



## Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 11:01 PM JST

PDB ID : 8ZWB / pdb\_00008zwb  
EMDB ID : EMD-60522  
Title : 1.8 Å resolution structure of the Photosystem I assembly intermediate lacking stromal subunits.  
Authors : Naschberger, A.; Komenda, J.  
Deposited on : 2024-06-12  
Resolution : 1.83 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:

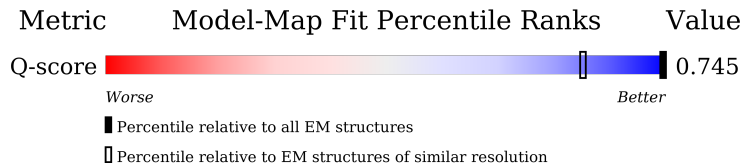
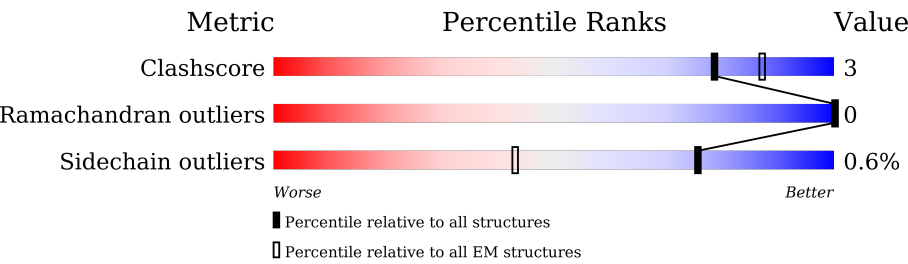
EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 1.83 Å.

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



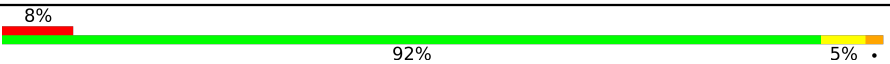
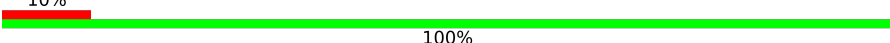
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 903 ( 1.33 - 2.33 )                                      |

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

| Mol | Chain | Length | Quality of chain                                                  |
|-----|-------|--------|-------------------------------------------------------------------|
| 1   | A     | 751    | <div><div>5%</div><div>92%</div><div>6%</div><div>.</div></div>   |
| 2   | B     | 731    | <div><div>6%</div><div>95%</div><div>5%</div></div>               |
| 3   | F     | 165    | <div><div>6%</div><div>79%</div><div>.</div><div>17%</div></div>  |
| 4   | I     | 40     | <div><div>62%</div><div>85%</div><div>8%</div><div>8%</div></div> |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 5   | J     | 40     |  |
| 6   | K     | 86     |  |
| 7   | M     | 31     |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 17  | SF4  | B     | 805 | -         | -        | X       | -                |

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 41672 atoms, of which 20603 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 1   | A     | 734      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 11352 | 3770 | 5602 | 973 | 980 | 27 |         |       |

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 2   | B     | 729      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 11317 | 3798 | 5547 | 967 | 990 | 15 |         |       |

- Molecule 3 is a protein called Photosystem I reaction center subunit III.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 3   | F     | 137      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2116  | 689 | 1051 | 175 | 196 | 5 |         |       |

- Molecule 4 is a protein called Photosystem I reaction center subunit VIII.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 4   | I     | 37       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 585   | 200 | 292 | 41 | 49 | 3 |         |       |

- Molecule 5 is a protein called Photosystem I reaction center subunit IX.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 5   | J     | 40       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 647   | 215 | 328 | 47 | 54 | 3 |         |       |

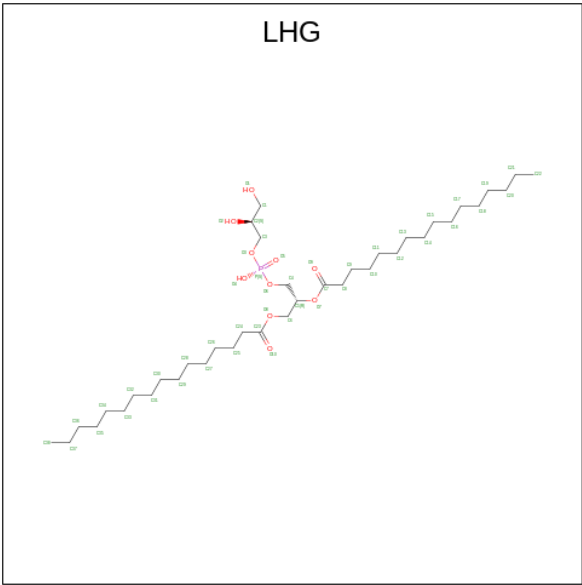
- Molecule 6 is a protein called Photosystem I reaction center subunit Psak 1.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 6   | K     | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1114  | 356 | 570 | 90 | 94 | 4 |         |       |

- Molecule 7 is a protein called Photosystem I reaction center subunit XII.

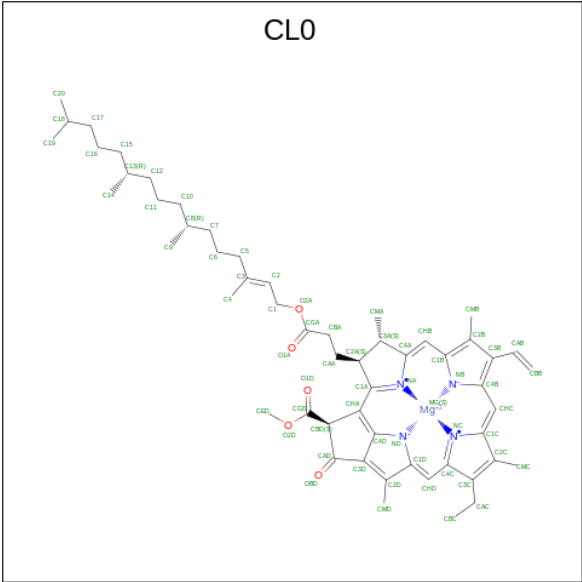
| Mol | Chain | Residues | Atoms |     |     |    |    |   |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|--|---------|-------|
|     |       |          | Total | C   | H   | N  | O  | S |  |         |       |
| 7   | M     | 31       | 498   | 159 | 260 | 36 | 42 | 1 |  | 0       | 0     |

- Molecule 8 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



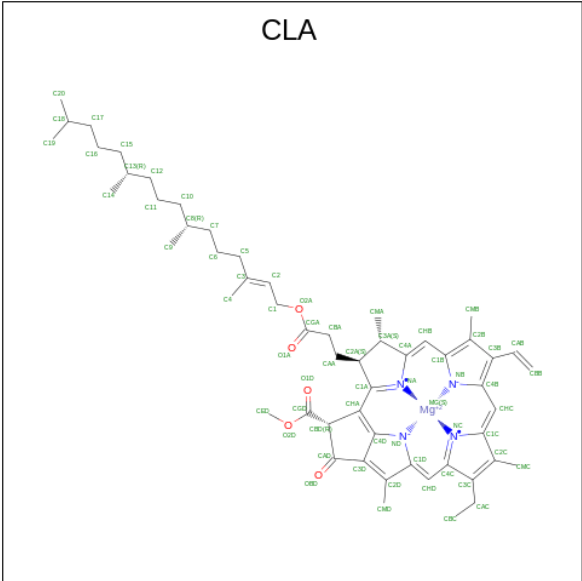
| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|----|---|---------|
|     |       |          | Total | C  | H  | O  | P |         |
| 8   | A     | 1        | 123   | 38 | 74 | 10 | 1 | 0       |
| 8   | A     | 1        | 69    | 22 | 36 | 10 | 1 | 0       |
| 8   | B     | 1        | 90    | 28 | 51 | 10 | 1 | 0       |

- Molecule 9 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 9   | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

- Molecule 10 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 89    | 40 | 39 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 79    | 36 | 33 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 89    | 40 | 39 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 102   | 44 | 48 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 104   | 45 | 49 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 119   | 50 | 59 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 88    | 39 | 39 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 92    | 41 | 41 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 117   | 49 | 58 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 104   | 45 | 49 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 102   | 44 | 48 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 92    | 41 | 41 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 104   | 45 | 49 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 82    | 37 | 35 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | A     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 119   | 50 | 59 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 104   | 45 | 49 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 125   | 52 | 63 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |

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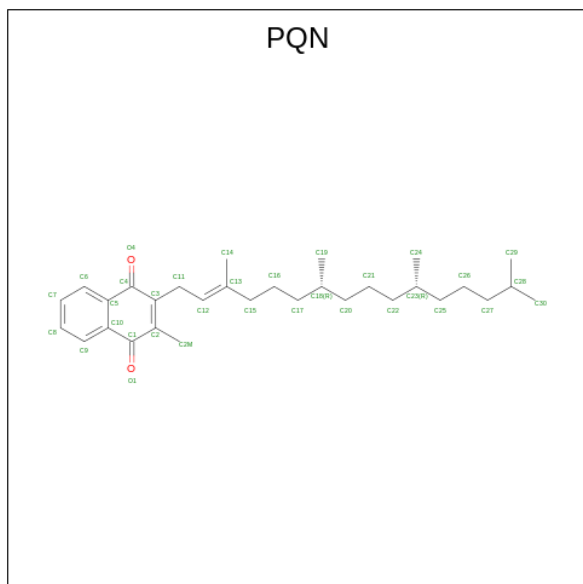
| Mol | Chain | Residues | Atoms |    |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 119   | 50 | 59 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 104   | 45 | 49 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 89    | 40 | 39 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 119   | 50 | 59 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 104   | 45 | 49 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 137   | 55 | 72 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 122   | 51 | 61 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 89    | 40 | 39 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 125   | 52 | 63 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 92    | 41 | 41 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | B     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 30    | 22 | 3  | 1  | 4 |   |         |
| 10  | F     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |

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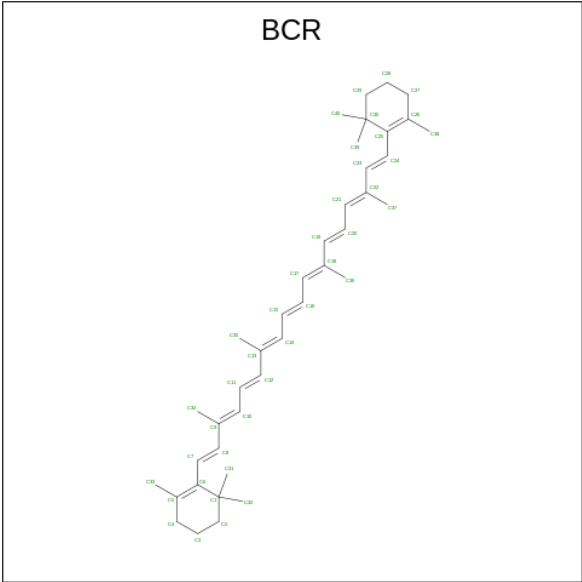
| Mol | Chain | Residues | Atoms |    |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|
| 10  | F     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | J     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | J     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | K     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | K     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 10  | K     | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 119   | 50 | 59 | 1  | 4 | 5 |         |

- Molecule 11 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ).



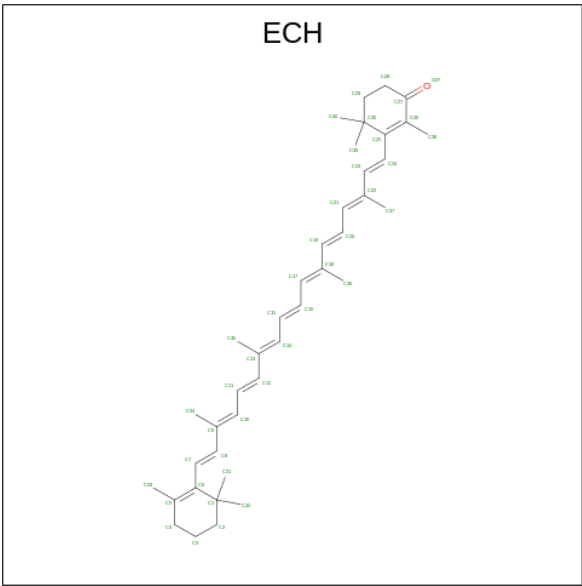
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 11  | A     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 79    | 31 | 46 | 2 |         |
| 11  | B     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 79    | 31 | 46 | 2 |         |

- Molecule 12 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



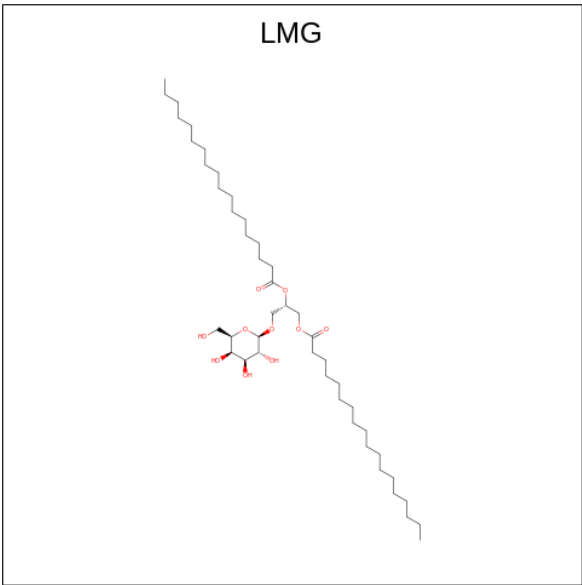
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 12  | A     | 1        | Total | C  | H  | 0       |
|     |       |          | 96    | 40 | 56 |         |
| 12  | A     | 1        | Total | C  | H  | 0       |
|     |       |          | 96    | 40 | 56 |         |
| 12  | A     | 1        | Total | C  | H  | 0       |
|     |       |          | 96    | 40 | 56 |         |
| 12  | A     | 1        | Total | C  | H  | 0       |
|     |       |          | 96    | 40 | 56 |         |
| 12  | A     | 1        | Total | C  | H  | 0       |
|     |       |          | 96    | 40 | 56 |         |
| 12  | B     | 1        | Total | C  | H  | 0       |
|     |       |          | 96    | 40 | 56 |         |
| 12  | B     | 1        | Total | C  | H  | 0       |
|     |       |          | 96    | 40 | 56 |         |
| 12  | B     | 1        | Total | C  | H  | 0       |
|     |       |          | 96    | 40 | 56 |         |
| 12  | B     | 1        | Total | C  | H  | 0       |
|     |       |          | 96    | 40 | 56 |         |
| 12  | F     | 1        | Total | C  | H  | 0       |
|     |       |          | 96    | 40 | 56 |         |
| 12  | I     | 1        | Total | C  | H  | 0       |
|     |       |          | 96    | 40 | 56 |         |
| 12  | J     | 1        | Total | C  | H  | 0       |
|     |       |          | 96    | 40 | 56 |         |
| 12  | K     | 1        | Total | C  | H  | 0       |
|     |       |          | 96    | 40 | 56 |         |

- Molecule 13 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: C<sub>40</sub>H<sub>54</sub>O).



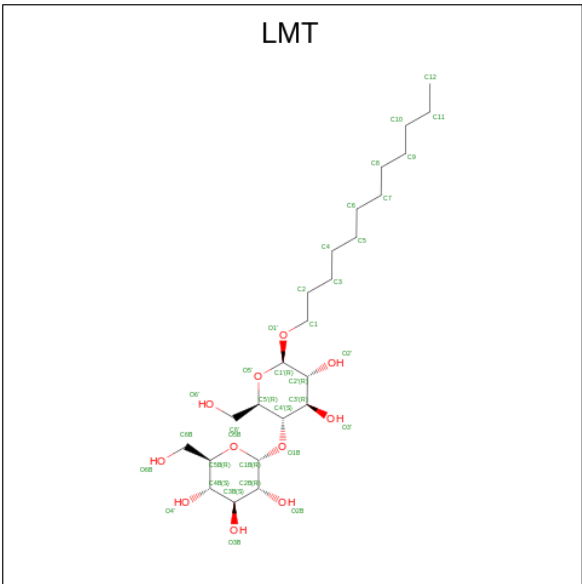
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 13  | A     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 95    | 40 | 54 | 1 |         |
| 13  | A     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 95    | 40 | 54 | 1 |         |
| 13  | B     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 95    | 40 | 54 | 1 |         |
| 13  | F     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 95    | 40 | 54 | 1 |         |
| 13  | M     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 95    | 40 | 54 | 1 |         |

- Molecule 14 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |    | AltConf |
|-----|-------|----------|-------|----|----|----|---------|
| 14  | A     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 66    | 22 | 34 | 10 |         |
| 14  | B     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 114   | 38 | 66 | 10 |         |

- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |    | AltConf |
|-----|-------|----------|-------|----|----|----|---------|
| 15  | A     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 81    | 24 | 46 | 11 |         |

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| Mol | Chain | Residues | Atoms |    |    |    | AltConf |
|-----|-------|----------|-------|----|----|----|---------|
| 15  | A     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 31    | 10 | 15 | 6  |         |
| 15  | A     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 38    | 12 | 25 | 1  |         |
| 15  | A     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 29    | 10 | 18 | 1  |         |
| 15  | A     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 38    | 12 | 25 | 1  |         |
| 15  | A     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 57    | 18 | 33 | 6  |         |
| 15  | A     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 38    | 12 | 25 | 1  |         |
| 15  | A     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 57    | 18 | 33 | 6  |         |
| 15  | A     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 81    | 24 | 46 | 11 |         |
| 15  | B     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 58    | 18 | 34 | 6  |         |
| 15  | B     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 52    | 16 | 25 | 11 |         |
| 15  | B     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 64    | 20 | 33 | 11 |         |
| 15  | B     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 38    | 12 | 25 | 1  |         |
| 15  | B     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 38    | 12 | 25 | 1  |         |
| 15  | B     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 43    | 14 | 23 | 6  |         |
| 15  | B     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 38    | 12 | 25 | 1  |         |
| 15  | B     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 38    | 12 | 25 | 1  |         |
| 15  | B     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 38    | 12 | 25 | 1  |         |
| 15  | F     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 61    | 19 | 31 | 11 |         |
| 15  | F     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 38    | 12 | 25 | 1  |         |
| 15  | F     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 72    | 23 | 38 | 11 |         |
| 15  | I     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 51    | 15 | 25 | 11 |         |

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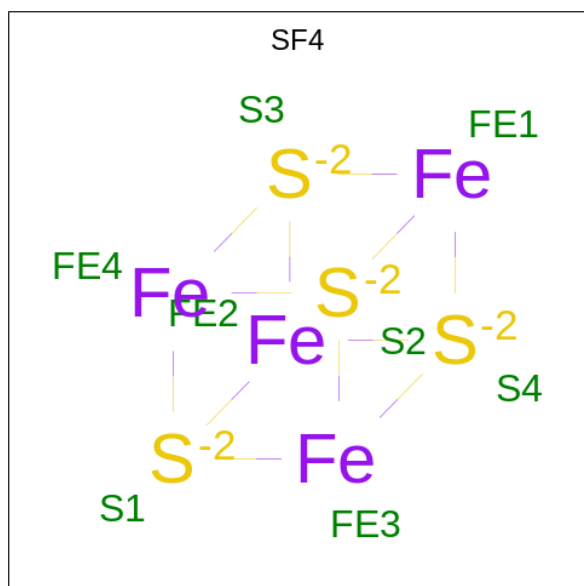
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| Mol | Chain | Residues | Atoms |    |    |    | AltConf |
|-----|-------|----------|-------|----|----|----|---------|
| 15  | I     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 64    | 20 | 33 | 11 |         |
| 15  | J     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 38    | 12 | 25 | 1  |         |
| 15  | J     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 38    | 12 | 25 | 1  |         |
| 15  | M     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 38    | 12 | 25 | 1  |         |

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

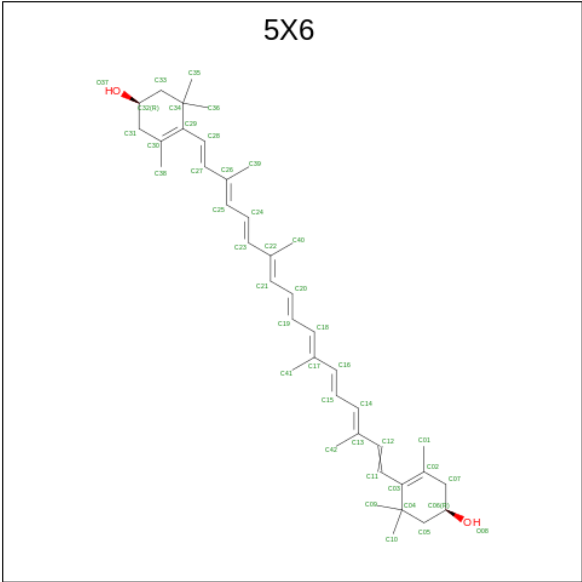
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 16  | A     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 17  | B     | 1        | Total | Fe | S | 0       |
|     |       |          | 6     | 2  | 4 |         |

- Molecule 18 is Zeaxanthin (CCD ID: 5X6) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 18  | B     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 98    | 40 | 56 | 2 |         |

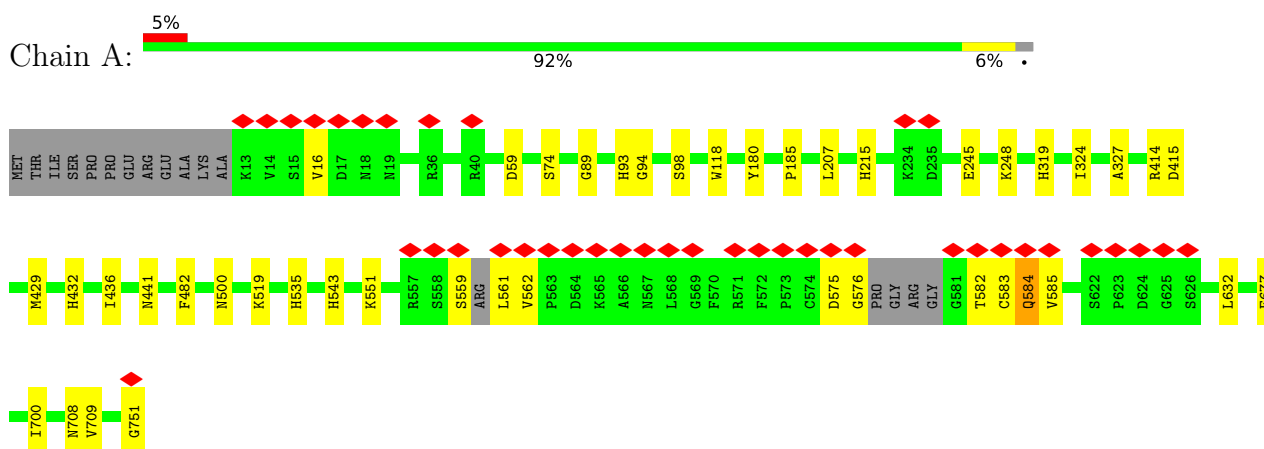
- Molecule 19 is water.

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 19  | A     | 171      | Total | O   | 0       |
|     |       |          | 171   | 171 |         |
| 19  | B     | 150      | Total | O   | 0       |
|     |       |          | 150   | 150 |         |
| 19  | F     | 17       | Total | O   | 0       |
|     |       |          | 17    | 17  |         |
| 19  | J     | 5        | Total | O   | 0       |
|     |       |          | 5     | 5   |         |
| 19  | K     | 11       | Total | O   | 0       |
|     |       |          | 11    | 11  |         |
| 19  | M     | 1        | Total | O   | 0       |
|     |       |          | 1     | 1   |         |

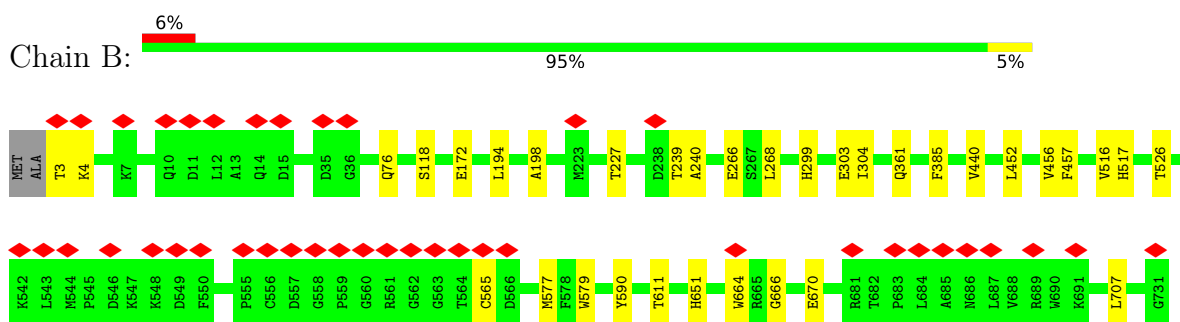
### 3 Residue-property plots

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

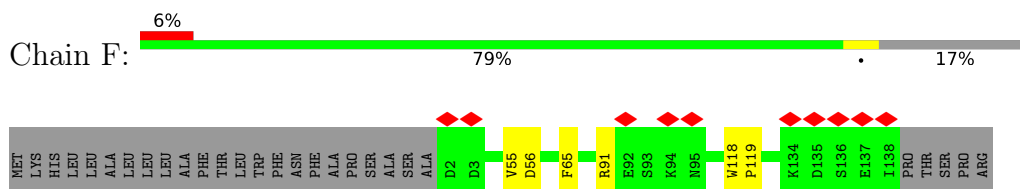
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



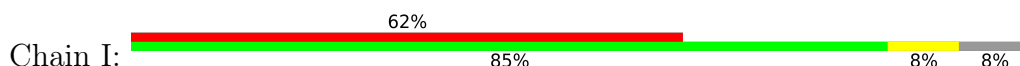
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

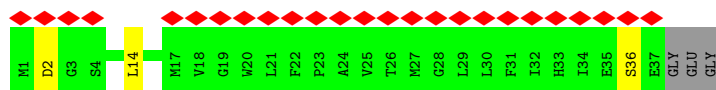


- Molecule 3: Photosystem I reaction center subunit III

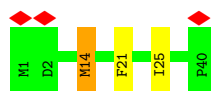


- Molecule 4: Photosystem I reaction center subunit VIII

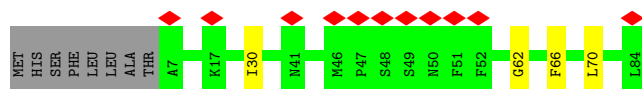
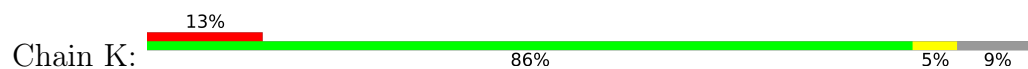




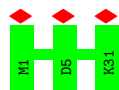
- Molecule 5: Photosystem I reaction center subunit IX



- Molecule 6: Photosystem I reaction center subunit PsaK 1



- Molecule 7: Photosystem I reaction center subunit XII



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 333941                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 1                                       | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 1900                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 0.047                                   | Depositor |
| Minimum map value                    | -0.012                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.001                                   | Depositor |
| Recommended contour level            | 0.01                                    | Depositor |
| Map size (Å)                         | 255.15, 255.15, 255.15                  | wwPDB     |
| Map dimensions                       | 350, 350, 350                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.729, 0.729, 0.729                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, BCR, SF4, 5X6, LMG, CL0, PQN, CL, LHG, CLA, ECH

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

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | A     | 0.09         | 0/5945  | 0.21        | 0/8102  |
| 2   | B     | 0.08         | 0/5981  | 0.21        | 0/8178  |
| 3   | F     | 0.08         | 0/1093  | 0.22        | 0/1486  |
| 4   | I     | 0.07         | 0/304   | 0.21        | 0/416   |
| 5   | J     | 0.08         | 0/328   | 0.21        | 0/443   |
| 6   | K     | 0.07         | 0/555   | 0.18        | 0/752   |
| 7   | M     | 0.06         | 0/241   | 0.15        | 0/326   |
| All | All   | 0.08         | 0/14447 | 0.21        | 0/19703 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5750  | 5602     | 5606     | 33      | 0            |
| 2   | B     | 5770  | 5547     | 5549     | 25      | 0            |
| 3   | F     | 1065  | 1051     | 1050     | 4       | 0            |
| 4   | I     | 293   | 292      | 292      | 3       | 0            |
| 5   | J     | 319   | 328      | 328      | 3       | 0            |
| 6   | K     | 544   | 570      | 570      | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | M     | 238   | 260      | 260      | 0       | 0            |
| 8   | A     | 82    | 110      | 110      | 0       | 0            |
| 8   | B     | 39    | 51       | 51       | 0       | 0            |
| 9   | A     | 65    | 0        | 72       | 2       | 0            |
| 10  | A     | 2466  | 2358     | 2358     | 20      | 0            |
| 10  | B     | 2269  | 2142     | 2142     | 23      | 0            |
| 10  | F     | 90    | 66       | 66       | 0       | 0            |
| 10  | J     | 90    | 66       | 66       | 0       | 0            |
| 10  | K     | 150   | 125      | 125      | 3       | 0            |
| 11  | A     | 33    | 46       | 46       | 0       | 0            |
| 11  | B     | 33    | 46       | 46       | 0       | 0            |
| 12  | A     | 200   | 280      | 280      | 8       | 0            |
| 12  | B     | 200   | 280      | 280      | 11      | 0            |
| 12  | F     | 40    | 56       | 56       | 3       | 0            |
| 12  | I     | 40    | 56       | 56       | 0       | 0            |
| 12  | J     | 40    | 56       | 56       | 1       | 0            |
| 12  | K     | 40    | 56       | 56       | 0       | 0            |
| 13  | A     | 82    | 108      | 108      | 7       | 0            |
| 13  | B     | 41    | 54       | 54       | 0       | 0            |
| 13  | F     | 41    | 54       | 54       | 2       | 0            |
| 13  | M     | 41    | 54       | 54       | 1       | 0            |
| 14  | A     | 32    | 34       | 34       | 0       | 0            |
| 14  | B     | 48    | 66       | 66       | 0       | 0            |
| 15  | A     | 184   | 266      | 271      | 0       | 0            |
| 15  | B     | 167   | 240      | 246      | 0       | 0            |
| 15  | F     | 77    | 94       | 99       | 0       | 0            |
| 15  | I     | 57    | 58       | 60       | 1       | 0            |
| 15  | J     | 26    | 50       | 50       | 0       | 0            |
| 15  | M     | 13    | 25       | 25       | 0       | 0            |
| 16  | A     | 1     | 0        | 0        | 0       | 0            |
| 17  | B     | 6     | 0        | 0        | 2       | 0            |
| 18  | B     | 42    | 56       | 0        | 0       | 0            |
| 19  | A     | 171   | 0        | 0        | 2       | 0            |
| 19  | B     | 150   | 0        | 0        | 0       | 0            |
| 19  | F     | 17    | 0        | 0        | 0       | 0            |
| 19  | J     | 5     | 0        | 0        | 0       | 0            |
| 19  | K     | 11    | 0        | 0        | 0       | 0            |
| 19  | M     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 21069 | 20603    | 20642    | 116     | 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 3.

All (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:575:ASP:O     | 1:A:582:THR:OG1   | 2.00                     | 0.79              |
| 1:A:432:HIS:CE1   | 1:A:436:ILE:HD11  | 2.20                     | 0.76              |
| 10:B:810:CLA:H43  | 10:B:829:CLA:H42  | 1.67                     | 0.75              |
| 1:A:415:ASP:OD2   | 19:A:901:HOH:O    | 2.10                     | 0.70              |
| 1:A:575:ASP:OD1   | 1:A:576:GLY:N     | 2.25                     | 0.69              |
| 1:A:94:GLY:O      | 1:A:98:SER:OG     | 2.11                     | 0.68              |
| 1:A:245:GLU:OE1   | 1:A:248:LYS:NZ    | 2.30                     | 0.64              |
| 10:B:828:CLA:H143 | 12:B:847:BCR:C18  | 2.28                     | 0.64              |
| 2:B:456:VAL:HG11  | 3:F:56:ASP:HB3    | 1.79                     | 0.63              |
| 2:B:565:CYS:SG    | 17:B:805:SF4:S2   | 2.87                     | 0.61              |
| 12:B:844:BCR:H321 | 12:B:844:BCR:HC8  | 1.84                     | 0.60              |
| 2:B:3:THR:OG1     | 4:I:36:SER:O      | 2.21                     | 0.58              |
| 12:A:850:BCR:H23C | 12:A:850:BCR:H403 | 1.85                     | 0.58              |
| 10:A:804:CLA:HMB1 | 10:A:804:CLA:HBB1 | 1.85                     | 0.57              |
| 1:A:677:PHE:CG    | 13:A:851:ECH:H36B | 2.41                     | 0.56              |
| 10:B:802:CLA:HBB1 | 10:B:802:CLA:HMB1 | 1.87                     | 0.56              |
| 10:B:825:CLA:H51  | 10:B:826:CLA:H142 | 1.86                     | 0.56              |
| 10:A:813:CLA:H141 | 10:A:813:CLA:H171 | 1.88                     | 0.55              |
| 1:A:482:PHE:CE2   | 10:A:842:CLA:H42  | 2.42                     | 0.54              |
| 10:K:102:CLA:HMC3 | 10:K:102:CLA:HBC2 | 1.90                     | 0.54              |
| 1:A:709:VAL:HG22  | 1:A:709:VAL:O     | 2.09                     | 0.53              |
| 13:M:101:ECH:H23  | 13:M:101:ECH:H40B | 1.91                     | 0.53              |
| 1:A:519:LYS:NZ    | 1:A:751:GLY:OXT   | 2.42                     | 0.52              |
| 10:A:814:CLA:HMB1 | 10:A:814:CLA:HBB1 | 1.92                     | 0.51              |
| 13:A:851:ECH:H36A | 10:B:802:CLA:H2   | 1.92                     | 0.51              |
| 2:B:268:LEU:HD13  | 10:B:819:CLA:HMA2 | 1.93                     | 0.51              |
| 10:K:102:CLA:HBC2 | 10:K:102:CLA:CMC  | 2.41                     | 0.50              |
| 1:A:118:TRP:CD2   | 10:A:814:CLA:HED3 | 2.47                     | 0.50              |
| 10:B:808:CLA:C4   | 10:B:808:CLA:HED3 | 2.42                     | 0.50              |
| 10:A:844:CLA:H43  | 10:B:834:CLA:HAA2 | 1.94                     | 0.50              |
| 10:B:821:CLA:H203 | 10:B:826:CLA:H141 | 1.92                     | 0.50              |
| 10:B:821:CLA:HMB2 | 10:B:826:CLA:CED  | 2.42                     | 0.49              |
| 12:F:202:BCR:C8   | 12:F:202:BCR:H331 | 2.42                     | 0.49              |
| 10:B:828:CLA:H143 | 12:B:847:BCR:C17  | 2.42                     | 0.49              |
| 4:I:2:ASP:OD1     | 15:I:102:LMT:O6B  | 2.28                     | 0.49              |
| 2:B:76:GLN:N      | 2:B:76:GLN:OE1    | 2.45                     | 0.49              |
| 1:A:583:CYS:O     | 2:B:666:GLY:N     | 2.44                     | 0.49              |
| 10:B:810:CLA:H112 | 12:B:849:BCR:H342 | 1.96                     | 0.48              |
| 1:A:559:SER:OG    | 1:A:562:VAL:N     | 2.46                     | 0.48              |
| 10:B:823:CLA:OBD  | 12:B:844:BCR:H332 | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:319:HIS:HB3   | 1:A:324:ILE:HD11  | 1.95                     | 0.47              |
| 1:A:677:PHE:CD2   | 13:A:851:ECH:H36B | 2.48                     | 0.47              |
| 2:B:385:PHE:CE2   | 12:B:848:BCR:H373 | 2.49                     | 0.47              |
| 1:A:16:VAL:HG12   | 1:A:185:PRO:HA    | 1.97                     | 0.47              |
| 2:B:577:MET:HG3   | 2:B:707:LEU:HD21  | 1.97                     | 0.47              |
| 10:B:810:CLA:C11  | 12:B:849:BCR:H342 | 2.44                     | 0.47              |
| 2:B:303:GLU:OE1   | 2:B:303:GLU:N     | 2.48                     | 0.47              |
| 12:B:845:BCR:H382 | 12:B:845:BCR:H23C | 1.97                     | 0.47              |
| 6:K:66:PHE:CE2    | 6:K:70:LEU:HD11   | 2.49                     | 0.47              |
| 10:A:813:CLA:H71  | 12:J:103:BCR:H372 | 1.98                     | 0.46              |
| 3:F:55:VAL:HG12   | 3:F:65:PHE:HB2    | 1.95                     | 0.46              |
| 1:A:583:CYS:HB3   | 17:B:805:SF4:S4   | 2.55                     | 0.46              |
| 10:B:810:CLA:CGA  | 10:B:810:CLA:C1A  | 2.94                     | 0.46              |
| 12:A:866:BCR:H372 | 6:K:62:GLY:HA2    | 1.96                     | 0.46              |
| 9:A:803:CL0:H8    | 9:A:803:CL0:CGD   | 2.47                     | 0.45              |
| 5:J:14:MET:HA     | 5:J:14:MET:HE2    | 1.99                     | 0.45              |
| 9:A:803:CL0:H12   | 10:B:802:CLA:OBD  | 2.17                     | 0.45              |
| 1:A:327:ALA:CB    | 10:A:828:CLA:HED2 | 2.46                     | 0.45              |
| 2:B:194:LEU:HA    | 2:B:198:ALA:HB3   | 1.99                     | 0.45              |
| 1:A:89:GLY:O      | 1:A:93:HIS:HD2    | 2.00                     | 0.44              |
| 1:A:429:MET:HA    | 1:A:432:HIS:CE1   | 2.53                     | 0.44              |
| 1:A:500:ASN:HB2   | 10:A:840:CLA:HED2 | 1.98                     | 0.44              |
| 10:A:827:CLA:CHD  | 12:A:866:BCR:H382 | 2.48                     | 0.44              |
| 10:A:805:CLA:H152 | 10:A:805:CLA:H203 | 1.99                     | 0.44              |
| 13:A:851:ECH:C8   | 13:A:851:ECH:H33  | 2.47                     | 0.44              |
| 2:B:239:THR:HG22  | 2:B:240:ALA:N     | 2.33                     | 0.44              |
| 10:B:809:CLA:HMD3 | 4:I:14:LEU:CD1    | 2.48                     | 0.44              |
| 1:A:632:LEU:HD22  | 1:A:632:LEU:N     | 2.33                     | 0.43              |
| 12:B:844:BCR:HC7  | 12:B:844:BCR:H331 | 1.88                     | 0.43              |
| 2:B:227:THR:O     | 2:B:227:THR:HG22  | 2.17                     | 0.43              |
| 2:B:452:LEU:HD22  | 2:B:611:THR:HG21  | 2.01                     | 0.43              |
| 1:A:441:ASN:ND2   | 10:B:803:CLA:HED2 | 2.33                     | 0.43              |
| 2:B:456:VAL:HG13  | 2:B:457:PHE:CD1   | 2.54                     | 0.43              |
| 6:K:30:ILE:HD11   | 10:K:102:CLA:HBC3 | 2.01                     | 0.43              |
| 10:A:813:CLA:H143 | 13:A:865:ECH:C34  | 2.49                     | 0.43              |
| 1:A:207:LEU:HD22  | 12:A:847:BCR:H361 | 2.01                     | 0.43              |
| 12:A:866:BCR:C8   | 12:A:866:BCR:H331 | 2.48                     | 0.42              |
| 10:A:810:CLA:O1A  | 10:A:810:CLA:H43  | 2.19                     | 0.42              |
| 10:A:838:CLA:HED3 | 19:A:902:HOH:O    | 2.19                     | 0.42              |
| 13:A:851:ECH:H23  | 13:A:851:ECH:H40B | 2.01                     | 0.42              |
| 13:F:205:ECH:H20  | 13:F:205:ECH:H36  | 1.91                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:327:ALA:HB2   | 10:A:828:CLA:HED2 | 2.01                     | 0.42              |
| 1:A:708:ASN:OD1   | 3:F:91:ARG:NH1    | 2.49                     | 0.42              |
| 3:F:118:TRP:N     | 3:F:119:PRO:HD2   | 2.33                     | 0.42              |
| 12:F:202:BCR:H24C | 12:F:202:BCR:H371 | 1.91                     | 0.42              |
| 10:A:828:CLA:CGA  | 10:A:828:CLA:C1A  | 2.97                     | 0.42              |
| 2:B:266:GLU:OE1   | 2:B:361:GLN:NE2   | 2.45                     | 0.42              |
| 5:J:21:PHE:CZ     | 5:J:25:ILE:HD11   | 2.55                     | 0.42              |
| 10:A:845:CLA:C7   | 10:A:845:CLA:H41  | 2.50                     | 0.42              |
| 10:B:821:CLA:HMB2 | 10:B:826:CLA:HED1 | 2.02                     | 0.42              |
| 12:B:844:BCR:H24C | 12:B:844:BCR:H371 | 1.89                     | 0.42              |
| 1:A:551:LYS:NZ    | 2:B:670:GLU:OE2   | 2.52                     | 0.42              |
| 12:F:202:BCR:H20C | 12:F:202:BCR:H361 | 1.93                     | 0.42              |
| 2:B:3:THR:OG1     | 2:B:4:LYS:N       | 2.53                     | 0.41              |
| 1:A:74:SER:OG     | 1:A:180:TYR:HB2   | 2.19                     | 0.41              |
| 1:A:584:GLN:HB2   | 2:B:664:TRP:HB2   | 2.03                     | 0.41              |
| 10:B:808:CLA:HED3 | 10:B:808:CLA:H42  | 2.02                     | 0.41              |
| 1:A:319:HIS:CB    | 1:A:324:ILE:HD11  | 2.50                     | 0.41              |
| 12:A:848:BCR:H24C | 12:A:848:BCR:H371 | 1.88                     | 0.41              |
| 13:F:205:ECH:H24  | 13:F:205:ECH:H37  | 1.89                     | 0.41              |
| 12:A:850:BCR:H24C | 12:A:850:BCR:H371 | 1.90                     | 0.41              |
| 2:B:385:PHE:CZ    | 12:B:848:BCR:H373 | 2.56                     | 0.41              |
| 1:A:215:HIS:HE1   | 10:A:819:CLA:C1A  | 2.32                     | 0.41              |
| 2:B:440:VAL:HG21  | 10:B:835:CLA:HAC2 | 2.02                     | 0.41              |
| 2:B:526:THR:HG21  | 2:B:579:TRP:CE2   | 2.56                     | 0.41              |
| 1:A:59:ASP:OD1    | 1:A:414:ARG:NH1   | 2.54                     | 0.40              |
| 2:B:172:GLU:OE1   | 2:B:172:GLU:N     | 2.50                     | 0.40              |
| 2:B:118:SER:HB2   | 10:B:829:CLA:HED3 | 2.02                     | 0.40              |
| 5:J:21:PHE:CE2    | 5:J:25:ILE:HD11   | 2.56                     | 0.40              |
| 1:A:700:ILE:HD13  | 10:A:844:CLA:HMD1 | 2.03                     | 0.40              |
| 10:A:830:CLA:HAA2 | 10:A:830:CLA:HBD  | 2.02                     | 0.40              |
| 13:A:865:ECH:H24  | 13:A:865:ECH:H37  | 1.88                     | 0.40              |
| 12:A:866:BCR:H371 | 12:A:866:BCR:H24C | 1.87                     | 0.40              |
| 2:B:516:VAL:HG21  | 2:B:590:TYR:HB2   | 2.03                     | 0.40              |
| 2:B:299:HIS:HB3   | 2:B:304:ILE:HD11  | 2.02                     | 0.40              |
| 10:B:826:CLA:HMA2 | 10:B:826:CLA:CGA  | 2.51                     | 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   | A     | 728/751 (97%)   | 713 (98%)  | 15 (2%) | 0        | 100         | 100 |
| 2   | B     | 727/731 (100%)  | 716 (98%)  | 11 (2%) | 0        | 100         | 100 |
| 3   | F     | 135/165 (82%)   | 134 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 4   | I     | 35/40 (88%)     | 35 (100%)  | 0       | 0        | 100         | 100 |
| 5   | J     | 38/40 (95%)     | 38 (100%)  | 0       | 0        | 100         | 100 |
| 6   | K     | 76/86 (88%)     | 75 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 7   | M     | 29/31 (94%)     | 29 (100%)  | 0       | 0        | 100         | 100 |
| All | All   | 1768/1844 (96%) | 1740 (98%) | 28 (2%) | 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   | A     | 590/603 (98%)  | 585 (99%)  | 5 (1%)   | 73          | 65  |
| 2   | B     | 582/583 (100%) | 580 (100%) | 2 (0%)   | 86          | 81  |
| 3   | F     | 113/137 (82%)  | 113 (100%) | 0        | 100         | 100 |
| 4   | I     | 31/32 (97%)    | 31 (100%)  | 0        | 100         | 100 |
| 5   | J     | 35/35 (100%)   | 34 (97%)   | 1 (3%)   | 37          | 20  |
| 6   | K     | 55/62 (89%)    | 55 (100%)  | 0        | 100         | 100 |
| 7   | M     | 25/25 (100%)   | 25 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| All | All   | 1431/1477 (97%) | 1423 (99%) | 8 (1%)   | 76          | 72 |

All (8) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 535 | HIS  |
| 1   | A     | 543 | HIS  |
| 1   | A     | 561 | LEU  |
| 1   | A     | 584 | GLN  |
| 1   | A     | 585 | VAL  |
| 2   | B     | 517 | HIS  |
| 2   | B     | 651 | HIS  |
| 5   | J     | 14  | MET  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 216 | GLN  |
| 1   | A     | 441 | ASN  |
| 2   | B     | 34  | HIS  |
| 2   | B     | 701 | GLN  |
| 3   | F     | 31  | ASN  |
| 3   | F     | 99  | GLN  |
| 4   | I     | 33  | HIS  |

