



## Full wwPDB EM Validation Report ⓘ

Oct 15, 2024 – 03:03 AM JST

PDB ID : 8HG6  
EMDB ID : EMD-34736  
Title : Cryo-EM structure of the prasinophyte-specific light-harvesting complex (Lhcp) from *Ostreococcus tauri*  
Authors : Shan, J.; Sheng, X.; Ishii, A.; Watanabe, A.; Song, C.; Murata, K.; Minagawa, J.; Liu, Z.  
Deposited on : 2022-11-13  
Resolution : 3.44 Å (reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

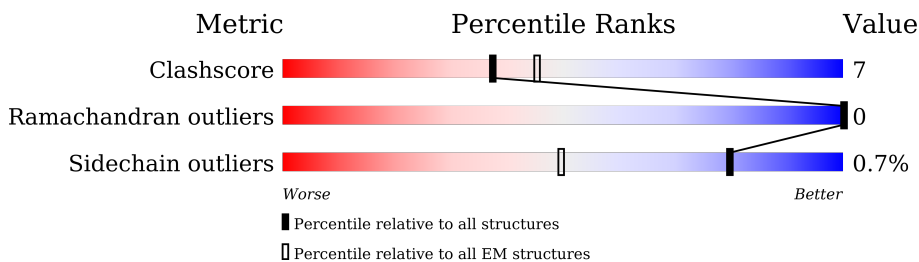
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.44 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 210492                      | 15764                       |
| Ramachandran outliers | 207382                      | 16835                       |
| Sidechain outliers    | 206894                      | 16415                       |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | V     | 233    |                  |
| 1   | W     | 233    |                  |
| 1   | X     | 233    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | CLA  | V     | 301 | X         | -        | -       | -                |
| 2   | CLA  | V     | 302 | X         | -        | -       | -                |
| 2   | CLA  | V     | 303 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | CLA  | V     | 309 | X         | -        | -       | -                |
| 2   | CLA  | V     | 310 | X         | -        | -       | -                |
| 2   | CLA  | V     | 311 | X         | -        | -       | -                |
| 2   | CLA  | V     | 313 | X         | -        | -       | -                |
| 2   | CLA  | W     | 301 | X         | -        | -       | -                |
| 2   | CLA  | W     | 302 | X         | -        | -       | -                |
| 2   | CLA  | W     | 303 | X         | -        | -       | -                |
| 2   | CLA  | W     | 309 | X         | -        | -       | -                |
| 2   | CLA  | W     | 310 | X         | -        | -       | -                |
| 2   | CLA  | W     | 311 | X         | -        | -       | -                |
| 2   | CLA  | W     | 312 | X         | -        | -       | -                |
| 2   | CLA  | W     | 313 | X         | -        | -       | -                |
| 2   | CLA  | X     | 302 | X         | -        | -       | -                |
| 2   | CLA  | X     | 303 | X         | -        | -       | -                |
| 2   | CLA  | X     | 304 | X         | -        | -       | -                |
| 2   | CLA  | X     | 310 | X         | -        | -       | -                |
| 2   | CLA  | X     | 311 | X         | -        | -       | -                |
| 2   | CLA  | X     | 312 | X         | -        | -       | -                |
| 2   | CLA  | X     | 313 | X         | -        | -       | -                |
| 2   | CLA  | X     | 314 | X         | -        | -       | -                |
| 3   | CHL  | V     | 304 | X         | -        | -       | -                |
| 3   | CHL  | V     | 305 | X         | -        | -       | -                |
| 3   | CHL  | V     | 306 | X         | -        | -       | -                |
| 3   | CHL  | V     | 307 | X         | -        | -       | -                |
| 3   | CHL  | V     | 314 | X         | -        | -       | -                |
| 3   | CHL  | W     | 304 | X         | -        | -       | -                |
| 3   | CHL  | W     | 305 | X         | -        | -       | -                |
| 3   | CHL  | W     | 306 | X         | -        | -       | -                |
| 3   | CHL  | W     | 307 | X         | -        | -       | -                |
| 3   | CHL  | W     | 314 | X         | -        | -       | -                |
| 3   | CHL  | X     | 305 | X         | -        | -       | -                |
| 3   | CHL  | X     | 306 | X         | -        | -       | -                |
| 3   | CHL  | X     | 307 | X         | -        | -       | -                |
| 3   | CHL  | X     | 308 | X         | -        | -       | -                |
| 3   | CHL  | X     | 315 | X         | -        | -       | -                |

## 2 Entry composition [i](#)

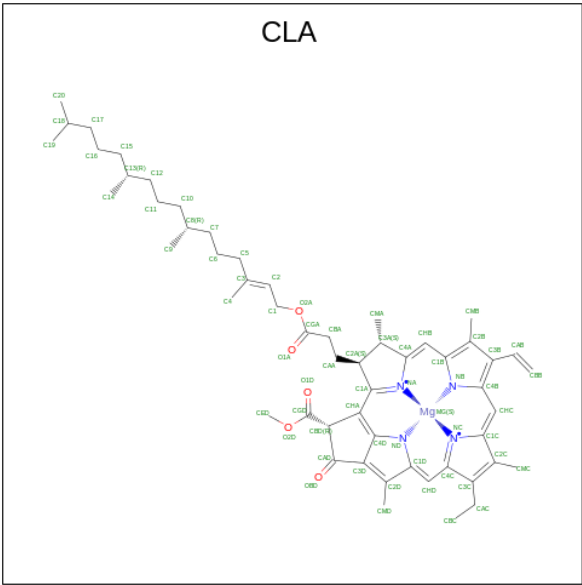
There are 7 unique types of molecules in this entry. The entry contains 7259 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | V     | 197      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1484  | 956 | 242 | 280 | 6 |         |       |
| 1   | W     | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1499  | 964 | 245 | 284 | 6 |         |       |
| 1   | X     | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1474  | 949 | 241 | 278 | 6 |         |       |

- Molecule 2 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



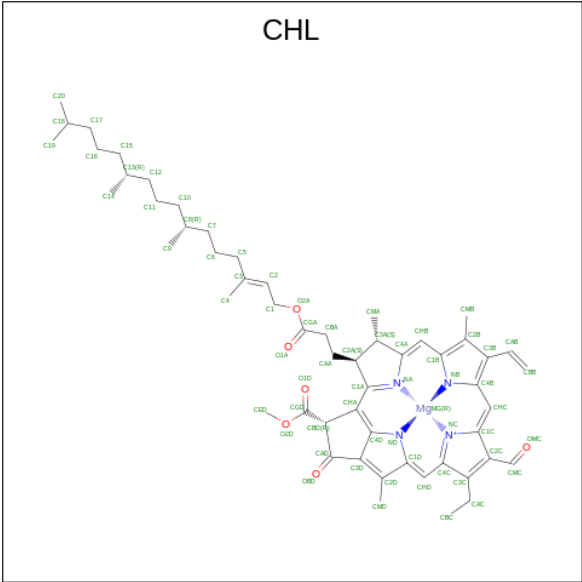
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 2   | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 2   | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 2   | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 2   | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 2   | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 2   | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 2   | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 2   | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 38 | 1  | 4 | 5 |         |
| 2   | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 2   | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 2   | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 2   | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 64    | 54 | 1  | 4 | 5 |         |
| 2   | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 2   | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 2   | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 2   | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 35 | 1  | 4 | 3 |         |
| 2   | X     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 2   | X     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 2   | X     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 2   | X     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 2   | X     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 2   | X     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 2   | X     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 2   | X     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |

- Molecule 3 is CHLOROPHYLL B (three-letter code: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ).



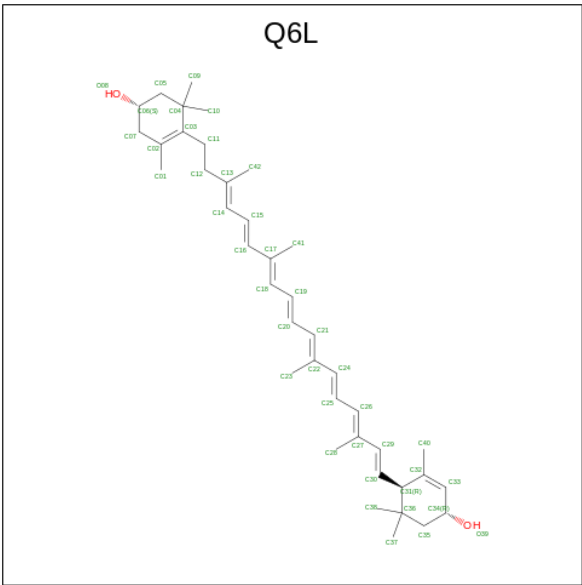
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 3   | V     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 3   | V     | 1        | Total<br>43 | C<br>34 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | V     | 1        | Total<br>44 | C<br>35 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | V     | 1        | Total<br>44 | C<br>35 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | V     | 1        | Total<br>44 | C<br>35 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | W     | 1        | Total<br>42 | C<br>33 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | W     | 1        | Total<br>42 | C<br>33 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | W     | 1        | Total<br>52 | C<br>41 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 3   | W     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 3   | W     | 1        | Total<br>41 | C<br>32 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | X     | 1        | Total<br>42 | C<br>33 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | X     | 1        | Total<br>42 | C<br>33 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | X     | 1        | Total<br>52 | C<br>41 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 3   | X     | 1        | Total<br>44 | C<br>35 | Mg<br>1 | N<br>4 | O<br>4 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 3   | X     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

- [illegible]

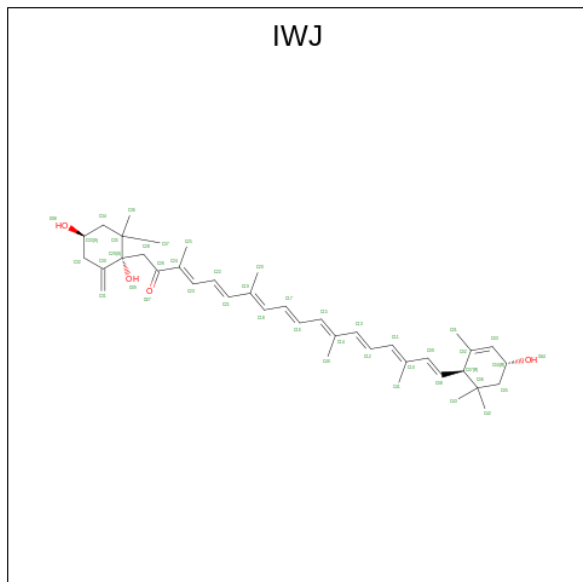
- Molecule 5 is (1 {S}-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaenyl]cyclohex-3-en-1-ol (three-letter code: Q6L) (formula: C<sub>40</sub>H<sub>58</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 5   | V     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 5   | V     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 5   | V     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 5   | V     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 5   | W     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 5   | W     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 5   | W     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 5   | W     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 5   | X     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 5   | X     | 1        | Total | C  |   | 0       |
|     |       |          | 40    | 40 |   |         |
| 5   | X     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 5   | X     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

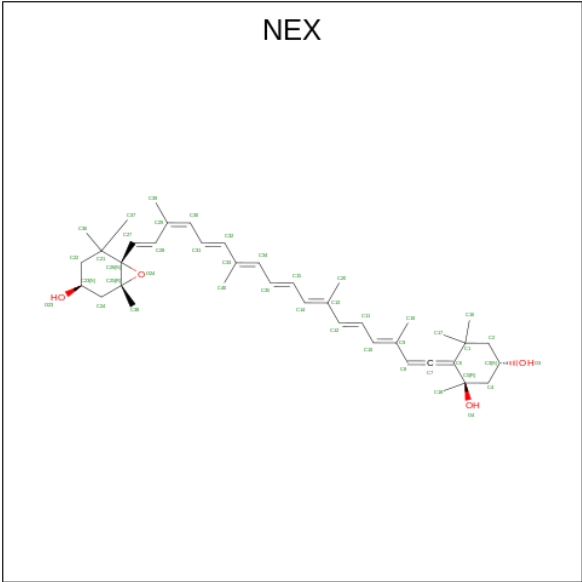
- Molecule 6 is (3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-1-[(1 {S},4 {S})-2,2-dimethyl-6-methylidene-1,4-bis(oxidanyl)cyclohexyl]-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octa

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



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 6   | V     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 6   | V     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 6   | V     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 6   | W     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 6   | X     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

- Molecule 7 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-TETRAMETHYLOCTA DECA-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>).

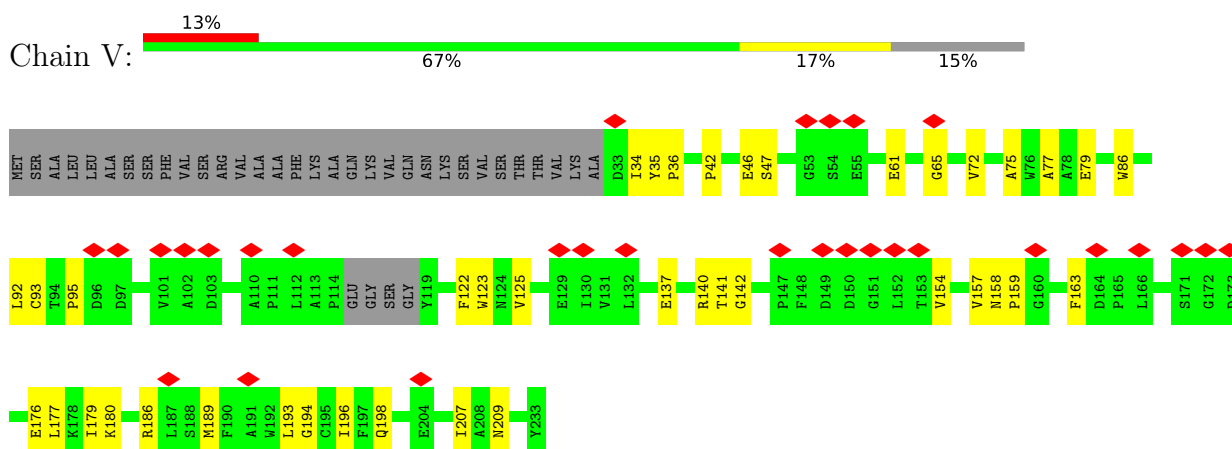


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 7   | W     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

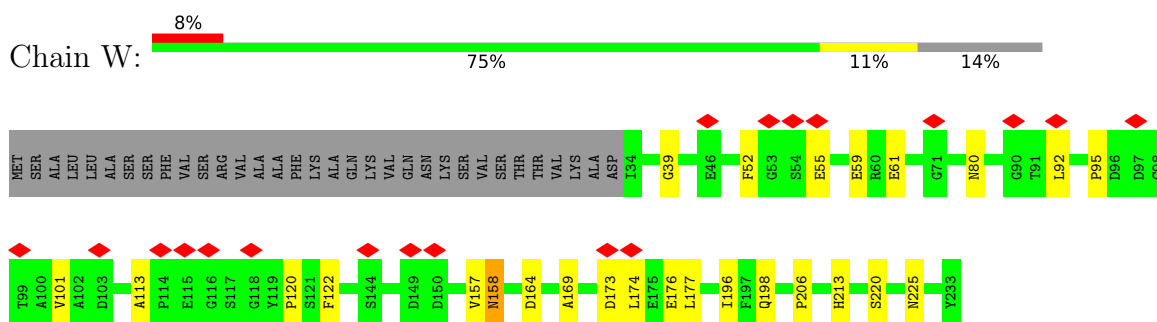
### 3 Residue-property plots [i](#)

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

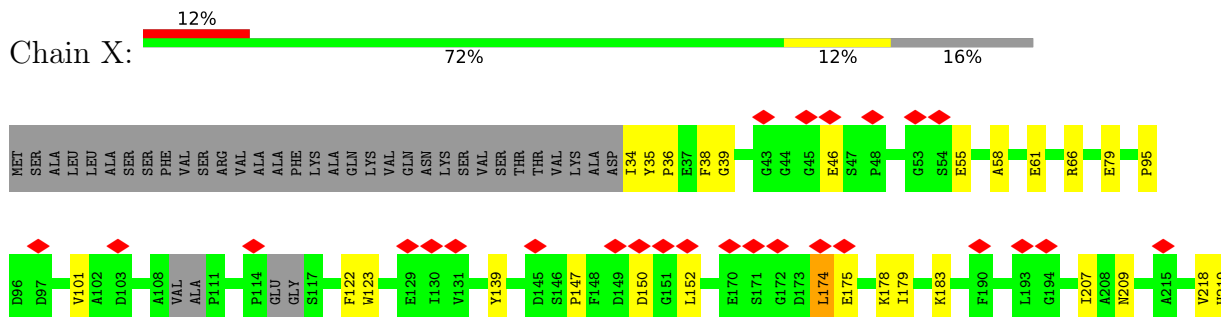
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

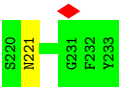


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



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





## 4 Experimental information

| Property                             | Value                      | Source    |
|--------------------------------------|----------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE            | Depositor |
| Imposed symmetry                     | POINT, Not provided        |           |
| Number of particles used             | 80573                      | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF          | Depositor |
| CTF correction method                | NONE                       | Depositor |
| Microscope                           | FEI TITAN KRIOS            | Depositor |
| Voltage (kV)                         | 300                        | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                         | Depositor |
| Minimum defocus (nm)                 | 1800                       | Depositor |
| Maximum defocus (nm)                 | 2200                       | Depositor |
| Magnification                        | Not provided               |           |
| Image detector                       | GATAN K2 QUANTUM (4k x 4k) | Depositor |
| Maximum map value                    | 0.070                      | Depositor |
| Minimum map value                    | -0.044                     | Depositor |
| Average map value                    | 0.000                      | Depositor |
| Map value standard deviation         | 0.002                      | Depositor |
| Recommended contour level            | 0.0154                     | Depositor |
| Map size ( $\text{\AA}$ )            | 399.36, 399.36, 399.36     | wwPDB     |
| Map dimensions                       | 384, 384, 384              | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0           | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.04, 1.04, 1.04           | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CHL, KC2, NEX, CLA, IWJ, Q6L

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   | V     | 0.55         | 1/1529 (0.1%) | 0.70        | 2/2089 (0.1%) |
| 1   | W     | 0.56         | 1/1545 (0.1%) | 0.67        | 1/2111 (0.0%) |
| 1   | X     | 0.50         | 0/1518        | 0.68        | 1/2070 (0.0%) |
| All | All   | 0.54         | 2/4592 (0.0%) | 0.68        | 4/6270 (0.1%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | W     | 55  | GLU  | CB-CG | 5.45  | 1.62        | 1.52     |
| 1   | V     | 93  | CYS  | CB-SG | -5.04 | 1.73        | 1.81     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | W     | 55  | GLU  | OE1-CD-OE2 | -6.73 | 115.22      | 123.30   |
| 1   | X     | 174 | LEU  | CA-CB-CG   | 5.33  | 127.56      | 115.30   |
| 1   | V     | 36  | PRO  | CA-N-CD    | -5.28 | 104.11      | 111.50   |
| 1   | V     | 92  | LEU  | CB-CG-CD1  | -5.25 | 102.07      | 111.00   |

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   | V     | 1484  | 0        | 1411     | 35      | 0            |
| 1   | W     | 1499  | 0        | 1425     | 22      | 0            |
| 1   | X     | 1474  | 0        | 1401     | 26      | 0            |
| 2   | V     | 412   | 0        | 347      | 15      | 0            |
| 2   | W     | 427   | 0        | 379      | 11      | 0            |
| 2   | X     | 373   | 0        | 290      | 9       | 0            |
| 3   | V     | 221   | 0        | 153      | 2       | 0            |
| 3   | W     | 243   | 0        | 189      | 0       | 0            |
| 3   | X     | 225   | 0        | 155      | 2       | 0            |
| 4   | V     | 45    | 0        | 0        | 1       | 0            |
| 4   | W     | 45    | 0        | 0        | 0       | 0            |
| 4   | X     | 45    | 0        | 0        | 0       | 0            |
| 5   | V     | 168   | 0        | 0        | 1       | 0            |
| 5   | W     | 168   | 0        | 0        | 2       | 0            |
| 5   | X     | 166   | 0        | 0        | 1       | 0            |
| 6   | V     | 132   | 0        | 0        | 2       | 0            |
| 6   | W     | 44    | 0        | 0        | 2       | 0            |
| 6   | X     | 44    | 0        | 0        | 0       | 0            |
| 7   | W     | 44    | 0        | 56       | 0       | 0            |
| All | All   | 7259  | 0        | 5806     | 93      | 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 7.

All (93) 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:V:177:LEU:HG   | 2:V:309:CLA:H3A  | 1.62                     | 0.80              |
| 1:W:174:LEU:HD12 | 2:W:309:CLA:HMA2 | 1.65                     | 0.78              |
| 1:V:137:GLU:OE1  | 4:V:308:KC2:C4C  | 2.34                     | 0.73              |
| 1:W:169:ALA:HB1  | 1:W:174:LEU:HD13 | 1.70                     | 0.72              |
| 3:V:307:CHL:HBB1 | 3:V:307:CHL:HMB1 | 1.75                     | 0.68              |
| 1:X:36:PRO:HD2   | 1:X:183:LYS:NZ   | 2.09                     | 0.68              |
| 1:W:169:ALA:CB   | 1:W:174:LEU:HD13 | 2.24                     | 0.67              |
| 1:V:180:LYS:HZ1  | 2:V:311:CLA:HBD  | 1.59                     | 0.66              |
| 1:X:39:GLY:HA3   | 2:X:302:CLA:HMD1 | 1.78                     | 0.65              |
| 1:W:92:LEU:CD2   | 2:W:303:CLA:H2A  | 2.26                     | 0.65              |
| 1:X:36:PRO:HD2   | 1:X:183:LYS:HZ1  | 1.60                     | 0.65              |
| 1:V:198:GLN:HE21 | 1:V:209:ASN:HD22 | 1.44                     | 0.64              |
| 1:W:61:GLU:OE1   | 2:W:301:CLA:C4A  | 2.46                     | 0.63              |
| 1:X:35:TYR:CD2   | 1:X:183:LYS:HE2  | 2.34                     | 0.63              |
| 1:X:35:TYR:HD2   | 1:X:183:LYS:HE2  | 1.64                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:V:301:CLA:H72  | 2:V:302:CLA:HMD1 | 1.82                     | 0.62              |
| 1:V:163:PHE:CD2  | 2:V:309:CLA:HMD1 | 2.34                     | 0.62              |
| 6:W:318:IWJ:O27  | 6:W:318:IWJ:O39  | 2.15                     | 0.60              |
| 1:W:92:LEU:HG    | 1:W:101:VAL:HG22 | 1.84                     | 0.59              |
| 1:X:174:LEU:HG   | 1:X:178:LYS:HZ2  | 1.68                     | 0.59              |
| 1:V:194:GLY:O    | 1:V:198:GLN:HG3  | 2.03                     | 0.58              |
| 1:W:39:GLY:HA3   | 2:W:301:CLA:HMD1 | 1.85                     | 0.58              |
| 1:W:173:ASP:HB2  | 1:W:176:GLU:HB2  | 1.85                     | 0.57              |
| 1:W:206:PRO:O    | 5:W:315:Q6L:O08  | 2.23                     | 0.57              |
| 1:X:34:ILE:HG12  | 1:X:36:PRO:HD3   | 1.87                     | 0.57              |
| 1:X:209:ASN:N    | 1:X:209:ASN:OD1  | 2.36                     | 0.56              |
| 2:V:301:CLA:O1A  | 2:V:301:CLA:H3A  | 2.06                     | 0.56              |
| 1:X:61:GLU:OE1   | 2:X:302:CLA:C4A  | 2.53                     | 0.56              |
| 1:V:86:TRP:CH2   | 1:V:196:ILE:HG22 | 2.41                     | 0.56              |
| 2:X:304:CLA:H2A  | 2:X:304:CLA:HED3 | 1.87                     | 0.56              |
| 1:X:101:VAL:HG11 | 3:X:306:CHL:HBC1 | 1.88                     | 0.55              |
| 1:W:80:ASN:ND2   | 6:W:318:IWJ:O44  | 2.39                     | 0.55              |
| 1:X:218:VAL:O    | 1:X:221:ASN:ND2  | 2.39                     | 0.55              |
| 1:V:86:TRP:HH2   | 1:V:196:ILE:HG22 | 1.70                     | 0.54              |
| 1:V:61:GLU:OE2   | 1:V:186:ARG:NE   | 2.40                     | 0.54              |
| 1:V:35:TYR:OH    | 1:V:186:ARG:NH1  | 2.41                     | 0.53              |
| 1:V:177:LEU:CG   | 2:V:309:CLA:H3A  | 2.35                     | 0.53              |
| 1:W:52:PHE:HA    | 2:W:301:CLA:HBA1 | 1.90                     | 0.53              |
| 1:V:79:GLU:OE1   | 1:V:207:ILE:HB   | 2.10                     | 0.52              |
| 1:V:176:GLU:O    | 1:V:180:LYS:HG3  | 2.11                     | 0.51              |
| 1:V:198:GLN:HG2  | 2:V:312:CLA:ND   | 2.26                     | 0.50              |
| 1:V:34:ILE:HD11  | 1:V:179:ILE:HG21 | 1.94                     | 0.50              |
| 2:X:311:CLA:HED3 | 2:X:311:CLA:H2A  | 1.93                     | 0.50              |
| 1:X:36:PRO:HG3   | 2:X:311:CLA:HMA3 | 1.93                     | 0.49              |
| 1:V:42:PRO:HD3   | 1:V:186:ARG:NH2  | 2.27                     | 0.49              |
| 1:V:46:GLU:OE2   | 1:V:47:SER:OG    | 2.30                     | 0.49              |
| 6:V:317:IWJ:O39  | 6:V:317:IWJ:O27  | 2.30                     | 0.49              |
| 2:W:309:CLA:H2A  | 2:W:309:CLA:O1D  | 2.12                     | 0.49              |
| 1:V:189:MET:HB3  | 2:V:301:CLA:HMC3 | 1.94                     | 0.48              |
| 1:W:158:ASN:HB2  | 2:W:309:CLA:CGD  | 2.44                     | 0.48              |
| 1:X:66:ARG:NH1   | 3:X:308:CHL:OBD  | 2.45                     | 0.48              |
| 1:V:125:VAL:HG21 | 3:V:305:CHL:C3D  | 2.44                     | 0.47              |
| 1:V:142:GLY:HA2  | 1:V:154:VAL:HG11 | 1.95                     | 0.47              |
| 1:X:36:PRO:HG3   | 2:X:311:CLA:CMA  | 2.45                     | 0.47              |
| 1:V:61:GLU:OE1   | 2:V:301:CLA:C4A  | 2.57                     | 0.47              |
| 1:V:142:GLY:CA   | 1:V:154:VAL:HG11 | 2.45                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:72:VAL:O     | 1:V:75:ALA:HB3   | 2.15                     | 0.46              |
| 1:W:198:GLN:HG2  | 2:W:312:CLA:ND   | 2.30                     | 0.46              |
| 1:W:113:ALA:HB3  | 1:W:120:PRO:HG3  | 1.96                     | 0.46              |
| 1:W:164:ASP:OD1  | 5:W:315:Q6L:O39  | 2.33                     | 0.46              |
| 6:V:320:IWJ:O27  | 6:V:320:IWJ:O39  | 2.34                     | 0.46              |
| 1:W:213:HIS:HA   | 1:W:220:SER:HB2  | 1.98                     | 0.46              |
| 1:W:95:PRO:HA    | 1:W:122:PHE:HB3  | 1.97                     | 0.46              |
| 1:X:34:ILE:N     | 1:X:179:ILE:HG21 | 2.31                     | 0.45              |
| 1:X:79:GLU:OE2   | 1:X:207:ILE:N    | 2.46                     | 0.45              |
| 1:V:123:TRP:HZ2  | 1:X:218:VAL:HG21 | 1.82                     | 0.45              |
| 1:V:137:GLU:HA   | 1:V:140:ARG:HG2  | 1.98                     | 0.45              |
| 1:X:174:LEU:HD11 | 2:X:310:CLA:HED2 | 1.98                     | 0.45              |
| 1:X:46:GLU:HA    | 2:X:302:CLA:HED1 | 1.99                     | 0.44              |
| 1:X:175:GLU:HA   | 1:X:178:LYS:HZ3  | 1.83                     | 0.44              |
| 1:V:65:GLY:HA2   | 1:V:189:MET:HG3  | 1.99                     | 0.44              |
| 1:W:59:GLU:OE2   | 1:W:157:VAL:HG13 | 2.18                     | 0.44              |
| 1:X:139:TYR:CE2  | 1:X:147:PRO:HB3  | 2.53                     | 0.44              |
| 1:X:175:GLU:HA   | 1:X:178:LYS:NZ   | 2.33                     | 0.44              |
| 2:V:301:CLA:H3A  | 2:V:301:CLA:CGA  | 2.48                     | 0.43              |
| 1:W:225:ASN:ND2  | 2:W:312:CLA:OBD  | 2.51                     | 0.43              |
| 1:V:158:ASN:ND2  | 2:V:309:CLA:O1D  | 2.51                     | 0.43              |
| 1:V:193:LEU:O    | 1:V:196:ILE:HG12 | 2.18                     | 0.43              |
| 5:V:321:Q6L:C28  | 1:W:196:ILE:HG23 | 2.48                     | 0.43              |
| 1:V:95:PRO:HA    | 1:V:122:PHE:CD2  | 2.54                     | 0.42              |
| 1:V:140:ARG:HG3  | 1:V:141:THR:HG23 | 2.01                     | 0.42              |
| 1:X:150:ASP:HB3  | 1:X:152:LEU:HD23 | 2.02                     | 0.42              |
| 1:X:95:PRO:HA    | 1:X:122:PHE:HB3  | 2.01                     | 0.42              |
| 1:V:198:GLN:HG2  | 2:V:312:CLA:C1D  | 2.50                     | 0.42              |
| 1:V:180:LYS:NZ   | 2:V:311:CLA:HAA2 | 2.35                     | 0.42              |
| 2:X:313:CLA:H2A  | 2:X:313:CLA:O2D  | 2.20                     | 0.41              |
| 1:W:177:LEU:HD13 | 2:W:309:CLA:O1A  | 2.21                     | 0.41              |
| 1:X:38:PHE:O     | 5:X:319:Q6L:O39  | 2.38                     | 0.41              |
| 1:V:77:ALA:O     | 2:V:303:CLA:HMD3 | 2.20                     | 0.41              |
| 1:W:177:LEU:HB3  | 2:W:309:CLA:H3A  | 2.03                     | 0.41              |
| 1:X:55:GLU:O     | 1:X:58:ALA:N     | 2.54                     | 0.41              |
| 1:V:157:VAL:C    | 1:V:159:PRO:HD3  | 2.42                     | 0.40              |
| 1:V:180:LYS:NZ   | 2:V:311:CLA:HBD  | 2.30                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | V     | 193/233 (83%) | 188 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | W     | 198/233 (85%) | 188 (95%) | 10 (5%) | 0        | 100         | 100 |
| 1   | X     | 190/233 (82%) | 184 (97%) | 6 (3%)  | 0        | 100         | 100 |
| All | All   | 581/699 (83%) | 560 (96%) | 21 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | V     | 151/179 (84%) | 151 (100%) | 0        | 100         | 100 |
| 1   | W     | 152/179 (85%) | 151 (99%)  | 1 (1%)   | 81          | 89  |
| 1   | X     | 150/179 (84%) | 148 (99%)  | 2 (1%)   | 65          | 80  |
| All | All   | 453/537 (84%) | 450 (99%)  | 3 (1%)   | 80          | 89  |

All (3) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | W     | 158 | ASN  |
| 1   | X     | 123 | TRP  |
| 1   | X     | 219 | HIS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | V     | 209 | ASN  |
| 1   | W     | 209 | 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

60 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 5   | Q6L  | X     | 316 | -    | 40,41,43     | 1.86 | 5 (12%)     | 46,56,60    | 1.61 | 6 (13%)     |
| 2   | CLA  | W     | 301 | 1    | 55,63,73     | 1.59 | 9 (16%)     | 64,101,113  | 1.53 | 9 (14%)     |
| 6   | IWJ  | V     | 320 | -    | 43,45,45     | 1.16 | 5 (11%)     | 43,65,65    | 1.13 | 2 (4%)      |
| 5   | Q6L  | X     | 301 | -    | 42,43,43     | 1.90 | 7 (16%)     | 47,60,60    | 1.52 | 5 (10%)     |
| 2   | CLA  | X     | 314 | -    | 41,49,73     | 1.85 | 7 (17%)     | 47,84,113   | 1.55 | 8 (17%)     |
| 3   | CHL  | X     | 307 | -    | 52,60,74     | 1.58 | 10 (19%)    | 56,97,114   | 2.51 | 18 (32%)    |
| 3   | CHL  | X     | 305 | 1    | 42,50,74     | 1.85 | 5 (11%)     | 44,85,114   | 1.43 | 8 (18%)     |
| 3   | CHL  | X     | 306 | -    | 42,50,74     | 1.79 | 6 (14%)     | 44,85,114   | 1.84 | 8 (18%)     |
| 2   | CLA  | X     | 311 | 1    | 50,58,73     | 1.65 | 7 (14%)     | 58,95,113   | 1.41 | 8 (13%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | CLA  | X     | 312 | -    | 51,59,73     | 1.66 | 8 (15%)  | 59,96,113   | 1.56 | 11 (18%) |
| 5   | Q6L  | W     | 319 | -    | 42,43,43     | 1.88 | 7 (16%)  | 47,60,60    | 1.45 | 7 (14%)  |
| 2   | CLA  | V     | 309 | 1    | 42,50,73     | 2.12 | 9 (21%)  | 48,85,113   | 2.06 | 14 (29%) |
| 2   | CLA  | W     | 302 | -    | 55,63,73     | 1.61 | 8 (14%)  | 64,101,113  | 1.34 | 8 (12%)  |
| 2   | CLA  | W     | 309 | 1    | 64,72,73     | 1.51 | 6 (9%)   | 74,111,113  | 1.59 | 14 (18%) |
| 4   | KC2  | W     | 308 | 1    | 48,53,53     | 2.57 | 16 (33%) | 54,89,89    | 2.32 | 20 (37%) |
| 2   | CLA  | X     | 304 | -    | 42,50,73     | 1.86 | 8 (19%)  | 48,85,113   | 1.74 | 9 (18%)  |
| 3   | CHL  | W     | 314 | 1    | 40,49,74     | 1.84 | 6 (15%)  | 42,83,114   | 1.99 | 10 (23%) |
| 6   | IWJ  | V     | 317 | -    | 43,45,45     | 1.17 | 4 (9%)   | 43,65,65    | 1.20 | 2 (4%)   |
| 6   | IWJ  | V     | 318 | -    | 43,45,45     | 1.14 | 4 (9%)   | 43,65,65    | 1.43 | 8 (18%)  |
| 2   | CLA  | W     | 303 | -    | 50,58,73     | 1.65 | 8 (16%)  | 58,95,113   | 1.68 | 11 (18%) |
| 3   | CHL  | V     | 314 | 1    | 44,52,74     | 1.79 | 7 (15%)  | 46,87,114   | 1.66 | 10 (21%) |
| 5   | Q6L  | V     | 315 | -    | 42,43,43     | 1.91 | 7 (16%)  | 47,60,60    | 1.45 | 6 (12%)  |
| 2   | CLA  | V     | 310 | 1    | 47,55,73     | 1.74 | 8 (17%)  | 54,91,113   | 1.48 | 10 (18%) |
| 2   | CLA  | X     | 310 | 1    | 42,50,73     | 1.82 | 7 (16%)  | 48,85,113   | 1.58 | 9 (18%)  |
| 4   | KC2  | V     | 308 | 1    | 48,53,53     | 2.53 | 16 (33%) | 54,89,89    | 2.21 | 19 (35%) |
| 5   | Q6L  | V     | 321 | -    | 42,43,43     | 1.86 | 7 (16%)  | 47,60,60    | 1.57 | 4 (8%)   |
| 3   | CHL  | V     | 306 | -    | 44,52,74     | 1.75 | 7 (15%)  | 46,87,114   | 1.96 | 12 (26%) |
| 3   | CHL  | X     | 315 | 1    | 45,53,74     | 1.83 | 6 (13%)  | 46,88,114   | 1.36 | 5 (10%)  |
| 3   | CHL  | W     | 304 | 1    | 42,50,74     | 1.88 | 5 (11%)  | 44,85,114   | 1.58 | 7 (15%)  |
| 3   | CHL  | X     | 308 | -    | 44,52,74     | 1.72 | 6 (13%)  | 46,87,114   | 1.77 | 10 (21%) |
| 4   | KC2  | X     | 309 | 1    | 48,53,53     | 2.57 | 16 (33%) | 54,89,89    | 2.54 | 21 (38%) |
| 5   | Q6L  | X     | 317 | -    | 42,43,43     | 1.86 | 7 (16%)  | 47,60,60    | 1.57 | 5 (10%)  |
| 2   | CLA  | V     | 313 | -    | 48,56,73     | 1.70 | 7 (14%)  | 55,92,113   | 1.37 | 8 (14%)  |
| 6   | IWJ  | X     | 318 | -    | 43,45,45     | 1.18 | 7 (16%)  | 43,65,65    | 1.39 | 7 (16%)  |
| 3   | CHL  | W     | 307 | -    | 66,74,74     | 1.46 | 6 (9%)   | 73,114,114  | 1.53 | 10 (13%) |
| 2   | CLA  | X     | 302 | 1    | 55,63,73     | 1.64 | 10 (18%) | 64,101,113  | 1.48 | 13 (20%) |
| 2   | CLA  | W     | 311 | -    | 45,53,73     | 1.68 | 6 (13%)  | 52,89,113   | 1.62 | 8 (15%)  |
| 7   | NEX  | W     | 317 | -    | 38,46,46     | 1.13 | 4 (10%)  | 50,70,70    | 2.59 | 13 (26%) |
| 2   | CLA  | W     | 312 | 1    | 55,63,73     | 1.60 | 7 (12%)  | 64,101,113  | 1.79 | 13 (20%) |
| 2   | CLA  | V     | 301 | 1    | 60,68,73     | 1.48 | 5 (8%)   | 70,107,113  | 1.74 | 11 (15%) |
| 2   | CLA  | X     | 303 | -    | 51,59,73     | 1.72 | 8 (15%)  | 59,96,113   | 1.32 | 7 (11%)  |
| 5   | Q6L  | V     | 319 | -    | 42,43,43     | 1.81 | 7 (16%)  | 47,60,60    | 1.79 | 12 (25%) |
| 2   | CLA  | X     | 313 | 1    | 41,49,73     | 1.86 | 8 (19%)  | 47,84,113   | 1.60 | 9 (19%)  |
| 6   | IWJ  | W     | 318 | -    | 43,45,45     | 1.15 | 4 (9%)   | 43,65,65    | 1.36 | 6 (13%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | CHL  | V     | 305 | 1    | 43,51,74     | 1.74 | 7 (16%)  | 45,86,114   | 1.76 | 7 (15%)  |
| 3   | CHL  | V     | 304 | 1    | 46,54,74     | 1.78 | 8 (17%)  | 49,90,114   | 1.49 | 8 (16%)  |
| 5   | Q6L  | W     | 320 | -    | 42,43,43     | 1.88 | 7 (16%)  | 47,60,60    | 1.72 | 5 (10%)  |
| 3   | CHL  | W     | 306 | -    | 52,60,74     | 1.60 | 8 (15%)  | 56,97,114   | 2.11 | 14 (25%) |
| 2   | CLA  | V     | 311 | -    | 60,68,73     | 1.51 | 7 (11%)  | 70,107,113  | 1.40 | 11 (15%) |
| 5   | Q6L  | X     | 319 | -    | 42,43,43     | 1.92 | 6 (14%)  | 47,60,60    | 1.77 | 7 (14%)  |
| 2   | CLA  | V     | 303 | -    | 50,58,73     | 1.72 | 8 (16%)  | 58,95,113   | 1.73 | 8 (13%)  |
| 5   | Q6L  | W     | 315 | -    | 42,43,43     | 1.84 | 7 (16%)  | 47,60,60    | 1.54 | 7 (14%)  |
| 2   | CLA  | W     | 313 | -    | 43,51,73     | 1.77 | 6 (13%)  | 49,86,113   | 1.41 | 7 (14%)  |
| 3   | CHL  | V     | 307 | -    | 44,52,74     | 1.74 | 5 (11%)  | 46,87,114   | 1.53 | 9 (19%)  |
| 5   | Q6L  | V     | 316 | -    | 42,43,43     | 1.94 | 7 (16%)  | 47,60,60    | 1.60 | 5 (10%)  |
| 5   | Q6L  | W     | 316 | -    | 42,43,43     | 1.91 | 9 (21%)  | 47,60,60    | 1.54 | 6 (12%)  |
| 2   | CLA  | V     | 312 | 1    | 55,63,73     | 1.60 | 9 (16%)  | 64,101,113  | 1.47 | 9 (14%)  |
| 2   | CLA  | W     | 310 | 1    | 60,68,73     | 1.55 | 6 (10%)  | 70,107,113  | 1.30 | 8 (11%)  |
| 2   | CLA  | V     | 302 | -    | 50,58,73     | 1.70 | 9 (18%)  | 58,95,113   | 1.47 | 11 (18%) |
| 3   | CHL  | W     | 305 | -    | 42,50,74     | 1.81 | 6 (14%)  | 44,85,114   | 1.83 | 10 (22%) |

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   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 5   | Q6L  | X     | 316 | -    | -         | 7/29/63/67    | 0/2/2/2 |
| 2   | CLA  | W     | 301 | 1    | 1/1/13/20 | 10/25/103/115 | -       |
| 6   | IWJ  | V     | 320 | -    | -         | 5/33/76/76    | 1/2/2/2 |
| 5   | Q6L  | X     | 301 | -    | -         | 8/29/67/67    | 0/2/2/2 |
| 2   | CLA  | X     | 314 | -    | 1/1/10/20 | 5/8/86/115    | -       |
| 3   | CHL  | X     | 307 | -    | 3/3/17/26 | 10/23/121/137 | -       |
| 3   | CHL  | X     | 305 | 1    | 3/3/15/26 | 1/10/108/137  | -       |
| 3   | CHL  | X     | 306 | -    | 3/3/15/26 | 2/10/108/137  | -       |
| 2   | CLA  | X     | 311 | 1    | 1/1/12/20 | 8/19/97/115   | -       |
| 2   | CLA  | X     | 312 | -    | 1/1/12/20 | 4/21/99/115   | -       |
| 5   | Q6L  | W     | 319 | -    | -         | 9/29/67/67    | 0/2/2/2 |
| 2   | CLA  | V     | 309 | 1    | 1/1/10/20 | 4/10/88/115   | -       |
| 2   | CLA  | W     | 302 | -    | 1/1/13/20 | 5/25/103/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 2   | CLA  | W     | 309 | 1    | 1/1/14/20 | 7/36/114/115  | -       |
| 4   | KC2  | W     | 308 | 1    | -         | 10/15/71/71   | -       |
| 2   | CLA  | X     | 304 | -    | 1/1/10/20 | 5/10/88/115   | -       |
| 3   | CHL  | W     | 314 | 1    | 3/3/14/26 | 5/10/104/137  | -       |
| 6   | IWJ  | V     | 317 | -    | -         | 6/33/76/76    | 0/2/2/2 |
| 6   | IWJ  | V     | 318 | -    | -         | 4/33/76/76    | 0/2/2/2 |
| 2   | CLA  | W     | 303 | -    | 1/1/12/20 | 4/19/97/115   | -       |
| 3   | CHL  | V     | 314 | 1    | 3/3/15/26 | 5/13/111/137  | -       |
| 5   | Q6L  | V     | 315 | -    | -         | 11/29/67/67   | 0/2/2/2 |
| 2   | CLA  | V     | 310 | 1    | 1/1/11/20 | 8/16/94/115   | -       |
| 2   | CLA  | X     | 310 | 1    | 1/1/10/20 | 3/10/88/115   | -       |
| 4   | KC2  | V     | 308 | 1    | -         | 10/15/71/71   | -       |
| 5   | Q6L  | V     | 321 | -    | -         | 6/29/67/67    | 0/2/2/2 |
| 3   | CHL  | V     | 306 | -    | 3/3/15/26 | 0/13/111/137  | -       |
| 3   | CHL  | X     | 315 | 1    | 3/3/15/26 | 4/13/112/137  | -       |
| 3   | CHL  | W     | 304 | 1    | 3/3/15/26 | 0/10/108/137  | -       |
| 3   | CHL  | X     | 308 | -    | 3/3/15/26 | 8/13/111/137  | -       |
| 4   | KC2  | X     | 309 | 1    | -         | 10/15/71/71   | -       |
| 5   | Q6L  | X     | 317 | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 2   | CLA  | V     | 313 | -    | 1/1/11/20 | 4/17/95/115   | -       |
| 6   | IWJ  | X     | 318 | -    | -         | 6/33/76/76    | 1/2/2/2 |
| 3   | CHL  | W     | 307 | -    | 3/3/20/26 | 13/39/137/137 | -       |
| 2   | CLA  | X     | 302 | 1    | 1/1/13/20 | 8/25/103/115  | -       |
| 2   | CLA  | W     | 311 | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 7   | NEX  | W     | 317 | -    | -         | 2/27/83/83    | 0/3/3/3 |
| 2   | CLA  | W     | 312 | 1    | 1/1/13/20 | 9/25/103/115  | -       |
| 2   | CLA  | V     | 301 | 1    | 1/1/14/20 | 10/31/109/115 | -       |
| 2   | CLA  | X     | 303 | -    | 1/1/12/20 | 9/21/99/115   | -       |
| 5   | Q6L  | V     | 319 | -    | -         | 9/29/67/67    | 0/2/2/2 |
| 2   | CLA  | X     | 313 | 1    | 1/1/10/20 | 3/8/86/115    | -       |
| 6   | IWJ  | W     | 318 | -    | -         | 10/33/76/76   | 0/2/2/2 |
| 3   | CHL  | V     | 305 | 1    | 3/3/15/26 | 2/12/110/137  | -       |
| 3   | CHL  | V     | 304 | 1    | 3/3/16/26 | 8/15/113/137  | -       |
| 5   | Q6L  | W     | 320 | -    | -         | 7/29/67/67    | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 3   | CHL  | W     | 306 | -    | 3/3/17/26 | 5/23/121/137  | -       |
| 2   | CLA  | V     | 311 | -    | 1/1/14/20 | 10/31/109/115 | -       |
| 5   | Q6L  | X     | 319 | -    | -         | 10/29/67/67   | 0/2/2/2 |
| 2   | CLA  | V     | 303 | -    | 1/1/12/20 | 5/19/97/115   | -       |
| 5   | Q6L  | W     | 315 | -    | -         | 4/29/67/67    | 0/2/2/2 |
| 2   | CLA  | W     | 313 | -    | 1/1/10/20 | 2/11/89/115   | -       |
| 3   | CHL  | V     | 307 | -    | 3/3/15/26 | 5/13/111/137  | -       |
| 5   | Q6L  | V     | 316 | -    | -         | 8/29/67/67    | 0/2/2/2 |
| 5   | Q6L  | W     | 316 | -    | -         | 5/29/67/67    | 0/2/2/2 |
| 2   | CLA  | V     | 312 | 1    | -         | 7/25/103/115  | -       |
| 2   | CLA  | W     | 310 | 1    | 1/1/14/20 | 9/31/109/115  | -       |
| 2   | CLA  | V     | 302 | -    | 1/1/12/20 | 9/19/97/115   | -       |
| 3   | CHL  | W     | 305 | -    | 3/3/15/26 | 2/10/108/137  | -       |

