -3.79 | 104.11      | 107.11   |
| 2   | A     | 301 | 0IE  | C21-C7-C8   | -3.79 | 117.62      | 122.92   |
| 6   | E     | 307 | CLA  | CMB-C2B-C3B | 3.79  | 131.76      | 124.68   |
| 5   | A     | 306 | CHL  | CMD-C2D-C3D | 3.78  | 136.32      | 127.61   |
| 2   | C     | 302 | 0IE  | C10-C9-C8   | 3.78  | 131.22      | 123.47   |
| 5   | B     | 314 | CHL  | CHD-C1D-ND  | 3.78  | 127.93      | 124.45   |
| 5   | F     | 317 | CHL  | CHA-C4D-ND  | 3.78  | 140.40      | 132.50   |
| 5   | B     | 314 | CHL  | CHC-C1C-NC  | 3.77  | 129.93      | 124.20   |
| 5   | A     | 306 | CHL  | C4D-CHA-C1A | -3.77 | 116.66      | 121.25   |
| 6   | D     | 314 | CLA  | CMB-C2B-C3B | 3.77  | 131.73      | 124.68   |
| 5   | F     | 304 | CHL  | C2C-C3C-C4C | -3.77 | 103.80      | 106.49   |
| 5   | D     | 310 | CHL  | C2C-C3C-C4C | -3.76 | 103.81      | 106.49   |
| 5   | D     | 306 | CHL  | C3A-C2A-C1A | -3.75 | 95.72       | 101.34   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | C     | 313 | CHL  | CHD-C4C-C3C | -3.75 | 119.33      | 124.84   |
| 6   | A     | 314 | CLA  | CMB-C2B-C3B | 3.74  | 131.68      | 124.68   |
| 5   | F     | 305 | CHL  | CAA-C2A-C1A | 3.74  | 124.22      | 111.97   |
| 5   | E     | 317 | CHL  | C1C-C2C-C3C | -3.74 | 104.15      | 107.11   |
| 5   | E     | 304 | CHL  | CHD-C4C-C3C | -3.73 | 119.35      | 124.84   |
| 5   | C     | 305 | CHL  | C1-C2-C3    | -3.73 | 119.59      | 126.04   |
| 4   | B     | 304 | LMU  | C1B-O1B-C4' | -3.73 | 108.74      | 117.96   |
| 5   | A     | 310 | CHL  | C1-C2-C3    | -3.72 | 120.72      | 126.75   |
| 5   | A     | 305 | CHL  | CHA-C4D-ND  | 3.72  | 140.29      | 132.50   |
| 6   | B     | 318 | CLA  | CMB-C2B-C1B | -3.72 | 122.74      | 128.46   |
| 5   | A     | 310 | CHL  | CHD-C1D-C2D | -3.72 | 117.68      | 125.48   |
| 5   | E     | 305 | CHL  | C2C-C3C-C4C | -3.72 | 103.84      | 106.49   |
| 4   | A     | 304 | LMU  | C1B-O1B-C4' | -3.71 | 108.77      | 117.96   |
| 5   | F     | 309 | CHL  | CHB-C4A-NA  | 3.71  | 129.65      | 124.51   |
| 5   | A     | 305 | CHL  | C2C-C3C-C4C | -3.71 | 103.84      | 106.49   |
| 2   | E     | 302 | OIE  | C20-C3-C4   | -3.71 | 120.06      | 124.83   |
| 5   | D     | 306 | CHL  | C1C-C2C-C3C | -3.71 | 104.17      | 107.11   |
| 2   | A     | 301 | OIE  | C23-C16-C15 | -3.70 | 117.74      | 122.92   |
| 9   | F     | 320 | OURL | O44-C45-C46 | 3.70  | 121.38      | 111.55   |
| 5   | C     | 305 | CHL  | C4D-CHA-C1A | -3.70 | 116.75      | 121.25   |
| 6   | E     | 316 | CLA  | CMB-C2B-C1B | -3.69 | 122.78      | 128.46   |
| 5   | B     | 313 | CHL  | C2C-C3C-C4C | -3.69 | 103.86      | 106.49   |
| 5   | C     | 309 | CHL  | C3A-C2A-C1A | -3.69 | 95.39       | 101.64   |
| 2   | D     | 302 | OIE  | C21-C7-C8   | -3.69 | 117.75      | 122.92   |
| 5   | F     | 310 | CHL  | C1-O2A-CGA  | 3.69  | 126.12      | 116.44   |
| 5   | A     | 318 | CHL  | CHA-C4D-ND  | 3.69  | 140.21      | 132.50   |
| 5   | A     | 313 | CHL  | CMD-C2D-C1D | 3.69  | 131.21      | 124.71   |
| 5   | E     | 310 | CHL  | CHA-C4D-ND  | 3.69  | 140.21      | 132.50   |
| 2   | D     | 301 | OIE  | C10-C9-C8   | 3.68  | 131.02      | 123.47   |
| 5   | D     | 306 | CHL  | CHD-C4C-NC  | 3.68  | 130.00      | 124.20   |
| 5   | C     | 306 | CHL  | C3A-C2A-C1A | -3.68 | 95.83       | 101.34   |
| 7   | B     | 324 | LHG  | O8-C23-C24  | 3.68  | 123.45      | 111.91   |
| 2   | B     | 301 | OIE  | C10-C9-C8   | 3.68  | 131.00      | 123.47   |
| 5   | C     | 310 | CHL  | CMD-C2D-C3D | -3.68 | 119.16      | 127.61   |
| 5   | E     | 309 | CHL  | C2C-C3C-C4C | -3.67 | 103.87      | 106.49   |
| 5   | C     | 305 | CHL  | CHD-C4C-NC  | 3.67  | 129.99      | 124.20   |
| 5   | C     | 311 | CHL  | CHD-C1D-C2D | -3.67 | 117.78      | 125.48   |
| 6   | C     | 308 | CLA  | CMB-C2B-C3B | 3.66  | 131.52      | 124.68   |
| 5   | E     | 317 | CHL  | CHA-C4D-ND  | 3.66  | 140.15      | 132.50   |
| 5   | D     | 306 | CHL  | C4A-NA-C1A  | 3.65  | 108.35      | 106.71   |
| 9   | B     | 325 | OURL | C10-C11-C12 | -3.65 | 122.09      | 127.31   |
| 9   | C     | 321 | OURL | C5-C4-C3    | -3.65 | 122.62      | 127.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | B     | 319 | CHL  | CHA-C4D-ND  | 3.65  | 140.13      | 132.50   |
| 6   | E     | 313 | CLA  | CMB-C2B-C3B | 3.65  | 131.50      | 124.68   |
| 5   | B     | 311 | CHL  | CHD-C4C-C3C | -3.65 | 119.48      | 124.84   |
| 2   | D     | 302 | 0IE  | C6-C7-C8    | 3.64  | 124.53      | 118.94   |
| 5   | C     | 313 | CHL  | CMD-C2D-C3D | -3.64 | 119.25      | 127.61   |
| 4   | E     | 319 | LMU  | C1B-O1B-C4' | -3.64 | 108.97      | 117.96   |
| 2   | E     | 301 | 0IE  | C9-C10-C11  | 3.63  | 130.92      | 123.47   |
| 5   | B     | 307 | CHL  | C4D-CHA-C1A | -3.63 | 116.83      | 121.25   |
| 5   | E     | 308 | CHL  | CHA-C4D-ND  | 3.63  | 140.10      | 132.50   |
| 5   | B     | 313 | CHL  | C4D-CHA-C1A | -3.63 | 116.84      | 121.25   |
| 5   | C     | 309 | CHL  | C1C-C2C-C3C | -3.62 | 104.24      | 107.11   |
| 5   | E     | 310 | CHL  | C3A-C2A-C1A | -3.62 | 95.91       | 101.34   |
| 5   | F     | 304 | CHL  | C4D-CHA-C1A | -3.62 | 116.84      | 121.25   |
| 3   | B     | 303 | NEX  | C35-C15-C14 | 3.62  | 130.89      | 123.47   |
| 5   | C     | 313 | CHL  | CHC-C1C-NC  | 3.62  | 129.69      | 124.20   |
| 5   | D     | 306 | CHL  | C1D-ND-C4D  | 3.61  | 108.90      | 106.33   |
| 5   | F     | 305 | CHL  | C3A-C2A-C1A | -3.60 | 95.95       | 101.34   |
| 2   | E     | 302 | 0IE  | C22-C12-C11 | -3.60 | 117.88      | 122.92   |
| 5   | F     | 305 | CHL  | C1-C2-C3    | -3.59 | 119.83      | 126.04   |
| 5   | A     | 312 | CHL  | C4D-CHA-C1A | -3.59 | 116.88      | 121.25   |
| 6   | B     | 315 | CLA  | CMB-C2B-C3B | 3.59  | 131.39      | 124.68   |
| 2   | F     | 301 | 0IE  | C21-C7-C8   | -3.59 | 117.90      | 122.92   |
| 6   | E     | 315 | CLA  | CMB-C2B-C1B | -3.58 | 122.95      | 128.46   |
| 5   | B     | 310 | CHL  | CHD-C4C-C3C | -3.58 | 119.58      | 124.84   |
| 5   | D     | 309 | CHL  | C3A-C2A-C1A | -3.58 | 95.59       | 101.64   |
| 5   | C     | 306 | CHL  | CHC-C1C-NC  | 3.58  | 129.63      | 124.20   |
| 5   | B     | 310 | CHL  | C2C-C3C-C4C | -3.57 | 103.94      | 106.49   |
| 5   | C     | 309 | CHL  | CHD-C4C-C3C | -3.56 | 119.60      | 124.84   |
| 5   | B     | 311 | CHL  | C2C-C3C-C4C | -3.56 | 103.95      | 106.49   |
| 2   | D     | 301 | 0IE  | C21-C7-C8   | -3.56 | 117.93      | 122.92   |
| 5   | B     | 312 | CHL  | CHA-C4D-ND  | 3.56  | 139.95      | 132.50   |
| 5   | D     | 306 | CHL  | C4D-CHA-C1A | -3.56 | 116.92      | 121.25   |
| 6   | C     | 317 | CLA  | CMB-C2B-C1B | -3.56 | 123.00      | 128.46   |
| 5   | A     | 312 | CHL  | C1-C2-C3    | -3.56 | 119.89      | 126.04   |
| 5   | F     | 309 | CHL  | C1C-C2C-C3C | -3.56 | 104.29      | 107.11   |
| 5   | F     | 310 | CHL  | C4-C3-C5    | 3.55  | 121.25      | 115.27   |
| 9   | A     | 322 | 0UR  | C43-C3-C2   | 3.55  | 125.00      | 116.66   |
| 5   | E     | 312 | CHL  | C4D-CHA-C1A | -3.55 | 116.93      | 121.25   |
| 5   | E     | 304 | CHL  | CHD-C4C-NC  | 3.55  | 129.79      | 124.20   |
| 5   | D     | 313 | CHL  | C2C-C3C-C4C | -3.55 | 103.96      | 106.49   |
| 2   | B     | 301 | 0IE  | C9-C10-C11  | 3.55  | 130.74      | 123.47   |
| 5   | A     | 311 | CHL  | CHA-C4D-ND  | 3.54  | 139.91      | 132.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | C     | 306 | CHL  | C4-C3-C5    | 3.54  | 121.23      | 115.27   |
| 5   | F     | 305 | CHL  | C2A-C1A-CHA | -3.54 | 117.67      | 123.86   |
| 9   | F     | 320 | OUR  | C5-C4-C3    | -3.54 | 122.75      | 127.00   |
| 5   | D     | 311 | CHL  | CHA-C4D-ND  | 3.54  | 139.90      | 132.50   |
| 5   | C     | 312 | CHL  | CHA-C4D-ND  | 3.53  | 139.89      | 132.50   |
| 5   | E     | 311 | CHL  | C4D-CHA-C1A | -3.52 | 116.96      | 121.25   |
| 5   | C     | 306 | CHL  | C2C-C3C-C4C | -3.52 | 103.98      | 106.49   |
| 2   | A     | 301 | OIE  | C10-C9-C8   | 3.52  | 130.68      | 123.47   |
| 6   | A     | 317 | CLA  | CMB-C2B-C1B | -3.52 | 123.06      | 128.46   |
| 2   | E     | 302 | OIE  | C21-C7-C8   | -3.51 | 118.00      | 122.92   |
| 4   | D     | 304 | LMU  | C1'-C2'-C3' | 3.51  | 117.31      | 110.00   |
| 5   | E     | 312 | CHL  | CHD-C4C-C3C | -3.51 | 119.68      | 124.84   |
| 9   | E     | 320 | OUR  | C9-C8-C7    | -3.51 | 122.31      | 127.31   |
| 5   | F     | 308 | CHL  | C3A-C2A-C1A | -3.50 | 95.71       | 101.64   |
| 5   | B     | 312 | CHL  | CHD-C4C-C3C | -3.50 | 119.69      | 124.84   |
| 2   | C     | 302 | OIE  | C21-C7-C8   | -3.50 | 118.02      | 122.92   |
| 2   | F     | 302 | OIE  | C21-C7-C8   | -3.50 | 118.02      | 122.92   |
| 9   | D     | 321 | OUR  | C10-C11-C12 | -3.50 | 122.32      | 127.31   |
| 5   | A     | 306 | CHL  | CHC-C1C-NC  | 3.50  | 129.51      | 124.20   |
| 6   | F     | 315 | CLA  | CMB-C2B-C3B | 3.49  | 131.22      | 124.68   |
| 5   | E     | 310 | CHL  | CHD-C1D-C2D | -3.49 | 118.16      | 125.48   |
| 5   | A     | 310 | CHL  | CHC-C1C-NC  | 3.49  | 129.50      | 124.20   |
| 2   | C     | 301 | OIE  | C21-C7-C8   | -3.49 | 118.04      | 122.92   |
| 5   | B     | 310 | CHL  | C4D-CHA-C1A | -3.49 | 117.01      | 121.25   |
| 2   | A     | 301 | OIE  | C22-C12-C11 | -3.48 | 118.05      | 122.92   |
| 2   | E     | 301 | OIE  | C21-C7-C8   | -3.48 | 118.05      | 122.92   |
| 5   | A     | 306 | CHL  | C4-C3-C5    | 3.48  | 121.12      | 115.27   |
| 6   | C     | 314 | CLA  | CMB-C2B-C3B | 3.48  | 131.18      | 124.68   |
| 5   | F     | 305 | CHL  | OBD-CAD-C3D | 3.47  | 136.88      | 128.52   |
| 5   | D     | 311 | CHL  | C1-C2-C3    | -3.47 | 120.04      | 126.04   |
| 5   | C     | 311 | CHL  | C4D-CHA-C1A | -3.47 | 117.02      | 121.25   |
| 5   | F     | 310 | CHL  | O2A-CGA-CBA | 3.47  | 122.80      | 111.91   |
| 9   | C     | 321 | OUR  | O44-C45-C46 | 3.47  | 120.77      | 111.55   |
| 5   | F     | 308 | CHL  | CHD-C4C-C3C | -3.46 | 119.75      | 124.84   |
| 5   | C     | 313 | CHL  | CHD-C4C-NC  | 3.46  | 129.65      | 124.20   |
| 6   | A     | 308 | CLA  | CAA-C2A-C3A | -3.45 | 103.32      | 112.78   |
| 9   | D     | 321 | OUR  | C5-C4-C3    | -3.45 | 122.85      | 127.00   |
| 6   | A     | 316 | CLA  | CMB-C2B-C1B | -3.45 | 123.16      | 128.46   |
| 9   | E     | 320 | OUR  | C43-C3-C2   | 3.45  | 124.76      | 116.66   |
| 5   | F     | 312 | CHL  | CMD-C2D-C1D | 3.45  | 130.79      | 124.71   |
| 9   | B     | 325 | OUR  | C43-C3-C2   | 3.45  | 124.75      | 116.66   |
| 2   | C     | 301 | OIE  | C22-C12-C11 | -3.45 | 118.10      | 122.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | B     | 306 | CHL  | CHD-C4C-C3C | -3.45 | 119.78      | 124.84   |
| 6   | C     | 316 | CLA  | CMB-C2B-C3B | 3.44  | 131.12      | 124.68   |
| 5   | B     | 311 | CHL  | CHB-C4A-NA  | 3.44  | 129.26      | 124.51   |
| 5   | A     | 306 | CHL  | C3A-C2A-C1A | -3.43 | 96.20       | 101.34   |
| 5   | F     | 317 | CHL  | C3A-C2A-C1A | -3.43 | 96.20       | 101.34   |
| 6   | D     | 308 | CLA  | CMB-C2B-C3B | 3.43  | 131.09      | 124.68   |
| 5   | C     | 311 | CHL  | CHC-C1C-NC  | 3.43  | 129.40      | 124.20   |
| 2   | D     | 301 | 0IE  | C22-C12-C11 | -3.42 | 118.13      | 122.92   |
| 9   | B     | 302 | 0UR  | O44-C45-C46 | 3.42  | 120.65      | 111.55   |
| 5   | F     | 310 | CHL  | C4D-CHA-C1A | -3.42 | 117.09      | 121.25   |
| 5   | E     | 305 | CHL  | C4D-CHA-C1A | -3.42 | 117.09      | 121.25   |
| 5   | F     | 304 | CHL  | CHA-C4D-ND  | 3.42  | 139.65      | 132.50   |
| 5   | E     | 308 | CHL  | CHC-C1C-NC  | 3.41  | 129.38      | 124.20   |
| 2   | E     | 301 | 0IE  | C22-C12-C11 | -3.41 | 118.15      | 122.92   |
| 2   | E     | 302 | 0IE  | C6-C7-C8    | 3.41  | 124.17      | 118.94   |
| 5   | C     | 310 | CHL  | CHA-C4D-ND  | 3.41  | 139.62      | 132.50   |
| 5   | C     | 313 | CHL  | C2C-C3C-C4C | -3.40 | 104.06      | 106.49   |
| 5   | F     | 309 | CHL  | C4D-CHA-C1A | -3.40 | 117.11      | 121.25   |
| 5   | C     | 310 | CHL  | CHD-C4C-C3C | -3.40 | 119.84      | 124.84   |
| 5   | D     | 310 | CHL  | CHA-C4D-ND  | 3.40  | 139.60      | 132.50   |
| 5   | D     | 305 | CHL  | CHD-C1D-C2D | -3.39 | 118.36      | 125.48   |
| 6   | E     | 306 | CLA  | O2D-CGD-O1D | -3.39 | 117.21      | 123.84   |
| 6   | B     | 317 | CLA  | CMB-C2B-C3B | 3.39  | 131.02      | 124.68   |
| 5   | E     | 305 | CHL  | CHC-C1C-NC  | 3.39  | 129.34      | 124.20   |
| 5   | D     | 311 | CHL  | C1C-C2C-C3C | -3.38 | 104.43      | 107.11   |
| 5   | E     | 305 | CHL  | C4A-NA-C1A  | 3.38  | 108.23      | 106.71   |
| 5   | A     | 313 | CHL  | C2C-C3C-C4C | -3.38 | 104.08      | 106.49   |
| 5   | E     | 309 | CHL  | CHA-C4D-ND  | 3.38  | 139.56      | 132.50   |
| 5   | A     | 306 | CHL  | C2C-C3C-C4C | -3.37 | 104.08      | 106.49   |
| 5   | D     | 305 | CHL  | C3A-C2A-C1A | -3.37 | 96.29       | 101.34   |
| 2   | F     | 302 | 0IE  | C22-C12-C11 | -3.37 | 118.20      | 122.92   |
| 2   | E     | 302 | 0IE  | C13-C12-C11 | 3.37  | 124.11      | 118.94   |
| 2   | F     | 302 | 0IE  | C10-C9-C8   | 3.36  | 130.37      | 123.47   |
| 5   | C     | 318 | CHL  | CHB-C4A-NA  | 3.36  | 129.16      | 124.51   |
| 5   | B     | 307 | CHL  | C2A-C1A-CHA | -3.36 | 117.98      | 123.86   |
| 2   | D     | 301 | 0IE  | C9-C10-C11  | 3.36  | 130.36      | 123.47   |
| 6   | D     | 315 | CLA  | CMB-C2B-C3B | 3.36  | 130.96      | 124.68   |
| 5   | A     | 309 | CHL  | CHA-C4D-ND  | 3.35  | 139.52      | 132.50   |
| 5   | E     | 309 | CHL  | C4D-CHA-C1A | -3.35 | 117.17      | 121.25   |
| 5   | A     | 305 | CHL  | CHD-C4C-C3C | -3.35 | 119.91      | 124.84   |
| 2   | B     | 301 | 0IE  | C21-C7-C8   | -3.35 | 118.23      | 122.92   |
| 5   | B     | 307 | CHL  | C3A-C2A-C1A | -3.35 | 96.32       | 101.34   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | C     | 305 | CHL  | CHA-C4D-ND  | 3.35  | 139.51      | 132.50   |
| 5   | D     | 305 | CHL  | CAA-C2A-C1A | -3.35 | 101.00      | 111.97   |
| 2   | C     | 302 | 0IE  | C22-C12-C11 | -3.35 | 118.23      | 122.92   |
| 6   | E     | 307 | CLA  | CAA-C2A-C3A | -3.35 | 103.61      | 112.78   |
| 5   | A     | 309 | CHL  | C4D-CHA-C1A | -3.34 | 117.18      | 121.25   |
| 6   | D     | 307 | CLA  | O2D-CGD-O1D | -3.34 | 117.30      | 123.84   |
| 5   | A     | 310 | CHL  | CHA-C4D-ND  | 3.34  | 139.49      | 132.50   |
| 5   | C     | 318 | CHL  | CHD-C4C-C3C | -3.34 | 119.93      | 124.84   |
| 2   | A     | 301 | 0IE  | C17-C16-C15 | 3.34  | 124.06      | 118.94   |
| 6   | B     | 316 | CLA  | CMB-C2B-C1B | -3.34 | 123.33      | 128.46   |
| 5   | F     | 311 | CHL  | C4-C3-C5    | 3.33  | 120.88      | 115.27   |
| 2   | F     | 301 | 0IE  | C9-C10-C11  | 3.33  | 130.30      | 123.47   |
| 5   | D     | 313 | CHL  | CHA-C4D-ND  | 3.33  | 139.47      | 132.50   |
| 5   | E     | 309 | CHL  | CHD-C1D-C2D | -3.33 | 118.51      | 125.48   |
| 2   | F     | 302 | 0IE  | C6-C7-C8    | 3.32  | 124.04      | 118.94   |
| 5   | C     | 309 | CHL  | CHC-C1C-NC  | 3.32  | 129.24      | 124.20   |
| 5   | B     | 310 | CHL  | CHA-C4D-ND  | 3.32  | 139.44      | 132.50   |
| 5   | C     | 318 | CHL  | CHA-C4D-ND  | 3.32  | 139.44      | 132.50   |
| 6   | B     | 309 | CLA  | CMB-C2B-C3B | 3.32  | 130.88      | 124.68   |
| 6   | F     | 313 | CLA  | O2D-CGD-O1D | -3.32 | 117.35      | 123.84   |
| 5   | A     | 312 | CHL  | CHA-C4D-ND  | 3.32  | 139.44      | 132.50   |
| 5   | F     | 309 | CHL  | CHD-C1D-C2D | -3.31 | 118.53      | 125.48   |
| 5   | E     | 305 | CHL  | C1-C2-C3    | -3.31 | 120.31      | 126.04   |
| 5   | A     | 311 | CHL  | CHD-C1D-C2D | -3.31 | 118.55      | 125.48   |
| 6   | A     | 315 | CLA  | CMB-C2B-C1B | -3.31 | 123.38      | 128.46   |
| 5   | A     | 311 | CHL  | C3A-C2A-C1A | -3.30 | 96.40       | 101.34   |
| 6   | D     | 316 | CLA  | CMB-C2B-C3B | 3.30  | 130.85      | 124.68   |
| 5   | F     | 305 | CHL  | C2C-C3C-C4C | -3.29 | 104.14      | 106.49   |
| 5   | B     | 312 | CHL  | C3A-C2A-C1A | -3.29 | 96.41       | 101.34   |
| 3   | B     | 303 | NEX  | C11-C12-C13 | 3.29  | 135.66      | 126.42   |
| 5   | E     | 311 | CHL  | C1-C2-C3    | -3.29 | 120.36      | 126.04   |
| 6   | C     | 314 | CLA  | O2D-CGD-O1D | -3.29 | 117.41      | 123.84   |
| 5   | E     | 310 | CHL  | C1-C2-C3    | -3.29 | 120.36      | 126.04   |
| 6   | D     | 317 | CLA  | CMB-C2B-C1B | -3.28 | 123.42      | 128.46   |
| 6   | B     | 315 | CLA  | O2D-CGD-O1D | -3.28 | 117.42      | 123.84   |
| 5   | D     | 309 | CHL  | CHA-C4D-ND  | 3.28  | 139.37      | 132.50   |
| 5   | F     | 308 | CHL  | CHA-C4D-ND  | 3.28  | 139.37      | 132.50   |
| 3   | B     | 303 | NEX  | C27-C28-C29 | -3.28 | 120.44      | 125.53   |
| 9   | E     | 320 | 0UR  | C10-C11-C12 | -3.28 | 122.62      | 127.31   |
| 5   | D     | 305 | CHL  | CHC-C1C-NC  | 3.28  | 129.18      | 124.20   |
| 9   | F     | 320 | 0UR  | C24-C25-C26 | -3.28 | 105.81      | 110.30   |
| 2   | D     | 302 | 0IE  | C22-C12-C11 | -3.28 | 118.33      | 122.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | D     | 305 | CHL  | C4D-CHA-C1A | -3.28 | 117.26      | 121.25   |
| 5   | B     | 311 | CHL  | CHA-C4D-ND  | 3.27  | 139.34      | 132.50   |
| 5   | F     | 311 | CHL  | CHD-C4C-C3C | -3.26 | 120.04      | 124.84   |
| 5   | B     | 319 | CHL  | C4D-CHA-C1A | -3.26 | 117.28      | 121.25   |
| 5   | D     | 318 | CHL  | CHD-C1D-C2D | -3.26 | 118.65      | 125.48   |
| 2   | F     | 301 | 0IE  | C22-C12-C11 | -3.26 | 118.36      | 122.92   |
| 6   | F     | 316 | CLA  | CMB-C2B-C3B | 3.25  | 130.77      | 124.68   |
| 6   | F     | 306 | CLA  | CMB-C2B-C1B | -3.25 | 123.47      | 128.46   |
| 5   | A     | 311 | CHL  | C1C-C2C-C3C | -3.25 | 104.53      | 107.11   |
| 5   | D     | 313 | CHL  | CHB-C4A-NA  | 3.25  | 129.00      | 124.51   |
| 6   | A     | 315 | CLA  | O2D-CGD-O1D | -3.25 | 117.49      | 123.84   |
| 5   | A     | 306 | CHL  | C1-C2-C3    | -3.25 | 120.43      | 126.04   |
| 5   | E     | 305 | CHL  | C4-C3-C5    | 3.25  | 120.73      | 115.27   |
| 5   | E     | 309 | CHL  | CHD-C4C-C3C | -3.24 | 120.08      | 124.84   |
| 6   | A     | 308 | CLA  | CMB-C2B-C3B | 3.24  | 130.74      | 124.68   |
| 5   | F     | 309 | CHL  | C2A-C3A-C4A | 3.23  | 105.91      | 101.78   |
| 5   | C     | 306 | CHL  | CHD-C4C-NC  | 3.22  | 129.28      | 124.20   |
| 6   | A     | 307 | CLA  | O2D-CGD-O1D | -3.22 | 117.54      | 123.84   |
| 5   | D     | 309 | CHL  | CHD-C4C-C3C | -3.22 | 120.11      | 124.84   |
| 5   | F     | 310 | CHL  | O2D-CGD-O1D | -3.22 | 117.55      | 123.84   |
| 2   | A     | 302 | 0IE  | C22-C12-C11 | -3.22 | 118.42      | 122.92   |
| 6   | C     | 315 | CLA  | CMB-C2B-C3B | 3.21  | 130.68      | 124.68   |
| 6   | E     | 314 | CLA  | CMB-C2B-C1B | -3.21 | 123.53      | 128.46   |
| 2   | C     | 302 | 0IE  | C6-C7-C8    | 3.21  | 123.86      | 118.94   |
| 5   | E     | 311 | CHL  | CHA-C4D-ND  | 3.21  | 139.21      | 132.50   |
| 5   | C     | 311 | CHL  | CAA-C2A-C1A | 3.20  | 122.48      | 111.97   |
| 5   | B     | 312 | CHL  | C1-C2-C3    | -3.20 | 120.50      | 126.04   |
| 5   | F     | 317 | CHL  | CAC-C3C-C4C | 3.20  | 128.96      | 124.81   |
| 6   | D     | 307 | CLA  | CMB-C2B-C3B | 3.20  | 130.66      | 124.68   |
| 6   | B     | 308 | CLA  | CMB-C2B-C1B | -3.20 | 123.55      | 128.46   |
| 4   | D     | 304 | LMU  | O5'-C5'-C4' | -3.19 | 103.02      | 109.75   |
| 5   | D     | 313 | CHL  | CMD-C2D-C3D | -3.19 | 120.28      | 127.61   |
| 9   | E     | 320 | 0UR  | O44-C45-C46 | 3.19  | 120.03      | 111.55   |
| 5   | F     | 305 | CHL  | CHD-C1D-ND  | 3.19  | 127.38      | 124.45   |
| 5   | D     | 310 | CHL  | CHD-C4C-C3C | -3.19 | 120.15      | 124.84   |
| 5   | B     | 314 | CHL  | OMC-CMC-C2C | -3.18 | 118.49      | 125.69   |
| 5   | A     | 312 | CHL  | CAC-C3C-C4C | 3.18  | 128.94      | 124.81   |
| 5   | B     | 312 | CHL  | C1-O2A-CGA  | 3.18  | 124.79      | 116.44   |
| 5   | F     | 310 | CHL  | CHA-C4D-ND  | 3.18  | 139.15      | 132.50   |
| 6   | A     | 315 | CLA  | C1-C2-C3    | -3.18 | 120.54      | 126.04   |
| 5   | A     | 310 | CHL  | O2D-CGD-O1D | -3.18 | 117.62      | 123.84   |
| 5   | E     | 310 | CHL  | O2A-CGA-CBA | 3.18  | 121.88      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | B     | 316 | CLA  | O2D-CGD-O1D | -3.18 | 117.63      | 123.84   |
| 2   | F     | 301 | 0IE  | C6-C7-C8    | 3.18  | 123.81      | 118.94   |
| 5   | E     | 312 | CHL  | C3A-C2A-C1A | -3.17 | 96.58       | 101.34   |
| 5   | C     | 310 | CHL  | OBD-CAD-C3D | -3.17 | 120.88      | 128.52   |
| 5   | E     | 317 | CHL  | C4D-CHA-C1A | -3.17 | 117.39      | 121.25   |
| 6   | B     | 315 | CLA  | CAC-C3C-C4C | 3.17  | 128.93      | 124.81   |
| 2   | C     | 301 | 0IE  | C6-C7-C8    | 3.17  | 123.81      | 118.94   |
| 6   | E     | 316 | CLA  | CMB-C2B-C3B | 3.17  | 130.61      | 124.68   |
| 5   | D     | 310 | CHL  | C4D-CHA-C1A | -3.17 | 117.39      | 121.25   |
| 6   | B     | 318 | CLA  | O2D-CGD-O1D | -3.17 | 117.64      | 123.84   |
| 5   | E     | 312 | CHL  | CHA-C4D-ND  | 3.17  | 139.13      | 132.50   |
| 2   | A     | 302 | 0IE  | C9-C10-C11  | 3.17  | 129.96      | 123.47   |
| 6   | F     | 307 | CLA  | CMB-C2B-C3B | 3.17  | 130.60      | 124.68   |
| 5   | D     | 309 | CHL  | CHC-C1C-NC  | 3.17  | 129.01      | 124.20   |
| 6   | F     | 314 | CLA  | CMB-C2B-C3B | 3.17  | 130.60      | 124.68   |
| 6   | C     | 317 | CLA  | O2D-CGD-O1D | -3.17 | 117.65      | 123.84   |
| 5   | F     | 311 | CHL  | CHC-C1C-NC  | 3.16  | 129.00      | 124.20   |
| 5   | F     | 310 | CHL  | C3A-C2A-C1A | -3.16 | 96.60       | 101.34   |
| 9   | E     | 320 | 0UR  | C5-C4-C3    | -3.16 | 123.20      | 127.00   |
| 9   | D     | 321 | 0UR  | O44-C45-C46 | 3.16  | 119.96      | 111.55   |
| 5   | C     | 318 | CHL  | O2D-CGD-O1D | -3.16 | 117.66      | 123.84   |
| 9   | E     | 320 | 0UR  | O42-C2-C3   | -3.16 | 114.89      | 120.66   |
| 5   | E     | 311 | CHL  | C1C-C2C-C3C | -3.16 | 104.61      | 107.11   |
| 6   | A     | 307 | CLA  | CMB-C2B-C1B | -3.15 | 123.62      | 128.46   |
| 5   | C     | 309 | CHL  | CHA-C4D-ND  | 3.15  | 139.09      | 132.50   |
| 2   | B     | 301 | 0IE  | C22-C12-C11 | -3.15 | 118.51      | 122.92   |
| 6   | B     | 318 | CLA  | CMB-C2B-C3B | 3.14  | 130.56      | 124.68   |
| 5   | E     | 305 | CHL  | CHD-C4C-NC  | 3.14  | 129.15      | 124.20   |
| 6   | C     | 307 | CLA  | O2D-CGD-CBD | 3.13  | 116.83      | 111.27   |
| 5   | C     | 312 | CHL  | CHC-C1C-NC  | 3.13  | 128.95      | 124.20   |
| 5   | B     | 312 | CHL  | CHC-C1C-NC  | 3.13  | 128.95      | 124.20   |
| 3   | E     | 303 | NEX  | C38-C25-C24 | -3.13 | 110.76      | 114.28   |
| 5   | F     | 317 | CHL  | CHC-C1C-NC  | 3.12  | 128.94      | 124.20   |
| 5   | E     | 308 | CHL  | C4D-CHA-C1A | -3.12 | 117.45      | 121.25   |
| 5   | F     | 305 | CHL  | O2D-CGD-O1D | -3.11 | 117.75      | 123.84   |
| 5   | F     | 317 | CHL  | CHD-C1D-C2D | -3.11 | 118.96      | 125.48   |
| 5   | C     | 305 | CHL  | O2A-CGA-CBA | 3.11  | 121.65      | 111.91   |
| 6   | A     | 314 | CLA  | O2D-CGD-O1D | -3.10 | 117.77      | 123.84   |
| 6   | E     | 315 | CLA  | CMB-C2B-C3B | 3.10  | 130.48      | 124.68   |
| 5   | D     | 311 | CHL  | C4-C3-C5    | 3.09  | 120.48      | 115.27   |
| 6   | F     | 314 | CLA  | O2D-CGD-O1D | -3.09 | 117.79      | 123.84   |
| 5   | B     | 307 | CHL  | CAC-C3C-C4C | 3.09  | 128.82      | 124.81   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | B     | 313 | CHL  | C4-C3-C5    | 3.09  | 120.46      | 115.27   |
| 5   | E     | 310 | CHL  | C1C-C2C-C3C | -3.09 | 104.67      | 107.11   |
| 5   | E     | 312 | CHL  | C1-C2-C3    | -3.08 | 120.71      | 126.04   |
| 5   | C     | 313 | CHL  | CHA-C4D-ND  | 3.08  | 138.95      | 132.50   |
| 5   | F     | 311 | CHL  | CHD-C4C-NC  | 3.08  | 129.05      | 124.20   |
| 6   | A     | 314 | CLA  | C1-C2-C3    | -3.08 | 120.72      | 126.04   |
| 5   | E     | 317 | CHL  | CHC-C1C-NC  | 3.08  | 128.87      | 124.20   |
| 9   | F     | 320 | OUR  | O42-C2-C3   | -3.08 | 115.04      | 120.66   |
| 5   | D     | 306 | CHL  | C6-C7-C8    | -3.07 | 105.98      | 115.92   |
| 2   | D     | 301 | OIE  | C13-C12-C11 | 3.07  | 123.65      | 118.94   |
| 9   | C     | 321 | OUR  | C48-C47-C46 | -3.07 | 119.27      | 125.85   |
| 9   | A     | 322 | OUR  | C29-C30-C31 | -3.07 | 108.25      | 111.74   |
| 6   | C     | 317 | CLA  | CMB-C2B-C3B | 3.06  | 130.41      | 124.68   |
| 9   | A     | 322 | OUR  | O44-C45-O57 | -3.06 | 116.20      | 122.93   |
| 5   | F     | 317 | CHL  | C4D-CHA-C1A | -3.06 | 117.52      | 121.25   |
| 5   | C     | 311 | CHL  | CAC-C3C-C4C | 3.06  | 128.78      | 124.81   |
| 2   | C     | 301 | OIE  | C13-C12-C11 | 3.06  | 123.63      | 118.94   |
| 5   | B     | 313 | CHL  | CHC-C1C-NC  | 3.06  | 128.84      | 124.20   |
| 5   | B     | 306 | CHL  | CHD-C1D-C2D | -3.05 | 119.08      | 125.48   |
| 5   | E     | 305 | CHL  | C2A-C1A-CHA | -3.05 | 118.53      | 123.86   |
| 5   | F     | 311 | CHL  | C2C-C3C-C4C | -3.05 | 104.32      | 106.49   |
| 5   | B     | 307 | CHL  | C4-C3-C5    | 3.05  | 120.40      | 115.27   |
| 5   | D     | 309 | CHL  | C4D-CHA-C1A | -3.05 | 117.54      | 121.25   |
| 2   | D     | 302 | OIE  | C9-C10-C11  | 3.05  | 129.72      | 123.47   |
| 5   | F     | 312 | CHL  | C2C-C3C-C4C | -3.05 | 104.32      | 106.49   |
| 5   | D     | 312 | CHL  | CHD-C4C-NC  | 3.04  | 129.00      | 124.20   |
| 5   | B     | 310 | CHL  | CHC-C1C-NC  | 3.04  | 128.82      | 124.20   |
| 5   | B     | 319 | CHL  | CAC-C3C-C4C | 3.04  | 128.76      | 124.81   |
| 9   | C     | 321 | OUR  | C34-C27-C1  | -3.04 | 120.50      | 124.49   |
| 5   | B     | 312 | CHL  | CHD-C1D-C2D | -3.04 | 119.11      | 125.48   |
| 5   | F     | 312 | CHL  | CHC-C1C-NC  | 3.03  | 128.80      | 124.20   |
| 2   | A     | 301 | OIE  | C14-C15-C16 | 3.03  | 131.63      | 127.31   |
| 5   | C     | 311 | CHL  | O2A-CGA-CBA | 3.03  | 121.42      | 111.91   |
| 5   | B     | 314 | CHL  | C2C-C3C-C4C | -3.03 | 104.33      | 106.49   |
| 5   | E     | 311 | CHL  | CHD-C4C-C3C | -3.03 | 120.39      | 124.84   |
| 5   | C     | 312 | CHL  | CHD-C1D-C2D | -3.02 | 119.14      | 125.48   |
| 2   | E     | 301 | OIE  | C13-C12-C11 | 3.02  | 123.57      | 118.94   |
| 9   | D     | 321 | OUR  | C43-C3-C2   | 3.02  | 123.75      | 116.66   |
| 5   | D     | 311 | CHL  | O2A-CGA-CBA | 3.02  | 121.37      | 111.91   |
| 6   | F     | 306 | CLA  | O2D-CGD-O1D | -3.01 | 117.95      | 123.84   |
| 3   | F     | 303 | NEX  | C12-C13-C14 | 3.01  | 123.56      | 118.94   |
| 5   | A     | 305 | CHL  | O2A-CGA-CBA | 3.01  | 121.35      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | A     | 317 | CLA  | CMB-C2B-C3B | 3.01  | 130.31      | 124.68   |
| 5   | B     | 313 | CHL  | CHA-C4D-ND  | 3.01  | 138.79      | 132.50   |
| 5   | C     | 311 | CHL  | C1C-C2C-C3C | -3.00 | 104.73      | 107.11   |
| 5   | A     | 310 | CHL  | CBA-CAA-C2A | -3.00 | 105.00      | 113.86   |
| 5   | D     | 306 | CHL  | C2A-C1A-CHA | -3.00 | 118.61      | 123.86   |
| 6   | D     | 317 | CLA  | O2D-CGD-O1D | -3.00 | 117.97      | 123.84   |
| 5   | D     | 312 | CHL  | C6-C5-C3    | -3.00 | 105.59      | 113.45   |
| 6   | F     | 315 | CLA  | O2D-CGD-O1D | -3.00 | 117.97      | 123.84   |
| 5   | A     | 309 | CHL  | CHD-C4C-C3C | -2.99 | 120.44      | 124.84   |
| 5   | C     | 312 | CHL  | C3A-C2A-C1A | -2.99 | 96.86       | 101.34   |
| 5   | A     | 318 | CHL  | CHD-C4C-C3C | -2.99 | 120.44      | 124.84   |
| 5   | C     | 310 | CHL  | CHD-C1D-C2D | -2.99 | 119.22      | 125.48   |
| 6   | E     | 314 | CLA  | O2D-CGD-O1D | -2.98 | 118.00      | 123.84   |
| 5   | C     | 311 | CHL  | C2A-C3A-C4A | 2.98  | 106.68      | 101.87   |
| 5   | D     | 313 | CHL  | C1-C2-C3    | -2.98 | 120.89      | 126.04   |
| 5   | A     | 318 | CHL  | CHD-C1D-C2D | -2.98 | 119.24      | 125.48   |
| 5   | E     | 311 | CHL  | OMC-CMC-C2C | -2.97 | 118.96      | 125.69   |
| 5   | F     | 305 | CHL  | C1D-ND-C4D  | 2.97  | 108.45      | 106.33   |
| 5   | F     | 310 | CHL  | CHD-C1D-C2D | -2.97 | 119.24      | 125.48   |
| 2   | E     | 301 | 0IE  | C6-C7-C8    | 2.97  | 123.50      | 118.94   |
| 5   | D     | 311 | CHL  | C3A-C2A-C1A | -2.97 | 96.89       | 101.34   |
| 6   | A     | 316 | CLA  | CMB-C2B-C3B | 2.97  | 130.24      | 124.68   |
| 5   | D     | 311 | CHL  | C3B-C4B-NB  | 2.97  | 113.05      | 109.21   |
| 3   | D     | 303 | NEX  | C24-C23-C22 | -2.97 | 105.04      | 110.77   |
| 5   | A     | 311 | CHL  | O2A-CGA-CBA | 2.97  | 121.23      | 111.91   |
| 5   | D     | 312 | CHL  | CHA-C4D-ND  | 2.97  | 138.71      | 132.50   |
| 5   | F     | 304 | CHL  | CHD-C4C-NC  | 2.97  | 128.88      | 124.20   |
| 6   | B     | 315 | CLA  | C1B-CHB-C4A | -2.96 | 124.25      | 130.12   |
| 6   | E     | 306 | CLA  | CMB-C2B-C1B | -2.96 | 123.91      | 128.46   |
| 5   | D     | 311 | CHL  | CHD-C1D-C2D | -2.96 | 119.27      | 125.48   |
| 5   | F     | 311 | CHL  | C2A-C1A-CHA | -2.96 | 118.68      | 123.86   |
| 3   | F     | 303 | NEX  | C39-C29-C30 | -2.96 | 118.78      | 122.92   |
| 2   | B     | 301 | 0IE  | C6-C7-C8    | 2.96  | 123.48      | 118.94   |
| 5   | D     | 310 | CHL  | CHC-C1C-NC  | 2.95  | 128.69      | 124.20   |
| 5   | B     | 311 | CHL  | CHD-C4C-NC  | 2.95  | 128.86      | 124.20   |
| 6   | F     | 307 | CLA  | O2D-CGD-O1D | -2.95 | 118.07      | 123.84   |
| 5   | D     | 312 | CHL  | O2A-CGA-CBA | 2.94  | 121.14      | 111.91   |
| 9   | A     | 322 | 0UR  | C9-C8-C7    | -2.94 | 123.11      | 127.31   |
| 2   | D     | 301 | 0IE  | C6-C7-C8    | 2.94  | 123.45      | 118.94   |
| 5   | B     | 306 | CHL  | C4-C3-C5    | 2.94  | 120.22      | 115.27   |
| 5   | F     | 309 | CHL  | CHC-C1C-NC  | 2.94  | 128.66      | 124.20   |
| 5   | F     | 310 | CHL  | CHD-C4C-C3C | -2.94 | 120.52      | 124.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | E     | 308 | CHL  | CHD-C4C-C3C | -2.93 | 120.53      | 124.84   |
| 2   | E     | 302 | 0IE  | C17-C16-C15 | 2.93  | 123.44      | 118.94   |
| 5   | F     | 304 | CHL  | CHD-C1D-C2D | -2.93 | 119.33      | 125.48   |
| 5   | B     | 306 | CHL  | C3A-C2A-C1A | -2.93 | 96.95       | 101.34   |
| 5   | B     | 319 | CHL  | CHC-C1C-NC  | 2.93  | 128.65      | 124.20   |
| 5   | C     | 311 | CHL  | C4-C3-C5    | 2.93  | 120.20      | 115.27   |
| 5   | F     | 304 | CHL  | C3A-C2A-C1A | -2.93 | 96.96       | 101.34   |
| 5   | C     | 312 | CHL  | CAC-C3C-C4C | 2.92  | 128.60      | 124.81   |
| 5   | C     | 313 | CHL  | C1-C2-C3    | -2.92 | 120.98      | 126.04   |
| 5   | A     | 306 | CHL  | C2A-C1A-CHA | -2.92 | 118.75      | 123.86   |
| 5   | D     | 312 | CHL  | CHC-C1C-NC  | 2.92  | 128.64      | 124.20   |
| 2   | F     | 302 | 0IE  | C13-C12-C11 | 2.92  | 123.42      | 118.94   |
| 5   | A     | 312 | CHL  | O2A-CGA-CBA | 2.92  | 121.07      | 111.91   |
| 6   | F     | 313 | CLA  | O2A-CGA-O1A | -2.92 | 116.22      | 123.59   |
| 5   | D     | 318 | CHL  | CAA-C2A-C1A | 2.92  | 121.54      | 111.97   |
| 5   | C     | 306 | CHL  | C4D-CHA-C1A | -2.92 | 117.70      | 121.25   |
| 5   | C     | 310 | CHL  | O2D-CGD-O1D | -2.92 | 118.14      | 123.84   |
| 5   | A     | 305 | CHL  | C1-C2-C3    | -2.92 | 121.00      | 126.04   |
| 5   | A     | 310 | CHL  | CHD-C4C-C3C | -2.91 | 120.56      | 124.84   |
| 5   | B     | 312 | CHL  | O2A-CGA-CBA | 2.91  | 121.05      | 111.91   |
| 6   | A     | 316 | CLA  | O2D-CGD-O1D | -2.91 | 118.14      | 123.84   |
| 5   | E     | 311 | CHL  | CHD-C1D-C2D | -2.91 | 119.38      | 125.48   |
| 6   | D     | 314 | CLA  | O2D-CGD-O1D | -2.91 | 118.15      | 123.84   |
| 6   | A     | 308 | CLA  | O2D-CGD-O1D | -2.91 | 118.15      | 123.84   |
| 5   | D     | 312 | CHL  | CHD-C4C-C3C | -2.91 | 120.57      | 124.84   |
| 5   | B     | 312 | CHL  | C2A-C3A-C4A | 2.90  | 106.56      | 101.87   |
| 5   | B     | 319 | CHL  | O2D-CGD-O1D | -2.90 | 118.16      | 123.84   |
| 5   | C     | 311 | CHL  | CMD-C2D-C3D | 2.90  | 134.29      | 127.61   |
| 6   | C     | 307 | CLA  | CHB-C4A-NA  | 2.90  | 128.52      | 124.51   |
| 6   | A     | 314 | CLA  | C1B-CHB-C4A | -2.90 | 124.38      | 130.12   |
| 5   | D     | 309 | CHL  | C2A-C3A-C4A | 2.90  | 105.48      | 101.78   |
| 5   | C     | 305 | CHL  | C6-C5-C3    | -2.90 | 105.86      | 113.45   |
| 6   | C     | 307 | CLA  | O2A-CGA-O1A | -2.90 | 116.28      | 123.59   |
| 5   | F     | 312 | CHL  | C3A-C2A-C1A | -2.90 | 97.00       | 101.34   |
| 5   | E     | 317 | CHL  | CHD-C1D-C2D | -2.89 | 119.41      | 125.48   |
| 5   | E     | 304 | CHL  | C2C-C3C-C4C | -2.89 | 104.43      | 106.49   |
| 5   | E     | 304 | CHL  | CHA-C4D-ND  | 2.89  | 138.54      | 132.50   |
| 5   | A     | 311 | CHL  | CAC-C3C-C4C | 2.89  | 128.55      | 124.81   |
| 6   | F     | 306 | CLA  | CHB-C4A-NA  | 2.88  | 128.50      | 124.51   |
| 5   | B     | 313 | CHL  | OMC-CMC-C2C | -2.88 | 119.17      | 125.69   |
| 6   | B     | 315 | CLA  | CHB-C4A-NA  | 2.88  | 128.50      | 124.51   |
| 6   | B     | 308 | CLA  | C4-C3-C5    | 2.88  | 120.12      | 115.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | A     | 318 | CHL  | C3A-C2A-C1A | -2.88 | 96.76       | 101.64   |
| 6   | D     | 315 | CLA  | O2D-CGD-O1D | -2.88 | 118.21      | 123.84   |
| 7   | B     | 320 | LHG  | C5-O7-C7    | -2.88 | 110.71      | 117.79   |
| 5   | C     | 309 | CHL  | CMD-C2D-C1D | 2.88  | 129.78      | 124.71   |
| 5   | A     | 306 | CHL  | CHA-C4D-ND  | 2.87  | 138.51      | 132.50   |
| 2   | C     | 302 | 0IE  | C13-C12-C11 | 2.87  | 123.35      | 118.94   |
| 5   | B     | 313 | CHL  | CHD-C1D-C2D | -2.87 | 119.45      | 125.48   |
| 6   | C     | 317 | CLA  | O1D-CGD-CBD | 2.87  | 130.36      | 124.48   |
| 5   | F     | 310 | CHL  | CHC-C1C-NC  | 2.87  | 128.56      | 124.20   |
| 5   | B     | 313 | CHL  | O2A-CGA-CBA | 2.87  | 120.91      | 111.91   |
| 6   | B     | 309 | CLA  | O2D-CGD-O1D | -2.87 | 118.23      | 123.84   |
| 5   | F     | 305 | CHL  | C4D-CHA-C1A | -2.87 | 117.76      | 121.25   |
| 5   | C     | 306 | CHL  | CHA-C4D-ND  | 2.86  | 138.49      | 132.50   |
| 5   | D     | 312 | CHL  | CAC-C3C-C4C | 2.86  | 128.53      | 124.81   |
| 5   | A     | 313 | CHL  | CHA-C4D-ND  | 2.86  | 138.48      | 132.50   |
| 5   | D     | 310 | CHL  | CHD-C1D-C2D | -2.86 | 119.49      | 125.48   |
| 6   | B     | 309 | CLA  | C1B-CHB-C4A | -2.85 | 124.47      | 130.12   |
| 2   | A     | 301 | 0IE  | C6-C7-C8    | 2.85  | 123.32      | 118.94   |
| 6   | E     | 307 | CLA  | O2D-CGD-O1D | -2.85 | 118.26      | 123.84   |
| 5   | A     | 312 | CHL  | OMC-CMC-C2C | -2.85 | 119.24      | 125.69   |
| 7   | A     | 319 | LHG  | O8-C23-C24  | 2.85  | 120.85      | 111.91   |
| 5   | D     | 305 | CHL  | C2A-C3A-C4A | 2.85  | 106.47      | 101.87   |
| 5   | D     | 313 | CHL  | CHC-C1C-NC  | 2.85  | 128.52      | 124.20   |
| 5   | A     | 313 | CHL  | C4-C3-C5    | 2.84  | 120.06      | 115.27   |
| 2   | D     | 301 | 0IE  | C17-C16-C15 | 2.84  | 123.30      | 118.94   |
| 5   | C     | 318 | CHL  | OMC-CMC-C2C | -2.84 | 119.27      | 125.69   |
| 3   | A     | 303 | NEX  | C26-C27-C28 | 2.84  | 131.99      | 125.99   |
| 5   | A     | 309 | CHL  | C2A-C3A-C4A | 2.84  | 106.45      | 101.87   |
| 5   | D     | 311 | CHL  | CAC-C3C-C4C | 2.84  | 128.49      | 124.81   |
| 5   | E     | 304 | CHL  | O2A-CGA-CBA | 2.83  | 120.79      | 111.91   |
| 5   | E     | 310 | CHL  | C2A-C3A-C4A | 2.83  | 106.44      | 101.87   |
| 5   | B     | 313 | CHL  | CHD-C4C-C3C | -2.83 | 120.68      | 124.84   |
| 5   | A     | 305 | CHL  | CHD-C1D-C2D | -2.83 | 119.55      | 125.48   |
| 6   | D     | 316 | CLA  | O2D-CGD-O1D | -2.83 | 118.31      | 123.84   |
| 9   | C     | 321 | 0UR  | C24-C25-C26 | -2.82 | 106.44      | 110.30   |
| 5   | F     | 309 | CHL  | C3A-C2A-C1A | -2.82 | 96.87       | 101.64   |
| 5   | B     | 307 | CHL  | CHC-C1C-C2C | -2.82 | 115.89      | 126.11   |
| 7   | D     | 319 | LHG  | O8-C23-C24  | 2.82  | 120.75      | 111.91   |
| 5   | E     | 305 | CHL  | CHA-C4D-ND  | 2.82  | 138.39      | 132.50   |
| 9   | C     | 321 | 0UR  | C43-C3-C2   | 2.82  | 123.28      | 116.66   |
| 5   | E     | 312 | CHL  | O2A-CGA-CBA | 2.81  | 120.73      | 111.91   |
| 6   | B     | 308 | CLA  | O2D-CGD-O1D | -2.81 | 118.34      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | C     | 318 | CHL  | CHD-C1D-C2D | -2.81 | 119.58      | 125.48   |
| 9   | D     | 321 | 0UR  | C48-C47-C46 | -2.81 | 119.82      | 125.85   |
| 5   | A     | 311 | CHL  | CHD-C4C-C3C | -2.81 | 120.71      | 124.84   |
| 5   | E     | 317 | CHL  | O2D-CGD-O1D | -2.81 | 118.35      | 123.84   |
| 5   | B     | 307 | CHL  | O2D-CGD-O1D | -2.81 | 118.35      | 123.84   |
| 5   | A     | 318 | CHL  | C4D-CHA-C1A | -2.80 | 117.84      | 121.25   |
| 6   | B     | 308 | CLA  | CHB-C4A-NA  | 2.80  | 128.39      | 124.51   |
| 5   | A     | 318 | CHL  | CAA-C2A-C3A | -2.80 | 109.56      | 116.10   |
| 2   | D     | 302 | 0IE  | C20-C3-C4   | -2.80 | 121.23      | 124.83   |
| 5   | E     | 312 | CHL  | CHD-C1D-C2D | -2.80 | 119.61      | 125.48   |
| 6   | C     | 315 | CLA  | O2D-CGD-O1D | -2.80 | 118.37      | 123.84   |
| 5   | A     | 311 | CHL  | C4-C3-C5    | 2.80  | 119.98      | 115.27   |
| 6   | B     | 316 | CLA  | CMB-C2B-C3B | 2.80  | 129.91      | 124.68   |
| 5   | B     | 319 | CHL  | CHD-C1D-C2D | -2.79 | 119.62      | 125.48   |
| 2   | D     | 302 | 0IE  | C4-C3-C2    | -2.79 | 117.68      | 120.08   |
| 5   | D     | 313 | CHL  | C3A-C2A-C1A | -2.79 | 97.16       | 101.34   |
| 5   | A     | 313 | CHL  | C3A-C2A-C1A | -2.79 | 97.16       | 101.34   |
| 5   | F     | 311 | CHL  | OMC-CMC-C2C | -2.79 | 119.38      | 125.69   |
| 5   | E     | 311 | CHL  | CAC-C3C-C4C | 2.79  | 128.43      | 124.81   |
| 5   | F     | 311 | CHL  | O2A-CGA-CBA | 2.79  | 120.66      | 111.91   |
| 6   | A     | 316 | CLA  | CHB-C4A-NA  | 2.79  | 128.37      | 124.51   |
| 5   | C     | 312 | CHL  | C4-C3-C5    | 2.79  | 119.96      | 115.27   |
| 6   | D     | 317 | CLA  | CMB-C2B-C3B | 2.78  | 129.89      | 124.68   |
| 6   | B     | 317 | CLA  | O2D-CGD-O1D | -2.78 | 118.39      | 123.84   |
| 5   | C     | 309 | CHL  | OMC-CMC-C2C | -2.78 | 119.39      | 125.69   |
| 2   | A     | 302 | 0IE  | C13-C12-C11 | 2.78  | 123.21      | 118.94   |
| 5   | A     | 306 | CHL  | O2A-CGA-CBA | 2.78  | 120.64      | 111.91   |
| 5   | F     | 309 | CHL  | CHD-C4C-C3C | -2.78 | 120.75      | 124.84   |
| 5   | E     | 310 | CHL  | CHD-C4C-C3C | -2.78 | 120.75      | 124.84   |
| 5   | D     | 306 | CHL  | O2A-CGA-CBA | 2.78  | 120.63      | 111.91   |
| 5   | A     | 310 | CHL  | O2A-CGA-CBA | 2.78  | 120.62      | 111.91   |
| 2   | E     | 301 | 0IE  | C17-C16-C15 | 2.78  | 123.20      | 118.94   |
| 5   | A     | 318 | CHL  | CAA-C2A-C1A | 2.77  | 118.65      | 111.81   |
| 5   | E     | 317 | CHL  | OMC-CMC-C2C | -2.77 | 119.42      | 125.69   |
| 5   | B     | 314 | CHL  | C3A-C2A-C1A | -2.77 | 97.19       | 101.34   |
| 6   | A     | 315 | CLA  | CMB-C2B-C3B | 2.76  | 129.85      | 124.68   |
| 5   | C     | 313 | CHL  | C3A-C2A-C1A | -2.76 | 97.20       | 101.34   |
| 5   | C     | 306 | CHL  | C2A-C1A-CHA | -2.76 | 119.03      | 123.86   |
| 5   | B     | 314 | CHL  | C1-C2-C3    | -2.76 | 121.27      | 126.04   |
| 5   | B     | 313 | CHL  | C1-C2-C3    | -2.76 | 121.28      | 126.04   |
| 5   | B     | 311 | CHL  | CHD-C1D-C2D | -2.76 | 119.70      | 125.48   |
| 2   | F     | 301 | 0IE  | C13-C12-C11 | 2.76  | 123.17      | 118.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | F     | 316 | CLA  | O2D-CGD-O1D | -2.75 | 118.46      | 123.84   |
| 6   | D     | 316 | CLA  | CHB-C4A-NA  | 2.75  | 128.31      | 124.51   |
| 5   | E     | 304 | CHL  | C3A-C2A-C1A | -2.75 | 97.22       | 101.34   |
| 5   | C     | 305 | CHL  | C2C-C3C-C4C | -2.75 | 104.53      | 106.49   |
| 6   | C     | 308 | CLA  | C1B-CHB-C4A | -2.75 | 124.67      | 130.12   |
| 6   | C     | 307 | CLA  | C1-C2-C3    | -2.75 | 121.29      | 126.04   |
| 5   | D     | 305 | CHL  | CAC-C3C-C4C | 2.74  | 128.37      | 124.81   |
| 5   | E     | 308 | CHL  | CAC-C3C-C4C | 2.74  | 128.37      | 124.81   |
| 2   | B     | 301 | 0IE  | C13-C12-C11 | 2.74  | 123.15      | 118.94   |
| 5   | E     | 310 | CHL  | CAC-C3C-C4C | 2.74  | 128.37      | 124.81   |
| 5   | D     | 309 | CHL  | O2D-CGD-O1D | -2.74 | 118.48      | 123.84   |
| 6   | E     | 315 | CLA  | O2D-CGD-O1D | -2.73 | 118.49      | 123.84   |
| 6   | E     | 313 | CLA  | O2D-CGD-O1D | -2.73 | 118.50      | 123.84   |
| 6   | D     | 308 | CLA  | O2D-CGD-O1D | -2.73 | 118.50      | 123.84   |
| 5   | D     | 318 | CHL  | CHC-C1C-NC  | 2.73  | 128.34      | 124.20   |
| 5   | D     | 312 | CHL  | OMC-CMC-C2C | -2.72 | 119.53      | 125.69   |
| 5   | E     | 308 | CHL  | OMC-CMC-C2C | -2.72 | 119.53      | 125.69   |
| 5   | C     | 309 | CHL  | CHD-C4C-NC  | 2.72  | 128.49      | 124.20   |
| 7   | B     | 324 | LHG  | O7-C7-O9    | -2.72 | 117.14      | 123.70   |
| 5   | E     | 312 | CHL  | CHD-C4C-NC  | 2.72  | 128.48      | 124.20   |
| 3   | E     | 303 | NEX  | C31-C32-C33 | -2.71 | 118.80      | 126.42   |
| 2   | D     | 302 | 0IE  | C13-C12-C11 | 2.71  | 123.10      | 118.94   |
| 5   | B     | 307 | CHL  | O2A-CGA-CBA | 2.71  | 120.42      | 111.91   |
| 6   | A     | 317 | CLA  | C1B-CHB-C4A | -2.71 | 124.75      | 130.12   |
| 3   | F     | 303 | NEX  | C40-C33-C34 | -2.71 | 119.13      | 122.92   |
| 5   | F     | 305 | CHL  | C16-C15-C13 | -2.71 | 107.17      | 115.92   |
| 5   | B     | 311 | CHL  | O2A-CGA-CBA | 2.71  | 120.40      | 111.91   |
| 6   | C     | 307 | CLA  | CMB-C2B-C1B | -2.71 | 124.31      | 128.46   |
| 6   | D     | 314 | CLA  | C1B-CHB-C4A | -2.70 | 124.76      | 130.12   |
| 5   | A     | 313 | CHL  | OMC-CMC-C2C | -2.70 | 119.58      | 125.69   |
| 9   | E     | 320 | 0UR  | C48-C47-C46 | -2.70 | 120.05      | 125.85   |
| 5   | E     | 317 | CHL  | CHD-C4C-NC  | 2.70  | 128.46      | 124.20   |
| 4   | D     | 304 | LMU  | C3'-C4'-C5' | -2.70 | 104.74      | 110.93   |
| 5   | C     | 310 | CHL  | CHC-C1C-NC  | 2.70  | 128.30      | 124.20   |
| 6   | E     | 307 | CLA  | C1B-CHB-C4A | -2.70 | 124.77      | 130.12   |
| 7   | F     | 318 | LHG  | C11-C10-C9  | -2.70 | 100.74      | 114.42   |
| 5   | E     | 309 | CHL  | C3A-C2A-C1A | -2.70 | 97.30       | 101.34   |
| 9   | F     | 320 | 0UR  | C10-C11-C12 | -2.69 | 123.46      | 127.31   |
| 5   | A     | 312 | CHL  | C4-C3-C5    | 2.69  | 119.80      | 115.27   |
| 5   | C     | 312 | CHL  | O2A-CGA-CBA | 2.69  | 120.36      | 111.91   |
| 9   | F     | 320 | 0UR  | C43-C3-C2   | 2.69  | 122.98      | 116.66   |
| 5   | F     | 308 | CHL  | CHC-C1C-NC  | 2.69  | 128.28      | 124.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | E     | 310 | CHL  | C4-C3-C5    | 2.69  | 119.80      | 115.27   |
| 5   | B     | 319 | CHL  | C3A-C2A-C1A | -2.69 | 97.31       | 101.34   |
| 6   | E     | 306 | CLA  | O2A-CGA-O1A | -2.69 | 116.81      | 123.59   |
| 5   | E     | 311 | CHL  | C3A-C2A-C1A | -2.69 | 97.31       | 101.34   |
| 3   | F     | 303 | NEX  | C17-C1-C6   | -2.69 | 108.07      | 110.47   |
| 5   | A     | 309 | CHL  | O2D-CGD-O1D | -2.69 | 118.59      | 123.84   |
| 5   | B     | 310 | CHL  | O2D-CGD-O1D | -2.69 | 118.59      | 123.84   |
| 5   | E     | 305 | CHL  | O2A-CGA-CBA | 2.69  | 120.33      | 111.91   |
| 5   | C     | 312 | CHL  | O2D-CGD-O1D | -2.68 | 118.59      | 123.84   |
| 5   | F     | 311 | CHL  | C4D-CHA-C1A | -2.68 | 117.98      | 121.25   |
| 5   | B     | 306 | CHL  | OMC-CMC-C2C | -2.68 | 119.62      | 125.69   |
| 5   | F     | 310 | CHL  | CMD-C2D-C3D | 2.68  | 133.78      | 127.61   |
| 5   | D     | 310 | CHL  | CAC-C3C-C4C | 2.68  | 128.29      | 124.81   |
| 5   | B     | 313 | CHL  | C6-C5-C3    | -2.68 | 106.43      | 113.45   |
| 5   | B     | 310 | CHL  | CHD-C4C-NC  | 2.68  | 128.42      | 124.20   |
| 6   | F     | 306 | CLA  | CMB-C2B-C3B | 2.68  | 129.69      | 124.68   |
| 5   | B     | 307 | CHL  | CHA-C4D-ND  | 2.68  | 138.10      | 132.50   |
| 5   | A     | 306 | CHL  | CMD-C2D-C1D | -2.68 | 120.00      | 124.71   |
| 5   | B     | 313 | CHL  | C3A-C2A-C1A | -2.67 | 97.33       | 101.34   |
| 5   | A     | 312 | CHL  | CHD-C1D-C2D | -2.67 | 119.87      | 125.48   |
| 2   | B     | 301 | OIE  | C39-C32-C31 | 2.67  | 113.53      | 109.71   |
| 5   | E     | 304 | CHL  | C2A-C1A-CHA | -2.67 | 119.19      | 123.86   |
| 5   | F     | 308 | CHL  | CHD-C1D-C2D | -2.67 | 119.88      | 125.48   |
| 5   | F     | 308 | CHL  | C4D-CHA-C1A | -2.67 | 118.00      | 121.25   |
| 7   | C     | 319 | LHG  | O8-C23-C24  | 2.67  | 120.28      | 111.91   |
| 6   | E     | 313 | CLA  | C1B-CHB-C4A | -2.67 | 124.83      | 130.12   |
| 5   | D     | 306 | CHL  | C11-C10-C8  | -2.67 | 107.30      | 115.92   |
| 6   | B     | 315 | CLA  | CHD-C1D-ND  | -2.67 | 122.00      | 124.45   |
| 2   | A     | 301 | OIE  | C9-C10-C11  | 2.67  | 128.94      | 123.47   |
| 6   | B     | 308 | CLA  | O2D-CGD-CBD | 2.66  | 116.00      | 111.27   |
| 5   | A     | 305 | CHL  | OMC-CMC-C2C | -2.66 | 119.67      | 125.69   |
| 5   | F     | 308 | CHL  | C2A-C3A-C4A | 2.66  | 105.18      | 101.78   |
| 9   | F     | 320 | OUR  | C21-C12-C11 | -2.66 | 119.20      | 122.92   |
| 5   | F     | 311 | CHL  | C3A-C2A-C1A | -2.66 | 97.35       | 101.34   |
| 5   | F     | 304 | CHL  | C2A-C1A-CHA | -2.66 | 119.21      | 123.86   |
| 6   | B     | 315 | CLA  | C3C-C4C-NC  | -2.66 | 107.59      | 110.57   |
| 5   | F     | 317 | CHL  | OMC-CMC-C2C | -2.66 | 119.68      | 125.69   |
| 5   | A     | 305 | CHL  | CHD-C4C-NC  | 2.65  | 128.39      | 124.20   |
| 9   | F     | 320 | OUR  | C48-C47-C46 | -2.65 | 120.16      | 125.85   |
| 6   | F     | 306 | CLA  | C1-C2-C3    | -2.65 | 121.46      | 126.04   |
| 5   | F     | 304 | CHL  | OMC-CMC-C2C | -2.65 | 119.70      | 125.69   |
| 5   | B     | 306 | CHL  | C2A-C3A-C4A | 2.65  | 106.15      | 101.87   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | F     | 313 | CLA  | CHB-C4A-NA  | 2.65  | 128.17      | 124.51   |
| 6   | E     | 314 | CLA  | CMB-C2B-C3B | 2.65  | 129.63      | 124.68   |
| 5   | C     | 312 | CHL  | C2A-C1A-CHA | -2.64 | 119.24      | 123.86   |
| 6   | A     | 314 | CLA  | C7-C6-C5    | -2.64 | 106.19      | 113.36   |
| 5   | A     | 311 | CHL  | O2D-CGD-O1D | -2.64 | 118.68      | 123.84   |
| 5   | E     | 311 | CHL  | O2A-CGA-CBA | 2.64  | 120.18      | 111.91   |
| 5   | E     | 304 | CHL  | C4D-CHA-C1A | -2.64 | 118.04      | 121.25   |
| 5   | B     | 313 | CHL  | C2A-C1A-CHA | -2.63 | 119.25      | 123.86   |
| 5   | D     | 313 | CHL  | OBD-CAD-C3D | -2.63 | 122.18      | 128.52   |
| 6   | F     | 313 | CLA  | CHD-C1D-ND  | -2.63 | 122.03      | 124.45   |
| 9   | E     | 320 | OUR  | C23-C24-C25 | -2.63 | 107.70      | 113.64   |
| 5   | E     | 312 | CHL  | CAC-C3C-C4C | 2.63  | 128.22      | 124.81   |
| 9   | B     | 325 | OUR  | C10-C9-C8   | -2.63 | 118.08      | 123.47   |
| 5   | D     | 313 | CHL  | O2D-CGD-O1D | -2.63 | 118.69      | 123.84   |
| 11  | F     | 319 | LMG  | O6-C1-O1    | -2.63 | 103.75      | 109.97   |
| 5   | B     | 312 | CHL  | CMD-C2D-C3D | -2.63 | 121.56      | 127.61   |
| 6   | E     | 307 | CLA  | CHB-C4A-NA  | 2.63  | 128.15      | 124.51   |
| 5   | B     | 311 | CHL  | C5-C3-C4    | 2.63  | 120.41      | 114.60   |
| 5   | A     | 313 | CHL  | O2A-CGA-CBA | 2.63  | 120.15      | 111.91   |
| 5   | D     | 318 | CHL  | CAC-C3C-C4C | 2.63  | 128.22      | 124.81   |
| 5   | D     | 318 | CHL  | O2D-CGD-O1D | -2.63 | 118.70      | 123.84   |
| 5   | B     | 311 | CHL  | CHC-C1C-NC  | 2.63  | 128.19      | 124.20   |
| 5   | A     | 311 | CHL  | C2A-C3A-C4A | 2.62  | 106.11      | 101.87   |
| 5   | C     | 306 | CHL  | O2D-CGD-O1D | -2.62 | 118.72      | 123.84   |
| 7   | A     | 319 | LHG  | C11-C10-C9  | -2.62 | 101.15      | 114.42   |
| 5   | E     | 304 | CHL  | OMC-CMC-C2C | -2.62 | 119.77      | 125.69   |
| 6   | B     | 316 | CLA  | CHB-C4A-NA  | 2.61  | 128.13      | 124.51   |
| 5   | F     | 311 | CHL  | O2D-CGD-O1D | -2.61 | 118.73      | 123.84   |
| 6   | A     | 307 | CLA  | CMB-C2B-C3B | 2.61  | 129.57      | 124.68   |
| 5   | A     | 311 | CHL  | O2A-C1-C2   | -2.61 | 101.77      | 108.64   |
| 6   | D     | 308 | CLA  | C1B-CHB-C4A | -2.61 | 124.95      | 130.12   |
| 6   | B     | 317 | CLA  | CHB-C4A-NA  | 2.61  | 128.12      | 124.51   |
| 5   | A     | 309 | CHL  | CHD-C1D-C2D | -2.60 | 120.02      | 125.48   |
| 6   | D     | 314 | CLA  | CHB-C4A-NA  | 2.60  | 128.11      | 124.51   |
| 5   | F     | 308 | CHL  | CHD-C4C-NC  | 2.60  | 128.30      | 124.20   |
| 5   | D     | 318 | CHL  | CHD-C4C-C3C | -2.60 | 121.02      | 124.84   |
| 7   | B     | 320 | LHG  | C11-C10-C9  | -2.59 | 101.25      | 114.42   |
| 5   | A     | 309 | CHL  | CAC-C3C-C4C | 2.59  | 128.18      | 124.81   |
| 6   | F     | 315 | CLA  | CHB-C4A-NA  | 2.59  | 128.10      | 124.51   |
| 9   | A     | 322 | OUR  | O42-C2-C41  | -2.59 | 116.83      | 120.58   |
| 5   | F     | 312 | CHL  | C2A-C1A-CHA | -2.59 | 119.33      | 123.86   |
| 6   | B     | 318 | CLA  | C1B-CHB-C4A | -2.59 | 124.98      | 130.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | B     | 306 | CHL  | CHD-C4C-NC  | 2.59  | 128.28      | 124.20   |
| 5   | C     | 306 | CHL  | CAC-C3C-C4C | 2.59  | 128.17      | 124.81   |
| 9   | A     | 322 | OUR  | C33-C32-C31 | -2.59 | 118.03      | 123.56   |
| 6   | C     | 317 | CLA  | C1B-CHB-C4A | -2.59 | 125.00      | 130.12   |
| 5   | B     | 313 | CHL  | CAC-C3C-C4C | 2.58  | 128.16      | 124.81   |
| 7   | C     | 319 | LHG  | C11-C10-C9  | -2.58 | 101.32      | 114.42   |
| 5   | F     | 312 | CHL  | C4-C3-C5    | 2.58  | 119.61      | 115.27   |
| 5   | B     | 314 | CHL  | CHA-C4D-ND  | 2.58  | 137.90      | 132.50   |
| 5   | D     | 313 | CHL  | OMC-CMC-C2C | -2.58 | 119.85      | 125.69   |
| 9   | C     | 321 | OUR  | O42-C2-C3   | -2.58 | 115.94      | 120.66   |
| 6   | B     | 309 | CLA  | CHD-C1D-ND  | -2.58 | 122.08      | 124.45   |
| 5   | B     | 310 | CHL  | CHD-C1D-C2D | -2.58 | 120.07      | 125.48   |
| 5   | C     | 311 | CHL  | CHD-C4C-C3C | -2.58 | 121.05      | 124.84   |
| 6   | E     | 306 | CLA  | CHB-C4A-NA  | 2.58  | 128.07      | 124.51   |
| 3   | E     | 303 | NEX  | C11-C12-C13 | 2.58  | 133.65      | 126.42   |
| 5   | C     | 318 | CHL  | CAC-C3C-C4C | 2.57  | 128.15      | 124.81   |
| 7   | F     | 318 | LHG  | O8-C23-O10  | -2.57 | 117.10      | 123.59   |
| 6   | E     | 314 | CLA  | C1B-CHB-C4A | -2.57 | 125.02      | 130.12   |
| 5   | A     | 312 | CHL  | C3A-C2A-C1A | -2.57 | 97.49       | 101.34   |
| 2   | A     | 301 | OIE  | C13-C12-C11 | 2.57  | 122.89      | 118.94   |
| 5   | E     | 312 | CHL  | OMC-CMC-C2C | -2.57 | 119.88      | 125.69   |
| 9   | B     | 302 | OUR  | O42-C2-C41  | -2.56 | 116.87      | 120.58   |
| 6   | F     | 313 | CLA  | C1B-CHB-C4A | -2.56 | 125.05      | 130.12   |
| 9   | C     | 321 | OUR  | C10-C11-C12 | -2.56 | 123.66      | 127.31   |
| 6   | B     | 315 | CLA  | O2A-CGA-O1A | -2.56 | 117.14      | 123.59   |
| 5   | D     | 306 | CHL  | CHA-C4D-ND  | 2.56  | 137.85      | 132.50   |
| 7   | F     | 318 | LHG  | C5-O7-C7    | -2.56 | 111.50      | 117.79   |
| 5   | E     | 310 | CHL  | CAA-C2A-C1A | 2.55  | 120.34      | 111.97   |
| 2   | E     | 301 | OIE  | C4-C3-C2    | 2.55  | 122.27      | 120.08   |
| 5   | C     | 309 | CHL  | C4D-CHA-C1A | -2.55 | 118.14      | 121.25   |
| 3   | B     | 303 | NEX  | C20-C13-C14 | -2.55 | 119.35      | 122.92   |
| 4   | D     | 304 | LMU  | O5'-C1'-C2' | 2.54  | 115.73      | 110.35   |
| 6   | F     | 314 | CLA  | C1B-CHB-C4A | -2.54 | 125.08      | 130.12   |
| 5   | C     | 305 | CHL  | O2A-CGA-O1A | -2.54 | 117.17      | 123.59   |
| 5   | F     | 309 | CHL  | CAC-C3C-C4C | 2.54  | 128.11      | 124.81   |
| 6   | A     | 308 | CLA  | C1B-CHB-C4A | -2.54 | 125.08      | 130.12   |
| 6   | C     | 314 | CLA  | C1B-CHB-C4A | -2.54 | 125.08      | 130.12   |
| 9   | B     | 302 | OUR  | C4-C3-C2    | 2.54  | 122.26      | 120.08   |
| 5   | B     | 307 | CHL  | CHD-C1D-ND  | 2.54  | 126.78      | 124.45   |
| 5   | C     | 309 | CHL  | CAC-C3C-C4C | 2.54  | 128.10      | 124.81   |
| 5   | E     | 311 | CHL  | C4-C3-C5    | 2.54  | 119.54      | 115.27   |
| 5   | C     | 311 | CHL  | OMC-CMC-C2C | -2.54 | 119.95      | 125.69   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 9   | A     | 322 | 0UR  | O42-C2-C3   | -2.53 | 116.03      | 120.66   |
| 5   | A     | 318 | CHL  | CHC-C1C-NC  | 2.53  | 128.04      | 124.20   |
| 9   | F     | 320 | 0UR  | C22-C16-C15 | -2.53 | 119.38      | 122.92   |
| 5   | E     | 312 | CHL  | C4-C3-C5    | 2.53  | 119.52      | 115.27   |
| 5   | E     | 308 | CHL  | CHD-C1D-C2D | -2.53 | 120.18      | 125.48   |
| 6   | A     | 317 | CLA  | C1-C2-C3    | -2.53 | 121.67      | 126.04   |
| 4   | B     | 304 | LMU  | C4B-C3B-C2B | 2.53  | 115.23      | 110.82   |
| 5   | C     | 305 | CHL  | OMC-CMC-C2C | -2.53 | 119.98      | 125.69   |
| 5   | E     | 309 | CHL  | C2A-C1A-CHA | -2.52 | 119.44      | 123.86   |
| 5   | A     | 305 | CHL  | CAC-C3C-C4C | 2.52  | 128.08      | 124.81   |
| 6   | C     | 316 | CLA  | CHB-C4A-NA  | 2.52  | 128.00      | 124.51   |
| 2   | A     | 301 | 0IE  | C5-C4-C3    | 2.52  | 130.03      | 127.00   |
| 5   | A     | 306 | CHL  | C1-O2A-CGA  | 2.52  | 123.05      | 116.44   |
| 9   | D     | 321 | 0UR  | C33-C32-C31 | -2.51 | 118.18      | 123.56   |
| 6   | F     | 306 | CLA  | C1B-CHB-C4A | -2.51 | 125.14      | 130.12   |
| 6   | C     | 317 | CLA  | CHB-C4A-NA  | 2.51  | 127.98      | 124.51   |
| 6   | E     | 316 | CLA  | O2D-CGD-O1D | -2.51 | 118.93      | 123.84   |
| 6   | E     | 316 | CLA  | CHB-C4A-NA  | 2.51  | 127.98      | 124.51   |
| 5   | C     | 310 | CHL  | CHD-C4C-NC  | 2.51  | 128.15      | 124.20   |
| 5   | C     | 305 | CHL  | C4-C3-C5    | 2.51  | 119.49      | 115.27   |
| 6   | D     | 315 | CLA  | C1B-CHB-C4A | -2.50 | 125.16      | 130.12   |
| 5   | E     | 310 | CHL  | O2D-CGD-O1D | -2.50 | 118.94      | 123.84   |
| 6   | A     | 315 | CLA  | C1B-CHB-C4A | -2.50 | 125.17      | 130.12   |
| 5   | B     | 312 | CHL  | C2A-C1A-CHA | -2.49 | 119.50      | 123.86   |
| 2   | F     | 301 | 0IE  | C4-C3-C2    | 2.49  | 122.22      | 120.08   |
| 7   | D     | 319 | LHG  | C11-C10-C9  | -2.49 | 101.77      | 114.42   |
| 9   | B     | 325 | 0UR  | C33-C32-C31 | -2.49 | 118.23      | 123.56   |
| 5   | F     | 312 | CHL  | CHA-C4D-ND  | 2.49  | 137.71      | 132.50   |
| 6   | D     | 307 | CLA  | O2A-CGA-O1A | -2.49 | 117.31      | 123.59   |
| 4   | B     | 305 | LMU  | O5'-C1'-C2' | -2.49 | 105.08      | 110.35   |
| 5   | B     | 319 | CHL  | CHD-C4C-C3C | -2.49 | 121.19      | 124.84   |
| 5   | F     | 312 | CHL  | O2A-CGA-CBA | 2.49  | 119.71      | 111.91   |
| 4   | B     | 305 | LMU  | C1B-O1B-C4' | -2.48 | 111.81      | 117.96   |
| 6   | D     | 314 | CLA  | CHD-C1D-ND  | -2.48 | 122.17      | 124.45   |
| 6   | D     | 307 | CLA  | CHB-C4A-NA  | 2.48  | 127.95      | 124.51   |
| 5   | C     | 313 | CHL  | OMC-CMC-C2C | -2.48 | 120.07      | 125.69   |
| 9   | D     | 321 | 0UR  | C21-C12-C11 | -2.48 | 119.44      | 122.92   |
| 5   | B     | 306 | CHL  | CAC-C3C-C4C | 2.48  | 128.03      | 124.81   |
| 3   | C     | 303 | NEX  | C39-C29-C30 | -2.48 | 119.45      | 122.92   |
| 5   | C     | 310 | CHL  | C4D-CHA-C1A | -2.48 | 118.23      | 121.25   |
| 7   | D     | 319 | LHG  | C20-C19-C18 | -2.48 | 101.85      | 114.42   |
| 5   | A     | 312 | CHL  | CHD-C4C-C3C | -2.48 | 121.20      | 124.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | B     | 316 | CLA  | C1B-CHB-C4A | -2.47 | 125.22      | 130.12   |
| 9   | A     | 322 | 0UR  | C10-C9-C8   | -2.47 | 118.41      | 123.47   |
| 9   | A     | 322 | 0UR  | C15-C14-C13 | -2.47 | 115.50      | 123.22   |
| 5   | C     | 318 | CHL  | C3A-C2A-C1A | -2.47 | 97.64       | 101.34   |
| 5   | A     | 318 | CHL  | O2D-CGD-O1D | -2.47 | 119.01      | 123.84   |
| 5   | B     | 319 | CHL  | OMC-CMC-C2C | -2.47 | 120.11      | 125.69   |
| 5   | C     | 311 | CHL  | C3C-C4C-NC  | 2.46  | 113.33      | 110.57   |
| 5   | E     | 312 | CHL  | C2A-C3A-C4A | 2.46  | 105.85      | 101.87   |
| 7   | E     | 318 | LHG  | C11-C10-C9  | -2.46 | 101.93      | 114.42   |
| 5   | D     | 306 | CHL  | CHD-C1D-C2D | -2.46 | 120.32      | 125.48   |
| 5   | C     | 311 | CHL  | C1-O2A-CGA  | 2.46  | 122.90      | 116.44   |
| 5   | A     | 318 | CHL  | C2A-C3A-C4A | 2.46  | 104.92      | 101.78   |
| 6   | A     | 314 | CLA  | CHB-C4A-NA  | 2.46  | 127.91      | 124.51   |
| 6   | C     | 314 | CLA  | C1-C2-C3    | -2.46 | 121.80      | 126.04   |
| 6   | E     | 316 | CLA  | C1B-CHB-C4A | -2.45 | 125.25      | 130.12   |
| 6   | F     | 307 | CLA  | C1B-CHB-C4A | -2.45 | 125.26      | 130.12   |
| 5   | F     | 305 | CHL  | CAC-C3C-C4C | 2.45  | 127.99      | 124.81   |
| 9   | B     | 302 | 0UR  | C28-C19-C18 | -2.45 | 109.60      | 112.70   |
| 5   | F     | 304 | CHL  | O2A-CGA-CBA | 2.45  | 119.60      | 111.91   |
| 6   | E     | 307 | CLA  | O2A-CGA-O1A | -2.45 | 117.41      | 123.59   |
| 5   | D     | 305 | CHL  | O2D-CGD-O1D | -2.45 | 119.05      | 123.84   |
| 5   | F     | 304 | CHL  | C2A-C3A-C4A | 2.45  | 105.83      | 101.87   |
| 6   | A     | 307 | CLA  | CHB-C4A-NA  | 2.45  | 127.90      | 124.51   |
| 5   | A     | 313 | CHL  | C2A-C1A-CHA | -2.45 | 119.57      | 123.86   |
| 5   | F     | 317 | CHL  | O2D-CGD-O1D | -2.45 | 119.05      | 123.84   |
| 6   | E     | 306 | CLA  | O2D-CGD-CBD | 2.45  | 115.61      | 111.27   |
| 5   | D     | 318 | CHL  | OMC-CMC-C2C | -2.44 | 120.16      | 125.69   |
| 5   | A     | 305 | CHL  | CAA-CBA-CGA | -2.44 | 106.11      | 113.25   |
| 3   | D     | 303 | NEX  | C40-C33-C34 | -2.44 | 119.50      | 122.92   |
| 9   | B     | 325 | 0UR  | C47-C46-C45 | -2.44 | 116.69      | 122.92   |
| 5   | E     | 309 | CHL  | O2D-CGD-O1D | -2.44 | 119.06      | 123.84   |
| 6   | F     | 316 | CLA  | C1B-CHB-C4A | -2.44 | 125.28      | 130.12   |
| 6   | E     | 315 | CLA  | CHB-C4A-NA  | 2.44  | 127.89      | 124.51   |
| 5   | C     | 309 | CHL  | O2D-CGD-O1D | -2.44 | 119.06      | 123.84   |
| 5   | D     | 306 | CHL  | OMC-CMC-C2C | -2.44 | 120.17      | 125.69   |
| 3   | F     | 303 | NEX  | C20-C13-C14 | -2.44 | 119.51      | 122.92   |
| 6   | C     | 316 | CLA  | O2D-CGD-O1D | -2.44 | 119.08      | 123.84   |
| 5   | D     | 309 | CHL  | CHD-C4C-NC  | 2.43  | 128.04      | 124.20   |
| 6   | B     | 318 | CLA  | CHB-C4A-NA  | 2.43  | 127.87      | 124.51   |
| 4   | B     | 304 | LMU  | C1B-O5B-C5B | -2.43 | 108.92      | 113.69   |
| 3   | C     | 303 | NEX  | O24-C25-C26 | -2.43 | 56.95       | 58.96    |
| 9   | C     | 321 | 0UR  | O42-C2-C41  | -2.43 | 117.07      | 120.58   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 9   | B     | 325 | 0UR  | O42-C2-C41  | -2.42 | 117.07      | 120.58   |
| 2   | A     | 302 | 0IE  | C14-C15-C16 | 2.42  | 130.77      | 127.31   |
| 5   | F     | 309 | CHL  | CMD-C2D-C3D | -2.42 | 122.04      | 127.61   |
| 9   | F     | 320 | 0UR  | C25-C26-C27 | -2.42 | 107.03      | 111.85   |
| 6   | A     | 314 | CLA  | O2A-CGA-O1A | -2.42 | 117.49      | 123.59   |
| 6   | A     | 314 | CLA  | CAC-C3C-C4C | 2.42  | 127.95      | 124.81   |
| 3   | F     | 303 | NEX  | O24-C25-C26 | -2.42 | 56.96       | 58.96    |
| 6   | D     | 316 | CLA  | C1B-CHB-C4A | -2.42 | 125.33      | 130.12   |
| 5   | D     | 309 | CHL  | CHD-C1D-C2D | -2.41 | 120.42      | 125.48   |
| 5   | B     | 311 | CHL  | O2D-CGD-O1D | -2.41 | 119.12      | 123.84   |
| 5   | D     | 305 | CHL  | CHD-C4C-C3C | -2.41 | 121.29      | 124.84   |
| 5   | D     | 310 | CHL  | CHD-C4C-NC  | 2.41  | 128.00      | 124.20   |
| 6   | A     | 308 | CLA  | CHB-C4A-NA  | 2.41  | 127.85      | 124.51   |
| 4   | B     | 305 | LMU  | C3'-C4'-C5' | 2.41  | 116.45      | 110.93   |
| 5   | F     | 312 | CHL  | OBD-CAD-C3D | 2.41  | 134.32      | 128.52   |
| 5   | D     | 313 | CHL  | CHD-C1D-C2D | -2.41 | 120.42      | 125.48   |
| 5   | A     | 312 | CHL  | C2A-C1A-CHA | -2.41 | 119.64      | 123.86   |
| 5   | F     | 308 | CHL  | OMC-CMC-C2C | -2.41 | 120.24      | 125.69   |
| 6   | B     | 317 | CLA  | C1B-CHB-C4A | -2.41 | 125.35      | 130.12   |
| 5   | C     | 313 | CHL  | O2A-CGA-CBA | 2.41  | 119.46      | 111.91   |
| 5   | D     | 310 | CHL  | O2D-CGD-O1D | -2.41 | 119.13      | 123.84   |
| 6   | D     | 317 | CLA  | C1B-CHB-C4A | -2.40 | 125.36      | 130.12   |
| 5   | D     | 305 | CHL  | C1-C2-C3    | -2.40 | 121.89      | 126.04   |
| 5   | A     | 313 | CHL  | CED-O2D-CGD | 2.40  | 121.36      | 115.94   |
| 5   | F     | 311 | CHL  | CHD-C1D-C2D | -2.40 | 120.45      | 125.48   |
| 5   | A     | 312 | CHL  | O2D-CGD-O1D | -2.39 | 119.16      | 123.84   |
| 5   | C     | 306 | CHL  | O2A-CGA-CBA | 2.39  | 119.42      | 111.91   |
| 6   | C     | 315 | CLA  | CHB-C4A-NA  | 2.39  | 127.82      | 124.51   |
| 5   | D     | 312 | CHL  | C1-C2-C3    | -2.39 | 121.91      | 126.04   |
| 7   | F     | 318 | LHG  | C20-C19-C18 | -2.39 | 102.31      | 114.42   |
| 9   | E     | 320 | 0UR  | O44-C43-C3  | 2.38  | 115.49      | 109.11   |
| 5   | C     | 305 | CHL  | O2D-CGD-O1D | -2.38 | 119.18      | 123.84   |
| 6   | D     | 314 | CLA  | C1-C2-C3    | -2.38 | 121.92      | 126.04   |
| 9   | B     | 302 | 0UR  | C35-C23-C1  | -2.38 | 106.31      | 109.71   |
| 5   | A     | 318 | CHL  | OMC-CMC-C2C | -2.38 | 120.31      | 125.69   |
| 5   | F     | 304 | CHL  | CAC-C3C-C4C | 2.38  | 127.90      | 124.81   |
| 5   | E     | 312 | CHL  | C2A-C1A-CHA | -2.38 | 119.70      | 123.86   |
| 5   | D     | 312 | CHL  | C2C-C3C-C4C | -2.38 | 104.79      | 106.49   |
| 5   | B     | 312 | CHL  | C4-C3-C5    | 2.38  | 119.27      | 115.27   |
| 5   | C     | 313 | CHL  | O1D-CGD-CBD | -2.38 | 119.62      | 124.48   |
| 5   | F     | 312 | CHL  | OMC-CMC-C2C | -2.38 | 120.32      | 125.69   |
| 5   | D     | 311 | CHL  | CHD-C4C-C3C | -2.38 | 121.35      | 124.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | D     | 317 | CLA  | O2A-CGA-O1A | -2.37 | 117.61      | 123.59   |
| 5   | D     | 306 | CHL  | C4-C3-C5    | 2.37  | 119.26      | 115.27   |
| 5   | E     | 308 | CHL  | O2D-CGD-O1D | -2.37 | 119.20      | 123.84   |
| 9   | B     | 325 | 0UR  | C21-C12-C11 | -2.37 | 119.61      | 122.92   |
| 6   | F     | 307 | CLA  | CHD-C1D-ND  | -2.37 | 122.28      | 124.45   |
| 9   | A     | 322 | 0UR  | C20-C7-C6   | 2.37  | 121.81      | 118.08   |
| 6   | C     | 308 | CLA  | CHB-C4A-NA  | 2.37  | 127.78      | 124.51   |
| 6   | B     | 308 | CLA  | CMB-C2B-C3B | 2.36  | 129.10      | 124.68   |
| 5   | E     | 309 | CHL  | CHD-C4C-NC  | 2.36  | 127.93      | 124.20   |
| 6   | A     | 314 | CLA  | C2D-C1D-ND  | -2.36 | 108.36      | 110.10   |
| 5   | A     | 309 | CHL  | CHD-C4C-NC  | 2.36  | 127.93      | 124.20   |
| 9   | E     | 320 | 0UR  | C28-C19-C18 | -2.36 | 109.72      | 112.70   |
| 6   | A     | 317 | CLA  | O2D-CGD-O1D | -2.36 | 119.22      | 123.84   |
| 5   | F     | 304 | CHL  | C4-C3-C5    | 2.36  | 119.24      | 115.27   |
| 9   | B     | 325 | 0UR  | C48-C47-C46 | -2.36 | 120.79      | 125.85   |
| 5   | C     | 310 | CHL  | OMC-CMC-C2C | -2.36 | 120.36      | 125.69   |
| 5   | D     | 306 | CHL  | O2D-CGD-O1D | -2.36 | 119.23      | 123.84   |
| 3   | B     | 303 | NEX  | C39-C29-C30 | -2.36 | 119.62      | 122.92   |
| 4   | B     | 305 | LMU  | C1'-O5'-C5' | -2.36 | 109.06      | 113.69   |
| 5   | B     | 312 | CHL  | O2D-CGD-O1D | -2.35 | 119.23      | 123.84   |
| 5   | D     | 318 | CHL  | C2D-C1D-ND  | -2.35 | 108.37      | 110.10   |
| 6   | D     | 308 | CLA  | CHD-C1D-ND  | -2.35 | 122.29      | 124.45   |
| 5   | D     | 311 | CHL  | C2A-C1A-CHA | -2.35 | 119.75      | 123.86   |
| 5   | E     | 311 | CHL  | C2A-C1A-CHA | -2.35 | 119.75      | 123.86   |
| 6   | B     | 316 | CLA  | O2A-CGA-O1A | -2.35 | 117.67      | 123.59   |
| 5   | D     | 311 | CHL  | O2D-CGD-O1D | -2.35 | 119.25      | 123.84   |
| 6   | B     | 318 | CLA  | O2A-CGA-O1A | -2.34 | 117.68      | 123.59   |
| 5   | D     | 311 | CHL  | CMB-C2B-C3B | 2.34  | 129.06      | 124.68   |
| 5   | A     | 311 | CHL  | CMB-C2B-C3B | 2.34  | 129.06      | 124.68   |
| 5   | C     | 318 | CHL  | CHC-C1C-NC  | 2.34  | 127.76      | 124.20   |
| 5   | E     | 304 | CHL  | C2A-C3A-C4A | 2.34  | 105.65      | 101.87   |
| 9   | E     | 320 | 0UR  | O44-C45-O57 | -2.34 | 117.78      | 122.93   |
| 5   | B     | 314 | CHL  | C3D-C2D-C1D | -2.34 | 102.64      | 105.83   |
| 5   | D     | 313 | CHL  | C4D-CHA-C1A | -2.34 | 118.40      | 121.25   |
| 6   | F     | 315 | CLA  | C1B-CHB-C4A | -2.34 | 125.48      | 130.12   |
| 5   | F     | 311 | CHL  | CHA-C4D-ND  | 2.34  | 137.39      | 132.50   |
| 6   | D     | 315 | CLA  | CHB-C4A-NA  | 2.34  | 127.74      | 124.51   |
| 6   | A     | 317 | CLA  | CHD-C1D-ND  | -2.33 | 122.31      | 124.45   |
| 6   | E     | 313 | CLA  | O2A-CGA-O1A | -2.33 | 117.70      | 123.59   |
| 5   | A     | 305 | CHL  | C2A-C1A-CHA | -2.33 | 119.78      | 123.86   |
| 5   | F     | 304 | CHL  | CAA-CBA-CGA | -2.33 | 106.44      | 113.25   |
| 6   | D     | 314 | CLA  | O1D-CGD-CBD | 2.33  | 129.25      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | F     | 316 | CLA  | CHB-C4A-NA  | 2.33  | 127.73      | 124.51   |
| 5   | E     | 305 | CHL  | O2A-CGA-O1A | -2.33 | 117.71      | 123.59   |
| 5   | A     | 309 | CHL  | OMC-CMC-C2C | -2.33 | 120.42      | 125.69   |
| 9   | B     | 325 | OUR  | O44-C43-C3  | 2.33  | 115.34      | 109.11   |
| 5   | A     | 305 | CHL  | O2D-CGD-O1D | -2.33 | 119.29      | 123.84   |
| 6   | A     | 315 | CLA  | O2D-CGD-CBD | 2.33  | 115.40      | 111.27   |
| 6   | C     | 315 | CLA  | CHD-C1D-ND  | -2.32 | 122.32      | 124.45   |
| 5   | E     | 304 | CHL  | CAC-C3C-C4C | 2.32  | 127.82      | 124.81   |
| 7   | F     | 318 | LHG  | C18-C17-C16 | -2.32 | 102.64      | 114.42   |
| 6   | F     | 316 | CLA  | O2A-CGA-O1A | -2.32 | 117.73      | 123.59   |
| 5   | E     | 311 | CHL  | CHD-C4C-NC  | 2.32  | 127.86      | 124.20   |
| 5   | A     | 306 | CHL  | OMC-CMC-C2C | -2.32 | 120.44      | 125.69   |
| 6   | E     | 306 | CLA  | CMB-C2B-C3B | 2.32  | 129.02      | 124.68   |
| 5   | A     | 312 | CHL  | C6-C5-C3    | -2.32 | 107.37      | 113.45   |
| 5   | D     | 313 | CHL  | C2A-C1A-CHA | -2.32 | 119.80      | 123.86   |
| 6   | E     | 315 | CLA  | C1B-CHB-C4A | -2.32 | 125.52      | 130.12   |
| 5   | B     | 307 | CHL  | OMC-CMC-C2C | -2.32 | 120.44      | 125.69   |
| 5   | C     | 318 | CHL  | CHD-C4C-NC  | 2.32  | 127.86      | 124.20   |
| 5   | F     | 308 | CHL  | O2D-CGD-O1D | -2.32 | 119.31      | 123.84   |
| 6   | C     | 317 | CLA  | O2A-CGA-O1A | -2.31 | 117.76      | 123.59   |
| 3   | B     | 303 | NEX  | C20-C13-C12 | 2.31  | 121.72      | 118.08   |
| 6   | A     | 308 | CLA  | O2A-CGA-O1A | -2.31 | 117.76      | 123.59   |
| 5   | A     | 313 | CHL  | O1D-CGD-CBD | -2.31 | 119.76      | 124.48   |
| 9   | F     | 320 | OUR  | C21-C12-C13 | 2.31  | 121.71      | 118.08   |
| 6   | D     | 308 | CLA  | CHB-C4A-NA  | 2.31  | 127.70      | 124.51   |
| 5   | F     | 305 | CHL  | CBC-CAC-C3C | -2.31 | 106.07      | 112.43   |
| 5   | E     | 305 | CHL  | OMC-CMC-C2C | -2.31 | 120.47      | 125.69   |
| 5   | E     | 304 | CHL  | CAA-CBA-CGA | -2.30 | 106.52      | 113.25   |
| 5   | A     | 305 | CHL  | CHC-C1C-C2C | -2.30 | 117.76      | 126.11   |
| 5   | F     | 309 | CHL  | CMA-C3A-C2A | -2.30 | 110.72      | 116.10   |
| 6   | E     | 313 | CLA  | CHB-C4A-NA  | 2.30  | 127.70      | 124.51   |
| 2   | C     | 301 | OIE  | C17-C16-C15 | 2.30  | 122.47      | 118.94   |
| 5   | F     | 311 | CHL  | C1-C2-C3    | -2.30 | 122.06      | 126.04   |
| 5   | D     | 312 | CHL  | CBC-CAC-C3C | -2.30 | 106.09      | 112.43   |
| 6   | C     | 315 | CLA  | C1B-CHB-C4A | -2.30 | 125.56      | 130.12   |
| 7   | E     | 318 | LHG  | O8-C23-O10  | -2.30 | 117.79      | 123.59   |
| 3   | F     | 303 | NEX  | C31-C32-C33 | -2.30 | 119.96      | 126.42   |
| 5   | C     | 318 | CHL  | C4D-CHA-C1A | -2.30 | 118.45      | 121.25   |
| 9   | C     | 321 | OUR  | C28-C19-C32 | -2.30 | 107.30      | 111.42   |
| 5   | C     | 306 | CHL  | OMC-CMC-C2C | -2.30 | 120.50      | 125.69   |
| 5   | B     | 313 | CHL  | CHD-C4C-NC  | 2.30  | 127.82      | 124.20   |
| 6   | E     | 314 | CLA  | CHB-C4A-NA  | 2.29  | 127.68      | 124.51   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | E     | 305 | CHL  | C16-C15-C13 | -2.29 | 108.50      | 115.92   |
| 2   | C     | 302 | OIE  | C17-C16-C15 | 2.29  | 122.46      | 118.94   |
| 9   | B     | 325 | OUR  | C15-C14-C13 | -2.29 | 116.07      | 123.22   |
| 11  | B     | 323 | LMG  | C1-O6-C5    | -2.29 | 109.19      | 113.69   |
| 5   | A     | 310 | CHL  | OMC-CMC-C2C | -2.29 | 120.51      | 125.69   |
| 5   | E     | 305 | CHL  | O2D-CGD-O1D | -2.29 | 119.36      | 123.84   |
| 6   | B     | 316 | CLA  | C1-C2-C3    | -2.29 | 122.09      | 126.04   |
| 5   | C     | 305 | CHL  | CMA-C3A-C4A | -2.29 | 105.63      | 111.77   |
| 5   | D     | 312 | CHL  | CHD-C1D-C2D | -2.29 | 120.69      | 125.48   |
| 5   | A     | 311 | CHL  | OMC-CMC-C2C | -2.29 | 120.52      | 125.69   |
| 6   | F     | 307 | CLA  | CHB-C4A-NA  | 2.29  | 127.67      | 124.51   |
| 7   | C     | 319 | LHG  | C27-C26-C25 | -2.28 | 102.83      | 114.42   |
| 5   | A     | 305 | CHL  | C3A-C2A-C1A | -2.28 | 97.92       | 101.34   |
| 5   | F     | 312 | CHL  | C1-C2-C3    | -2.28 | 122.09      | 126.04   |
| 5   | C     | 309 | CHL  | C2A-C3A-C4A | 2.28  | 104.69      | 101.78   |
| 5   | A     | 311 | CHL  | C1-C2-C3    | -2.28 | 122.10      | 126.04   |
| 3   | A     | 303 | NEX  | C39-C29-C30 | -2.28 | 119.73      | 122.92   |
| 6   | F     | 314 | CLA  | CHB-C4A-NA  | 2.28  | 127.67      | 124.51   |
| 5   | A     | 306 | CHL  | O2A-CGA-O1A | -2.28 | 117.84      | 123.59   |
| 5   | C     | 313 | CHL  | CAC-C3C-C4C | 2.28  | 127.77      | 124.81   |
| 5   | F     | 304 | CHL  | O2A-CGA-O1A | -2.28 | 117.85      | 123.59   |
| 5   | E     | 305 | CHL  | C11-C12-C13 | -2.28 | 108.56      | 115.92   |
| 5   | B     | 314 | CHL  | C4-C3-C5    | 2.27  | 119.10      | 115.27   |
| 5   | C     | 311 | CHL  | O2D-CGD-O1D | -2.27 | 119.39      | 123.84   |
| 5   | D     | 306 | CHL  | C16-C15-C13 | -2.27 | 108.57      | 115.92   |
| 6   | C     | 315 | CLA  | C1-C2-C3    | -2.27 | 122.11      | 126.04   |
| 6   | A     | 315 | CLA  | CHB-C4A-NA  | 2.27  | 127.66      | 124.51   |
| 5   | C     | 306 | CHL  | CHD-C1D-C2D | -2.27 | 120.71      | 125.48   |
| 5   | D     | 311 | CHL  | C2A-C3A-C4A | 2.27  | 105.54      | 101.87   |
| 5   | C     | 313 | CHL  | CHD-C1D-C2D | -2.27 | 120.72      | 125.48   |
| 5   | D     | 312 | CHL  | C3A-C2A-C1A | -2.27 | 97.94       | 101.34   |
| 2   | D     | 302 | OIE  | C39-C32-C31 | 2.27  | 112.95      | 109.71   |
| 5   | F     | 317 | CHL  | O1D-CGD-CBD | -2.27 | 119.84      | 124.48   |
| 6   | C     | 316 | CLA  | C1B-CHB-C4A | -2.27 | 125.62      | 130.12   |
| 6   | C     | 308 | CLA  | O2D-CGD-O1D | -2.27 | 119.40      | 123.84   |
| 6   | C     | 307 | CLA  | CMB-C2B-C3B | 2.27  | 128.92      | 124.68   |
| 3   | C     | 303 | NEX  | C31-C32-C33 | -2.27 | 120.05      | 126.42   |
| 7   | C     | 304 | LHG  | O8-C23-C24  | 2.27  | 119.02      | 111.91   |
| 5   | D     | 318 | CHL  | C3A-C2A-C1A | -2.26 | 97.95       | 101.34   |
| 5   | B     | 306 | CHL  | O2D-CGD-O1D | -2.26 | 119.42      | 123.84   |
| 7   | B     | 320 | LHG  | C20-C19-C18 | -2.26 | 102.97      | 114.42   |
| 5   | F     | 311 | CHL  | C6-C5-C3    | -2.26 | 107.54      | 113.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | A     | 318 | CHL  | CAC-C3C-C4C | 2.25  | 127.73      | 124.81   |
| 6   | A     | 316 | CLA  | C1B-CHB-C4A | -2.25 | 125.66      | 130.12   |
| 9   | B     | 325 | OUR  | C9-C8-C7    | -2.25 | 124.10      | 127.31   |
| 3   | D     | 303 | NEX  | C20-C13-C14 | -2.25 | 119.77      | 122.92   |
| 7   | B     | 324 | LHG  | O8-C23-O10  | -2.25 | 117.92      | 123.59   |
| 5   | F     | 309 | CHL  | C2A-C1A-CHA | -2.24 | 119.94      | 123.85   |
| 5   | F     | 310 | CHL  | C2A-C3A-C4A | 2.24  | 105.49      | 101.87   |
| 5   | C     | 312 | CHL  | OMC-CMC-C2C | -2.24 | 120.62      | 125.69   |
| 3   | F     | 303 | NEX  | C11-C12-C13 | 2.24  | 132.71      | 126.42   |
| 5   | F     | 312 | CHL  | C4D-CHA-C1A | -2.24 | 118.53      | 121.25   |
| 5   | E     | 305 | CHL  | C11-C10-C8  | -2.24 | 108.69      | 115.92   |
| 5   | D     | 312 | CHL  | O2D-CGD-O1D | -2.23 | 119.47      | 123.84   |
| 6   | F     | 313 | CLA  | C3A-C2A-C1A | 2.23  | 104.68      | 101.34   |
| 7   | E     | 318 | LHG  | C18-C17-C16 | -2.23 | 103.10      | 114.42   |
| 5   | D     | 305 | CHL  | C2D-C1D-ND  | -2.23 | 108.46      | 110.10   |
| 3   | D     | 303 | NEX  | C39-C29-C30 | -2.23 | 119.80      | 122.92   |
| 5   | F     | 305 | CHL  | C2A-C3A-C4A | 2.23  | 105.47      | 101.87   |
| 5   | B     | 306 | CHL  | O2A-CGA-CBA | 2.23  | 118.90      | 111.91   |
| 5   | B     | 311 | CHL  | C2A-C1A-CHA | -2.23 | 119.96      | 123.86   |
| 5   | C     | 312 | CHL  | C2A-C3A-C4A | 2.23  | 105.47      | 101.87   |
| 9   | A     | 322 | OUR  | C47-C46-C45 | -2.23 | 117.24      | 122.92   |
| 5   | B     | 307 | CHL  | C16-C15-C13 | -2.22 | 108.74      | 115.92   |
| 9   | C     | 321 | OUR  | C21-C12-C13 | 2.22  | 121.58      | 118.08   |
| 6   | A     | 317 | CLA  | CHB-C4A-NA  | 2.22  | 127.58      | 124.51   |
| 5   | D     | 309 | CHL  | CAA-C2A-C3A | -2.22 | 110.92      | 116.10   |
| 5   | D     | 305 | CHL  | OMC-CMC-C2C | -2.22 | 120.67      | 125.69   |
| 6   | C     | 314 | CLA  | O2A-CGA-O1A | -2.22 | 118.00      | 123.59   |
| 7   | E     | 318 | LHG  | O8-C23-C24  | 2.21  | 118.86      | 111.91   |
| 5   | D     | 309 | CHL  | CMA-C3A-C2A | -2.21 | 110.93      | 116.10   |
| 5   | F     | 311 | CHL  | CAC-C3C-C4C | 2.21  | 127.68      | 124.81   |
| 5   | F     | 305 | CHL  | OMC-CMC-C2C | -2.21 | 120.69      | 125.69   |
| 5   | D     | 309 | CHL  | CAC-C3C-C4C | 2.21  | 127.67      | 124.81   |
| 9   | A     | 322 | OUR  | C23-C24-C25 | -2.21 | 108.66      | 113.64   |
| 7   | D     | 319 | LHG  | C18-C17-C16 | -2.21 | 103.22      | 114.42   |
| 3   | A     | 303 | NEX  | C31-C32-C33 | -2.21 | 120.22      | 126.42   |
| 6   | E     | 314 | CLA  | CHD-C1D-ND  | -2.21 | 122.43      | 124.45   |
| 5   | E     | 304 | CHL  | CHD-C1D-C2D | -2.21 | 120.85      | 125.48   |
| 5   | A     | 306 | CHL  | CHD-C1D-C2D | -2.21 | 120.85      | 125.48   |
| 5   | B     | 310 | CHL  | C2A-C3A-C4A | 2.20  | 105.43      | 101.87   |
| 3   | F     | 303 | NEX  | C24-C23-C22 | -2.20 | 106.52      | 110.77   |
| 5   | D     | 318 | CHL  | O2A-CGA-CBA | 2.20  | 121.11      | 114.03   |
| 5   | B     | 314 | CHL  | O2A-CGA-CBA | 2.20  | 118.81      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | E     | 304 | CHL  | C6-C5-C3    | -2.20 | 107.69      | 113.45   |
| 5   | B     | 310 | CHL  | OMC-CMC-C2C | -2.20 | 120.72      | 125.69   |
| 5   | F     | 305 | CHL  | O2A-CGA-CBA | 2.20  | 118.80      | 111.91   |
| 5   | B     | 311 | CHL  | C4D-CHA-C1A | -2.20 | 118.58      | 121.25   |
| 5   | F     | 312 | CHL  | CHD-C1D-C2D | -2.20 | 120.87      | 125.48   |
| 2   | D     | 302 | OIE  | C4-C5-C6    | 2.20  | 130.07      | 123.22   |
| 5   | A     | 310 | CHL  | C5-C3-C4    | 2.19  | 119.45      | 114.60   |
| 5   | D     | 312 | CHL  | C4-C3-C5    | 2.19  | 118.96      | 115.27   |
| 5   | E     | 309 | CHL  | C2A-C3A-C4A | 2.19  | 105.41      | 101.87   |
| 5   | C     | 305 | CHL  | CHD-C1D-C2D | -2.19 | 120.88      | 125.48   |
| 5   | A     | 306 | CHL  | O2D-CGD-O1D | -2.19 | 119.55      | 123.84   |
| 5   | E     | 309 | CHL  | CHC-C1C-NC  | 2.19  | 127.53      | 124.20   |
| 5   | A     | 310 | CHL  | CBC-CAC-C3C | -2.19 | 106.39      | 112.43   |
| 5   | F     | 312 | CHL  | C2A-C3A-C4A | 2.19  | 105.41      | 101.87   |
| 5   | B     | 311 | CHL  | OMC-CMC-C2C | -2.19 | 120.74      | 125.69   |
| 5   | F     | 310 | CHL  | O2A-CGA-O1A | -2.19 | 118.07      | 123.59   |
| 6   | A     | 307 | CLA  | O2D-CGD-CBD | 2.19  | 115.16      | 111.27   |
| 6   | E     | 306 | CLA  | C1-C2-C3    | -2.19 | 122.26      | 126.04   |
| 7   | D     | 319 | LHG  | C5-O7-C7    | -2.19 | 112.41      | 117.79   |
| 11  | B     | 323 | LMG  | O6-C1-O1    | -2.18 | 104.80      | 109.97   |
| 3   | B     | 303 | NEX  | O24-C25-C26 | -2.18 | 57.15       | 58.96    |
| 5   | D     | 306 | CHL  | O2A-CGA-O1A | -2.18 | 118.08      | 123.59   |
| 5   | F     | 317 | CHL  | O2A-CGA-CBA | 2.18  | 121.05      | 114.03   |
| 5   | E     | 304 | CHL  | C4-C3-C5    | 2.18  | 118.94      | 115.27   |
| 6   | C     | 314 | CLA  | CHB-C4A-NA  | 2.18  | 127.53      | 124.51   |
| 5   | A     | 313 | CHL  | CAC-C3C-C4C | 2.18  | 127.64      | 124.81   |
| 5   | E     | 305 | CHL  | CHD-C1D-C2D | -2.18 | 120.91      | 125.48   |
| 6   | B     | 309 | CLA  | CHB-C4A-NA  | 2.18  | 127.52      | 124.51   |
| 5   | A     | 306 | CHL  | C2A-C3A-C4A | 2.17  | 105.38      | 101.87   |
| 6   | C     | 315 | CLA  | O2A-CGA-O1A | -2.17 | 118.11      | 123.59   |
| 4   | B     | 305 | LMU  | C2'-C3'-C4' | 2.17  | 114.64      | 109.68   |
| 5   | C     | 313 | CHL  | C4D-CHA-C1A | -2.17 | 118.61      | 121.25   |
| 9   | A     | 322 | OUR  | C4-C5-C6    | -2.17 | 116.45      | 123.22   |
| 5   | C     | 311 | CHL  | O2A-CGA-O1A | -2.17 | 118.12      | 123.59   |
| 5   | F     | 309 | CHL  | O2D-CGD-O1D | -2.17 | 119.60      | 123.84   |
| 5   | F     | 309 | CHL  | C3C-C4C-NC  | 2.16  | 113.00      | 110.57   |
| 5   | F     | 310 | CHL  | CAC-C3C-C4C | 2.16  | 127.62      | 124.81   |
| 5   | B     | 311 | CHL  | C1-C2-C3    | -2.16 | 123.25      | 126.75   |
| 6   | D     | 314 | CLA  | C7-C6-C5    | -2.16 | 107.49      | 113.36   |
| 5   | F     | 305 | CHL  | CHC-C1C-C2C | -2.16 | 118.28      | 126.11   |
| 6   | F     | 313 | CLA  | O2D-CGD-CBD | 2.16  | 115.11      | 111.27   |
| 6   | B     | 318 | CLA  | CHD-C1D-ND  | -2.16 | 122.47      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | F     | 315 | CLA  | O2A-CGA-O1A | -2.16 | 117.92      | 123.30   |
| 5   | E     | 311 | CHL  | C2A-C3A-C4A | 2.16  | 105.36      | 101.87   |
| 6   | B     | 308 | CLA  | C1B-CHB-C4A | -2.16 | 125.84      | 130.12   |
| 5   | F     | 308 | CHL  | O1D-CGD-CBD | -2.16 | 120.07      | 124.48   |
| 6   | D     | 317 | CLA  | CHB-C4A-NA  | 2.16  | 127.49      | 124.51   |
| 3   | D     | 303 | NEX  | C31-C32-C33 | -2.16 | 120.36      | 126.42   |
| 9   | B     | 302 | OUR  | C33-C32-C31 | -2.16 | 118.95      | 123.56   |
| 3   | E     | 303 | NEX  | C39-C29-C30 | -2.16 | 119.90      | 122.92   |
| 6   | B     | 317 | CLA  | O2A-CGA-O1A | -2.15 | 117.93      | 123.30   |
| 5   | C     | 312 | CHL  | C2D-C1D-ND  | -2.15 | 108.52      | 110.10   |
| 5   | C     | 312 | CHL  | CMD-C2D-C3D | -2.15 | 122.66      | 127.61   |
| 9   | E     | 320 | OUR  | C22-C16-C15 | -2.15 | 119.91      | 122.92   |
| 6   | D     | 316 | CLA  | O2A-CGA-O1A | -2.15 | 117.94      | 123.30   |
| 6   | C     | 317 | CLA  | CHD-C1D-ND  | -2.15 | 122.48      | 124.45   |
| 5   | A     | 318 | CHL  | CHD-C4C-NC  | 2.15  | 127.59      | 124.20   |
| 5   | C     | 311 | CHL  | CHA-C1A-NA  | -2.15 | 121.48      | 126.40   |
| 5   | F     | 304 | CHL  | CHC-C1C-C2C | -2.15 | 118.33      | 126.11   |
| 6   | B     | 315 | CLA  | CAC-C3C-C2C | -2.15 | 123.86      | 127.53   |
| 7   | B     | 320 | LHG  | O8-C23-C24  | 2.15  | 118.64      | 111.91   |
| 5   | F     | 305 | CHL  | CHA-C4D-ND  | 2.14  | 136.98      | 132.50   |
| 6   | D     | 315 | CLA  | O2D-CGD-CBD | 2.14  | 115.08      | 111.27   |
| 6   | D     | 314 | CLA  | C3C-C4C-NC  | -2.14 | 108.17      | 110.57   |
| 5   | D     | 306 | CHL  | CHC-C1C-C2C | -2.14 | 118.36      | 126.11   |
| 5   | A     | 311 | CHL  | C2A-C1A-CHA | -2.14 | 120.12      | 123.86   |
| 5   | C     | 309 | CHL  | CAA-C2A-C3A | -2.14 | 111.11      | 116.10   |
| 9   | C     | 321 | OUR  | C28-C19-C18 | -2.14 | 110.00      | 112.70   |
| 5   | C     | 306 | CHL  | CMB-C2B-C3B | 2.13  | 128.67      | 124.68   |
| 7   | C     | 319 | LHG  | C20-C19-C18 | -2.13 | 103.60      | 114.42   |
| 5   | E     | 310 | CHL  | CHC-C1C-C2C | -2.13 | 118.38      | 126.11   |
| 6   | A     | 317 | CLA  | O2A-CGA-O1A | -2.13 | 118.22      | 123.59   |
| 5   | E     | 310 | CHL  | O2A-CGA-O1A | -2.13 | 118.22      | 123.59   |
| 5   | A     | 311 | CHL  | C3C-C4C-NC  | 2.13  | 112.96      | 110.57   |
| 9   | B     | 325 | OUR  | C21-C12-C13 | 2.13  | 121.43      | 118.08   |
| 5   | E     | 311 | CHL  | O2D-CGD-O1D | -2.13 | 119.68      | 123.84   |
| 5   | F     | 308 | CHL  | CAA-C2A-C3A | -2.13 | 111.14      | 116.10   |
| 6   | E     | 306 | CLA  | C11-C12-C13 | -2.13 | 109.05      | 115.92   |
| 5   | B     | 311 | CHL  | C3A-C2A-C1A | -2.13 | 98.16       | 101.34   |
| 6   | D     | 314 | CLA  | O2A-CGA-O1A | -2.13 | 118.23      | 123.59   |
| 7   | C     | 319 | LHG  | C18-C17-C16 | -2.12 | 103.65      | 114.42   |
| 9   | A     | 322 | OUR  | C28-C19-C18 | -2.12 | 110.02      | 112.70   |
| 5   | D     | 305 | CHL  | O2A-CGA-CBA | 2.12  | 118.57      | 111.91   |
| 5   | A     | 305 | CHL  | CBC-CAC-C3C | -2.12 | 106.59      | 112.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 9   | B     | 302 | 0UR  | O44-C45-O57 | -2.12 | 118.28      | 122.93   |
| 5   | D     | 306 | CHL  | CAC-C3C-C4C | 2.12  | 127.56      | 124.81   |
| 11  | F     | 319 | LMG  | O2-C2-C1    | -2.12 | 104.91      | 110.05   |
| 2   | A     | 301 | 0IE  | C5-C6-C7    | 2.12  | 132.36      | 126.42   |
| 5   | F     | 312 | CHL  | C1-O2A-CGA  | 2.12  | 122.00      | 116.44   |
| 3   | B     | 303 | NEX  | C31-C32-C33 | -2.12 | 120.47      | 126.42   |
| 6   | F     | 313 | CLA  | C3C-C4C-NC  | -2.12 | 108.20      | 110.57   |
| 5   | A     | 310 | CHL  | CAC-C3C-C4C | 2.11  | 127.55      | 124.81   |
| 6   | C     | 307 | CLA  | C1B-CHB-C4A | -2.11 | 125.93      | 130.12   |
| 5   | D     | 311 | CHL  | O2A-CGA-O1A | -2.11 | 118.26      | 123.59   |
| 5   | C     | 305 | CHL  | CAC-C3C-C4C | 2.11  | 127.55      | 124.81   |
| 2   | F     | 301 | 0IE  | C23-C16-C17 | 2.11  | 121.40      | 118.08   |
| 5   | E     | 304 | CHL  | CHC-C1C-C2C | -2.11 | 118.46      | 126.11   |
| 11  | B     | 323 | LMG  | O3-C3-C2    | -2.11 | 105.48      | 110.35   |
| 5   | F     | 317 | CHL  | C2D-C1D-ND  | -2.11 | 108.55      | 110.10   |
| 5   | F     | 308 | CHL  | CAC-C3C-C4C | 2.10  | 127.54      | 124.81   |
| 9   | C     | 321 | 0UR  | C9-C8-C7    | -2.10 | 124.31      | 127.31   |
| 5   | D     | 311 | CHL  | O1D-CGD-CBD | -2.10 | 120.18      | 124.48   |
| 7   | F     | 318 | LHG  | C27-C26-C25 | -2.10 | 103.75      | 114.42   |
| 9   | D     | 321 | 0UR  | C15-C14-C13 | -2.10 | 116.66      | 123.22   |
| 11  | F     | 319 | LMG  | O3-C3-C2    | -2.10 | 105.49      | 110.35   |
| 6   | A     | 314 | CLA  | CHD-C1D-ND  | -2.10 | 122.52      | 124.45   |
| 5   | A     | 306 | CHL  | CED-O2D-CGD | 2.10  | 120.69      | 115.94   |
| 5   | C     | 309 | CHL  | CHD-C1D-C2D | -2.10 | 121.08      | 125.48   |
| 5   | D     | 310 | CHL  | O1D-CGD-CBD | -2.10 | 120.19      | 124.48   |
| 6   | C     | 314 | CLA  | O2D-CGD-CBD | 2.10  | 115.00      | 111.27   |
| 6   | A     | 307 | CLA  | C4-C3-C5    | 2.10  | 118.80      | 115.27   |
| 9   | E     | 320 | 0UR  | C21-C12-C11 | -2.10 | 119.98      | 122.92   |
| 9   | F     | 320 | 0UR  | C34-C27-C1  | -2.10 | 121.74      | 124.49   |
| 6   | D     | 315 | CLA  | CHD-C1D-ND  | -2.10 | 122.53      | 124.45   |
| 6   | E     | 314 | CLA  | C1-C2-C3    | -2.09 | 122.42      | 126.04   |
| 5   | D     | 313 | CHL  | O1D-CGD-CBD | -2.09 | 120.20      | 124.48   |
| 5   | C     | 312 | CHL  | O2A-CGA-O1A | -2.09 | 118.31      | 123.59   |
| 5   | E     | 305 | CHL  | CED-O2D-CGD | 2.09  | 120.67      | 115.94   |
| 5   | E     | 312 | CHL  | C1-O2A-CGA  | 2.09  | 121.94      | 116.44   |
| 5   | B     | 307 | CHL  | C6-C5-C3    | -2.09 | 107.97      | 113.45   |
| 5   | F     | 309 | CHL  | OMC-CMC-C2C | -2.09 | 120.96      | 125.69   |
| 11  | B     | 323 | LMG  | O2-C2-C1    | -2.09 | 104.97      | 110.05   |
| 5   | C     | 313 | CHL  | C2A-C1A-CHA | -2.09 | 120.21      | 123.86   |
| 6   | A     | 314 | CLA  | O1D-CGD-CBD | 2.09  | 128.75      | 124.48   |
| 3   | F     | 303 | NEX  | C19-C9-C10  | -2.08 | 120.00      | 122.92   |
| 5   | B     | 314 | CHL  | C11-C10-C8  | -2.08 | 109.18      | 115.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | B     | 319 | CHL  | O1D-CGD-CBD | -2.08 | 120.22      | 124.48   |
| 5   | C     | 312 | CHL  | C6-C5-C3    | -2.08 | 108.00      | 113.45   |
| 5   | F     | 312 | CHL  | CED-O2D-CGD | 2.08  | 120.64      | 115.94   |
| 3   | B     | 303 | NEX  | C40-C33-C34 | -2.08 | 120.01      | 122.92   |
| 9   | A     | 322 | OUR  | C4-C3-C2    | -2.08 | 118.29      | 120.08   |
| 9   | F     | 320 | OUR  | O42-C2-C41  | -2.08 | 117.57      | 120.58   |
| 6   | A     | 316 | CLA  | O2A-CGA-O1A | -2.08 | 118.12      | 123.30   |
| 10  | B     | 321 | BET  | C-CA-N      | -2.08 | 113.48      | 116.34   |
| 6   | F     | 314 | CLA  | CHD-C1D-ND  | -2.08 | 122.55      | 124.45   |
| 6   | B     | 315 | CLA  | C3A-C2A-C1A | 2.08  | 104.45      | 101.34   |
| 5   | F     | 312 | CHL  | C3D-C2D-C1D | -2.08 | 103.00      | 105.83   |
| 6   | A     | 314 | CLA  | C6-C5-C3    | 2.08  | 118.90      | 113.45   |
| 9   | B     | 302 | OUR  | C17-C16-C15 | 2.07  | 122.12      | 118.94   |
| 9   | D     | 321 | OUR  | C28-C19-C18 | -2.07 | 110.08      | 112.70   |
| 5   | D     | 313 | CHL  | C2A-C3A-C4A | 2.07  | 105.22      | 101.87   |
| 5   | B     | 319 | CHL  | O2A-CGA-CBA | 2.07  | 120.42      | 112.23   |
| 5   | D     | 311 | CHL  | CED-O2D-CGD | 2.07  | 120.62      | 115.94   |
| 3   | B     | 303 | NEX  | C19-C9-C10  | -2.07 | 120.02      | 122.92   |
| 3   | A     | 303 | NEX  | C40-C33-C34 | -2.07 | 120.02      | 122.92   |
| 5   | B     | 312 | CHL  | CHD-C4C-NC  | 2.07  | 127.47      | 124.20   |
| 5   | E     | 317 | CHL  | CAC-C3C-C4C | 2.07  | 127.49      | 124.81   |
| 7   | D     | 319 | LHG  | C27-C26-C25 | -2.07 | 103.93      | 114.42   |
| 5   | A     | 305 | CHL  | C6-C5-C3    | -2.07 | 108.03      | 113.45   |
| 6   | D     | 315 | CLA  | O2A-CGA-O1A | -2.07 | 118.37      | 123.59   |
| 5   | F     | 317 | CHL  | CHD-C4C-C3C | -2.07 | 121.80      | 124.84   |
| 5   | D     | 318 | CHL  | C2A-C1A-CHA | -2.07 | 120.25      | 123.86   |
| 9   | B     | 302 | OUR  | O42-C2-C3   | -2.06 | 116.89      | 120.66   |
| 6   | B     | 308 | CLA  | O2A-CGA-O1A | -2.06 | 118.39      | 123.59   |
| 5   | F     | 304 | CHL  | CBC-CAC-C3C | -2.06 | 106.75      | 112.43   |
| 9   | E     | 320 | OUR  | C15-C14-C13 | -2.06 | 116.79      | 123.22   |
| 5   | A     | 305 | CHL  | C2A-C3A-C4A | 2.06  | 105.19      | 101.87   |
| 5   | A     | 311 | CHL  | O2A-CGA-O1A | -2.06 | 118.40      | 123.59   |
| 6   | F     | 314 | CLA  | C1-C2-C3    | -2.06 | 122.49      | 126.04   |
| 7   | B     | 320 | LHG  | C18-C17-C16 | -2.06 | 103.99      | 114.42   |
| 5   | D     | 312 | CHL  | C1-O2A-CGA  | 2.06  | 121.84      | 116.44   |
| 3   | D     | 303 | NEX  | C19-C9-C10  | -2.05 | 120.05      | 122.92   |
| 3   | E     | 303 | NEX  | C19-C9-C10  | -2.05 | 120.05      | 122.92   |
| 9   | E     | 320 | OUR  | C21-C12-C13 | 2.05  | 121.31      | 118.08   |
| 6   | E     | 307 | CLA  | C2A-C1A-CHA | 2.05  | 127.44      | 123.86   |
| 5   | E     | 310 | CHL  | OMC-CMC-C2C | -2.05 | 121.06      | 125.69   |
| 6   | A     | 307 | CLA  | C1B-CHB-C4A | -2.05 | 126.06      | 130.12   |
| 5   | E     | 304 | CHL  | C1-C2-C3    | -2.05 | 122.50      | 126.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 9   | F     | 320 | 0UR  | C33-C32-C31 | -2.05 | 119.18      | 123.56   |
| 6   | E     | 306 | CLA  | C1B-CHB-C4A | -2.05 | 126.06      | 130.12   |
| 5   | B     | 312 | CHL  | O2A-CGA-O1A | -2.05 | 118.43      | 123.59   |
| 5   | D     | 311 | CHL  | C1-O2A-CGA  | 2.05  | 121.81      | 116.44   |
| 7   | C     | 319 | LHG  | C5-O7-C7    | -2.05 | 112.75      | 117.79   |
| 5   | D     | 309 | CHL  | OMC-CMC-C2C | -2.05 | 121.06      | 125.69   |
| 5   | A     | 312 | CHL  | CMB-C2B-C3B | 2.04  | 128.50      | 124.68   |
| 6   | E     | 316 | CLA  | O2A-CGA-O1A | -2.04 | 118.44      | 123.59   |
| 5   | E     | 309 | CHL  | OMC-CMC-C2C | -2.04 | 121.07      | 125.69   |
| 5   | B     | 311 | CHL  | O1D-CGD-CBD | -2.04 | 120.31      | 124.48   |
| 9   | D     | 321 | 0UR  | O42-C2-C41  | -2.04 | 117.62      | 120.58   |
| 6   | E     | 313 | CLA  | CHD-C1D-ND  | -2.04 | 122.58      | 124.45   |
| 9   | A     | 322 | 0UR  | C21-C12-C11 | -2.04 | 120.07      | 122.92   |
| 5   | C     | 306 | CHL  | C4-C3-C2    | -2.04 | 118.45      | 123.68   |
| 5   | D     | 305 | CHL  | CHA-C1A-NA  | -2.04 | 121.73      | 126.40   |
| 7   | E     | 318 | LHG  | C27-C26-C25 | -2.03 | 104.09      | 114.42   |
| 5   | D     | 312 | CHL  | C2A-C1A-CHA | -2.03 | 120.30      | 123.86   |
| 5   | B     | 306 | CHL  | CHC-C1C-C2C | -2.03 | 118.75      | 126.11   |
| 5   | B     | 306 | CHL  | C2A-C1A-CHA | -2.03 | 120.31      | 123.86   |
| 6   | F     | 313 | CLA  | C1-C2-C3    | -2.03 | 122.53      | 126.04   |
| 5   | E     | 308 | CHL  | CHD-C4C-NC  | 2.03  | 127.40      | 124.20   |
| 5   | E     | 310 | CHL  | C3C-C4C-NC  | 2.03  | 112.84      | 110.57   |
| 5   | C     | 306 | CHL  | C11-C12-C13 | -2.03 | 109.36      | 115.92   |
| 5   | C     | 313 | CHL  | C4-C3-C5    | 2.03  | 118.68      | 115.27   |
| 6   | D     | 317 | CLA  | CHD-C1D-ND  | -2.02 | 122.59      | 124.45   |
| 5   | C     | 306 | CHL  | C11-C10-C8  | -2.02 | 109.38      | 115.92   |
| 5   | D     | 309 | CHL  | C2A-C1A-CHA | -2.02 | 120.32      | 123.85   |
| 9   | D     | 321 | 0UR  | C25-C26-C27 | 2.02  | 115.88      | 111.85   |
| 6   | B     | 315 | CLA  | C2D-C1D-ND  | -2.02 | 108.61      | 110.10   |
| 5   | F     | 310 | CHL  | C2A-C1A-CHA | -2.02 | 120.32      | 123.86   |
| 9   | B     | 325 | 0UR  | O44-C45-O57 | -2.02 | 118.49      | 122.93   |
| 5   | B     | 312 | CHL  | C3C-C4C-NC  | 2.02  | 112.84      | 110.57   |
| 3   | B     | 303 | NEX  | C24-C23-C22 | -2.02 | 106.87      | 110.77   |
| 5   | B     | 314 | CHL  | O1D-CGD-CBD | -2.02 | 120.36      | 124.48   |
| 5   | E     | 312 | CHL  | CHC-C1C-C2C | -2.02 | 118.80      | 126.11   |
| 5   | B     | 314 | CHL  | C2A-C1A-CHA | -2.02 | 120.33      | 123.86   |
| 5   | E     | 312 | CHL  | O1D-CGD-CBD | -2.02 | 120.36      | 124.48   |
| 5   | B     | 314 | CHL  | CBC-CAC-C3C | -2.01 | 106.88      | 112.43   |
| 5   | B     | 311 | CHL  | C2A-C3A-C4A | 2.01  | 105.12      | 101.87   |
| 5   | A     | 309 | CHL  | C2A-C1A-CHA | -2.01 | 120.34      | 123.86   |
| 5   | D     | 305 | CHL  | C4-C3-C5    | 2.01  | 118.65      | 115.27   |
| 6   | D     | 307 | CLA  | C1B-CHB-C4A | -2.01 | 126.14      | 130.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | D     | 311 | CHL  | OMC-CMC-C2C | -2.01 | 121.14      | 125.69   |
| 5   | A     | 310 | CHL  | CMA-C3A-C4A | -2.01 | 106.37      | 111.77   |
| 5   | C     | 306 | CHL  | C2A-C3A-C4A | 2.01  | 105.11      | 101.87   |
| 6   | C     | 314 | CLA  | CHD-C1D-ND  | -2.01 | 122.61      | 124.45   |
| 9   | C     | 321 | OUR  | C15-C14-C13 | -2.01 | 116.95      | 123.22   |
| 11  | B     | 323 | LMG  | O1-C7-C8    | -2.01 | 106.06      | 110.90   |
| 6   | C     | 317 | CLA  | C3A-C2A-C1A | 2.01  | 104.34      | 101.34   |
| 2   | F     | 302 | OIE  | C23-C16-C17 | 2.01  | 121.24      | 118.08   |
| 5   | A     | 312 | CHL  | CHD-C4C-NC  | 2.01  | 127.36      | 124.20   |
| 10  | B     | 322 | BET  | OXT-C-O     | -2.01 | 118.30      | 123.30   |
| 5   | E     | 304 | CHL  | C4-C3-C2    | -2.00 | 118.54      | 123.68   |
| 9   | B     | 302 | OUR  | C28-C19-C32 | -2.00 | 107.83      | 111.42   |
| 5   | F     | 317 | CHL  | O2A-CGA-O1A | -2.00 | 118.30      | 123.30   |
| 3   | D     | 303 | NEX  | O24-C25-C38 | 2.00  | 117.46      | 115.06   |
| 5   | A     | 318 | CHL  | CED-O2D-CGD | 2.00  | 120.47      | 115.94   |
| 7   | F     | 318 | LHG  | O8-C23-C24  | 2.00  | 118.19      | 111.91   |
| 5   | B     | 313 | CHL  | O2D-CGD-O1D | -2.00 | 119.92      | 123.84   |
| 5   | D     | 313 | CHL  | O2A-CGA-CBA | 2.00  | 118.19      | 111.91   |
| 6   | B     | 316 | CLA  | C11-C10-C8  | -2.00 | 109.45      | 115.92   |