### 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

Of 148 ligands modelled in this entry, 1 is monoatomic - leaving 147 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 10  | CLA  | B     | 823 | 2    | 49,53,73     | 1.39 | 4 (8%)   | 59,89,113   | 1.05 | 3 (5%)   |
| 10  | CLA  | B     | 806 | 2    | 49,53,73     | 1.36 | 4 (8%)   | 59,89,113   | 1.03 | 3 (5%)   |
| 10  | CLA  | B     | 808 | 2    | 69,73,73     | 1.16 | 4 (5%)   | 83,113,113  | 0.86 | 3 (3%)   |
| 10  | CLA  | A     | 812 | 1    | 50,54,73     | 1.33 | 4 (8%)   | 60,90,113   | 1.02 | 3 (5%)   |
| 10  | CLA  | A     | 825 | 1    | 64,68,73     | 1.19 | 4 (6%)   | 77,107,113  | 0.92 | 3 (3%)   |
| 10  | CLA  | B     | 831 | 2    | 64,68,73     | 1.19 | 4 (6%)   | 77,107,113  | 0.91 | 3 (3%)   |
| 12  | BCR  | A     | 847 | -    | 41,41,41     | 0.12 | 0        | 56,56,56    | 0.28 | 0        |
| 13  | ECH  | F     | 205 | -    | 42,42,42     | 0.10 | 0        | 55,58,58    | 0.32 | 0        |
| 10  | CLA  | A     | 836 | 1    | 49,53,73     | 1.38 | 4 (8%)   | 59,89,113   | 1.05 | 3 (5%)   |
| 10  | CLA  | B     | 828 | 2    | 69,73,73     | 1.17 | 4 (5%)   | 83,113,113  | 0.89 | 3 (3%)   |
| 10  | CLA  | A     | 826 | 19   | 69,73,73     | 1.18 | 4 (5%)   | 83,113,113  | 0.88 | 3 (3%)   |
| 12  | BCR  | I     | 101 | -    | 41,41,41     | 0.12 | 0        | 56,56,56    | 0.39 | 0        |
| 10  | CLA  | A     | 844 | 1    | 69,73,73     | 1.14 | 4 (5%)   | 83,113,113  | 0.88 | 3 (3%)   |
| 10  | CLA  | B     | 827 | 19   | 54,58,73     | 1.33 | 4 (7%)   | 65,95,113   | 0.98 | 4 (6%)   |
| 12  | BCR  | A     | 850 | -    | 41,41,41     | 0.13 | 0        | 56,56,56    | 0.32 | 0        |
| 15  | LMT  | A     | 860 | -    | 24,24,36     | 0.52 | 0        | 29,29,47    | 0.55 | 0        |
| 10  | CLA  | B     | 843 | 8    | 28,35,73     | 1.95 | 6 (21%)  | 32,60,113   | 1.73 | 6 (18%)  |
| 10  | CLA  | A     | 810 | 1    | 69,73,73     | 1.13 | 4 (5%)   | 83,113,113  | 0.92 | 4 (4%)   |
| 10  | CLA  | A     | 863 | 19   | 69,73,73     | 1.17 | 4 (5%)   | 83,113,113  | 0.87 | 3 (3%)   |
| 10  | CLA  | B     | 841 | 19   | 49,53,73     | 1.40 | 4 (8%)   | 59,89,113   | 1.05 | 3 (5%)   |
| 17  | SF4  | B     | 805 | 1    | 0,6,12       | -    | -        | -           | -    | -        |
| 15  | LMT  | B     | 860 | -    | 12,12,36     | 0.27 | 0        | 11,11,47    | 0.32 | 0        |
| 8   | LHG  | A     | 801 | -    | 48,48,48     | 0.22 | 0        | 51,54,54    | 0.26 | 0        |
| 10  | CLA  | B     | 826 | 19   | 69,73,73     | 1.21 | 4 (5%)   | 83,113,113  | 0.86 | 4 (4%)   |
| 10  | CLA  | B     | 818 | 2    | 59,63,73     | 1.24 | 4 (6%)   | 71,101,113  | 1.01 | 3 (4%)   |
| 15  | LMT  | B     | 858 | -    | 20,20,36     | 0.57 | 0        | 25,25,47    | 0.60 | 0        |
| 10  | CLA  | A     | 817 | 1    | 58,62,73     | 1.26 | 4 (6%)   | 69,99,113   | 0.96 | 3 (4%)   |
| 15  | LMT  | F     | 207 | -    | 35,35,36     | 0.55 | 0        | 46,46,47    | 0.66 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 12  | BCR  | B     | 845 | -    | 41,41,41     | 0.13 | 0        | 56,56,56    | 0.40 | 0        |
| 13  | ECH  | B     | 846 | -    | 42,42,42     | 0.12 | 0        | 55,58,58    | 0.29 | 0        |
| 15  | LMT  | B     | 859 | -    | 12,12,36     | 0.26 | 0        | 11,11,47    | 0.31 | 0        |
| 10  | CLA  | B     | 809 | 2    | 64,68,73     | 1.20 | 4 (6%)   | 77,107,113  | 0.91 | 3 (3%)   |
| 14  | LMG  | A     | 852 | -    | 32,32,55     | 0.21 | 0        | 40,40,63    | 0.17 | 0        |
| 10  | CLA  | A     | 834 | 1    | 69,73,73     | 1.16 | 4 (5%)   | 83,113,113  | 0.87 | 3 (3%)   |
| 10  | CLA  | B     | 829 | 2    | 69,73,73     | 1.17 | 4 (5%)   | 83,113,113  | 0.90 | 4 (4%)   |
| 13  | ECH  | A     | 865 | -    | 42,42,42     | 0.10 | 0        | 55,58,58    | 0.24 | 0        |
| 11  | PQN  | B     | 804 | -    | 34,34,34     | 0.32 | 0        | 42,45,45    | 0.34 | 0        |
| 10  | CLA  | A     | 846 | 19   | 49,53,73     | 1.40 | 4 (8%)   | 59,89,113   | 1.05 | 3 (5%)   |
| 10  | CLA  | A     | 813 | 1    | 69,73,73     | 1.16 | 4 (5%)   | 83,113,113  | 0.85 | 3 (3%)   |
| 15  | LMT  | A     | 859 | -    | 12,12,36     | 0.26 | 0        | 11,11,47    | 0.31 | 0        |
| 15  | LMT  | A     | 853 | -    | 36,36,36     | 0.56 | 0        | 47,47,47    | 0.79 | 1 (2%)   |
| 12  | BCR  | F     | 202 | -    | 41,41,41     | 0.15 | 0        | 56,56,56    | 0.46 | 0        |
| 10  | CLA  | B     | 832 | 2    | 49,53,73     | 1.36 | 4 (8%)   | 59,89,113   | 1.07 | 3 (5%)   |
| 15  | LMT  | I     | 103 | -    | 32,32,36     | 0.55 | 0        | 43,43,47    | 0.66 | 0        |
| 12  | BCR  | A     | 866 | -    | 41,41,41     | 0.13 | 0        | 56,56,56    | 0.25 | 0        |
| 10  | CLA  | B     | 810 | 2    | 69,73,73     | 1.15 | 4 (5%)   | 83,113,113  | 0.90 | 3 (3%)   |
| 15  | LMT  | B     | 857 | -    | 12,12,36     | 0.27 | 0        | 11,11,47    | 0.33 | 0        |
| 10  | CLA  | A     | 818 | 1    | 59,63,73     | 1.23 | 4 (6%)   | 71,101,113  | 0.93 | 3 (4%)   |
| 10  | CLA  | B     | 803 | -    | 69,73,73     | 1.19 | 4 (5%)   | 83,113,113  | 0.86 | 3 (3%)   |
| 10  | CLA  | K     | 103 | 19   | 64,68,73     | 1.22 | 4 (6%)   | 77,107,113  | 0.93 | 3 (3%)   |
| 15  | LMT  | B     | 854 | -    | 28,28,36     | 0.60 | 0        | 39,39,47    | 0.68 | 0        |
| 10  | CLA  | A     | 807 | 8    | 49,53,73     | 1.40 | 4 (8%)   | 59,89,113   | 1.02 | 3 (5%)   |
| 12  | BCR  | B     | 848 | -    | 41,41,41     | 0.15 | 0        | 56,56,56    | 0.50 | 0        |
| 10  | CLA  | B     | 838 | 2    | 54,58,73     | 1.29 | 4 (7%)   | 65,95,113   | 0.97 | 3 (4%)   |
| 12  | BCR  | B     | 849 | -    | 41,41,41     | 0.12 | 0        | 56,56,56    | 0.47 | 0        |
| 10  | CLA  | A     | 831 | 19   | 59,63,73     | 1.25 | 4 (6%)   | 71,101,113  | 0.95 | 3 (4%)   |
| 10  | CLA  | B     | 817 | 2    | 49,53,73     | 1.37 | 4 (8%)   | 59,89,113   | 1.04 | 3 (5%)   |
| 15  | LMT  | B     | 855 | -    | 32,32,36     | 0.58 | 0        | 43,43,47    | 0.66 | 0        |
| 15  | LMT  | B     | 853 | -    | 24,24,36     | 0.52 | 0        | 29,29,47    | 0.55 | 0        |
| 10  | CLA  | A     | 835 | 1    | 69,73,73     | 1.15 | 4 (5%)   | 83,113,113  | 0.87 | 3 (3%)   |
| 10  | CLA  | A     | 828 | 1    | 55,59,73     | 1.31 | 4 (7%)   | 66,96,113   | 0.99 | 3 (4%)   |
| 10  | CLA  | J     | 101 | 5    | 49,53,73     | 1.42 | 4 (8%)   | 59,89,113   | 1.04 | 3 (5%)   |
| 10  | CLA  | A     | 821 | 19   | 49,53,73     | 1.39 | 4 (8%)   | 59,89,113   | 1.06 | 3 (5%)   |
| 10  | CLA  | A     | 830 | 19   | 69,73,73     | 1.19 | 4 (5%)   | 83,113,113  | 0.86 | 3 (3%)   |
| 10  | CLA  | A     | 837 | 1    | 49,53,73     | 1.39 | 4 (8%)   | 59,89,113   | 1.05 | 3 (5%)   |
| 10  | CLA  | B     | 801 | 2    | 69,73,73     | 1.13 | 4 (5%)   | 83,113,113  | 0.89 | 4 (4%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 10  | CLA  | A     | 822 | 1    | 69,73,73     | 1.13 | 4 (5%)   | 83,113,113  | 0.88 | 3 (3%)   |
| 10  | CLA  | B     | 840 | 2    | 55,59,73     | 1.31 | 4 (7%)   | 66,96,113   | 0.97 | 3 (4%)   |
| 10  | CLA  | F     | 203 | 19   | 49,53,73     | 1.39 | 4 (8%)   | 59,89,113   | 1.02 | 3 (5%)   |
| 10  | CLA  | B     | 819 | 2    | 69,73,73     | 1.13 | 4 (5%)   | 83,113,113  | 0.88 | 3 (3%)   |
| 15  | LMT  | A     | 854 | -    | 16,16,36     | 0.60 | 0        | 21,21,47    | 0.63 | 0        |
| 15  | LMT  | J     | 104 | -    | 12,12,36     | 0.27 | 0        | 11,11,47    | 0.36 | 0        |
| 10  | CLA  | B     | 813 | 2    | 49,53,73     | 1.35 | 4 (8%)   | 59,89,113   | 1.04 | 3 (5%)   |
| 15  | LMT  | B     | 861 | -    | 12,12,36     | 0.26 | 0        | 11,11,47    | 0.33 | 0        |
| 15  | LMT  | A     | 857 | -    | 12,12,36     | 0.26 | 0        | 11,11,47    | 0.31 | 0        |
| 10  | CLA  | B     | 811 | 2    | 49,53,73     | 1.40 | 4 (8%)   | 59,89,113   | 1.02 | 3 (5%)   |
| 12  | BCR  | B     | 844 | -    | 41,41,41     | 0.24 | 0        | 56,56,56    | 0.44 | 0        |
| 15  | LMT  | A     | 855 | -    | 12,12,36     | 0.27 | 0        | 11,11,47    | 0.31 | 0        |
| 10  | CLA  | B     | 835 | 2    | 65,69,73     | 1.17 | 4 (6%)   | 78,108,113  | 0.92 | 3 (3%)   |
| 15  | LMT  | I     | 102 | -    | 27,27,36     | 0.59 | 0        | 37,38,47    | 0.76 | 0        |
| 10  | CLA  | A     | 820 | 1    | 49,53,73     | 1.36 | 4 (8%)   | 59,89,113   | 1.04 | 3 (5%)   |
| 10  | CLA  | B     | 812 | 2    | 49,53,73     | 1.39 | 4 (8%)   | 59,89,113   | 1.05 | 3 (5%)   |
| 10  | CLA  | A     | 861 | 1    | 49,53,73     | 1.40 | 4 (8%)   | 59,89,113   | 1.04 | 3 (5%)   |
| 10  | CLA  | B     | 839 | 2    | 66,70,73     | 1.18 | 4 (6%)   | 79,109,113  | 0.91 | 3 (3%)   |
| 10  | CLA  | K     | 101 | 6    | 49,53,73     | 1.39 | 4 (8%)   | 59,89,113   | 1.03 | 3 (5%)   |
| 15  | LMT  | F     | 201 | -    | 31,31,36     | 0.58 | 0        | 42,42,47    | 0.65 | 0        |
| 10  | CLA  | B     | 815 | 2    | 69,73,73     | 1.15 | 4 (5%)   | 83,113,113  | 0.88 | 3 (3%)   |
| 10  | CLA  | A     | 832 | 1    | 69,73,73     | 1.17 | 4 (5%)   | 83,113,113  | 0.84 | 3 (3%)   |
| 13  | ECH  | M     | 101 | -    | 42,42,42     | 0.12 | 0        | 55,58,58    | 0.26 | 0        |
| 15  | LMT  | F     | 206 | -    | 12,12,36     | 0.26 | 0        | 11,11,47    | 0.31 | 0        |
| 8   | LHG  | A     | 802 | 10   | 32,32,48     | 0.27 | 0        | 35,38,54    | 0.32 | 0        |
| 10  | CLA  | A     | 809 | 10,1 | 54,58,73     | 1.28 | 4 (7%)   | 65,95,113   | 0.99 | 3 (4%)   |
| 10  | CLA  | B     | 824 | 2    | 64,68,73     | 1.20 | 4 (6%)   | 77,107,113  | 0.90 | 3 (3%)   |
| 10  | CLA  | A     | 840 | 1    | 49,53,73     | 1.39 | 4 (8%)   | 59,89,113   | 1.03 | 3 (5%)   |
| 10  | CLA  | A     | 845 | 1    | 69,73,73     | 1.13 | 4 (5%)   | 83,113,113  | 0.89 | 3 (3%)   |
| 10  | CLA  | B     | 820 | 2    | 69,73,73     | 1.16 | 4 (5%)   | 83,113,113  | 0.87 | 3 (3%)   |
| 10  | CLA  | A     | 819 | 1    | 49,53,73     | 1.37 | 4 (8%)   | 59,89,113   | 1.03 | 4 (6%)   |
| 15  | LMT  | A     | 858 | -    | 24,24,36     | 0.52 | 0        | 29,29,47    | 0.61 | 0        |
| 15  | LMT  | J     | 105 | -    | 12,12,36     | 0.27 | 0        | 11,11,47    | 0.30 | 0        |
| 10  | CLA  | A     | 843 | 1    | 51,55,73     | 1.35 | 4 (7%)   | 61,91,113   | 1.03 | 3 (4%)   |
| 12  | BCR  | A     | 849 | -    | 41,41,41     | 0.12 | 0        | 56,56,56    | 0.26 | 0        |
| 12  | BCR  | J     | 103 | -    | 41,41,41     | 0.13 | 0        | 56,56,56    | 0.30 | 0        |
| 10  | CLA  | A     | 811 | 1    | 69,73,73     | 1.15 | 4 (5%)   | 83,113,113  | 0.85 | 3 (3%)   |
| 10  | CLA  | J     | 102 | 5    | 49,53,73     | 1.39 | 4 (8%)   | 59,89,113   | 1.04 | 3 (5%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 10  | CLA  | B     | 802 | 19   | 69,73,73     | 1.21 | 4 (5%)   | 83,113,113  | 0.87 | 3 (3%)   |
| 10  | CLA  | A     | 824 | 1    | 69,73,73     | 1.14 | 4 (5%)   | 83,113,113  | 0.91 | 4 (4%)   |
| 15  | LMT  | A     | 864 | -    | 36,36,36     | 0.57 | 0        | 47,47,47    | 0.70 | 0        |
| 10  | CLA  | A     | 814 | 1    | 54,58,73     | 1.35 | 4 (7%)   | 65,95,113   | 1.00 | 3 (4%)   |
| 10  | CLA  | A     | 808 | 1    | 69,73,73     | 1.14 | 4 (5%)   | 83,113,113  | 0.88 | 4 (4%)   |
| 10  | CLA  | A     | 841 | 1    | 55,59,73     | 1.27 | 4 (7%)   | 66,96,113   | 0.98 | 3 (4%)   |
| 10  | CLA  | B     | 833 | 2    | 59,63,73     | 1.25 | 4 (6%)   | 71,101,113  | 0.94 | 3 (4%)   |
| 10  | CLA  | B     | 807 | 2    | 69,73,73     | 1.17 | 4 (5%)   | 83,113,113  | 0.90 | 3 (3%)   |
| 10  | CLA  | B     | 842 | 2    | 49,53,73     | 1.37 | 4 (8%)   | 59,89,113   | 1.04 | 4 (6%)   |
| 12  | BCR  | K     | 104 | -    | 41,41,41     | 0.12 | 0        | 56,56,56    | 0.29 | 0        |
| 10  | CLA  | A     | 827 | 1    | 53,57,73     | 1.34 | 4 (7%)   | 62,93,113   | 1.04 | 3 (4%)   |
| 10  | CLA  | A     | 842 | 1    | 59,63,73     | 1.26 | 4 (6%)   | 71,101,113  | 0.97 | 3 (4%)   |
| 10  | CLA  | A     | 815 | 1    | 49,53,73     | 1.37 | 4 (8%)   | 59,89,113   | 1.03 | 3 (5%)   |
| 10  | CLA  | B     | 816 | 2    | 50,54,73     | 1.34 | 4 (8%)   | 60,90,113   | 1.02 | 3 (5%)   |
| 15  | LMT  | A     | 856 | -    | 10,10,36     | 0.28 | 0        | 9,9,47      | 0.35 | 0        |
| 8   | LHG  | B     | 851 | 10   | 38,38,48     | 0.25 | 0        | 41,44,54    | 0.28 | 0        |
| 10  | CLA  | K     | 102 | 6    | 49,53,73     | 1.41 | 4 (8%)   | 59,89,113   | 1.03 | 3 (5%)   |
| 10  | CLA  | B     | 830 | 2    | 69,73,73     | 1.14 | 4 (5%)   | 83,113,113  | 0.87 | 3 (3%)   |
| 11  | PQN  | A     | 806 | -    | 34,34,34     | 0.31 | 0        | 42,45,45    | 0.35 | 0        |
| 18  | 5X6  | B     | 852 | -    | 43,43,43     | 0.12 | 0        | 58,60,60    | 0.48 | 2 (3%)   |
| 9   | CL0  | A     | 803 | 1    | 69,73,73     | 1.59 | 8 (11%)  | 83,113,113  | 1.21 | 9 (10%)  |
| 15  | LMT  | M     | 102 | -    | 12,12,36     | 0.27 | 0        | 11,11,47    | 0.32 | 0        |
| 10  | CLA  | B     | 814 | 2    | 49,53,73     | 1.40 | 4 (8%)   | 59,89,113   | 1.03 | 3 (5%)   |
| 12  | BCR  | A     | 848 | -    | 41,41,41     | 0.15 | 0        | 56,56,56    | 0.30 | 0        |
| 10  | CLA  | A     | 833 | 1    | 69,73,73     | 1.16 | 4 (5%)   | 83,113,113  | 0.87 | 3 (3%)   |
| 10  | CLA  | A     | 838 | 1    | 49,53,73     | 1.36 | 4 (8%)   | 59,89,113   | 1.05 | 3 (5%)   |
| 10  | CLA  | A     | 805 | -    | 69,73,73     | 1.15 | 4 (5%)   | 83,113,113  | 0.84 | 3 (3%)   |
| 12  | BCR  | B     | 847 | -    | 41,41,41     | 0.12 | 0        | 56,56,56    | 0.32 | 0        |
| 10  | CLA  | A     | 804 | 19   | 69,73,73     | 1.24 | 4 (5%)   | 83,113,113  | 0.88 | 4 (4%)   |
| 13  | ECH  | A     | 851 | -    | 42,42,42     | 0.13 | 0        | 55,58,58    | 0.33 | 0        |
| 10  | CLA  | B     | 834 | 2    | 69,73,73     | 1.14 | 4 (5%)   | 83,113,113  | 0.86 | 3 (3%)   |
| 15  | LMT  | B     | 856 | -    | 12,12,36     | 0.26 | 0        | 11,11,47    | 0.31 | 0        |
| 10  | CLA  | B     | 825 | 2    | 59,63,73     | 1.27 | 4 (6%)   | 71,101,113  | 0.95 | 3 (4%)   |
| 10  | CLA  | A     | 829 | 1    | 63,67,73     | 1.21 | 4 (6%)   | 75,105,113  | 0.93 | 3 (4%)   |
| 10  | CLA  | B     | 837 | 19   | 49,53,73     | 1.41 | 4 (8%)   | 59,89,113   | 1.03 | 3 (5%)   |
| 10  | CLA  | B     | 822 | 2    | 66,70,73     | 1.20 | 4 (6%)   | 79,109,113  | 0.92 | 3 (3%)   |
| 10  | CLA  | B     | 836 | 19   | 49,53,73     | 1.40 | 4 (8%)   | 59,89,113   | 1.06 | 3 (5%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | LMG  | B     | 850 | -    | 48,48,55     | 0.19 | 0        | 56,56,63    | 0.14 | 0        |
| 10  | CLA  | A     | 839 | 1    | 58,62,73     | 1.27 | 4 (6%)   | 69,99,113   | 0.97 | 3 (4%)   |
| 10  | CLA  | B     | 821 | 19   | 69,73,73     | 1.19 | 4 (5%)   | 83,113,113  | 0.87 | 3 (3%)   |
| 10  | CLA  | A     | 823 | 1    | 69,73,73     | 1.16 | 4 (5%)   | 83,113,113  | 0.92 | 3 (3%)   |
| 10  | CLA  | F     | 204 | 3    | 49,53,73     | 1.39 | 4 (8%)   | 59,89,113   | 1.03 | 3 (5%)   |
| 10  | CLA  | A     | 816 | 10,1 | 69,73,73     | 1.14 | 4 (5%)   | 83,113,113  | 0.87 | 3 (3%)   |

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   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 10  | CLA  | B     | 823 | 2    | -       | 4/15/91/115  | -       |
| 10  | CLA  | B     | 806 | 2    | -       | 3/15/91/115  | -       |
| 10  | CLA  | B     | 808 | 2    | -       | 2/39/115/115 | -       |
| 10  | CLA  | A     | 812 | 1    | -       | 1/17/93/115  | -       |
| 10  | CLA  | A     | 825 | 1    | -       | 2/33/109/115 | -       |
| 10  | CLA  | B     | 831 | 2    | -       | 5/33/109/115 | -       |
| 12  | BCR  | A     | 847 | -    | -       | 2/29/63/63   | 0/2/2/2 |
| 13  | ECH  | F     | 205 | -    | -       | 2/29/66/66   | 0/2/2/2 |
| 10  | CLA  | A     | 836 | 1    | -       | 3/15/91/115  | -       |
| 10  | CLA  | B     | 828 | 2    | -       | 3/39/115/115 | -       |
| 10  | CLA  | A     | 826 | 19   | -       | 1/39/115/115 | -       |
| 12  | BCR  | I     | 101 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 10  | CLA  | A     | 844 | 1    | -       | 5/39/115/115 | -       |
| 10  | CLA  | B     | 827 | 19   | -       | 2/21/97/115  | -       |
| 12  | BCR  | A     | 850 | -    | -       | 2/29/63/63   | 0/2/2/2 |
| 15  | LMT  | A     | 860 | -    | -       | 3/15/35/61   | 0/1/1/2 |
| 10  | CLA  | A     | 810 | 1    | -       | 4/39/115/115 | -       |
| 10  | CLA  | A     | 863 | 19   | -       | 6/39/115/115 | -       |
| 10  | CLA  | B     | 841 | 19   | -       | 3/15/91/115  | -       |
| 17  | SF4  | B     | 805 | 1    | -       | -            | 0/1/1/5 |
| 15  | LMT  | B     | 860 | -    | -       | 0/10/10/61   | -       |
| 8   | LHG  | A     | 801 | -    | -       | 15/53/53/53  | -       |
| 10  | CLA  | B     | 826 | 19   | -       | 2/39/115/115 | -       |
| 10  | CLA  | B     | 818 | 2    | -       | 4/27/103/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 15  | LMT  | B     | 858 | -    | -       | 1/11/31/61   | 0/1/1/2 |
| 10  | CLA  | A     | 817 | 1    | -       | 1/26/102/115 | -       |
| 15  | LMT  | F     | 207 | -    | -       | 5/20/60/61   | 0/2/2/2 |
| 12  | BCR  | B     | 845 | -    | -       | 2/29/63/63   | 0/2/2/2 |
| 13  | ECH  | B     | 846 | -    | -       | 5/29/66/66   | 0/2/2/2 |
| 15  | LMT  | B     | 859 | -    | -       | 1/10/10/61   | -       |
| 10  | CLA  | B     | 809 | 2    | -       | 2/33/109/115 | -       |
| 14  | LMG  | A     | 852 | -    | -       | 5/27/47/70   | 0/1/1/1 |
| 10  | CLA  | A     | 834 | 1    | -       | 2/39/115/115 | -       |
| 10  | CLA  | B     | 829 | 2    | -       | 7/39/115/115 | -       |
| 13  | ECH  | A     | 865 | -    | -       | 0/29/66/66   | 0/2/2/2 |
| 11  | PQN  | B     | 804 | -    | -       | 0/23/43/43   | 0/2/2/2 |
| 10  | CLA  | A     | 846 | 19   | -       | 4/15/91/115  | -       |
| 10  | CLA  | A     | 813 | 1    | -       | 4/39/115/115 | -       |
| 15  | LMT  | A     | 859 | -    | -       | 0/10/10/61   | -       |
| 15  | LMT  | A     | 853 | -    | -       | 4/21/61/61   | 0/2/2/2 |
| 12  | BCR  | F     | 202 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 10  | CLA  | B     | 832 | 2    | -       | 1/15/91/115  | -       |
| 15  | LMT  | I     | 103 | -    | -       | 4/17/57/61   | 0/2/2/2 |
| 12  | BCR  | A     | 866 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 10  | CLA  | B     | 810 | 2    | -       | 5/39/115/115 | -       |
| 15  | LMT  | B     | 857 | -    | -       | 1/10/10/61   | -       |
| 10  | CLA  | A     | 818 | 1    | -       | 3/27/103/115 | -       |
| 10  | CLA  | B     | 803 | -    | -       | 3/39/115/115 | -       |
| 10  | CLA  | K     | 103 | 19   | -       | 6/33/109/115 | -       |
| 15  | LMT  | B     | 854 | -    | -       | 1/13/53/61   | 0/2/2/2 |
| 10  | CLA  | A     | 807 | 8    | -       | 2/15/91/115  | -       |
| 12  | BCR  | B     | 848 | -    | -       | 2/29/63/63   | 0/2/2/2 |
| 10  | CLA  | B     | 838 | 2    | -       | 1/21/97/115  | -       |
| 12  | BCR  | B     | 849 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 10  | CLA  | A     | 831 | 19   | -       | 1/27/103/115 | -       |
| 10  | CLA  | B     | 817 | 2    | -       | 0/15/91/115  | -       |
| 15  | LMT  | B     | 855 | -    | -       | 0/17/57/61   | 0/2/2/2 |
| 15  | LMT  | B     | 853 | -    | -       | 3/15/35/61   | 0/1/1/2 |
| 10  | CLA  | A     | 835 | 1    | -       | 3/39/115/115 | -       |
| 10  | CLA  | A     | 828 | 1    | -       | 3/23/99/115  | -       |
| 10  | CLA  | J     | 101 | 5    | -       | 4/15/91/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 10  | CLA  | A     | 821 | 19   | -       | 3/15/91/115  | -       |
| 10  | CLA  | A     | 830 | 19   | -       | 6/39/115/115 | -       |
| 10  | CLA  | A     | 837 | 1    | -       | 5/15/91/115  | -       |
| 10  | CLA  | B     | 801 | 2    | -       | 4/39/115/115 | -       |
| 10  | CLA  | A     | 822 | 1    | -       | 0/39/115/115 | -       |
| 10  | CLA  | B     | 840 | 2    | -       | 2/23/99/115  | -       |
| 10  | CLA  | F     | 203 | 19   | -       | 2/15/91/115  | -       |
| 10  | CLA  | B     | 819 | 2    | -       | 5/39/115/115 | -       |
| 15  | LMT  | A     | 854 | -    | -       | 1/7/27/61    | 0/1/1/2 |
| 15  | LMT  | J     | 104 | -    | -       | 2/10/10/61   | -       |
| 10  | CLA  | B     | 813 | 2    | -       | 1/15/91/115  | -       |
| 15  | LMT  | B     | 861 | -    | -       | 0/10/10/61   | -       |
| 15  | LMT  | A     | 857 | -    | -       | 0/10/10/61   | -       |
| 10  | CLA  | B     | 811 | 2    | -       | 2/15/91/115  | -       |
| 12  | BCR  | B     | 844 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 15  | LMT  | A     | 855 | -    | -       | 1/10/10/61   | -       |
| 10  | CLA  | B     | 835 | 2    | -       | 2/35/111/115 | -       |
| 15  | LMT  | I     | 102 | -    | -       | 3/12/52/61   | 0/2/2/2 |
| 10  | CLA  | A     | 820 | 1    | -       | 3/15/91/115  | -       |
| 10  | CLA  | B     | 812 | 2    | -       | 4/15/91/115  | -       |
| 10  | CLA  | A     | 861 | 1    | -       | 0/15/91/115  | -       |
| 10  | CLA  | B     | 839 | 2    | -       | 0/36/112/115 | -       |
| 10  | CLA  | K     | 101 | 6    | -       | 5/15/91/115  | -       |
| 15  | LMT  | F     | 201 | -    | -       | 0/16/56/61   | 0/2/2/2 |
| 10  | CLA  | B     | 815 | 2    | -       | 4/39/115/115 | -       |
| 10  | CLA  | A     | 832 | 1    | -       | 3/39/115/115 | -       |
| 13  | ECH  | M     | 101 | -    | -       | 4/29/66/66   | 0/2/2/2 |
| 15  | LMT  | F     | 206 | -    | -       | 0/10/10/61   | -       |
| 8   | LHG  | A     | 802 | 10   | -       | 11/37/37/53  | -       |
| 10  | CLA  | A     | 809 | 10,1 | -       | 1/21/97/115  | -       |
| 10  | CLA  | B     | 824 | 2    | -       | 5/33/109/115 | -       |
| 10  | CLA  | A     | 840 | 1    | -       | 7/15/91/115  | -       |
| 10  | CLA  | A     | 845 | 1    | -       | 4/39/115/115 | -       |
| 10  | CLA  | B     | 820 | 2    | -       | 4/39/115/115 | -       |
| 10  | CLA  | A     | 819 | 1    | -       | 3/15/91/115  | -       |
| 15  | LMT  | A     | 858 | -    | -       | 6/15/35/61   | 0/1/1/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 15  | LMT  | J     | 105 | -    | -       | 2/10/10/61   | -       |
| 10  | CLA  | A     | 843 | 1    | -       | 4/18/94/115  | -       |
| 12  | BCR  | A     | 849 | -    | -       | 2/29/63/63   | 0/2/2/2 |
| 12  | BCR  | J     | 103 | -    | -       | 2/29/63/63   | 0/2/2/2 |
| 10  | CLA  | A     | 811 | 1    | -       | 2/39/115/115 | -       |
| 10  | CLA  | J     | 102 | 5    | -       | 4/15/91/115  | -       |
| 10  | CLA  | B     | 802 | 19   | -       | 7/39/115/115 | -       |
| 10  | CLA  | A     | 824 | 1    | -       | 4/39/115/115 | -       |
| 15  | LMT  | A     | 864 | -    | -       | 1/21/61/61   | 0/2/2/2 |
| 10  | CLA  | A     | 814 | 1    | -       | 1/21/97/115  | -       |
| 10  | CLA  | A     | 808 | 1    | -       | 2/39/115/115 | -       |
| 10  | CLA  | A     | 841 | 1    | -       | 2/23/99/115  | -       |
| 10  | CLA  | B     | 833 | 2    | -       | 3/27/103/115 | -       |
| 10  | CLA  | B     | 807 | 2    | -       | 8/39/115/115 | -       |
| 10  | CLA  | B     | 842 | 2    | -       | 5/15/91/115  | -       |
| 12  | BCR  | K     | 104 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 10  | CLA  | A     | 827 | 1    | -       | 3/20/96/115  | -       |
| 10  | CLA  | A     | 842 | 1    | -       | 2/27/103/115 | -       |
| 10  | CLA  | A     | 815 | 1    | -       | 1/15/91/115  | -       |
| 10  | CLA  | B     | 816 | 2    | -       | 1/17/93/115  | -       |
| 15  | LMT  | A     | 856 | -    | -       | 0/8/8/61     | -       |
| 8   | LHG  | B     | 851 | 10   | -       | 8/43/43/53   | -       |
| 10  | CLA  | K     | 102 | 6    | -       | 7/15/91/115  | -       |
| 10  | CLA  | B     | 830 | 2    | -       | 2/39/115/115 | -       |
| 11  | PQN  | A     | 806 | -    | -       | 0/23/43/43   | 0/2/2/2 |
| 18  | 5X6  | B     | 852 | -    | -       | 2/29/67/67   | 0/2/2/2 |
| 9   | CL0  | A     | 803 | 1    | -       | 2/39/115/115 | -       |
| 15  | LMT  | M     | 102 | -    | -       | 0/10/10/61   | -       |
| 10  | CLA  | B     | 814 | 2    | -       | 3/15/91/115  | -       |
| 12  | BCR  | A     | 848 | -    | -       | 2/29/63/63   | 0/2/2/2 |
| 10  | CLA  | A     | 833 | 1    | -       | 1/39/115/115 | -       |
| 10  | CLA  | A     | 838 | 1    | -       | 2/15/91/115  | -       |
| 10  | CLA  | A     | 805 | -    | -       | 5/39/115/115 | -       |
| 12  | BCR  | B     | 847 | -    | -       | 2/29/63/63   | 0/2/2/2 |
| 10  | CLA  | A     | 804 | 19   | -       | 2/39/115/115 | -       |
| 13  | ECH  | A     | 851 | -    | -       | 6/29/66/66   | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 10  | CLA  | B     | 834 | 2    | -       | 2/39/115/115 | -       |
| 15  | LMT  | B     | 856 | -    | -       | 0/10/10/61   | -       |
| 10  | CLA  | B     | 825 | 2    | -       | 5/27/103/115 | -       |
| 10  | CLA  | A     | 829 | 1    | -       | 6/32/108/115 | -       |
| 10  | CLA  | B     | 837 | 19   | -       | 2/15/91/115  | -       |
| 10  | CLA  | B     | 822 | 2    | -       | 7/36/112/115 | -       |
| 10  | CLA  | B     | 836 | 19   | -       | 0/15/91/115  | -       |
| 14  | LMG  | B     | 850 | -    | -       | 4/43/63/70   | 0/1/1/1 |
| 10  | CLA  | A     | 839 | 1    | -       | 3/26/102/115 | -       |
| 10  | CLA  | B     | 821 | 19   | -       | 2/39/115/115 | -       |
| 10  | CLA  | A     | 823 | 1    | -       | 6/39/115/115 | -       |
| 10  | CLA  | F     | 204 | 3    | -       | 2/15/91/115  | -       |
| 10  | CLA  | A     | 816 | 10,1 | -       | 8/39/115/115 | -       |