All (438) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | V     | 309 | CLA  | C4B-NB  | 10.02 | 1.44        | 1.35     |
| 5   | V     | 316 | Q6L  | C29-C30 | 8.77  | 1.53        | 1.32     |
| 4   | V     | 308 | KC2  | C2A-C3A | 8.64  | 1.54        | 1.37     |
| 4   | X     | 309 | KC2  | C2A-C3A | 8.61  | 1.54        | 1.37     |
| 5   | X     | 319 | Q6L  | C29-C30 | 8.50  | 1.52        | 1.32     |
| 5   | X     | 301 | Q6L  | C29-C30 | 8.42  | 1.52        | 1.32     |
| 5   | W     | 319 | Q6L  | C29-C30 | 8.41  | 1.52        | 1.32     |
| 5   | W     | 316 | Q6L  | C29-C30 | 8.39  | 1.52        | 1.32     |
| 5   | X     | 316 | Q6L  | C29-C30 | 8.38  | 1.52        | 1.32     |
| 5   | X     | 317 | Q6L  | C29-C30 | 8.37  | 1.52        | 1.32     |
| 5   | W     | 320 | Q6L  | C29-C30 | 8.31  | 1.51        | 1.32     |
| 5   | V     | 321 | Q6L  | C29-C30 | 8.29  | 1.51        | 1.32     |
| 3   | X     | 305 | CHL  | C4B-NB  | 8.25  | 1.42        | 1.35     |
| 5   | V     | 315 | Q6L  | C29-C30 | 8.17  | 1.51        | 1.32     |
| 5   | W     | 315 | Q6L  | C29-C30 | 8.06  | 1.51        | 1.32     |
| 3   | W     | 304 | CHL  | C4B-NB  | 8.05  | 1.42        | 1.35     |
| 4   | W     | 308 | KC2  | C2A-C3A | 7.90  | 1.53        | 1.37     |
| 3   | X     | 315 | CHL  | C4B-NB  | 7.80  | 1.42        | 1.35     |
| 3   | X     | 308 | CHL  | C4B-NB  | 7.71  | 1.42        | 1.35     |
| 3   | W     | 307 | CHL  | C4B-NB  | 7.70  | 1.42        | 1.35     |
| 3   | W     | 314 | CHL  | C4B-NB  | 7.67  | 1.42        | 1.35     |
| 5   | V     | 319 | Q6L  | C29-C30 | 7.59  | 1.50        | 1.32     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | W     | 305 | CHL  | C4B-NB  | 7.59  | 1.42        | 1.35     |
| 3   | V     | 314 | CHL  | C4B-NB  | 7.52  | 1.41        | 1.35     |
| 2   | X     | 313 | CLA  | C4B-NB  | 7.51  | 1.41        | 1.35     |
| 2   | W     | 309 | CLA  | C4B-NB  | 7.47  | 1.41        | 1.35     |
| 2   | W     | 312 | CLA  | C4B-NB  | 7.46  | 1.41        | 1.35     |
| 3   | V     | 307 | CHL  | C4B-NB  | 7.35  | 1.41        | 1.35     |
| 2   | X     | 310 | CLA  | C4B-NB  | 7.33  | 1.41        | 1.35     |
| 2   | W     | 310 | CLA  | C4B-NB  | 7.32  | 1.41        | 1.35     |
| 3   | W     | 306 | CHL  | C4B-NB  | 7.31  | 1.41        | 1.35     |
| 3   | V     | 306 | CHL  | C4B-NB  | 7.30  | 1.41        | 1.35     |
| 2   | X     | 314 | CLA  | C4B-NB  | 7.17  | 1.41        | 1.35     |
| 3   | V     | 304 | CHL  | C4B-NB  | 7.12  | 1.41        | 1.35     |
| 2   | V     | 302 | CLA  | C4B-NB  | 7.11  | 1.41        | 1.35     |
| 2   | X     | 312 | CLA  | C4B-NB  | 7.11  | 1.41        | 1.35     |
| 2   | V     | 303 | CLA  | C4B-NB  | 7.06  | 1.41        | 1.35     |
| 2   | V     | 313 | CLA  | C4B-NB  | 7.04  | 1.41        | 1.35     |
| 2   | X     | 303 | CLA  | C4B-NB  | 7.03  | 1.41        | 1.35     |
| 3   | X     | 306 | CHL  | C4B-NB  | 7.03  | 1.41        | 1.35     |
| 3   | V     | 305 | CHL  | C4B-NB  | 6.90  | 1.41        | 1.35     |
| 2   | X     | 304 | CLA  | C4B-NB  | 6.85  | 1.41        | 1.35     |
| 4   | X     | 309 | KC2  | C3D-C4D | 6.80  | 1.46        | 1.40     |
| 2   | V     | 311 | CLA  | C4B-NB  | 6.78  | 1.41        | 1.35     |
| 2   | W     | 313 | CLA  | C4B-NB  | 6.78  | 1.41        | 1.35     |
| 2   | W     | 302 | CLA  | C4B-NB  | 6.77  | 1.41        | 1.35     |
| 2   | V     | 312 | CLA  | C4B-NB  | 6.70  | 1.41        | 1.35     |
| 4   | W     | 308 | KC2  | C1D-ND  | 6.68  | 1.41        | 1.35     |
| 2   | V     | 310 | CLA  | C4B-NB  | 6.65  | 1.41        | 1.35     |
| 2   | W     | 311 | CLA  | C4B-NB  | 6.56  | 1.41        | 1.35     |
| 4   | W     | 308 | KC2  | C3D-C4D | 6.56  | 1.46        | 1.40     |
| 2   | X     | 311 | CLA  | C4B-NB  | 6.51  | 1.41        | 1.35     |
| 2   | V     | 301 | CLA  | C4B-NB  | 6.39  | 1.40        | 1.35     |
| 2   | W     | 303 | CLA  | C4B-NB  | 6.37  | 1.40        | 1.35     |
| 4   | V     | 308 | KC2  | CBA-CAA | 6.28  | 1.52        | 1.33     |
| 4   | X     | 309 | KC2  | C1D-ND  | 6.24  | 1.40        | 1.35     |
| 2   | W     | 301 | CLA  | C4B-NB  | 6.14  | 1.40        | 1.35     |
| 4   | W     | 308 | KC2  | CBA-CAA | 6.05  | 1.51        | 1.33     |
| 3   | X     | 307 | CHL  | C4B-NB  | 6.04  | 1.40        | 1.35     |
| 4   | X     | 309 | KC2  | CBA-CAA | 5.98  | 1.51        | 1.33     |
| 2   | X     | 302 | CLA  | C4B-NB  | 5.83  | 1.40        | 1.35     |
| 5   | V     | 315 | Q6L  | C12-C11 | -5.73 | 1.33        | 1.52     |
| 5   | W     | 320 | Q6L  | C12-C11 | -5.53 | 1.34        | 1.52     |
| 5   | W     | 315 | Q6L  | C12-C11 | -5.51 | 1.34        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | X     | 319 | Q6L  | C12-C11 | -5.51 | 1.34        | 1.52     |
| 5   | V     | 316 | Q6L  | C12-C11 | -5.47 | 1.34        | 1.52     |
| 5   | W     | 316 | Q6L  | C12-C11 | -5.46 | 1.34        | 1.52     |
| 5   | V     | 321 | Q6L  | C12-C11 | -5.45 | 1.34        | 1.52     |
| 5   | V     | 319 | Q6L  | C12-C11 | -5.44 | 1.34        | 1.52     |
| 5   | W     | 319 | Q6L  | C12-C11 | -5.40 | 1.34        | 1.52     |
| 5   | X     | 301 | Q6L  | C12-C11 | -5.40 | 1.34        | 1.52     |
| 4   | V     | 308 | KC2  | C1D-ND  | 5.26  | 1.39        | 1.35     |
| 5   | X     | 316 | Q6L  | C12-C11 | -5.24 | 1.35        | 1.52     |
| 5   | X     | 317 | Q6L  | C12-C11 | -5.16 | 1.35        | 1.52     |
| 4   | V     | 308 | KC2  | C3D-C4D | 4.97  | 1.44        | 1.40     |
| 2   | X     | 302 | CLA  | C4D-ND  | -4.43 | 1.31        | 1.37     |
| 4   | X     | 309 | KC2  | CMD-C2D | -4.19 | 1.42        | 1.51     |
| 4   | W     | 308 | KC2  | C4A-C3A | 4.11  | 1.52        | 1.44     |
| 4   | V     | 308 | KC2  | CMD-C2D | -4.07 | 1.43        | 1.51     |
| 2   | V     | 309 | CLA  | CHC-C1C | 4.03  | 1.45        | 1.35     |
| 2   | V     | 301 | CLA  | C4D-ND  | -4.03 | 1.32        | 1.37     |
| 2   | X     | 303 | CLA  | C1D-ND  | 3.94  | 1.42        | 1.37     |
| 3   | W     | 304 | CHL  | C1D-ND  | 3.93  | 1.42        | 1.37     |
| 3   | V     | 304 | CHL  | C1D-ND  | 3.92  | 1.42        | 1.37     |
| 2   | W     | 303 | CLA  | C4D-ND  | -3.91 | 1.32        | 1.37     |
| 2   | W     | 302 | CLA  | C1D-ND  | 3.90  | 1.42        | 1.37     |
| 3   | X     | 306 | CHL  | C1D-ND  | 3.86  | 1.42        | 1.37     |
| 2   | W     | 312 | CLA  | C4D-ND  | -3.84 | 1.32        | 1.37     |
| 2   | W     | 310 | CLA  | C1D-ND  | 3.83  | 1.42        | 1.37     |
| 2   | X     | 304 | CLA  | CMB-C2B | -3.83 | 1.43        | 1.51     |
| 2   | V     | 311 | CLA  | C1D-ND  | 3.82  | 1.42        | 1.37     |
| 4   | V     | 308 | KC2  | C4A-C3A | 3.81  | 1.51        | 1.44     |
| 2   | W     | 313 | CLA  | C1D-ND  | 3.81  | 1.42        | 1.37     |
| 2   | X     | 314 | CLA  | C1D-ND  | 3.80  | 1.42        | 1.37     |
| 2   | W     | 301 | CLA  | C1D-ND  | 3.79  | 1.42        | 1.37     |
| 4   | X     | 309 | KC2  | C4A-C3A | 3.76  | 1.51        | 1.44     |
| 3   | W     | 314 | CHL  | C1D-ND  | 3.74  | 1.42        | 1.37     |
| 3   | X     | 315 | CHL  | C1D-ND  | 3.73  | 1.42        | 1.37     |
| 2   | V     | 310 | CLA  | C1D-ND  | 3.70  | 1.42        | 1.37     |
| 2   | W     | 309 | CLA  | C1D-ND  | 3.67  | 1.42        | 1.37     |
| 2   | X     | 303 | CLA  | C4D-ND  | -3.64 | 1.32        | 1.37     |
| 4   | W     | 308 | KC2  | CMD-C2D | -3.62 | 1.44        | 1.51     |
| 3   | X     | 307 | CHL  | C1D-ND  | 3.61  | 1.42        | 1.37     |
| 3   | X     | 306 | CHL  | C4D-ND  | -3.61 | 1.32        | 1.37     |
| 2   | X     | 311 | CLA  | C1D-ND  | 3.60  | 1.42        | 1.37     |
| 3   | V     | 307 | CHL  | C1D-ND  | 3.60  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | V     | 301 | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 2   | V     | 313 | CLA  | C1D-ND  | 3.57  | 1.42        | 1.37     |
| 2   | X     | 312 | CLA  | C1D-ND  | 3.56  | 1.42        | 1.37     |
| 2   | W     | 301 | CLA  | C4D-ND  | -3.55 | 1.32        | 1.37     |
| 3   | W     | 304 | CHL  | CHC-C1C | 3.54  | 1.44        | 1.35     |
| 3   | V     | 305 | CHL  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 3   | V     | 314 | CHL  | C4D-ND  | -3.45 | 1.33        | 1.37     |
| 2   | X     | 313 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 2   | W     | 311 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 3   | V     | 314 | CHL  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 2   | V     | 302 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 2   | X     | 304 | CLA  | C3B-C2B | -3.40 | 1.35        | 1.40     |
| 2   | W     | 313 | CLA  | C4D-ND  | -3.40 | 1.33        | 1.37     |
| 3   | W     | 307 | CHL  | C1D-ND  | 3.39  | 1.41        | 1.37     |
| 6   | V     | 317 | IWJ  | C09-C10 | 3.38  | 1.53        | 1.45     |
| 3   | V     | 306 | CHL  | CHC-C1C | 3.38  | 1.43        | 1.35     |
| 2   | X     | 304 | CLA  | C1D-ND  | 3.37  | 1.41        | 1.37     |
| 3   | W     | 306 | CHL  | C4D-ND  | -3.37 | 1.33        | 1.37     |
| 6   | V     | 320 | IWJ  | C09-C10 | 3.35  | 1.53        | 1.45     |
| 5   | V     | 315 | Q6L  | C12-C13 | -3.35 | 1.44        | 1.51     |
| 3   | V     | 306 | CHL  | C1D-ND  | 3.35  | 1.41        | 1.37     |
| 3   | X     | 308 | CHL  | C1D-ND  | 3.34  | 1.41        | 1.37     |
| 6   | V     | 318 | IWJ  | C09-C10 | 3.33  | 1.53        | 1.45     |
| 2   | V     | 303 | CLA  | CHC-C1C | 3.33  | 1.43        | 1.35     |
| 3   | V     | 307 | CHL  | C4D-ND  | -3.30 | 1.33        | 1.37     |
| 2   | V     | 309 | CLA  | C1D-ND  | 3.30  | 1.41        | 1.37     |
| 6   | W     | 318 | IWJ  | C09-C10 | 3.30  | 1.53        | 1.45     |
| 2   | X     | 310 | CLA  | C1D-ND  | 3.30  | 1.41        | 1.37     |
| 2   | V     | 302 | CLA  | C4D-ND  | -3.29 | 1.33        | 1.37     |
| 3   | X     | 305 | CHL  | CHC-C1C | 3.25  | 1.43        | 1.35     |
| 2   | V     | 312 | CLA  | C4D-ND  | -3.22 | 1.33        | 1.37     |
| 3   | V     | 304 | CHL  | CHC-C1C | 3.21  | 1.43        | 1.35     |
| 3   | X     | 315 | CHL  | C4D-ND  | -3.19 | 1.33        | 1.37     |
| 4   | V     | 308 | KC2  | MG-NA   | 3.19  | 2.13        | 2.06     |
| 3   | X     | 308 | CHL  | CHC-C1C | 3.18  | 1.43        | 1.35     |
| 3   | X     | 305 | CHL  | C4D-ND  | -3.18 | 1.33        | 1.37     |
| 3   | W     | 304 | CHL  | C4D-ND  | -3.16 | 1.33        | 1.37     |
| 3   | W     | 307 | CHL  | CHC-C1C | 3.16  | 1.43        | 1.35     |
| 3   | W     | 305 | CHL  | C4D-ND  | -3.14 | 1.33        | 1.37     |
| 2   | X     | 314 | CLA  | C4D-ND  | -3.13 | 1.33        | 1.37     |
| 2   | V     | 303 | CLA  | C4D-ND  | -3.13 | 1.33        | 1.37     |
| 4   | V     | 308 | KC2  | C4D-ND  | -3.12 | 1.32        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | X     | 310 | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 2   | X     | 311 | CLA  | C4D-ND  | -3.12 | 1.33        | 1.37     |
| 3   | V     | 306 | CHL  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 3   | W     | 305 | CHL  | C1D-ND  | 3.10  | 1.41        | 1.37     |
| 3   | W     | 314 | CHL  | C4D-ND  | -3.10 | 1.33        | 1.37     |
| 2   | W     | 309 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 2   | X     | 302 | CLA  | C3B-CAB | -3.08 | 1.41        | 1.47     |
| 2   | W     | 302 | CLA  | C4D-ND  | -3.08 | 1.33        | 1.37     |
| 2   | V     | 310 | CLA  | C4D-ND  | -3.07 | 1.33        | 1.37     |
| 2   | X     | 312 | CLA  | C4D-ND  | -3.07 | 1.33        | 1.37     |
| 3   | X     | 315 | CHL  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 2   | W     | 311 | CLA  | C4D-ND  | -3.07 | 1.33        | 1.37     |
| 2   | X     | 303 | CLA  | C3B-C2B | -3.06 | 1.36        | 1.40     |
| 2   | X     | 302 | CLA  | C1D-ND  | 3.05  | 1.41        | 1.37     |
| 6   | X     | 318 | IWJ  | C09-C10 | 3.05  | 1.52        | 1.45     |
| 2   | W     | 301 | CLA  | CHC-C1C | 3.05  | 1.42        | 1.35     |
| 2   | V     | 312 | CLA  | C1D-ND  | 3.04  | 1.41        | 1.37     |
| 2   | V     | 303 | CLA  | C3B-C2B | -3.04 | 1.36        | 1.40     |
| 2   | V     | 313 | CLA  | CHC-C1C | 3.03  | 1.42        | 1.35     |
| 4   | W     | 308 | KC2  | C4B-NB  | 3.02  | 1.41        | 1.37     |
| 2   | V     | 303 | CLA  | CMB-C2B | -3.02 | 1.45        | 1.51     |
| 5   | V     | 319 | Q6L  | C34-C33 | 3.02  | 1.54        | 1.50     |
| 2   | W     | 303 | CLA  | C1D-ND  | 3.01  | 1.41        | 1.37     |
| 2   | W     | 310 | CLA  | CHC-C1C | 3.01  | 1.42        | 1.35     |
| 2   | W     | 303 | CLA  | CMB-C2B | -3.01 | 1.45        | 1.51     |
| 5   | X     | 319 | Q6L  | C34-C33 | 3.01  | 1.54        | 1.50     |
| 2   | X     | 311 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 2   | X     | 313 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 2   | X     | 313 | CLA  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 2   | X     | 302 | CLA  | CHC-C1C | 2.99  | 1.42        | 1.35     |
| 2   | V     | 313 | CLA  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 3   | V     | 304 | CHL  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 2   | X     | 304 | CLA  | C4D-ND  | -2.98 | 1.33        | 1.37     |
| 6   | V     | 317 | IWJ  | C29-C35 | -2.97 | 1.51        | 1.56     |
| 2   | W     | 313 | CLA  | CHC-C1C | 2.97  | 1.42        | 1.35     |
| 4   | X     | 309 | KC2  | C2A-C1A | 2.96  | 1.53        | 1.44     |
| 3   | X     | 308 | CHL  | C4D-ND  | -2.95 | 1.33        | 1.37     |
| 6   | X     | 318 | IWJ  | C04-C03 | 2.95  | 1.54        | 1.50     |
| 3   | V     | 314 | CHL  | CHC-C1C | 2.95  | 1.42        | 1.35     |
| 2   | V     | 311 | CLA  | CHC-C1C | 2.94  | 1.42        | 1.35     |
| 3   | V     | 305 | CHL  | CHC-C1C | 2.93  | 1.42        | 1.35     |
| 3   | W     | 314 | CHL  | CHC-C1C | 2.92  | 1.42        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | X     | 306 | CHL  | CHC-C1C | 2.91  | 1.42        | 1.35     |
| 7   | W     | 317 | NEX  | C7-C8   | -2.90 | 1.27        | 1.32     |
| 3   | V     | 305 | CHL  | C4D-ND  | -2.89 | 1.33        | 1.37     |
| 6   | V     | 320 | IWJ  | C04-C03 | 2.89  | 1.54        | 1.50     |
| 4   | V     | 308 | KC2  | C4B-NB  | 2.89  | 1.41        | 1.37     |
| 3   | V     | 307 | CHL  | CHC-C1C | 2.89  | 1.42        | 1.35     |
| 4   | V     | 308 | KC2  | C2A-C1A | 2.88  | 1.53        | 1.44     |
| 2   | V     | 312 | CLA  | CMB-C2B | -2.87 | 1.45        | 1.51     |
| 2   | V     | 312 | CLA  | CHC-C1C | 2.87  | 1.42        | 1.35     |
| 2   | V     | 310 | CLA  | C3B-C2B | -2.87 | 1.36        | 1.40     |
| 5   | X     | 319 | Q6L  | C12-C13 | -2.87 | 1.45        | 1.51     |
| 2   | V     | 301 | CLA  | CMB-C2B | -2.87 | 1.45        | 1.51     |
| 2   | W     | 302 | CLA  | CHC-C1C | 2.86  | 1.42        | 1.35     |
| 2   | X     | 314 | CLA  | CHC-C1C | 2.86  | 1.42        | 1.35     |
| 2   | V     | 311 | CLA  | C4D-ND  | -2.86 | 1.33        | 1.37     |
| 2   | V     | 310 | CLA  | CMB-C2B | -2.85 | 1.45        | 1.51     |
| 5   | W     | 316 | Q6L  | C12-C13 | -2.83 | 1.45        | 1.51     |
| 4   | W     | 308 | KC2  | C2A-C1A | 2.83  | 1.53        | 1.44     |
| 2   | W     | 310 | CLA  | C4D-ND  | -2.81 | 1.33        | 1.37     |
| 4   | W     | 308 | KC2  | CMC-C2C | -2.81 | 1.44        | 1.50     |
| 2   | X     | 313 | CLA  | CMB-C2B | -2.80 | 1.45        | 1.51     |
| 2   | X     | 310 | CLA  | C4D-ND  | -2.77 | 1.33        | 1.37     |
| 2   | X     | 312 | CLA  | CHC-C1C | 2.77  | 1.42        | 1.35     |
| 6   | V     | 318 | IWJ  | C04-C03 | 2.77  | 1.54        | 1.50     |
| 3   | W     | 305 | CHL  | CHC-C1C | 2.76  | 1.42        | 1.35     |
| 2   | W     | 312 | CLA  | C1D-ND  | 2.76  | 1.41        | 1.37     |
| 2   | V     | 302 | CLA  | CMB-C2B | -2.76 | 1.45        | 1.51     |
| 3   | X     | 305 | CHL  | C1D-ND  | 2.76  | 1.41        | 1.37     |
| 3   | W     | 307 | CHL  | C4D-ND  | -2.74 | 1.33        | 1.37     |
| 5   | V     | 321 | Q6L  | C12-C13 | -2.74 | 1.45        | 1.51     |
| 3   | X     | 307 | CHL  | C4D-ND  | -2.74 | 1.33        | 1.37     |
| 5   | W     | 315 | Q6L  | C12-C13 | -2.73 | 1.45        | 1.51     |
| 5   | W     | 320 | Q6L  | C34-C33 | 2.73  | 1.54        | 1.50     |
| 5   | W     | 320 | Q6L  | C12-C13 | -2.73 | 1.45        | 1.51     |
| 6   | V     | 317 | IWJ  | C04-C03 | 2.72  | 1.54        | 1.50     |
| 5   | V     | 316 | Q6L  | C34-C33 | 2.71  | 1.54        | 1.50     |
| 5   | X     | 301 | Q6L  | C33-C32 | 2.71  | 1.36        | 1.33     |
| 2   | X     | 314 | CLA  | CMB-C2B | -2.71 | 1.46        | 1.51     |
| 5   | W     | 319 | Q6L  | C12-C13 | -2.70 | 1.45        | 1.51     |
| 2   | X     | 311 | CLA  | CMB-C2B | -2.70 | 1.46        | 1.51     |
| 2   | W     | 303 | CLA  | CHC-C1C | 2.69  | 1.41        | 1.35     |
| 2   | W     | 302 | CLA  | C3B-C2B | -2.69 | 1.36        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | W     | 316 | Q6L  | C34-C33 | 2.68  | 1.54        | 1.50     |
| 6   | W     | 318 | IWJ  | C04-C03 | 2.68  | 1.54        | 1.50     |
| 3   | W     | 305 | CHL  | CMD-C2D | -2.67 | 1.45        | 1.50     |
| 5   | X     | 301 | Q6L  | C34-C33 | 2.67  | 1.54        | 1.50     |
| 2   | X     | 310 | CLA  | CMB-C2B | -2.67 | 1.46        | 1.51     |
| 3   | V     | 305 | CHL  | CMD-C2D | -2.67 | 1.45        | 1.50     |
| 2   | W     | 312 | CLA  | CMB-C2B | -2.67 | 1.46        | 1.51     |
| 5   | V     | 319 | Q6L  | C12-C13 | -2.66 | 1.45        | 1.51     |
| 2   | V     | 312 | CLA  | CMD-C2D | -2.66 | 1.45        | 1.50     |
| 5   | X     | 316 | Q6L  | C02-C03 | 2.66  | 1.37        | 1.34     |
| 5   | X     | 317 | Q6L  | C02-C03 | 2.65  | 1.37        | 1.34     |
| 2   | V     | 310 | CLA  | C4B-CHC | -2.65 | 1.33        | 1.41     |
| 4   | X     | 309 | KC2  | CMC-C2C | -2.65 | 1.45        | 1.50     |
| 3   | X     | 307 | CHL  | CMB-C2B | -2.64 | 1.46        | 1.51     |
| 2   | W     | 311 | CLA  | CHC-C1C | 2.64  | 1.41        | 1.35     |
| 4   | X     | 309 | KC2  | C4B-NB  | 2.64  | 1.41        | 1.37     |
| 6   | W     | 318 | IWJ  | C03-C02 | 2.63  | 1.36        | 1.33     |
| 2   | W     | 309 | CLA  | C4D-ND  | -2.62 | 1.34        | 1.37     |
| 2   | X     | 312 | CLA  | CMB-C2B | -2.62 | 1.46        | 1.51     |
| 4   | V     | 308 | KC2  | CMC-C2C | -2.62 | 1.45        | 1.50     |
| 5   | X     | 317 | Q6L  | C34-C33 | 2.62  | 1.53        | 1.50     |
| 3   | V     | 314 | CHL  | CMD-C2D | -2.61 | 1.45        | 1.50     |
| 2   | V     | 302 | CLA  | C3B-C2B | -2.60 | 1.36        | 1.40     |
| 5   | X     | 301 | Q6L  | C12-C13 | -2.59 | 1.45        | 1.51     |
| 3   | W     | 306 | CHL  | C1D-ND  | 2.58  | 1.41        | 1.37     |
| 5   | W     | 319 | Q6L  | C34-C33 | 2.58  | 1.53        | 1.50     |
| 3   | V     | 304 | CHL  | C3B-C2B | -2.58 | 1.36        | 1.40     |
| 2   | V     | 311 | CLA  | CMB-C2B | -2.58 | 1.46        | 1.51     |
| 5   | V     | 316 | Q6L  | C12-C13 | -2.58 | 1.45        | 1.51     |
| 2   | X     | 303 | CLA  | CHC-C1C | 2.58  | 1.41        | 1.35     |
| 2   | W     | 302 | CLA  | CMB-C2B | -2.58 | 1.46        | 1.51     |
| 2   | V     | 303 | CLA  | C1D-ND  | 2.57  | 1.40        | 1.37     |
| 5   | V     | 315 | Q6L  | C34-C33 | 2.57  | 1.53        | 1.50     |
| 5   | W     | 316 | Q6L  | C02-C03 | 2.56  | 1.37        | 1.34     |
| 2   | X     | 304 | CLA  | CHC-C1C | 2.56  | 1.41        | 1.35     |
| 5   | V     | 319 | Q6L  | C02-C03 | 2.55  | 1.37        | 1.34     |
| 2   | W     | 309 | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 2   | W     | 310 | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 6   | W     | 318 | IWJ  | C29-C35 | -2.54 | 1.52        | 1.56     |
| 2   | W     | 313 | CLA  | CMB-C2B | -2.54 | 1.46        | 1.51     |
| 3   | W     | 306 | CHL  | CHC-C1C | 2.53  | 1.41        | 1.35     |
| 5   | W     | 315 | Q6L  | C34-C33 | 2.53  | 1.53        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | V     | 304 | CHL  | C3B-CAB | -2.53 | 1.42        | 1.47     |
| 2   | W     | 311 | CLA  | CMB-C2B | -2.52 | 1.46        | 1.51     |
| 2   | X     | 310 | CLA  | CMD-C2D | -2.52 | 1.45        | 1.50     |
| 6   | V     | 320 | IWJ  | C03-C02 | 2.52  | 1.36        | 1.33     |
| 3   | X     | 315 | CHL  | CMB-C2B | -2.52 | 1.46        | 1.51     |
| 6   | X     | 318 | IWJ  | C29-C35 | -2.52 | 1.52        | 1.56     |
| 6   | V     | 318 | IWJ  | C03-C02 | 2.51  | 1.36        | 1.33     |
| 3   | W     | 306 | CHL  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 3   | W     | 304 | CHL  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 4   | V     | 308 | KC2  | O2A-CGA | 2.50  | 1.36        | 1.30     |
| 4   | V     | 308 | KC2  | CHD-C4C | 2.50  | 1.41        | 1.35     |
| 4   | X     | 309 | KC2  | CMB-C2B | -2.49 | 1.45        | 1.50     |
| 5   | X     | 319 | Q6L  | C02-C03 | 2.49  | 1.37        | 1.34     |
| 5   | V     | 321 | Q6L  | C34-C33 | 2.48  | 1.53        | 1.50     |
| 5   | W     | 320 | Q6L  | C02-C03 | 2.48  | 1.37        | 1.34     |
| 3   | W     | 306 | CHL  | CAC-C3C | -2.48 | 1.44        | 1.51     |
| 3   | X     | 307 | CHL  | CHC-C1C | 2.48  | 1.41        | 1.35     |
| 3   | X     | 307 | CHL  | C4B-CHC | -2.48 | 1.34        | 1.41     |
| 5   | V     | 315 | Q6L  | C11-C03 | -2.48 | 1.47        | 1.51     |
| 5   | V     | 315 | Q6L  | C02-C03 | 2.47  | 1.37        | 1.34     |
| 5   | W     | 315 | Q6L  | C02-C03 | 2.47  | 1.37        | 1.34     |
| 2   | X     | 302 | CLA  | C3B-C2B | -2.47 | 1.36        | 1.40     |
| 5   | V     | 316 | Q6L  | C02-C03 | 2.46  | 1.37        | 1.34     |
| 2   | X     | 302 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 3   | X     | 305 | CHL  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 3   | W     | 314 | CHL  | CMD-C2D | -2.46 | 1.45        | 1.50     |
| 2   | V     | 313 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 2   | V     | 309 | CLA  | C1A-CHA | -2.45 | 1.32        | 1.43     |
| 5   | X     | 316 | Q6L  | C12-C13 | -2.44 | 1.46        | 1.51     |
| 5   | X     | 319 | Q6L  | C33-C32 | 2.43  | 1.36        | 1.33     |
| 6   | X     | 318 | IWJ  | C03-C02 | 2.43  | 1.36        | 1.33     |
| 2   | V     | 312 | CLA  | C3B-C2B | -2.43 | 1.37        | 1.40     |
| 2   | W     | 301 | CLA  | C3B-C2B | -2.43 | 1.37        | 1.40     |
| 2   | W     | 309 | CLA  | C3B-C2B | -2.42 | 1.37        | 1.40     |
| 5   | V     | 316 | Q6L  | C33-C32 | 2.42  | 1.36        | 1.33     |
| 2   | X     | 303 | CLA  | CMB-C2B | -2.41 | 1.46        | 1.51     |
| 2   | V     | 302 | CLA  | C4B-CHC | -2.41 | 1.34        | 1.41     |
| 4   | W     | 308 | KC2  | C4D-ND  | -2.41 | 1.33        | 1.35     |
| 2   | V     | 309 | CLA  | C1C-C2C | 2.41  | 1.49        | 1.44     |
| 4   | X     | 309 | KC2  | C1B-NB  | -2.40 | 1.34        | 1.37     |
| 5   | V     | 315 | Q6L  | C01-C02 | 2.39  | 1.54        | 1.50     |
| 5   | X     | 301 | Q6L  | C02-C03 | 2.39  | 1.37        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | W     | 307 | CHL  | CMB-C2B | -2.39 | 1.46        | 1.51     |
| 2   | V     | 302 | CLA  | CHC-C1C | 2.39  | 1.41        | 1.35     |
| 3   | V     | 306 | CHL  | CMB-C2B | -2.38 | 1.46        | 1.51     |
| 5   | W     | 319 | Q6L  | C01-C02 | 2.38  | 1.54        | 1.50     |
| 4   | X     | 309 | KC2  | O2A-CGA | 2.38  | 1.36        | 1.30     |
| 2   | W     | 312 | CLA  | C4B-CHC | -2.37 | 1.34        | 1.41     |
| 5   | V     | 316 | Q6L  | C29-C27 | 2.37  | 1.51        | 1.45     |
| 2   | X     | 312 | CLA  | C3B-C2B | -2.37 | 1.37        | 1.40     |
| 4   | W     | 308 | KC2  | O2A-CGA | 2.37  | 1.36        | 1.30     |
| 5   | V     | 321 | Q6L  | C02-C03 | 2.37  | 1.37        | 1.34     |
| 5   | X     | 317 | Q6L  | C12-C13 | -2.36 | 1.46        | 1.51     |
| 2   | X     | 303 | CLA  | C3B-CAB | -2.35 | 1.43        | 1.47     |
| 5   | W     | 316 | Q6L  | C33-C32 | 2.35  | 1.36        | 1.33     |
| 2   | X     | 314 | CLA  | C3B-C2B | -2.35 | 1.37        | 1.40     |
| 2   | V     | 309 | CLA  | CMB-C2B | -2.34 | 1.46        | 1.51     |
| 5   | X     | 301 | Q6L  | C01-C02 | 2.32  | 1.54        | 1.50     |
| 3   | V     | 305 | CHL  | CMB-C2B | -2.32 | 1.46        | 1.51     |
| 5   | W     | 319 | Q6L  | C02-C03 | 2.32  | 1.37        | 1.34     |
| 2   | W     | 303 | CLA  | O2D-CED | -2.32 | 1.39        | 1.45     |
| 4   | V     | 308 | KC2  | CAA-C2A | 2.31  | 1.53        | 1.46     |
| 3   | W     | 305 | CHL  | CMB-C2B | -2.31 | 1.46        | 1.51     |
| 2   | V     | 301 | CLA  | CHC-C1C | 2.30  | 1.40        | 1.35     |
| 5   | V     | 319 | Q6L  | C01-C02 | 2.29  | 1.54        | 1.50     |
| 5   | X     | 316 | Q6L  | C01-C02 | 2.28  | 1.54        | 1.50     |
| 2   | V     | 310 | CLA  | CHC-C1C | 2.27  | 1.40        | 1.35     |
| 4   | W     | 308 | KC2  | CMB-C2B | -2.27 | 1.46        | 1.50     |
| 2   | W     | 303 | CLA  | C3B-C2B | -2.27 | 1.37        | 1.40     |
| 3   | X     | 307 | CHL  | CAC-C3C | -2.26 | 1.45        | 1.51     |
| 3   | V     | 314 | CHL  | MG-ND   | -2.26 | 2.01        | 2.05     |
| 5   | W     | 316 | Q6L  | C01-C02 | 2.25  | 1.54        | 1.50     |
| 5   | W     | 319 | Q6L  | C33-C32 | 2.25  | 1.35        | 1.33     |
| 3   | W     | 314 | CHL  | CMB-C2B | -2.25 | 1.47        | 1.51     |
| 3   | V     | 304 | CHL  | CMB-C2B | -2.25 | 1.47        | 1.51     |
| 2   | W     | 301 | CLA  | CMC-C2C | -2.24 | 1.46        | 1.50     |
| 2   | V     | 309 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 6   | V     | 320 | IWJ  | C29-C35 | -2.23 | 1.53        | 1.56     |
| 2   | V     | 303 | CLA  | C3B-CAB | -2.23 | 1.43        | 1.47     |
| 4   | V     | 308 | KC2  | MG-NC   | 2.23  | 2.11        | 2.06     |
| 2   | W     | 312 | CLA  | CHC-C1C | 2.23  | 1.40        | 1.35     |
| 2   | V     | 313 | CLA  | C3B-C2B | -2.23 | 1.37        | 1.40     |
| 2   | X     | 302 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 2   | V     | 311 | CLA  | C3B-C2B | -2.22 | 1.37        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | V     | 314 | CHL  | CMB-C2B | -2.22 | 1.47        | 1.51     |
| 3   | V     | 306 | CHL  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 6   | V     | 317 | IWJ  | C03-C02 | 2.22  | 1.35        | 1.33     |
| 7   | W     | 317 | NEX  | C35-C15 | -2.21 | 1.30        | 1.36     |
| 3   | X     | 315 | CHL  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 2   | X     | 304 | CLA  | C4B-CHC | -2.21 | 1.34        | 1.41     |
| 3   | W     | 307 | CHL  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 2   | W     | 302 | CLA  | C4B-CHC | -2.20 | 1.34        | 1.41     |
| 3   | X     | 307 | CHL  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 4   | V     | 308 | KC2  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 3   | W     | 306 | CHL  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 4   | X     | 309 | KC2  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 2   | X     | 312 | CLA  | C4B-CHC | -2.18 | 1.34        | 1.41     |
| 5   | W     | 320 | Q6L  | C01-C02 | 2.18  | 1.54        | 1.50     |
| 4   | X     | 309 | KC2  | C4D-ND  | -2.18 | 1.33        | 1.35     |
| 2   | W     | 301 | CLA  | C3B-CAB | -2.18 | 1.43        | 1.47     |
| 5   | X     | 317 | Q6L  | C01-C02 | 2.18  | 1.54        | 1.50     |
| 3   | X     | 308 | CHL  | CMB-C2B | -2.18 | 1.47        | 1.51     |
| 2   | V     | 312 | CLA  | C4B-CHC | -2.18 | 1.34        | 1.41     |
| 2   | V     | 302 | CLA  | C3B-CAB | -2.18 | 1.43        | 1.47     |
| 6   | V     | 318 | IWJ  | C29-C35 | -2.17 | 1.53        | 1.56     |
| 2   | V     | 309 | CLA  | C1B-NB  | 2.17  | 1.37        | 1.35     |
| 5   | W     | 315 | Q6L  | C01-C02 | 2.17  | 1.54        | 1.50     |
| 3   | W     | 306 | CHL  | MG-ND   | -2.16 | 2.01        | 2.05     |
| 2   | W     | 312 | CLA  | MG-NC   | 2.16  | 2.11        | 2.06     |
| 2   | X     | 302 | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 5   | V     | 321 | Q6L  | C01-C02 | 2.16  | 1.54        | 1.50     |
| 2   | W     | 301 | CLA  | CMB-C2B | -2.15 | 1.47        | 1.51     |
| 3   | V     | 304 | CHL  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 3   | V     | 307 | CHL  | CMB-C2B | -2.15 | 1.47        | 1.51     |
| 2   | W     | 303 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 5   | V     | 319 | Q6L  | C33-C32 | 2.14  | 1.35        | 1.33     |
| 6   | X     | 318 | IWJ  | O39-C29 | -2.14 | 1.39        | 1.43     |
| 2   | X     | 313 | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 3   | X     | 308 | CHL  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 3   | V     | 305 | CHL  | MG-ND   | -2.13 | 2.01        | 2.05     |
| 4   | X     | 309 | KC2  | MG-NA   | 2.13  | 2.11        | 2.06     |
| 3   | X     | 306 | CHL  | CMB-C2B | -2.13 | 1.47        | 1.51     |
| 2   | X     | 303 | CLA  | C4B-CHC | -2.13 | 1.35        | 1.41     |
| 4   | W     | 308 | KC2  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 6   | X     | 318 | IWJ  | C26-C24 | -2.13 | 1.45        | 1.49     |
| 4   | W     | 308 | KC2  | MG-NA   | 2.12  | 2.11        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | W     | 317 | NEX  | O24-C25 | -2.12 | 1.43        | 1.46     |
| 2   | X     | 313 | CLA  | C3B-C2B | -2.11 | 1.37        | 1.40     |
| 3   | X     | 306 | CHL  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 2   | V     | 303 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 3   | V     | 306 | CHL  | MG-ND   | -2.10 | 2.01        | 2.05     |
| 5   | W     | 316 | Q6L  | C29-C27 | 2.09  | 1.50        | 1.45     |
| 4   | W     | 308 | KC2  | MG-NC   | 2.08  | 2.11        | 2.06     |
| 2   | X     | 312 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 4   | X     | 309 | KC2  | MG-NC   | 2.08  | 2.11        | 2.06     |
| 5   | X     | 317 | Q6L  | C33-C32 | 2.07  | 1.35        | 1.33     |
| 2   | W     | 302 | CLA  | C3B-CAB | -2.06 | 1.43        | 1.47     |
| 2   | V     | 310 | CLA  | C3B-CAB | -2.06 | 1.43        | 1.47     |
| 2   | V     | 313 | CLA  | C4B-CHC | -2.05 | 1.35        | 1.41     |
| 2   | W     | 310 | CLA  | C3B-C2B | -2.05 | 1.37        | 1.40     |
| 5   | W     | 316 | Q6L  | C11-C03 | -2.05 | 1.48        | 1.51     |
| 2   | W     | 311 | CLA  | C4B-CHC | -2.05 | 1.35        | 1.41     |
| 6   | X     | 318 | IWJ  | C32-C30 | 2.05  | 1.55        | 1.51     |
| 2   | X     | 311 | CLA  | C3B-C2B | -2.05 | 1.37        | 1.40     |
| 2   | X     | 314 | CLA  | C4B-CHC | -2.04 | 1.35        | 1.41     |
| 5   | V     | 321 | Q6L  | C33-C32 | 2.04  | 1.35        | 1.33     |
| 2   | V     | 311 | CLA  | C4B-CHC | -2.04 | 1.35        | 1.41     |
| 2   | X     | 311 | CLA  | C4B-CHC | -2.04 | 1.35        | 1.41     |
| 2   | V     | 309 | CLA  | C4D-ND  | -2.04 | 1.34        | 1.37     |
| 2   | X     | 302 | CLA  | CMA-C3A | -2.04 | 1.48        | 1.53     |
| 7   | W     | 317 | NEX  | C22-C21 | -2.03 | 1.51        | 1.54     |
| 4   | W     | 308 | KC2  | C1A-NA  | 2.03  | 1.42        | 1.38     |
| 5   | W     | 315 | Q6L  | C33-C32 | 2.03  | 1.35        | 1.33     |
| 5   | W     | 320 | Q6L  | C33-C32 | 2.03  | 1.35        | 1.33     |
| 2   | V     | 302 | CLA  | MG-NC   | 2.02  | 2.11        | 2.06     |
| 6   | V     | 320 | IWJ  | C32-C30 | 2.02  | 1.55        | 1.51     |
| 2   | W     | 301 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 2   | W     | 313 | CLA  | C3B-C2B | -2.01 | 1.37        | 1.40     |
| 3   | X     | 307 | CHL  | O2A-CGA | 2.01  | 1.39        | 1.33     |
| 2   | X     | 310 | CLA  | C3B-C2B | -2.01 | 1.37        | 1.40     |
| 2   | V     | 312 | CLA  | MG-ND   | -2.01 | 2.01        | 2.05     |
| 3   | X     | 307 | CHL  | C4C-C3C | 2.01  | 1.48        | 1.45     |
| 2   | X     | 313 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 2   | X     | 304 | CLA  | C3B-CAB | -2.01 | 1.43        | 1.47     |

All (553) bond angle outliers are listed below:

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | W     | 317 | NEX  | O24-C25-C24 | 13.18 | 123.28      | 113.38   |
| 4   | X     | 309 | KC2  | CMA-C3A-C4A | -8.51 | 112.08      | 125.04   |
| 3   | X     | 307 | CHL  | C4A-NA-C1A  | 7.68  | 110.16      | 106.71   |
| 4   | W     | 308 | KC2  | C1A-C2A-C3A | -7.54 | 101.13      | 107.11   |
| 3   | X     | 307 | CHL  | OMC-CMC-C2C | -7.18 | 109.46      | 125.69   |
| 5   | W     | 320 | Q6L  | C11-C12-C13 | 6.89  | 132.26      | 112.69   |
| 3   | W     | 314 | CHL  | CMB-C2B-C1B | -6.79 | 118.03      | 128.46   |
| 4   | X     | 309 | KC2  | C1A-NA-C4A  | 6.72  | 109.73      | 106.71   |
| 5   | X     | 319 | Q6L  | C11-C12-C13 | 6.72  | 131.77      | 112.69   |
| 5   | V     | 316 | Q6L  | C11-C12-C13 | 6.53  | 131.23      | 112.69   |
| 5   | V     | 319 | Q6L  | C11-C12-C13 | 6.45  | 131.02      | 112.69   |
| 5   | V     | 321 | Q6L  | C11-C12-C13 | 6.44  | 130.98      | 112.69   |
| 2   | V     | 301 | CLA  | CMB-C2B-C1B | -6.40 | 118.63      | 128.46   |
| 2   | X     | 312 | CLA  | C4A-NA-C1A  | 6.37  | 109.57      | 106.71   |
| 3   | W     | 306 | CHL  | C4A-NA-C1A  | 6.32  | 109.55      | 106.71   |
| 3   | X     | 308 | CHL  | CMB-C2B-C1B | -6.32 | 118.75      | 128.46   |
| 2   | W     | 303 | CLA  | CMB-C2B-C1B | -6.31 | 118.77      | 128.46   |
| 5   | W     | 315 | Q6L  | C11-C12-C13 | 6.18  | 130.25      | 112.69   |
| 4   | V     | 308 | KC2  | C1A-C2A-C3A | -6.09 | 102.28      | 107.11   |
| 3   | W     | 305 | CHL  | C4A-NA-C1A  | 6.01  | 109.41      | 106.71   |
| 2   | W     | 312 | CLA  | C4A-NA-C1A  | 5.98  | 109.39      | 106.71   |
| 2   | X     | 304 | CLA  | CMB-C2B-C1B | -5.95 | 119.33      | 128.46   |
| 4   | W     | 308 | KC2  | C1A-NA-C4A  | 5.92  | 109.37      | 106.71   |
| 3   | W     | 306 | CHL  | CMB-C2B-C1B | -5.88 | 119.42      | 128.46   |
| 5   | X     | 301 | Q6L  | C11-C12-C13 | 5.87  | 129.37      | 112.69   |
| 3   | W     | 307 | CHL  | CMB-C2B-C1B | -5.85 | 119.48      | 128.46   |
| 2   | V     | 309 | CLA  | CMC-C2C-C1C | 5.73  | 133.77      | 125.04   |
| 4   | X     | 309 | KC2  | CMD-C2D-C1D | -5.69 | 119.72      | 128.46   |
| 2   | V     | 303 | CLA  | CMB-C2B-C1B | -5.60 | 119.86      | 128.46   |
| 2   | V     | 303 | CLA  | CAC-C3C-C4C | 5.53  | 131.98      | 124.81   |
| 3   | V     | 306 | CHL  | CMB-C2B-C1B | -5.49 | 120.03      | 128.46   |
| 5   | X     | 316 | Q6L  | C11-C12-C13 | 5.49  | 128.28      | 112.69   |
| 2   | X     | 314 | CLA  | C4A-NA-C1A  | 5.45  | 109.16      | 106.71   |
| 3   | V     | 314 | CHL  | CMB-C2B-C1B | -5.37 | 120.21      | 128.46   |
| 3   | V     | 306 | CHL  | C4A-NA-C1A  | 5.35  | 109.11      | 106.71   |
| 7   | W     | 317 | NEX  | C26-C27-C28 | -5.31 | 114.76      | 125.99   |
| 4   | W     | 308 | KC2  | CMA-C3A-C2A | -5.22 | 115.52      | 128.30   |
| 2   | W     | 311 | CLA  | C4A-NA-C1A  | 5.21  | 109.05      | 106.71   |
| 2   | V     | 311 | CLA  | C4A-NA-C1A  | 5.14  | 109.02      | 106.71   |
| 3   | W     | 306 | CHL  | C2C-C3C-C4C | 5.11  | 110.13      | 106.49   |
| 5   | X     | 317 | Q6L  | C11-C12-C13 | 5.06  | 127.06      | 112.69   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | V     | 301 | CLA  | CMB-C2B-C3B | 5.05  | 134.12      | 124.68   |
| 3   | W     | 314 | CHL  | CMB-C2B-C3B | 5.04  | 134.12      | 124.68   |
| 2   | W     | 312 | CLA  | CMB-C2B-C1B | -5.04 | 120.72      | 128.46   |
| 2   | V     | 312 | CLA  | C4A-NA-C1A  | 5.03  | 108.97      | 106.71   |
| 5   | W     | 316 | Q6L  | C11-C12-C13 | 5.03  | 126.98      | 112.69   |
| 4   | V     | 308 | KC2  | CMA-C3A-C2A | -5.03 | 115.99      | 128.30   |
| 2   | W     | 303 | CLA  | CMB-C2B-C3B | 5.02  | 134.08      | 124.68   |
| 3   | X     | 306 | CHL  | CMB-C2B-C1B | -5.01 | 120.76      | 128.46   |
| 2   | W     | 309 | CLA  | O2D-CGD-O1D | -5.00 | 114.07      | 123.84   |
| 4   | X     | 309 | KC2  | CMA-C3A-C2A | -4.93 | 116.24      | 128.30   |
| 3   | V     | 305 | CHL  | CMB-C2B-C1B | -4.90 | 120.94      | 128.46   |
| 2   | W     | 301 | CLA  | C4A-NA-C1A  | 4.83  | 108.88      | 106.71   |
| 5   | V     | 321 | Q6L  | C40-C32-C33 | -4.82 | 113.25      | 123.56   |
| 3   | X     | 308 | CHL  | CMB-C2B-C3B | 4.74  | 133.54      | 124.68   |
| 2   | V     | 313 | CLA  | C4A-NA-C1A  | 4.74  | 108.83      | 106.71   |
| 3   | V     | 305 | CHL  | C4A-NA-C1A  | 4.70  | 108.82      | 106.71   |
| 3   | X     | 306 | CHL  | CMA-C3A-C2A | -4.68 | 105.17      | 116.10   |
| 2   | V     | 303 | CLA  | CMB-C2B-C3B | 4.67  | 133.42      | 124.68   |
| 2   | W     | 311 | CLA  | CMB-C2B-C1B | -4.66 | 121.30      | 128.46   |
| 5   | V     | 315 | Q6L  | C11-C12-C13 | 4.66  | 125.93      | 112.69   |
| 5   | X     | 301 | Q6L  | C40-C32-C33 | -4.66 | 113.60      | 123.56   |
| 3   | W     | 305 | CHL  | CMB-C2B-C1B | -4.64 | 121.33      | 128.46   |
| 5   | W     | 319 | Q6L  | C11-C12-C13 | 4.60  | 125.76      | 112.69   |
| 5   | W     | 316 | Q6L  | C40-C32-C33 | -4.57 | 113.78      | 123.56   |
| 2   | W     | 313 | CLA  | C4A-NA-C1A  | 4.53  | 108.74      | 106.71   |
| 4   | W     | 308 | KC2  | CMA-C3A-C4A | -4.49 | 118.19      | 125.04   |
| 2   | X     | 313 | CLA  | CMB-C2B-C1B | -4.48 | 121.58      | 128.46   |
| 4   | X     | 309 | KC2  | C1A-C2A-C3A | -4.43 | 103.59      | 107.11   |
| 4   | V     | 308 | KC2  | CMD-C2D-C1D | -4.43 | 121.65      | 128.46   |
| 2   | X     | 313 | CLA  | C4A-NA-C1A  | 4.43  | 108.70      | 106.71   |
| 5   | W     | 320 | Q6L  | C40-C32-C33 | -4.42 | 114.10      | 123.56   |
| 3   | X     | 307 | CHL  | CHB-C4A-NA  | 4.40  | 130.59      | 124.51   |
| 2   | V     | 309 | CLA  | CMB-C2B-C1B | -4.39 | 121.72      | 128.46   |
| 3   | X     | 307 | CHL  | C2C-C3C-C4C | 4.37  | 109.61      | 106.49   |
| 2   | X     | 304 | CLA  | CMB-C2B-C3B | 4.36  | 132.83      | 124.68   |
| 6   | V     | 317 | IWJ  | C01-C02-C03 | -4.33 | 114.29      | 123.56   |
| 3   | X     | 306 | CHL  | CMA-C3A-C4A | 4.33  | 123.42      | 111.77   |
| 3   | W     | 304 | CHL  | C4A-NA-C1A  | 4.33  | 108.65      | 106.71   |
| 3   | X     | 307 | CHL  | C1-O2A-CGA  | 4.32  | 127.79      | 116.44   |
| 4   | V     | 308 | KC2  | C2A-C3A-C4A | -4.32 | 103.28      | 106.49   |
| 5   | V     | 316 | Q6L  | C40-C32-C33 | -4.32 | 114.32      | 123.56   |
| 2   | V     | 309 | CLA  | C1D-ND-C4D  | -4.28 | 103.30      | 106.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | X     | 310 | CLA  | CMB-C2B-C1B | -4.27 | 121.90      | 128.46   |
| 3   | W     | 306 | CHL  | CMB-C2B-C3B | 4.25  | 132.64      | 124.68   |
| 3   | W     | 307 | CHL  | CMB-C2B-C3B | 4.23  | 132.59      | 124.68   |
| 6   | W     | 318 | IWJ  | C01-C02-C03 | -4.22 | 114.54      | 123.56   |
| 6   | V     | 320 | IWJ  | C01-C02-C03 | -4.20 | 114.56      | 123.56   |
| 6   | V     | 318 | IWJ  | C01-C02-C03 | -4.20 | 114.57      | 123.56   |
| 3   | V     | 306 | CHL  | CMB-C2B-C3B | 4.20  | 132.54      | 124.68   |
| 6   | X     | 318 | IWJ  | C01-C02-C03 | -4.19 | 114.59      | 123.56   |
| 2   | V     | 309 | CLA  | CMB-C2B-C3B | 4.18  | 132.50      | 124.68   |
| 4   | X     | 309 | KC2  | C2A-C3A-C4A | -4.15 | 103.41      | 106.49   |
| 2   | V     | 309 | CLA  | O2D-CGD-O1D | -4.14 | 115.74      | 123.84   |
| 2   | W     | 301 | CLA  | C1B-CHB-C4A | -4.14 | 121.92      | 130.12   |
| 5   | X     | 317 | Q6L  | C40-C32-C33 | -4.13 | 114.72      | 123.56   |
| 2   | V     | 301 | CLA  | C4A-NA-C1A  | 4.12  | 108.56      | 106.71   |
| 4   | V     | 308 | KC2  | CMA-C3A-C4A | -4.11 | 118.78      | 125.04   |
| 3   | W     | 306 | CHL  | C1C-C2C-C3C | -4.11 | 103.85      | 107.11   |
| 3   | V     | 314 | CHL  | CMB-C2B-C3B | 4.08  | 132.30      | 124.68   |
| 2   | X     | 302 | CLA  | C1B-CHB-C4A | -4.05 | 122.09      | 130.12   |
| 3   | V     | 306 | CHL  | C1B-CHB-C4A | -4.04 | 122.11      | 130.12   |
| 5   | X     | 316 | Q6L  | C05-C04-C03 | 4.04  | 116.28      | 109.92   |
| 2   | V     | 301 | CLA  | C4-C3-C5    | 4.04  | 122.06      | 115.27   |
| 2   | W     | 311 | CLA  | CMB-C2B-C3B | 4.03  | 132.22      | 124.68   |
| 3   | X     | 307 | CHL  | CMB-C2B-C1B | -4.02 | 122.29      | 128.46   |
| 2   | V     | 312 | CLA  | CMB-C2B-C1B | -4.00 | 122.32      | 128.46   |
| 3   | X     | 307 | CHL  | C1C-C2C-C3C | -3.99 | 103.94      | 107.11   |
| 5   | X     | 319 | Q6L  | C05-C06-C07 | 3.98  | 115.75      | 110.30   |
| 3   | V     | 305 | CHL  | CMB-C2B-C3B | 3.98  | 132.12      | 124.68   |
| 4   | X     | 309 | KC2  | CMD-C2D-C3D | 3.97  | 132.11      | 124.68   |
| 5   | V     | 316 | Q6L  | C38-C36-C31 | -3.95 | 103.55      | 109.55   |
| 5   | X     | 316 | Q6L  | C34-C33-C32 | -3.94 | 121.07      | 124.85   |
| 3   | W     | 304 | CHL  | CMB-C2B-C1B | -3.93 | 122.43      | 128.46   |
| 2   | W     | 301 | CLA  | CHB-C4A-NA  | 3.92  | 129.94      | 124.51   |
| 2   | W     | 310 | CLA  | CMB-C2B-C1B | -3.91 | 122.45      | 128.46   |
| 2   | X     | 311 | CLA  | CMB-C2B-C1B | -3.91 | 122.46      | 128.46   |
| 2   | W     | 312 | CLA  | CMB-C2B-C3B | 3.90  | 131.97      | 124.68   |
| 7   | W     | 317 | NEX  | C38-C25-C26 | -3.88 | 115.77      | 122.26   |
| 2   | V     | 301 | CLA  | C1B-CHB-C4A | -3.87 | 122.45      | 130.12   |
| 2   | W     | 309 | CLA  | O2D-CGD-CBD | 3.87  | 118.14      | 111.27   |
| 5   | W     | 319 | Q6L  | C40-C32-C33 | -3.86 | 115.30      | 123.56   |
| 2   | W     | 313 | CLA  | CMB-C2B-C1B | -3.86 | 122.53      | 128.46   |
| 2   | W     | 310 | CLA  | C4A-NA-C1A  | 3.85  | 108.44      | 106.71   |
| 4   | W     | 308 | KC2  | CMD-C2D-C1D | -3.85 | 122.55      | 128.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | X     | 307 | CHL  | C3C-C4C-NC  | -3.81 | 106.30      | 110.57   |
| 5   | W     | 315 | Q6L  | C40-C32-C33 | -3.81 | 115.41      | 123.56   |
| 2   | W     | 309 | CLA  | C4-C3-C5    | 3.80  | 121.67      | 115.27   |
| 3   | V     | 304 | CHL  | C1B-CHB-C4A | -3.80 | 122.59      | 130.12   |
| 5   | W     | 320 | Q6L  | C38-C36-C35 | -3.79 | 102.26      | 109.44   |
| 3   | X     | 306 | CHL  | CMB-C2B-C3B | 3.78  | 131.75      | 124.68   |
| 3   | V     | 314 | CHL  | C1B-CHB-C4A | -3.77 | 122.65      | 130.12   |
| 3   | X     | 315 | CHL  | CMB-C2B-C1B | -3.77 | 122.67      | 128.46   |
| 3   | V     | 307 | CHL  | C4A-NA-C1A  | 3.76  | 108.40      | 106.71   |
| 6   | X     | 318 | IWJ  | C16-C15-C14 | -3.75 | 121.96      | 127.31   |
| 3   | W     | 306 | CHL  | C3C-C4C-NC  | -3.73 | 106.39      | 110.57   |
| 5   | X     | 319 | Q6L  | C40-C32-C33 | -3.72 | 115.61      | 123.56   |
| 7   | W     | 317 | NEX  | C39-C29-C30 | -3.69 | 117.75      | 122.92   |
| 5   | V     | 315 | Q6L  | C40-C32-C33 | -3.68 | 115.68      | 123.56   |
| 4   | V     | 308 | KC2  | CBA-CAA-C2A | -3.67 | 111.26      | 125.27   |
| 3   | W     | 307 | CHL  | C4A-NA-C1A  | 3.65  | 108.35      | 106.71   |
| 5   | X     | 317 | Q6L  | C19-C18-C17 | -3.63 | 122.13      | 127.31   |
| 4   | V     | 308 | KC2  | O2D-CGD-O1D | -3.63 | 116.74      | 123.84   |
| 2   | X     | 313 | CLA  | CMB-C2B-C3B | 3.58  | 131.37      | 124.68   |
| 2   | X     | 304 | CLA  | C4A-NA-C1A  | 3.57  | 108.31      | 106.71   |
| 2   | X     | 310 | CLA  | CMB-C2B-C3B | 3.55  | 131.31      | 124.68   |
| 2   | W     | 309 | CLA  | CMB-C2B-C1B | -3.54 | 123.02      | 128.46   |
| 4   | X     | 309 | KC2  | O2D-CGD-O1D | -3.54 | 116.92      | 123.84   |
| 3   | X     | 305 | CHL  | C1B-CHB-C4A | -3.54 | 123.11      | 130.12   |
| 7   | W     | 317 | NEX  | C28-C29-C30 | 3.53  | 124.36      | 118.94   |
| 3   | W     | 306 | CHL  | C1B-CHB-C4A | -3.52 | 123.14      | 130.12   |
| 3   | X     | 307 | CHL  | O2D-CGD-O1D | -3.52 | 116.95      | 123.84   |
| 4   | V     | 308 | KC2  | C3A-C4A-NA  | 3.48  | 114.37      | 110.57   |
| 2   | V     | 311 | CLA  | CMB-C2B-C1B | -3.47 | 123.13      | 128.46   |
| 2   | W     | 309 | CLA  | C4A-NA-C1A  | 3.46  | 108.26      | 106.71   |
| 3   | X     | 308 | CHL  | C4A-NA-C1A  | 3.44  | 108.25      | 106.71   |
| 3   | X     | 315 | CHL  | C1B-CHB-C4A | -3.43 | 123.32      | 130.12   |
| 3   | X     | 307 | CHL  | CAA-C2A-C3A | 3.43  | 122.17      | 112.78   |
| 2   | V     | 309 | CLA  | C1B-CHB-C4A | -3.42 | 123.33      | 130.12   |
| 3   | W     | 304 | CHL  | C1B-CHB-C4A | -3.42 | 123.34      | 130.12   |
| 2   | X     | 302 | CLA  | C4A-NA-C1A  | 3.40  | 108.23      | 106.71   |
| 4   | V     | 308 | KC2  | O2D-CGD-CBD | 3.40  | 117.30      | 111.27   |
| 2   | W     | 302 | CLA  | CMB-C2B-C1B | -3.39 | 123.25      | 128.46   |
| 2   | V     | 302 | CLA  | CMB-C2B-C1B | -3.39 | 123.26      | 128.46   |
| 2   | X     | 312 | CLA  | CMB-C2B-C1B | -3.38 | 123.26      | 128.46   |
| 2   | W     | 302 | CLA  | C4A-NA-C1A  | 3.37  | 108.22      | 106.71   |
| 3   | X     | 305 | CHL  | CMB-C2B-C1B | -3.37 | 123.28      | 128.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | X     | 307 | CHL  | O2D-CGD-CBD | 3.37  | 117.25      | 111.27   |
| 3   | X     | 307 | CHL  | C1B-CHB-C4A | -3.37 | 123.45      | 130.12   |
| 5   | X     | 316 | Q6L  | C25-C26-C27 | 3.36  | 132.10      | 127.31   |
| 4   | W     | 308 | KC2  | O2D-CGD-O1D | -3.36 | 117.28      | 123.84   |
| 3   | V     | 307 | CHL  | CHB-C4A-NA  | 3.35  | 129.15      | 124.51   |
| 2   | V     | 309 | CLA  | O2D-CGD-CBD | 3.34  | 117.20      | 111.27   |
| 2   | X     | 310 | CLA  | C4A-NA-C1A  | 3.34  | 108.21      | 106.71   |
| 2   | W     | 303 | CLA  | C1B-CHB-C4A | -3.34 | 123.51      | 130.12   |
| 2   | W     | 302 | CLA  | C1B-CHB-C4A | -3.33 | 123.51      | 130.12   |
| 3   | W     | 306 | CHL  | CHB-C4A-NA  | 3.32  | 129.11      | 124.51   |
| 2   | X     | 310 | CLA  | O2D-CGD-O1D | -3.31 | 117.36      | 123.84   |
| 5   | W     | 320 | Q6L  | C35-C34-C33 | 3.31  | 115.51      | 111.74   |
| 2   | W     | 310 | CLA  | CMB-C2B-C3B | 3.29  | 130.84      | 124.68   |
| 3   | X     | 307 | CHL  | C2D-C1D-ND  | -3.29 | 107.68      | 110.10   |
| 2   | X     | 303 | CLA  | C1B-CHB-C4A | -3.28 | 123.62      | 130.12   |
| 3   | W     | 304 | CHL  | O2D-CGD-O1D | -3.28 | 117.43      | 123.84   |
| 2   | V     | 310 | CLA  | CMB-C2B-C1B | -3.27 | 123.44      | 128.46   |
| 2   | X     | 311 | CLA  | CMB-C2B-C3B | 3.25  | 130.76      | 124.68   |
| 4   | V     | 308 | KC2  | CHB-C4A-C3A | -3.25 | 119.90      | 124.98   |
| 2   | V     | 302 | CLA  | O2D-CGD-O1D | -3.24 | 117.51      | 123.84   |
| 7   | W     | 317 | NEX  | C15-C35-C34 | -3.23 | 116.85      | 123.47   |
| 2   | X     | 311 | CLA  | C4A-NA-C1A  | 3.23  | 108.16      | 106.71   |
| 2   | V     | 301 | CLA  | O2D-CGD-O1D | -3.22 | 117.53      | 123.84   |
| 2   | W     | 303 | CLA  | O2D-CGD-O1D | -3.22 | 117.55      | 123.84   |
| 3   | V     | 306 | CHL  | O2D-CGD-O1D | -3.21 | 117.56      | 123.84   |
| 2   | X     | 302 | CLA  | CMB-C2B-C3B | 3.21  | 130.68      | 124.68   |
| 2   | W     | 312 | CLA  | C1D-ND-C4D  | -3.21 | 104.06      | 106.33   |
| 3   | V     | 304 | CHL  | CHB-C4A-NA  | 3.20  | 128.94      | 124.51   |
| 2   | X     | 314 | CLA  | CMB-C2B-C1B | -3.19 | 123.56      | 128.46   |
| 2   | V     | 302 | CLA  | C1B-CHB-C4A | -3.18 | 123.81      | 130.12   |
| 2   | V     | 312 | CLA  | C1B-CHB-C4A | -3.18 | 123.83      | 130.12   |
| 2   | W     | 309 | CLA  | C1B-CHB-C4A | -3.17 | 123.83      | 130.12   |
| 2   | V     | 309 | CLA  | C3A-C2A-C1A | -3.17 | 96.59       | 101.34   |
| 2   | V     | 309 | CLA  | CHD-C1D-ND  | -3.16 | 121.55      | 124.45   |
| 3   | V     | 305 | CHL  | C1B-CHB-C4A | -3.16 | 123.86      | 130.12   |
| 3   | W     | 306 | CHL  | O2D-CGD-O1D | -3.16 | 117.67      | 123.84   |
| 3   | X     | 307 | CHL  | CHD-C4C-C3C | 3.16  | 129.48      | 124.84   |
| 3   | W     | 314 | CHL  | C4A-NA-C1A  | 3.15  | 108.12      | 106.71   |
| 2   | W     | 313 | CLA  | CMB-C2B-C3B | 3.14  | 130.56      | 124.68   |
| 3   | W     | 314 | CHL  | C1B-CHB-C4A | -3.14 | 123.91      | 130.12   |
| 2   | V     | 312 | CLA  | O2A-CGA-O1A | -3.13 | 115.69      | 123.59   |
| 3   | X     | 306 | CHL  | O2D-CGD-O1D | -3.10 | 117.78      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | V     | 314 | CHL  | C4A-NA-C1A  | 3.10  | 108.10      | 106.71   |
| 2   | V     | 310 | CLA  | C1B-CHB-C4A | -3.09 | 124.00      | 130.12   |
| 3   | W     | 305 | CHL  | CMB-C2B-C3B | 3.08  | 130.44      | 124.68   |
| 5   | X     | 319 | Q6L  | C42-C13-C12 | 3.08  | 120.45      | 115.27   |
| 4   | W     | 308 | KC2  | C3C-C2C-C1C | 3.08  | 108.77      | 106.49   |
| 2   | X     | 302 | CLA  | C4D-CHA-C1A | 3.08  | 124.99      | 121.25   |
| 2   | X     | 310 | CLA  | C1B-CHB-C4A | -3.08 | 124.02      | 130.12   |
| 2   | W     | 301 | CLA  | CMB-C2B-C3B | 3.07  | 130.43      | 124.68   |
| 2   | X     | 312 | CLA  | O2D-CGD-O1D | -3.07 | 117.83      | 123.84   |
| 3   | W     | 314 | CHL  | CBD-CHA-C1A | 3.07  | 132.12      | 128.50   |
| 5   | V     | 319 | Q6L  | C28-C27-C26 | 3.06  | 127.21      | 122.92   |
| 2   | V     | 302 | CLA  | C1-C2-C3    | -3.06 | 121.80      | 126.75   |
| 2   | V     | 311 | CLA  | CMB-C2B-C3B | 3.06  | 130.40      | 124.68   |
| 2   | V     | 303 | CLA  | O2D-CGD-O1D | -3.06 | 117.86      | 123.84   |
| 3   | X     | 307 | CHL  | CAC-C3C-C4C | 3.06  | 128.78      | 124.81   |
| 2   | V     | 303 | CLA  | CAC-C3C-C2C | -3.05 | 122.31      | 127.53   |
| 2   | V     | 312 | CLA  | CMB-C2B-C3B | 3.04  | 130.37      | 124.68   |
| 3   | X     | 307 | CHL  | O2A-CGA-O1A | -3.04 | 115.92      | 123.59   |
| 2   | X     | 304 | CLA  | O2D-CGD-O1D | -3.04 | 117.90      | 123.84   |
| 3   | X     | 308 | CHL  | C1B-CHB-C4A | -3.03 | 124.11      | 130.12   |
| 3   | V     | 304 | CHL  | CMB-C2B-C1B | -3.02 | 123.82      | 128.46   |
| 2   | W     | 312 | CLA  | CAC-C3C-C4C | 3.02  | 128.72      | 124.81   |
| 2   | V     | 301 | CLA  | CAA-C2A-C1A | -3.02 | 102.09      | 111.97   |
| 2   | V     | 313 | CLA  | CMB-C2B-C1B | -3.01 | 123.83      | 128.46   |
| 4   | W     | 308 | KC2  | CMD-C2D-C3D | 3.01  | 130.31      | 124.68   |
| 2   | W     | 303 | CLA  | C1-C2-C3    | -3.00 | 121.89      | 126.75   |
| 4   | X     | 309 | KC2  | CAA-C2A-C1A | -3.00 | 110.96      | 124.75   |
| 3   | W     | 305 | CHL  | C1C-C2C-C3C | -3.00 | 104.73      | 107.11   |
| 2   | W     | 309 | CLA  | CMB-C2B-C3B | 3.00  | 130.29      | 124.68   |
| 2   | V     | 302 | CLA  | C4A-NA-C1A  | 2.99  | 108.05      | 106.71   |
| 3   | V     | 305 | CHL  | CHB-C4A-NA  | 2.98  | 128.64      | 124.51   |
| 2   | W     | 310 | CLA  | C1B-CHB-C4A | -2.98 | 124.22      | 130.12   |
| 5   | V     | 319 | Q6L  | C26-C25-C24 | -2.97 | 113.94      | 123.22   |
| 3   | V     | 307 | CHL  | C2C-C3C-C4C | 2.96  | 108.60      | 106.49   |
| 2   | W     | 312 | CLA  | C1B-CHB-C4A | -2.95 | 124.27      | 130.12   |
| 2   | V     | 311 | CLA  | CHB-C4A-NA  | 2.95  | 128.59      | 124.51   |
| 2   | X     | 303 | CLA  | O2D-CGD-O1D | -2.95 | 118.08      | 123.84   |
| 2   | V     | 303 | CLA  | CHD-C1D-ND  | -2.94 | 121.75      | 124.45   |
| 4   | W     | 308 | KC2  | CAC-C3C-C2C | -2.93 | 118.96      | 128.60   |
| 2   | V     | 311 | CLA  | O2D-CGD-O1D | -2.92 | 118.12      | 123.84   |
| 7   | W     | 317 | NEX  | C16-C1-C6   | 2.92  | 113.09      | 110.47   |
| 5   | X     | 319 | Q6L  | C12-C13-C14 | -2.92 | 113.14      | 121.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | V     | 304 | CHL  | O2A-CGA-O1A | -2.91 | 116.06      | 123.30   |
| 3   | X     | 306 | CHL  | C4A-NA-C1A  | 2.90  | 108.01      | 106.71   |
| 2   | V     | 303 | CLA  | C1B-CHB-C4A | -2.90 | 124.38      | 130.12   |
| 5   | V     | 319 | Q6L  | C40-C32-C33 | -2.90 | 117.36      | 123.56   |
| 3   | V     | 305 | CHL  | O2D-CGD-O1D | -2.89 | 118.18      | 123.84   |
| 2   | X     | 313 | CLA  | C1B-CHB-C4A | -2.89 | 124.39      | 130.12   |
| 4   | W     | 308 | KC2  | CBA-CAA-C2A | -2.89 | 114.25      | 125.27   |
| 5   | W     | 320 | Q6L  | C01-C02-C07 | -2.89 | 109.00      | 114.36   |
| 5   | X     | 301 | Q6L  | C19-C18-C17 | -2.89 | 123.19      | 127.31   |
| 2   | W     | 302 | CLA  | CMB-C2B-C3B | 2.88  | 130.07      | 124.68   |
| 4   | W     | 308 | KC2  | CMC-C2C-C1C | 2.88  | 129.43      | 125.04   |
| 3   | V     | 307 | CHL  | C1B-CHB-C4A | -2.88 | 124.42      | 130.12   |
| 3   | X     | 307 | CHL  | CMB-C2B-C3B | 2.88  | 130.06      | 124.68   |
| 3   | V     | 304 | CHL  | CMB-C2B-C3B | 2.87  | 130.05      | 124.68   |
| 7   | W     | 317 | NEX  | C19-C9-C10  | 2.87  | 126.94      | 122.92   |
| 2   | X     | 311 | CLA  | C1B-CHB-C4A | -2.86 | 124.45      | 130.12   |
| 3   | W     | 314 | CHL  | O2D-CGD-O1D | -2.86 | 118.25      | 123.84   |
| 2   | V     | 312 | CLA  | CHB-C4A-NA  | 2.86  | 128.46      | 124.51   |
| 3   | W     | 307 | CHL  | CHB-C4A-NA  | 2.86  | 128.46      | 124.51   |
| 3   | V     | 306 | CHL  | CHB-C4A-NA  | 2.86  | 128.46      | 124.51   |
| 5   | V     | 319 | Q6L  | C29-C27-C26 | -2.85 | 114.57      | 118.94   |
| 2   | X     | 314 | CLA  | C1B-CHB-C4A | -2.84 | 124.49      | 130.12   |
| 2   | X     | 302 | CLA  | CMB-C2B-C1B | -2.83 | 124.11      | 128.46   |
| 7   | W     | 317 | NEX  | C15-C14-C13 | -2.83 | 123.27      | 127.31   |
| 5   | V     | 321 | Q6L  | C38-C36-C35 | -2.83 | 104.08      | 109.44   |
| 2   | V     | 313 | CLA  | CHD-C1D-ND  | -2.82 | 121.86      | 124.45   |
| 4   | X     | 309 | KC2  | CBD-CHA-C1A | 2.82  | 134.14      | 128.88   |
| 3   | V     | 305 | CHL  | C2D-C1D-ND  | -2.82 | 108.03      | 110.10   |
| 3   | X     | 308 | CHL  | O2D-CGD-O1D | -2.82 | 118.33      | 123.84   |
| 3   | W     | 305 | CHL  | CHB-C4A-NA  | 2.80  | 128.38      | 124.51   |
| 4   | V     | 308 | KC2  | CAC-C3C-C2C | -2.79 | 119.40      | 128.60   |
| 4   | X     | 309 | KC2  | CBA-CAA-C2A | -2.79 | 114.62      | 125.27   |
| 3   | X     | 308 | CHL  | C2A-C1A-CHA | 2.79  | 128.74      | 123.86   |
| 2   | W     | 313 | CLA  | C1B-CHB-C4A | -2.79 | 124.59      | 130.12   |
| 5   | X     | 319 | Q6L  | C35-C34-C33 | 2.79  | 114.92      | 111.74   |
| 5   | X     | 301 | Q6L  | C19-C20-C21 | -2.79 | 117.76      | 123.47   |
| 5   | W     | 316 | Q6L  | C41-C17-C18 | 2.79  | 126.83      | 122.92   |
| 2   | W     | 310 | CLA  | O2D-CGD-O1D | -2.79 | 118.39      | 123.84   |
| 3   | W     | 305 | CHL  | C2C-C3C-C4C | 2.78  | 108.47      | 106.49   |
| 3   | W     | 307 | CHL  | C1B-CHB-C4A | -2.78 | 124.61      | 130.12   |
| 5   | X     | 317 | Q6L  | C19-C20-C21 | -2.78 | 117.78      | 123.47   |
| 5   | W     | 316 | Q6L  | C19-C20-C21 | -2.78 | 117.78      | 123.47   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | W     | 311 | CLA  | CHB-C4A-NA  | 2.77  | 128.35      | 124.51   |
| 2   | V     | 303 | CLA  | CHB-C4A-NA  | 2.77  | 128.34      | 124.51   |
| 3   | V     | 314 | CHL  | O2D-CGD-O1D | -2.77 | 118.42      | 123.84   |
| 5   | V     | 319 | Q6L  | C19-C20-C21 | -2.77 | 117.80      | 123.47   |
| 2   | V     | 302 | CLA  | O2D-CGD-CBD | 2.77  | 116.18      | 111.27   |
| 2   | X     | 313 | CLA  | CHB-C4A-NA  | 2.76  | 128.33      | 124.51   |
| 5   | V     | 319 | Q6L  | C42-C13-C12 | 2.76  | 119.91      | 115.27   |
| 2   | X     | 312 | CLA  | CMB-C2B-C3B | 2.76  | 129.84      | 124.68   |
| 2   | V     | 310 | CLA  | O2D-CGD-O1D | -2.76 | 118.45      | 123.84   |
| 3   | X     | 306 | CHL  | C1B-CHB-C4A | -2.75 | 124.66      | 130.12   |
| 3   | V     | 307 | CHL  | C3C-C4C-NC  | -2.75 | 107.49      | 110.57   |
| 2   | V     | 313 | CLA  | O2D-CGD-O1D | -2.75 | 118.47      | 123.84   |
| 3   | X     | 307 | CHL  | O2A-CGA-CBA | 2.74  | 120.51      | 111.91   |
| 2   | V     | 313 | CLA  | C1B-CHB-C4A | -2.74 | 124.69      | 130.12   |
| 2   | W     | 303 | CLA  | CHD-C1D-ND  | -2.74 | 121.94      | 124.45   |
| 3   | W     | 305 | CHL  | C1B-CHB-C4A | -2.74 | 124.70      | 130.12   |
| 2   | W     | 301 | CLA  | CMB-C2B-C1B | -2.73 | 124.27      | 128.46   |
| 4   | X     | 309 | KC2  | CAA-CBA-CGA | -2.73 | 113.23      | 127.26   |
| 2   | X     | 311 | CLA  | O2D-CGD-O1D | -2.73 | 118.51      | 123.84   |
| 2   | X     | 314 | CLA  | CHD-C1D-ND  | -2.73 | 121.95      | 124.45   |
| 2   | V     | 302 | CLA  | CMB-C2B-C3B | 2.72  | 129.76      | 124.68   |
| 2   | W     | 302 | CLA  | CHB-C4A-NA  | 2.72  | 128.27      | 124.51   |
| 2   | X     | 313 | CLA  | O2D-CGD-O1D | -2.71 | 118.53      | 123.84   |
| 3   | V     | 304 | CHL  | O2D-CGD-O1D | -2.71 | 118.54      | 123.84   |
| 4   | W     | 308 | KC2  | CAA-CBA-CGA | -2.71 | 113.34      | 127.26   |
| 3   | W     | 304 | CHL  | CHB-C4A-NA  | 2.71  | 128.26      | 124.51   |
| 6   | V     | 318 | IWJ  | O27-C26-C28 | -2.70 | 116.17      | 121.66   |
| 2   | W     | 311 | CLA  | O2D-CGD-O1D | -2.70 | 118.55      | 123.84   |
| 2   | W     | 312 | CLA  | C4-C3-C5    | 2.70  | 119.82      | 115.27   |
| 3   | V     | 306 | CHL  | C2D-C1D-ND  | -2.70 | 108.11      | 110.10   |
| 4   | V     | 308 | KC2  | CMD-C2D-C3D | 2.70  | 129.73      | 124.68   |
| 2   | W     | 303 | CLA  | CED-O2D-CGD | -2.69 | 109.84      | 115.94   |
| 5   | W     | 319 | Q6L  | C05-C06-C07 | 2.69  | 113.99      | 110.30   |
| 2   | W     | 310 | CLA  | CHB-C4A-NA  | 2.69  | 128.22      | 124.51   |
| 5   | W     | 319 | Q6L  | C42-C13-C12 | 2.68  | 119.79      | 115.27   |
| 2   | V     | 310 | CLA  | C4A-NA-C1A  | 2.68  | 107.91      | 106.71   |
| 4   | V     | 308 | KC2  | O2A-CGA-O1A | -2.68 | 117.10      | 122.67   |
| 3   | X     | 315 | CHL  | O2D-CGD-O1D | -2.67 | 118.61      | 123.84   |
| 3   | W     | 305 | CHL  | CMA-C3A-C2A | -2.67 | 109.87      | 116.10   |
| 2   | W     | 302 | CLA  | CHD-C1D-ND  | -2.66 | 122.01      | 124.45   |
| 2   | X     | 303 | CLA  | CHD-C1D-ND  | -2.66 | 122.01      | 124.45   |
| 4   | W     | 308 | KC2  | CMC-C2C-C3C | -2.65 | 121.80      | 128.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | W     | 301 | CLA  | C4-C3-C5    | 2.65  | 119.73      | 115.27   |
| 2   | W     | 312 | CLA  | CBC-CAC-C3C | 2.65  | 119.74      | 112.43   |
| 6   | W     | 318 | IWJ  | C21-C19-C18 | -2.65 | 114.88      | 118.94   |
| 2   | X     | 310 | CLA  | CHB-C4A-NA  | 2.65  | 128.18      | 124.51   |
| 3   | V     | 306 | CHL  | O2D-CGD-CBD | 2.65  | 115.97      | 111.27   |
| 5   | W     | 315 | Q6L  | C42-C13-C12 | 2.65  | 119.72      | 115.27   |
| 4   | X     | 309 | KC2  | CAC-C3C-C2C | -2.65 | 119.89      | 128.60   |
| 5   | V     | 315 | Q6L  | C24-C22-C21 | -2.64 | 114.90      | 118.94   |
| 2   | W     | 312 | CLA  | CHB-C4A-NA  | 2.63  | 128.15      | 124.51   |
| 3   | W     | 307 | CHL  | C4-C3-C2    | -2.63 | 116.92      | 123.68   |
| 3   | V     | 307 | CHL  | CHD-C1D-ND  | -2.63 | 122.04      | 124.45   |
| 2   | V     | 309 | CLA  | CHB-C4A-NA  | 2.63  | 128.15      | 124.51   |
| 3   | V     | 314 | CHL  | C1D-CHD-C4C | -2.63 | 120.39      | 126.06   |
| 6   | V     | 318 | IWJ  | C22-C21-C19 | 2.62  | 133.77      | 126.42   |
| 2   | X     | 303 | CLA  | C4A-NA-C1A  | 2.62  | 107.88      | 106.71   |
| 2   | W     | 309 | CLA  | CHB-C4A-NA  | 2.61  | 128.12      | 124.51   |
| 3   | X     | 305 | CHL  | O2D-CGD-O1D | -2.61 | 118.74      | 123.84   |
| 3   | W     | 307 | CHL  | C1-C2-C3    | -2.60 | 121.54      | 126.04   |
| 2   | V     | 310 | CLA  | CMB-C2B-C3B | 2.60  | 129.54      | 124.68   |
| 2   | X     | 302 | CLA  | CHB-C4A-NA  | 2.59  | 128.10      | 124.51   |
| 2   | W     | 303 | CLA  | C4A-NA-C1A  | 2.59  | 107.87      | 106.71   |
| 3   | X     | 306 | CHL  | CAA-C2A-C3A | -2.59 | 110.05      | 116.10   |
| 4   | X     | 309 | KC2  | O1A-CGA-CBA | 2.59  | 129.08      | 120.99   |
| 2   | X     | 304 | CLA  | C1B-CHB-C4A | -2.58 | 125.00      | 130.12   |
| 3   | W     | 306 | CHL  | C1-C2-C3    | -2.58 | 121.59      | 126.04   |
| 5   | V     | 321 | Q6L  | C01-C02-C07 | -2.57 | 109.59      | 114.36   |
| 5   | W     | 315 | Q6L  | C12-C13-C14 | -2.57 | 114.19      | 121.98   |
| 5   | X     | 319 | Q6L  | C01-C02-C07 | -2.57 | 109.59      | 114.36   |
| 4   | X     | 309 | KC2  | C4C-C3C-C2C | -2.56 | 105.08      | 107.11   |
| 2   | V     | 311 | CLA  | C1B-CHB-C4A | -2.56 | 125.05      | 130.12   |
| 7   | W     | 317 | NEX  | C31-C30-C29 | -2.55 | 123.66      | 127.31   |
| 4   | W     | 308 | KC2  | O1A-CGA-CBA | 2.55  | 128.97      | 120.99   |
| 2   | W     | 312 | CLA  | C2C-C1C-NC  | 2.55  | 112.36      | 109.97   |
| 2   | X     | 310 | CLA  | CHD-C1D-ND  | -2.55 | 122.11      | 124.45   |
| 2   | X     | 302 | CLA  | O2A-CGA-O1A | -2.54 | 117.18      | 123.59   |
| 2   | W     | 313 | CLA  | CHD-C1D-ND  | -2.54 | 122.12      | 124.45   |
| 3   | V     | 307 | CHL  | C1C-C2C-C3C | -2.54 | 105.10      | 107.11   |
| 2   | V     | 309 | CLA  | CMC-C2C-C3C | -2.54 | 119.23      | 126.12   |
| 2   | V     | 310 | CLA  | CHB-C4A-NA  | 2.53  | 128.02      | 124.51   |
| 3   | X     | 305 | CHL  | CHD-C1D-ND  | -2.53 | 122.12      | 124.45   |
| 5   | V     | 315 | Q6L  | C35-C34-C33 | 2.53  | 114.62      | 111.74   |
| 3   | X     | 305 | CHL  | C4A-NA-C1A  | 2.53  | 107.84      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | W     | 305 | CHL  | O2D-CGD-O1D | -2.52 | 118.91      | 123.84   |
| 2   | V     | 301 | CLA  | CHB-C4A-NA  | 2.52  | 127.99      | 124.51   |
| 4   | V     | 308 | KC2  | CAA-CBA-CGA | -2.51 | 114.36      | 127.26   |
| 5   | V     | 315 | Q6L  | C19-C20-C21 | -2.50 | 118.35      | 123.47   |
| 5   | V     | 316 | Q6L  | C01-C02-C07 | -2.50 | 109.72      | 114.36   |
| 4   | X     | 309 | KC2  | O2D-CGD-CBD | 2.50  | 115.71      | 111.27   |
| 2   | X     | 312 | CLA  | CHB-C4A-NA  | 2.50  | 127.97      | 124.51   |
| 5   | V     | 316 | Q6L  | C37-C36-C31 | 2.49  | 113.32      | 109.55   |
| 2   | W     | 312 | CLA  | O2D-CGD-O1D | -2.49 | 118.97      | 123.84   |
| 3   | W     | 304 | CHL  | CMB-C2B-C3B | 2.49  | 129.34      | 124.68   |
| 5   | X     | 317 | Q6L  | C05-C06-C07 | 2.49  | 113.71      | 110.30   |
| 2   | X     | 302 | CLA  | O1D-CGD-CBD | 2.48  | 129.57      | 124.48   |
| 2   | W     | 302 | CLA  | O2D-CGD-O1D | -2.48 | 118.99      | 123.84   |
| 5   | V     | 319 | Q6L  | C12-C13-C14 | -2.48 | 114.48      | 121.98   |
| 6   | W     | 318 | IWJ  | C17-C18-C19 | 2.47  | 130.84      | 127.31   |
| 2   | X     | 314 | CLA  | O2D-CGD-O1D | -2.47 | 119.02      | 123.84   |
| 3   | V     | 307 | CHL  | O2D-CGD-O1D | -2.46 | 119.02      | 123.84   |
| 3   | W     | 307 | CHL  | O2D-CGD-O1D | -2.45 | 119.05      | 123.84   |
| 2   | V     | 311 | CLA  | C2A-C1A-CHA | 2.44  | 128.13      | 123.86   |
| 5   | V     | 319 | Q6L  | C24-C22-C21 | -2.44 | 115.19      | 118.94   |
| 3   | X     | 308 | CHL  | CHB-C4A-NA  | 2.44  | 127.89      | 124.51   |
| 2   | X     | 312 | CLA  | C1B-CHB-C4A | -2.44 | 125.29      | 130.12   |
| 6   | V     | 318 | IWJ  | C36-C35-C34 | -2.43 | 104.75      | 108.98   |
| 5   | W     | 319 | Q6L  | C06-C07-C02 | 2.43  | 116.70      | 111.85   |
| 2   | X     | 313 | CLA  | CAA-C2A-C3A | -2.43 | 110.43      | 116.10   |
| 2   | X     | 314 | CLA  | CMB-C2B-C3B | 2.43  | 129.22      | 124.68   |
| 2   | V     | 312 | CLA  | O2D-CGD-O1D | -2.43 | 119.09      | 123.84   |
| 7   | W     | 317 | NEX  | C11-C10-C9  | -2.43 | 123.85      | 127.31   |
| 4   | W     | 308 | KC2  | CBD-CHA-C1A | 2.41  | 133.38      | 128.88   |
| 3   | V     | 306 | CHL  | C3C-C4C-NC  | -2.41 | 107.87      | 110.57   |
| 5   | W     | 319 | Q6L  | C12-C13-C14 | -2.41 | 114.69      | 121.98   |
| 3   | W     | 314 | CHL  | CHB-C4A-NA  | 2.40  | 127.84      | 124.51   |
| 4   | W     | 308 | KC2  | CAC-C3C-C4C | 2.40  | 135.66      | 124.47   |
| 4   | W     | 308 | KC2  | C4C-C3C-C2C | -2.40 | 105.21      | 107.11   |
| 7   | W     | 317 | NEX  | C32-C33-C34 | -2.39 | 115.27      | 118.94   |
| 2   | X     | 302 | CLA  | O2D-CGD-O1D | -2.39 | 119.17      | 123.84   |
| 2   | W     | 301 | CLA  | CHD-C1D-ND  | -2.38 | 122.26      | 124.45   |
| 4   | W     | 308 | KC2  | O2D-CGD-CBD | 2.38  | 115.50      | 111.27   |
| 3   | W     | 314 | CHL  | C2D-C1D-ND  | -2.38 | 108.35      | 110.10   |
| 2   | X     | 311 | CLA  | CHD-C1D-ND  | -2.37 | 122.27      | 124.45   |
| 3   | W     | 314 | CHL  | C2A-C1A-CHA | 2.37  | 126.38      | 122.71   |
| 3   | X     | 305 | CHL  | CHB-C4A-NA  | 2.37  | 127.78      | 124.51   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | V     | 308 | KC2  | O1A-CGA-CBA | 2.36  | 128.37      | 120.99   |
| 2   | V     | 313 | CLA  | CHB-C4A-NA  | 2.36  | 127.78      | 124.51   |
| 2   | V     | 313 | CLA  | CMB-C2B-C3B | 2.36  | 129.10      | 124.68   |
| 4   | V     | 308 | KC2  | CAA-C2A-C1A | -2.36 | 113.90      | 124.75   |
| 3   | W     | 306 | CHL  | CHD-C1D-ND  | -2.35 | 122.29      | 124.45   |
| 3   | W     | 306 | CHL  | CAA-C2A-C3A | 2.35  | 119.22      | 112.78   |
| 3   | X     | 315 | CHL  | CMB-C2B-C3B | 2.35  | 129.08      | 124.68   |
| 2   | V     | 310 | CLA  | C2C-C1C-NC  | 2.35  | 112.17      | 109.97   |
| 5   | W     | 319 | Q6L  | C19-C20-C21 | -2.35 | 118.66      | 123.47   |
| 5   | V     | 319 | Q6L  | C16-C17-C18 | -2.35 | 115.34      | 118.94   |
| 2   | X     | 312 | CLA  | O2A-CGA-O1A | -2.34 | 117.67      | 123.59   |
| 2   | X     | 314 | CLA  | CHB-C4A-NA  | 2.34  | 127.75      | 124.51   |
| 4   | V     | 308 | KC2  | OBD-CAD-CBD | -2.34 | 122.56      | 125.89   |
| 5   | V     | 319 | Q6L  | C23-C22-C21 | 2.34  | 126.20      | 122.92   |
| 6   | V     | 318 | IWJ  | C21-C19-C18 | -2.33 | 115.36      | 118.94   |
| 2   | X     | 302 | CLA  | CHD-C1D-ND  | -2.33 | 122.31      | 124.45   |
| 3   | W     | 304 | CHL  | CHD-C1D-ND  | -2.33 | 122.31      | 124.45   |
| 2   | X     | 303 | CLA  | CHB-C4A-NA  | 2.33  | 127.73      | 124.51   |
| 2   | X     | 314 | CLA  | CAA-C2A-C3A | -2.33 | 110.67      | 116.10   |
| 2   | X     | 310 | CLA  | O2D-CGD-CBD | 2.32  | 115.39      | 111.27   |
| 2   | W     | 311 | CLA  | C1B-CHB-C4A | -2.32 | 125.52      | 130.12   |
| 6   | W     | 318 | IWJ  | C25-C24-C26 | 2.32  | 119.92      | 116.02   |
| 3   | X     | 315 | CHL  | CHB-C4A-NA  | 2.31  | 127.70      | 124.51   |
| 5   | W     | 315 | Q6L  | C01-C02-C07 | -2.30 | 110.09      | 114.36   |
| 2   | V     | 301 | CLA  | C4-C3-C2    | -2.30 | 117.78      | 123.68   |
| 3   | W     | 306 | CHL  | O2D-CGD-CBD | 2.29  | 115.34      | 111.27   |
| 2   | W     | 310 | CLA  | O2A-CGA-O1A | -2.29 | 117.81      | 123.59   |
| 2   | W     | 310 | CLA  | CHD-C1D-ND  | -2.28 | 122.36      | 124.45   |
| 5   | X     | 316 | Q6L  | C29-C27-C26 | -2.28 | 115.44      | 118.94   |
| 2   | W     | 309 | CLA  | CHD-C1D-ND  | -2.28 | 122.36      | 124.45   |
| 2   | V     | 302 | CLA  | CAC-C3C-C4C | 2.27  | 127.76      | 124.81   |
| 2   | X     | 304 | CLA  | CHD-C1D-ND  | -2.27 | 122.37      | 124.45   |
| 4   | X     | 309 | KC2  | CAC-C3C-C4C | 2.26  | 135.01      | 124.47   |
| 3   | V     | 306 | CHL  | C2C-C3C-C4C | 2.26  | 108.10      | 106.49   |
| 6   | V     | 318 | IWJ  | C37-C35-C34 | -2.26 | 105.06      | 108.98   |
| 2   | W     | 301 | CLA  | O2A-C1-C2   | -2.25 | 102.71      | 108.64   |
| 2   | V     | 310 | CLA  | CHD-C1D-ND  | -2.25 | 122.39      | 124.45   |
| 2   | W     | 312 | CLA  | O2D-CGD-CBD | 2.24  | 115.25      | 111.27   |
| 3   | V     | 314 | CHL  | CHB-C4A-NA  | 2.24  | 127.61      | 124.51   |
| 2   | X     | 312 | CLA  | C5-C3-C2    | 2.24  | 126.04      | 120.50   |
| 2   | V     | 310 | CLA  | CAC-C3C-C4C | 2.23  | 127.71      | 124.81   |
| 2   | W     | 309 | CLA  | C6-C5-C3    | 2.23  | 119.31      | 113.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | X     | 313 | CLA  | CHD-C1D-ND  | -2.23 | 122.40      | 124.45   |
| 2   | V     | 302 | CLA  | CHB-C4A-NA  | 2.23  | 127.60      | 124.51   |
| 4   | V     | 308 | KC2  | C2A-C1A-NA  | 2.22  | 112.97      | 109.40   |
| 5   | X     | 316 | Q6L  | C28-C27-C26 | 2.22  | 126.03      | 122.92   |
| 6   | W     | 318 | IWJ  | C32-C30-C31 | 2.21  | 125.47      | 121.10   |
| 2   | V     | 309 | CLA  | C4A-NA-C1A  | 2.21  | 107.70      | 106.71   |
| 2   | V     | 302 | CLA  | C2C-C1C-NC  | 2.21  | 112.04      | 109.97   |
| 6   | W     | 318 | IWJ  | C36-C35-C34 | -2.21 | 105.15      | 108.98   |
| 2   | W     | 311 | CLA  | CHA-C1A-NA  | -2.20 | 121.35      | 126.40   |
| 2   | V     | 310 | CLA  | CMC-C2C-C1C | 2.20  | 128.39      | 125.04   |
| 5   | V     | 319 | Q6L  | C01-C02-C07 | -2.20 | 110.28      | 114.36   |
| 6   | V     | 318 | IWJ  | C23-C22-C21 | -2.20 | 116.35      | 123.22   |
| 2   | W     | 313 | CLA  | O2D-CGD-O1D | -2.20 | 119.54      | 123.84   |
| 5   | W     | 315 | Q6L  | C05-C06-C07 | 2.20  | 113.31      | 110.30   |
| 2   | V     | 311 | CLA  | CHD-C1D-ND  | -2.19 | 122.44      | 124.45   |
| 6   | X     | 318 | IWJ  | C23-C22-C21 | -2.19 | 116.37      | 123.22   |
| 2   | V     | 301 | CLA  | CHD-C1D-ND  | -2.19 | 122.44      | 124.45   |
| 2   | W     | 302 | CLA  | CAC-C3C-C4C | 2.18  | 127.64      | 124.81   |
| 2   | X     | 303 | CLA  | O2A-CGA-O1A | -2.18 | 118.09      | 123.59   |
| 2   | V     | 311 | CLA  | C1-C2-C3    | -2.17 | 122.29      | 126.04   |
| 4   | W     | 308 | KC2  | O2A-CGA-O1A | -2.17 | 118.17      | 122.67   |
| 2   | V     | 309 | CLA  | CAA-C2A-C3A | 2.17  | 119.67      | 114.26   |
| 3   | V     | 304 | CHL  | C4A-NA-C1A  | 2.16  | 107.68      | 106.71   |
| 3   | V     | 314 | CHL  | C2D-C1D-ND  | -2.16 | 108.51      | 110.10   |
| 4   | X     | 309 | KC2  | C3C-C2C-C1C | 2.16  | 108.09      | 106.49   |
| 2   | V     | 311 | CLA  | O2A-CGA-O1A | -2.16 | 118.15      | 123.59   |
| 4   | W     | 308 | KC2  | CAA-C2A-C1A | -2.15 | 114.84      | 124.75   |
| 3   | X     | 308 | CHL  | OMC-CMC-C2C | -2.15 | 120.82      | 125.69   |
| 2   | W     | 312 | CLA  | C3A-C2A-C1A | 2.15  | 104.56      | 101.34   |
| 3   | V     | 314 | CHL  | C1C-C2C-C3C | -2.15 | 105.41      | 107.11   |
| 3   | W     | 307 | CHL  | CBA-CAA-C2A | 2.14  | 120.19      | 113.86   |
| 5   | V     | 315 | Q6L  | C05-C06-C07 | 2.14  | 113.23      | 110.30   |
| 2   | X     | 304 | CLA  | CAC-C3C-C4C | 2.14  | 127.58      | 124.81   |
| 2   | W     | 303 | CLA  | C3A-C2A-C1A | 2.14  | 104.54      | 101.34   |
| 2   | X     | 304 | CLA  | CMA-C3A-C4A | -2.13 | 106.04      | 111.77   |
| 4   | X     | 309 | KC2  | CHB-C4A-C3A | -2.13 | 121.65      | 124.98   |
| 2   | X     | 302 | CLA  | CMC-C2C-C1C | 2.13  | 128.29      | 125.04   |
| 3   | X     | 305 | CHL  | CAA-C2A-C3A | -2.13 | 111.12      | 116.10   |
| 2   | W     | 309 | CLA  | C2D-C1D-ND  | -2.13 | 108.54      | 110.10   |
| 2   | W     | 309 | CLA  | C1-C2-C3    | -2.13 | 122.36      | 126.04   |
| 6   | V     | 320 | IWJ  | C22-C21-C19 | 2.13  | 132.39      | 126.42   |
| 3   | W     | 307 | CHL  | C5-C3-C2    | 2.12  | 125.42      | 121.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | W     | 311 | CLA  | C2A-C1A-CHA | 2.12  | 127.57      | 123.86   |
| 4   | V     | 308 | KC2  | CAC-C3C-C4C | 2.12  | 134.35      | 124.47   |
| 2   | V     | 312 | CLA  | O1D-CGD-CBD | 2.12  | 128.82      | 124.48   |
| 2   | W     | 303 | CLA  | CHB-C4A-NA  | 2.12  | 127.44      | 124.51   |
| 2   | W     | 313 | CLA  | CHB-C4A-NA  | 2.12  | 127.44      | 124.51   |
| 2   | W     | 301 | CLA  | CAA-C2A-C1A | -2.12 | 105.04      | 111.97   |
| 2   | X     | 302 | CLA  | CHA-C1A-NA  | -2.12 | 121.55      | 126.40   |
| 2   | V     | 301 | CLA  | C4D-CHA-C1A | 2.11  | 123.82      | 121.25   |
| 2   | X     | 312 | CLA  | CHD-C1D-ND  | -2.11 | 122.52      | 124.45   |
| 3   | X     | 308 | CHL  | C2A-C3A-C4A | -2.11 | 98.47       | 101.87   |
| 6   | V     | 318 | IWJ  | C34-C33-C32 | 2.10  | 113.18      | 110.30   |
| 3   | X     | 305 | CHL  | CMB-C2B-C3B | 2.10  | 128.61      | 124.68   |
| 6   | X     | 318 | IWJ  | C25-C24-C26 | 2.10  | 119.55      | 116.02   |
| 2   | V     | 309 | CLA  | C3D-C4D-ND  | 2.10  | 113.63      | 110.24   |
| 4   | X     | 309 | KC2  | C1B-CHB-C4A | 2.10  | 130.58      | 126.06   |
| 2   | X     | 312 | CLA  | C2A-C1A-CHA | 2.10  | 127.52      | 123.86   |
| 3   | W     | 314 | CHL  | OMC-CMC-C2C | -2.10 | 120.95      | 125.69   |
| 2   | V     | 313 | CLA  | O2A-CGA-O1A | -2.09 | 118.31      | 123.59   |
| 2   | X     | 313 | CLA  | CMA-C3A-C2A | -2.09 | 111.22      | 116.10   |
| 3   | V     | 306 | CHL  | C2A-C1A-CHA | 2.09  | 127.51      | 123.86   |
| 2   | W     | 309 | CLA  | CAA-CBA-CGA | -2.08 | 107.16      | 113.25   |
| 2   | V     | 311 | CLA  | CHA-C1A-NA  | -2.08 | 121.63      | 126.40   |
| 5   | W     | 315 | Q6L  | C19-C20-C21 | -2.08 | 119.21      | 123.47   |
| 2   | X     | 311 | CLA  | CHB-C4A-NA  | 2.07  | 127.38      | 124.51   |
| 2   | X     | 312 | CLA  | C4-C3-C2    | -2.07 | 118.38      | 123.68   |
| 3   | W     | 306 | CHL  | CHD-C4C-C3C | 2.06  | 127.87      | 124.84   |
| 7   | W     | 317 | NEX  | C40-C33-C32 | 2.06  | 121.33      | 118.08   |
| 2   | W     | 309 | CLA  | C5-C3-C2    | -2.06 | 116.96      | 121.12   |
| 2   | X     | 303 | CLA  | C2C-C1C-NC  | 2.05  | 111.89      | 109.97   |
| 2   | X     | 302 | CLA  | C4-C3-C2    | -2.05 | 118.42      | 123.68   |
| 6   | X     | 318 | IWJ  | C36-C35-C34 | -2.05 | 105.42      | 108.98   |
| 6   | X     | 318 | IWJ  | C22-C23-C24 | 2.04  | 132.61      | 126.61   |
| 6   | X     | 318 | IWJ  | C33-C32-C30 | 2.04  | 115.53      | 112.04   |
| 5   | X     | 301 | Q6L  | C24-C22-C21 | -2.04 | 115.82      | 118.94   |
| 2   | X     | 304 | CLA  | O2D-CGD-CBD | 2.03  | 114.88      | 111.27   |
| 3   | V     | 307 | CHL  | CMB-C2B-C1B | -2.03 | 125.35      | 128.46   |
| 2   | X     | 311 | CLA  | O2A-CGA-O1A | -2.03 | 118.48      | 123.59   |
| 5   | W     | 316 | Q6L  | C41-C17-C16 | -2.02 | 114.89      | 118.08   |
| 6   | V     | 317 | IWJ  | C33-C32-C30 | 2.02  | 115.49      | 112.04   |
| 2   | V     | 312 | CLA  | CBA-CAA-C2A | 2.02  | 119.82      | 113.86   |
| 2   | V     | 302 | CLA  | O2A-CGA-O1A | -2.02 | 118.50      | 123.59   |
| 3   | V     | 306 | CHL  | C1D-CHD-C4C | -2.02 | 121.71      | 126.06   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | X     | 310 | CLA  | C2D-C1D-ND  | -2.01 | 108.62      | 110.10   |
| 4   | X     | 309 | KC2  | O2A-CGA-O1A | -2.01 | 118.50      | 122.67   |
| 3   | V     | 314 | CHL  | CHA-C1A-NA  | -2.00 | 121.81      | 126.40   |
| 3   | X     | 308 | CHL  | O1D-CGD-CBD | 2.00  | 128.59      | 124.48   |
| 2   | W     | 303 | CLA  | O2A-CGA-O1A | -2.00 | 118.54      | 123.59   |
| 5   | W     | 316 | Q6L  | C29-C27-C26 | -2.00 | 115.87      | 118.94   |
| 3   | V     | 304 | CHL  | C2D-C1D-ND  | -2.00 | 108.63      | 110.10   |
| 3   | W     | 305 | CHL  | C3C-C4C-NC  | -2.00 | 108.33      | 110.57   |