All (180) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 5   | A     | 305 | CHL  | NA   |
| 5   | A     | 305 | CHL  | NC   |
| 5   | A     | 305 | CHL  | ND   |
| 5   | A     | 306 | CHL  | NA   |
| 5   | A     | 306 | CHL  | NC   |
| 5   | A     | 306 | CHL  | ND   |
| 5   | A     | 309 | CHL  | NA   |
| 5   | A     | 309 | CHL  | NC   |
| 5   | A     | 309 | CHL  | ND   |
| 5   | A     | 310 | CHL  | NA   |
| 5   | A     | 310 | CHL  | NC   |
| 5   | A     | 310 | CHL  | ND   |
| 5   | A     | 311 | CHL  | NA   |
| 5   | A     | 311 | CHL  | NC   |
| 5   | A     | 311 | CHL  | ND   |
| 5   | A     | 312 | CHL  | NA   |
| 5   | A     | 312 | CHL  | NC   |
| 5   | A     | 312 | CHL  | ND   |
| 5   | A     | 313 | CHL  | NA   |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Atom</b> |
|------------|--------------|------------|-------------|-------------|
| 5          | A            | 313        | CHL         | NC          |
| 5          | A            | 313        | CHL         | ND          |
| 5          | A            | 318        | CHL         | NA          |
| 5          | A            | 318        | CHL         | NC          |
| 5          | A            | 318        | CHL         | ND          |
| 5          | B            | 306        | CHL         | NA          |
| 5          | B            | 306        | CHL         | NC          |
| 5          | B            | 306        | CHL         | ND          |
| 5          | B            | 307        | CHL         | NA          |
| 5          | B            | 307        | CHL         | NC          |
| 5          | B            | 307        | CHL         | ND          |
| 5          | B            | 310        | CHL         | NA          |
| 5          | B            | 310        | CHL         | NC          |
| 5          | B            | 310        | CHL         | ND          |
| 5          | B            | 311        | CHL         | NA          |
| 5          | B            | 311        | CHL         | NC          |
| 5          | B            | 311        | CHL         | ND          |
| 5          | B            | 312        | CHL         | NA          |
| 5          | B            | 312        | CHL         | NC          |
| 5          | B            | 312        | CHL         | ND          |
| 5          | B            | 313        | CHL         | NA          |
| 5          | B            | 313        | CHL         | NC          |
| 5          | B            | 313        | CHL         | ND          |
| 5          | B            | 314        | CHL         | NA          |
| 5          | B            | 314        | CHL         | NC          |
| 5          | B            | 314        | CHL         | ND          |
| 5          | B            | 319        | CHL         | NA          |
| 5          | B            | 319        | CHL         | NC          |
| 5          | B            | 319        | CHL         | ND          |
| 5          | C            | 305        | CHL         | NA          |
| 5          | C            | 305        | CHL         | NC          |
| 5          | C            | 305        | CHL         | ND          |
| 5          | C            | 306        | CHL         | NA          |
| 5          | C            | 306        | CHL         | NC          |
| 5          | C            | 306        | CHL         | ND          |
| 5          | C            | 309        | CHL         | NA          |
| 5          | C            | 309        | CHL         | NC          |
| 5          | C            | 309        | CHL         | ND          |
| 5          | C            | 310        | CHL         | NA          |
| 5          | C            | 310        | CHL         | NC          |
| 5          | C            | 310        | CHL         | ND          |
| 5          | C            | 311        | CHL         | NA          |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Atom</b> |
|------------|--------------|------------|-------------|-------------|
| 5          | C            | 311        | CHL         | NC          |
| 5          | C            | 311        | CHL         | ND          |
| 5          | C            | 312        | CHL         | NA          |
| 5          | C            | 312        | CHL         | NC          |
| 5          | C            | 312        | CHL         | ND          |
| 5          | C            | 313        | CHL         | NA          |
| 5          | C            | 313        | CHL         | NC          |
| 5          | C            | 313        | CHL         | ND          |
| 5          | C            | 318        | CHL         | NA          |
| 5          | C            | 318        | CHL         | NC          |
| 5          | C            | 318        | CHL         | ND          |
| 5          | D            | 305        | CHL         | NA          |
| 5          | D            | 305        | CHL         | NC          |
| 5          | D            | 305        | CHL         | ND          |
| 5          | D            | 306        | CHL         | NA          |
| 5          | D            | 306        | CHL         | NC          |
| 5          | D            | 306        | CHL         | ND          |
| 5          | D            | 309        | CHL         | NA          |
| 5          | D            | 309        | CHL         | NC          |
| 5          | D            | 309        | CHL         | ND          |
| 5          | D            | 310        | CHL         | NA          |
| 5          | D            | 310        | CHL         | NC          |
| 5          | D            | 310        | CHL         | ND          |
| 5          | D            | 311        | CHL         | NA          |
| 5          | D            | 311        | CHL         | NC          |
| 5          | D            | 311        | CHL         | ND          |
| 5          | D            | 312        | CHL         | NA          |
| 5          | D            | 312        | CHL         | NC          |
| 5          | D            | 312        | CHL         | ND          |
| 5          | D            | 313        | CHL         | NA          |
| 5          | D            | 313        | CHL         | NC          |
| 5          | D            | 313        | CHL         | ND          |
| 5          | D            | 318        | CHL         | NA          |
| 5          | D            | 318        | CHL         | NC          |
| 5          | D            | 318        | CHL         | ND          |
| 5          | E            | 304        | CHL         | NA          |
| 5          | E            | 304        | CHL         | NC          |
| 5          | E            | 304        | CHL         | ND          |
| 5          | E            | 305        | CHL         | NA          |
| 5          | E            | 305        | CHL         | NC          |
| 5          | E            | 305        | CHL         | ND          |
| 5          | E            | 308        | CHL         | NA          |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Atom</b> |
|------------|--------------|------------|-------------|-------------|
| 5          | E            | 308        | CHL         | NC          |
| 5          | E            | 308        | CHL         | ND          |
| 5          | E            | 309        | CHL         | NA          |
| 5          | E            | 309        | CHL         | NC          |
| 5          | E            | 309        | CHL         | ND          |
| 5          | E            | 310        | CHL         | NA          |
| 5          | E            | 310        | CHL         | NC          |
| 5          | E            | 310        | CHL         | ND          |
| 5          | E            | 311        | CHL         | NA          |
| 5          | E            | 311        | CHL         | NC          |
| 5          | E            | 311        | CHL         | ND          |
| 5          | E            | 312        | CHL         | NA          |
| 5          | E            | 312        | CHL         | NC          |
| 5          | E            | 312        | CHL         | ND          |
| 5          | E            | 317        | CHL         | NA          |
| 5          | E            | 317        | CHL         | NC          |
| 5          | E            | 317        | CHL         | ND          |
| 5          | F            | 304        | CHL         | NA          |
| 5          | F            | 304        | CHL         | NC          |
| 5          | F            | 304        | CHL         | ND          |
| 5          | F            | 305        | CHL         | NA          |
| 5          | F            | 305        | CHL         | NC          |
| 5          | F            | 305        | CHL         | ND          |
| 5          | F            | 308        | CHL         | NA          |
| 5          | F            | 308        | CHL         | NC          |
| 5          | F            | 308        | CHL         | ND          |
| 5          | F            | 309        | CHL         | NA          |
| 5          | F            | 309        | CHL         | NC          |
| 5          | F            | 309        | CHL         | ND          |
| 5          | F            | 310        | CHL         | NA          |
| 5          | F            | 310        | CHL         | NC          |
| 5          | F            | 310        | CHL         | ND          |
| 5          | F            | 311        | CHL         | NA          |
| 5          | F            | 311        | CHL         | NC          |
| 5          | F            | 311        | CHL         | ND          |
| 5          | F            | 312        | CHL         | NA          |
| 5          | F            | 312        | CHL         | NC          |
| 5          | F            | 312        | CHL         | ND          |
| 5          | F            | 317        | CHL         | NA          |
| 5          | F            | 317        | CHL         | NC          |
| 5          | F            | 317        | CHL         | ND          |
| 6          | A            | 307        | CLA         | ND          |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 6   | A     | 308 | CLA  | ND   |
| 6   | A     | 314 | CLA  | ND   |
| 6   | A     | 315 | CLA  | ND   |
| 6   | A     | 316 | CLA  | ND   |
| 6   | A     | 317 | CLA  | ND   |
| 6   | B     | 308 | CLA  | ND   |
| 6   | B     | 309 | CLA  | ND   |
| 6   | B     | 315 | CLA  | ND   |
| 6   | B     | 316 | CLA  | ND   |
| 6   | B     | 317 | CLA  | ND   |
| 6   | B     | 318 | CLA  | ND   |
| 6   | C     | 307 | CLA  | ND   |
| 6   | C     | 308 | CLA  | ND   |
| 6   | C     | 314 | CLA  | ND   |
| 6   | C     | 315 | CLA  | ND   |
| 6   | C     | 316 | CLA  | ND   |
| 6   | C     | 317 | CLA  | ND   |
| 6   | D     | 307 | CLA  | ND   |
| 6   | D     | 308 | CLA  | ND   |
| 6   | D     | 314 | CLA  | ND   |
| 6   | D     | 315 | CLA  | ND   |
| 6   | D     | 316 | CLA  | ND   |
| 6   | D     | 317 | CLA  | ND   |
| 6   | E     | 306 | CLA  | ND   |
| 6   | E     | 307 | CLA  | ND   |
| 6   | E     | 313 | CLA  | ND   |
| 6   | E     | 314 | CLA  | ND   |
| 6   | E     | 315 | CLA  | ND   |
| 6   | E     | 316 | CLA  | ND   |
| 6   | F     | 306 | CLA  | ND   |
| 6   | F     | 307 | CLA  | ND   |
| 6   | F     | 313 | CLA  | ND   |
| 6   | F     | 314 | CLA  | ND   |
| 6   | F     | 315 | CLA  | ND   |
| 6   | F     | 316 | CLA  | ND   |

All (1237) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 2   | A     | 302 | 0IE  | C5-C6-C7-C21 |
| 2   | A     | 302 | 0IE  | C5-C6-C7-C8  |
| 2   | A     | 302 | 0IE  | C3-C4-C5-C6  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 302 | 0IE  | C15-C16-C17-C18 |
| 2   | A     | 302 | 0IE  | C23-C16-C17-C18 |
| 2   | B     | 301 | 0IE  | C11-C12-C13-C14 |
| 2   | B     | 301 | 0IE  | C22-C12-C13-C14 |
| 2   | C     | 301 | 0IE  | C15-C16-C17-C18 |
| 2   | C     | 301 | 0IE  | C23-C16-C17-C18 |
| 2   | C     | 302 | 0IE  | C5-C6-C7-C21    |
| 2   | C     | 302 | 0IE  | C2-C3-C4-C5     |
| 2   | C     | 302 | 0IE  | C20-C3-C4-C5    |
| 2   | C     | 302 | 0IE  | C15-C16-C17-C18 |
| 2   | C     | 302 | 0IE  | C23-C16-C17-C18 |
| 2   | D     | 301 | 0IE  | C6-C7-C8-C9     |
| 2   | D     | 301 | 0IE  | C21-C7-C8-C9    |
| 2   | D     | 301 | 0IE  | O1-C2-C3-C20    |
| 2   | D     | 301 | 0IE  | C15-C16-C17-C18 |
| 2   | D     | 301 | 0IE  | C23-C16-C17-C18 |
| 2   | D     | 302 | 0IE  | C5-C6-C7-C21    |
| 2   | D     | 302 | 0IE  | C5-C6-C7-C8     |
| 2   | D     | 302 | 0IE  | C3-C4-C5-C6     |
| 2   | D     | 302 | 0IE  | C20-C3-C4-C5    |
| 2   | D     | 302 | 0IE  | O29-C20-C3-C2   |
| 2   | D     | 302 | 0IE  | C22-C12-C13-C14 |
| 2   | D     | 302 | 0IE  | C15-C16-C17-C18 |
| 2   | D     | 302 | 0IE  | C23-C16-C17-C18 |
| 2   | E     | 301 | 0IE  | C15-C16-C17-C18 |
| 2   | E     | 301 | 0IE  | C23-C16-C17-C18 |
| 2   | E     | 302 | 0IE  | C6-C7-C8-C9     |
| 2   | E     | 302 | 0IE  | C21-C7-C8-C9    |
| 2   | E     | 302 | 0IE  | C2-C3-C4-C5     |
| 2   | E     | 302 | 0IE  | C20-C3-C4-C5    |
| 2   | E     | 302 | 0IE  | C11-C10-C9-C8   |
| 2   | E     | 302 | 0IE  | C15-C16-C17-C18 |
| 2   | E     | 302 | 0IE  | C23-C16-C17-C18 |
| 2   | F     | 301 | 0IE  | C5-C6-C7-C21    |
| 2   | F     | 301 | 0IE  | C5-C6-C7-C8     |
| 2   | F     | 301 | 0IE  | O1-C2-C3-C20    |
| 2   | F     | 302 | 0IE  | C5-C6-C7-C21    |
| 2   | F     | 302 | 0IE  | C5-C6-C7-C8     |
| 2   | F     | 302 | 0IE  | C11-C12-C13-C14 |
| 2   | F     | 302 | 0IE  | C22-C12-C13-C14 |
| 2   | F     | 302 | 0IE  | C15-C16-C17-C18 |
| 2   | F     | 302 | 0IE  | C23-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | A     | 303 | NEX  | O24-C26-C27-C28 |
| 4   | A     | 304 | LMU  | C2'-C1'-O1'-C1  |
| 4   | A     | 304 | LMU  | O5'-C1'-O1'-C1  |
| 4   | B     | 304 | LMU  | C2'-C1'-O1'-C1  |
| 4   | B     | 304 | LMU  | O5'-C1'-O1'-C1  |
| 4   | B     | 305 | LMU  | O5'-C1'-O1'-C1  |
| 4   | D     | 304 | LMU  | C2'-C1'-O1'-C1  |
| 4   | D     | 304 | LMU  | C2-C1-O1'-C1'   |
| 4   | E     | 319 | LMU  | C2'-C1'-O1'-C1  |
| 4   | E     | 319 | LMU  | O5'-C1'-O1'-C1  |
| 5   | A     | 305 | CHL  | C3A-C2A-CAA-CBA |
| 5   | A     | 305 | CHL  | C1C-C2C-CMC-OMC |
| 5   | A     | 305 | CHL  | C3C-C2C-CMC-OMC |
| 5   | A     | 305 | CHL  | CHA-CBD-CGD-O1D |
| 5   | A     | 305 | CHL  | CHA-CBD-CGD-O2D |
| 5   | A     | 305 | CHL  | C2-C3-C5-C6     |
| 5   | A     | 305 | CHL  | C4-C3-C5-C6     |
| 5   | A     | 309 | CHL  | C1A-C2A-CAA-CBA |
| 5   | A     | 309 | CHL  | C3A-C2A-CAA-CBA |
| 5   | A     | 309 | CHL  | C1C-C2C-CMC-OMC |
| 5   | A     | 309 | CHL  | C3C-C2C-CMC-OMC |
| 5   | A     | 311 | CHL  | C1A-C2A-CAA-CBA |
| 5   | A     | 311 | CHL  | C3C-C2C-CMC-OMC |
| 5   | A     | 312 | CHL  | C2A-CAA-CBA-CGA |
| 5   | A     | 313 | CHL  | C3C-C2C-CMC-OMC |
| 5   | A     | 318 | CHL  | C1C-C2C-CMC-OMC |
| 5   | A     | 318 | CHL  | C3C-C2C-CMC-OMC |
| 5   | B     | 306 | CHL  | C1A-C2A-CAA-CBA |
| 5   | B     | 306 | CHL  | C3A-C2A-CAA-CBA |
| 5   | B     | 306 | CHL  | C3C-C2C-CMC-OMC |
| 5   | B     | 310 | CHL  | C1A-C2A-CAA-CBA |
| 5   | B     | 310 | CHL  | C1C-C2C-CMC-OMC |
| 5   | B     | 310 | CHL  | C3C-C2C-CMC-OMC |
| 5   | B     | 312 | CHL  | C1A-C2A-CAA-CBA |
| 5   | B     | 312 | CHL  | C1C-C2C-CMC-OMC |
| 5   | B     | 312 | CHL  | CHA-CBD-CGD-O1D |
| 5   | B     | 312 | CHL  | CHA-CBD-CGD-O2D |
| 5   | B     | 314 | CHL  | C1C-C2C-CMC-OMC |
| 5   | B     | 314 | CHL  | CBD-CGD-O2D-CED |
| 5   | B     | 314 | CHL  | C14-C13-C15-C16 |
| 5   | C     | 305 | CHL  | C1C-C2C-CMC-OMC |
| 5   | C     | 305 | CHL  | C3C-C2C-CMC-OMC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | C     | 306 | CHL  | C3C-C2C-CMC-OMC |
| 5   | C     | 306 | CHL  | C2-C3-C5-C6     |
| 5   | C     | 306 | CHL  | C4-C3-C5-C6     |
| 5   | C     | 309 | CHL  | C1C-C2C-CMC-OMC |
| 5   | C     | 309 | CHL  | C3C-C2C-CMC-OMC |
| 5   | C     | 310 | CHL  | C1A-C2A-CAA-CBA |
| 5   | C     | 310 | CHL  | C3C-C2C-CMC-OMC |
| 5   | C     | 311 | CHL  | C1A-C2A-CAA-CBA |
| 5   | C     | 311 | CHL  | C3A-C2A-CAA-CBA |
| 5   | C     | 312 | CHL  | C1C-C2C-CMC-OMC |
| 5   | C     | 312 | CHL  | C3C-C2C-CMC-OMC |
| 5   | D     | 305 | CHL  | C1C-C2C-CMC-OMC |
| 5   | D     | 305 | CHL  | C3C-C2C-CMC-OMC |
| 5   | D     | 305 | CHL  | CHA-CBD-CGD-O1D |
| 5   | D     | 305 | CHL  | CHA-CBD-CGD-O2D |
| 5   | D     | 305 | CHL  | C2-C3-C5-C6     |
| 5   | D     | 305 | CHL  | C4-C3-C5-C6     |
| 5   | D     | 306 | CHL  | C3C-C2C-CMC-OMC |
| 5   | D     | 309 | CHL  | C1C-C2C-CMC-OMC |
| 5   | D     | 309 | CHL  | C3C-C2C-CMC-OMC |
| 5   | D     | 311 | CHL  | C1A-C2A-CAA-CBA |
| 5   | D     | 311 | CHL  | C1C-C2C-CMC-OMC |
| 5   | D     | 311 | CHL  | C3C-C2C-CMC-OMC |
| 5   | D     | 313 | CHL  | C1C-C2C-CMC-OMC |
| 5   | D     | 318 | CHL  | CHA-CBD-CGD-O1D |
| 5   | E     | 304 | CHL  | C3A-C2A-CAA-CBA |
| 5   | E     | 308 | CHL  | C1C-C2C-CMC-OMC |
| 5   | E     | 308 | CHL  | C3C-C2C-CMC-OMC |
| 5   | E     | 309 | CHL  | C3A-C2A-CAA-CBA |
| 5   | E     | 310 | CHL  | C1A-C2A-CAA-CBA |
| 5   | E     | 310 | CHL  | C3A-C2A-CAA-CBA |
| 5   | E     | 310 | CHL  | C3C-C2C-CMC-OMC |
| 5   | F     | 304 | CHL  | C1A-C2A-CAA-CBA |
| 5   | F     | 305 | CHL  | C2-C3-C5-C6     |
| 5   | F     | 305 | CHL  | C4-C3-C5-C6     |
| 5   | F     | 308 | CHL  | C1C-C2C-CMC-OMC |
| 5   | F     | 308 | CHL  | C3C-C2C-CMC-OMC |
| 5   | F     | 309 | CHL  | C1C-C2C-CMC-OMC |
| 5   | F     | 309 | CHL  | C3C-C2C-CMC-OMC |
| 5   | F     | 310 | CHL  | C1A-C2A-CAA-CBA |
| 5   | F     | 310 | CHL  | C3A-C2A-CAA-CBA |
| 5   | F     | 310 | CHL  | C1C-C2C-CMC-OMC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | F     | 310 | CHL  | C3C-C2C-CMC-OMC |
| 5   | F     | 310 | CHL  | C2-C3-C5-C6     |
| 5   | F     | 310 | CHL  | C4-C3-C5-C6     |
| 5   | F     | 311 | CHL  | C1C-C2C-CMC-OMC |
| 5   | F     | 311 | CHL  | C3C-C2C-CMC-OMC |
| 5   | F     | 312 | CHL  | C3C-C2C-CMC-OMC |
| 6   | A     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 6   | A     | 317 | CLA  | CBD-CGD-O2D-CED |
| 6   | D     | 314 | CLA  | CBD-CGD-O2D-CED |
| 6   | D     | 317 | CLA  | CHA-CBD-CGD-O1D |
| 6   | D     | 317 | CLA  | CHA-CBD-CGD-O2D |
| 6   | D     | 317 | CLA  | CBD-CGD-O2D-CED |
| 6   | F     | 306 | CLA  | C1A-C2A-CAA-CBA |
| 6   | F     | 306 | CLA  | C3A-C2A-CAA-CBA |
| 6   | F     | 306 | CLA  | C11-C12-C13-C14 |
| 6   | F     | 313 | CLA  | C4-C3-C5-C6     |
| 7   | A     | 319 | LHG  | C3-O3-P-O4      |
| 7   | A     | 319 | LHG  | C3-O3-P-O6      |
| 7   | A     | 319 | LHG  | C4-O6-P-O5      |
| 7   | B     | 320 | LHG  | O1-C1-C2-O2     |
| 7   | B     | 320 | LHG  | O1-C1-C2-C3     |
| 7   | B     | 320 | LHG  | O2-C2-C3-O3     |
| 7   | B     | 320 | LHG  | C4-O6-P-O5      |
| 7   | B     | 320 | LHG  | O6-C4-C5-O7     |
| 7   | B     | 324 | LHG  | O1-C1-C2-C3     |
| 7   | B     | 324 | LHG  | C3-O3-P-O5      |
| 7   | B     | 324 | LHG  | C4-O6-P-O4      |
| 7   | B     | 324 | LHG  | O9-C7-O7-C5     |
| 7   | C     | 304 | LHG  | C3-O3-P-O4      |
| 7   | C     | 304 | LHG  | C3-O3-P-O5      |
| 7   | C     | 304 | LHG  | C3-O3-P-O6      |
| 7   | C     | 304 | LHG  | C4-O6-P-O4      |
| 7   | C     | 319 | LHG  | C4-O6-P-O5      |
| 7   | F     | 318 | LHG  | C1-C2-C3-O3     |
| 7   | F     | 318 | LHG  | C4-O6-P-O3      |
| 7   | F     | 318 | LHG  | C4-O6-P-O4      |
| 9   | A     | 322 | OUR  | C2-C3-C43-O44   |
| 9   | A     | 322 | OUR  | C4-C3-C43-O44   |
| 9   | A     | 322 | OUR  | C46-C45-O44-C43 |
| 9   | A     | 322 | OUR  | O57-C45-O44-C43 |
| 9   | B     | 302 | OUR  | C2-C3-C43-O44   |
| 9   | B     | 302 | OUR  | C4-C3-C43-O44   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 9   | B     | 302 | 0UR  | C5-C6-C7-C20    |
| 9   | B     | 302 | 0UR  | C5-C6-C7-C8     |
| 9   | B     | 302 | 0UR  | C17-C18-C19-C28 |
| 9   | B     | 302 | 0UR  | C17-C18-C19-C32 |
| 9   | B     | 302 | 0UR  | C46-C45-O44-C43 |
| 9   | B     | 302 | 0UR  | O57-C45-O44-C43 |
| 9   | B     | 302 | 0UR  | C7-C8-C9-C10    |
| 9   | B     | 325 | 0UR  | C2-C3-C43-O44   |
| 9   | B     | 325 | 0UR  | C4-C3-C43-O44   |
| 9   | B     | 325 | 0UR  | C46-C45-O44-C43 |
| 9   | B     | 325 | 0UR  | O57-C45-O44-C43 |
| 9   | C     | 321 | 0UR  | O57-C45-O44-C43 |
| 9   | E     | 320 | 0UR  | C2-C3-C43-O44   |
| 9   | E     | 320 | 0UR  | C4-C3-C43-O44   |
| 9   | E     | 320 | 0UR  | C46-C45-O44-C43 |
| 9   | E     | 320 | 0UR  | O57-C45-O44-C43 |
| 9   | F     | 320 | 0UR  | O57-C45-O44-C43 |
| 10  | B     | 321 | BET  | C-CA-N-C1       |
| 10  | B     | 321 | BET  | C-CA-N-C2       |
| 10  | B     | 321 | BET  | C-CA-N-C3       |
| 10  | B     | 321 | BET  | O-C-CA-N        |
| 10  | B     | 321 | BET  | OXT-C-CA-N      |
| 10  | B     | 322 | BET  | O-C-CA-N        |
| 10  | B     | 322 | BET  | OXT-C-CA-N      |
| 10  | C     | 320 | BET  | OXT-C-CA-N      |
| 11  | B     | 323 | LMG  | O9-C10-O7-C8    |
| 11  | B     | 323 | LMG  | C11-C10-O7-C8   |
| 11  | F     | 319 | LMG  | C2-C1-O1-C7     |
| 11  | F     | 319 | LMG  | O6-C1-O1-C7     |
| 11  | F     | 319 | LMG  | O7-C8-C9-O8     |
| 11  | F     | 319 | LMG  | O9-C10-O7-C8    |
| 11  | F     | 319 | LMG  | C11-C10-O7-C8   |
| 5   | C     | 313 | CHL  | CBD-CGD-O2D-CED |
| 5   | D     | 313 | CHL  | CBD-CGD-O2D-CED |
| 5   | F     | 312 | CHL  | CBD-CGD-O2D-CED |
| 6   | A     | 314 | CLA  | CBD-CGD-O2D-CED |
| 6   | C     | 308 | CLA  | CBD-CGD-O2D-CED |
| 6   | E     | 314 | CLA  | CBD-CGD-O2D-CED |
| 6   | E     | 315 | CLA  | CBD-CGD-O2D-CED |
| 6   | F     | 313 | CLA  | CBD-CGD-O2D-CED |
| 11  | F     | 319 | LMG  | O10-C28-O8-C9   |
| 4   | D     | 304 | LMU  | O5B-C1B-O1B-C4' |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | E     | 319 | LMU  | C4'-C5'-C6'-O6' |
| 6   | E     | 314 | CLA  | O1D-CGD-O2D-CED |
| 5   | B     | 314 | CHL  | O1D-CGD-O2D-CED |
| 6   | C     | 315 | CLA  | CBA-CGA-O2A-C1  |
| 11  | F     | 319 | LMG  | C29-C28-O8-C9   |
| 5   | A     | 313 | CHL  | CBD-CGD-O2D-CED |
| 5   | B     | 306 | CHL  | CBD-CGD-O2D-CED |
| 5   | D     | 310 | CHL  | CBD-CGD-O2D-CED |
| 5   | E     | 309 | CHL  | CBD-CGD-O2D-CED |
| 5   | E     | 311 | CHL  | CBD-CGD-O2D-CED |
| 5   | E     | 312 | CHL  | CBD-CGD-O2D-CED |
| 6   | B     | 315 | CLA  | CBD-CGD-O2D-CED |
| 6   | B     | 316 | CLA  | CBD-CGD-O2D-CED |
| 6   | C     | 315 | CLA  | O1A-CGA-O2A-C1  |
| 7   | A     | 319 | LHG  | O10-C23-O8-C6   |
| 7   | E     | 318 | LHG  | O10-C23-O8-C6   |
| 7   | F     | 318 | LHG  | O10-C23-O8-C6   |
| 6   | A     | 317 | CLA  | O1D-CGD-O2D-CED |
| 6   | D     | 314 | CLA  | O1D-CGD-O2D-CED |
| 6   | D     | 317 | CLA  | O1D-CGD-O2D-CED |
| 6   | C     | 317 | CLA  | CBD-CGD-O2D-CED |
| 4   | E     | 319 | LMU  | C4B-C5B-C6B-O6B |
| 6   | D     | 308 | CLA  | CBA-CGA-O2A-C1  |
| 6   | D     | 308 | CLA  | O1A-CGA-O2A-C1  |
| 9   | D     | 321 | OUR  | O57-C45-O44-C43 |
| 5   | A     | 311 | CHL  | C3-C5-C6-C7     |
| 5   | B     | 306 | CHL  | C3-C5-C6-C7     |
| 5   | D     | 312 | CHL  | C3-C5-C6-C7     |
| 5   | E     | 310 | CHL  | C3-C5-C6-C7     |
| 5   | F     | 310 | CHL  | C3-C5-C6-C7     |
| 6   | A     | 315 | CLA  | C3-C5-C6-C7     |
| 6   | D     | 315 | CLA  | C3-C5-C6-C7     |
| 6   | E     | 314 | CLA  | C3-C5-C6-C7     |
| 9   | C     | 321 | OUR  | C46-C45-O44-C43 |
| 9   | F     | 320 | OUR  | C46-C45-O44-C43 |
| 7   | B     | 324 | LHG  | C8-C7-O7-C5     |
| 6   | C     | 308 | CLA  | CBA-CGA-O2A-C1  |
| 4   | E     | 319 | LMU  | O5'-C5'-C6'-O6' |
| 6   | F     | 313 | CLA  | C2-C3-C5-C6     |
| 6   | A     | 307 | CLA  | CBD-CGD-O2D-CED |
| 6   | D     | 307 | CLA  | CBD-CGD-O2D-CED |
| 5   | A     | 305 | CHL  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | B     | 313 | CHL  | C2A-CAA-CBA-CGA |
| 5   | D     | 305 | CHL  | C2A-CAA-CBA-CGA |
| 5   | E     | 311 | CHL  | C2A-CAA-CBA-CGA |
| 6   | F     | 306 | CLA  | C2A-CAA-CBA-CGA |
| 5   | A     | 305 | CHL  | C3-C5-C6-C7     |
| 5   | D     | 305 | CHL  | C3-C5-C6-C7     |
| 5   | C     | 310 | CHL  | C2A-CAA-CBA-CGA |
| 6   | B     | 316 | CLA  | CBA-CGA-O2A-C1  |
| 6   | F     | 313 | CLA  | CBA-CGA-O2A-C1  |
| 7   | A     | 319 | LHG  | C24-C23-O8-C6   |
| 7   | B     | 320 | LHG  | C24-C23-O8-C6   |
| 7   | E     | 318 | LHG  | C24-C23-O8-C6   |
| 7   | F     | 318 | LHG  | C24-C23-O8-C6   |
| 4   | B     | 304 | LMU  | O5B-C5B-C6B-O6B |
| 4   | A     | 304 | LMU  | C4-C5-C6-C7     |
| 6   | E     | 315 | CLA  | O1D-CGD-O2D-CED |
| 6   | F     | 313 | CLA  | O1A-CGA-O2A-C1  |
| 5   | A     | 311 | CHL  | CBD-CGD-O2D-CED |
| 5   | A     | 318 | CHL  | CBD-CGD-O2D-CED |
| 5   | B     | 313 | CHL  | CBD-CGD-O2D-CED |
| 5   | C     | 311 | CHL  | CBD-CGD-O2D-CED |
| 5   | C     | 318 | CHL  | CBD-CGD-O2D-CED |
| 5   | D     | 311 | CHL  | CBD-CGD-O2D-CED |
| 5   | F     | 311 | CHL  | CBD-CGD-O2D-CED |
| 6   | D     | 315 | CLA  | CBD-CGD-O2D-CED |
| 6   | E     | 316 | CLA  | CBD-CGD-O2D-CED |
| 6   | F     | 307 | CLA  | CBD-CGD-O2D-CED |
| 5   | A     | 312 | CHL  | C3-C5-C6-C7     |
| 5   | C     | 311 | CHL  | C3-C5-C6-C7     |
| 6   | B     | 318 | CLA  | C3-C5-C6-C7     |
| 6   | C     | 317 | CLA  | C3-C5-C6-C7     |
| 6   | B     | 316 | CLA  | O1A-CGA-O2A-C1  |
| 4   | E     | 319 | LMU  | O5B-C5B-C6B-O6B |
| 9   | D     | 321 | OUR  | C46-C45-O44-C43 |
| 6   | A     | 314 | CLA  | O1D-CGD-O2D-CED |
| 6   | F     | 313 | CLA  | O1D-CGD-O2D-CED |
| 4   | E     | 319 | LMU  | C1-C2-C3-C4     |
| 4   | A     | 304 | LMU  | O5B-C1B-O1B-C4' |
| 5   | D     | 313 | CHL  | O1D-CGD-O2D-CED |
| 5   | C     | 312 | CHL  | CBD-CGD-O2D-CED |
| 6   | A     | 315 | CLA  | CBD-CGD-O2D-CED |
| 6   | C     | 308 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | B     | 324 | LHG  | C24-C25-C26-C27 |
| 7   | B     | 324 | LHG  | C26-C27-C28-C29 |
| 4   | B     | 305 | LMU  | O5B-C5B-C6B-O6B |
| 11  | B     | 323 | LMG  | C4-C5-C6-O5     |
| 6   | C     | 308 | CLA  | O1A-CGA-O2A-C1  |
| 5   | C     | 305 | CHL  | C4-C3-C5-C6     |
| 5   | E     | 304 | CHL  | C4-C3-C5-C6     |
| 5   | C     | 305 | CHL  | C2-C3-C5-C6     |
| 5   | E     | 304 | CHL  | C2-C3-C5-C6     |
| 5   | F     | 308 | CHL  | CBD-CGD-O2D-CED |
| 5   | D     | 312 | CHL  | C2A-CAA-CBA-CGA |
| 5   | F     | 312 | CHL  | O1D-CGD-O2D-CED |
| 4   | B     | 304 | LMU  | C4B-C5B-C6B-O6B |
| 6   | B     | 315 | CLA  | C2C-C3C-CAC-CBC |
| 6   | F     | 315 | CLA  | CBD-CGD-O2D-CED |
| 11  | B     | 323 | LMG  | O6-C5-C6-O5     |
| 5   | C     | 313 | CHL  | O1D-CGD-O2D-CED |
| 5   | D     | 310 | CHL  | O1D-CGD-O2D-CED |
| 5   | E     | 311 | CHL  | O1D-CGD-O2D-CED |
| 6   | B     | 316 | CLA  | O1D-CGD-O2D-CED |
| 10  | C     | 320 | BET  | C-CA-N-C3       |
| 5   | E     | 312 | CHL  | O1D-CGD-O2D-CED |
| 7   | B     | 320 | LHG  | C1-C2-C3-O3     |
| 7   | C     | 304 | LHG  | C1-C2-C3-O3     |
| 5   | B     | 313 | CHL  | C3-C5-C6-C7     |
| 6   | A     | 315 | CLA  | CBA-CGA-O2A-C1  |
| 6   | D     | 315 | CLA  | CBA-CGA-O2A-C1  |
| 7   | B     | 324 | LHG  | C24-C23-O8-C6   |
| 5   | C     | 309 | CHL  | CBD-CGD-O2D-CED |
| 2   | E     | 302 | OIE  | C3-C4-C5-C6     |
| 5   | E     | 311 | CHL  | C5-C6-C7-C8     |
| 6   | B     | 315 | CLA  | O1D-CGD-O2D-CED |
| 7   | B     | 320 | LHG  | C29-C30-C31-C32 |
| 4   | A     | 304 | LMU  | C11-C10-C9-C8   |
| 5   | F     | 305 | CHL  | C8-C10-C11-C12  |
| 6   | D     | 317 | CLA  | C8-C10-C11-C12  |
| 7   | C     | 304 | LHG  | O2-C2-C3-O3     |
| 6   | D     | 315 | CLA  | O1A-CGA-O2A-C1  |
| 5   | B     | 307 | CHL  | C11-C12-C13-C14 |
| 5   | C     | 305 | CHL  | C14-C13-C15-C16 |
| 5   | C     | 306 | CHL  | C14-C13-C15-C16 |
| 5   | C     | 311 | CHL  | C11-C10-C8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | C     | 313 | CHL  | C11-C12-C13-C14 |
| 5   | E     | 310 | CHL  | C11-C10-C8-C9   |
| 5   | F     | 304 | CHL  | C14-C13-C15-C16 |
| 5   | F     | 305 | CHL  | C11-C12-C13-C14 |
| 5   | F     | 310 | CHL  | C11-C10-C8-C9   |
| 5   | F     | 312 | CHL  | C11-C10-C8-C9   |
| 6   | B     | 316 | CLA  | C6-C7-C8-C9     |
| 6   | B     | 318 | CLA  | C11-C10-C8-C9   |
| 6   | D     | 317 | CLA  | C5-C6-C7-C8     |
| 6   | F     | 313 | CLA  | C5-C6-C7-C8     |
| 5   | A     | 310 | CHL  | C2A-CAA-CBA-CGA |
| 2   | A     | 301 | 0IE  | C5-C6-C7-C21    |
| 2   | B     | 301 | 0IE  | C5-C6-C7-C21    |
| 2   | C     | 302 | 0IE  | C5-C6-C7-C8     |
| 9   | B     | 302 | 0UR  | C15-C16-C17-C18 |
| 4   | D     | 304 | LMU  | O5B-C5B-C6B-O6B |
| 4   | A     | 304 | LMU  | C6-C7-C8-C9     |
| 7   | A     | 319 | LHG  | C24-C25-C26-C27 |
| 7   | B     | 320 | LHG  | O10-C23-O8-C6   |
| 7   | B     | 324 | LHG  | O10-C23-O8-C6   |
| 5   | C     | 311 | CHL  | C5-C6-C7-C8     |
| 5   | F     | 304 | CHL  | C13-C15-C16-C17 |
| 6   | C     | 315 | CLA  | C13-C15-C16-C17 |
| 5   | B     | 311 | CHL  | CBD-CGD-O2D-CED |
| 5   | D     | 309 | CHL  | CBD-CGD-O2D-CED |
| 5   | C     | 312 | CHL  | C3-C5-C6-C7     |
| 5   | B     | 314 | CHL  | C13-C15-C16-C17 |
| 5   | E     | 305 | CHL  | C5-C6-C7-C8     |
| 6   | F     | 306 | CLA  | C10-C11-C12-C13 |
| 5   | A     | 312 | CHL  | C5-C6-C7-C8     |
| 5   | D     | 311 | CHL  | C8-C10-C11-C12  |
| 5   | E     | 304 | CHL  | C5-C6-C7-C8     |
| 5   | E     | 312 | CHL  | C15-C16-C17-C18 |
| 5   | F     | 310 | CHL  | C5-C6-C7-C8     |
| 5   | F     | 311 | CHL  | C5-C6-C7-C8     |
| 7   | B     | 324 | LHG  | O1-C1-C2-O2     |
| 7   | B     | 320 | LHG  | C23-C24-C25-C26 |
| 7   | B     | 324 | LHG  | C23-C24-C25-C26 |
| 7   | D     | 319 | LHG  | C7-C8-C9-C10    |
| 5   | E     | 308 | CHL  | CBD-CGD-O2D-CED |
| 5   | B     | 313 | CHL  | C5-C6-C7-C8     |
| 5   | C     | 311 | CHL  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | E     | 304 | CHL  | C15-C16-C17-C18 |
| 5   | F     | 312 | CHL  | C15-C16-C17-C18 |
| 6   | B     | 318 | CLA  | C10-C11-C12-C13 |
| 6   | C     | 307 | CLA  | C10-C11-C12-C13 |
| 6   | D     | 317 | CLA  | C10-C11-C12-C13 |
| 7   | C     | 304 | LHG  | C24-C23-O8-C6   |
| 5   | A     | 313 | CHL  | O1D-CGD-O2D-CED |
| 5   | B     | 306 | CHL  | O1D-CGD-O2D-CED |
| 4   | D     | 304 | LMU  | O1'-C1-C2-C3    |
| 5   | E     | 310 | CHL  | C5-C6-C7-C8     |
| 5   | F     | 310 | CHL  | C10-C11-C12-C13 |
| 5   | F     | 312 | CHL  | C13-C15-C16-C17 |
| 6   | D     | 315 | CLA  | C8-C10-C11-C12  |
| 7   | C     | 304 | LHG  | C5-C4-O6-P      |
| 7   | A     | 319 | LHG  | C7-C8-C9-C10    |
| 5   | E     | 317 | CHL  | CBD-CGD-O2D-CED |
| 5   | C     | 318 | CHL  | C2A-CAA-CBA-CGA |
| 5   | A     | 305 | CHL  | C13-C15-C16-C17 |
| 5   | B     | 313 | CHL  | C6-C7-C8-C10    |
| 5   | D     | 312 | CHL  | C6-C7-C8-C10    |
| 6   | B     | 308 | CLA  | C12-C13-C15-C16 |
| 6   | F     | 313 | CLA  | C6-C7-C8-C10    |
| 9   | B     | 302 | OUR  | C9-C10-C11-C12  |
| 5   | A     | 312 | CHL  | CBD-CGD-O2D-CED |
| 6   | F     | 314 | CLA  | CBA-CGA-O2A-C1  |
| 5   | C     | 312 | CHL  | C2A-CAA-CBA-CGA |
| 5   | F     | 311 | CHL  | C2A-CAA-CBA-CGA |
| 5   | E     | 309 | CHL  | O1D-CGD-O2D-CED |
| 6   | D     | 307 | CLA  | O1D-CGD-O2D-CED |
| 5   | A     | 311 | CHL  | C5-C6-C7-C8     |
| 5   | B     | 314 | CHL  | C10-C11-C12-C13 |
| 5   | C     | 311 | CHL  | C10-C11-C12-C13 |
| 5   | F     | 310 | CHL  | C8-C10-C11-C12  |
| 6   | A     | 315 | CLA  | O1A-CGA-O2A-C1  |
| 5   | D     | 305 | CHL  | CBD-CGD-O2D-CED |
| 4   | D     | 304 | LMU  | O5'-C1'-O1'-C1  |
| 2   | D     | 301 | OIE  | C4-C5-C6-C7     |
| 4   | A     | 304 | LMU  | O1'-C1-C2-C3    |
| 4   | E     | 319 | LMU  | C7-C8-C9-C10    |
| 7   | F     | 318 | LHG  | O2-C2-C3-O3     |
| 5   | F     | 311 | CHL  | C3-C5-C6-C7     |
| 5   | F     | 312 | CHL  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | E     | 318 | LHG  | C24-C25-C26-C27 |
| 5   | B     | 307 | CHL  | C5-C6-C7-C8     |
| 5   | B     | 307 | CHL  | C13-C15-C16-C17 |
| 5   | C     | 306 | CHL  | C15-C16-C17-C18 |
| 5   | D     | 312 | CHL  | C5-C6-C7-C8     |
| 6   | A     | 307 | CLA  | C15-C16-C17-C18 |
| 4   | B     | 305 | LMU  | C5'-C4'-O1B-C1B |
| 6   | C     | 317 | CLA  | O1D-CGD-O2D-CED |
| 5   | C     | 305 | CHL  | CBD-CGD-O2D-CED |
| 7   | F     | 318 | LHG  | C24-C25-C26-C27 |
| 5   | C     | 312 | CHL  | C5-C6-C7-C8     |
| 5   | C     | 313 | CHL  | C15-C16-C17-C18 |
| 5   | D     | 313 | CHL  | C13-C15-C16-C17 |
| 6   | C     | 315 | CLA  | C8-C10-C11-C12  |
| 6   | E     | 306 | CLA  | C10-C11-C12-C13 |
| 7   | B     | 320 | LHG  | C4-O6-P-O3      |
| 7   | B     | 324 | LHG  | C3-O3-P-O6      |
| 7   | C     | 304 | LHG  | C4-O6-P-O3      |
| 5   | C     | 306 | CHL  | C3-C5-C6-C7     |
| 6   | A     | 317 | CLA  | C3-C5-C6-C7     |
| 6   | F     | 313 | CLA  | C3-C5-C6-C7     |
| 4   | B     | 305 | LMU  | C3'-C4'-O1B-C1B |
| 5   | E     | 305 | CHL  | CBA-CGA-O2A-C1  |
| 6   | E     | 314 | CLA  | CBA-CGA-O2A-C1  |
| 10  | C     | 320 | BET  | C-CA-N-C2       |
| 5   | C     | 310 | CHL  | CBD-CGD-O2D-CED |
| 5   | A     | 306 | CHL  | C8-C10-C11-C12  |
| 6   | B     | 318 | CLA  | C4-C3-C5-C6     |
| 5   | A     | 306 | CHL  | C5-C6-C7-C8     |
| 5   | F     | 304 | CHL  | C15-C16-C17-C18 |
| 5   | D     | 305 | CHL  | C2C-C3C-CAC-CBC |
| 5   | F     | 304 | CHL  | C2A-CAA-CBA-CGA |
| 6   | E     | 306 | CLA  | C16-C17-C18-C19 |
| 6   | C     | 307 | CLA  | C3-C5-C6-C7     |
| 5   | C     | 306 | CHL  | C10-C11-C12-C13 |
| 6   | B     | 308 | CLA  | C13-C15-C16-C17 |
| 4   | B     | 305 | LMU  | C3-C4-C5-C6     |
| 2   | F     | 302 | OIE  | C3-C4-C5-C6     |
| 9   | C     | 321 | OUR  | C47-C48-C49-C50 |
| 2   | A     | 301 | OIE  | C21-C7-C8-C9    |
| 2   | A     | 302 | OIE  | C21-C7-C8-C9    |
| 2   | A     | 302 | OIE  | C14-C15-C16-C23 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | B     | 301 | OIE  | C21-C7-C8-C9    |
| 2   | C     | 302 | OIE  | C10-C11-C12-C22 |
| 2   | D     | 301 | OIE  | C14-C15-C16-C23 |
| 2   | D     | 302 | OIE  | C10-C11-C12-C22 |
| 2   | E     | 301 | OIE  | C14-C15-C16-C23 |
| 2   | F     | 301 | OIE  | C21-C7-C8-C9    |
| 2   | F     | 302 | OIE  | C14-C15-C16-C23 |
| 5   | D     | 306 | CHL  | C3-C5-C6-C7     |
| 5   | D     | 313 | CHL  | C3-C5-C6-C7     |
| 7   | D     | 319 | LHG  | C15-C16-C17-C18 |
| 7   | F     | 318 | LHG  | C13-C14-C15-C16 |
| 5   | A     | 311 | CHL  | O1D-CGD-O2D-CED |
| 5   | A     | 305 | CHL  | C16-C17-C18-C19 |
| 5   | F     | 304 | CHL  | C16-C17-C18-C19 |
| 5   | E     | 310 | CHL  | C10-C11-C12-C13 |
| 6   | A     | 307 | CLA  | O1D-CGD-O2D-CED |
| 5   | A     | 305 | CHL  | C15-C16-C17-C18 |
| 4   | A     | 304 | LMU  | C5-C6-C7-C8     |
| 7   | A     | 319 | LHG  | C12-C13-C14-C15 |
| 7   | C     | 319 | LHG  | C11-C10-C9-C8   |
| 7   | E     | 318 | LHG  | C13-C14-C15-C16 |
| 6   | F     | 314 | CLA  | O1A-CGA-O2A-C1  |
| 4   | D     | 304 | LMU  | C3-C4-C5-C6     |
| 4   | B     | 305 | LMU  | C4B-C5B-C6B-O6B |
| 4   | B     | 305 | LMU  | C6-C7-C8-C9     |
| 4   | E     | 319 | LMU  | O1'-C1-C2-C3    |
| 7   | D     | 319 | LHG  | C11-C10-C9-C8   |
| 2   | A     | 301 | OIE  | C6-C7-C8-C9     |
| 2   | A     | 302 | OIE  | C6-C7-C8-C9     |
| 2   | A     | 302 | OIE  | C14-C15-C16-C17 |
| 2   | B     | 301 | OIE  | C6-C7-C8-C9     |
| 2   | C     | 302 | OIE  | C10-C11-C12-C13 |
| 2   | D     | 301 | OIE  | C14-C15-C16-C17 |
| 2   | D     | 302 | OIE  | C10-C11-C12-C13 |
| 2   | E     | 301 | OIE  | C14-C15-C16-C17 |
| 2   | F     | 301 | OIE  | C6-C7-C8-C9     |
| 2   | F     | 302 | OIE  | C10-C11-C12-C13 |
| 2   | F     | 302 | OIE  | C14-C15-C16-C17 |
| 5   | C     | 305 | CHL  | C13-C15-C16-C17 |
| 6   | E     | 316 | CLA  | C4-C3-C5-C6     |
| 7   | D     | 319 | LHG  | C26-C27-C28-C29 |
| 7   | F     | 318 | LHG  | C25-C26-C27-C28 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | B     | 318 | CLA  | C2-C3-C5-C6     |
| 6   | F     | 306 | CLA  | C2-C3-C5-C6     |
| 5   | D     | 305 | CHL  | C6-C7-C8-C9     |
| 6   | C     | 315 | CLA  | C11-C12-C13-C14 |
| 6   | D     | 314 | CLA  | C11-C10-C8-C9   |
| 6   | F     | 313 | CLA  | C6-C7-C8-C9     |
| 10  | B     | 322 | BET  | C-CA-N-C3       |
| 4   | A     | 304 | LMU  | C3-C4-C5-C6     |
| 7   | C     | 319 | LHG  | C24-C25-C26-C27 |
| 5   | E     | 305 | CHL  | C13-C15-C16-C17 |
| 6   | E     | 306 | CLA  | C2A-CAA-CBA-CGA |
| 6   | F     | 307 | CLA  | C2A-CAA-CBA-CGA |
| 5   | D     | 311 | CHL  | O1D-CGD-O2D-CED |
| 5   | E     | 305 | CHL  | O1A-CGA-O2A-C1  |
| 2   | E     | 302 | OIE  | C5-C6-C7-C21    |
| 9   | B     | 302 | OUR  | C22-C16-C17-C18 |
| 7   | C     | 319 | LHG  | C16-C17-C18-C19 |
| 10  | C     | 320 | BET  | O-C-CA-N        |
| 2   | D     | 302 | OIE  | C11-C12-C13-C14 |
| 2   | E     | 302 | OIE  | C5-C6-C7-C8     |
| 6   | B     | 318 | CLA  | C8-C10-C11-C12  |
| 4   | D     | 304 | LMU  | C4-C5-C6-C7     |
| 4   | E     | 319 | LMU  | C4-C5-C6-C7     |
| 7   | B     | 320 | LHG  | C27-C28-C29-C30 |
| 7   | C     | 319 | LHG  | C17-C18-C19-C20 |
| 5   | C     | 311 | CHL  | O1D-CGD-O2D-CED |
| 6   | E     | 316 | CLA  | O1D-CGD-O2D-CED |
| 4   | B     | 305 | LMU  | C5-C6-C7-C8     |
| 7   | B     | 320 | LHG  | C9-C10-C11-C12  |
| 7   | C     | 319 | LHG  | C27-C28-C29-C30 |
| 7   | E     | 318 | LHG  | C12-C13-C14-C15 |
| 7   | F     | 318 | LHG  | C9-C10-C11-C12  |
| 4   | A     | 304 | LMU  | O5B-C5B-C6B-O6B |
| 4   | B     | 304 | LMU  | O5'-C5'-C6'-O6' |
| 5   | A     | 312 | CHL  | C6-C7-C8-C9     |
| 6   | C     | 307 | CLA  | C16-C17-C18-C19 |
| 6   | C     | 307 | CLA  | C16-C17-C18-C20 |
| 6   | C     | 315 | CLA  | C16-C17-C18-C19 |
| 6   | C     | 315 | CLA  | C16-C17-C18-C20 |
| 6   | E     | 306 | CLA  | C16-C17-C18-C20 |
| 5   | C     | 318 | CHL  | O1D-CGD-O2D-CED |
| 4   | E     | 319 | LMU  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | B     | 324 | LHG  | C25-C26-C27-C28 |
| 6   | E     | 313 | CLA  | CBD-CGD-O2D-CED |
| 6   | D     | 315 | CLA  | O1D-CGD-O2D-CED |
| 7   | D     | 319 | LHG  | C9-C10-C11-C12  |
| 7   | D     | 319 | LHG  | C10-C11-C12-C13 |
| 6   | E     | 314 | CLA  | O1A-CGA-O2A-C1  |
| 4   | D     | 304 | LMU  | C5-C6-C7-C8     |
| 5   | A     | 311 | CHL  | C3A-C2A-CAA-CBA |
| 5   | B     | 312 | CHL  | C3A-C2A-CAA-CBA |
| 5   | C     | 310 | CHL  | C3A-C2A-CAA-CBA |
| 5   | D     | 311 | CHL  | C3A-C2A-CAA-CBA |
| 4   | E     | 319 | LMU  | C2-C1-O1'-C1'   |
| 5   | A     | 318 | CHL  | O1D-CGD-O2D-CED |
| 6   | F     | 307 | CLA  | O1D-CGD-O2D-CED |
| 4   | D     | 304 | LMU  | C4B-C5B-C6B-O6B |
| 5   | B     | 313 | CHL  | O1D-CGD-O2D-CED |
| 11  | F     | 319 | LMG  | O1-C7-C8-C9     |
| 7   | F     | 318 | LHG  | C28-C29-C30-C31 |
| 3   | F     | 303 | NEX  | C14-C15-C35-C34 |
| 6   | C     | 315 | CLA  | C3-C5-C6-C7     |
| 7   | B     | 324 | LHG  | C27-C28-C29-C30 |
| 6   | F     | 306 | CLA  | C4-C3-C5-C6     |
| 6   | E     | 316 | CLA  | C2-C3-C5-C6     |
| 6   | F     | 316 | CLA  | C2-C3-C5-C6     |
| 5   | E     | 305 | CHL  | C2A-CAA-CBA-CGA |
| 5   | F     | 305 | CHL  | C15-C16-C17-C18 |
| 7   | C     | 304 | LHG  | C23-C24-C25-C26 |
| 10  | C     | 320 | BET  | C-CA-N-C1       |
| 6   | A     | 315 | CLA  | C10-C11-C12-C13 |
| 4   | E     | 319 | LMU  | C2-C3-C4-C5     |
| 5   | A     | 305 | CHL  | CBA-CGA-O2A-C1  |
| 6   | C     | 315 | CLA  | C15-C16-C17-C18 |
| 5   | A     | 309 | CHL  | CBD-CGD-O2D-CED |
| 5   | F     | 305 | CHL  | C2-C1-O2A-CGA   |
| 4   | A     | 304 | LMU  | O5'-C5'-C6'-O6' |
| 5   | A     | 310 | CHL  | CBA-CGA-O2A-C1  |
| 5   | C     | 311 | CHL  | CBA-CGA-O2A-C1  |
| 5   | F     | 312 | CHL  | CBA-CGA-O2A-C1  |
| 5   | B     | 306 | CHL  | C8-C10-C11-C12  |
| 6   | A     | 307 | CLA  | C10-C11-C12-C13 |
| 7   | F     | 318 | LHG  | C29-C30-C31-C32 |
| 11  | F     | 319 | LMG  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | B     | 306 | CHL  | C10-C11-C12-C13 |
| 5   | E     | 312 | CHL  | C4-C3-C5-C6     |
| 5   | A     | 305 | CHL  | C11-C12-C13-C15 |
| 5   | A     | 311 | CHL  | C2-C3-C5-C6     |
| 5   | B     | 314 | CHL  | C2-C3-C5-C6     |
| 5   | C     | 305 | CHL  | C6-C7-C8-C10    |
| 5   | C     | 305 | CHL  | C12-C13-C15-C16 |
| 5   | D     | 305 | CHL  | C6-C7-C8-C10    |
| 5   | D     | 305 | CHL  | C12-C13-C15-C16 |
| 5   | E     | 312 | CHL  | C2-C3-C5-C6     |
| 5   | F     | 304 | CHL  | C12-C13-C15-C16 |
| 5   | F     | 305 | CHL  | C11-C12-C13-C15 |
| 6   | C     | 315 | CLA  | C11-C12-C13-C15 |
| 6   | D     | 314 | CLA  | C6-C7-C8-C10    |
| 5   | C     | 311 | CHL  | O1A-CGA-O2A-C1  |
| 2   | F     | 302 | 0IE  | C9-C10-C11-C12  |
| 6   | F     | 314 | CLA  | CBD-CGD-O2D-CED |
| 5   | C     | 305 | CHL  | C16-C17-C18-C20 |
| 5   | C     | 312 | CHL  | C6-C7-C8-C9     |
| 5   | F     | 311 | CHL  | C6-C7-C8-C9     |
| 5   | C     | 312 | CHL  | O1D-CGD-O2D-CED |
| 5   | F     | 311 | CHL  | O1D-CGD-O2D-CED |
| 9   | B     | 325 | 0UR  | C47-C48-C49-C50 |
| 5   | A     | 313 | CHL  | CBA-CGA-O2A-C1  |
| 5   | D     | 313 | CHL  | CBA-CGA-O2A-C1  |
| 5   | E     | 304 | CHL  | CBA-CGA-O2A-C1  |
| 5   | E     | 304 | CHL  | C2A-CAA-CBA-CGA |
| 6   | A     | 315 | CLA  | O1D-CGD-O2D-CED |
| 6   | D     | 307 | CLA  | C8-C10-C11-C12  |
| 6   | B     | 315 | CLA  | C4C-C3C-CAC-CBC |
| 5   | A     | 313 | CHL  | C8-C10-C11-C12  |
| 4   | E     | 319 | LMU  | C5-C6-C7-C8     |
| 5   | B     | 307 | CHL  | C15-C16-C17-C18 |
| 5   | F     | 308 | CHL  | O1D-CGD-O2D-CED |
| 4   | D     | 304 | LMU  | C11-C10-C9-C8   |
| 7   | A     | 319 | LHG  | C8-C7-O7-C5     |
| 4   | A     | 304 | LMU  | C1-C2-C3-C4     |
| 5   | A     | 305 | CHL  | O1A-CGA-O2A-C1  |
| 5   | F     | 312 | CHL  | O1A-CGA-O2A-C1  |
| 7   | C     | 304 | LHG  | O7-C5-C6-O8     |
| 4   | D     | 304 | LMU  | O5'-C5'-C6'-O6' |
| 6   | F     | 315 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | F     | 304 | CHL  | C16-C17-C18-C20 |
| 4   | B     | 305 | LMU  | C4-C5-C6-C7     |
| 5   | B     | 314 | CHL  | C15-C16-C17-C18 |
| 9   | A     | 322 | OUR  | C47-C48-C49-C50 |
| 9   | D     | 321 | OUR  | C47-C48-C49-C50 |
| 5   | A     | 306 | CHL  | C4-C3-C5-C6     |
| 5   | B     | 314 | CHL  | C4-C3-C5-C6     |
| 6   | F     | 316 | CLA  | C4-C3-C5-C6     |
| 5   | A     | 305 | CHL  | C11-C12-C13-C14 |
| 5   | B     | 313 | CHL  | C6-C7-C8-C9     |
| 5   | C     | 305 | CHL  | C6-C7-C8-C9     |
| 5   | D     | 305 | CHL  | C14-C13-C15-C16 |
| 5   | D     | 312 | CHL  | C6-C7-C8-C9     |
| 5   | E     | 305 | CHL  | C11-C10-C8-C9   |
| 5   | E     | 312 | CHL  | C11-C12-C13-C14 |
| 6   | A     | 307 | CLA  | C11-C10-C8-C9   |
| 6   | A     | 315 | CLA  | C6-C7-C8-C9     |
| 2   | C     | 302 | OIE  | C22-C12-C13-C14 |
| 2   | F     | 301 | OIE  | C22-C12-C13-C14 |
| 3   | A     | 303 | NEX  | C31-C32-C33-C40 |
| 5   | A     | 305 | CHL  | C10-C11-C12-C13 |
| 5   | A     | 305 | CHL  | C1A-C2A-CAA-CBA |
| 5   | A     | 313 | CHL  | C1A-C2A-CAA-CBA |
| 5   | D     | 313 | CHL  | C1A-C2A-CAA-CBA |
| 5   | D     | 318 | CHL  | C1A-C2A-CAA-CBA |
| 5   | E     | 304 | CHL  | C1A-C2A-CAA-CBA |
| 5   | F     | 305 | CHL  | C1A-C2A-CAA-CBA |
| 5   | F     | 312 | CHL  | C1A-C2A-CAA-CBA |
| 6   | C     | 315 | CLA  | C1A-C2A-CAA-CBA |
| 6   | D     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 6   | D     | 314 | CLA  | C1A-C2A-CAA-CBA |
| 6   | D     | 315 | CLA  | C1A-C2A-CAA-CBA |
| 5   | A     | 312 | CHL  | C6-C7-C8-C10    |
| 7   | B     | 320 | LHG  | C8-C7-O7-C5     |
| 4   | B     | 305 | LMU  | C11-C10-C9-C8   |
| 9   | F     | 320 | OUR  | C46-C47-C48-C49 |
| 2   | C     | 302 | OIE  | C9-C10-C11-C12  |
| 6   | E     | 306 | CLA  | C15-C16-C17-C18 |
| 5   | E     | 312 | CHL  | C3-C5-C6-C7     |
| 5   | C     | 309 | CHL  | O1D-CGD-O2D-CED |
| 5   | D     | 311 | CHL  | C10-C11-C12-C13 |
| 7   | B     | 320 | LHG  | O6-C4-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | F     | 318 | LHG  | O6-C4-C5-C6     |
| 7   | A     | 319 | LHG  | C34-C35-C36-C37 |
| 5   | D     | 306 | CHL  | C13-C15-C16-C17 |
| 5   | D     | 313 | CHL  | C8-C10-C11-C12  |
| 7   | D     | 319 | LHG  | C24-C25-C26-C27 |
| 6   | C     | 314 | CLA  | CBA-CGA-O2A-C1  |
| 5   | A     | 311 | CHL  | C4-C3-C5-C6     |
| 5   | B     | 310 | CHL  | C3A-C2A-CAA-CBA |
| 6   | D     | 307 | CLA  | C15-C16-C17-C18 |
| 7   | C     | 319 | LHG  | C9-C10-C11-C12  |
| 7   | E     | 318 | LHG  | C11-C10-C9-C8   |
| 5   | C     | 305 | CHL  | C16-C17-C18-C19 |
| 11  | F     | 319 | LMG  | C7-C8-C9-O8     |
| 4   | B     | 304 | LMU  | C7-C8-C9-C10    |
| 5   | E     | 310 | CHL  | C12-C13-C15-C16 |
| 7   | F     | 318 | LHG  | C23-C24-C25-C26 |
| 5   | B     | 311 | CHL  | O1D-CGD-O2D-CED |
| 6   | A     | 317 | CLA  | C5-C6-C7-C8     |
| 5   | A     | 311 | CHL  | CAA-CBA-CGA-O2A |
| 5   | A     | 310 | CHL  | O1A-CGA-O2A-C1  |
| 5   | D     | 313 | CHL  | O1A-CGA-O2A-C1  |
| 4   | D     | 304 | LMU  | C1-C2-C3-C4     |
| 6   | E     | 316 | CLA  | C3-C5-C6-C7     |
| 5   | F     | 309 | CHL  | CBD-CGD-O2D-CED |
| 9   | A     | 322 | OUR  | C46-C47-C48-C49 |
| 11  | B     | 323 | LMG  | C13-C14-C15-C16 |
| 7   | B     | 324 | LHG  | C7-C8-C9-C10    |
| 5   | B     | 307 | CHL  | C16-C17-C18-C19 |
| 5   | E     | 305 | CHL  | C15-C16-C17-C18 |
| 2   | D     | 302 | OIE  | C14-C15-C16-C23 |
| 2   | F     | 302 | OIE  | C10-C11-C12-C22 |
| 5   | E     | 310 | CHL  | C4-C3-C5-C6     |
| 6   | A     | 317 | CLA  | C4-C3-C5-C6     |
| 7   | D     | 319 | LHG  | C32-C33-C34-C35 |
| 6   | A     | 317 | CLA  | C2-C3-C5-C6     |
| 6   | F     | 306 | CLA  | C16-C17-C18-C19 |
| 5   | A     | 311 | CHL  | C12-C13-C15-C16 |
| 6   | C     | 315 | CLA  | C10-C11-C12-C13 |
| 6   | B     | 308 | CLA  | C2-C1-O2A-CGA   |
| 7   | B     | 320 | LHG  | C11-C12-C13-C14 |
| 5   | D     | 309 | CHL  | O1D-CGD-O2D-CED |
| 5   | E     | 308 | CHL  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | A     | 319 | LHG  | C28-C29-C30-C31 |
| 5   | C     | 305 | CHL  | O1D-CGD-O2D-CED |
| 9   | C     | 321 | OUR  | C46-C47-C48-C49 |
| 7   | C     | 304 | LHG  | O6-C4-C5-O7     |
| 5   | A     | 313 | CHL  | O1A-CGA-O2A-C1  |
| 5   | E     | 304 | CHL  | O1A-CGA-O2A-C1  |
| 6   | A     | 317 | CLA  | C6-C7-C8-C10    |
| 2   | D     | 302 | OIE  | C14-C15-C16-C17 |
| 11  | B     | 323 | LMG  | C2-C1-O1-C7     |
| 4   | B     | 304 | LMU  | C11-C10-C9-C8   |
| 7   | D     | 319 | LHG  | C27-C28-C29-C30 |
| 5   | C     | 305 | CHL  | C5-C6-C7-C8     |
| 5   | F     | 310 | CHL  | C11-C12-C13-C15 |
| 5   | D     | 305 | CHL  | O1D-CGD-O2D-CED |
| 5   | A     | 313 | CHL  | C4-C3-C5-C6     |
| 5   | B     | 307 | CHL  | C4-C3-C5-C6     |
| 6   | E     | 313 | CLA  | O1D-CGD-O2D-CED |
| 5   | F     | 305 | CHL  | C13-C15-C16-C17 |
| 5   | D     | 306 | CHL  | C12-C13-C15-C16 |
| 5   | D     | 313 | CHL  | C11-C12-C13-C15 |
| 5   | E     | 305 | CHL  | C11-C10-C8-C7   |
| 5   | E     | 310 | CHL  | C2-C3-C5-C6     |
| 5   | E     | 310 | CHL  | C11-C10-C8-C7   |
| 5   | F     | 310 | CHL  | C11-C10-C8-C7   |
| 6   | A     | 307 | CLA  | C11-C10-C8-C7   |
| 6   | A     | 315 | CLA  | C6-C7-C8-C10    |
| 6   | D     | 307 | CLA  | C12-C13-C15-C16 |
| 6   | E     | 314 | CLA  | C6-C7-C8-C10    |
| 5   | A     | 313 | CHL  | C3-C5-C6-C7     |
| 5   | A     | 306 | CHL  | C11-C10-C8-C9   |
| 5   | B     | 306 | CHL  | C14-C13-C15-C16 |
| 5   | B     | 314 | CHL  | C11-C12-C13-C14 |
| 5   | D     | 313 | CHL  | C11-C12-C13-C14 |
| 5   | F     | 304 | CHL  | C11-C12-C13-C14 |
| 6   | B     | 308 | CLA  | C14-C13-C15-C16 |
| 6   | B     | 318 | CLA  | C11-C12-C13-C14 |
| 6   | E     | 306 | CLA  | C11-C10-C8-C9   |
| 6   | E     | 314 | CLA  | C6-C7-C8-C9     |
| 10  | B     | 322 | BET  | C-CA-N-C1       |
| 5   | E     | 317 | CHL  | O1D-CGD-O2D-CED |
| 5   | D     | 306 | CHL  | C2A-CAA-CBA-CGA |
| 5   | F     | 317 | CHL  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | C     | 310 | CHL  | O1D-CGD-O2D-CED |
| 2   | A     | 301 | OIE  | C22-C12-C13-C14 |
| 7   | C     | 319 | LHG  | C7-C8-C9-C10    |
| 5   | B     | 306 | CHL  | C13-C15-C16-C17 |
| 5   | D     | 305 | CHL  | C5-C6-C7-C8     |
| 5   | D     | 305 | CHL  | C4C-C3C-CAC-CBC |
| 6   | C     | 314 | CLA  | O1A-CGA-O2A-C1  |
| 4   | E     | 319 | LMU  | C3-C4-C5-C6     |
| 5   | E     | 312 | CHL  | C13-C15-C16-C17 |
| 4   | A     | 304 | LMU  | C7-C8-C9-C10    |
| 7   | F     | 318 | LHG  | C10-C11-C12-C13 |
| 5   | D     | 313 | CHL  | C16-C17-C18-C19 |
| 7   | C     | 304 | LHG  | O6-C4-C5-C6     |
| 5   | A     | 313 | CHL  | C2-C3-C5-C6     |
| 5   | B     | 307 | CHL  | C2-C3-C5-C6     |
| 5   | A     | 312 | CHL  | O1D-CGD-O2D-CED |
| 5   | F     | 310 | CHL  | C11-C12-C13-C14 |
| 6   | D     | 307 | CLA  | C16-C17-C18-C19 |
| 7   | E     | 318 | LHG  | C11-C12-C13-C14 |
| 5   | D     | 306 | CHL  | CBA-CGA-O2A-C1  |
| 7   | C     | 319 | LHG  | C24-C23-O8-C6   |
| 10  | B     | 322 | BET  | C-CA-N-C2       |
| 5   | F     | 317 | CHL  | CBD-CGD-O2D-CED |
| 4   | B     | 304 | LMU  | C2-C1-O1'-C1'   |
| 6   | D     | 307 | CLA  | C16-C17-C18-C20 |
| 7   | C     | 304 | LHG  | C4-C5-C6-O8     |
| 7   | C     | 319 | LHG  | C4-C5-C6-O8     |
| 7   | D     | 319 | LHG  | C4-C5-C6-O8     |
| 5   | D     | 311 | CHL  | CAA-CBA-CGA-O2A |
| 6   | C     | 314 | CLA  | C5-C6-C7-C8     |
| 5   | B     | 307 | CHL  | C3C-C2C-CMC-OMC |
| 5   | B     | 312 | CHL  | C3C-C2C-CMC-OMC |
| 5   | B     | 314 | CHL  | C3C-C2C-CMC-OMC |
| 5   | D     | 313 | CHL  | C3C-C2C-CMC-OMC |
| 5   | A     | 309 | CHL  | O1D-CGD-O2D-CED |
| 6   | F     | 306 | CLA  | C8-C10-C11-C12  |
| 5   | C     | 306 | CHL  | C2C-C3C-CAC-CBC |
| 7   | F     | 318 | LHG  | O6-C4-C5-O7     |
| 5   | C     | 313 | CHL  | CBA-CGA-O2A-C1  |
| 6   | F     | 306 | CLA  | C16-C17-C18-C20 |
| 7   | D     | 319 | LHG  | C31-C32-C33-C34 |
| 7   | B     | 324 | LHG  | O7-C5-C6-O8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 7   | C     | 319 | LHG  | O7-C5-C6-O8     |
| 7   | D     | 319 | LHG  | O7-C5-C6-O8     |
| 11  | B     | 323 | LMG  | O1-C7-C8-O7     |
| 5   | F     | 310 | CHL  | CAA-CBA-CGA-O2A |
| 6   | E     | 316 | CLA  | C11-C10-C8-C7   |
| 5   | D     | 313 | CHL  | C16-C17-C18-C20 |
| 5   | E     | 312 | CHL  | C2-C1-O2A-CGA   |
| 5   | E     | 304 | CHL  | C13-C15-C16-C17 |
| 5   | A     | 306 | CHL  | C6-C7-C8-C9     |
| 5   | A     | 311 | CHL  | C11-C10-C8-C9   |
| 5   | A     | 313 | CHL  | C11-C12-C13-C14 |
| 6   | C     | 315 | CLA  | C14-C13-C15-C16 |
| 6   | F     | 316 | CLA  | C6-C7-C8-C9     |
| 5   | A     | 305 | CHL  | C8-C10-C11-C12  |
| 7   | C     | 304 | LHG  | C2-C3-O3-P      |
| 6   | D     | 314 | CLA  | C2A-CAA-CBA-CGA |
| 5   | C     | 312 | CHL  | C6-C7-C8-C10    |
| 5   | F     | 311 | CHL  | C6-C7-C8-C10    |
| 5   | B     | 319 | CHL  | CAA-CBA-CGA-O2A |
| 2   | B     | 301 | 0IE  | C5-C6-C7-C8     |
| 6   | B     | 308 | CLA  | C15-C16-C17-C18 |
| 7   | A     | 319 | LHG  | O9-C7-O7-C5     |
| 2   | D     | 301 | 0IE  | C11-C10-C9-C8   |
| 3   | E     | 303 | NEX  | C14-C15-C35-C34 |
| 5   | A     | 305 | CHL  | C16-C17-C18-C20 |
| 5   | D     | 311 | CHL  | C14-C13-C15-C16 |
| 5   | A     | 305 | CHL  | C5-C6-C7-C8     |
| 5   | F     | 304 | CHL  | C5-C6-C7-C8     |
| 7   | E     | 318 | LHG  | O6-C4-C5-C6     |
| 5   | D     | 311 | CHL  | C4-C3-C5-C6     |
| 5   | A     | 306 | CHL  | C11-C10-C8-C7   |
| 5   | A     | 313 | CHL  | C11-C12-C13-C15 |
| 5   | B     | 306 | CHL  | C12-C13-C15-C16 |
| 5   | B     | 314 | CHL  | C11-C12-C13-C15 |
| 5   | C     | 306 | CHL  | C12-C13-C15-C16 |
| 5   | C     | 311 | CHL  | C11-C10-C8-C7   |
| 5   | E     | 304 | CHL  | C11-C12-C13-C15 |
| 5   | E     | 304 | CHL  | C12-C13-C15-C16 |
| 5   | F     | 304 | CHL  | C11-C12-C13-C15 |
| 6   | B     | 318 | CLA  | C11-C10-C8-C7   |
| 6   | B     | 318 | CLA  | C11-C12-C13-C15 |
| 6   | E     | 306 | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | F     | 306 | CLA  | C11-C12-C13-C15 |
| 6   | F     | 316 | CLA  | C6-C7-C8-C10    |
| 6   | A     | 307 | CLA  | C8-C10-C11-C12  |
| 2   | A     | 302 | 0IE  | C9-C10-C11-C12  |
| 2   | A     | 302 | 0IE  | C7-C8-C9-C10    |
| 2   | D     | 301 | 0IE  | C13-C14-C15-C16 |
| 2   | E     | 301 | 0IE  | C13-C14-C15-C16 |
| 5   | B     | 312 | CHL  | CAA-CBA-CGA-O2A |
| 2   | A     | 301 | 0IE  | O1-C2-C3-C4     |
| 2   | B     | 301 | 0IE  | C20-C3-C4-C5    |
| 2   | B     | 301 | 0IE  | O1-C2-C3-C4     |
| 2   | C     | 301 | 0IE  | O1-C2-C3-C4     |
| 2   | C     | 301 | 0IE  | C14-C15-C16-C23 |
| 2   | C     | 302 | 0IE  | C14-C15-C16-C23 |
| 2   | D     | 301 | 0IE  | O1-C2-C3-C4     |
| 2   | E     | 301 | 0IE  | O1-C2-C3-C4     |
| 2   | F     | 301 | 0IE  | O1-C2-C3-C4     |
| 9   | A     | 322 | 0UR  | O42-C2-C3-C4    |
| 9   | B     | 302 | 0UR  | O42-C2-C3-C4    |
| 9   | B     | 325 | 0UR  | O42-C2-C3-C4    |
| 9   | C     | 321 | 0UR  | O42-C2-C3-C4    |
| 9   | D     | 321 | 0UR  | O42-C2-C3-C4    |
| 9   | E     | 320 | 0UR  | O42-C2-C3-C4    |
| 9   | F     | 320 | 0UR  | O42-C2-C3-C4    |
| 5   | B     | 314 | CHL  | C3-C5-C6-C7     |
| 5   | B     | 310 | CHL  | CBD-CGD-O2D-CED |
| 5   | D     | 313 | CHL  | C15-C16-C17-C18 |
| 5   | D     | 311 | CHL  | C12-C13-C15-C16 |
| 5   | A     | 310 | CHL  | CAD-CBD-CGD-O2D |
| 5   | B     | 311 | CHL  | CAD-CBD-CGD-O2D |
| 6   | A     | 314 | CLA  | CAD-CBD-CGD-O2D |
| 6   | E     | 306 | CLA  | CAD-CBD-CGD-O2D |
| 6   | E     | 314 | CLA  | CAD-CBD-CGD-O2D |
| 6   | F     | 313 | CLA  | CAD-CBD-CGD-O2D |
| 5   | F     | 309 | CHL  | O1D-CGD-O2D-CED |
| 11  | B     | 323 | LMG  | O1-C7-C8-C9     |
| 7   | E     | 318 | LHG  | O6-C4-C5-O7     |
| 6   | B     | 318 | CLA  | C15-C16-C17-C18 |
| 7   | E     | 318 | LHG  | C27-C28-C29-C30 |
| 6   | C     | 315 | CLA  | C2A-CAA-CBA-CGA |
| 5   | B     | 319 | CHL  | CHA-CBD-CGD-O1D |
| 5   | B     | 319 | CHL  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | D     | 318 | CHL  | CHA-CBD-CGD-O2D |
| 5   | E     | 305 | CHL  | CHA-CBD-CGD-O1D |
| 5   | E     | 305 | CHL  | CHA-CBD-CGD-O2D |
| 5   | E     | 311 | CHL  | CHA-CBD-CGD-O1D |
| 5   | E     | 311 | CHL  | CHA-CBD-CGD-O2D |
| 5   | F     | 305 | CHL  | CHA-CBD-CGD-O1D |
| 6   | A     | 308 | CLA  | CHA-CBD-CGD-O1D |
| 6   | B     | 309 | CLA  | CHA-CBD-CGD-O1D |
| 6   | B     | 309 | CLA  | CHA-CBD-CGD-O2D |
| 6   | D     | 308 | CLA  | CHA-CBD-CGD-O1D |
| 6   | D     | 308 | CLA  | CHA-CBD-CGD-O2D |
| 6   | F     | 314 | CLA  | O1D-CGD-O2D-CED |
| 5   | C     | 313 | CHL  | O1A-CGA-O2A-C1  |
| 5   | D     | 306 | CHL  | O1A-CGA-O2A-C1  |
| 7   | C     | 319 | LHG  | C25-C26-C27-C28 |
| 2   | C     | 302 | 0IE  | C14-C15-C16-C17 |
| 11  | F     | 319 | LMG  | O1-C7-C8-O7     |
| 6   | A     | 307 | CLA  | C3-C5-C6-C7     |
| 5   | C     | 305 | CHL  | C15-C16-C17-C18 |
| 7   | F     | 318 | LHG  | O9-C7-O7-C5     |
| 5   | C     | 305 | CHL  | C11-C12-C13-C14 |
| 5   | F     | 317 | CHL  | O1D-CGD-O2D-CED |
| 3   | D     | 303 | NEX  | C31-C32-C33-C40 |
| 6   | A     | 307 | CLA  | C13-C15-C16-C17 |
| 2   | A     | 301 | 0IE  | C5-C6-C7-C8     |
| 5   | B     | 314 | CHL  | C1A-C2A-CAA-CBA |
| 5   | D     | 306 | CHL  | C1A-C2A-CAA-CBA |
| 6   | C     | 314 | CLA  | C1A-C2A-CAA-CBA |
| 6   | E     | 313 | CLA  | C1A-C2A-CAA-CBA |
| 6   | A     | 307 | CLA  | C2-C1-O2A-CGA   |
| 6   | D     | 307 | CLA  | C2-C1-O2A-CGA   |
| 2   | C     | 302 | 0IE  | C3-C4-C5-C6     |
| 4   | A     | 304 | LMU  | C9-C10-C11-C12  |
| 5   | D     | 306 | CHL  | C4-C3-C5-C6     |
| 6   | F     | 316 | CLA  | C3-C5-C6-C7     |
| 5   | A     | 306 | CHL  | C2-C3-C5-C6     |
| 7   | C     | 304 | LHG  | O10-C23-O8-C6   |
| 7   | B     | 324 | LHG  | C3-O3-P-O4      |
| 7   | F     | 318 | LHG  | C4-O6-P-O5      |
| 7   | A     | 319 | LHG  | C11-C12-C13-C14 |
| 5   | B     | 319 | CHL  | CAD-CBD-CGD-O1D |
| 5   | D     | 318 | CHL  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | B     | 309 | CLA  | CAD-CBD-CGD-O1D |
| 6   | D     | 308 | CLA  | CAD-CBD-CGD-O1D |
| 5   | B     | 310 | CHL  | O1D-CGD-O2D-CED |
| 6   | B     | 308 | CLA  | C4-C3-C5-C6     |
| 2   | B     | 301 | 0IE  | O1-C2-C3-C20    |
| 2   | B     | 301 | 0IE  | C3-C2-C30-C31   |
| 2   | D     | 302 | 0IE  | C2-C3-C4-C5     |
| 5   | B     | 307 | CHL  | C6-C7-C8-C10    |
| 5   | B     | 307 | CHL  | C11-C12-C13-C15 |
| 5   | C     | 305 | CHL  | C11-C10-C8-C7   |
| 5   | C     | 305 | CHL  | C11-C12-C13-C15 |
| 5   | C     | 313 | CHL  | C11-C12-C13-C15 |
| 5   | D     | 306 | CHL  | C11-C10-C8-C7   |
| 6   | B     | 316 | CLA  | C6-C7-C8-C10    |
| 6   | B     | 308 | CLA  | C10-C11-C12-C13 |
| 5   | A     | 306 | CHL  | C2A-CAA-CBA-CGA |
| 6   | C     | 317 | CLA  | C2A-CAA-CBA-CGA |
| 5   | A     | 311 | CHL  | C1C-C2C-CMC-OMC |
| 5   | A     | 313 | CHL  | C1C-C2C-CMC-OMC |
| 5   | B     | 306 | CHL  | C1C-C2C-CMC-OMC |
| 5   | D     | 306 | CHL  | C1C-C2C-CMC-OMC |
| 5   | E     | 310 | CHL  | C1C-C2C-CMC-OMC |
| 5   | F     | 312 | CHL  | C1C-C2C-CMC-OMC |
| 7   | B     | 324 | LHG  | C4-C5-C6-O8     |
| 2   | F     | 301 | 0IE  | C11-C10-C9-C8   |
| 5   | C     | 313 | CHL  | C4-C3-C5-C6     |
| 5   | D     | 311 | CHL  | C2-C3-C5-C6     |
| 6   | E     | 314 | CLA  | C10-C11-C12-C13 |
| 5   | B     | 307 | CHL  | C6-C7-C8-C9     |
| 5   | C     | 306 | CHL  | C11-C10-C8-C9   |
| 5   | D     | 306 | CHL  | C14-C13-C15-C16 |
| 5   | E     | 304 | CHL  | C11-C12-C13-C14 |
| 5   | E     | 304 | CHL  | C14-C13-C15-C16 |
| 5   | F     | 305 | CHL  | C11-C10-C8-C9   |
| 6   | B     | 318 | CLA  | C14-C13-C15-C16 |
| 9   | B     | 302 | 0UR  | C4-C5-C6-C7     |
| 2   | F     | 301 | 0IE  | C11-C12-C13-C14 |
| 5   | B     | 314 | CHL  | O1A-CGA-O2A-C1  |
| 5   | F     | 304 | CHL  | CAA-CBA-CGA-O2A |
| 7   | B     | 324 | LHG  | C4-C5-O7-C7     |
| 5   | C     | 306 | CHL  | C2A-CAA-CBA-CGA |
| 6   | B     | 309 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | C     | 311 | CHL  | C2-C1-O2A-CGA   |
| 5   | D     | 313 | CHL  | C2-C1-O2A-CGA   |
| 4   | B     | 305 | LMU  | C7-C8-C9-C10    |
| 2   | E     | 302 | 0IE  | C16-C17-C18-C19 |
| 5   | B     | 314 | CHL  | CBA-CGA-O2A-C1  |
| 4   | D     | 304 | LMU  | C9-C10-C11-C12  |
| 2   | C     | 301 | 0IE  | C14-C15-C16-C17 |
| 7   | F     | 318 | LHG  | C11-C10-C9-C8   |
| 7   | A     | 319 | LHG  | C4-O6-P-O3      |
| 7   | B     | 320 | LHG  | C3-O3-P-O6      |
| 7   | C     | 319 | LHG  | C3-O3-P-O6      |
| 7   | D     | 319 | LHG  | C3-O3-P-O6      |
| 7   | E     | 318 | LHG  | C4-O6-P-O3      |
| 7   | B     | 320 | LHG  | C10-C11-C12-C13 |
| 5   | A     | 306 | CHL  | C13-C15-C16-C17 |
| 5   | C     | 306 | CHL  | C11-C10-C8-C7   |
| 5   | D     | 306 | CHL  | C2-C3-C5-C6     |
| 5   | F     | 305 | CHL  | C11-C10-C8-C7   |
| 5   | F     | 312 | CHL  | C11-C10-C8-C7   |
| 6   | B     | 308 | CLA  | C11-C10-C8-C7   |
| 5   | D     | 306 | CHL  | C11-C10-C8-C9   |
| 6   | B     | 308 | CLA  | C16-C17-C18-C20 |
| 5   | F     | 312 | CHL  | C10-C11-C12-C13 |
| 7   | B     | 324 | LHG  | C2-C3-O3-P      |
| 5   | E     | 310 | CHL  | CAA-CBA-CGA-O2A |
| 2   | C     | 302 | 0IE  | C11-C12-C13-C14 |
| 5   | F     | 305 | CHL  | CBA-CGA-O2A-C1  |
| 9   | F     | 320 | 0UR  | C47-C48-C49-C50 |
| 7   | C     | 319 | LHG  | C18-C19-C20-C21 |
| 6   | E     | 316 | CLA  | C2A-CAA-CBA-CGA |
| 2   | D     | 302 | 0IE  | C9-C10-C11-C12  |
| 9   | F     | 320 | 0UR  | C3-C4-C5-C6     |
| 6   | A     | 308 | CLA  | CAA-CBA-CGA-O2A |
| 5   | A     | 313 | CHL  | C5-C6-C7-C8     |
| 5   | F     | 305 | CHL  | C5-C6-C7-C8     |
| 6   | B     | 318 | CLA  | C13-C15-C16-C17 |
| 6   | F     | 313 | CLA  | C2A-CAA-CBA-CGA |
| 5   | C     | 306 | CHL  | C4C-C3C-CAC-CBC |
| 6   | C     | 307 | CLA  | C6-C7-C8-C9     |
| 6   | F     | 306 | CLA  | C15-C16-C17-C18 |
| 2   | E     | 302 | 0IE  | C14-C15-C16-C23 |
| 3   | A     | 303 | NEX  | C39-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | B     | 303 | NEX  | C39-C29-C30-C31 |
| 3   | C     | 303 | NEX  | C39-C29-C30-C31 |
| 3   | D     | 303 | NEX  | C39-C29-C30-C31 |
| 3   | E     | 303 | NEX  | C39-C29-C30-C31 |
| 3   | F     | 303 | NEX  | C39-C29-C30-C31 |
| 6   | A     | 308 | CLA  | C2A-CAA-CBA-CGA |
| 7   | A     | 319 | LHG  | C33-C34-C35-C36 |
| 5   | A     | 311 | CHL  | CAA-CBA-CGA-O1A |
| 2   | A     | 301 | OIE  | C23-C16-C17-C18 |
| 2   | D     | 301 | OIE  | C22-C12-C13-C14 |
| 6   | E     | 306 | CLA  | C5-C6-C7-C8     |
| 6   | E     | 315 | CLA  | CAA-CBA-CGA-O1A |
| 7   | B     | 324 | LHG  | C6-C5-O7-C7     |
| 5   | B     | 314 | CHL  | C8-C10-C11-C12  |
| 5   | C     | 306 | CHL  | C5-C6-C7-C8     |
| 5   | A     | 306 | CHL  | C1A-C2A-CAA-CBA |
| 5   | C     | 313 | CHL  | C1A-C2A-CAA-CBA |
| 5   | E     | 305 | CHL  | C1A-C2A-CAA-CBA |
| 6   | A     | 314 | CLA  | C1A-C2A-CAA-CBA |
| 5   | F     | 305 | CHL  | C12-C13-C15-C16 |
| 6   | B     | 308 | CLA  | C6-C7-C8-C10    |
| 7   | D     | 319 | LHG  | C30-C31-C32-C33 |
| 6   | D     | 315 | CLA  | C10-C11-C12-C13 |
| 9   | D     | 321 | OUR  | C48-C49-C50-C51 |
| 6   | A     | 317 | CLA  | C2A-CAA-CBA-CGA |
| 7   | E     | 318 | LHG  | C29-C30-C31-C32 |
| 6   | C     | 316 | CLA  | CAA-CBA-CGA-O2A |
| 6   | C     | 316 | CLA  | CAA-CBA-CGA-O1A |
| 5   | C     | 305 | CHL  | C3-C5-C6-C7     |
| 3   | A     | 303 | NEX  | C28-C29-C30-C31 |
| 3   | B     | 303 | NEX  | C28-C29-C30-C31 |
| 3   | C     | 303 | NEX  | C28-C29-C30-C31 |
| 3   | D     | 303 | NEX  | C28-C29-C30-C31 |
| 3   | E     | 303 | NEX  | C28-C29-C30-C31 |
| 3   | F     | 303 | NEX  | C28-C29-C30-C31 |
| 5   | C     | 305 | CHL  | C8-C10-C11-C12  |
| 7   | F     | 318 | LHG  | C16-C17-C18-C19 |
| 7   | E     | 318 | LHG  | C9-C10-C11-C12  |
| 5   | B     | 314 | CHL  | C2-C1-O2A-CGA   |
| 5   | C     | 313 | CHL  | C2-C3-C5-C6     |
| 5   | C     | 305 | CHL  | O1A-CGA-O2A-C1  |
| 4   | B     | 305 | LMU  | C2B-C1B-O1B-C4' |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | E     | 315 | CLA  | CAA-CBA-CGA-O2A |
| 7   | A     | 319 | LHG  | C13-C14-C15-C16 |
| 6   | D     | 316 | CLA  | O1D-CGD-O2D-CED |
| 2   | C     | 301 | 0IE  | C3-C4-C5-C6     |
| 2   | F     | 301 | 0IE  | C7-C8-C9-C10    |
| 6   | A     | 314 | CLA  | C4-C3-C5-C6     |
| 3   | A     | 303 | NEX  | C31-C32-C33-C34 |
| 3   | D     | 303 | NEX  | C31-C32-C33-C34 |
| 5   | E     | 309 | CHL  | C1A-C2A-CAA-CBA |
| 7   | B     | 320 | LHG  | C13-C14-C15-C16 |
| 6   | E     | 306 | CLA  | C3-C5-C6-C7     |
| 6   | A     | 314 | CLA  | C6-C7-C8-C10    |
| 5   | E     | 305 | CHL  | C8-C10-C11-C12  |
| 6   | C     | 307 | CLA  | C15-C16-C17-C18 |
| 6   | E     | 307 | CLA  | C2A-CAA-CBA-CGA |
| 9   | B     | 302 | 0UR  | C46-C47-C48-C49 |
| 5   | C     | 305 | CHL  | CBA-CGA-O2A-C1  |
| 4   | B     | 305 | LMU  | O5B-C1B-O1B-C4' |
| 5   | F     | 304 | CHL  | C4-C3-C5-C6     |
| 5   | F     | 311 | CHL  | C4-C3-C5-C6     |
| 5   | B     | 314 | CHL  | C12-C13-C15-C16 |
| 5   | F     | 305 | CHL  | O1A-CGA-O2A-C1  |
| 5   | A     | 306 | CHL  | O1A-CGA-O2A-C1  |
| 7   | D     | 319 | LHG  | C11-C12-C13-C14 |
| 5   | C     | 306 | CHL  | C13-C15-C16-C17 |
| 2   | F     | 301 | 0IE  | C20-C3-C4-C5    |
| 5   | D     | 311 | CHL  | CAA-CBA-CGA-O1A |
| 5   | F     | 312 | CHL  | C4-C3-C5-C6     |
| 5   | D     | 311 | CHL  | C5-C6-C7-C8     |
| 6   | B     | 308 | CLA  | C2-C3-C5-C6     |
| 5   | C     | 305 | CHL  | C11-C10-C8-C9   |
| 5   | C     | 313 | CHL  | C11-C10-C8-C9   |
| 5   | F     | 305 | CHL  | C14-C13-C15-C16 |
| 6   | D     | 307 | CLA  | C5-C6-C7-C8     |
| 5   | E     | 311 | CHL  | O1A-CGA-O2A-C1  |
| 5   | F     | 311 | CHL  | O1A-CGA-O2A-C1  |
| 5   | B     | 307 | CHL  | CAD-CBD-CGD-O2D |
| 5   | C     | 310 | CHL  | CAD-CBD-CGD-O2D |
| 5   | C     | 318 | CHL  | CAD-CBD-CGD-O2D |
| 5   | D     | 313 | CHL  | CAD-CBD-CGD-O2D |
| 5   | E     | 317 | CHL  | CAD-CBD-CGD-O2D |
| 5   | F     | 309 | CHL  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | A     | 315 | CLA  | CAD-CBD-CGD-O2D |
| 6   | B     | 315 | CLA  | CAD-CBD-CGD-O2D |
| 6   | C     | 315 | CLA  | CAD-CBD-CGD-O2D |
| 6   | D     | 307 | CLA  | CAD-CBD-CGD-O2D |
| 6   | D     | 314 | CLA  | CAD-CBD-CGD-O2D |
| 6   | D     | 315 | CLA  | CAD-CBD-CGD-O2D |
| 6   | F     | 307 | CLA  | CAD-CBD-CGD-O2D |
| 6   | D     | 314 | CLA  | C10-C11-C12-C13 |
| 7   | B     | 320 | LHG  | C32-C33-C34-C35 |
| 5   | D     | 305 | CHL  | C13-C15-C16-C17 |
| 5   | C     | 311 | CHL  | C2A-CAA-CBA-CGA |
| 4   | B     | 305 | LMU  | C1-C2-C3-C4     |
| 7   | A     | 319 | LHG  | C26-C27-C28-C29 |
| 5   | E     | 304 | CHL  | C16-C17-C18-C20 |
| 5   | F     | 317 | CHL  | CAA-CBA-CGA-O2A |
| 5   | C     | 311 | CHL  | CAA-CBA-CGA-O2A |
| 7   | F     | 318 | LHG  | C14-C15-C16-C17 |
| 2   | A     | 301 | 0IE  | C11-C12-C13-C14 |
| 2   | D     | 301 | 0IE  | C11-C12-C13-C14 |
| 4   | B     | 304 | LMU  | C5-C6-C7-C8     |
| 3   | D     | 303 | NEX  | O24-C26-C27-C28 |
| 3   | E     | 303 | NEX  | O24-C26-C27-C28 |
| 9   | D     | 321 | 0UR  | C4-C3-C43-O44   |
| 6   | A     | 316 | CLA  | CAA-CBA-CGA-O2A |
| 9   | C     | 321 | 0UR  | C48-C49-C50-C51 |
| 5   | C     | 305 | CHL  | C2A-CAA-CBA-CGA |
| 6   | B     | 318 | CLA  | C2A-CAA-CBA-CGA |
| 6   | F     | 316 | CLA  | C2A-CAA-CBA-CGA |
| 2   | C     | 301 | 0IE  | C11-C10-C9-C8   |
| 5   | F     | 310 | CHL  | CAA-CBA-CGA-O1A |
| 5   | F     | 317 | CHL  | CAA-CBA-CGA-O1A |
| 6   | A     | 316 | CLA  | CAA-CBA-CGA-O1A |
| 6   | B     | 317 | CLA  | CAA-CBA-CGA-O2A |
| 6   | F     | 315 | CLA  | CAA-CBA-CGA-O2A |
| 2   | C     | 301 | 0IE  | C13-C14-C15-C16 |
| 5   | A     | 306 | CHL  | CHA-CBD-CGD-O1D |
| 5   | B     | 306 | CHL  | CHA-CBD-CGD-O1D |
| 5   | B     | 306 | CHL  | CHA-CBD-CGD-O2D |
| 5   | B     | 307 | CHL  | CHA-CBD-CGD-O2D |
| 5   | C     | 306 | CHL  | CHA-CBD-CGD-O1D |
| 5   | D     | 306 | CHL  | CHA-CBD-CGD-O1D |
| 5   | E     | 304 | CHL  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | E     | 304 | CHL  | CHA-CBD-CGD-O2D |
| 5   | F     | 304 | CHL  | CHA-CBD-CGD-O1D |
| 5   | F     | 304 | CHL  | CHA-CBD-CGD-O2D |
| 5   | F     | 305 | CHL  | CHA-CBD-CGD-O2D |
| 6   | A     | 307 | CLA  | CHA-CBD-CGD-O1D |
| 6   | A     | 307 | CLA  | CHA-CBD-CGD-O2D |
| 6   | A     | 308 | CLA  | CHA-CBD-CGD-O2D |
| 6   | A     | 316 | CLA  | CHA-CBD-CGD-O1D |
| 6   | A     | 316 | CLA  | CHA-CBD-CGD-O2D |
| 6   | A     | 317 | CLA  | CHA-CBD-CGD-O1D |
| 6   | A     | 317 | CLA  | CHA-CBD-CGD-O2D |
| 6   | B     | 308 | CLA  | CHA-CBD-CGD-O1D |
| 6   | B     | 308 | CLA  | CHA-CBD-CGD-O2D |
| 6   | B     | 318 | CLA  | CHA-CBD-CGD-O1D |
| 6   | B     | 318 | CLA  | CHA-CBD-CGD-O2D |
| 6   | C     | 307 | CLA  | CHA-CBD-CGD-O2D |
| 6   | C     | 308 | CLA  | CHA-CBD-CGD-O1D |
| 6   | C     | 316 | CLA  | CHA-CBD-CGD-O1D |
| 6   | C     | 316 | CLA  | CHA-CBD-CGD-O2D |
| 6   | E     | 315 | CLA  | CHA-CBD-CGD-O1D |
| 6   | E     | 315 | CLA  | CHA-CBD-CGD-O2D |
| 6   | F     | 306 | CLA  | CHA-CBD-CGD-O1D |
| 6   | F     | 306 | CLA  | CHA-CBD-CGD-O2D |
| 5   | F     | 312 | CHL  | C2-C3-C5-C6     |
| 7   | B     | 320 | LHG  | O7-C7-C8-C9     |
| 7   | F     | 318 | LHG  | O7-C7-C8-C9     |
| 6   | A     | 307 | CLA  | C2A-CAA-CBA-CGA |
| 6   | D     | 317 | CLA  | C2A-CAA-CBA-CGA |
| 5   | C     | 312 | CHL  | CBA-CGA-O2A-C1  |
| 5   | D     | 313 | CHL  | C2-C3-C5-C6     |
| 6   | B     | 308 | CLA  | C6-C7-C8-C9     |
| 6   | D     | 314 | CLA  | C6-C7-C8-C9     |
| 3   | D     | 303 | NEX  | C13-C14-C15-C35 |
| 5   | A     | 306 | CHL  | CBA-CGA-O2A-C1  |
| 5   | F     | 311 | CHL  | CBA-CGA-O2A-C1  |
| 7   | C     | 319 | LHG  | C28-C29-C30-C31 |
| 6   | B     | 317 | CLA  | CAA-CBA-CGA-O1A |
| 6   | F     | 315 | CLA  | CAA-CBA-CGA-O1A |
| 5   | B     | 312 | CHL  | CAA-CBA-CGA-O1A |
| 5   | B     | 319 | CHL  | CAA-CBA-CGA-O1A |
| 5   | E     | 311 | CHL  | CBA-CGA-O2A-C1  |
| 5   | C     | 312 | CHL  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | C     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 5   | F     | 310 | CHL  | C2A-CAA-CBA-CGA |
| 6   | C     | 314 | CLA  | C2A-CAA-CBA-CGA |
| 6   | E     | 313 | CLA  | C2A-CAA-CBA-CGA |
| 7   | B     | 324 | LHG  | C4-O6-P-O3      |
| 7   | B     | 320 | LHG  | O10-C23-C24-C25 |
| 5   | D     | 305 | CHL  | CAA-CBA-CGA-O2A |
| 2   | D     | 302 | 0IE  | C11-C10-C9-C8   |
| 7   | B     | 320 | LHG  | C3-O3-P-O5      |
| 7   | B     | 324 | LHG  | C4-O6-P-O5      |
| 7   | C     | 319 | LHG  | C3-O3-P-O5      |
| 7   | D     | 319 | LHG  | C3-O3-P-O4      |
| 7   | E     | 318 | LHG  | C4-O6-P-O5      |
| 7   | C     | 319 | LHG  | O9-C7-C8-C9     |
| 5   | B     | 311 | CHL  | O1A-CGA-O2A-C1  |
| 2   | D     | 301 | 0IE  | C10-C11-C12-C22 |
| 7   | A     | 319 | LHG  | C9-C10-C11-C12  |
| 5   | D     | 306 | CHL  | C5-C6-C7-C8     |
| 6   | C     | 317 | CLA  | C5-C6-C7-C8     |
| 5   | B     | 312 | CHL  | O1A-CGA-O2A-C1  |
| 5   | E     | 310 | CHL  | C2A-CAA-CBA-CGA |
| 5   | A     | 318 | CHL  | CAD-CBD-CGD-O1D |
| 5   | F     | 304 | CHL  | CAD-CBD-CGD-O1D |
| 6   | A     | 308 | CLA  | CAD-CBD-CGD-O1D |
| 6   | B     | 318 | CLA  | CAD-CBD-CGD-O1D |
| 6   | C     | 308 | CLA  | CAD-CBD-CGD-O1D |
| 5   | B     | 306 | CHL  | C11-C12-C13-C14 |
| 5   | F     | 312 | CHL  | C14-C13-C15-C16 |
| 5   | B     | 311 | CHL  | CBA-CGA-O2A-C1  |
| 11  | B     | 323 | LMG  | O8-C28-C29-C30  |
| 6   | F     | 306 | CLA  | CAA-CBA-CGA-O2A |
| 7   | C     | 319 | LHG  | O7-C7-C8-C9     |
| 2   | A     | 301 | 0IE  | O1-C2-C3-C20    |
| 2   | B     | 301 | 0IE  | C2-C3-C4-C5     |
| 2   | C     | 301 | 0IE  | O1-C2-C3-C20    |
| 2   | E     | 301 | 0IE  | O1-C2-C3-C20    |
| 2   | F     | 301 | 0IE  | C2-C3-C4-C5     |
| 5   | B     | 306 | CHL  | C11-C12-C13-C15 |
| 6   | E     | 307 | CLA  | C3A-C2A-CAA-CBA |
| 9   | A     | 322 | 0UR  | O42-C2-C3-C43   |
| 9   | B     | 302 | 0UR  | O42-C2-C3-C43   |
| 9   | B     | 325 | 0UR  | O42-C2-C3-C43   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 9   | C     | 321 | 0UR  | O42-C2-C3-C43   |
| 9   | D     | 321 | 0UR  | O42-C2-C3-C43   |
| 9   | E     | 320 | 0UR  | O42-C2-C3-C43   |
| 9   | F     | 320 | 0UR  | O42-C2-C3-C43   |
| 5   | A     | 306 | CHL  | CAA-CBA-CGA-O2A |
| 5   | D     | 306 | CHL  | CAA-CBA-CGA-O2A |
| 2   | A     | 301 | 0IE  | C15-C16-C17-C18 |
| 5   | D     | 305 | CHL  | CAA-CBA-CGA-O1A |
| 7   | F     | 318 | LHG  | O10-C23-C24-C25 |
| 6   | B     | 315 | CLA  | C10-C11-C12-C13 |
| 7   | B     | 324 | LHG  | O7-C7-C8-C9     |
| 5   | A     | 306 | CHL  | CAA-CBA-CGA-O1A |
| 7   | E     | 318 | LHG  | O10-C23-C24-C25 |
| 6   | D     | 316 | CLA  | CBD-CGD-O2D-CED |
| 7   | B     | 320 | LHG  | C16-C17-C18-C19 |
| 5   | D     | 306 | CHL  | CAA-CBA-CGA-O1A |