All (378) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 10  | A     | 804 | CLA  | MG-NB  | -5.87 | 1.94        | 2.05     |
| 10  | B     | 829 | CLA  | C1D-ND | 5.79  | 1.44        | 1.37     |
| 10  | A     | 841 | CLA  | C1D-ND | 5.76  | 1.44        | 1.37     |
| 10  | A     | 833 | CLA  | C1D-ND | 5.72  | 1.44        | 1.37     |
| 10  | J     | 102 | CLA  | C1D-ND | 5.70  | 1.44        | 1.37     |
| 10  | B     | 826 | CLA  | C1D-ND | 5.70  | 1.44        | 1.37     |
| 10  | B     | 810 | CLA  | C1D-ND | 5.68  | 1.44        | 1.37     |
| 10  | B     | 802 | CLA  | C1D-ND | 5.66  | 1.44        | 1.37     |
| 10  | K     | 101 | CLA  | C1D-ND | 5.66  | 1.44        | 1.37     |
| 10  | A     | 810 | CLA  | C1D-ND | 5.65  | 1.44        | 1.37     |
| 10  | A     | 843 | CLA  | C1D-ND | 5.65  | 1.44        | 1.37     |
| 10  | B     | 812 | CLA  | C1D-ND | 5.64  | 1.44        | 1.37     |
| 10  | B     | 815 | CLA  | C1D-ND | 5.63  | 1.44        | 1.37     |
| 10  | A     | 832 | CLA  | C1D-ND | 5.61  | 1.44        | 1.37     |
| 10  | F     | 203 | CLA  | C1D-ND | 5.60  | 1.44        | 1.37     |
| 10  | J     | 101 | CLA  | C1D-ND | 5.60  | 1.44        | 1.37     |
| 10  | B     | 818 | CLA  | C1D-ND | 5.59  | 1.44        | 1.37     |
| 10  | A     | 830 | CLA  | C1D-ND | 5.59  | 1.44        | 1.37     |
| 10  | B     | 832 | CLA  | C1D-ND | 5.56  | 1.44        | 1.37     |
| 10  | A     | 812 | CLA  | C1D-ND | 5.56  | 1.44        | 1.37     |
| 10  | B     | 840 | CLA  | C1D-ND | 5.56  | 1.44        | 1.37     |
| 10  | A     | 842 | CLA  | C1D-ND | 5.56  | 1.44        | 1.37     |
| 10  | A     | 820 | CLA  | C1D-ND | 5.55  | 1.44        | 1.37     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 10  | B     | 806 | CLA  | C1D-ND | 5.53  | 1.44        | 1.37     |
| 10  | B     | 822 | CLA  | C1D-ND | 5.53  | 1.44        | 1.37     |
| 10  | B     | 801 | CLA  | C1D-ND | 5.52  | 1.44        | 1.37     |
| 10  | A     | 829 | CLA  | C1D-ND | 5.52  | 1.44        | 1.37     |
| 10  | A     | 818 | CLA  | C1D-ND | 5.50  | 1.44        | 1.37     |
| 10  | B     | 828 | CLA  | C1D-ND | 5.50  | 1.44        | 1.37     |
| 10  | A     | 840 | CLA  | C1D-ND | 5.49  | 1.44        | 1.37     |
| 10  | A     | 825 | CLA  | C1D-ND | 5.48  | 1.44        | 1.37     |
| 9   | A     | 803 | CL0  | C4B-NB | 5.48  | 1.44        | 1.37     |
| 10  | B     | 807 | CLA  | C1D-ND | 5.47  | 1.44        | 1.37     |
| 10  | B     | 820 | CLA  | C1D-ND | 5.47  | 1.44        | 1.37     |
| 10  | B     | 816 | CLA  | C1D-ND | 5.47  | 1.44        | 1.37     |
| 10  | A     | 846 | CLA  | C1D-ND | 5.46  | 1.44        | 1.37     |
| 10  | B     | 837 | CLA  | C1D-ND | 5.46  | 1.44        | 1.37     |
| 10  | A     | 863 | CLA  | C1D-ND | 5.46  | 1.44        | 1.37     |
| 10  | A     | 807 | CLA  | C1D-ND | 5.46  | 1.44        | 1.37     |
| 10  | A     | 836 | CLA  | C1D-ND | 5.46  | 1.44        | 1.37     |
| 10  | B     | 833 | CLA  | C1D-ND | 5.46  | 1.44        | 1.37     |
| 10  | A     | 835 | CLA  | C1D-ND | 5.46  | 1.44        | 1.37     |
| 10  | A     | 809 | CLA  | C1D-ND | 5.45  | 1.44        | 1.37     |
| 10  | A     | 822 | CLA  | C1D-ND | 5.45  | 1.44        | 1.37     |
| 10  | B     | 843 | CLA  | C4C-NC | 5.45  | 1.46        | 1.37     |
| 10  | A     | 823 | CLA  | C1D-ND | 5.44  | 1.44        | 1.37     |
| 10  | B     | 838 | CLA  | C1D-ND | 5.44  | 1.44        | 1.37     |
| 10  | A     | 819 | CLA  | C1D-ND | 5.44  | 1.44        | 1.37     |
| 10  | B     | 808 | CLA  | C1D-ND | 5.44  | 1.44        | 1.37     |
| 10  | A     | 837 | CLA  | C1D-ND | 5.44  | 1.44        | 1.37     |
| 10  | A     | 804 | CLA  | C1D-ND | 5.44  | 1.44        | 1.37     |
| 10  | B     | 839 | CLA  | C1D-ND | 5.43  | 1.44        | 1.37     |
| 10  | B     | 827 | CLA  | C1D-ND | 5.43  | 1.44        | 1.37     |
| 10  | A     | 815 | CLA  | C1D-ND | 5.43  | 1.44        | 1.37     |
| 10  | B     | 817 | CLA  | C1D-ND | 5.42  | 1.44        | 1.37     |
| 10  | B     | 836 | CLA  | C1D-ND | 5.42  | 1.44        | 1.37     |
| 10  | A     | 814 | CLA  | MG-NB  | -5.41 | 1.95        | 2.05     |
| 10  | A     | 861 | CLA  | C1D-ND | 5.41  | 1.44        | 1.37     |
| 10  | B     | 823 | CLA  | C1D-ND | 5.40  | 1.44        | 1.37     |
| 10  | A     | 824 | CLA  | C1D-ND | 5.40  | 1.44        | 1.37     |
| 10  | A     | 834 | CLA  | C1D-ND | 5.40  | 1.44        | 1.37     |
| 10  | B     | 813 | CLA  | C1D-ND | 5.39  | 1.44        | 1.37     |
| 10  | B     | 802 | CLA  | MG-NB  | -5.39 | 1.95        | 2.05     |
| 10  | A     | 828 | CLA  | C1D-ND | 5.39  | 1.44        | 1.37     |
| 10  | F     | 204 | CLA  | C1D-ND | 5.38  | 1.44        | 1.37     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 10  | K     | 102 | CLA  | C1D-ND | 5.38  | 1.44        | 1.37     |
| 10  | B     | 841 | CLA  | C1D-ND | 5.37  | 1.44        | 1.37     |
| 10  | B     | 831 | CLA  | C1D-ND | 5.37  | 1.44        | 1.37     |
| 10  | B     | 834 | CLA  | C1D-ND | 5.37  | 1.44        | 1.37     |
| 10  | B     | 811 | CLA  | C1D-ND | 5.35  | 1.44        | 1.37     |
| 10  | B     | 842 | CLA  | C1D-ND | 5.35  | 1.44        | 1.37     |
| 10  | A     | 808 | CLA  | C1D-ND | 5.34  | 1.44        | 1.37     |
| 10  | A     | 826 | CLA  | C1D-ND | 5.34  | 1.44        | 1.37     |
| 10  | A     | 821 | CLA  | C1D-ND | 5.34  | 1.44        | 1.37     |
| 10  | A     | 844 | CLA  | C1D-ND | 5.34  | 1.44        | 1.37     |
| 10  | A     | 827 | CLA  | C1D-ND | 5.33  | 1.44        | 1.37     |
| 10  | B     | 830 | CLA  | C1D-ND | 5.32  | 1.44        | 1.37     |
| 10  | A     | 811 | CLA  | C1D-ND | 5.32  | 1.44        | 1.37     |
| 10  | B     | 821 | CLA  | MG-NB  | -5.32 | 1.95        | 2.05     |
| 10  | B     | 843 | CLA  | MG-NB  | -5.31 | 1.95        | 2.05     |
| 10  | A     | 816 | CLA  | C1D-ND | 5.30  | 1.44        | 1.37     |
| 10  | A     | 839 | CLA  | C1D-ND | 5.29  | 1.44        | 1.37     |
| 10  | B     | 803 | CLA  | MG-NB  | -5.28 | 1.95        | 2.05     |
| 10  | A     | 838 | CLA  | C1D-ND | 5.28  | 1.44        | 1.37     |
| 10  | B     | 814 | CLA  | C1D-ND | 5.27  | 1.44        | 1.37     |
| 10  | A     | 813 | CLA  | C1D-ND | 5.27  | 1.44        | 1.37     |
| 10  | B     | 824 | CLA  | C1D-ND | 5.26  | 1.44        | 1.37     |
| 10  | B     | 825 | CLA  | C1D-ND | 5.25  | 1.44        | 1.37     |
| 10  | B     | 809 | CLA  | C1D-ND | 5.25  | 1.44        | 1.37     |
| 10  | K     | 103 | CLA  | C1D-ND | 5.24  | 1.44        | 1.37     |
| 10  | B     | 803 | CLA  | C1D-ND | 5.24  | 1.44        | 1.37     |
| 10  | A     | 845 | CLA  | C1D-ND | 5.24  | 1.44        | 1.37     |
| 10  | B     | 821 | CLA  | C1D-ND | 5.21  | 1.44        | 1.37     |
| 10  | A     | 826 | CLA  | MG-NB  | -5.19 | 1.95        | 2.05     |
| 10  | J     | 101 | CLA  | MG-NB  | -5.18 | 1.95        | 2.05     |
| 10  | A     | 817 | CLA  | C1D-ND | 5.17  | 1.44        | 1.37     |
| 10  | B     | 819 | CLA  | C1D-ND | 5.16  | 1.44        | 1.37     |
| 10  | B     | 837 | CLA  | MG-NB  | -5.15 | 1.95        | 2.05     |
| 10  | B     | 826 | CLA  | MG-NB  | -5.15 | 1.95        | 2.05     |
| 10  | K     | 102 | CLA  | MG-NB  | -5.13 | 1.95        | 2.05     |
| 10  | B     | 811 | CLA  | MG-NB  | -5.13 | 1.95        | 2.05     |
| 9   | A     | 803 | CL0  | MG-NB  | -5.12 | 1.95        | 2.05     |
| 10  | B     | 807 | CLA  | MG-NB  | -5.08 | 1.95        | 2.05     |
| 10  | A     | 831 | CLA  | C1D-ND | 5.07  | 1.44        | 1.37     |
| 10  | A     | 846 | CLA  | MG-NB  | -5.07 | 1.95        | 2.05     |
| 10  | B     | 841 | CLA  | MG-NB  | -5.05 | 1.95        | 2.05     |
| 10  | A     | 805 | CLA  | MG-NB  | -5.05 | 1.95        | 2.05     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 10  | A     | 821 | CLA  | MG-NB  | -5.04 | 1.95        | 2.05     |
| 10  | B     | 828 | CLA  | MG-NB  | -5.04 | 1.95        | 2.05     |
| 10  | B     | 825 | CLA  | MG-NB  | -5.04 | 1.95        | 2.05     |
| 10  | B     | 836 | CLA  | MG-NB  | -5.03 | 1.95        | 2.05     |
| 10  | A     | 830 | CLA  | MG-NB  | -5.01 | 1.95        | 2.05     |
| 10  | A     | 831 | CLA  | MG-NB  | -5.01 | 1.95        | 2.05     |
| 10  | B     | 823 | CLA  | MG-NB  | -5.01 | 1.95        | 2.05     |
| 10  | A     | 827 | CLA  | MG-NB  | -5.01 | 1.95        | 2.05     |
| 10  | A     | 861 | CLA  | MG-NB  | -5.01 | 1.95        | 2.05     |
| 10  | A     | 807 | CLA  | MG-NB  | -5.01 | 1.95        | 2.05     |
| 10  | A     | 828 | CLA  | MG-NB  | -4.99 | 1.95        | 2.05     |
| 9   | A     | 803 | CL0  | C1D-ND | 4.99  | 1.43        | 1.37     |
| 10  | B     | 827 | CLA  | MG-NB  | -4.98 | 1.95        | 2.05     |
| 10  | B     | 814 | CLA  | MG-NB  | -4.98 | 1.95        | 2.05     |
| 10  | A     | 813 | CLA  | MG-NB  | -4.97 | 1.95        | 2.05     |
| 10  | B     | 809 | CLA  | MG-NB  | -4.97 | 1.95        | 2.05     |
| 10  | A     | 817 | CLA  | MG-NB  | -4.96 | 1.95        | 2.05     |
| 10  | A     | 837 | CLA  | MG-NB  | -4.96 | 1.96        | 2.05     |
| 10  | K     | 103 | CLA  | MG-NB  | -4.96 | 1.96        | 2.05     |
| 10  | B     | 812 | CLA  | MG-NB  | -4.95 | 1.96        | 2.05     |
| 10  | A     | 863 | CLA  | MG-NB  | -4.94 | 1.96        | 2.05     |
| 10  | F     | 204 | CLA  | MG-NB  | -4.93 | 1.96        | 2.05     |
| 10  | B     | 835 | CLA  | MG-NB  | -4.92 | 1.96        | 2.05     |
| 10  | B     | 822 | CLA  | MG-NB  | -4.92 | 1.96        | 2.05     |
| 10  | B     | 808 | CLA  | MG-NB  | -4.90 | 1.96        | 2.05     |
| 10  | A     | 839 | CLA  | MG-NB  | -4.89 | 1.96        | 2.05     |
| 10  | B     | 839 | CLA  | MG-NB  | -4.89 | 1.96        | 2.05     |
| 10  | B     | 840 | CLA  | MG-NB  | -4.89 | 1.96        | 2.05     |
| 10  | B     | 842 | CLA  | MG-NB  | -4.86 | 1.96        | 2.05     |
| 10  | A     | 840 | CLA  | MG-NB  | -4.85 | 1.96        | 2.05     |
| 10  | A     | 832 | CLA  | MG-NB  | -4.85 | 1.96        | 2.05     |
| 10  | B     | 835 | CLA  | C1D-ND | 4.84  | 1.43        | 1.37     |
| 10  | F     | 203 | CLA  | MG-NB  | -4.83 | 1.96        | 2.05     |
| 10  | J     | 102 | CLA  | MG-NB  | -4.82 | 1.96        | 2.05     |
| 10  | A     | 842 | CLA  | MG-NB  | -4.82 | 1.96        | 2.05     |
| 10  | A     | 845 | CLA  | MG-NB  | -4.82 | 1.96        | 2.05     |
| 10  | A     | 823 | CLA  | MG-NB  | -4.81 | 1.96        | 2.05     |
| 10  | A     | 815 | CLA  | MG-NB  | -4.80 | 1.96        | 2.05     |
| 10  | B     | 824 | CLA  | MG-NB  | -4.80 | 1.96        | 2.05     |
| 10  | B     | 833 | CLA  | MG-NB  | -4.79 | 1.96        | 2.05     |
| 10  | A     | 814 | CLA  | C1D-ND | 4.79  | 1.43        | 1.37     |
| 10  | A     | 829 | CLA  | MG-NB  | -4.77 | 1.96        | 2.05     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 10  | A     | 834 | CLA  | MG-NB  | -4.77 | 1.96        | 2.05     |
| 10  | A     | 811 | CLA  | MG-NB  | -4.77 | 1.96        | 2.05     |
| 10  | B     | 829 | CLA  | MG-NB  | -4.76 | 1.96        | 2.05     |
| 10  | A     | 838 | CLA  | MG-NB  | -4.76 | 1.96        | 2.05     |
| 10  | A     | 836 | CLA  | MG-NB  | -4.75 | 1.96        | 2.05     |
| 10  | B     | 820 | CLA  | MG-NB  | -4.75 | 1.96        | 2.05     |
| 10  | A     | 805 | CLA  | C1D-ND | 4.73  | 1.43        | 1.37     |
| 10  | A     | 808 | CLA  | MG-NB  | -4.73 | 1.96        | 2.05     |
| 10  | A     | 819 | CLA  | MG-NB  | -4.72 | 1.96        | 2.05     |
| 10  | A     | 835 | CLA  | MG-NB  | -4.72 | 1.96        | 2.05     |
| 10  | B     | 817 | CLA  | MG-NB  | -4.72 | 1.96        | 2.05     |
| 10  | A     | 833 | CLA  | MG-NB  | -4.71 | 1.96        | 2.05     |
| 10  | A     | 844 | CLA  | MG-NB  | -4.70 | 1.96        | 2.05     |
| 10  | K     | 101 | CLA  | MG-NB  | -4.69 | 1.96        | 2.05     |
| 10  | A     | 816 | CLA  | MG-NB  | -4.68 | 1.96        | 2.05     |
| 10  | A     | 809 | CLA  | MG-NB  | -4.68 | 1.96        | 2.05     |
| 10  | A     | 814 | CLA  | MG-ND  | -4.68 | 1.96        | 2.05     |
| 10  | B     | 838 | CLA  | MG-NB  | -4.67 | 1.96        | 2.05     |
| 10  | A     | 810 | CLA  | MG-NB  | -4.66 | 1.96        | 2.05     |
| 10  | B     | 806 | CLA  | MG-NB  | -4.66 | 1.96        | 2.05     |
| 10  | B     | 813 | CLA  | MG-NB  | -4.65 | 1.96        | 2.05     |
| 10  | A     | 843 | CLA  | MG-NB  | -4.64 | 1.96        | 2.05     |
| 10  | B     | 818 | CLA  | MG-NB  | -4.64 | 1.96        | 2.05     |
| 10  | B     | 834 | CLA  | MG-NB  | -4.63 | 1.96        | 2.05     |
| 10  | A     | 820 | CLA  | MG-NB  | -4.63 | 1.96        | 2.05     |
| 10  | B     | 831 | CLA  | MG-NB  | -4.62 | 1.96        | 2.05     |
| 10  | A     | 824 | CLA  | MG-NB  | -4.60 | 1.96        | 2.05     |
| 10  | B     | 830 | CLA  | MG-NB  | -4.60 | 1.96        | 2.05     |
| 9   | A     | 803 | CL0  | MG-NA  | -4.59 | 1.95        | 2.06     |
| 10  | B     | 816 | CLA  | MG-NB  | -4.58 | 1.96        | 2.05     |
| 10  | B     | 832 | CLA  | MG-NB  | -4.54 | 1.96        | 2.05     |
| 10  | B     | 810 | CLA  | MG-NB  | -4.54 | 1.96        | 2.05     |
| 10  | B     | 815 | CLA  | MG-NB  | -4.53 | 1.96        | 2.05     |
| 10  | A     | 818 | CLA  | MG-NB  | -4.45 | 1.97        | 2.05     |
| 10  | A     | 822 | CLA  | MG-NB  | -4.43 | 1.97        | 2.05     |
| 10  | B     | 801 | CLA  | MG-NB  | -4.42 | 1.97        | 2.05     |
| 10  | A     | 825 | CLA  | MG-NB  | -4.41 | 1.97        | 2.05     |
| 10  | B     | 819 | CLA  | MG-NB  | -4.37 | 1.97        | 2.05     |
| 9   | A     | 803 | CL0  | MG-ND  | -4.31 | 1.97        | 2.05     |
| 10  | A     | 841 | CLA  | MG-NB  | -4.29 | 1.97        | 2.05     |
| 10  | A     | 812 | CLA  | MG-NB  | -4.25 | 1.97        | 2.05     |
| 10  | B     | 843 | CLA  | MG-ND  | -4.23 | 1.97        | 2.05     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 10  | A     | 804 | CLA  | MG-ND | -4.21 | 1.97        | 2.05     |
| 10  | B     | 814 | CLA  | MG-ND | -4.20 | 1.97        | 2.05     |
| 10  | B     | 821 | CLA  | MG-ND | -4.18 | 1.97        | 2.05     |
| 10  | K     | 103 | CLA  | MG-ND | -4.18 | 1.97        | 2.05     |
| 10  | K     | 102 | CLA  | MG-ND | -4.17 | 1.97        | 2.05     |
| 10  | B     | 826 | CLA  | MG-ND | -4.17 | 1.97        | 2.05     |
| 10  | A     | 821 | CLA  | MG-ND | -4.16 | 1.97        | 2.05     |
| 10  | B     | 803 | CLA  | MG-ND | -4.16 | 1.97        | 2.05     |
| 10  | A     | 827 | CLA  | MG-ND | -4.15 | 1.97        | 2.05     |
| 10  | B     | 825 | CLA  | MG-ND | -4.14 | 1.97        | 2.05     |
| 10  | A     | 805 | CLA  | MG-ND | -4.13 | 1.97        | 2.05     |
| 10  | A     | 861 | CLA  | MG-ND | -4.13 | 1.97        | 2.05     |
| 10  | B     | 823 | CLA  | MG-ND | -4.13 | 1.97        | 2.05     |
| 10  | A     | 817 | CLA  | MG-ND | -4.12 | 1.97        | 2.05     |
| 10  | A     | 825 | CLA  | MG-ND | -4.12 | 1.97        | 2.05     |
| 10  | A     | 830 | CLA  | MG-ND | -4.12 | 1.97        | 2.05     |
| 10  | B     | 841 | CLA  | MG-ND | -4.11 | 1.97        | 2.05     |
| 10  | B     | 819 | CLA  | MG-ND | -4.10 | 1.97        | 2.05     |
| 10  | B     | 817 | CLA  | MG-ND | -4.08 | 1.97        | 2.05     |
| 10  | B     | 835 | CLA  | MG-ND | -4.08 | 1.97        | 2.05     |
| 10  | J     | 101 | CLA  | MG-ND | -4.08 | 1.97        | 2.05     |
| 10  | B     | 802 | CLA  | MG-ND | -4.08 | 1.97        | 2.05     |
| 10  | B     | 824 | CLA  | MG-ND | -4.07 | 1.97        | 2.05     |
| 10  | A     | 839 | CLA  | MG-ND | -4.06 | 1.97        | 2.05     |
| 10  | B     | 822 | CLA  | MG-ND | -4.06 | 1.97        | 2.05     |
| 10  | F     | 203 | CLA  | MG-ND | -4.06 | 1.97        | 2.05     |
| 10  | B     | 811 | CLA  | MG-ND | -4.05 | 1.97        | 2.05     |
| 10  | A     | 823 | CLA  | MG-ND | -4.05 | 1.97        | 2.05     |
| 10  | A     | 811 | CLA  | MG-ND | -4.04 | 1.97        | 2.05     |
| 10  | B     | 837 | CLA  | MG-ND | -4.04 | 1.97        | 2.05     |
| 10  | A     | 828 | CLA  | MG-ND | -4.03 | 1.97        | 2.05     |
| 10  | A     | 840 | CLA  | MG-ND | -4.03 | 1.97        | 2.05     |
| 10  | A     | 831 | CLA  | MG-ND | -4.03 | 1.97        | 2.05     |
| 10  | A     | 813 | CLA  | MG-ND | -4.03 | 1.97        | 2.05     |
| 10  | B     | 820 | CLA  | MG-ND | -4.02 | 1.97        | 2.05     |
| 10  | A     | 837 | CLA  | MG-ND | -4.01 | 1.97        | 2.05     |
| 10  | A     | 818 | CLA  | MG-ND | -4.01 | 1.97        | 2.05     |
| 10  | B     | 815 | CLA  | MG-ND | -4.00 | 1.97        | 2.05     |
| 10  | F     | 204 | CLA  | MG-ND | -4.00 | 1.97        | 2.05     |
| 10  | A     | 826 | CLA  | MG-ND | -3.99 | 1.97        | 2.05     |
| 10  | A     | 807 | CLA  | MG-ND | -3.99 | 1.97        | 2.05     |
| 10  | A     | 834 | CLA  | MG-ND | -3.98 | 1.97        | 2.05     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 10  | A     | 846 | CLA  | MG-ND | -3.98 | 1.97        | 2.05     |
| 10  | B     | 836 | CLA  | MG-ND | -3.98 | 1.97        | 2.05     |
| 10  | B     | 809 | CLA  | MG-ND | -3.98 | 1.97        | 2.05     |
| 10  | B     | 833 | CLA  | MG-ND | -3.97 | 1.97        | 2.05     |
| 10  | A     | 819 | CLA  | MG-ND | -3.96 | 1.97        | 2.05     |
| 10  | K     | 101 | CLA  | MG-ND | -3.96 | 1.97        | 2.05     |
| 10  | A     | 843 | CLA  | MG-ND | -3.96 | 1.97        | 2.05     |
| 10  | B     | 840 | CLA  | MG-ND | -3.95 | 1.98        | 2.05     |
| 10  | A     | 815 | CLA  | MG-ND | -3.95 | 1.98        | 2.05     |
| 10  | A     | 838 | CLA  | MG-ND | -3.95 | 1.98        | 2.05     |
| 10  | B     | 808 | CLA  | MG-ND | -3.94 | 1.98        | 2.05     |
| 10  | A     | 836 | CLA  | MG-ND | -3.93 | 1.98        | 2.05     |
| 10  | A     | 863 | CLA  | MG-ND | -3.93 | 1.98        | 2.05     |
| 10  | B     | 830 | CLA  | MG-ND | -3.93 | 1.98        | 2.05     |
| 10  | A     | 812 | CLA  | MG-ND | -3.92 | 1.98        | 2.05     |
| 10  | A     | 842 | CLA  | MG-ND | -3.92 | 1.98        | 2.05     |
| 10  | A     | 844 | CLA  | MG-ND | -3.90 | 1.98        | 2.05     |
| 10  | A     | 829 | CLA  | MG-ND | -3.90 | 1.98        | 2.05     |
| 10  | B     | 842 | CLA  | MG-ND | -3.89 | 1.98        | 2.05     |
| 10  | A     | 832 | CLA  | MG-ND | -3.89 | 1.98        | 2.05     |
| 10  | B     | 831 | CLA  | MG-ND | -3.89 | 1.98        | 2.05     |
| 10  | B     | 827 | CLA  | MG-ND | -3.89 | 1.98        | 2.05     |
| 10  | J     | 102 | CLA  | MG-ND | -3.88 | 1.98        | 2.05     |
| 10  | B     | 834 | CLA  | MG-ND | -3.88 | 1.98        | 2.05     |
| 10  | A     | 835 | CLA  | MG-ND | -3.86 | 1.98        | 2.05     |
| 10  | B     | 816 | CLA  | MG-ND | -3.86 | 1.98        | 2.05     |
| 10  | B     | 807 | CLA  | MG-ND | -3.83 | 1.98        | 2.05     |
| 9   | A     | 803 | CL0  | MG-NC | -3.82 | 1.97        | 2.06     |
| 10  | B     | 828 | CLA  | MG-ND | -3.80 | 1.98        | 2.05     |
| 10  | A     | 820 | CLA  | MG-ND | -3.80 | 1.98        | 2.05     |
| 10  | B     | 839 | CLA  | MG-ND | -3.80 | 1.98        | 2.05     |
| 10  | B     | 812 | CLA  | MG-ND | -3.79 | 1.98        | 2.05     |
| 10  | B     | 813 | CLA  | MG-ND | -3.78 | 1.98        | 2.05     |
| 10  | B     | 806 | CLA  | MG-ND | -3.78 | 1.98        | 2.05     |
| 10  | A     | 816 | CLA  | MG-ND | -3.77 | 1.98        | 2.05     |
| 10  | B     | 832 | CLA  | MG-ND | -3.77 | 1.98        | 2.05     |
| 10  | B     | 838 | CLA  | MG-ND | -3.76 | 1.98        | 2.05     |
| 10  | B     | 810 | CLA  | MG-ND | -3.75 | 1.98        | 2.05     |
| 10  | A     | 824 | CLA  | MG-ND | -3.74 | 1.98        | 2.05     |
| 10  | B     | 818 | CLA  | MG-ND | -3.73 | 1.98        | 2.05     |
| 10  | B     | 801 | CLA  | MG-ND | -3.73 | 1.98        | 2.05     |
| 10  | B     | 829 | CLA  | MG-ND | -3.73 | 1.98        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10  | A     | 808 | CLA  | MG-ND   | -3.69 | 1.98        | 2.05     |
| 10  | A     | 833 | CLA  | MG-ND   | -3.69 | 1.98        | 2.05     |
| 10  | A     | 845 | CLA  | MG-ND   | -3.66 | 1.98        | 2.05     |
| 10  | A     | 822 | CLA  | MG-ND   | -3.64 | 1.98        | 2.05     |
| 10  | A     | 841 | CLA  | MG-ND   | -3.58 | 1.98        | 2.05     |
| 10  | A     | 809 | CLA  | MG-ND   | -3.46 | 1.98        | 2.05     |
| 10  | B     | 843 | CLA  | C4D-C3D | -3.31 | 1.39        | 1.46     |
| 9   | A     | 803 | CL0  | C1B-NB  | 3.27  | 1.41        | 1.37     |
| 10  | A     | 810 | CLA  | MG-ND   | -3.00 | 1.99        | 2.05     |
| 10  | B     | 843 | CLA  | CAD-C3D | -2.54 | 1.45        | 1.50     |
| 10  | B     | 826 | CLA  | C1D-C2D | -2.50 | 1.40        | 1.45     |
| 10  | A     | 830 | CLA  | C1D-C2D | -2.46 | 1.40        | 1.45     |
| 10  | B     | 801 | CLA  | C1D-C2D | -2.43 | 1.40        | 1.45     |
| 10  | B     | 803 | CLA  | C1D-C2D | -2.42 | 1.40        | 1.45     |
| 10  | B     | 831 | CLA  | C1D-C2D | -2.41 | 1.40        | 1.45     |
| 10  | A     | 813 | CLA  | C1D-C2D | -2.40 | 1.40        | 1.45     |
| 10  | A     | 805 | CLA  | C1D-C2D | -2.40 | 1.40        | 1.45     |
| 10  | B     | 840 | CLA  | C1D-C2D | -2.40 | 1.40        | 1.45     |
| 10  | B     | 811 | CLA  | C1D-C2D | -2.39 | 1.40        | 1.45     |
| 10  | A     | 816 | CLA  | C1D-C2D | -2.39 | 1.40        | 1.45     |
| 10  | A     | 832 | CLA  | C1D-C2D | -2.39 | 1.40        | 1.45     |
| 10  | A     | 818 | CLA  | C1D-C2D | -2.38 | 1.40        | 1.45     |
| 10  | B     | 810 | CLA  | C1D-C2D | -2.38 | 1.40        | 1.45     |
| 10  | A     | 815 | CLA  | C1D-C2D | -2.38 | 1.40        | 1.45     |
| 10  | A     | 841 | CLA  | C1D-C2D | -2.38 | 1.40        | 1.45     |
| 10  | B     | 825 | CLA  | C1D-C2D | -2.37 | 1.40        | 1.45     |
| 10  | A     | 814 | CLA  | C1D-C2D | -2.37 | 1.40        | 1.45     |
| 10  | A     | 819 | CLA  | C1D-C2D | -2.37 | 1.40        | 1.45     |
| 10  | A     | 833 | CLA  | C1D-C2D | -2.37 | 1.40        | 1.45     |
| 10  | B     | 842 | CLA  | C1D-C2D | -2.37 | 1.40        | 1.45     |
| 10  | A     | 822 | CLA  | C1D-C2D | -2.36 | 1.40        | 1.45     |
| 10  | B     | 827 | CLA  | C1D-C2D | -2.36 | 1.40        | 1.45     |
| 10  | B     | 834 | CLA  | C1D-C2D | -2.36 | 1.40        | 1.45     |
| 10  | A     | 844 | CLA  | C1D-C2D | -2.36 | 1.40        | 1.45     |
| 10  | B     | 830 | CLA  | C1D-C2D | -2.36 | 1.40        | 1.45     |
| 10  | B     | 832 | CLA  | C1D-C2D | -2.36 | 1.40        | 1.45     |
| 10  | B     | 808 | CLA  | C1D-C2D | -2.36 | 1.40        | 1.45     |
| 10  | A     | 829 | CLA  | C1D-C2D | -2.36 | 1.40        | 1.45     |
| 10  | A     | 825 | CLA  | C1D-C2D | -2.35 | 1.40        | 1.45     |
| 10  | B     | 814 | CLA  | C1D-C2D | -2.35 | 1.40        | 1.45     |
| 10  | K     | 101 | CLA  | C1D-C2D | -2.35 | 1.40        | 1.45     |
| 10  | A     | 835 | CLA  | C1D-C2D | -2.35 | 1.40        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10  | A     | 820 | CLA  | C1D-C2D | -2.35 | 1.40        | 1.45     |
| 10  | B     | 815 | CLA  | C1D-C2D | -2.35 | 1.40        | 1.45     |
| 10  | B     | 829 | CLA  | C1D-C2D | -2.35 | 1.40        | 1.45     |
| 10  | A     | 836 | CLA  | C1D-C2D | -2.35 | 1.40        | 1.45     |
| 10  | A     | 863 | CLA  | C1D-C2D | -2.35 | 1.40        | 1.45     |
| 10  | A     | 837 | CLA  | C1D-C2D | -2.34 | 1.40        | 1.45     |
| 10  | B     | 823 | CLA  | C1D-C2D | -2.34 | 1.40        | 1.45     |
| 10  | J     | 101 | CLA  | C1D-C2D | -2.34 | 1.40        | 1.45     |
| 10  | B     | 806 | CLA  | C1D-C2D | -2.34 | 1.40        | 1.45     |
| 10  | B     | 816 | CLA  | C1D-C2D | -2.34 | 1.40        | 1.45     |
| 10  | K     | 103 | CLA  | C1D-C2D | -2.34 | 1.40        | 1.45     |
| 9   | A     | 803 | CL0  | C1D-C2D | -2.34 | 1.40        | 1.45     |
| 10  | A     | 811 | CLA  | C1D-C2D | -2.34 | 1.40        | 1.45     |
| 10  | A     | 827 | CLA  | C1D-C2D | -2.34 | 1.40        | 1.45     |
| 10  | A     | 817 | CLA  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 10  | B     | 807 | CLA  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 10  | F     | 204 | CLA  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 10  | B     | 820 | CLA  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 10  | F     | 203 | CLA  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 10  | B     | 837 | CLA  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 10  | B     | 833 | CLA  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 10  | B     | 818 | CLA  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 10  | B     | 838 | CLA  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 10  | A     | 834 | CLA  | C1D-C2D | -2.33 | 1.40        | 1.45     |
| 10  | A     | 845 | CLA  | C1D-C2D | -2.32 | 1.40        | 1.45     |
| 10  | B     | 828 | CLA  | C1D-C2D | -2.32 | 1.40        | 1.45     |
| 10  | A     | 807 | CLA  | C1D-C2D | -2.32 | 1.40        | 1.45     |
| 10  | B     | 839 | CLA  | C1D-C2D | -2.32 | 1.40        | 1.45     |
| 10  | B     | 813 | CLA  | C1D-C2D | -2.32 | 1.40        | 1.45     |
| 10  | B     | 802 | CLA  | C1D-C2D | -2.32 | 1.40        | 1.45     |
| 10  | A     | 821 | CLA  | C1D-C2D | -2.31 | 1.40        | 1.45     |
| 10  | A     | 823 | CLA  | C1D-C2D | -2.31 | 1.40        | 1.45     |
| 10  | A     | 826 | CLA  | C1D-C2D | -2.31 | 1.40        | 1.45     |
| 10  | A     | 804 | CLA  | C1D-C2D | -2.31 | 1.40        | 1.45     |
| 10  | A     | 828 | CLA  | C1D-C2D | -2.31 | 1.40        | 1.45     |
| 10  | B     | 817 | CLA  | C1D-C2D | -2.31 | 1.40        | 1.45     |
| 10  | A     | 842 | CLA  | C1D-C2D | -2.31 | 1.40        | 1.45     |
| 10  | B     | 822 | CLA  | C1D-C2D | -2.31 | 1.40        | 1.45     |
| 10  | A     | 838 | CLA  | C1D-C2D | -2.30 | 1.40        | 1.45     |
| 10  | A     | 843 | CLA  | C1D-C2D | -2.30 | 1.40        | 1.45     |
| 10  | A     | 846 | CLA  | C1D-C2D | -2.30 | 1.40        | 1.45     |
| 10  | J     | 102 | CLA  | C1D-C2D | -2.29 | 1.40        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10  | A     | 812 | CLA  | C1D-C2D | -2.29 | 1.40        | 1.45     |
| 10  | A     | 824 | CLA  | C1D-C2D | -2.29 | 1.40        | 1.45     |
| 10  | B     | 812 | CLA  | C1D-C2D | -2.29 | 1.40        | 1.45     |
| 10  | B     | 836 | CLA  | C1D-C2D | -2.29 | 1.40        | 1.45     |
| 10  | B     | 835 | CLA  | C1D-C2D | -2.28 | 1.40        | 1.45     |
| 10  | A     | 839 | CLA  | C1D-C2D | -2.28 | 1.40        | 1.45     |
| 10  | B     | 841 | CLA  | C1D-C2D | -2.28 | 1.40        | 1.45     |
| 10  | K     | 102 | CLA  | C1D-C2D | -2.28 | 1.40        | 1.45     |
| 10  | B     | 819 | CLA  | C1D-C2D | -2.28 | 1.40        | 1.45     |
| 10  | A     | 831 | CLA  | C1D-C2D | -2.28 | 1.40        | 1.45     |
| 10  | A     | 861 | CLA  | C1D-C2D | -2.28 | 1.40        | 1.45     |
| 10  | A     | 809 | CLA  | C1D-C2D | -2.27 | 1.40        | 1.45     |
| 10  | B     | 824 | CLA  | C1D-C2D | -2.27 | 1.40        | 1.45     |
| 10  | B     | 821 | CLA  | C1D-C2D | -2.26 | 1.40        | 1.45     |
| 10  | A     | 840 | CLA  | C1D-C2D | -2.26 | 1.40        | 1.45     |
| 10  | B     | 809 | CLA  | C1D-C2D | -2.26 | 1.40        | 1.45     |
| 10  | A     | 808 | CLA  | C1D-C2D | -2.25 | 1.40        | 1.45     |
| 10  | A     | 810 | CLA  | C1D-C2D | -2.25 | 1.40        | 1.45     |
| 10  | B     | 843 | CLA  | C2D-C3D | 2.09  | 1.42        | 1.36     |

All (301) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 10  | B     | 843 | CLA  | C1C-NC-C4C | -5.20 | 104.37      | 106.71   |
| 10  | A     | 810 | CLA  | C1D-ND-C4D | -4.50 | 103.14      | 106.33   |
| 10  | A     | 822 | CLA  | C1D-ND-C4D | -4.45 | 103.17      | 106.33   |
| 10  | A     | 808 | CLA  | C1D-ND-C4D | -4.41 | 103.20      | 106.33   |
| 10  | A     | 809 | CLA  | C1D-ND-C4D | -4.33 | 103.26      | 106.33   |
| 10  | B     | 810 | CLA  | C1D-ND-C4D | -4.32 | 103.27      | 106.33   |
| 10  | A     | 824 | CLA  | C1D-ND-C4D | -4.32 | 103.27      | 106.33   |
| 10  | A     | 841 | CLA  | C1D-ND-C4D | -4.30 | 103.28      | 106.33   |
| 10  | B     | 812 | CLA  | C1D-ND-C4D | -4.30 | 103.28      | 106.33   |
| 10  | B     | 818 | CLA  | C1D-ND-C4D | -4.30 | 103.28      | 106.33   |
| 10  | A     | 820 | CLA  | C1D-ND-C4D | -4.27 | 103.30      | 106.33   |
| 10  | B     | 816 | CLA  | C1D-ND-C4D | -4.27 | 103.30      | 106.33   |
| 10  | B     | 832 | CLA  | C1D-ND-C4D | -4.25 | 103.32      | 106.33   |
| 10  | B     | 836 | CLA  | C1D-ND-C4D | -4.25 | 103.32      | 106.33   |
| 10  | A     | 842 | CLA  | C1D-ND-C4D | -4.24 | 103.32      | 106.33   |
| 9   | A     | 803 | CL0  | CHB-C1B-NB | -4.21 | 119.80      | 124.26   |
| 10  | A     | 807 | CLA  | C1D-ND-C4D | -4.21 | 103.34      | 106.33   |
| 10  | A     | 843 | CLA  | C1D-ND-C4D | -4.21 | 103.35      | 106.33   |
| 10  | J     | 102 | CLA  | C1D-ND-C4D | -4.21 | 103.35      | 106.33   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 10  | A     | 845 | CLA  | C1D-ND-C4D | -4.21 | 103.35      | 106.33   |
| 10  | A     | 826 | CLA  | C1D-ND-C4D | -4.20 | 103.35      | 106.33   |
| 10  | A     | 836 | CLA  | C1D-ND-C4D | -4.20 | 103.35      | 106.33   |
| 10  | B     | 838 | CLA  | C1D-ND-C4D | -4.19 | 103.36      | 106.33   |
| 10  | A     | 839 | CLA  | C1D-ND-C4D | -4.19 | 103.36      | 106.33   |
| 10  | B     | 830 | CLA  | C1D-ND-C4D | -4.19 | 103.36      | 106.33   |
| 10  | B     | 817 | CLA  | C1D-ND-C4D | -4.18 | 103.37      | 106.33   |
| 10  | B     | 813 | CLA  | C1D-ND-C4D | -4.17 | 103.37      | 106.33   |
| 10  | B     | 806 | CLA  | C1D-ND-C4D | -4.17 | 103.38      | 106.33   |
| 10  | B     | 815 | CLA  | C1D-ND-C4D | -4.17 | 103.38      | 106.33   |
| 10  | A     | 827 | CLA  | C1D-ND-C4D | -4.16 | 103.38      | 106.33   |
| 10  | A     | 837 | CLA  | C1D-ND-C4D | -4.16 | 103.38      | 106.33   |
| 10  | A     | 825 | CLA  | C1D-ND-C4D | -4.15 | 103.39      | 106.33   |
| 10  | F     | 204 | CLA  | C1D-ND-C4D | -4.15 | 103.39      | 106.33   |
| 10  | K     | 101 | CLA  | C1D-ND-C4D | -4.15 | 103.39      | 106.33   |
| 10  | A     | 846 | CLA  | C1D-ND-C4D | -4.14 | 103.39      | 106.33   |
| 10  | B     | 839 | CLA  | C1D-ND-C4D | -4.14 | 103.39      | 106.33   |
| 10  | A     | 844 | CLA  | C1D-ND-C4D | -4.13 | 103.40      | 106.33   |
| 10  | A     | 812 | CLA  | C1D-ND-C4D | -4.13 | 103.40      | 106.33   |
| 10  | A     | 840 | CLA  | C1D-ND-C4D | -4.12 | 103.41      | 106.33   |
| 10  | B     | 822 | CLA  | C1D-ND-C4D | -4.12 | 103.41      | 106.33   |
| 10  | A     | 833 | CLA  | C1D-ND-C4D | -4.12 | 103.41      | 106.33   |
| 10  | B     | 833 | CLA  | C1D-ND-C4D | -4.11 | 103.41      | 106.33   |
| 10  | A     | 832 | CLA  | C1D-ND-C4D | -4.11 | 103.41      | 106.33   |
| 10  | A     | 816 | CLA  | C1D-ND-C4D | -4.11 | 103.41      | 106.33   |
| 10  | A     | 811 | CLA  | C1D-ND-C4D | -4.11 | 103.42      | 106.33   |
| 10  | A     | 815 | CLA  | C1D-ND-C4D | -4.11 | 103.42      | 106.33   |
| 10  | B     | 829 | CLA  | C1D-ND-C4D | -4.11 | 103.42      | 106.33   |
| 10  | A     | 861 | CLA  | C1D-ND-C4D | -4.10 | 103.42      | 106.33   |
| 10  | B     | 840 | CLA  | C1D-ND-C4D | -4.10 | 103.42      | 106.33   |
| 10  | B     | 841 | CLA  | C1D-ND-C4D | -4.10 | 103.42      | 106.33   |
| 10  | A     | 828 | CLA  | C1D-ND-C4D | -4.10 | 103.42      | 106.33   |
| 10  | B     | 814 | CLA  | C1D-ND-C4D | -4.10 | 103.42      | 106.33   |
| 10  | A     | 829 | CLA  | C1D-ND-C4D | -4.09 | 103.43      | 106.33   |
| 10  | A     | 835 | CLA  | C1D-ND-C4D | -4.09 | 103.43      | 106.33   |
| 10  | A     | 838 | CLA  | C1D-ND-C4D | -4.09 | 103.43      | 106.33   |
| 10  | A     | 863 | CLA  | C1D-ND-C4D | -4.07 | 103.44      | 106.33   |
| 10  | B     | 820 | CLA  | C1D-ND-C4D | -4.07 | 103.44      | 106.33   |
| 10  | K     | 103 | CLA  | C1D-ND-C4D | -4.07 | 103.45      | 106.33   |
| 10  | B     | 837 | CLA  | C1D-ND-C4D | -4.06 | 103.45      | 106.33   |
| 10  | B     | 828 | CLA  | C1D-ND-C4D | -4.05 | 103.46      | 106.33   |
| 10  | K     | 102 | CLA  | C1D-ND-C4D | -4.05 | 103.46      | 106.33   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 10  | A     | 821 | CLA  | C1D-ND-C4D | -4.04 | 103.47      | 106.33   |
| 10  | B     | 807 | CLA  | C1D-ND-C4D | -4.04 | 103.47      | 106.33   |
| 10  | B     | 823 | CLA  | C1D-ND-C4D | -4.04 | 103.47      | 106.33   |
| 10  | B     | 835 | CLA  | C1D-ND-C4D | -4.04 | 103.47      | 106.33   |
| 10  | A     | 823 | CLA  | C1D-ND-C4D | -4.03 | 103.47      | 106.33   |
| 10  | B     | 827 | CLA  | C1D-ND-C4D | -4.03 | 103.47      | 106.33   |
| 10  | B     | 809 | CLA  | C1D-ND-C4D | -4.03 | 103.47      | 106.33   |
| 10  | B     | 831 | CLA  | C1D-ND-C4D | -4.02 | 103.48      | 106.33   |
| 10  | B     | 842 | CLA  | C1D-ND-C4D | -4.01 | 103.48      | 106.33   |
| 10  | A     | 818 | CLA  | C1D-ND-C4D | -3.99 | 103.50      | 106.33   |
| 10  | B     | 819 | CLA  | C1D-ND-C4D | -3.99 | 103.50      | 106.33   |
| 10  | B     | 834 | CLA  | C1D-ND-C4D | -3.99 | 103.50      | 106.33   |
| 10  | A     | 834 | CLA  | C1D-ND-C4D | -3.99 | 103.50      | 106.33   |
| 10  | J     | 101 | CLA  | C1D-ND-C4D | -3.98 | 103.51      | 106.33   |
| 10  | A     | 817 | CLA  | C1D-ND-C4D | -3.98 | 103.51      | 106.33   |
| 10  | B     | 808 | CLA  | C1D-ND-C4D | -3.98 | 103.51      | 106.33   |
| 9   | A     | 803 | CL0  | CHD-C1D-ND | -3.97 | 120.80      | 124.45   |
| 10  | A     | 804 | CLA  | C1D-ND-C4D | -3.96 | 103.52      | 106.33   |
| 10  | F     | 203 | CLA  | C1D-ND-C4D | -3.96 | 103.52      | 106.33   |
| 10  | A     | 831 | CLA  | C1D-ND-C4D | -3.96 | 103.52      | 106.33   |
| 10  | B     | 801 | CLA  | C1D-ND-C4D | -3.95 | 103.53      | 106.33   |
| 10  | A     | 813 | CLA  | C1D-ND-C4D | -3.94 | 103.53      | 106.33   |
| 10  | B     | 821 | CLA  | C1D-ND-C4D | -3.94 | 103.53      | 106.33   |
| 10  | B     | 824 | CLA  | C1D-ND-C4D | -3.94 | 103.54      | 106.33   |
| 9   | A     | 803 | CL0  | C1D-ND-C4D | -3.94 | 103.54      | 106.33   |
| 10  | B     | 811 | CLA  | C1D-ND-C4D | -3.89 | 103.58      | 106.33   |
| 10  | B     | 843 | CLA  | C4D-ND-C1D | -3.88 | 103.58      | 106.33   |
| 9   | A     | 803 | CL0  | CHC-C1C-NC | 3.86  | 130.06      | 124.20   |
| 10  | B     | 802 | CLA  | C1D-ND-C4D | -3.85 | 103.60      | 106.33   |
| 10  | B     | 825 | CLA  | C1D-ND-C4D | -3.84 | 103.61      | 106.33   |
| 10  | A     | 819 | CLA  | C1D-ND-C4D | -3.81 | 103.63      | 106.33   |
| 10  | A     | 805 | CLA  | C1D-ND-C4D | -3.79 | 103.64      | 106.33   |
| 10  | B     | 826 | CLA  | C1D-ND-C4D | -3.79 | 103.64      | 106.33   |
| 10  | A     | 830 | CLA  | C1D-ND-C4D | -3.75 | 103.67      | 106.33   |
| 10  | B     | 803 | CLA  | C1D-ND-C4D | -3.74 | 103.67      | 106.33   |
| 10  | B     | 835 | CLA  | CHD-C1D-ND | -3.63 | 121.12      | 124.45   |
| 10  | A     | 835 | CLA  | CHD-C1D-ND | -3.62 | 121.12      | 124.45   |
| 10  | B     | 836 | CLA  | CHD-C1D-ND | -3.60 | 121.15      | 124.45   |
| 10  | B     | 819 | CLA  | CHD-C1D-ND | -3.53 | 121.21      | 124.45   |
| 10  | A     | 814 | CLA  | C1D-ND-C4D | -3.50 | 103.85      | 106.33   |
| 10  | B     | 821 | CLA  | CHD-C1D-ND | -3.49 | 121.24      | 124.45   |
| 10  | A     | 810 | CLA  | CHD-C1D-ND | -3.49 | 121.25      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10  | B     | 803 | CLA  | CHD-C1D-ND  | -3.49 | 121.25      | 124.45   |
| 10  | A     | 831 | CLA  | CHD-C1D-ND  | -3.48 | 121.25      | 124.45   |
| 10  | A     | 839 | CLA  | CHD-C1D-ND  | -3.43 | 121.30      | 124.45   |
| 10  | A     | 809 | CLA  | CHD-C1D-ND  | -3.43 | 121.31      | 124.45   |
| 10  | B     | 843 | CLA  | CHD-C1D-ND  | -3.42 | 121.21      | 124.52   |
| 10  | A     | 826 | CLA  | CHD-C1D-ND  | -3.42 | 121.31      | 124.45   |
| 10  | B     | 841 | CLA  | CHD-C1D-ND  | -3.42 | 121.31      | 124.45   |
| 10  | B     | 802 | CLA  | CHD-C1D-ND  | -3.41 | 121.32      | 124.45   |
| 10  | B     | 830 | CLA  | CHD-C1D-ND  | -3.41 | 121.32      | 124.45   |
| 10  | B     | 806 | CLA  | CHD-C1D-ND  | -3.40 | 121.33      | 124.45   |
| 10  | A     | 827 | CLA  | CHD-C1D-ND  | -3.39 | 121.34      | 124.45   |
| 10  | A     | 823 | CLA  | CHD-C1D-ND  | -3.38 | 121.34      | 124.45   |
| 10  | A     | 833 | CLA  | CHD-C1D-ND  | -3.38 | 121.34      | 124.45   |
| 10  | K     | 103 | CLA  | CHD-C1D-ND  | -3.38 | 121.35      | 124.45   |
| 10  | A     | 808 | CLA  | CHD-C1D-ND  | -3.38 | 121.35      | 124.45   |
| 10  | A     | 846 | CLA  | CHD-C1D-ND  | -3.38 | 121.35      | 124.45   |
| 10  | A     | 824 | CLA  | CHD-C1D-ND  | -3.37 | 121.36      | 124.45   |
| 10  | B     | 827 | CLA  | CHD-C1D-ND  | -3.37 | 121.36      | 124.45   |
| 10  | A     | 861 | CLA  | CHD-C1D-ND  | -3.37 | 121.36      | 124.45   |
| 10  | A     | 840 | CLA  | CHD-C1D-ND  | -3.35 | 121.38      | 124.45   |
| 10  | B     | 828 | CLA  | CHD-C1D-ND  | -3.34 | 121.39      | 124.45   |
| 10  | A     | 816 | CLA  | CHD-C1D-ND  | -3.34 | 121.39      | 124.45   |
| 10  | A     | 805 | CLA  | CHD-C1D-ND  | -3.33 | 121.39      | 124.45   |
| 10  | B     | 807 | CLA  | CHD-C1D-ND  | -3.33 | 121.40      | 124.45   |
| 10  | A     | 804 | CLA  | CHD-C1D-ND  | -3.33 | 121.40      | 124.45   |
| 10  | B     | 837 | CLA  | CHD-C1D-ND  | -3.32 | 121.41      | 124.45   |
| 10  | A     | 842 | CLA  | CHD-C1D-ND  | -3.31 | 121.41      | 124.45   |
| 10  | A     | 834 | CLA  | CHD-C1D-ND  | -3.31 | 121.41      | 124.45   |
| 10  | B     | 809 | CLA  | CHD-C1D-ND  | -3.31 | 121.42      | 124.45   |
| 10  | B     | 839 | CLA  | CHD-C1D-ND  | -3.31 | 121.42      | 124.45   |
| 10  | B     | 823 | CLA  | CHD-C1D-ND  | -3.29 | 121.43      | 124.45   |
| 10  | B     | 833 | CLA  | CHD-C1D-ND  | -3.29 | 121.43      | 124.45   |
| 10  | A     | 863 | CLA  | CHD-C1D-ND  | -3.29 | 121.43      | 124.45   |
| 10  | A     | 814 | CLA  | CHD-C1D-ND  | -3.29 | 121.43      | 124.45   |
| 10  | B     | 834 | CLA  | CHD-C1D-ND  | -3.28 | 121.44      | 124.45   |
| 10  | B     | 840 | CLA  | CHD-C1D-ND  | -3.28 | 121.44      | 124.45   |
| 9   | A     | 803 | CL0  | CHC-C1C-C2C | -3.28 | 117.63      | 126.73   |
| 10  | A     | 817 | CLA  | CHD-C1D-ND  | -3.28 | 121.44      | 124.45   |
| 10  | B     | 812 | CLA  | CHD-C1D-ND  | -3.27 | 121.45      | 124.45   |
| 10  | B     | 838 | CLA  | CHD-C1D-ND  | -3.27 | 121.45      | 124.45   |
| 10  | B     | 824 | CLA  | CHD-C1D-ND  | -3.27 | 121.45      | 124.45   |
| 10  | B     | 817 | CLA  | CHD-C1D-ND  | -3.26 | 121.45      | 124.45   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 10  | B     | 820 | CLA  | CHD-C1D-ND | -3.26 | 121.46      | 124.45   |
| 10  | F     | 204 | CLA  | CHD-C1D-ND | -3.25 | 121.47      | 124.45   |
| 10  | K     | 101 | CLA  | CHD-C1D-ND | -3.25 | 121.47      | 124.45   |
| 10  | A     | 838 | CLA  | CHD-C1D-ND | -3.25 | 121.47      | 124.45   |
| 10  | B     | 816 | CLA  | CHD-C1D-ND | -3.24 | 121.47      | 124.45   |
| 10  | A     | 807 | CLA  | CHD-C1D-ND | -3.24 | 121.47      | 124.45   |
| 10  | A     | 837 | CLA  | CHD-C1D-ND | -3.24 | 121.48      | 124.45   |
| 10  | B     | 822 | CLA  | CHD-C1D-ND | -3.24 | 121.48      | 124.45   |
| 10  | B     | 831 | CLA  | CHD-C1D-ND | -3.23 | 121.48      | 124.45   |
| 10  | A     | 821 | CLA  | CHD-C1D-ND | -3.23 | 121.49      | 124.45   |
| 10  | B     | 808 | CLA  | CHD-C1D-ND | -3.23 | 121.49      | 124.45   |
| 10  | B     | 829 | CLA  | CHD-C1D-ND | -3.23 | 121.49      | 124.45   |
| 10  | A     | 812 | CLA  | CHD-C1D-ND | -3.23 | 121.49      | 124.45   |
| 10  | A     | 845 | CLA  | CHD-C1D-ND | -3.23 | 121.49      | 124.45   |
| 10  | A     | 828 | CLA  | CHD-C1D-ND | -3.22 | 121.49      | 124.45   |
| 10  | A     | 813 | CLA  | CHD-C1D-ND | -3.22 | 121.50      | 124.45   |
| 10  | B     | 801 | CLA  | CHD-C1D-ND | -3.22 | 121.50      | 124.45   |
| 10  | A     | 825 | CLA  | CHD-C1D-ND | -3.21 | 121.50      | 124.45   |
| 10  | B     | 811 | CLA  | CHD-C1D-ND | -3.21 | 121.50      | 124.45   |
| 10  | A     | 815 | CLA  | CHD-C1D-ND | -3.21 | 121.50      | 124.45   |
| 10  | B     | 814 | CLA  | CHD-C1D-ND | -3.21 | 121.50      | 124.45   |
| 10  | A     | 820 | CLA  | CHD-C1D-ND | -3.20 | 121.51      | 124.45   |
| 10  | J     | 102 | CLA  | CHD-C1D-ND | -3.20 | 121.51      | 124.45   |
| 10  | A     | 829 | CLA  | CHD-C1D-ND | -3.19 | 121.52      | 124.45   |
| 10  | A     | 822 | CLA  | CHD-C1D-ND | -3.19 | 121.52      | 124.45   |
| 10  | B     | 813 | CLA  | CHD-C1D-ND | -3.19 | 121.52      | 124.45   |
| 10  | B     | 818 | CLA  | CHD-C1D-ND | -3.19 | 121.52      | 124.45   |
| 10  | A     | 841 | CLA  | CHD-C1D-ND | -3.19 | 121.53      | 124.45   |
| 10  | A     | 811 | CLA  | CHD-C1D-ND | -3.18 | 121.53      | 124.45   |
| 10  | B     | 825 | CLA  | CHD-C1D-ND | -3.17 | 121.54      | 124.45   |
| 10  | A     | 844 | CLA  | CHD-C1D-ND | -3.16 | 121.55      | 124.45   |
| 10  | A     | 832 | CLA  | CHD-C1D-ND | -3.16 | 121.55      | 124.45   |
| 10  | A     | 836 | CLA  | CHD-C1D-ND | -3.14 | 121.57      | 124.45   |
| 10  | B     | 832 | CLA  | CHD-C1D-ND | -3.14 | 121.57      | 124.45   |
| 10  | J     | 101 | CLA  | CHD-C1D-ND | -3.14 | 121.57      | 124.45   |
| 10  | A     | 843 | CLA  | CHD-C1D-ND | -3.13 | 121.58      | 124.45   |
| 10  | B     | 842 | CLA  | CHD-C1D-ND | -3.10 | 121.60      | 124.45   |
| 10  | K     | 102 | CLA  | CHD-C1D-ND | -3.10 | 121.61      | 124.45   |
| 10  | A     | 819 | CLA  | CHD-C1D-ND | -3.07 | 121.63      | 124.45   |
| 10  | F     | 203 | CLA  | CHD-C1D-ND | -3.06 | 121.64      | 124.45   |
| 10  | A     | 818 | CLA  | CHD-C1D-ND | -3.03 | 121.67      | 124.45   |
| 10  | B     | 810 | CLA  | CHD-C1D-ND | -2.99 | 121.70      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10  | B     | 815 | CLA  | CHD-C1D-ND  | -2.99 | 121.71      | 124.45   |
| 10  | B     | 826 | CLA  | CHD-C1D-ND  | -2.91 | 121.78      | 124.45   |
| 10  | A     | 836 | CLA  | CHC-C4B-NB  | 2.82  | 127.25      | 124.26   |
| 10  | B     | 832 | CLA  | CHC-C4B-NB  | 2.82  | 127.24      | 124.26   |
| 10  | A     | 830 | CLA  | CHD-C1D-ND  | -2.79 | 121.89      | 124.45   |
| 10  | A     | 838 | CLA  | CHC-C4B-NB  | 2.68  | 127.09      | 124.26   |
| 10  | A     | 825 | CLA  | CHC-C4B-NB  | 2.67  | 127.08      | 124.26   |
| 10  | B     | 818 | CLA  | CHC-C4B-NB  | 2.64  | 127.05      | 124.26   |
| 10  | B     | 801 | CLA  | CHC-C4B-NB  | 2.63  | 127.04      | 124.26   |
| 10  | A     | 846 | CLA  | CHC-C4B-NB  | 2.62  | 127.03      | 124.26   |
| 10  | B     | 843 | CLA  | C3A-C2A-C1A | -2.62 | 101.09      | 104.74   |
| 10  | A     | 842 | CLA  | CHC-C4B-NB  | 2.62  | 127.03      | 124.26   |
| 10  | A     | 816 | CLA  | CHC-C4B-NB  | 2.61  | 127.02      | 124.26   |
| 10  | B     | 842 | CLA  | CHC-C4B-NB  | 2.60  | 127.01      | 124.26   |
| 10  | B     | 843 | CLA  | CHC-C4B-NB  | 2.59  | 126.90      | 124.27   |
| 10  | B     | 817 | CLA  | CHC-C4B-NB  | 2.58  | 126.98      | 124.26   |
| 10  | B     | 801 | CLA  | CHB-C1B-NB  | -2.57 | 121.53      | 124.26   |
| 10  | B     | 822 | CLA  | CHC-C4B-NB  | 2.57  | 126.98      | 124.26   |
| 10  | A     | 813 | CLA  | CHC-C4B-NB  | 2.56  | 126.97      | 124.26   |
| 10  | B     | 825 | CLA  | CHC-C4B-NB  | 2.54  | 126.95      | 124.26   |
| 10  | A     | 829 | CLA  | CHC-C4B-NB  | 2.54  | 126.95      | 124.26   |
| 10  | B     | 810 | CLA  | CHC-C4B-NB  | 2.54  | 126.95      | 124.26   |
| 10  | A     | 817 | CLA  | CHC-C4B-NB  | 2.54  | 126.95      | 124.26   |
| 10  | A     | 863 | CLA  | CHC-C4B-NB  | 2.54  | 126.94      | 124.26   |
| 10  | K     | 102 | CLA  | CHC-C4B-NB  | 2.54  | 126.94      | 124.26   |
| 10  | K     | 103 | CLA  | CHC-C4B-NB  | 2.53  | 126.93      | 124.26   |
| 10  | A     | 845 | CLA  | CHC-C4B-NB  | 2.52  | 126.92      | 124.26   |
| 10  | A     | 844 | CLA  | CHC-C4B-NB  | 2.52  | 126.92      | 124.26   |
| 10  | A     | 839 | CLA  | CHC-C4B-NB  | 2.50  | 126.91      | 124.26   |
| 9   | A     | 803 | CL0  | C4A-NA-C1A  | -2.48 | 105.59      | 106.71   |
| 10  | A     | 815 | CLA  | CHC-C4B-NB  | 2.48  | 126.88      | 124.26   |
| 10  | B     | 813 | CLA  | CHC-C4B-NB  | 2.48  | 126.88      | 124.26   |
| 10  | B     | 819 | CLA  | CHC-C4B-NB  | 2.46  | 126.86      | 124.26   |
| 10  | A     | 837 | CLA  | CHC-C4B-NB  | 2.45  | 126.85      | 124.26   |
| 10  | B     | 812 | CLA  | CHC-C4B-NB  | 2.43  | 126.83      | 124.26   |
| 10  | B     | 837 | CLA  | CHC-C4B-NB  | 2.42  | 126.82      | 124.26   |
| 10  | A     | 821 | CLA  | CHC-C4B-NB  | 2.42  | 126.82      | 124.26   |
| 10  | A     | 823 | CLA  | CHC-C4B-NB  | 2.42  | 126.81      | 124.26   |
| 10  | B     | 839 | CLA  | CHC-C4B-NB  | 2.41  | 126.81      | 124.26   |
| 10  | A     | 818 | CLA  | CHC-C4B-NB  | 2.41  | 126.81      | 124.26   |
| 10  | A     | 810 | CLA  | CHC-C4B-NB  | 2.40  | 126.80      | 124.26   |
| 10  | B     | 816 | CLA  | CHC-C4B-NB  | 2.40  | 126.80      | 124.26   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10  | K     | 101 | CLA  | CHC-C4B-NB  | 2.40  | 126.80      | 124.26   |
| 10  | A     | 822 | CLA  | CHC-C4B-NB  | 2.40  | 126.80      | 124.26   |
| 9   | A     | 803 | CL0  | C2C-C1C-NC  | 2.40  | 112.22      | 109.97   |
| 18  | B     | 852 | 5X6  | C33-C32-C31 | -2.40 | 107.03      | 110.30   |
| 10  | B     | 814 | CLA  | CHC-C4B-NB  | 2.39  | 126.79      | 124.26   |
| 10  | B     | 833 | CLA  | CHC-C4B-NB  | 2.39  | 126.79      | 124.26   |
| 10  | B     | 811 | CLA  | CHC-C4B-NB  | 2.38  | 126.78      | 124.26   |
| 10  | B     | 841 | CLA  | CHC-C4B-NB  | 2.38  | 126.78      | 124.26   |
| 10  | A     | 820 | CLA  | CHC-C4B-NB  | 2.38  | 126.78      | 124.26   |
| 10  | A     | 827 | CLA  | CHC-C4B-NB  | 2.38  | 126.78      | 124.26   |
| 10  | B     | 815 | CLA  | CHC-C4B-NB  | 2.37  | 126.77      | 124.26   |
| 10  | A     | 819 | CLA  | CHC-C4B-NB  | 2.37  | 126.77      | 124.26   |
| 10  | A     | 861 | CLA  | CHC-C4B-NB  | 2.37  | 126.77      | 124.26   |
| 10  | B     | 806 | CLA  | CHC-C4B-NB  | 2.37  | 126.77      | 124.26   |
| 10  | B     | 835 | CLA  | CHC-C4B-NB  | 2.37  | 126.76      | 124.26   |
| 10  | F     | 204 | CLA  | CHC-C4B-NB  | 2.37  | 126.76      | 124.26   |
| 10  | B     | 807 | CLA  | CHC-C4B-NB  | 2.37  | 126.76      | 124.26   |
| 10  | A     | 828 | CLA  | CHC-C4B-NB  | 2.35  | 126.74      | 124.26   |
| 10  | J     | 102 | CLA  | CHC-C4B-NB  | 2.35  | 126.74      | 124.26   |
| 10  | A     | 824 | CLA  | C1-C2-C3    | -2.33 | 122.01      | 126.04   |
| 10  | A     | 831 | CLA  | CHC-C4B-NB  | 2.33  | 126.72      | 124.26   |
| 10  | B     | 831 | CLA  | CHC-C4B-NB  | 2.33  | 126.72      | 124.26   |
| 10  | A     | 826 | CLA  | CHC-C4B-NB  | 2.32  | 126.72      | 124.26   |
| 10  | B     | 826 | CLA  | CHC-C4B-NB  | 2.31  | 126.71      | 124.26   |
| 10  | B     | 836 | CLA  | CHC-C4B-NB  | 2.31  | 126.71      | 124.26   |
| 10  | A     | 812 | CLA  | CHC-C4B-NB  | 2.31  | 126.70      | 124.26   |
| 10  | A     | 833 | CLA  | CHB-C1B-NB  | -2.30 | 121.82      | 124.26   |
| 10  | B     | 808 | CLA  | CHC-C4B-NB  | 2.30  | 126.69      | 124.26   |
| 10  | A     | 808 | CLA  | CHC-C4B-NB  | 2.29  | 126.69      | 124.26   |
| 10  | B     | 830 | CLA  | CHC-C4B-NB  | 2.29  | 126.68      | 124.26   |
| 10  | F     | 203 | CLA  | CHC-C4B-NB  | 2.29  | 126.68      | 124.26   |
| 10  | B     | 802 | CLA  | CHB-C1B-NB  | -2.29 | 121.84      | 124.26   |
| 10  | B     | 820 | CLA  | CHC-C4B-NB  | 2.29  | 126.68      | 124.26   |
| 10  | A     | 841 | CLA  | CHC-C4B-NB  | 2.28  | 126.67      | 124.26   |
| 10  | B     | 823 | CLA  | CHC-C4B-NB  | 2.28  | 126.67      | 124.26   |
| 10  | A     | 834 | CLA  | CHC-C4B-NB  | 2.27  | 126.66      | 124.26   |
| 15  | A     | 853 | LMT  | O1'-C1'-C2' | 2.26  | 111.83      | 108.30   |
| 10  | B     | 828 | CLA  | C3B-C4B-NB  | -2.25 | 108.42      | 110.52   |
| 10  | J     | 101 | CLA  | CHC-C4B-NB  | 2.24  | 126.63      | 124.26   |
| 18  | B     | 852 | 5X6  | C05-C06-C07 | -2.24 | 107.24      | 110.30   |
| 10  | B     | 843 | CLA  | CBD-CAD-C3D | 2.23  | 108.84      | 105.94   |
| 10  | B     | 838 | CLA  | CHC-C4B-NB  | 2.22  | 126.61      | 124.26   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 10  | A     | 832 | CLA  | CHC-C4B-NB | 2.22  | 126.61      | 124.26   |
| 10  | B     | 840 | CLA  | CHC-C4B-NB | 2.21  | 126.59      | 124.26   |
| 10  | A     | 804 | CLA  | CHB-C1B-NB | -2.20 | 121.93      | 124.26   |
| 10  | A     | 807 | CLA  | CHC-C4B-NB | 2.19  | 126.58      | 124.26   |
| 10  | B     | 827 | CLA  | CHC-C4B-NB | 2.19  | 126.57      | 124.26   |
| 10  | B     | 824 | CLA  | CHC-C4B-NB | 2.18  | 126.57      | 124.26   |
| 10  | B     | 809 | CLA  | CHC-C4B-NB | 2.18  | 126.56      | 124.26   |
| 10  | A     | 840 | CLA  | CHC-C4B-NB | 2.15  | 126.53      | 124.26   |
| 10  | B     | 821 | CLA  | CHC-C4B-NB | 2.15  | 126.53      | 124.26   |
| 10  | A     | 835 | CLA  | CHC-C4B-NB | 2.15  | 126.53      | 124.26   |
| 10  | B     | 829 | CLA  | CHC-C4B-NB | 2.15  | 126.53      | 124.26   |
| 10  | B     | 826 | CLA  | CHB-C1B-NB | -2.13 | 122.00      | 124.26   |
| 10  | B     | 834 | CLA  | CHC-C4B-NB | 2.13  | 126.51      | 124.26   |
| 10  | A     | 808 | CLA  | C3D-C4D-ND | 2.12  | 113.67      | 110.24   |
| 10  | A     | 843 | CLA  | CHC-C4B-NB | 2.11  | 126.49      | 124.26   |
| 10  | A     | 814 | CLA  | CHB-C1B-NB | -2.10 | 122.03      | 124.26   |
| 10  | A     | 811 | CLA  | CHC-C4B-NB | 2.09  | 126.47      | 124.26   |
| 10  | B     | 842 | CLA  | CHB-C1B-NB | -2.08 | 122.05      | 124.26   |
| 9   | A     | 803 | CL0  | CHA-C1A-NA | -2.08 | 121.64      | 126.40   |
| 10  | A     | 824 | CLA  | C3D-C4D-ND | 2.07  | 113.59      | 110.24   |
| 10  | B     | 829 | CLA  | CHB-C1B-NB | -2.07 | 122.06      | 124.26   |
| 10  | A     | 805 | CLA  | CHC-C4B-NB | 2.06  | 126.44      | 124.26   |
| 10  | A     | 819 | CLA  | CHB-C1B-NB | -2.06 | 122.08      | 124.26   |
| 10  | A     | 809 | CLA  | CHC-C4B-NB | 2.06  | 126.43      | 124.26   |
| 10  | A     | 830 | CLA  | CHC-C4B-NB | 2.05  | 126.43      | 124.26   |
| 9   | A     | 803 | CL0  | C1-C2-C3   | -2.05 | 122.50      | 126.04   |
| 10  | A     | 804 | CLA  | C3B-C4B-NB | -2.04 | 108.62      | 110.52   |
| 10  | B     | 803 | CLA  | CHC-C4B-NB | 2.02  | 126.40      | 124.26   |
| 10  | B     | 827 | CLA  | CHB-C1B-NB | -2.01 | 122.13      | 124.26   |
| 10  | A     | 810 | CLA  | C3D-C4D-ND | 2.01  | 113.48      | 110.24   |