All (68) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 2   | V     | 301 | CLA  | ND   |
| 2   | V     | 302 | CLA  | ND   |
| 2   | V     | 303 | CLA  | ND   |
| 2   | V     | 309 | CLA  | ND   |
| 2   | V     | 310 | CLA  | ND   |
| 2   | V     | 311 | CLA  | ND   |
| 2   | V     | 313 | CLA  | ND   |
| 2   | W     | 301 | CLA  | ND   |
| 2   | W     | 302 | CLA  | ND   |
| 2   | W     | 303 | CLA  | ND   |
| 2   | W     | 309 | CLA  | ND   |
| 2   | W     | 310 | CLA  | ND   |
| 2   | W     | 311 | CLA  | ND   |
| 2   | W     | 312 | CLA  | ND   |
| 2   | W     | 313 | CLA  | ND   |
| 2   | X     | 302 | CLA  | ND   |
| 2   | X     | 303 | CLA  | ND   |
| 2   | X     | 304 | CLA  | ND   |
| 2   | X     | 310 | CLA  | ND   |
| 2   | X     | 311 | CLA  | ND   |
| 2   | X     | 312 | CLA  | ND   |
| 2   | X     | 313 | CLA  | ND   |
| 2   | X     | 314 | CLA  | ND   |
| 3   | V     | 304 | CHL  | NA   |
| 3   | V     | 304 | CHL  | NC   |
| 3   | V     | 304 | CHL  | ND   |
| 3   | V     | 305 | CHL  | NA   |
| 3   | V     | 305 | CHL  | NC   |
| 3   | V     | 305 | CHL  | ND   |
| 3   | V     | 306 | CHL  | NA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 3   | V     | 306 | CHL  | NC   |
| 3   | V     | 306 | CHL  | ND   |
| 3   | V     | 307 | CHL  | NA   |
| 3   | V     | 307 | CHL  | NC   |
| 3   | V     | 307 | CHL  | ND   |
| 3   | V     | 314 | CHL  | NA   |
| 3   | V     | 314 | CHL  | NC   |
| 3   | V     | 314 | CHL  | ND   |
| 3   | W     | 304 | CHL  | NA   |
| 3   | W     | 304 | CHL  | NC   |
| 3   | W     | 304 | CHL  | ND   |
| 3   | W     | 305 | CHL  | NA   |
| 3   | W     | 305 | CHL  | NC   |
| 3   | W     | 305 | CHL  | ND   |
| 3   | W     | 306 | CHL  | NA   |
| 3   | W     | 306 | CHL  | NC   |
| 3   | W     | 306 | CHL  | ND   |
| 3   | W     | 307 | CHL  | NA   |
| 3   | W     | 307 | CHL  | NC   |
| 3   | W     | 307 | CHL  | ND   |
| 3   | W     | 314 | CHL  | NA   |
| 3   | W     | 314 | CHL  | NC   |
| 3   | W     | 314 | CHL  | ND   |
| 3   | X     | 305 | CHL  | NA   |
| 3   | X     | 305 | CHL  | NC   |
| 3   | X     | 305 | CHL  | ND   |
| 3   | X     | 306 | CHL  | NA   |
| 3   | X     | 306 | CHL  | NC   |
| 3   | X     | 306 | CHL  | ND   |
| 3   | X     | 307 | CHL  | NA   |
| 3   | X     | 307 | CHL  | NC   |
| 3   | X     | 307 | CHL  | ND   |
| 3   | X     | 308 | CHL  | NA   |
| 3   | X     | 308 | CHL  | NC   |
| 3   | X     | 308 | CHL  | ND   |
| 3   | X     | 315 | CHL  | NA   |
| 3   | X     | 315 | CHL  | NC   |
| 3   | X     | 315 | CHL  | ND   |

All (372) torsion outliers are listed below:

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
|-----|-------|-----|------|-------|

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | V     | 302 | CLA  | CHA-CBD-CGD-O1D |
| 2   | V     | 302 | CLA  | CHA-CBD-CGD-O2D |
| 2   | V     | 303 | CLA  | CBD-CGD-O2D-CED |
| 2   | V     | 312 | CLA  | C1A-C2A-CAA-CBA |
| 2   | V     | 312 | CLA  | C3A-C2A-CAA-CBA |
| 2   | V     | 312 | CLA  | CHA-CBD-CGD-O1D |
| 2   | V     | 312 | CLA  | CHA-CBD-CGD-O2D |
| 2   | W     | 301 | CLA  | C1A-C2A-CAA-CBA |
| 2   | X     | 303 | CLA  | C1A-C2A-CAA-CBA |
| 2   | X     | 303 | CLA  | C3A-C2A-CAA-CBA |
| 2   | X     | 304 | CLA  | CHA-CBD-CGD-O1D |
| 2   | X     | 304 | CLA  | CHA-CBD-CGD-O2D |
| 2   | X     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 2   | X     | 311 | CLA  | C3A-C2A-CAA-CBA |
| 2   | X     | 311 | CLA  | CBD-CGD-O2D-CED |
| 2   | X     | 312 | CLA  | CBD-CGD-O2D-CED |
| 2   | X     | 313 | CLA  | CBD-CGD-O2D-CED |
| 2   | X     | 314 | CLA  | CHA-CBD-CGD-O1D |
| 2   | X     | 314 | CLA  | CHA-CBD-CGD-O2D |
| 2   | X     | 314 | CLA  | CAD-CBD-CGD-O1D |
| 2   | X     | 314 | CLA  | CBD-CGD-O2D-CED |
| 3   | V     | 304 | CHL  | CHA-CBD-CGD-O1D |
| 3   | V     | 304 | CHL  | CHA-CBD-CGD-O2D |
| 3   | V     | 304 | CHL  | CBD-CGD-O2D-CED |
| 3   | V     | 305 | CHL  | C3C-C2C-CMC-OMC |
| 3   | W     | 307 | CHL  | C1A-C2A-CAA-CBA |
| 3   | W     | 314 | CHL  | C3C-C2C-CMC-OMC |
| 3   | W     | 314 | CHL  | CHA-CBD-CGD-O1D |
| 3   | W     | 314 | CHL  | CHA-CBD-CGD-O2D |
| 3   | X     | 307 | CHL  | C3A-C2A-CAA-CBA |
| 3   | X     | 307 | CHL  | CBA-CGA-O2A-C1  |
| 3   | X     | 307 | CHL  | O1A-CGA-O2A-C1  |
| 3   | X     | 307 | CHL  | C1C-C2C-CMC-OMC |
| 3   | X     | 307 | CHL  | C3C-C2C-CMC-OMC |
| 3   | X     | 307 | CHL  | O2A-C1-C2-C3    |
| 3   | X     | 308 | CHL  | C1A-C2A-CAA-CBA |
| 3   | X     | 308 | CHL  | CHA-CBD-CGD-O1D |
| 3   | X     | 308 | CHL  | CHA-CBD-CGD-O2D |
| 3   | X     | 308 | CHL  | CAD-CBD-CGD-O1D |
| 3   | X     | 308 | CHL  | CBD-CGD-O2D-CED |
| 3   | X     | 315 | CHL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | V     | 308 | KC2  | C3A-C2A-CAA-CBA |
| 4   | V     | 308 | KC2  | C2A-CAA-CBA-CGA |
| 4   | V     | 308 | KC2  | CHA-CBD-CGD-O1D |
| 4   | V     | 308 | KC2  | CHA-CBD-CGD-O2D |
| 4   | W     | 308 | KC2  | C3A-C2A-CAA-CBA |
| 4   | W     | 308 | KC2  | C2A-CAA-CBA-CGA |
| 4   | X     | 309 | KC2  | C1A-C2A-CAA-CBA |
| 4   | X     | 309 | KC2  | C3A-C2A-CAA-CBA |
| 4   | X     | 309 | KC2  | C2A-CAA-CBA-CGA |
| 5   | V     | 315 | Q6L  | C02-C03-C11-C12 |
| 5   | V     | 315 | Q6L  | C21-C22-C24-C25 |
| 5   | V     | 315 | Q6L  | C23-C22-C24-C25 |
| 5   | V     | 315 | Q6L  | C29-C30-C31-C32 |
| 5   | V     | 315 | Q6L  | C27-C29-C30-C31 |
| 5   | V     | 315 | Q6L  | C15-C16-C17-C18 |
| 5   | V     | 315 | Q6L  | C15-C16-C17-C41 |
| 5   | V     | 316 | Q6L  | C04-C03-C11-C12 |
| 5   | V     | 316 | Q6L  | C29-C30-C31-C36 |
| 5   | V     | 316 | Q6L  | C29-C30-C31-C32 |
| 5   | V     | 316 | Q6L  | C27-C29-C30-C31 |
| 5   | V     | 316 | Q6L  | C19-C20-C21-C22 |
| 5   | V     | 319 | Q6L  | C02-C03-C11-C12 |
| 5   | V     | 319 | Q6L  | C28-C27-C29-C30 |
| 5   | V     | 319 | Q6L  | C26-C27-C29-C30 |
| 5   | V     | 321 | Q6L  | C04-C03-C11-C12 |
| 5   | W     | 315 | Q6L  | C15-C16-C17-C18 |
| 5   | W     | 315 | Q6L  | C15-C16-C17-C41 |
| 5   | W     | 319 | Q6L  | C28-C27-C29-C30 |
| 5   | W     | 319 | Q6L  | C26-C27-C29-C30 |
| 5   | W     | 320 | Q6L  | C02-C03-C11-C12 |
| 5   | W     | 320 | Q6L  | C11-C12-C13-C14 |
| 5   | W     | 320 | Q6L  | C11-C12-C13-C42 |
| 5   | W     | 320 | Q6L  | C28-C27-C29-C30 |
| 5   | W     | 320 | Q6L  | C29-C30-C31-C36 |
| 5   | W     | 320 | Q6L  | C29-C30-C31-C32 |
| 5   | X     | 301 | Q6L  | C29-C30-C31-C32 |
| 5   | X     | 301 | Q6L  | C27-C29-C30-C31 |
| 5   | X     | 317 | Q6L  | C04-C03-C11-C12 |
| 5   | X     | 319 | Q6L  | C11-C12-C13-C14 |
| 5   | X     | 319 | Q6L  | C11-C12-C13-C42 |
| 5   | X     | 319 | Q6L  | C21-C22-C24-C25 |
| 5   | X     | 319 | Q6L  | C23-C22-C24-C25 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | X     | 319 | Q6L  | C28-C27-C29-C30 |
| 5   | X     | 319 | Q6L  | C26-C27-C29-C30 |
| 5   | X     | 319 | Q6L  | C29-C30-C31-C36 |
| 5   | X     | 319 | Q6L  | C29-C30-C31-C32 |
| 5   | X     | 319 | Q6L  | C27-C29-C30-C31 |
| 5   | X     | 319 | Q6L  | C24-C25-C26-C27 |
| 6   | V     | 317 | IWJ  | C18-C19-C21-C22 |
| 6   | V     | 317 | IWJ  | C20-C19-C21-C22 |
| 6   | V     | 317 | IWJ  | C26-C28-C29-C30 |
| 6   | V     | 317 | IWJ  | C26-C28-C29-C35 |
| 6   | V     | 317 | IWJ  | C26-C28-C29-O39 |
| 6   | V     | 318 | IWJ  | C26-C28-C29-C30 |
| 6   | V     | 318 | IWJ  | C26-C28-C29-C35 |
| 6   | V     | 318 | IWJ  | C26-C28-C29-O39 |
| 6   | V     | 320 | IWJ  | C26-C28-C29-C30 |
| 6   | V     | 320 | IWJ  | C26-C28-C29-C35 |
| 6   | V     | 320 | IWJ  | C26-C28-C29-O39 |
| 6   | W     | 318 | IWJ  | C18-C19-C21-C22 |
| 6   | W     | 318 | IWJ  | C20-C19-C21-C22 |
| 6   | W     | 318 | IWJ  | C26-C28-C29-C30 |
| 6   | W     | 318 | IWJ  | C26-C28-C29-C35 |
| 6   | W     | 318 | IWJ  | C26-C28-C29-O39 |
| 6   | X     | 318 | IWJ  | C18-C19-C21-C22 |
| 6   | X     | 318 | IWJ  | C20-C19-C21-C22 |
| 6   | X     | 318 | IWJ  | C26-C28-C29-C30 |
| 6   | X     | 318 | IWJ  | C26-C28-C29-O39 |
| 2   | V     | 310 | CLA  | O1D-CGD-O2D-CED |
| 2   | W     | 303 | CLA  | O1D-CGD-O2D-CED |
| 3   | V     | 307 | CHL  | O1D-CGD-O2D-CED |
| 3   | X     | 308 | CHL  | O1D-CGD-O2D-CED |
| 3   | X     | 315 | CHL  | O1D-CGD-O2D-CED |
| 2   | W     | 311 | CLA  | O1D-CGD-O2D-CED |
| 2   | X     | 312 | CLA  | O1D-CGD-O2D-CED |
| 2   | V     | 301 | CLA  | CBD-CGD-O2D-CED |
| 2   | V     | 310 | CLA  | CBD-CGD-O2D-CED |
| 2   | W     | 301 | CLA  | CBD-CGD-O2D-CED |
| 2   | W     | 303 | CLA  | CBD-CGD-O2D-CED |
| 2   | W     | 311 | CLA  | CBD-CGD-O2D-CED |
| 2   | W     | 313 | CLA  | CBD-CGD-O2D-CED |
| 2   | X     | 303 | CLA  | CBD-CGD-O2D-CED |
| 2   | X     | 304 | CLA  | CBD-CGD-O2D-CED |
| 3   | V     | 307 | CHL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | W     | 307 | CHL  | CBD-CGD-O2D-CED |
| 4   | X     | 309 | KC2  | CBD-CGD-O2D-CED |
| 2   | V     | 302 | CLA  | O1A-CGA-O2A-C1  |
| 2   | V     | 303 | CLA  | O1D-CGD-O2D-CED |
| 2   | W     | 313 | CLA  | O1D-CGD-O2D-CED |
| 2   | X     | 313 | CLA  | O1D-CGD-O2D-CED |
| 2   | X     | 314 | CLA  | O1D-CGD-O2D-CED |
| 3   | V     | 304 | CHL  | O1D-CGD-O2D-CED |
| 3   | W     | 307 | CHL  | O1D-CGD-O2D-CED |
| 2   | X     | 303 | CLA  | O1D-CGD-O2D-CED |
| 2   | V     | 302 | CLA  | CBA-CGA-O2A-C1  |
| 2   | V     | 302 | CLA  | CBD-CGD-O2D-CED |
| 2   | V     | 309 | CLA  | CBD-CGD-O2D-CED |
| 3   | X     | 306 | CHL  | CBD-CGD-O2D-CED |
| 4   | W     | 308 | KC2  | CBD-CGD-O2D-CED |
| 2   | V     | 313 | CLA  | O1A-CGA-O2A-C1  |
| 2   | X     | 302 | CLA  | O1A-CGA-O2A-C1  |
| 2   | X     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 2   | X     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 3   | W     | 306 | CHL  | O1A-CGA-O2A-C1  |
| 3   | W     | 307 | CHL  | O1A-CGA-O2A-C1  |
| 2   | X     | 311 | CLA  | O1D-CGD-O2D-CED |
| 2   | V     | 312 | CLA  | C3-C5-C6-C7     |
| 2   | W     | 302 | CLA  | C3-C5-C6-C7     |
| 2   | W     | 312 | CLA  | C3-C5-C6-C7     |
| 2   | X     | 302 | CLA  | CBA-CGA-O2A-C1  |
| 2   | X     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 3   | W     | 307 | CHL  | CBA-CGA-O2A-C1  |
| 2   | V     | 311 | CLA  | CBD-CGD-O2D-CED |
| 2   | V     | 313 | CLA  | C2A-CAA-CBA-CGA |
| 2   | W     | 301 | CLA  | C2A-CAA-CBA-CGA |
| 3   | V     | 304 | CHL  | C2A-CAA-CBA-CGA |
| 2   | W     | 301 | CLA  | O1D-CGD-O2D-CED |
| 2   | W     | 301 | CLA  | C3-C5-C6-C7     |
| 2   | V     | 313 | CLA  | CBA-CGA-O2A-C1  |
| 2   | X     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 3   | W     | 306 | CHL  | CBA-CGA-O2A-C1  |
| 2   | V     | 301 | CLA  | O1D-CGD-O2D-CED |
| 5   | V     | 315 | Q6L  | C17-C18-C19-C20 |
| 6   | V     | 320 | IWJ  | C10-C11-C12-C13 |
| 2   | W     | 310 | CLA  | CBD-CGD-O2D-CED |
| 3   | X     | 307 | CHL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | X     | 309 | KC2  | O1D-CGD-O2D-CED |
| 2   | W     | 303 | CLA  | CBA-CGA-O2A-C1  |
| 2   | W     | 310 | CLA  | CBA-CGA-O2A-C1  |
| 2   | X     | 303 | CLA  | CBA-CGA-O2A-C1  |
| 3   | W     | 314 | CHL  | CBD-CGD-O2D-CED |
| 2   | V     | 311 | CLA  | C3-C5-C6-C7     |
| 2   | W     | 309 | CLA  | C3-C5-C6-C7     |
| 2   | X     | 302 | CLA  | C3-C5-C6-C7     |
| 2   | V     | 301 | CLA  | C4-C3-C5-C6     |
| 5   | V     | 315 | Q6L  | C11-C12-C13-C42 |
| 5   | V     | 319 | Q6L  | C11-C12-C13-C42 |
| 2   | V     | 301 | CLA  | C2-C3-C5-C6     |
| 5   | V     | 315 | Q6L  | C11-C12-C13-C14 |
| 5   | V     | 319 | Q6L  | C11-C12-C13-C14 |
| 2   | V     | 311 | CLA  | C2A-CAA-CBA-CGA |
| 2   | W     | 303 | CLA  | O1A-CGA-O2A-C1  |
| 2   | W     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 2   | X     | 303 | CLA  | O1A-CGA-O2A-C1  |
| 2   | V     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 2   | X     | 304 | CLA  | O1D-CGD-O2D-CED |
| 2   | V     | 309 | CLA  | O1D-CGD-O2D-CED |
| 3   | X     | 306 | CHL  | O1D-CGD-O2D-CED |
| 4   | W     | 308 | KC2  | O1D-CGD-O2D-CED |
| 2   | V     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 2   | W     | 301 | CLA  | CBA-CGA-O2A-C1  |
| 2   | W     | 302 | CLA  | CBA-CGA-O2A-C1  |
| 2   | W     | 310 | CLA  | C8-C10-C11-C12  |
| 4   | V     | 308 | KC2  | CAA-CBA-CGA-O1A |
| 4   | V     | 308 | KC2  | CAA-CBA-CGA-O2A |
| 4   | W     | 308 | KC2  | CAA-CBA-CGA-O1A |
| 3   | W     | 307 | CHL  | C5-C6-C7-C8     |
| 2   | V     | 301 | CLA  | C11-C10-C8-C9   |
| 3   | W     | 307 | CHL  | C6-C7-C8-C9     |
| 2   | V     | 302 | CLA  | O1D-CGD-O2D-CED |
| 5   | V     | 321 | Q6L  | C28-C27-C29-C30 |
| 5   | W     | 319 | Q6L  | C23-C22-C24-C25 |
| 5   | X     | 316 | Q6L  | C15-C16-C17-C41 |
| 5   | V     | 321 | Q6L  | C26-C27-C29-C30 |
| 5   | W     | 319 | Q6L  | C21-C22-C24-C25 |
| 5   | W     | 320 | Q6L  | C26-C27-C29-C30 |
| 4   | W     | 308 | KC2  | CAA-CBA-CGA-O2A |
| 2   | W     | 310 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | W     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 2   | X     | 310 | CLA  | CBD-CGD-O2D-CED |
| 2   | W     | 301 | CLA  | O1A-CGA-O2A-C1  |
| 5   | W     | 319 | Q6L  | C24-C25-C26-C27 |
| 6   | V     | 318 | IWJ  | C10-C11-C12-C13 |
| 2   | W     | 302 | CLA  | O1A-CGA-O2A-C1  |
| 2   | V     | 301 | CLA  | C10-C11-C12-C13 |
| 2   | W     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 5   | W     | 315 | Q6L  | C11-C12-C13-C42 |
| 2   | V     | 311 | CLA  | O1D-CGD-O2D-CED |
| 2   | W     | 310 | CLA  | O1D-CGD-O2D-CED |
| 5   | W     | 316 | Q6L  | C28-C27-C29-C30 |
| 5   | X     | 301 | Q6L  | C28-C27-C29-C30 |
| 5   | X     | 301 | Q6L  | C26-C27-C29-C30 |
| 2   | W     | 312 | CLA  | C6-C7-C8-C9     |
| 2   | X     | 302 | CLA  | C5-C6-C7-C8     |
| 2   | V     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 3   | V     | 314 | CHL  | C3A-C2A-CAA-CBA |
| 3   | W     | 307 | CHL  | C3A-C2A-CAA-CBA |
| 2   | W     | 312 | CLA  | C6-C7-C8-C10    |
| 5   | V     | 316 | Q6L  | C11-C12-C13-C14 |
| 2   | V     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 2   | W     | 309 | CLA  | C4-C3-C5-C6     |
| 3   | W     | 314 | CHL  | O1D-CGD-O2D-CED |
| 5   | W     | 319 | Q6L  | C11-C12-C13-C14 |
| 5   | V     | 319 | Q6L  | C24-C25-C26-C27 |
| 5   | X     | 301 | Q6L  | C24-C25-C26-C27 |
| 3   | X     | 307 | CHL  | O1D-CGD-O2D-CED |
| 4   | X     | 309 | KC2  | C4C-C3C-CAC-CBC |
| 5   | V     | 316 | Q6L  | C11-C12-C13-C42 |
| 5   | W     | 319 | Q6L  | C11-C12-C13-C42 |
| 5   | X     | 301 | Q6L  | C11-C12-C13-C42 |
| 5   | W     | 315 | Q6L  | C11-C12-C13-C14 |
| 2   | W     | 311 | CLA  | C2A-CAA-CBA-CGA |
| 3   | V     | 314 | CHL  | C1A-C2A-CAA-CBA |
| 3   | X     | 307 | CHL  | C1A-C2A-CAA-CBA |
| 3   | X     | 315 | CHL  | C1A-C2A-CAA-CBA |
| 5   | X     | 316 | Q6L  | C17-C18-C19-C20 |
| 3   | W     | 307 | CHL  | C15-C16-C17-C18 |
| 2   | X     | 310 | CLA  | O1D-CGD-O2D-CED |
| 2   | X     | 311 | CLA  | C4C-C3C-CAC-CBC |
| 2   | W     | 312 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | V     | 310 | CLA  | CBA-CGA-O2A-C1  |
| 3   | W     | 307 | CHL  | C11-C12-C13-C15 |
| 3   | W     | 307 | CHL  | C11-C12-C13-C14 |
| 3   | V     | 314 | CHL  | C2A-CAA-CBA-CGA |
| 2   | V     | 313 | CLA  | O2A-C1-C2-C3    |
| 5   | X     | 301 | Q6L  | C11-C12-C13-C14 |
| 2   | W     | 301 | CLA  | C3A-C2A-CAA-CBA |
| 6   | X     | 318 | IWJ  | C21-C22-C23-C24 |
| 6   | V     | 317 | IWJ  | O27-C26-C28-C29 |
| 6   | V     | 320 | IWJ  | O27-C26-C28-C29 |
| 6   | X     | 318 | IWJ  | O27-C26-C28-C29 |
| 5   | V     | 319 | Q6L  | C29-C30-C31-C36 |
| 2   | V     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 2   | X     | 302 | CLA  | C6-C7-C8-C10    |
| 2   | W     | 309 | CLA  | C2-C3-C5-C6     |
| 3   | V     | 304 | CHL  | C3C-C2C-CMC-OMC |
| 6   | W     | 318 | IWJ  | C23-C24-C26-C28 |
| 4   | W     | 308 | KC2  | C1A-C2A-CAA-CBA |
| 2   | V     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 2   | X     | 304 | CLA  | C1A-C2A-CAA-CBA |
| 5   | X     | 316 | Q6L  | C15-C16-C17-C18 |
| 2   | X     | 302 | CLA  | C6-C7-C8-C9     |
| 2   | W     | 309 | CLA  | C11-C10-C8-C7   |
| 5   | V     | 316 | Q6L  | C24-C25-C26-C27 |
| 5   | W     | 316 | Q6L  | C13-C14-C15-C16 |
| 5   | X     | 317 | Q6L  | C13-C14-C15-C16 |
| 2   | V     | 309 | CLA  | CAD-CBD-CGD-O2D |
| 2   | W     | 302 | CLA  | CAD-CBD-CGD-O2D |
| 2   | X     | 310 | CLA  | CAD-CBD-CGD-O2D |
| 3   | V     | 307 | CHL  | CAD-CBD-CGD-O2D |
| 3   | V     | 314 | CHL  | CAD-CBD-CGD-O2D |
| 3   | W     | 306 | CHL  | CAD-CBD-CGD-O2D |
| 3   | X     | 308 | CHL  | CAD-CBD-CGD-O2D |
| 4   | V     | 308 | KC2  | C2B-C3B-CAB-CBB |
| 4   | X     | 309 | KC2  | C2B-C3B-CAB-CBB |
| 5   | X     | 316 | Q6L  | C11-C12-C13-C14 |
| 6   | W     | 318 | IWJ  | C25-C24-C26-O27 |
| 4   | V     | 308 | KC2  | C4C-C3C-CAC-CBC |
| 4   | W     | 308 | KC2  | C4C-C3C-CAC-CBC |
| 2   | V     | 310 | CLA  | CHA-CBD-CGD-O1D |
| 6   | W     | 318 | IWJ  | C23-C24-C26-O27 |
| 2   | X     | 311 | CLA  | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | X     | 316 | Q6L  | C11-C12-C13-C42 |
| 5   | X     | 316 | Q6L  | C23-C22-C24-C25 |
| 2   | V     | 302 | CLA  | CAD-CBD-CGD-O1D |
| 2   | V     | 311 | CLA  | CAD-CBD-CGD-O1D |
| 2   | X     | 303 | CLA  | C2-C3-C5-C6     |
| 3   | W     | 307 | CHL  | C6-C7-C8-C10    |
| 5   | V     | 319 | Q6L  | C29-C30-C31-C32 |
| 5   | W     | 319 | Q6L  | C29-C30-C31-C32 |
| 2   | W     | 310 | CLA  | CAA-CBA-CGA-O2A |
| 3   | V     | 307 | CHL  | C2C-C3C-CAC-CBC |
| 3   | V     | 305 | CHL  | C1C-C2C-CMC-OMC |
| 2   | W     | 309 | CLA  | C11-C10-C8-C9   |
| 2   | V     | 311 | CLA  | C2-C1-O2A-CGA   |
| 5   | W     | 319 | Q6L  | C27-C29-C30-C31 |
| 6   | W     | 318 | IWJ  | C25-C24-C26-C28 |
| 3   | W     | 305 | CHL  | O1D-CGD-O2D-CED |
| 6   | W     | 318 | IWJ  | C16-C17-C18-C19 |
| 4   | V     | 308 | KC2  | C4B-C3B-CAB-CBB |
| 4   | X     | 309 | KC2  | C4B-C3B-CAB-CBB |
| 5   | V     | 321 | Q6L  | C24-C25-C26-C27 |
| 2   | W     | 312 | CLA  | C5-C6-C7-C8     |
| 7   | W     | 317 | NEX  | C39-C29-C30-C31 |
| 2   | V     | 311 | CLA  | C6-C7-C8-C10    |
| 5   | X     | 301 | Q6L  | C19-C20-C21-C22 |
| 2   | V     | 301 | CLA  | C5-C6-C7-C8     |
| 7   | W     | 317 | NEX  | C28-C29-C30-C31 |
| 3   | V     | 304 | CHL  | CAA-CBA-CGA-O2A |
| 5   | V     | 321 | Q6L  | C11-C12-C13-C42 |
| 5   | W     | 316 | Q6L  | C26-C27-C29-C30 |
| 3   | V     | 307 | CHL  | C4C-C3C-CAC-CBC |
| 2   | W     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 2   | W     | 311 | CLA  | CAA-CBA-CGA-O1A |
| 3   | V     | 314 | CHL  | O1D-CGD-O2D-CED |
| 4   | V     | 308 | KC2  | CBD-CGD-O2D-CED |
| 2   | V     | 301 | CLA  | CAA-CBA-CGA-O2A |
| 3   | W     | 306 | CHL  | C3A-C2A-CAA-CBA |
| 2   | X     | 302 | CLA  | CAD-CBD-CGD-O2D |
| 2   | X     | 313 | CLA  | CAD-CBD-CGD-O2D |
| 3   | X     | 305 | CHL  | CAD-CBD-CGD-O2D |
| 3   | X     | 307 | CHL  | CAD-CBD-CGD-O2D |
| 2   | V     | 310 | CLA  | CAA-CBA-CGA-O2A |
| 3   | W     | 305 | CHL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | V     | 304 | CHL  | CAA-CBA-CGA-O1A |
| 5   | X     | 316 | Q6L  | C21-C22-C24-C25 |
| 2   | V     | 303 | CLA  | O2A-C1-C2-C3    |
| 2   | W     | 302 | CLA  | O2A-C1-C2-C3    |
| 4   | W     | 308 | KC2  | C4B-C3B-CAB-CBB |
| 2   | X     | 302 | CLA  | C2A-CAA-CBA-CGA |
| 2   | V     | 303 | CLA  | CHA-CBD-CGD-O1D |
| 2   | V     | 303 | CLA  | CHA-CBD-CGD-O2D |
| 2   | V     | 310 | CLA  | CHA-CBD-CGD-O2D |
| 2   | W     | 301 | CLA  | CHA-CBD-CGD-O1D |
| 2   | W     | 301 | CLA  | CHA-CBD-CGD-O2D |
| 2   | W     | 310 | CLA  | CHA-CBD-CGD-O1D |
| 2   | W     | 310 | CLA  | CHA-CBD-CGD-O2D |
| 2   | W     | 312 | CLA  | CHA-CBD-CGD-O1D |
| 2   | W     | 312 | CLA  | CHA-CBD-CGD-O2D |
| 4   | X     | 309 | KC2  | CAA-CBA-CGA-O1A |
| 3   | W     | 306 | CHL  | C1A-C2A-CAA-CBA |
| 5   | V     | 315 | Q6L  | C04-C03-C11-C12 |
| 5   | W     | 316 | Q6L  | C04-C03-C11-C12 |
| 2   | V     | 301 | CLA  | CAA-CBA-CGA-O1A |
| 5   | W     | 316 | Q6L  | C19-C20-C21-C22 |
| 2   | W     | 309 | CLA  | C16-C17-C18-C19 |
| 2   | V     | 310 | CLA  | CAA-CBA-CGA-O1A |
| 3   | X     | 315 | CHL  | CAD-CBD-CGD-O1D |
| 4   | W     | 308 | KC2  | CAD-CBD-CGD-O1D |
| 2   | V     | 311 | CLA  | C6-C7-C8-C9     |
| 4   | X     | 309 | KC2  | CAA-CBA-CGA-O2A |
| 2   | X     | 303 | CLA  | CAA-CBA-CGA-O2A |
| 2   | V     | 302 | CLA  | CAA-CBA-CGA-O2A |
| 3   | W     | 307 | CHL  | C3-C5-C6-C7     |
| 2   | V     | 301 | CLA  | C11-C10-C8-C7   |
| 3   | X     | 308 | CHL  | C3A-C2A-CAA-CBA |
| 5   | V     | 321 | Q6L  | C29-C30-C31-C32 |
| 2   | V     | 302 | CLA  | CAA-CBA-CGA-O1A |
| 5   | V     | 319 | Q6L  | C19-C20-C21-C22 |
| 2   | X     | 303 | CLA  | CAA-CBA-CGA-O1A |
| 2   | W     | 309 | CLA  | O1A-CGA-O2A-C1  |

All (2) ring outliers are listed below:

| Mol | Chain | Res | Type | Atoms                   |
|-----|-------|-----|------|-------------------------|
| 6   | X     | 318 | IWJ  | C29-C30-C32-C33-C34-C35 |

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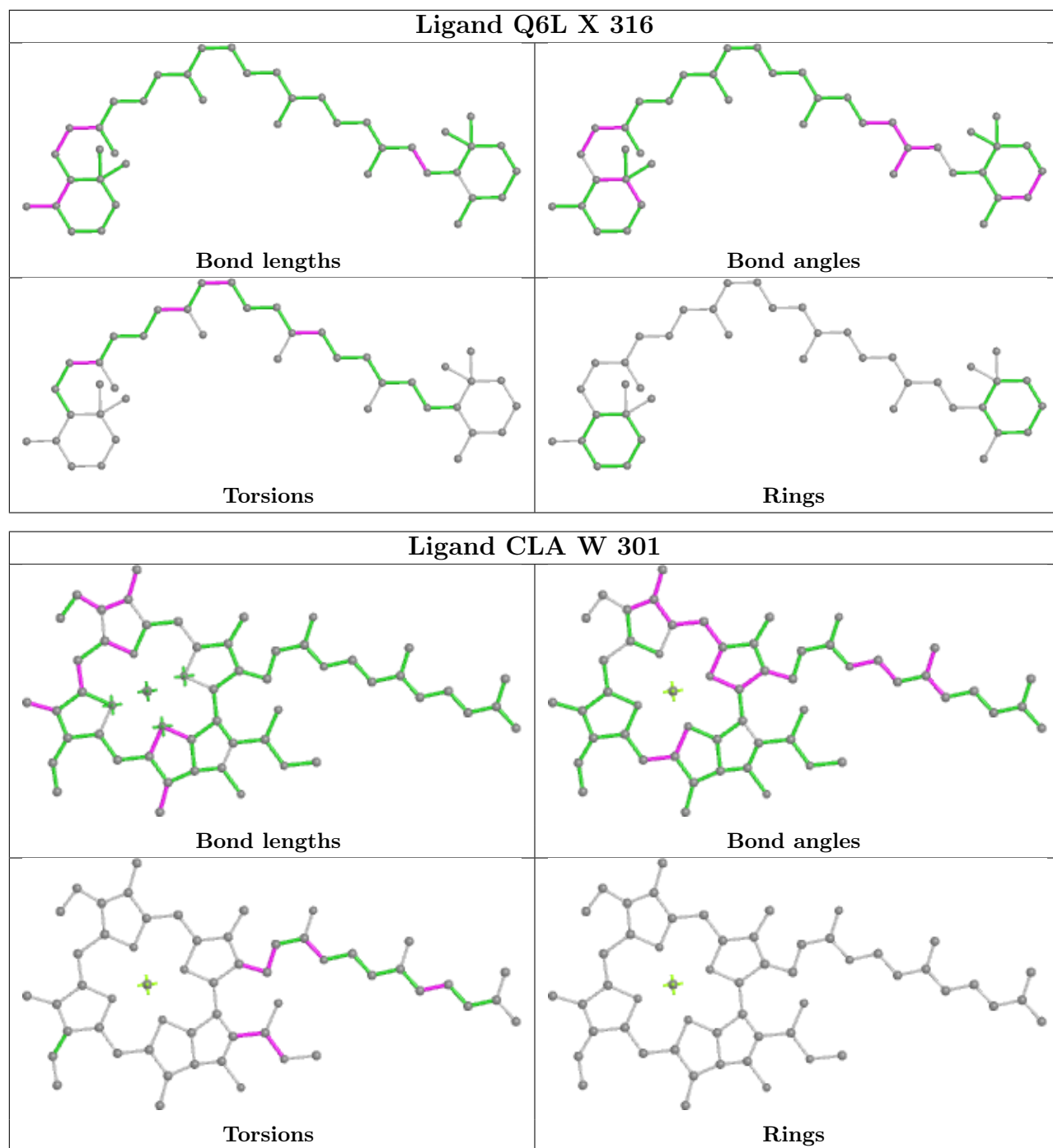
| Mol | Chain | Res | Type | Atoms                   |
|-----|-------|-----|------|-------------------------|
| 6   | V     | 320 | IWJ  | C29-C30-C32-C33-C34-C35 |

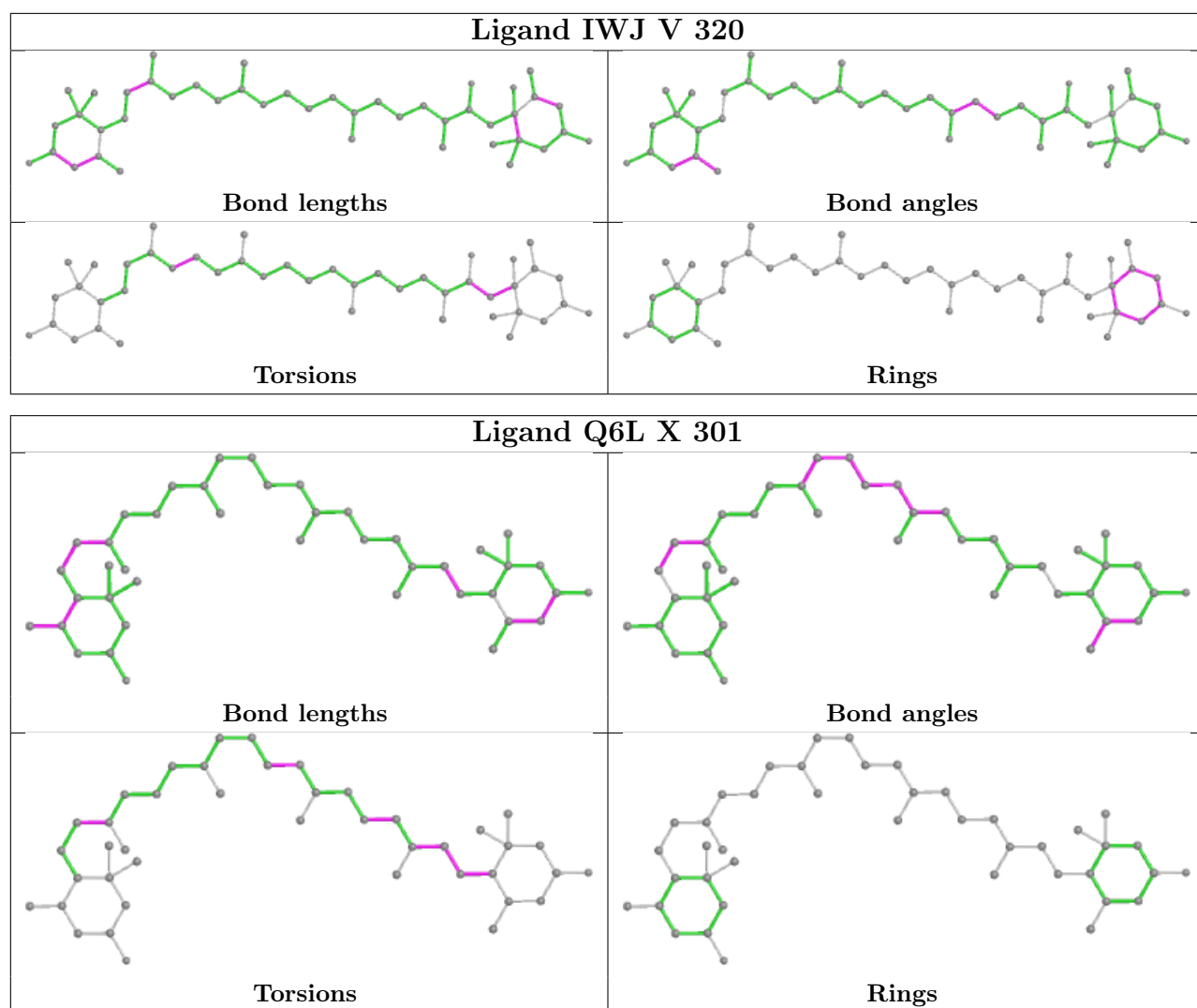
26 monomers are involved in 48 short contacts:

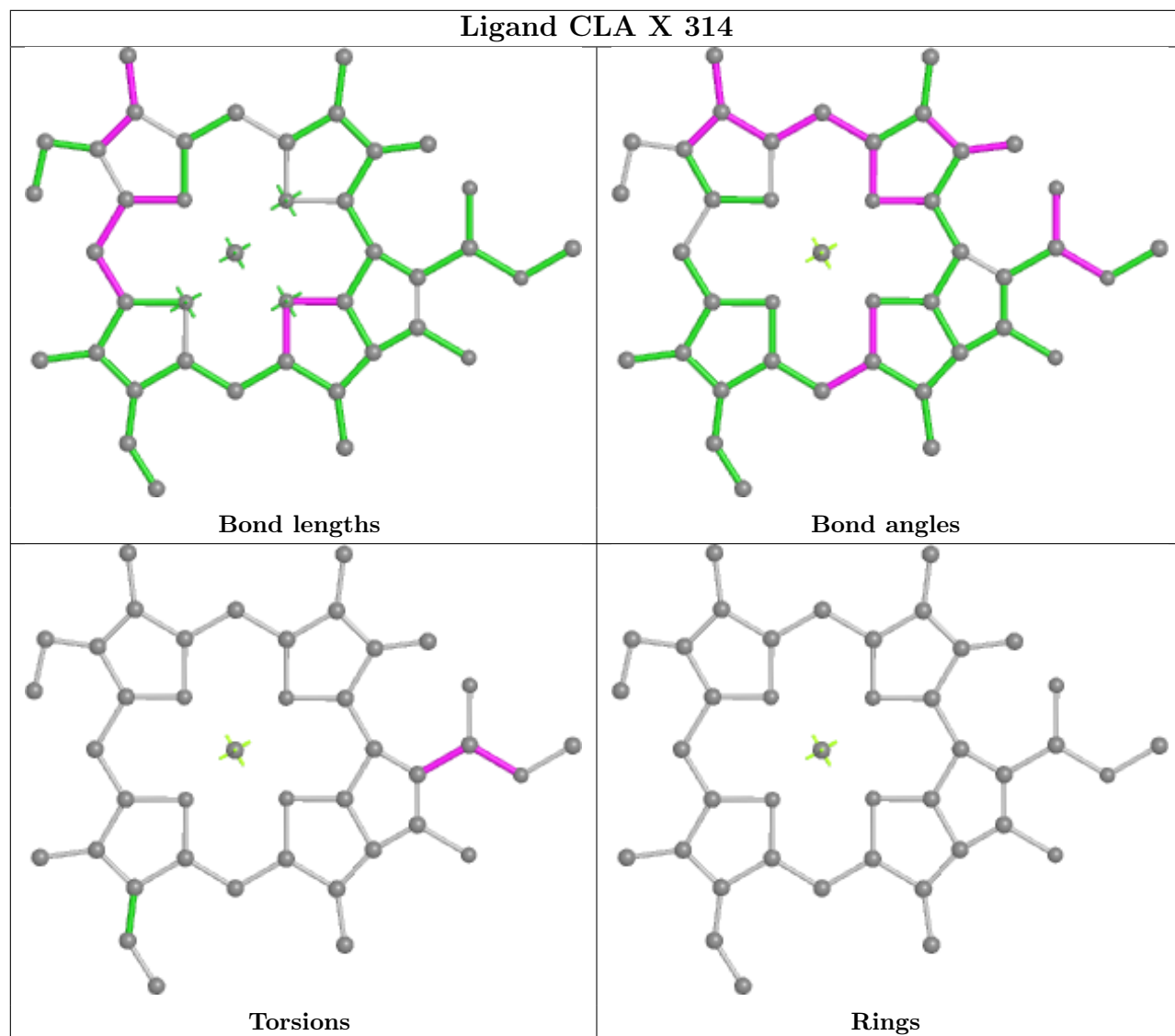
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | W     | 301 | CLA  | 3       | 0            |
| 6   | V     | 320 | IWJ  | 1       | 0            |
| 3   | X     | 306 | CHL  | 1       | 0            |
| 2   | X     | 311 | CLA  | 3       | 0            |
| 2   | V     | 309 | CLA  | 4       | 0            |
| 2   | W     | 309 | CLA  | 5       | 0            |
| 2   | X     | 304 | CLA  | 1       | 0            |
| 6   | V     | 317 | IWJ  | 1       | 0            |
| 2   | W     | 303 | CLA  | 1       | 0            |
| 2   | X     | 310 | CLA  | 1       | 0            |
| 4   | V     | 308 | KC2  | 1       | 0            |
| 5   | V     | 321 | Q6L  | 1       | 0            |
| 3   | X     | 308 | CHL  | 1       | 0            |
| 2   | X     | 302 | CLA  | 3       | 0            |
| 2   | W     | 312 | CLA  | 2       | 0            |
| 2   | V     | 301 | CLA  | 5       | 0            |
| 2   | X     | 313 | CLA  | 1       | 0            |
| 6   | W     | 318 | IWJ  | 2       | 0            |
| 3   | V     | 305 | CHL  | 1       | 0            |
| 2   | V     | 311 | CLA  | 3       | 0            |
| 5   | X     | 319 | Q6L  | 1       | 0            |
| 2   | V     | 303 | CLA  | 1       | 0            |
| 5   | W     | 315 | Q6L  | 2       | 0            |
| 3   | V     | 307 | CHL  | 1       | 0            |
| 2   | V     | 312 | CLA  | 2       | 0            |
| 2   | V     | 302 | CLA  | 1       | 0            |

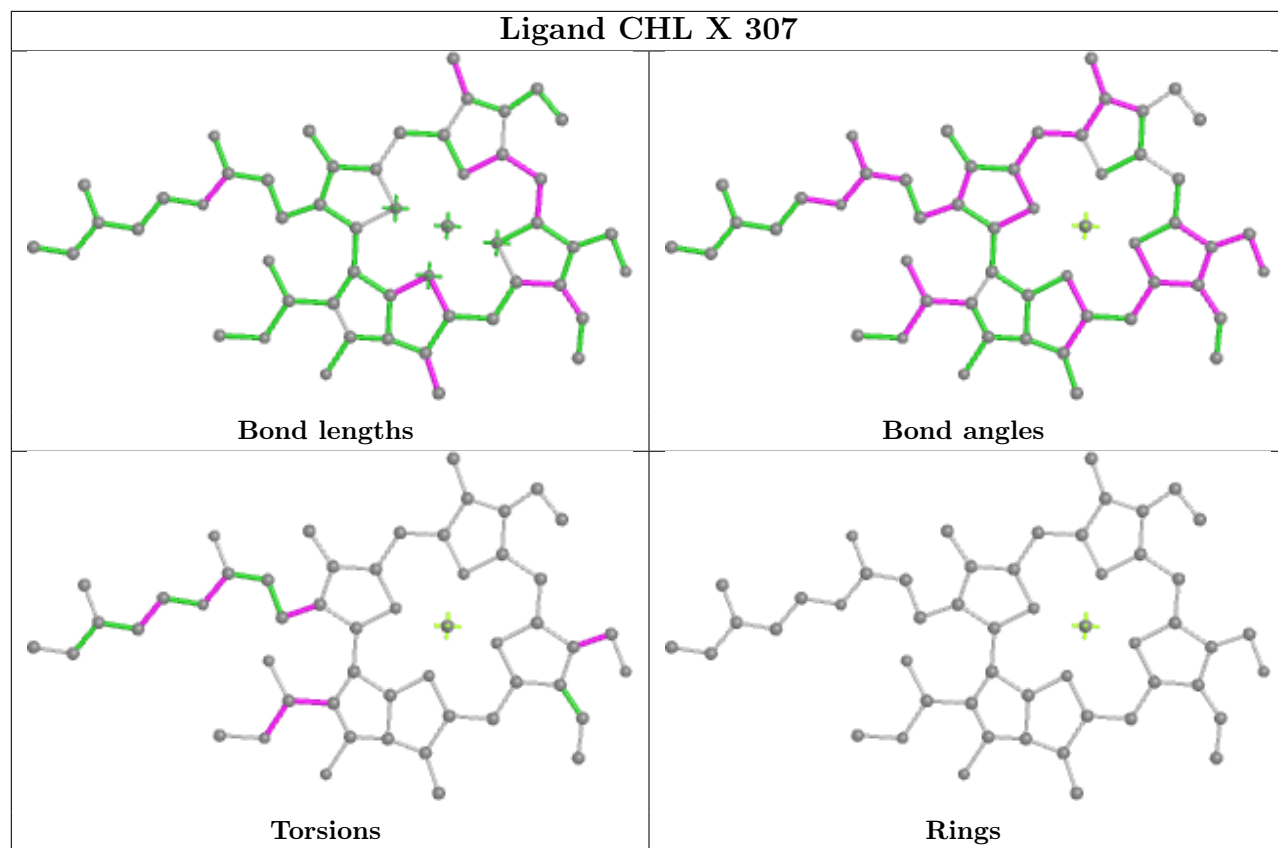
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

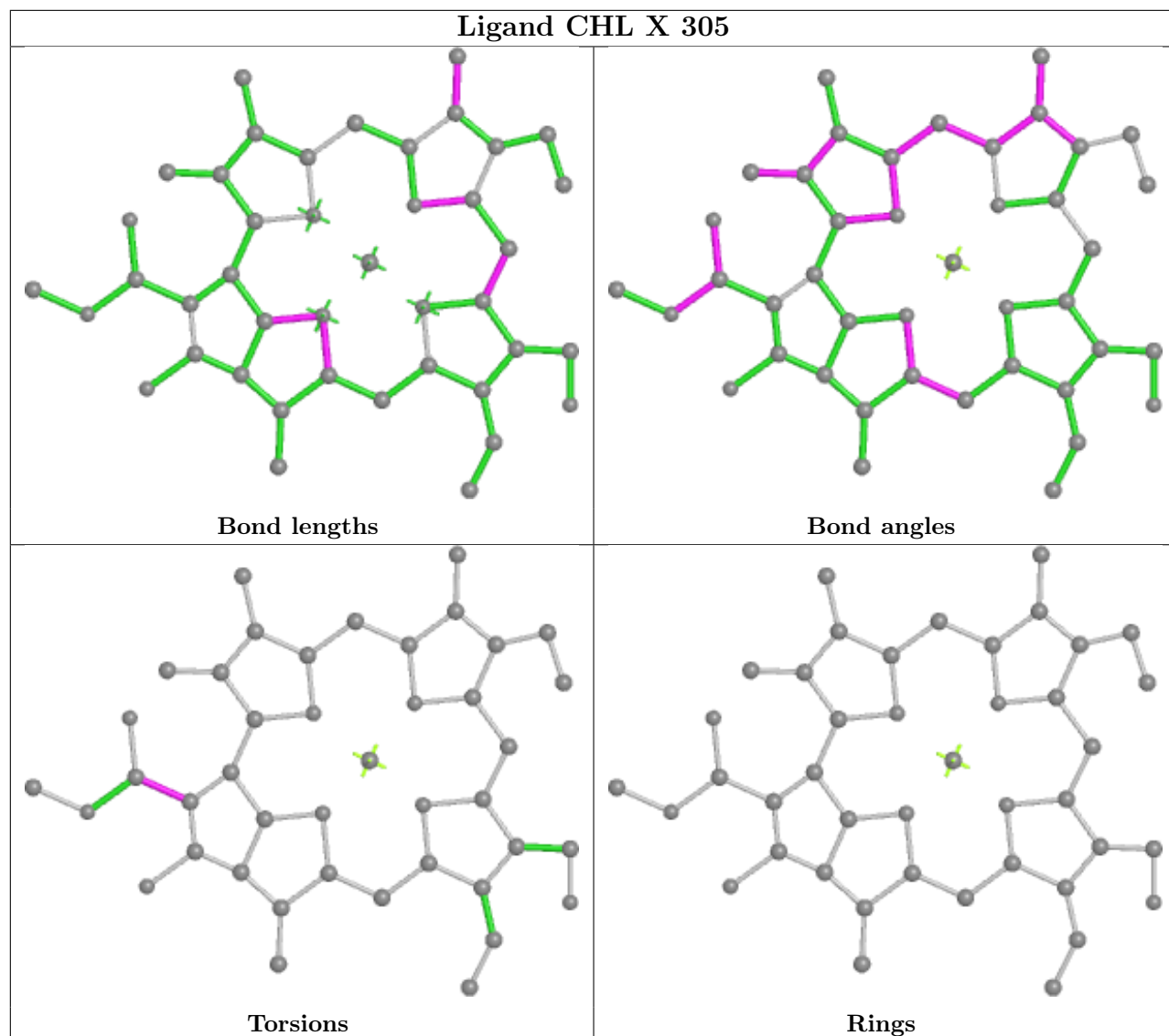
equivalents in the CSD to analyse the geometry.