All (1) ring outliers are listed below:

| Mol | Chain | Res | Type | Atoms                   |
|-----|-------|-----|------|-------------------------|
| 4   | B     | 304 | LMU  | C1'-C2'-C3'-C4'-C5'-O5' |

111 monomers are involved in 359 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | B     | 304 | LMU  | 2       | 0            |
| 3   | A     | 303 | NEX  | 3       | 0            |
| 5   | C     | 309 | CHL  | 5       | 0            |
| 5   | B     | 310 | CHL  | 1       | 0            |
| 5   | A     | 312 | CHL  | 2       | 0            |
| 9   | E     | 320 | 0UR  | 3       | 0            |
| 6   | D     | 314 | CLA  | 4       | 0            |
| 5   | C     | 305 | CHL  | 5       | 0            |
| 5   | D     | 312 | CHL  | 3       | 0            |
| 9   | B     | 325 | 0UR  | 5       | 0            |
| 6   | F     | 307 | CLA  | 3       | 0            |
| 6   | D     | 317 | CLA  | 10      | 0            |
| 5   | B     | 313 | CHL  | 6       | 0            |
| 5   | C     | 313 | CHL  | 10      | 0            |
| 6   | C     | 314 | CLA  | 3       | 0            |
| 5   | D     | 309 | CHL  | 2       | 0            |
| 5   | C     | 318 | CHL  | 3       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | C     | 311 | CHL  | 3       | 0            |
| 5   | B     | 312 | CHL  | 9       | 0            |
| 6   | D     | 307 | CLA  | 2       | 0            |
| 5   | E     | 311 | CHL  | 6       | 0            |
| 5   | D     | 313 | CHL  | 12      | 0            |
| 5   | E     | 305 | CHL  | 5       | 0            |
| 5   | B     | 306 | CHL  | 2       | 0            |
| 6   | A     | 314 | CLA  | 4       | 0            |
| 6   | F     | 306 | CLA  | 8       | 0            |
| 5   | A     | 318 | CHL  | 1       | 0            |
| 6   | A     | 308 | CLA  | 3       | 0            |
| 6   | B     | 316 | CLA  | 2       | 0            |
| 9   | C     | 321 | OUR  | 3       | 0            |
| 6   | E     | 306 | CLA  | 4       | 0            |
| 7   | E     | 318 | LHG  | 7       | 0            |
| 3   | C     | 303 | NEX  | 4       | 0            |
| 5   | F     | 311 | CHL  | 3       | 0            |
| 7   | F     | 318 | LHG  | 8       | 0            |
| 6   | E     | 316 | CLA  | 6       | 0            |
| 6   | A     | 307 | CLA  | 5       | 0            |
| 6   | A     | 317 | CLA  | 5       | 0            |
| 7   | B     | 324 | LHG  | 8       | 0            |
| 5   | F     | 305 | CHL  | 7       | 0            |
| 6   | B     | 309 | CLA  | 1       | 0            |
| 6   | E     | 315 | CLA  | 2       | 0            |
| 2   | E     | 302 | OIE  | 1       | 0            |
| 5   | E     | 312 | CHL  | 8       | 0            |
| 5   | B     | 319 | CHL  | 3       | 0            |
| 6   | B     | 308 | CLA  | 5       | 0            |
| 5   | D     | 306 | CHL  | 5       | 0            |
| 6   | F     | 316 | CLA  | 5       | 0            |
| 6   | E     | 313 | CLA  | 3       | 0            |
| 6   | C     | 315 | CLA  | 3       | 0            |
| 6   | D     | 316 | CLA  | 3       | 0            |
| 2   | C     | 302 | OIE  | 2       | 0            |
| 11  | F     | 319 | LMG  | 1       | 0            |
| 2   | B     | 301 | OIE  | 1       | 0            |
| 5   | A     | 306 | CHL  | 5       | 0            |
| 5   | A     | 311 | CHL  | 4       | 0            |
| 6   | B     | 317 | CLA  | 1       | 0            |
| 5   | E     | 317 | CHL  | 3       | 0            |
| 6   | D     | 315 | CLA  | 3       | 0            |

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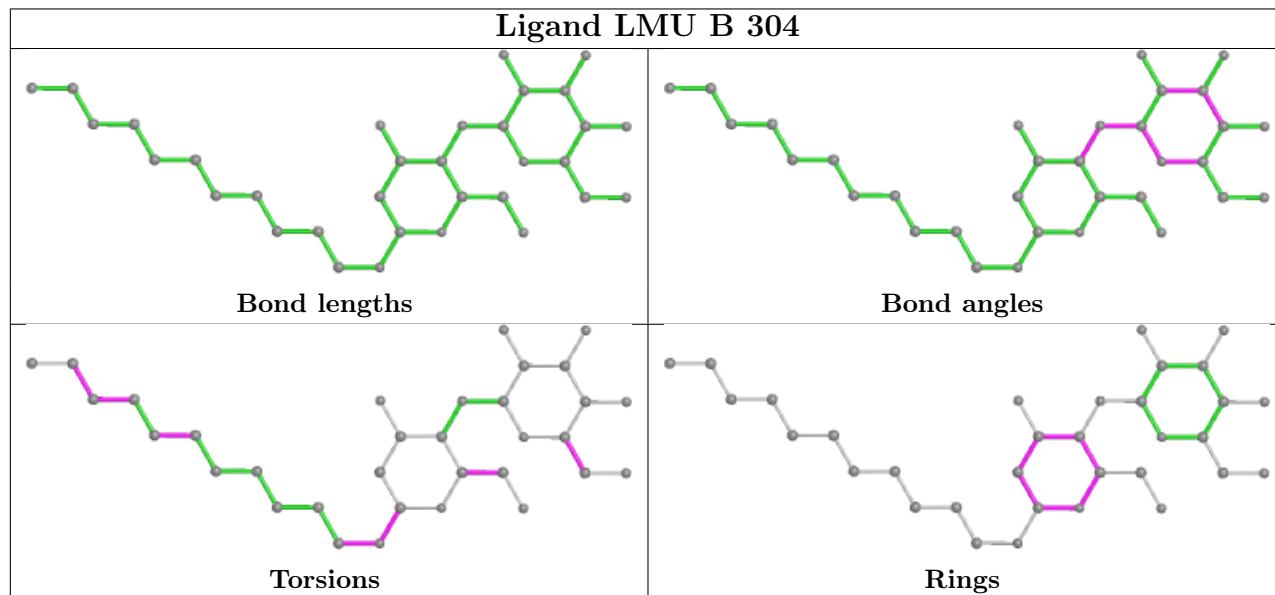
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | A     | 313 | CHL  | 6       | 0            |
| 3   | E     | 303 | NEX  | 3       | 0            |
| 6   | F     | 315 | CLA  | 2       | 0            |
| 3   | F     | 303 | NEX  | 2       | 0            |
| 5   | F     | 312 | CHL  | 5       | 0            |
| 5   | D     | 318 | CHL  | 1       | 0            |
| 2   | C     | 301 | OIE  | 1       | 0            |
| 7   | B     | 320 | LHG  | 5       | 0            |
| 3   | B     | 303 | NEX  | 4       | 0            |
| 6   | E     | 314 | CLA  | 3       | 0            |
| 6   | F     | 313 | CLA  | 7       | 0            |
| 5   | D     | 305 | CHL  | 3       | 0            |
| 6   | E     | 307 | CLA  | 4       | 0            |
| 6   | C     | 307 | CLA  | 11      | 0            |
| 5   | B     | 311 | CHL  | 4       | 0            |
| 5   | E     | 309 | CHL  | 3       | 0            |
| 5   | F     | 309 | CHL  | 2       | 0            |
| 5   | E     | 310 | CHL  | 3       | 0            |
| 5   | F     | 317 | CHL  | 2       | 0            |
| 6   | C     | 316 | CLA  | 4       | 0            |
| 10  | B     | 322 | BET  | 1       | 0            |
| 5   | D     | 311 | CHL  | 9       | 0            |
| 5   | A     | 305 | CHL  | 6       | 0            |
| 6   | A     | 316 | CLA  | 3       | 0            |
| 6   | C     | 317 | CLA  | 7       | 0            |
| 5   | C     | 306 | CHL  | 4       | 0            |
| 5   | C     | 310 | CHL  | 4       | 0            |
| 6   | B     | 315 | CLA  | 7       | 0            |
| 7   | D     | 319 | LHG  | 5       | 0            |
| 4   | D     | 304 | LMU  | 3       | 0            |
| 5   | C     | 312 | CHL  | 3       | 0            |
| 5   | B     | 307 | CHL  | 4       | 0            |
| 3   | D     | 303 | NEX  | 4       | 0            |
| 6   | B     | 318 | CLA  | 7       | 0            |
| 6   | F     | 314 | CLA  | 1       | 0            |
| 5   | A     | 310 | CHL  | 4       | 0            |
| 4   | E     | 319 | LMU  | 3       | 0            |
| 5   | B     | 314 | CHL  | 10      | 0            |
| 7   | A     | 319 | LHG  | 3       | 0            |
| 4   | A     | 304 | LMU  | 4       | 0            |
| 9   | F     | 320 | OUR  | 2       | 0            |
| 5   | F     | 304 | CHL  | 8       | 0            |

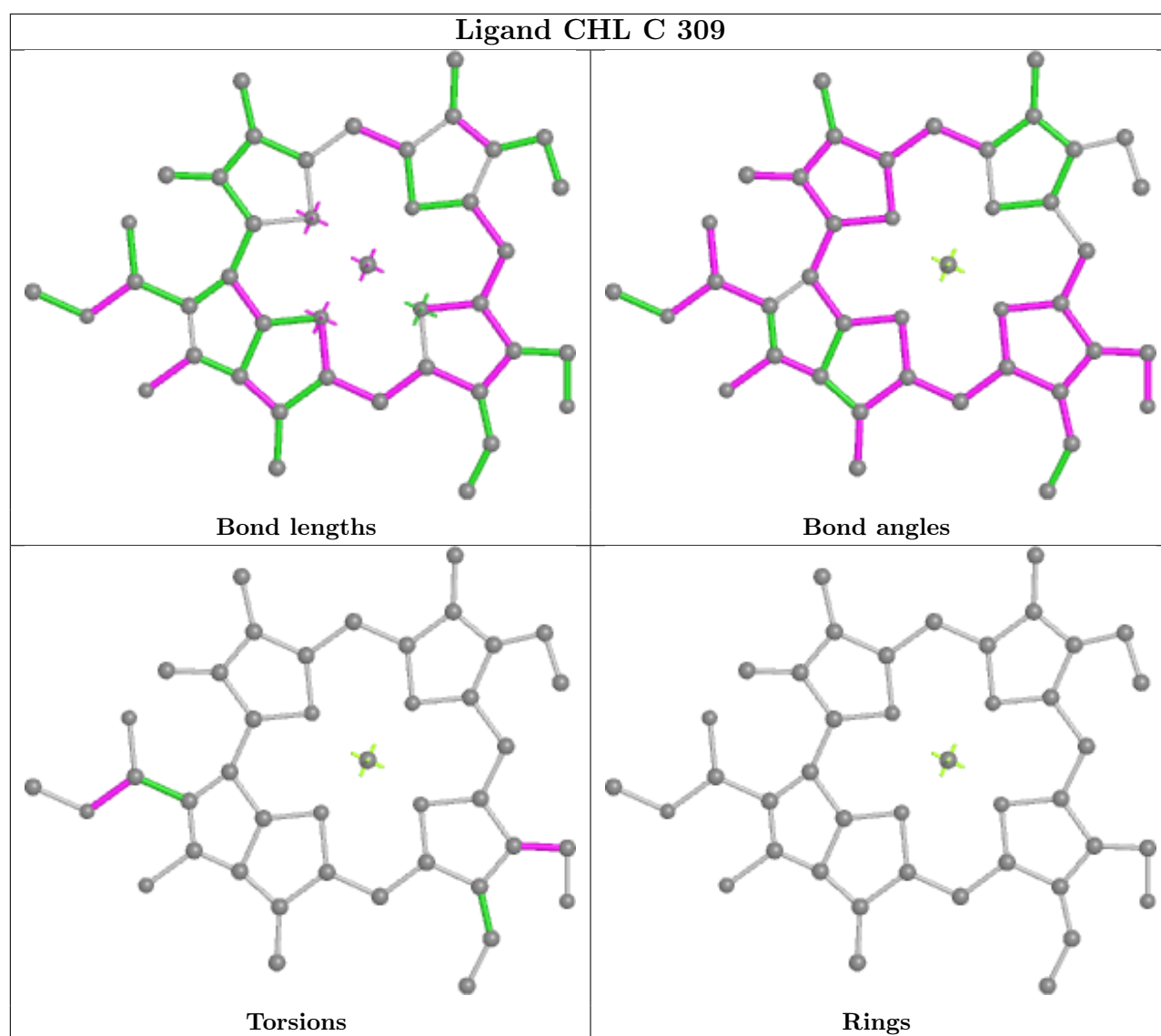
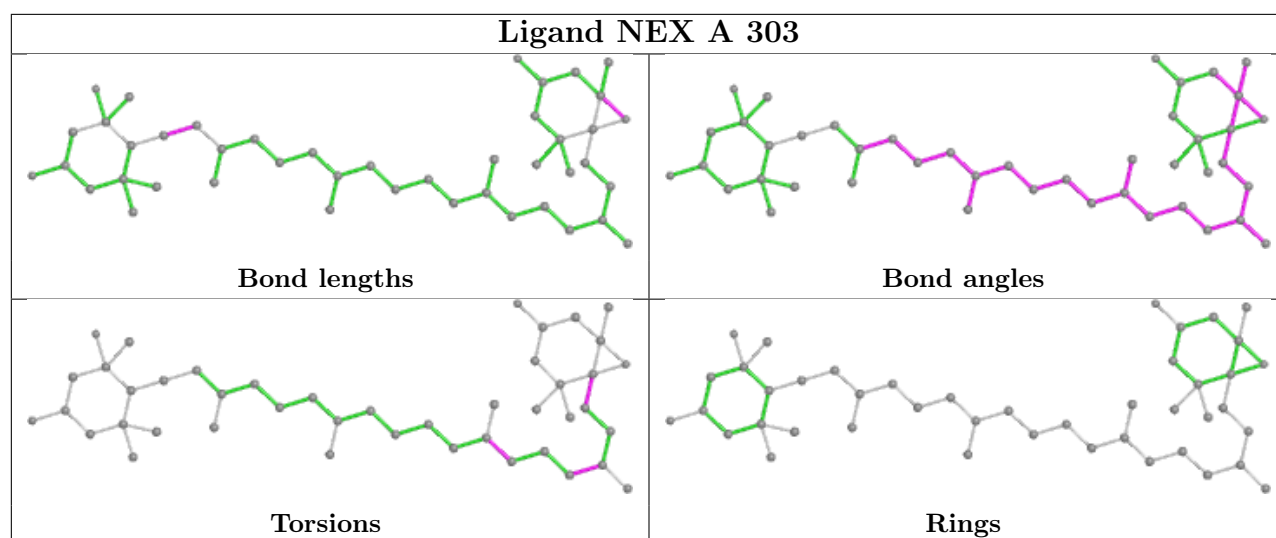
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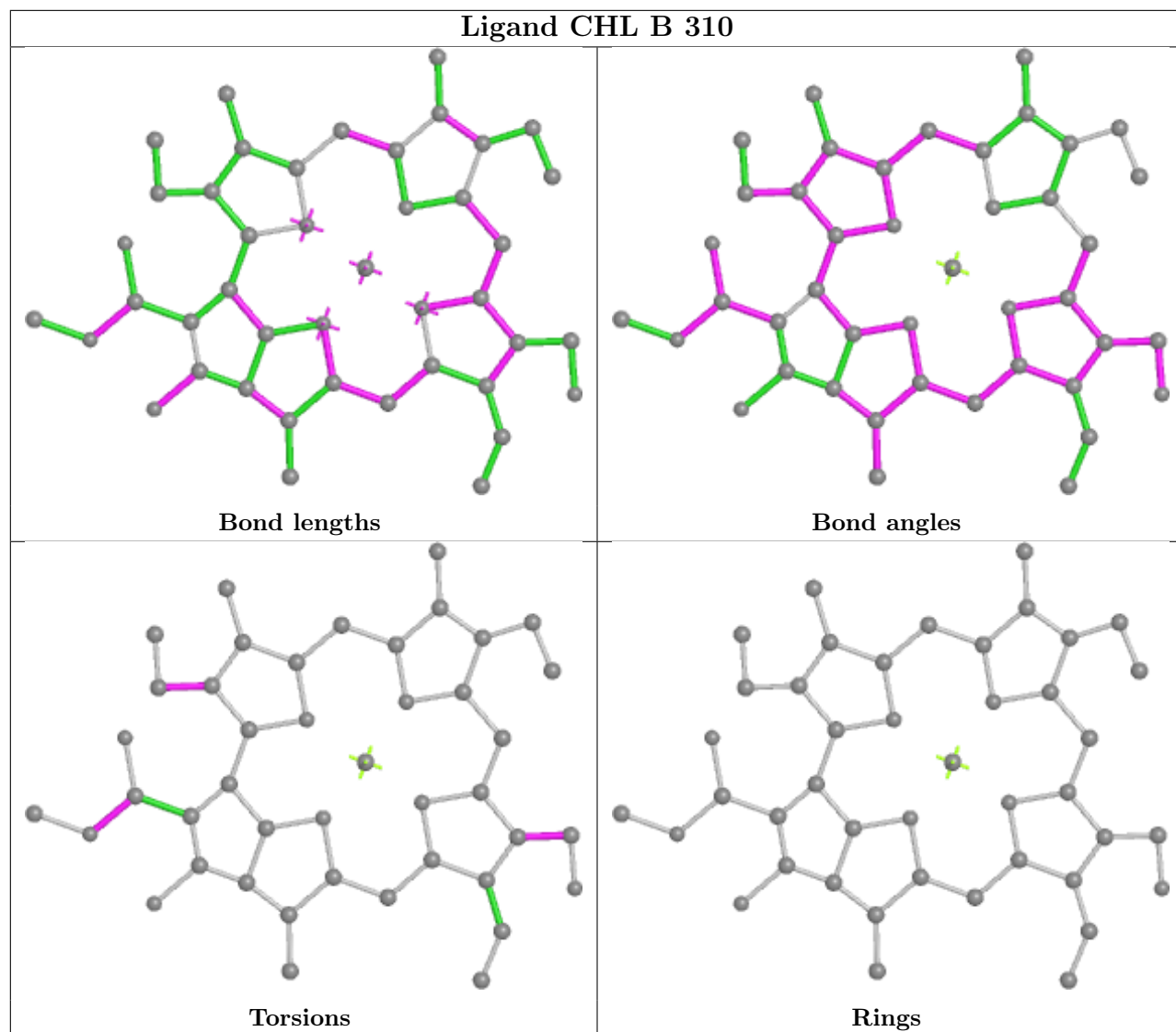
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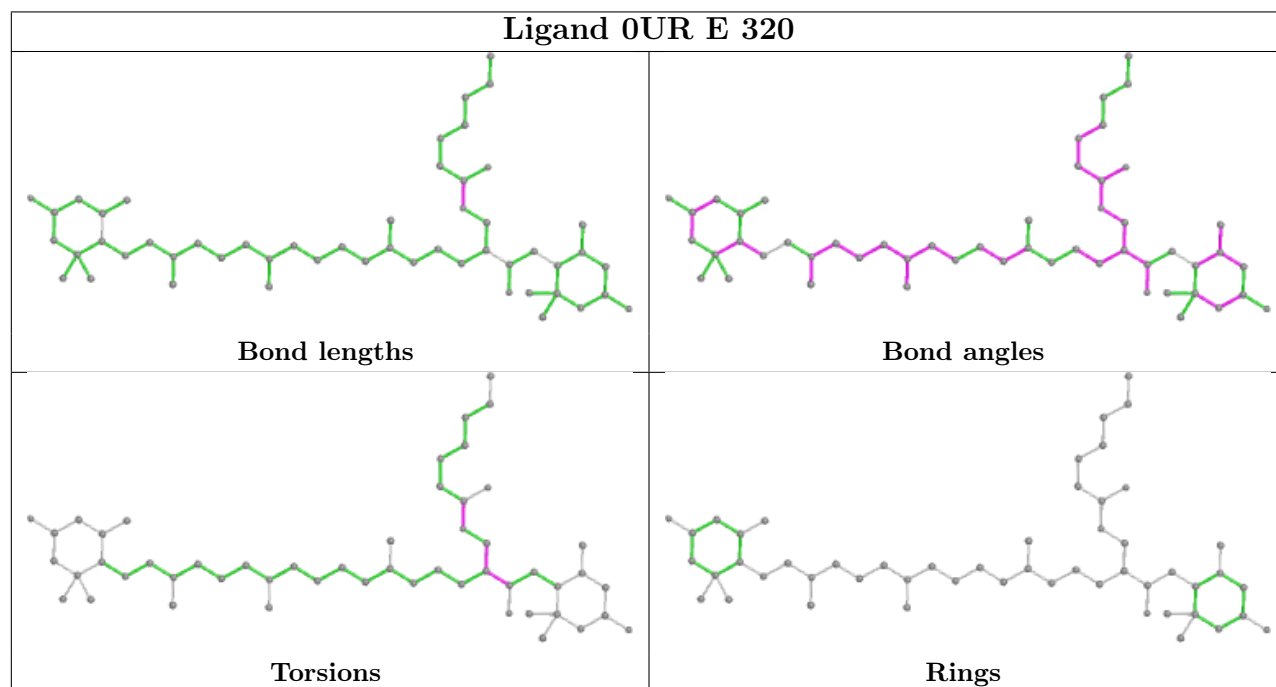
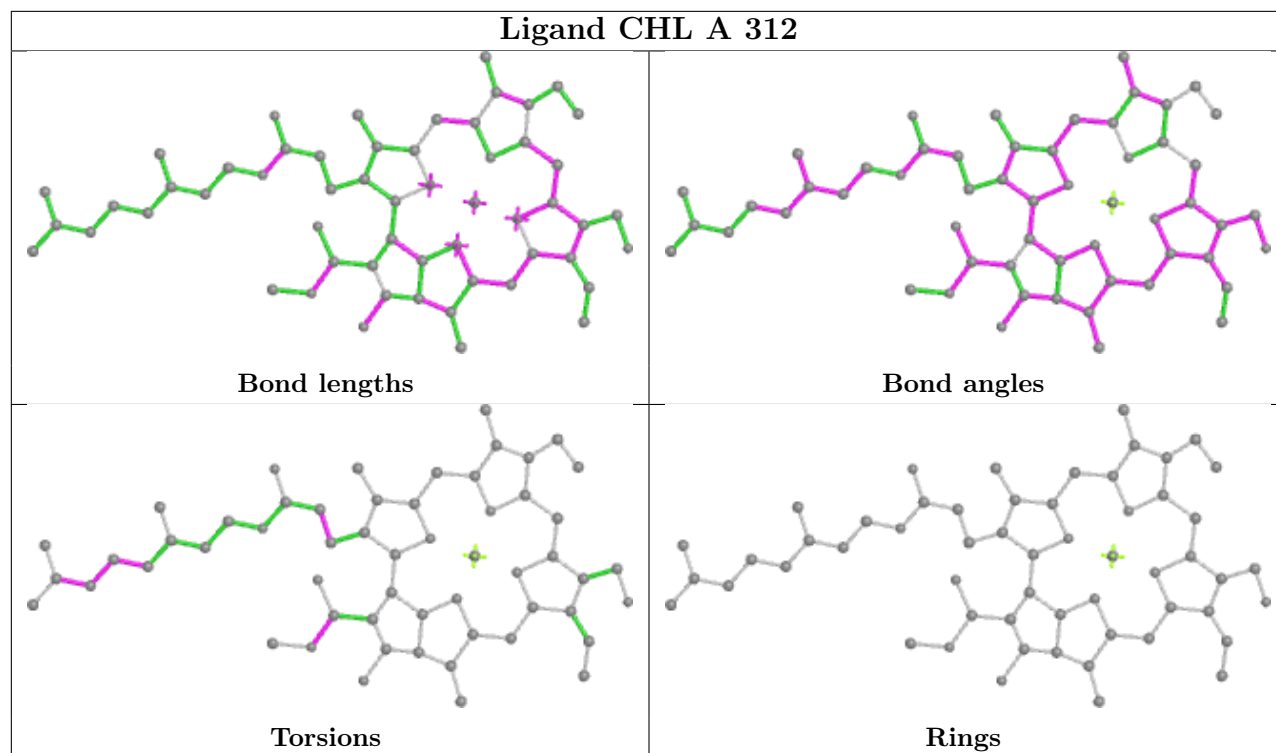
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | D     | 310 | CHL  | 5       | 0            |
| 6   | A     | 315 | CLA  | 3       | 0            |
| 6   | C     | 308 | CLA  | 3       | 0            |
| 5   | F     | 308 | CHL  | 1       | 0            |
| 2   | A     | 302 | OIE  | 1       | 0            |
| 5   | E     | 304 | CHL  | 4       | 0            |
| 5   | E     | 308 | CHL  | 3       | 0            |
| 7   | C     | 319 | LHG  | 4       | 0            |
| 4   | B     | 305 | LMU  | 1       | 0            |
| 5   | F     | 310 | CHL  | 7       | 0            |

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

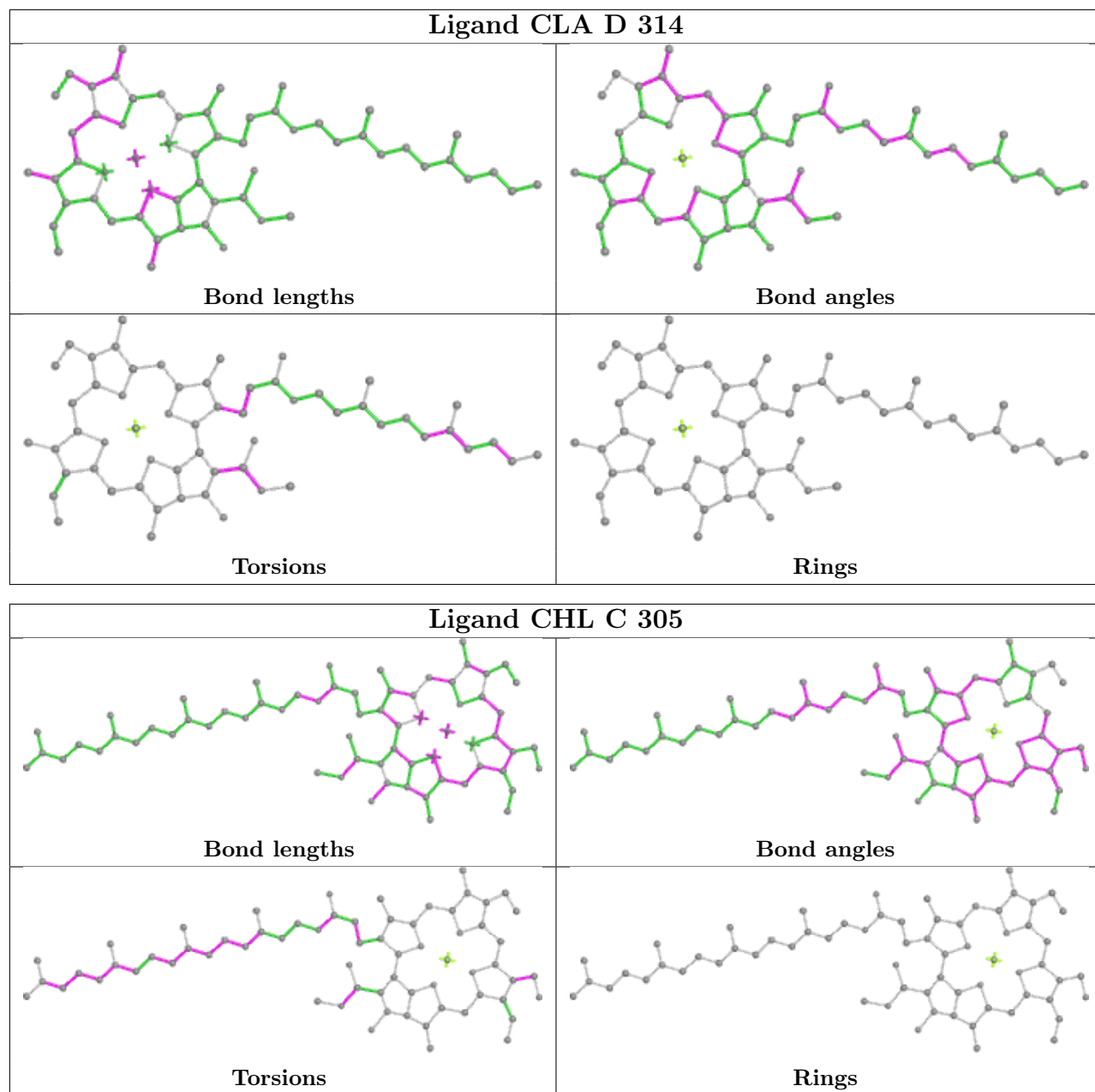


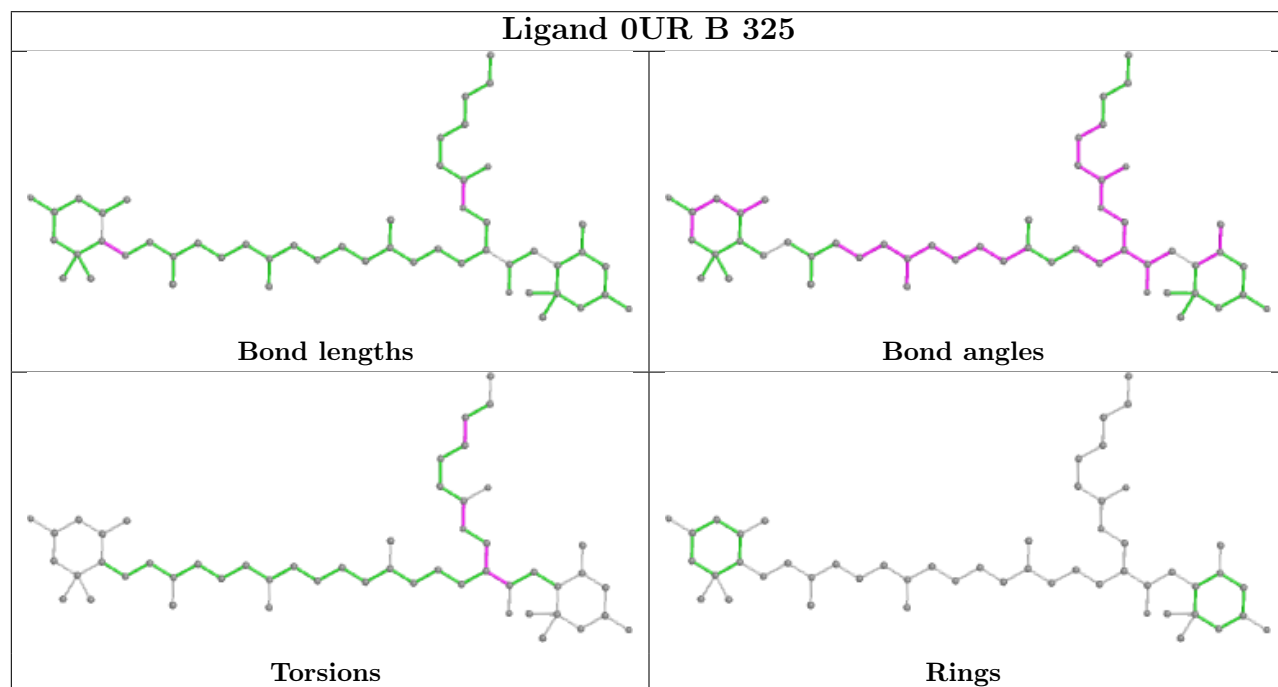
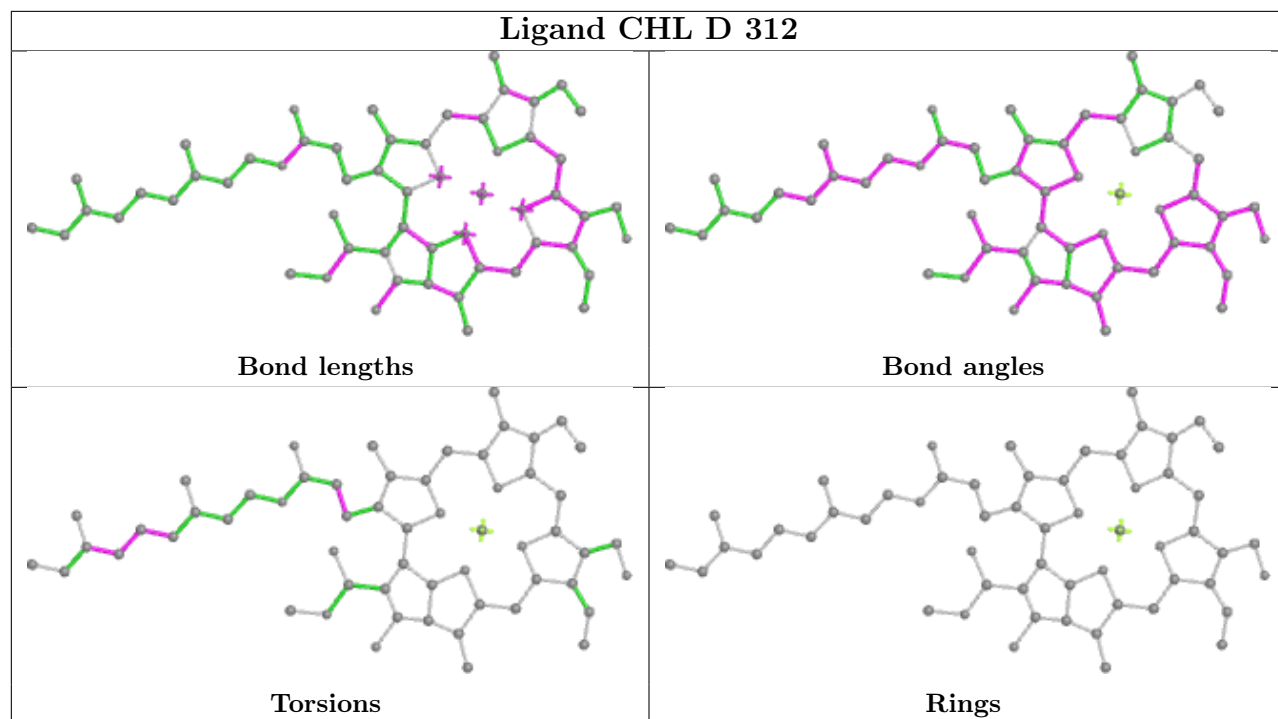


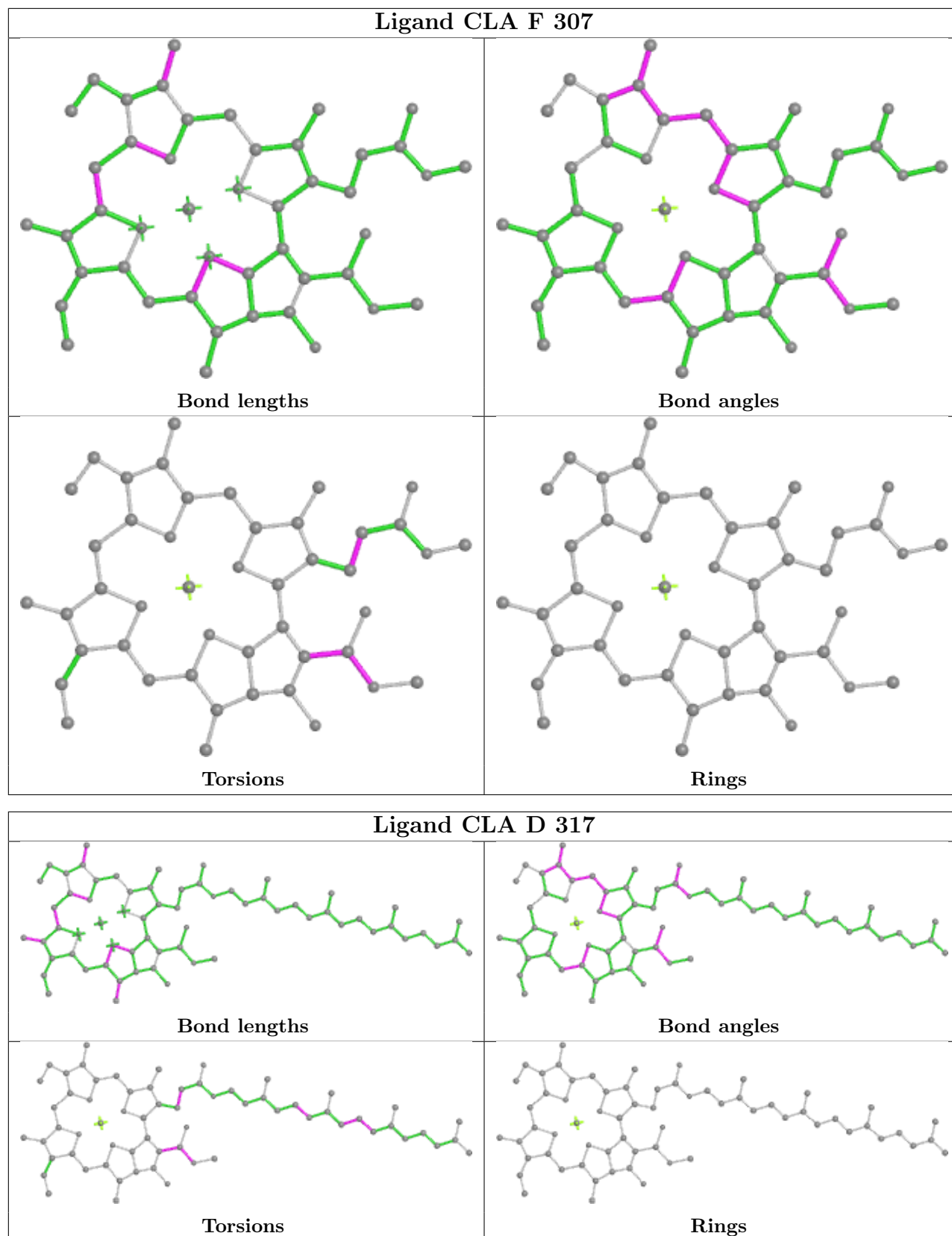


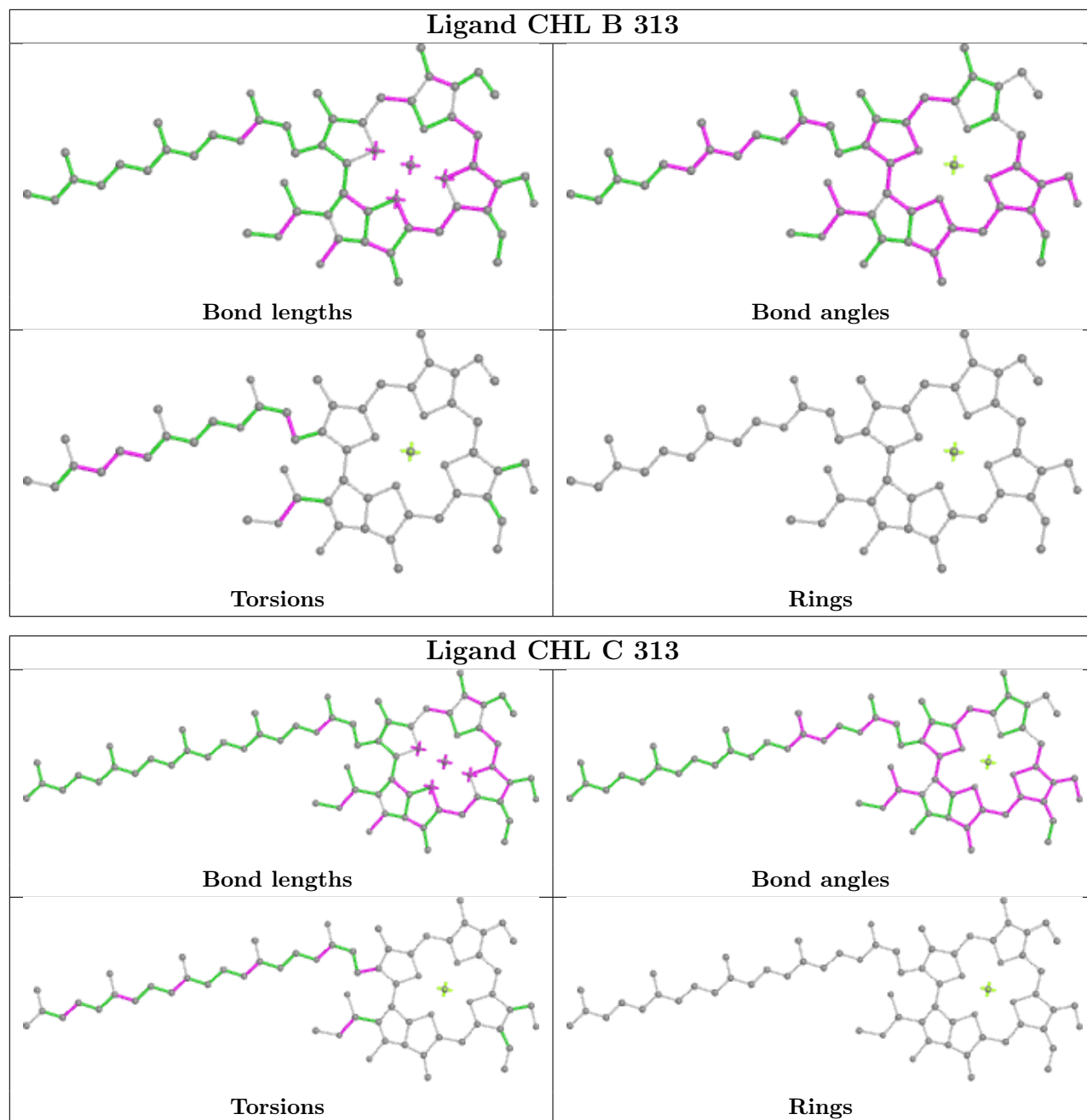


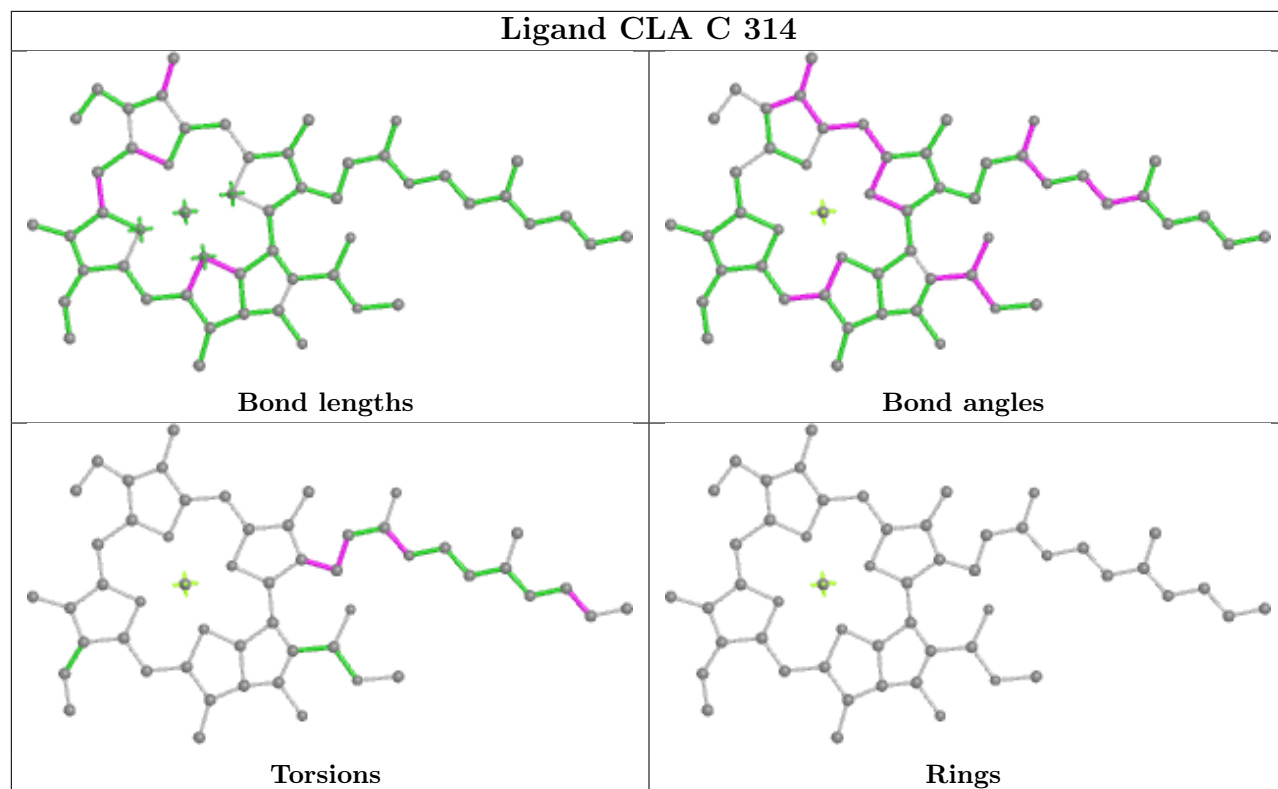


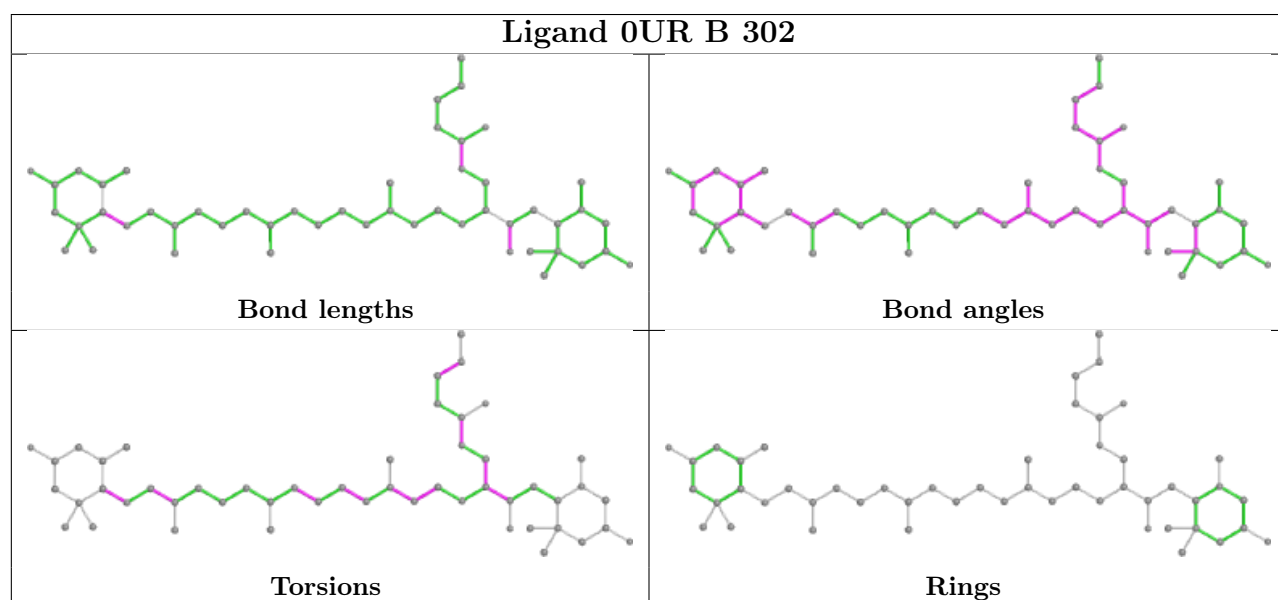
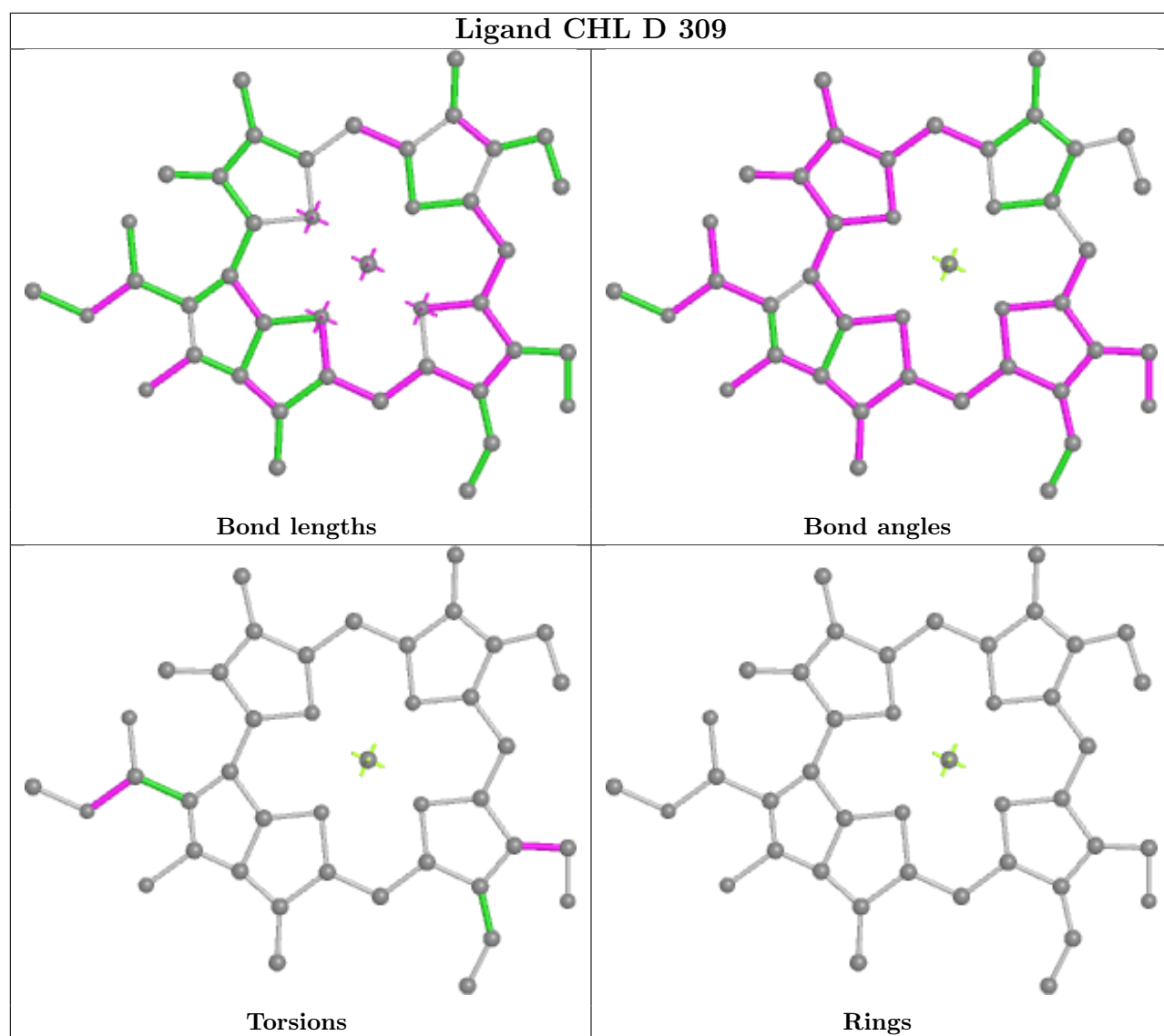