There are no chirality outliers.

All (410) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 8   | A     | 801 | LHG  | C4-O6-P-O4      |
| 8   | A     | 802 | LHG  | C3-O3-P-O5      |
| 8   | A     | 802 | LHG  | C4-O6-P-O4      |
| 8   | B     | 851 | LHG  | C4-O6-P-O5      |
| 10  | A     | 807 | CLA  | CHA-CBD-CGD-O1D |
| 10  | A     | 807 | CLA  | CHA-CBD-CGD-O2D |
| 10  | A     | 823 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | A     | 823 | CLA  | C3A-C2A-CAA-CBA |
| 10  | A     | 823 | CLA  | C2B-C3B-CAB-CBB |
| 10  | A     | 823 | CLA  | C4B-C3B-CAB-CBB |
| 10  | A     | 824 | CLA  | CHA-CBD-CGD-O1D |
| 10  | A     | 824 | CLA  | CHA-CBD-CGD-O2D |
| 10  | A     | 829 | CLA  | C2B-C3B-CAB-CBB |
| 10  | A     | 829 | CLA  | C4B-C3B-CAB-CBB |
| 10  | A     | 829 | CLA  | CHA-CBD-CGD-O1D |
| 10  | A     | 829 | CLA  | CHA-CBD-CGD-O2D |
| 10  | A     | 830 | CLA  | O2A-C1-C2-C3    |
| 10  | A     | 834 | CLA  | C2A-CAA-CBA-CGA |
| 10  | A     | 835 | CLA  | CHA-CBD-CGD-O1D |
| 10  | A     | 835 | CLA  | CHA-CBD-CGD-O2D |
| 10  | A     | 839 | CLA  | C4B-C3B-CAB-CBB |
| 10  | A     | 840 | CLA  | CHA-CBD-CGD-O1D |
| 10  | A     | 840 | CLA  | CHA-CBD-CGD-O2D |
| 10  | A     | 843 | CLA  | CHA-CBD-CGD-O1D |
| 10  | A     | 843 | CLA  | CHA-CBD-CGD-O2D |
| 10  | A     | 844 | CLA  | CHA-CBD-CGD-O1D |
| 10  | A     | 844 | CLA  | CHA-CBD-CGD-O2D |
| 10  | A     | 845 | CLA  | C2B-C3B-CAB-CBB |
| 10  | A     | 845 | CLA  | C4B-C3B-CAB-CBB |
| 10  | B     | 801 | CLA  | CHA-CBD-CGD-O1D |
| 10  | B     | 802 | CLA  | CHA-CBD-CGD-O1D |
| 10  | B     | 802 | CLA  | CHA-CBD-CGD-O2D |
| 10  | B     | 810 | CLA  | CHA-CBD-CGD-O2D |
| 10  | B     | 819 | CLA  | C2B-C3B-CAB-CBB |
| 10  | B     | 819 | CLA  | C4B-C3B-CAB-CBB |
| 10  | B     | 825 | CLA  | CHA-CBD-CGD-O1D |
| 10  | B     | 825 | CLA  | CHA-CBD-CGD-O2D |
| 10  | B     | 827 | CLA  | CHA-CBD-CGD-O1D |
| 10  | B     | 827 | CLA  | CHA-CBD-CGD-O2D |
| 10  | B     | 831 | CLA  | CHA-CBD-CGD-O1D |
| 10  | B     | 831 | CLA  | CHA-CBD-CGD-O2D |
| 10  | B     | 831 | CLA  | C2-C3-C5-C6     |
| 10  | B     | 831 | CLA  | C4-C3-C5-C6     |
| 10  | B     | 840 | CLA  | C4-C3-C5-C6     |
| 10  | B     | 841 | CLA  | C2B-C3B-CAB-CBB |
| 10  | B     | 841 | CLA  | C4B-C3B-CAB-CBB |
| 12  | A     | 848 | BCR  | C5-C6-C7-C8     |
| 12  | A     | 850 | BCR  | C23-C24-C25-C26 |
| 12  | A     | 850 | BCR  | C23-C24-C25-C30 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | B     | 845 | BCR  | C1-C6-C7-C8     |
| 12  | J     | 103 | BCR  | C5-C6-C7-C8     |
| 13  | A     | 851 | ECH  | C23-C24-C25-C26 |
| 13  | A     | 851 | ECH  | C23-C24-C25-C30 |
| 13  | M     | 101 | ECH  | C23-C24-C25-C26 |
| 13  | M     | 101 | ECH  | C23-C24-C25-C30 |
| 14  | A     | 852 | LMG  | C2-C1-O1-C7     |
| 14  | A     | 852 | LMG  | O6-C1-O1-C7     |
| 15  | A     | 858 | LMT  | O5'-C1'-O1'-C1  |
| 15  | A     | 858 | LMT  | C2-C1-O1'-C1'   |
| 10  | K     | 102 | CLA  | C4C-C3C-CAC-CBC |
| 10  | K     | 102 | CLA  | C2C-C3C-CAC-CBC |
| 15  | I     | 102 | LMT  | C3'-C4'-O1B-C1B |
| 15  | A     | 858 | LMT  | C2'-C1'-O1'-C1  |
| 10  | A     | 805 | CLA  | C14-C13-C15-C16 |
| 10  | B     | 824 | CLA  | C11-C10-C8-C9   |
| 10  | B     | 829 | CLA  | C11-C10-C8-C9   |
| 10  | A     | 845 | CLA  | C5-C6-C7-C8     |
| 10  | A     | 816 | CLA  | C12-C13-C15-C16 |
| 10  | B     | 802 | CLA  | C12-C13-C15-C16 |
| 10  | A     | 813 | CLA  | C2A-CAA-CBA-CGA |
| 15  | I     | 103 | LMT  | O5'-C1'-O1'-C1  |
| 15  | A     | 858 | LMT  | O1'-C1-C2-C3    |
| 10  | B     | 820 | CLA  | C5-C6-C7-C8     |
| 8   | A     | 801 | LHG  | C4-O6-P-O3      |
| 8   | A     | 802 | LHG  | C4-O6-P-O3      |
| 15  | A     | 860 | LMT  | O1'-C1-C2-C3    |
| 10  | A     | 810 | CLA  | C2A-CAA-CBA-CGA |
| 15  | F     | 207 | LMT  | C7-C8-C9-C10    |
| 8   | A     | 801 | LHG  | C28-C29-C30-C31 |
| 15  | A     | 858 | LMT  | C7-C8-C9-C10    |
| 15  | I     | 103 | LMT  | C2'-C1'-O1'-C1  |
| 10  | A     | 805 | CLA  | C11-C10-C8-C9   |
| 10  | A     | 863 | CLA  | C4B-C3B-CAB-CBB |
| 10  | B     | 842 | CLA  | C4B-C3B-CAB-CBB |
| 10  | J     | 101 | CLA  | C4B-C3B-CAB-CBB |
| 10  | K     | 102 | CLA  | C4B-C3B-CAB-CBB |
| 10  | K     | 103 | CLA  | C3A-C2A-CAA-CBA |
| 15  | B     | 854 | LMT  | C2-C1-O1'-C1'   |
| 15  | I     | 102 | LMT  | C2-C1-O1'-C1'   |
| 15  | A     | 853 | LMT  | C1-C2-C3-C4     |
| 14  | B     | 850 | LMG  | C31-C32-C33-C34 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | A     | 839 | CLA  | C2B-C3B-CAB-CBB |
| 10  | A     | 863 | CLA  | C2B-C3B-CAB-CBB |
| 10  | B     | 842 | CLA  | C2B-C3B-CAB-CBB |
| 10  | J     | 101 | CLA  | C2B-C3B-CAB-CBB |
| 10  | K     | 102 | CLA  | C2B-C3B-CAB-CBB |
| 10  | A     | 845 | CLA  | C3-C5-C6-C7     |
| 10  | B     | 818 | CLA  | C2-C1-O2A-CGA   |
| 12  | A     | 848 | BCR  | C1-C6-C7-C8     |
| 12  | A     | 849 | BCR  | C23-C24-C25-C26 |
| 12  | A     | 849 | BCR  | C23-C24-C25-C30 |
| 12  | B     | 845 | BCR  | C5-C6-C7-C8     |
| 12  | B     | 847 | BCR  | C23-C24-C25-C26 |
| 12  | B     | 847 | BCR  | C23-C24-C25-C30 |
| 12  | B     | 848 | BCR  | C23-C24-C25-C26 |
| 12  | B     | 848 | BCR  | C23-C24-C25-C30 |
| 12  | J     | 103 | BCR  | C1-C6-C7-C8     |
| 13  | M     | 101 | ECH  | C1-C6-C7-C8     |
| 13  | M     | 101 | ECH  | C5-C6-C7-C8     |
| 18  | B     | 852 | 5X6  | C27-C28-C29-C34 |
| 18  | B     | 852 | 5X6  | C27-C28-C29-C30 |
| 10  | A     | 805 | CLA  | C11-C10-C8-C7   |
| 10  | A     | 805 | CLA  | C12-C13-C15-C16 |
| 10  | A     | 863 | CLA  | C12-C13-C15-C16 |
| 10  | B     | 830 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 850 | LMG  | O6-C5-C6-O5     |
| 15  | A     | 854 | LMT  | O5'-C5'-C6'-O6' |
| 10  | B     | 830 | CLA  | C4-C3-C5-C6     |
| 10  | A     | 816 | CLA  | C14-C13-C15-C16 |
| 10  | A     | 863 | CLA  | C14-C13-C15-C16 |
| 10  | B     | 806 | CLA  | C2A-CAA-CBA-CGA |
| 15  | A     | 858 | LMT  | O5'-C5'-C6'-O6' |
| 15  | A     | 860 | LMT  | O5'-C5'-C6'-O6' |
| 10  | K     | 103 | CLA  | C1A-C2A-CAA-CBA |
| 8   | B     | 851 | LHG  | C4-O6-P-O3      |
| 14  | A     | 852 | LMG  | C8-C7-O1-C1     |
| 15  | I     | 103 | LMT  | O5'-C5'-C6'-O6' |
| 10  | A     | 816 | CLA  | C4-C3-C5-C6     |
| 10  | A     | 830 | CLA  | C4-C3-C5-C6     |
| 10  | A     | 816 | CLA  | C2-C3-C5-C6     |
| 10  | A     | 830 | CLA  | C2-C3-C5-C6     |
| 10  | A     | 832 | CLA  | C4-C3-C5-C6     |
| 10  | A     | 842 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | B     | 829 | CLA  | C4-C3-C5-C6     |
| 10  | K     | 103 | CLA  | C4-C3-C5-C6     |
| 10  | A     | 825 | CLA  | C2-C3-C5-C6     |
| 10  | B     | 822 | CLA  | C11-C10-C8-C7   |
| 10  | A     | 821 | CLA  | C4B-C3B-CAB-CBB |
| 10  | B     | 801 | CLA  | C4B-C3B-CAB-CBB |
| 10  | B     | 810 | CLA  | C4B-C3B-CAB-CBB |
| 8   | A     | 802 | LHG  | O6-C4-C5-C6     |
| 10  | A     | 825 | CLA  | C4-C3-C5-C6     |
| 10  | A     | 832 | CLA  | C2-C3-C5-C6     |
| 10  | A     | 842 | CLA  | C2-C3-C5-C6     |
| 10  | B     | 829 | CLA  | C2-C3-C5-C6     |
| 10  | K     | 103 | CLA  | C2-C3-C5-C6     |
| 10  | B     | 815 | CLA  | C2C-C3C-CAC-CBC |
| 15  | B     | 853 | LMT  | C2-C1-O1'-C1'   |
| 15  | F     | 207 | LMT  | C2-C1-O1'-C1'   |
| 15  | I     | 103 | LMT  | C2-C1-O1'-C1'   |
| 15  | B     | 853 | LMT  | C3-C4-C5-C6     |
| 15  | A     | 853 | LMT  | C3-C4-C5-C6     |
| 15  | B     | 857 | LMT  | C7-C8-C9-C10    |
| 15  | B     | 858 | LMT  | O1'-C1-C2-C3    |
| 8   | A     | 802 | LHG  | C3-O3-P-O6      |
| 8   | A     | 801 | LHG  | O6-C4-C5-O7     |
| 8   | A     | 802 | LHG  | O6-C4-C5-O7     |
| 10  | B     | 801 | CLA  | C2B-C3B-CAB-CBB |
| 10  | B     | 810 | CLA  | C2B-C3B-CAB-CBB |
| 10  | B     | 810 | CLA  | C11-C10-C8-C9   |
| 10  | B     | 822 | CLA  | C11-C12-C13-C14 |
| 15  | I     | 102 | LMT  | C5'-C4'-O1B-C1B |
| 15  | A     | 855 | LMT  | C7-C8-C9-C10    |
| 10  | A     | 816 | CLA  | C6-C7-C8-C10    |
| 10  | A     | 829 | CLA  | C11-C10-C8-C7   |
| 10  | B     | 824 | CLA  | C11-C10-C8-C7   |
| 15  | A     | 853 | LMT  | C6-C7-C8-C9     |
| 10  | A     | 812 | CLA  | CAD-CBD-CGD-O2D |
| 10  | A     | 819 | CLA  | CAD-CBD-CGD-O2D |
| 10  | A     | 821 | CLA  | CAD-CBD-CGD-O2D |
| 10  | B     | 814 | CLA  | CAD-CBD-CGD-O2D |
| 10  | B     | 842 | CLA  | CAD-CBD-CGD-O2D |
| 10  | K     | 101 | CLA  | CAD-CBD-CGD-O2D |
| 10  | B     | 822 | CLA  | C4-C3-C5-C6     |
| 15  | F     | 207 | LMT  | O5'-C1'-O1'-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | B     | 807 | CLA  | C2-C3-C5-C6     |
| 10  | A     | 823 | CLA  | CAA-CBA-CGA-O2A |
| 10  | A     | 810 | CLA  | CHA-CBD-CGD-O1D |
| 10  | A     | 810 | CLA  | CHA-CBD-CGD-O2D |
| 10  | A     | 813 | CLA  | CHA-CBD-CGD-O1D |
| 10  | A     | 813 | CLA  | CHA-CBD-CGD-O2D |
| 10  | A     | 828 | CLA  | CHA-CBD-CGD-O1D |
| 10  | A     | 828 | CLA  | CHA-CBD-CGD-O2D |
| 10  | B     | 807 | CLA  | CHA-CBD-CGD-O1D |
| 10  | B     | 810 | CLA  | CHA-CBD-CGD-O1D |
| 10  | B     | 807 | CLA  | C4-C3-C5-C6     |
| 10  | B     | 820 | CLA  | C4-C3-C5-C6     |
| 10  | B     | 825 | CLA  | C4-C3-C5-C6     |
| 10  | B     | 833 | CLA  | C4-C3-C5-C6     |
| 10  | A     | 829 | CLA  | C11-C10-C8-C9   |
| 15  | J     | 105 | LMT  | C7-C8-C9-C10    |
| 10  | A     | 814 | CLA  | C1A-C2A-CAA-CBA |
| 10  | A     | 827 | CLA  | C1A-C2A-CAA-CBA |
| 8   | A     | 802 | LHG  | O2-C2-C3-O3     |
| 15  | J     | 104 | LMT  | C2-C3-C4-C5     |
| 8   | A     | 802 | LHG  | C4-O6-P-O5      |
| 8   | B     | 851 | LHG  | C4-O6-P-O4      |
| 10  | A     | 840 | CLA  | C4B-C3B-CAB-CBB |
| 10  | A     | 843 | CLA  | C4B-C3B-CAB-CBB |
| 10  | B     | 821 | CLA  | C4B-C3B-CAB-CBB |
| 10  | B     | 824 | CLA  | C4B-C3B-CAB-CBB |
| 10  | B     | 828 | CLA  | C4B-C3B-CAB-CBB |
| 10  | K     | 101 | CLA  | C4B-C3B-CAB-CBB |
| 15  | J     | 104 | LMT  | C7-C8-C9-C10    |
| 10  | A     | 810 | CLA  | CAD-CBD-CGD-O1D |
| 10  | A     | 828 | CLA  | CAD-CBD-CGD-O1D |
| 10  | B     | 802 | CLA  | CAD-CBD-CGD-O1D |
| 10  | B     | 807 | CLA  | CAD-CBD-CGD-O1D |
| 10  | B     | 840 | CLA  | C2-C3-C5-C6     |
| 10  | A     | 844 | CLA  | C11-C10-C8-C7   |
| 10  | B     | 822 | CLA  | C2-C3-C5-C6     |
| 10  | B     | 819 | CLA  | CAA-CBA-CGA-O2A |
| 15  | J     | 105 | LMT  | C2-C3-C4-C5     |
| 10  | B     | 831 | CLA  | C5-C6-C7-C8     |
| 10  | A     | 816 | CLA  | C6-C7-C8-C9     |
| 10  | A     | 821 | CLA  | C2B-C3B-CAB-CBB |
| 10  | A     | 837 | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | A     | 838 | CLA  | C2B-C3B-CAB-CBB |
| 10  | B     | 821 | CLA  | C2B-C3B-CAB-CBB |
| 10  | F     | 204 | CLA  | C2B-C3B-CAB-CBB |
| 10  | K     | 101 | CLA  | C2B-C3B-CAB-CBB |
| 10  | A     | 813 | CLA  | C13-C15-C16-C17 |
| 10  | A     | 833 | CLA  | C2A-CAA-CBA-CGA |
| 10  | B     | 802 | CLA  | C2A-CAA-CBA-CGA |
| 10  | B     | 819 | CLA  | C2A-CAA-CBA-CGA |
| 8   | B     | 851 | LHG  | C26-C27-C28-C29 |
| 10  | B     | 820 | CLA  | C2-C3-C5-C6     |
| 10  | B     | 825 | CLA  | C2-C3-C5-C6     |
| 10  | B     | 833 | CLA  | C2-C3-C5-C6     |
| 10  | B     | 815 | CLA  | C4C-C3C-CAC-CBC |
| 15  | F     | 207 | LMT  | C2'-C1'-O1'-C1  |
| 8   | A     | 801 | LHG  | C3-O3-P-O6      |
| 8   | B     | 851 | LHG  | C3-O3-P-O6      |
| 10  | B     | 829 | CLA  | C11-C10-C8-C7   |
| 10  | B     | 822 | CLA  | C11-C10-C8-C9   |
| 10  | A     | 837 | CLA  | C4B-C3B-CAB-CBB |
| 10  | A     | 838 | CLA  | C4B-C3B-CAB-CBB |
| 10  | A     | 846 | CLA  | C4B-C3B-CAB-CBB |
| 10  | F     | 204 | CLA  | C4B-C3B-CAB-CBB |
| 10  | B     | 815 | CLA  | C5-C6-C7-C8     |
| 10  | A     | 824 | CLA  | C4-C3-C5-C6     |
| 10  | B     | 823 | CLA  | CAA-CBA-CGA-O1A |
| 10  | A     | 824 | CLA  | C2-C3-C5-C6     |
| 10  | J     | 101 | CLA  | CAA-CBA-CGA-O2A |
| 10  | B     | 842 | CLA  | CAA-CBA-CGA-O1A |
| 10  | A     | 804 | CLA  | C2A-CAA-CBA-CGA |
| 10  | K     | 101 | CLA  | CAA-CBA-CGA-O1A |
| 10  | B     | 823 | CLA  | CAA-CBA-CGA-O2A |
| 10  | B     | 842 | CLA  | CAA-CBA-CGA-O2A |
| 10  | A     | 830 | CLA  | C14-C13-C15-C16 |
| 10  | A     | 835 | CLA  | C6-C7-C8-C9     |
| 10  | B     | 814 | CLA  | CAA-CBA-CGA-O2A |
| 13  | A     | 851 | ECH  | C11-C10-C9-C34  |
| 13  | A     | 851 | ECH  | C16-C17-C18-C36 |
| 13  | B     | 846 | ECH  | C11-C10-C9-C34  |
| 13  | B     | 846 | ECH  | C20-C21-C22-C37 |
| 13  | F     | 205 | ECH  | C35-C13-C14-C15 |
| 10  | A     | 846 | CLA  | CAA-CBA-CGA-O1A |
| 10  | B     | 806 | CLA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | K     | 102 | CLA  | CAA-CBA-CGA-O1A |
| 10  | B     | 807 | CLA  | C2A-CAA-CBA-CGA |
| 10  | A     | 816 | CLA  | O2A-C1-C2-C3    |
| 10  | B     | 825 | CLA  | O2A-C1-C2-C3    |
| 10  | B     | 814 | CLA  | CAA-CBA-CGA-O1A |
| 8   | B     | 851 | LHG  | C6-C5-O7-C7     |
| 10  | B     | 807 | CLA  | C1A-C2A-CAA-CBA |
| 10  | B     | 818 | CLA  | C1A-C2A-CAA-CBA |
| 10  | B     | 822 | CLA  | C1A-C2A-CAA-CBA |
| 10  | B     | 823 | CLA  | C1A-C2A-CAA-CBA |
| 10  | B     | 829 | CLA  | C1A-C2A-CAA-CBA |
| 10  | A     | 863 | CLA  | C11-C10-C8-C7   |
| 10  | K     | 101 | CLA  | CAA-CBA-CGA-O2A |
| 10  | A     | 846 | CLA  | CAA-CBA-CGA-O2A |
| 10  | J     | 101 | CLA  | CAA-CBA-CGA-O1A |
| 15  | B     | 859 | LMT  | C7-C8-C9-C10    |
| 10  | K     | 102 | CLA  | CAA-CBA-CGA-O2A |
| 8   | A     | 801 | LHG  | C25-C26-C27-C28 |
| 10  | A     | 836 | CLA  | C2B-C3B-CAB-CBB |
| 10  | A     | 840 | CLA  | C2B-C3B-CAB-CBB |
| 10  | A     | 843 | CLA  | C2B-C3B-CAB-CBB |
| 10  | B     | 812 | CLA  | C2B-C3B-CAB-CBB |
| 10  | B     | 824 | CLA  | C2B-C3B-CAB-CBB |
| 10  | B     | 828 | CLA  | C2B-C3B-CAB-CBB |
| 13  | A     | 851 | ECH  | C11-C10-C9-C8   |
| 13  | A     | 851 | ECH  | C16-C17-C18-C19 |
| 13  | B     | 846 | ECH  | C11-C10-C9-C8   |
| 13  | B     | 846 | ECH  | C20-C21-C22-C23 |
| 13  | F     | 205 | ECH  | C12-C13-C14-C15 |
| 8   | A     | 802 | LHG  | C1-C2-C3-O3     |
| 10  | A     | 840 | CLA  | CAA-CBA-CGA-O1A |
| 10  | B     | 809 | CLA  | C4-C3-C5-C6     |
| 9   | A     | 803 | CL0  | CAA-CBA-CGA-O2A |
| 10  | B     | 820 | CLA  | C11-C10-C8-C9   |
| 12  | A     | 847 | BCR  | C1-C6-C7-C8     |
| 13  | B     | 846 | ECH  | C1-C6-C7-C8     |
| 10  | B     | 806 | CLA  | CAA-CBA-CGA-O2A |
| 10  | B     | 811 | CLA  | CAA-CBA-CGA-O2A |
| 9   | A     | 803 | CL0  | C5-C6-C7-C8     |
| 10  | A     | 819 | CLA  | CAA-CBA-CGA-O2A |
| 10  | B     | 837 | CLA  | CAA-CBA-CGA-O2A |
| 10  | A     | 836 | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | B     | 812 | CLA  | C4B-C3B-CAB-CBB |
| 10  | B     | 822 | CLA  | C4B-C3B-CAB-CBB |
| 10  | A     | 805 | CLA  | C15-C16-C17-C18 |
| 10  | A     | 804 | CLA  | C4-C3-C5-C6     |
| 10  | A     | 834 | CLA  | C11-C10-C8-C9   |
| 10  | A     | 844 | CLA  | C11-C12-C13-C14 |
| 10  | B     | 807 | CLA  | C3A-C2A-CAA-CBA |
| 10  | B     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 15  | A     | 853 | LMT  | C11-C10-C9-C8   |
| 10  | B     | 818 | CLA  | CAA-CBA-CGA-O2A |
| 10  | B     | 837 | CLA  | CAA-CBA-CGA-O1A |
| 10  | A     | 809 | CLA  | CAD-CBD-CGD-O2D |
| 10  | A     | 816 | CLA  | CAD-CBD-CGD-O2D |
| 10  | A     | 817 | CLA  | CAD-CBD-CGD-O2D |
| 10  | A     | 820 | CLA  | CAD-CBD-CGD-O2D |
| 10  | A     | 831 | CLA  | CAD-CBD-CGD-O2D |
| 10  | A     | 836 | CLA  | CAD-CBD-CGD-O2D |
| 10  | A     | 837 | CLA  | CAD-CBD-CGD-O2D |
| 10  | A     | 841 | CLA  | CAD-CBD-CGD-O2D |
| 10  | B     | 815 | CLA  | CAD-CBD-CGD-O2D |
| 10  | B     | 832 | CLA  | CAD-CBD-CGD-O2D |
| 10  | B     | 834 | CLA  | CAD-CBD-CGD-O2D |
| 10  | B     | 838 | CLA  | CAD-CBD-CGD-O2D |
| 10  | K     | 102 | CLA  | CAD-CBD-CGD-O2D |
| 10  | F     | 203 | CLA  | CAA-CBA-CGA-O2A |
| 10  | A     | 839 | CLA  | C4-C3-C5-C6     |
| 8   | A     | 801 | LHG  | O8-C23-C24-C25  |
| 10  | A     | 811 | CLA  | CAA-CBA-CGA-O2A |
| 10  | B     | 803 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 850 | LMG  | O7-C10-C11-C12  |
| 10  | A     | 819 | CLA  | CAA-CBA-CGA-O1A |
| 8   | A     | 801 | LHG  | O7-C7-C8-C9     |
| 14  | A     | 852 | LMG  | O8-C28-C29-C30  |
| 10  | B     | 819 | CLA  | O2A-C1-C2-C3    |
| 10  | B     | 829 | CLA  | O2A-C1-C2-C3    |
| 10  | B     | 803 | CLA  | C8-C10-C11-C12  |
| 10  | B     | 808 | CLA  | CAA-CBA-CGA-O2A |
| 10  | B     | 811 | CLA  | CAA-CBA-CGA-O1A |
| 10  | F     | 203 | CLA  | CAA-CBA-CGA-O1A |
| 10  | A     | 827 | CLA  | CHA-CBD-CGD-O1D |
| 10  | A     | 827 | CLA  | CHA-CBD-CGD-O2D |
| 10  | A     | 841 | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | B     | 801 | CLA  | CHA-CBD-CGD-O2D |
| 10  | B     | 807 | CLA  | CHA-CBD-CGD-O2D |
| 10  | B     | 823 | CLA  | CHA-CBD-CGD-O1D |
| 10  | B     | 826 | CLA  | CHA-CBD-CGD-O1D |
| 10  | B     | 826 | CLA  | CHA-CBD-CGD-O2D |
| 10  | B     | 828 | CLA  | CHA-CBD-CGD-O2D |
| 10  | B     | 835 | CLA  | CHA-CBD-CGD-O1D |
| 10  | B     | 835 | CLA  | CHA-CBD-CGD-O2D |
| 10  | J     | 102 | CLA  | CHA-CBD-CGD-O1D |
| 10  | J     | 102 | CLA  | CHA-CBD-CGD-O2D |
| 10  | A     | 837 | CLA  | CAA-CBA-CGA-O2A |
| 10  | B     | 812 | CLA  | CAA-CBA-CGA-O2A |
| 10  | J     | 102 | CLA  | CAA-CBA-CGA-O1A |
| 8   | A     | 801 | LHG  | O6-C4-C5-C6     |
| 8   | A     | 802 | LHG  | O7-C7-C8-C9     |
| 15  | F     | 207 | LMT  | O1'-C1-C2-C3    |
| 10  | A     | 840 | CLA  | CAA-CBA-CGA-O2A |
| 8   | A     | 801 | LHG  | C26-C27-C28-C29 |
| 10  | A     | 830 | CLA  | CAA-CBA-CGA-O2A |
| 10  | A     | 844 | CLA  | C11-C10-C8-C9   |
| 8   | A     | 801 | LHG  | C13-C14-C15-C16 |
| 10  | A     | 846 | CLA  | C2B-C3B-CAB-CBB |
| 14  | B     | 850 | LMG  | O9-C10-C11-C12  |
| 10  | B     | 803 | CLA  | CAA-CBA-CGA-O1A |
| 10  | A     | 830 | CLA  | CAA-CBA-CGA-O1A |
| 10  | A     | 808 | CLA  | C1A-C2A-CAA-CBA |
| 10  | A     | 840 | CLA  | C1A-C2A-CAA-CBA |
| 8   | A     | 801 | LHG  | O10-C23-C24-C25 |
| 10  | B     | 833 | CLA  | C2-C1-O2A-CGA   |
| 8   | A     | 801 | LHG  | O9-C7-C8-C9     |
| 10  | B     | 808 | CLA  | CAA-CBA-CGA-O1A |
| 10  | B     | 802 | CLA  | C16-C17-C18-C20 |
| 14  | A     | 852 | LMG  | O10-C28-C29-C30 |
| 10  | J     | 102 | CLA  | CAA-CBA-CGA-O2A |
| 8   | B     | 851 | LHG  | C3-O3-P-O5      |
| 10  | B     | 809 | CLA  | C4B-C3B-CAB-CBB |
| 12  | A     | 847 | BCR  | C5-C6-C7-C8     |
| 10  | A     | 811 | CLA  | CAA-CBA-CGA-O1A |
| 15  | A     | 860 | LMT  | C1-C2-C3-C4     |
| 10  | A     | 820 | CLA  | CAA-CBA-CGA-O2A |
| 10  | A     | 837 | CLA  | CAA-CBA-CGA-O1A |
| 8   | B     | 851 | LHG  | C4-C5-O7-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | A     | 818 | CLA  | CAD-CBD-CGD-O1D |
| 10  | A     | 832 | CLA  | CAD-CBD-CGD-O1D |
| 10  | B     | 816 | CLA  | CAD-CBD-CGD-O1D |
| 8   | A     | 802 | LHG  | O9-C7-C8-C9     |
| 10  | A     | 863 | CLA  | C11-C10-C8-C9   |
| 10  | B     | 802 | CLA  | C14-C13-C15-C16 |
| 10  | B     | 812 | CLA  | CAA-CBA-CGA-O1A |
| 10  | B     | 834 | CLA  | C5-C6-C7-C8     |
| 8   | A     | 801 | LHG  | C14-C15-C16-C17 |
| 8   | A     | 801 | LHG  | C24-C25-C26-C27 |
| 10  | A     | 808 | CLA  | C3A-C2A-CAA-CBA |
| 10  | A     | 826 | CLA  | C6-C7-C8-C10    |
| 10  | B     | 824 | CLA  | C3A-C2A-CAA-CBA |
| 10  | A     | 820 | CLA  | CAA-CBA-CGA-O1A |
| 10  | A     | 818 | CLA  | CAA-CBA-CGA-O2A |
| 10  | K     | 103 | CLA  | CAA-CBA-CGA-O2A |
| 10  | A     | 815 | CLA  | CAA-CBA-CGA-O2A |
| 10  | B     | 813 | CLA  | CAA-CBA-CGA-O2A |
| 10  | K     | 103 | CLA  | CAA-CBA-CGA-O1A |
| 10  | B     | 841 | CLA  | CAA-CBA-CGA-O2A |
| 10  | B     | 829 | CLA  | C8-C10-C11-C12  |
| 15  | B     | 853 | LMT  | C11-C10-C9-C8   |
| 10  | A     | 818 | CLA  | CAA-CBA-CGA-O1A |
| 10  | A     | 823 | CLA  | CAA-CBA-CGA-O1A |
| 15  | A     | 864 | LMT  | C3'-C4'-O1B-C1B |

There are no ring outliers.