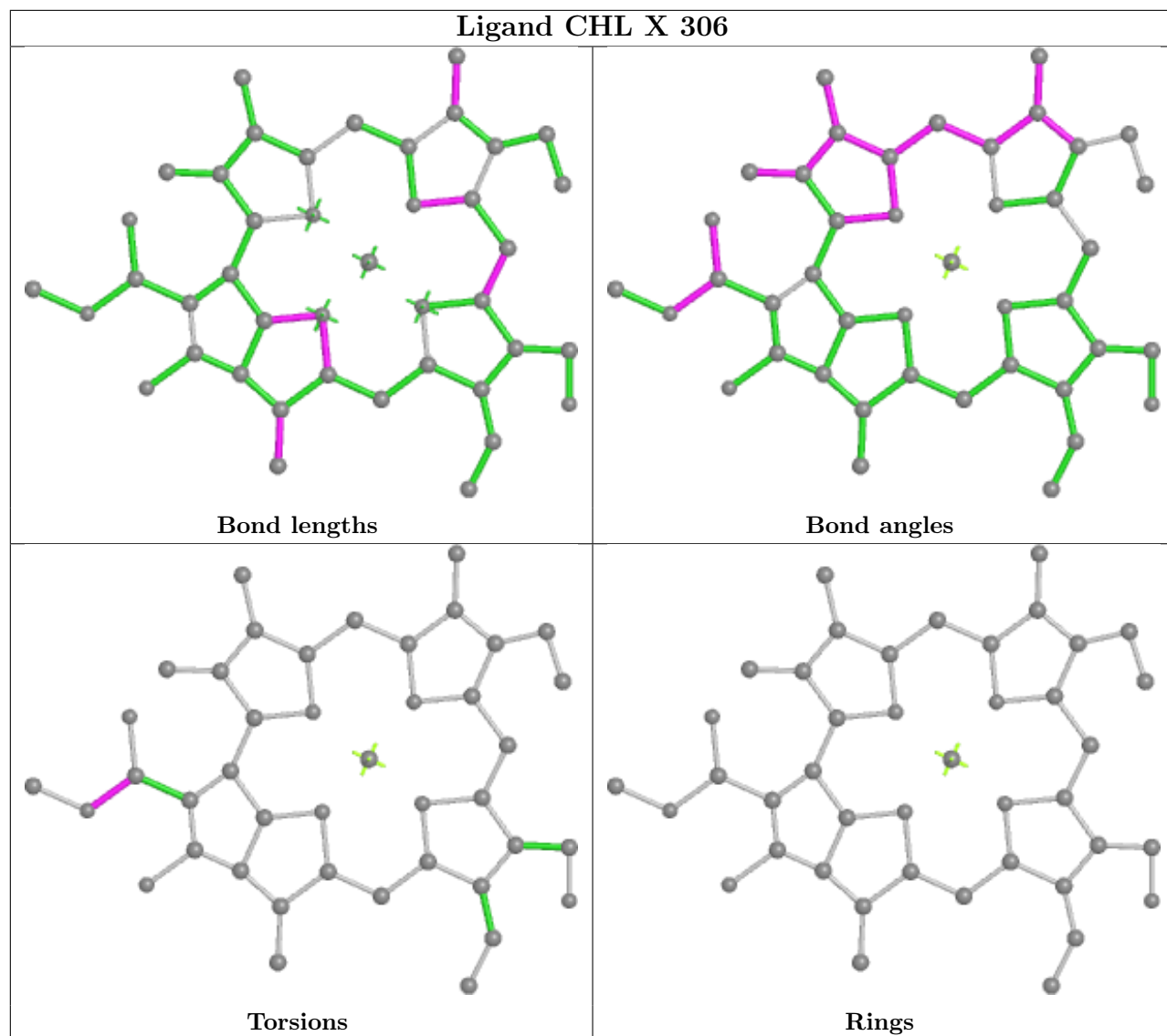




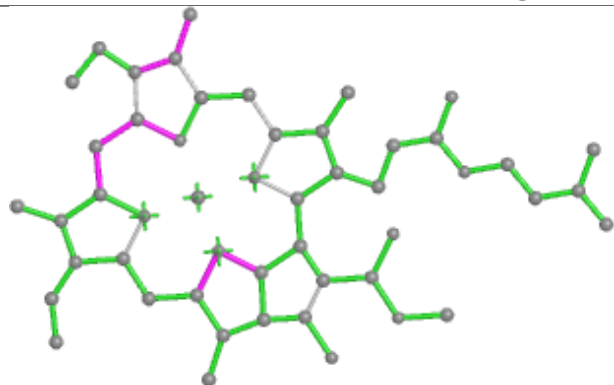




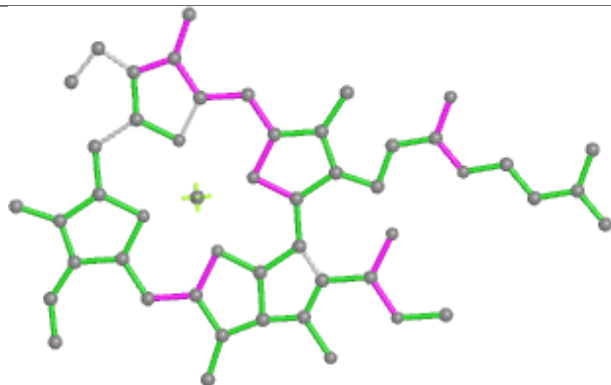




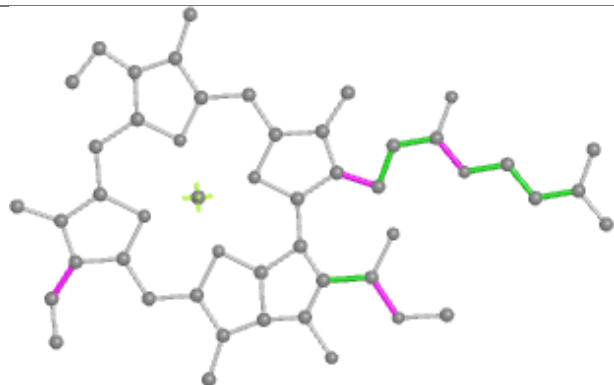
## Ligand CLA X 311



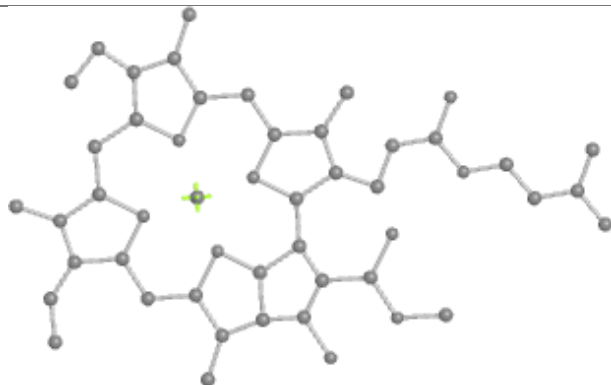
Bond lengths



Bond angles

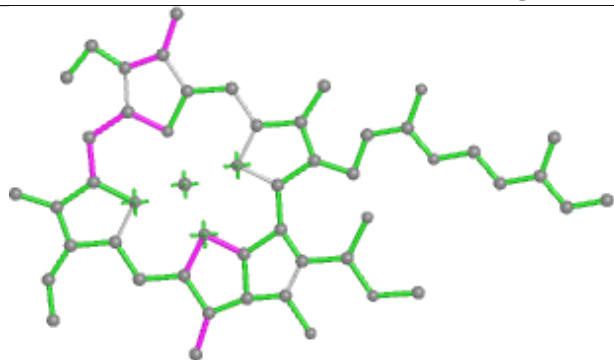


Torsions

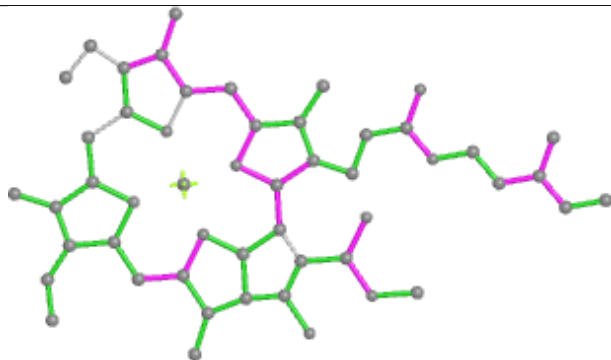


Rings

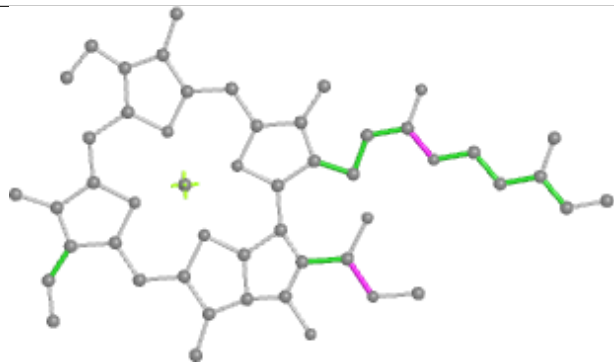
## Ligand CLA X 312



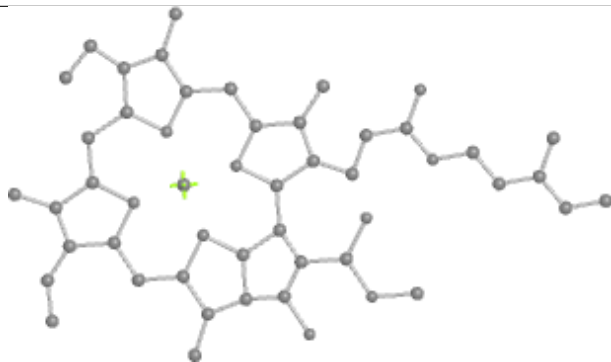
Bond lengths



Bond angles

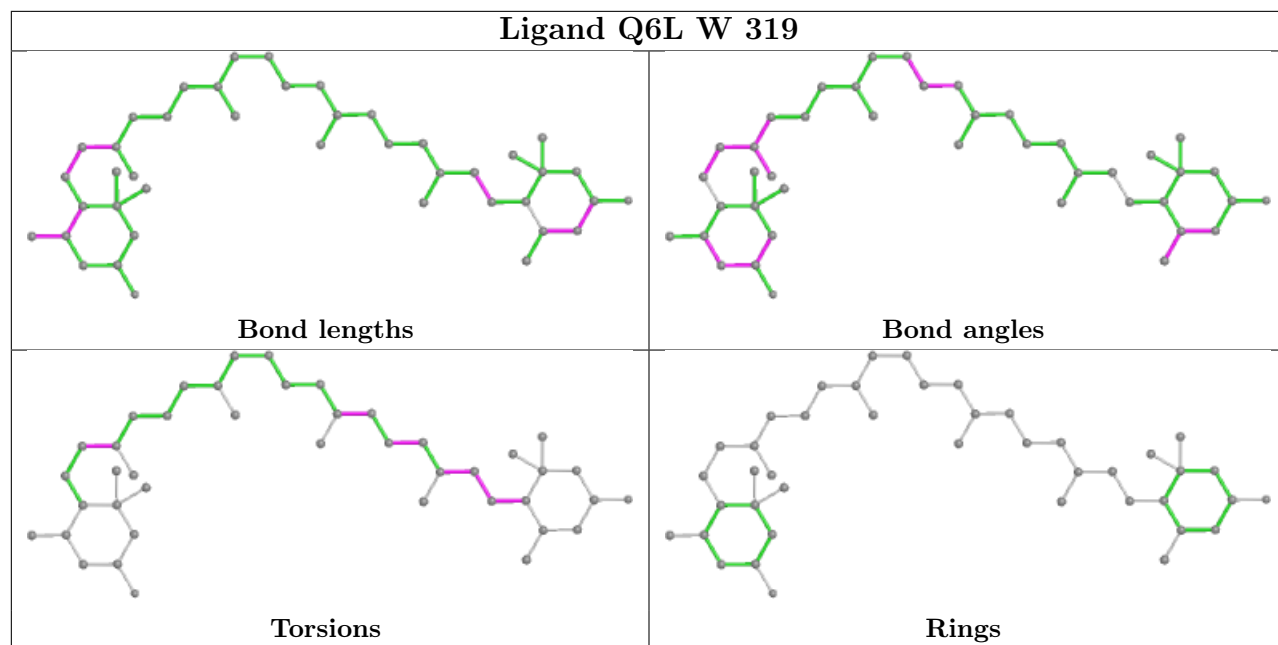


Torsions

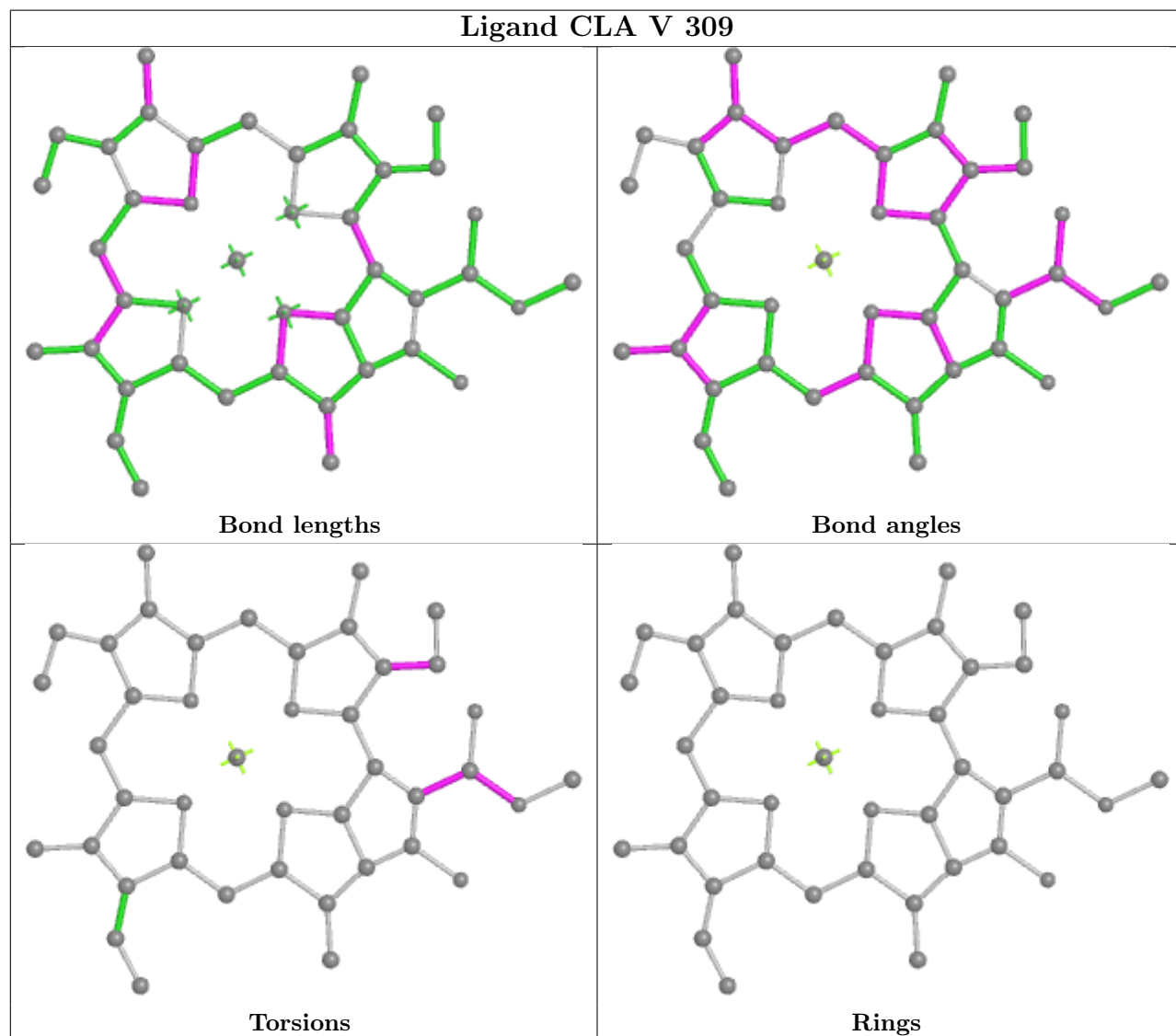


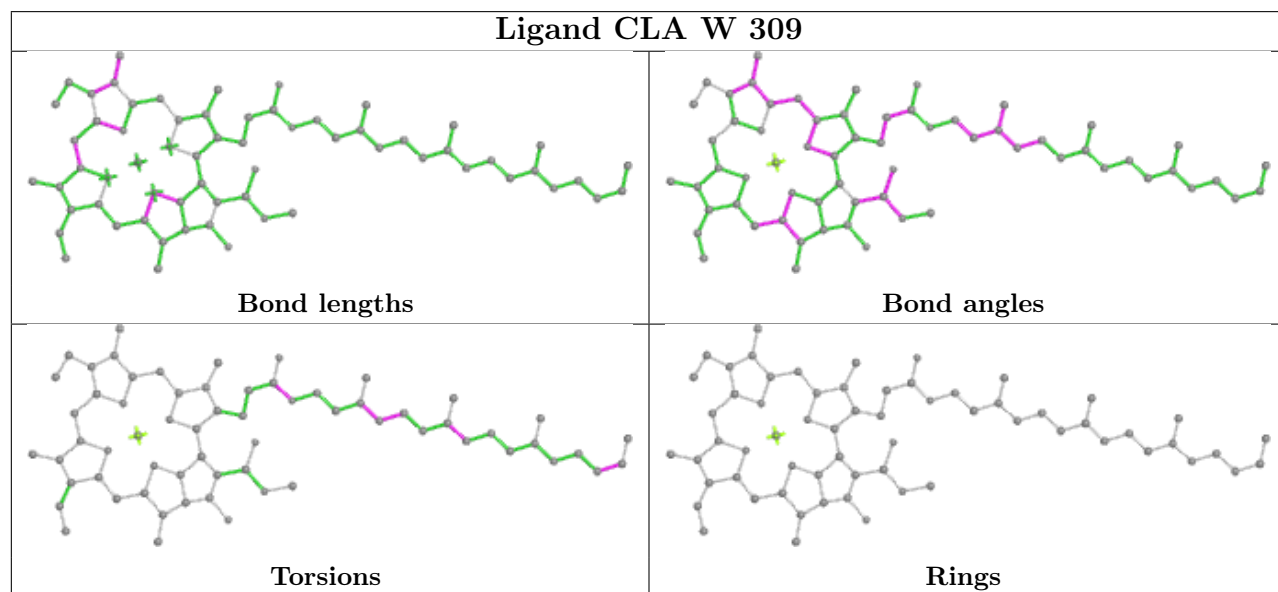
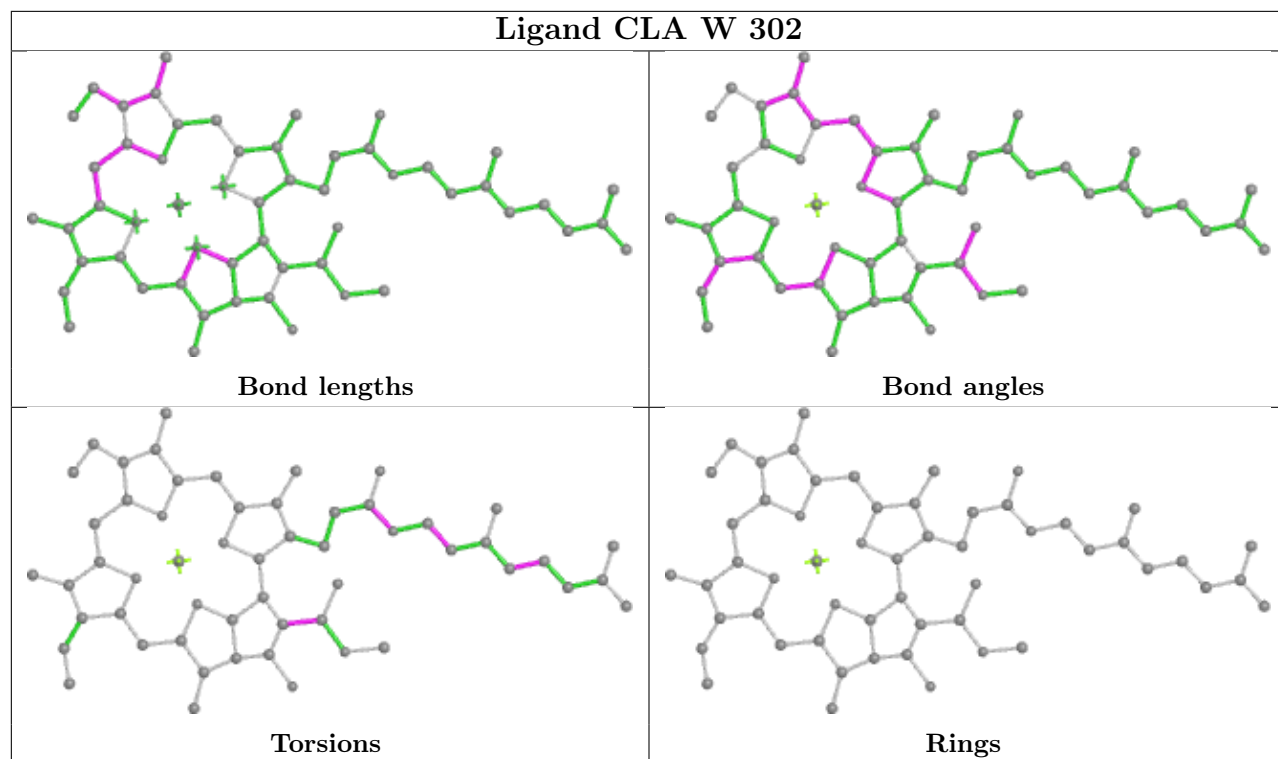
Rings

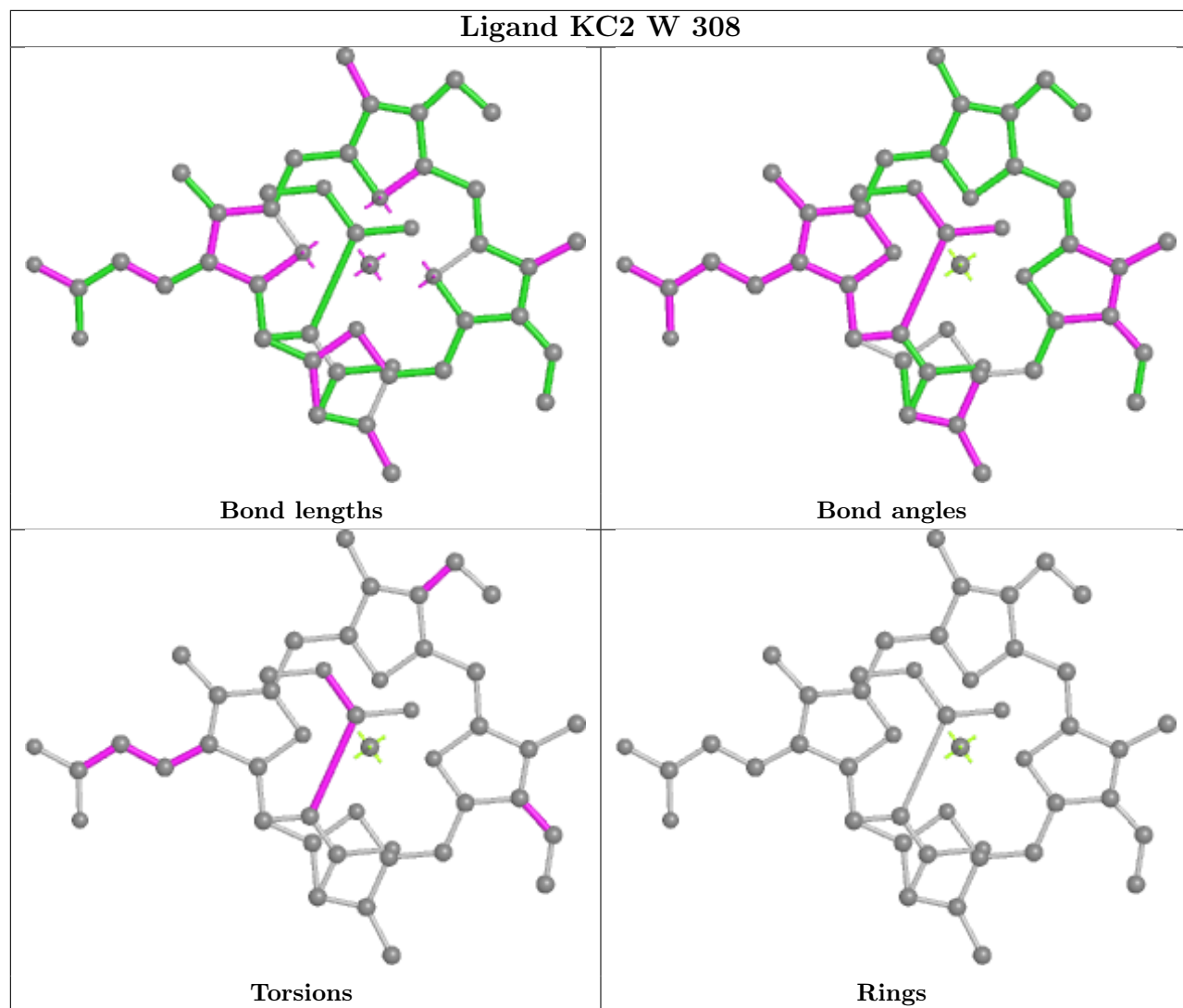
## Ligand Q6L W 319



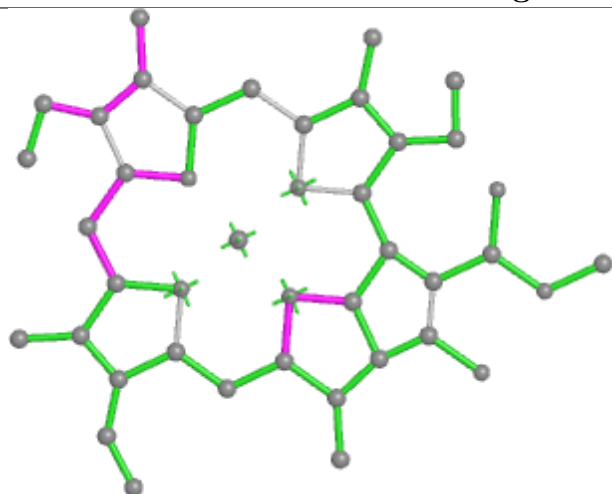
## Ligand CLA V 309



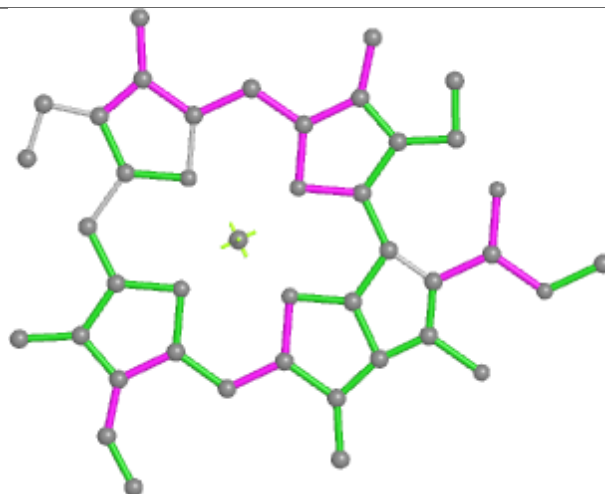




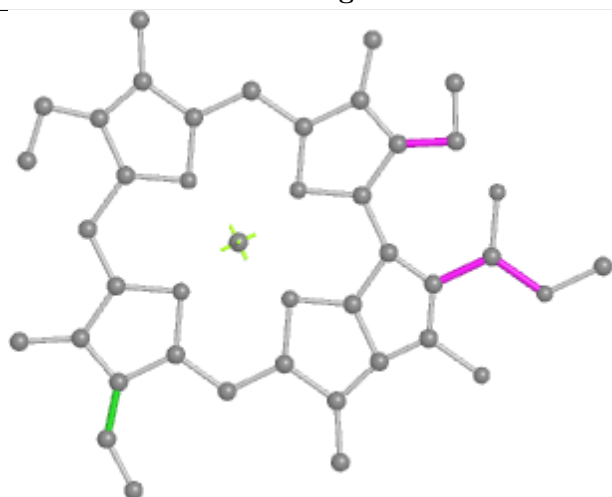
## Ligand CLA X 304



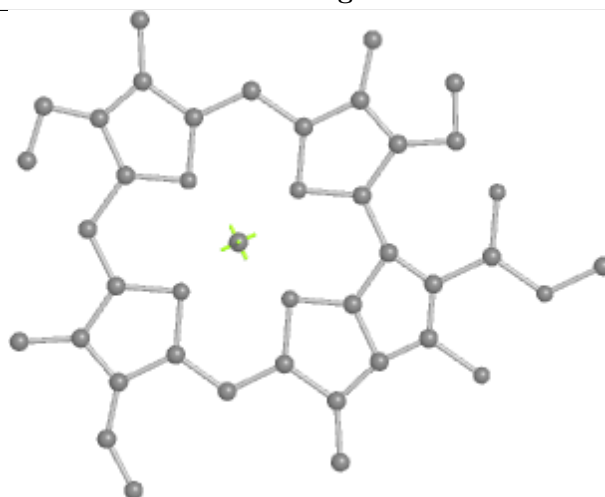
Bond lengths



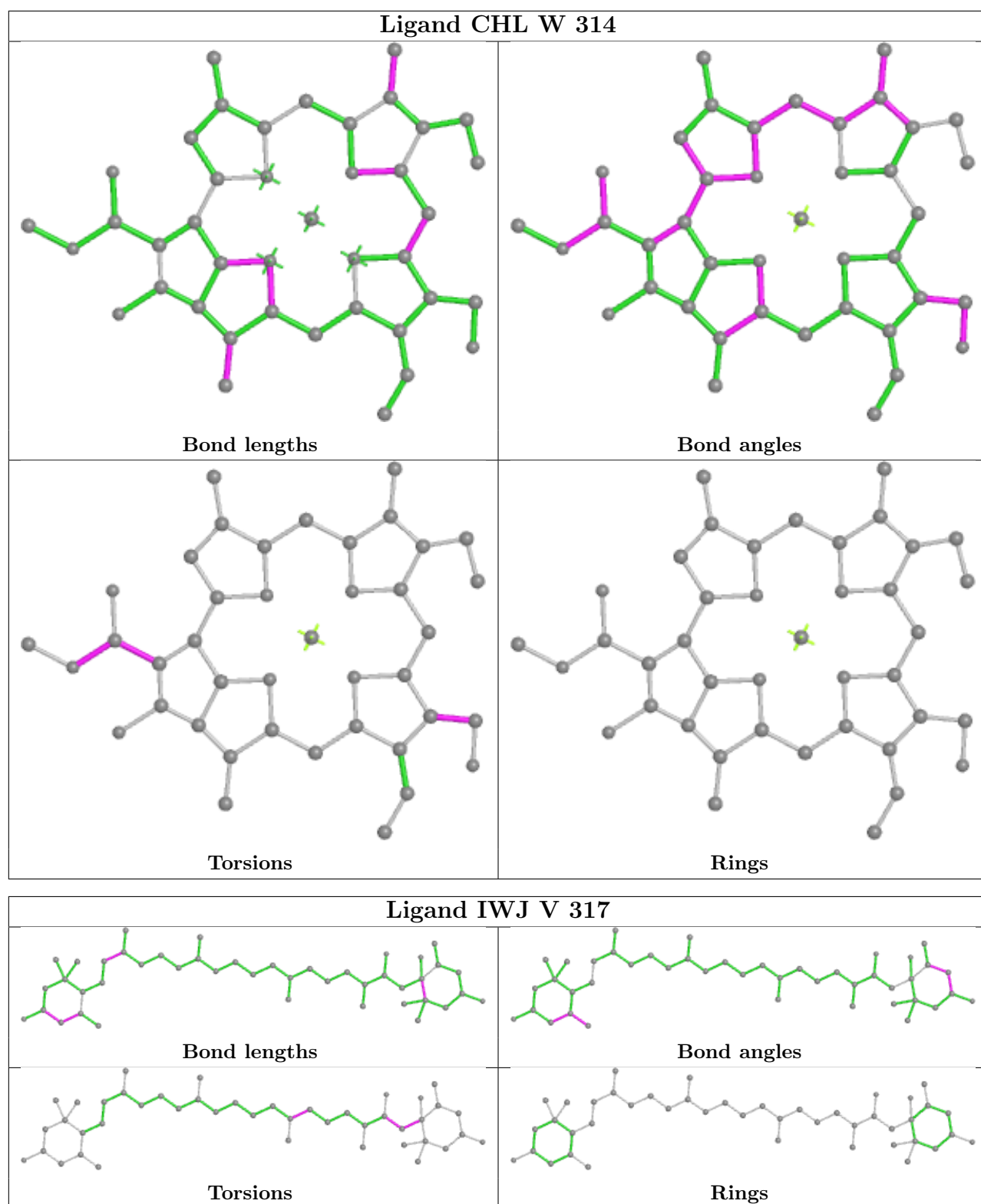
Bond angles

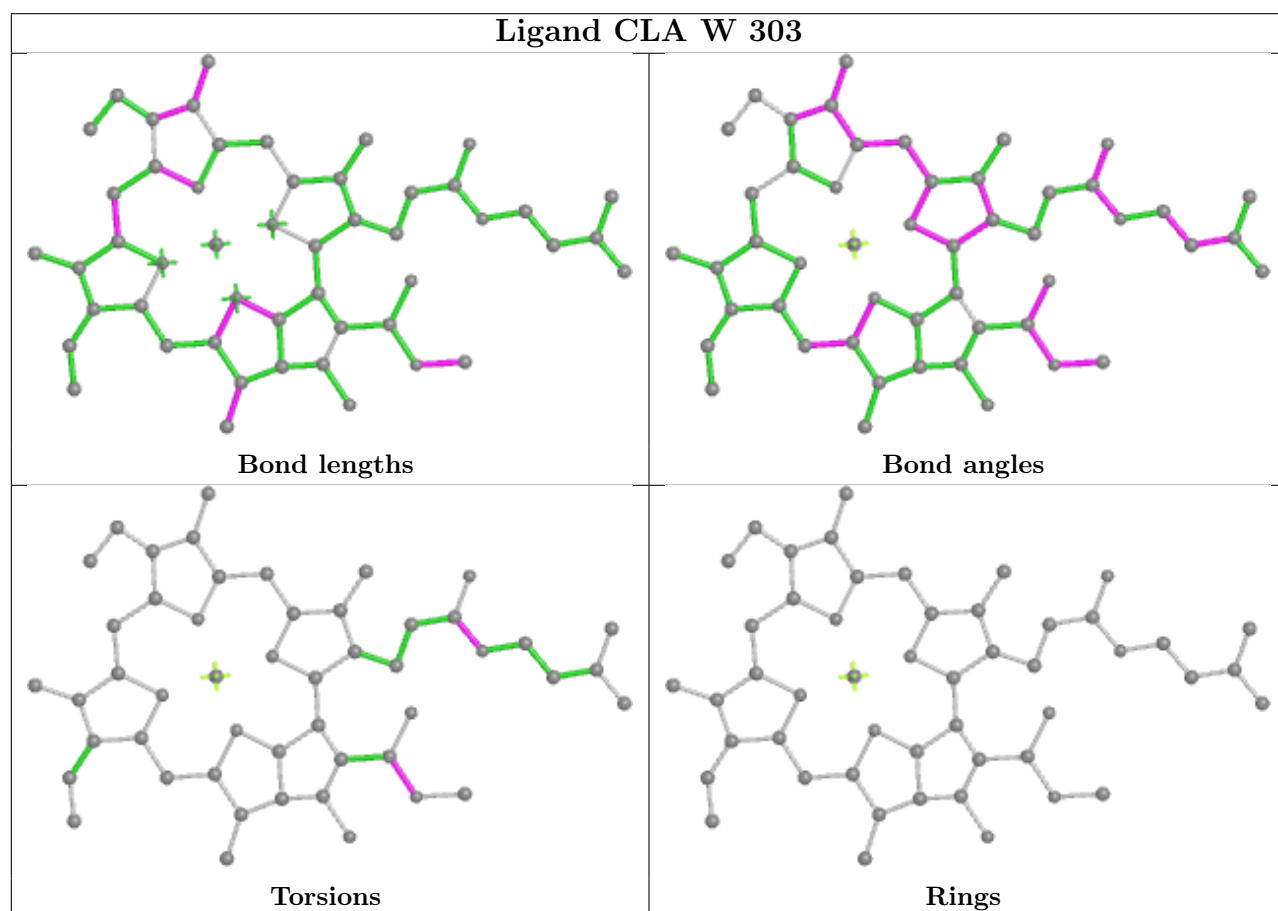
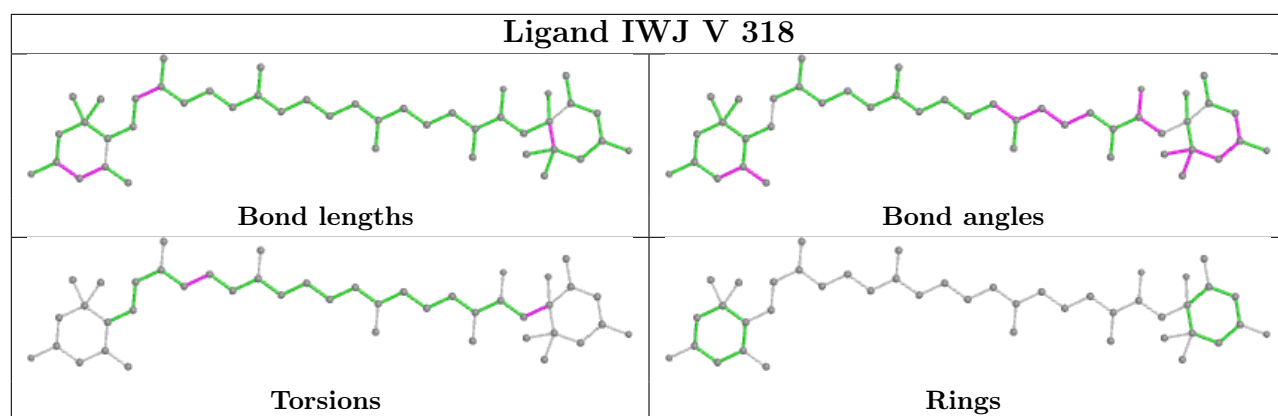