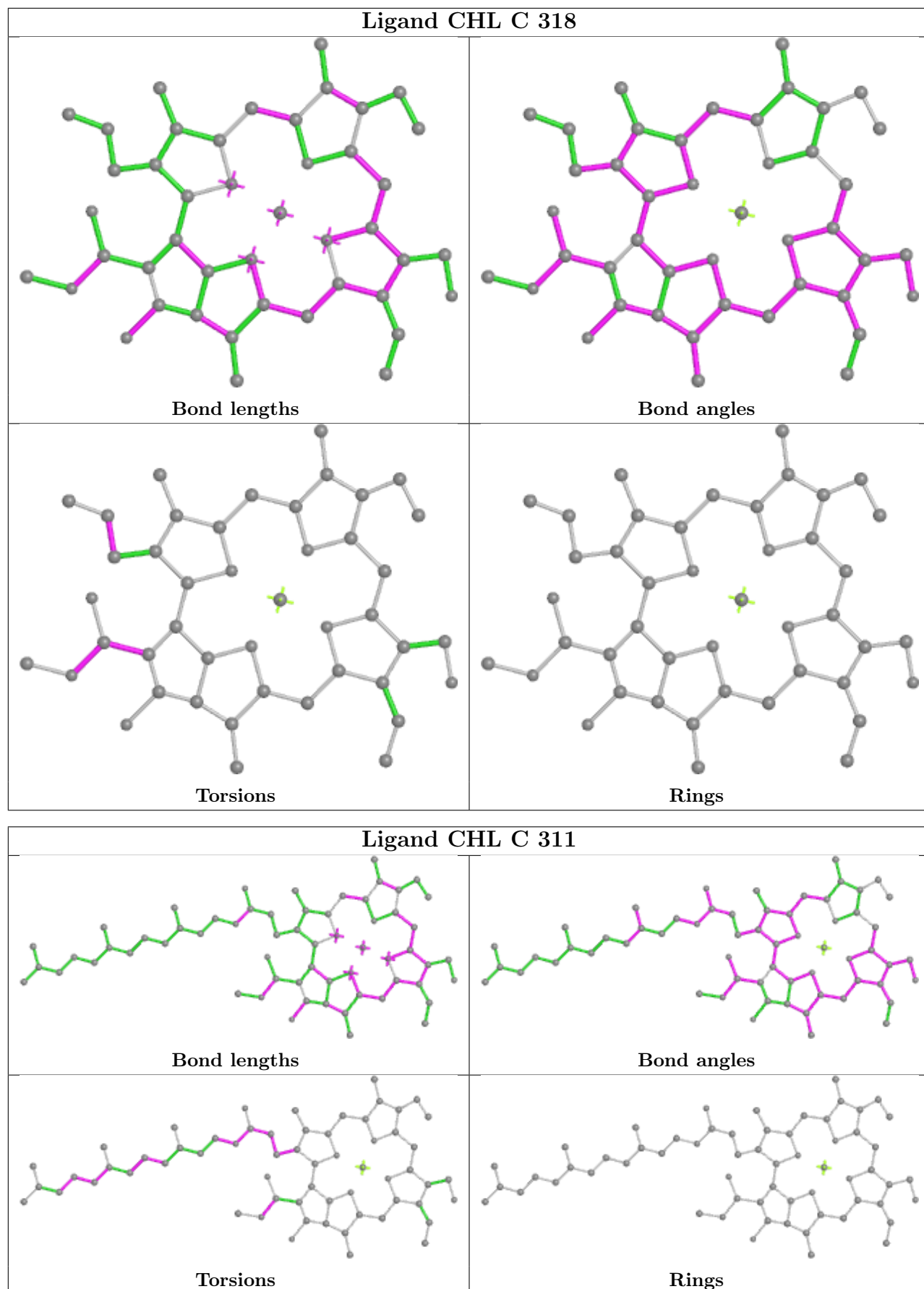


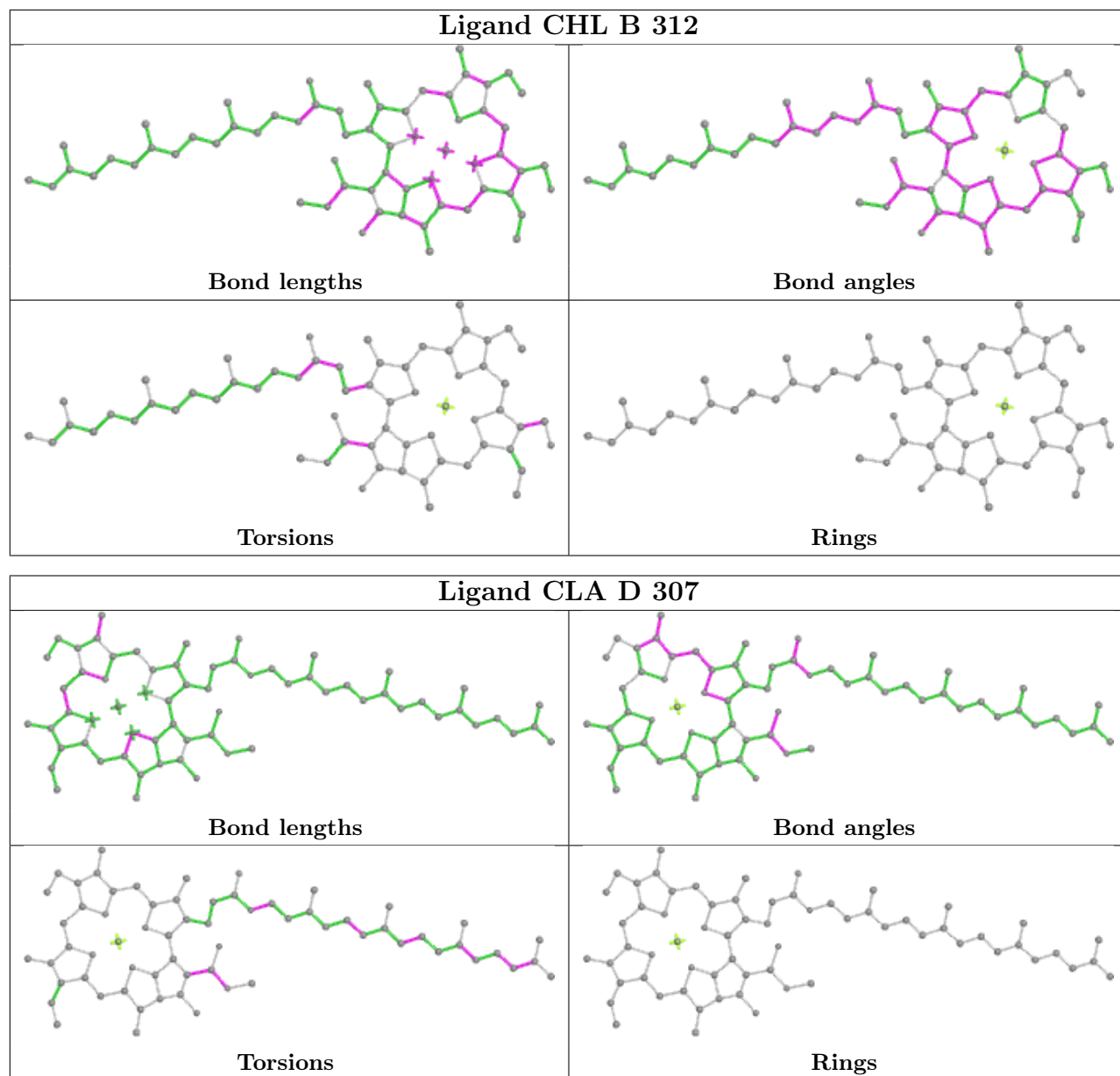




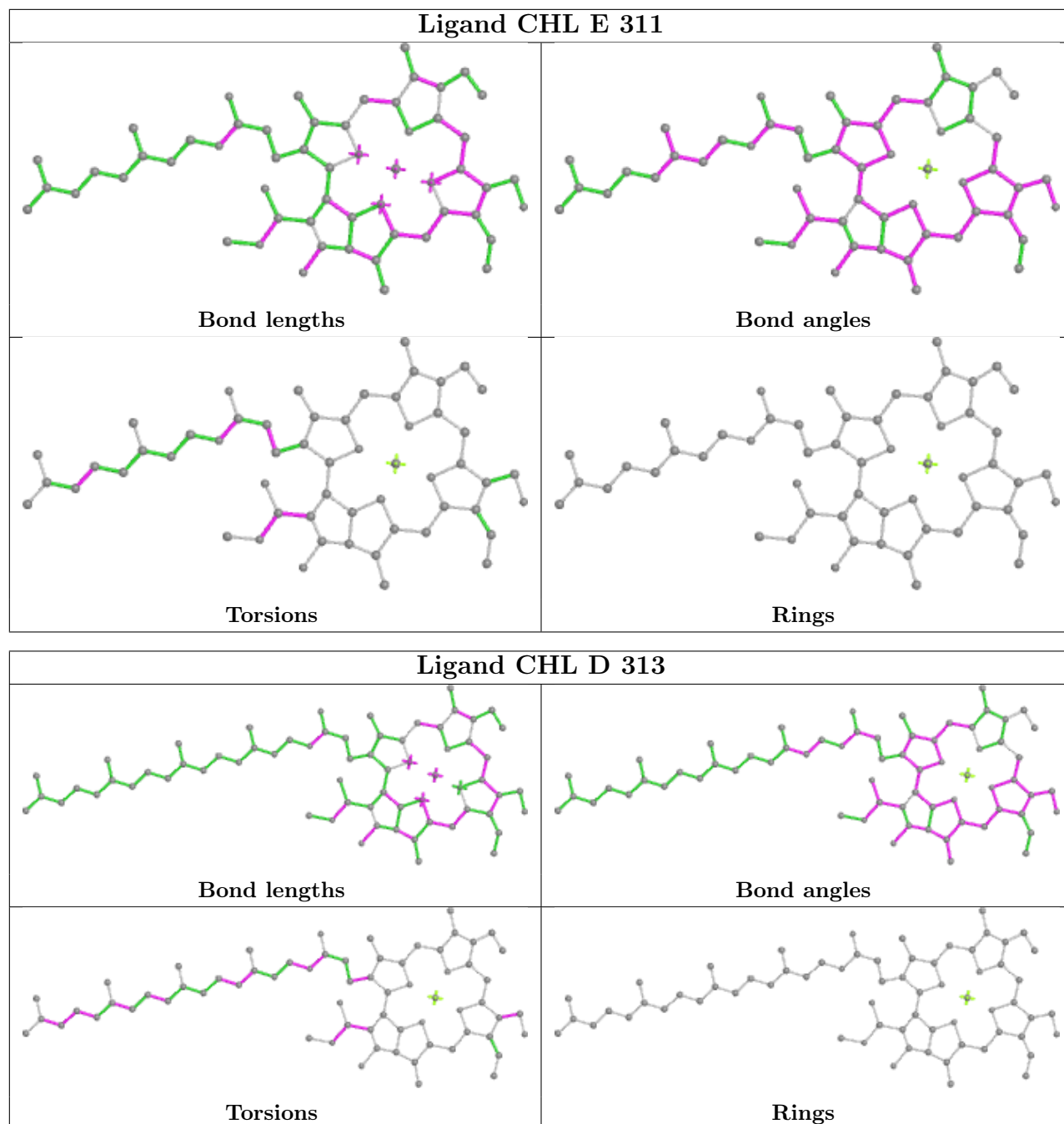


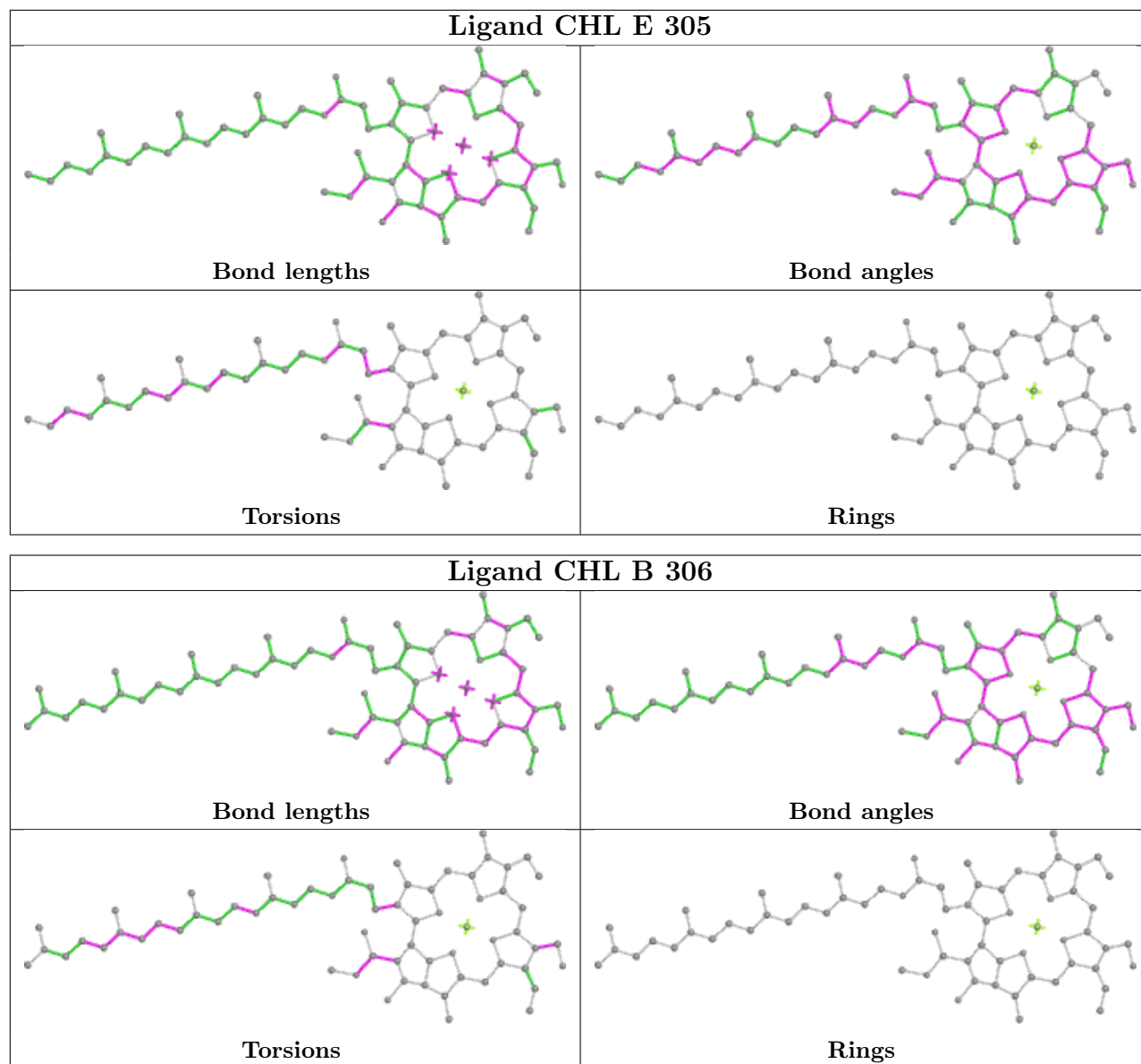


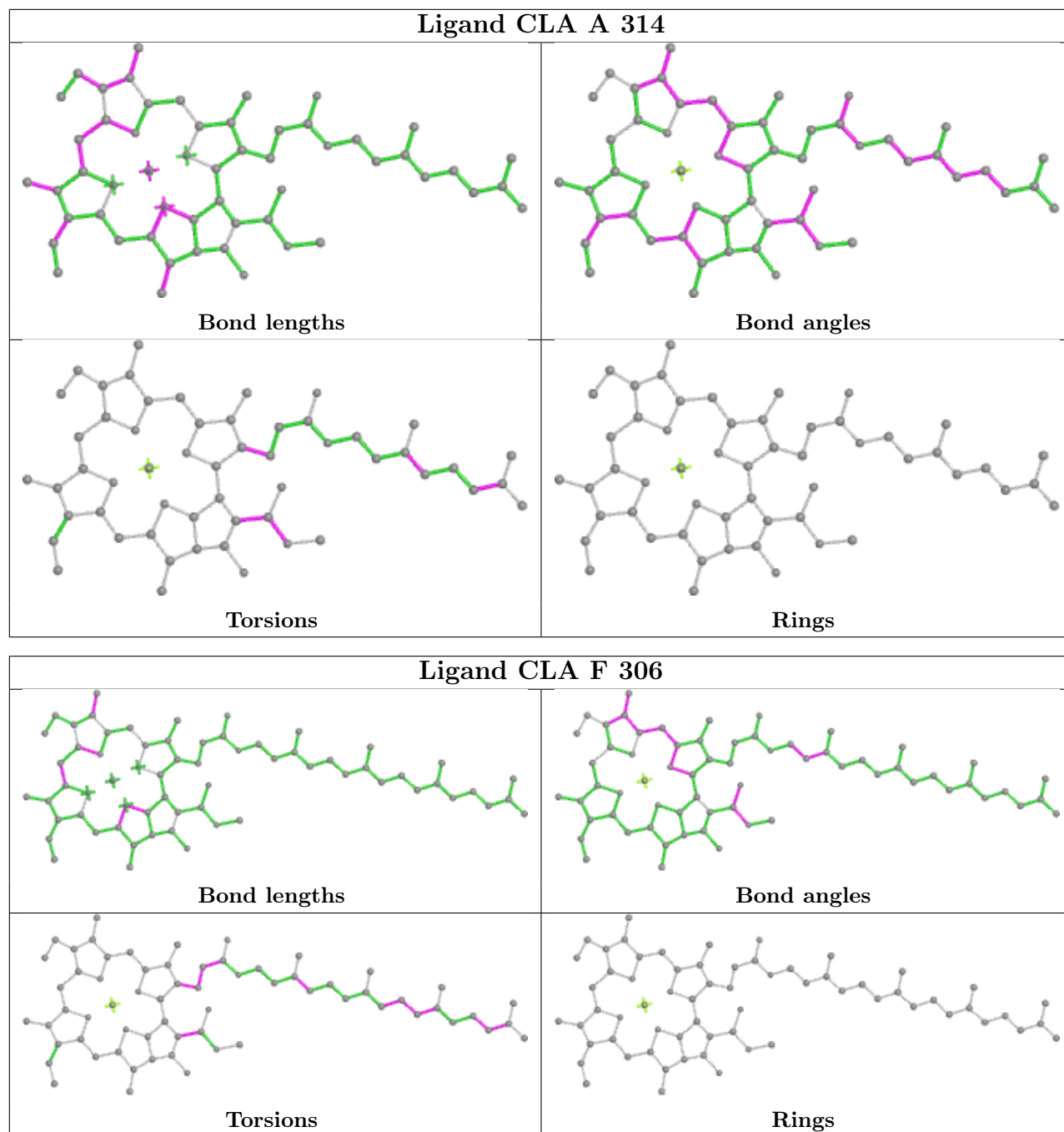


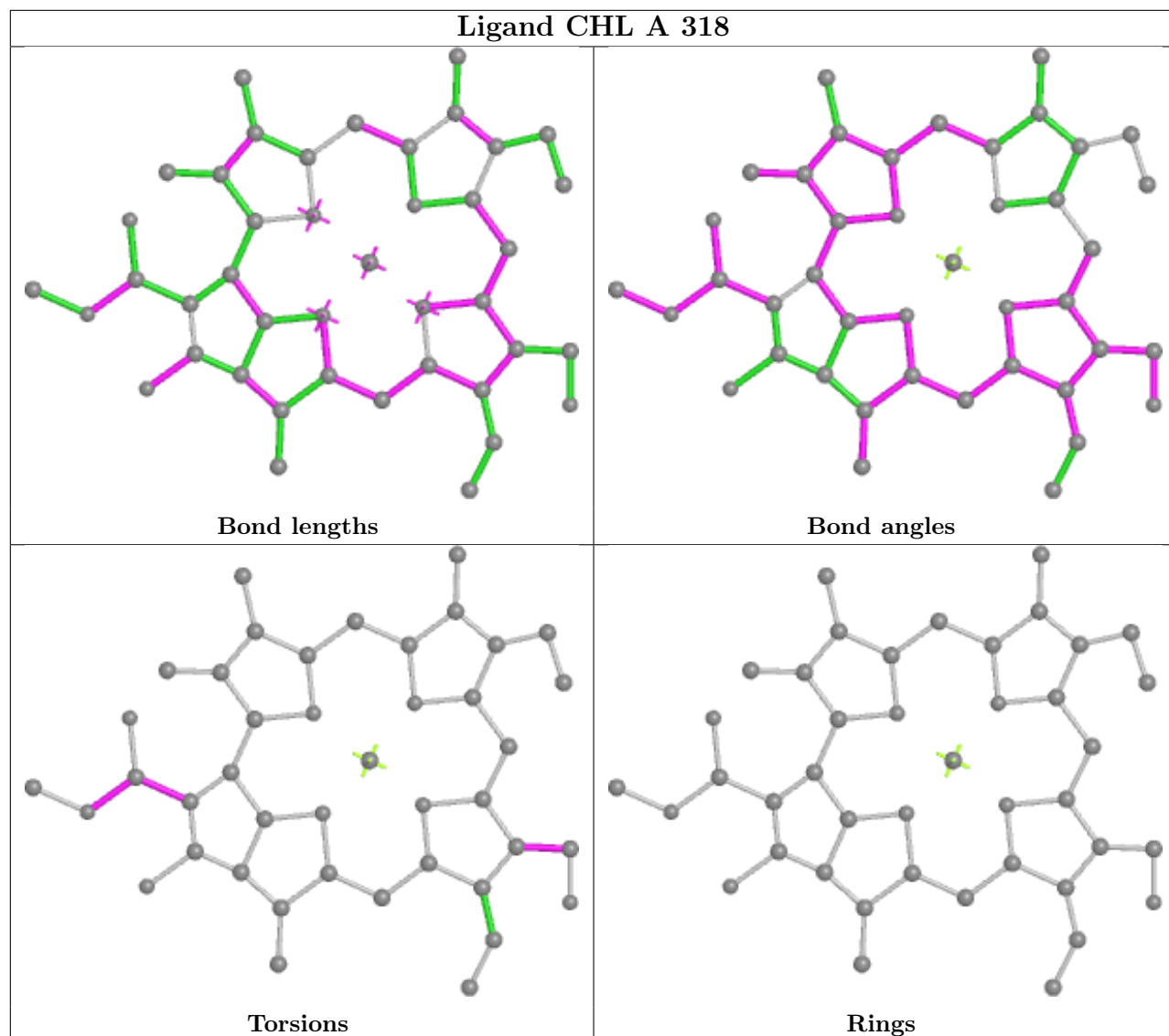


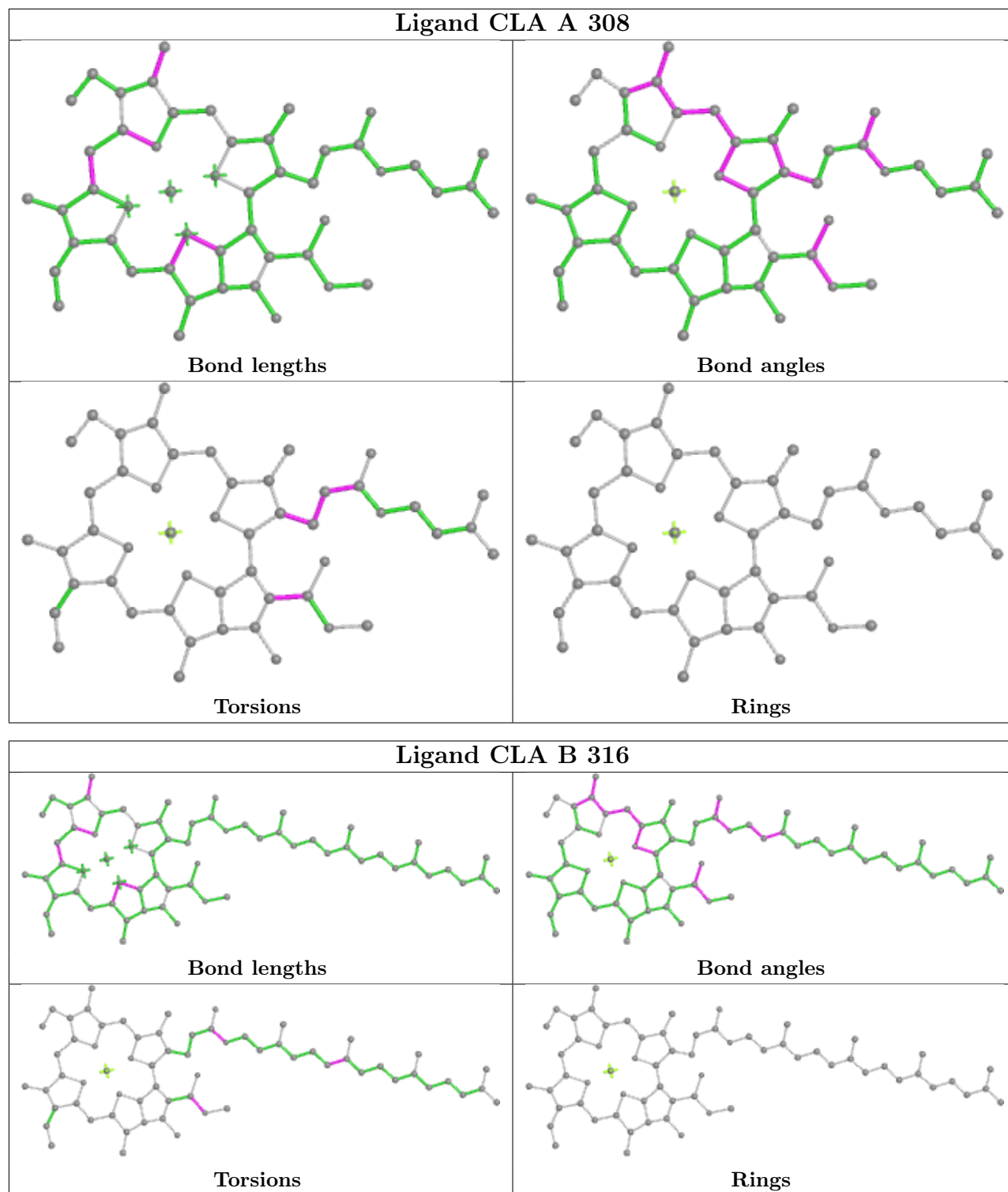


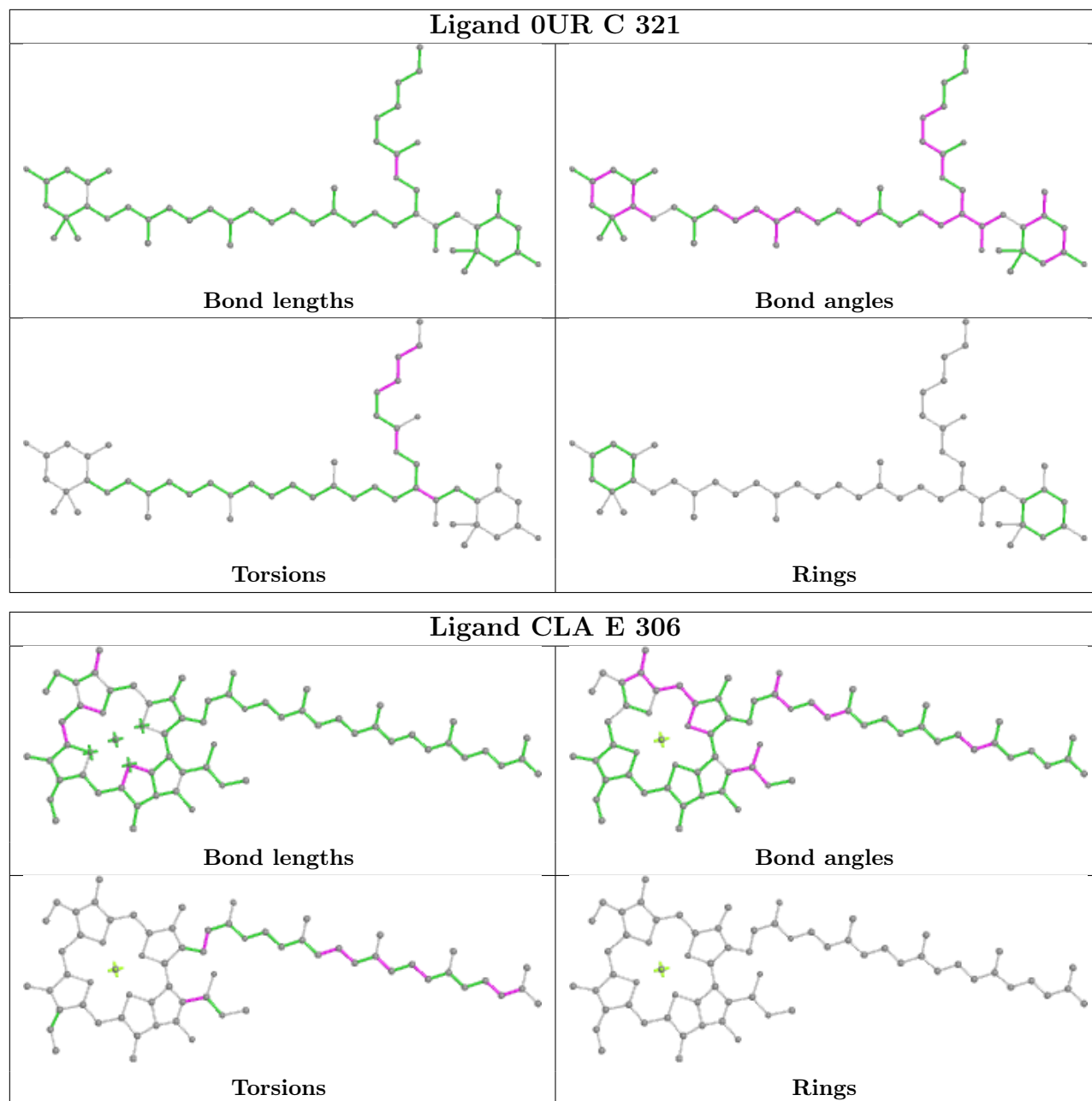


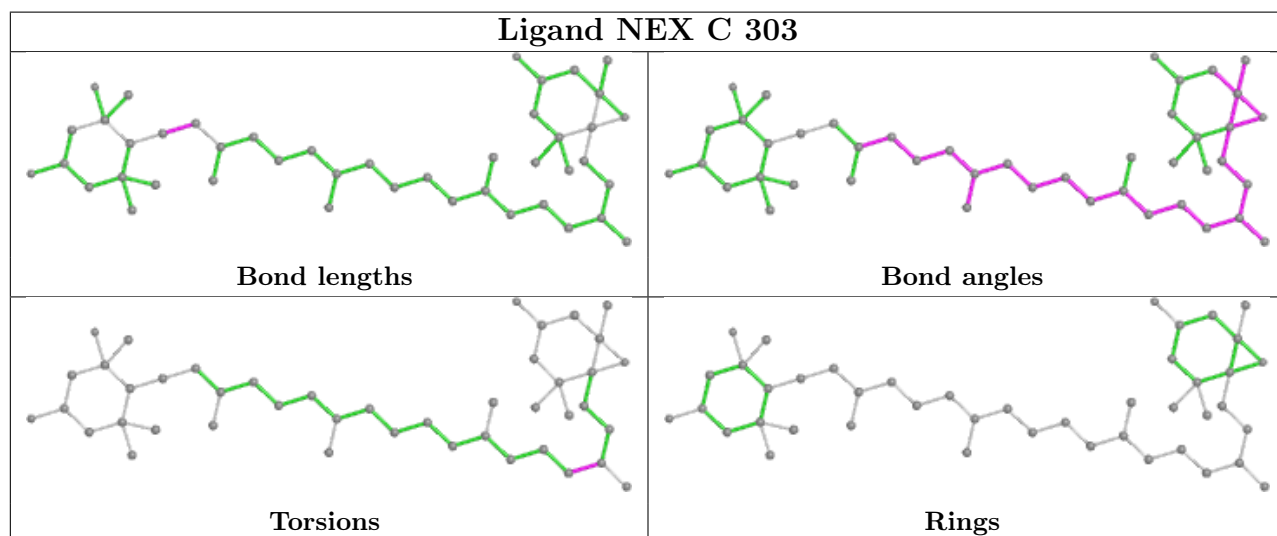
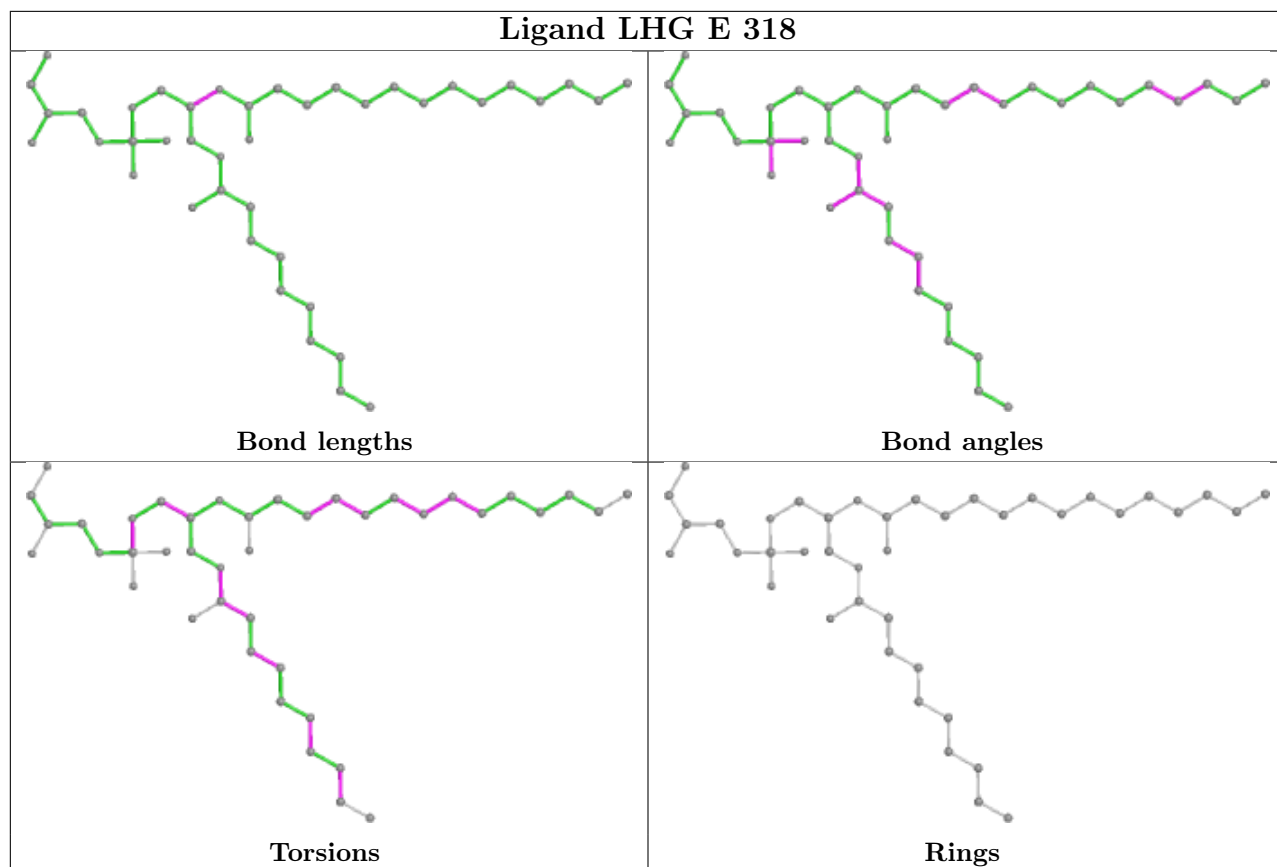


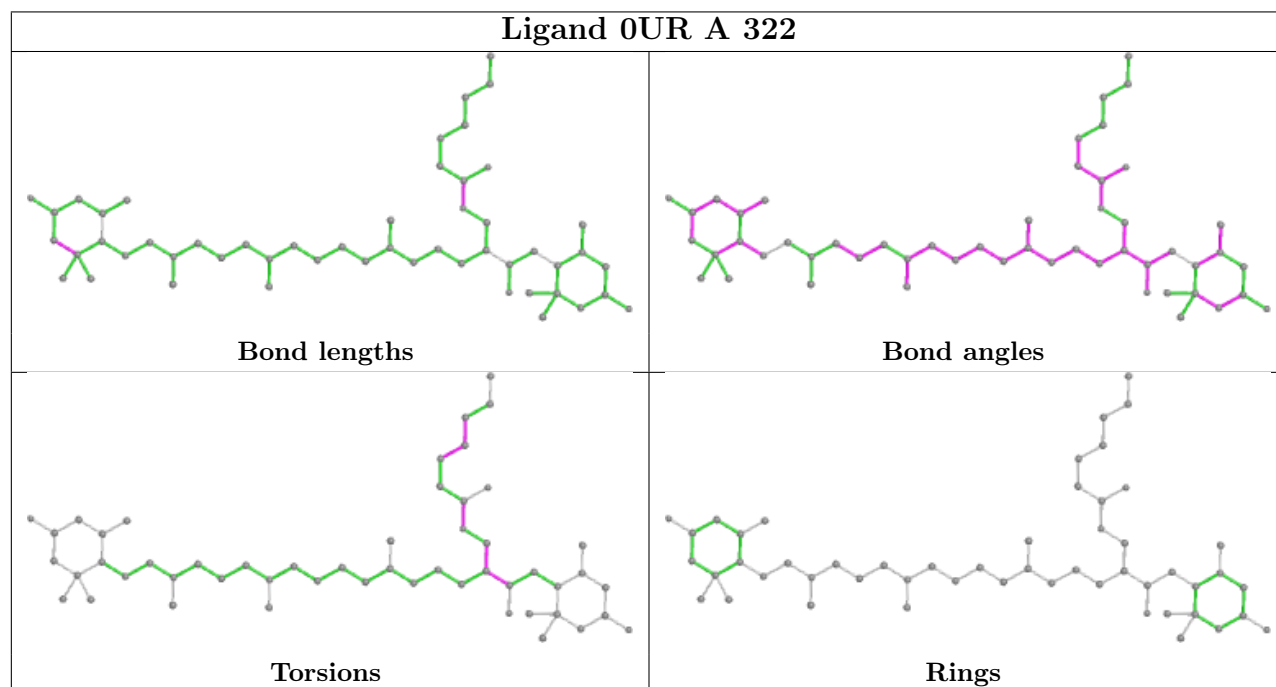
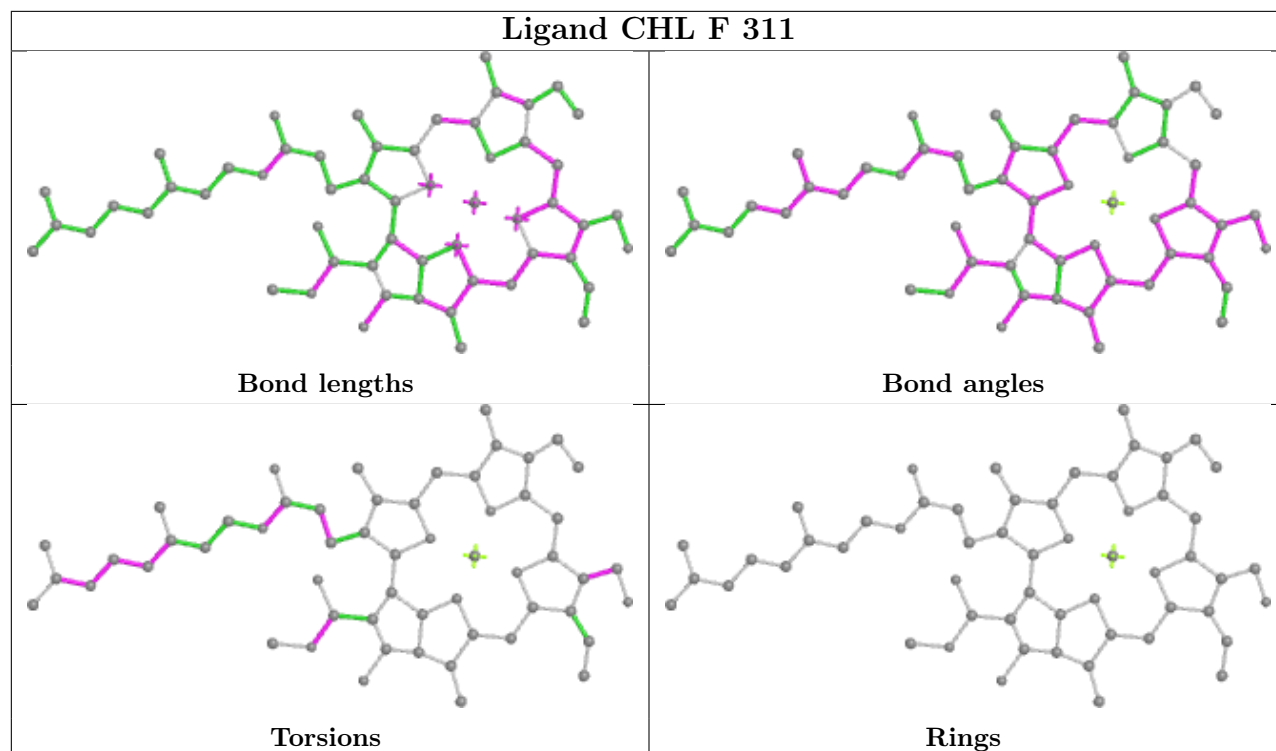




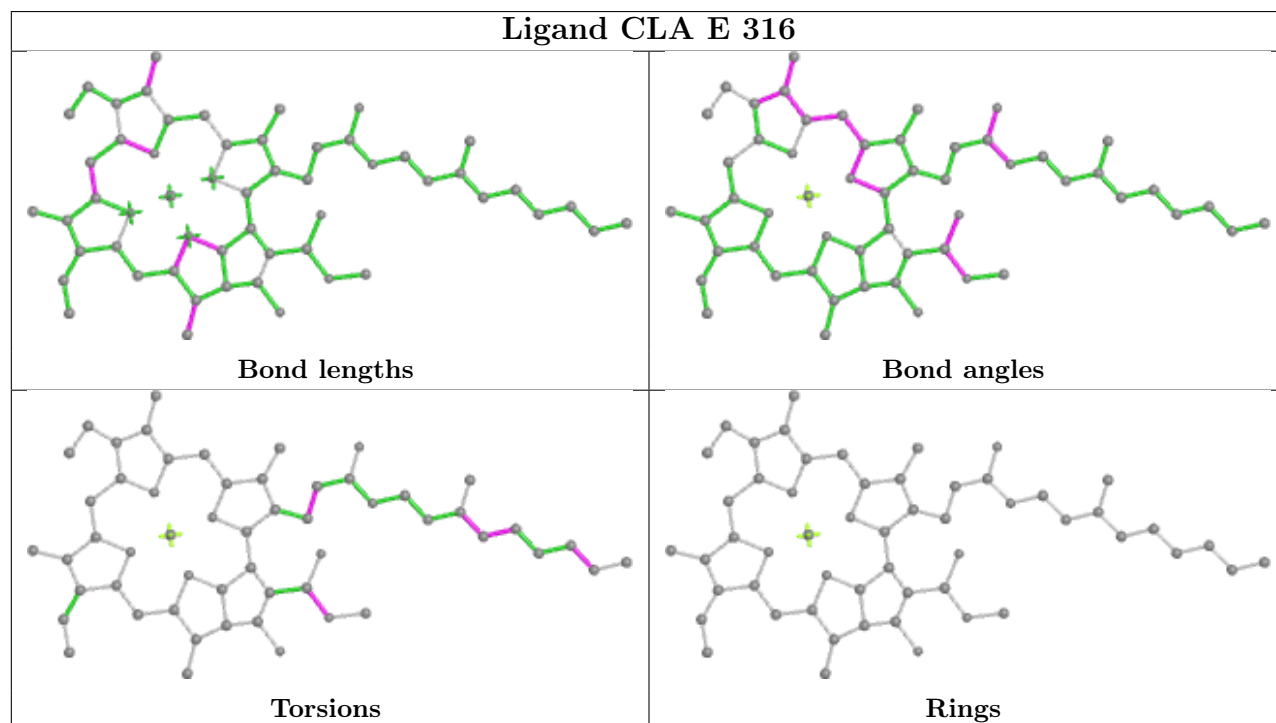
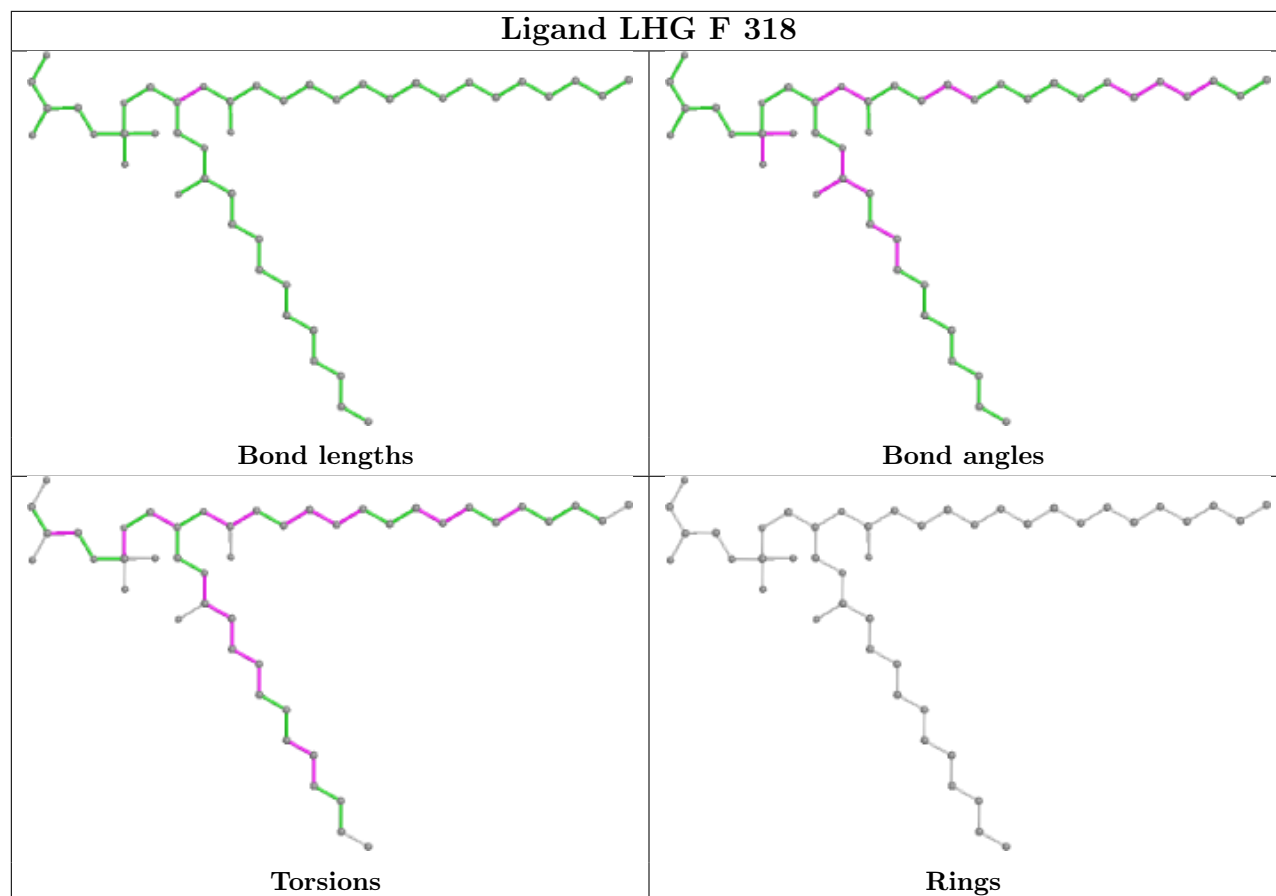


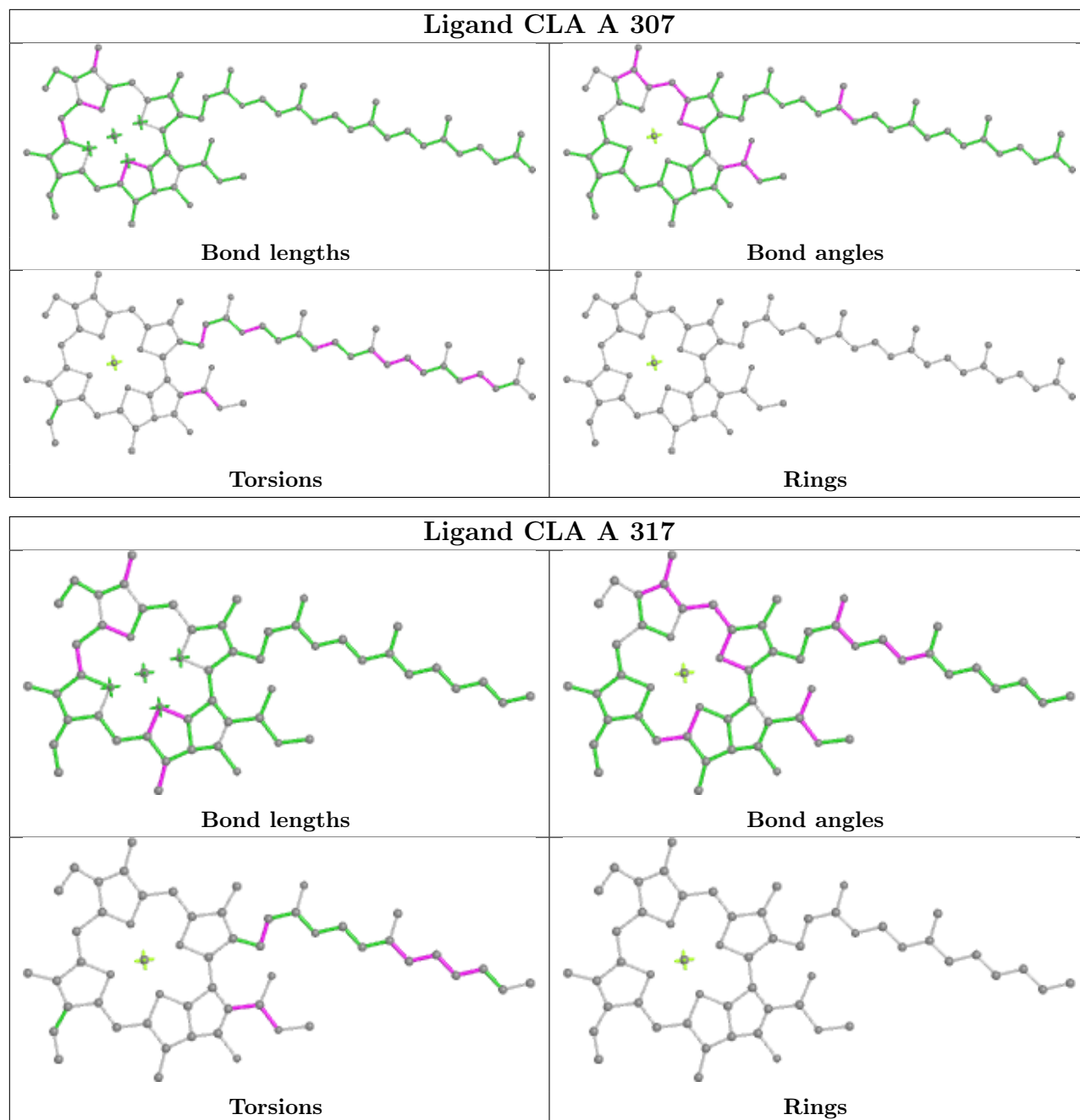


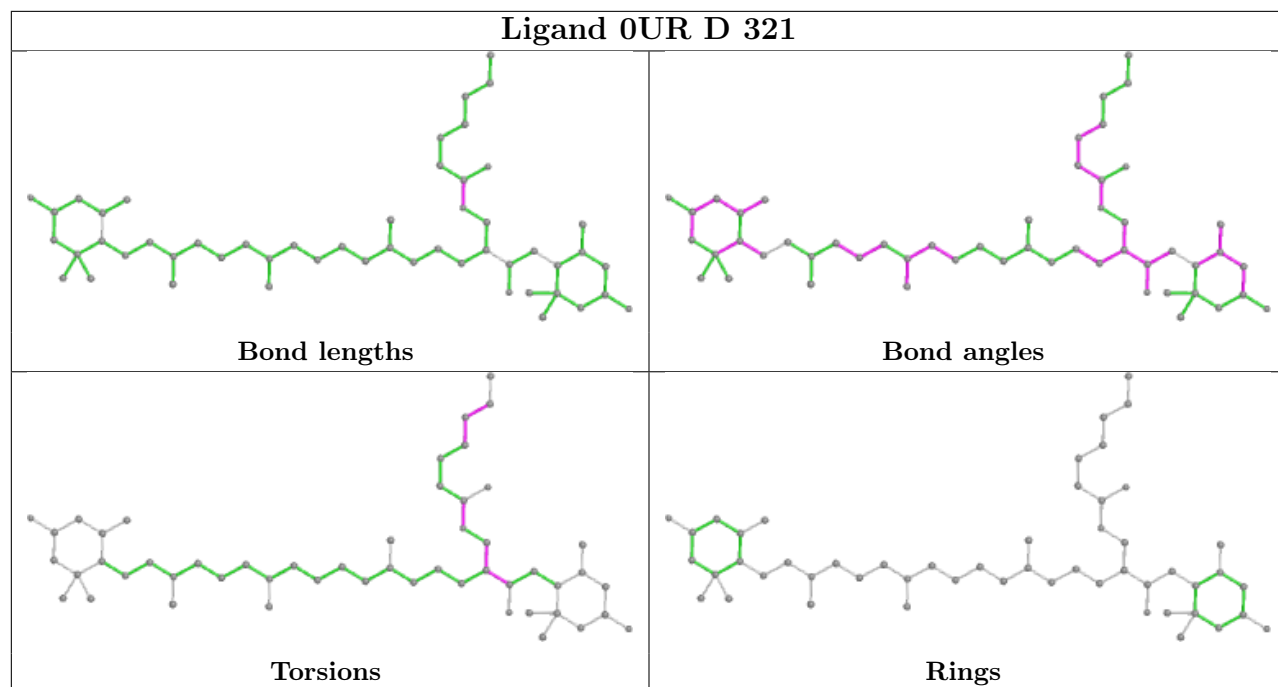


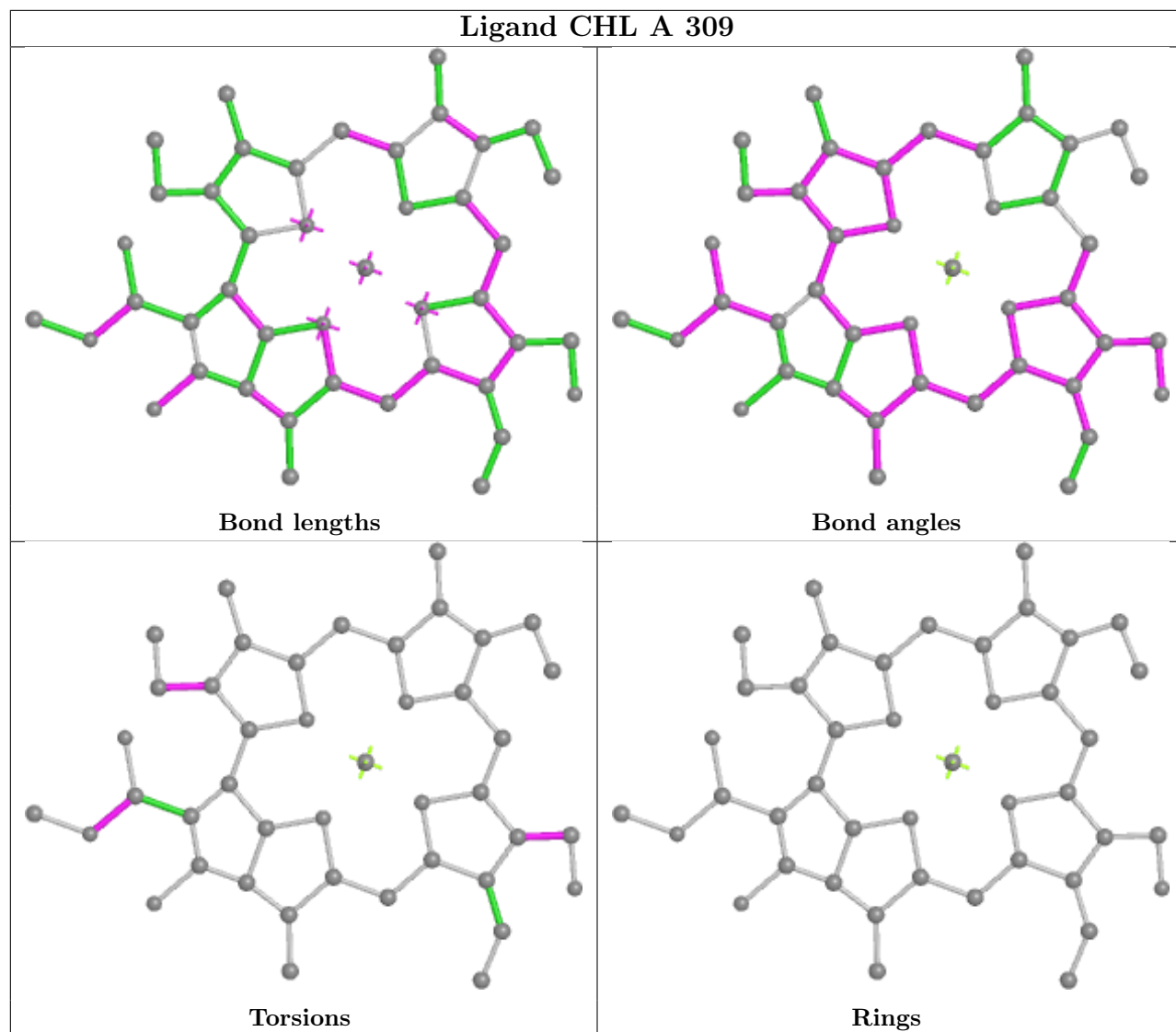


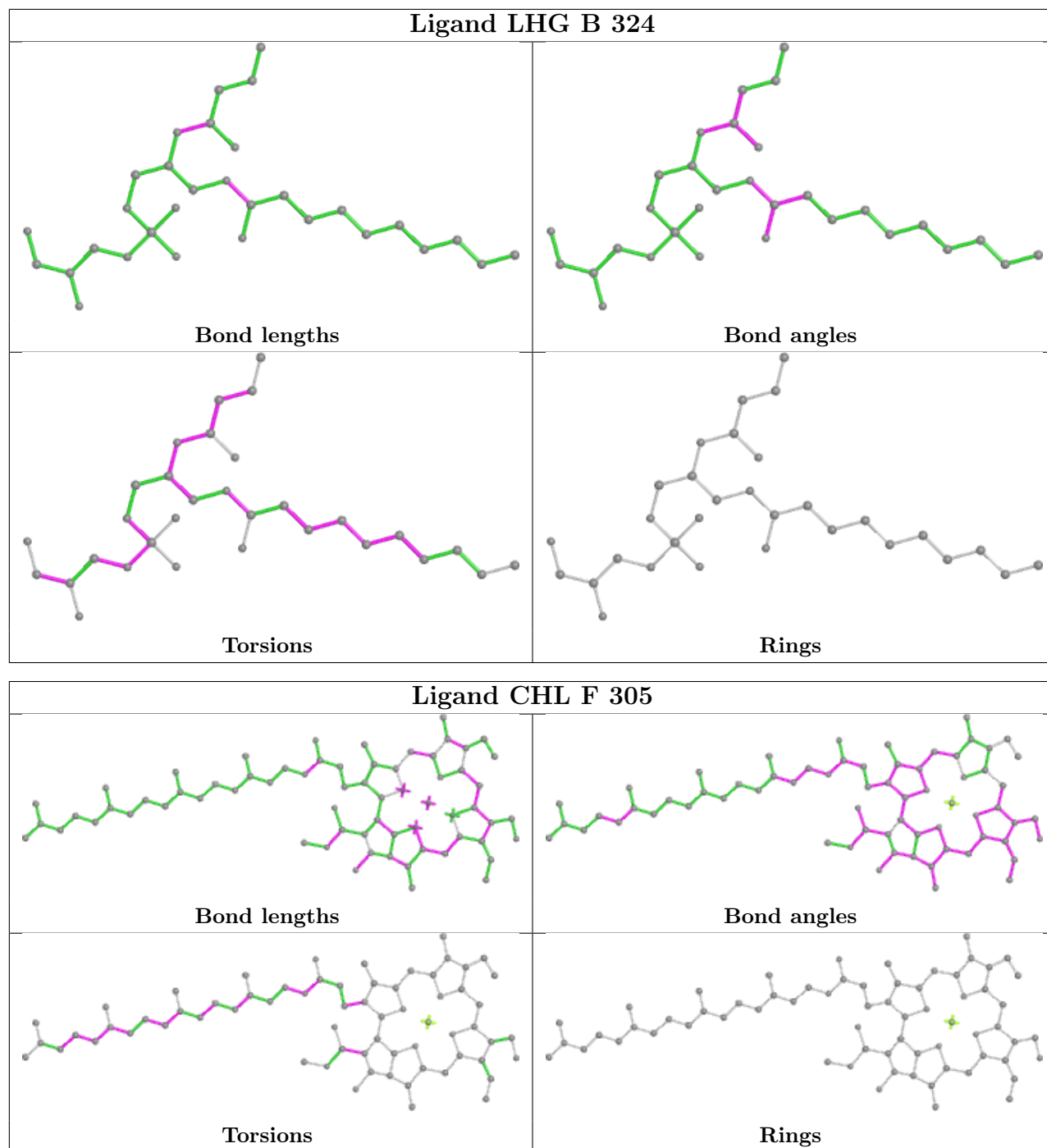


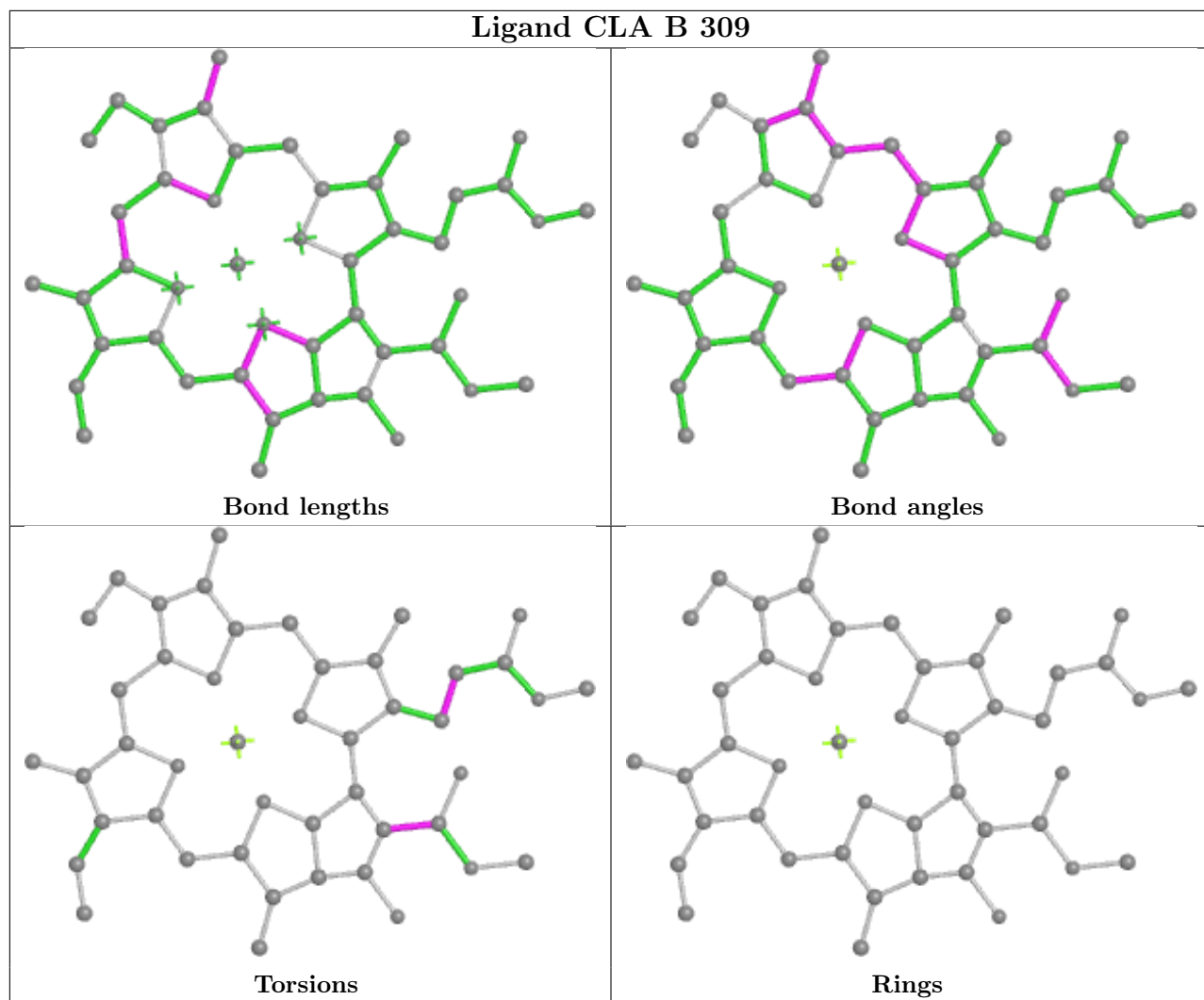


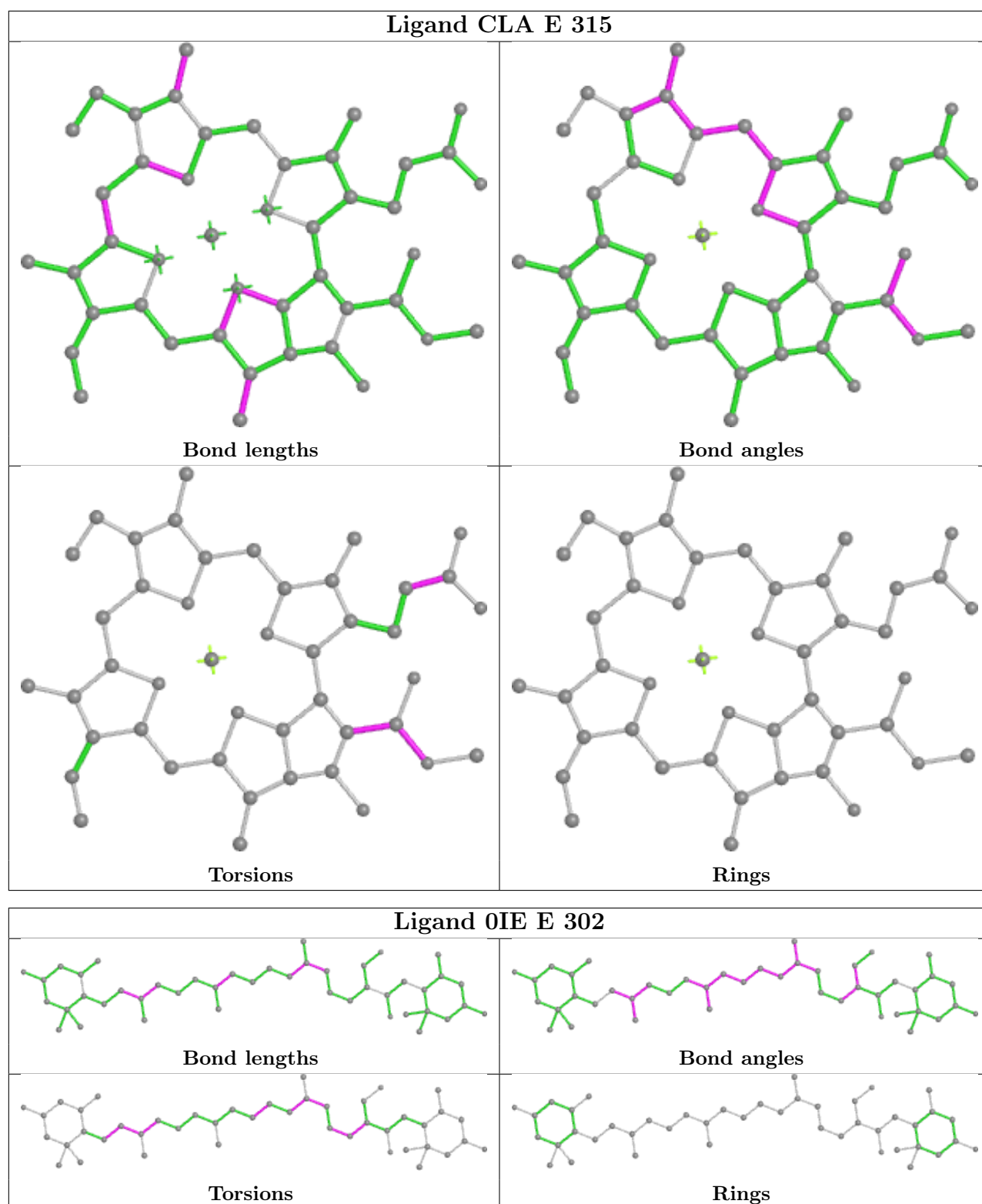


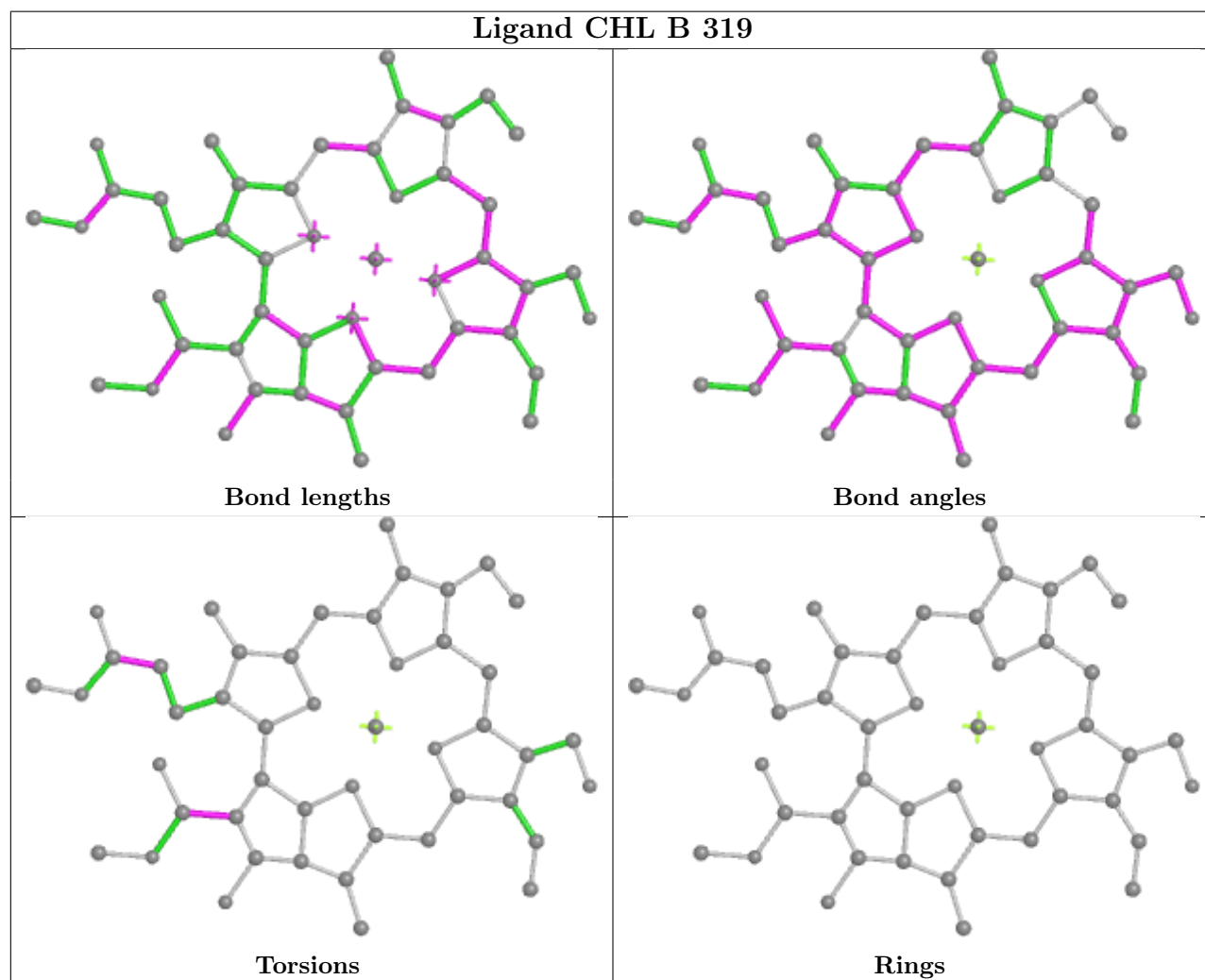
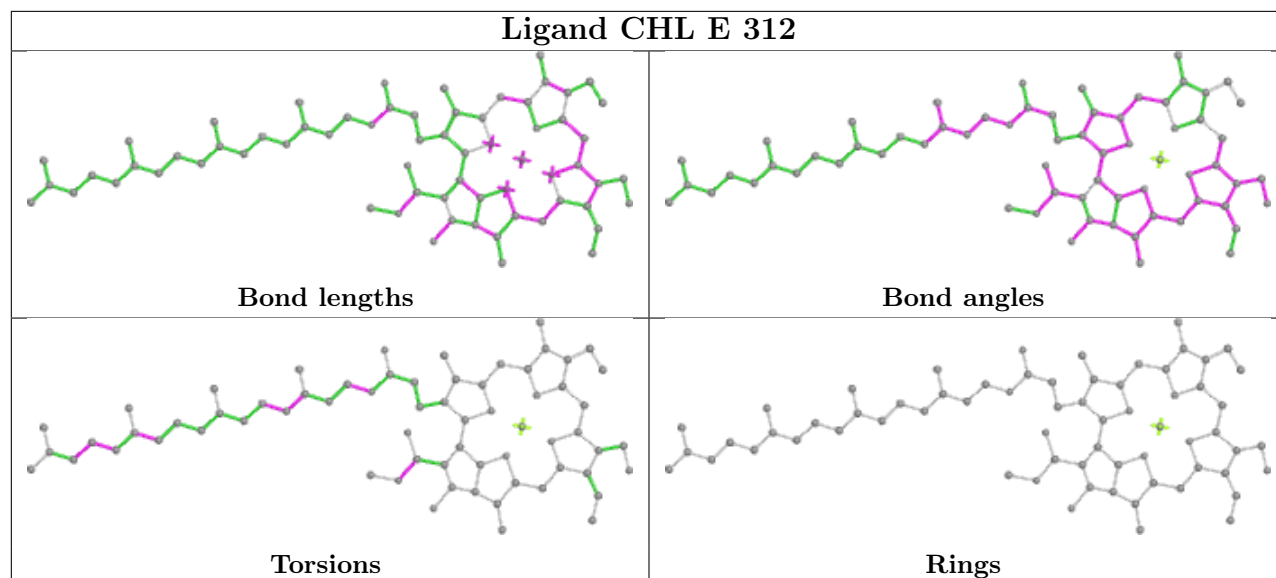




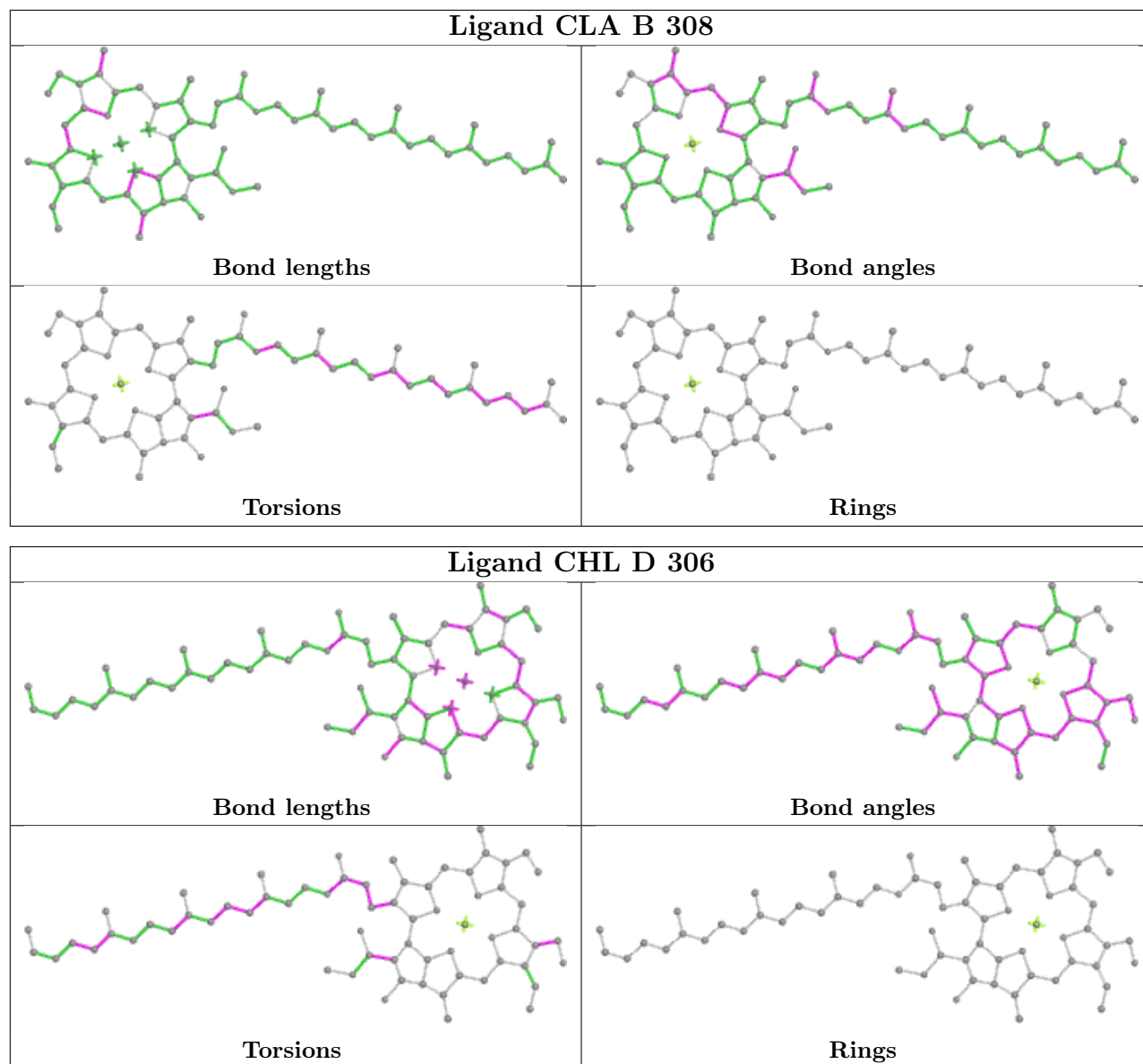


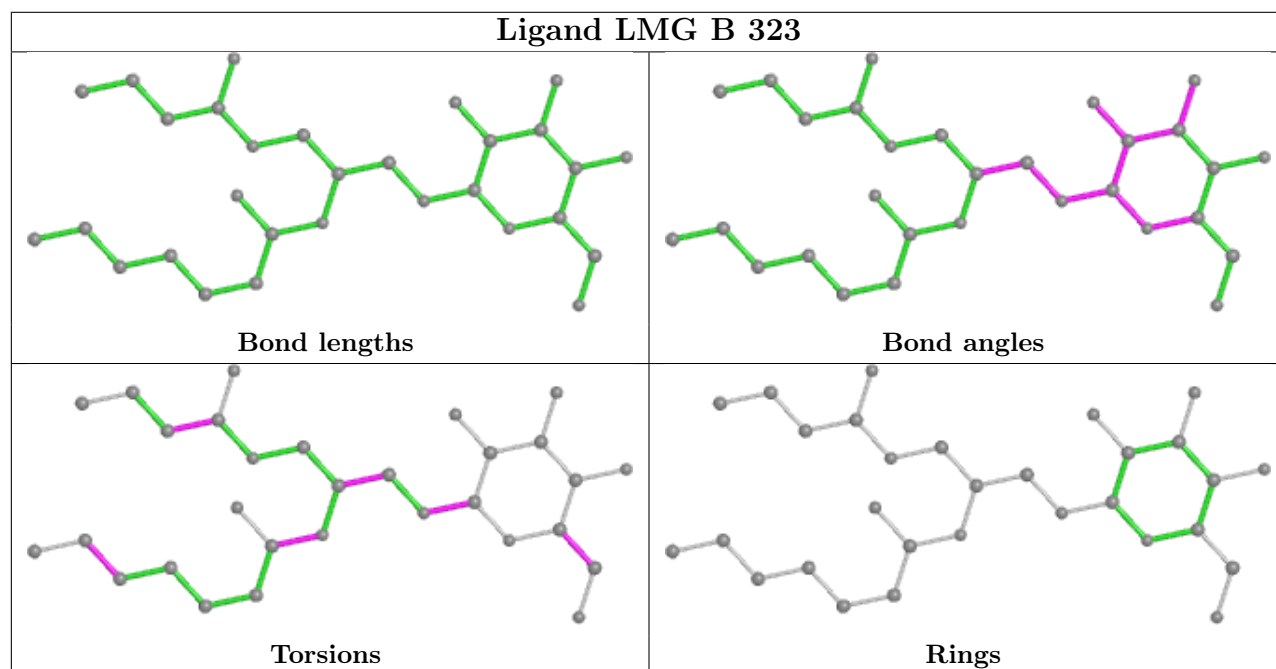
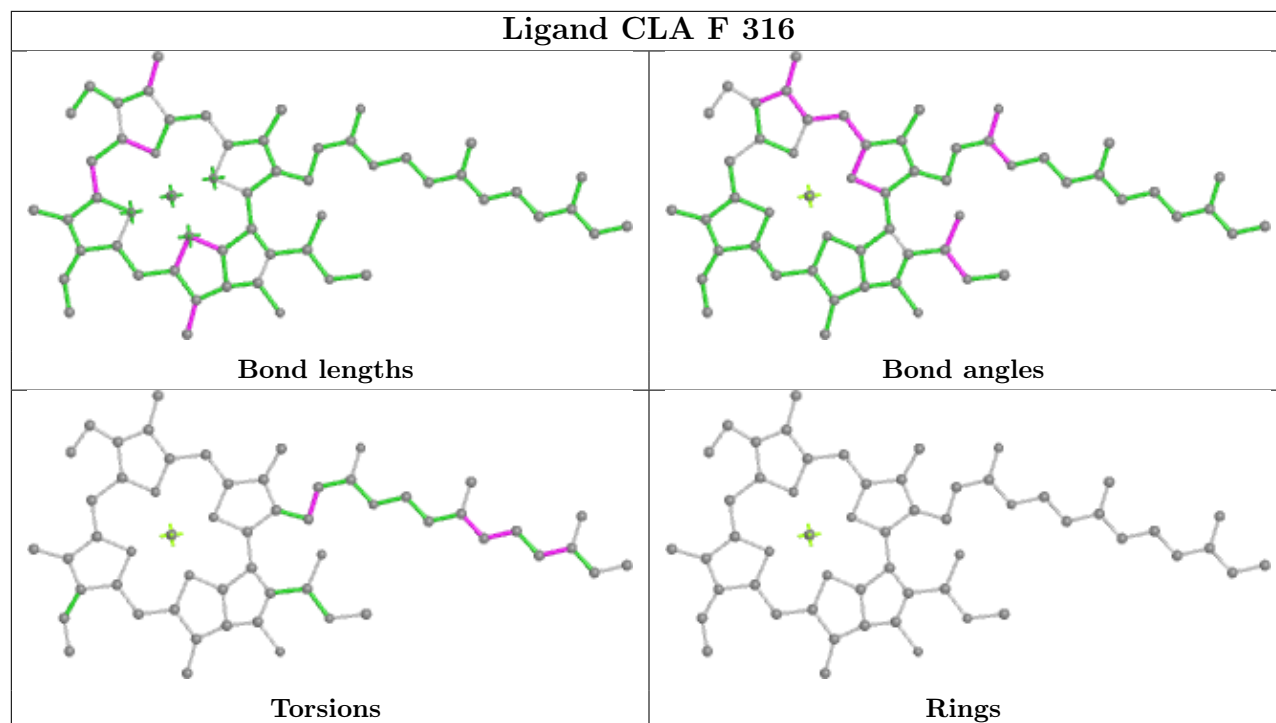


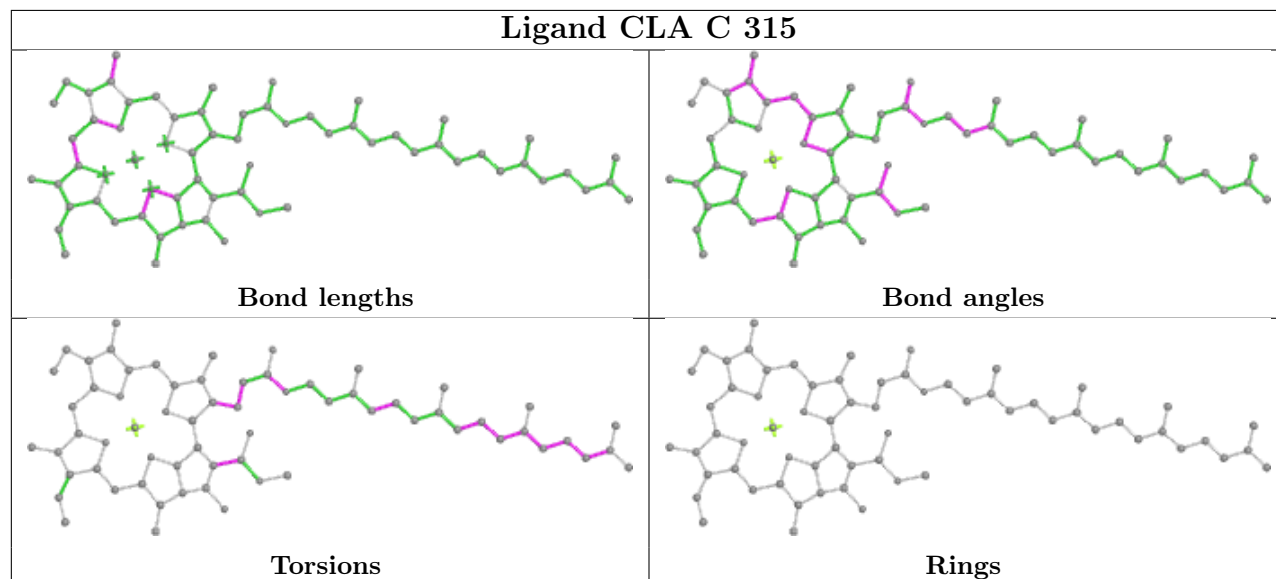
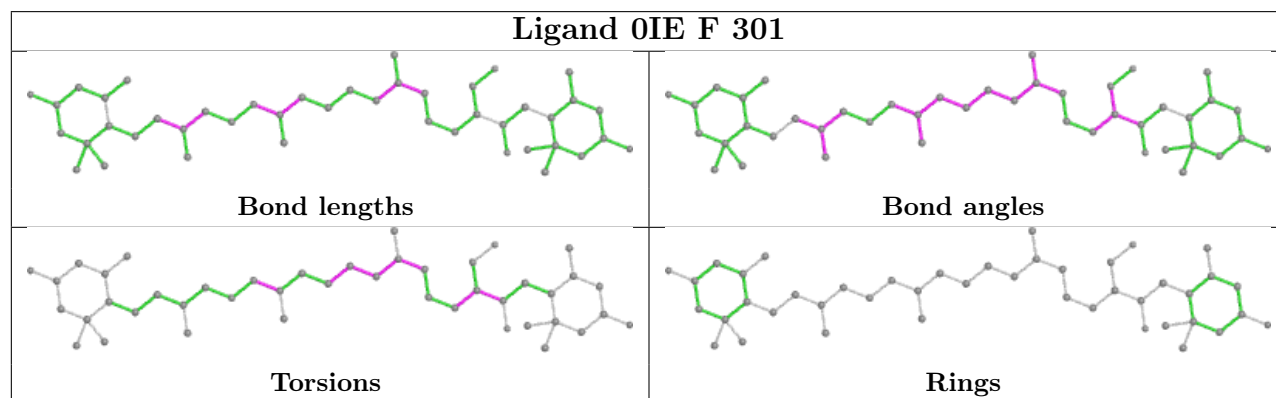
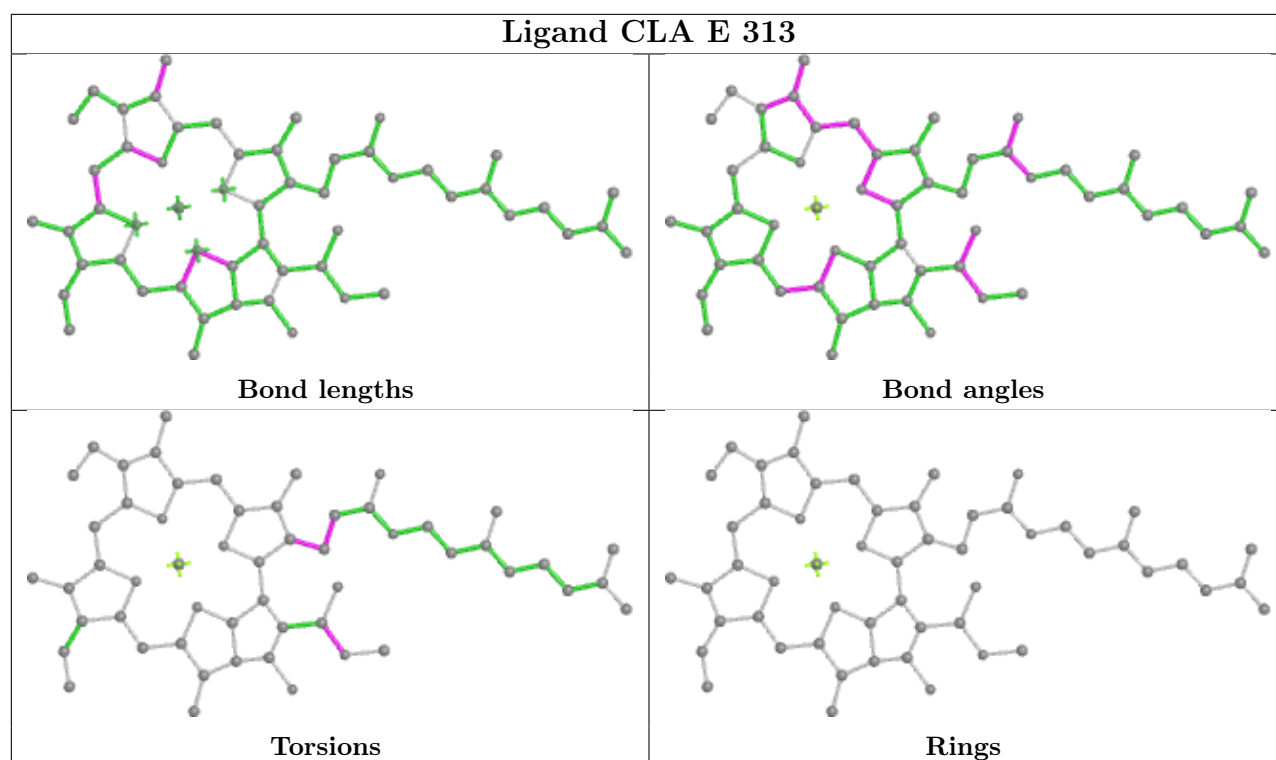


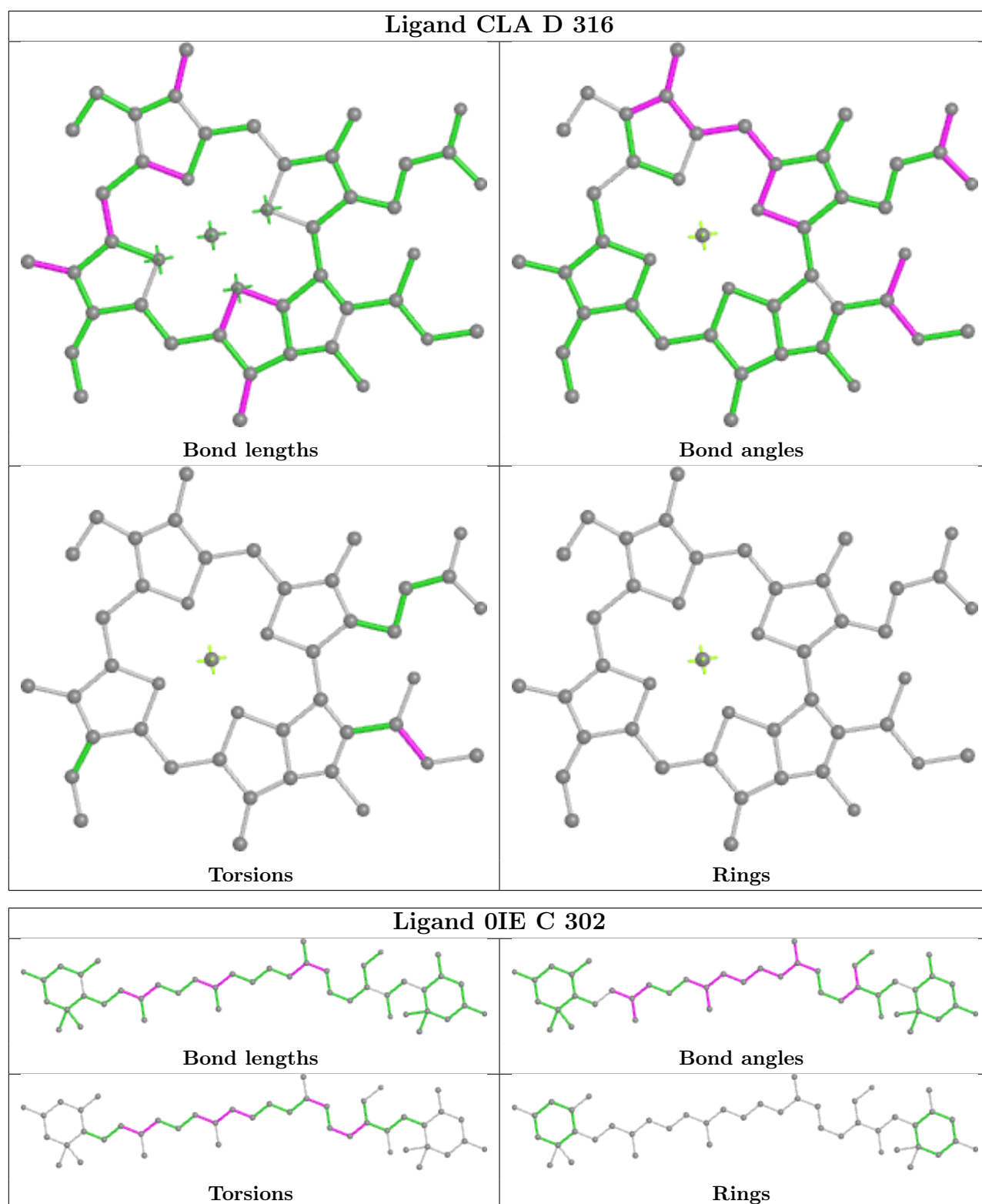


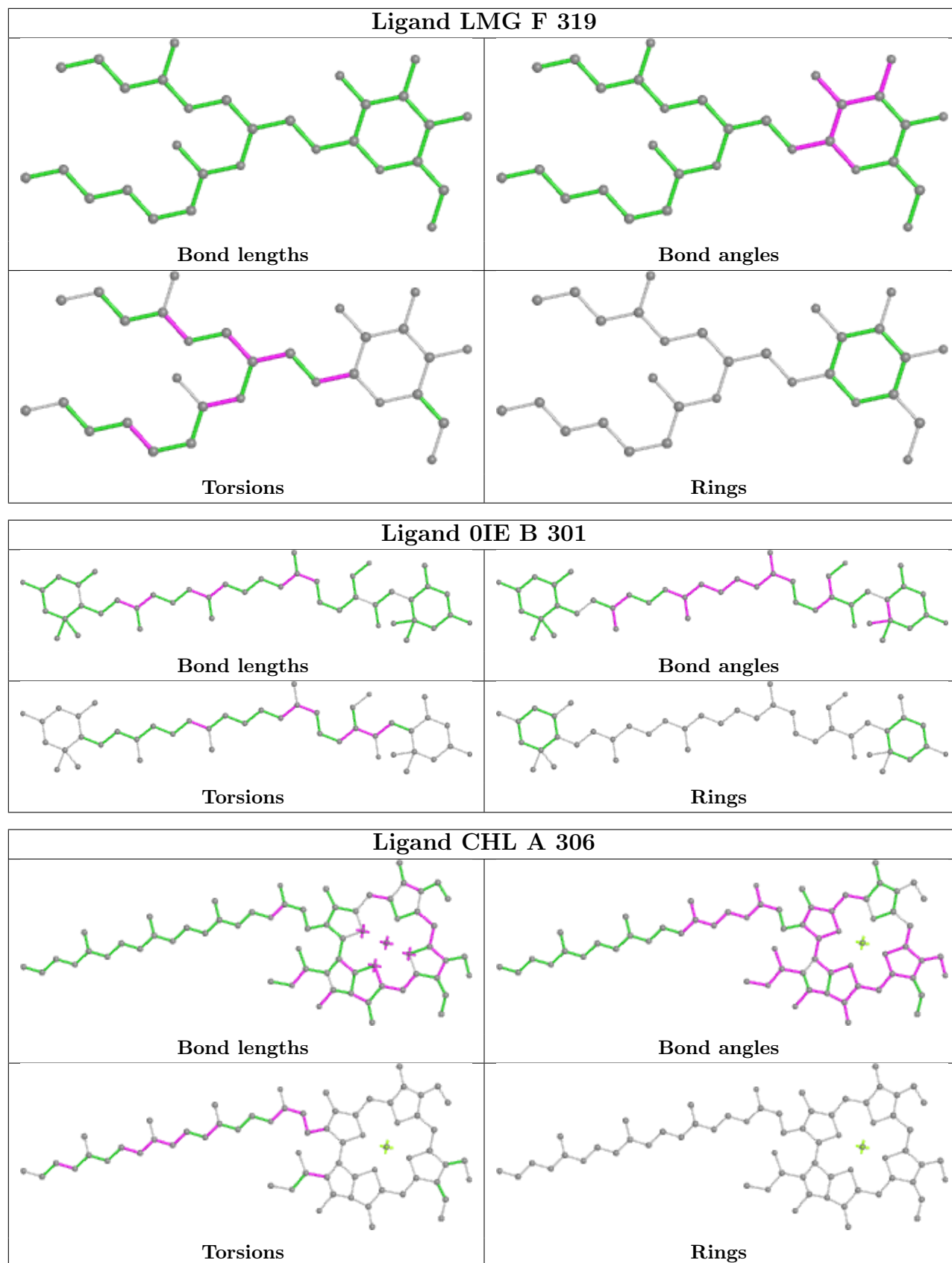


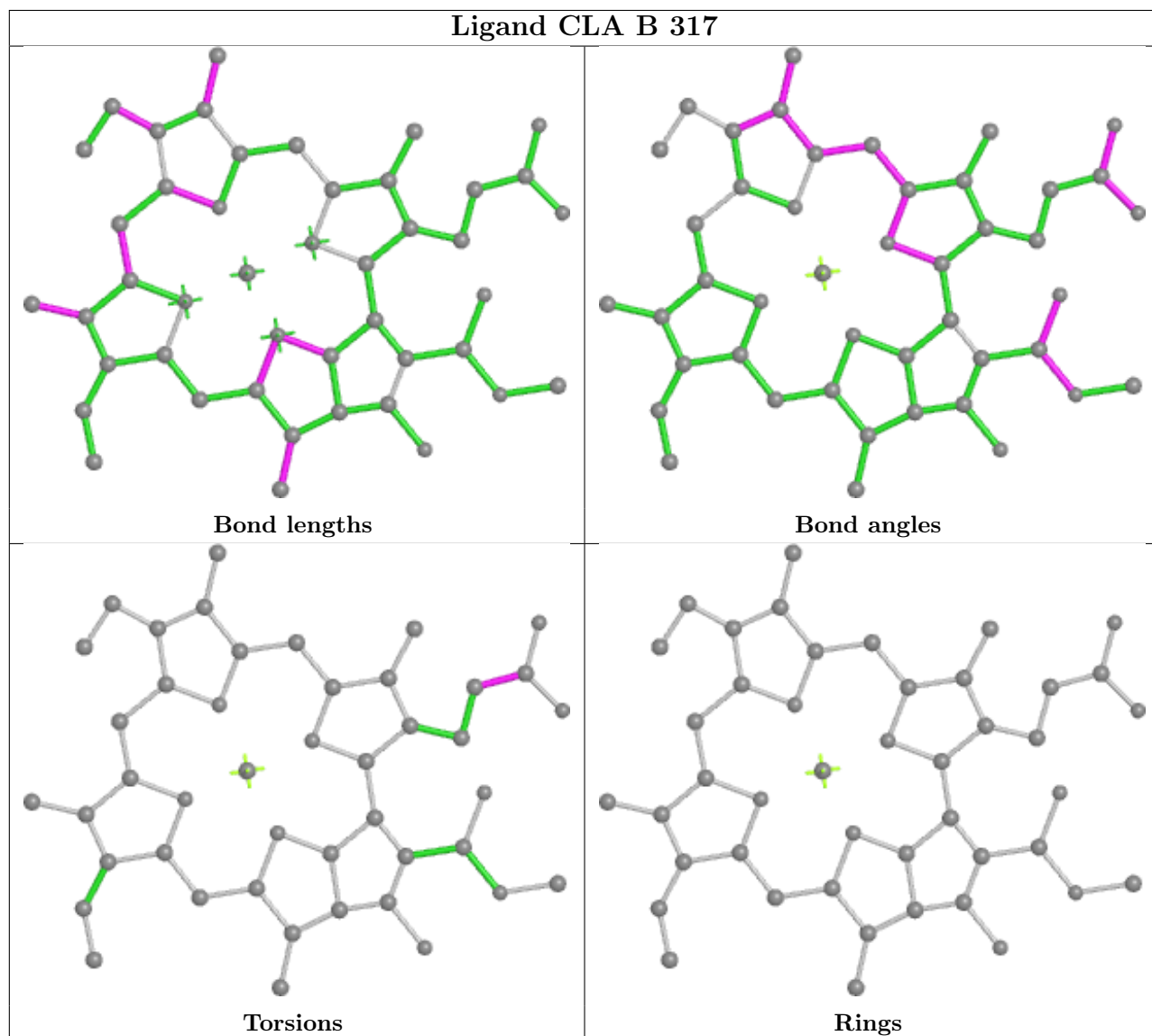
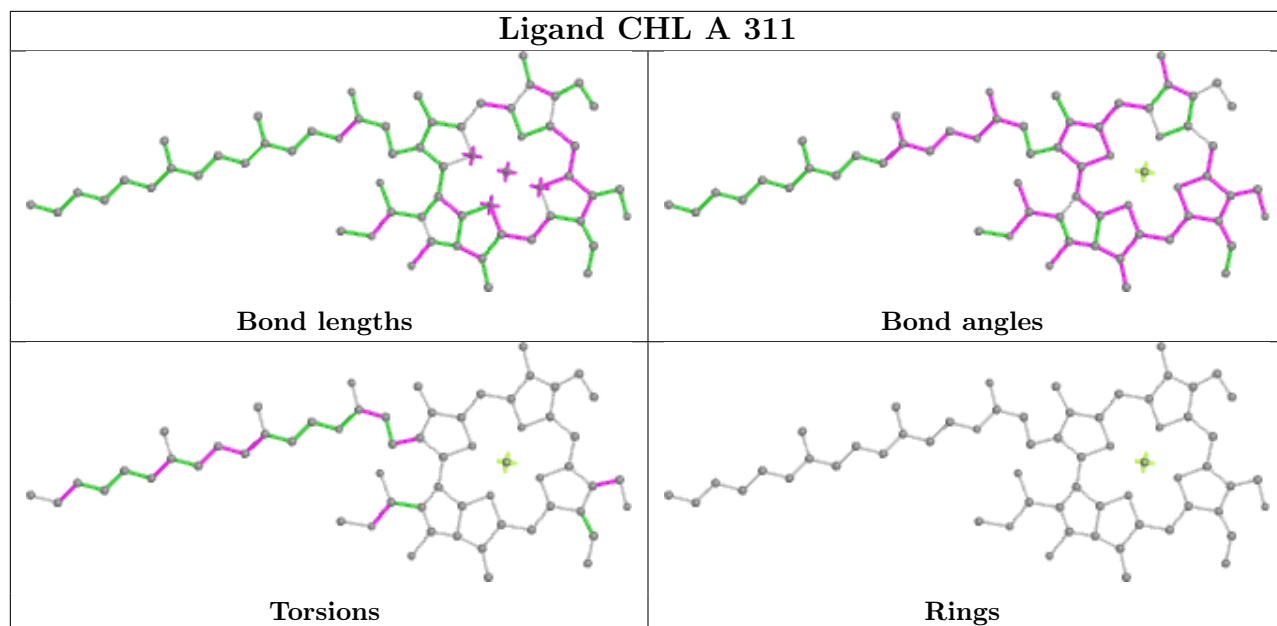


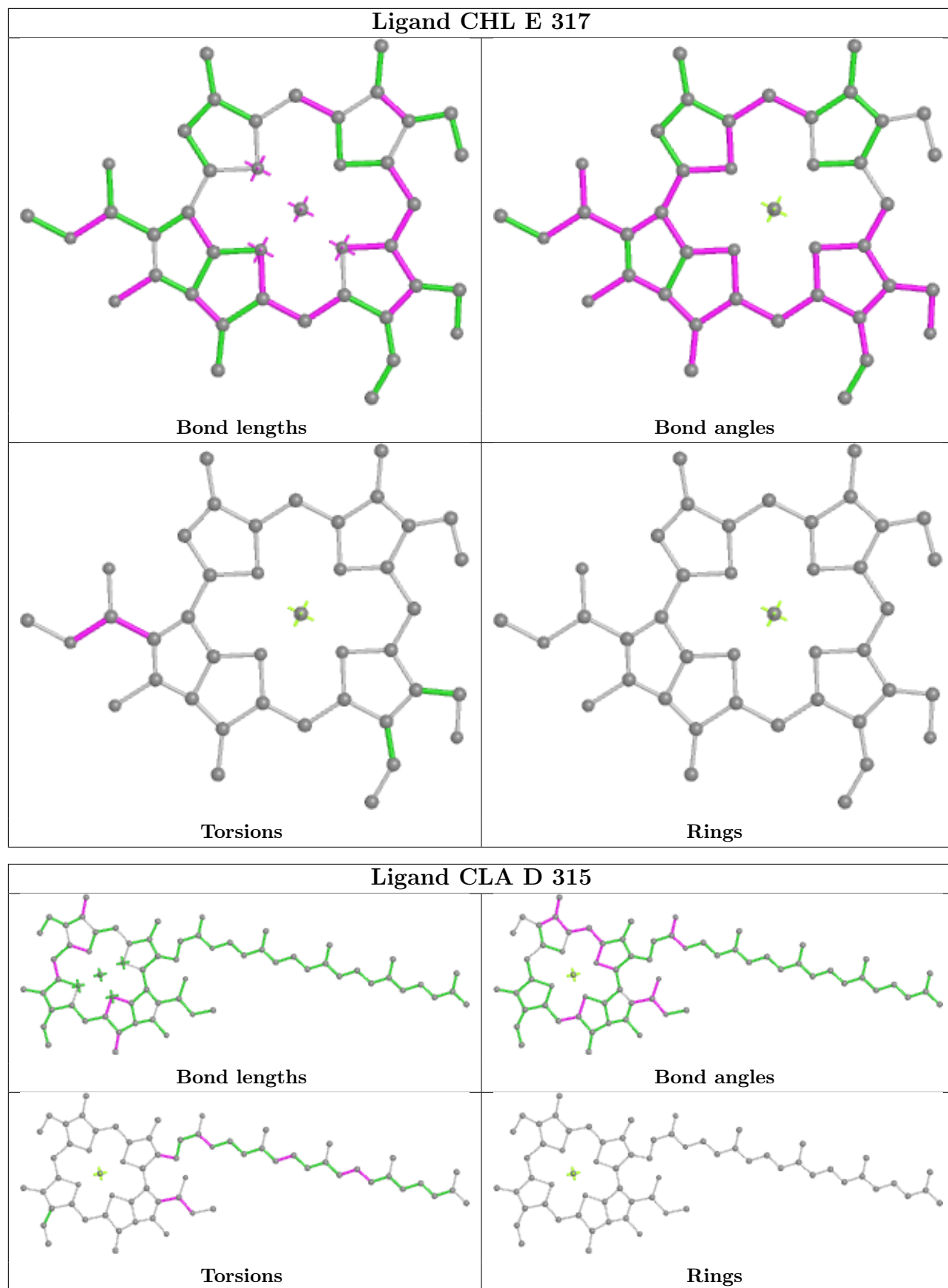


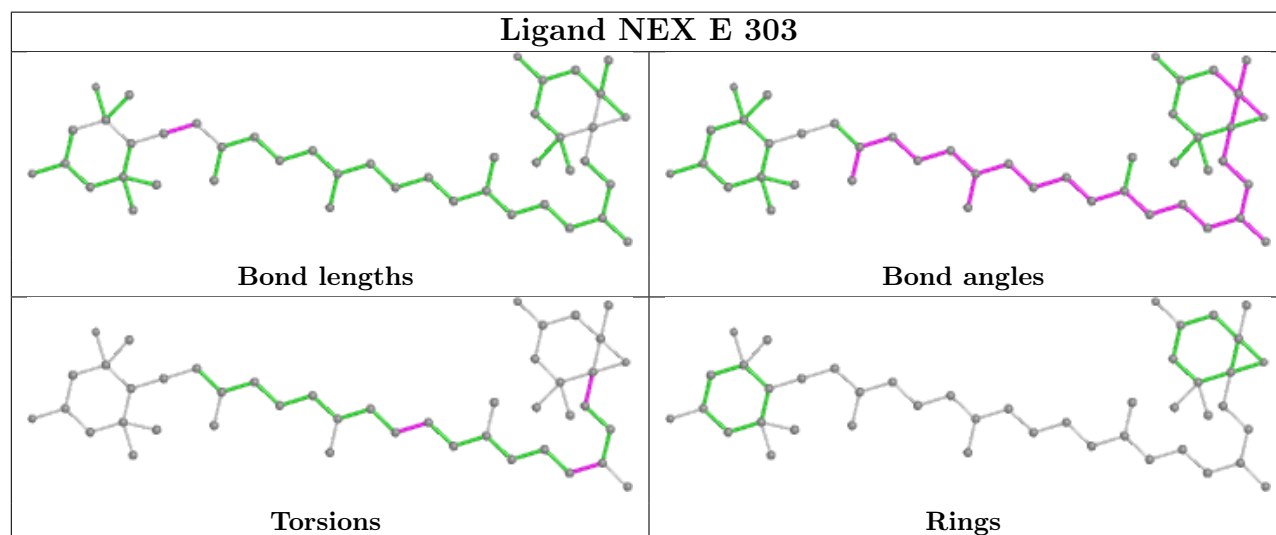
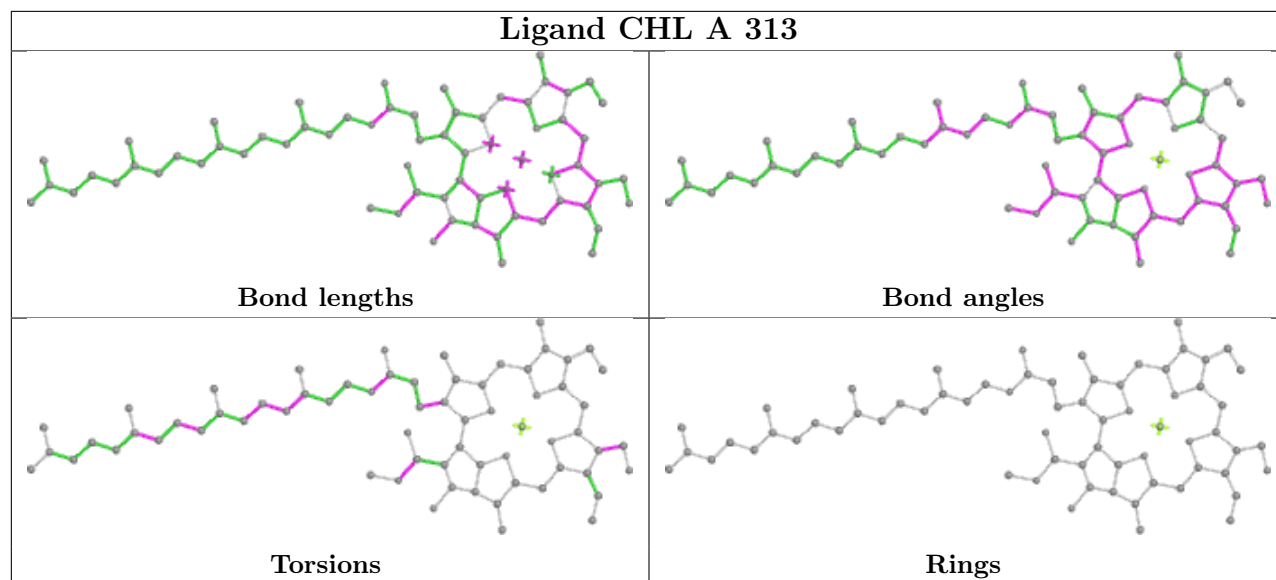




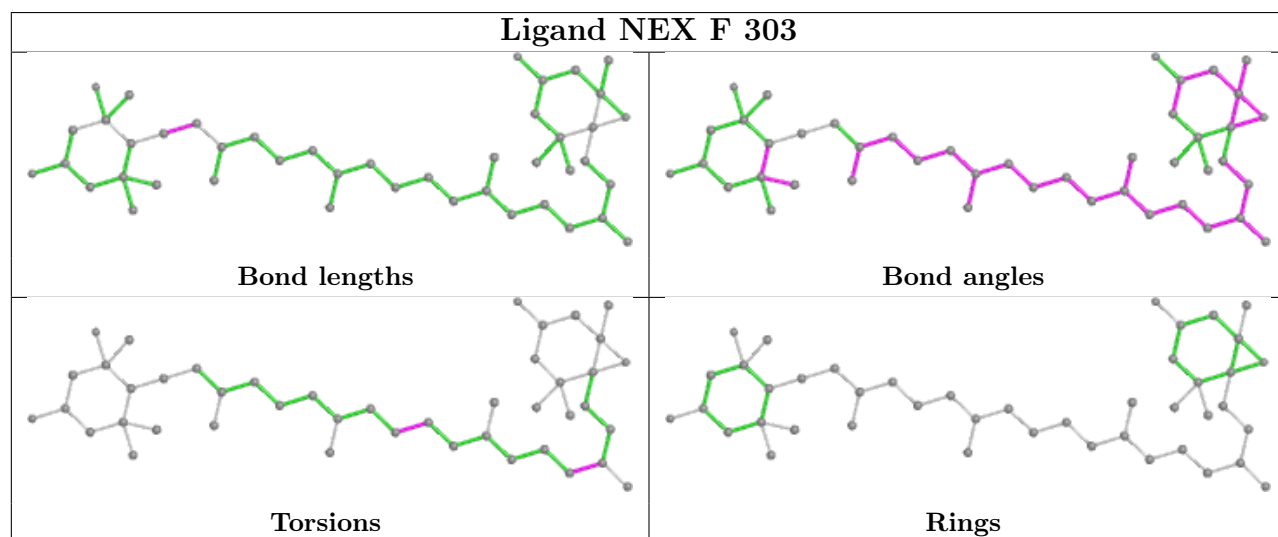
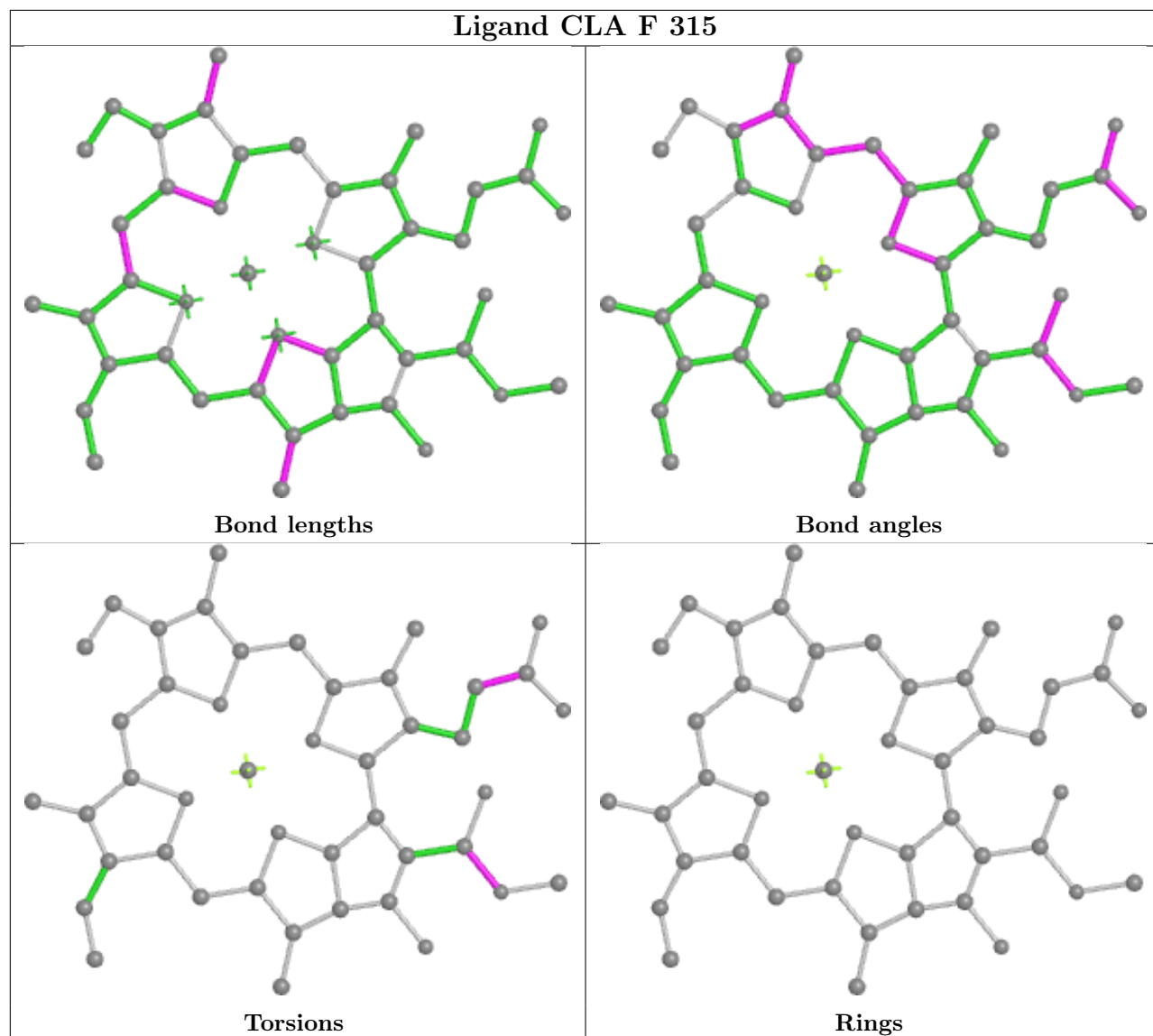