47 monomers are involved in 73 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 10  | B     | 823 | CLA  | 1       | 0            |
| 10  | B     | 808 | CLA  | 2       | 0            |
| 12  | A     | 847 | BCR  | 1       | 0            |
| 13  | F     | 205 | ECH  | 2       | 0            |
| 10  | B     | 828 | CLA  | 2       | 0            |
| 10  | A     | 844 | CLA  | 2       | 0            |
| 12  | A     | 850 | BCR  | 2       | 0            |
| 10  | A     | 810 | CLA  | 1       | 0            |
| 17  | B     | 805 | SF4  | 2       | 0            |
| 10  | B     | 826 | CLA  | 5       | 0            |
| 12  | B     | 845 | BCR  | 1       | 0            |
| 10  | B     | 809 | CLA  | 1       | 0            |

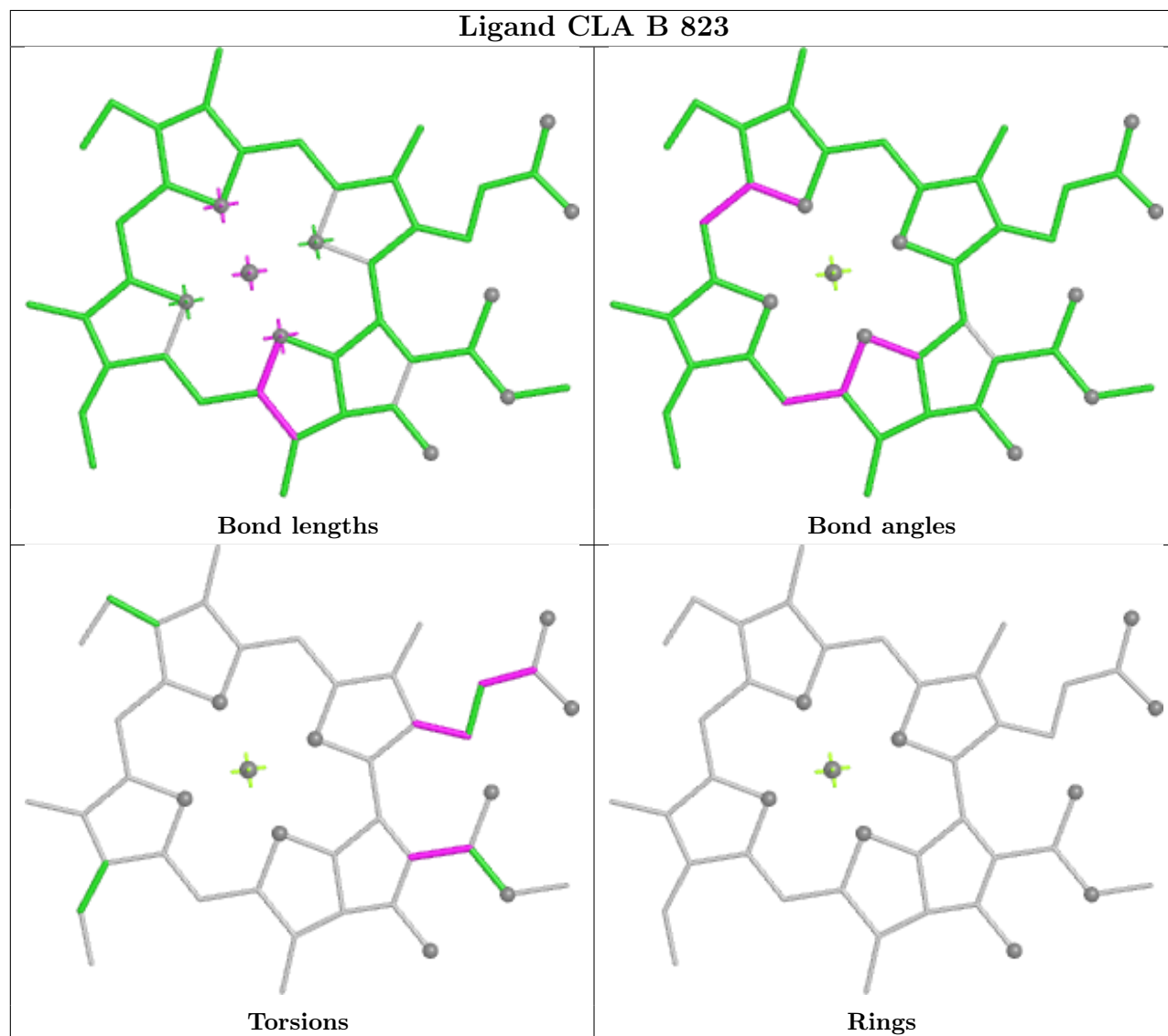
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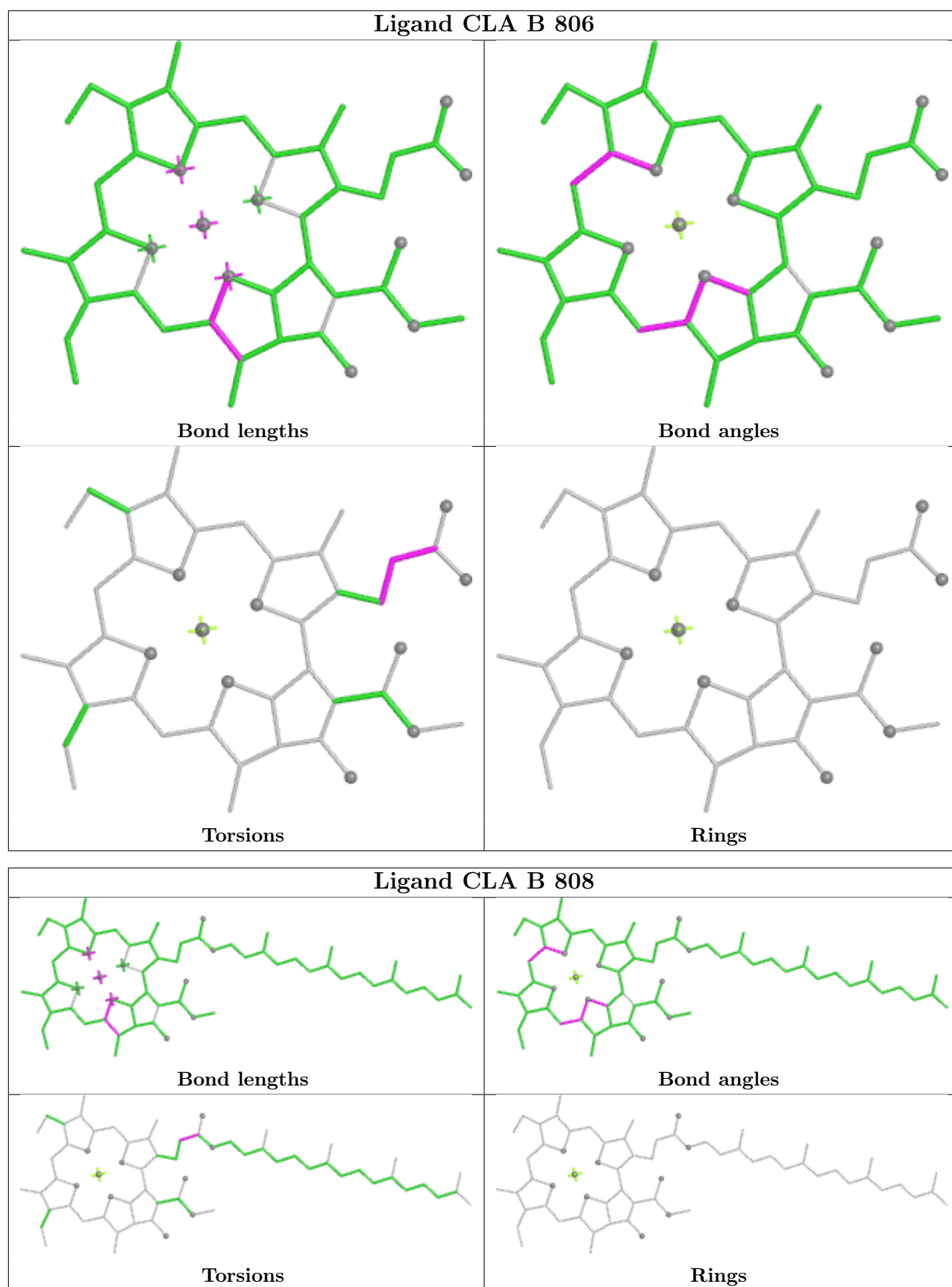
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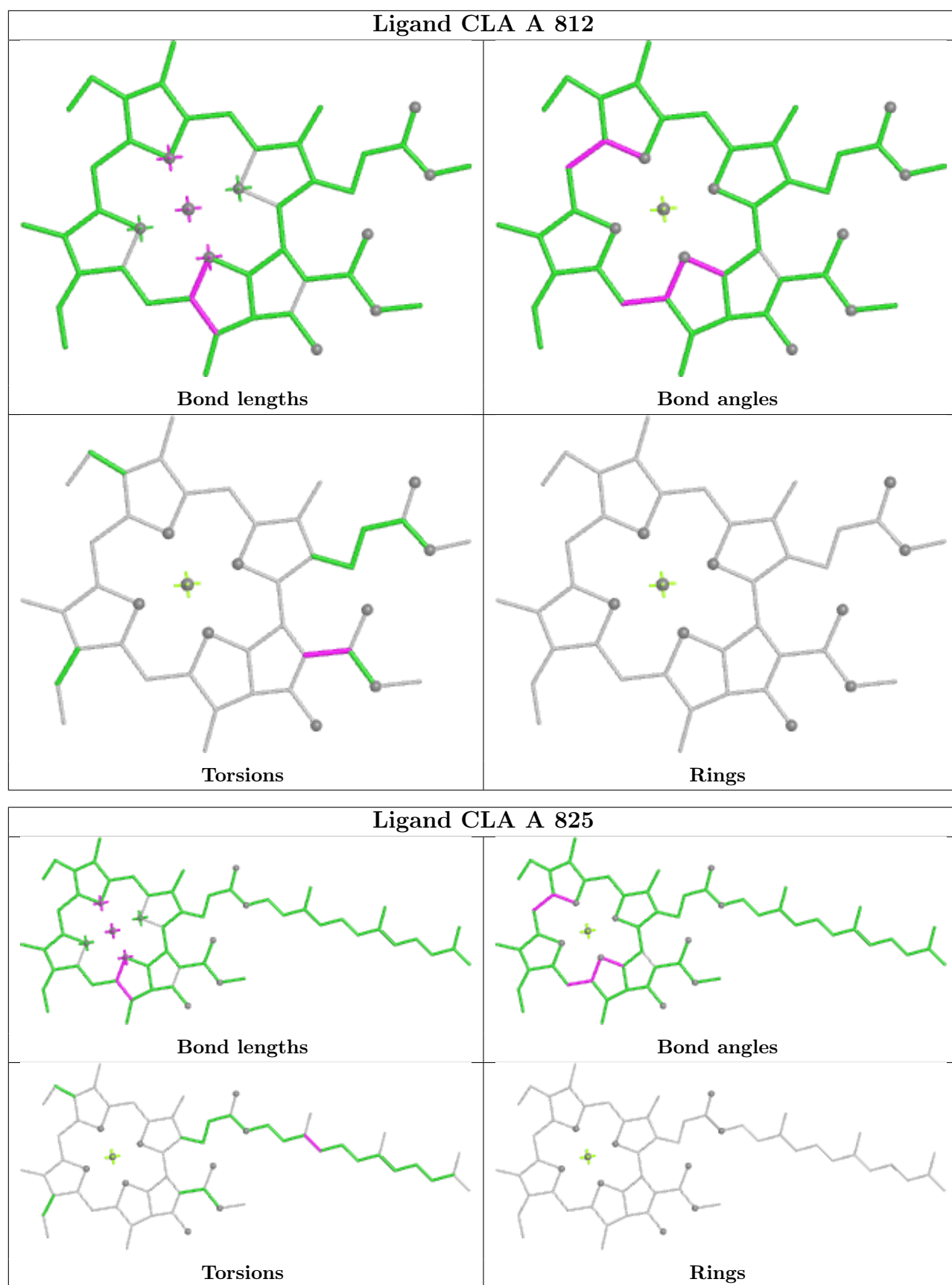
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 10  | B     | 829 | CLA  | 2       | 0            |
| 13  | A     | 865 | ECH  | 2       | 0            |
| 10  | A     | 813 | CLA  | 3       | 0            |
| 12  | F     | 202 | BCR  | 3       | 0            |
| 12  | A     | 866 | BCR  | 4       | 0            |
| 10  | B     | 810 | CLA  | 4       | 0            |
| 10  | B     | 803 | CLA  | 1       | 0            |
| 12  | B     | 848 | BCR  | 2       | 0            |
| 12  | B     | 849 | BCR  | 2       | 0            |
| 10  | A     | 828 | CLA  | 3       | 0            |
| 10  | A     | 830 | CLA  | 1       | 0            |
| 10  | B     | 819 | CLA  | 1       | 0            |
| 12  | B     | 844 | BCR  | 4       | 0            |
| 10  | B     | 835 | CLA  | 1       | 0            |
| 15  | I     | 102 | LMT  | 1       | 0            |
| 13  | M     | 101 | ECH  | 1       | 0            |
| 10  | A     | 840 | CLA  | 1       | 0            |
| 10  | A     | 845 | CLA  | 1       | 0            |
| 10  | A     | 819 | CLA  | 1       | 0            |
| 12  | J     | 103 | BCR  | 1       | 0            |
| 10  | B     | 802 | CLA  | 3       | 0            |
| 10  | A     | 814 | CLA  | 2       | 0            |
| 10  | A     | 827 | CLA  | 1       | 0            |
| 10  | A     | 842 | CLA  | 1       | 0            |
| 10  | K     | 102 | CLA  | 3       | 0            |
| 9   | A     | 803 | CL0  | 2       | 0            |
| 12  | A     | 848 | BCR  | 1       | 0            |
| 10  | A     | 838 | CLA  | 1       | 0            |
| 10  | A     | 805 | CLA  | 1       | 0            |
| 12  | B     | 847 | BCR  | 2       | 0            |
| 10  | A     | 804 | CLA  | 1       | 0            |
| 13  | A     | 851 | ECH  | 5       | 0            |
| 10  | B     | 834 | CLA  | 1       | 0            |
| 10  | B     | 825 | CLA  | 1       | 0            |
| 10  | B     | 821 | CLA  | 3       | 0            |

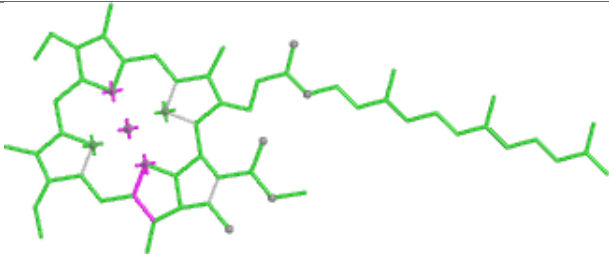
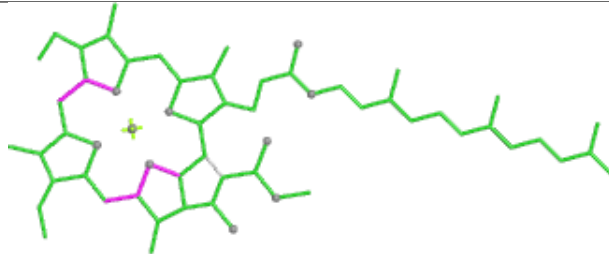
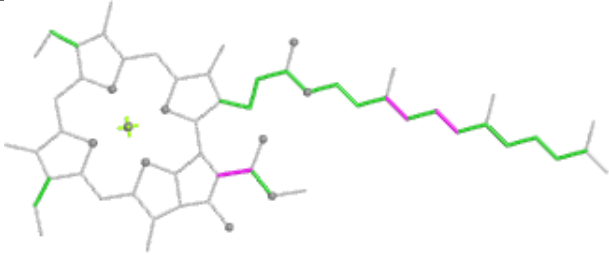
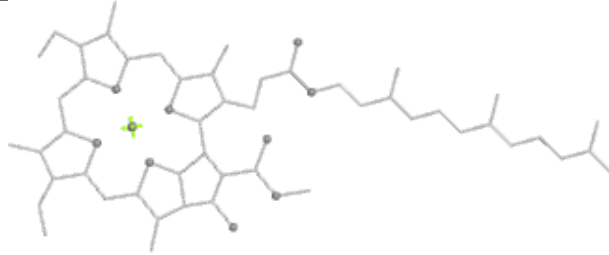
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

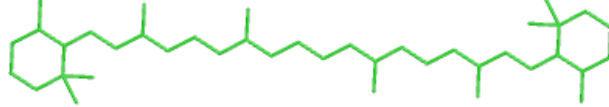
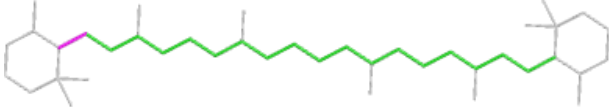
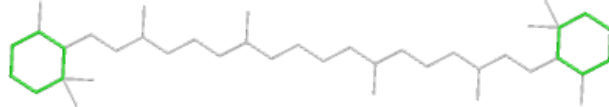
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

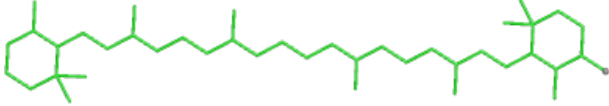
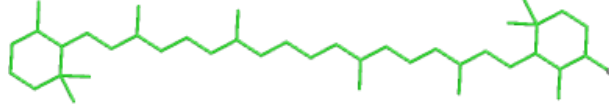
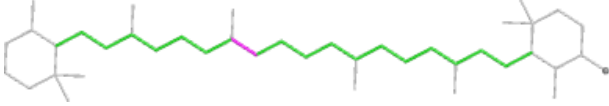
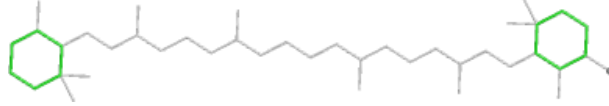


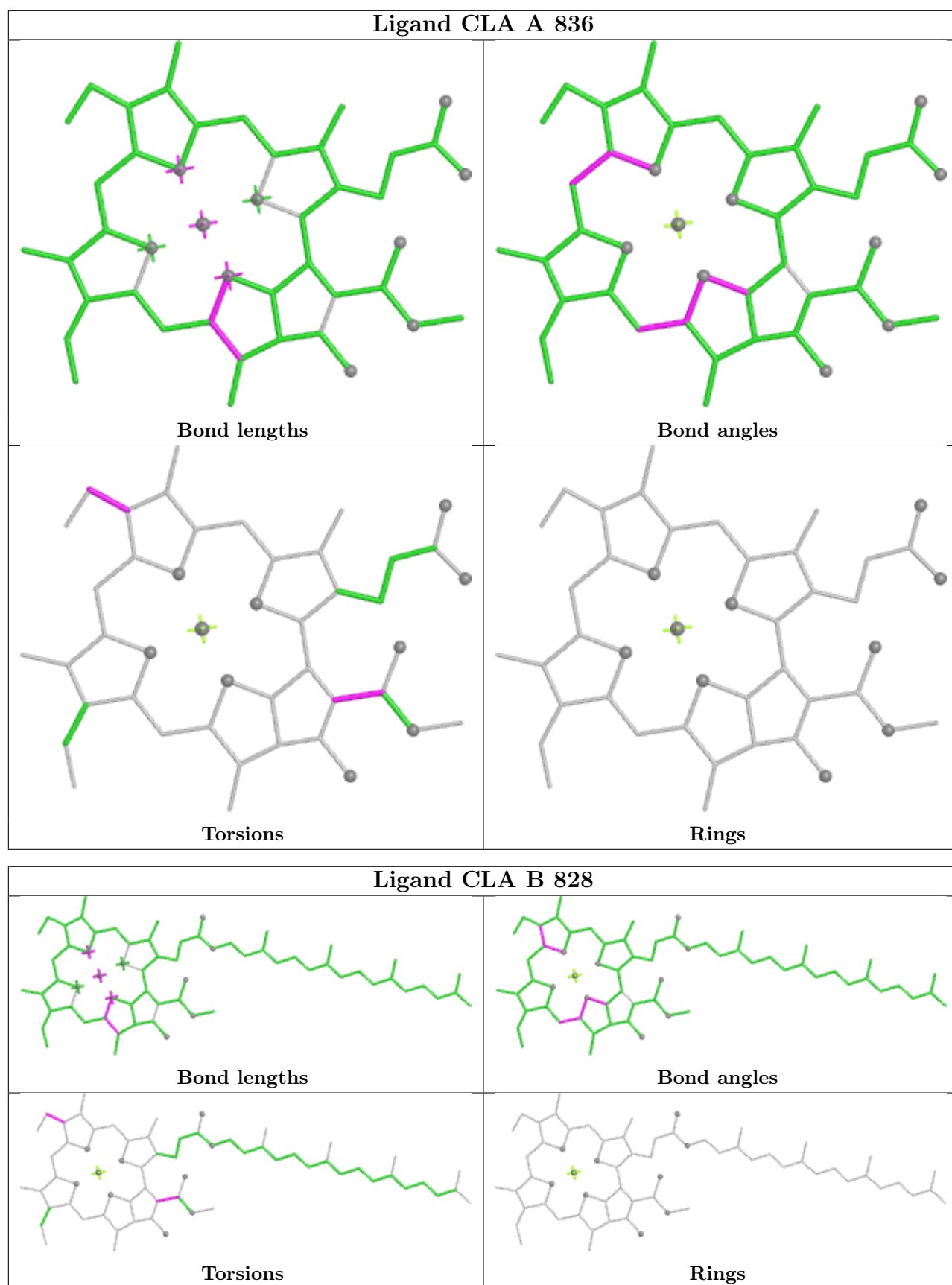


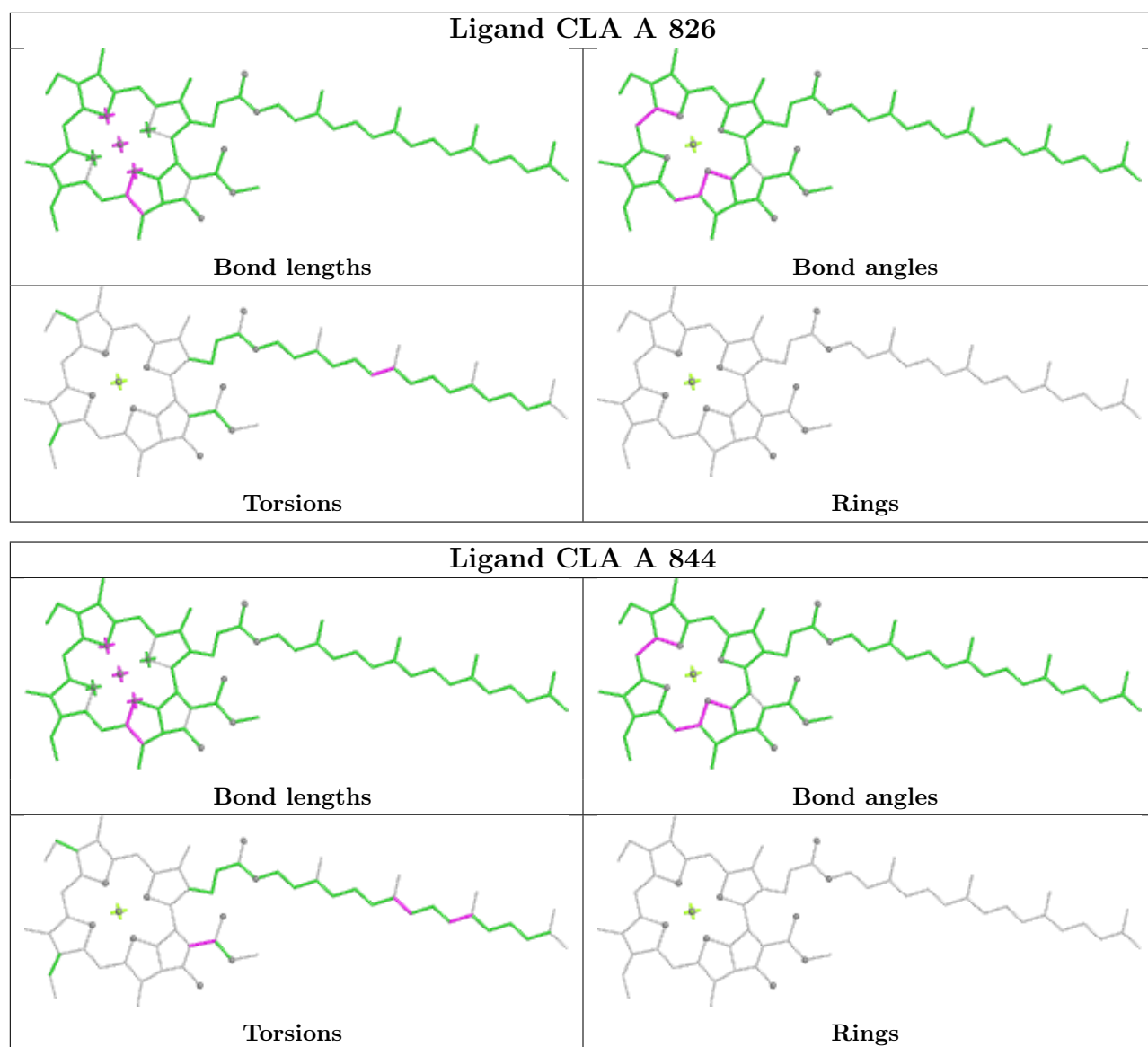


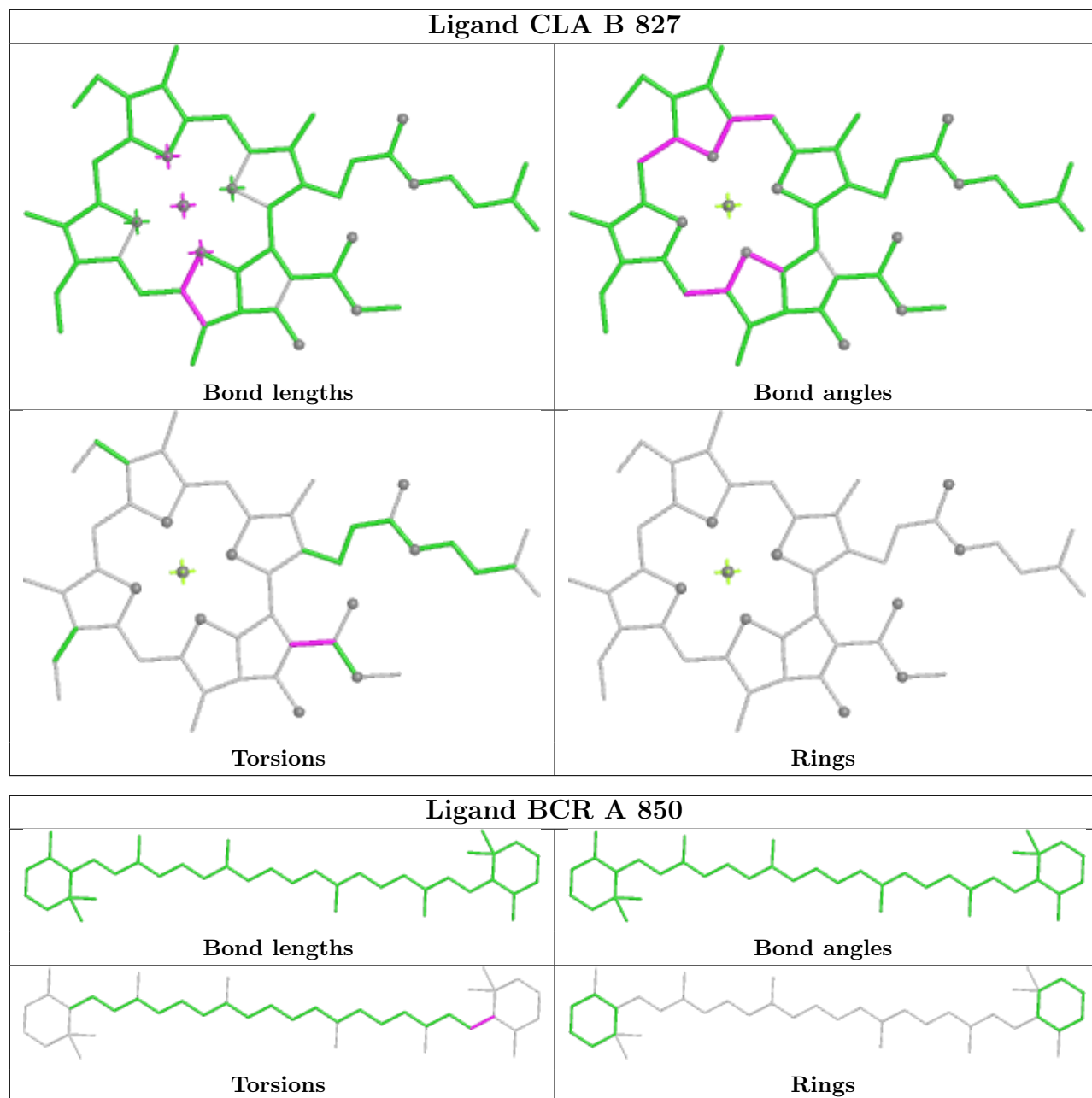
| Ligand CLA B 831                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

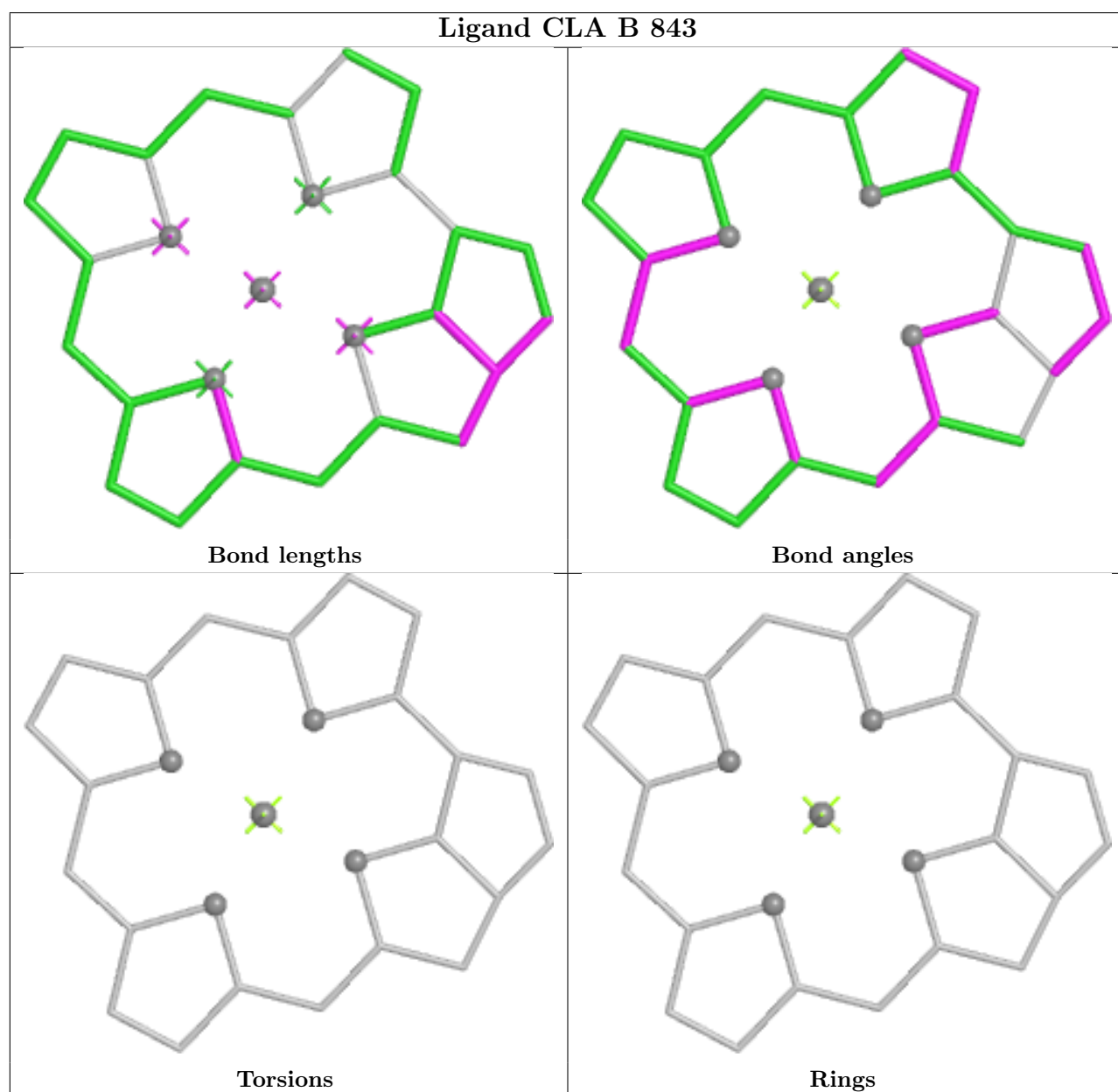
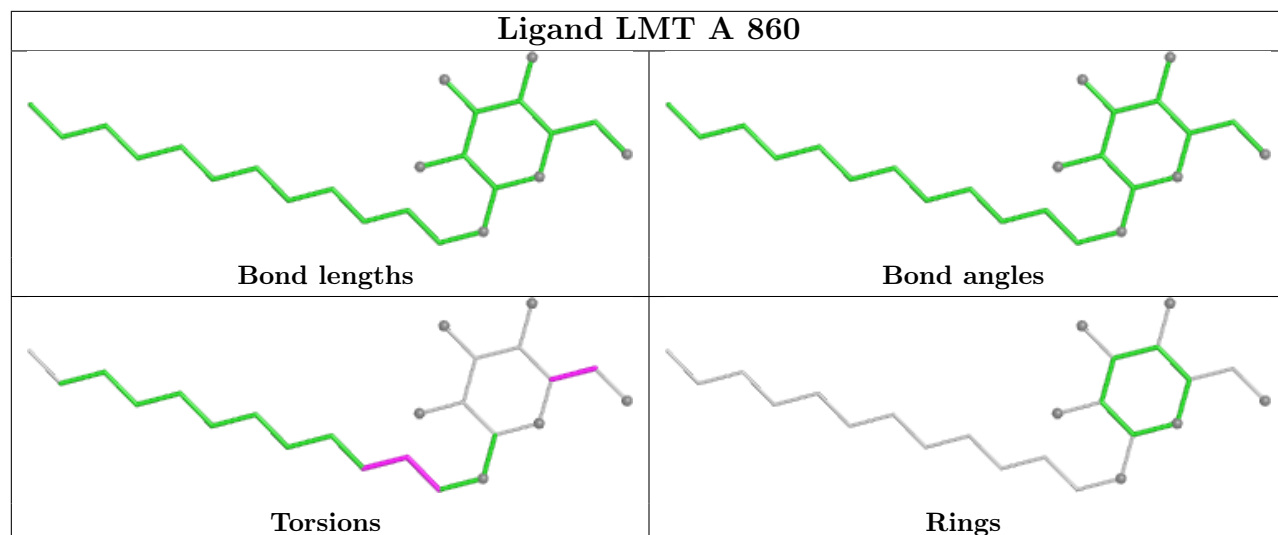
| Ligand BCR A 847                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

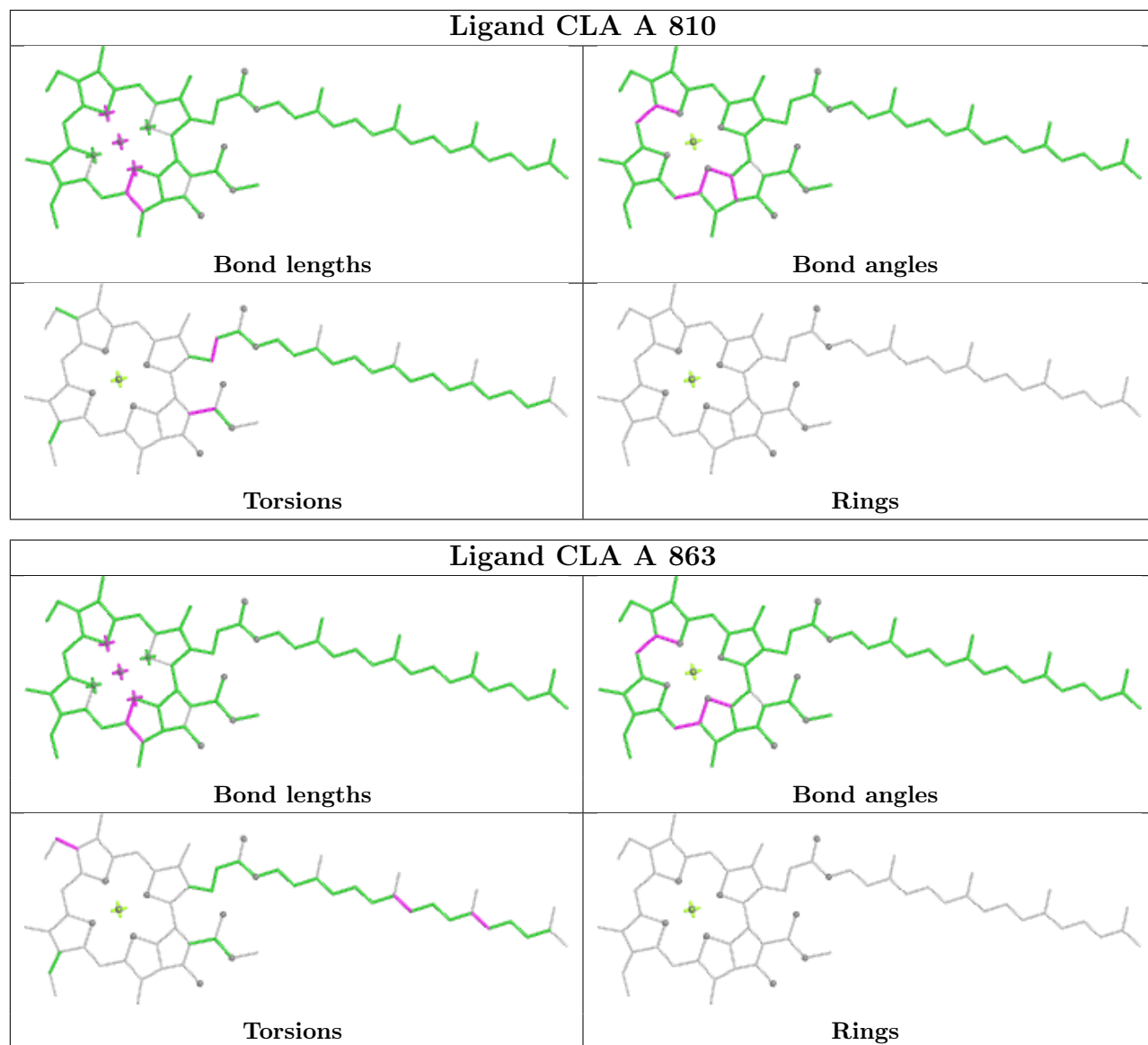
| Ligand ECH F 205                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

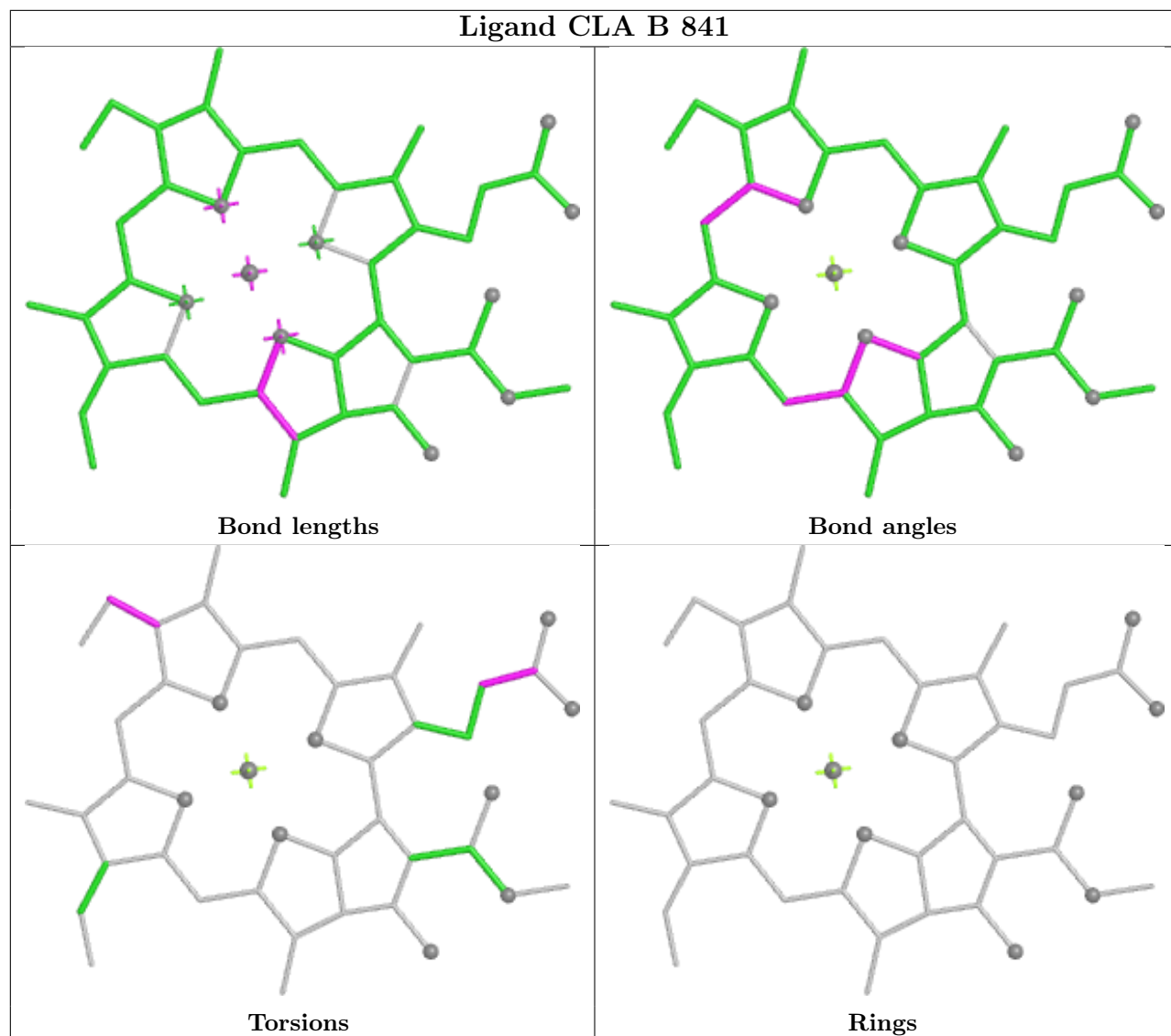


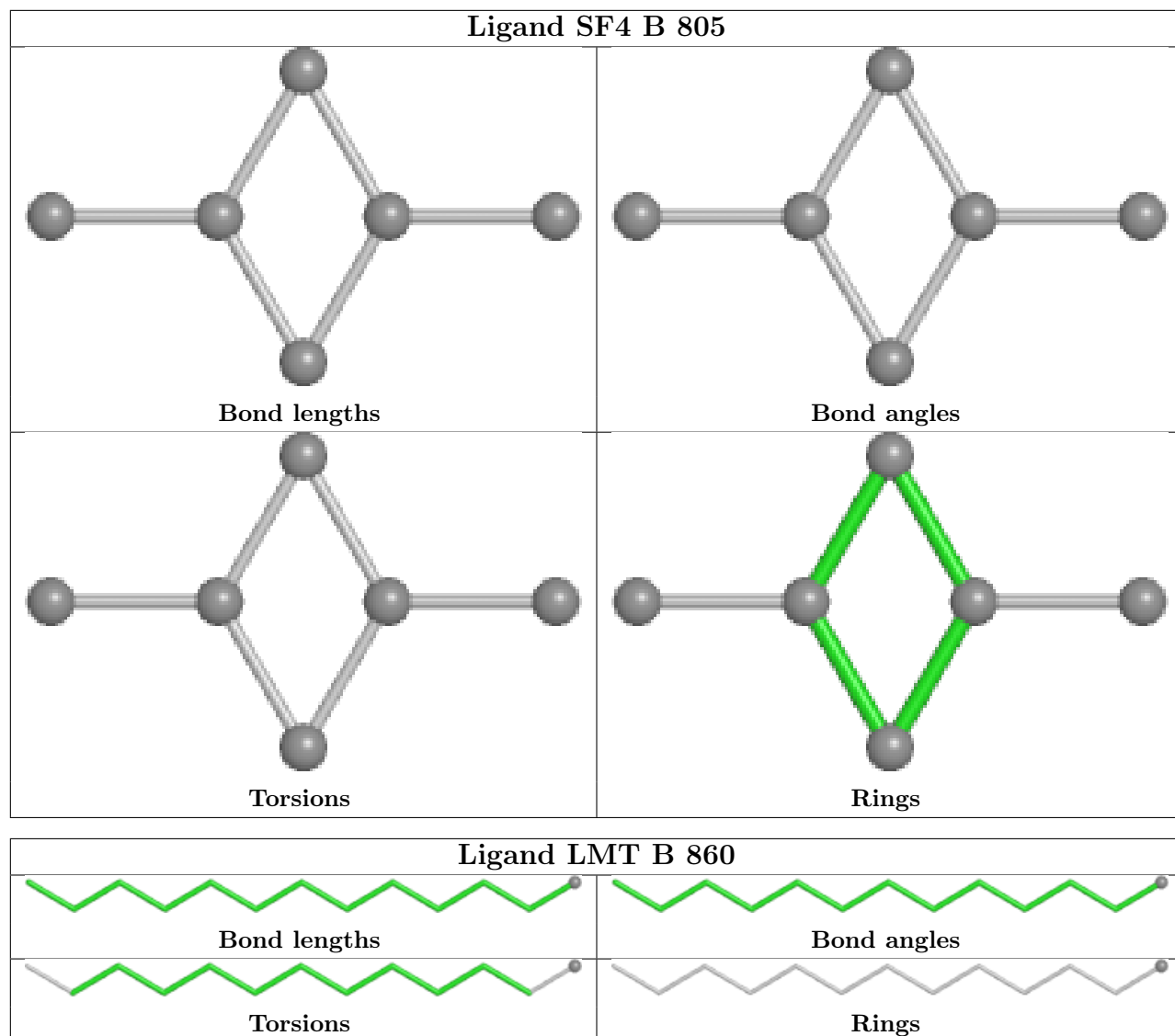


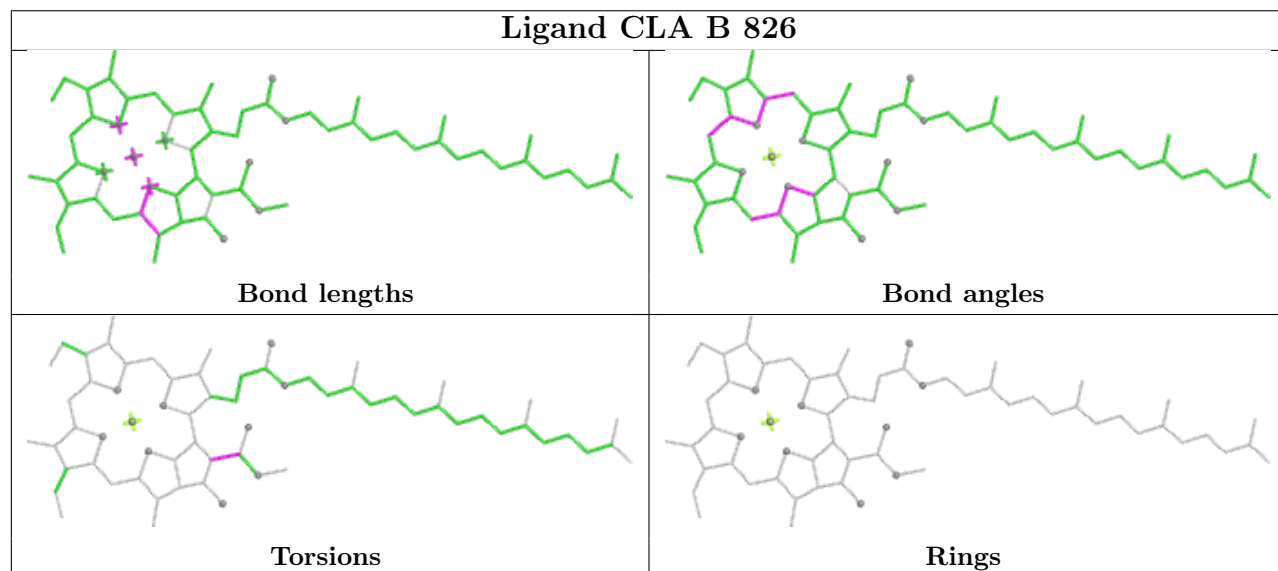
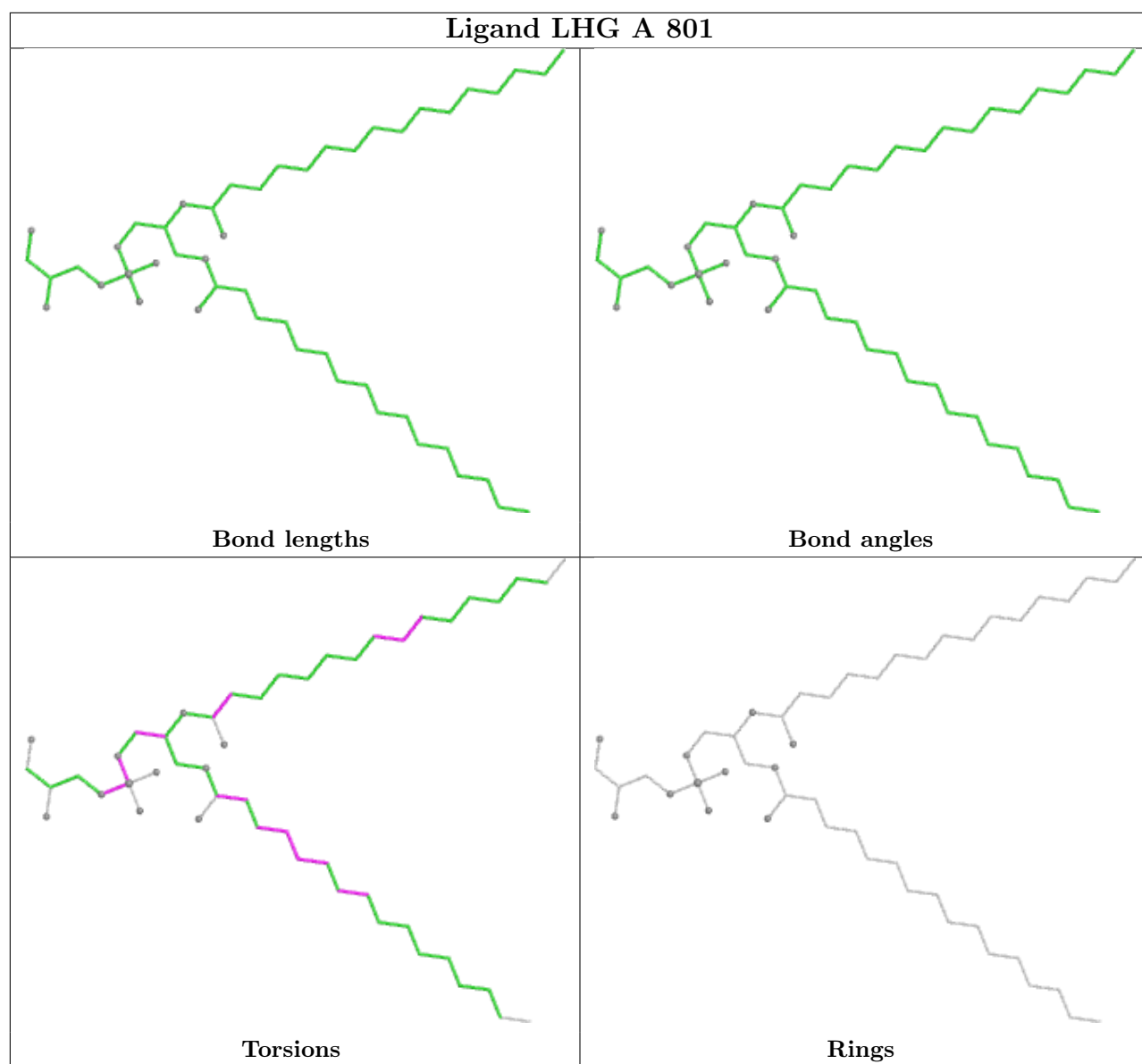