Torsions

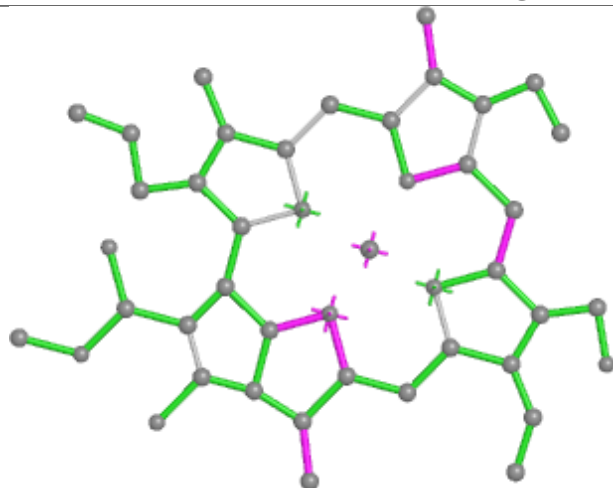


Rings

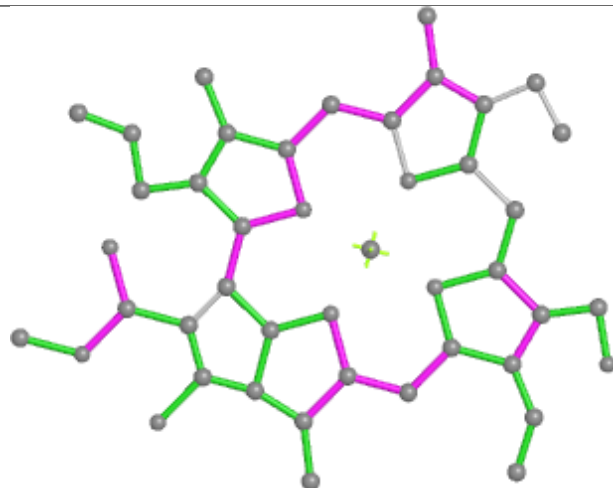




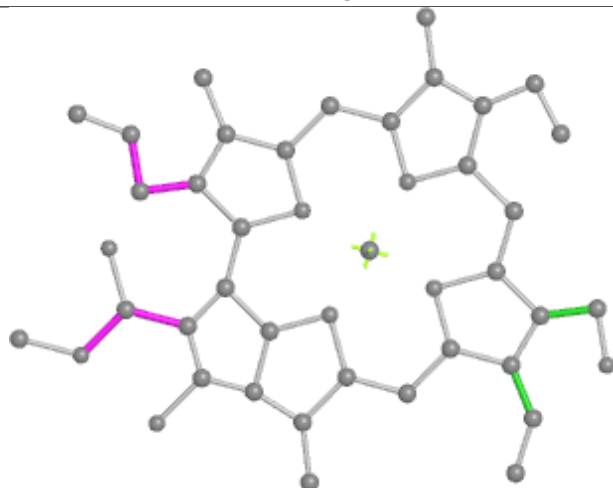
## Ligand CHL V 314



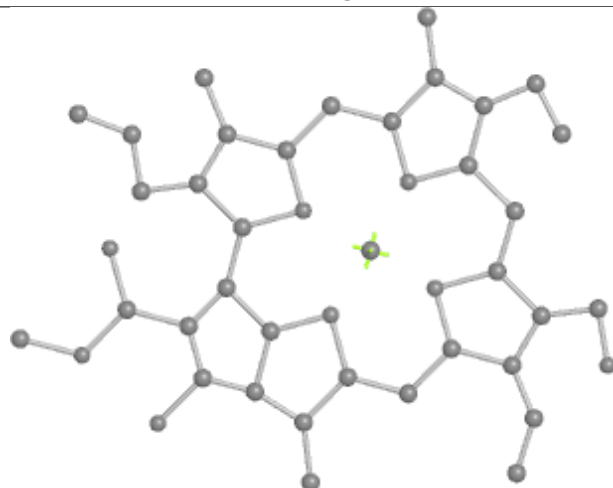
Bond lengths



Bond angles

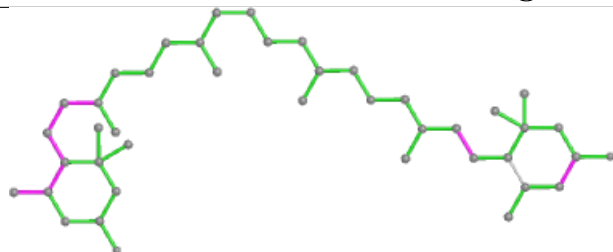


Torsions

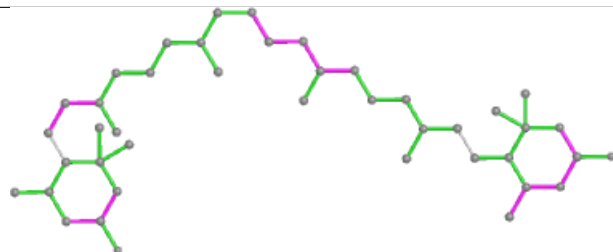


Rings

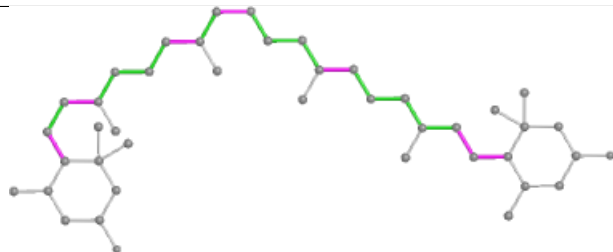
## Ligand Q6L V 315



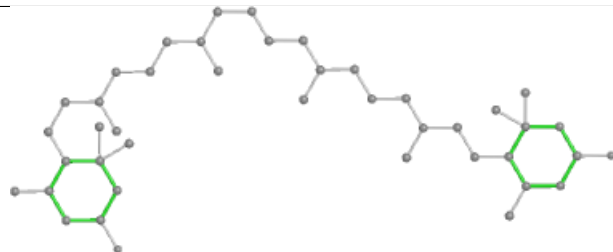
Bond lengths



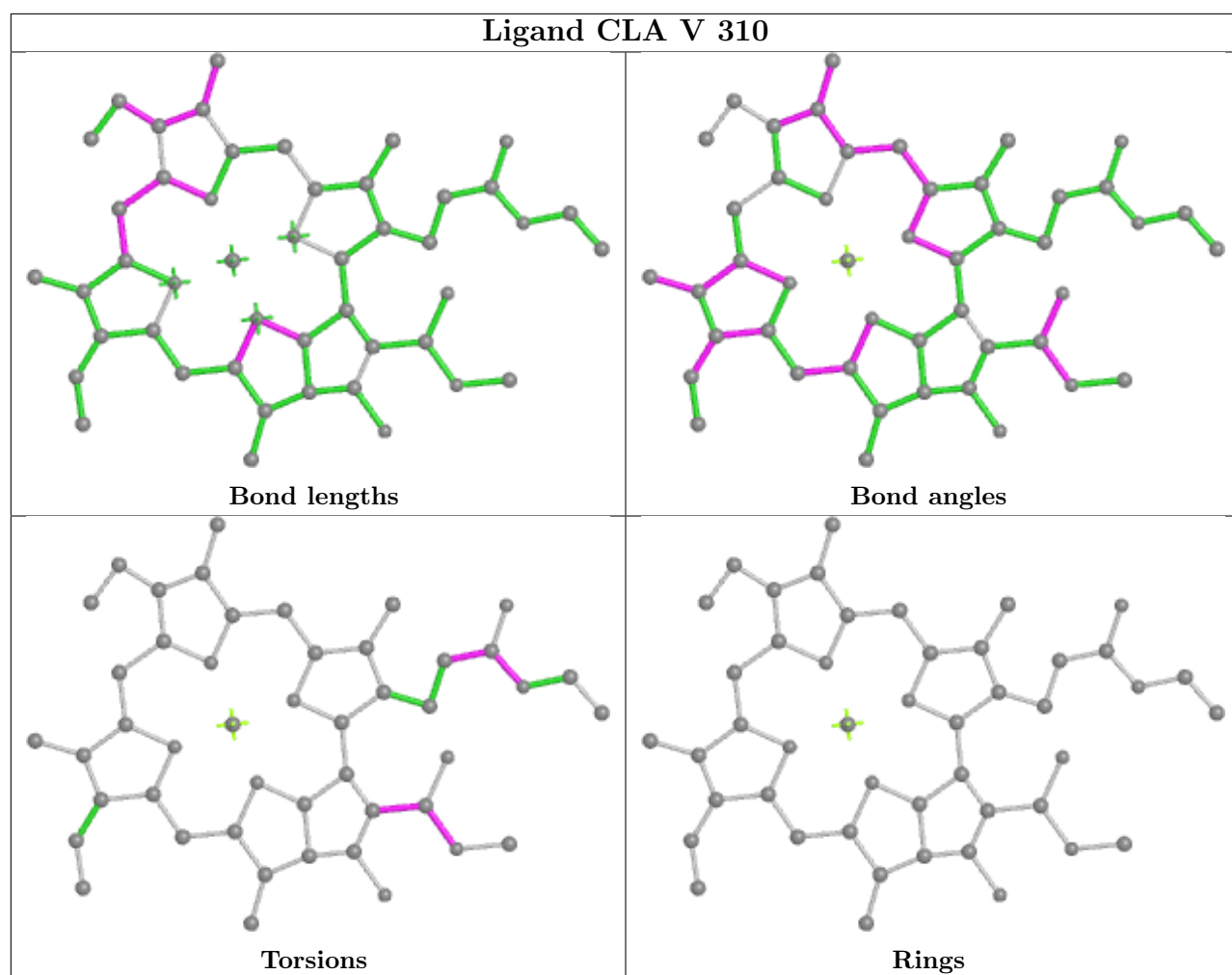
Bond angles



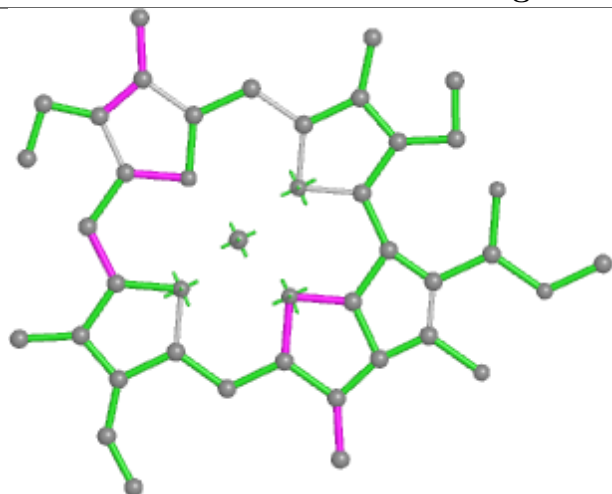
Torsions



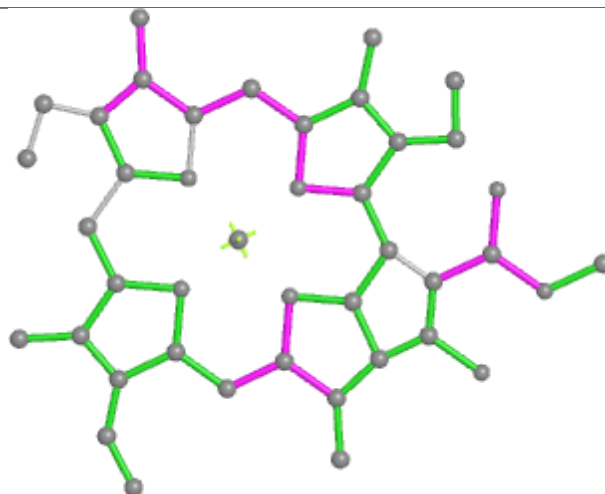
Rings



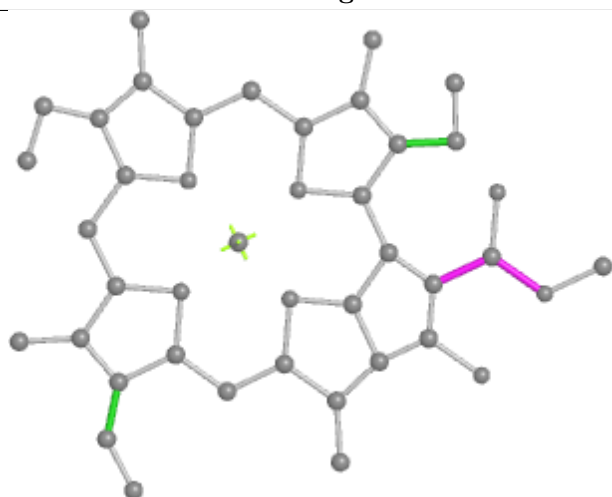
## Ligand CLA X 310



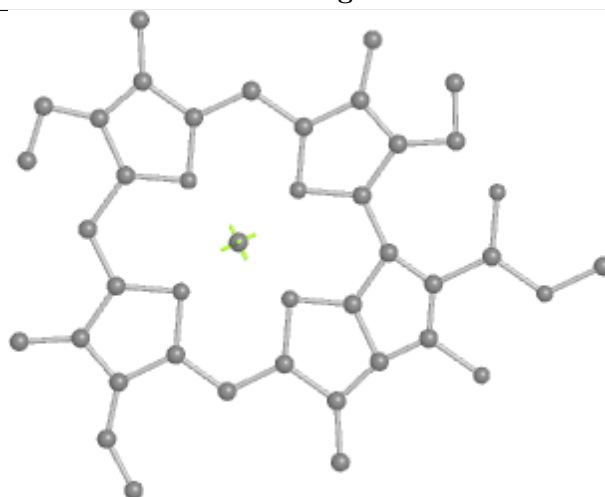
Bond lengths



Bond angles

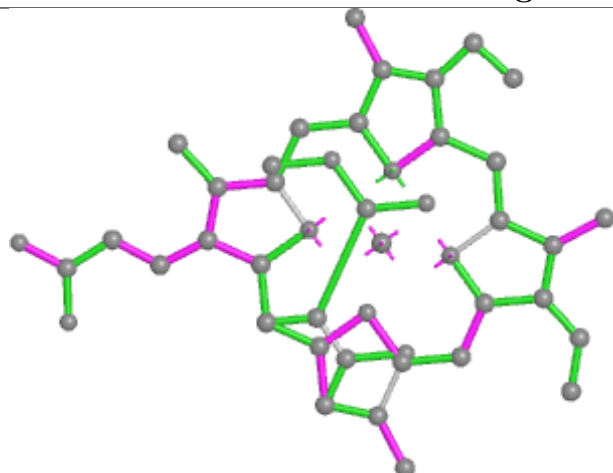


Torsions

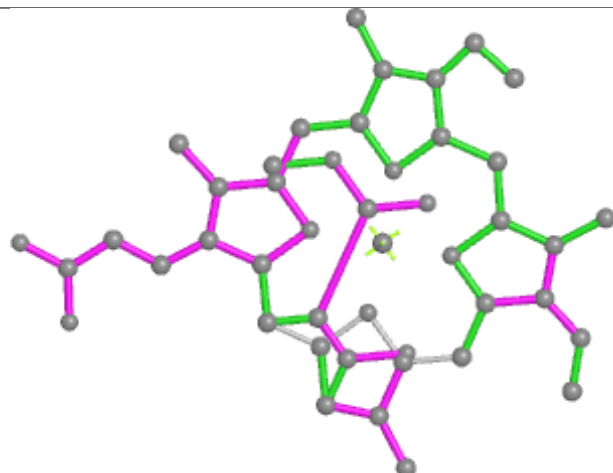


Rings

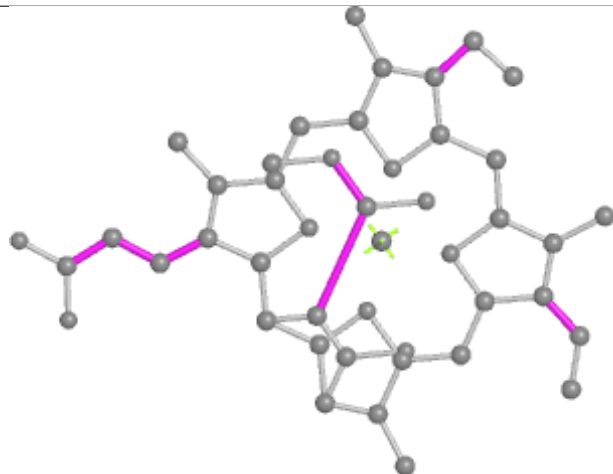
## Ligand KC2 V 308



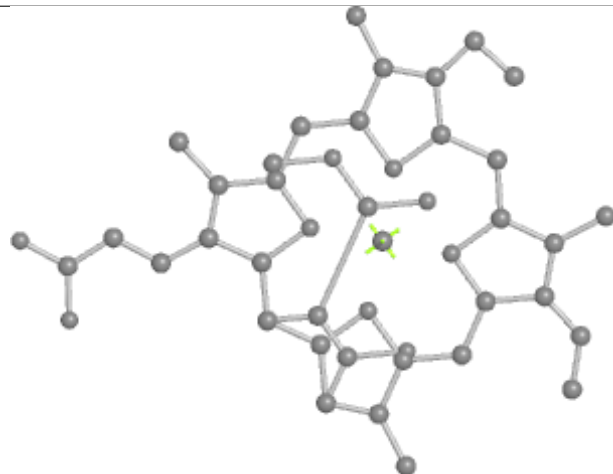
Bond lengths



Bond angles

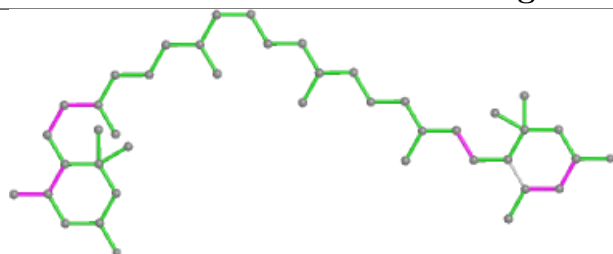


Torsions

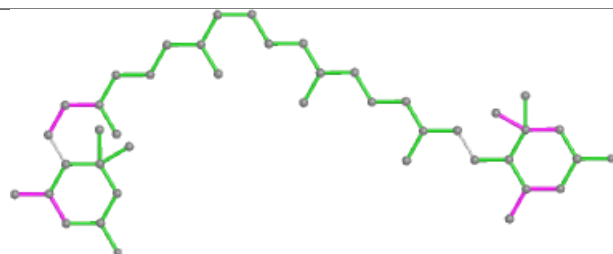


Rings

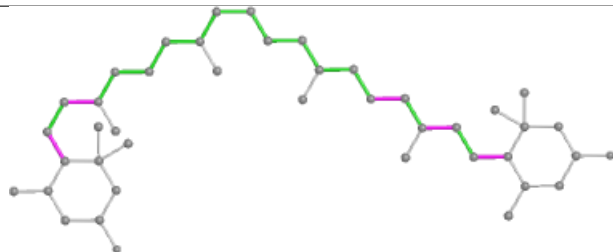
## Ligand Q6L V 321



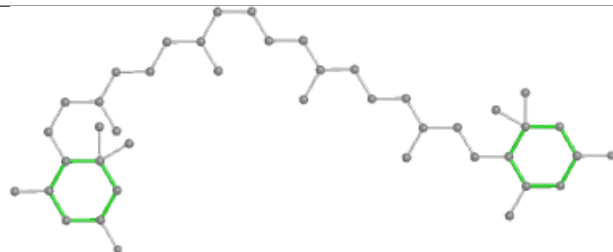
Bond lengths



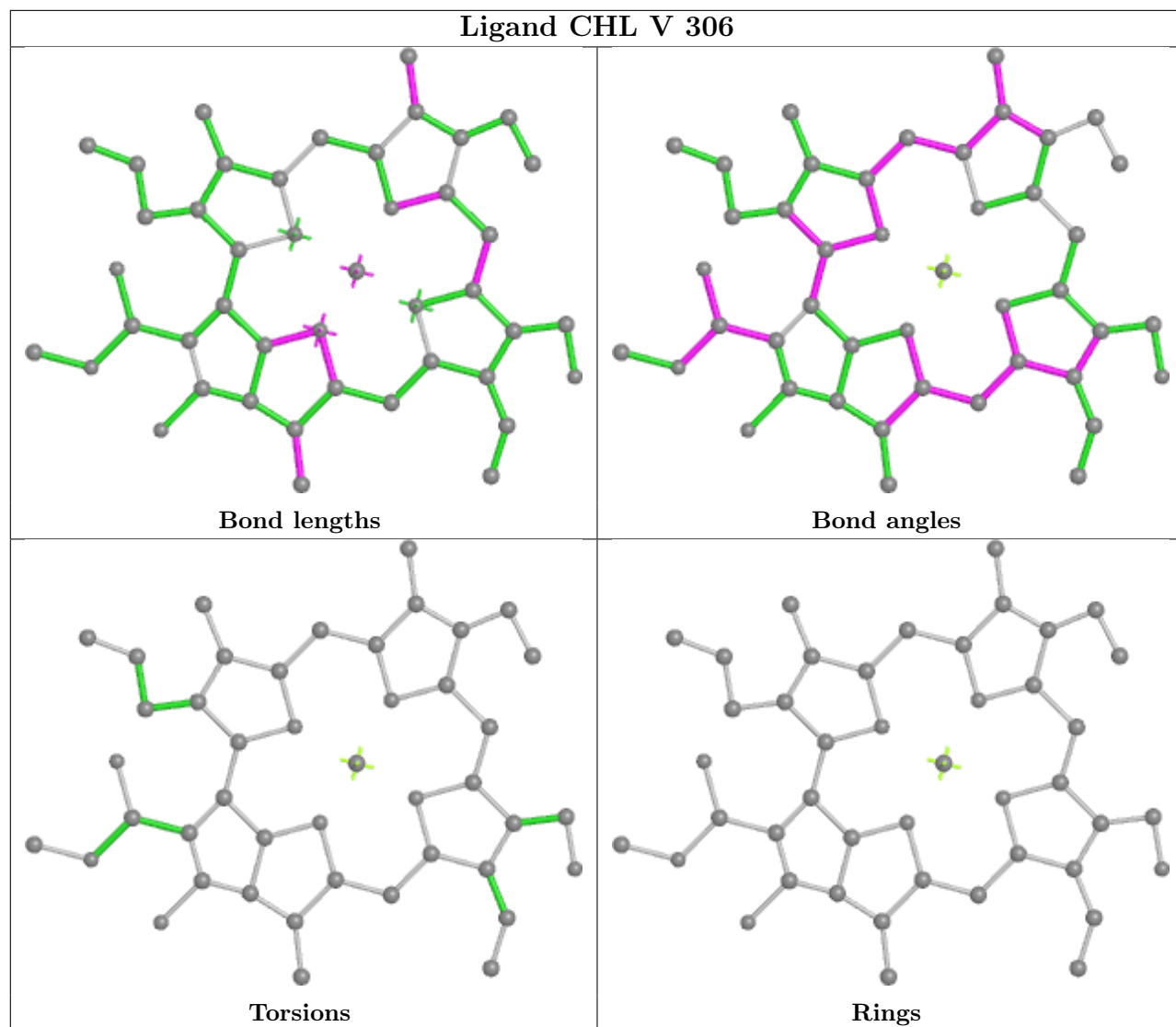
Bond angles

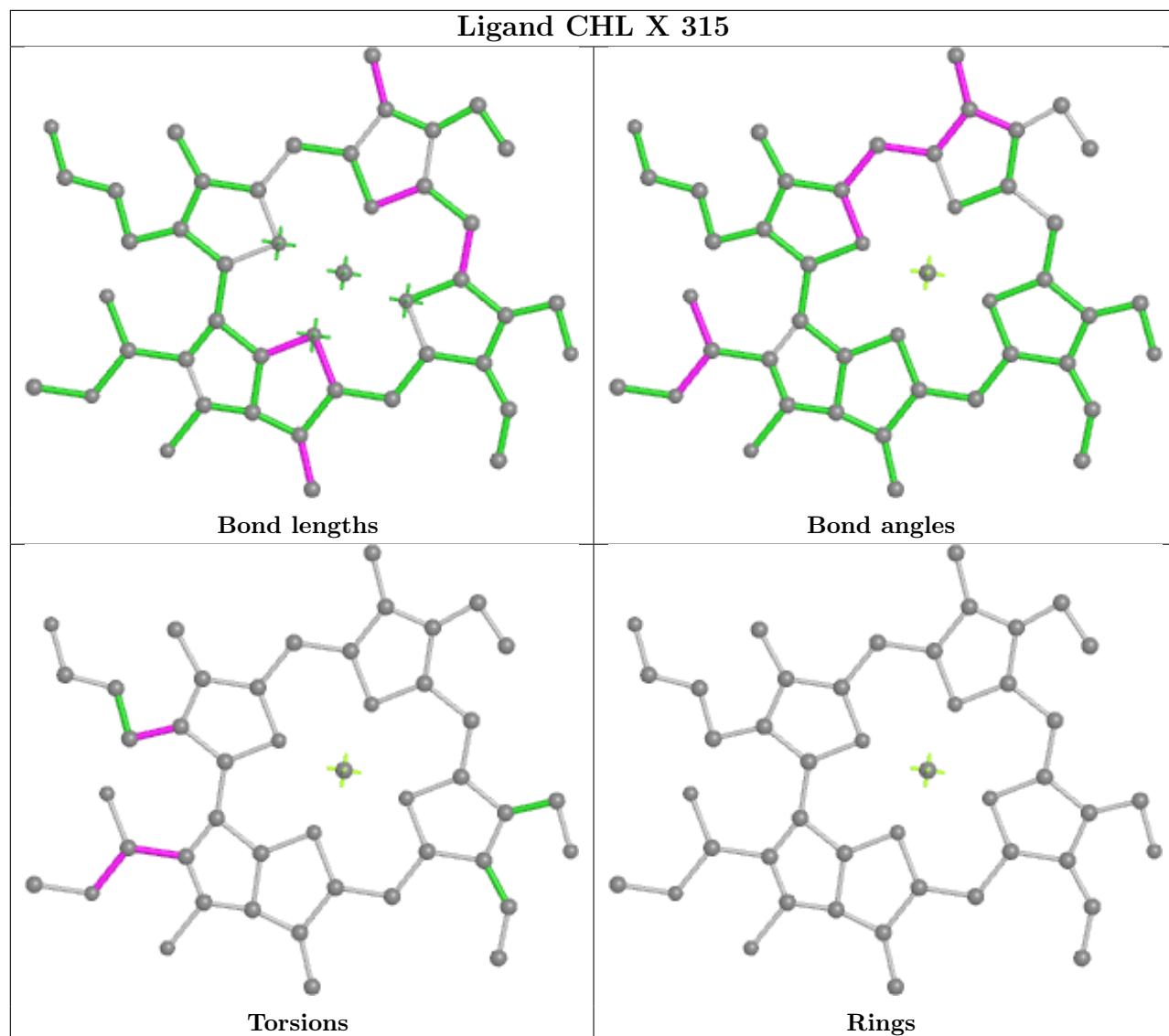


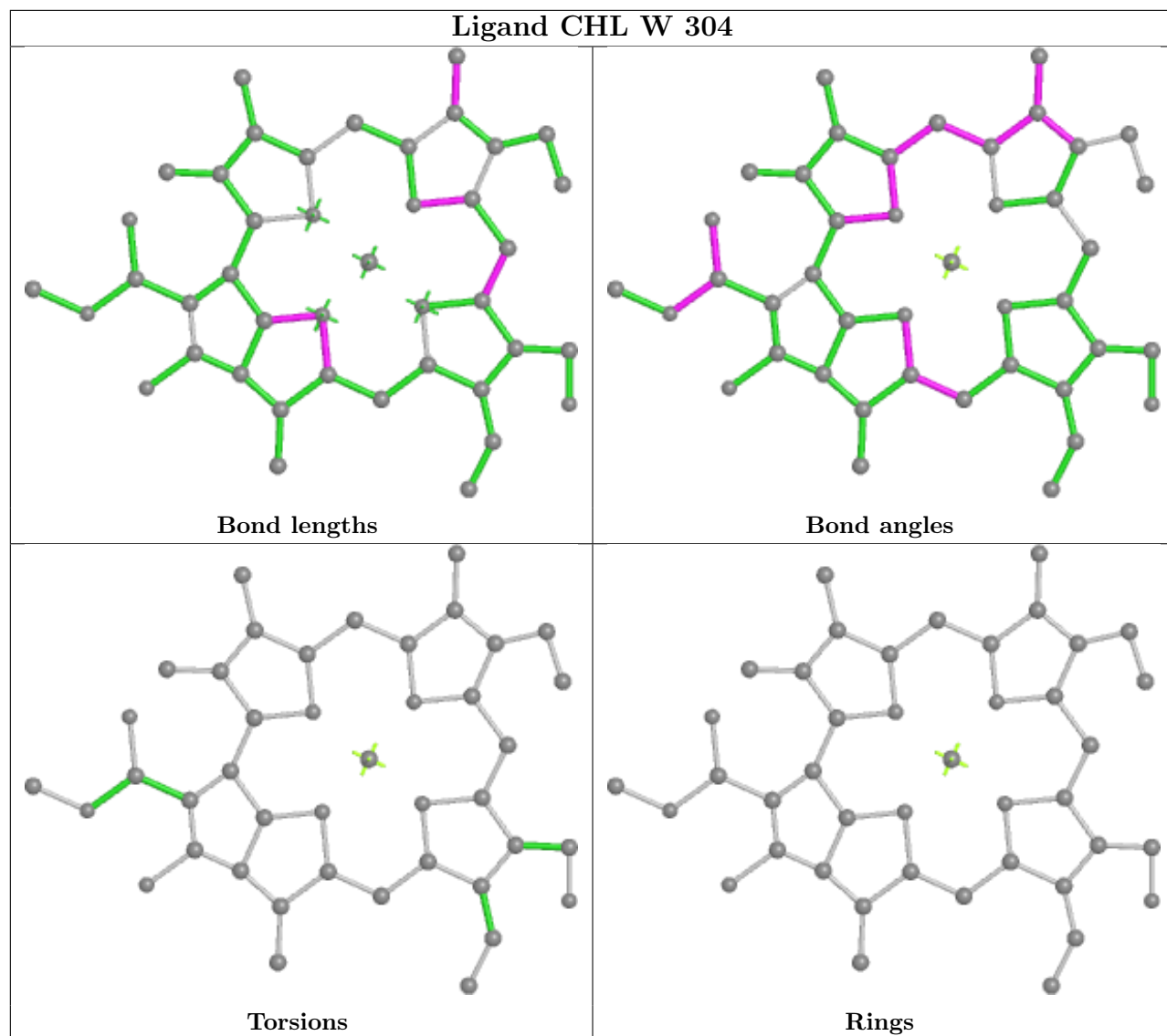
Torsions

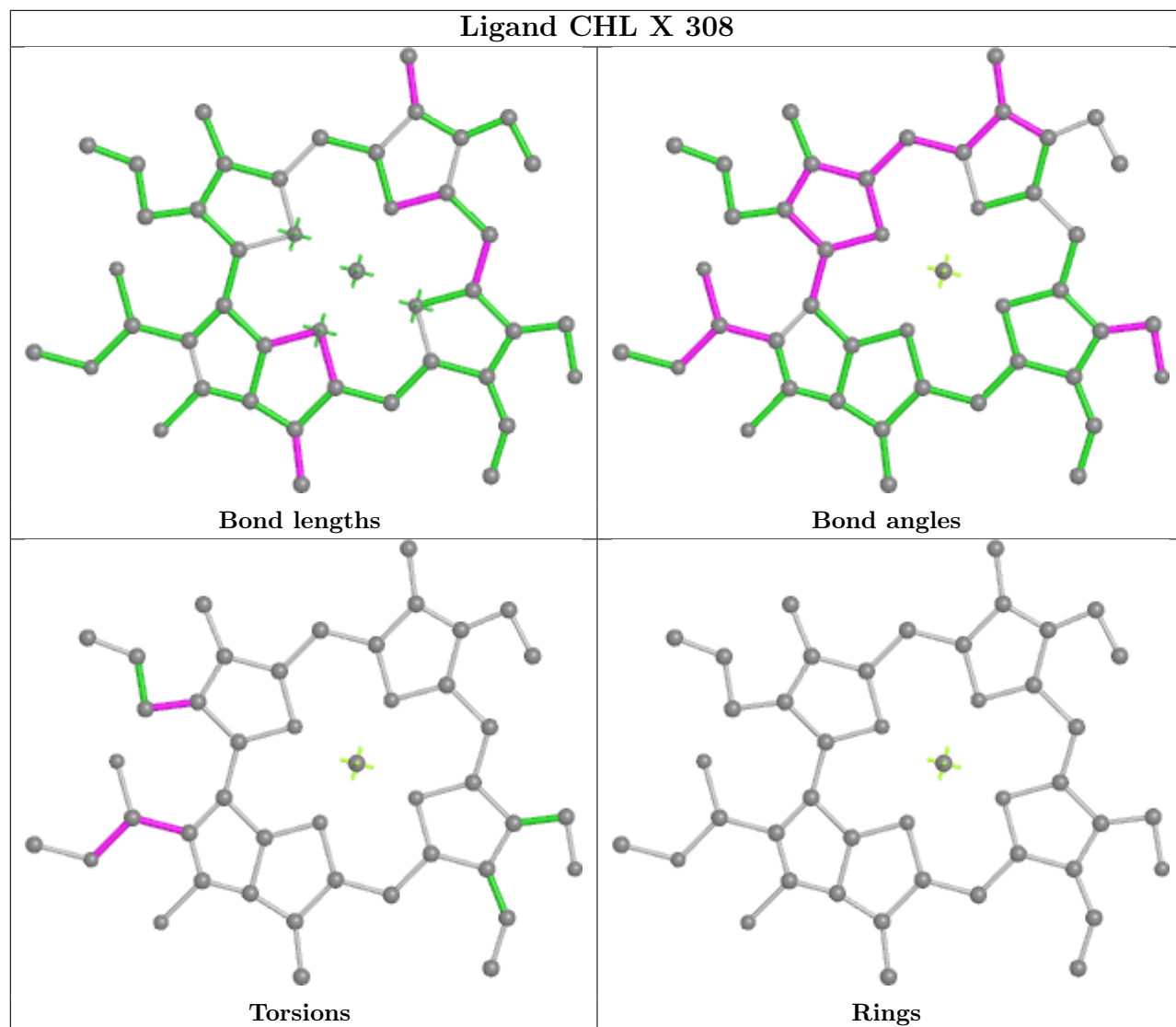


Rings

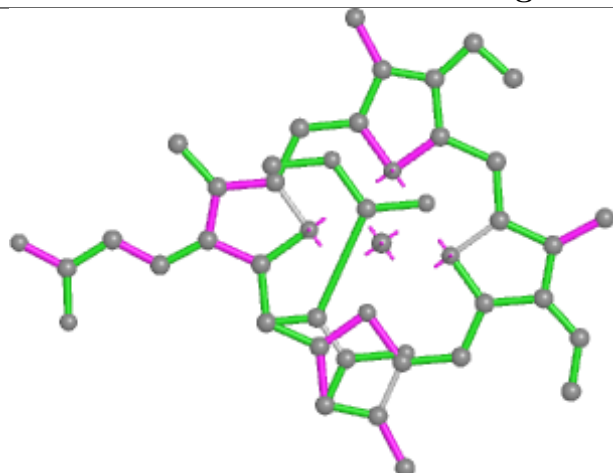




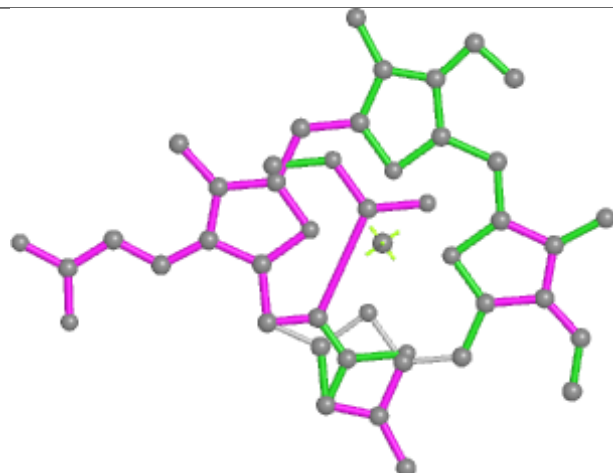




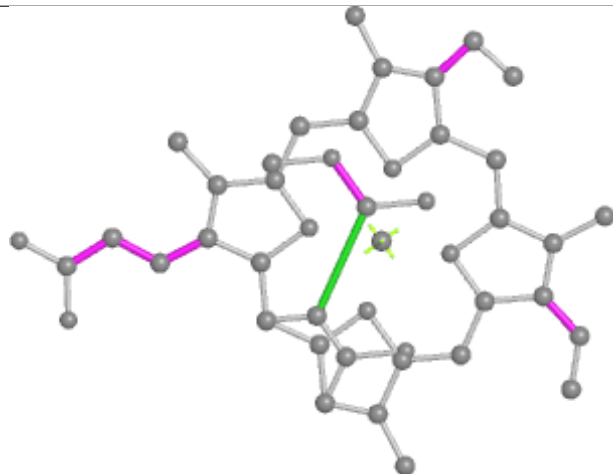
## Ligand KC2 X 309



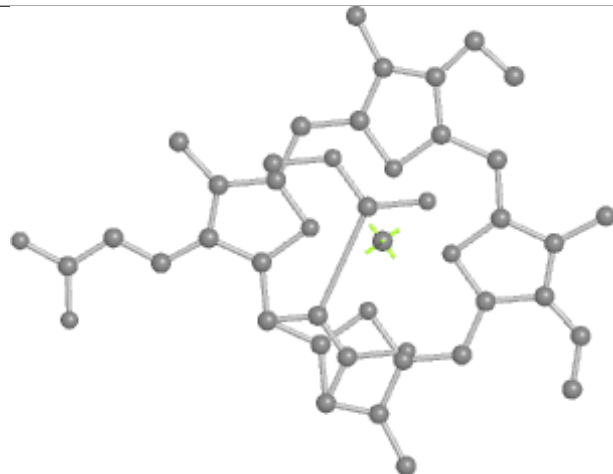
Bond lengths



Bond angles

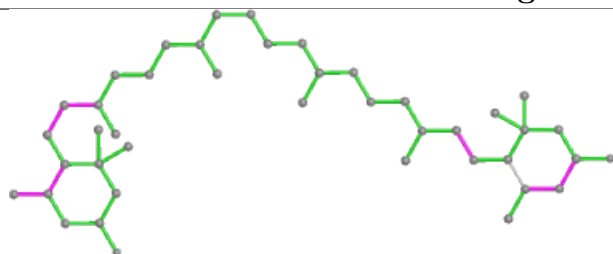


Torsions

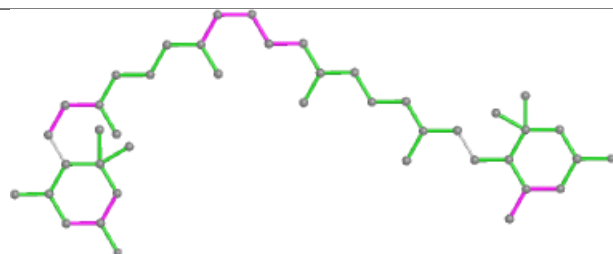


Rings

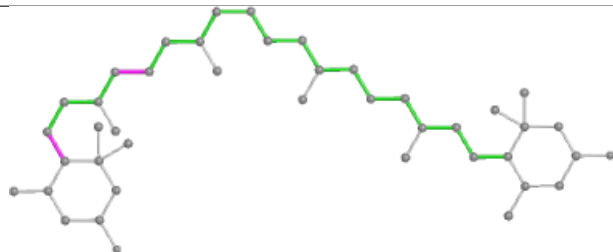
## Ligand Q6L X 317



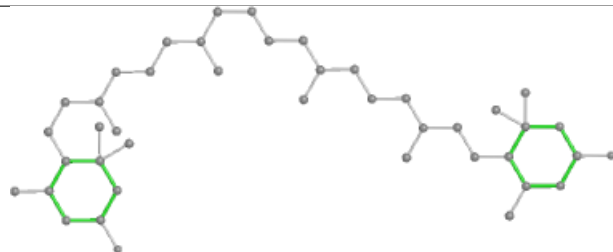
Bond lengths



Bond angles

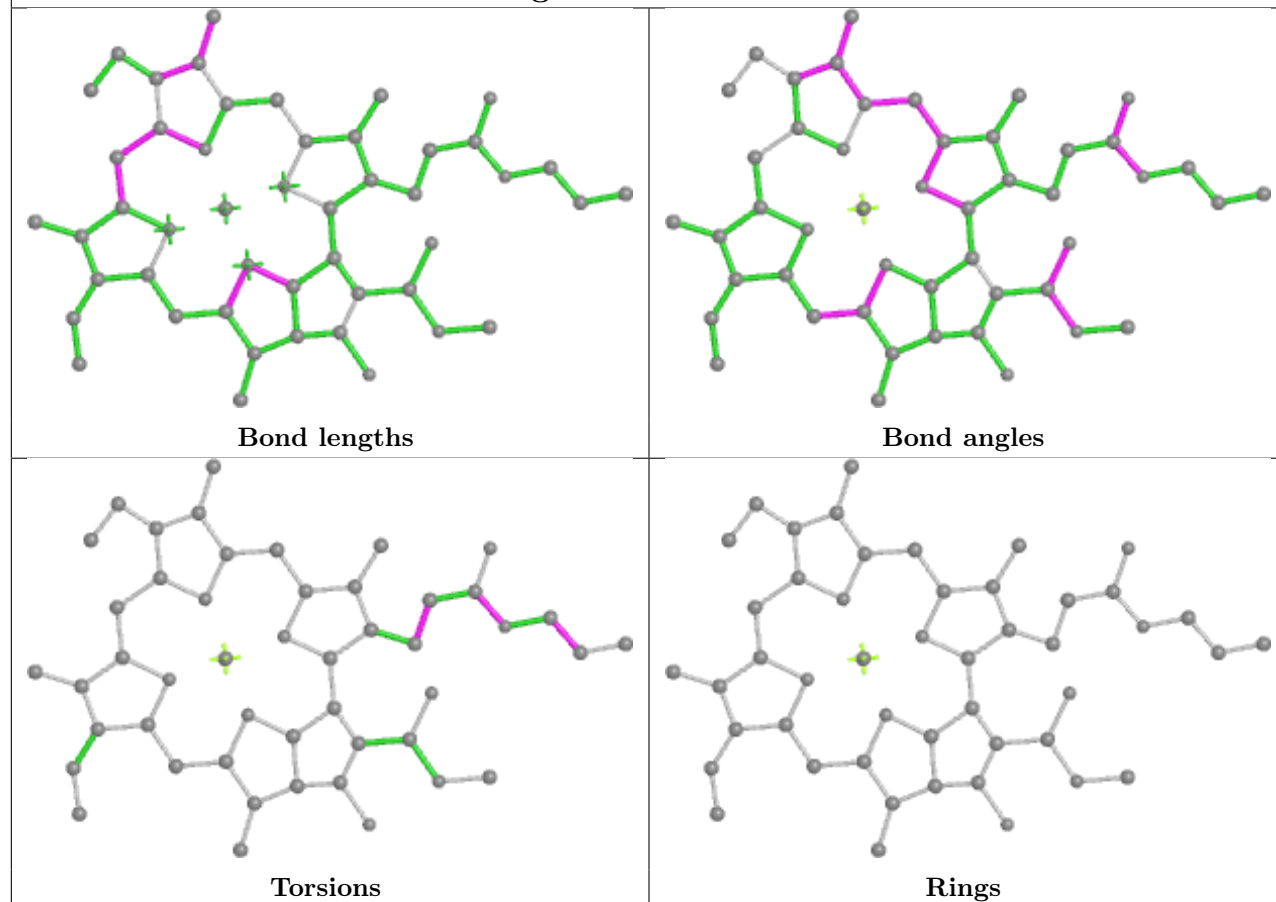


Torsions

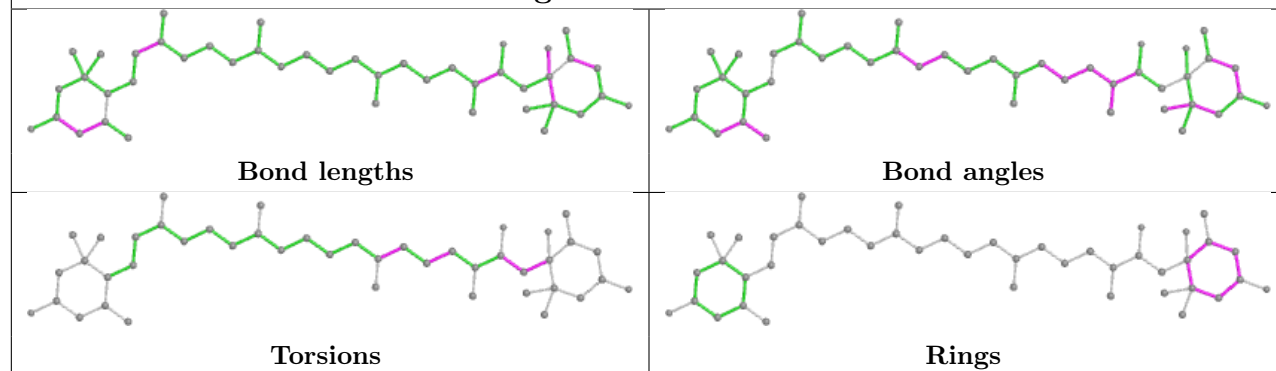


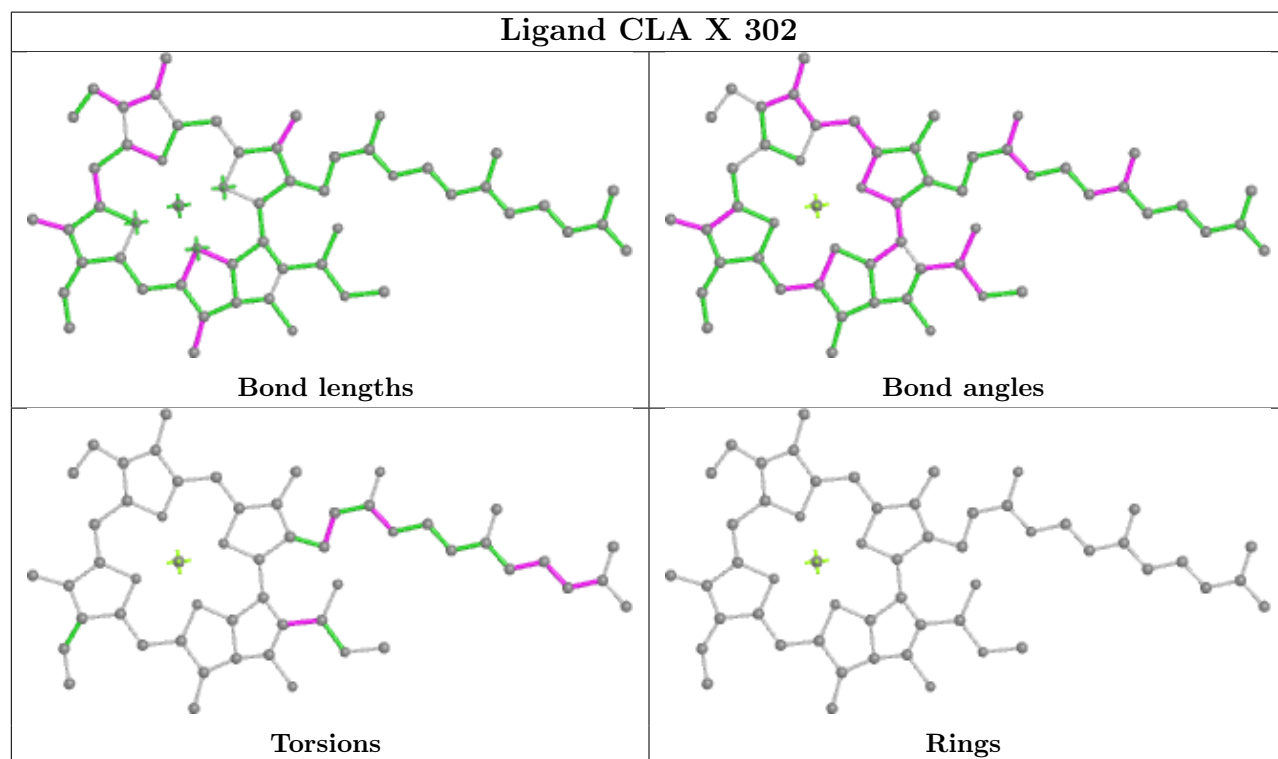
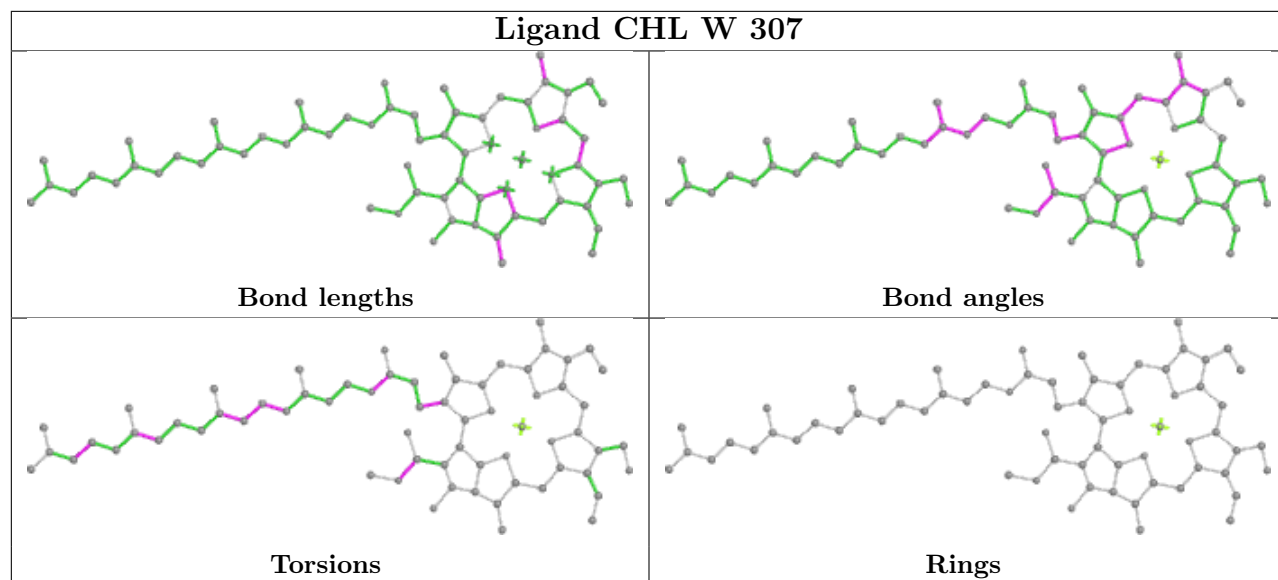
Rings

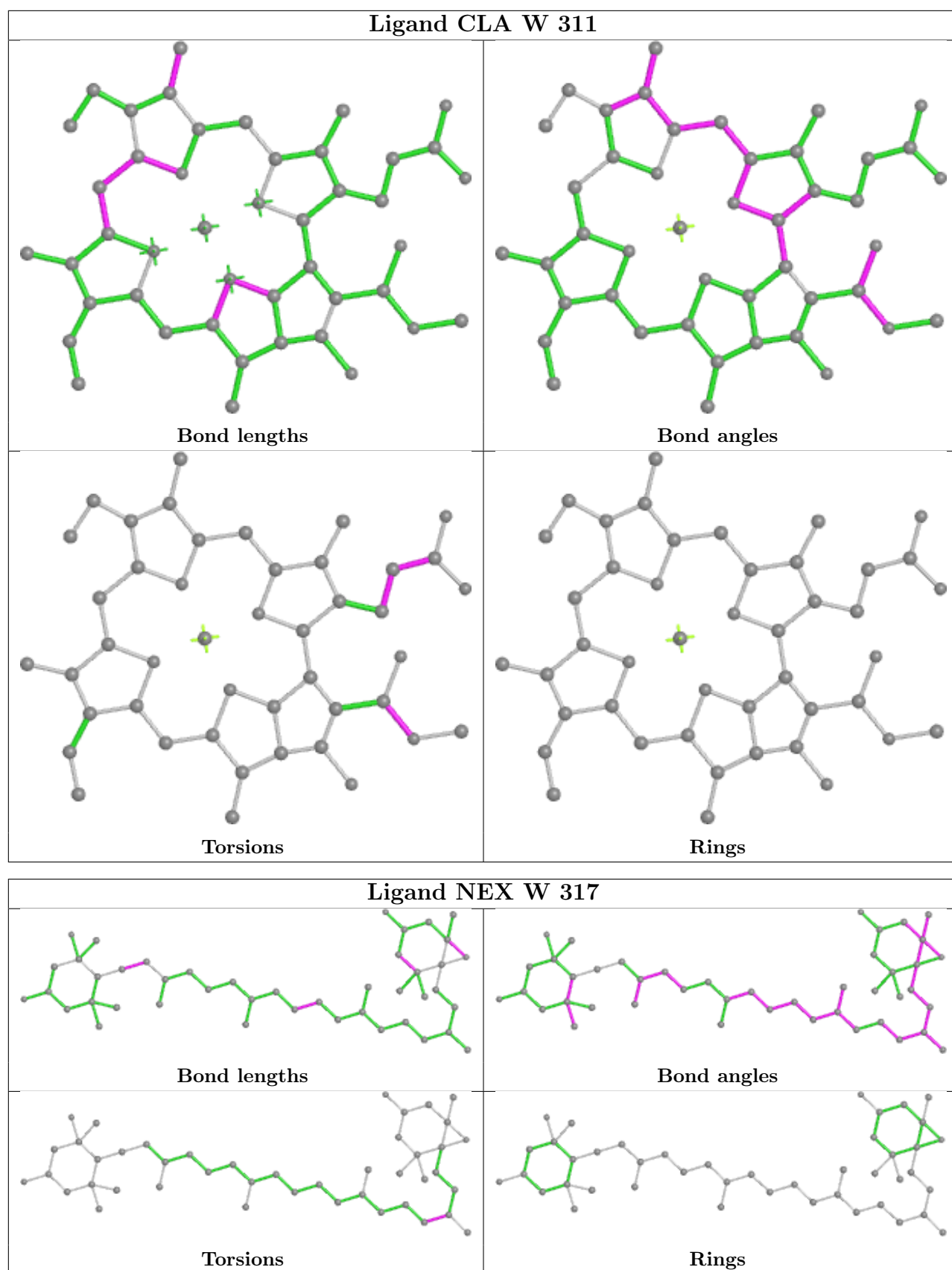
## Ligand CLA V 313

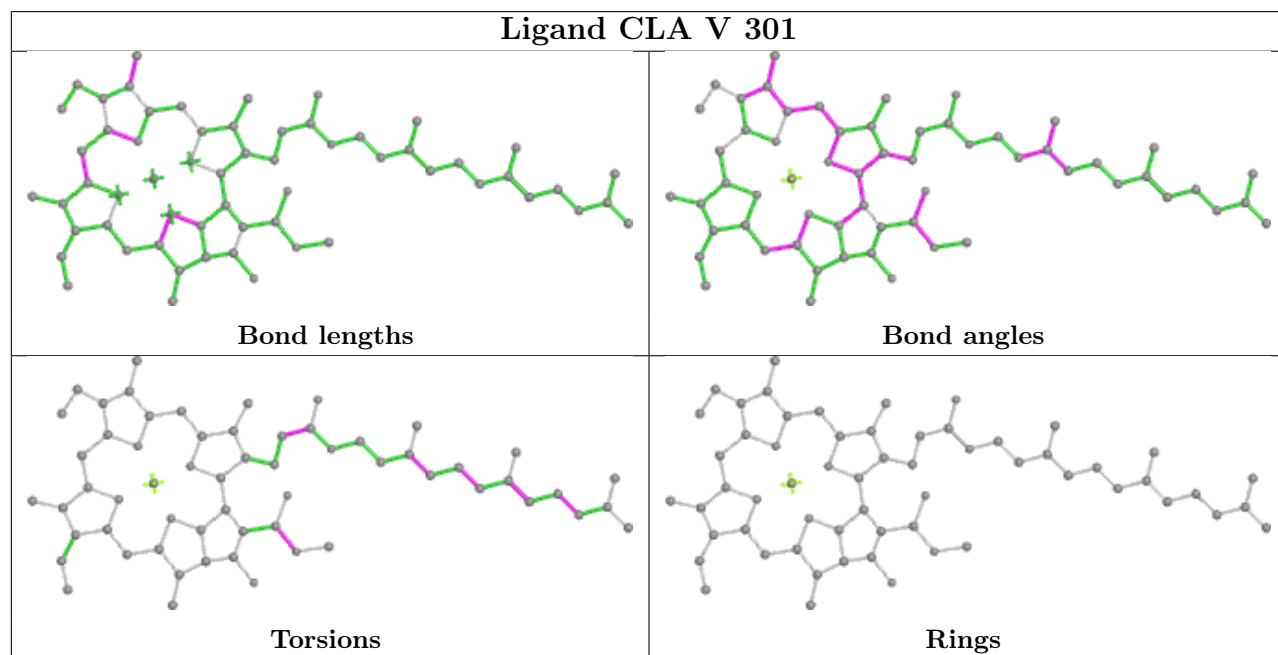
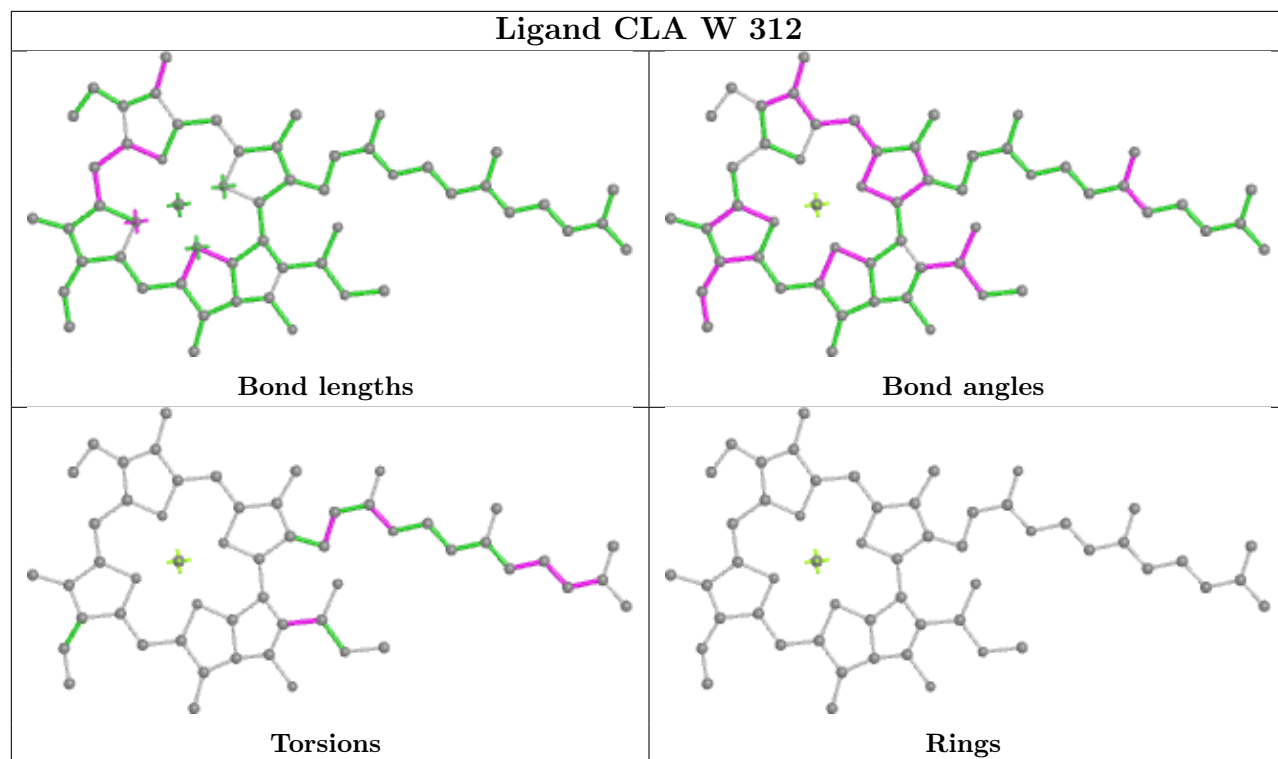