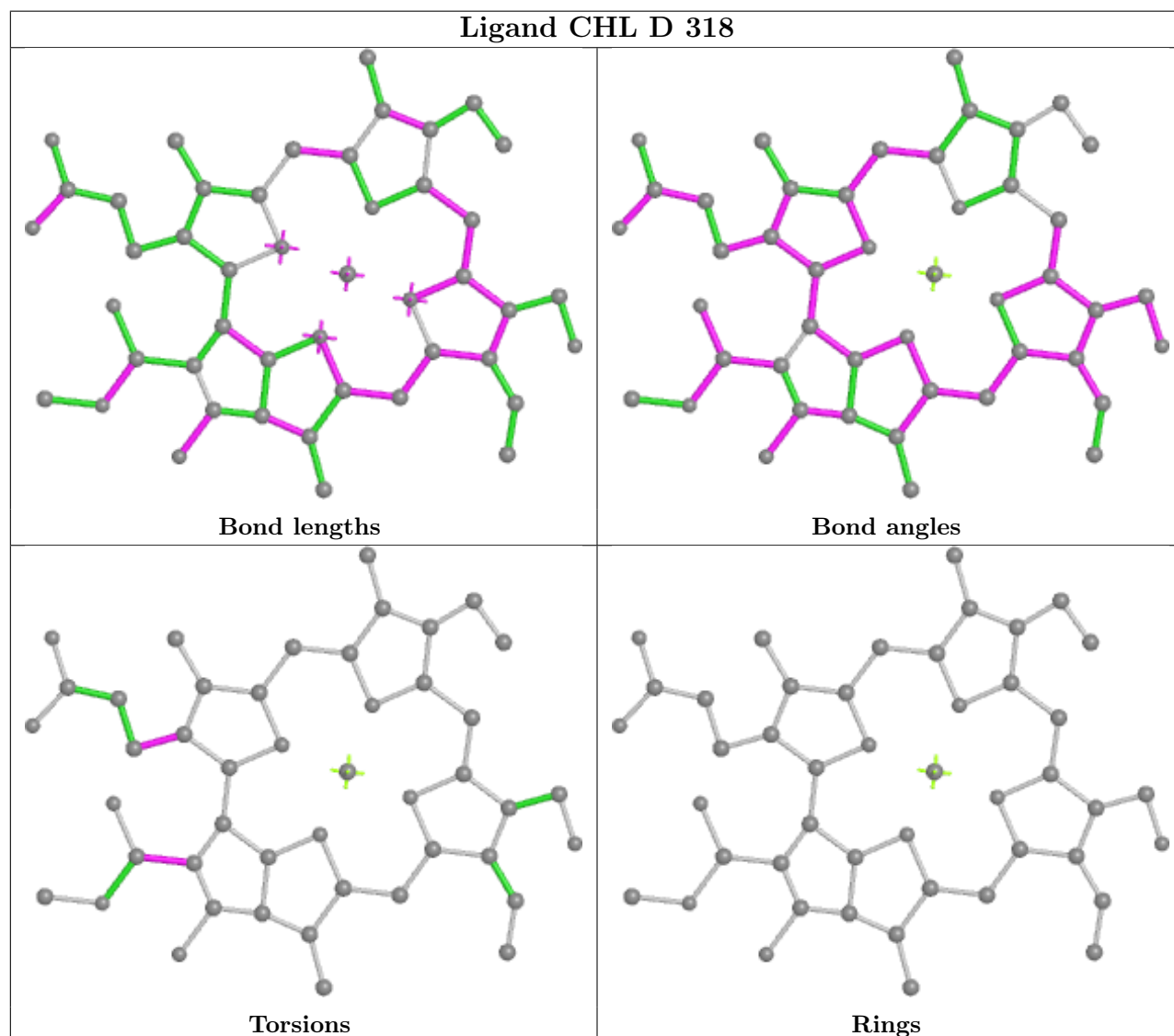
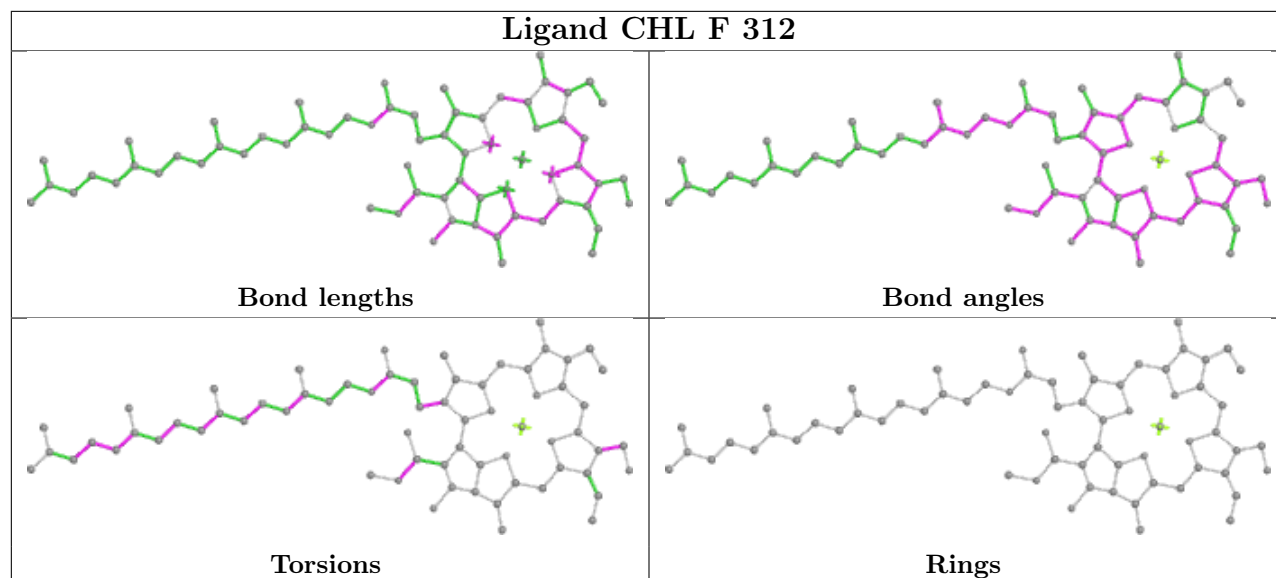


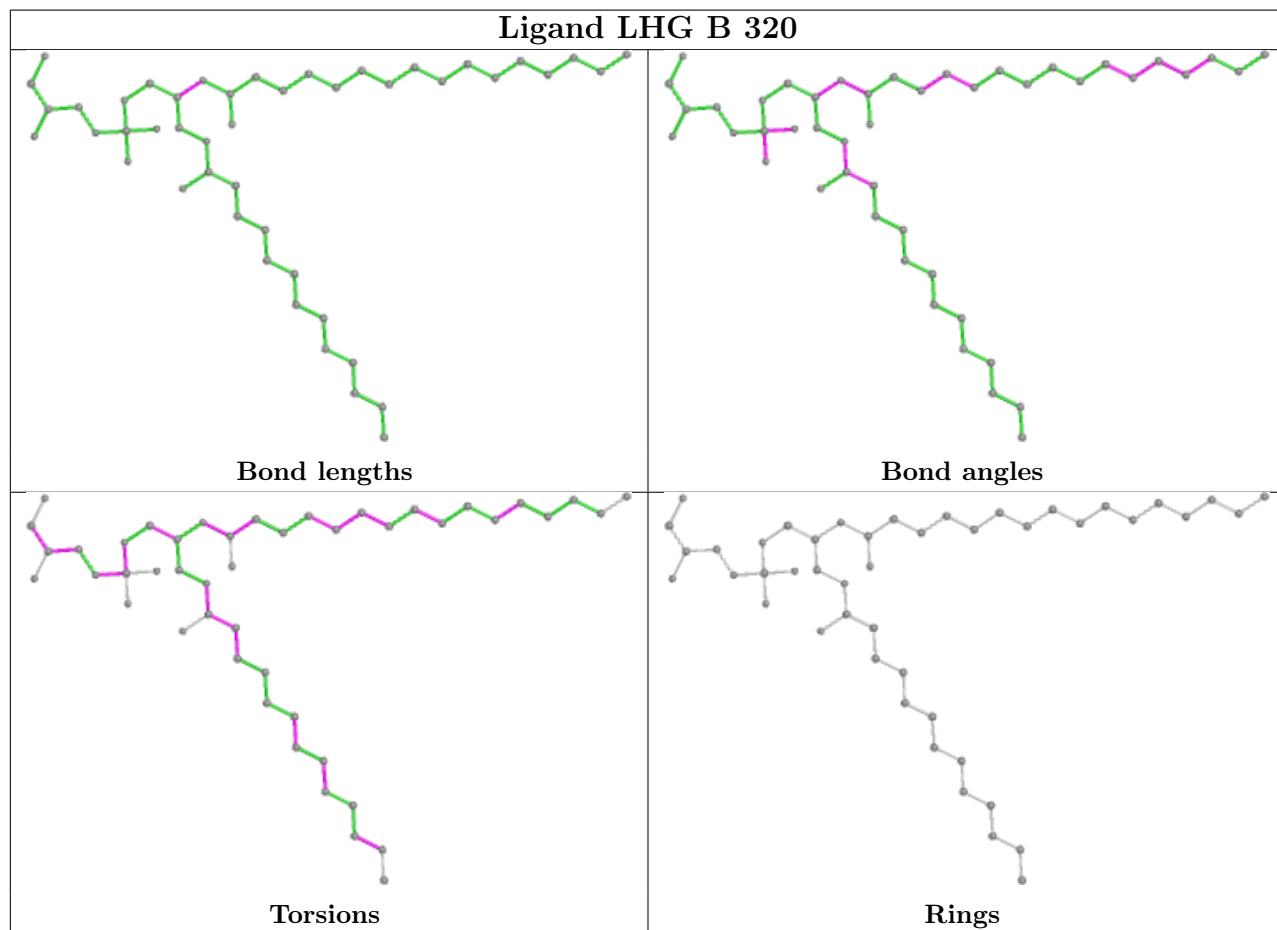
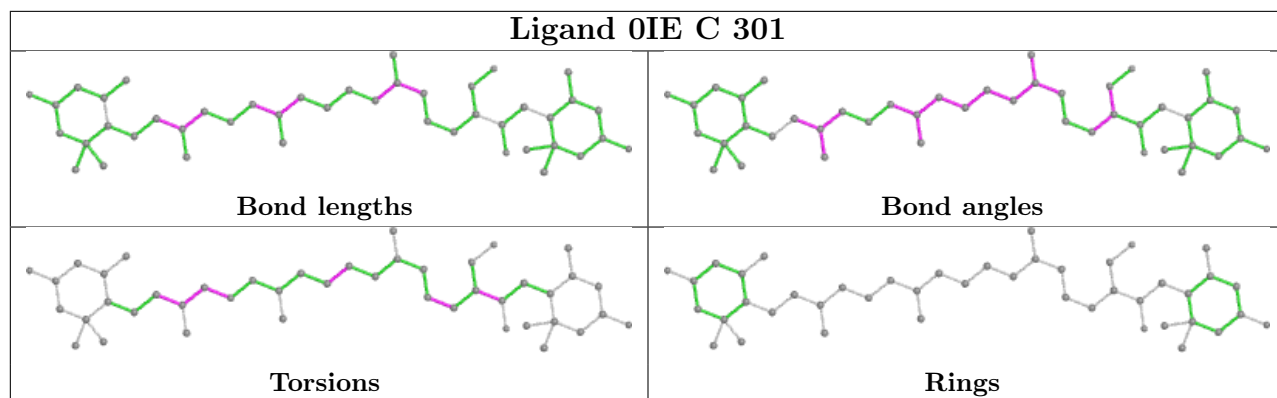


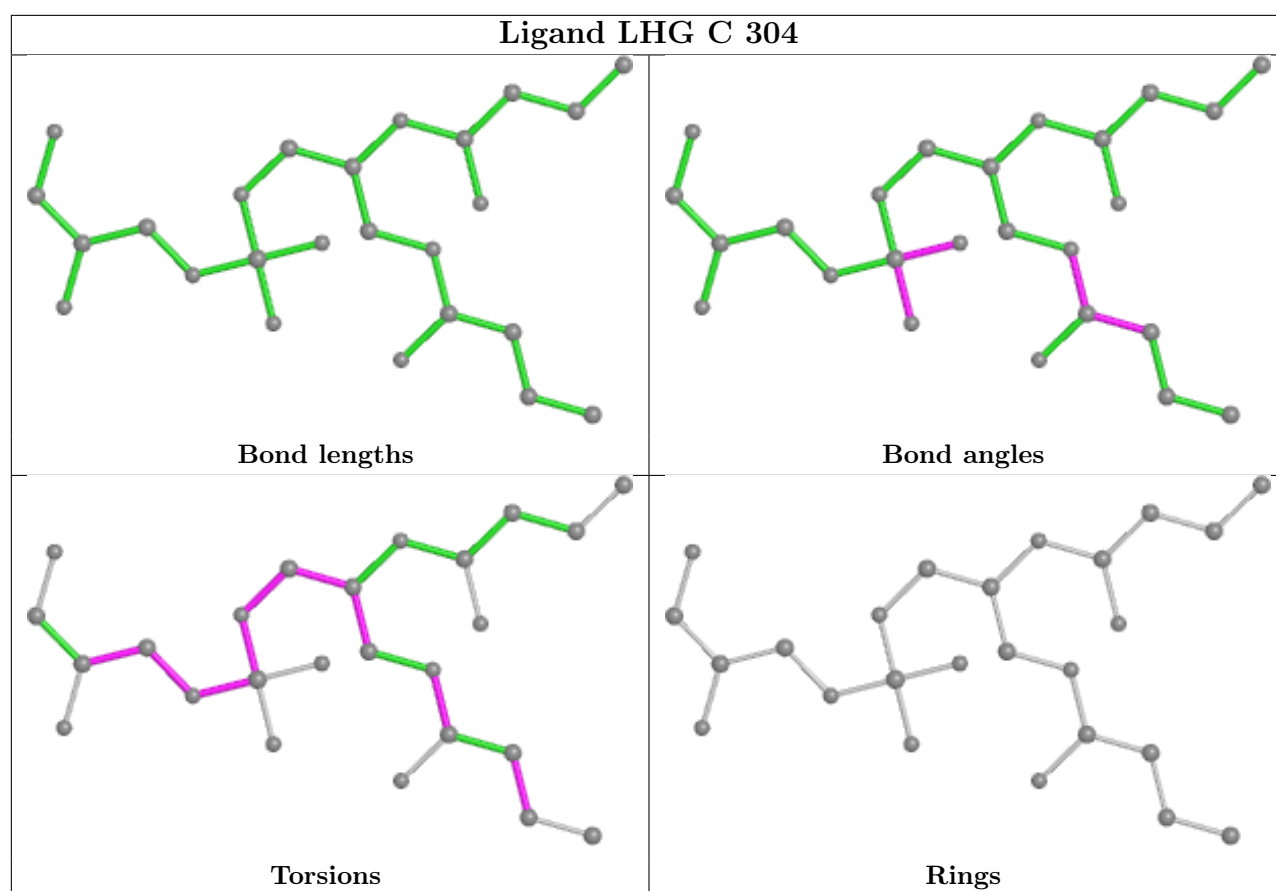
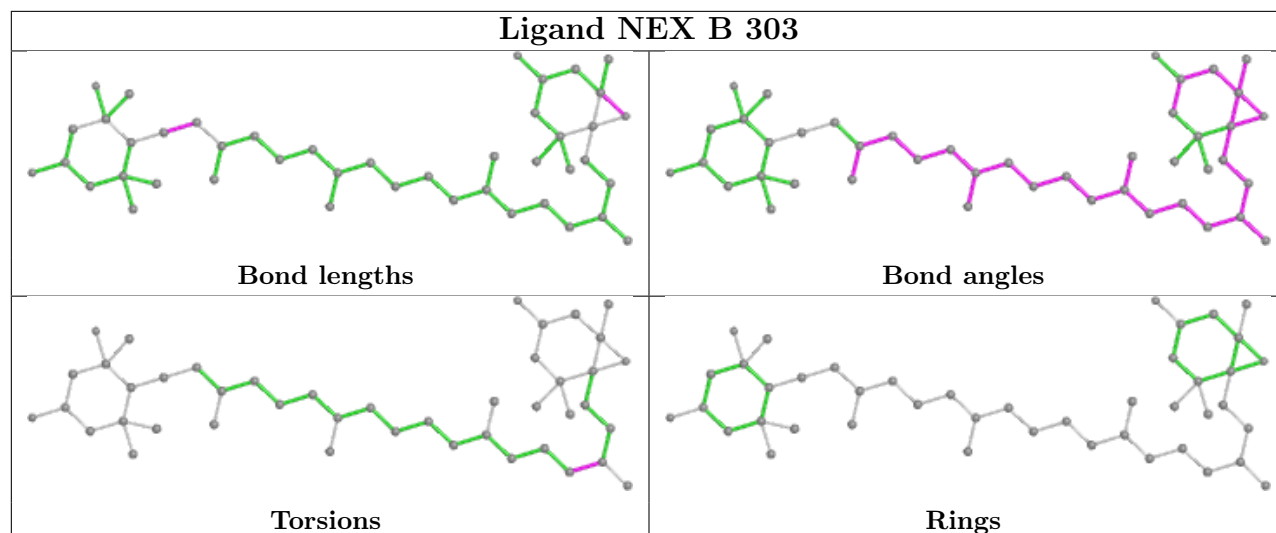


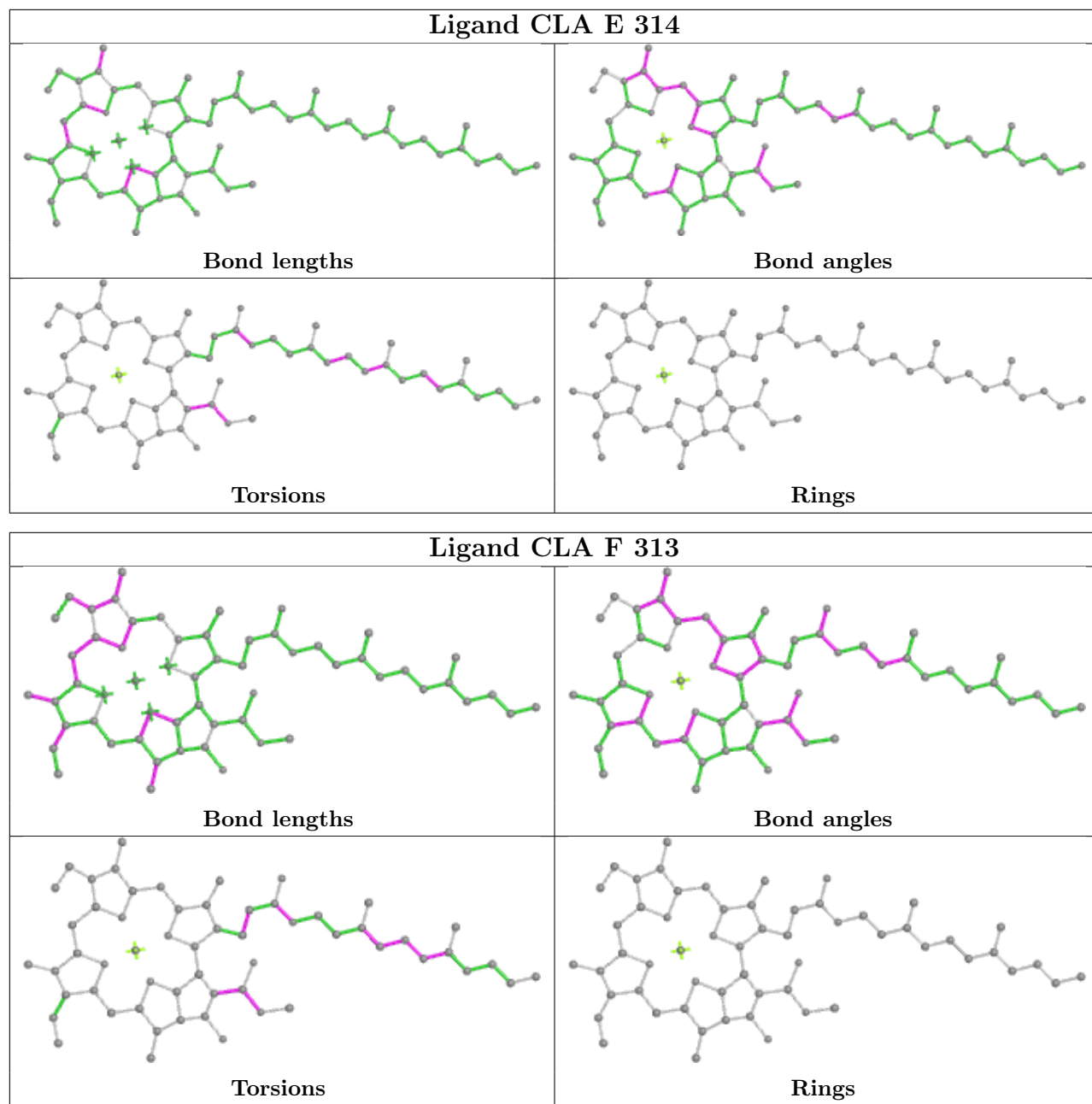


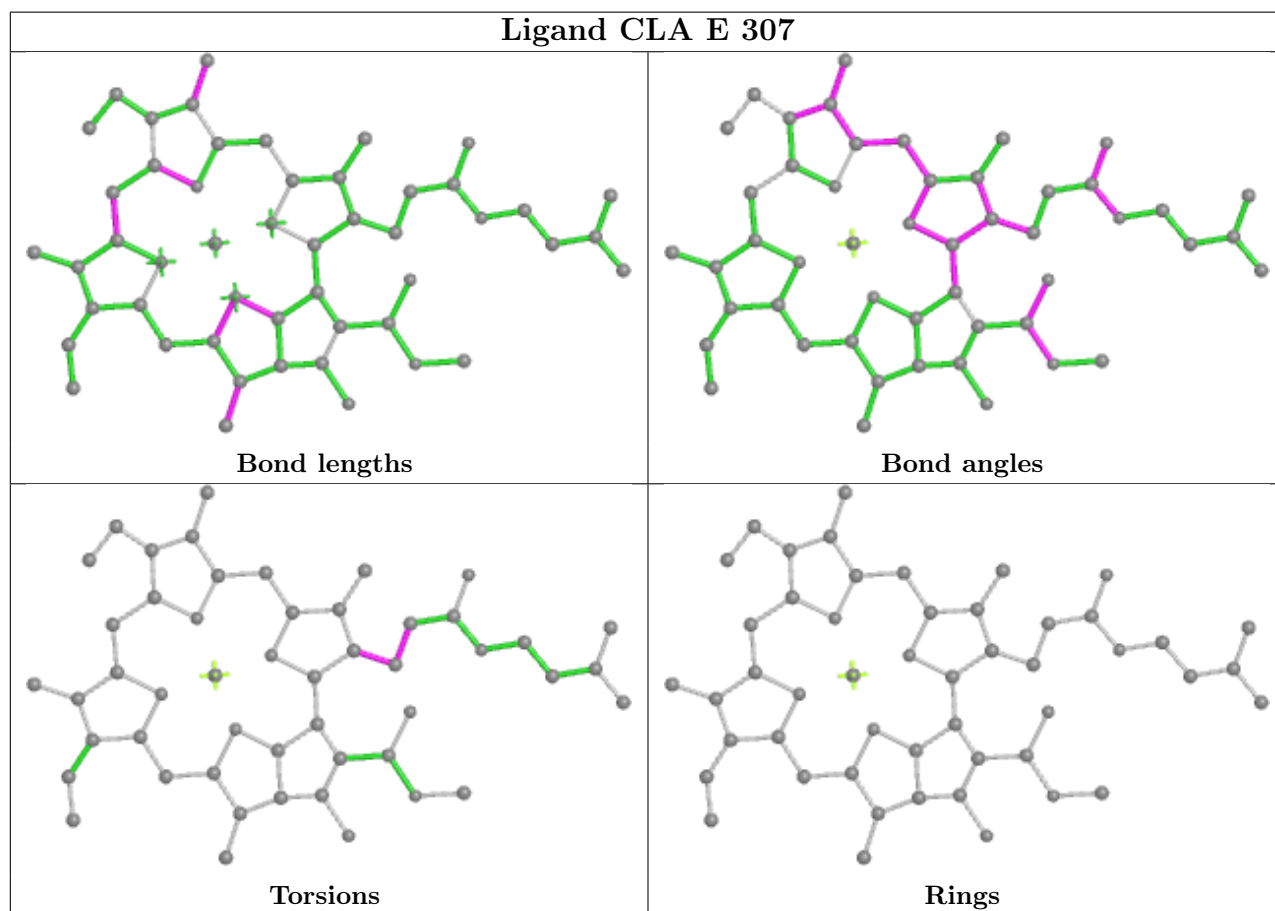
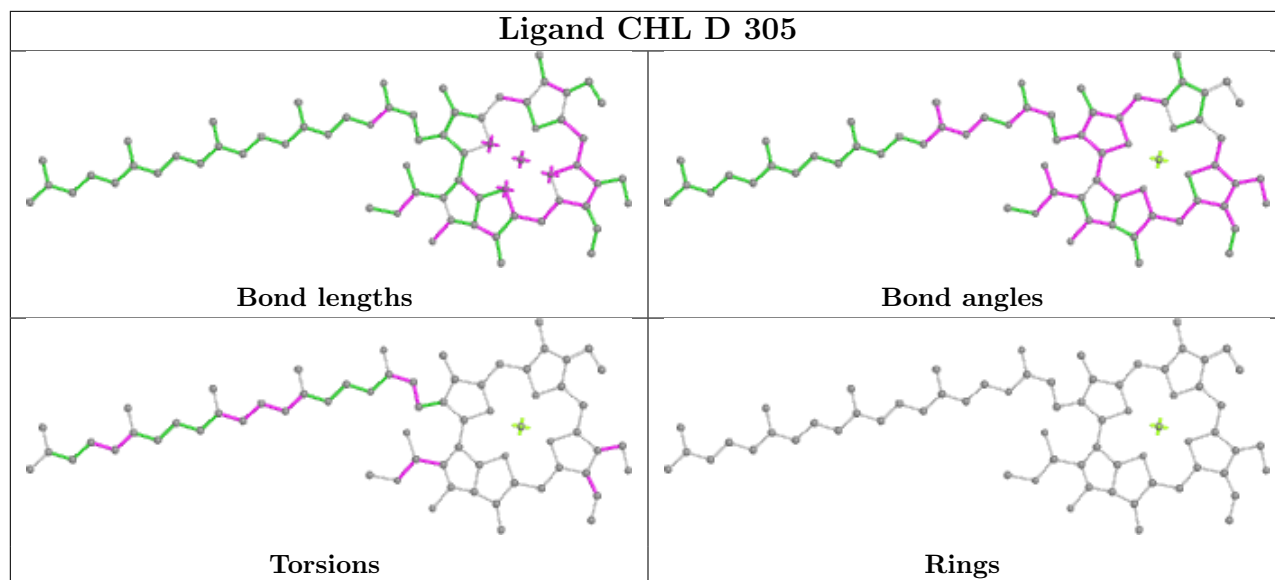


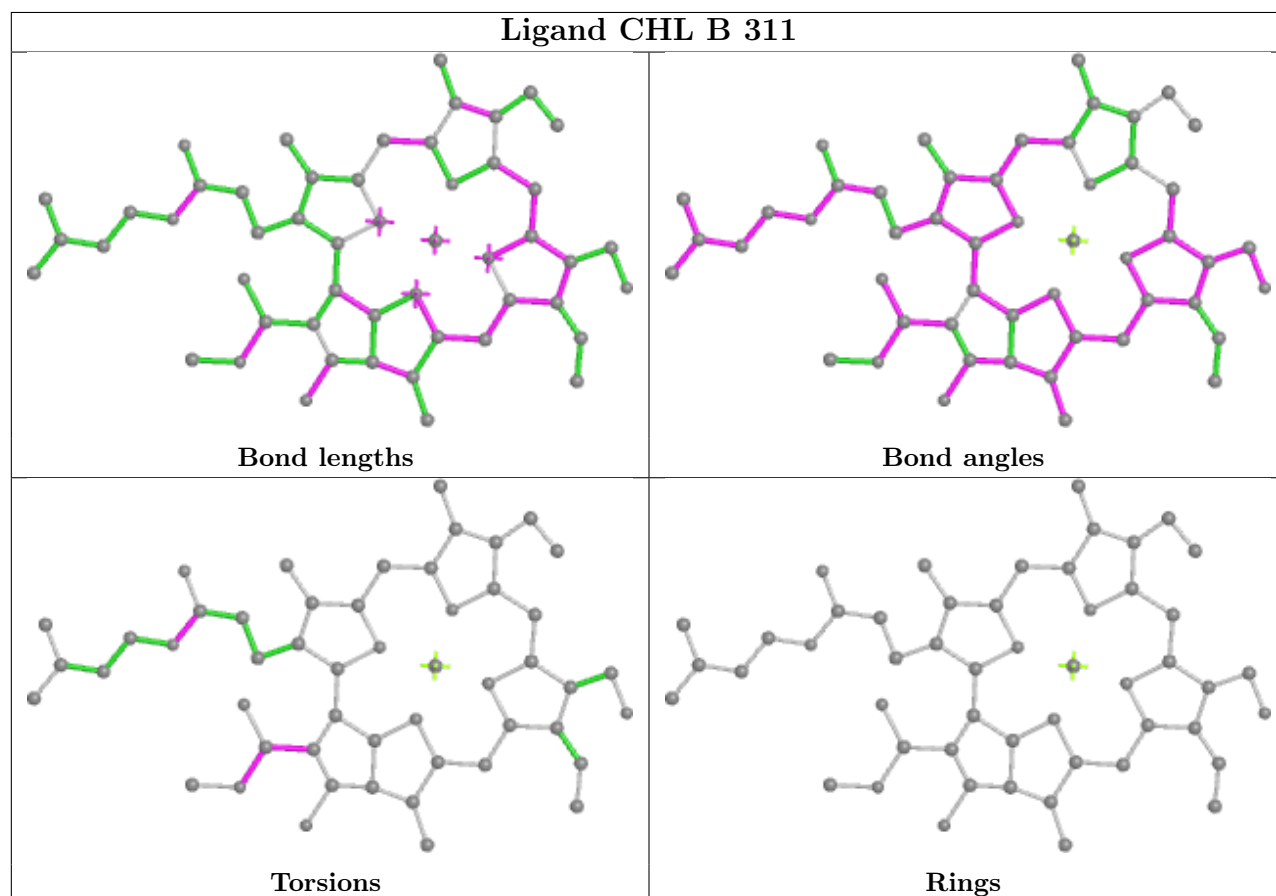
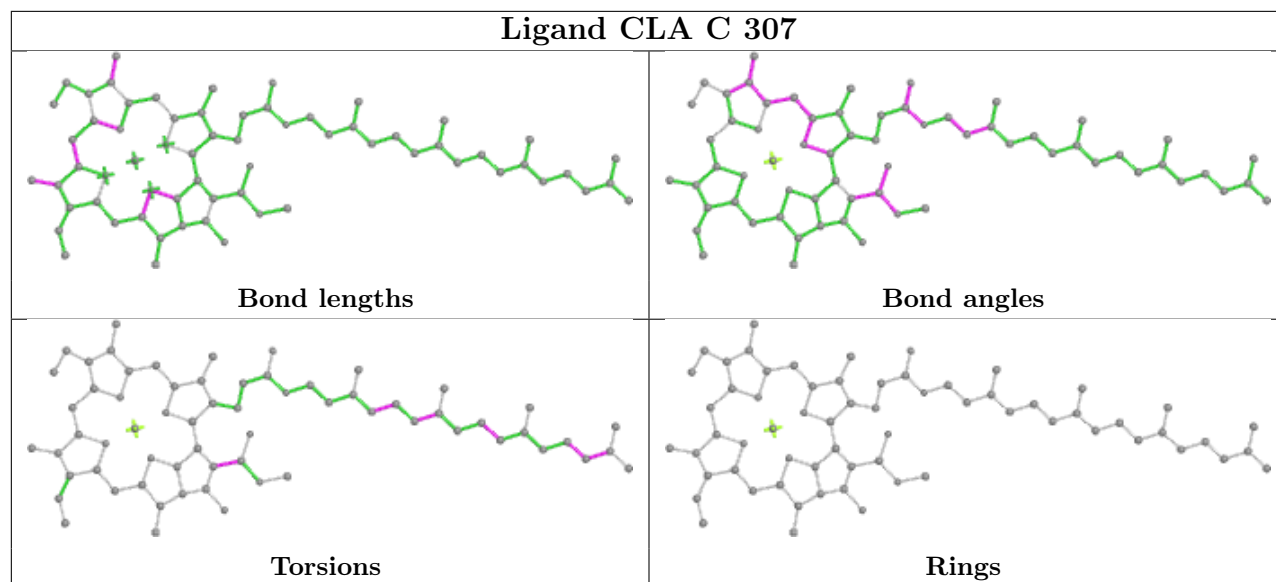


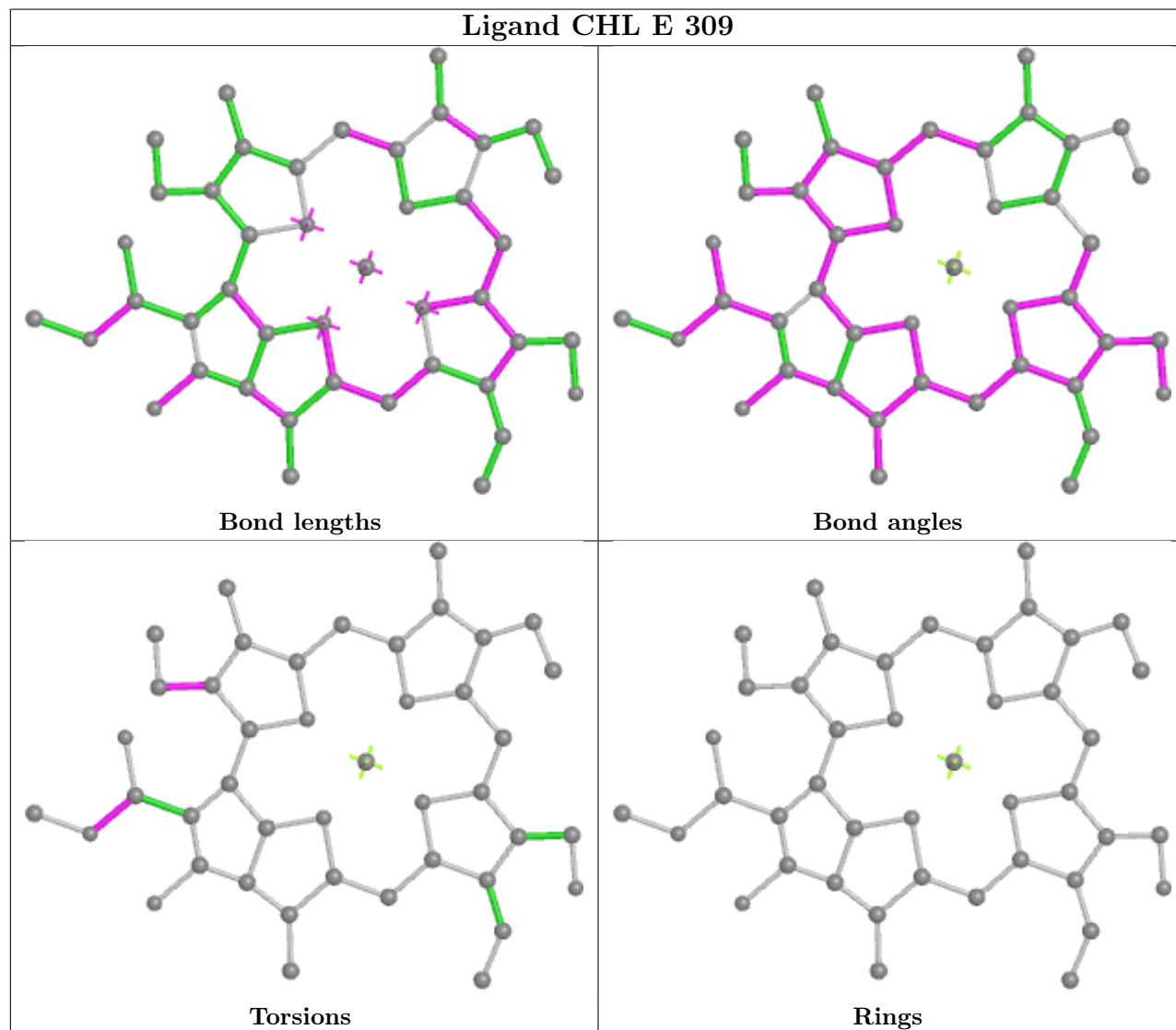
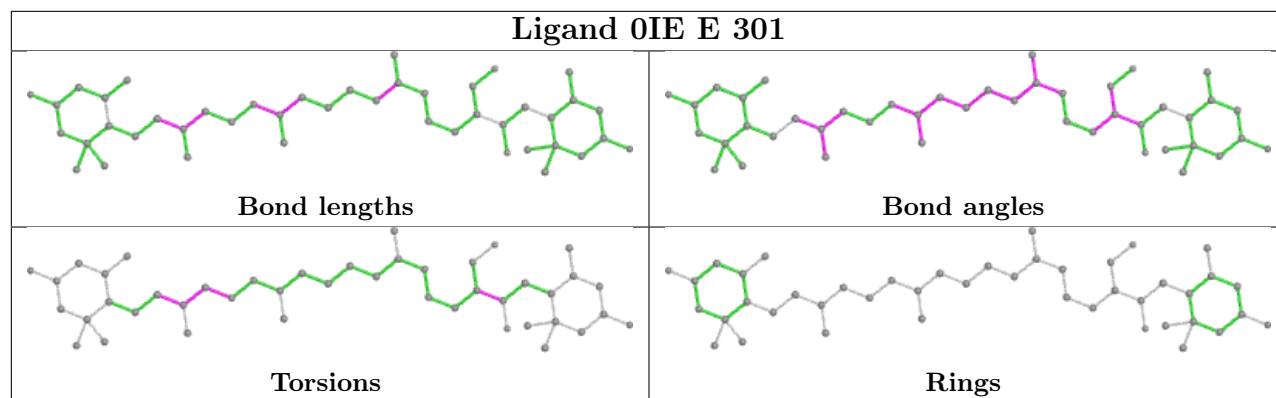




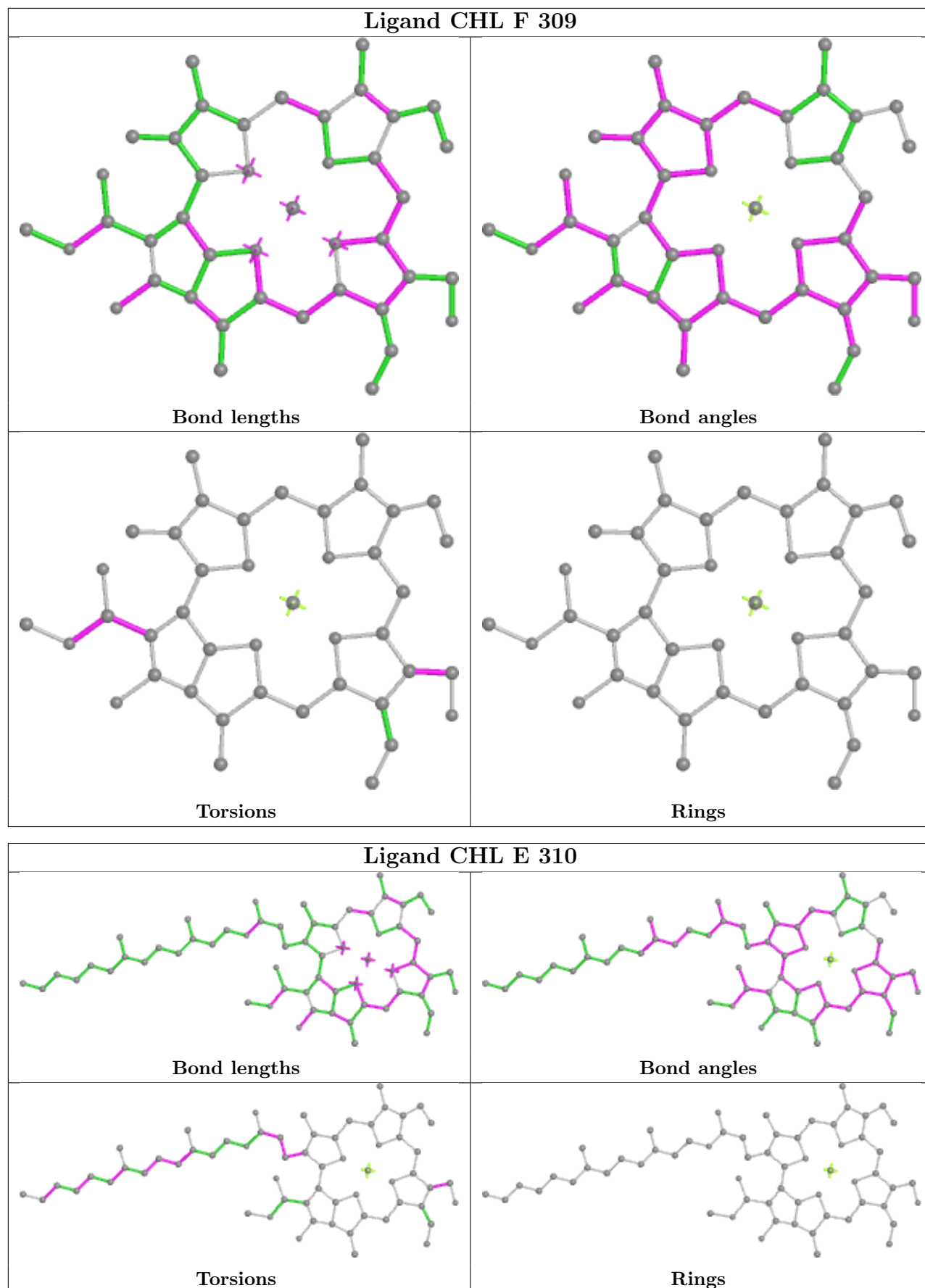


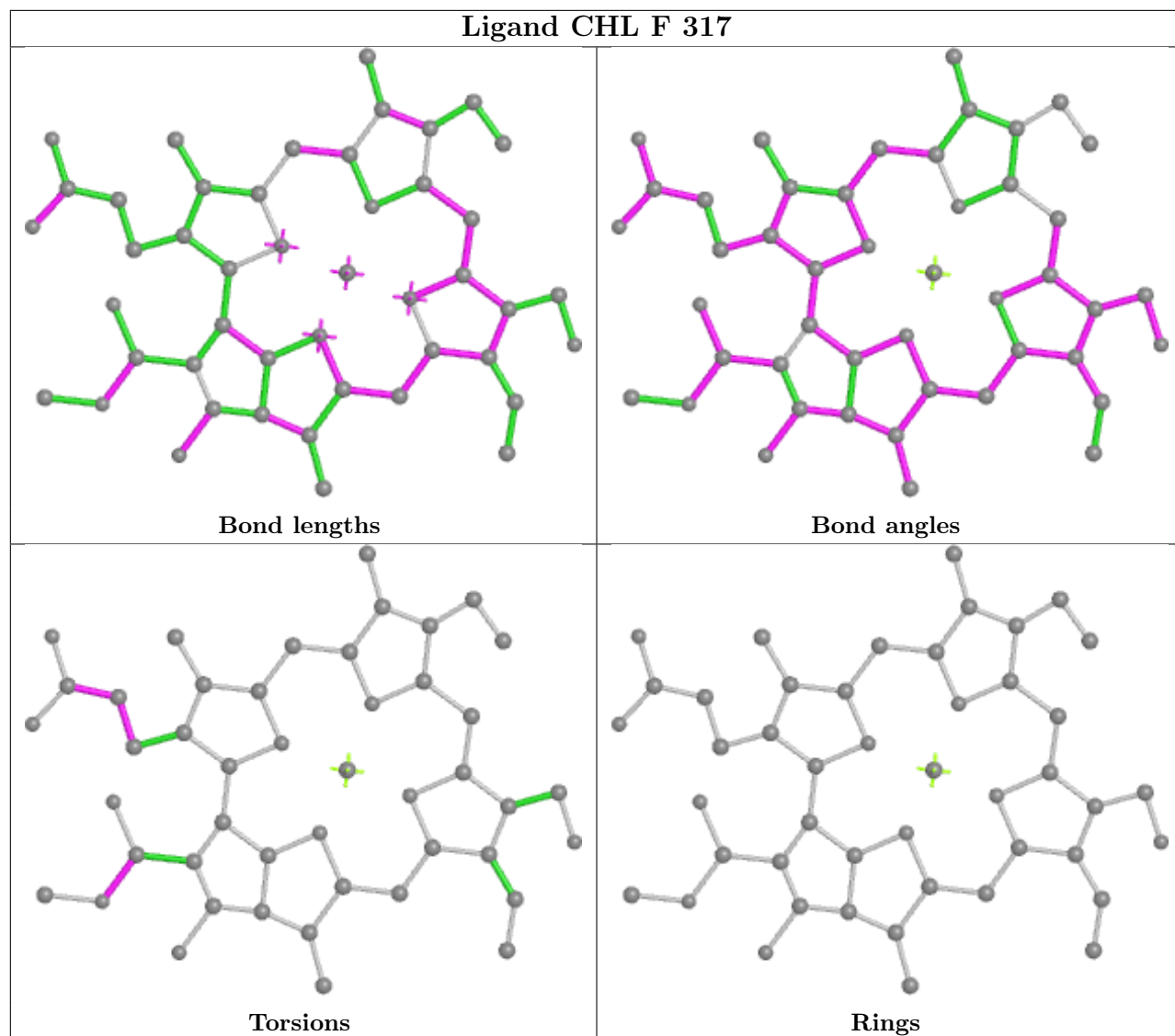


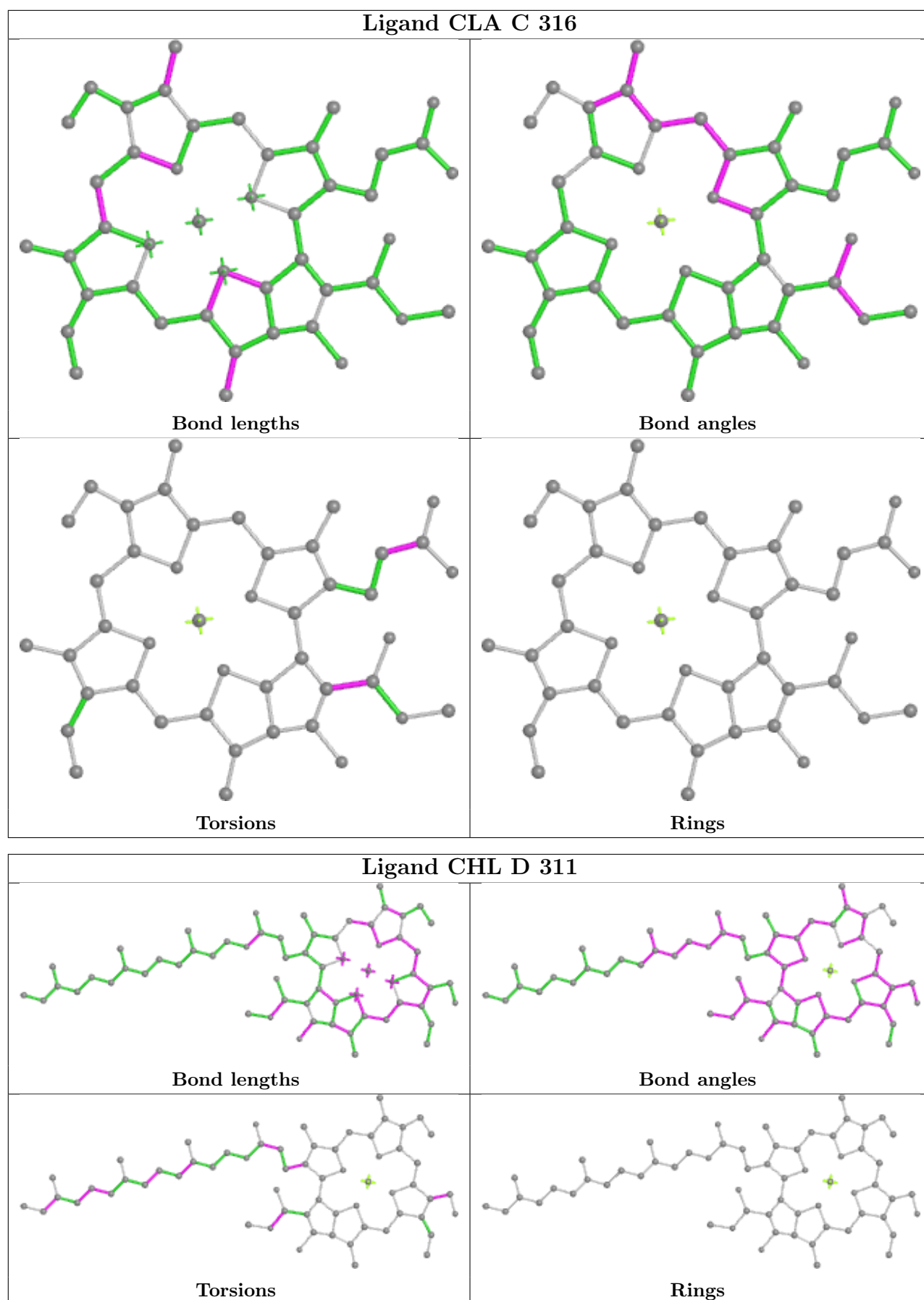


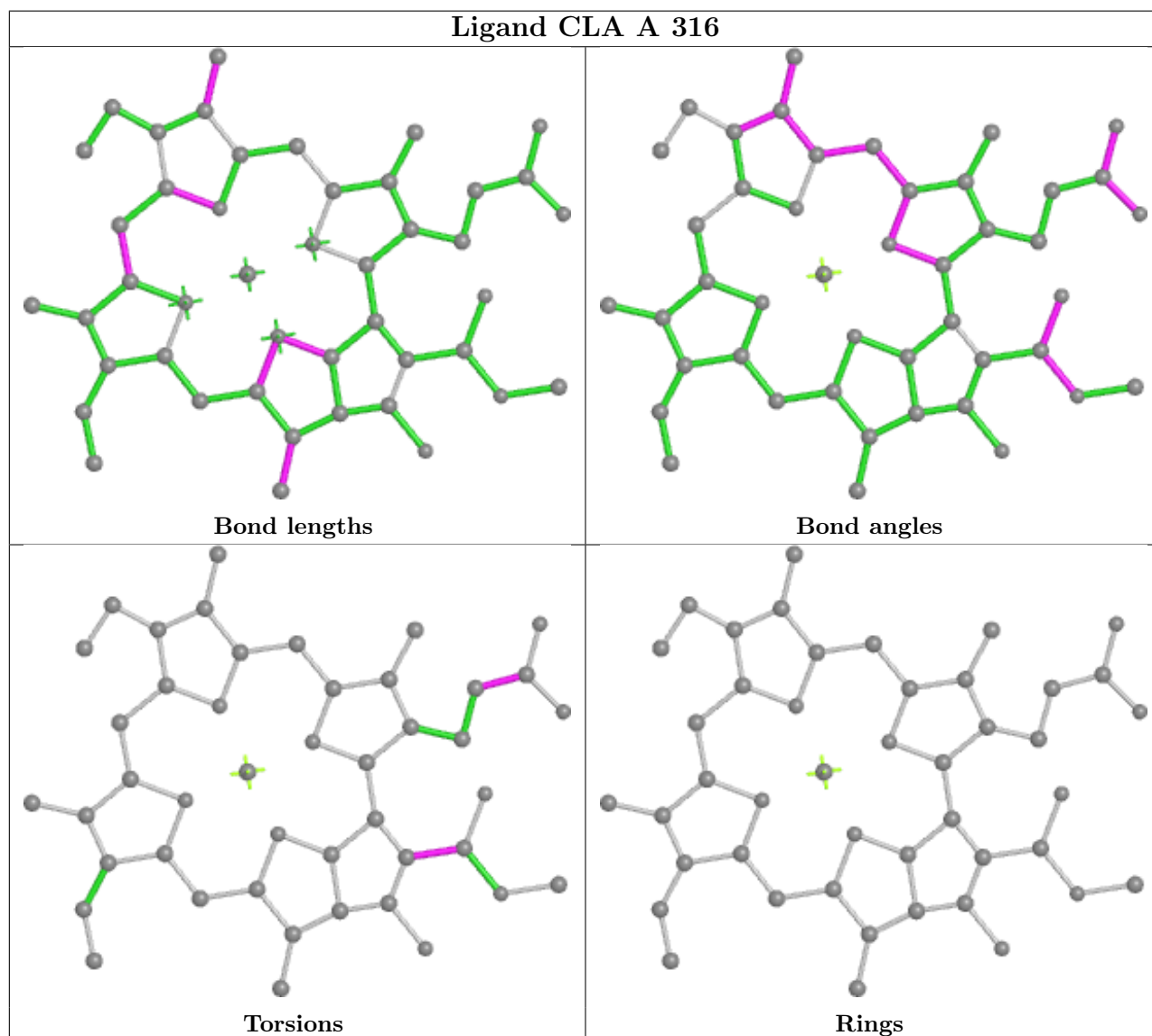
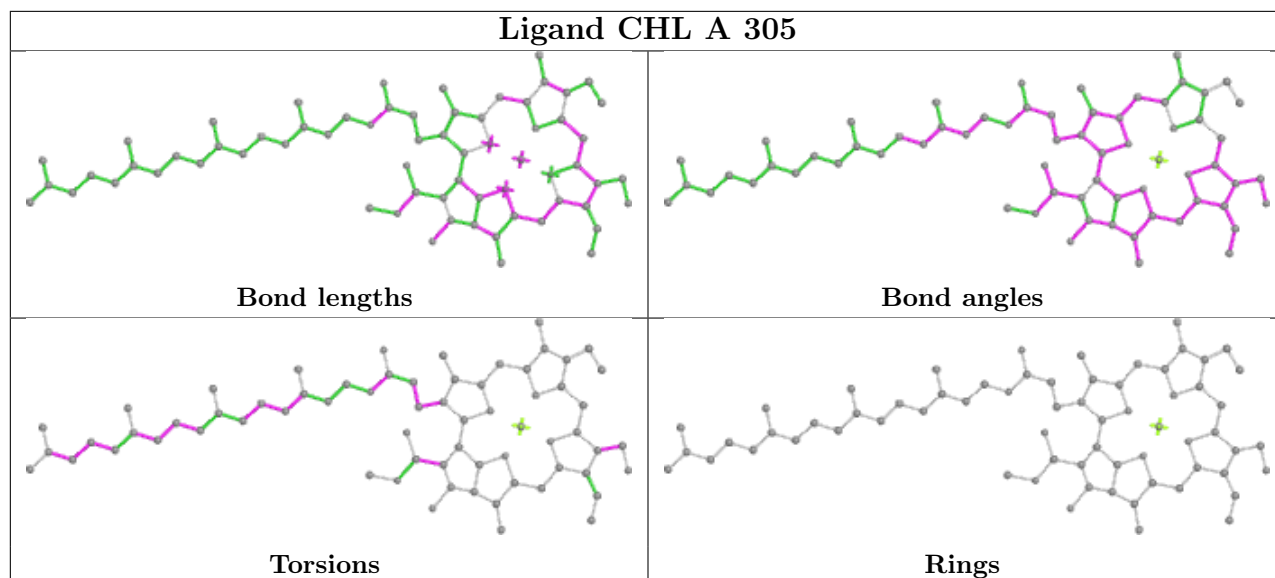


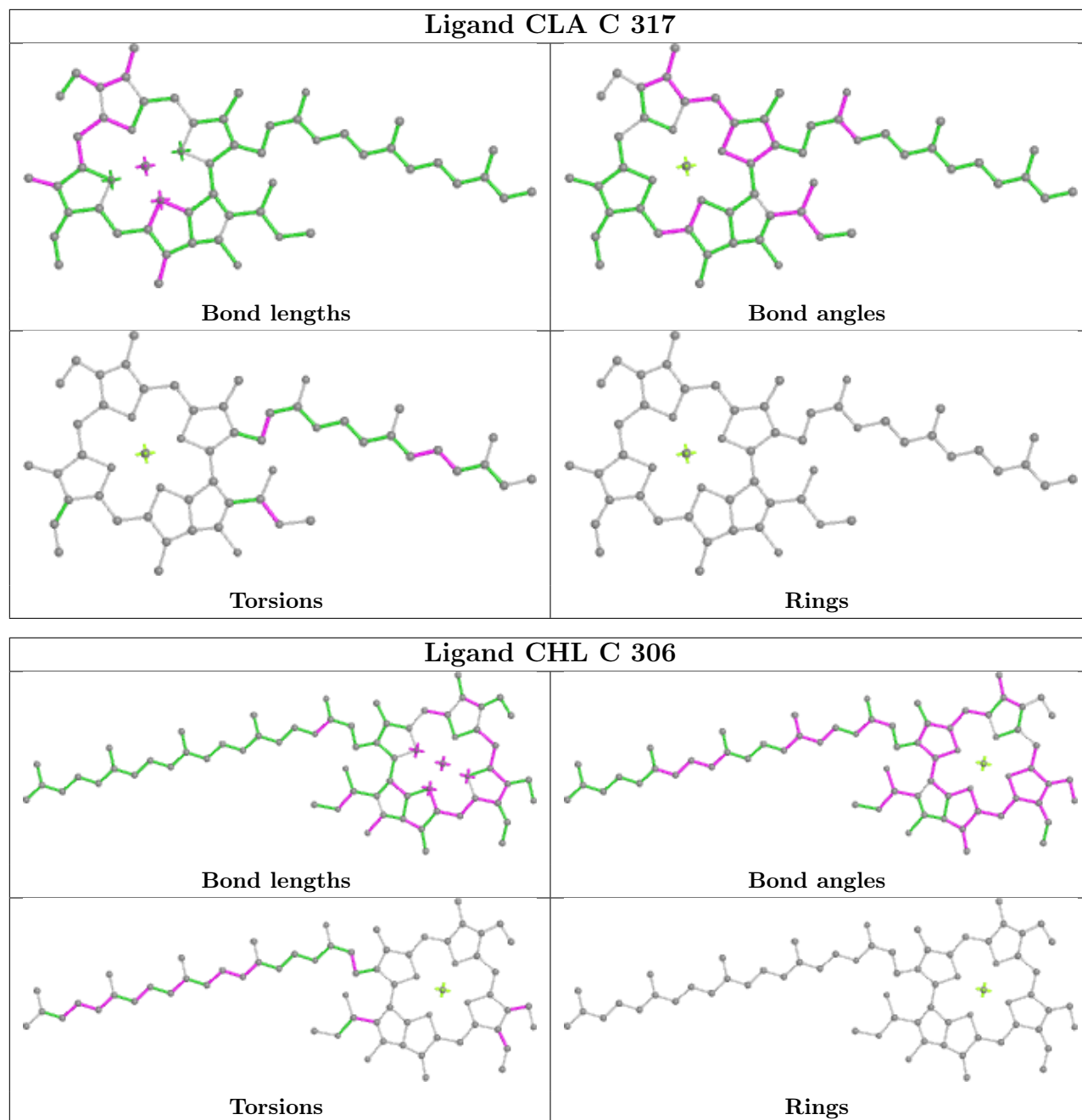


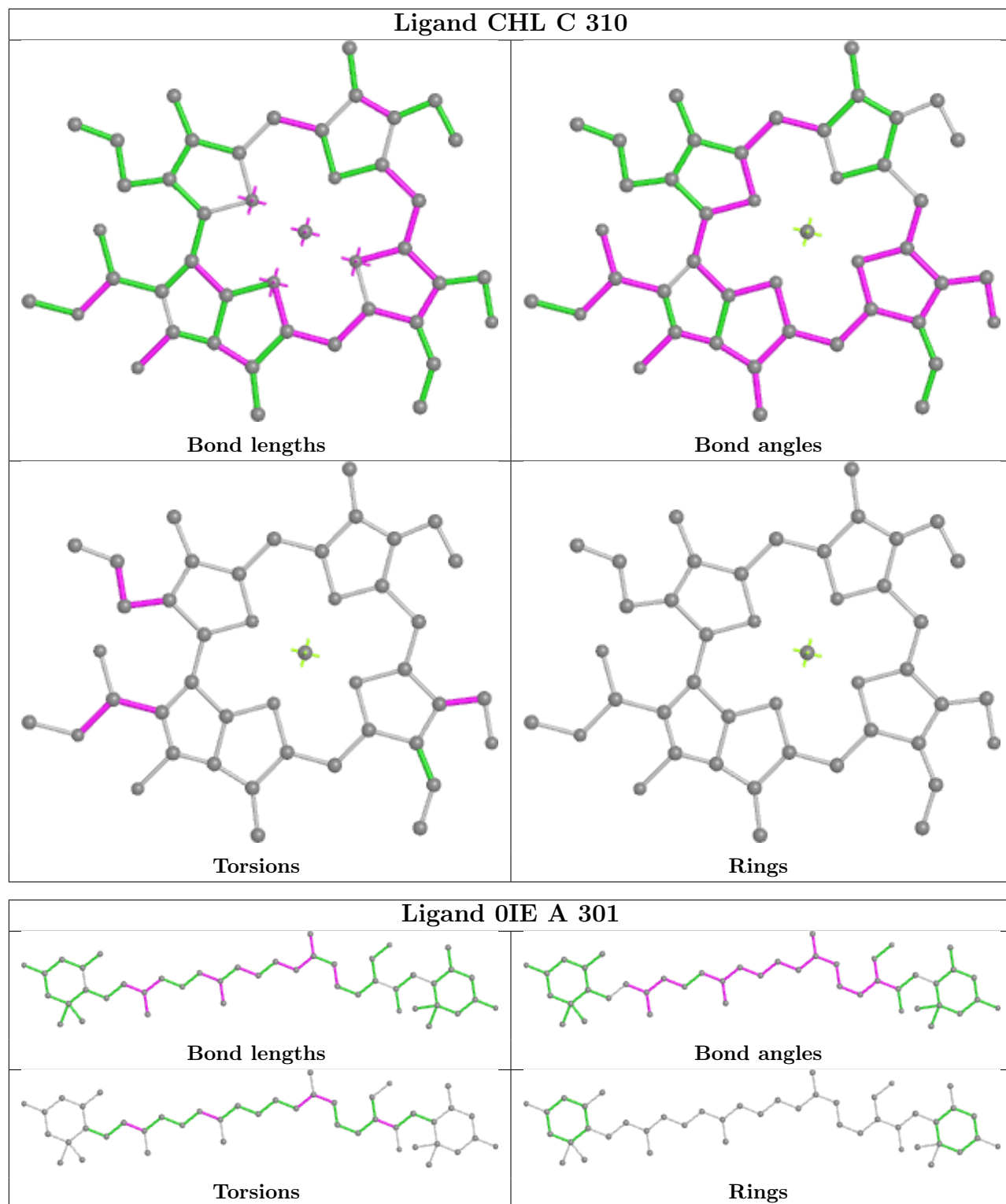


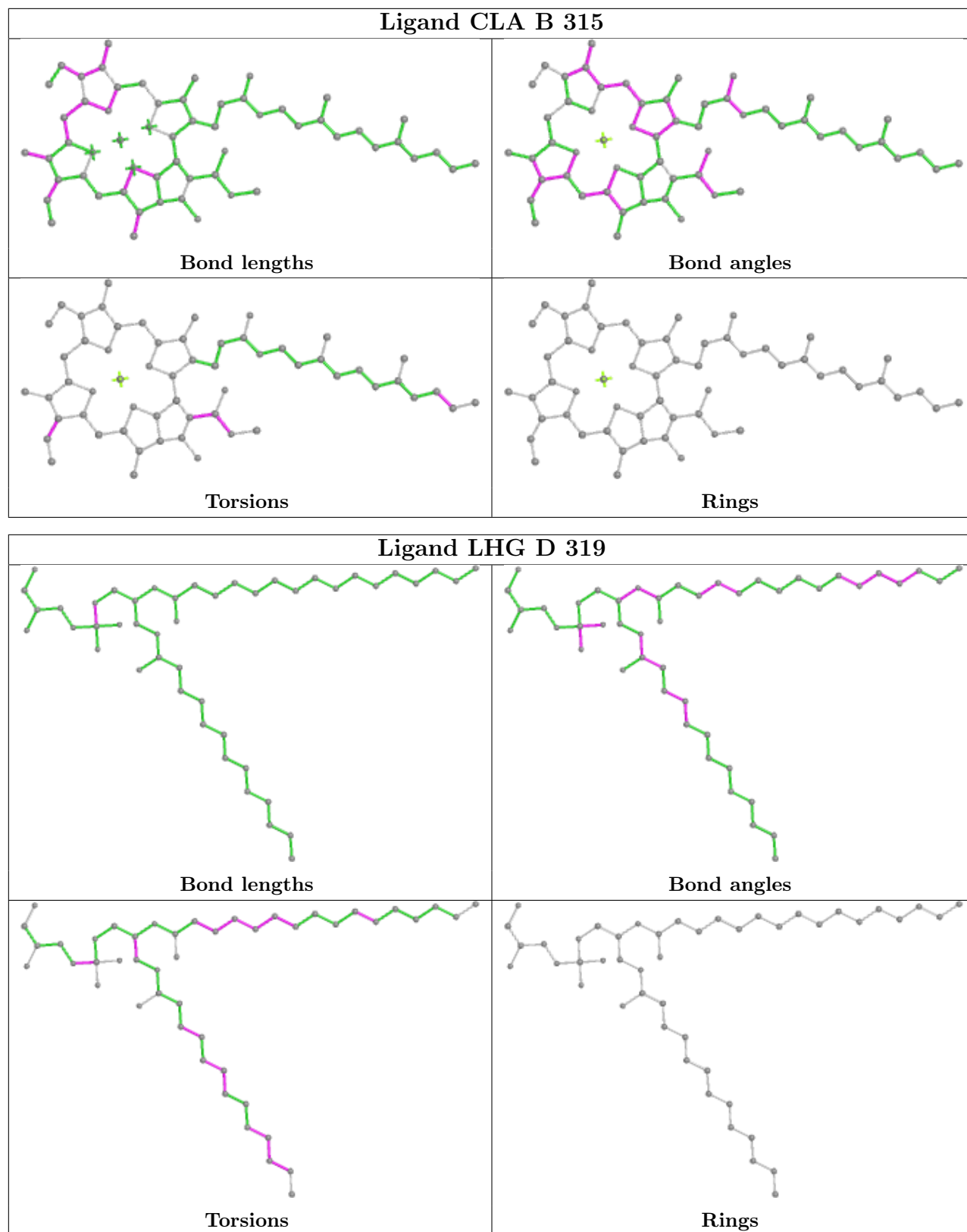


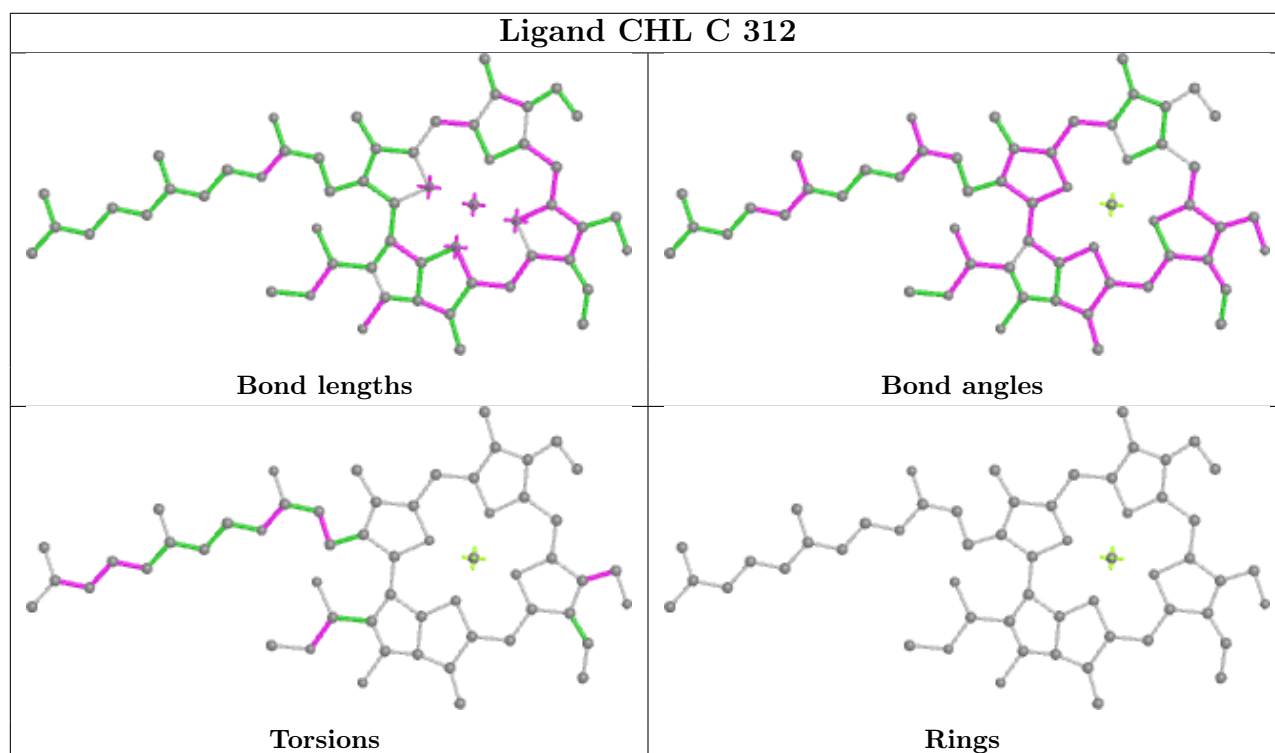
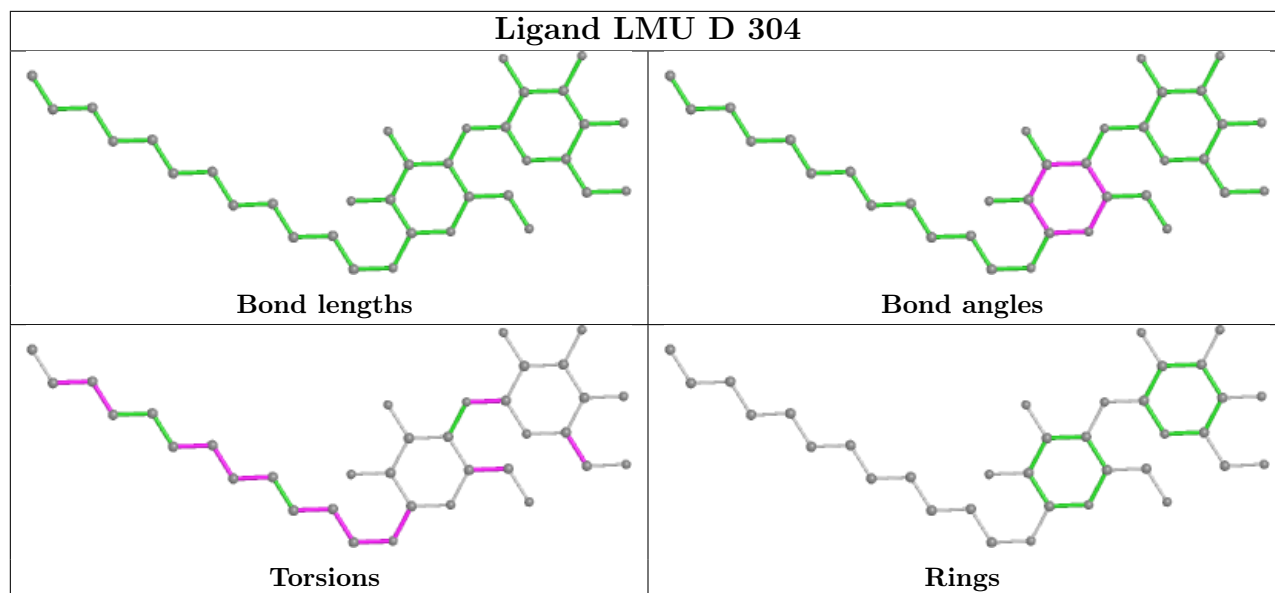




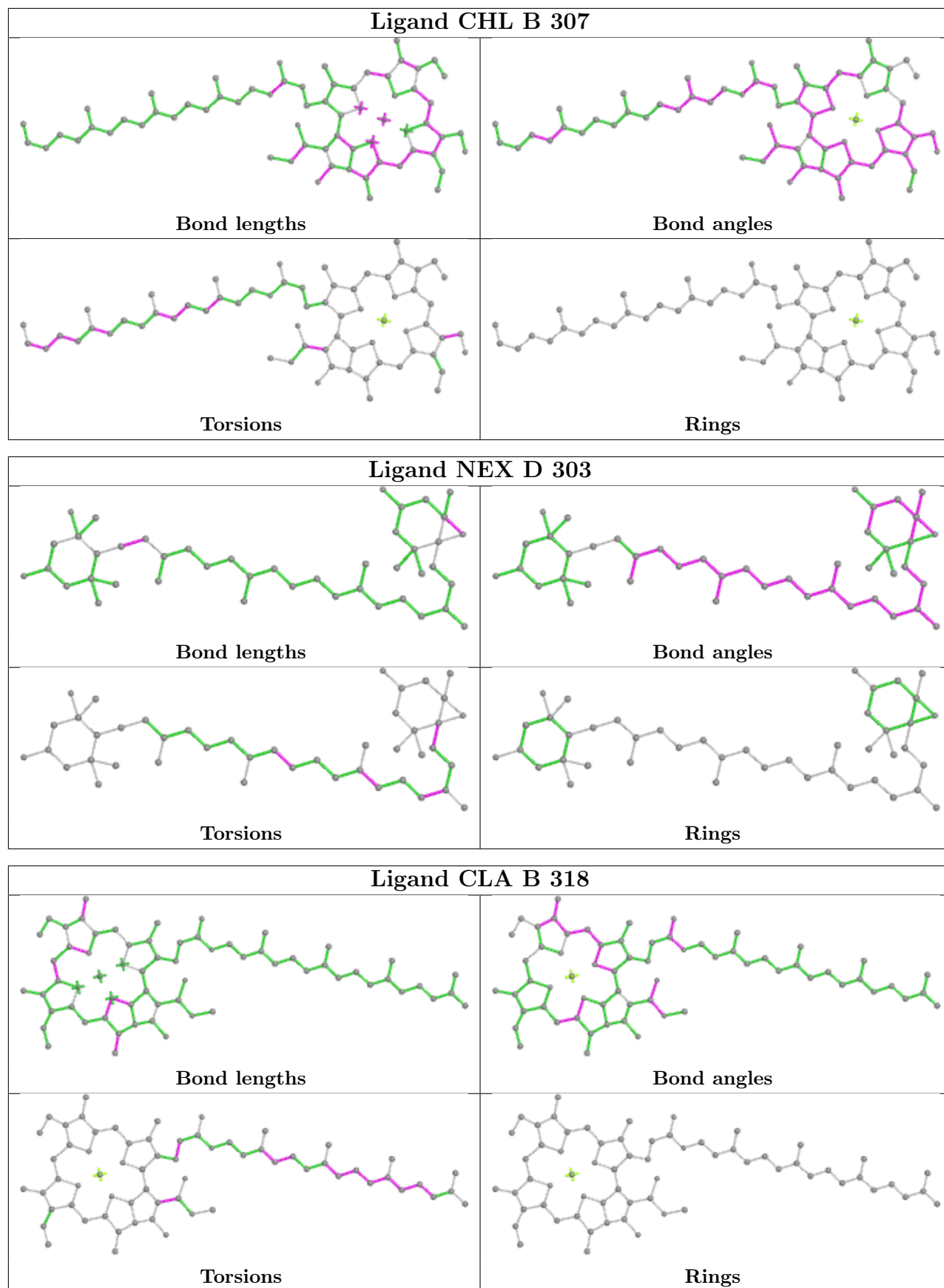


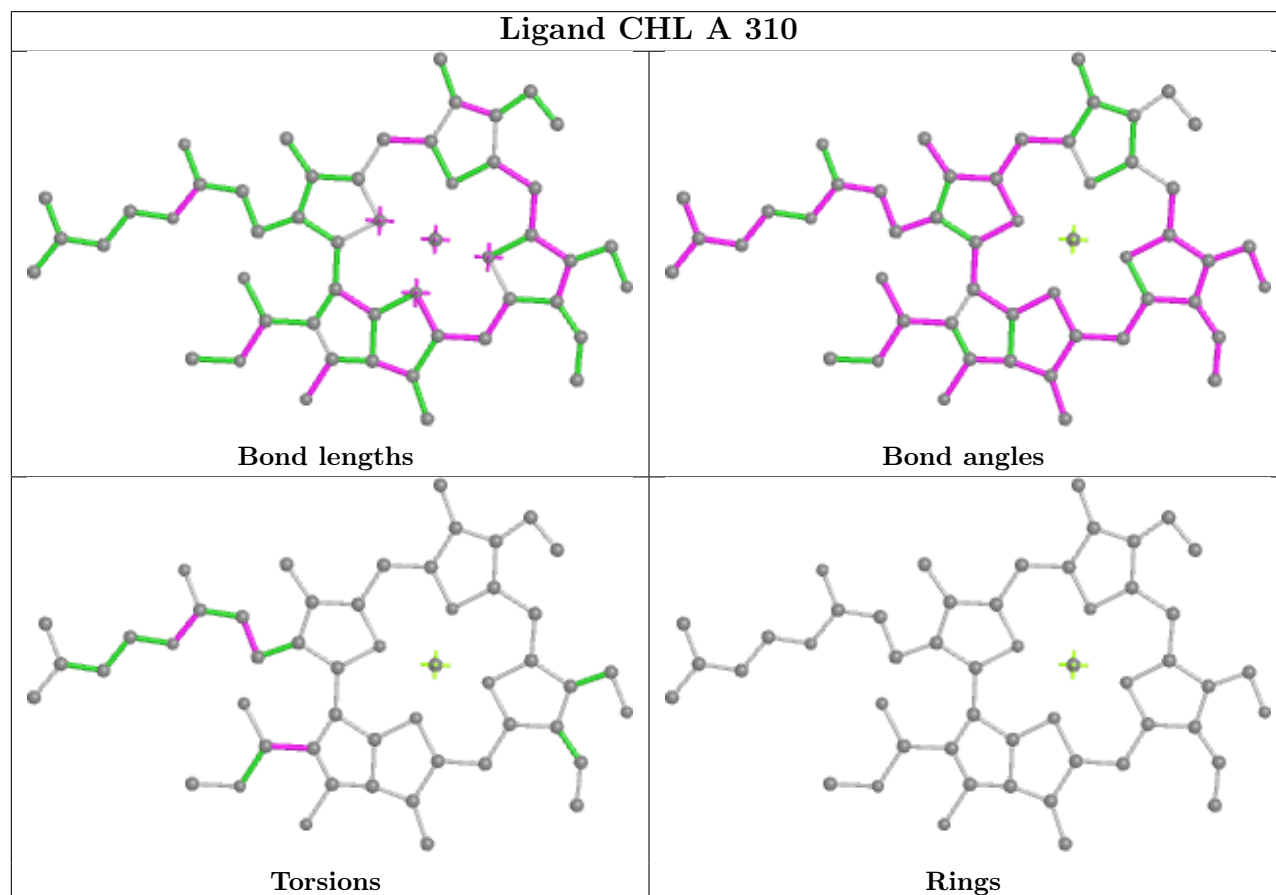
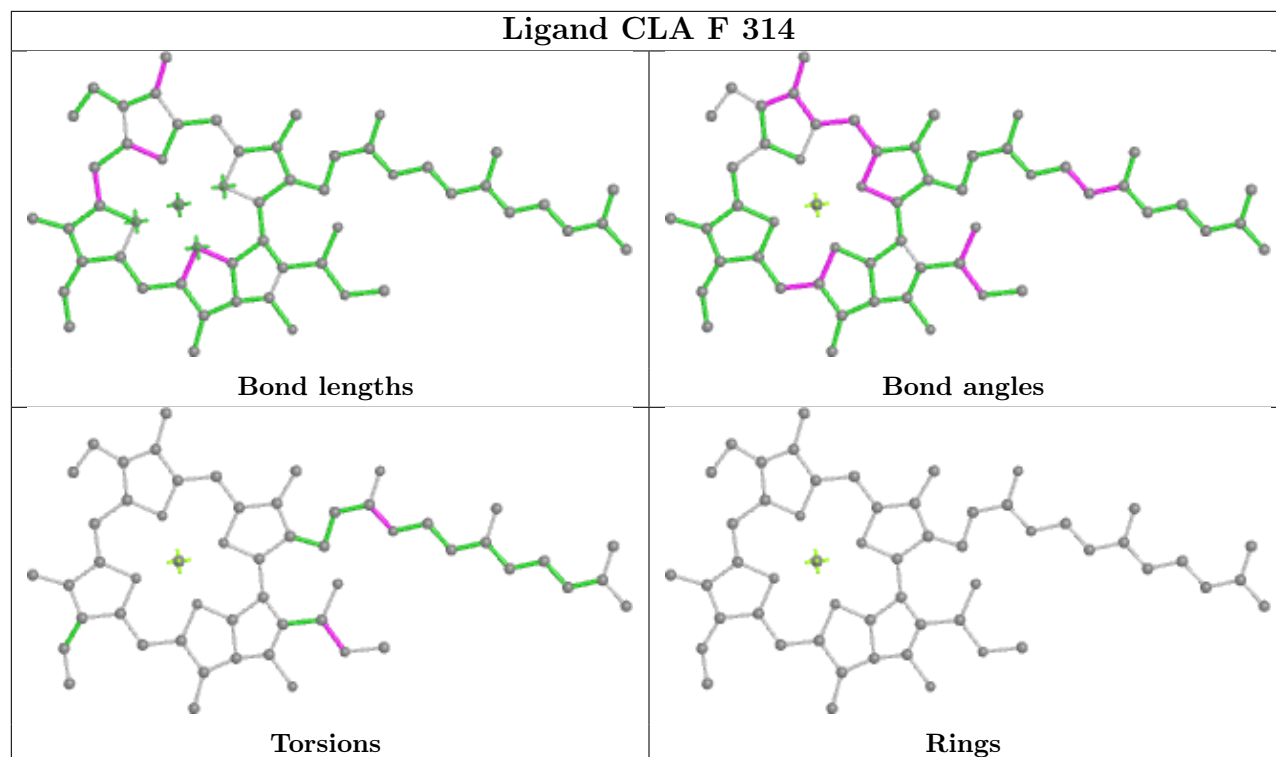


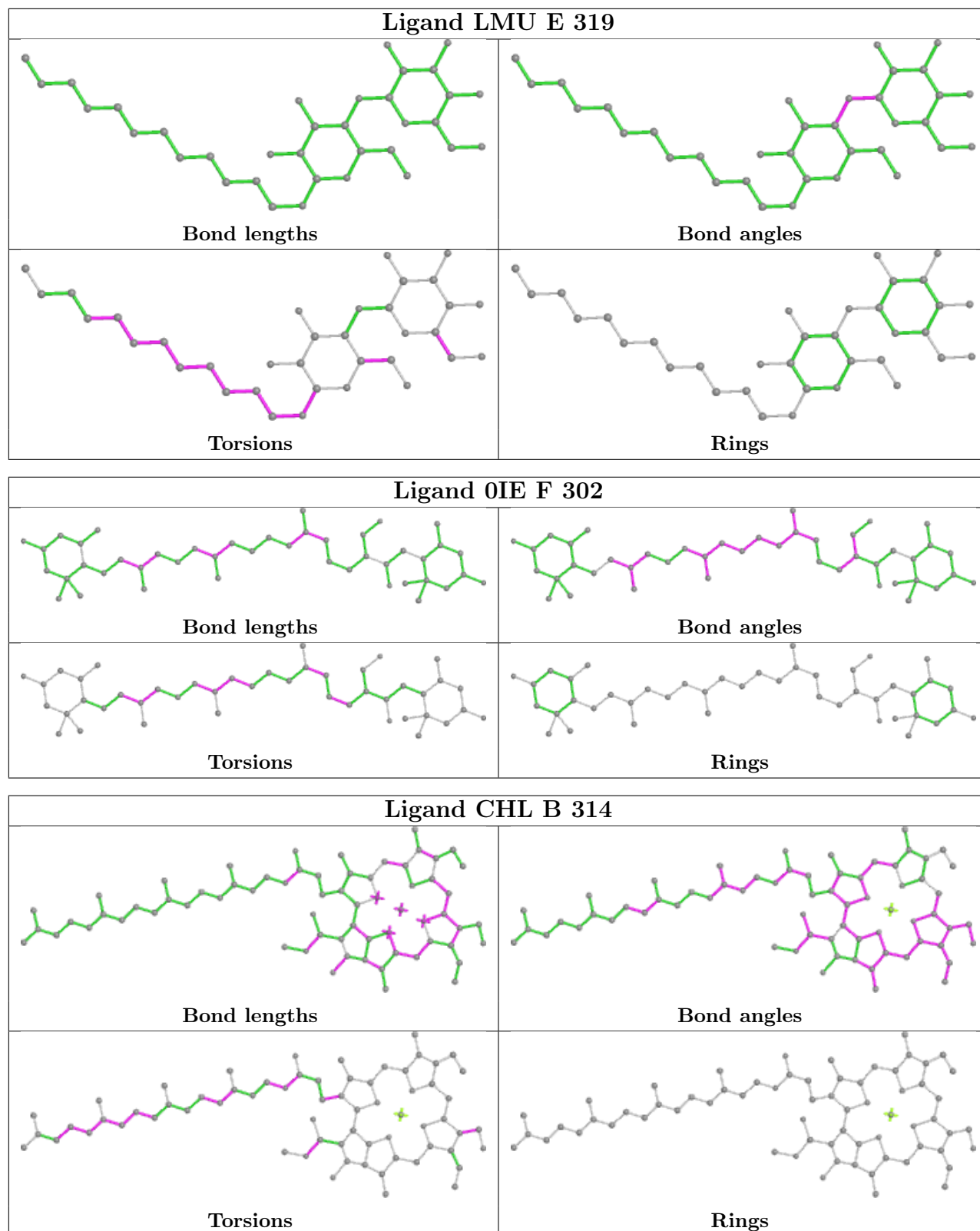


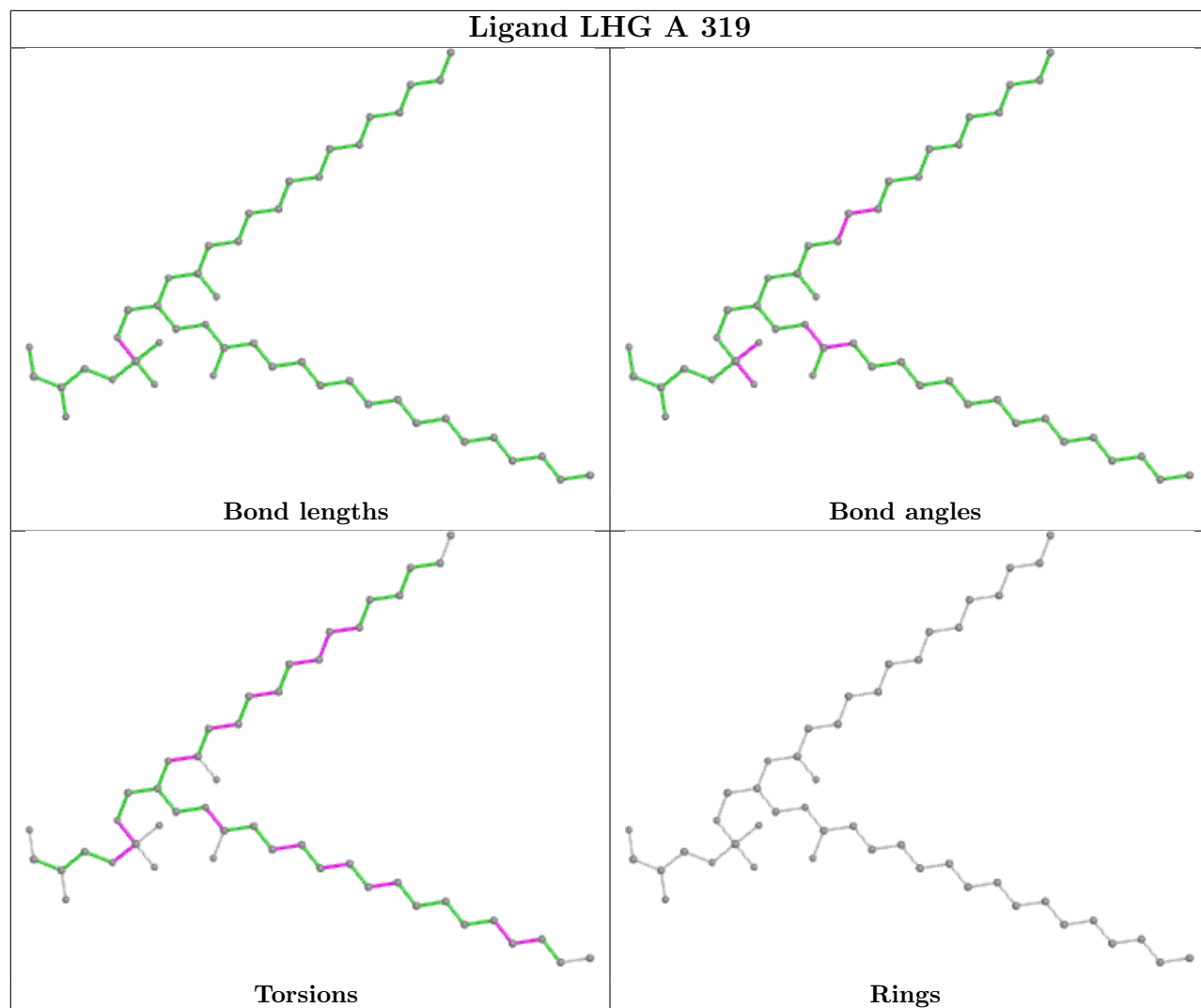


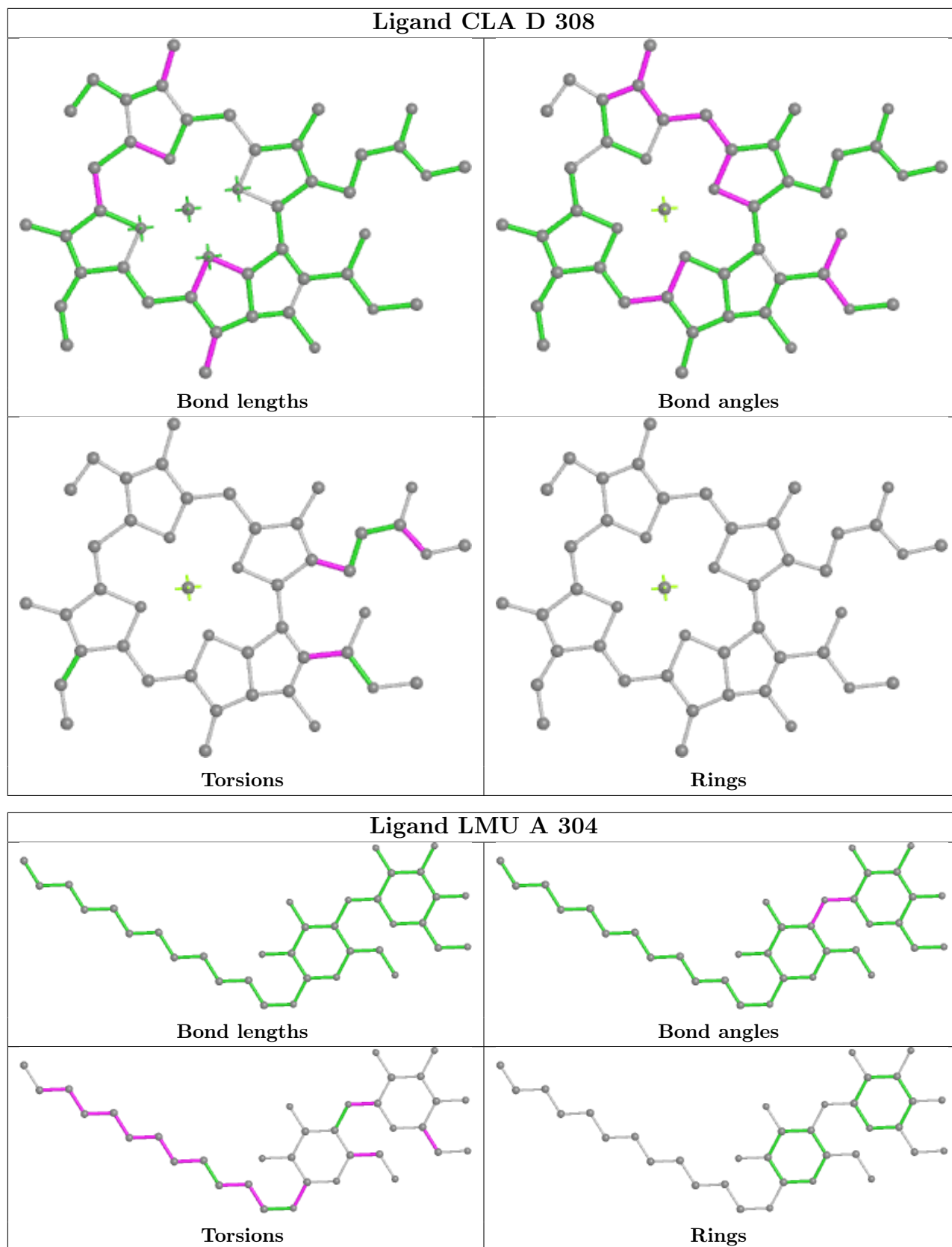


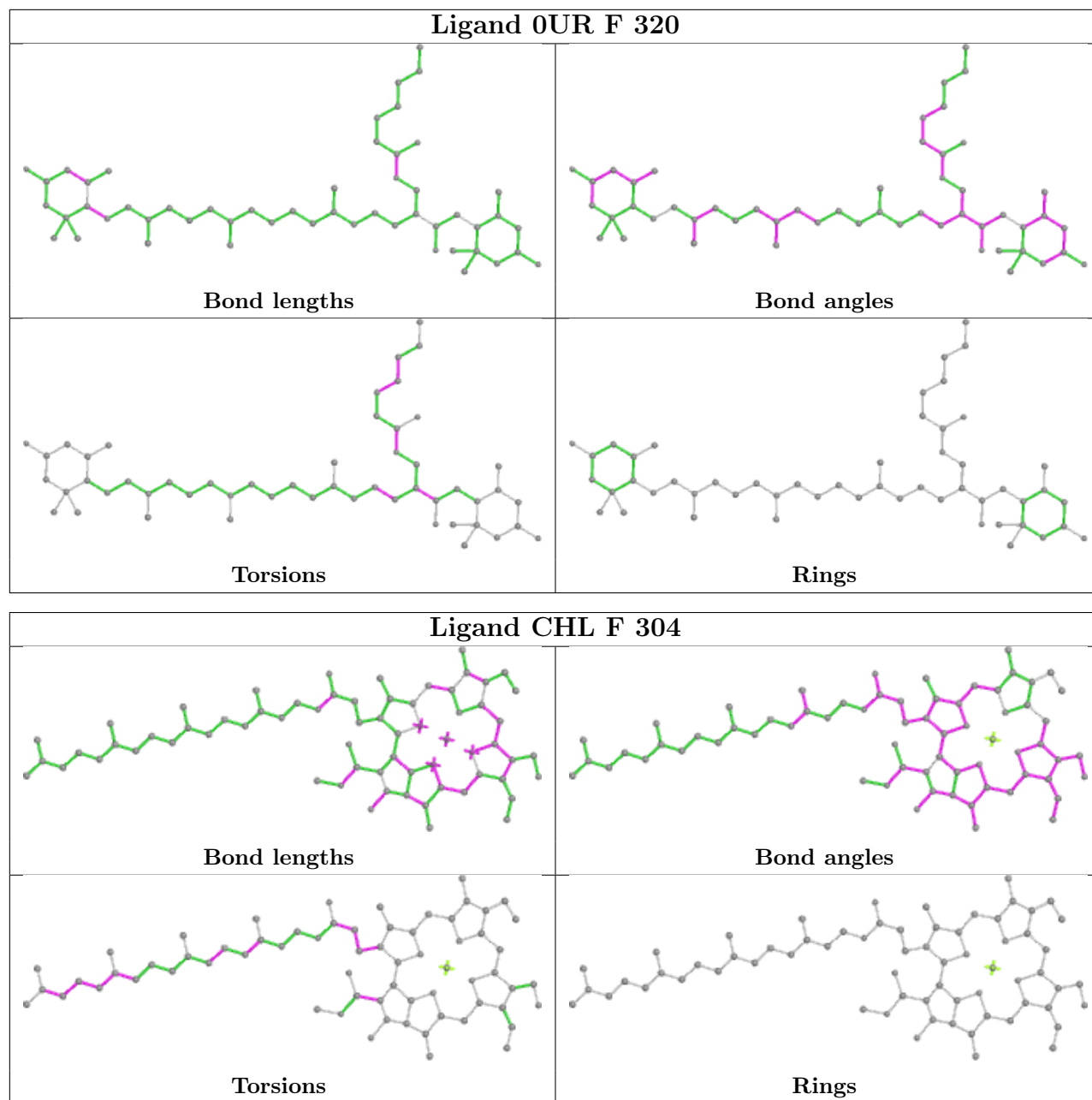


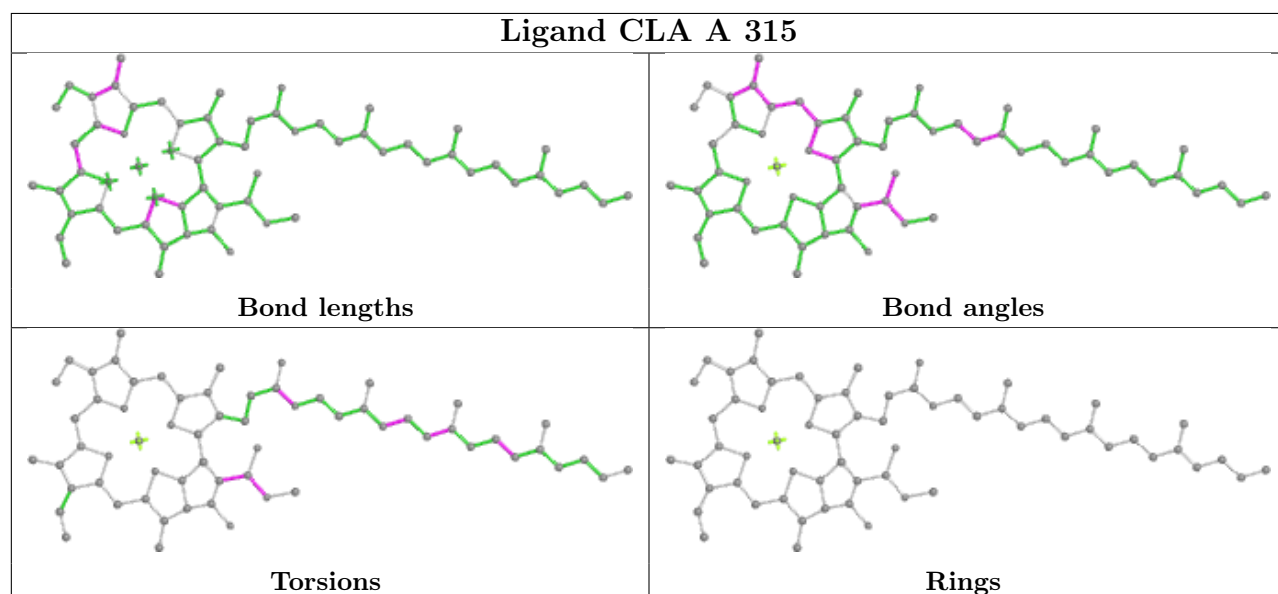
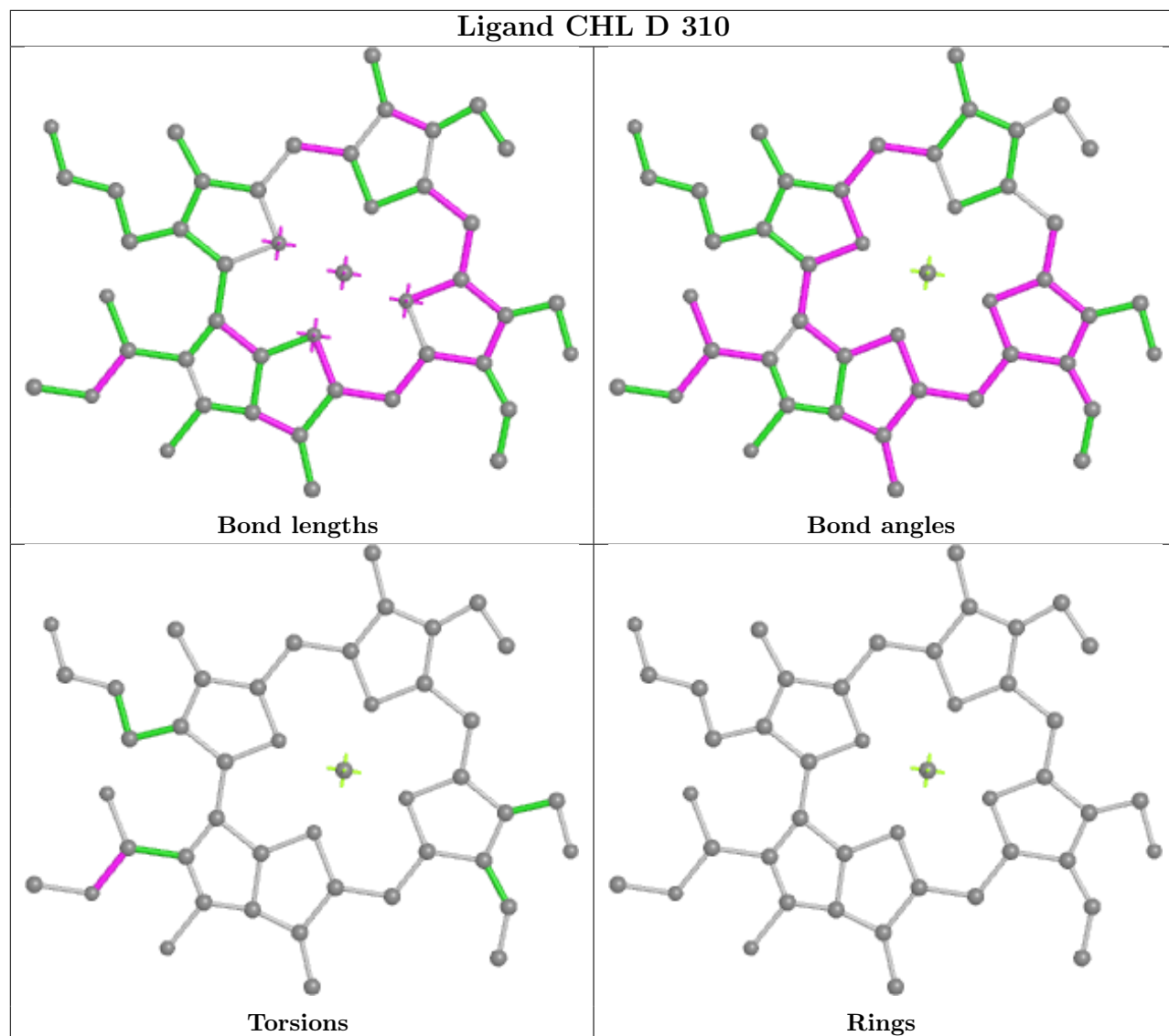