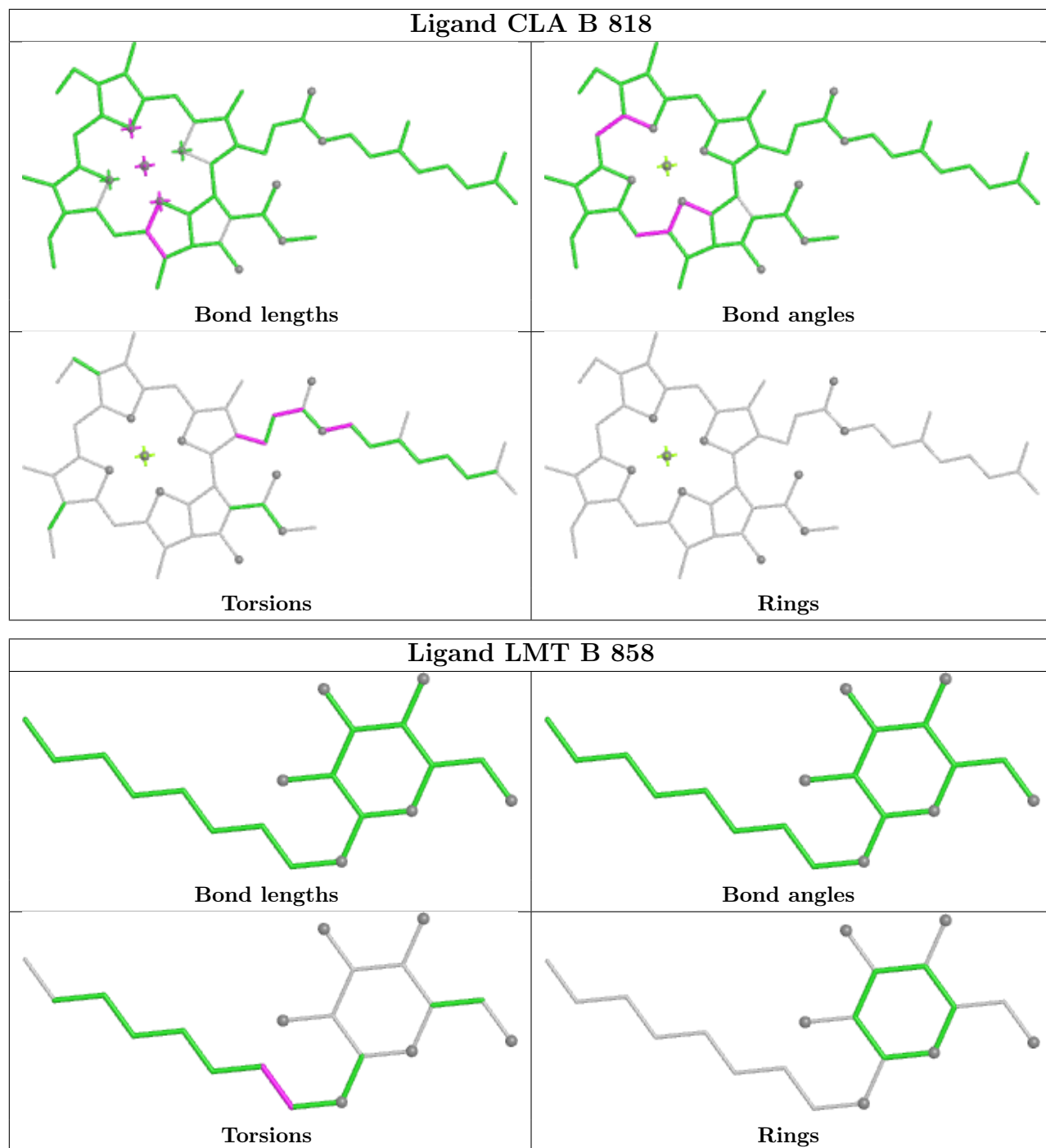


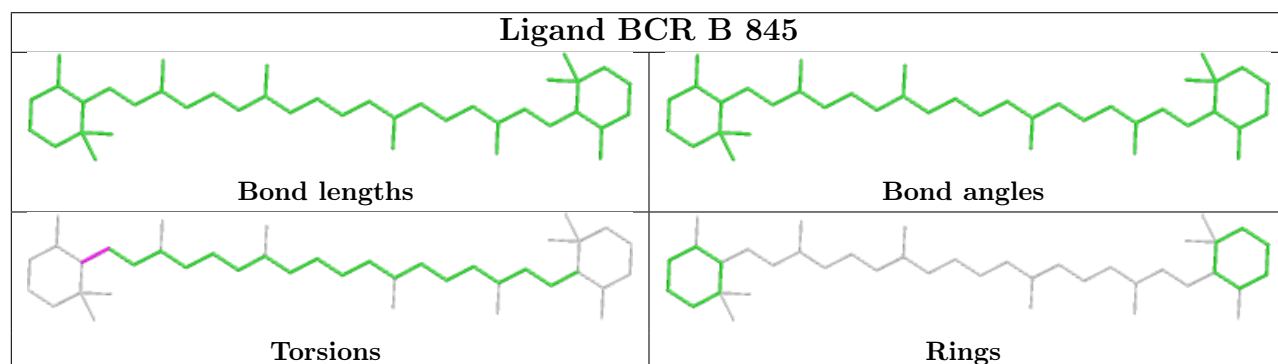
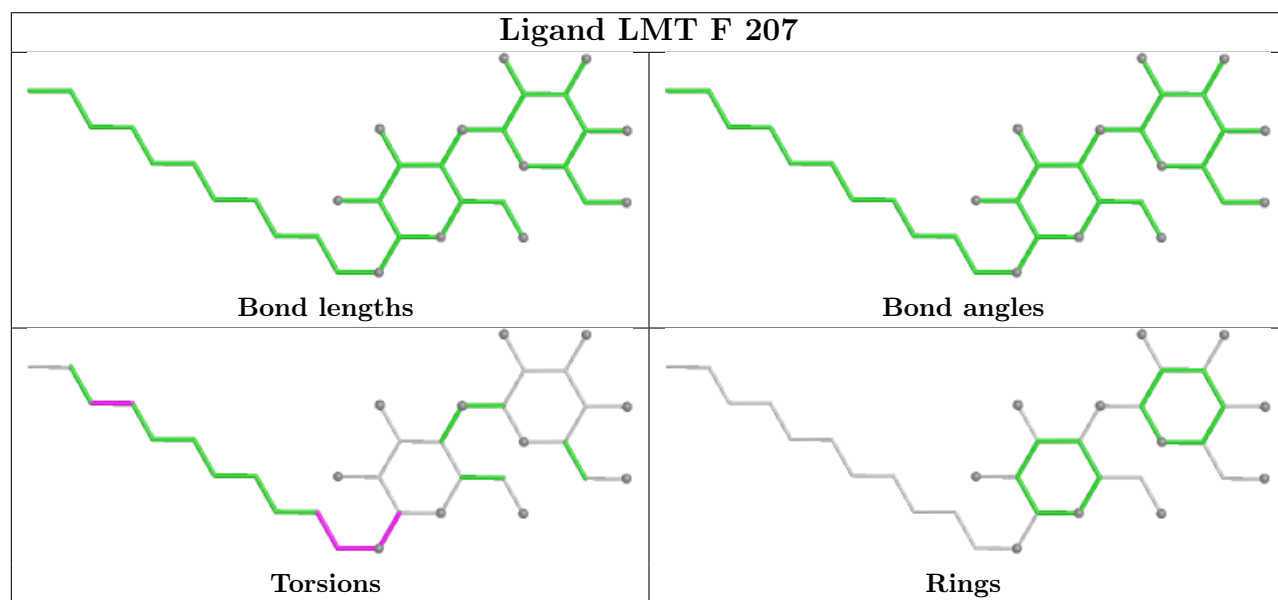
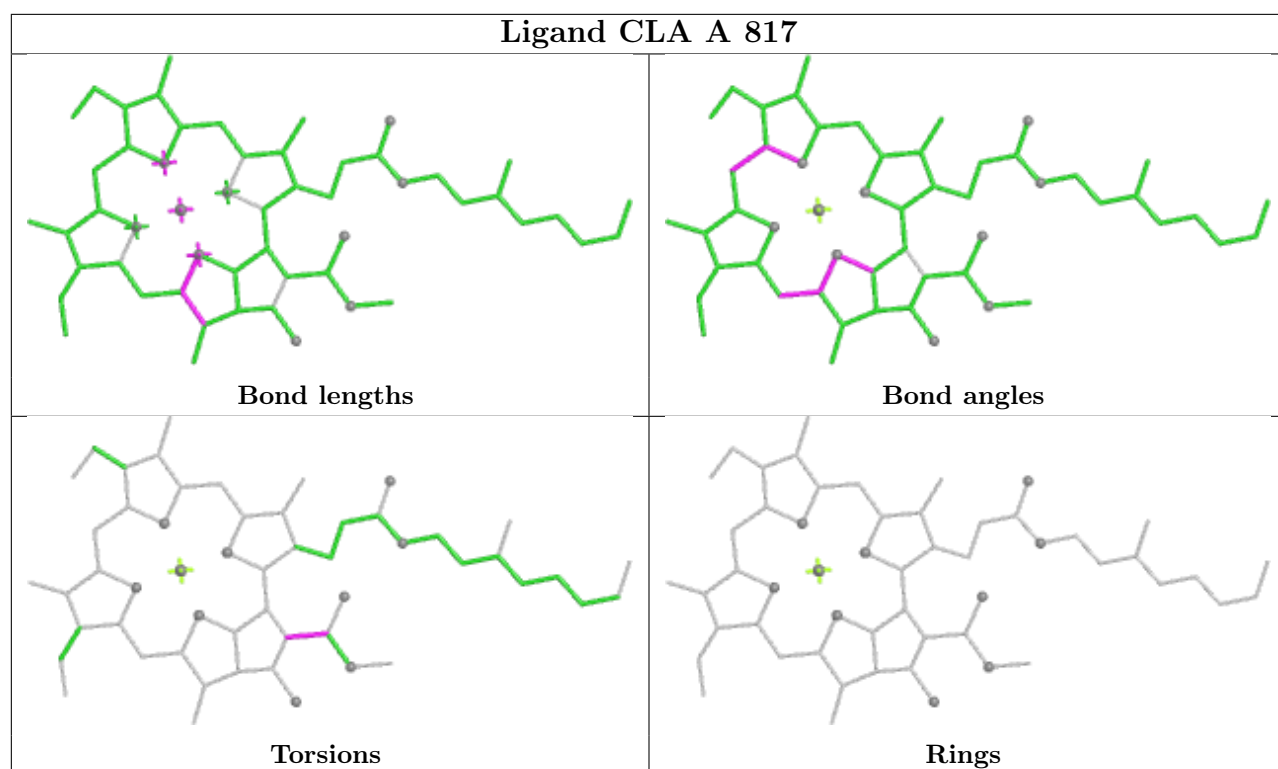


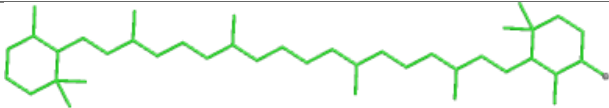
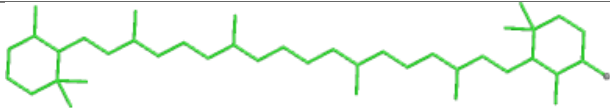
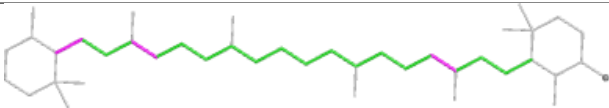
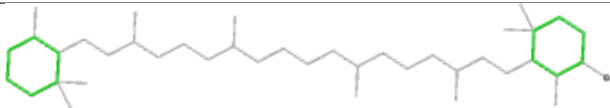




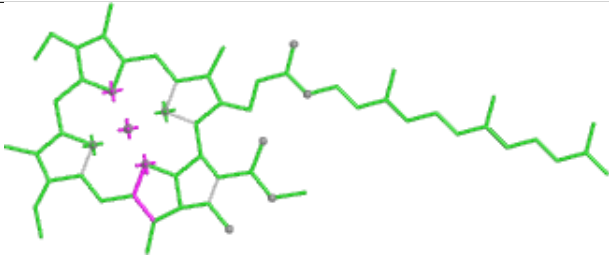
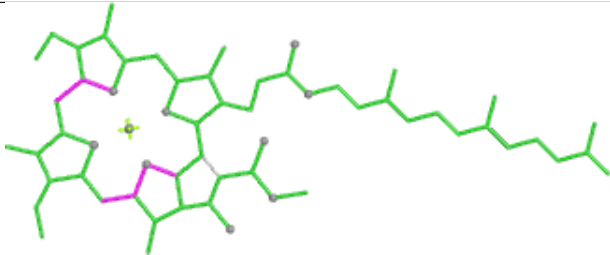
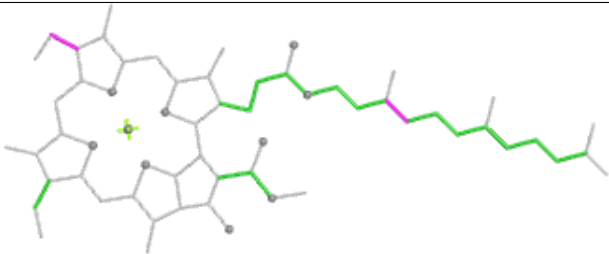
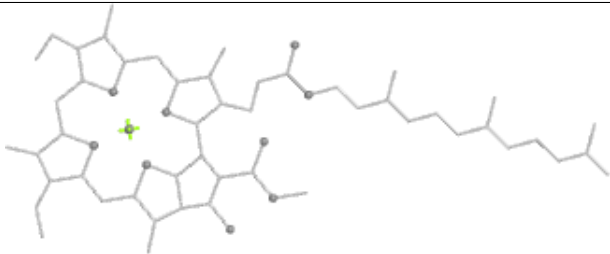


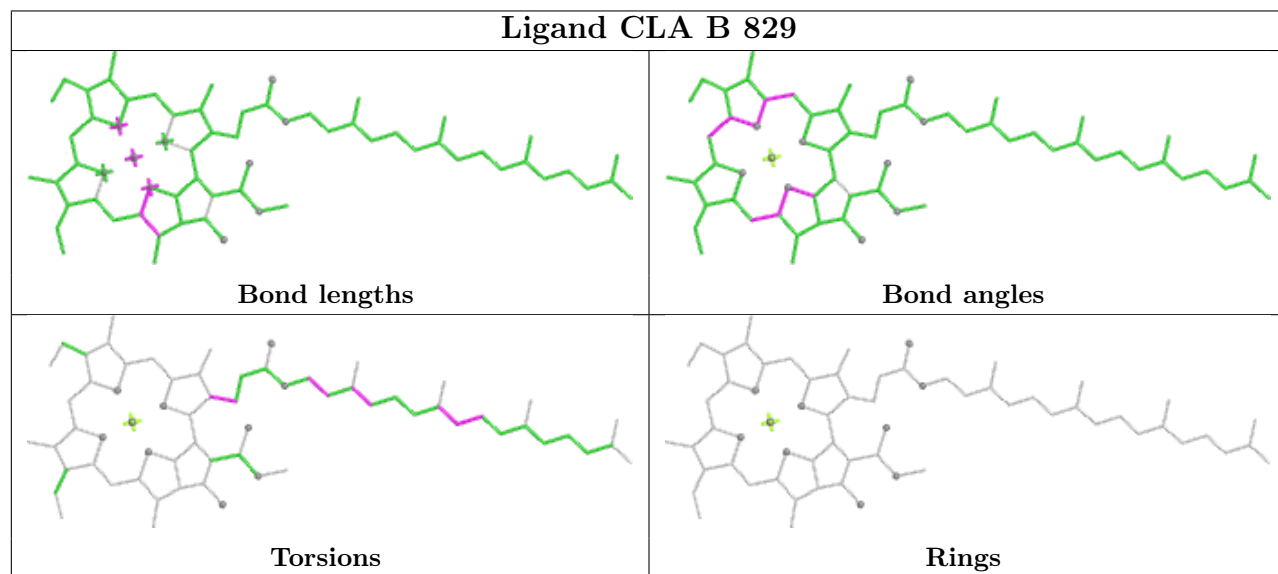
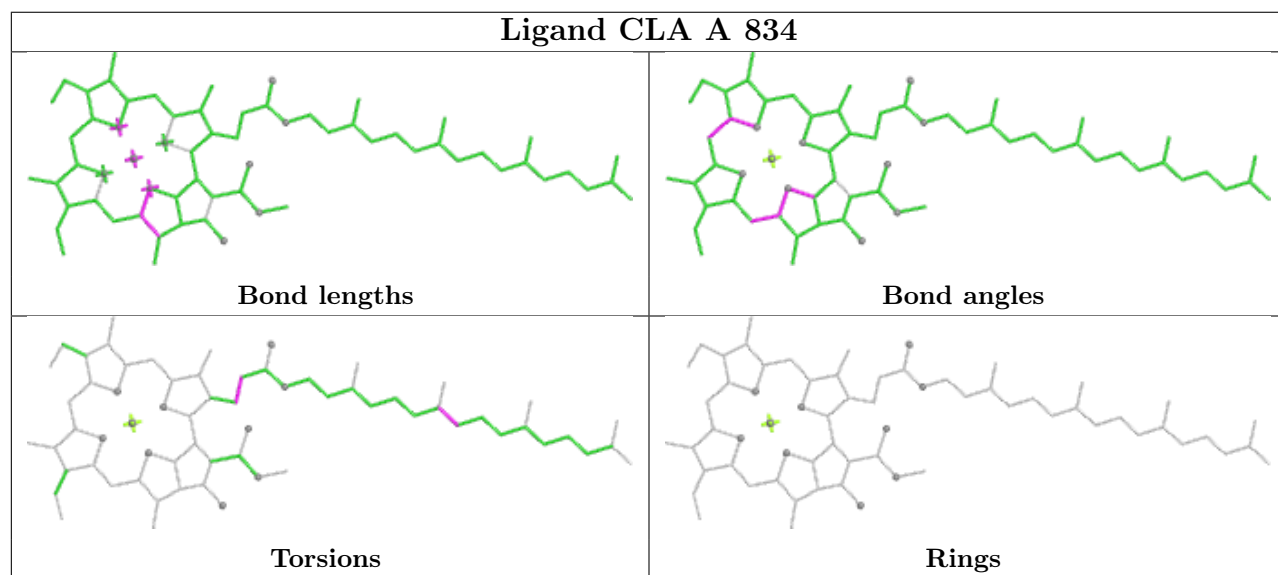
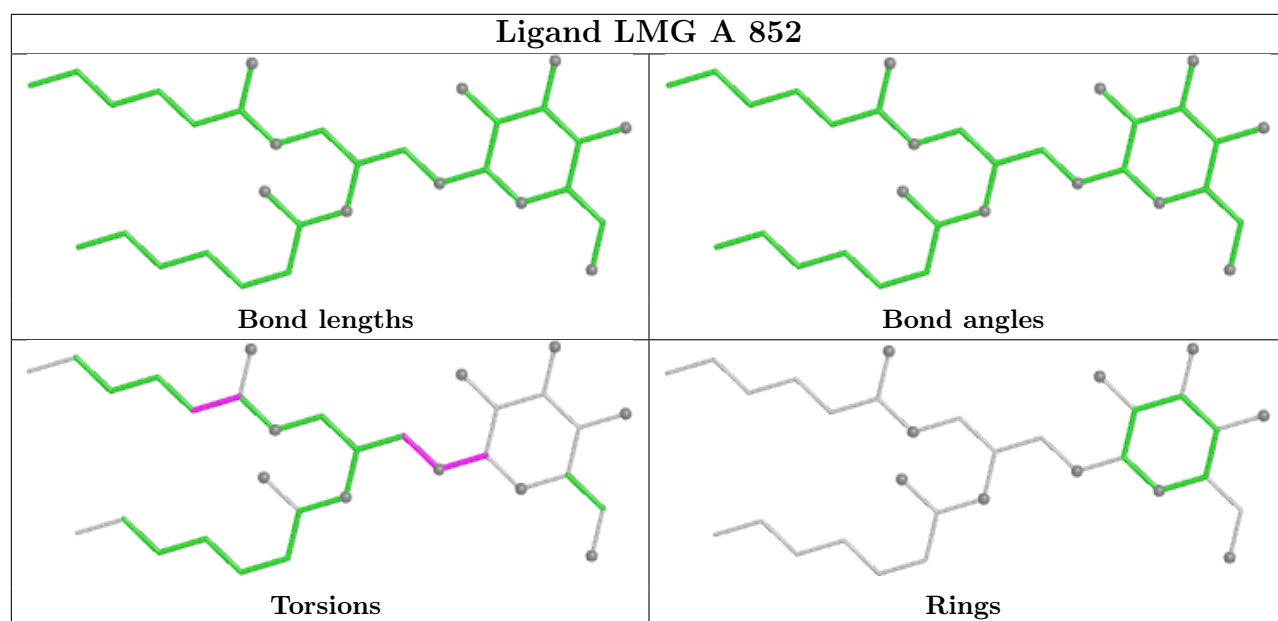


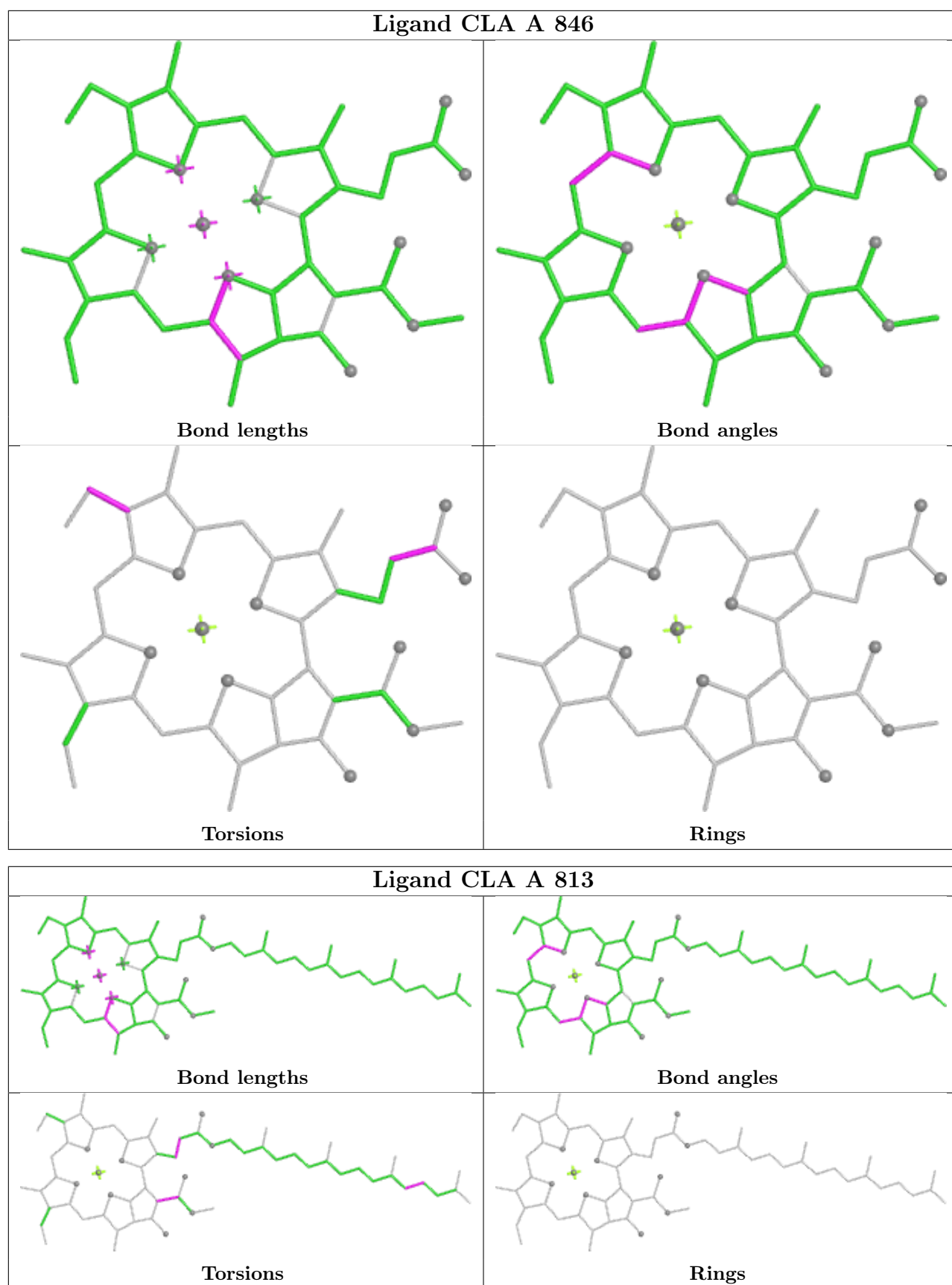


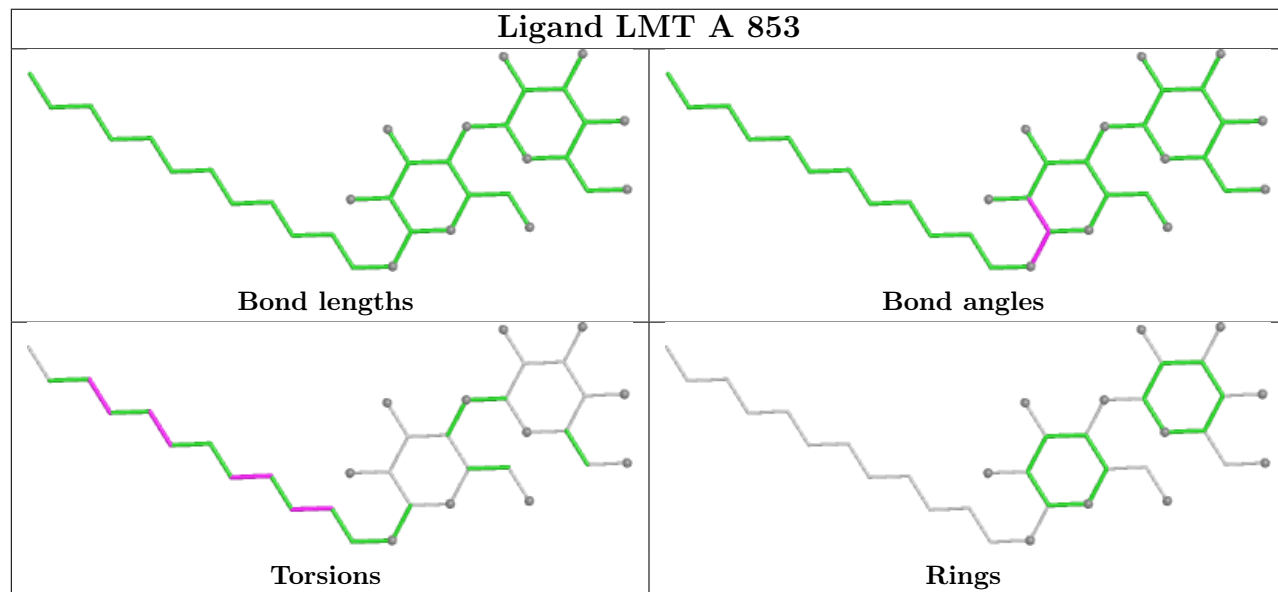
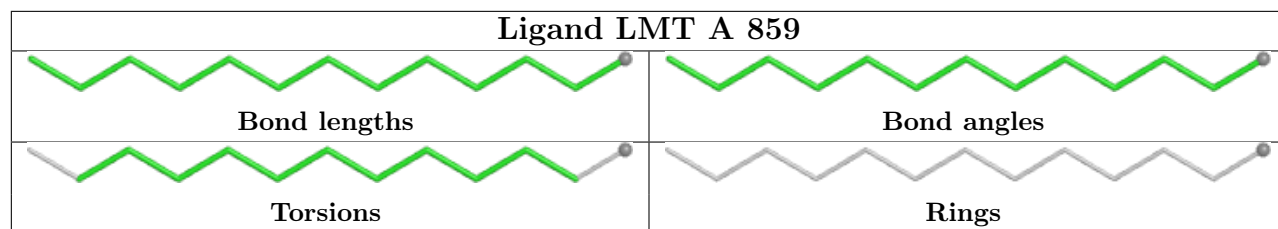
| Ligand ECH B 846                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

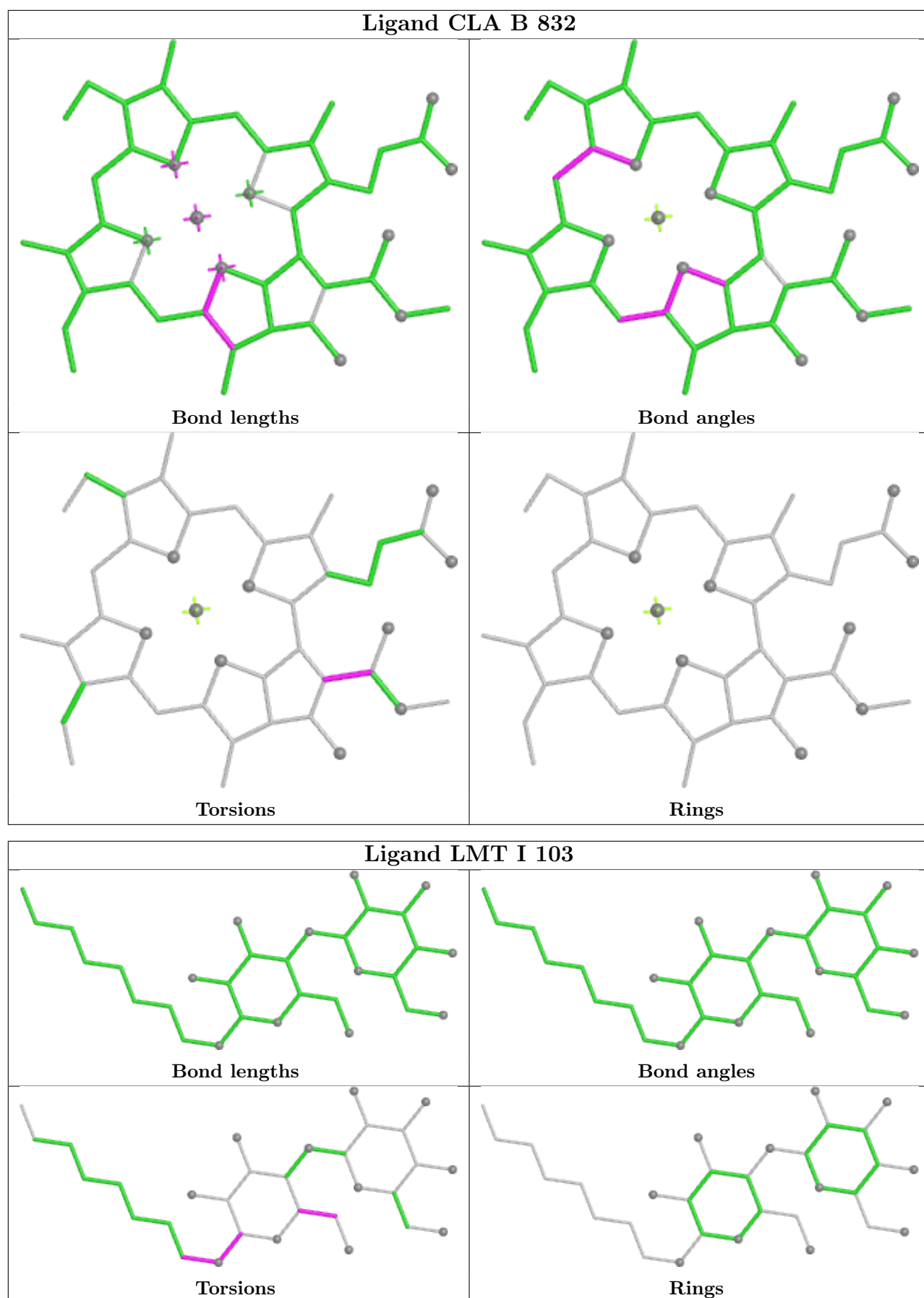
| Ligand LMT B 859                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

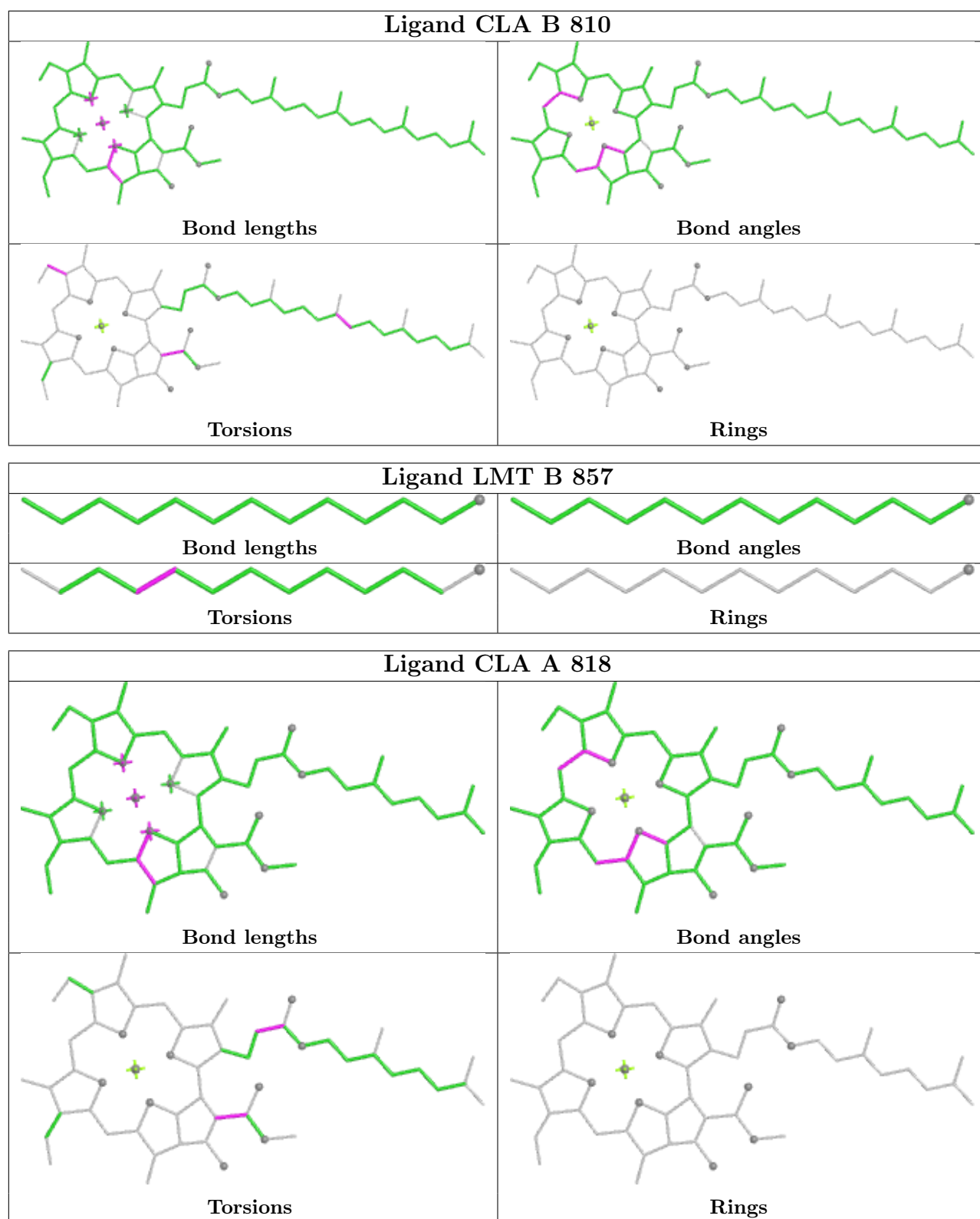
| Ligand CLA B 809                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

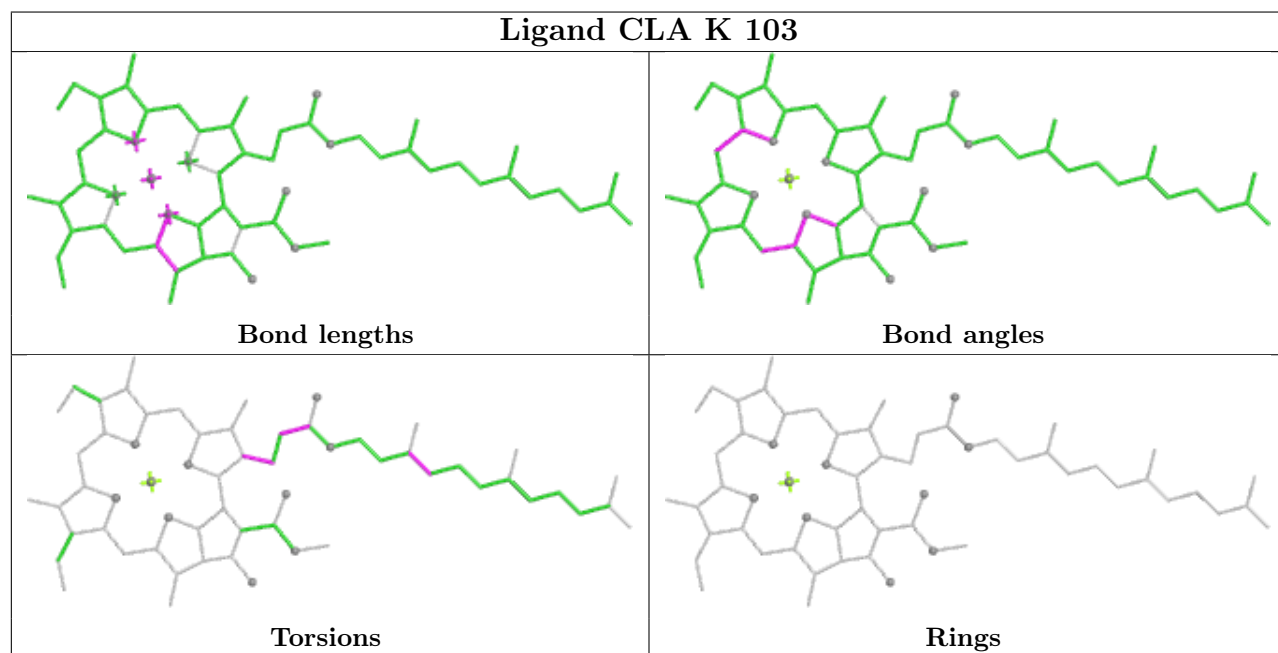
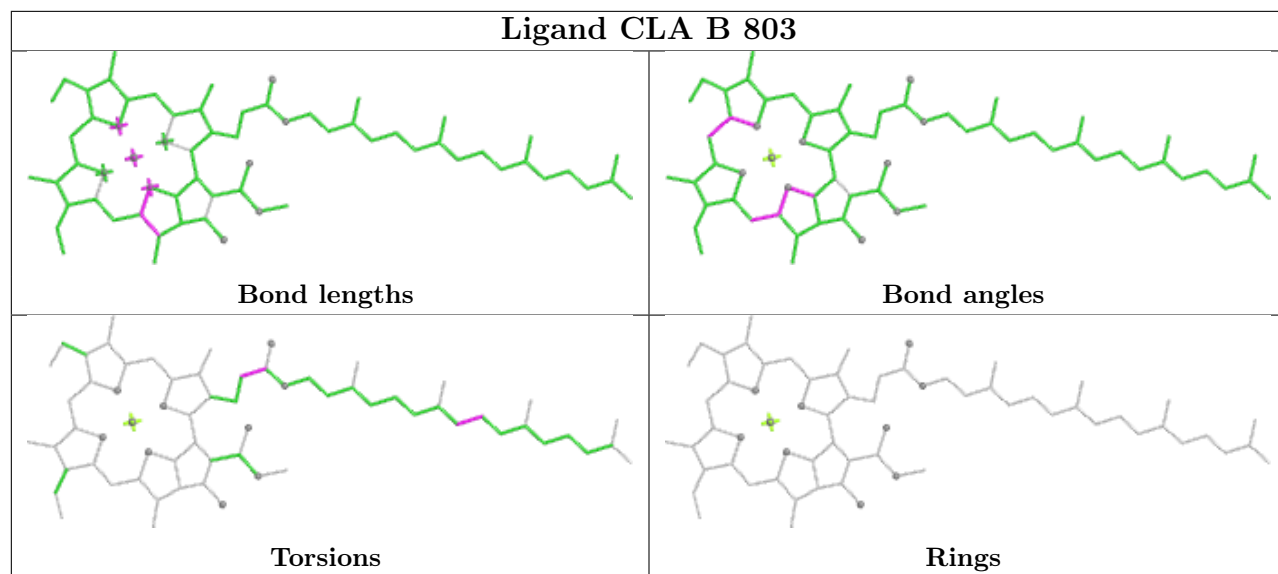