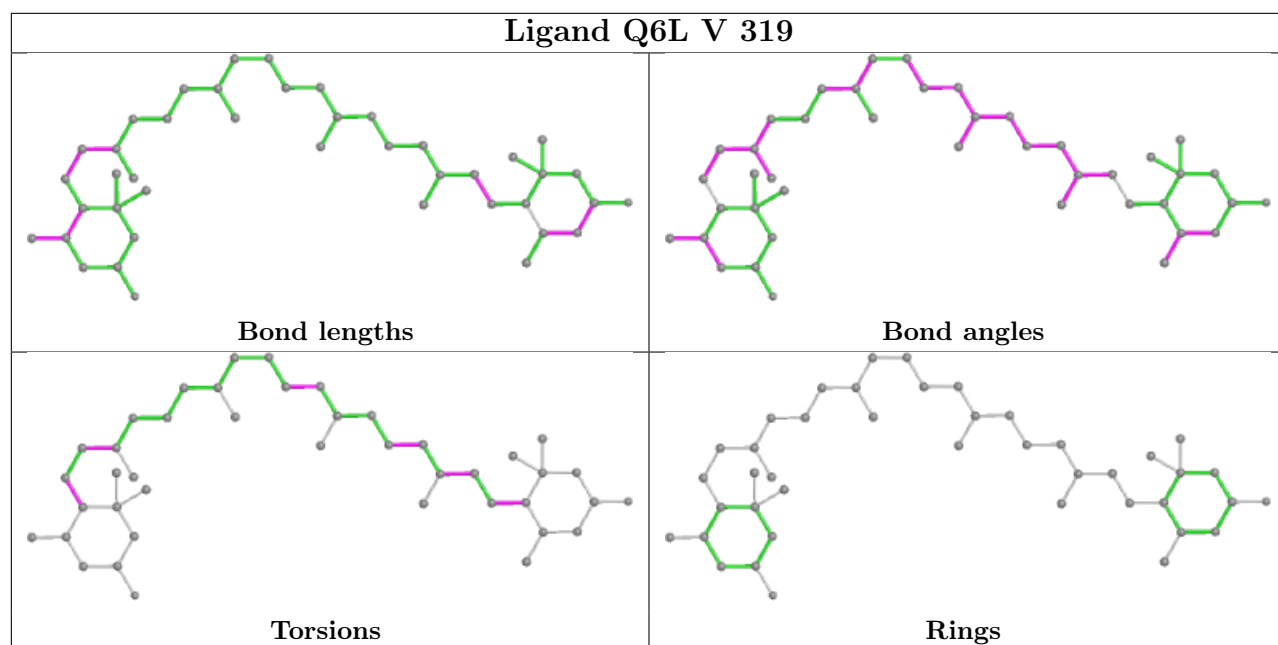
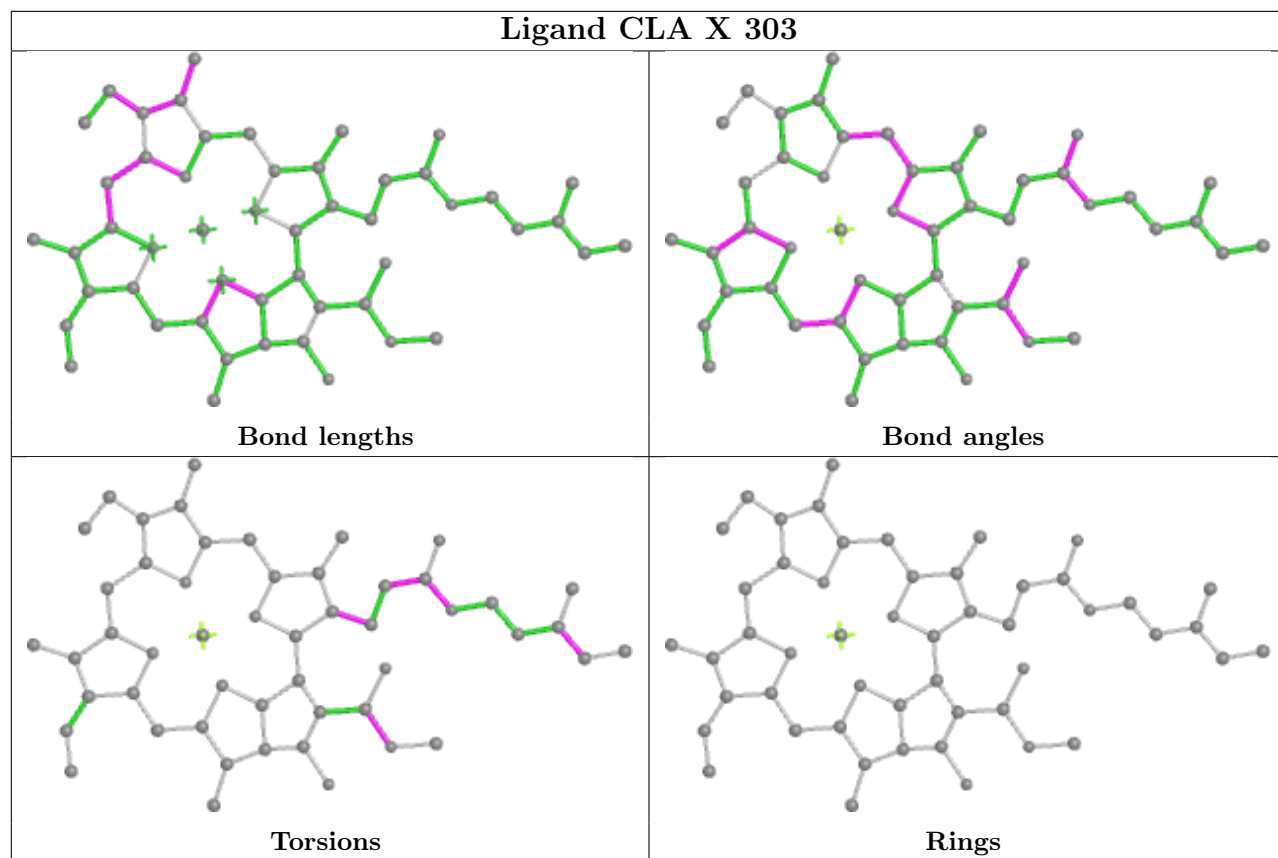
## Ligand IWJ X 318



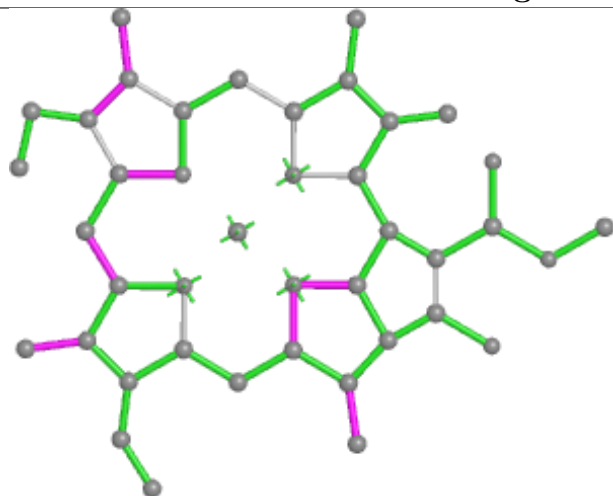




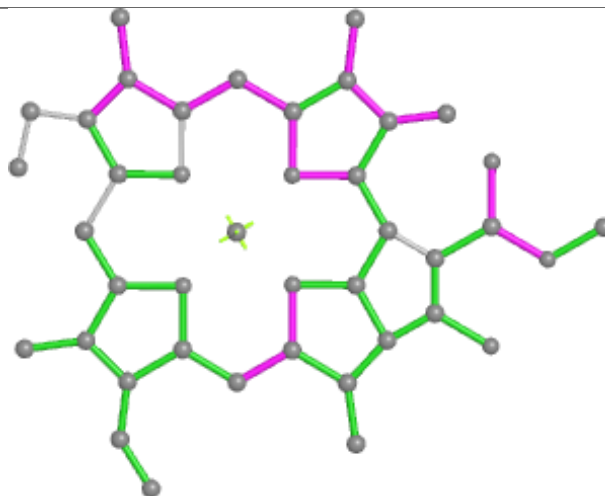




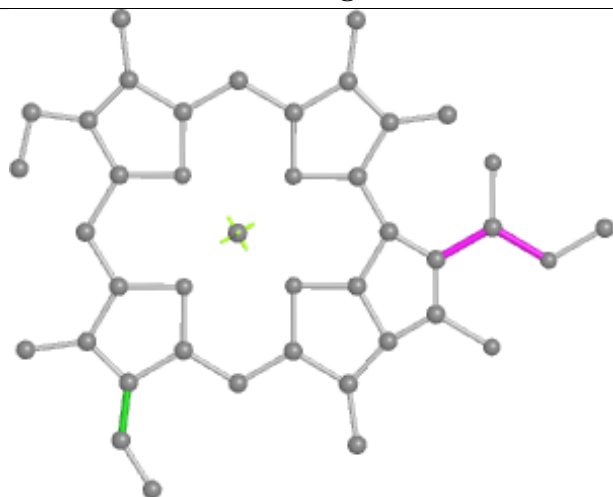
## Ligand CLA X 313



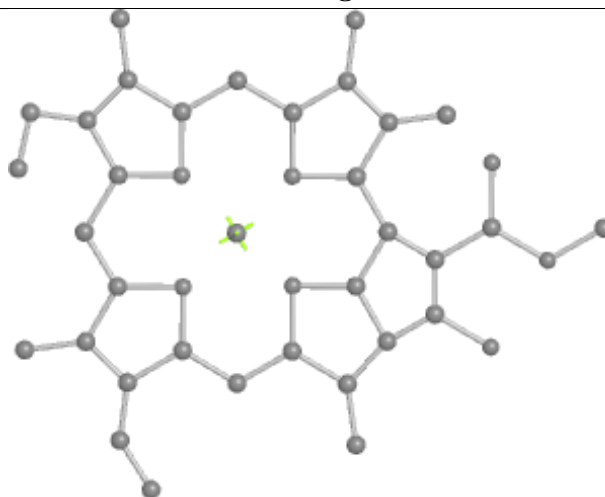
Bond lengths



Bond angles

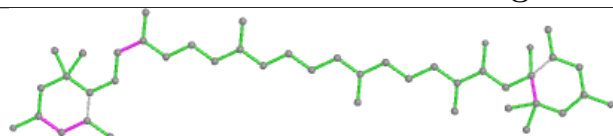


Torsions

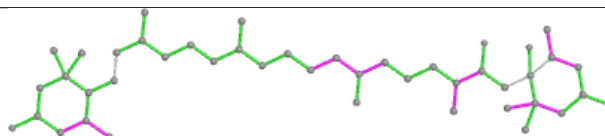


Rings

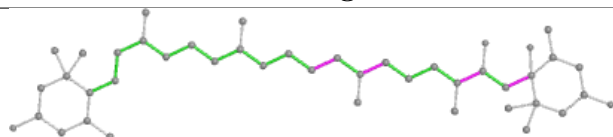
## Ligand IWJ W 318



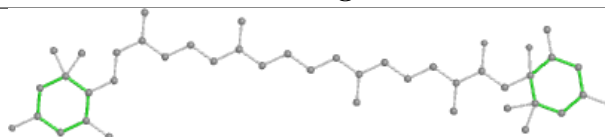
Bond lengths



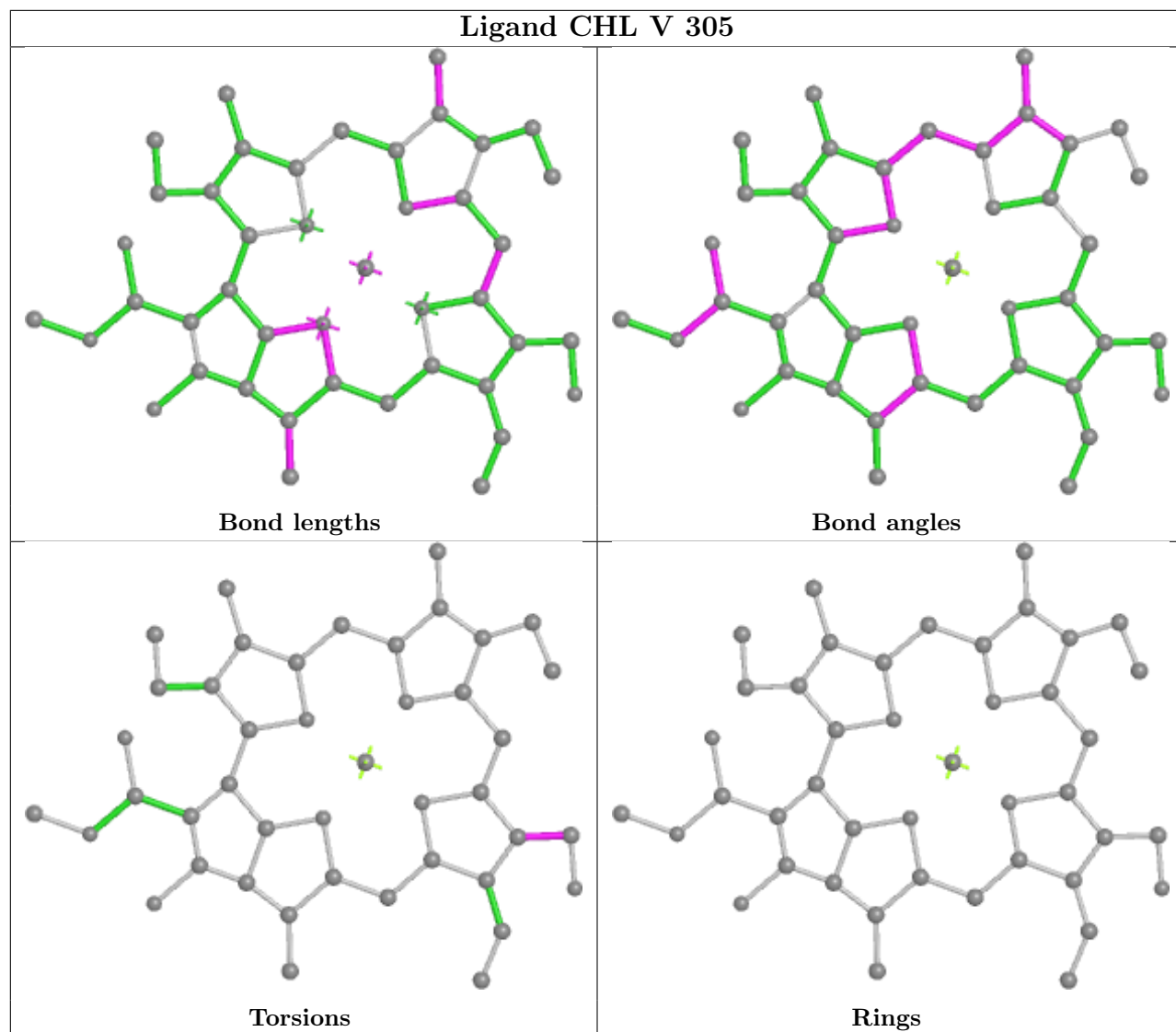
Bond angles

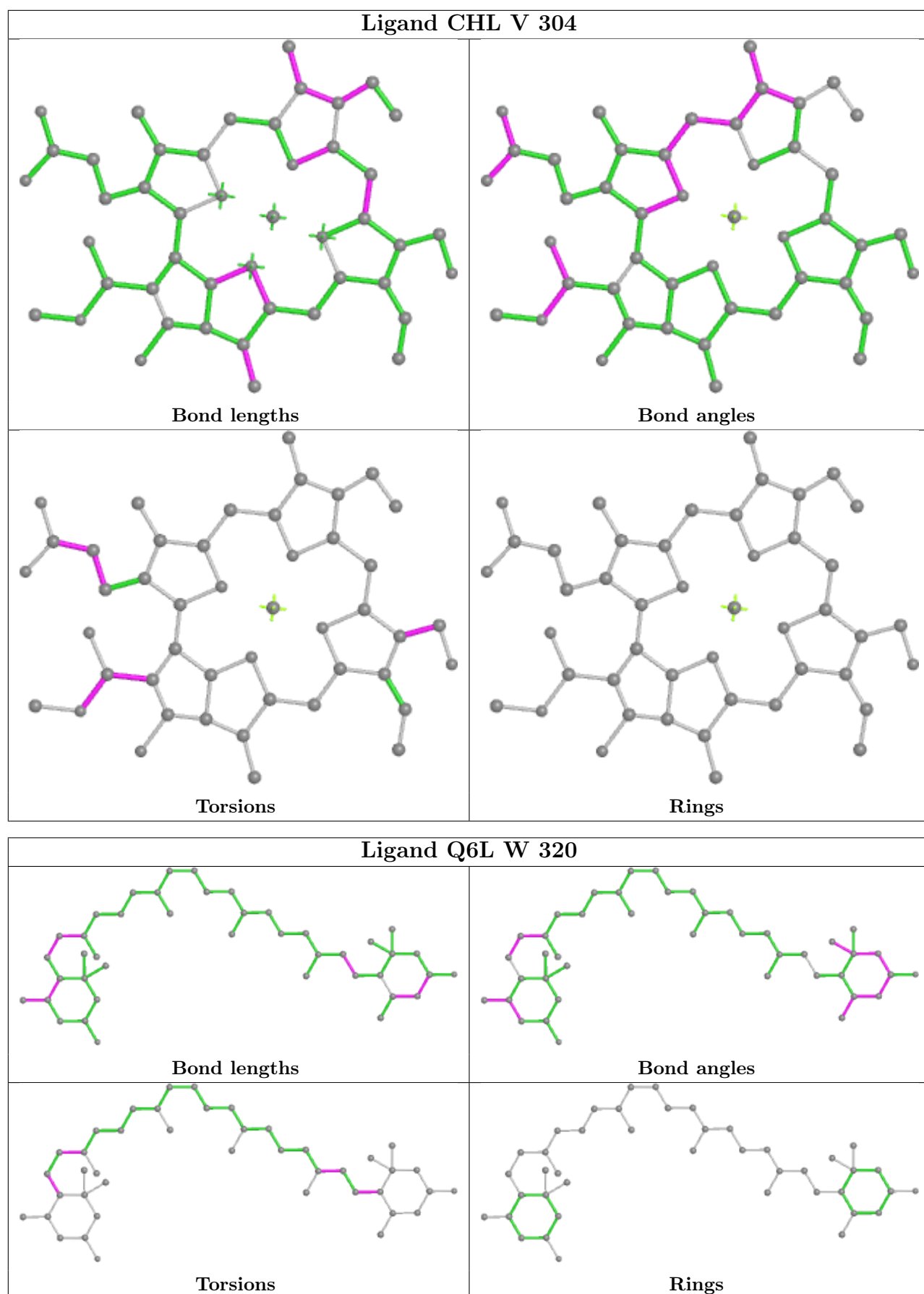


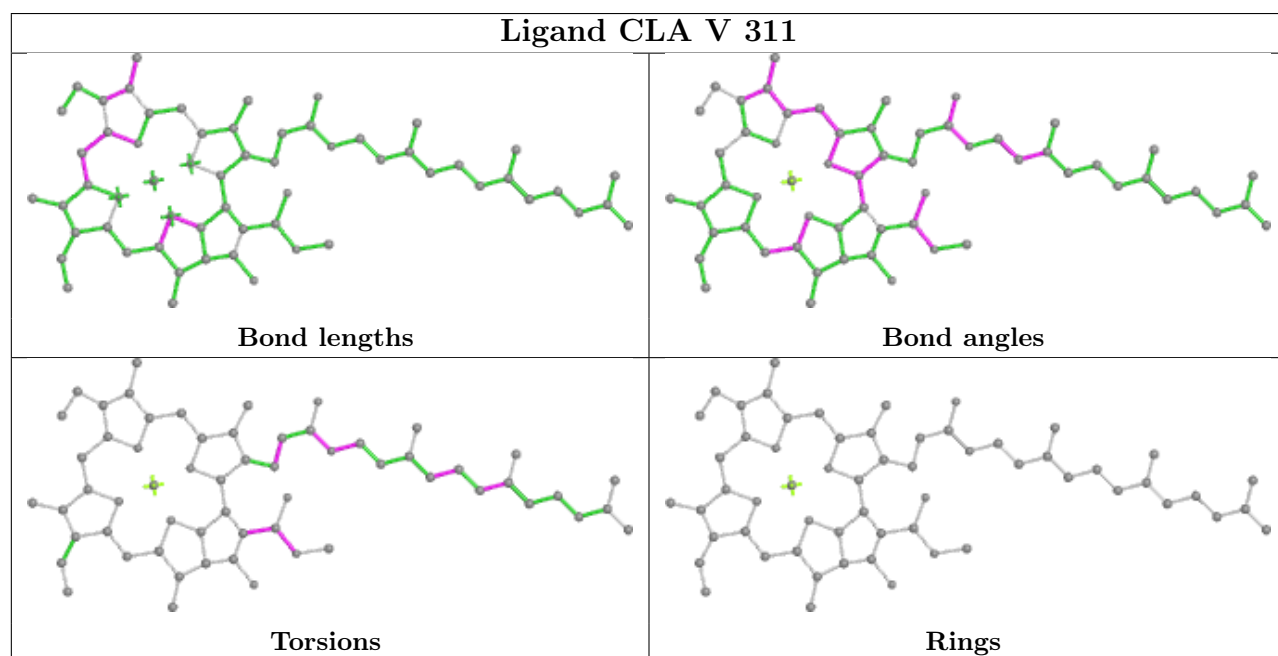
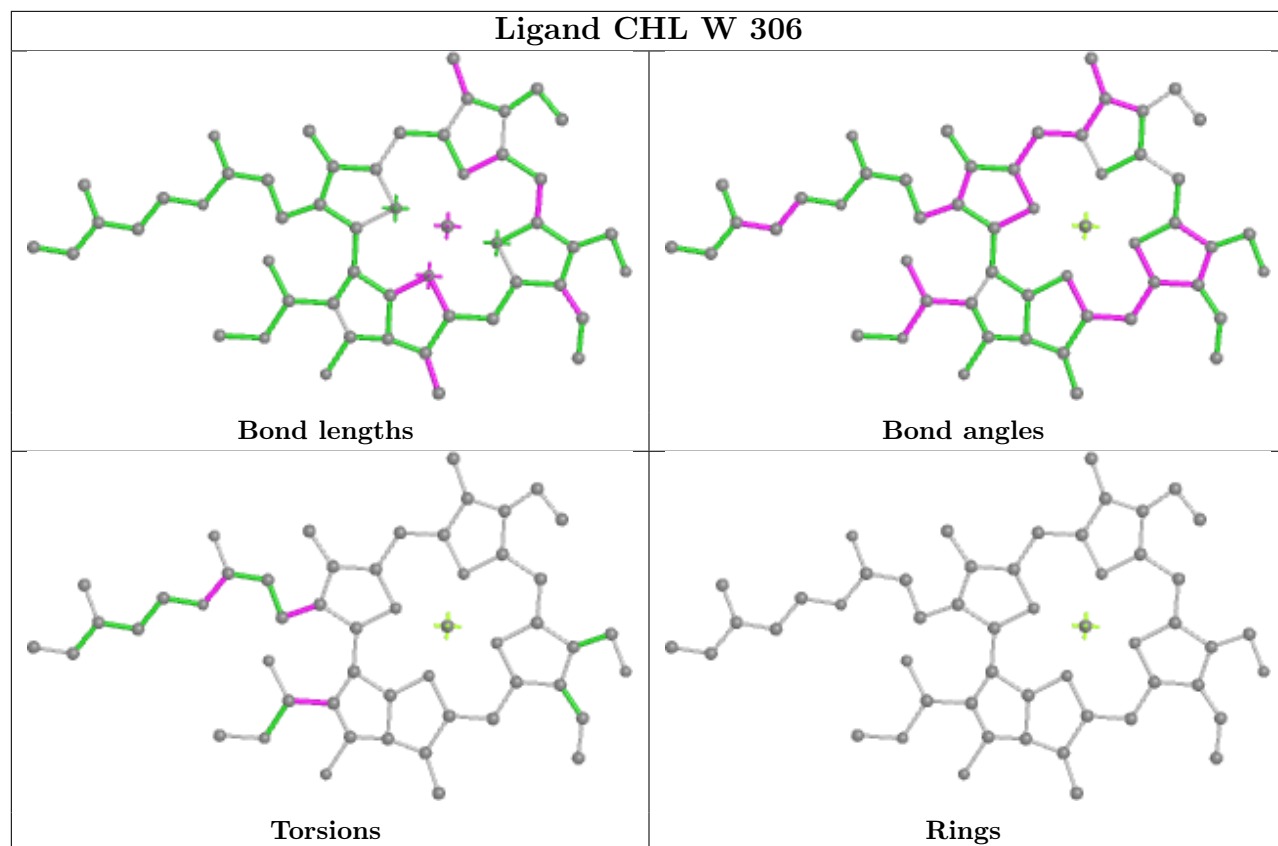
Torsions



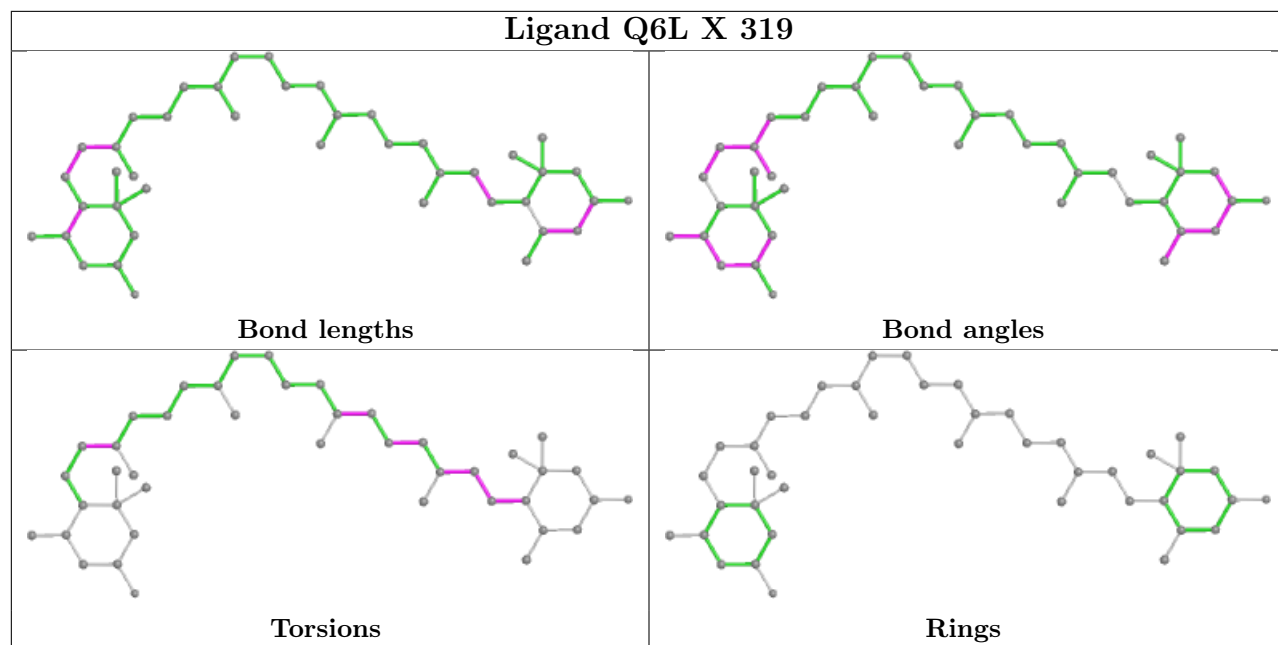
Rings



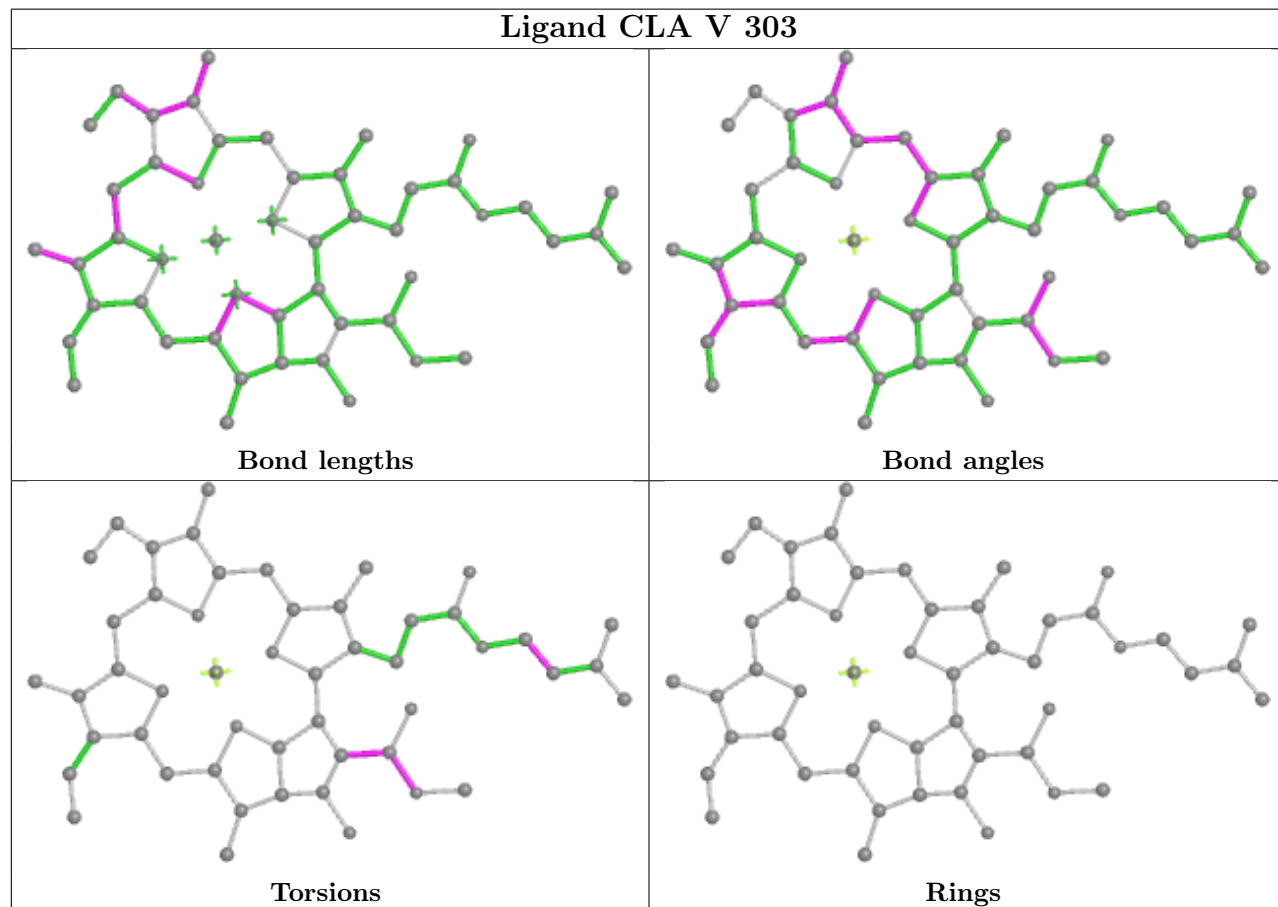




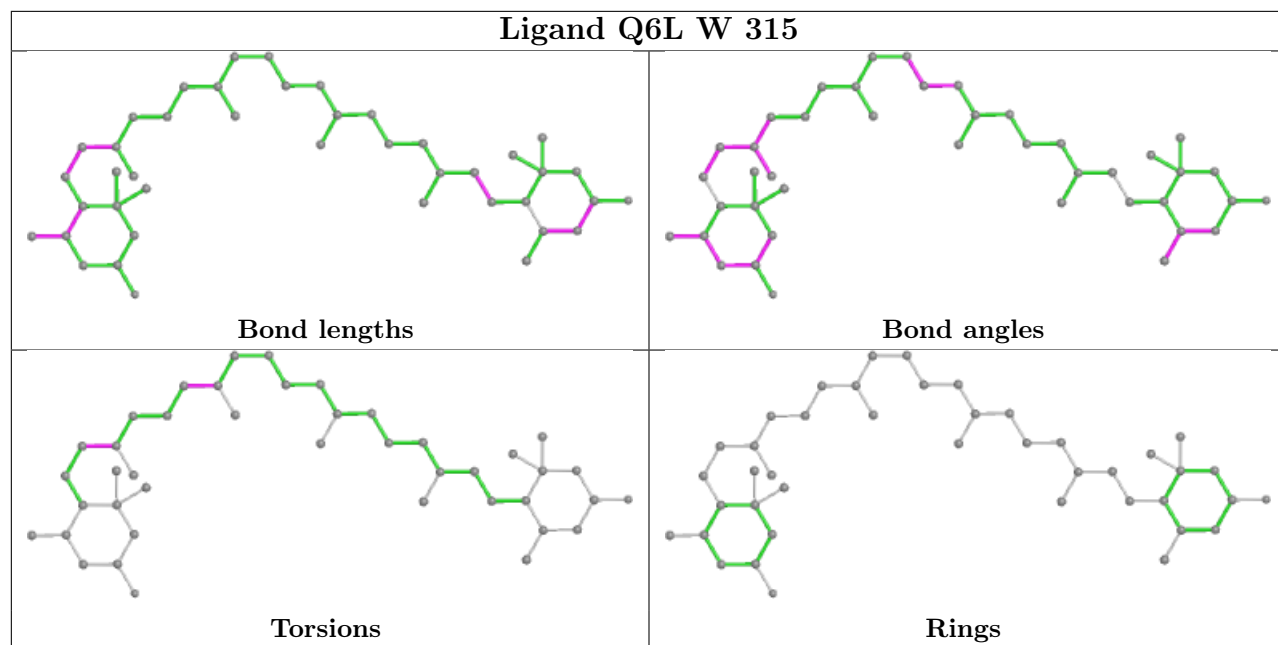
## Ligand Q6L X 319



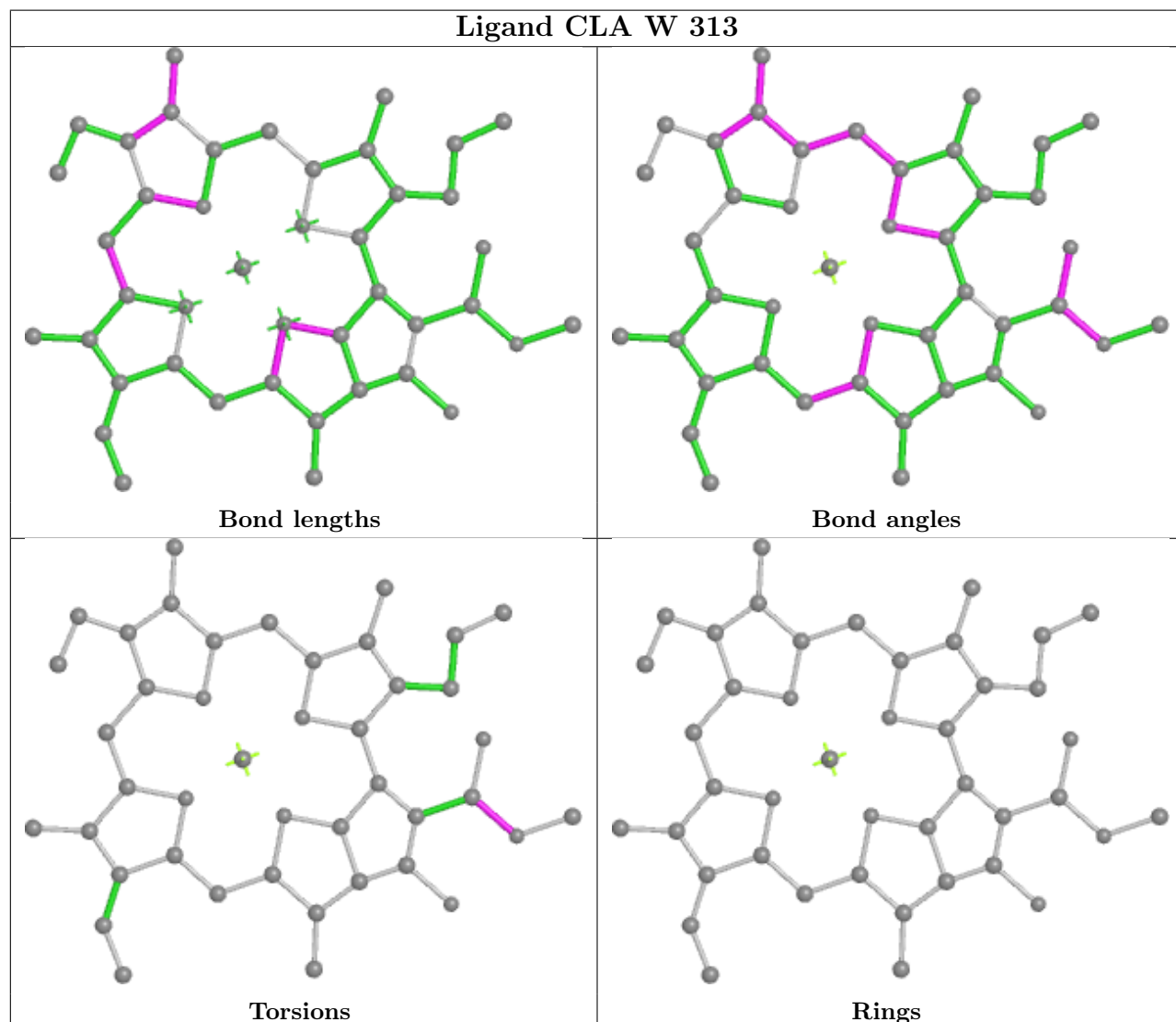
## Ligand CLA V 303



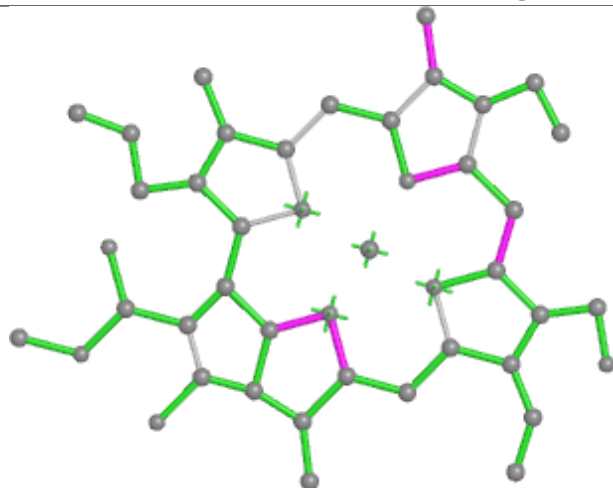
## Ligand Q6L W 315



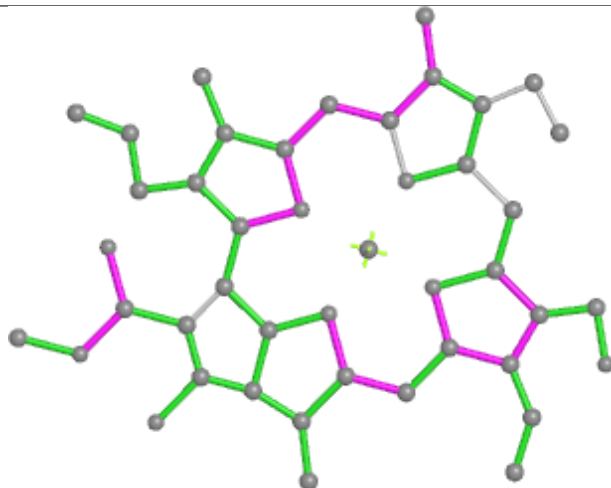
## Ligand CLA W 313



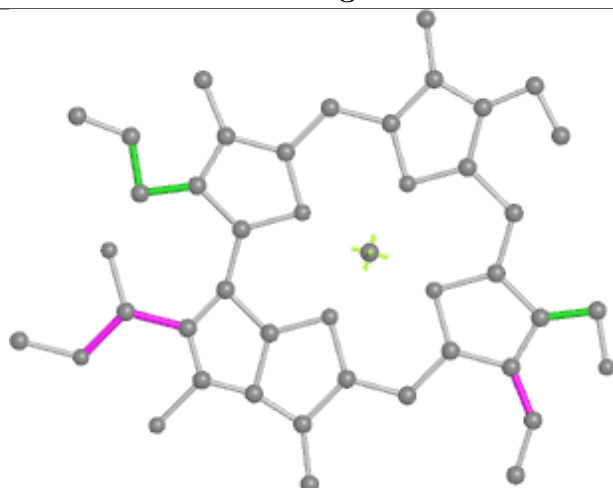
## Ligand CHL V 307



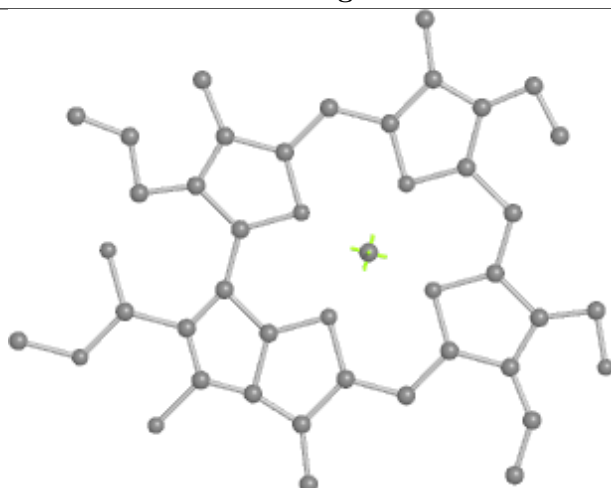
Bond lengths



Bond angles

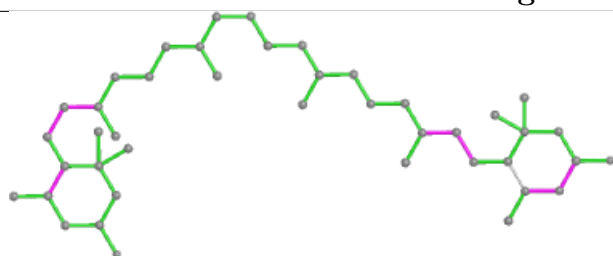


Torsions

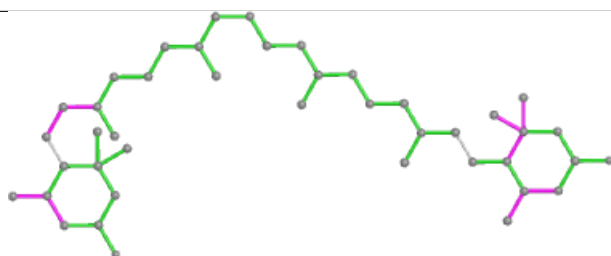


Rings

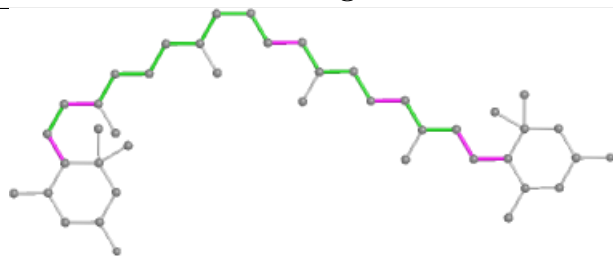
## Ligand Q6L V 316



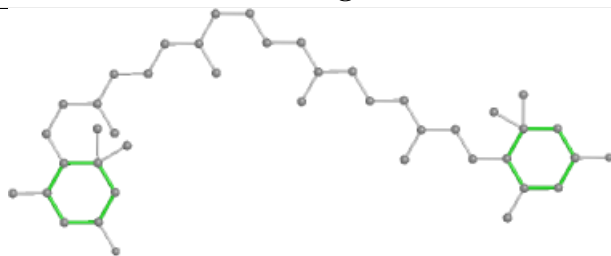
Bond lengths



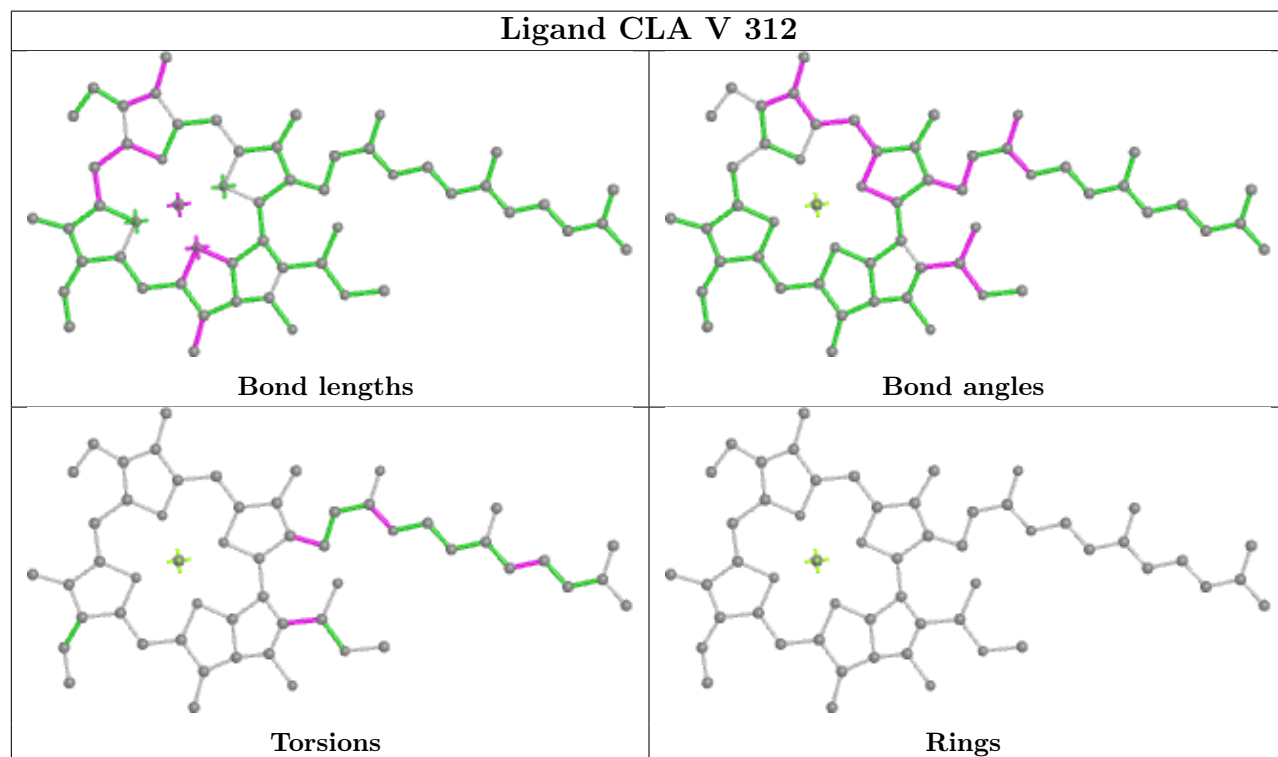
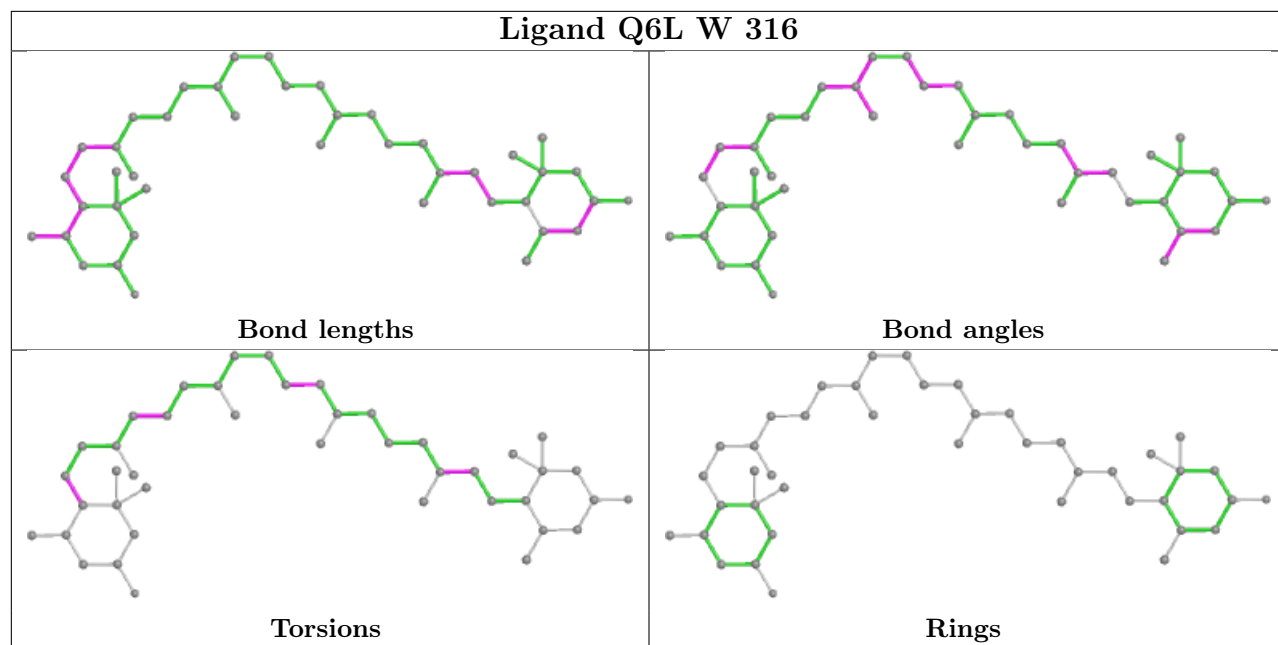
Bond angles