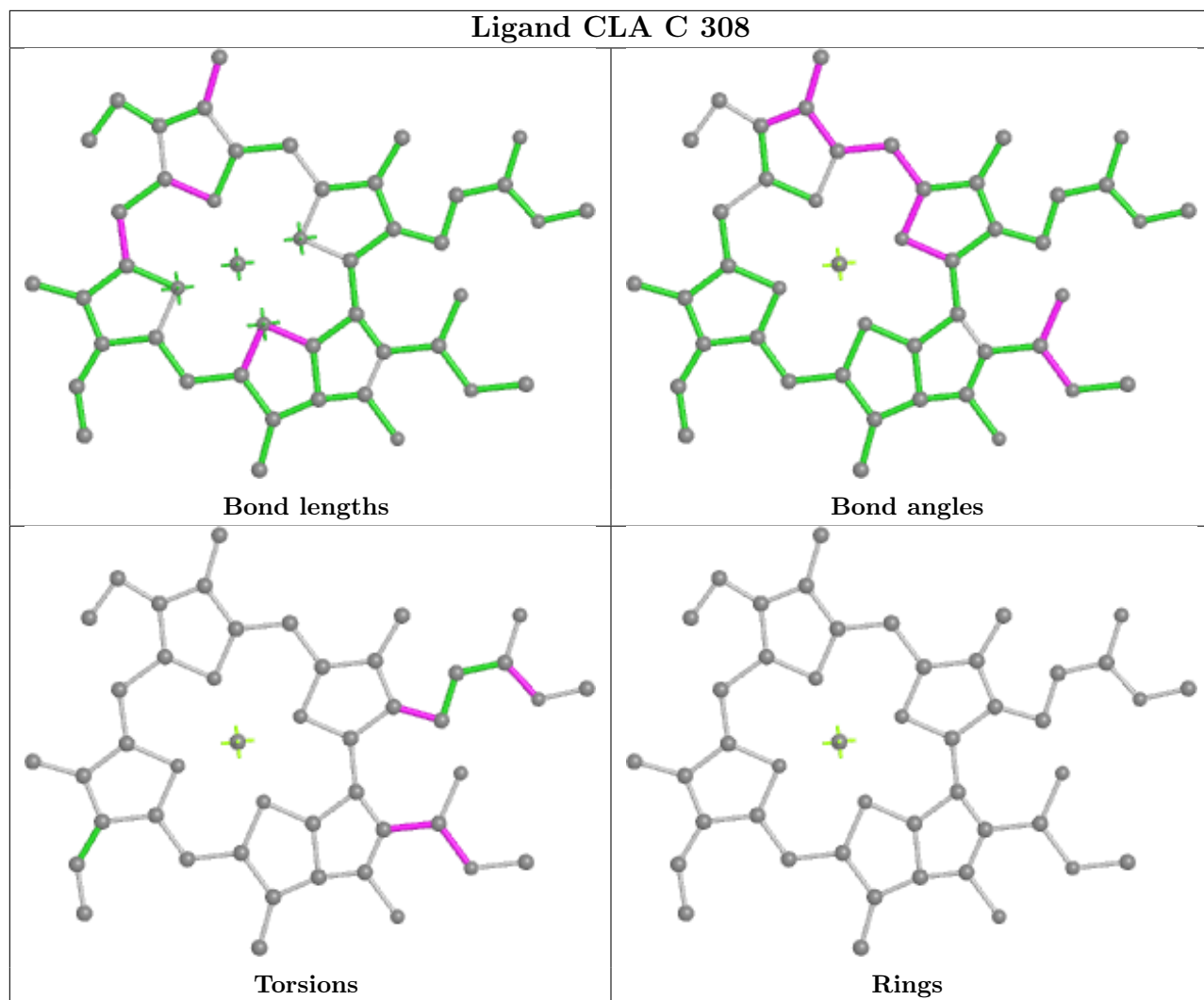




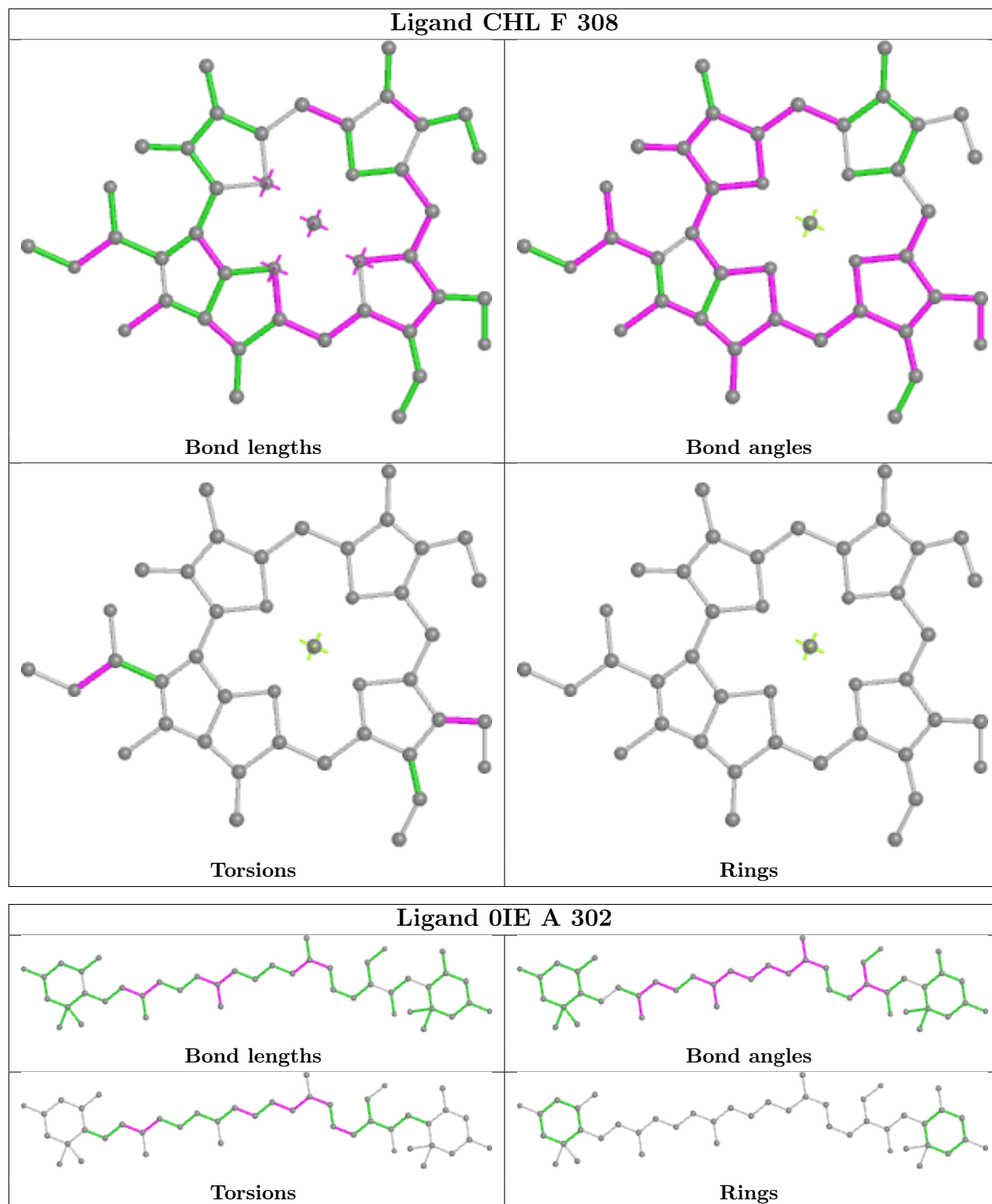


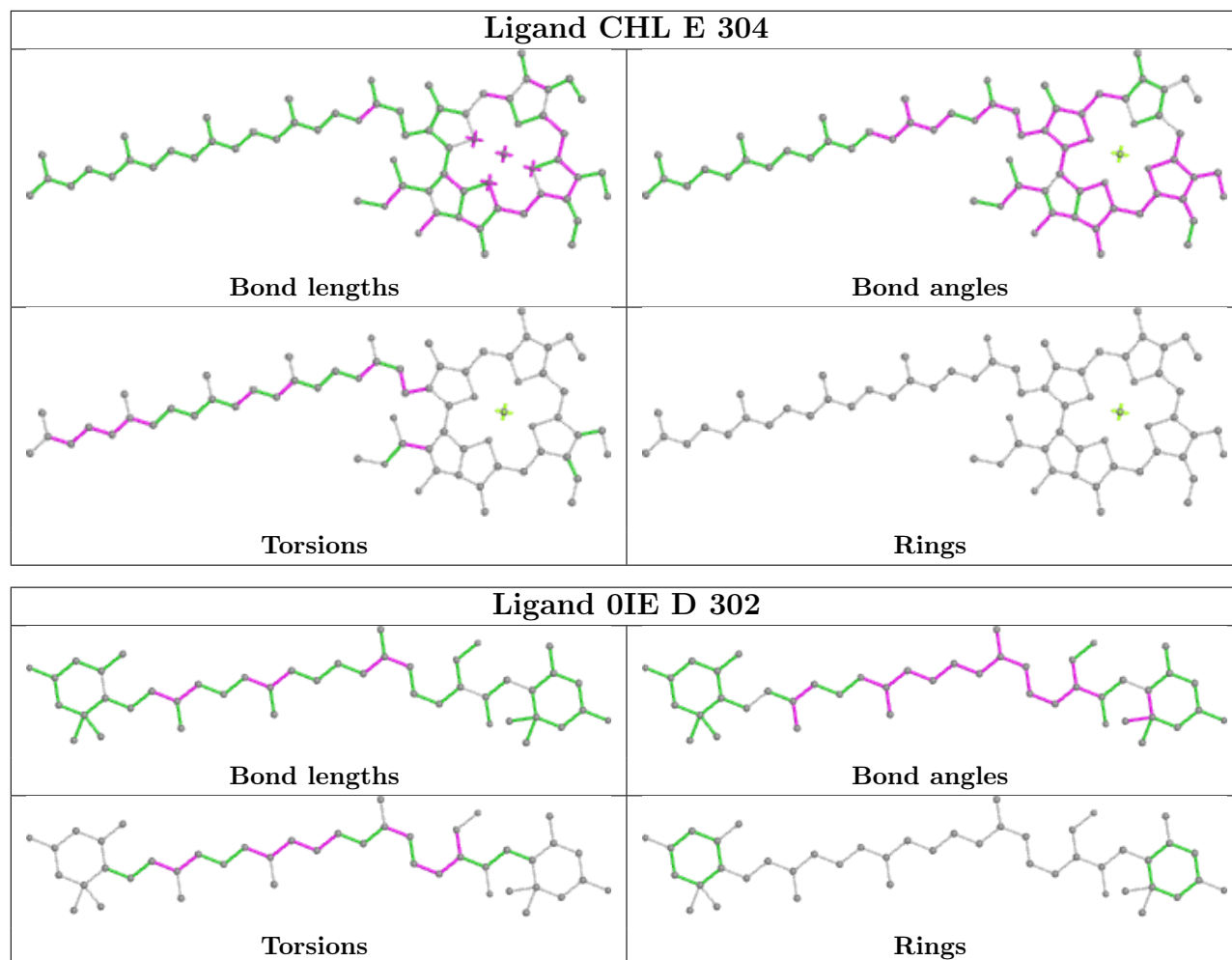


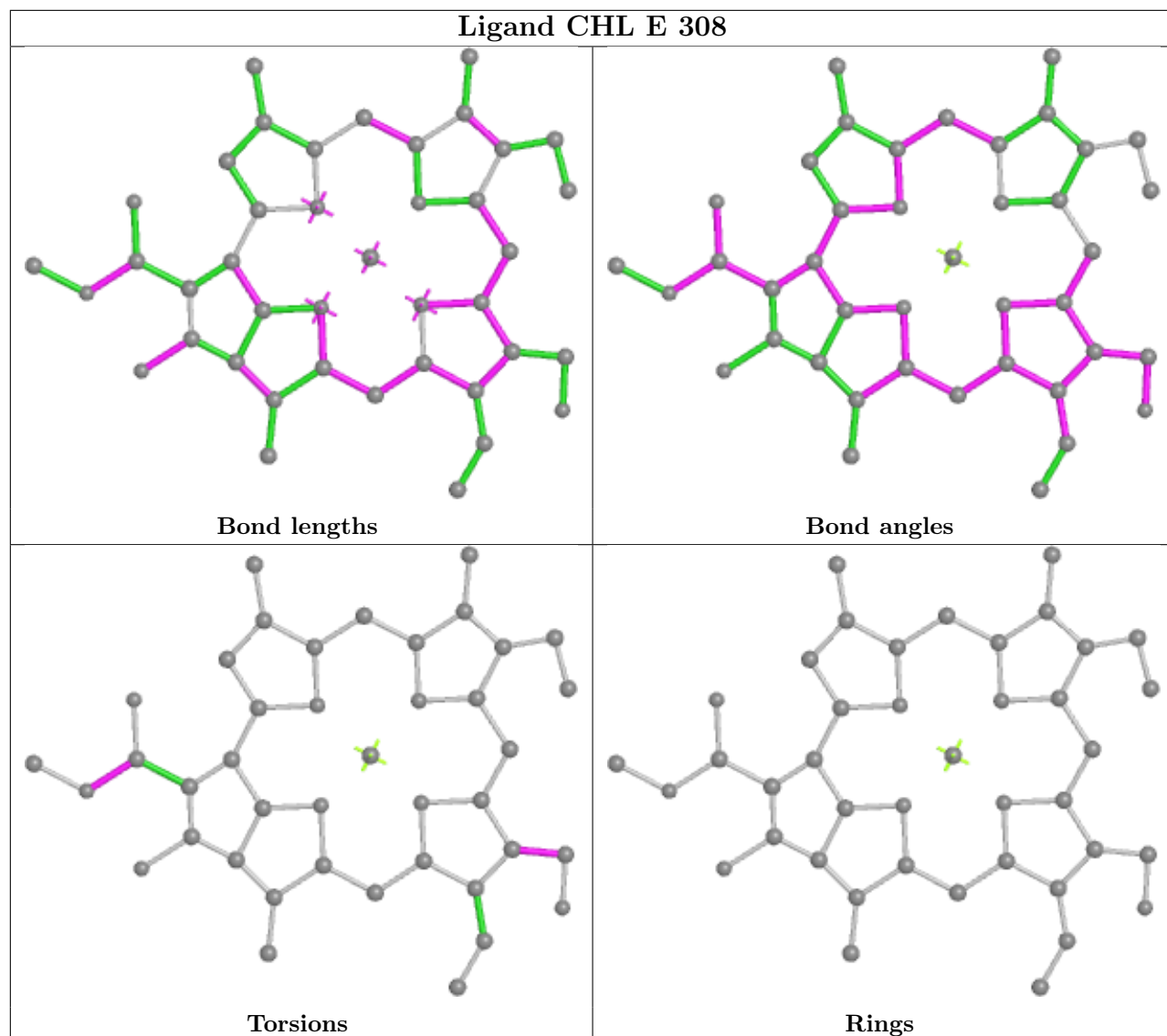


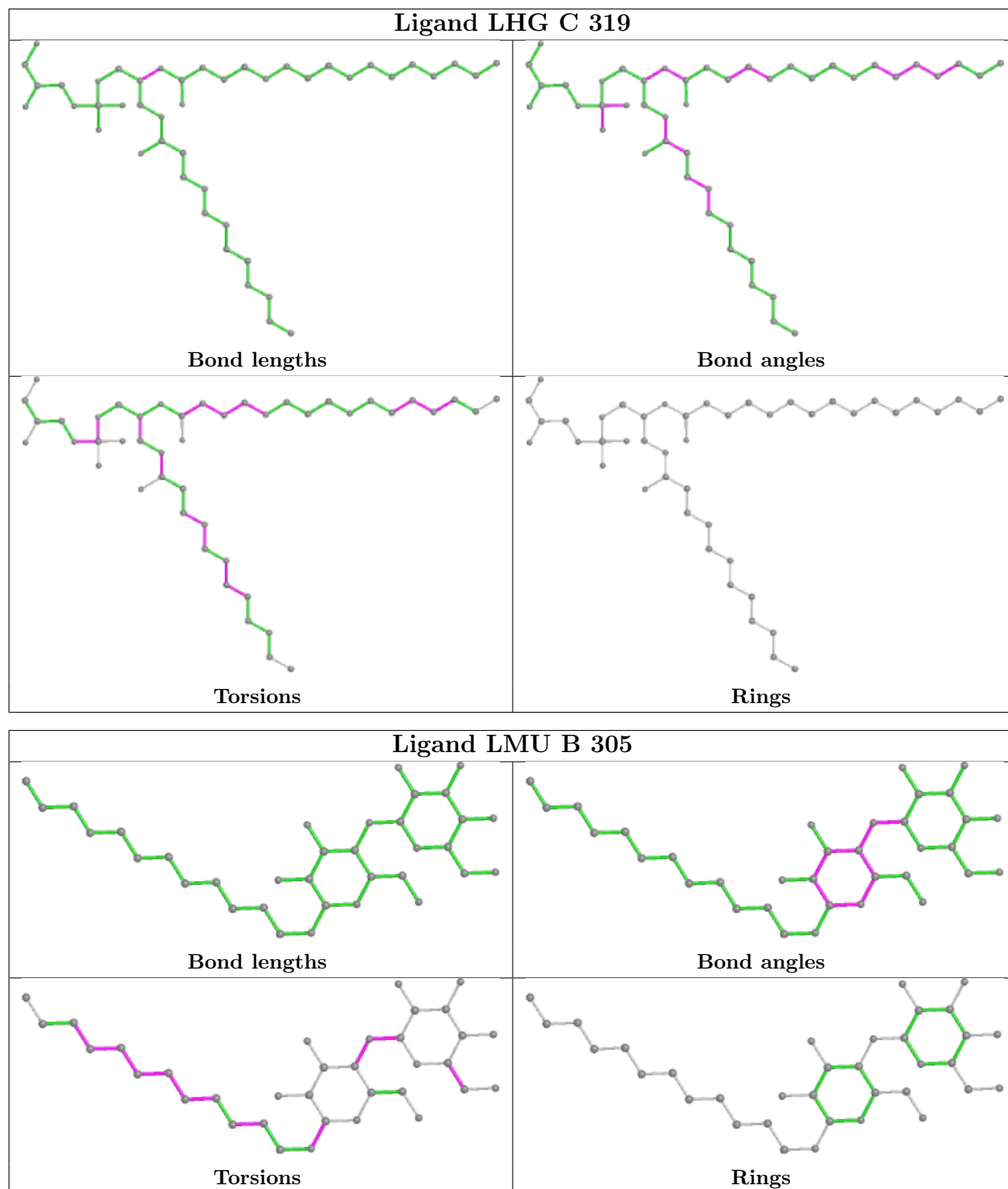


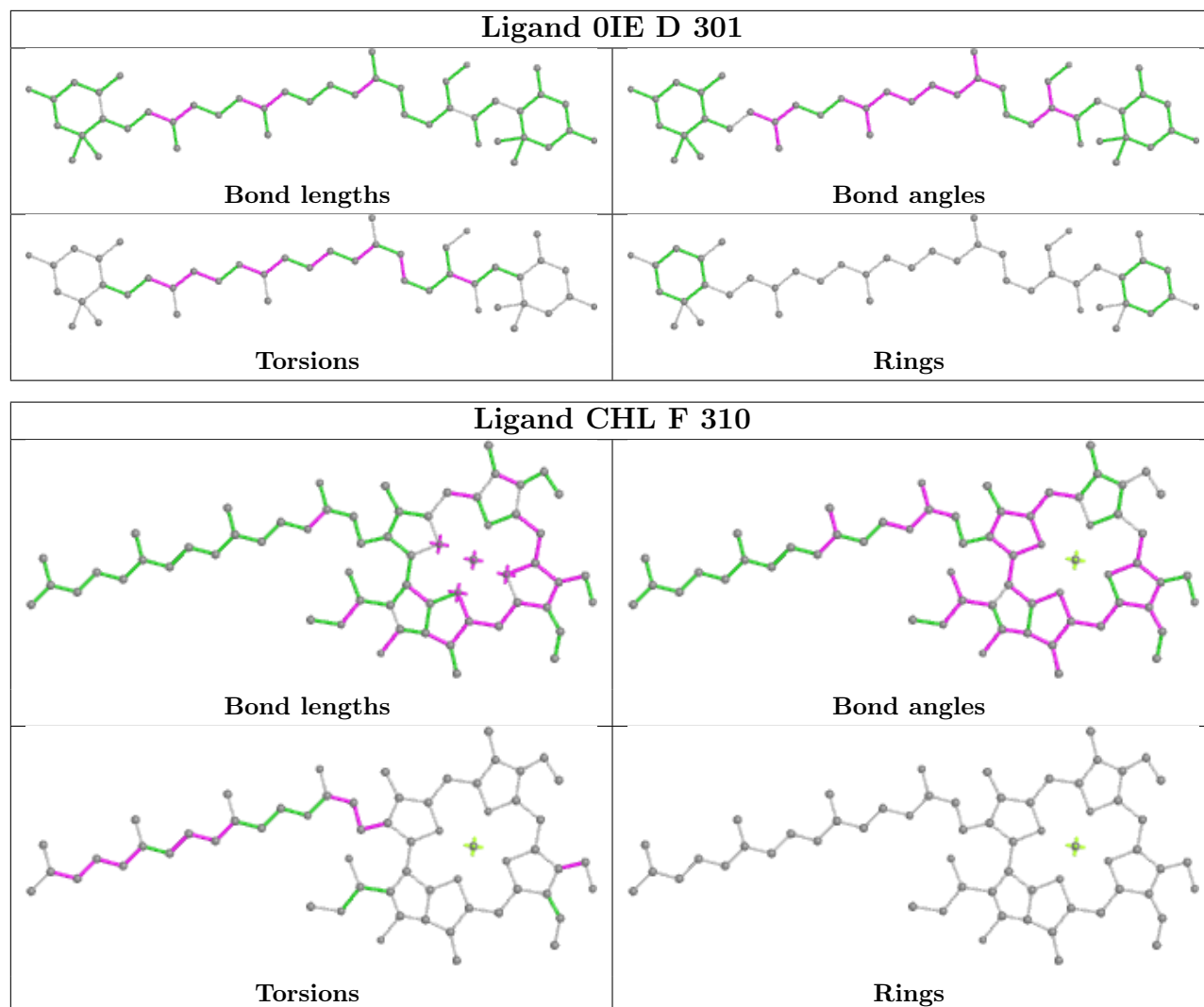












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 223/249 (89%)   | 0.39   | 15 (6%) 17 13 | 37, 79, 118, 154      | 0     |
| 1   | B     | 223/249 (89%)   | 0.19   | 14 (6%) 20 15 | 38, 79, 117, 137      | 0     |
| 1   | C     | 222/249 (89%)   | 0.15   | 18 (8%) 12 8  | 39, 84, 122, 158      | 0     |
| 1   | D     | 223/249 (89%)   | 0.32   | 18 (8%) 12 8  | 43, 80, 120, 151      | 0     |
| 1   | E     | 223/249 (89%)   | 0.55   | 34 (15%) 2 1  | 46, 100, 145, 161     | 0     |
| 1   | F     | 223/249 (89%)   | 0.25   | 14 (6%) 20 15 | 34, 76, 109, 126      | 0     |
| All | All   | 1337/1494 (89%) | 0.31   | 113 (8%) 10 7 | 34, 83, 127, 161      | 0     |

All (113) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 1   | VAL  | 17.1 |
| 1   | F     | 1   | VAL  | 12.1 |
| 1   | E     | 76  | TYR  | 8.3  |
| 1   | E     | 1   | VAL  | 7.4  |
| 1   | E     | 165 | LEU  | 6.7  |
| 1   | D     | 1   | VAL  | 6.3  |
| 1   | E     | 72  | ALA  | 5.8  |
| 1   | E     | 155 | MET  | 5.7  |
| 1   | E     | 77  | GLY  | 5.7  |
| 1   | E     | 137 | LEU  | 5.3  |
| 1   | E     | 73  | LEU  | 5.3  |
| 1   | A     | 134 | GLY  | 5.2  |
| 1   | C     | 76  | TYR  | 5.2  |
| 1   | E     | 74  | GLU  | 4.7  |
| 1   | D     | 203 | ALA  | 4.6  |
| 1   | E     | 79  | VAL  | 4.2  |
| 1   | E     | 81  | PHE  | 4.2  |
| 1   | A     | 203 | ALA  | 4.1  |
| 1   | E     | 149 | ALA  | 4.1  |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | A            | 162        | PHE         | 4.1         |
| 1          | E            | 84         | ALA         | 4.0         |
| 1          | E            | 107        | LEU         | 4.0         |
| 1          | B            | 223        | PHE         | 4.0         |
| 1          | A            | 1          | VAL         | 3.9         |
| 1          | F            | 106        | SER         | 3.8         |
| 1          | E            | 150        | PHE         | 3.7         |
| 1          | E            | 156        | ALA         | 3.6         |
| 1          | E            | 95         | ALA         | 3.6         |
| 1          | A            | 106        | SER         | 3.5         |
| 1          | E            | 136        | PRO         | 3.5         |
| 1          | B            | 78         | GLY         | 3.5         |
| 1          | E            | 154        | GLY         | 3.4         |
| 1          | E            | 157        | ASP         | 3.4         |
| 1          | D            | 6          | PRO         | 3.3         |
| 1          | C            | 78         | GLY         | 3.3         |
| 1          | D            | 159        | PRO         | 3.3         |
| 1          | D            | 3          | PHE         | 3.2         |
| 1          | F            | 115        | ALA         | 3.2         |
| 1          | B            | 152        | PRO         | 3.2         |
| 1          | A            | 107        | LEU         | 3.2         |
| 1          | C            | 208        | ASN         | 3.1         |
| 1          | C            | 103        | GLY         | 3.1         |
| 1          | A            | 137        | LEU         | 3.1         |
| 1          | D            | 196        | GLU         | 3.0         |
| 1          | D            | 200        | GLU         | 3.0         |
| 1          | C            | 105        | PRO         | 2.9         |
| 1          | D            | 199        | ALA         | 2.9         |
| 1          | E            | 168        | LYS         | 2.8         |
| 1          | F            | 95         | ALA         | 2.8         |
| 1          | E            | 135        | GLY         | 2.8         |
| 1          | C            | 107        | LEU         | 2.8         |
| 1          | A            | 104        | ASN         | 2.8         |
| 1          | E            | 161        | THR         | 2.7         |
| 1          | E            | 147        | GLY         | 2.7         |
| 1          | D            | 95         | ALA         | 2.7         |
| 1          | B            | 154        | GLY         | 2.7         |
| 1          | E            | 153        | MET         | 2.7         |
| 1          | C            | 202        | ILE         | 2.7         |
| 1          | F            | 110        | ALA         | 2.7         |
| 1          | F            | 156        | ALA         | 2.6         |
| 1          | D            | 5          | GLY         | 2.6         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | C            | 119        | THR         | 2.5         |
| 1          | A            | 77         | GLY         | 2.5         |
| 1          | E            | 134        | GLY         | 2.5         |
| 1          | A            | 7          | ASP         | 2.5         |
| 1          | B            | 105        | PRO         | 2.5         |
| 1          | B            | 106        | SER         | 2.5         |
| 1          | C            | 106        | SER         | 2.5         |
| 1          | E            | 160        | GLU         | 2.4         |
| 1          | E            | 105        | PRO         | 2.4         |
| 1          | B            | 156        | ALA         | 2.4         |
| 1          | F            | 107        | LEU         | 2.4         |
| 1          | D            | 7          | ASP         | 2.4         |
| 1          | F            | 177        | MET         | 2.4         |
| 1          | B            | 37         | ALA         | 2.4         |
| 1          | E            | 78         | GLY         | 2.4         |
| 1          | F            | 72         | ALA         | 2.3         |
| 1          | A            | 76         | TYR         | 2.3         |
| 1          | A            | 81         | PHE         | 2.3         |
| 1          | C            | 79         | VAL         | 2.3         |
| 1          | A            | 168        | LYS         | 2.3         |
| 1          | C            | 159        | PRO         | 2.3         |
| 1          | E            | 138        | GLY         | 2.2         |
| 1          | C            | 150        | PHE         | 2.2         |
| 1          | B            | 153        | MET         | 2.2         |
| 1          | C            | 149        | ALA         | 2.2         |
| 1          | D            | 162        | PHE         | 2.2         |
| 1          | B            | 39         | LEU         | 2.2         |
| 1          | F            | 39         | LEU         | 2.2         |
| 1          | E            | 158        | ASP         | 2.2         |
| 1          | F            | 160        | GLU         | 2.2         |
| 1          | D            | 156        | ALA         | 2.2         |
| 1          | F            | 153        | MET         | 2.2         |
| 1          | B            | 165        | LEU         | 2.2         |
| 1          | C            | 156        | ALA         | 2.1         |
| 1          | B            | 74         | GLU         | 2.1         |
| 1          | F            | 113        | ILE         | 2.1         |
| 1          | E            | 159        | PRO         | 2.1         |
| 1          | C            | 160        | GLU         | 2.1         |
| 1          | D            | 105        | PRO         | 2.1         |
| 1          | E            | 164        | GLU         | 2.1         |
| 1          | A            | 101        | TYR         | 2.1         |
| 1          | D            | 206        | VAL         | 2.1         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 159 | PRO  | 2.1  |
| 1   | B     | 77  | GLY  | 2.1  |
| 1   | D     | 10  | LEU  | 2.0  |
| 1   | D     | 14  | PRO  | 2.0  |
| 1   | E     | 80  | GLU  | 2.0  |
| 1   | C     | 73  | LEU  | 2.0  |
| 1   | C     | 74  | GLU  | 2.0  |
| 1   | C     | 152 | PRO  | 2.0  |
| 1   | A     | 156 | ALA  | 2.0  |
| 1   | D     | 181 | PHE  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 11  | LMG  | F     | 319 | 30/55 | 0.53 | 0.41 | 127,171,183,186            | 0     |
| 4   | LMU  | B     | 305 | 35/35 | 0.58 | 0.45 | 107,181,190,195            | 0     |
| 10  | BET  | B     | 322 | 8/8   | 0.66 | 0.21 | 90,114,123,132             | 0     |
| 4   | LMU  | E     | 319 | 35/35 | 0.67 | 0.33 | 117,171,194,195            | 0     |
| 7   | LHG  | C     | 304 | 25/49 | 0.68 | 0.35 | 132,176,208,243            | 0     |
| 4   | LMU  | A     | 304 | 35/35 | 0.69 | 0.50 | 115,156,181,187            | 0     |
| 4   | LMU  | B     | 304 | 33/35 | 0.70 | 0.35 | 116,148,174,180            | 0     |
| 10  | BET  | C     | 320 | 8/8   | 0.72 | 0.28 | 112,121,126,133            | 0     |
| 9   | OUR  | B     | 325 | 52/57 | 0.72 | 0.32 | 66,89,116,126              | 0     |
| 3   | NEX  | A     | 303 | 44/44 | 0.73 | 0.42 | 78,96,144,152              | 0     |
| 4   | LMU  | D     | 304 | 35/35 | 0.73 | 0.40 | 86,132,160,170             | 0     |
| 11  | LMG  | B     | 323 | 30/55 | 0.74 | 0.39 | 122,164,179,181            | 0     |
| 10  | BET  | B     | 321 | 8/8   | 0.75 | 0.49 | 85,102,109,114             | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | NEX  | D     | 303 | 44/44 | 0.76 | 0.46 | 65,81,126,145               | 0     |
| 9   | OUR  | D     | 321 | 52/57 | 0.77 | 0.26 | 66,89,116,126               | 0     |
| 9   | OUR  | E     | 320 | 52/57 | 0.80 | 0.32 | 66,89,116,126               | 0     |
| 3   | NEX  | E     | 303 | 44/44 | 0.80 | 0.36 | 101,120,167,186             | 0     |
| 9   | OUR  | A     | 322 | 52/57 | 0.80 | 0.24 | 66,89,116,126               | 0     |
| 9   | OUR  | F     | 320 | 52/57 | 0.81 | 0.26 | 66,89,116,126               | 0     |
| 7   | LHG  | B     | 324 | 31/49 | 0.81 | 0.26 | 56,98,121,145               | 0     |
| 8   | MG   | A     | 321 | 1/1   | 0.81 | 0.77 | 74,74,74,74                 | 0     |
| 8   | MG   | A     | 320 | 1/1   | 0.84 | 0.18 | 83,83,83,83                 | 0     |
| 9   | OUR  | C     | 321 | 52/57 | 0.84 | 0.22 | 66,89,116,126               | 0     |
| 3   | NEX  | B     | 303 | 44/44 | 0.85 | 0.24 | 76,95,144,165               | 0     |
| 2   | OIE  | A     | 301 | 44/44 | 0.85 | 0.32 | 37,50,66,77                 | 0     |
| 6   | CLA  | D     | 317 | 65/65 | 0.85 | 0.24 | 66,85,110,114               | 0     |
| 2   | OIE  | D     | 302 | 44/44 | 0.86 | 0.17 | 74,87,104,108               | 0     |
| 7   | LHG  | A     | 319 | 47/49 | 0.87 | 0.26 | 49,74,99,106                | 0     |
| 3   | NEX  | F     | 303 | 44/44 | 0.87 | 0.22 | 71,92,168,179               | 0     |
| 2   | OIE  | A     | 302 | 44/44 | 0.88 | 0.21 | 55,73,85,103                | 0     |
| 9   | OUR  | B     | 302 | 50/57 | 0.88 | 0.26 | 67,87,107,123               | 0     |
| 5   | CHL  | E     | 310 | 61/66 | 0.88 | 0.22 | 62,79,92,98                 | 0     |
| 5   | CHL  | E     | 312 | 66/66 | 0.88 | 0.24 | 46,76,90,100                | 0     |
| 7   | LHG  | C     | 319 | 45/49 | 0.89 | 0.20 | 59,84,108,139               | 0     |
| 5   | CHL  | A     | 312 | 56/66 | 0.89 | 0.23 | 51,74,104,117               | 0     |
| 2   | OIE  | F     | 301 | 44/44 | 0.89 | 0.26 | 29,43,65,81                 | 0     |
| 5   | CHL  | E     | 311 | 56/66 | 0.89 | 0.33 | 94,112,141,146              | 0     |
| 5   | CHL  | A     | 310 | 51/66 | 0.89 | 0.22 | 59,90,124,133               | 0     |
| 5   | CHL  | F     | 309 | 42/66 | 0.90 | 0.18 | 62,80,94,103                | 0     |
| 7   | LHG  | F     | 318 | 45/49 | 0.90 | 0.22 | 42,63,78,85                 | 0     |
| 6   | CLA  | A     | 308 | 50/65 | 0.90 | 0.20 | 68,88,102,119               | 0     |
| 6   | CLA  | A     | 315 | 63/65 | 0.90 | 0.26 | 66,86,99,109                | 0     |
| 5   | CHL  | D     | 306 | 65/66 | 0.90 | 0.29 | 42,58,76,89                 | 0     |
| 2   | OIE  | B     | 301 | 44/44 | 0.90 | 0.26 | 33,46,75,79                 | 0     |
| 5   | CHL  | B     | 310 | 43/66 | 0.90 | 0.38 | 95,121,136,143              | 0     |
| 5   | CHL  | C     | 311 | 61/66 | 0.90 | 0.24 | 51,68,84,92                 | 0     |
| 2   | OIE  | F     | 302 | 44/44 | 0.91 | 0.17 | 50,64,77,81                 | 0     |
| 5   | CHL  | D     | 318 | 46/66 | 0.91 | 0.16 | 86,105,120,121              | 0     |
| 5   | CHL  | A     | 318 | 42/66 | 0.91 | 0.18 | 66,89,100,101               | 0     |
| 2   | OIE  | E     | 302 | 44/44 | 0.91 | 0.27 | 57,75,105,125               | 0     |
| 5   | CHL  | B     | 311 | 51/66 | 0.91 | 0.22 | 71,90,122,134               | 0     |
| 5   | CHL  | C     | 310 | 44/66 | 0.91 | 0.20 | 66,86,104,107               | 0     |
| 2   | OIE  | E     | 301 | 44/44 | 0.91 | 0.20 | 44,68,86,99                 | 0     |
| 5   | CHL  | C     | 312 | 56/66 | 0.91 | 0.25 | 62,90,116,122               | 0     |
| 6   | CLA  | B     | 318 | 65/65 | 0.91 | 0.23 | 58,84,98,101                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 6   | CLA  | C     | 315 | 65/65 | 0.91 | 0.39 | 72,104,124,139              | 0     |
| 3   | NEX  | C     | 303 | 44/44 | 0.92 | 0.30 | 75,94,147,175               | 0     |
| 2   | OIE  | D     | 301 | 44/44 | 0.92 | 0.26 | 44,58,74,85                 | 0     |
| 5   | CHL  | F     | 308 | 42/66 | 0.92 | 0.43 | 93,110,123,128              | 0     |
| 5   | CHL  | D     | 305 | 66/66 | 0.92 | 0.20 | 59,85,100,108               | 0     |
| 7   | LHG  | D     | 319 | 46/49 | 0.92 | 0.19 | 66,87,101,108               | 0     |
| 5   | CHL  | B     | 313 | 57/66 | 0.92 | 0.20 | 59,84,104,105               | 0     |
| 5   | CHL  | D     | 313 | 66/66 | 0.92 | 0.24 | 33,50,74,96                 | 0     |
| 5   | CHL  | B     | 314 | 66/66 | 0.92 | 0.24 | 41,61,77,91                 | 0     |
| 5   | CHL  | E     | 305 | 64/66 | 0.92 | 0.23 | 44,65,79,95                 | 0     |
| 2   | OIE  | C     | 301 | 44/44 | 0.92 | 0.22 | 35,54,75,81                 | 0     |
| 5   | CHL  | A     | 313 | 66/66 | 0.93 | 0.34 | 43,58,76,95                 | 0     |
| 2   | OIE  | C     | 302 | 44/44 | 0.93 | 0.20 | 57,77,101,107               | 0     |
| 5   | CHL  | D     | 309 | 42/66 | 0.93 | 0.25 | 86,109,121,128              | 0     |
| 5   | CHL  | F     | 304 | 66/66 | 0.93 | 0.21 | 41,58,70,84                 | 0     |
| 5   | CHL  | D     | 310 | 45/66 | 0.93 | 0.15 | 52,77,90,91                 | 0     |
| 5   | CHL  | D     | 311 | 62/66 | 0.93 | 0.19 | 40,72,88,94                 | 0     |
| 5   | CHL  | F     | 310 | 61/66 | 0.93 | 0.20 | 49,65,80,89                 | 0     |
| 5   | CHL  | F     | 311 | 56/66 | 0.93 | 0.20 | 55,83,110,118               | 0     |
| 5   | CHL  | F     | 312 | 66/66 | 0.93 | 0.25 | 45,61,77,86                 | 0     |
| 5   | CHL  | F     | 317 | 46/66 | 0.93 | 0.20 | 63,83,106,122               | 0     |
| 5   | CHL  | A     | 311 | 61/66 | 0.93 | 0.19 | 51,70,82,97                 | 0     |
| 6   | CLA  | A     | 314 | 55/65 | 0.93 | 0.15 | 60,71,85,87                 | 0     |
| 5   | CHL  | A     | 309 | 43/66 | 0.93 | 0.28 | 103,123,135,140             | 0     |
| 6   | CLA  | B     | 315 | 58/65 | 0.93 | 0.23 | 65,76,100,107               | 0     |
| 5   | CHL  | E     | 304 | 66/66 | 0.93 | 0.21 | 54,75,102,137               | 0     |
| 5   | CHL  | B     | 312 | 62/66 | 0.93 | 0.19 | 51,68,84,93                 | 0     |
| 6   | CLA  | D     | 314 | 58/65 | 0.93 | 0.23 | 60,76,97,101                | 0     |
| 5   | CHL  | E     | 308 | 41/66 | 0.93 | 0.26 | 119,142,157,160             | 0     |
| 6   | CLA  | E     | 307 | 50/65 | 0.93 | 0.17 | 89,108,130,132              | 0     |
| 6   | CLA  | E     | 314 | 63/65 | 0.93 | 0.29 | 89,121,136,151              | 0     |
| 6   | CLA  | F     | 314 | 55/65 | 0.94 | 0.23 | 51,63,93,103                | 0     |
| 6   | CLA  | F     | 316 | 56/65 | 0.94 | 0.17 | 54,68,79,90                 | 0     |
| 5   | CHL  | C     | 309 | 42/66 | 0.94 | 0.34 | 92,113,122,129              | 0     |
| 7   | LHG  | B     | 320 | 46/49 | 0.94 | 0.18 | 50,74,88,106                | 0     |
| 5   | CHL  | F     | 305 | 66/66 | 0.94 | 0.29 | 29,43,59,71                 | 0     |
| 6   | CLA  | A     | 317 | 55/65 | 0.94 | 0.16 | 48,77,87,97                 | 0     |
| 6   | CLA  | B     | 309 | 46/65 | 0.94 | 0.16 | 72,88,99,103                | 0     |
| 5   | CHL  | A     | 305 | 66/66 | 0.94 | 0.20 | 45,73,91,106                | 0     |
| 7   | LHG  | E     | 318 | 41/49 | 0.94 | 0.16 | 55,85,121,144               | 0     |
| 6   | CLA  | B     | 317 | 45/65 | 0.94 | 0.19 | 74,82,99,112                | 0     |
| 5   | CHL  | C     | 305 | 66/66 | 0.94 | 0.19 | 51,71,86,102                | 0     |

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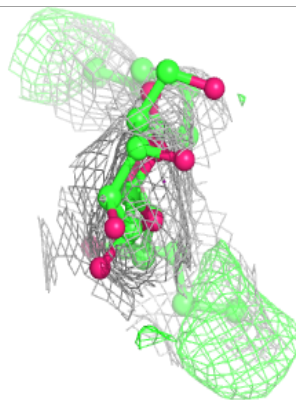
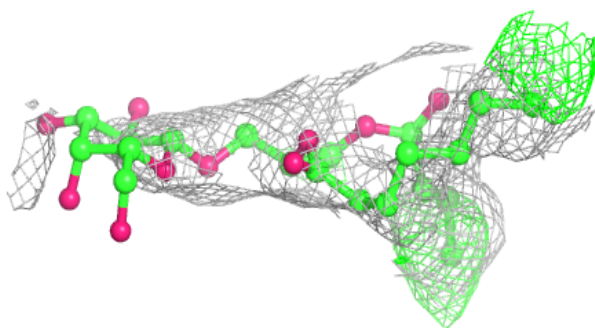
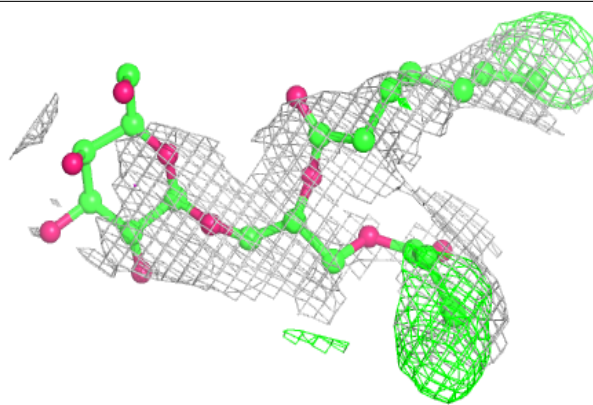
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 6   | CLA  | C     | 314 | 53/65 | 0.94 | 0.20 | 79,97,118,126              | 0     |
| 5   | CHL  | C     | 306 | 66/66 | 0.94 | 0.24 | 34,58,71,87                | 0     |
| 6   | CLA  | C     | 316 | 45/65 | 0.94 | 0.20 | 77,95,118,123              | 0     |
| 5   | CHL  | E     | 309 | 43/66 | 0.94 | 0.15 | 89,105,127,130             | 0     |
| 6   | CLA  | D     | 315 | 65/65 | 0.94 | 0.26 | 79,95,107,112              | 0     |
| 6   | CLA  | D     | 316 | 45/65 | 0.94 | 0.17 | 81,85,101,105              | 0     |
| 5   | CHL  | C     | 313 | 66/66 | 0.94 | 0.21 | 46,63,80,86                | 0     |
| 5   | CHL  | D     | 312 | 57/66 | 0.94 | 0.17 | 44,63,94,103               | 0     |
| 6   | CLA  | E     | 313 | 55/65 | 0.94 | 0.22 | 100,112,130,140            | 0     |
| 5   | CHL  | C     | 318 | 44/66 | 0.94 | 0.15 | 70,96,112,129              | 0     |
| 6   | CLA  | E     | 315 | 45/65 | 0.94 | 0.20 | 100,118,132,138            | 0     |
| 6   | CLA  | F     | 307 | 46/65 | 0.94 | 0.14 | 61,79,91,96                | 0     |
| 6   | CLA  | F     | 313 | 58/65 | 0.94 | 0.19 | 58,70,101,102              | 0     |
| 5   | CHL  | E     | 317 | 41/66 | 0.95 | 0.15 | 83,96,113,116              | 0     |
| 6   | CLA  | E     | 316 | 55/65 | 0.95 | 0.16 | 65,78,89,95                | 0     |
| 6   | CLA  | F     | 306 | 65/65 | 0.95 | 0.36 | 36,53,75,90                | 0     |
| 6   | CLA  | C     | 308 | 46/65 | 0.95 | 0.14 | 65,86,94,100               | 0     |
| 5   | CHL  | B     | 319 | 47/66 | 0.95 | 0.17 | 80,96,112,117              | 0     |
| 6   | CLA  | E     | 306 | 65/65 | 0.95 | 0.36 | 48,63,78,86                | 0     |
| 6   | CLA  | F     | 315 | 45/65 | 0.95 | 0.16 | 58,74,92,100               | 0     |
| 5   | CHL  | B     | 307 | 65/66 | 0.95 | 0.27 | 32,45,64,88                | 0     |
| 6   | CLA  | B     | 316 | 65/65 | 0.95 | 0.22 | 63,79,109,139              | 0     |
| 5   | CHL  | B     | 306 | 66/66 | 0.95 | 0.22 | 45,63,77,93                | 0     |
| 6   | CLA  | C     | 307 | 65/65 | 0.96 | 0.26 | 33,51,75,92                | 0     |
| 6   | CLA  | C     | 317 | 56/65 | 0.96 | 0.16 | 57,75,89,96                | 0     |
| 6   | CLA  | D     | 307 | 65/65 | 0.96 | 0.38 | 34,51,81,90                | 0     |
| 6   | CLA  | D     | 308 | 46/65 | 0.96 | 0.15 | 68,84,96,104               | 0     |
| 5   | CHL  | A     | 306 | 64/66 | 0.96 | 0.27 | 30,51,64,82                | 0     |
| 8   | MG   | D     | 320 | 1/1   | 0.96 | 0.21 | 63,63,63,63                | 0     |
| 6   | CLA  | A     | 307 | 65/65 | 0.97 | 0.42 | 31,47,79,85                | 0     |
| 6   | CLA  | B     | 308 | 65/65 | 0.97 | 0.35 | 35,49,75,84                | 0     |
| 6   | CLA  | A     | 316 | 45/65 | 0.97 | 0.14 | 74,80,98,116               | 0     |

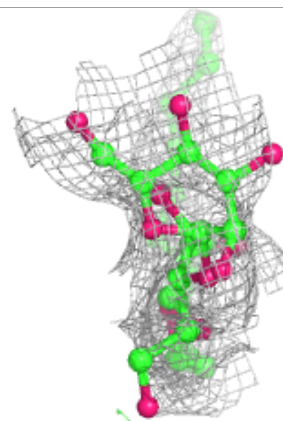
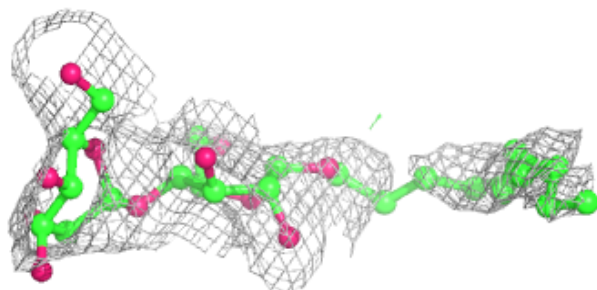
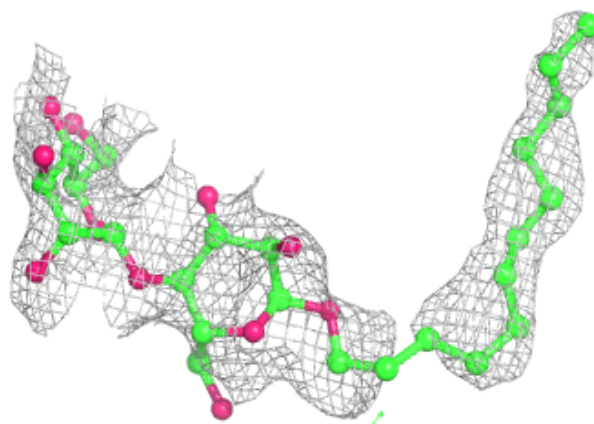
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around LMG F 319:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

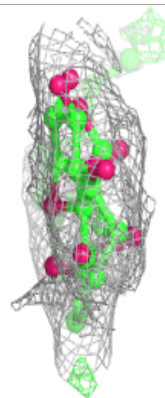
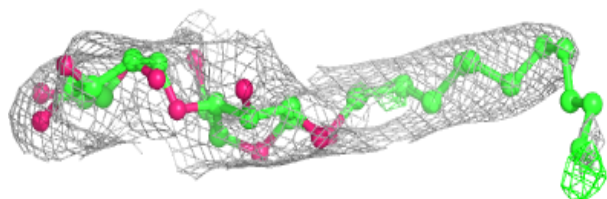
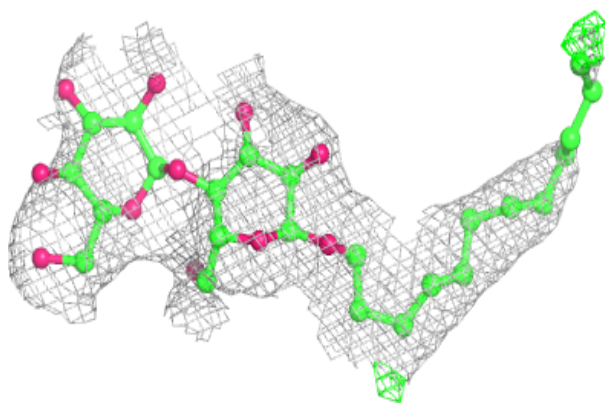
**Electron density around LMU B 305:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

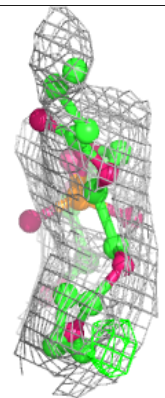
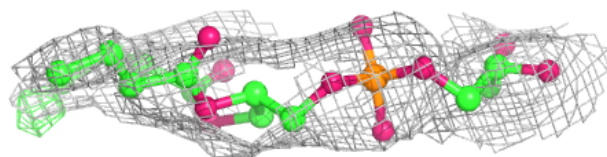
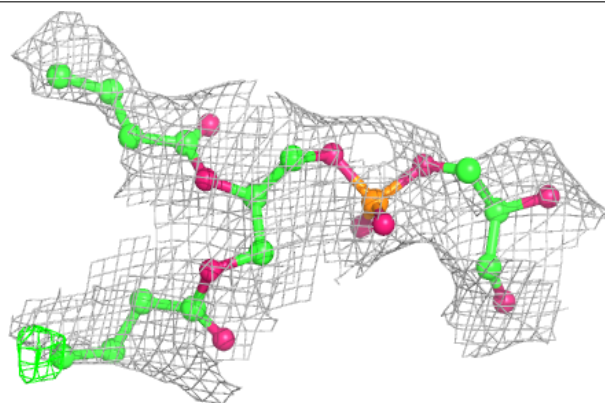


**Electron density around LMU E 319:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

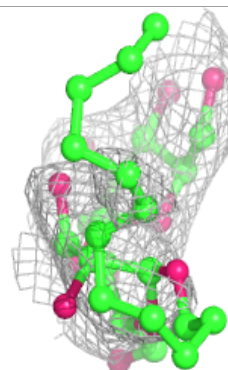
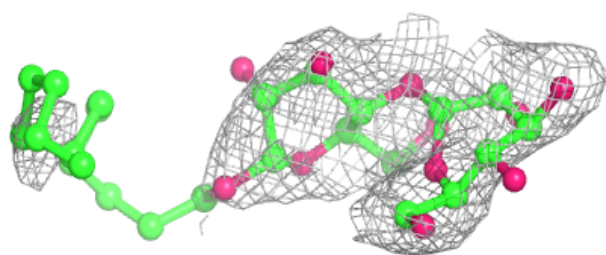
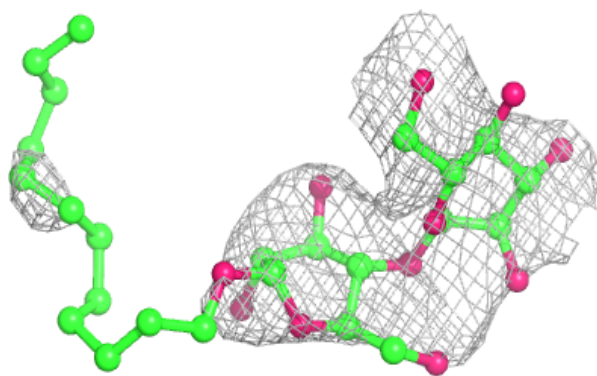
**Electron density around LHG C 304:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

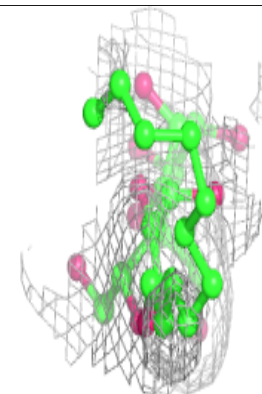
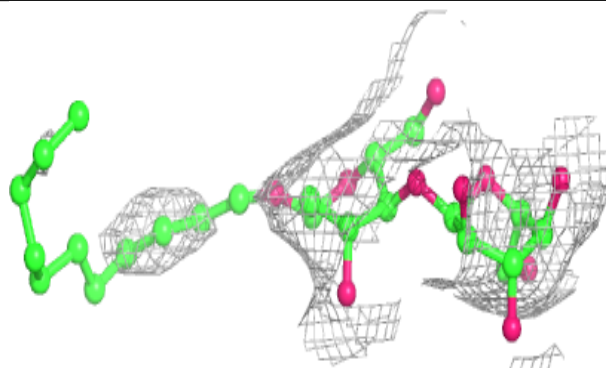
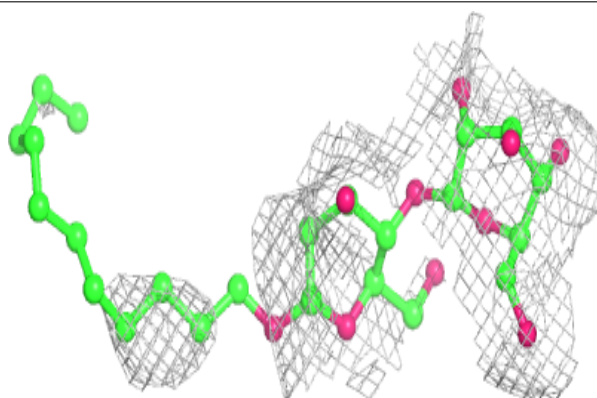


**Electron density around LMU A 304:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

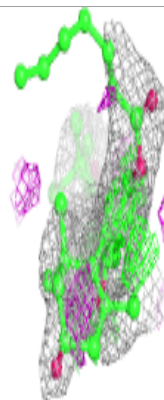
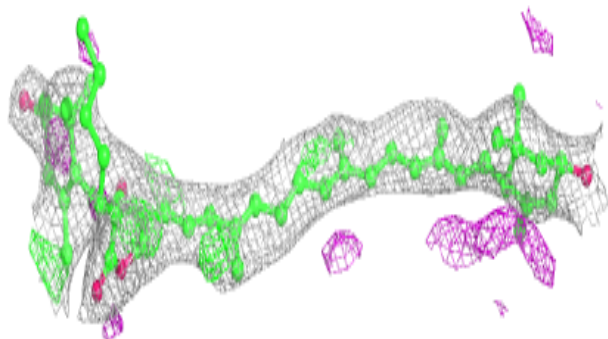
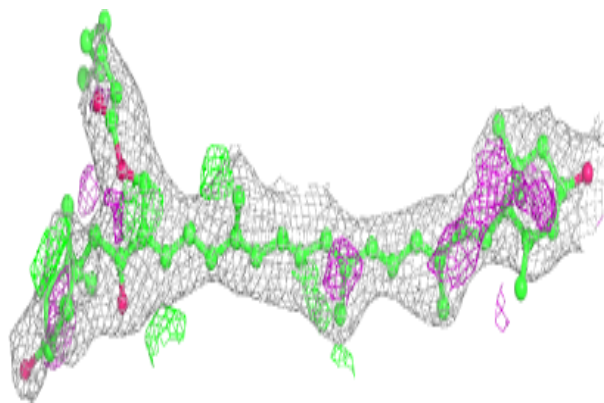
**Electron density around LMU B 304:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

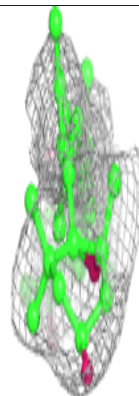
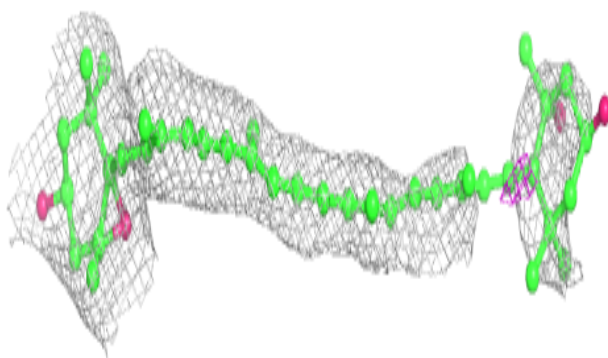
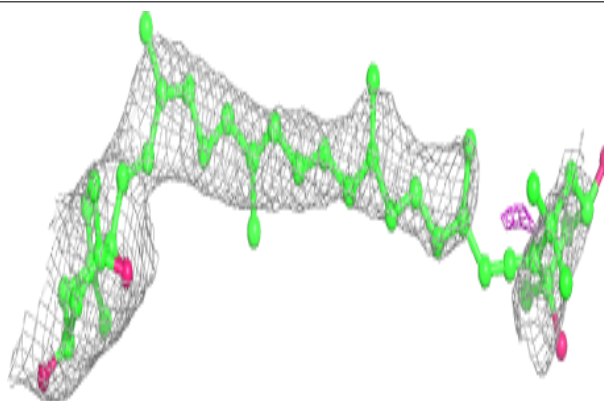


**Electron density around 0UR B 325:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NEX A 303:**

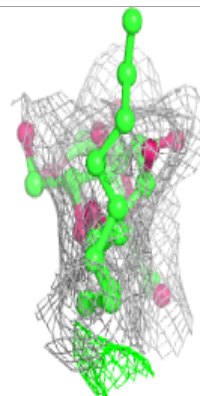
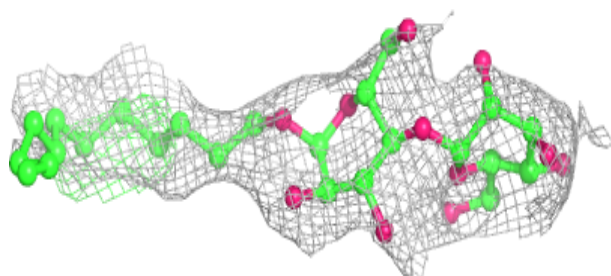
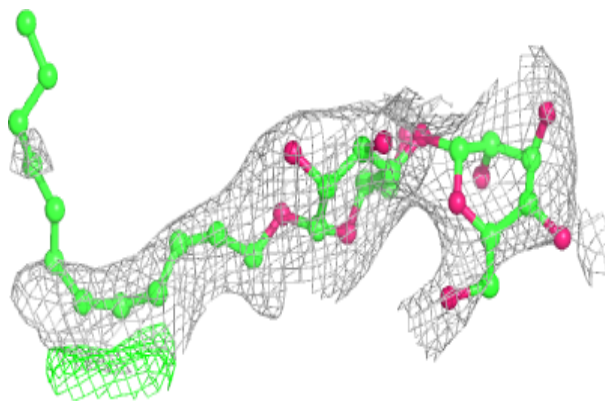
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



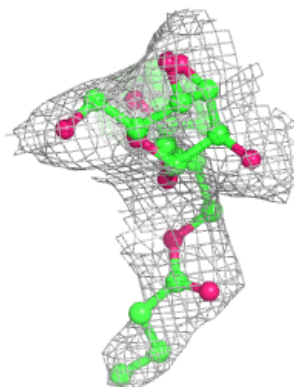
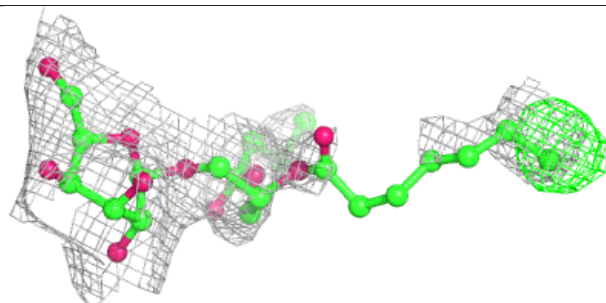
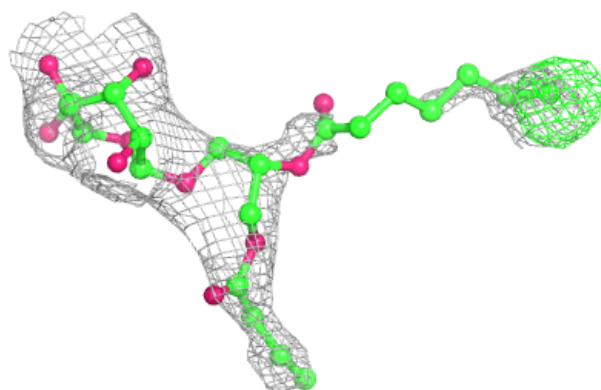


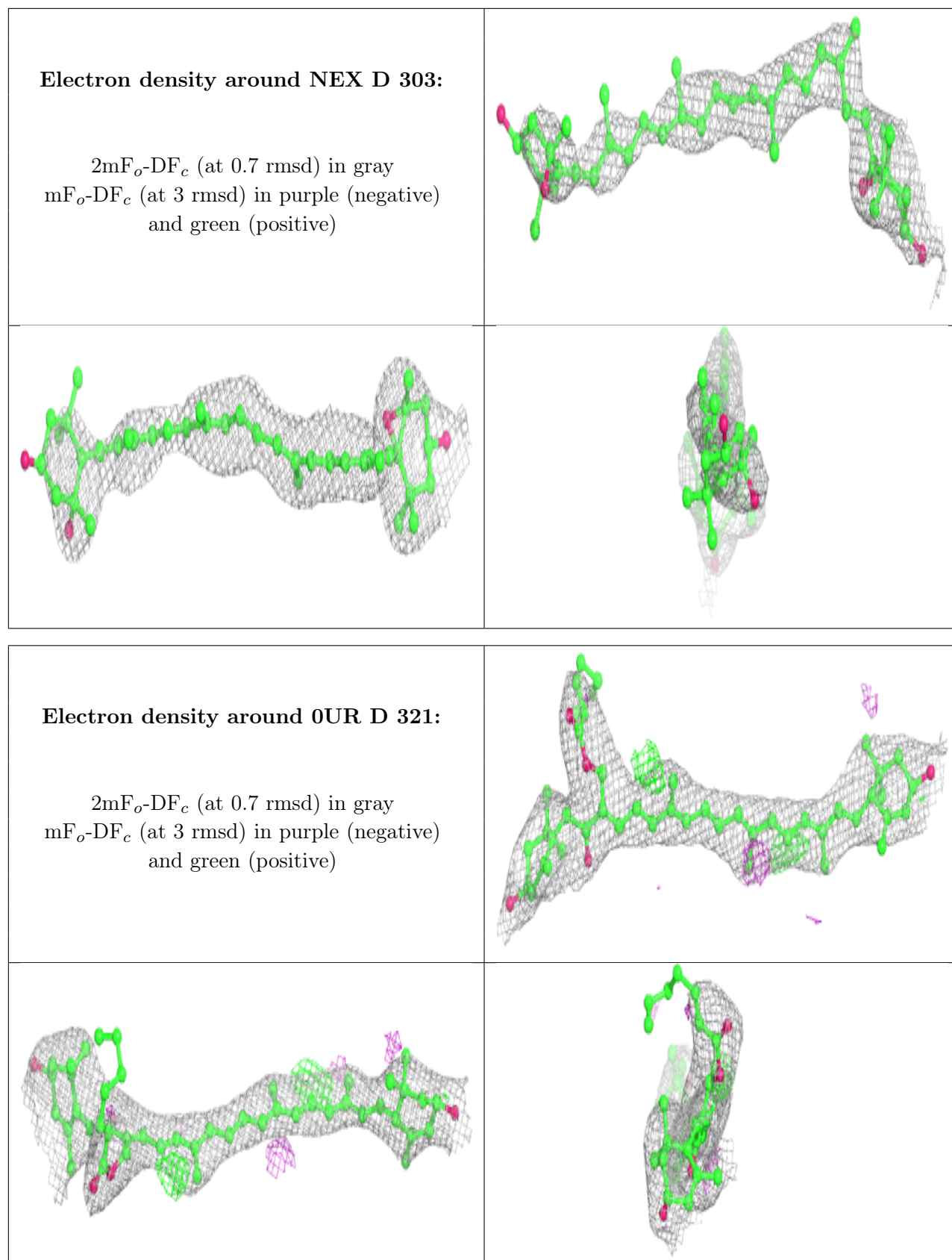
**Electron density around LMU D 304:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LMG B 323:**

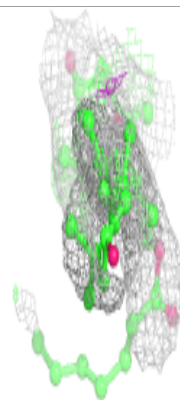
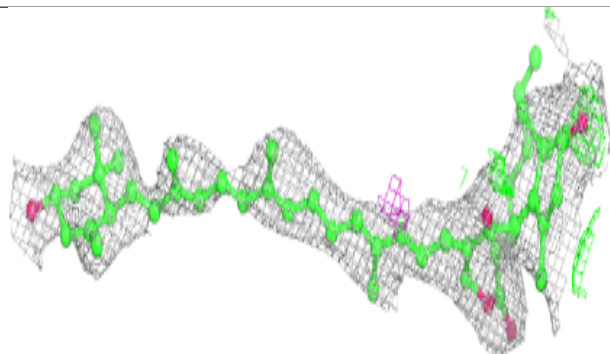
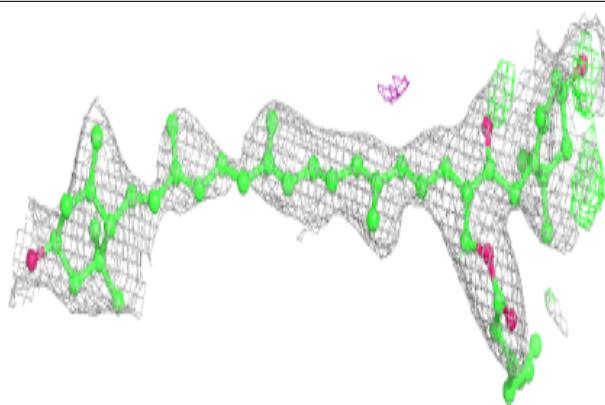
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



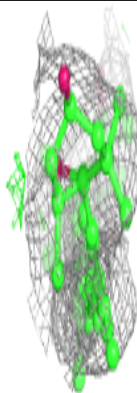
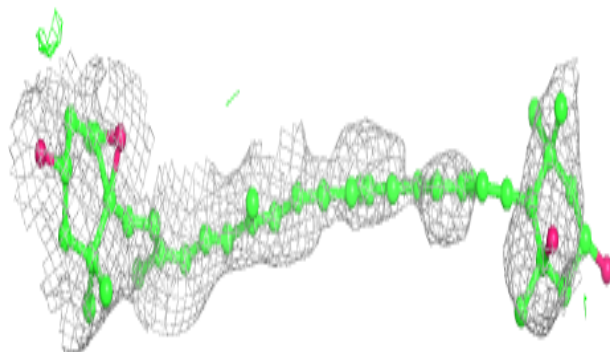
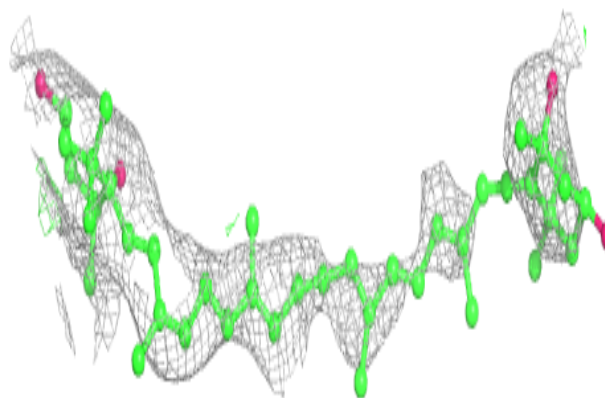


**Electron density around 0UR E 320:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

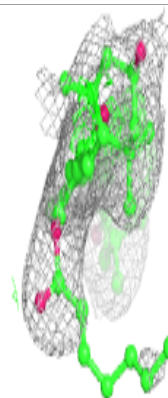
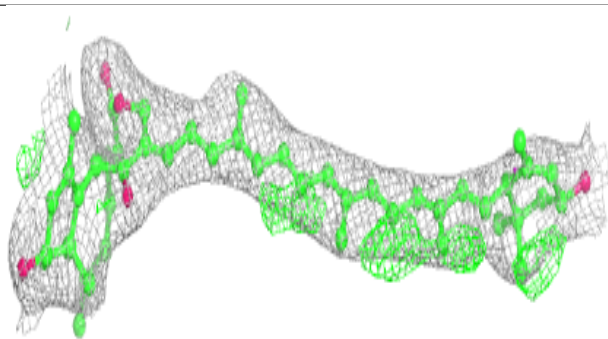
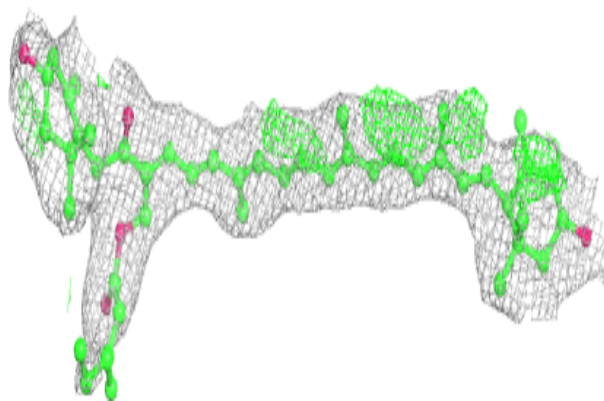
**Electron density around NEX E 303:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

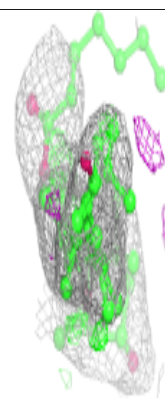
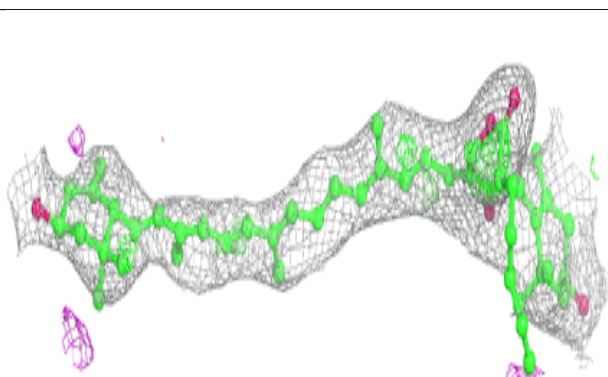
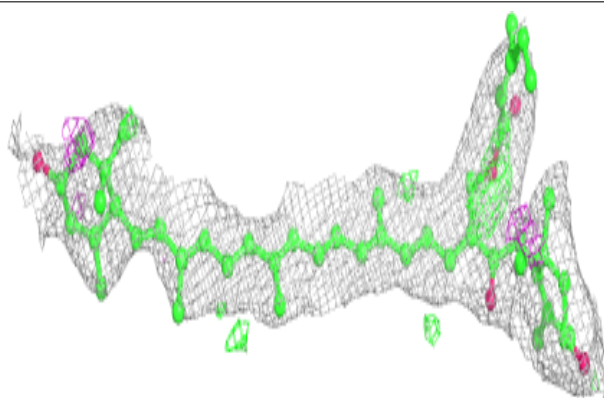


**Electron density around 0UR A 322:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

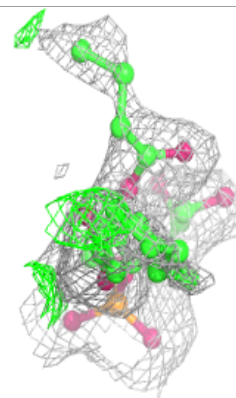
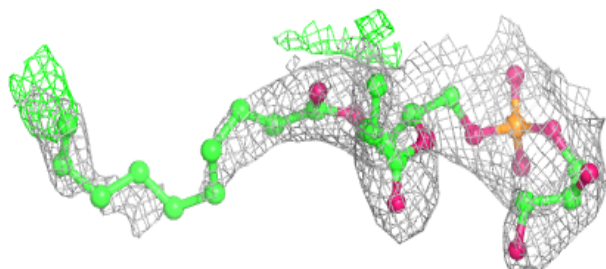
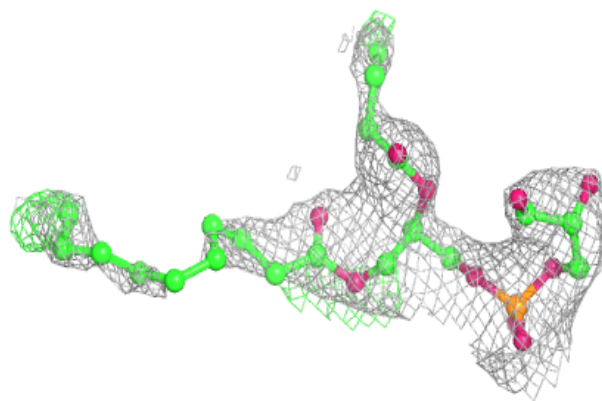
**Electron density around 0UR F 320:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

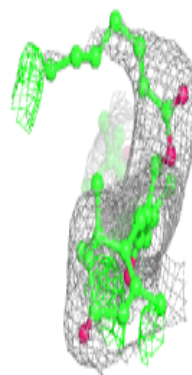
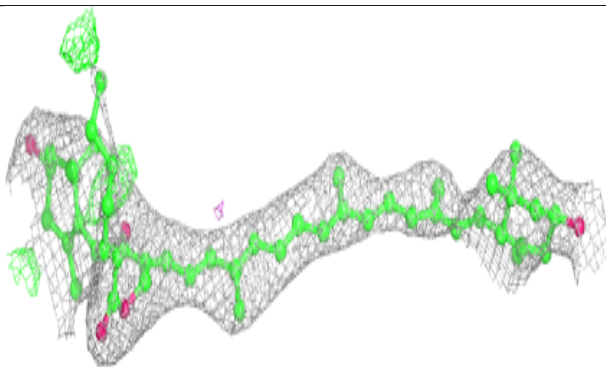
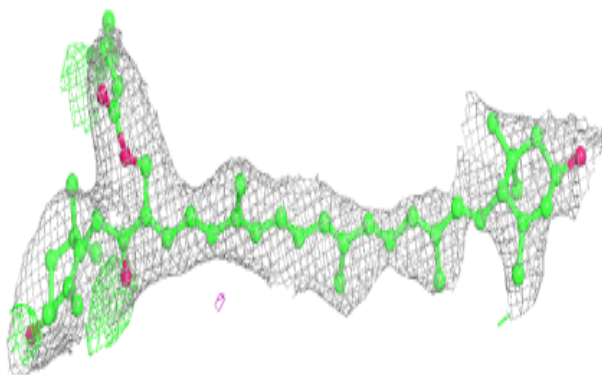


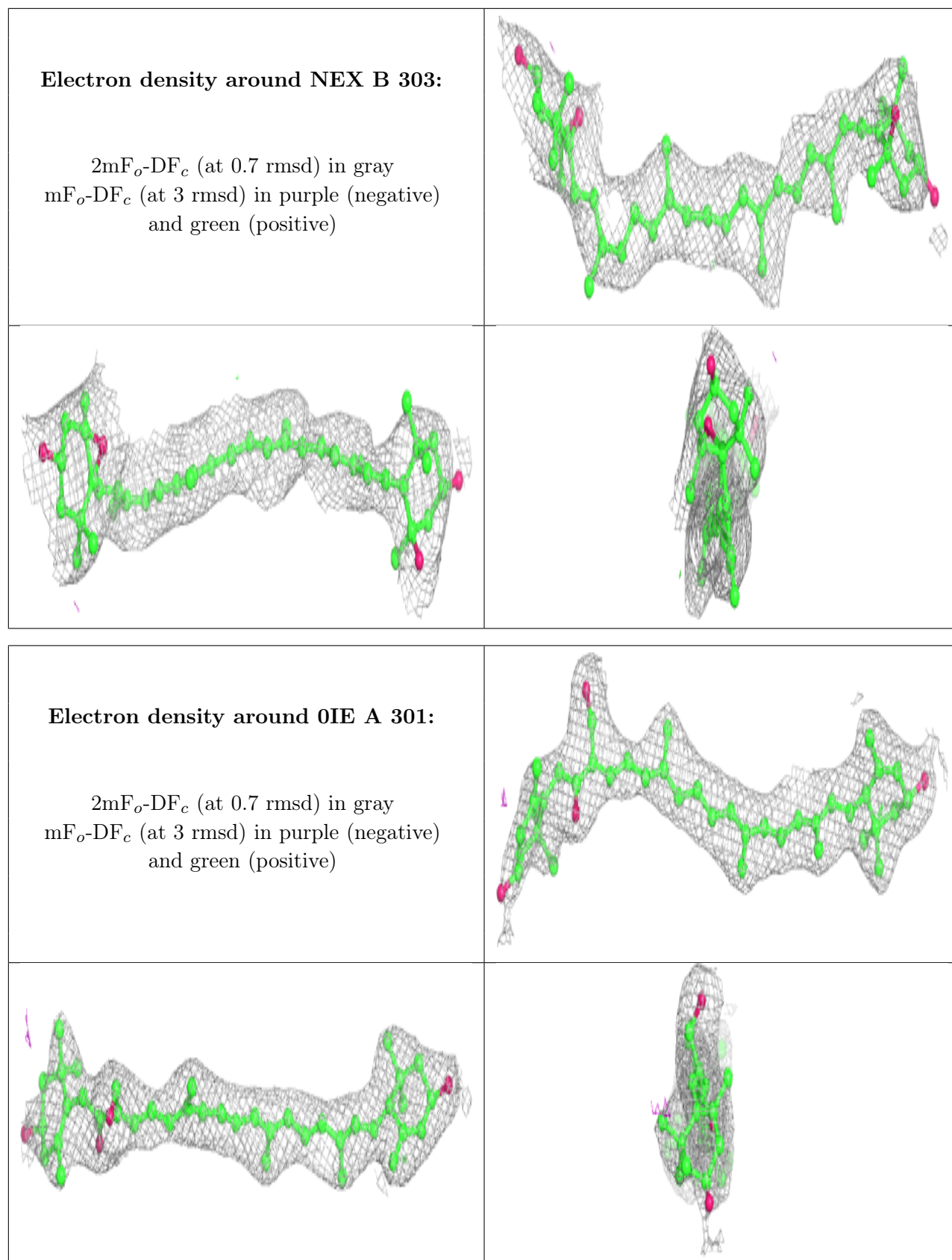
**Electron density around LHG B 324:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 0UR C 321:**

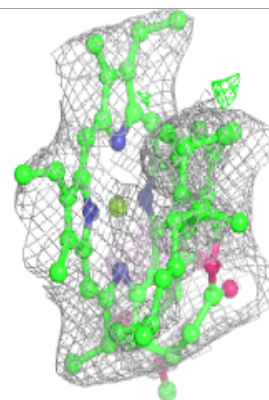
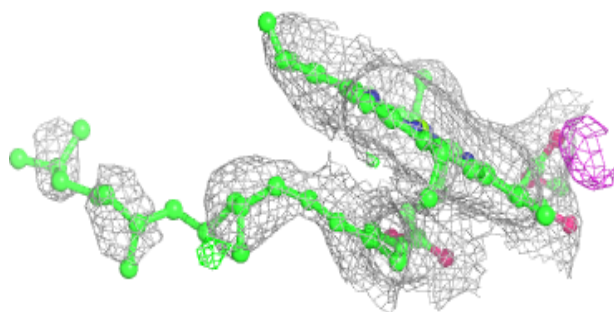
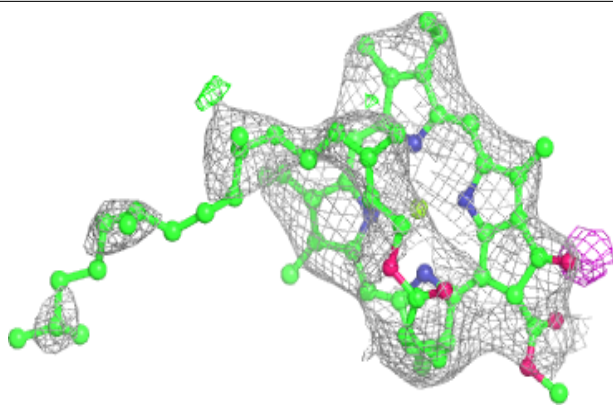
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



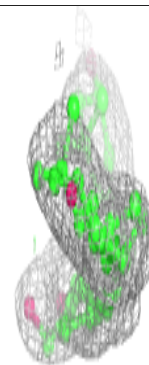
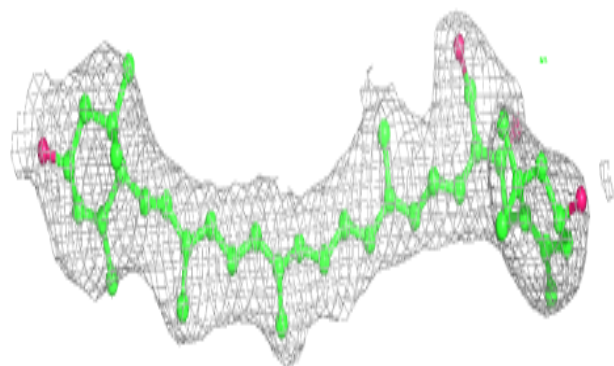
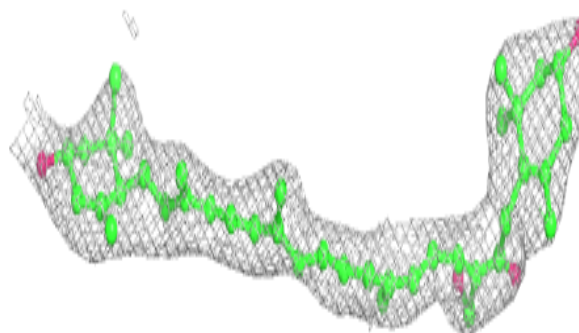


**Electron density around CLA D 317:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

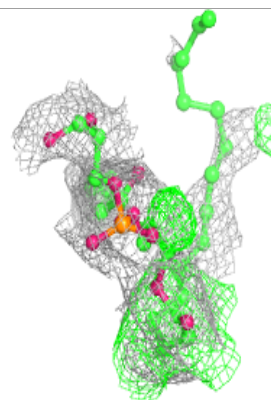
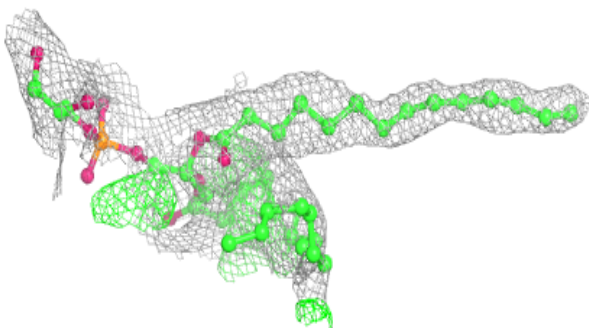
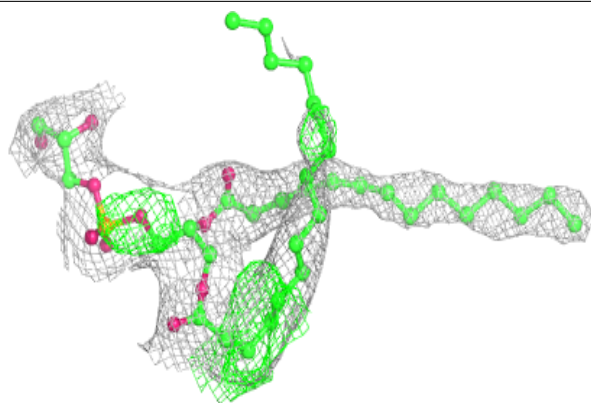
**Electron density around OIE D 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

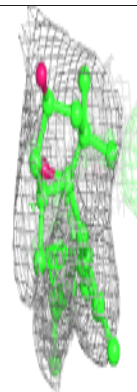
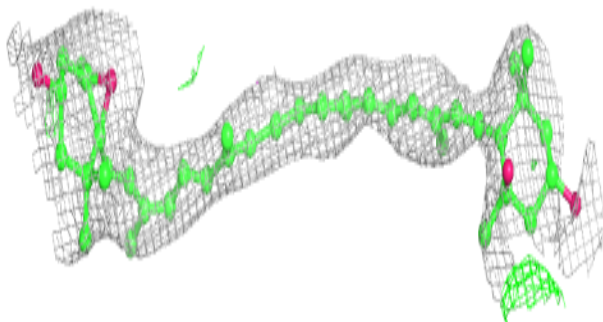
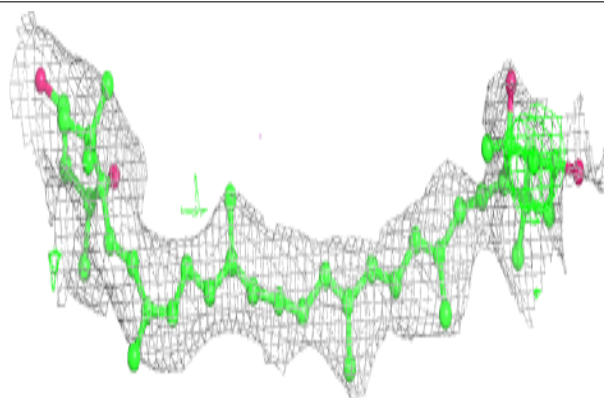


**Electron density around LHG A 319:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NEX F 303:**

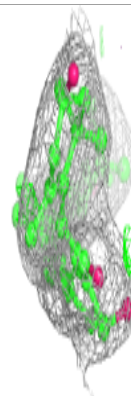
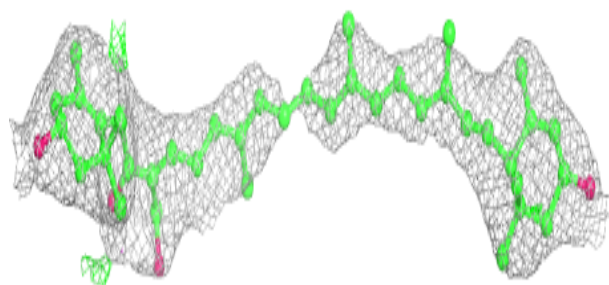
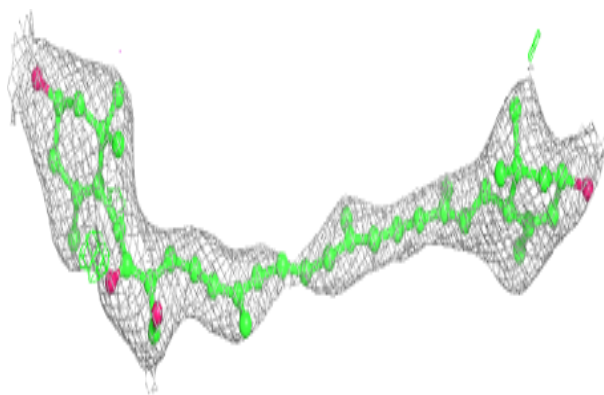
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



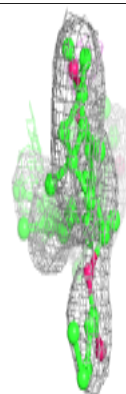
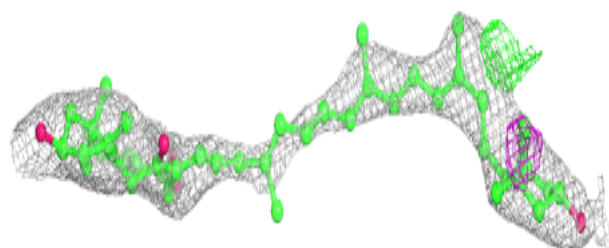
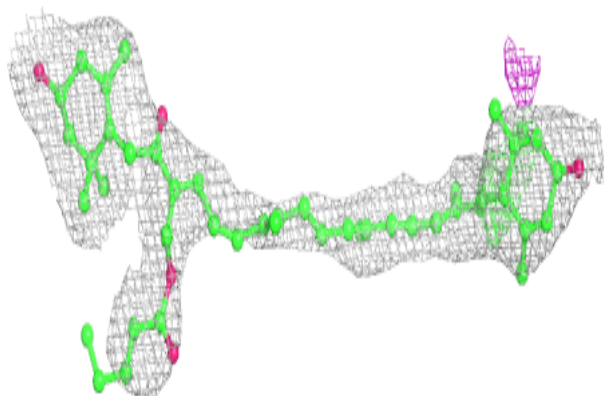


**Electron density around OIE A 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

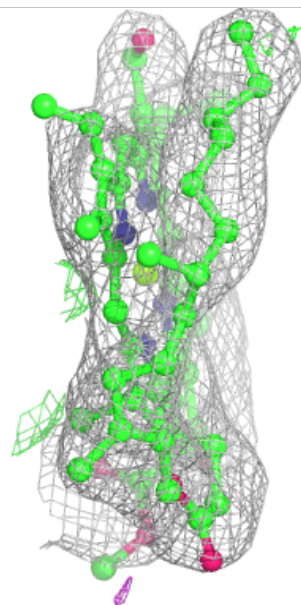
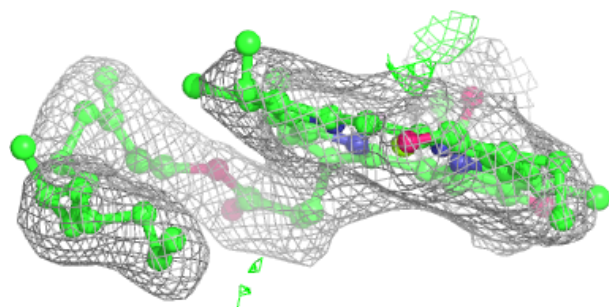
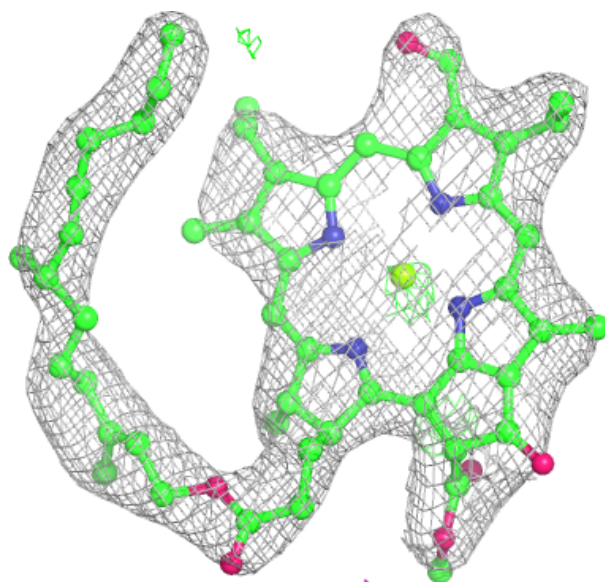
**Electron density around OUR B 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



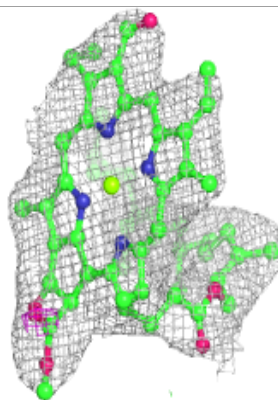
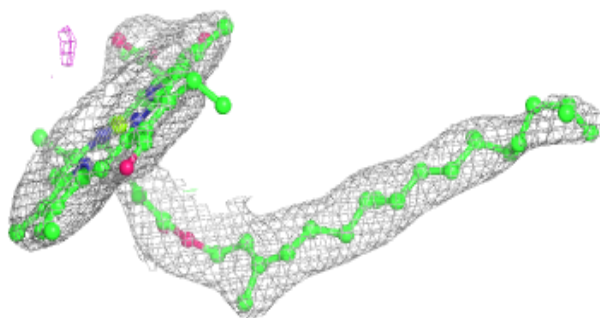
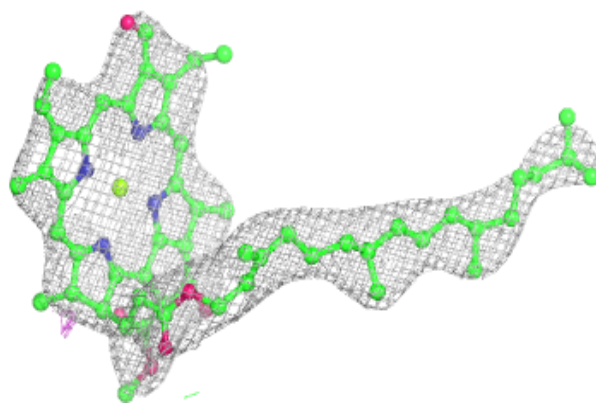
**Electron density around CHL E 310:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

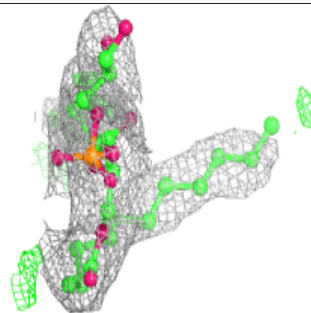
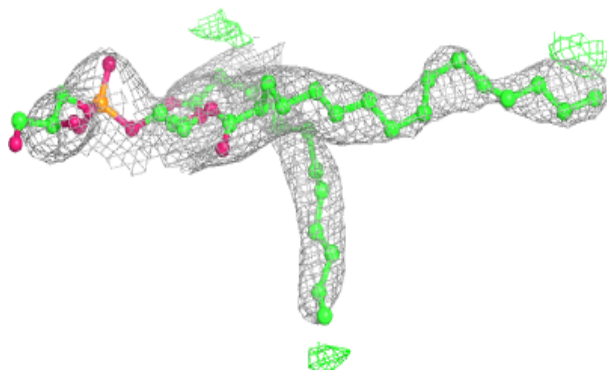
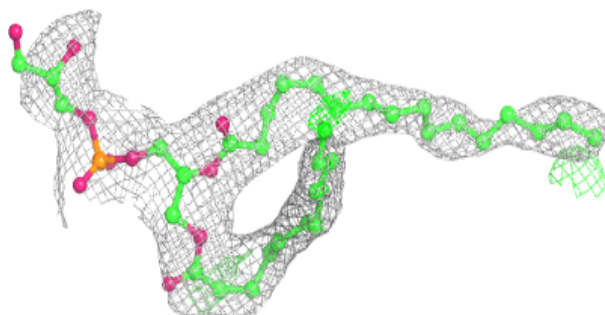


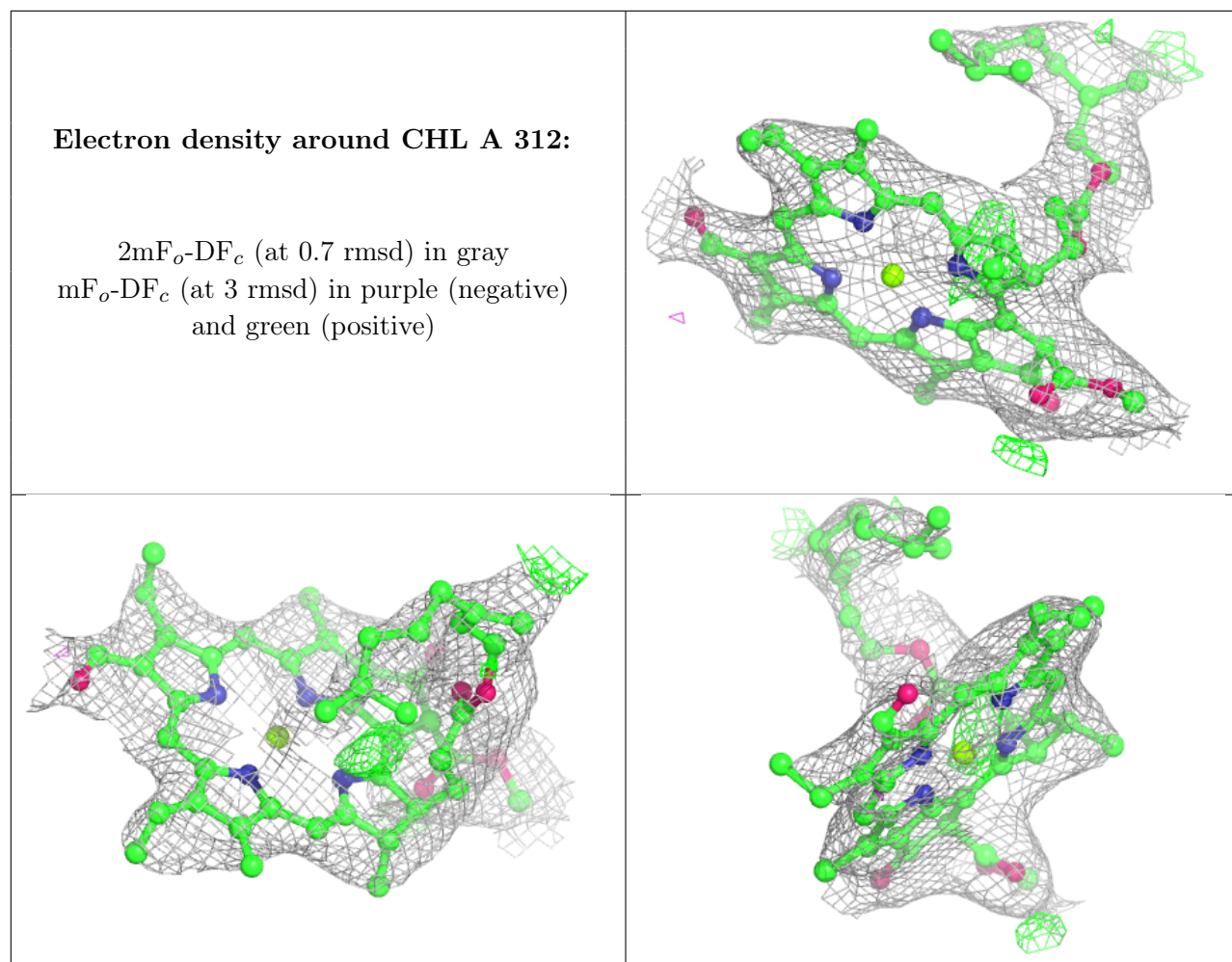
**Electron density around CHL E 312:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LHG C 319:**