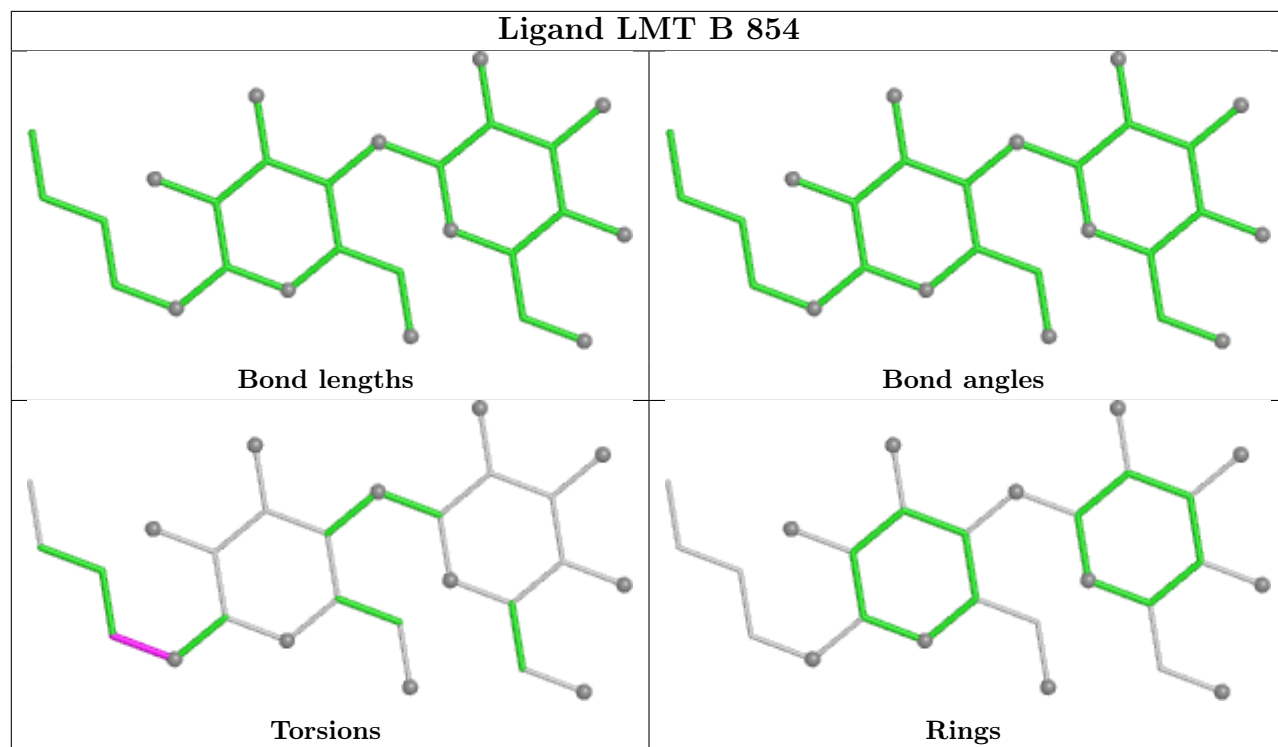


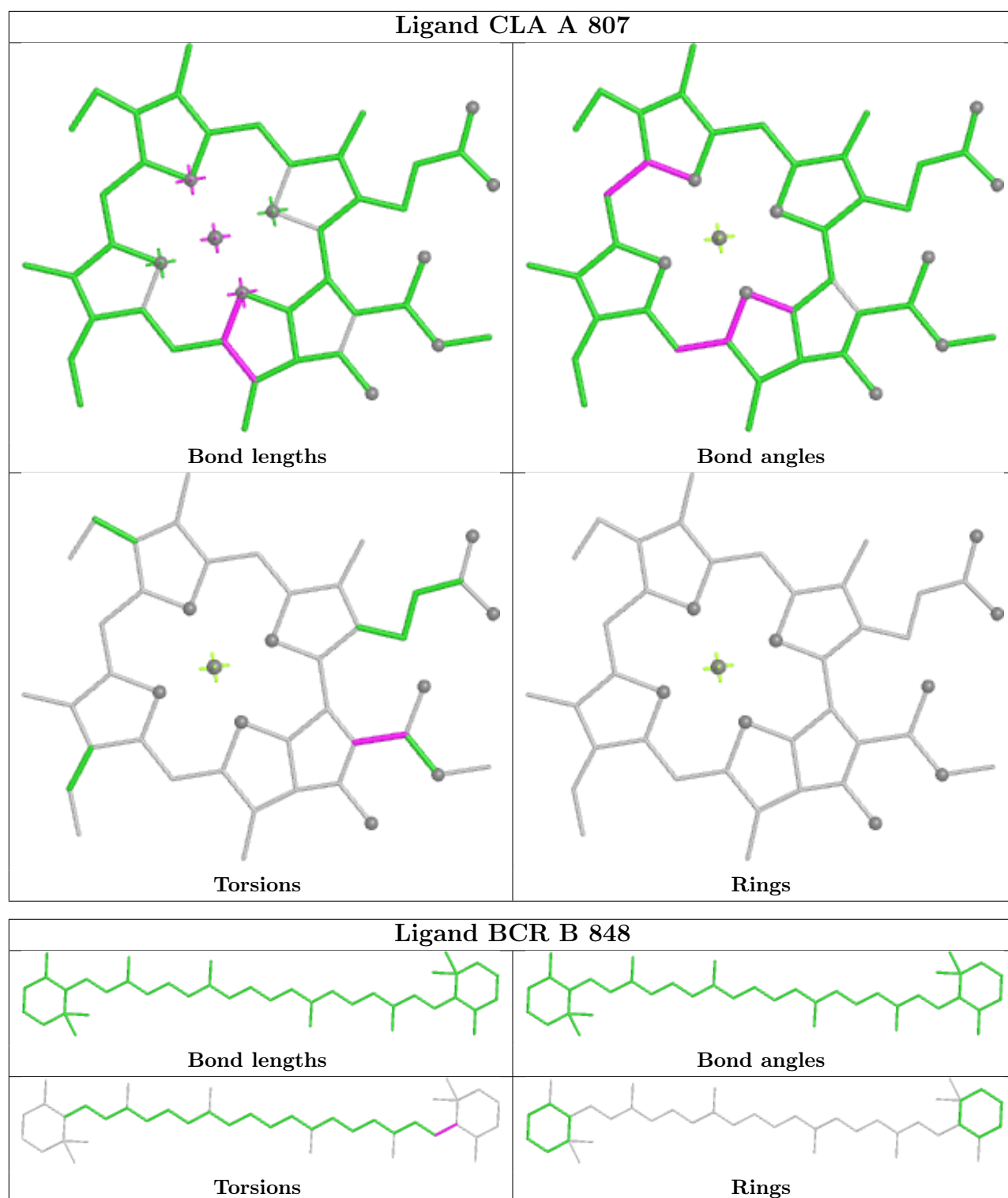




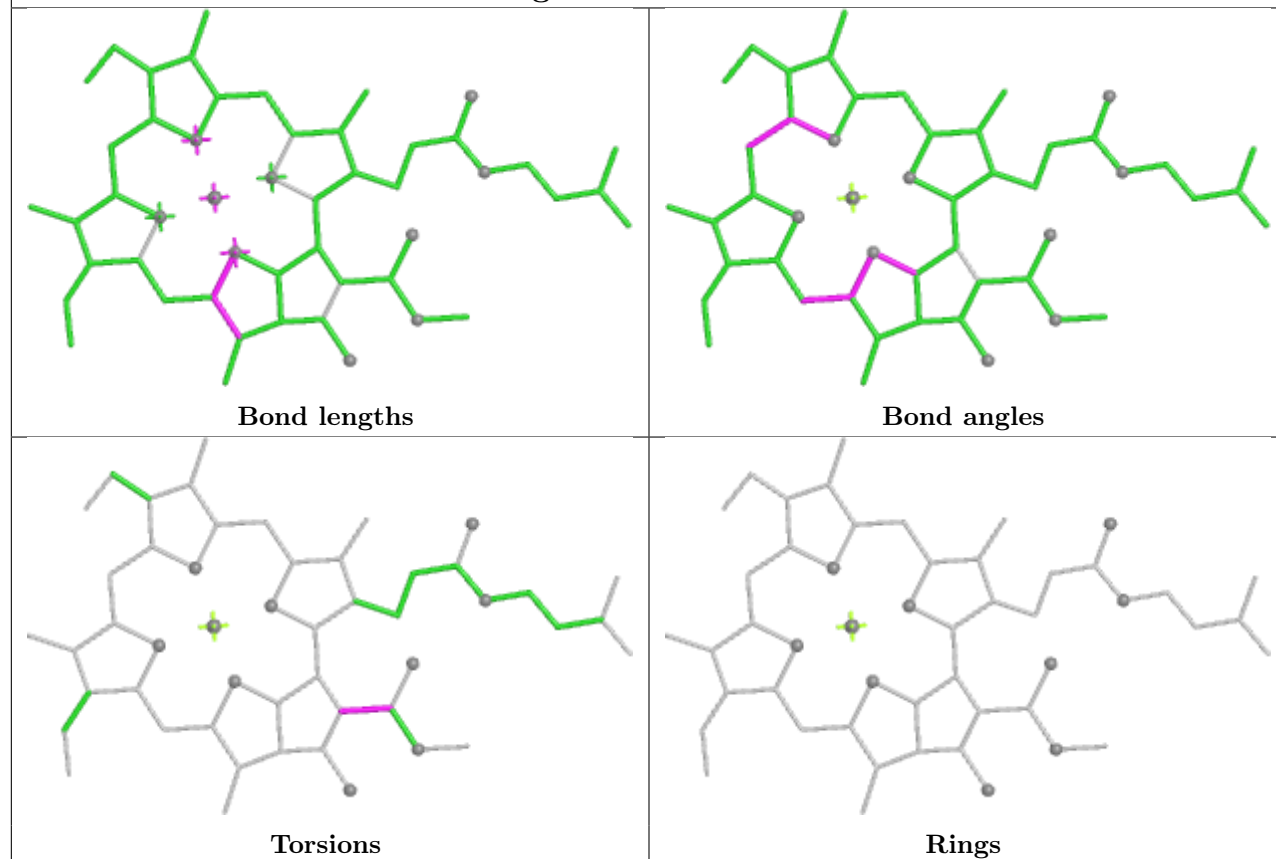




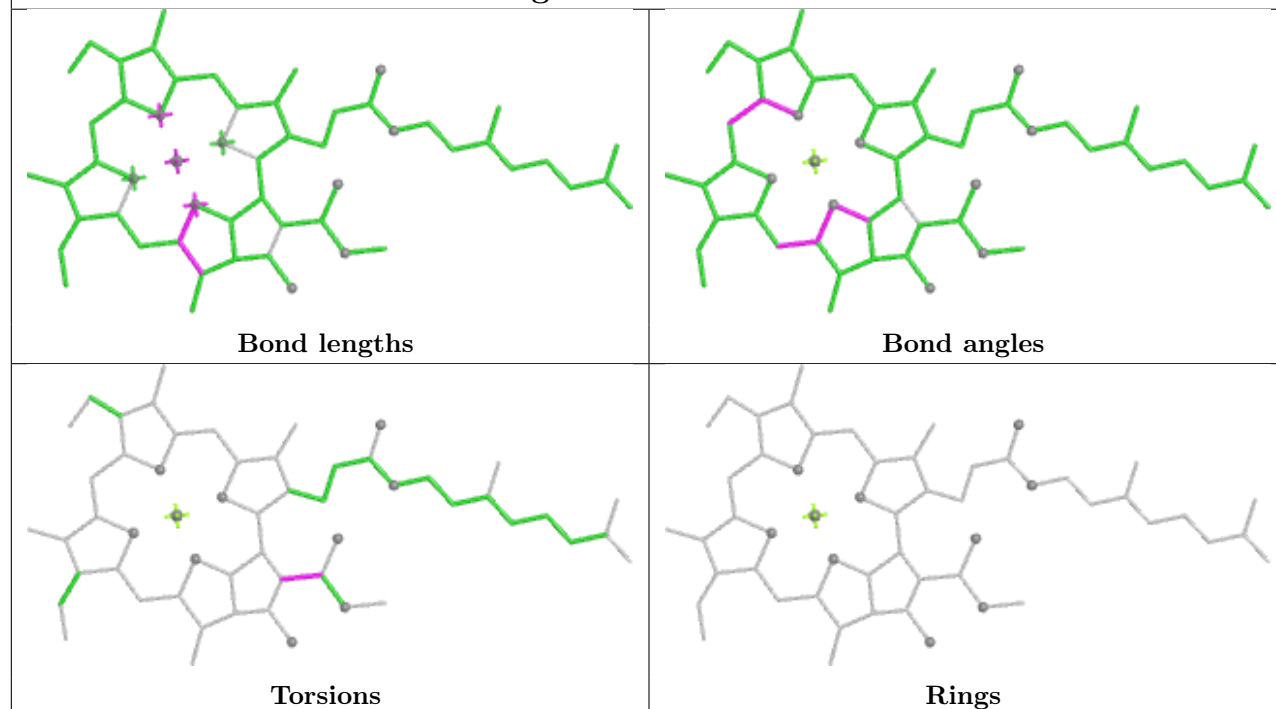


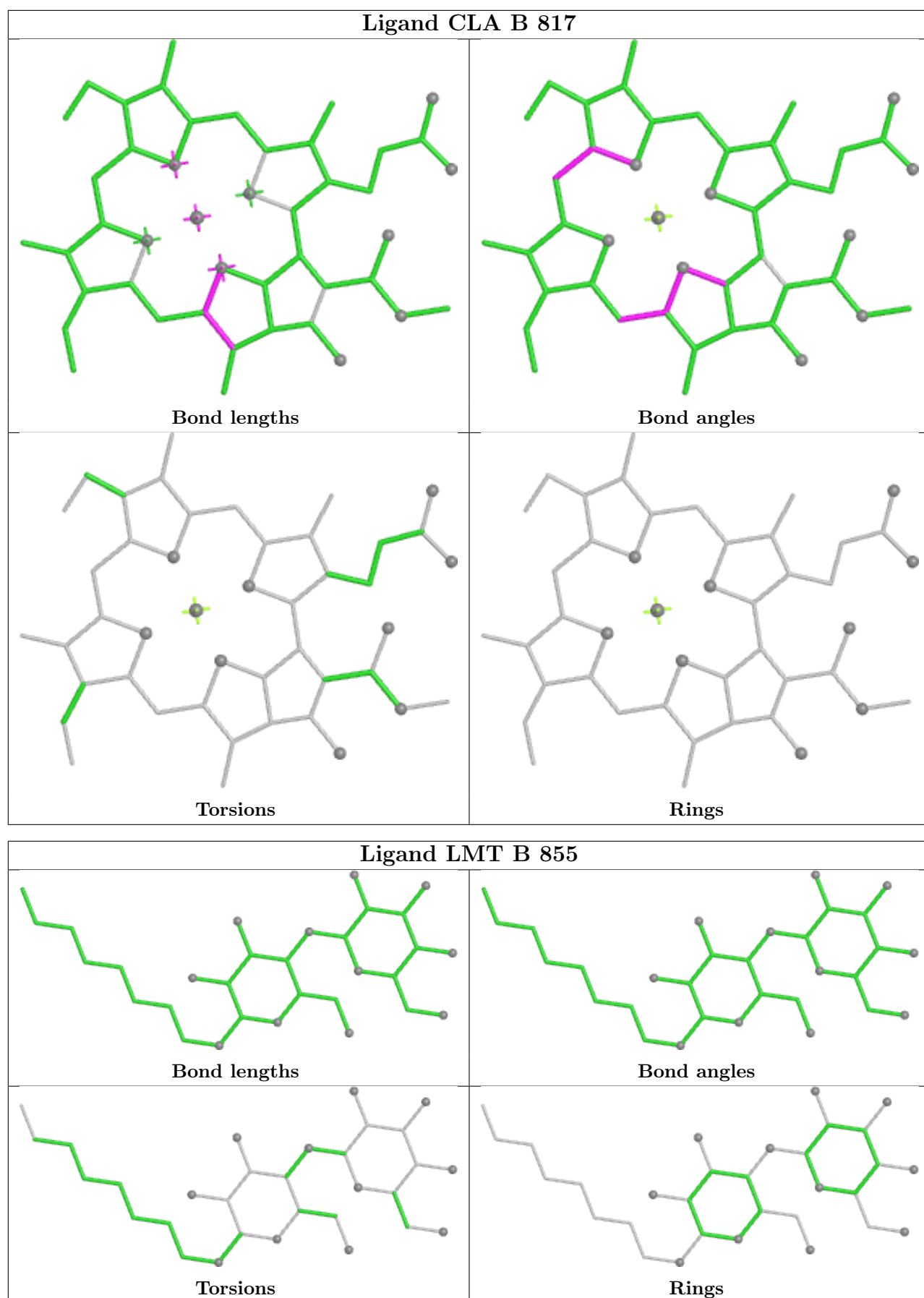


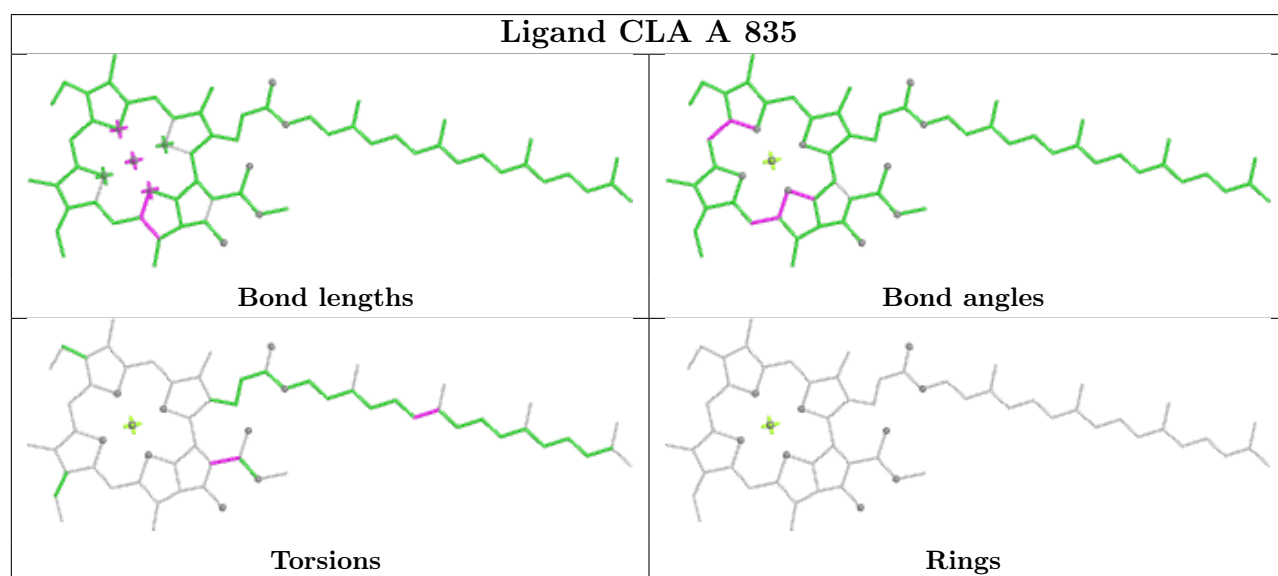
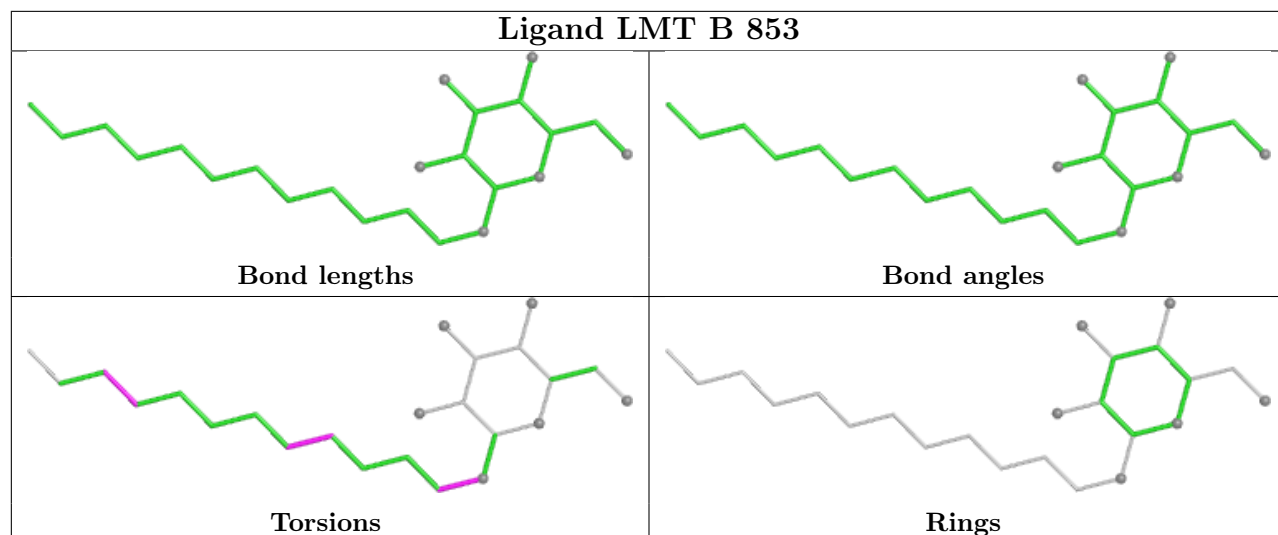
## Ligand CLA B 838

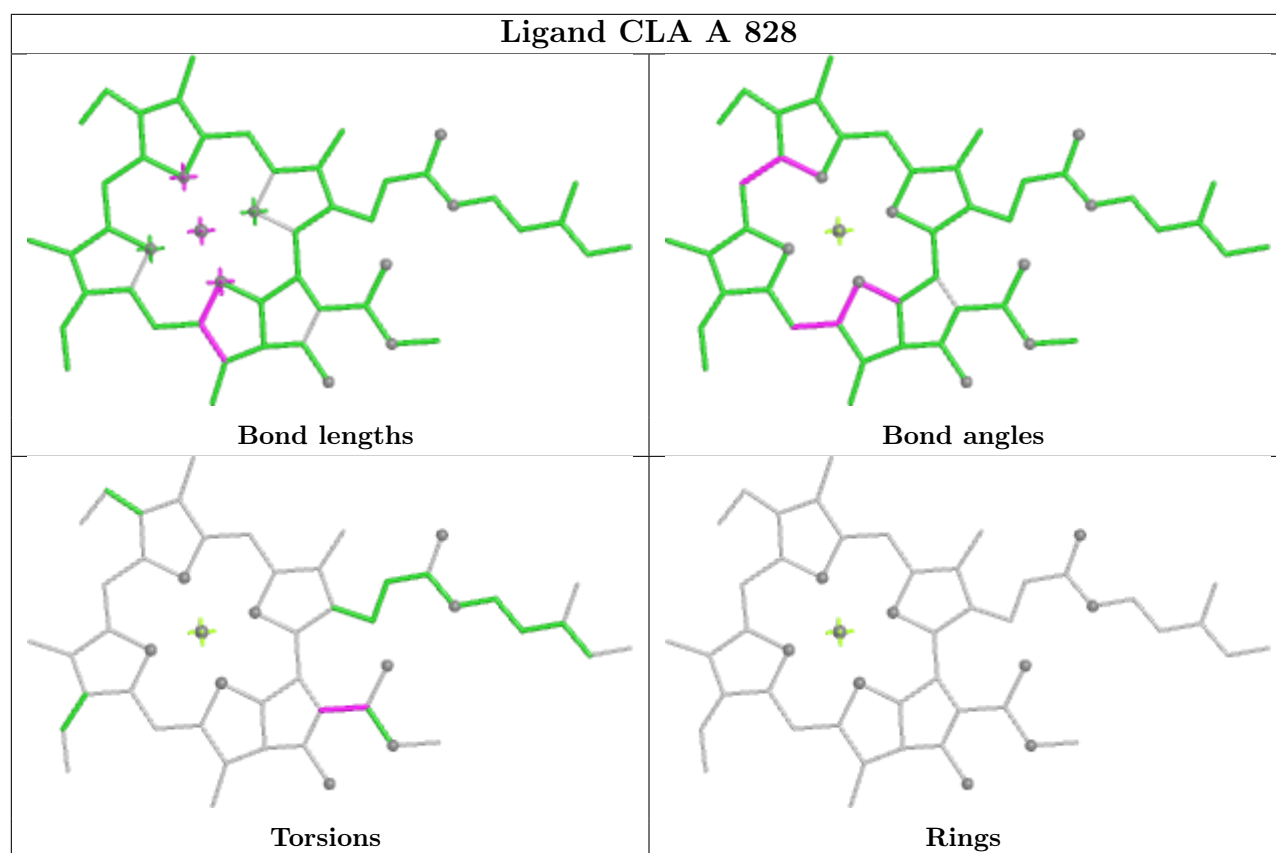


## Ligand CLA A 831

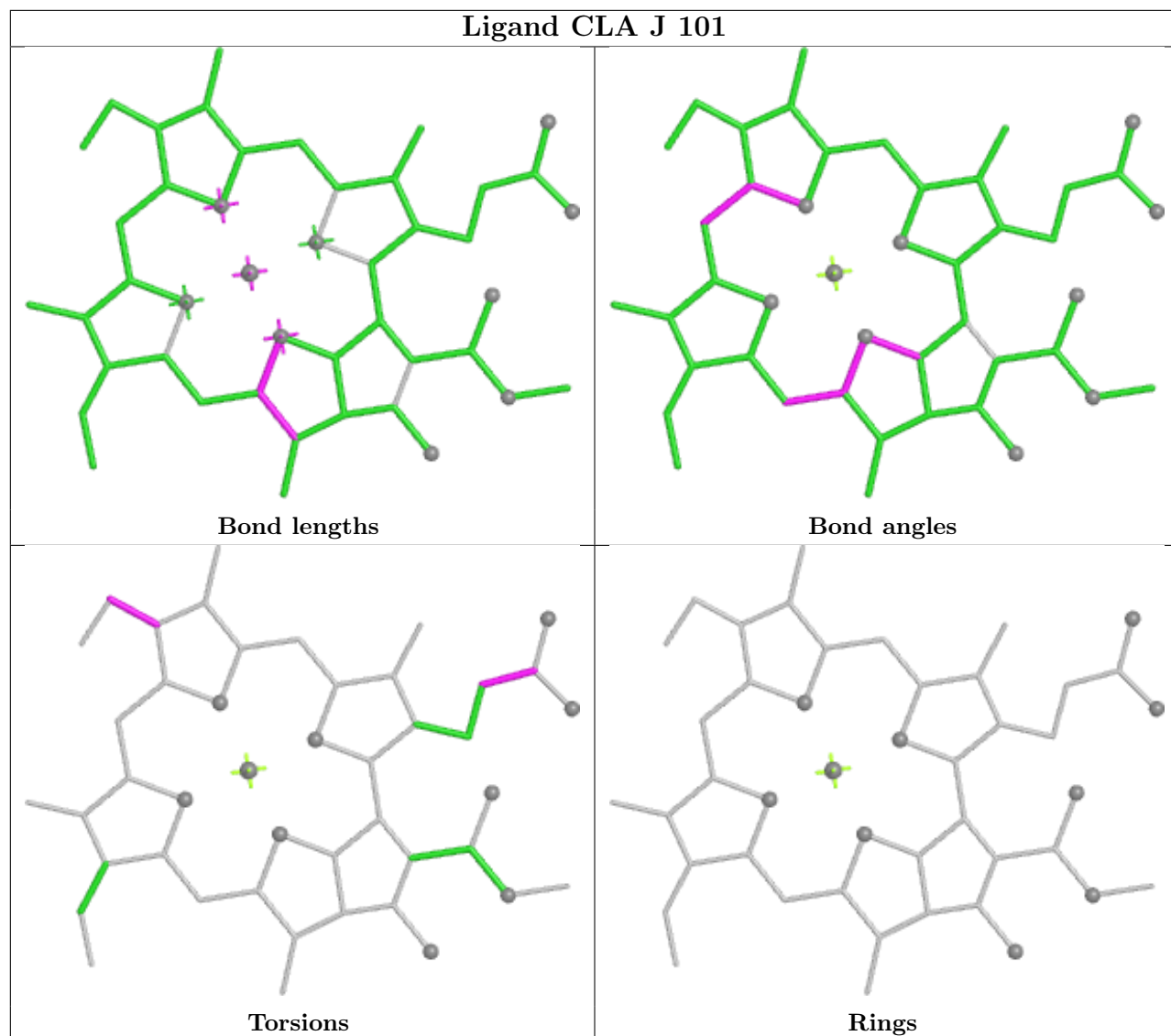


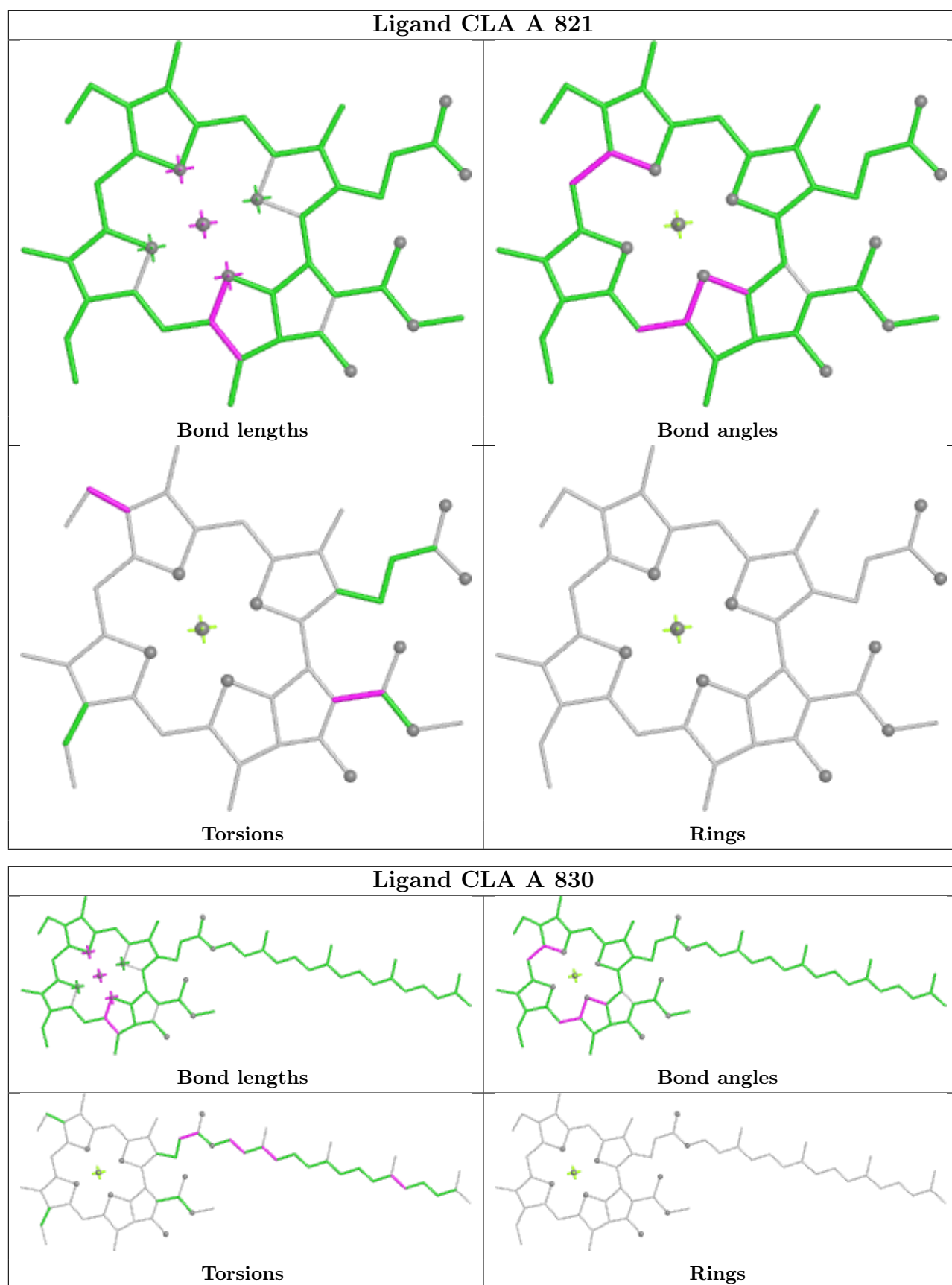




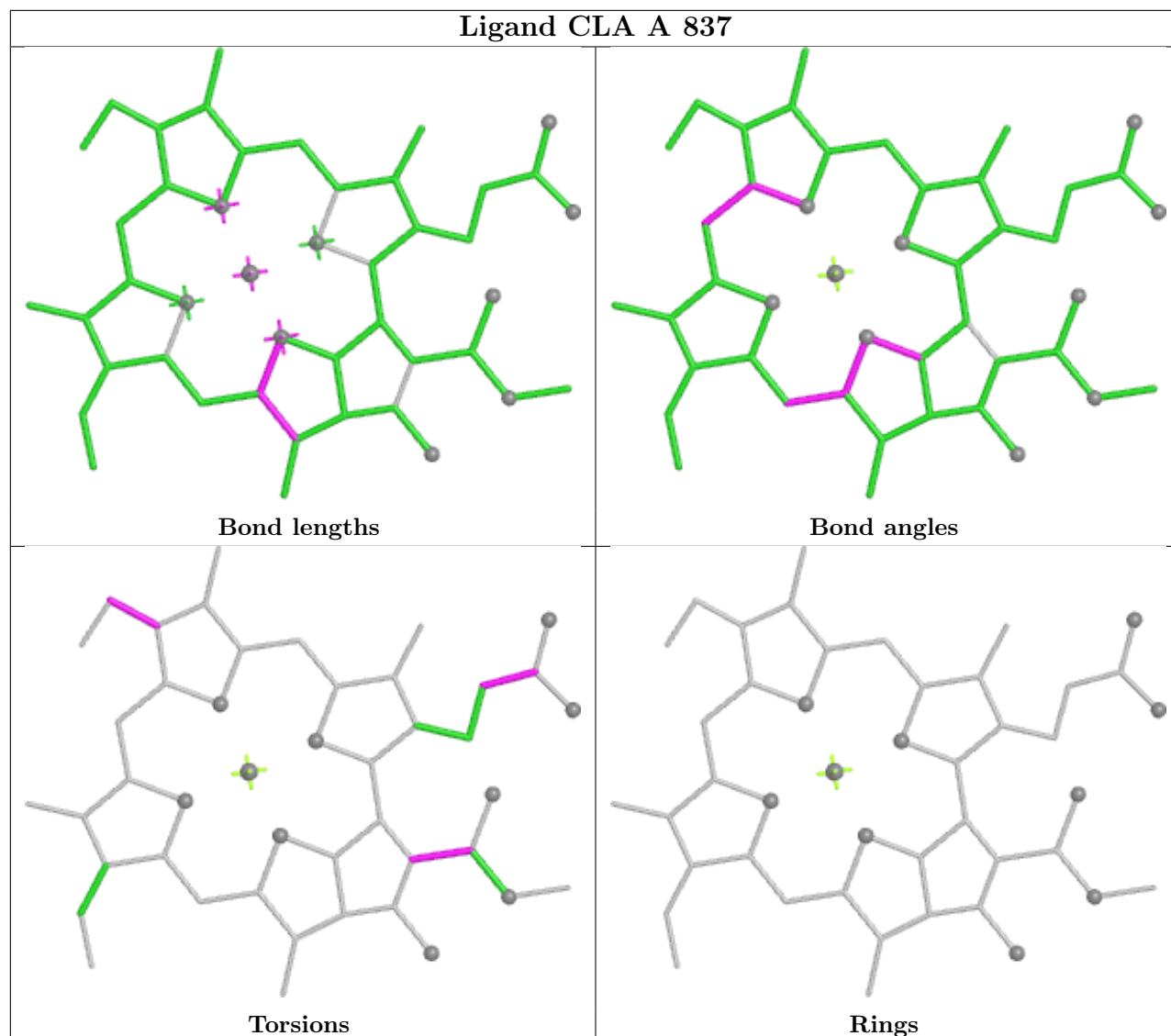


## Ligand CLA J 101

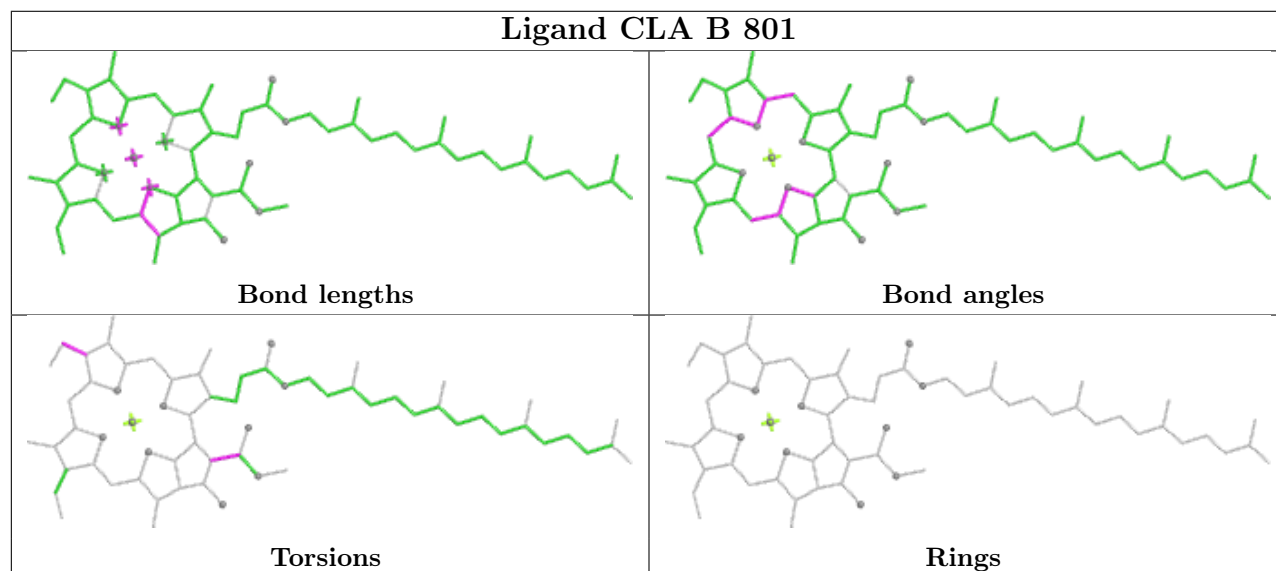


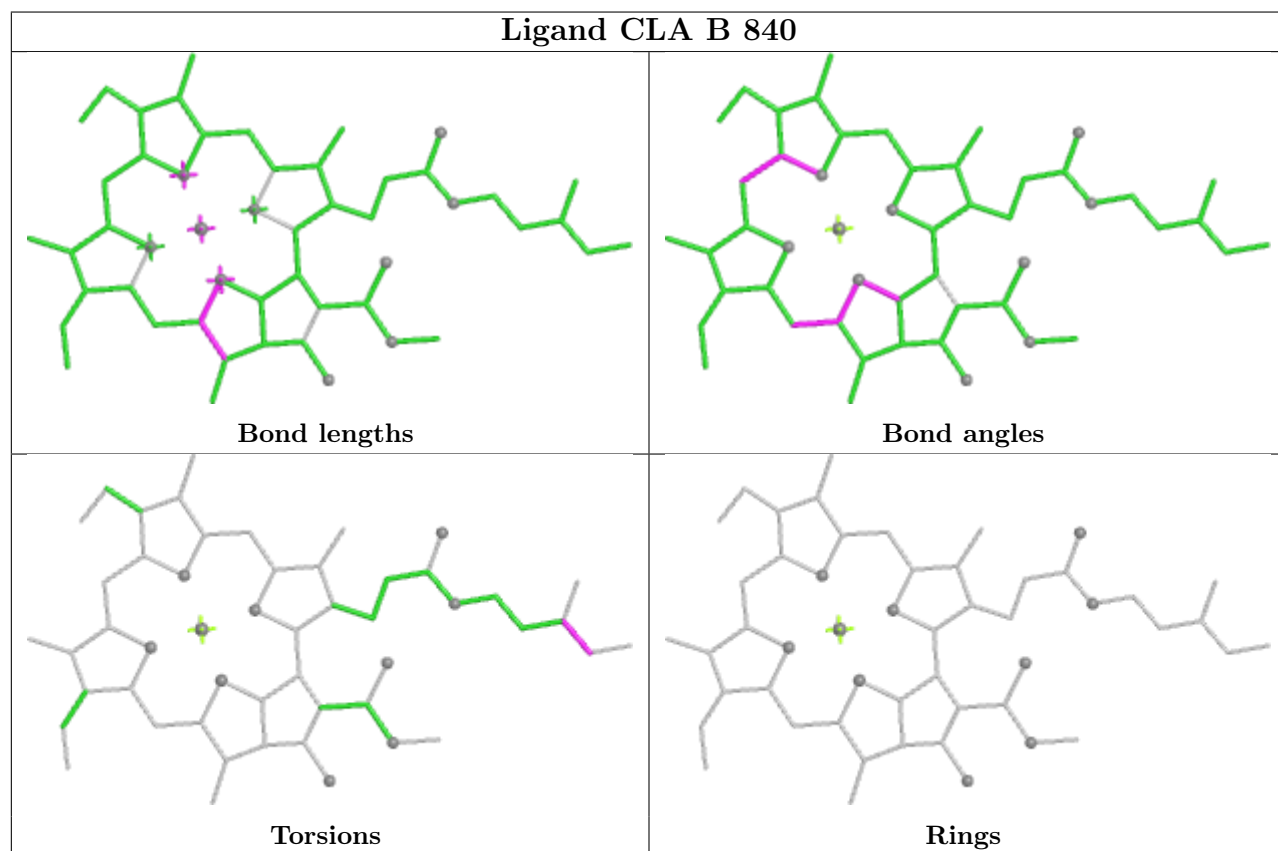
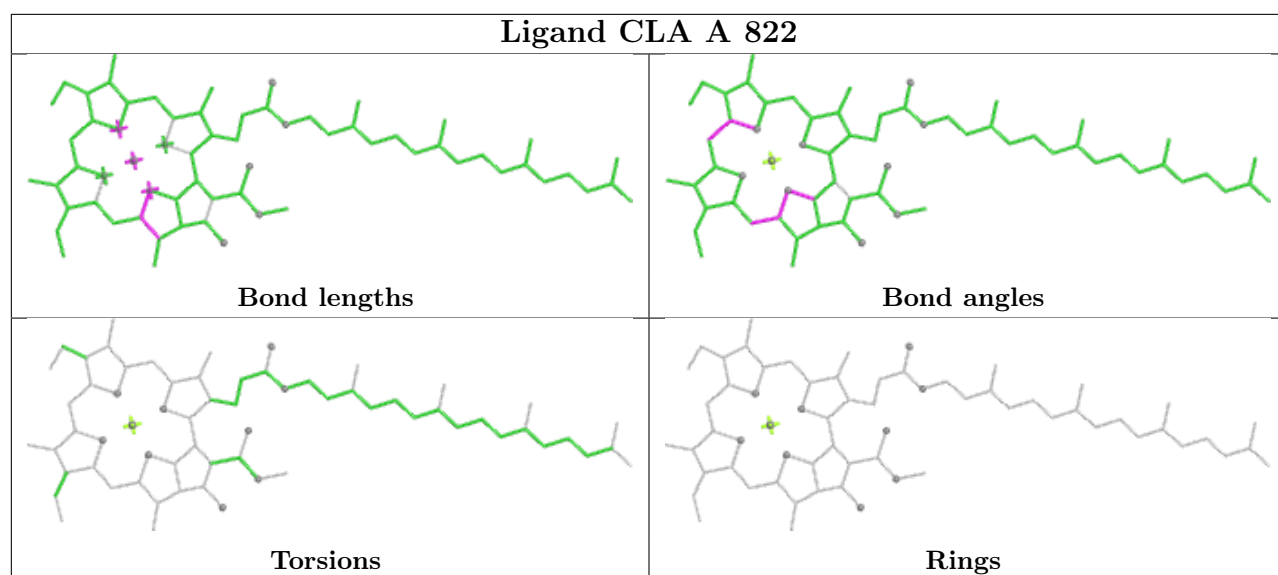