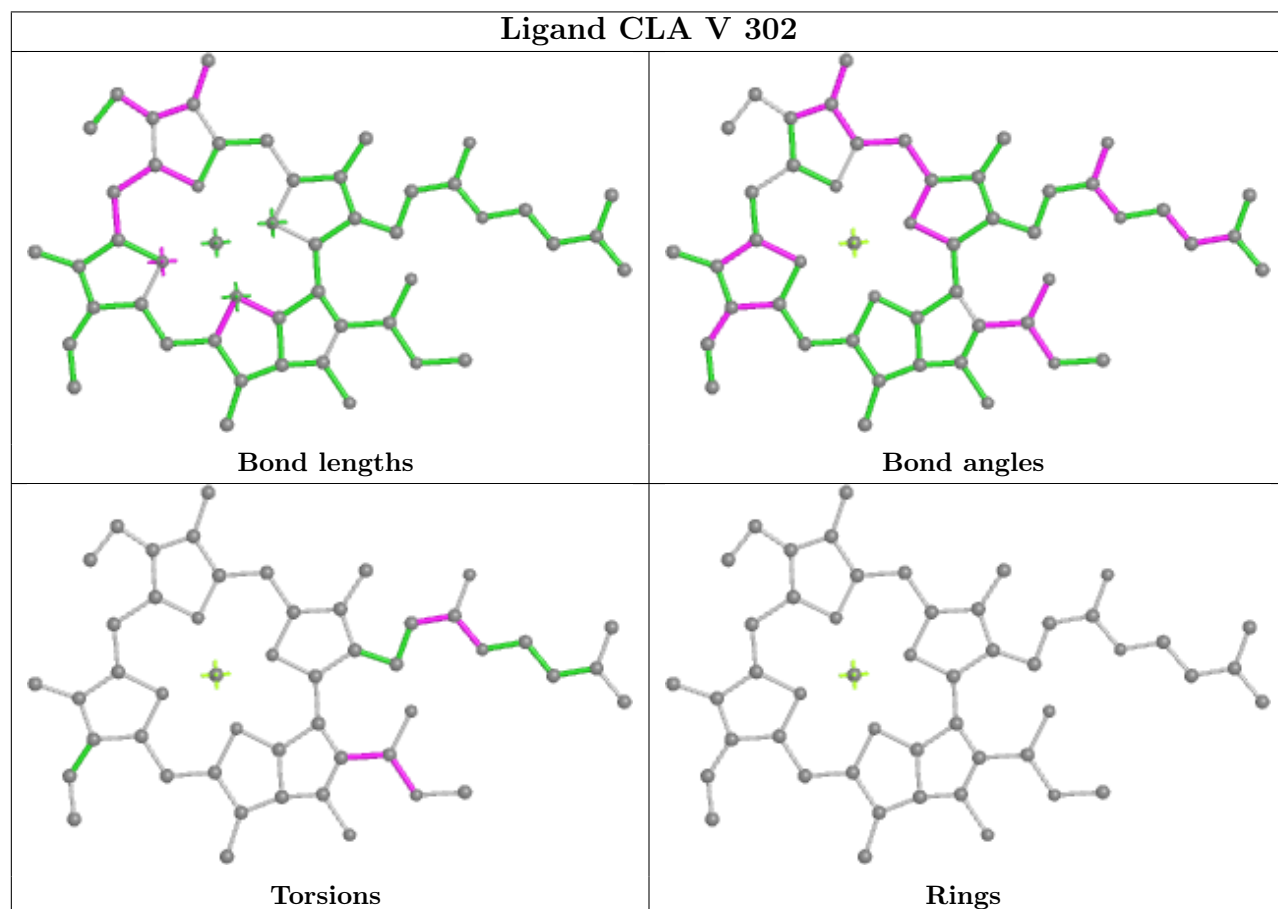
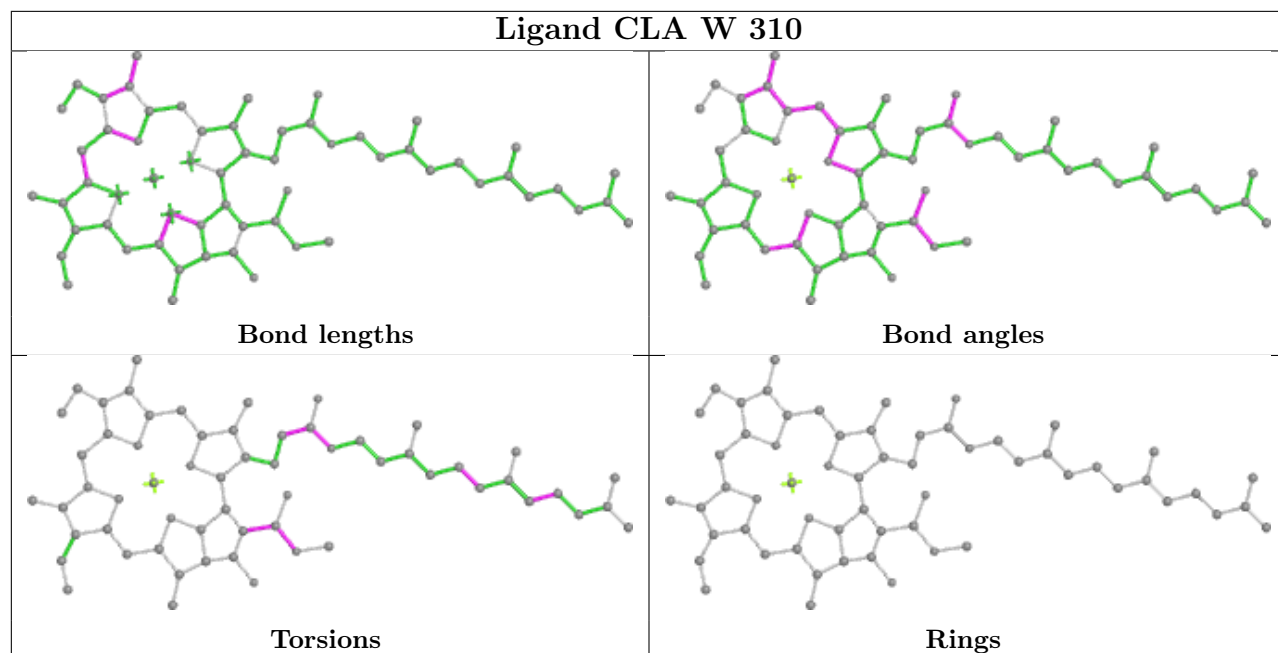


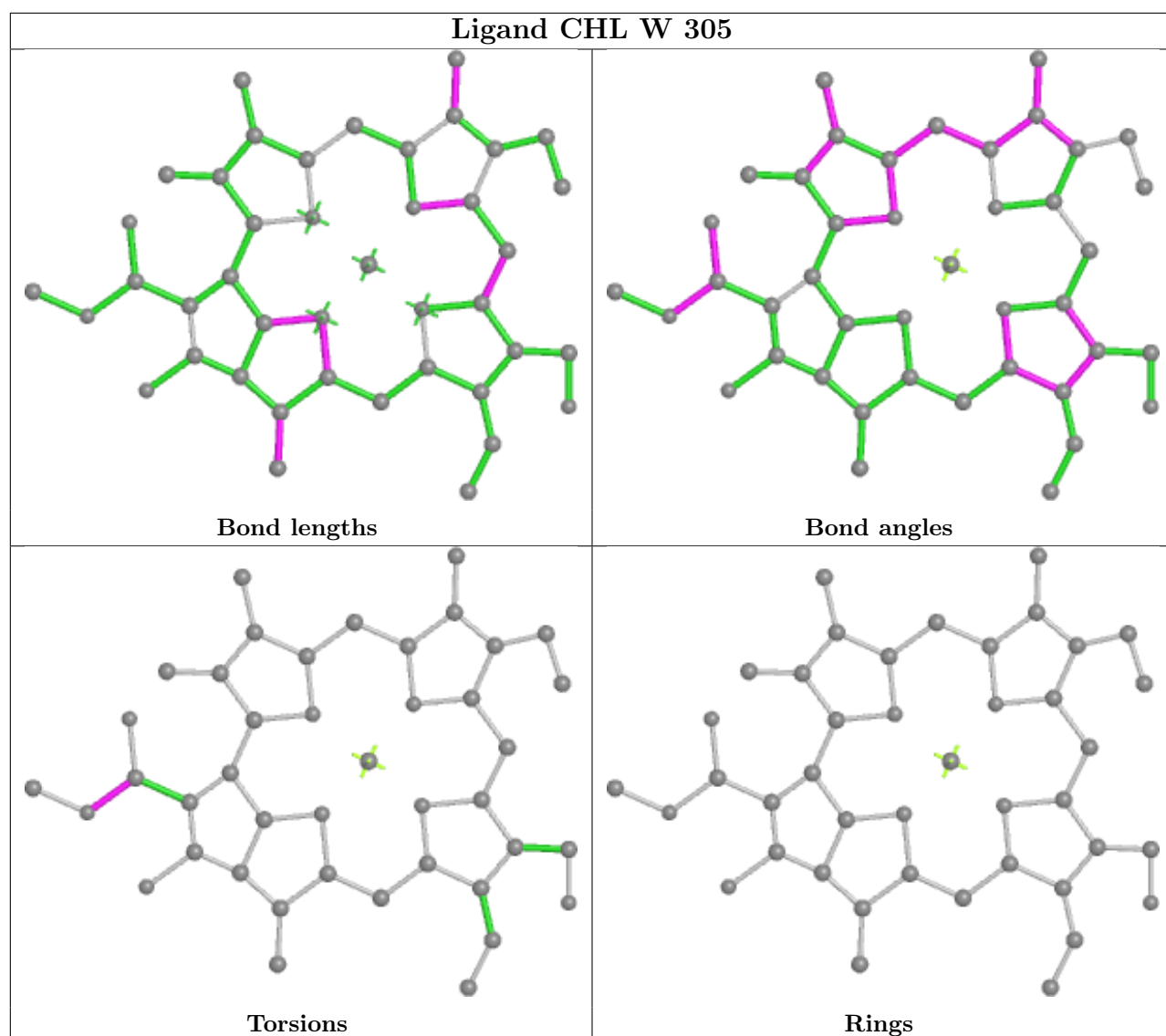
Torsions



Rings







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

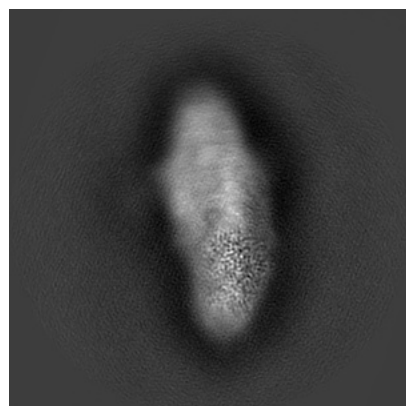
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34736. These allow visual inspection of the internal detail of the map and identification of artifacts.

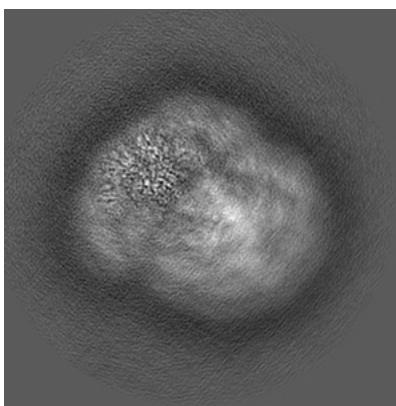
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

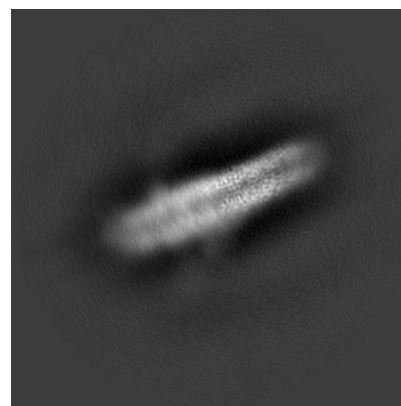
#### 6.1.1 Primary map



X

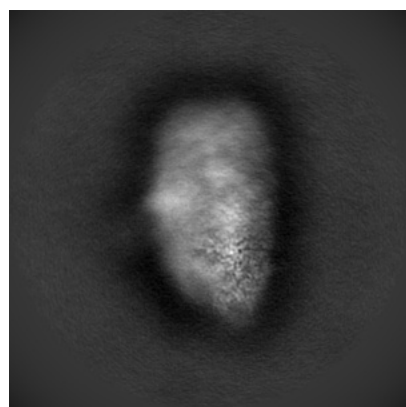


Y

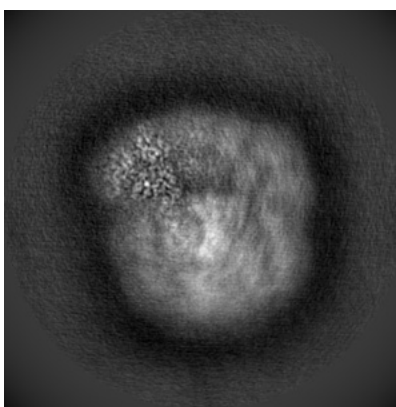


Z

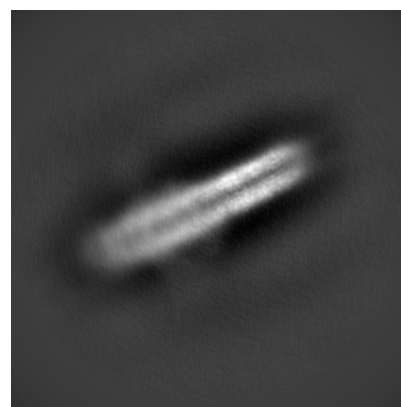
#### 6.1.2 Raw map



X



Y

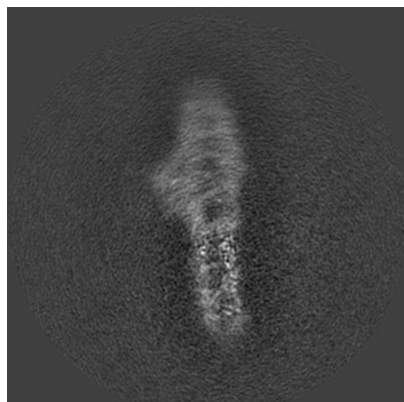


Z

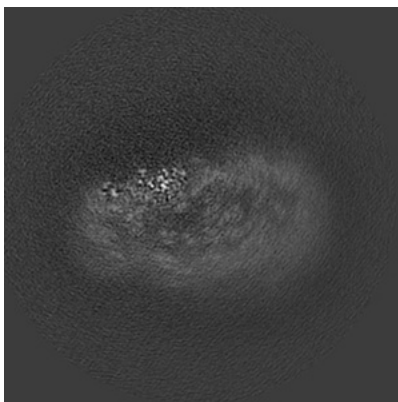
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

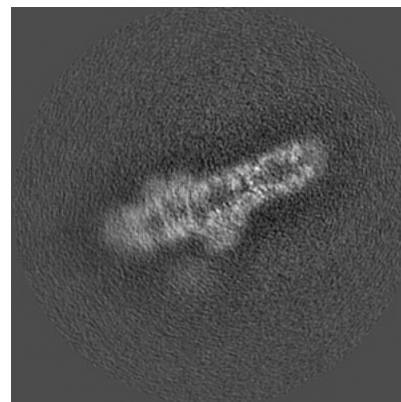
### 6.2.1 Primary map



X Index: 192

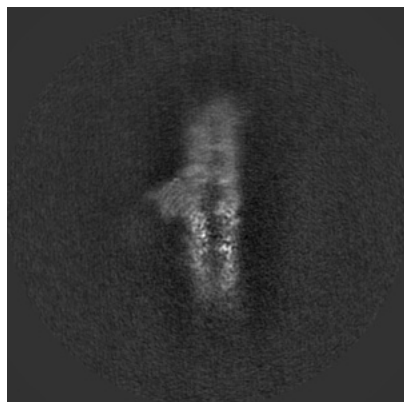


Y Index: 192

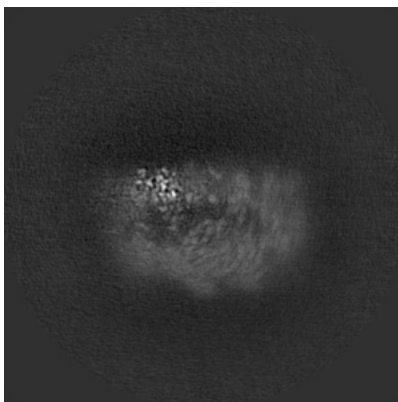


Z Index: 192

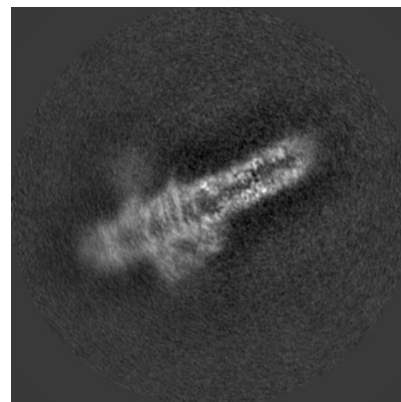
### 6.2.2 Raw map



X Index: 192



Y Index: 192

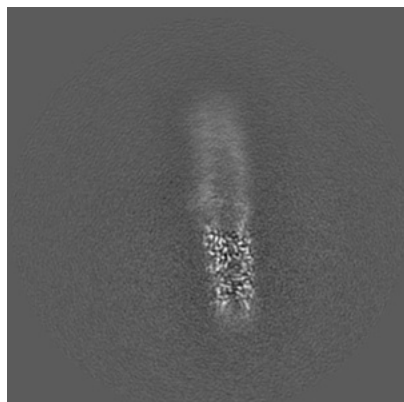


Z Index: 192

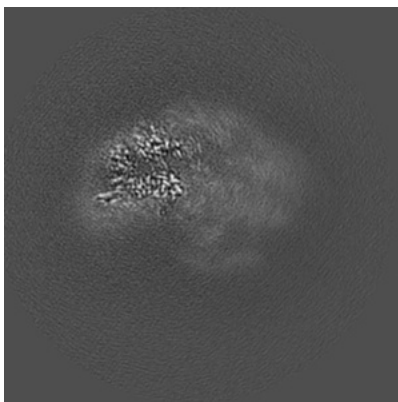
The images above show central slices of the map in three orthogonal directions.

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

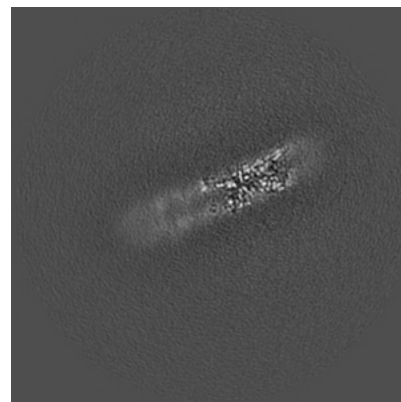
### 6.3.1 Primary map



X Index: 224

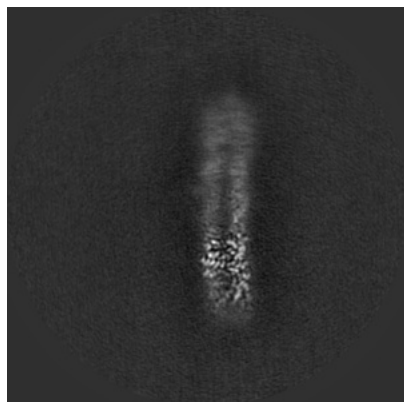


Y Index: 218

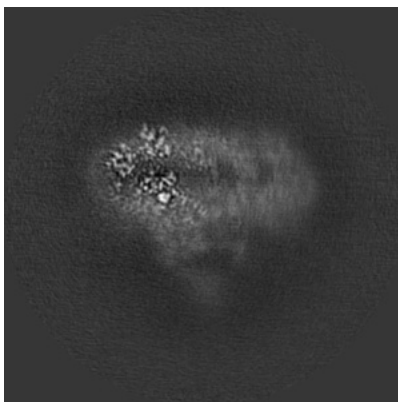


Z Index: 150

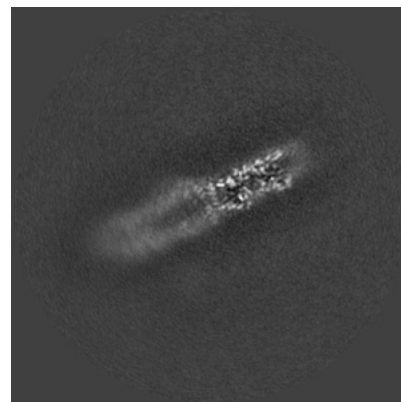
### 6.3.2 Raw map



X Index: 215



Y Index: 213

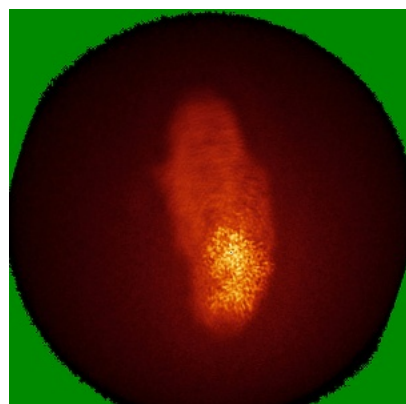


Z Index: 151

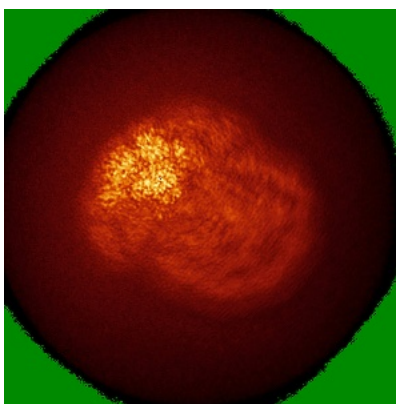
The images above show the largest variance slices of the map in three orthogonal directions.

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

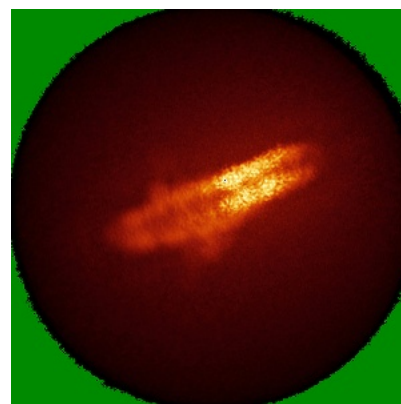
### 6.4.1 Primary map



X

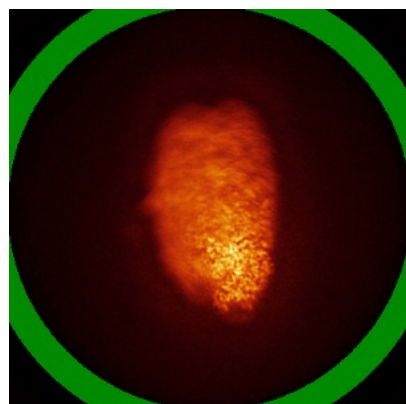


Y

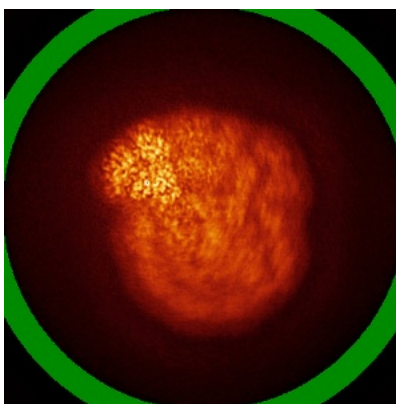


Z

### 6.4.2 Raw map



X



Y

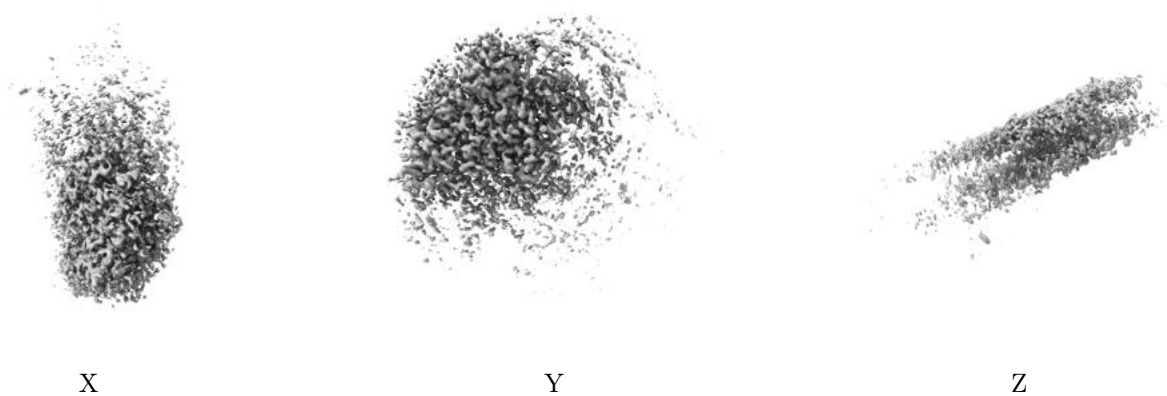


Z

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

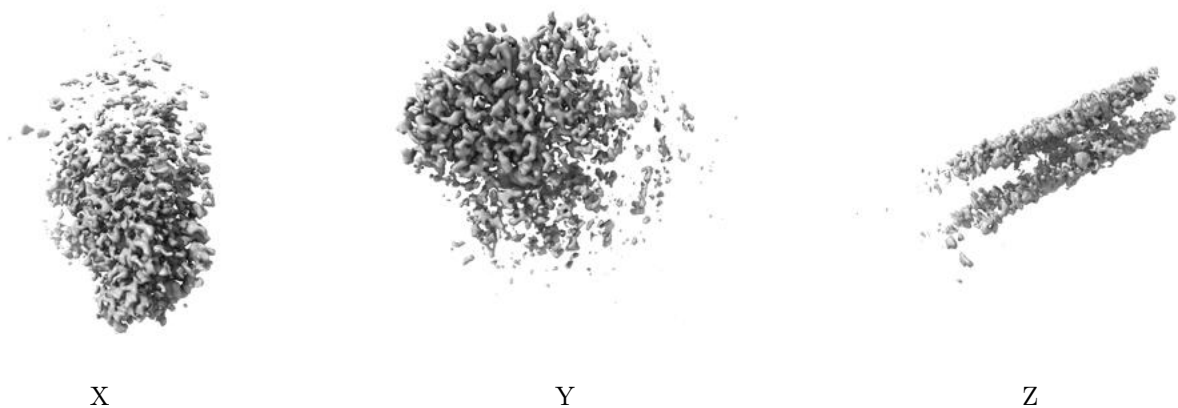
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0154. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

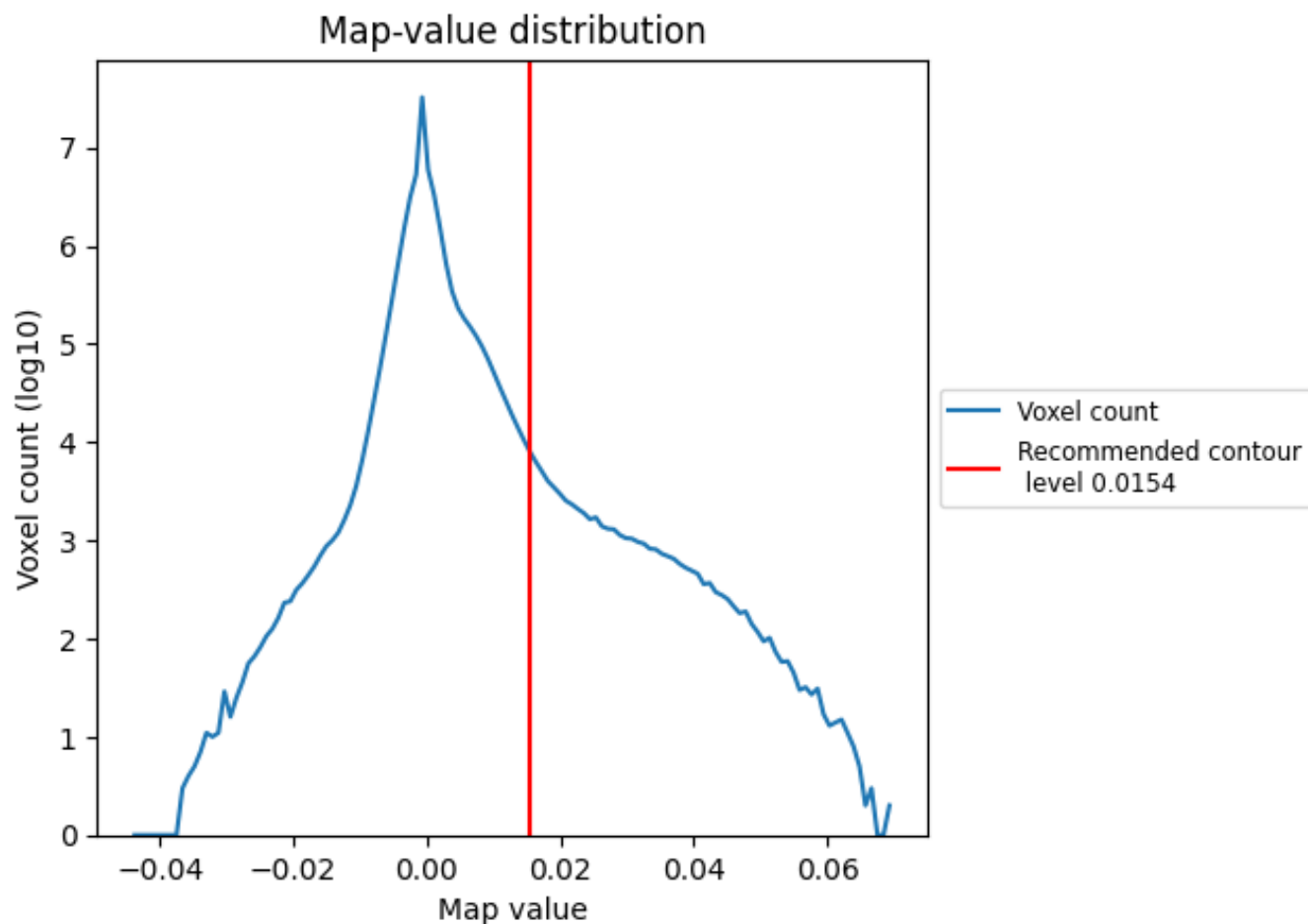
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

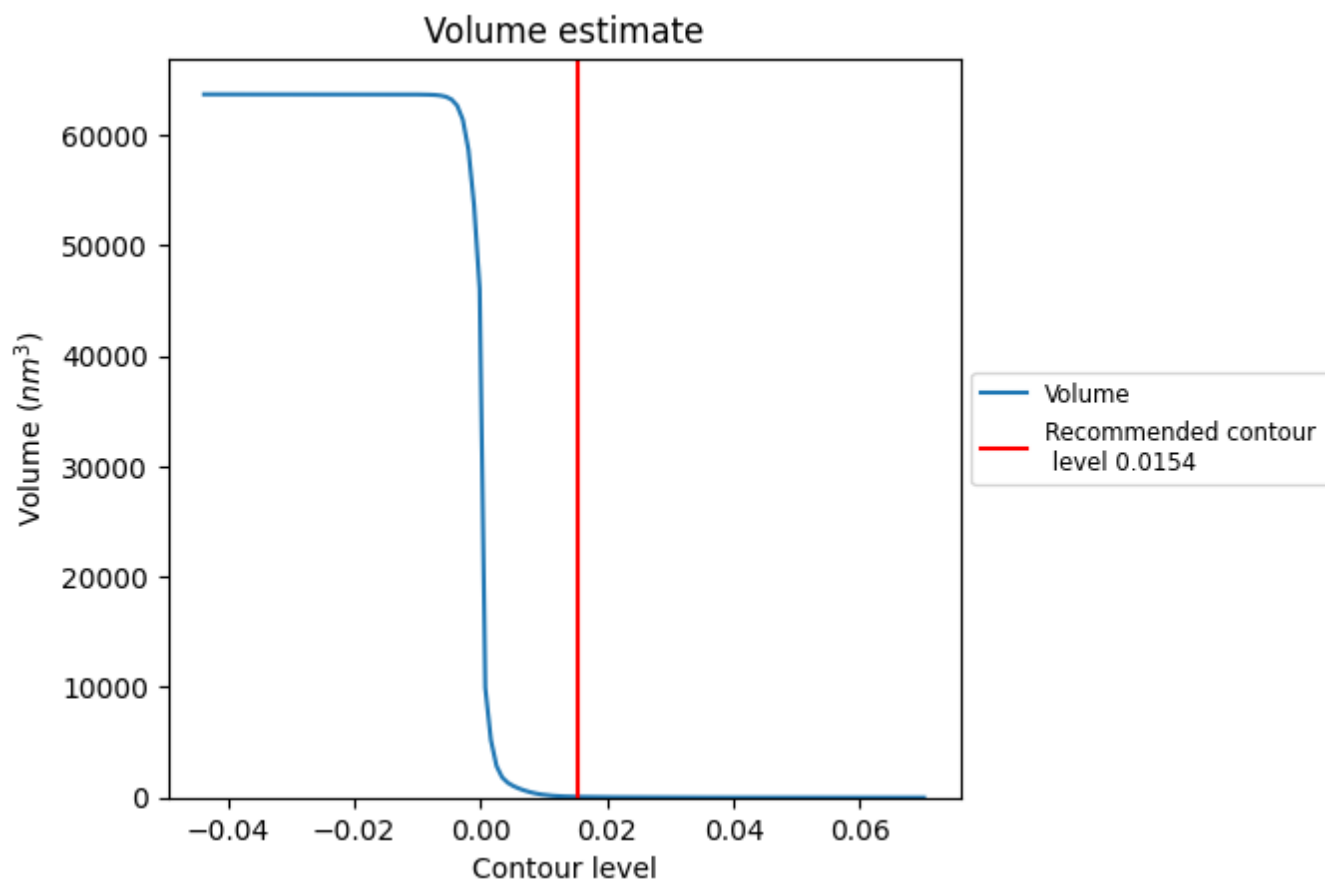
This section contains the results of statistical analysis of the map.

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



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

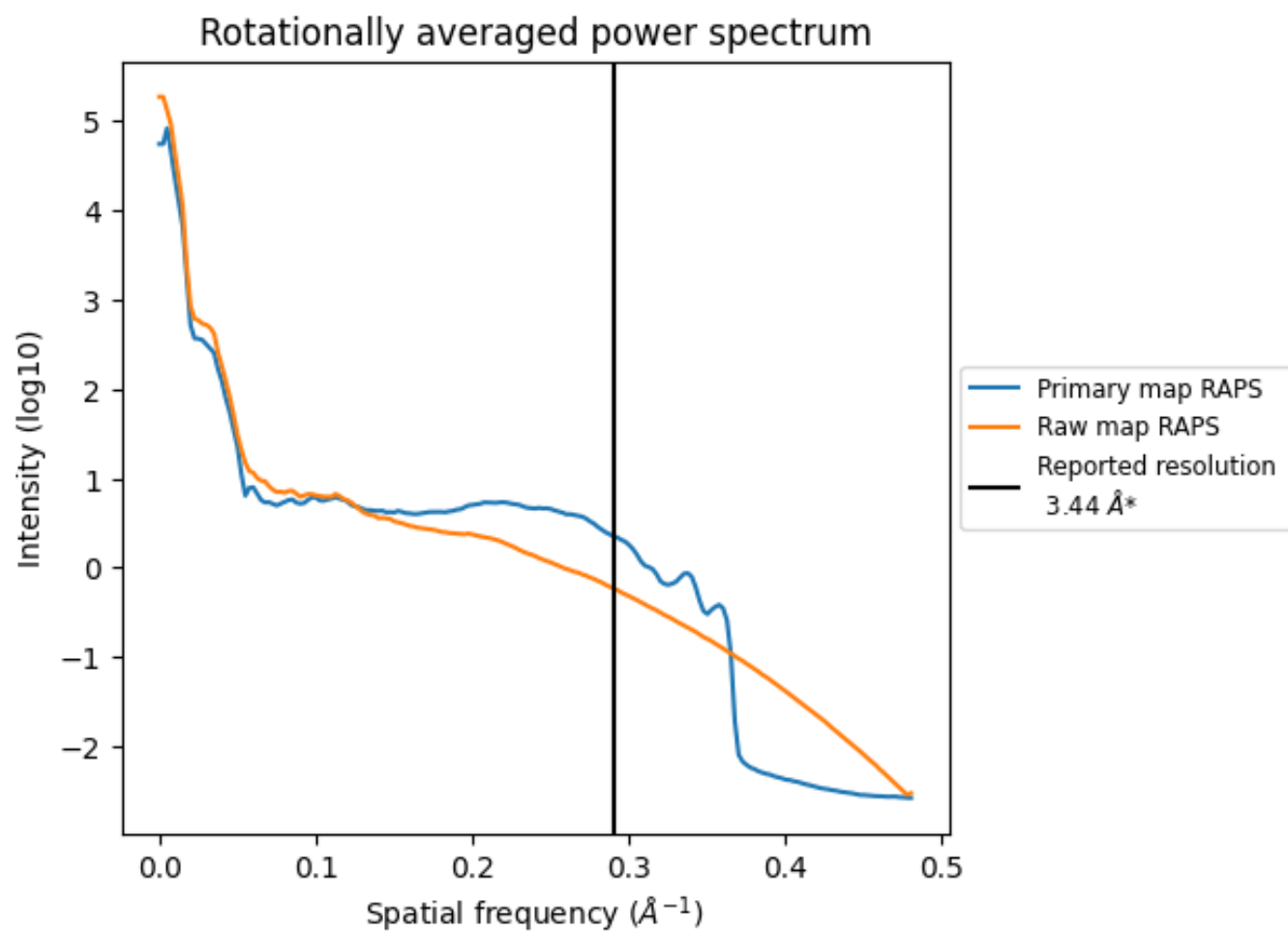
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 68 nm<sup>3</sup>; this corresponds to an approximate mass of 62 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

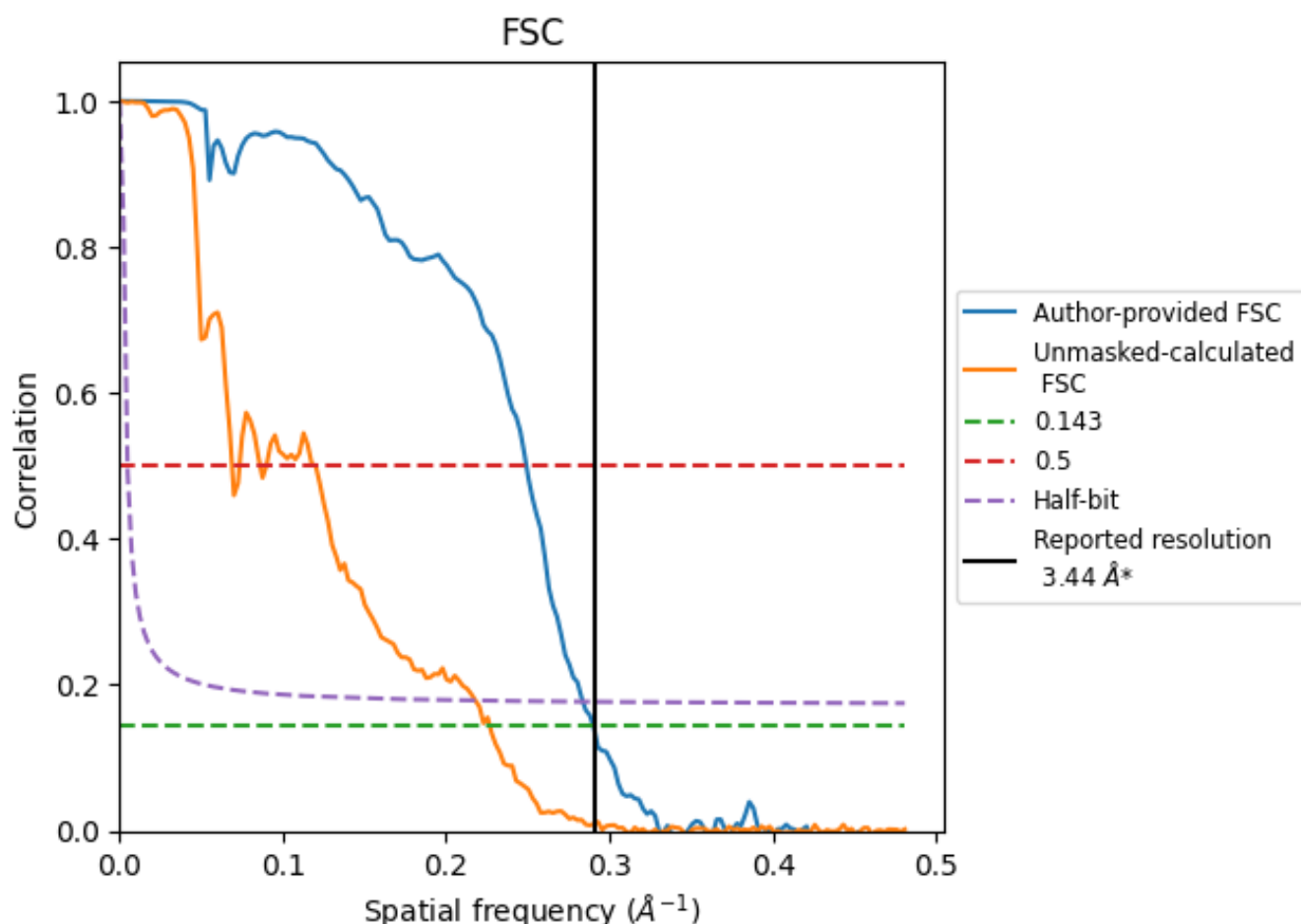


\*Reported resolution corresponds to spatial frequency of 0.291 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.291 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

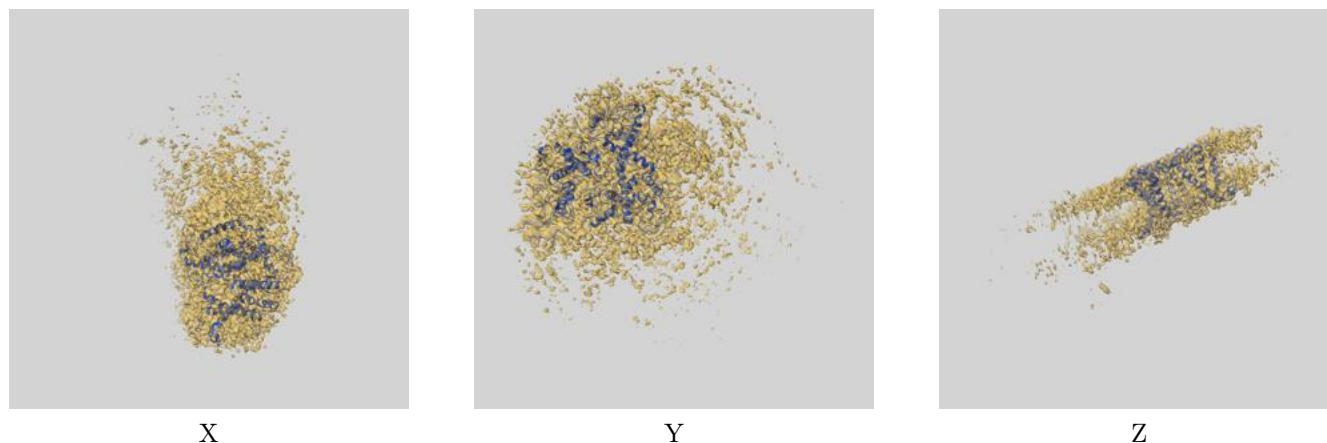
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 3.44                               | -     | -        |
| Author-provided FSC curve | 3.45                               | 4.01  | 3.52     |
| Unmasked-calculated*      | 4.41                               | 14.51 | 4.59     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.41 differs from the reported value 3.44 by more than 10 %

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

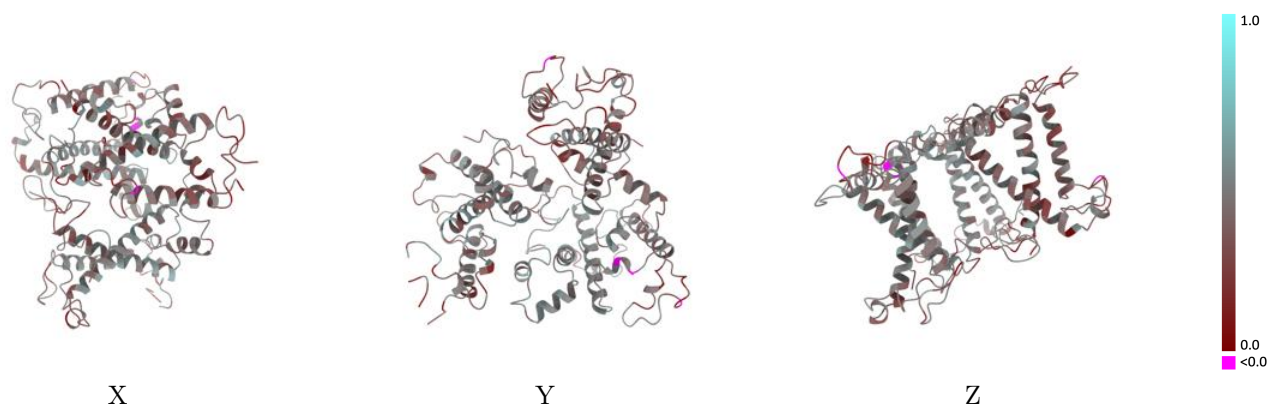
This section contains information regarding the fit between EMDB map EMD-34736 and PDB model 8HG6. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

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



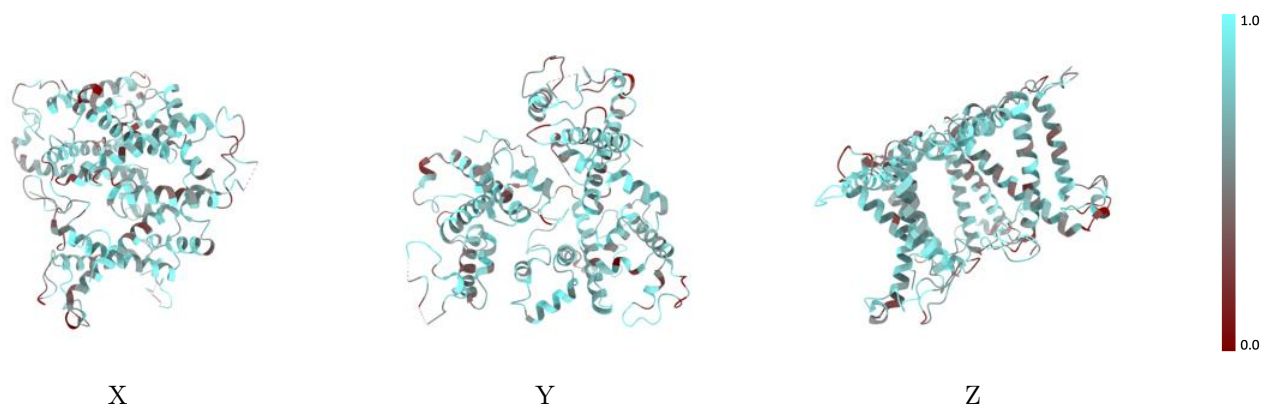
The images above show the 3D surface view of the map at the recommended contour level 0.0154 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



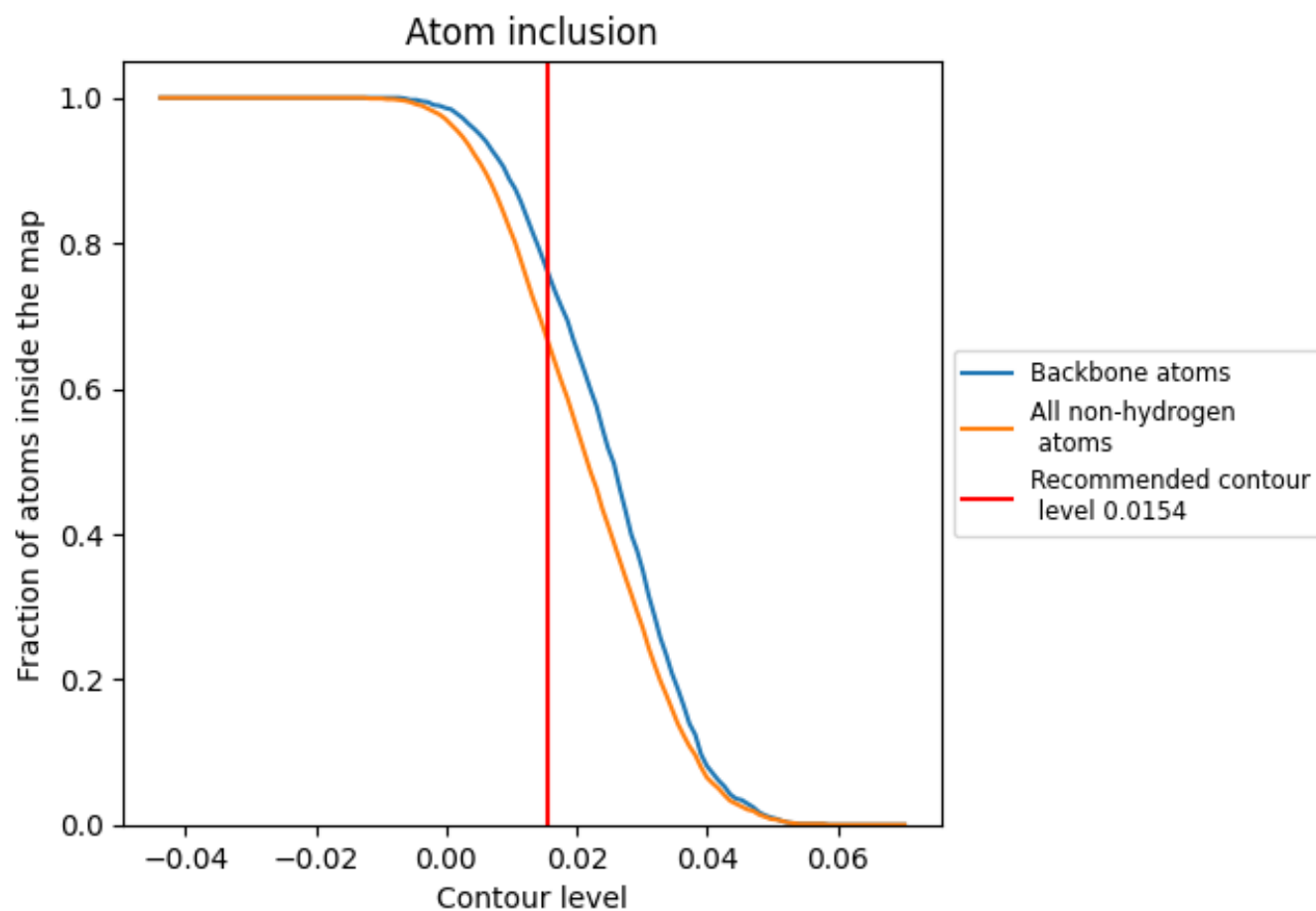
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0154).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0154) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.6690 | <div></div> 0.4120 |
| V     | <div></div> 0.6500 | <div></div> 0.3850 |
| W     | <div></div> 0.6930 | <div></div> 0.4400 |
| X     | <div></div> 0.6620 | <div></div> 0.4110 |