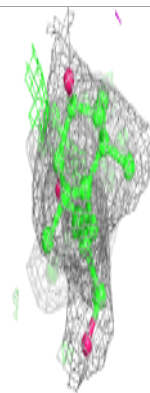
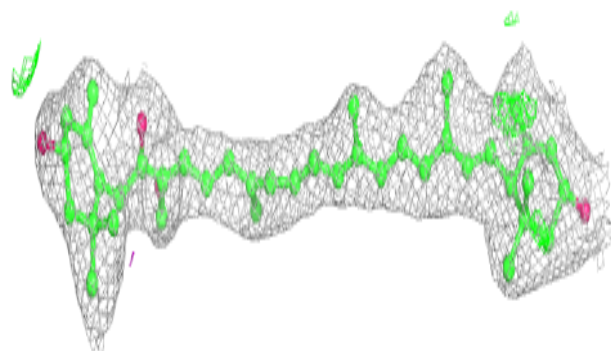
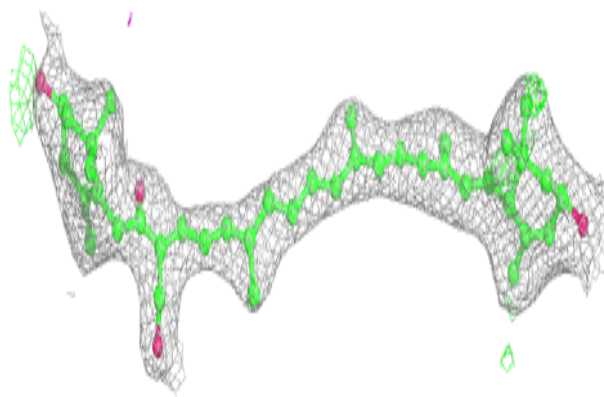
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





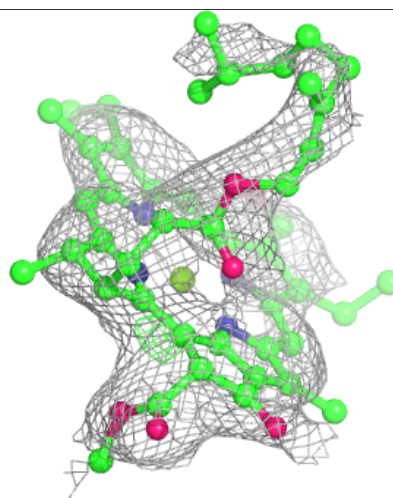
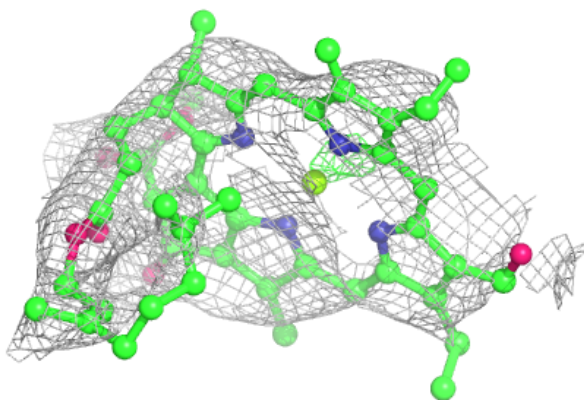
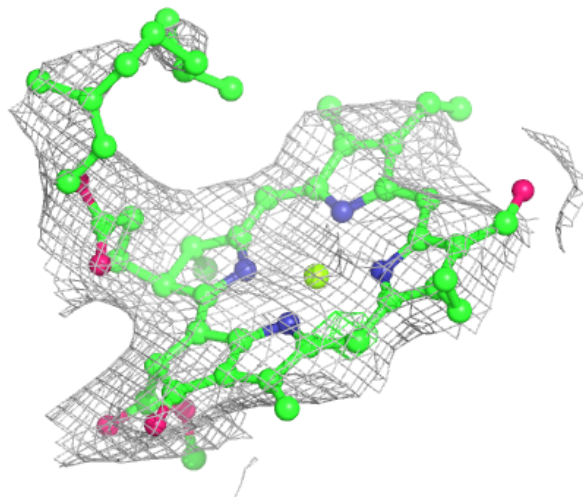
**Electron density around OIE F 301:**

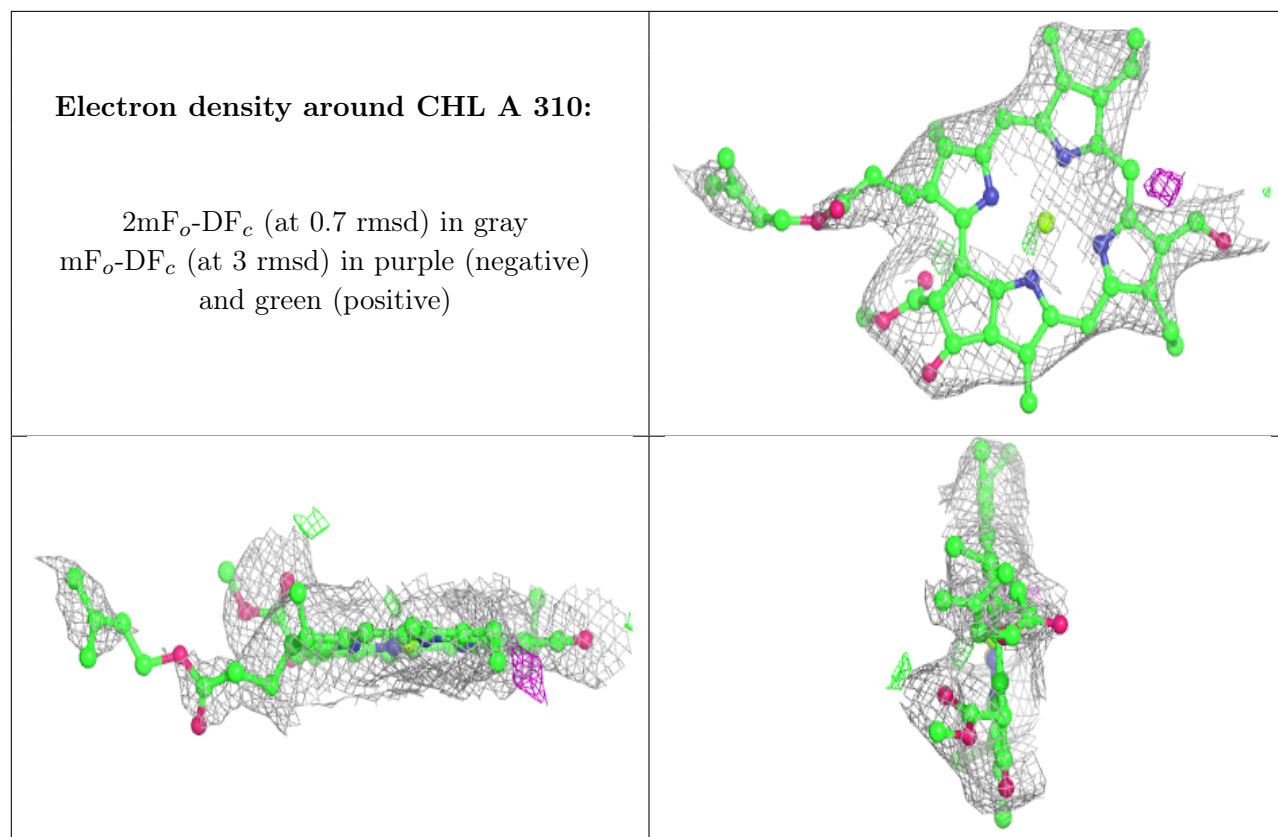
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CHL E 311:**

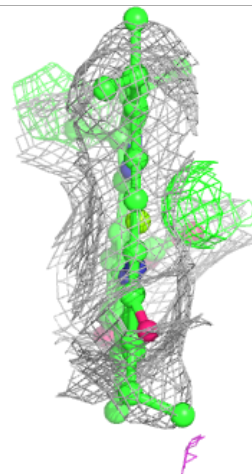
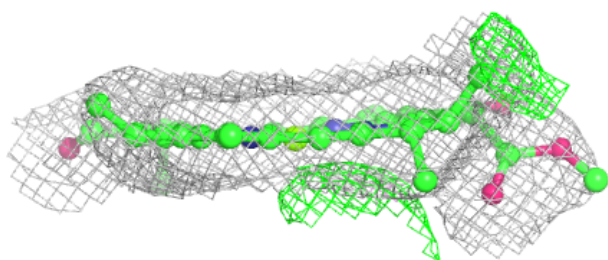
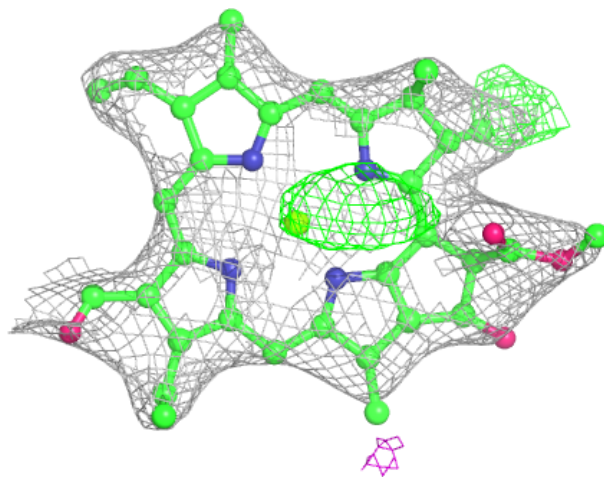
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



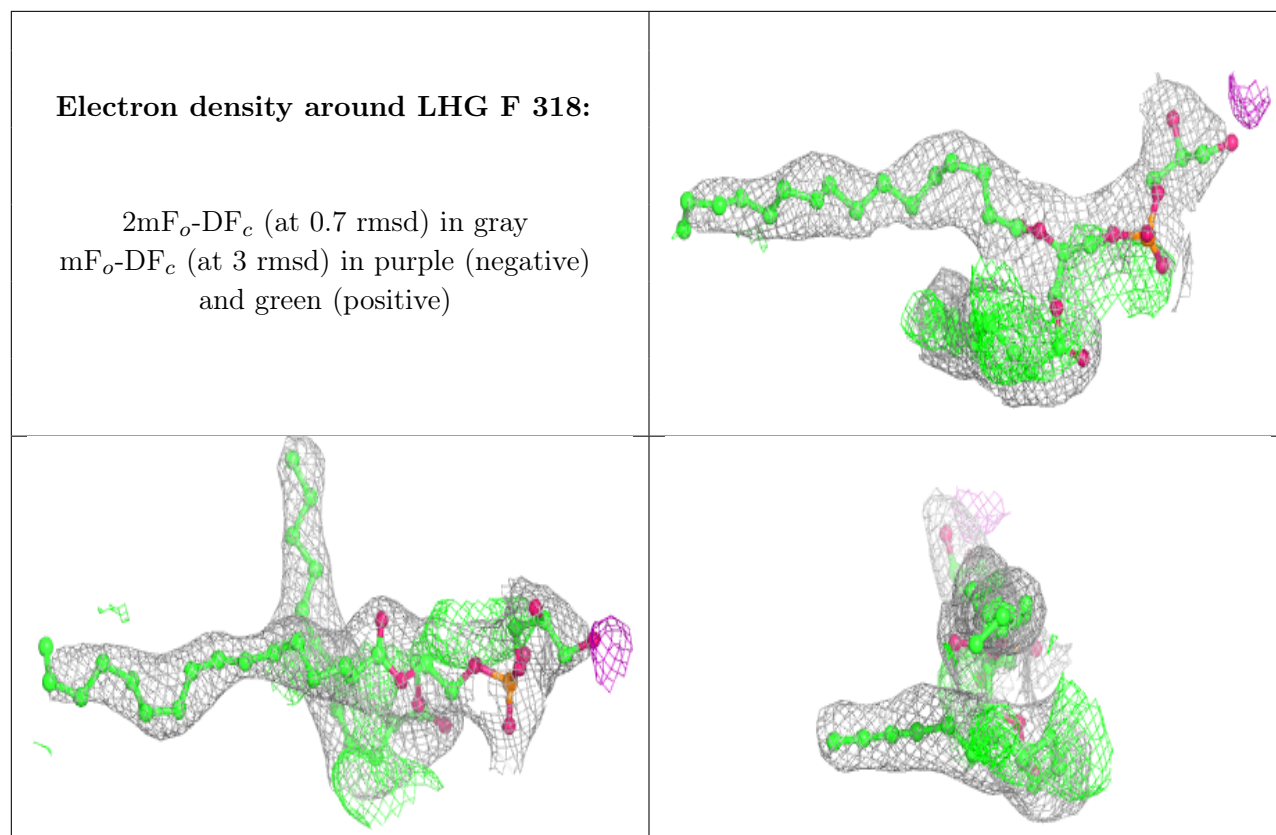


**Electron density around CHL F 309:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

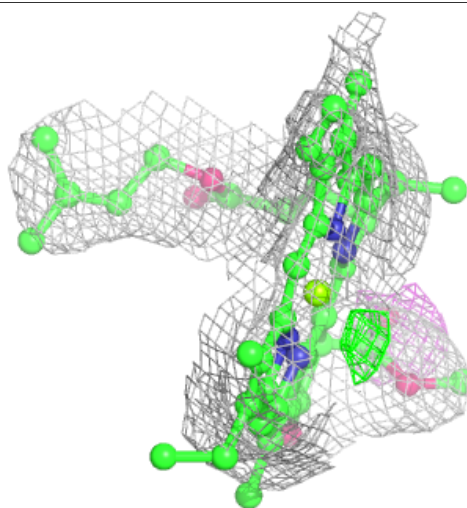
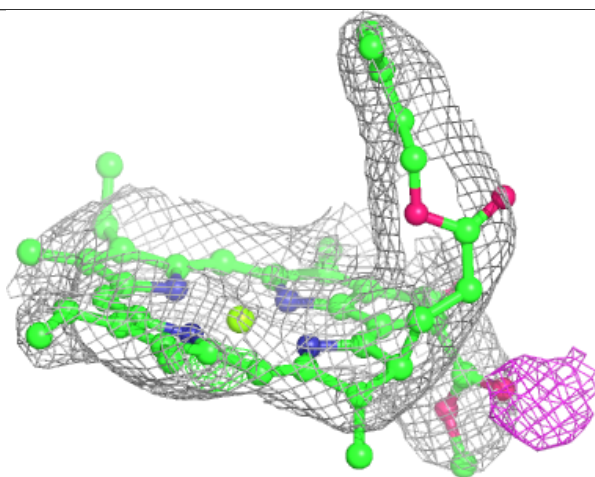
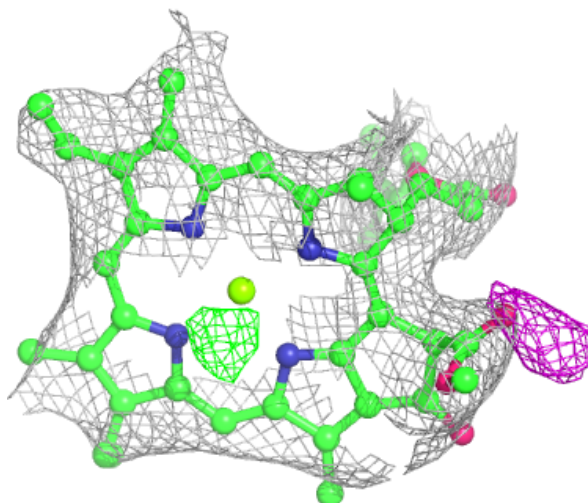






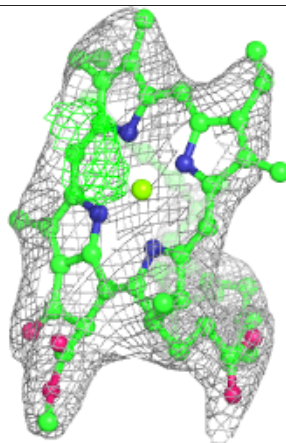
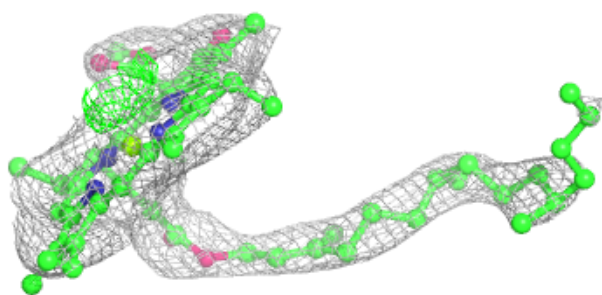
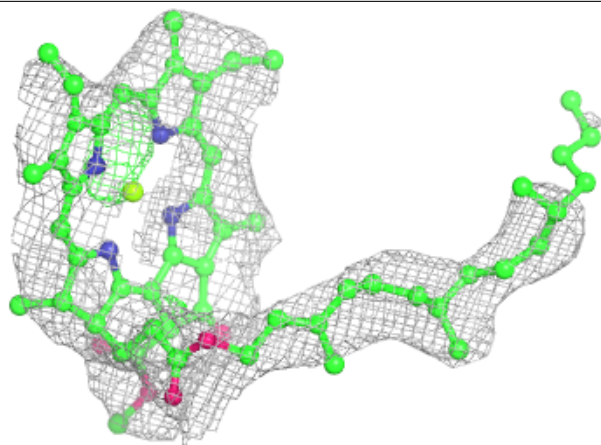
**Electron density around CLA A 308:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

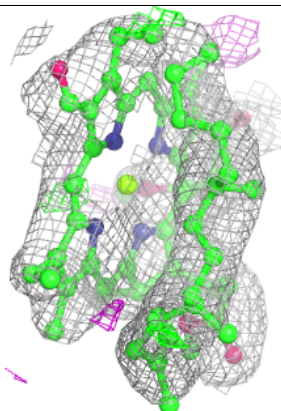
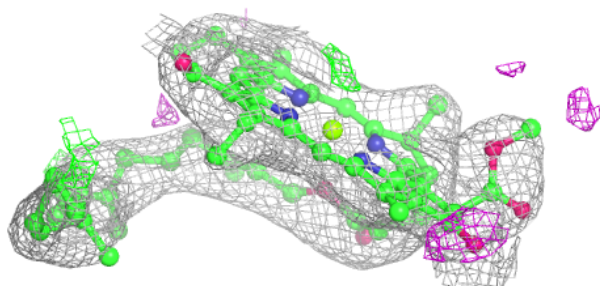
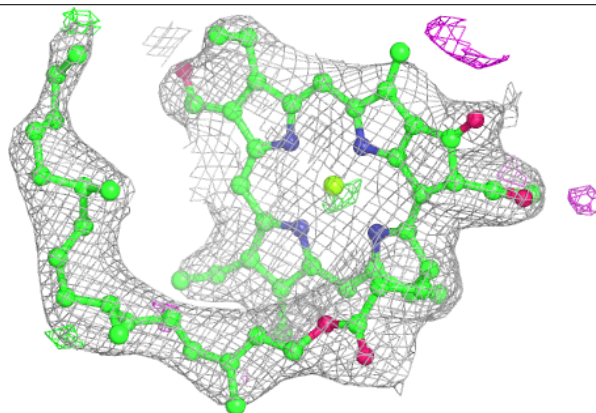


**Electron density around CLA A 315:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

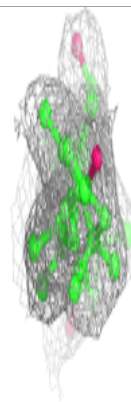
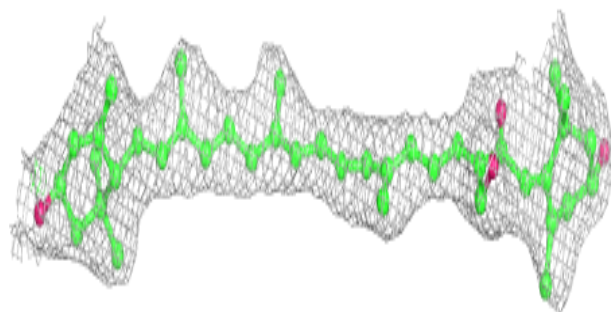
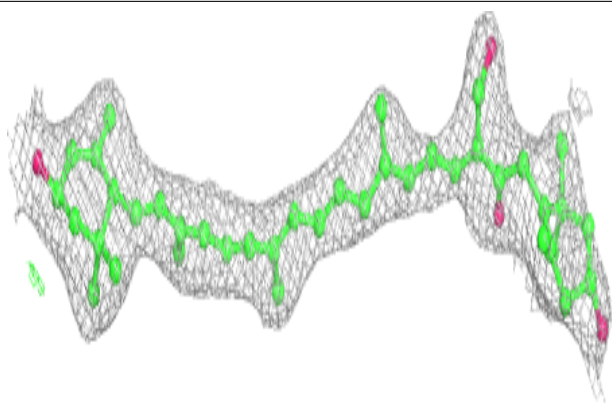
**Electron density around CHL D 306:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

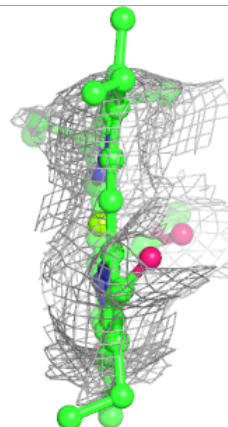
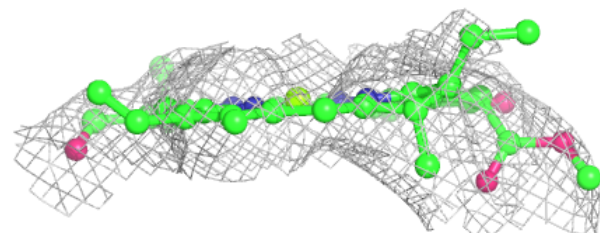
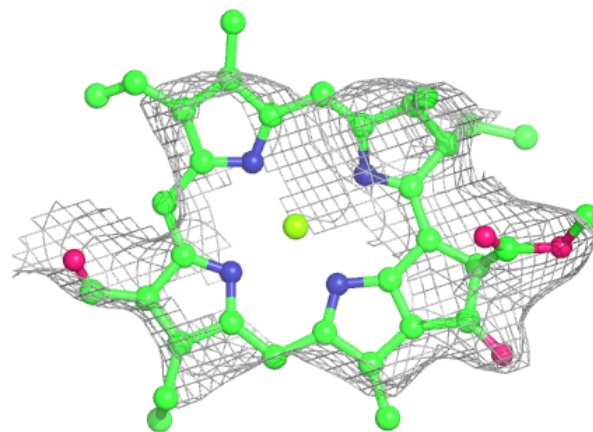


**Electron density around OIE B 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

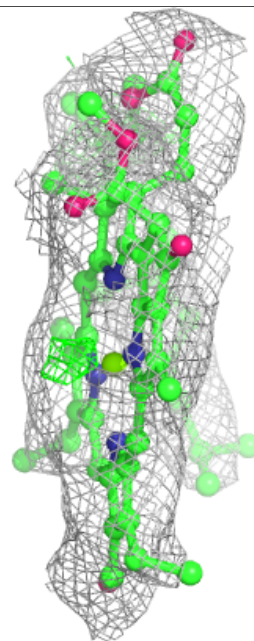
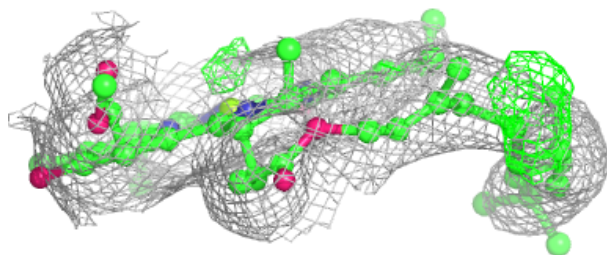
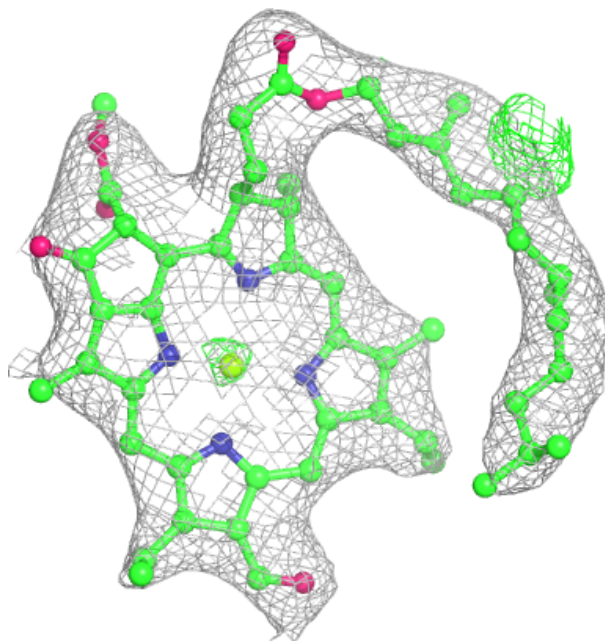
**Electron density around CHL B 310:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



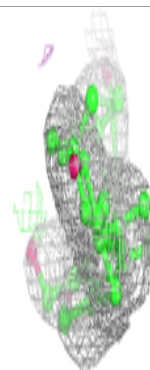
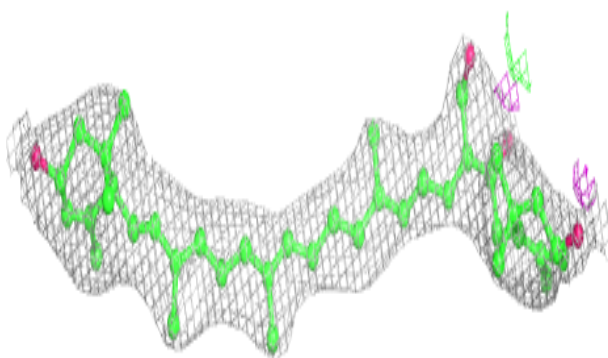
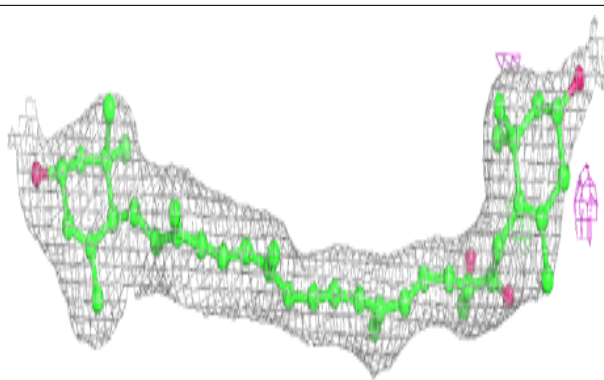
**Electron density around CHL C 311:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

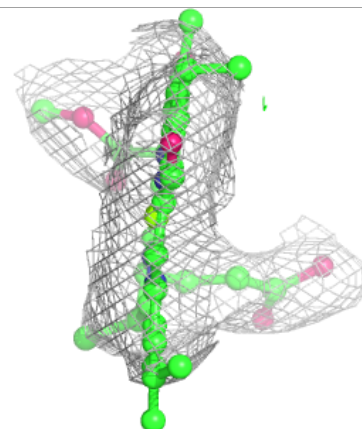
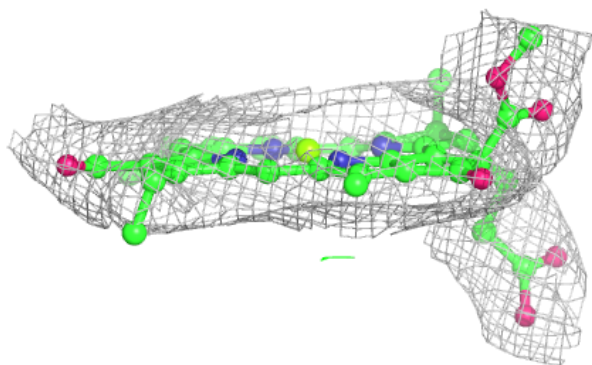
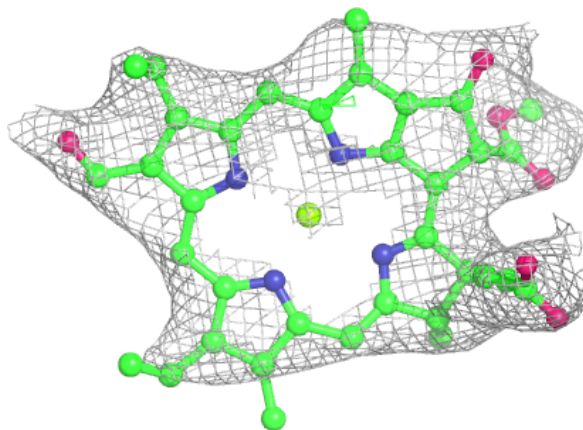


**Electron density around OIE F 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

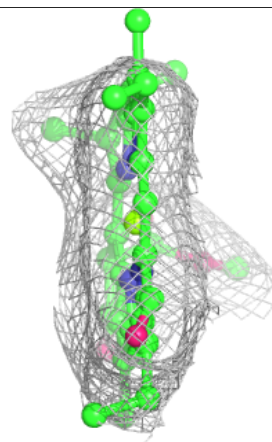
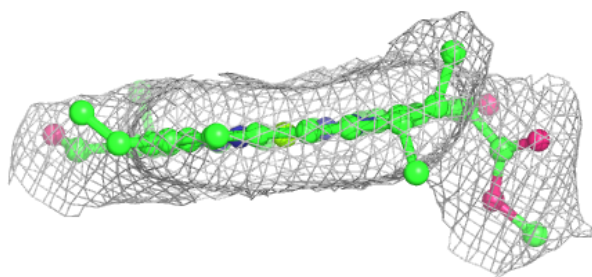
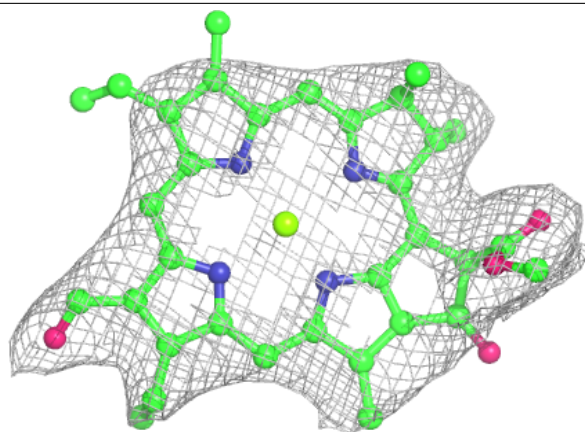
**Electron density around CHL D 318:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

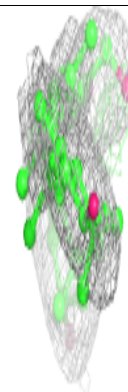
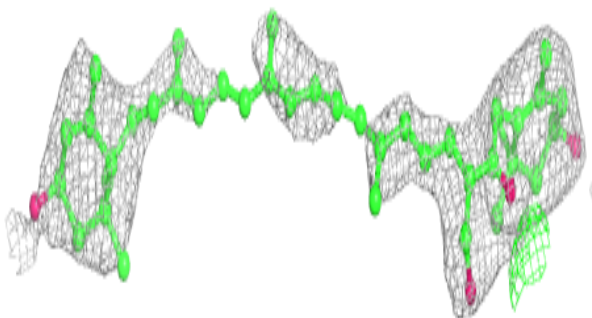
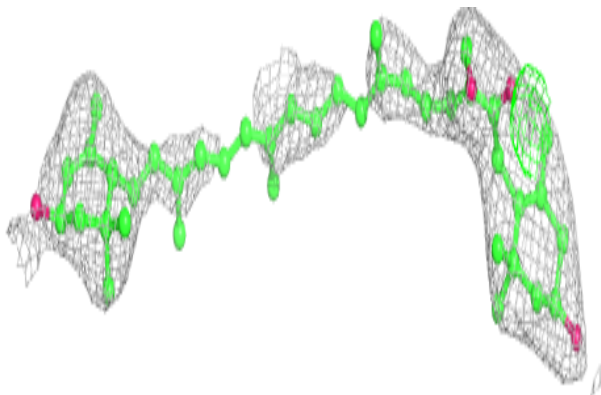


**Electron density around CHL A 318:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

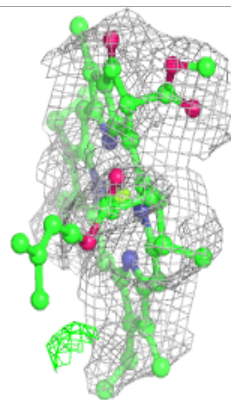
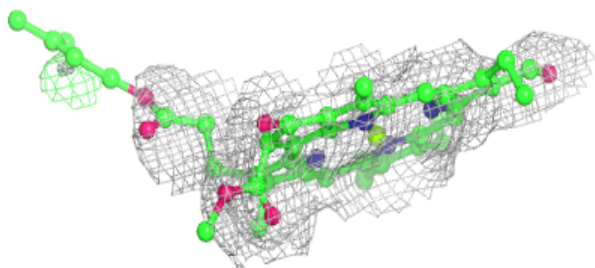
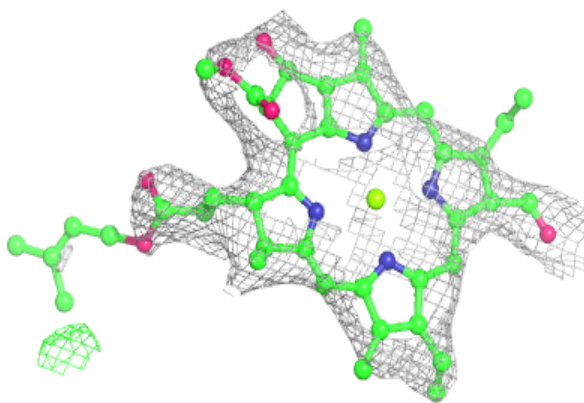
**Electron density around OIE E 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

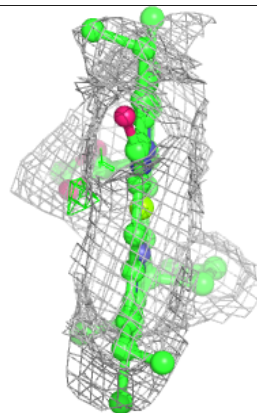
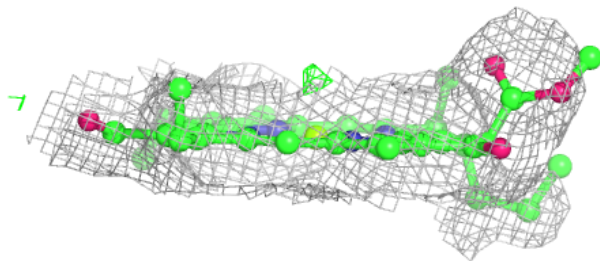
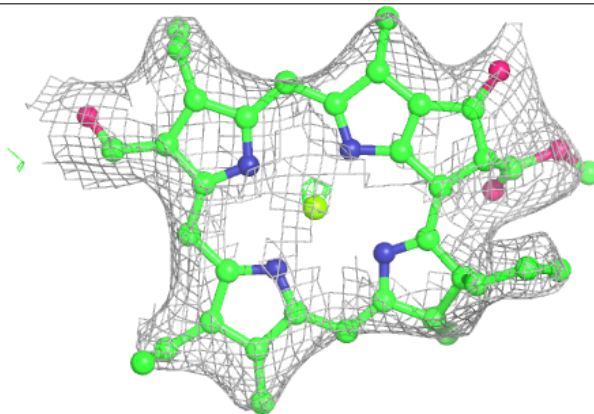


**Electron density around CHL B 311:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CHL C 310:**

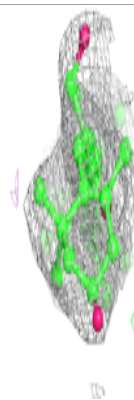
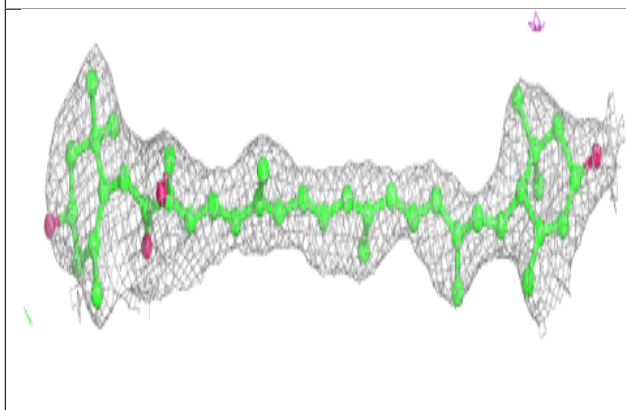
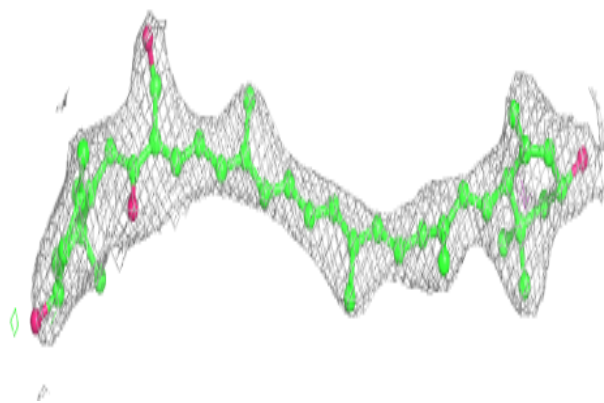
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





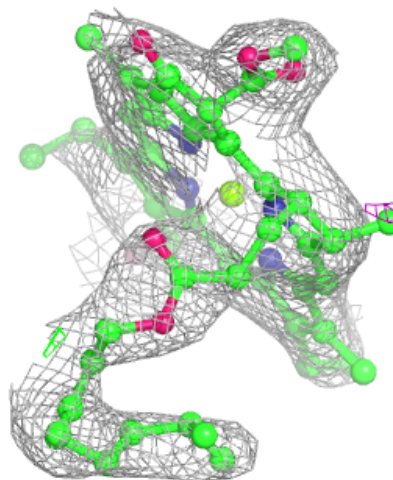
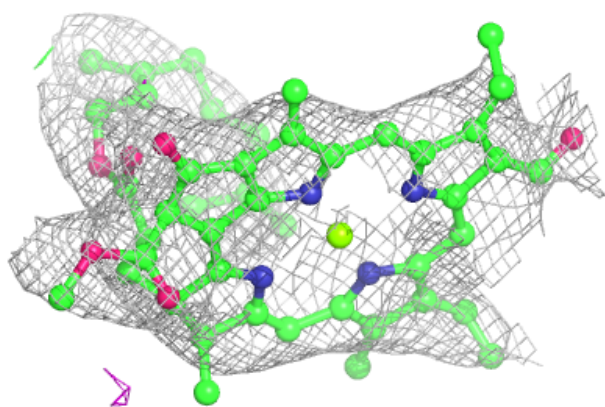
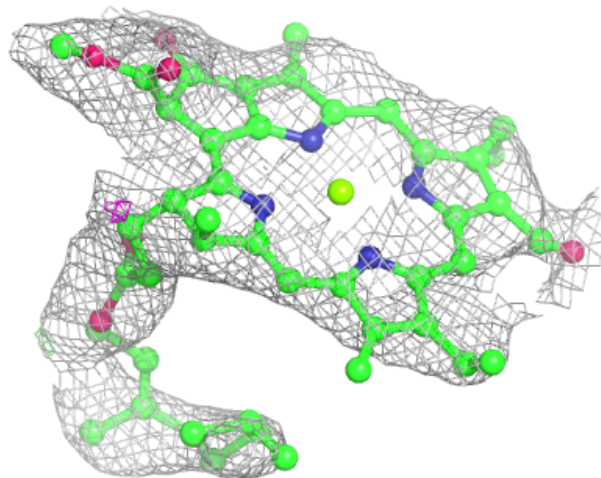
**Electron density around OIE E 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



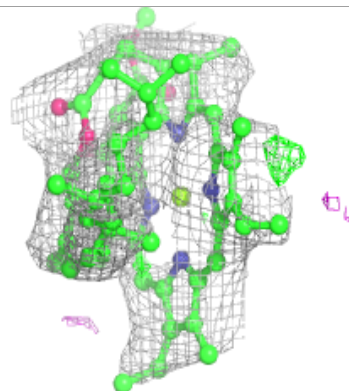
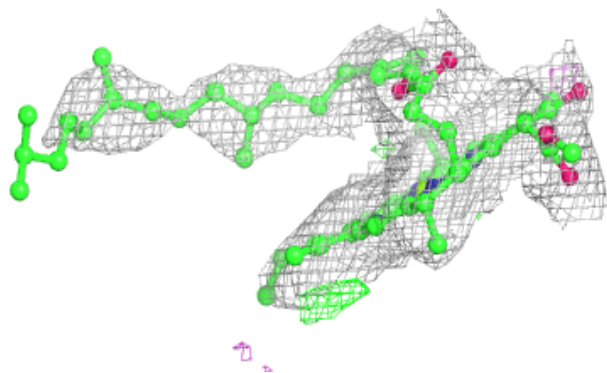
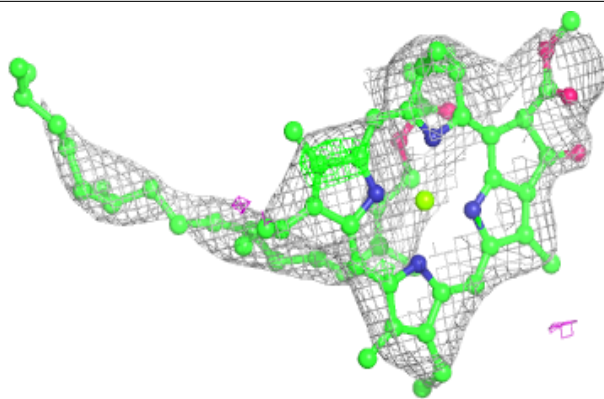
**Electron density around CHL C 312:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

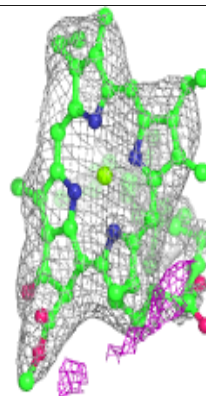
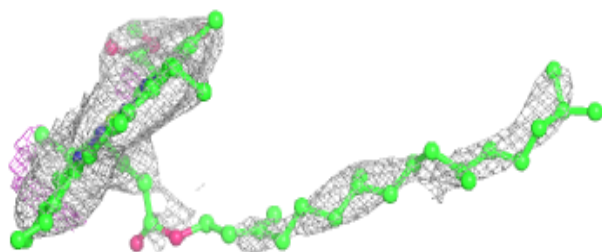
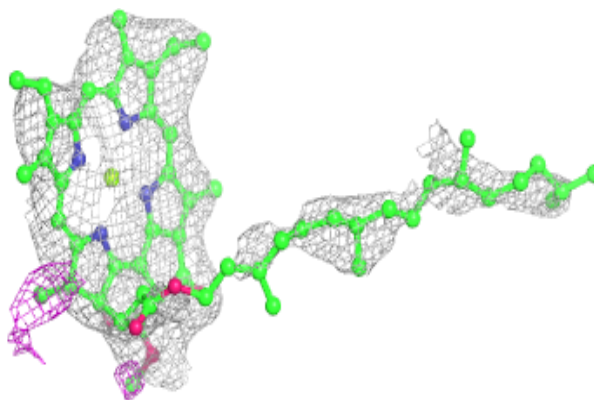


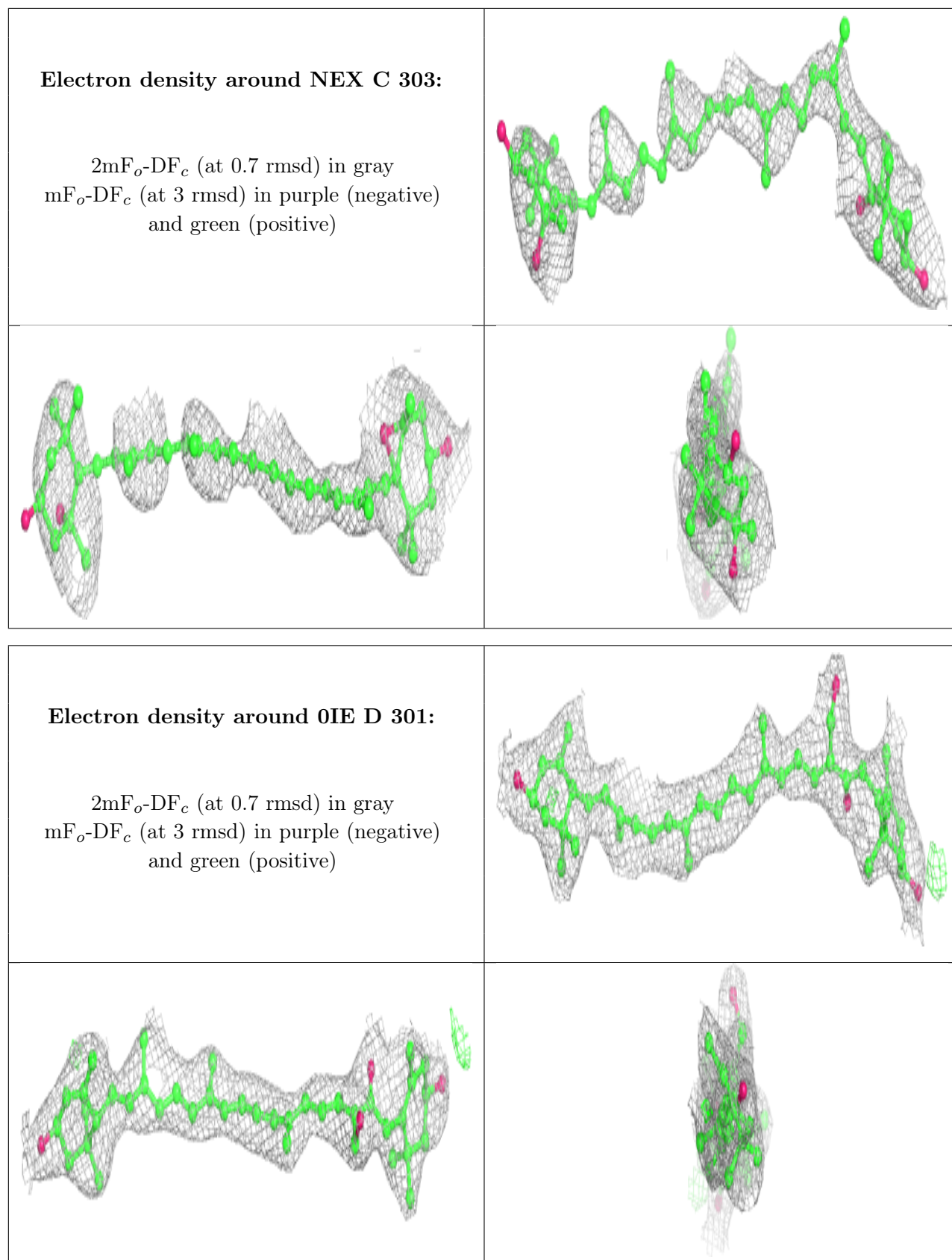
**Electron density around CLA B 318:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA C 315:**

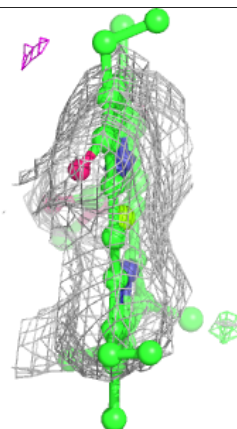
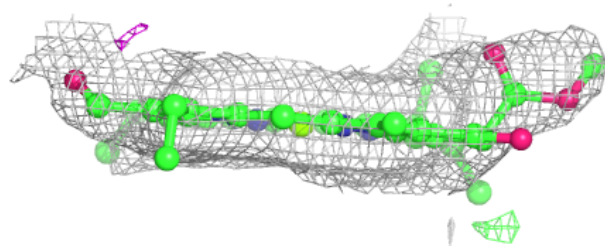
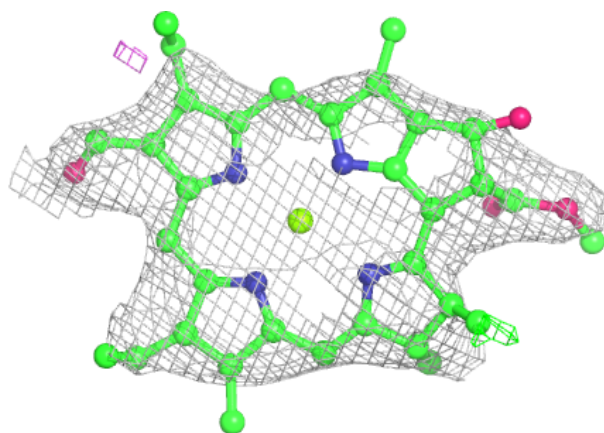
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



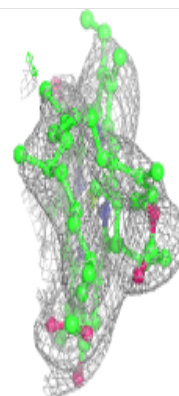
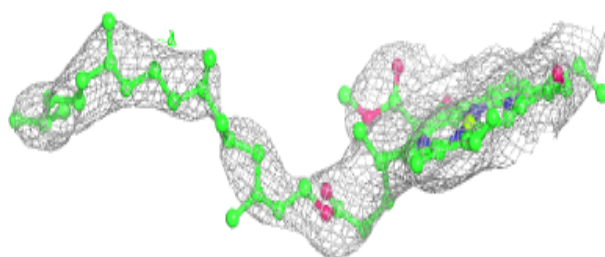
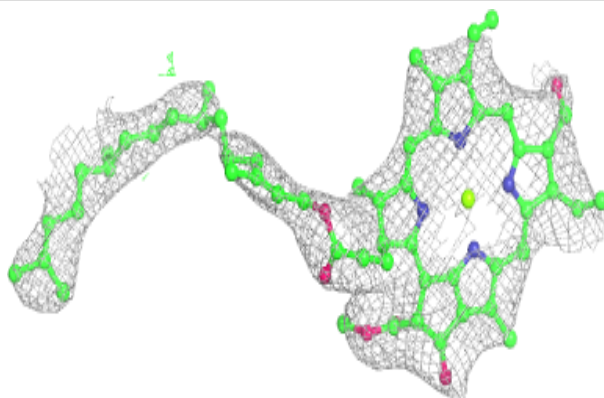


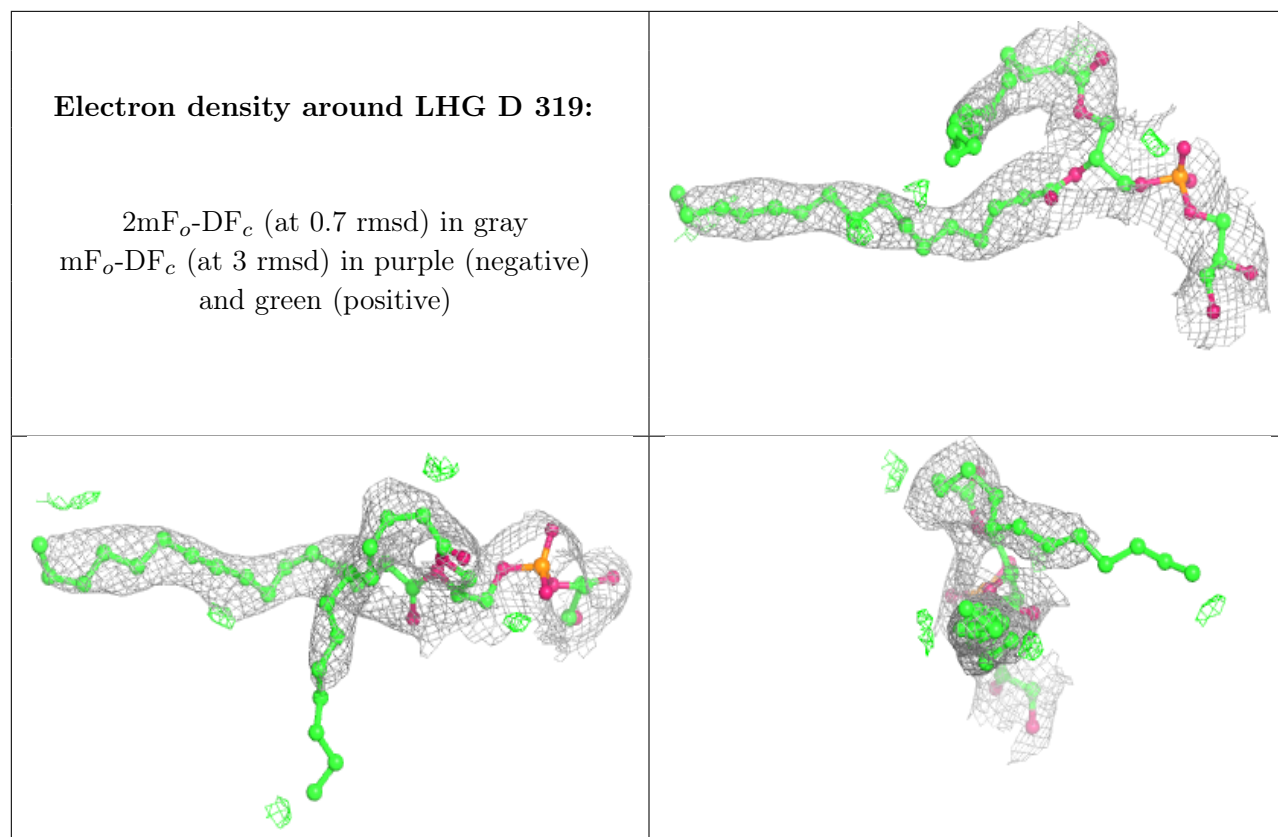
**Electron density around CHL F 308:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CHL D 305:**

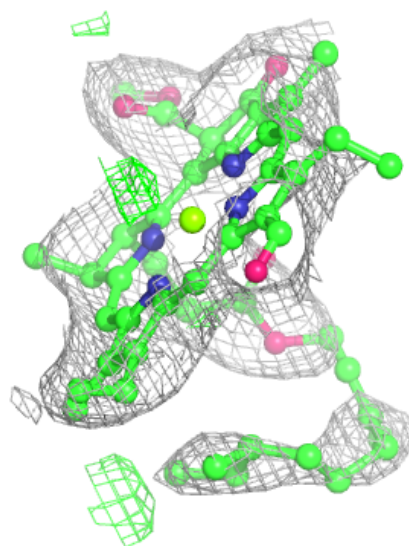
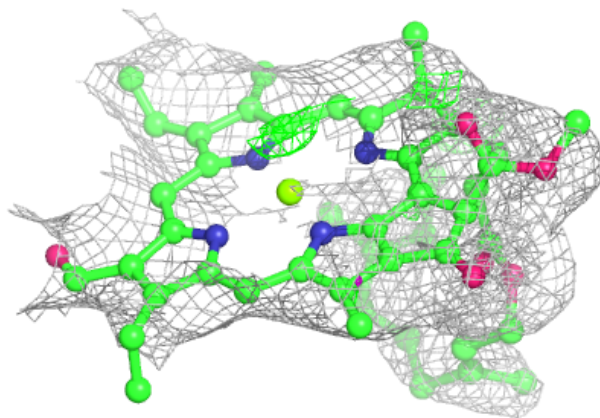
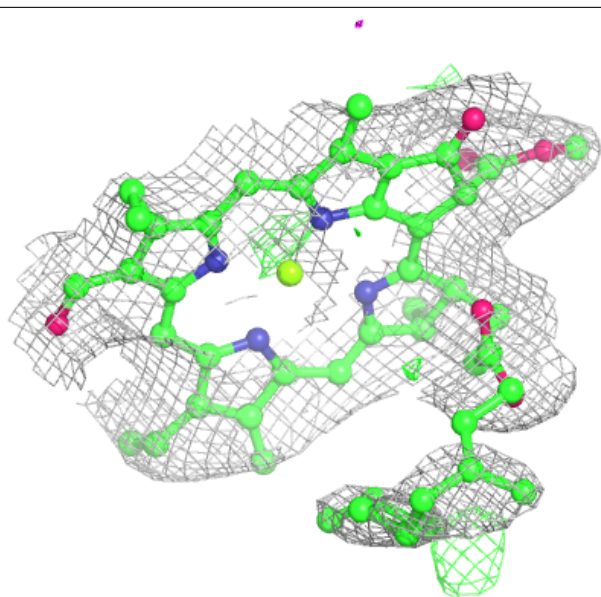
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

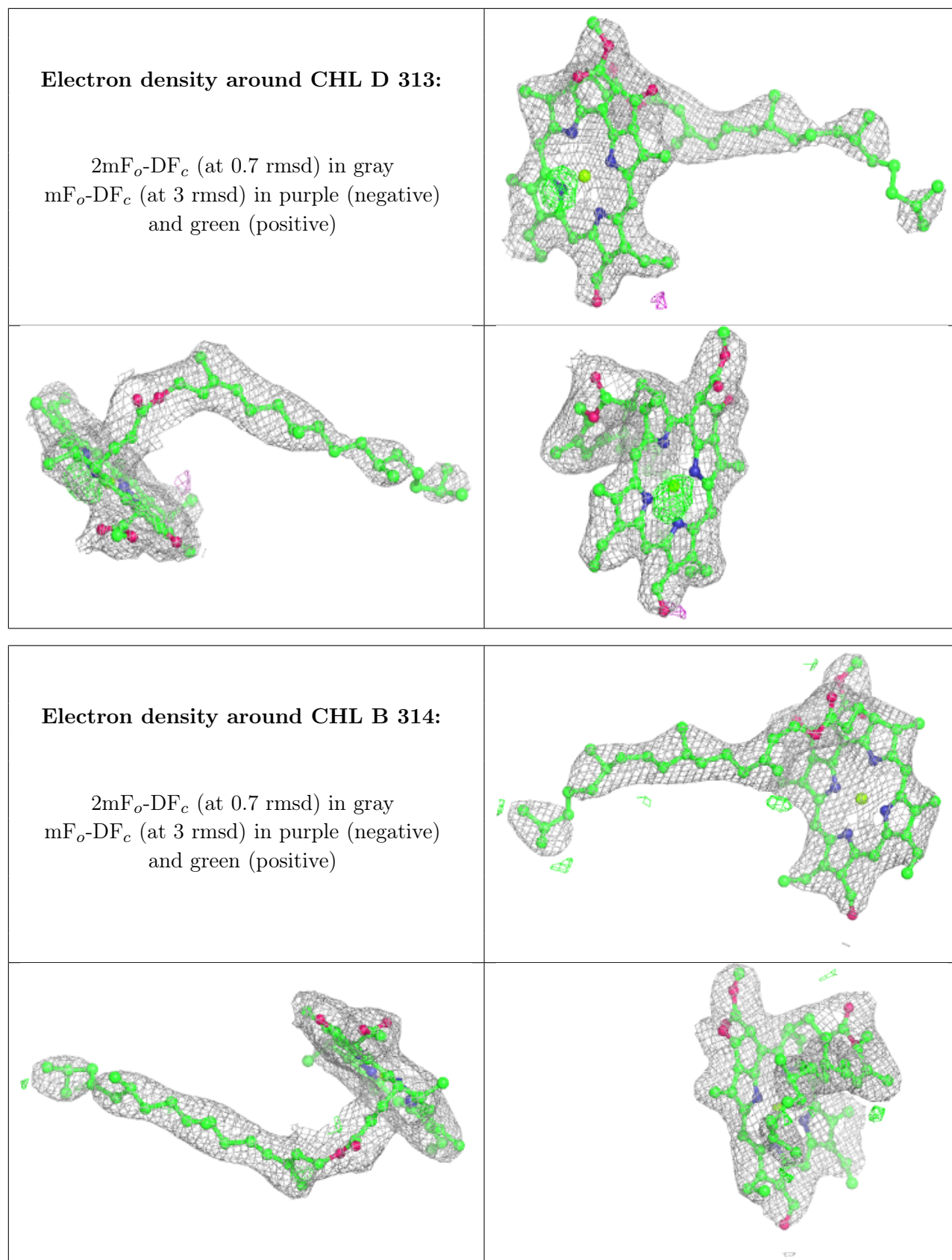




**Electron density around CHL B 313:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

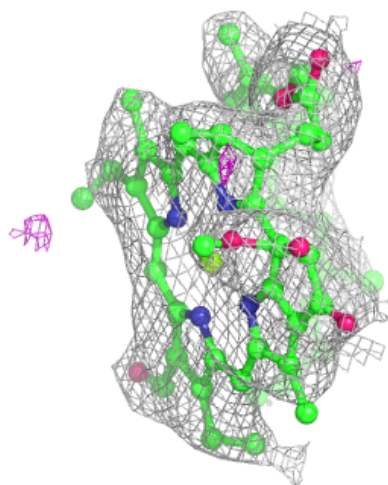
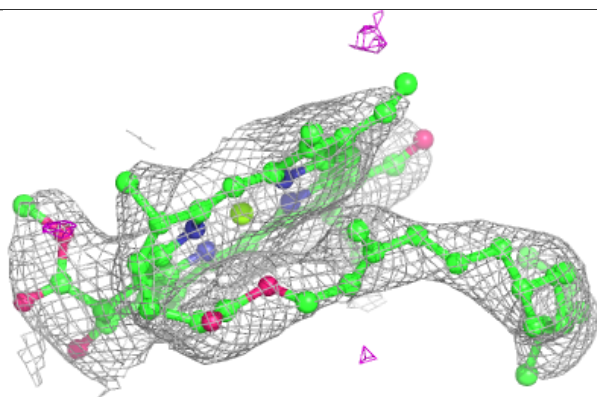
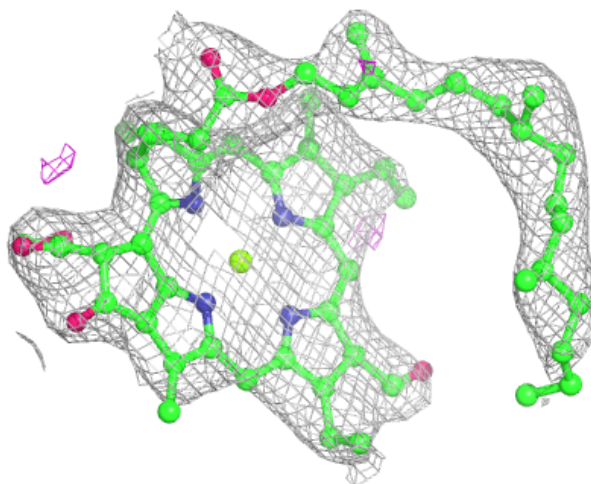






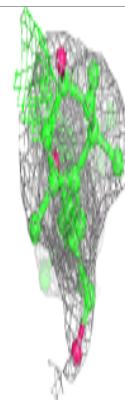
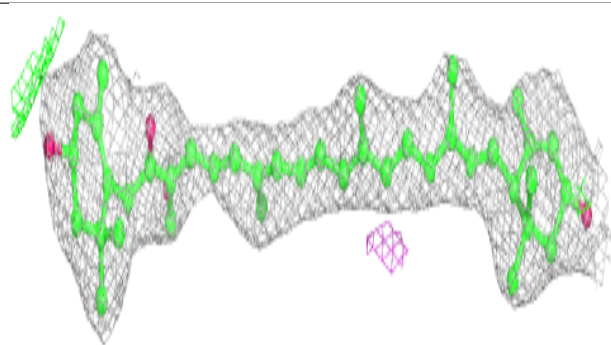
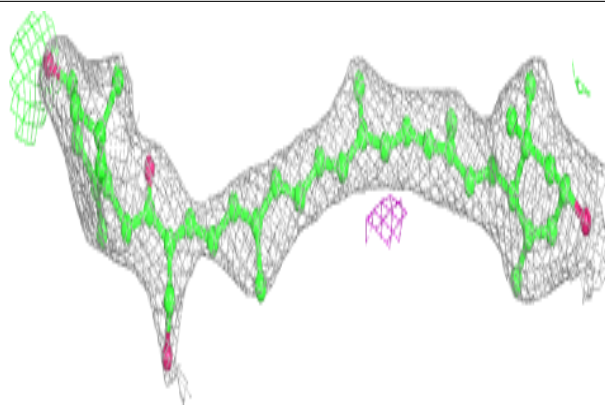
**Electron density around CHL E 305:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

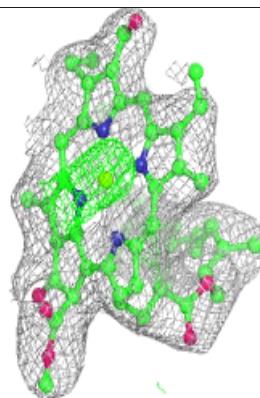
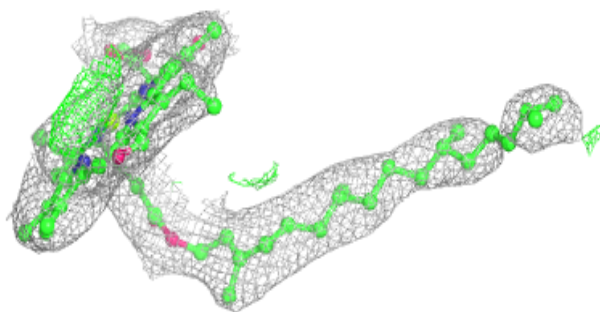
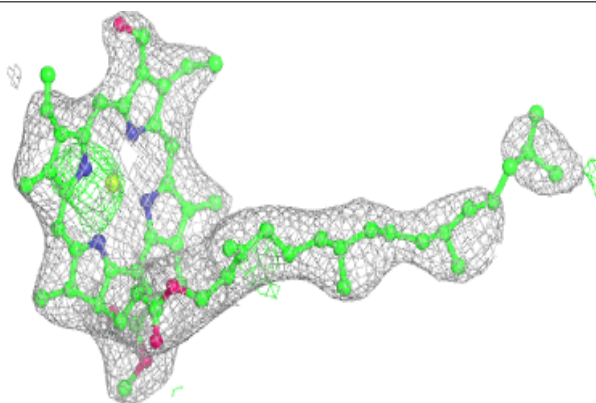


**Electron density around OIE C 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

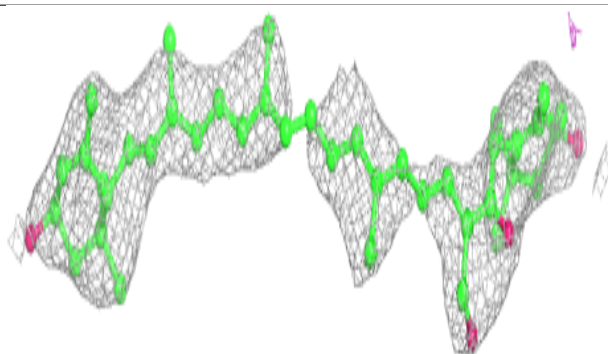
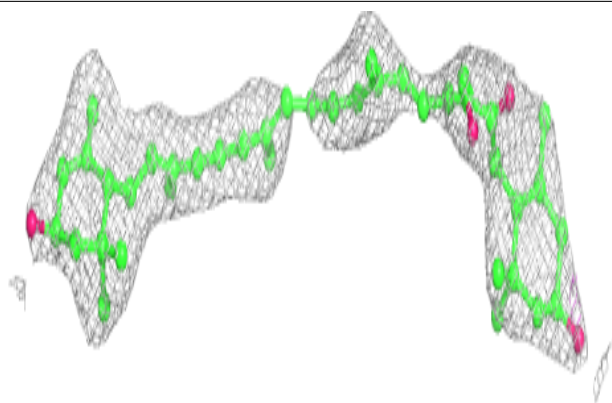
**Electron density around CHL A 313:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

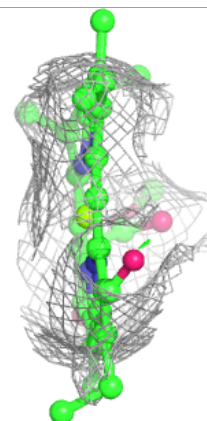
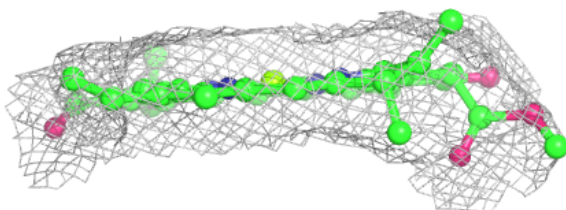
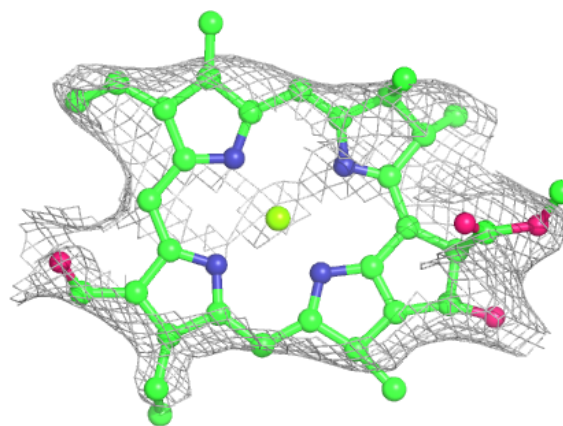


**Electron density around OIE C 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

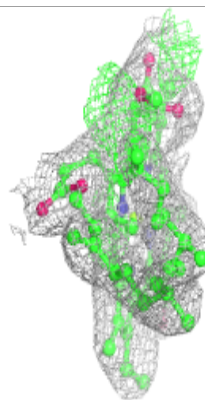
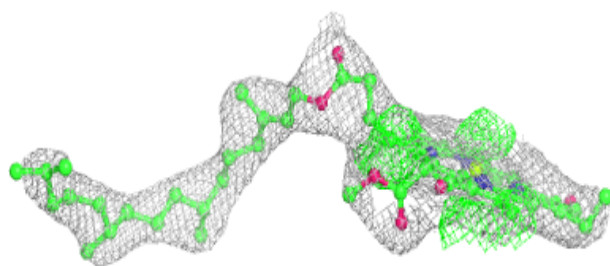
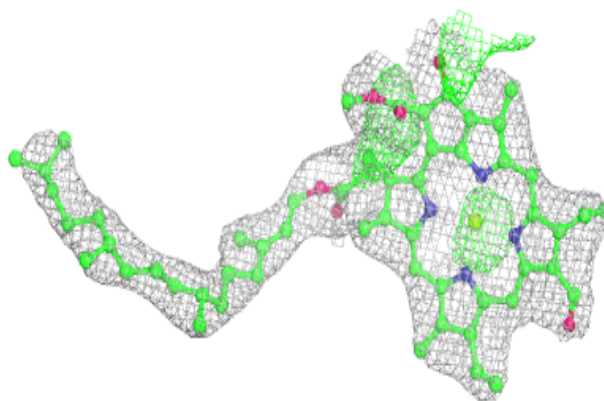
**Electron density around CHL D 309:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

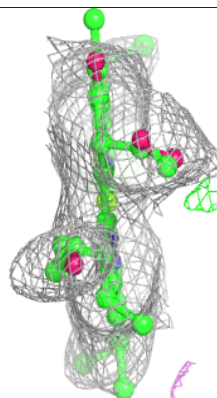
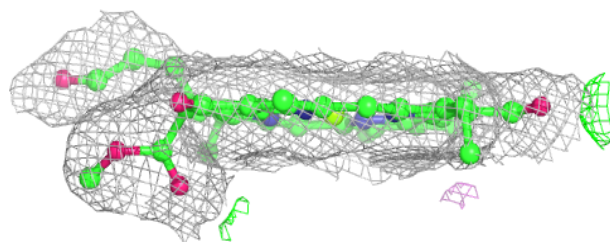
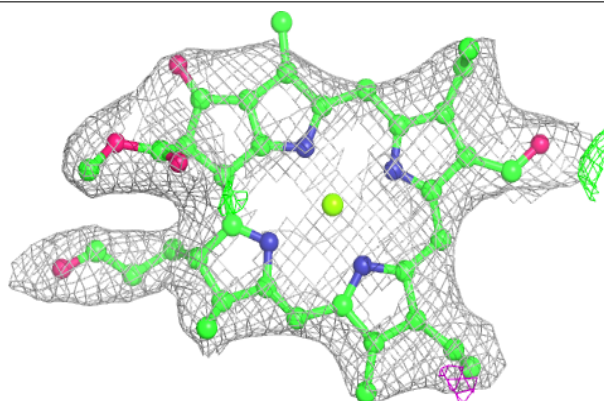


**Electron density around CHL F 304:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

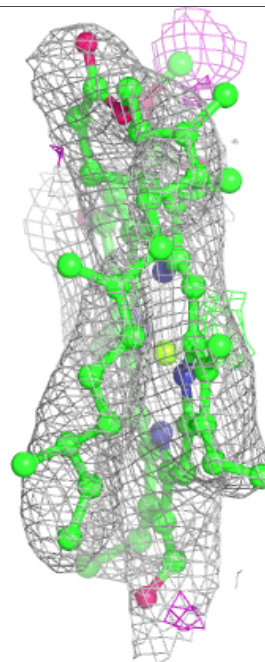
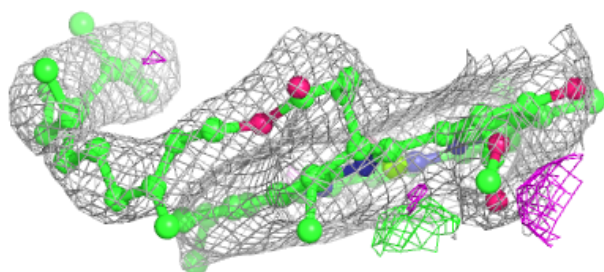
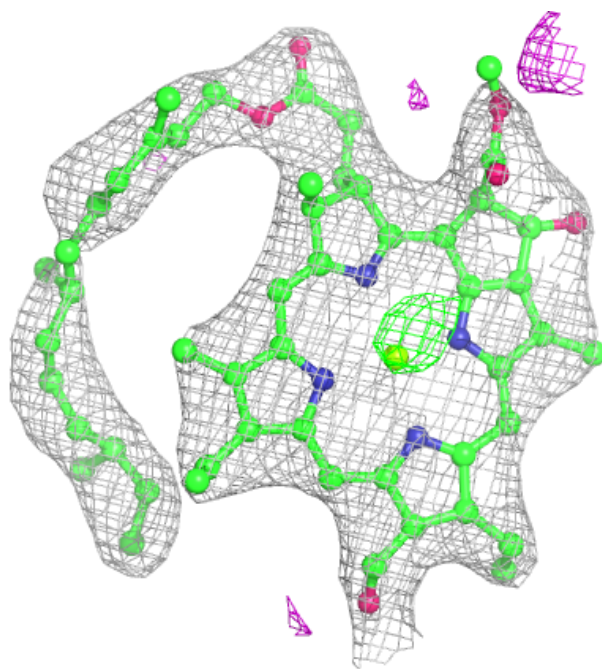
**Electron density around CHL D 310:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



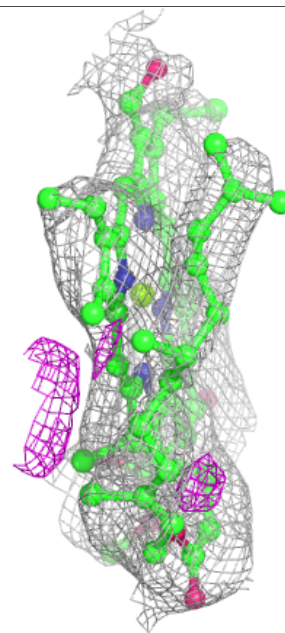
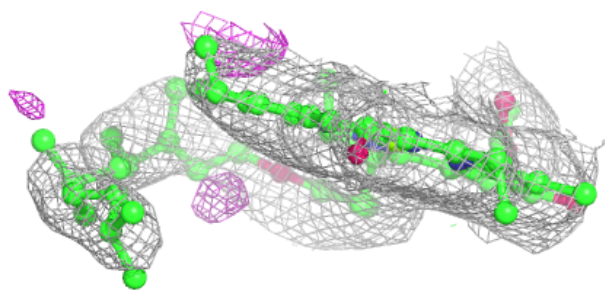
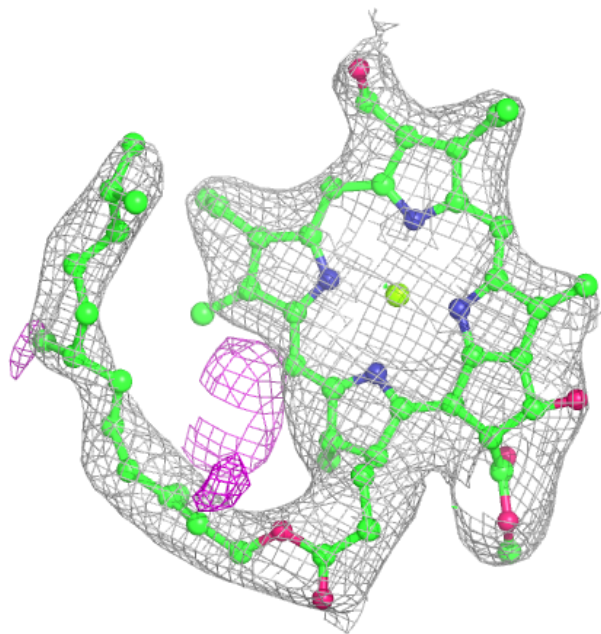
**Electron density around CHL D 311:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



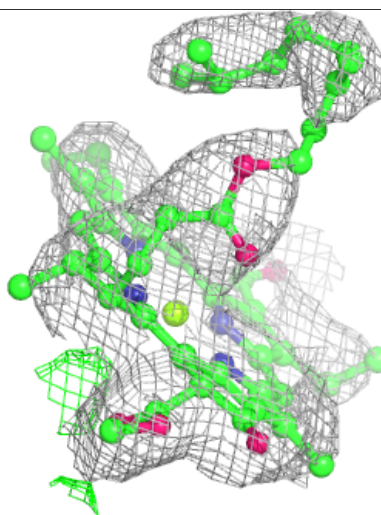
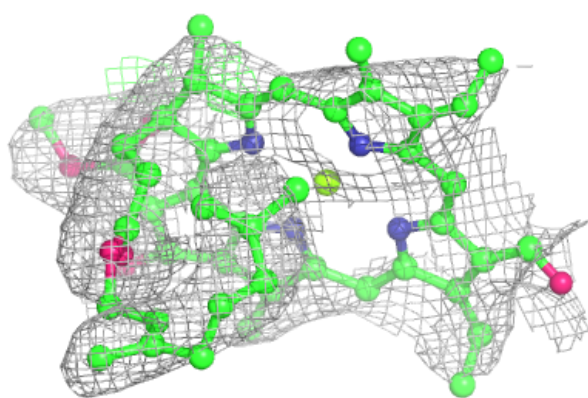
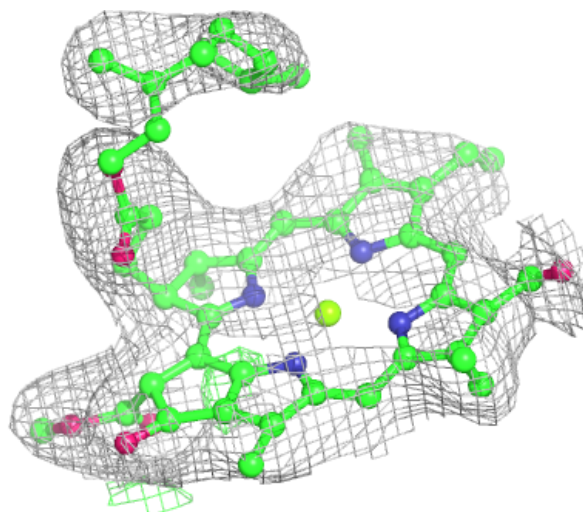
**Electron density around CHL F 310:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



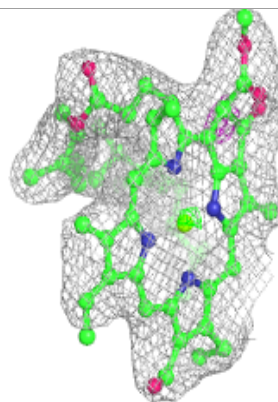
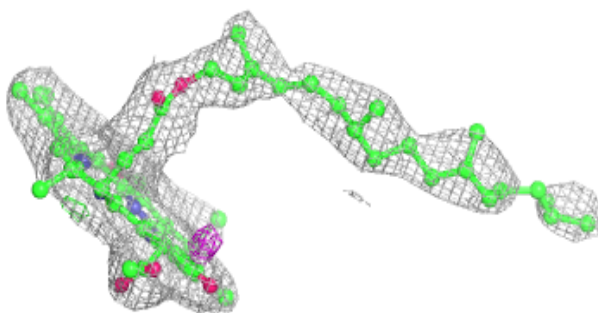
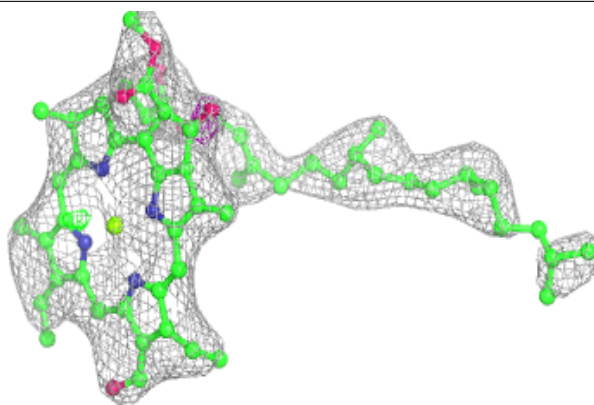
**Electron density around CHL F 311:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

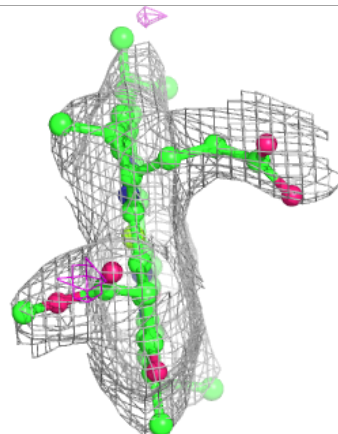
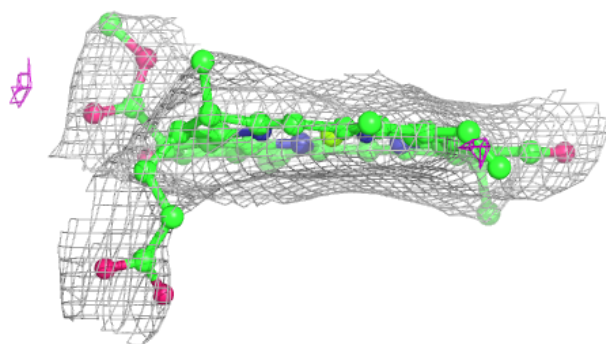
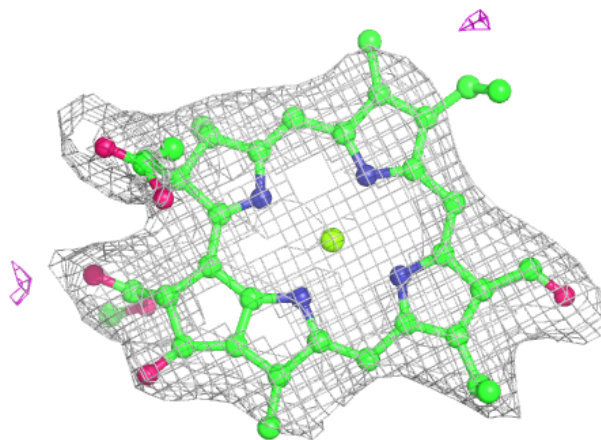


**Electron density around CHL F 312:**

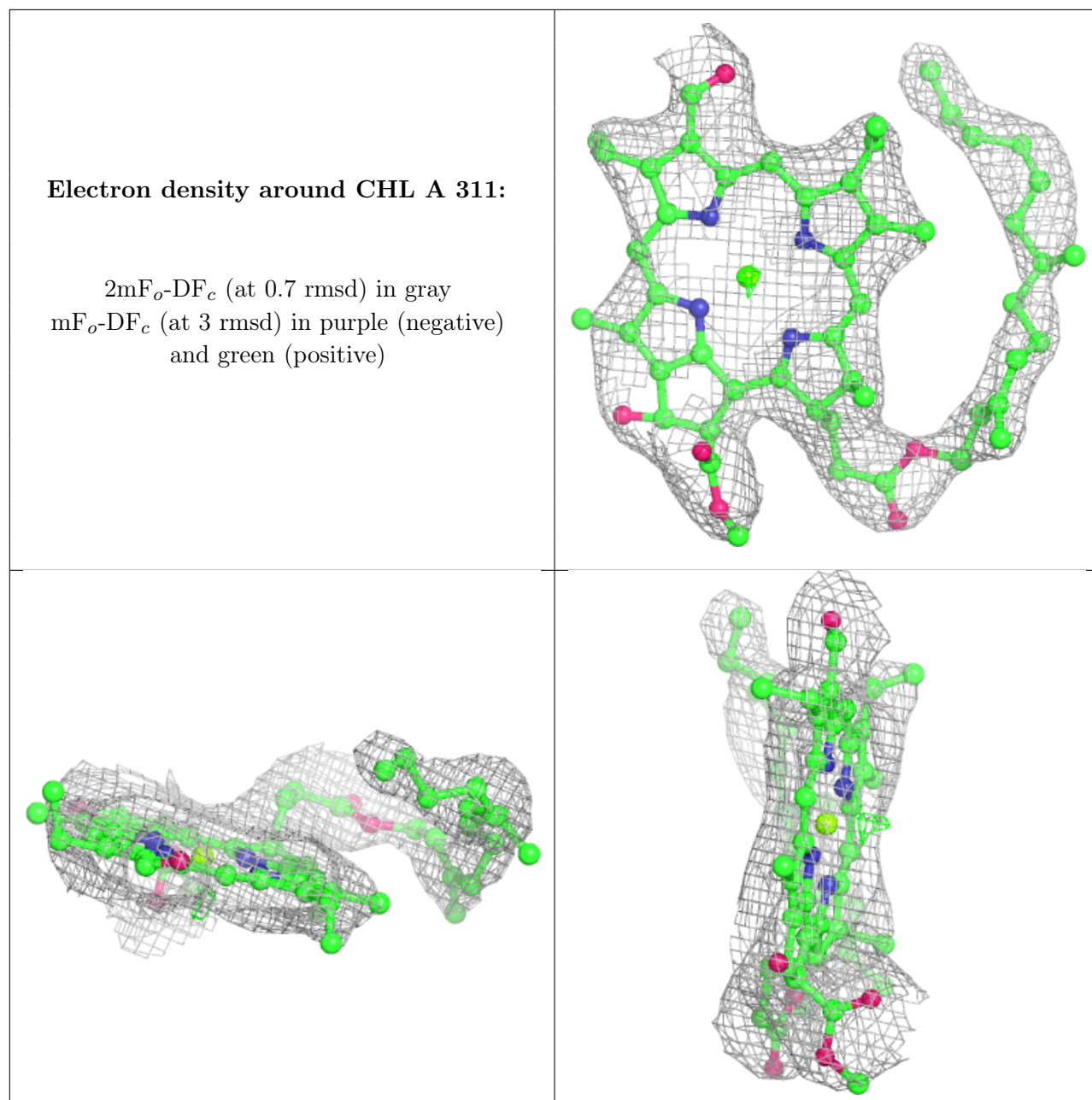
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CHL F 317:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

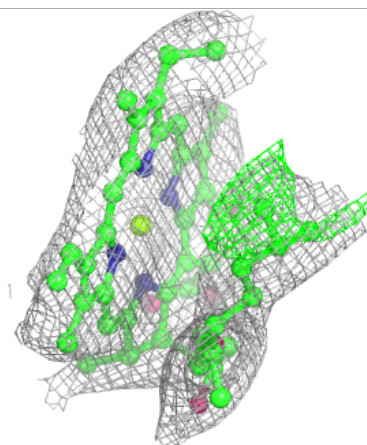
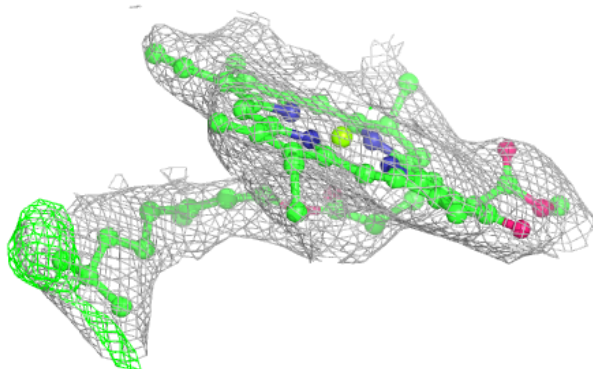
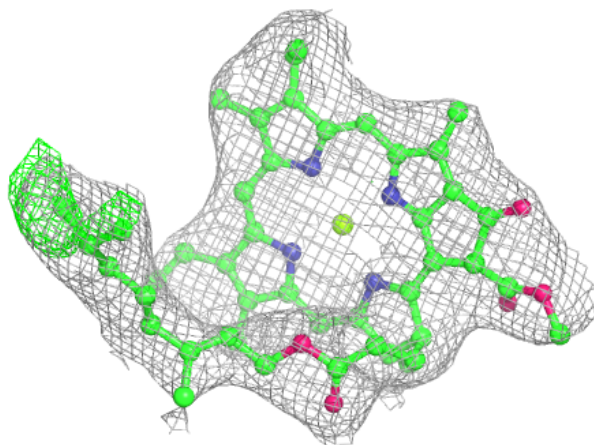


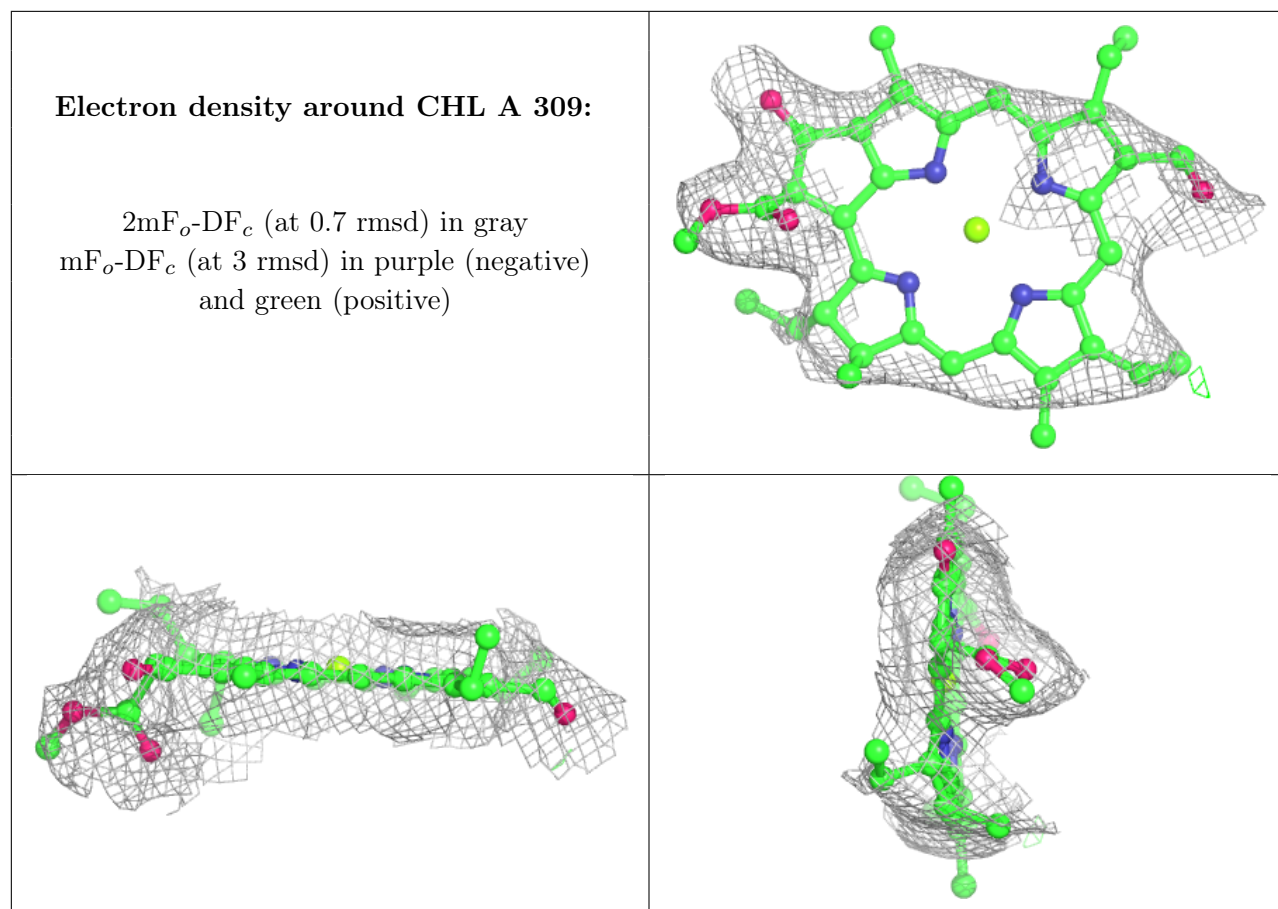




**Electron density around CLA A 314:**

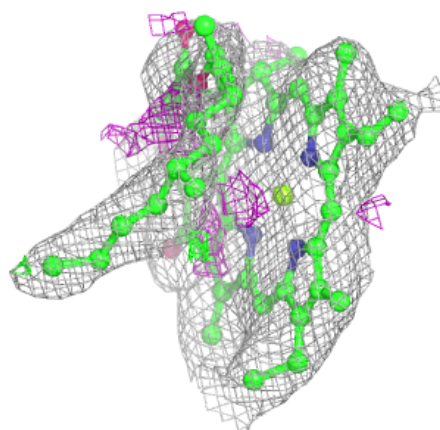
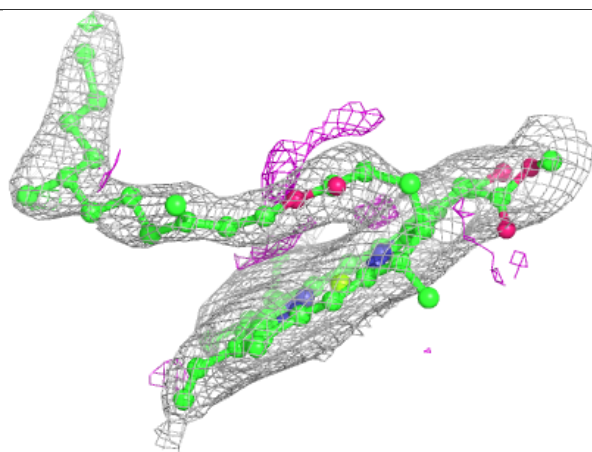
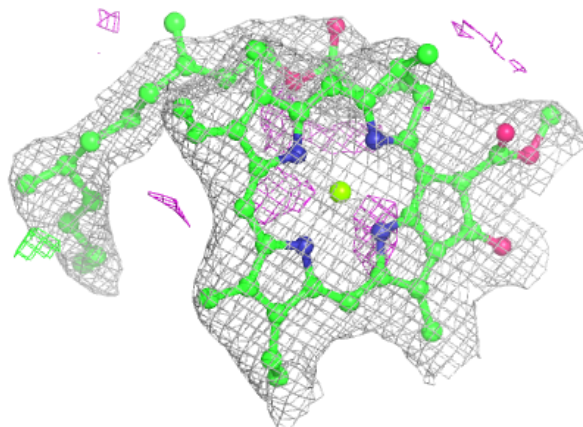
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





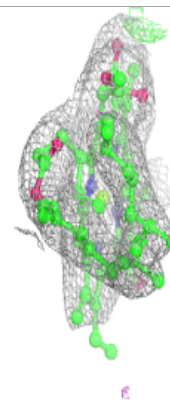
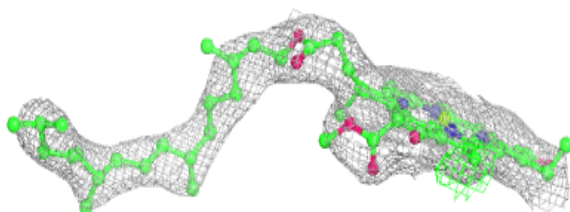
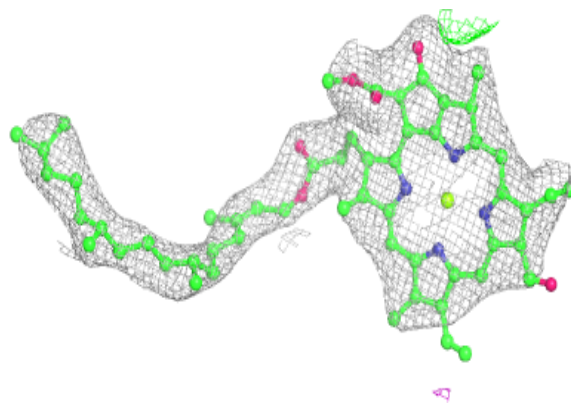
**Electron density around CLA B 315:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



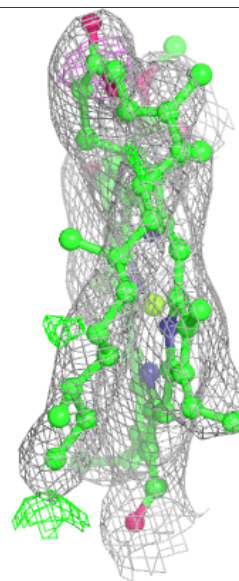
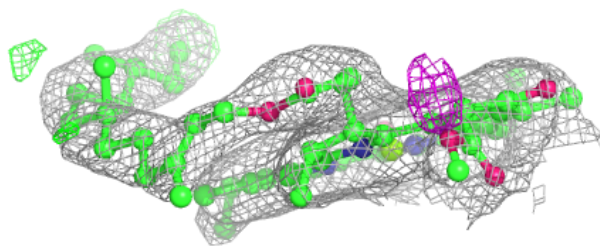
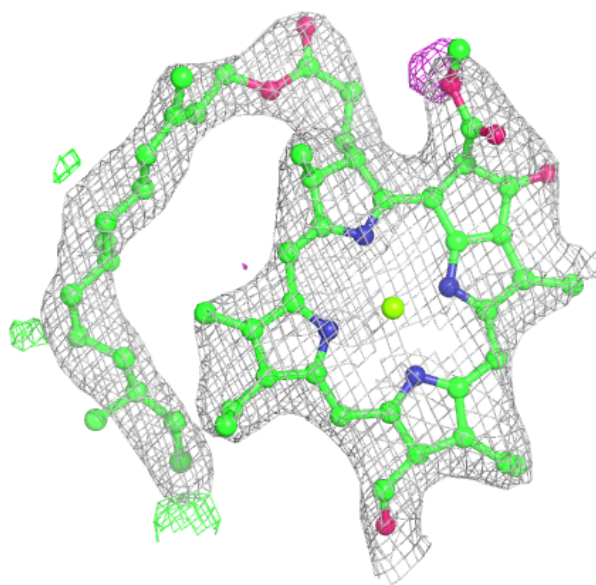
**Electron density around CHL E 304:**

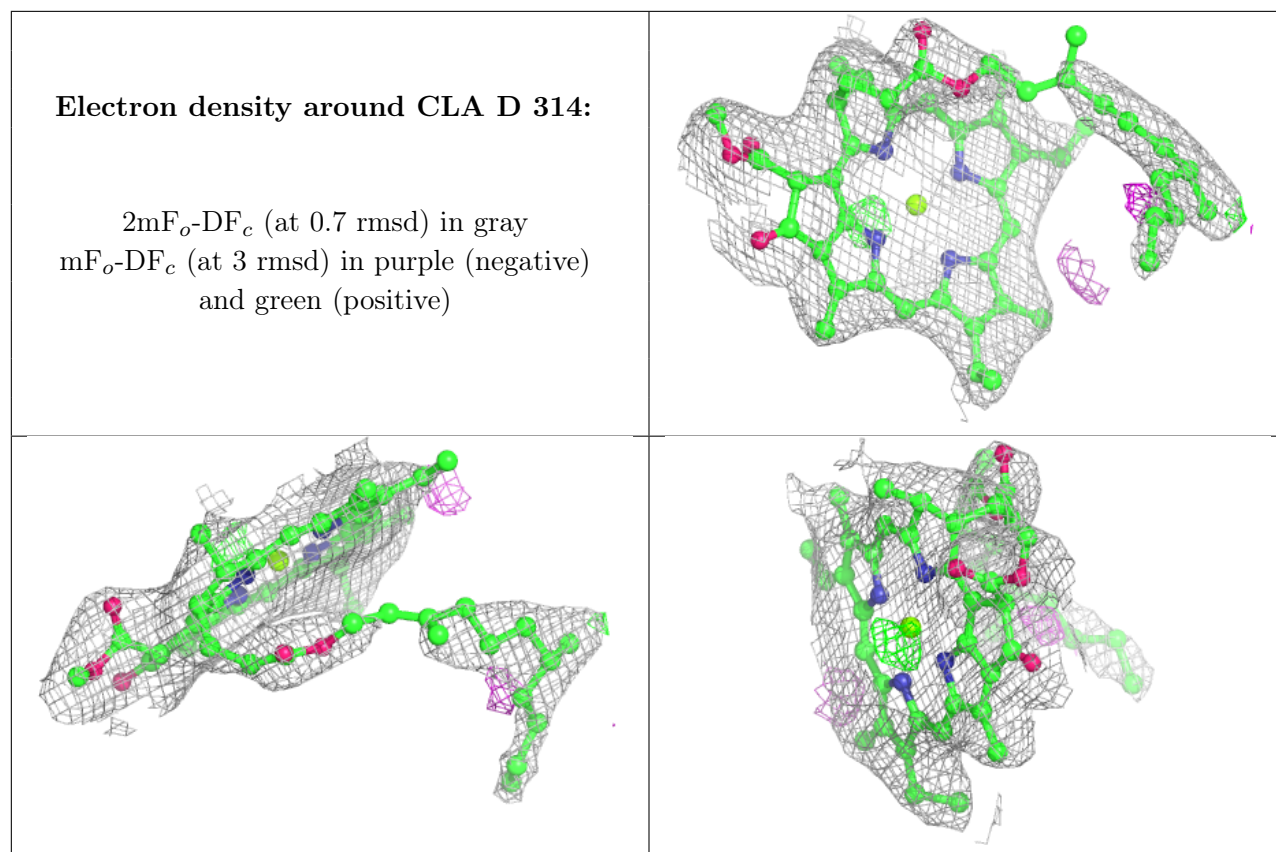
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CHL B 312:**

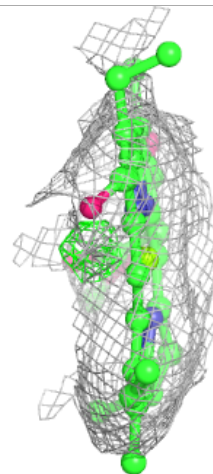
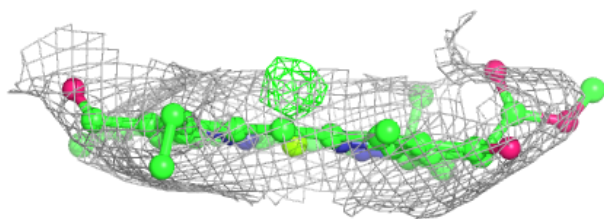
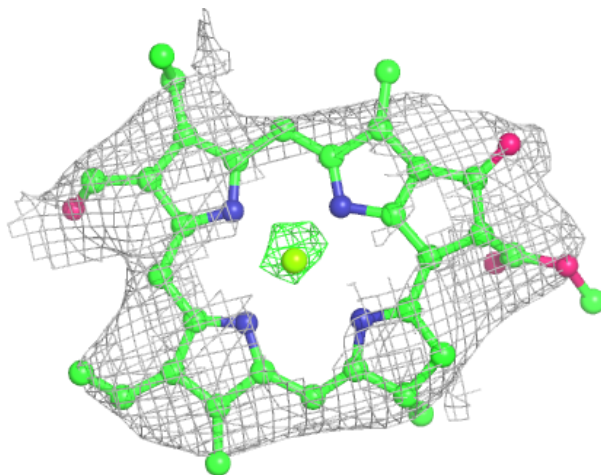
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CHL E 308:**

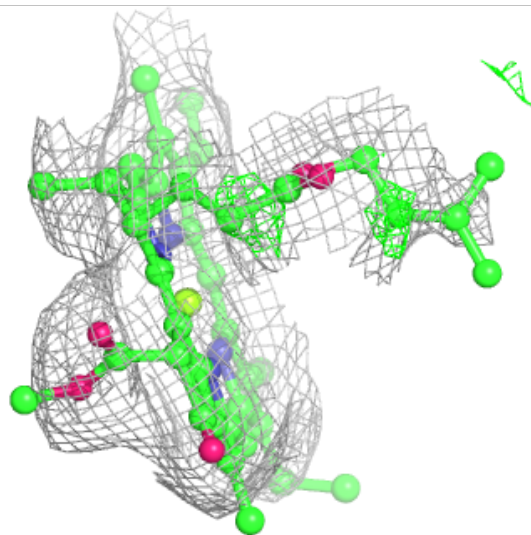
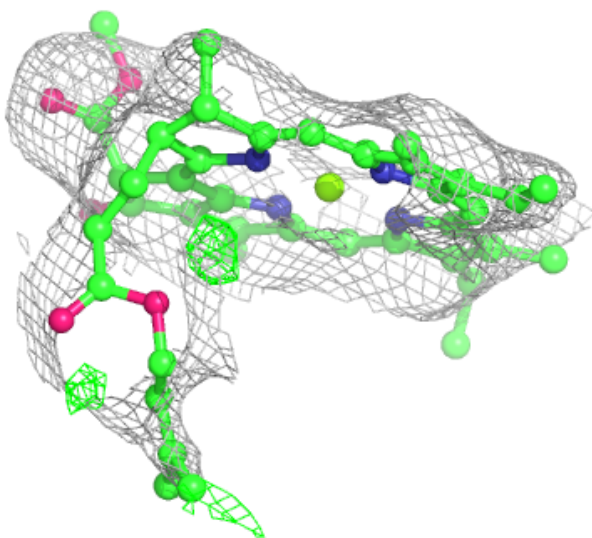
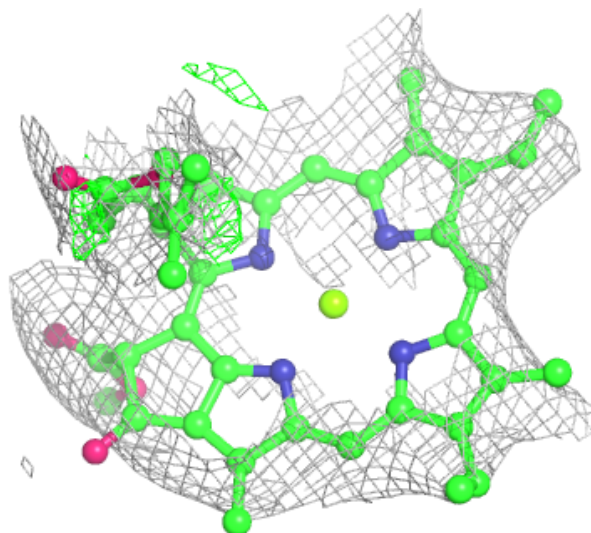
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





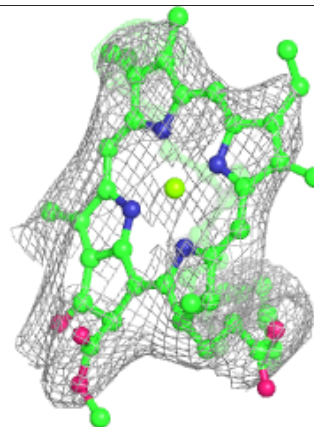
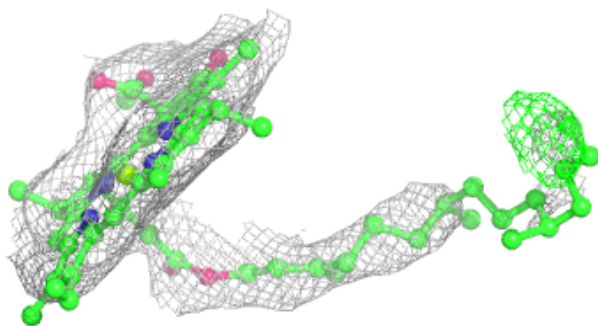
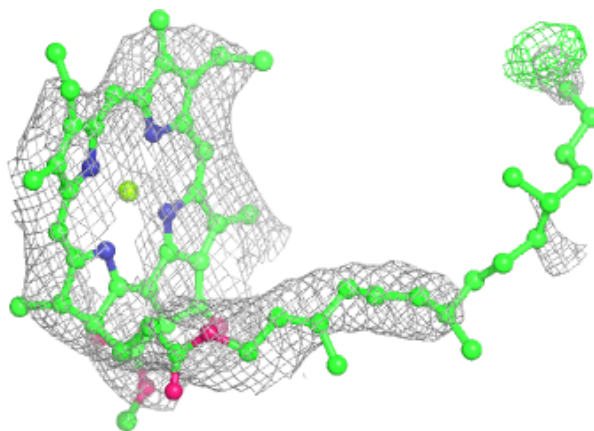
**Electron density around CLA E 307:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



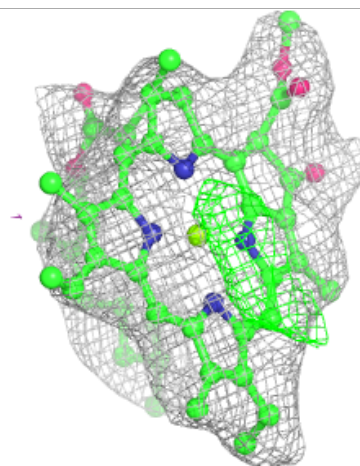
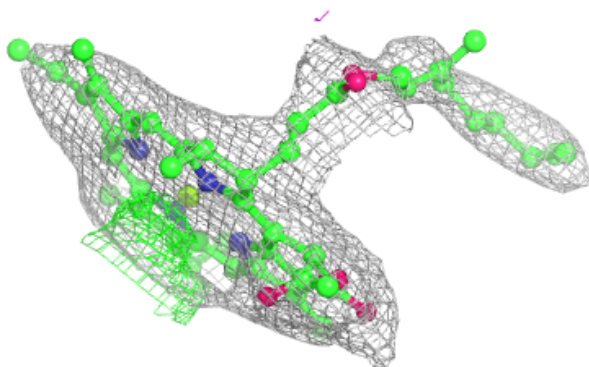
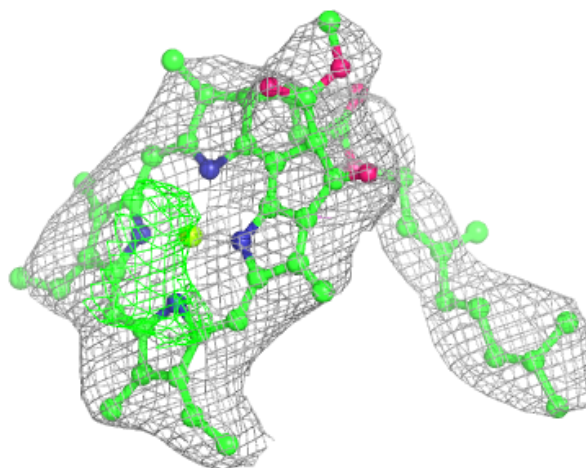
**Electron density around CLA E 314:**

$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) in purple (negative)  
and green (positive)



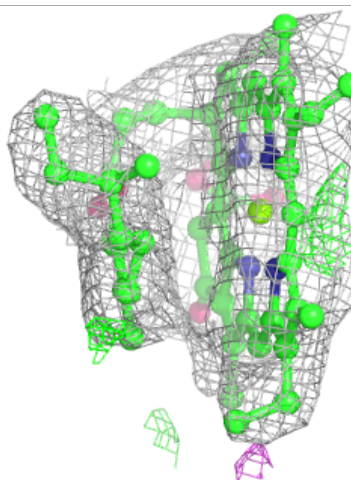
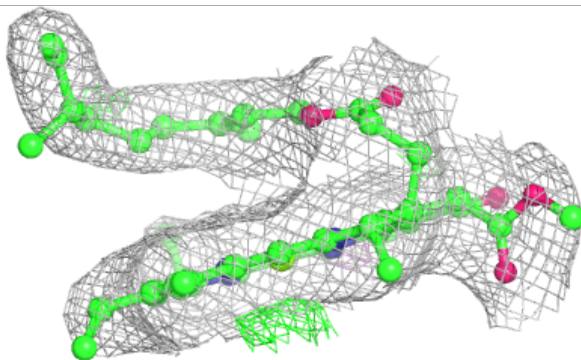
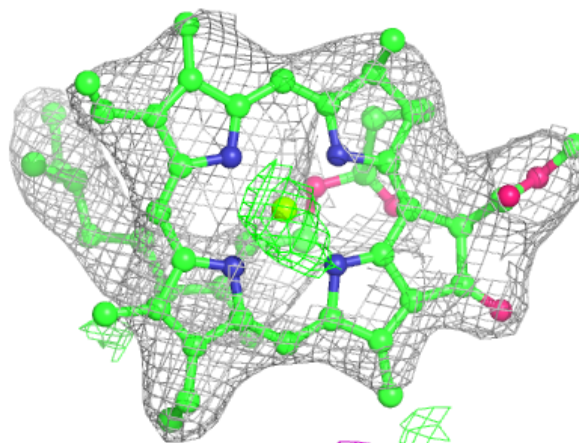
**Electron density around CLA F 314:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



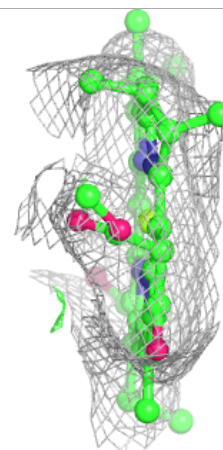
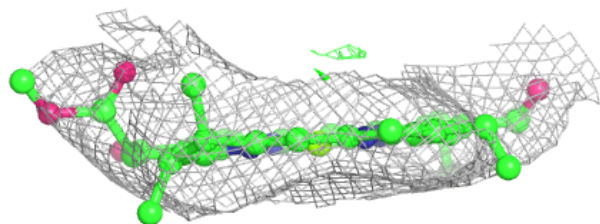
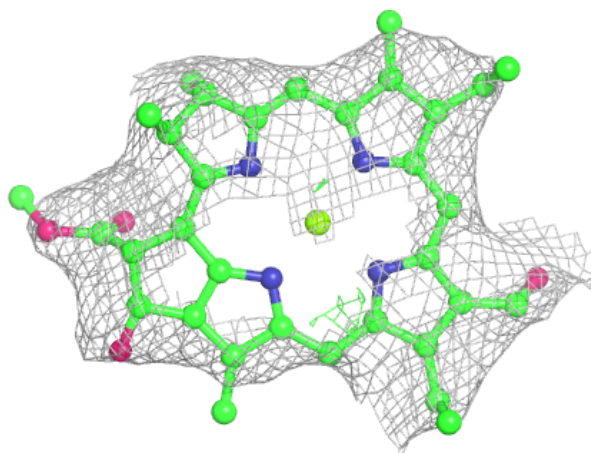
**Electron density around CLA F 316:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

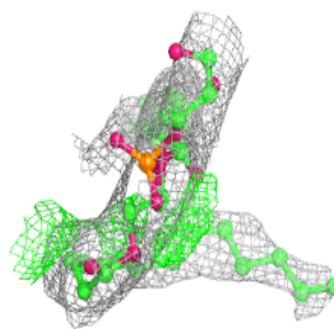
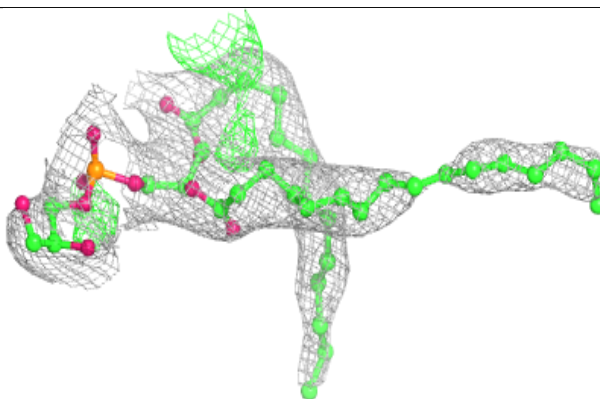
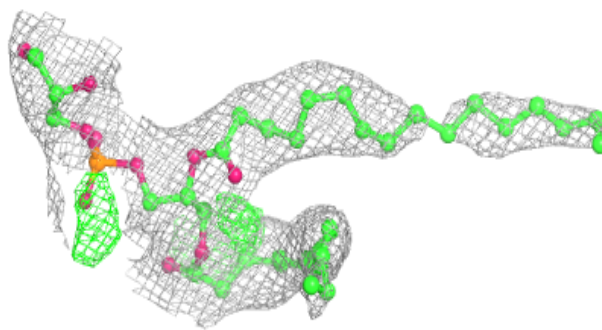


**Electron density around CHL C 309:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

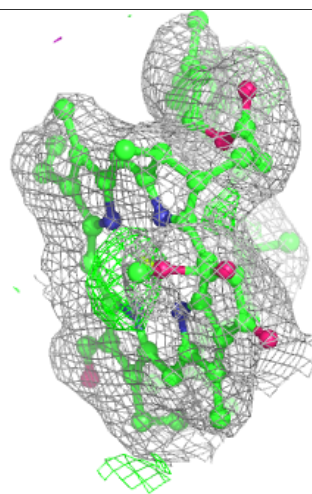
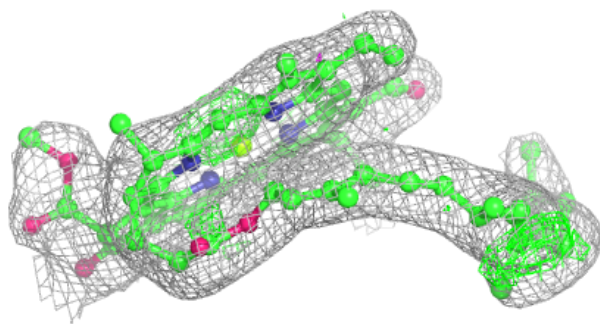
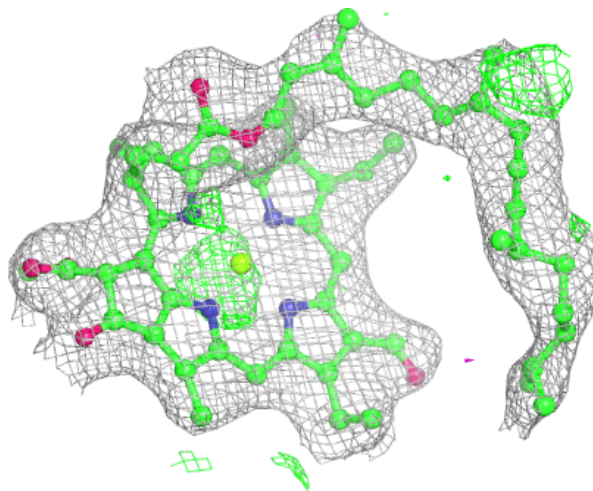
**Electron density around LHG B 320:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



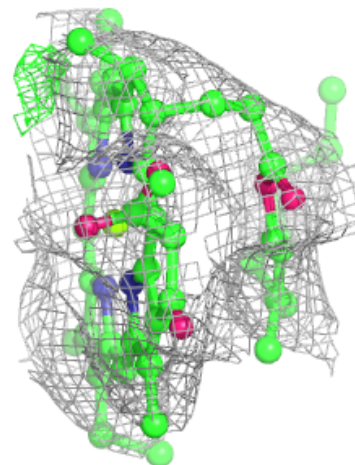
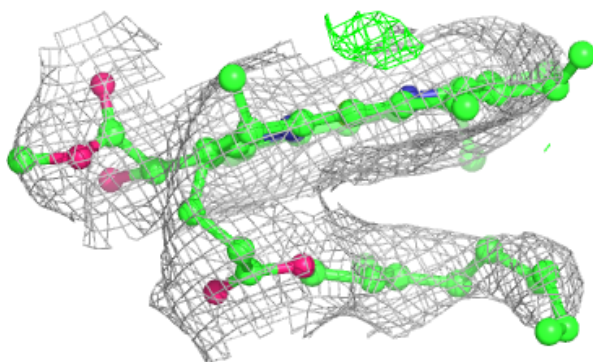
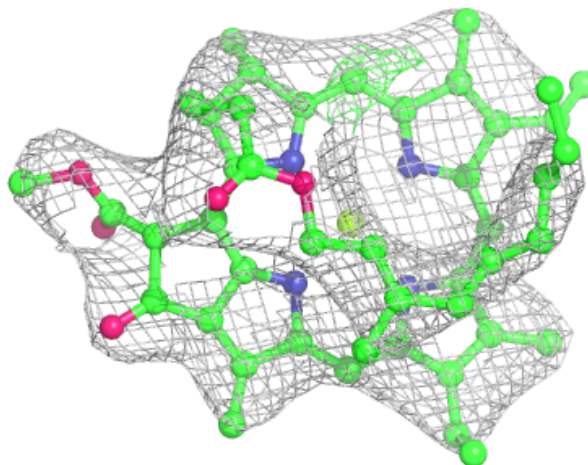
**Electron density around CHL F 305:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



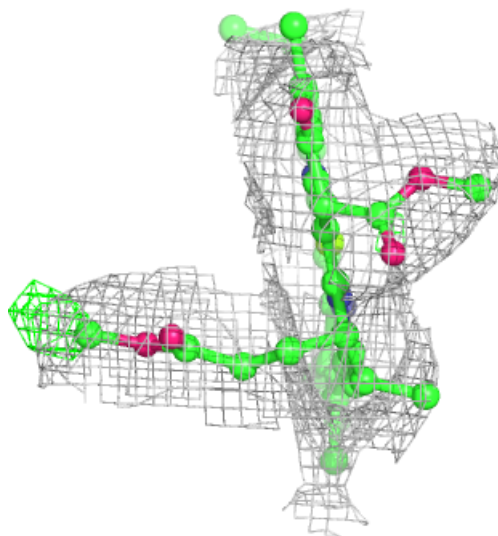
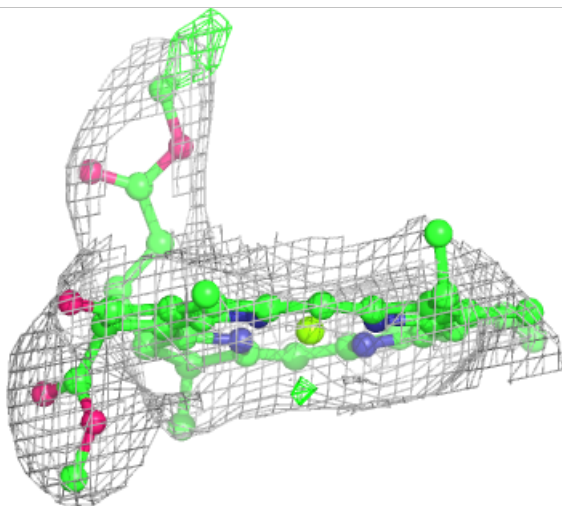
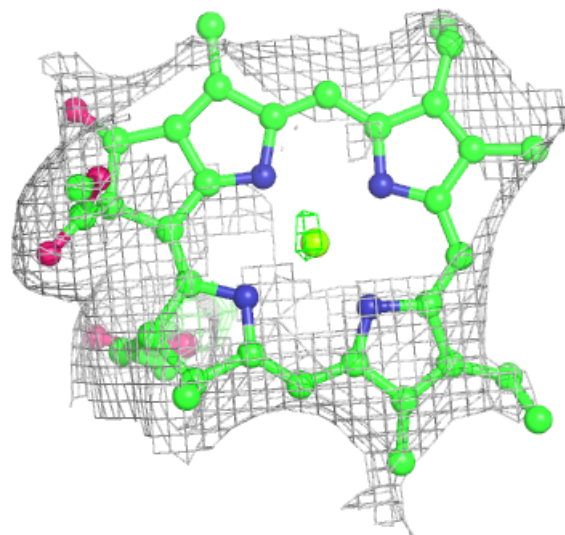
**Electron density around CLA A 317:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 309:**

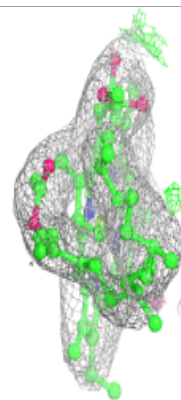
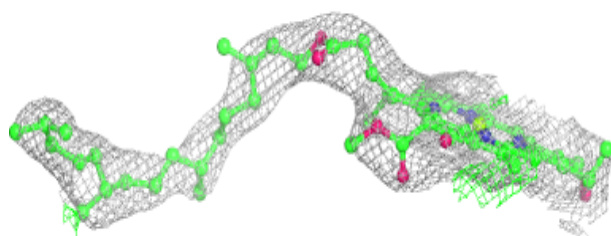
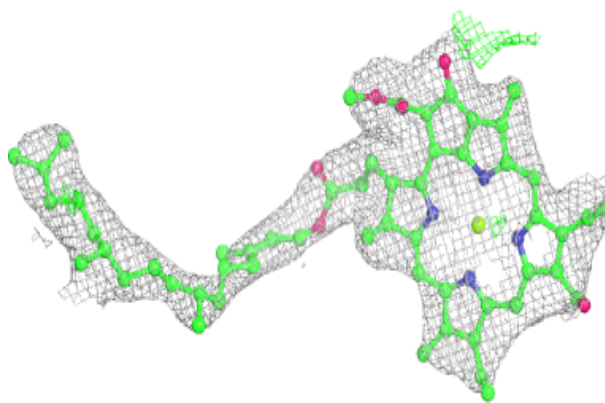
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



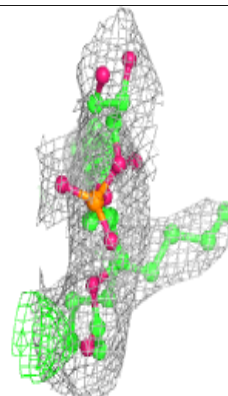
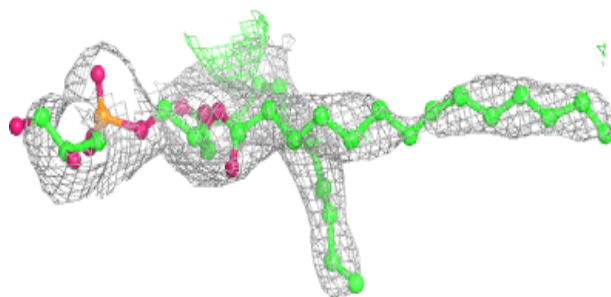
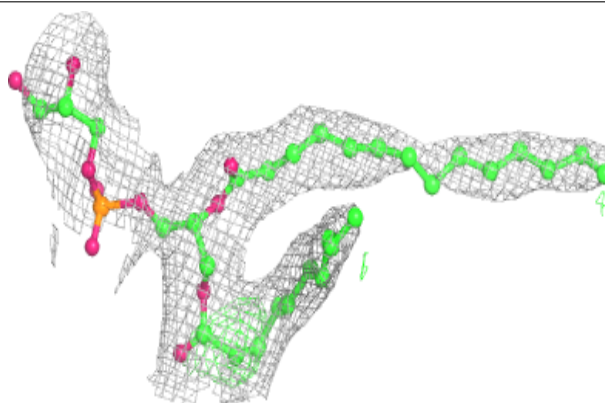


**Electron density around CHL A 305:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

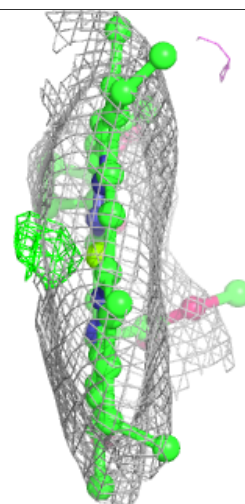
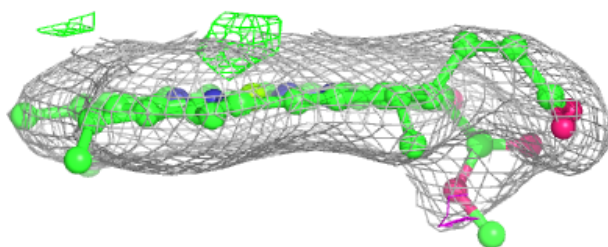
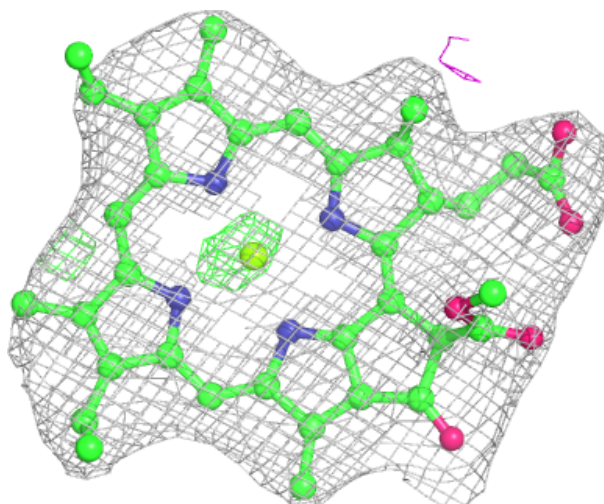
**Electron density around LHG E 318:**

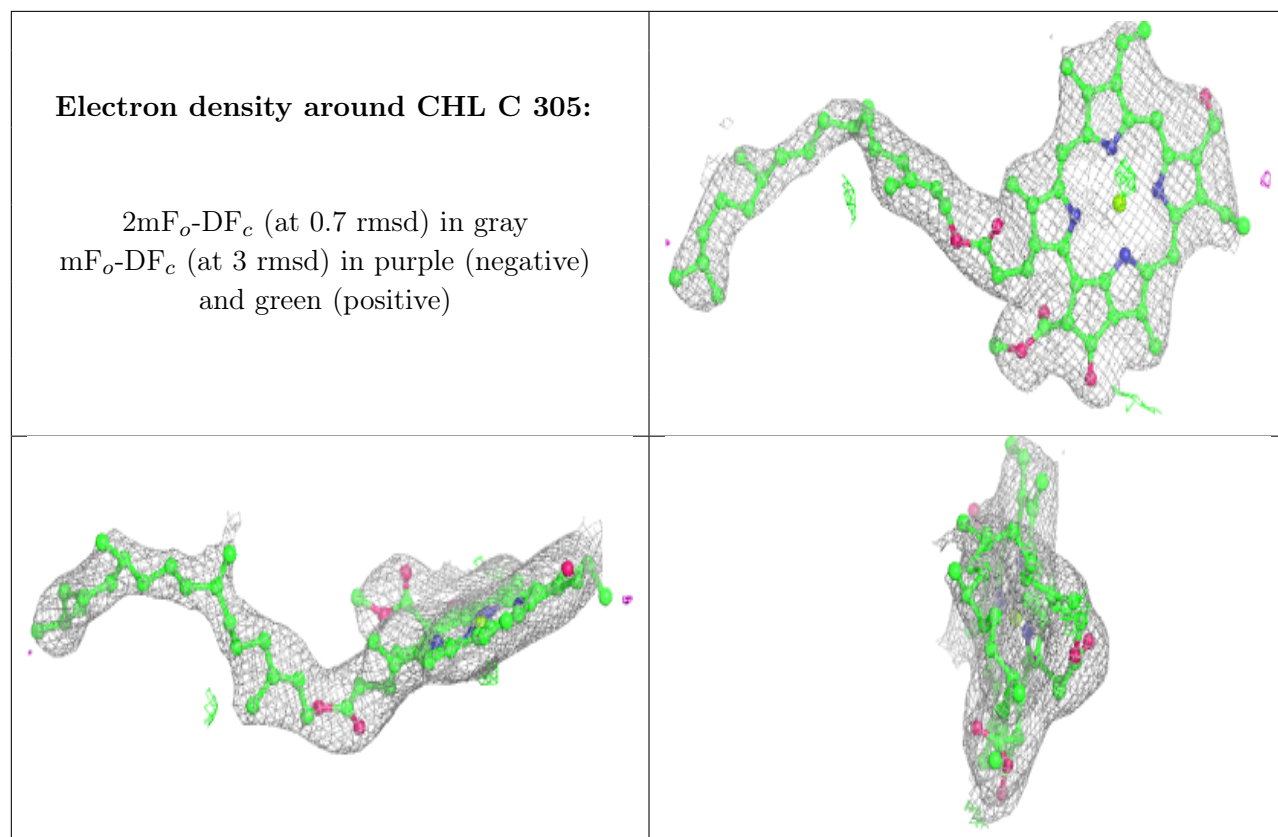
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 317:**

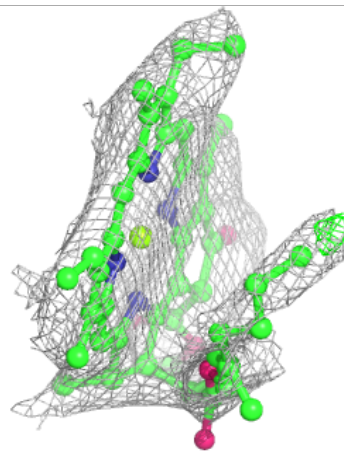
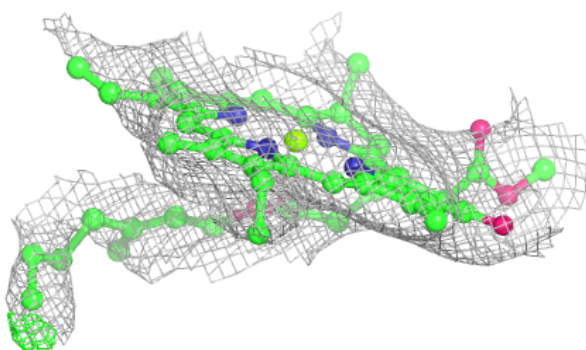
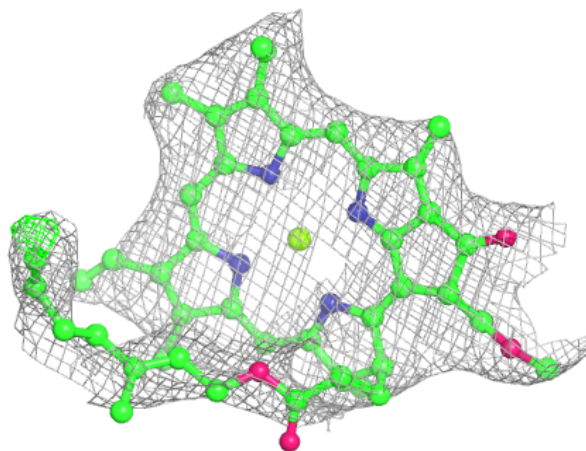
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





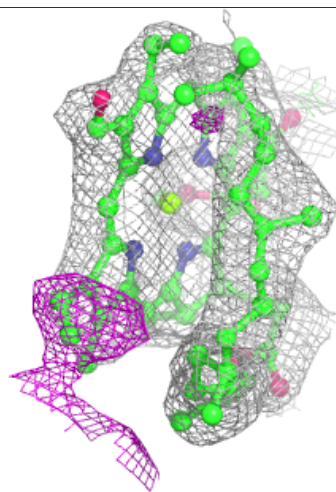
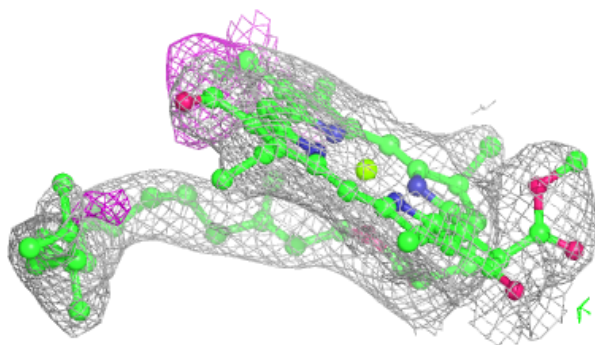
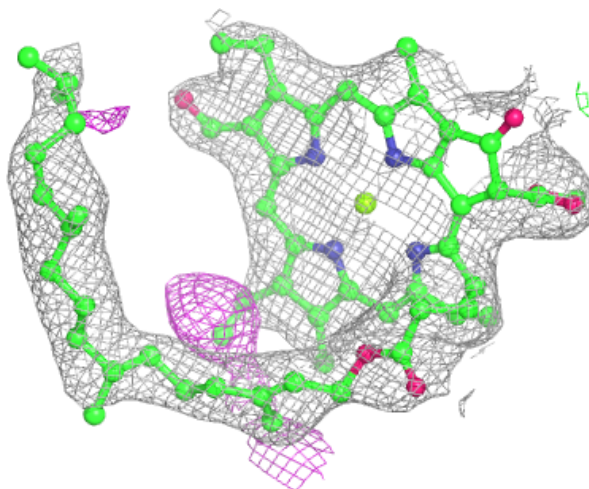
**Electron density around CLA C 314:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



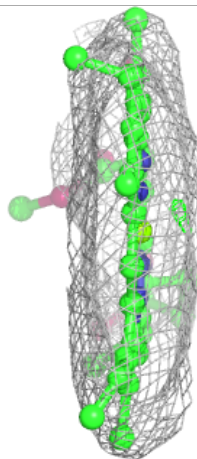
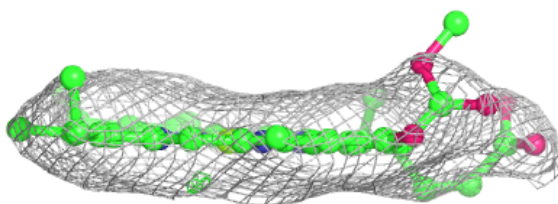
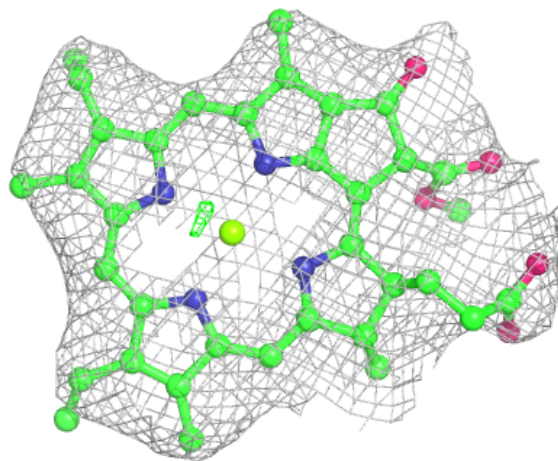
**Electron density around CHL C 306:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



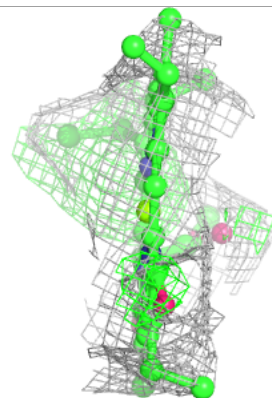
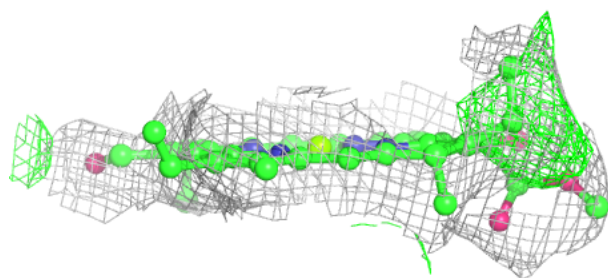
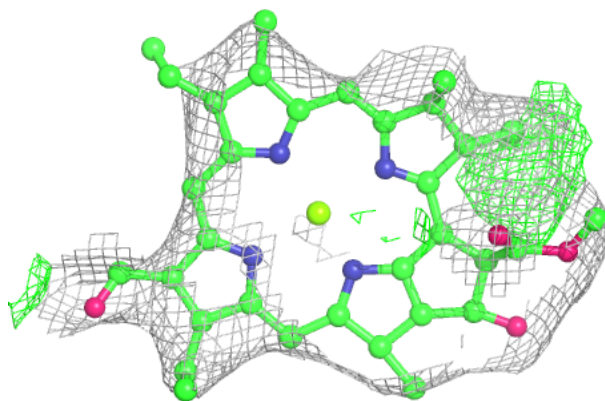
**Electron density around CLA C 316:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

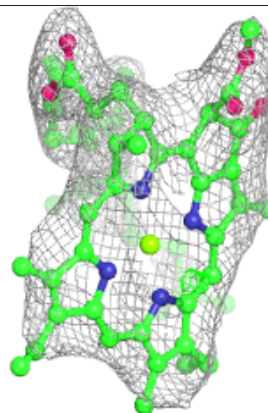
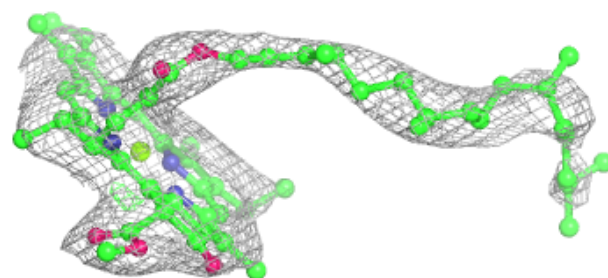
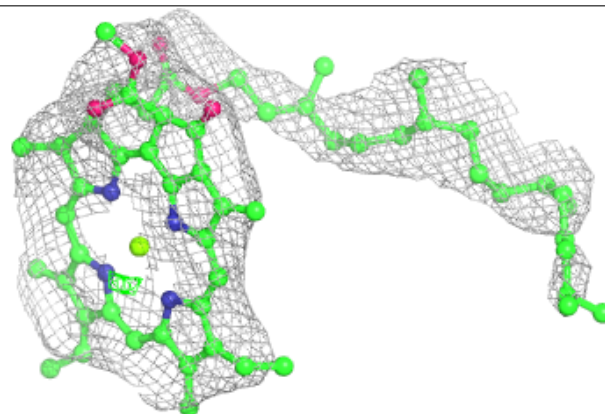


**Electron density around CHL E 309:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

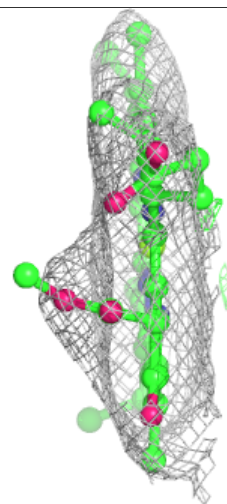
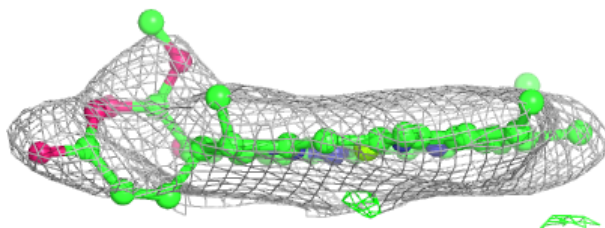
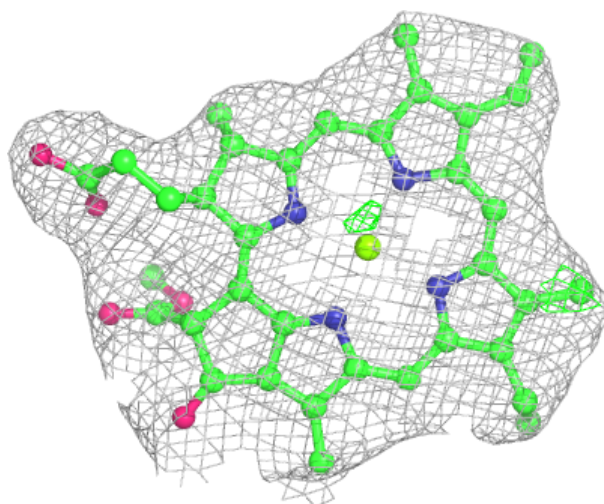
**Electron density around CLA D 315:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

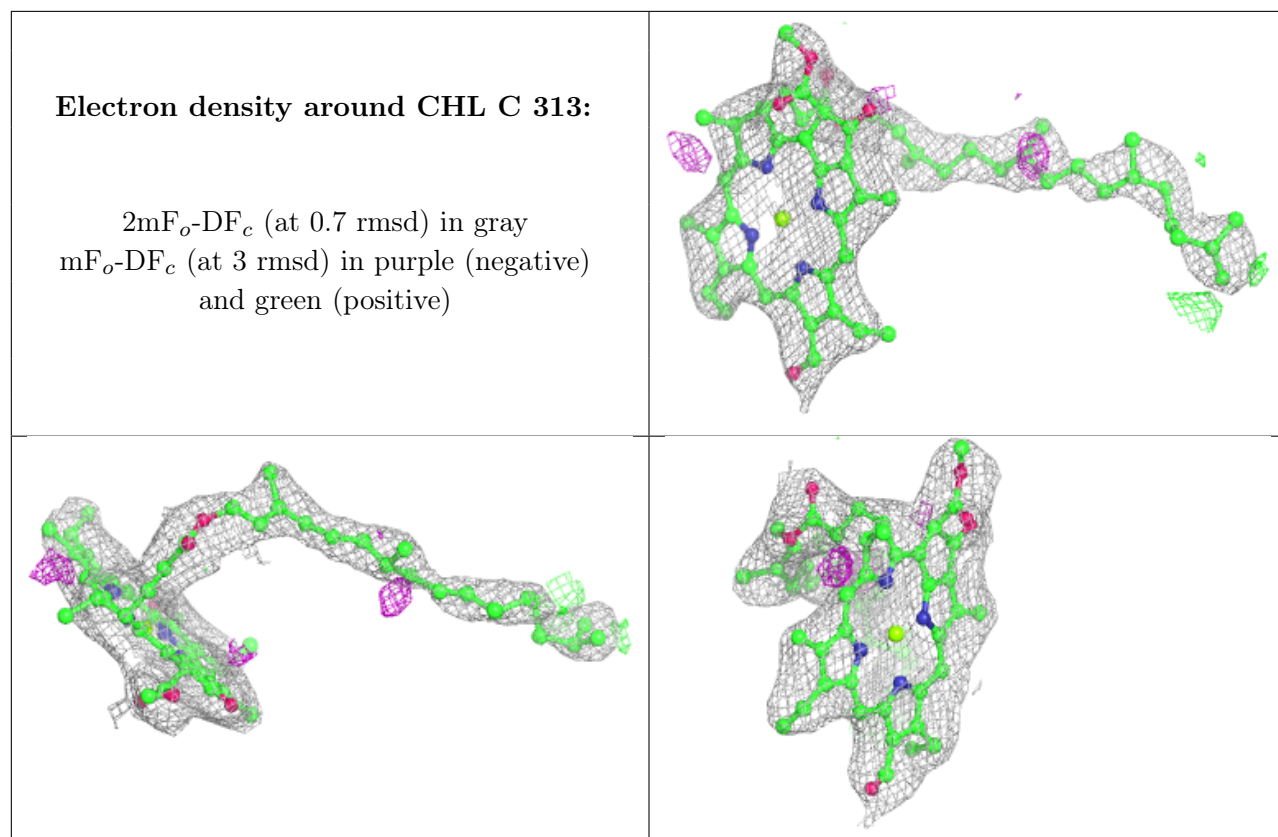


**Electron density around CLA D 316:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

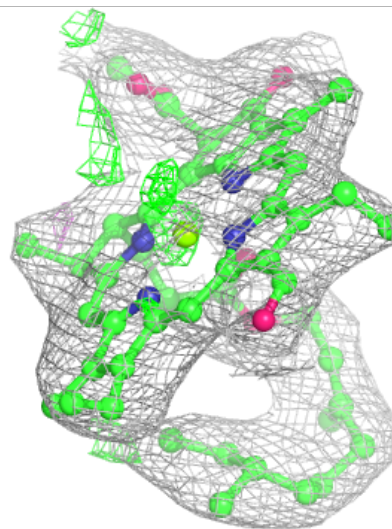
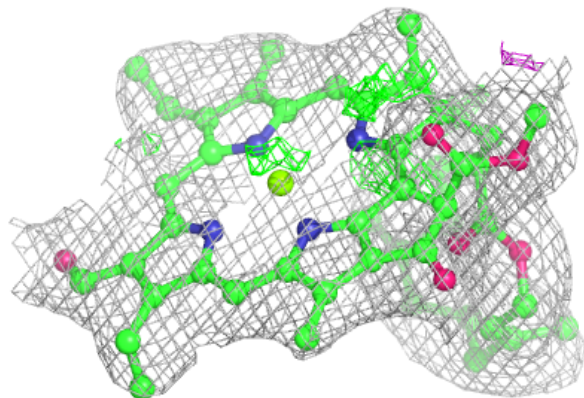
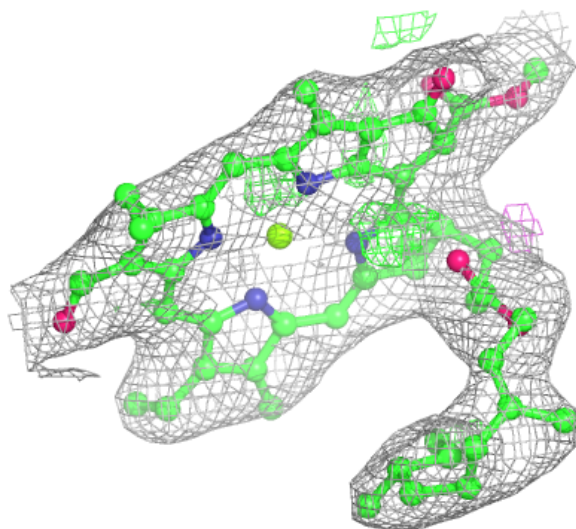






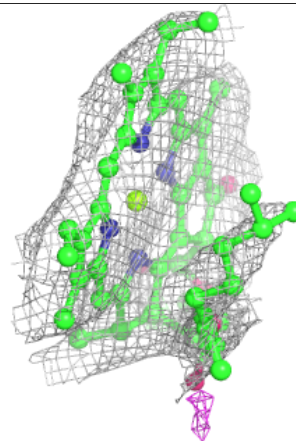
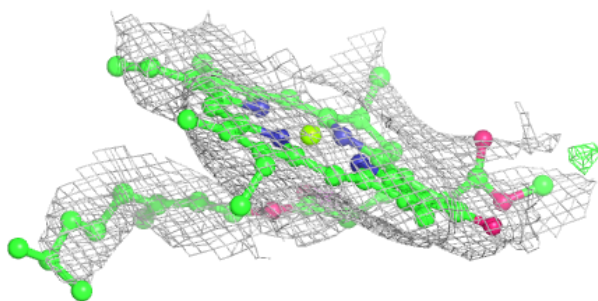
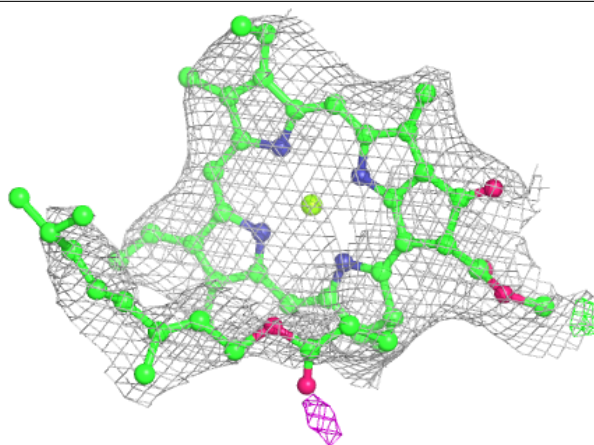
**Electron density around CHL D 312:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



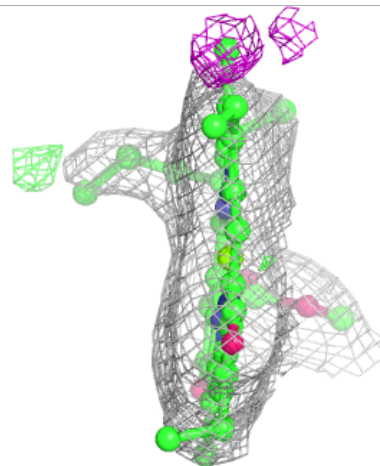
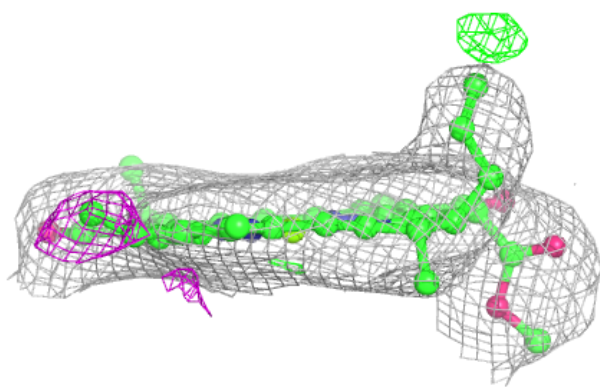
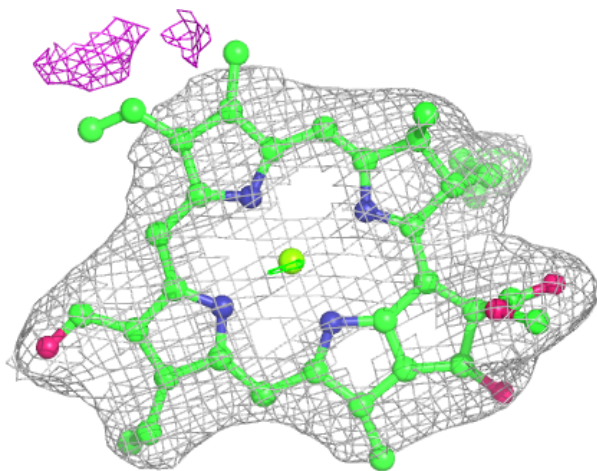
**Electron density around CLA E 313:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



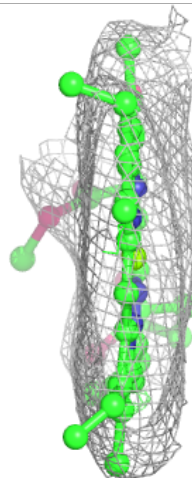
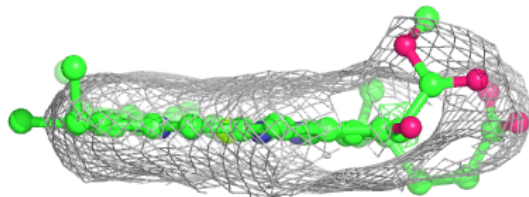
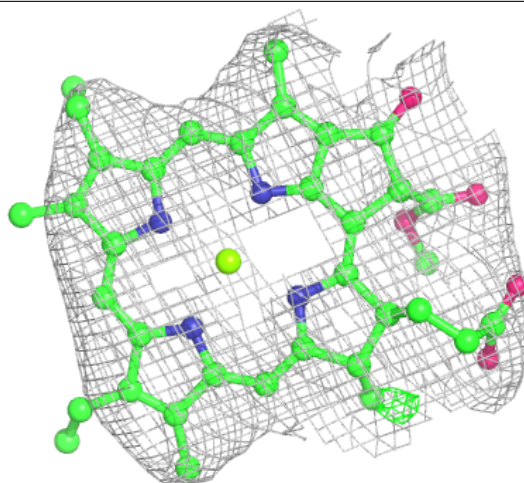
**Electron density around CHL C 318:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



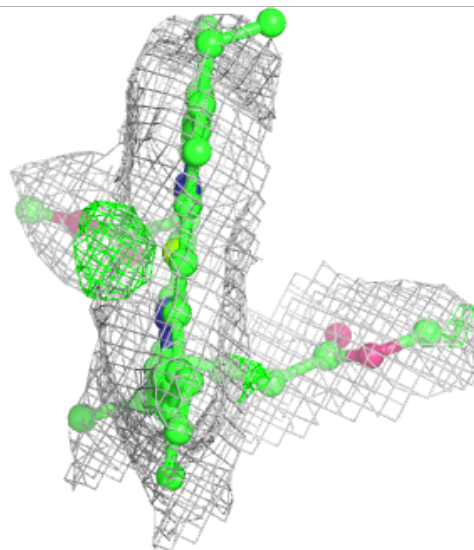
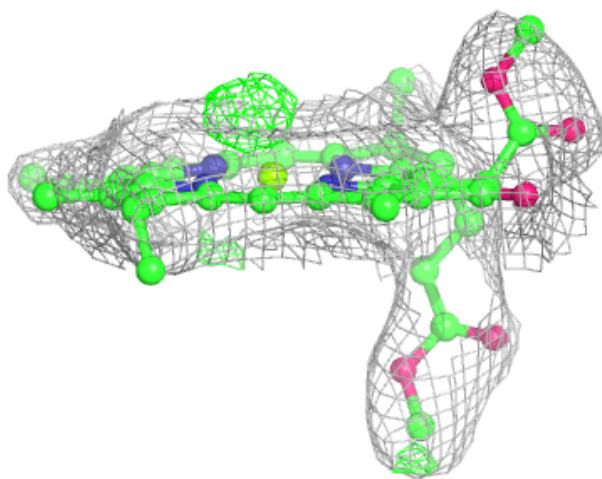
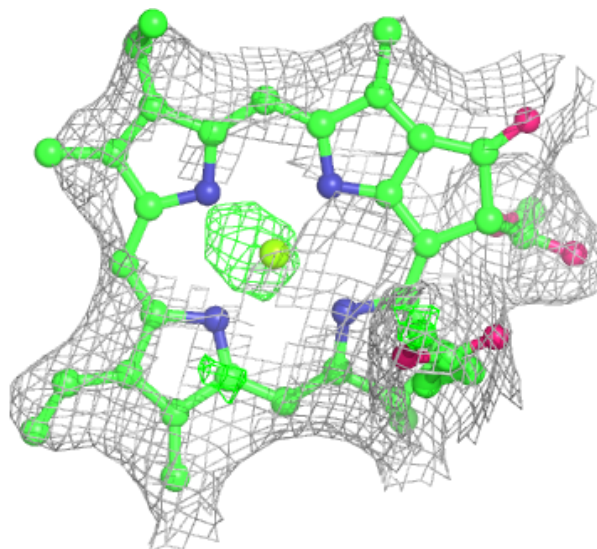
**Electron density around CLA E 315:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



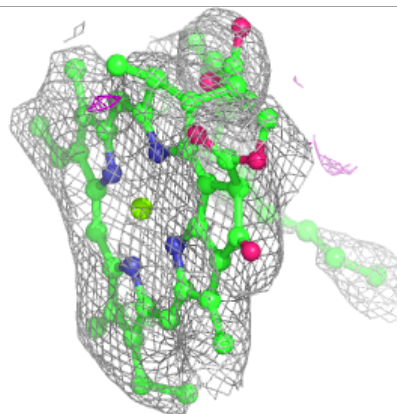
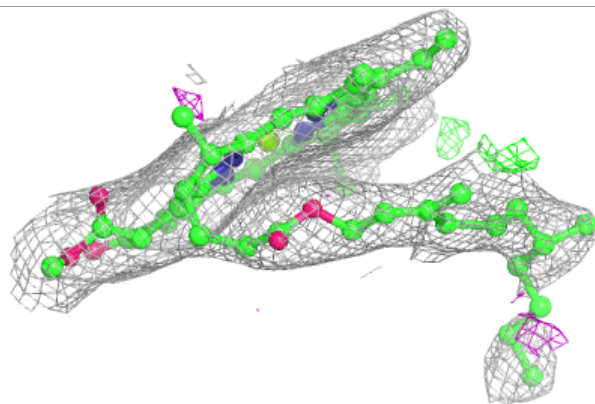
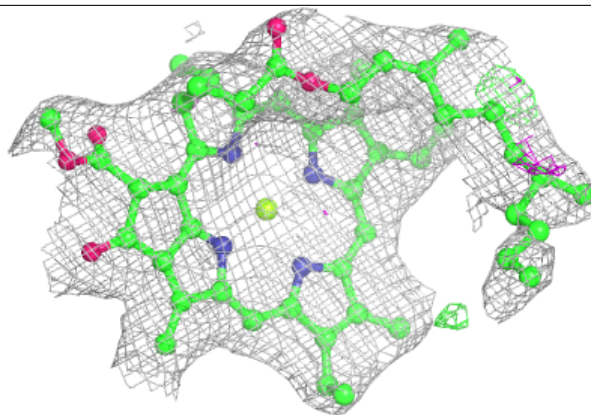
**Electron density around CLA F 307:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



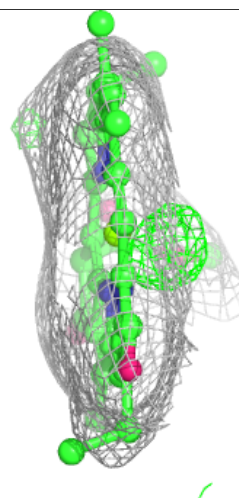
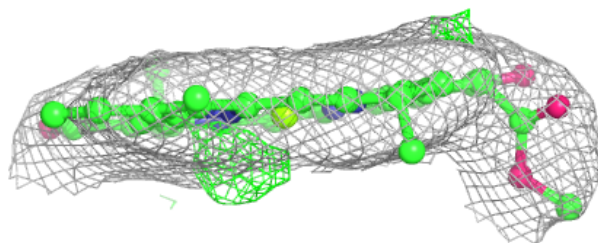
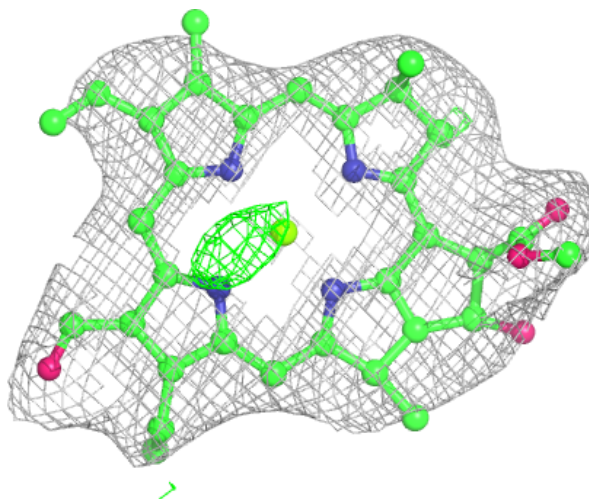
**Electron density around CLA F 313:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CHL E 317:**

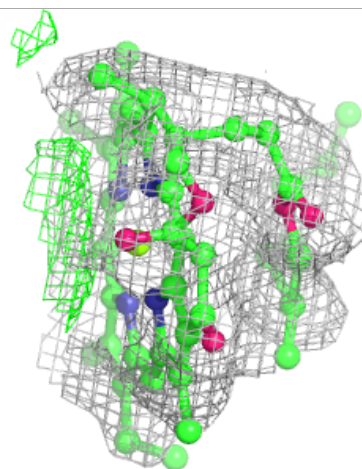
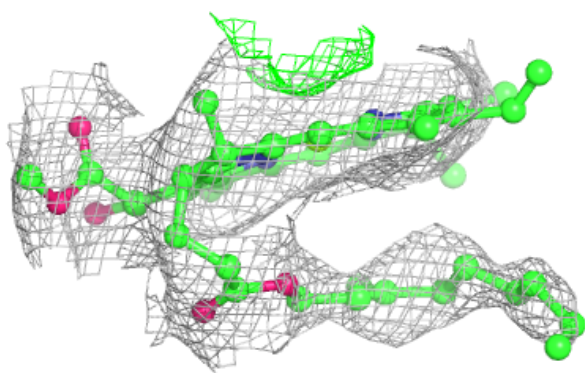
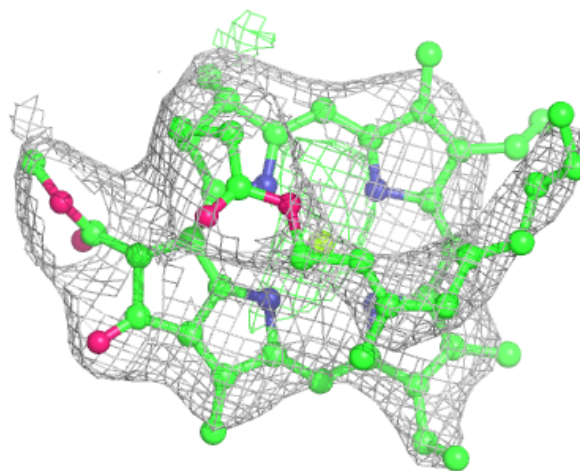
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





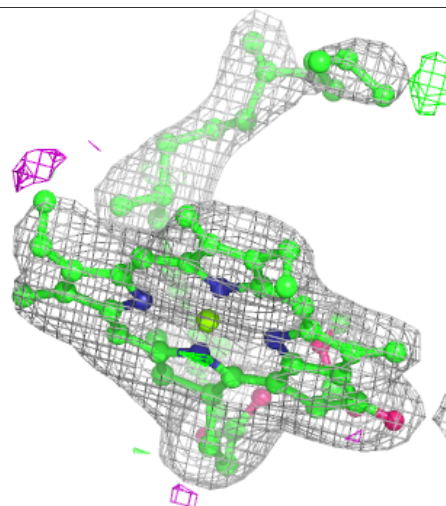
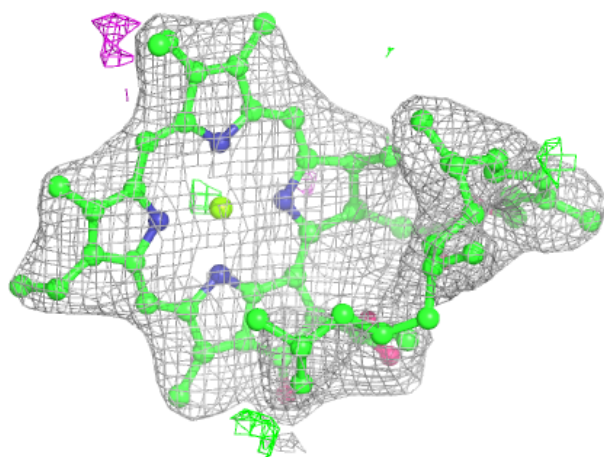
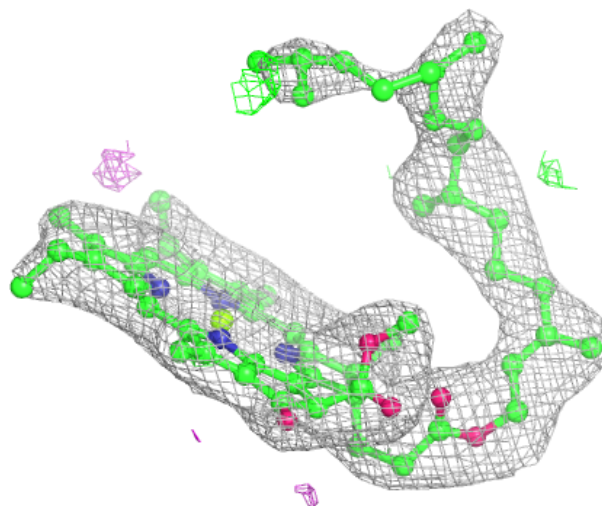
**Electron density around CLA E 316:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



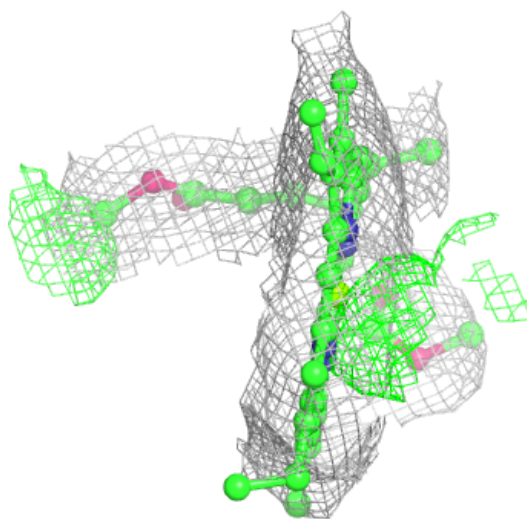
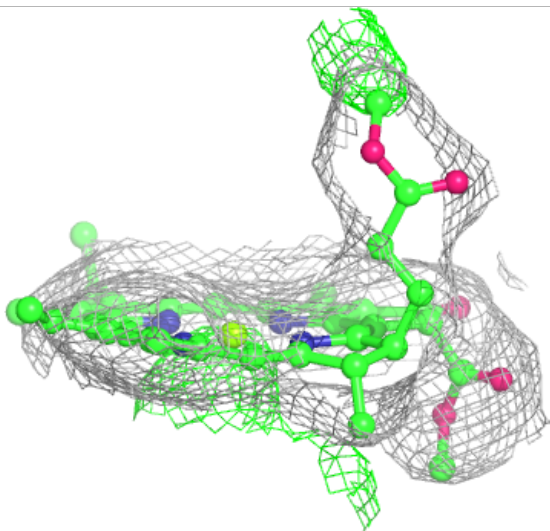
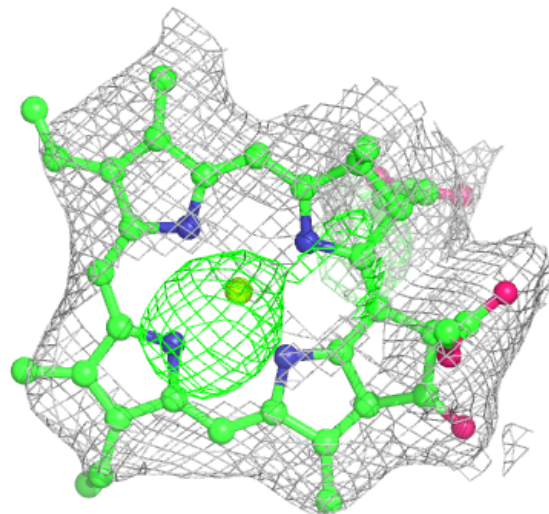
**Electron density around CLA F 306:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



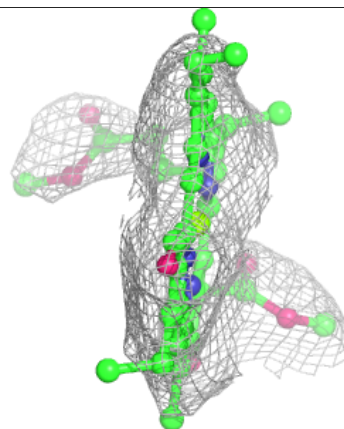
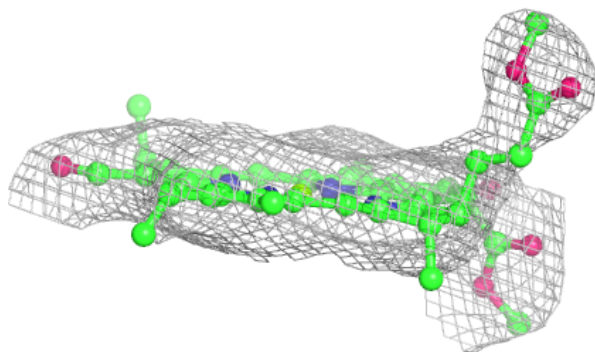
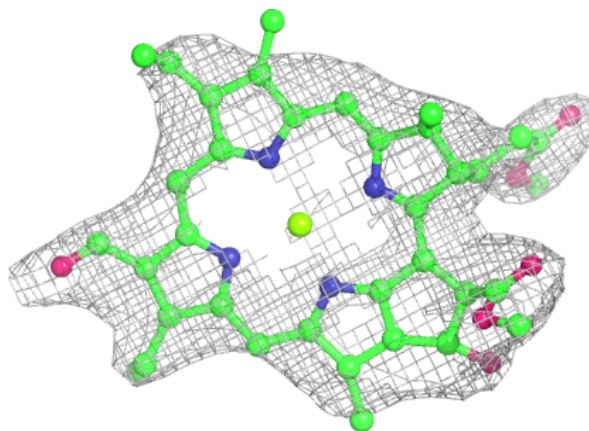
**Electron density around CLA C 308:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



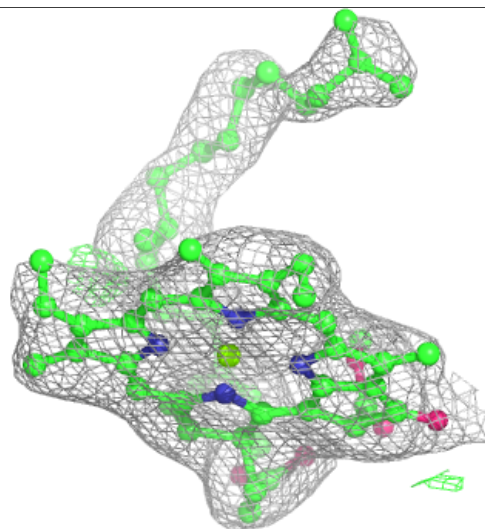
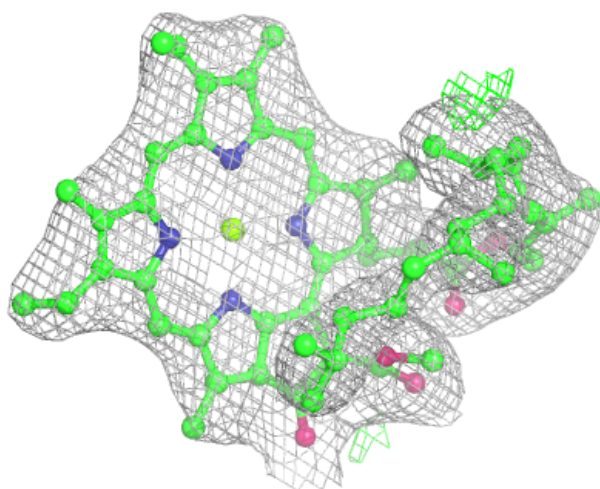
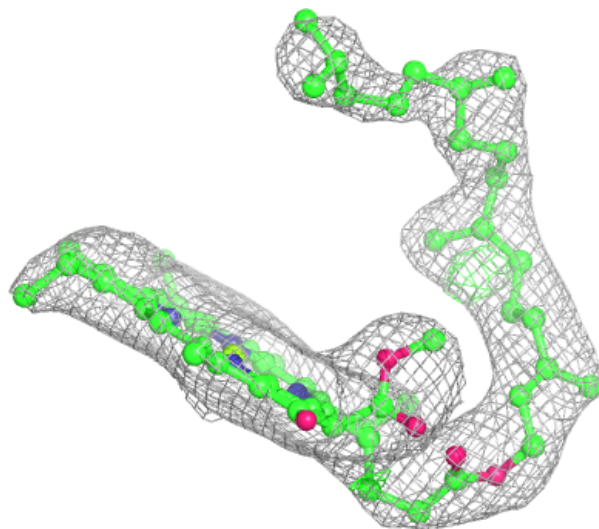
**Electron density around CHL B 319:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



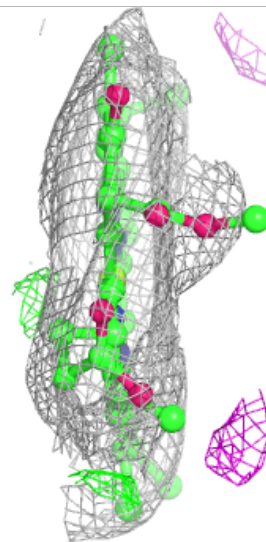
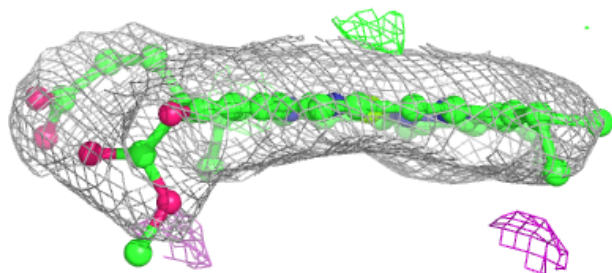
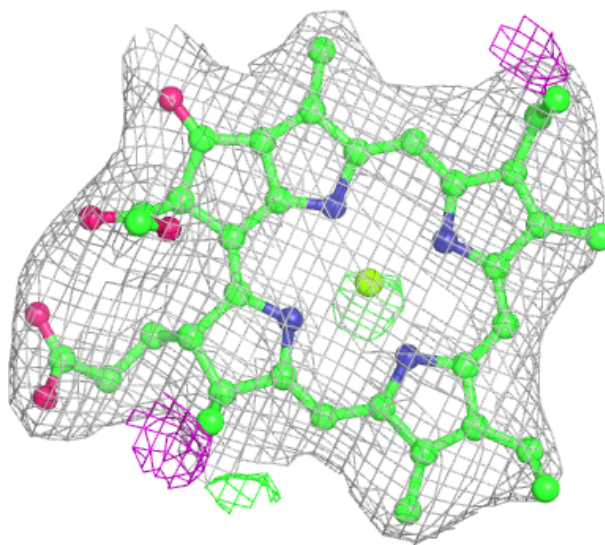
**Electron density around CLA E 306:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



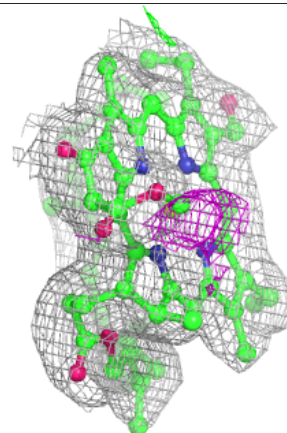
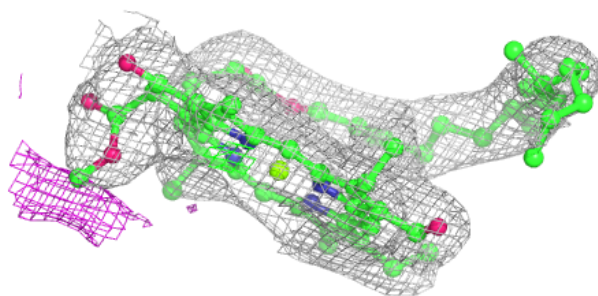
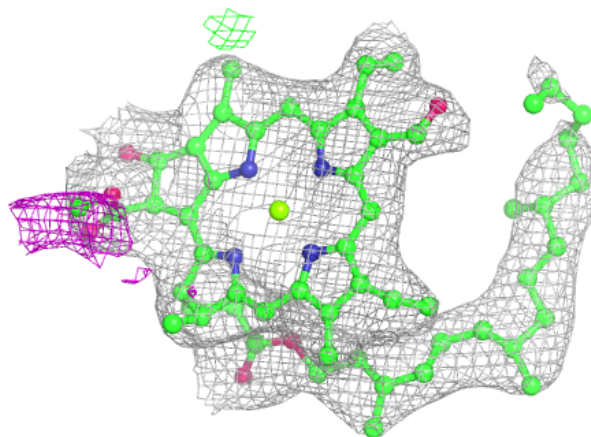
**Electron density around CLA F 315:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



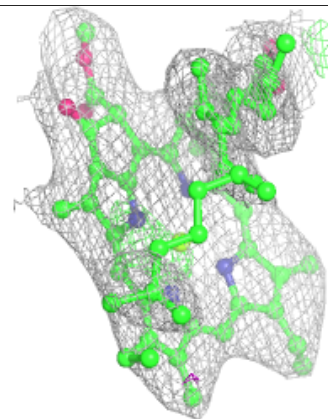
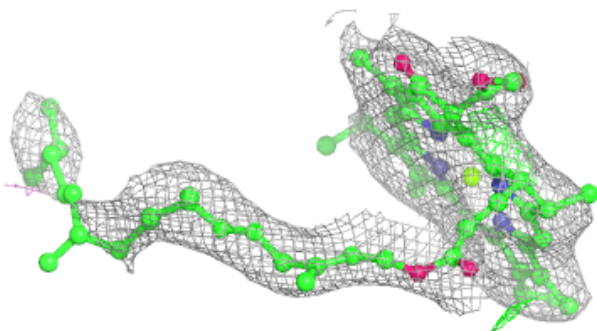
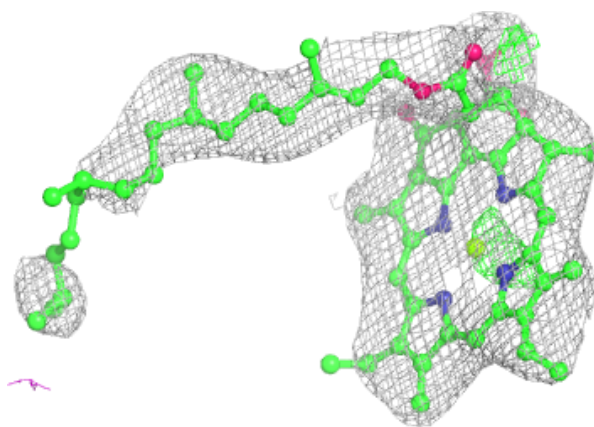
**Electron density around CHL B 307:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

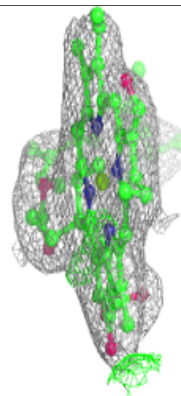
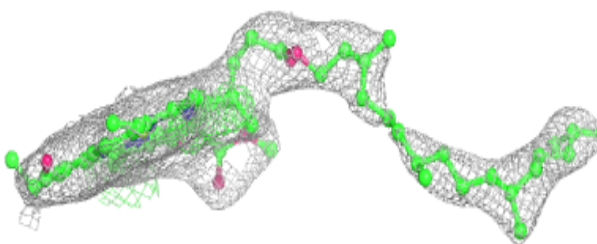
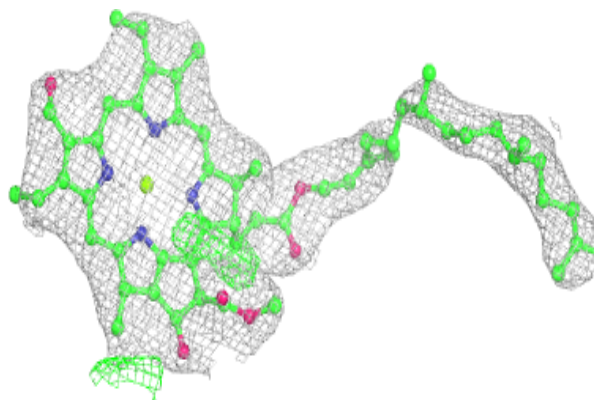


**Electron density around CLA B 316:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CHL B 306:**

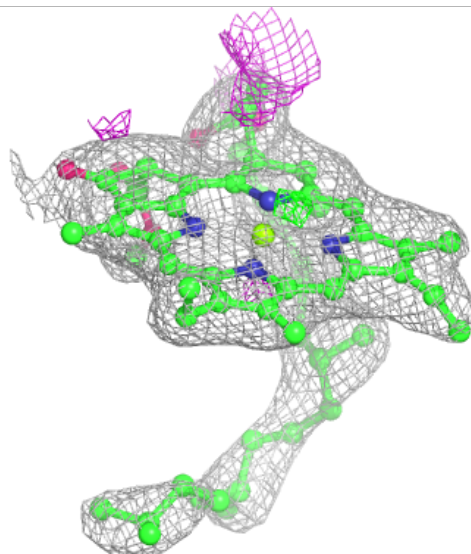
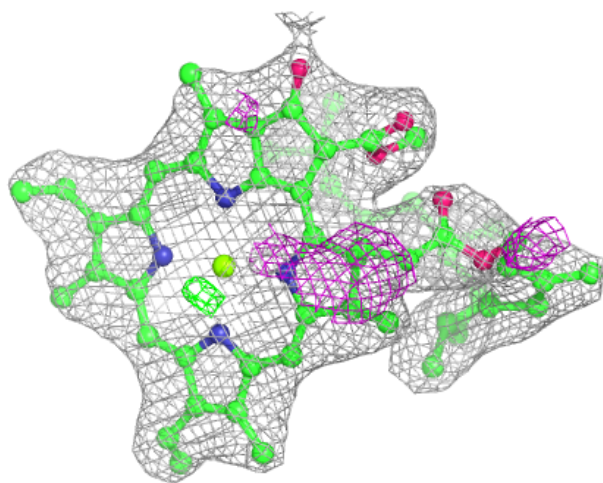
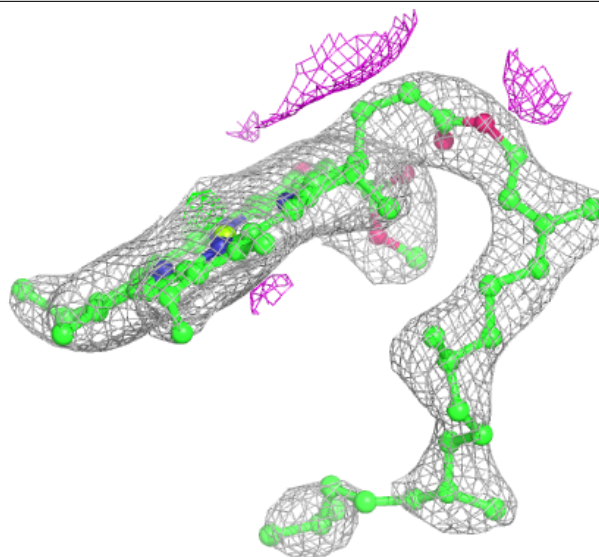
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





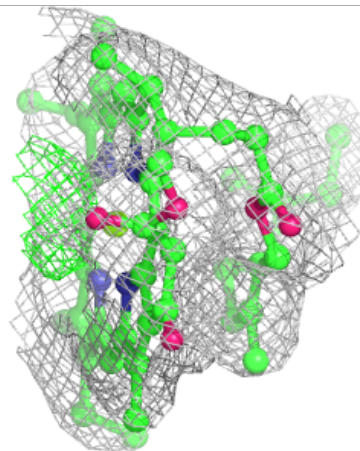
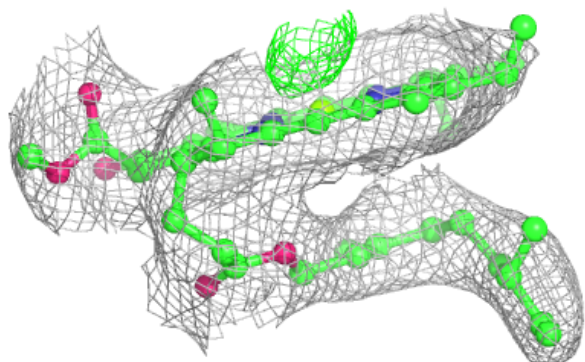
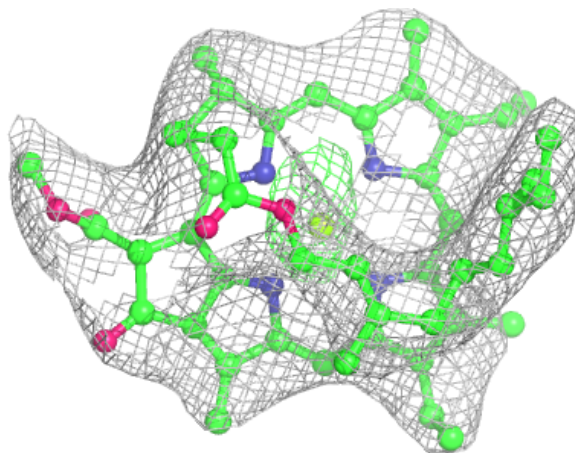
**Electron density around CLA C 307:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



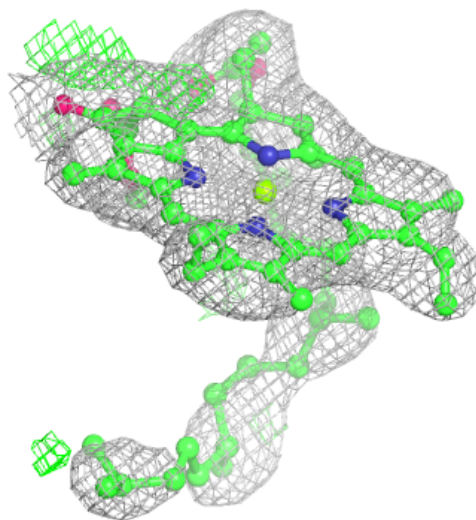
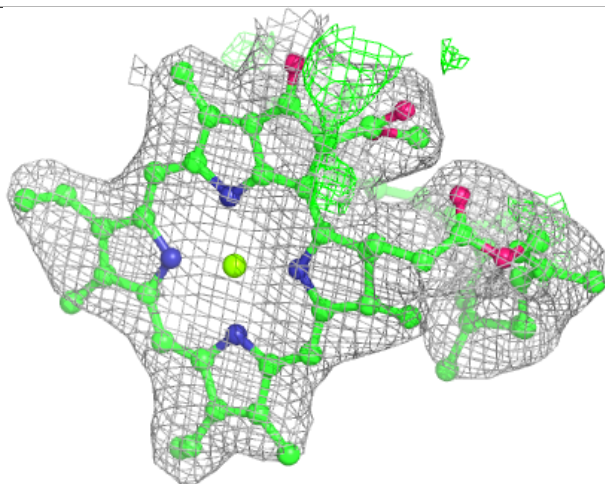
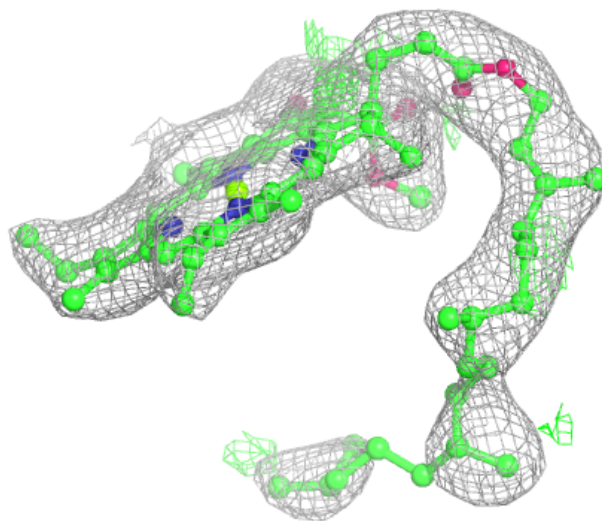
**Electron density around CLA C 317:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



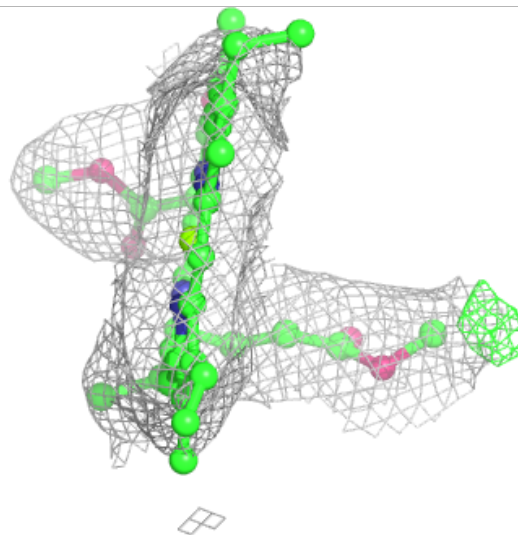
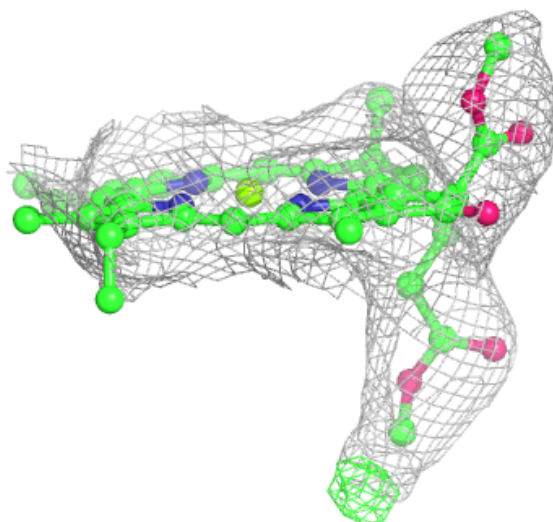
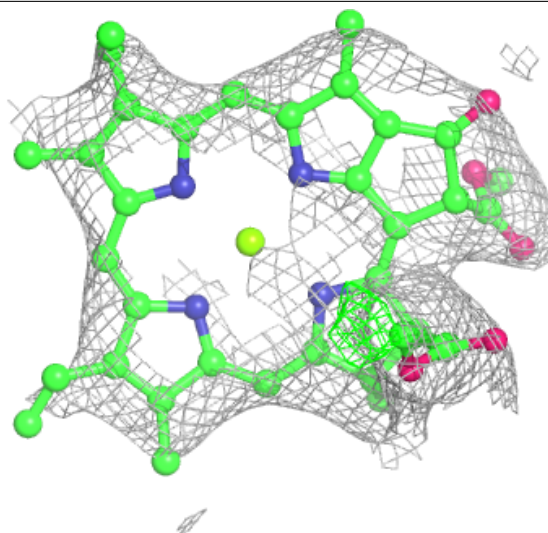
**Electron density around CLA D 307:**

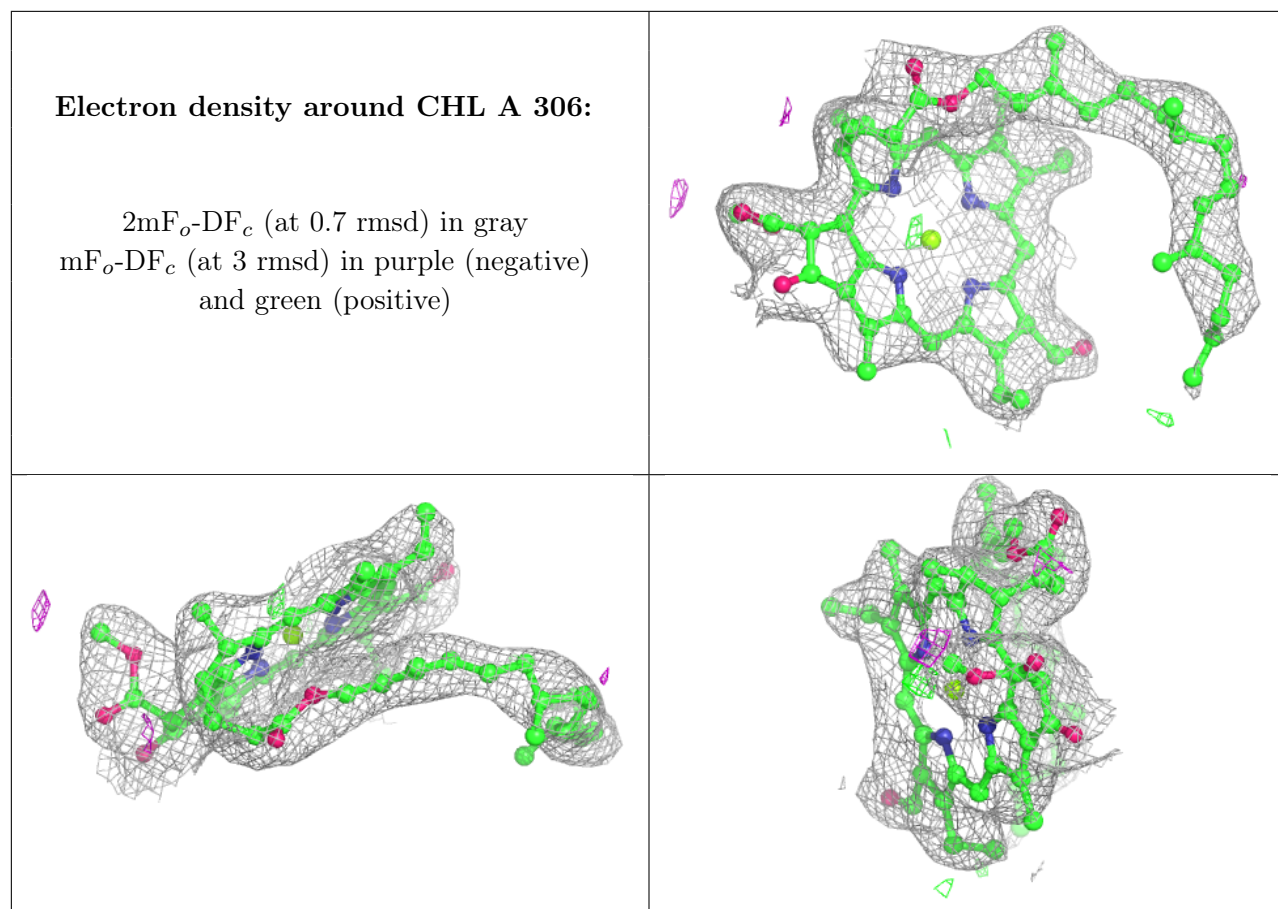
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA D 308:**

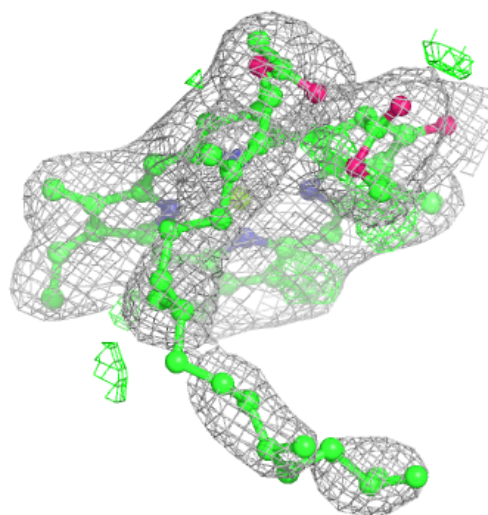
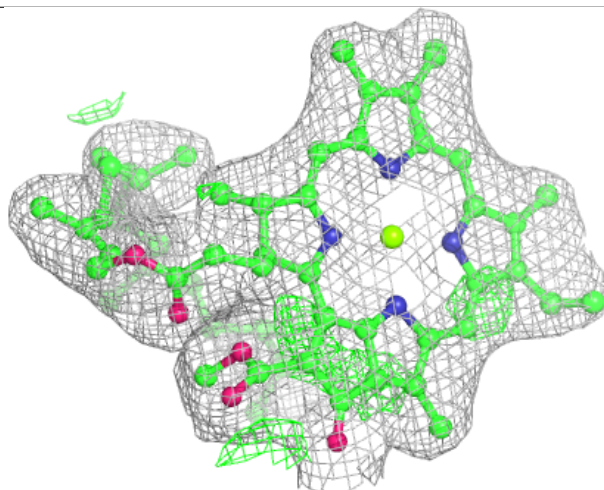
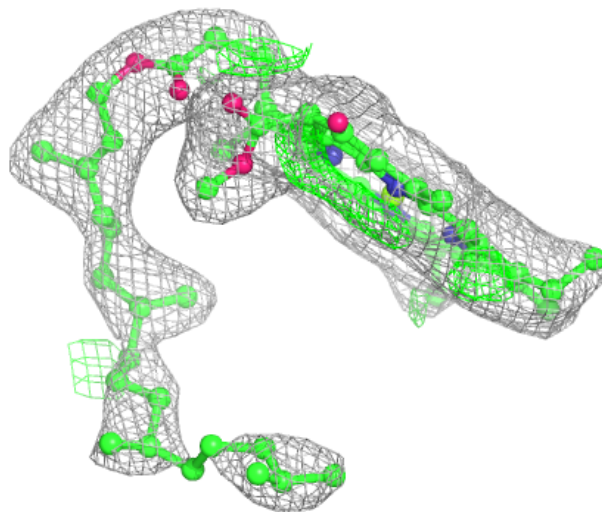
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





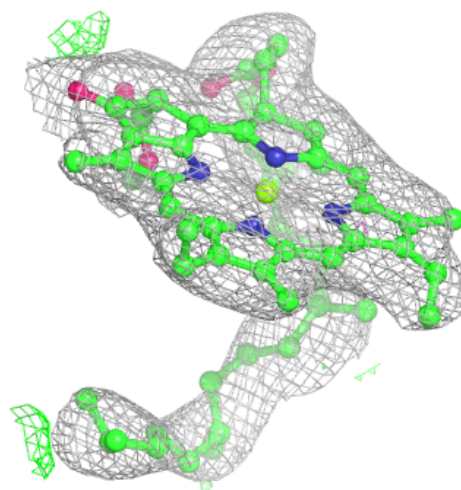
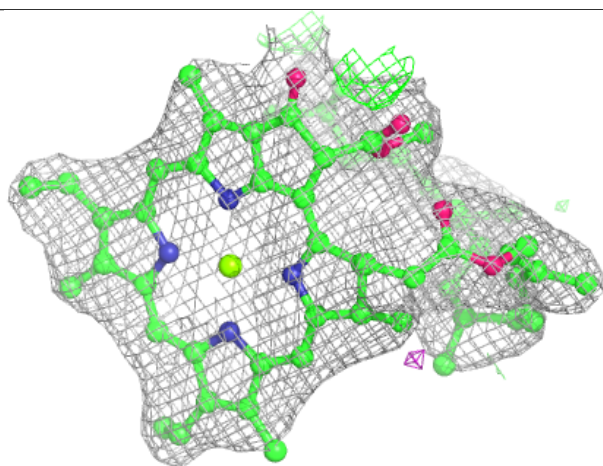
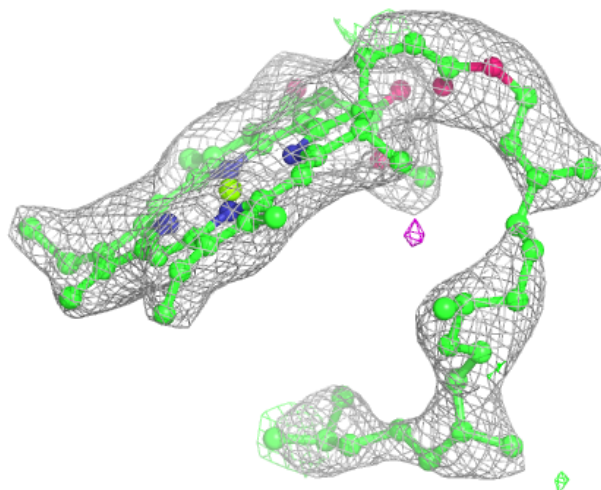
**Electron density around CLA A 307:**

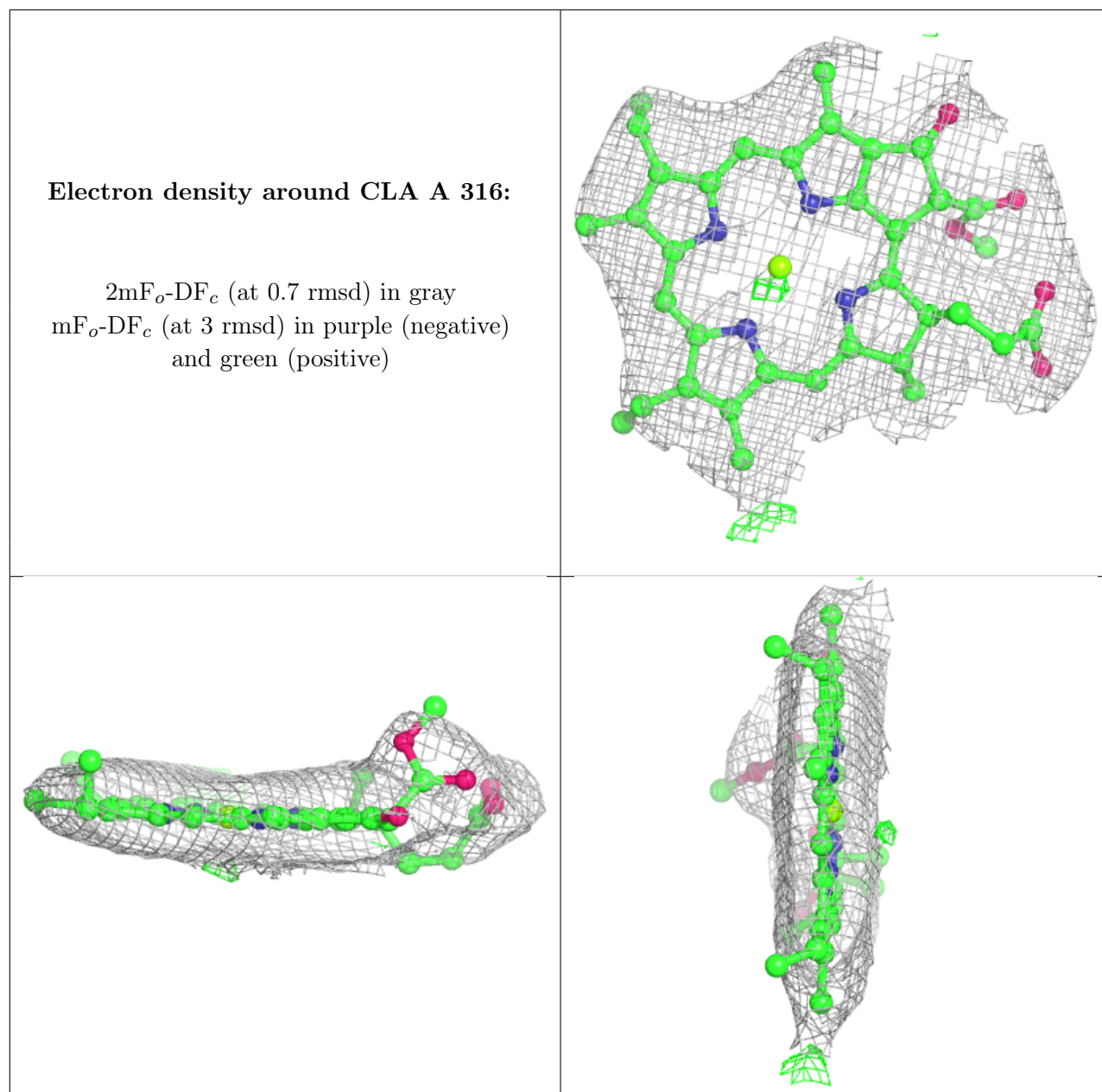
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 308:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.