## Ligand CLA A 837

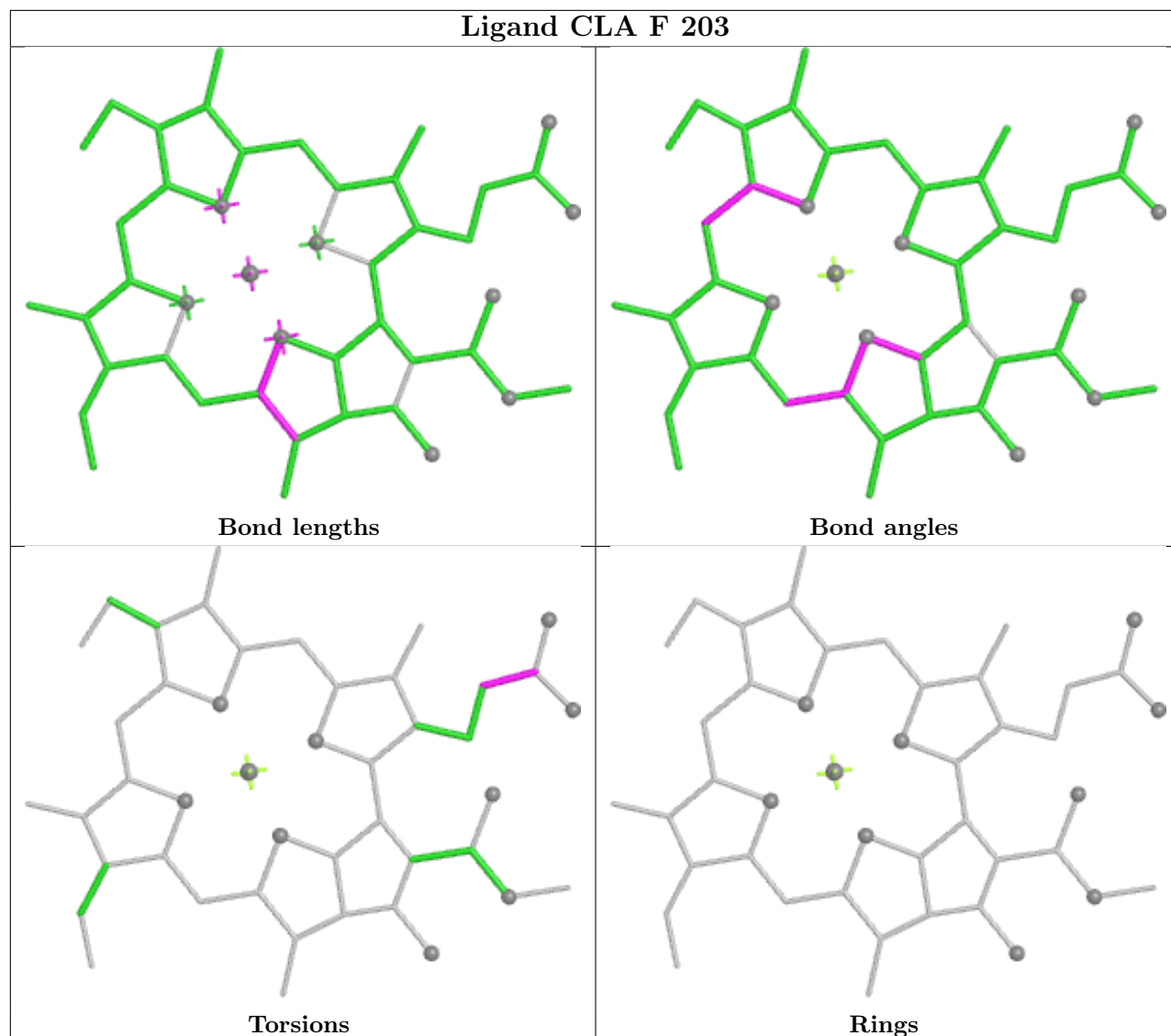


## Ligand CLA B 801

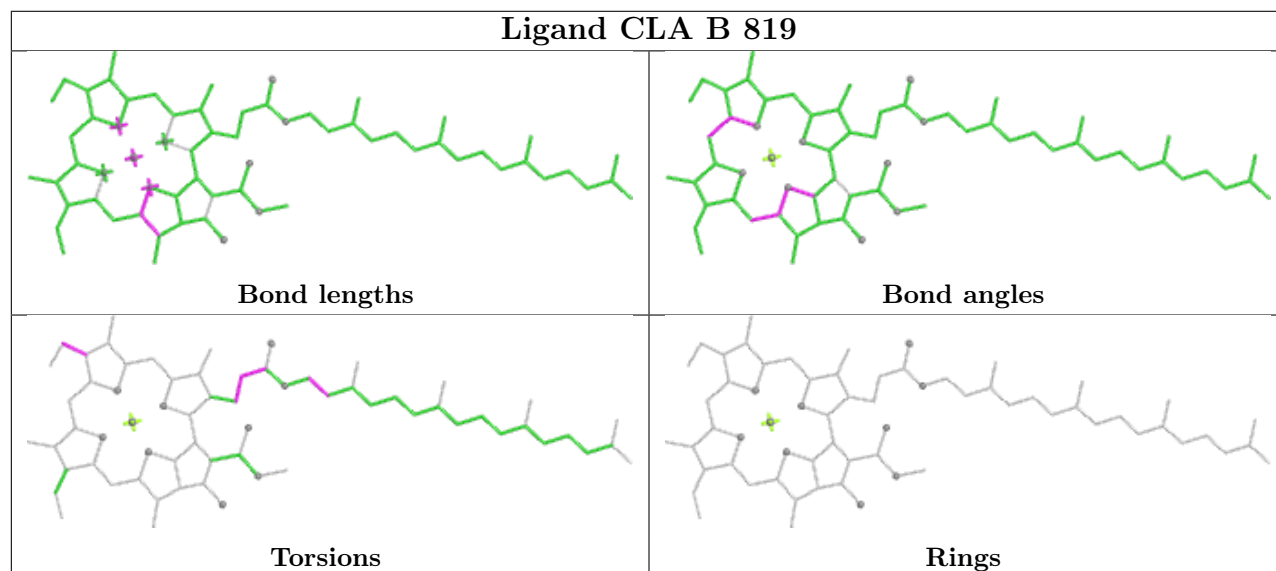


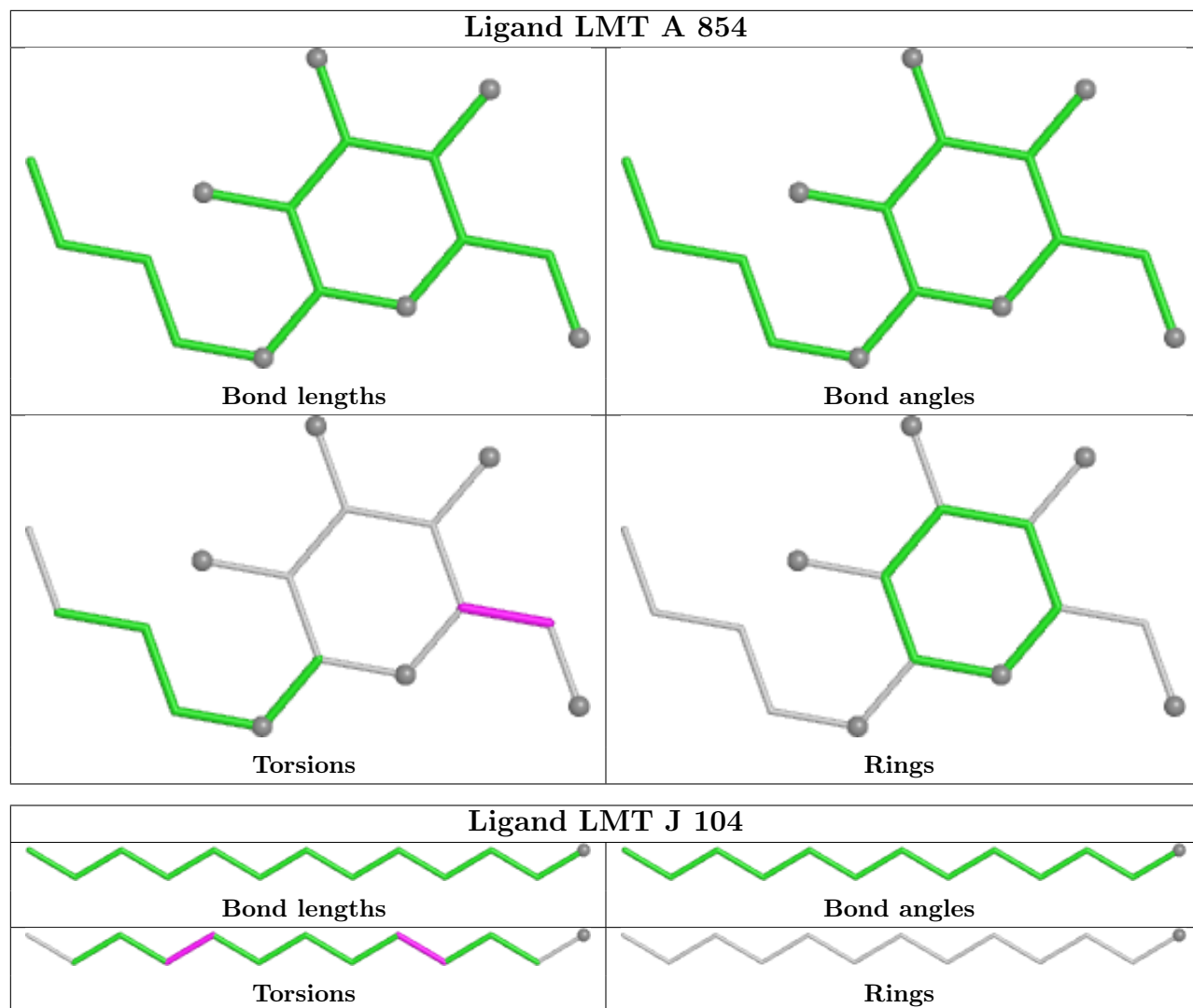


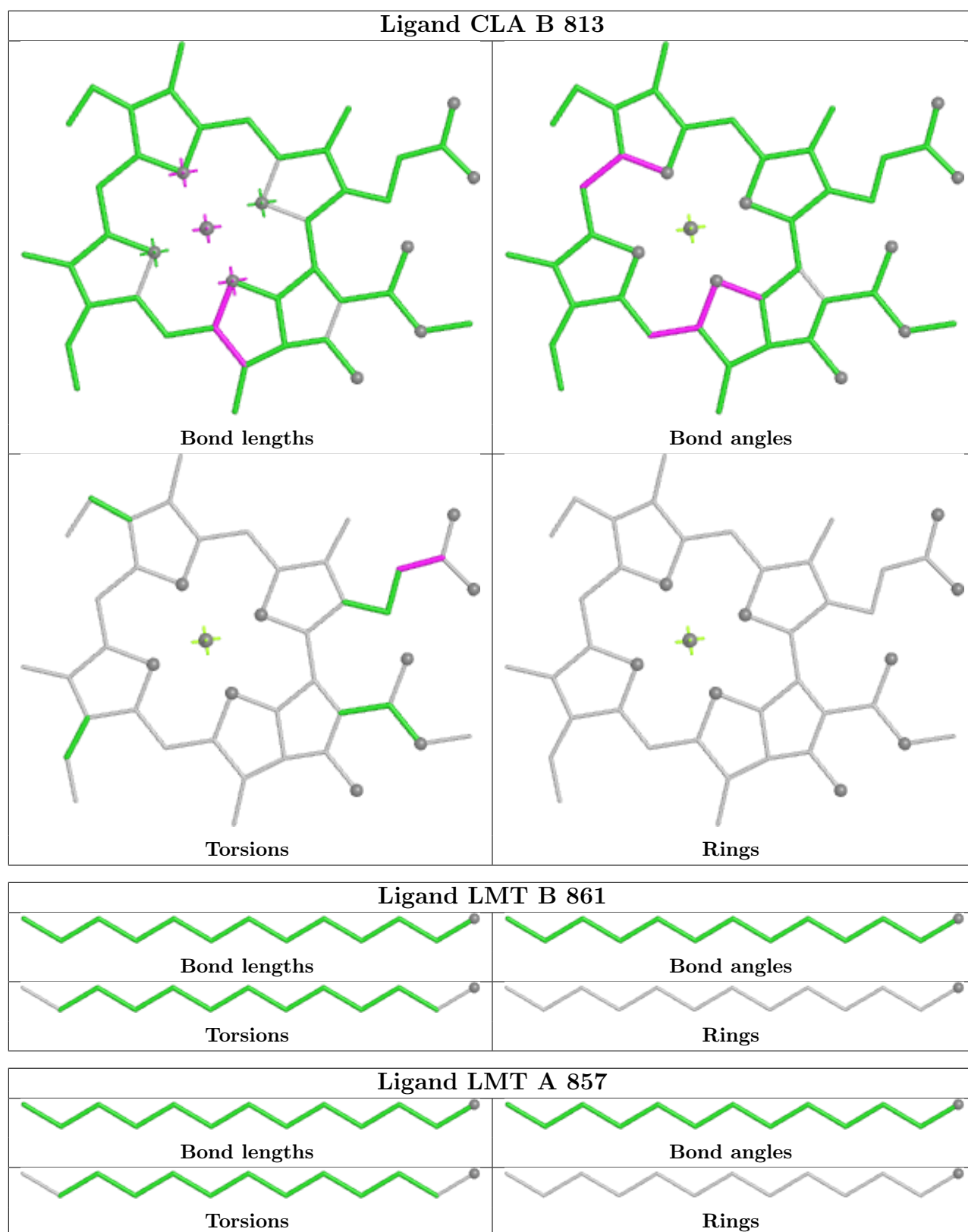
## Ligand CLA F 203

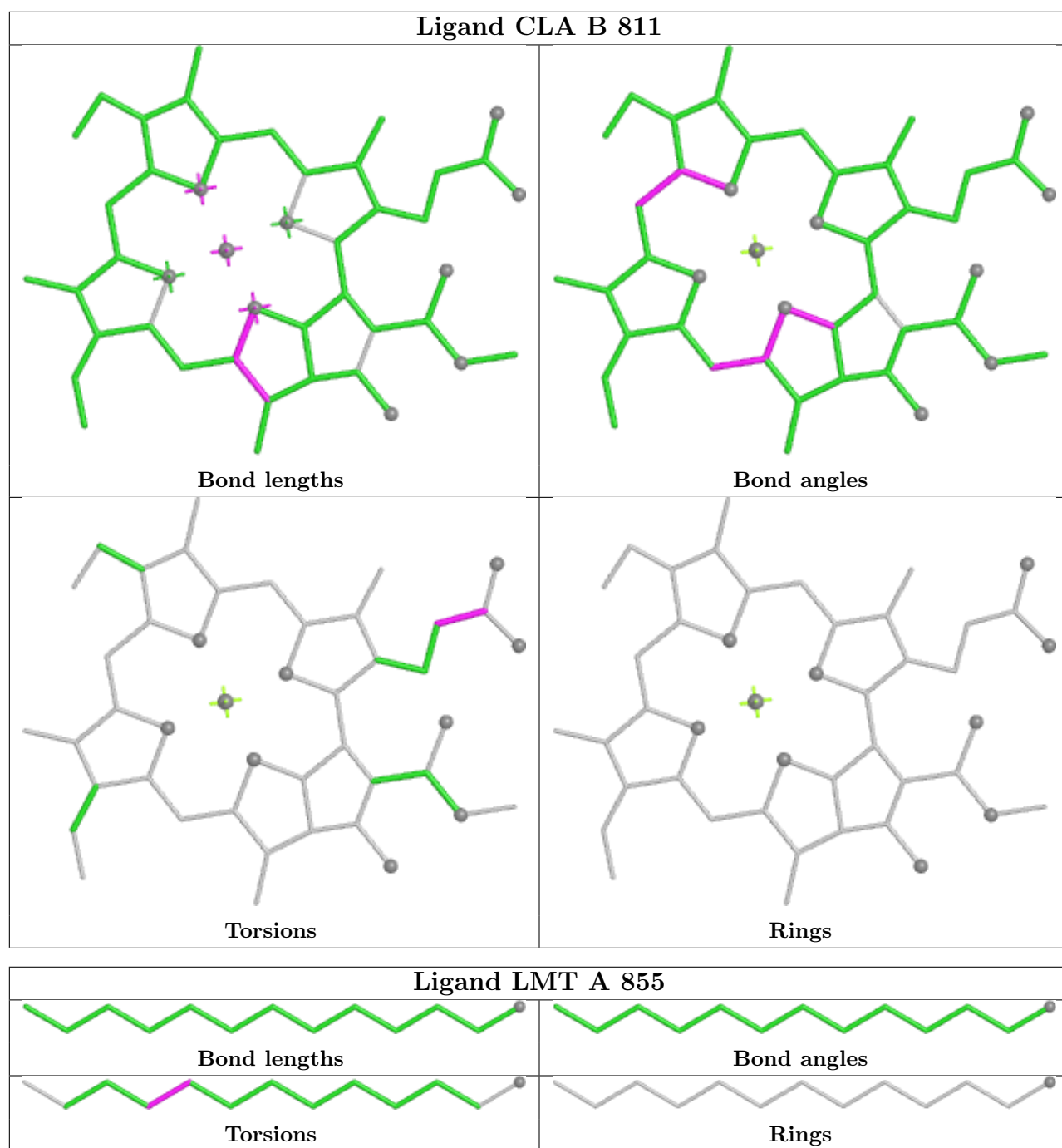


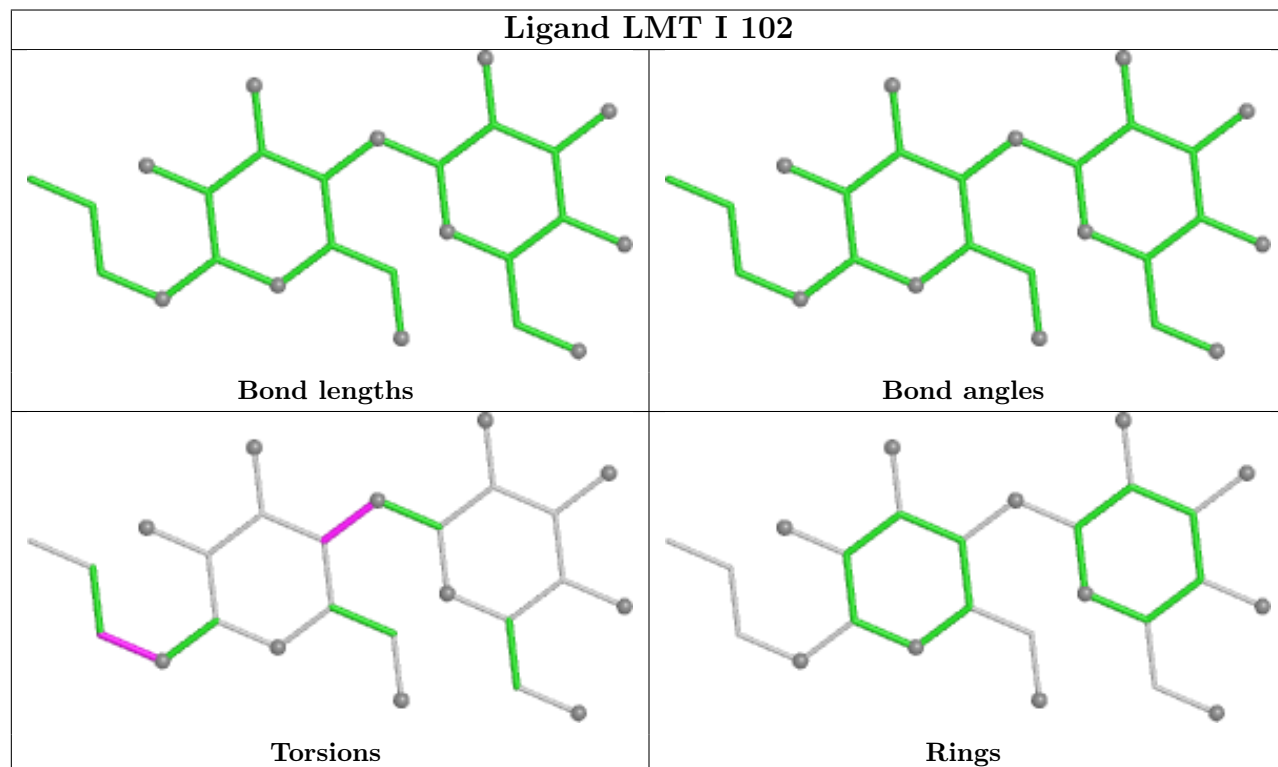
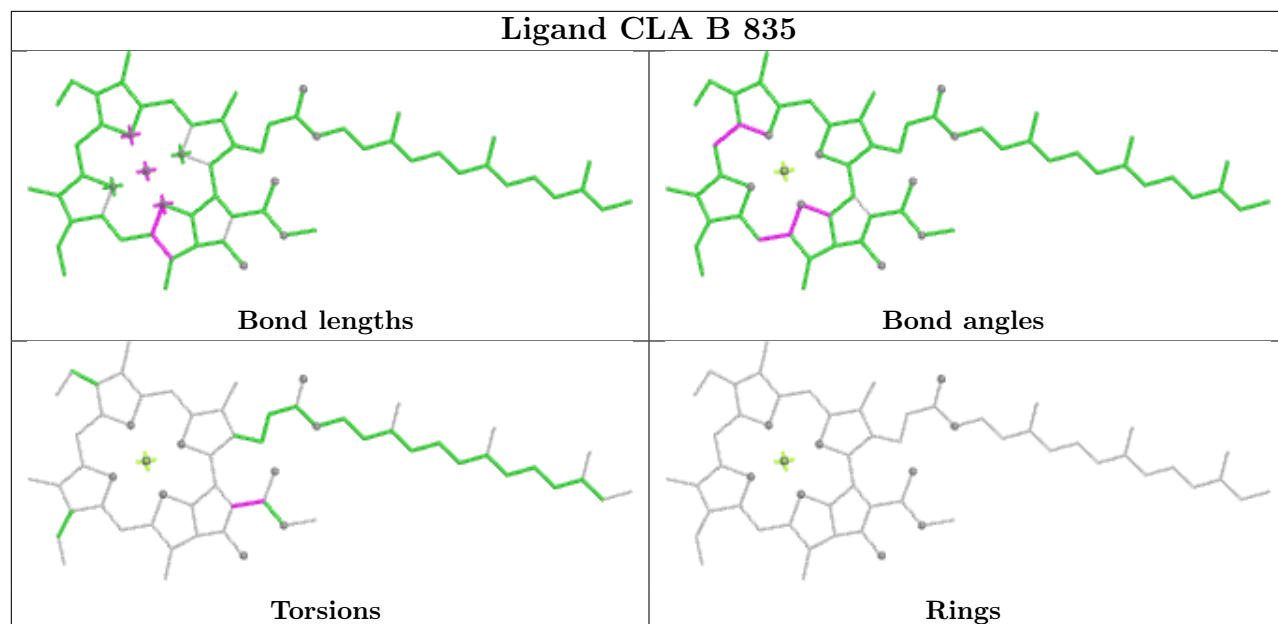
## Ligand CLA B 819

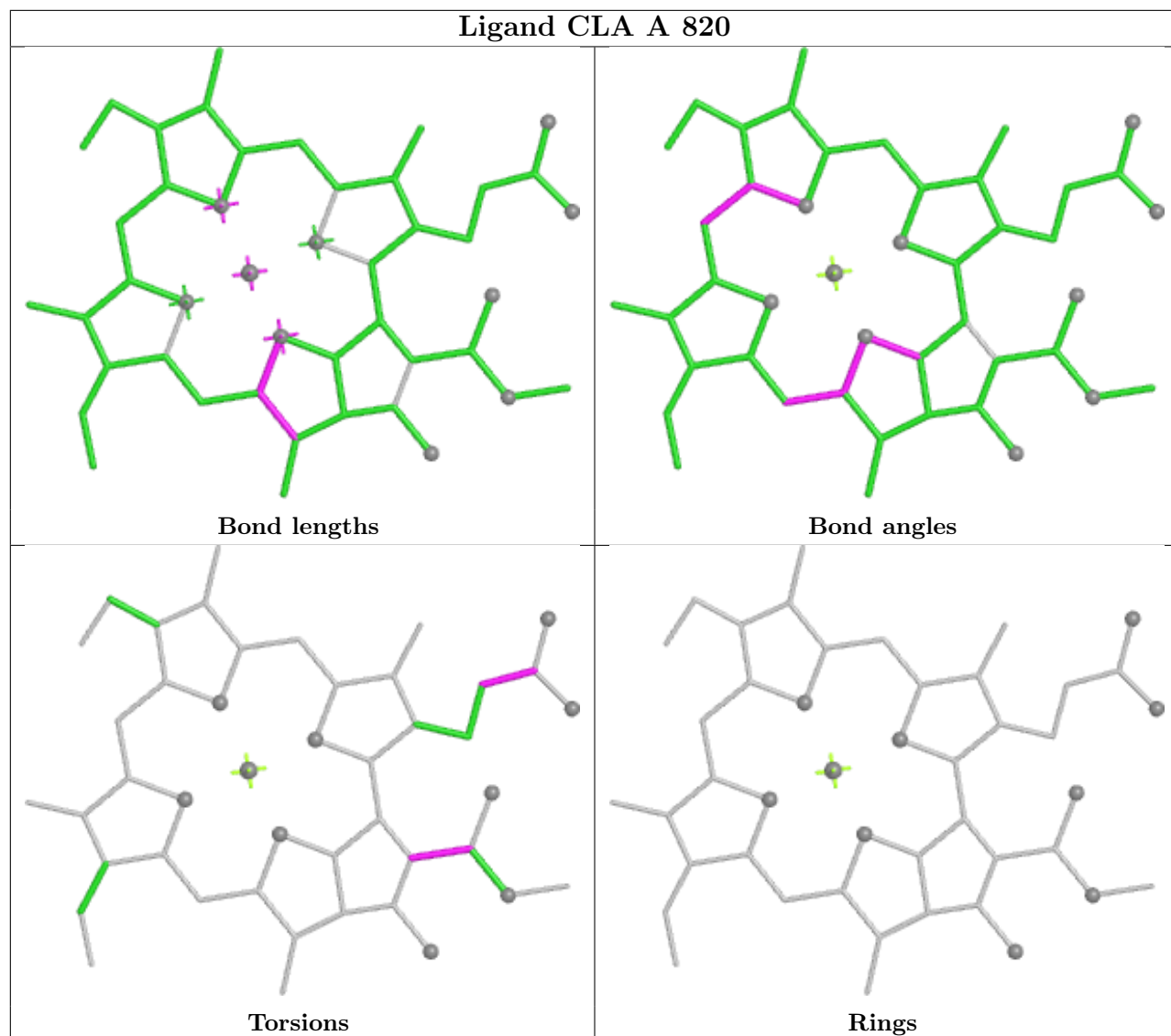




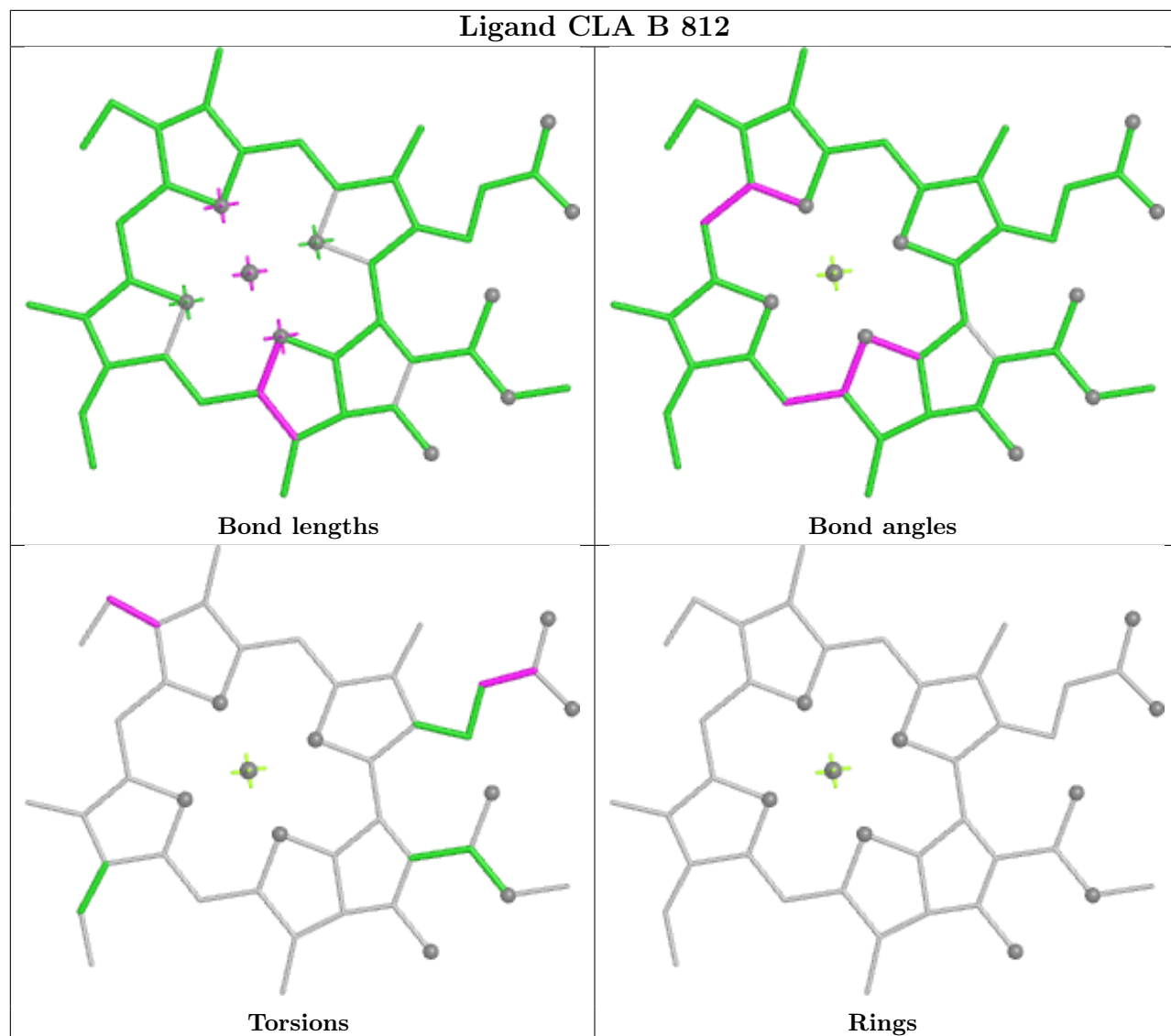


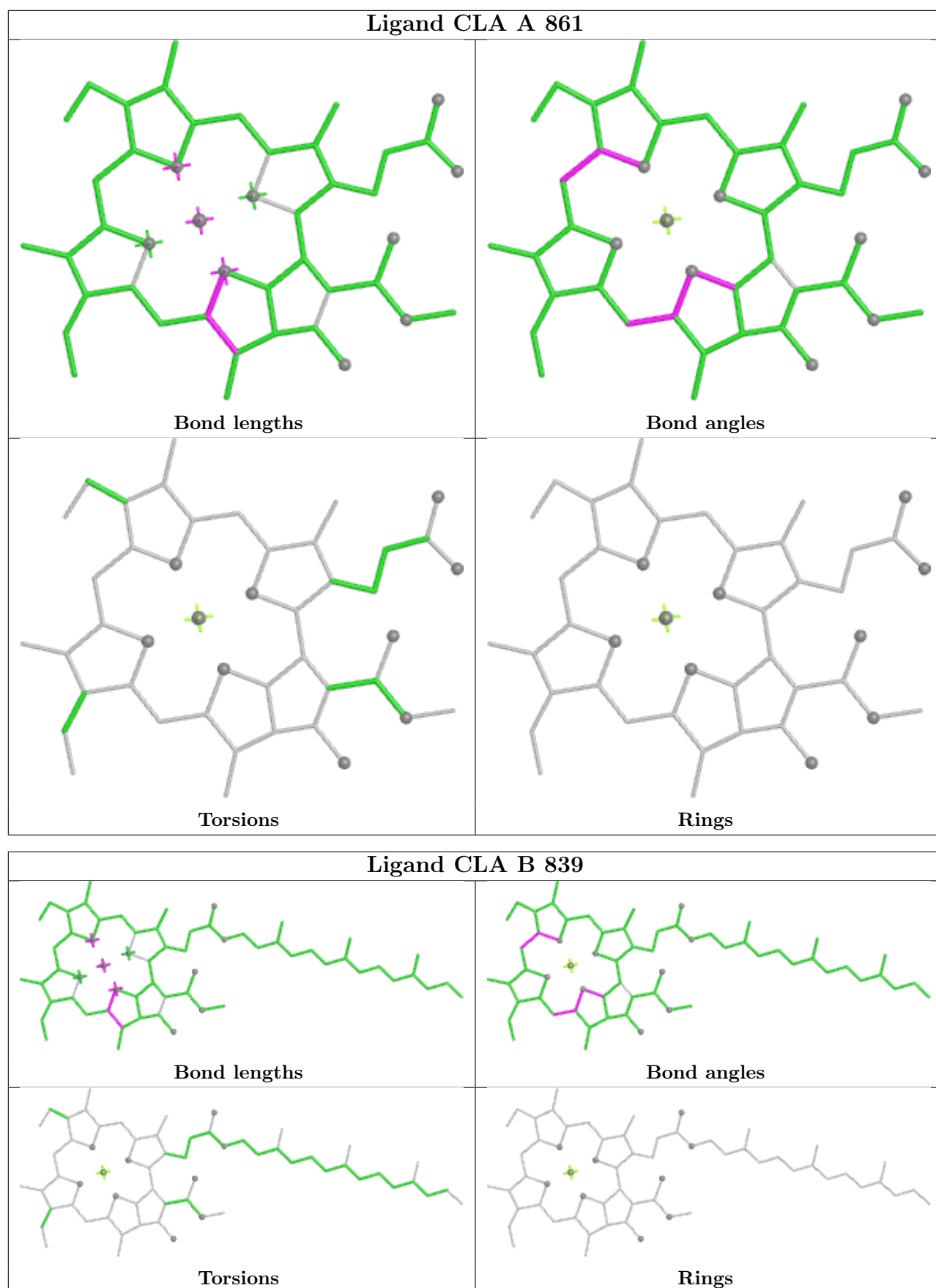


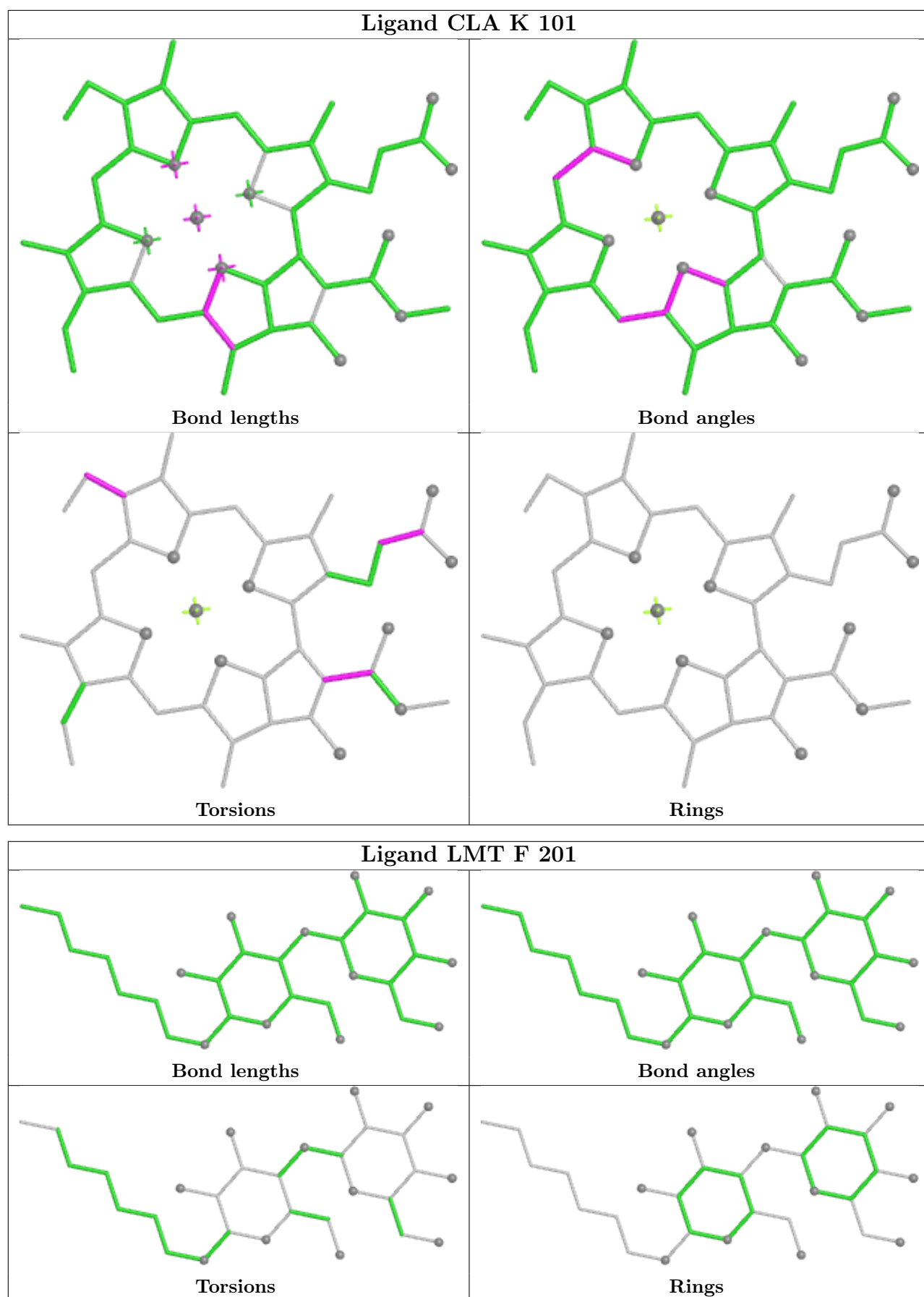


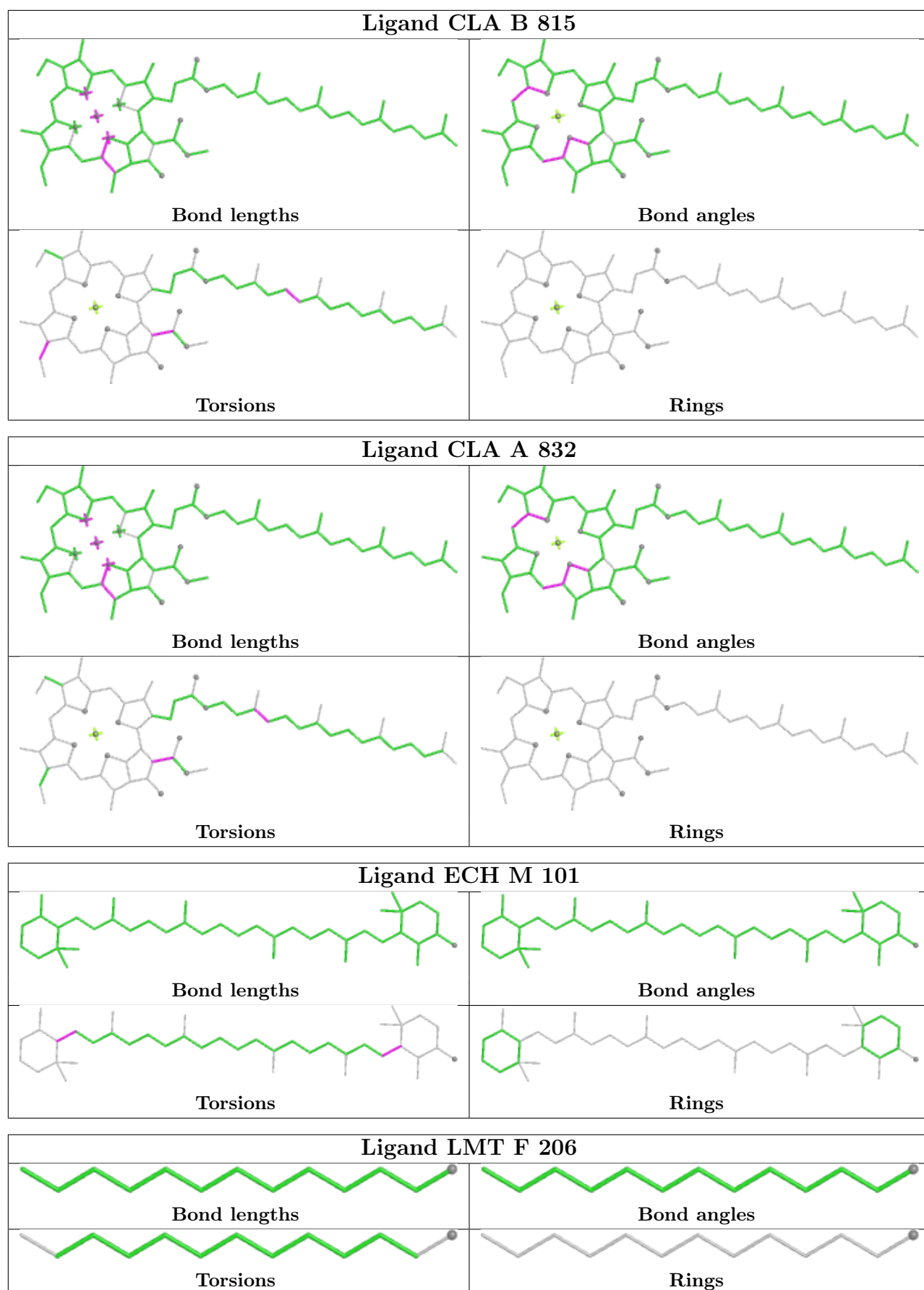


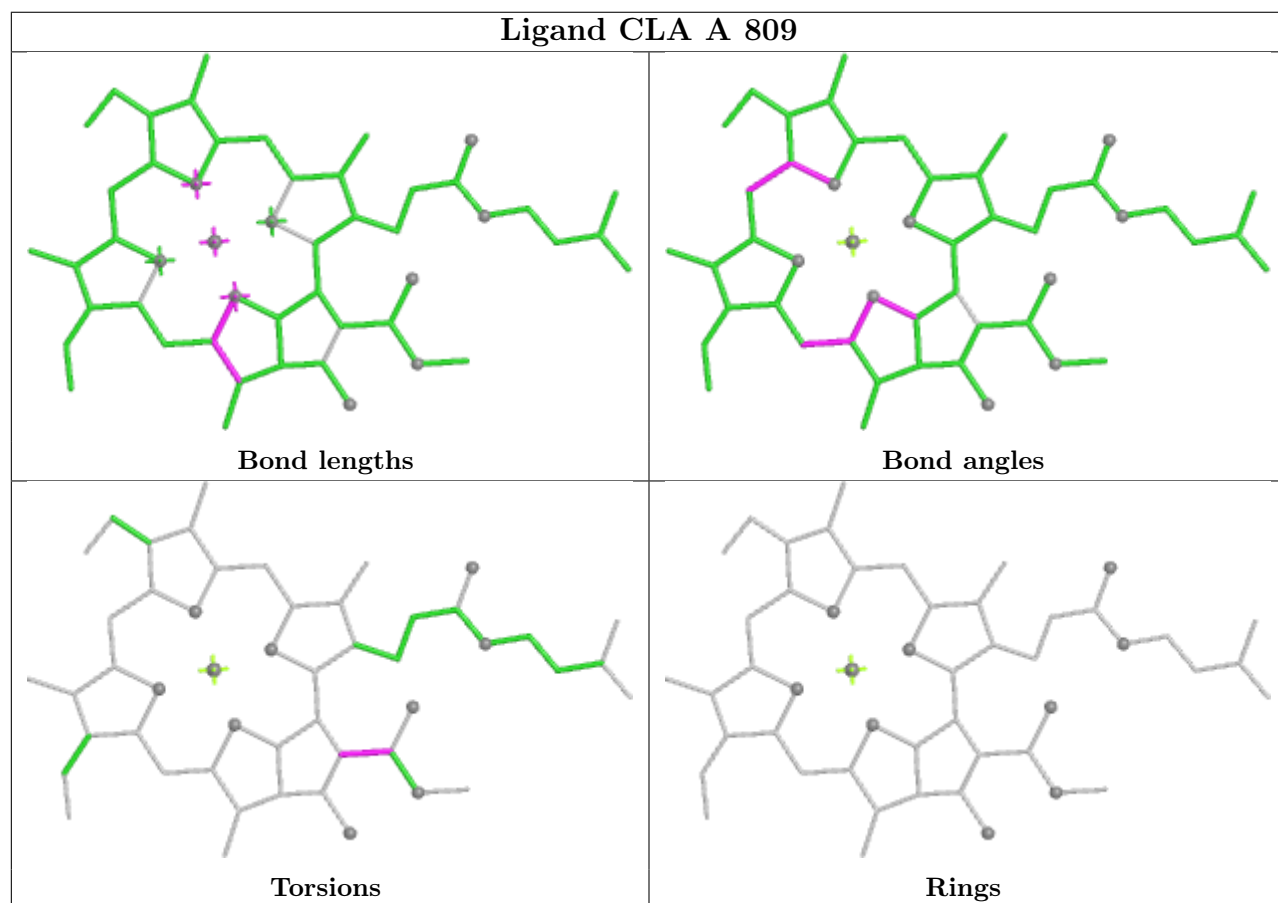
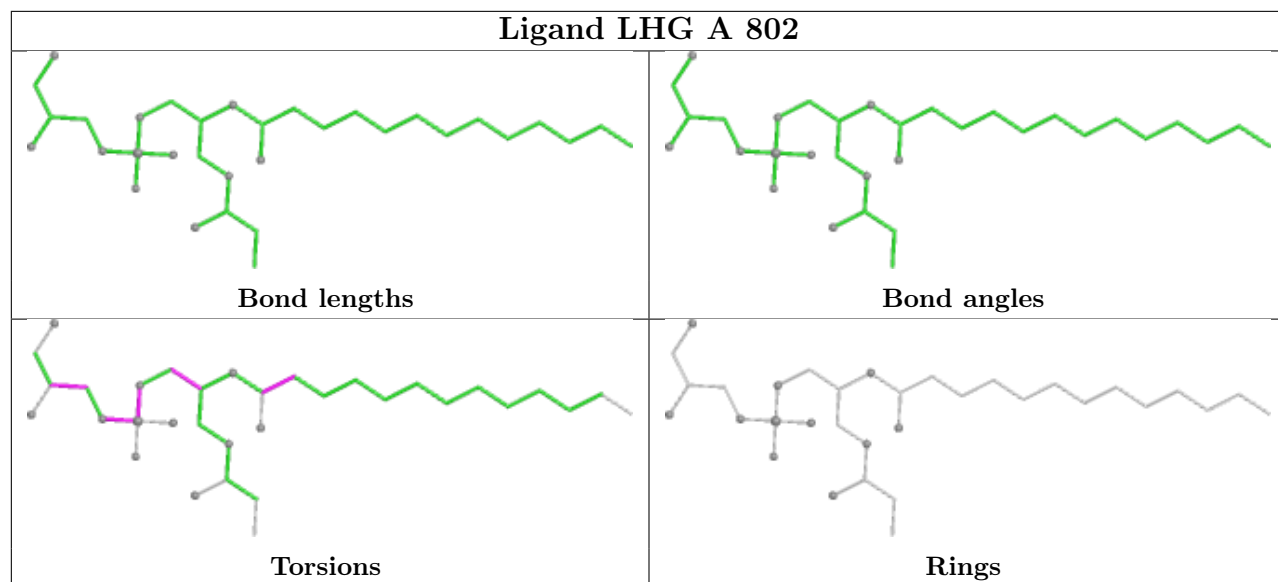
## Ligand CLA B 812



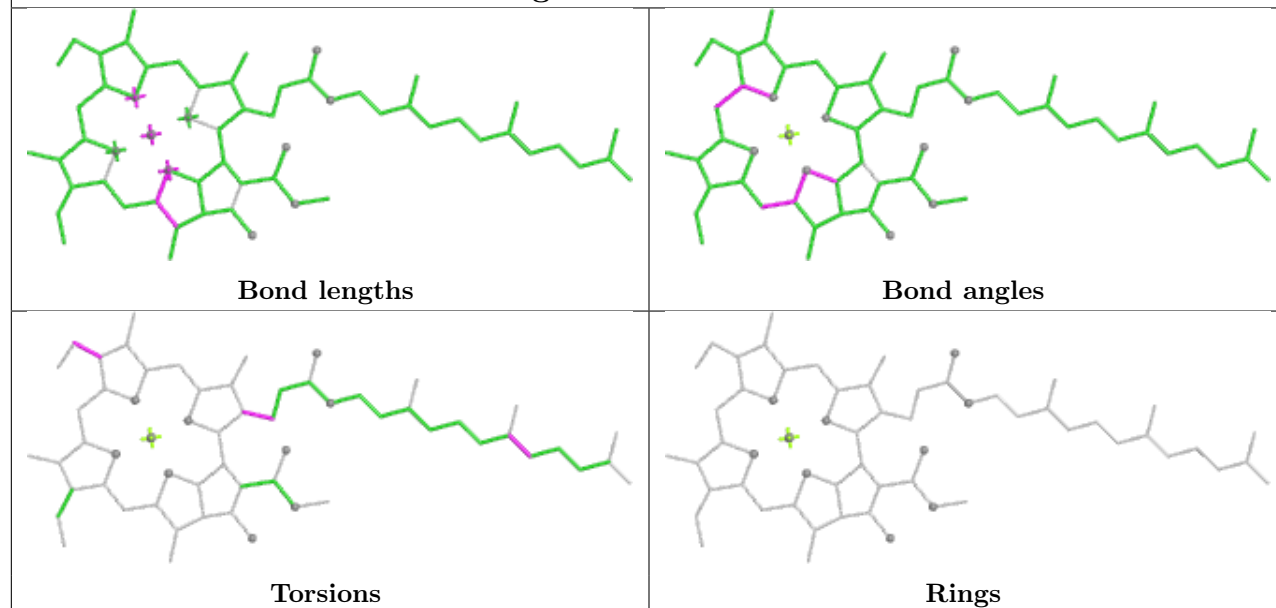




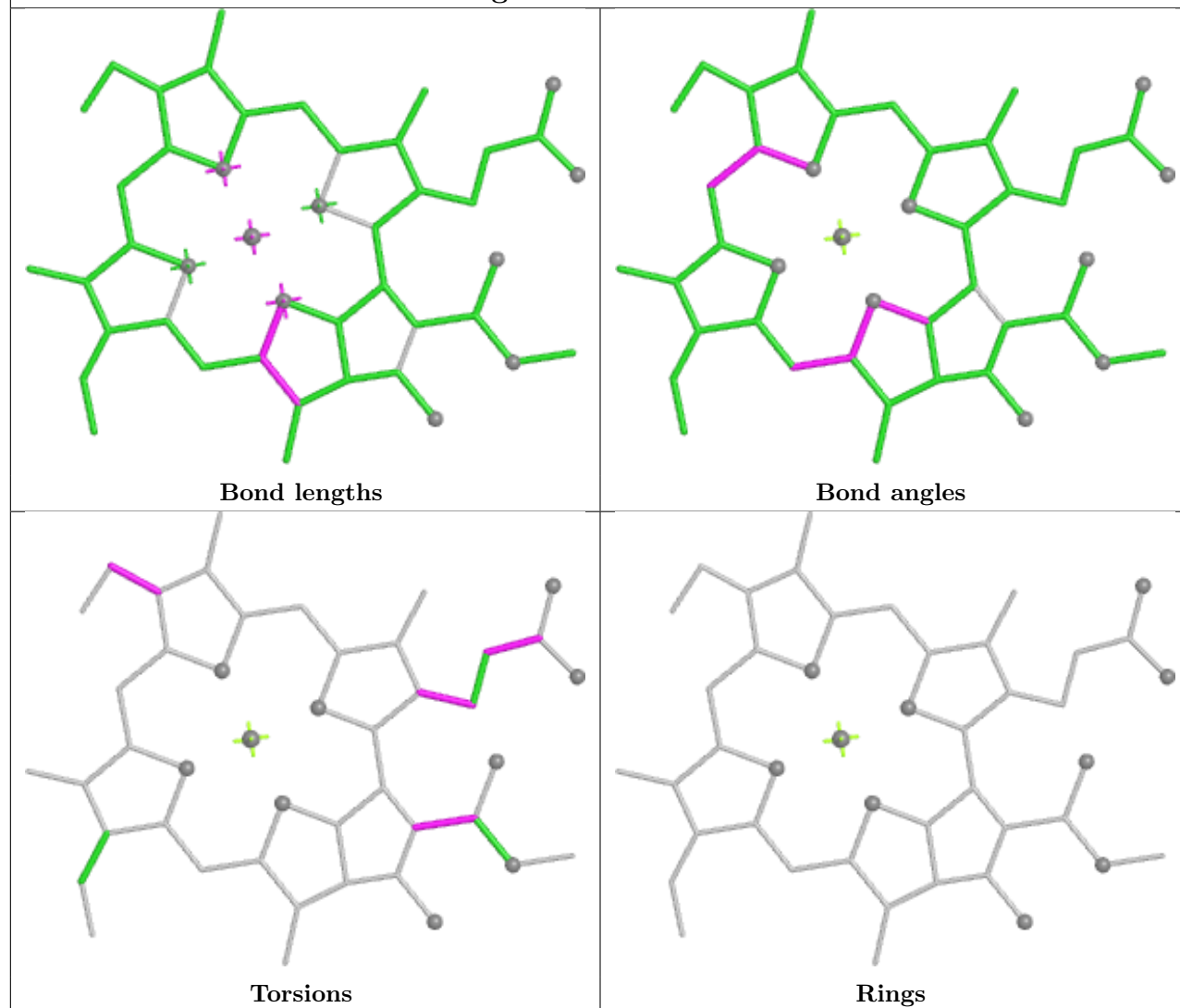


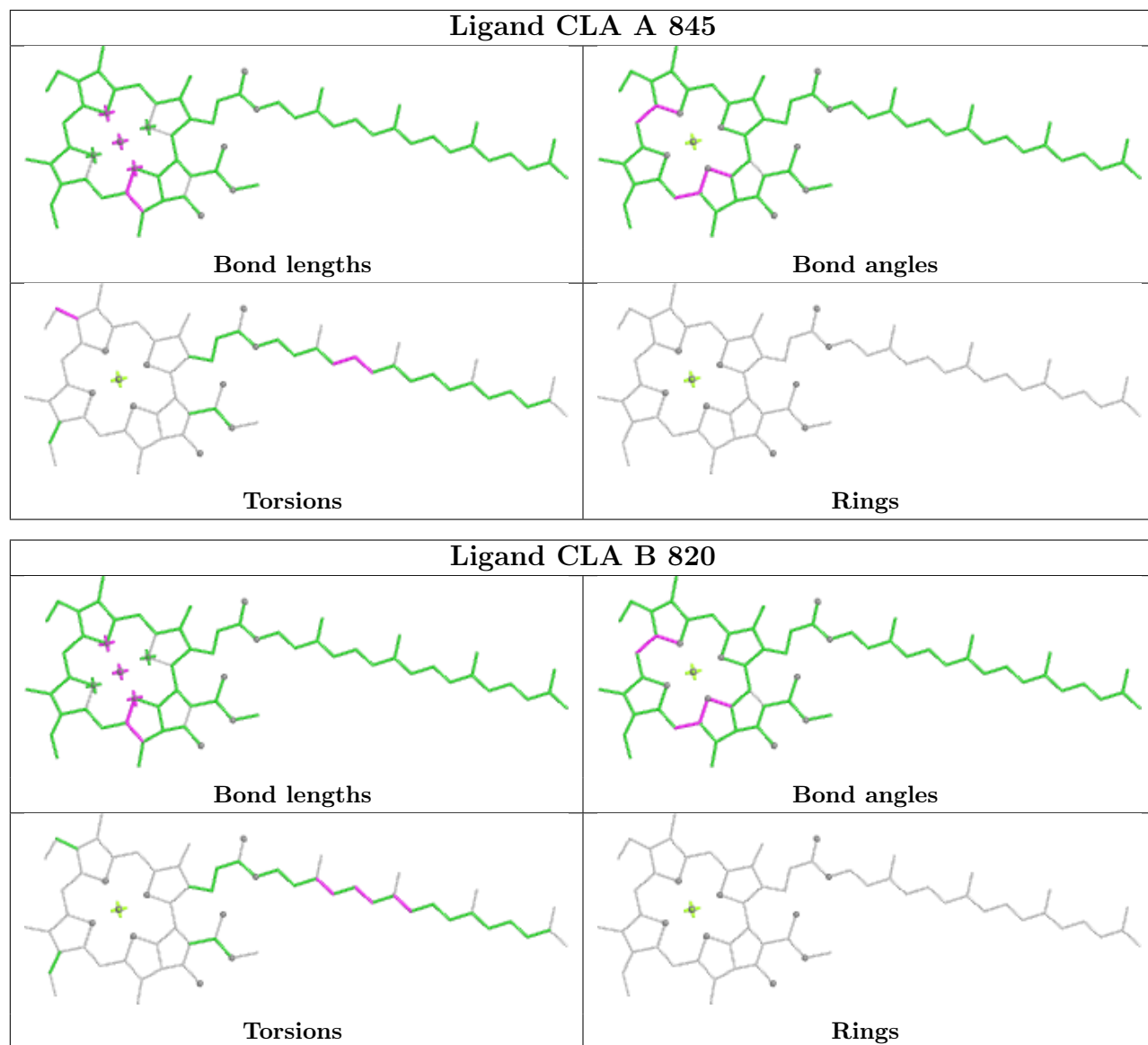


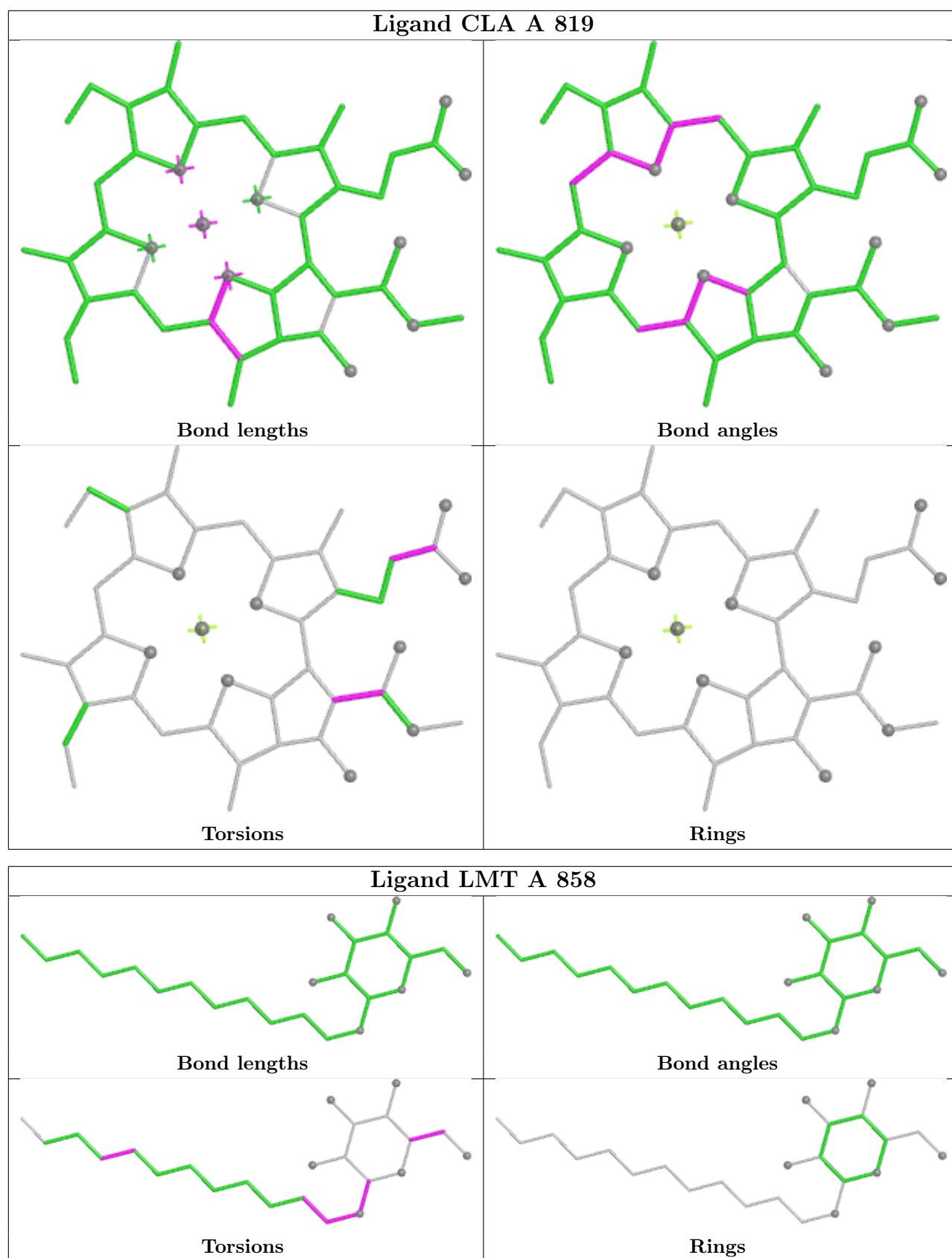
## Ligand CLA B 824

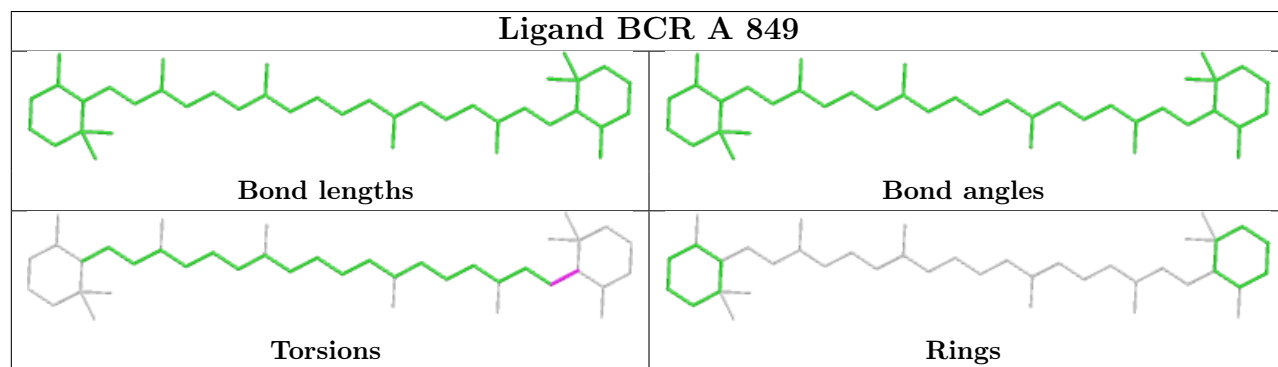
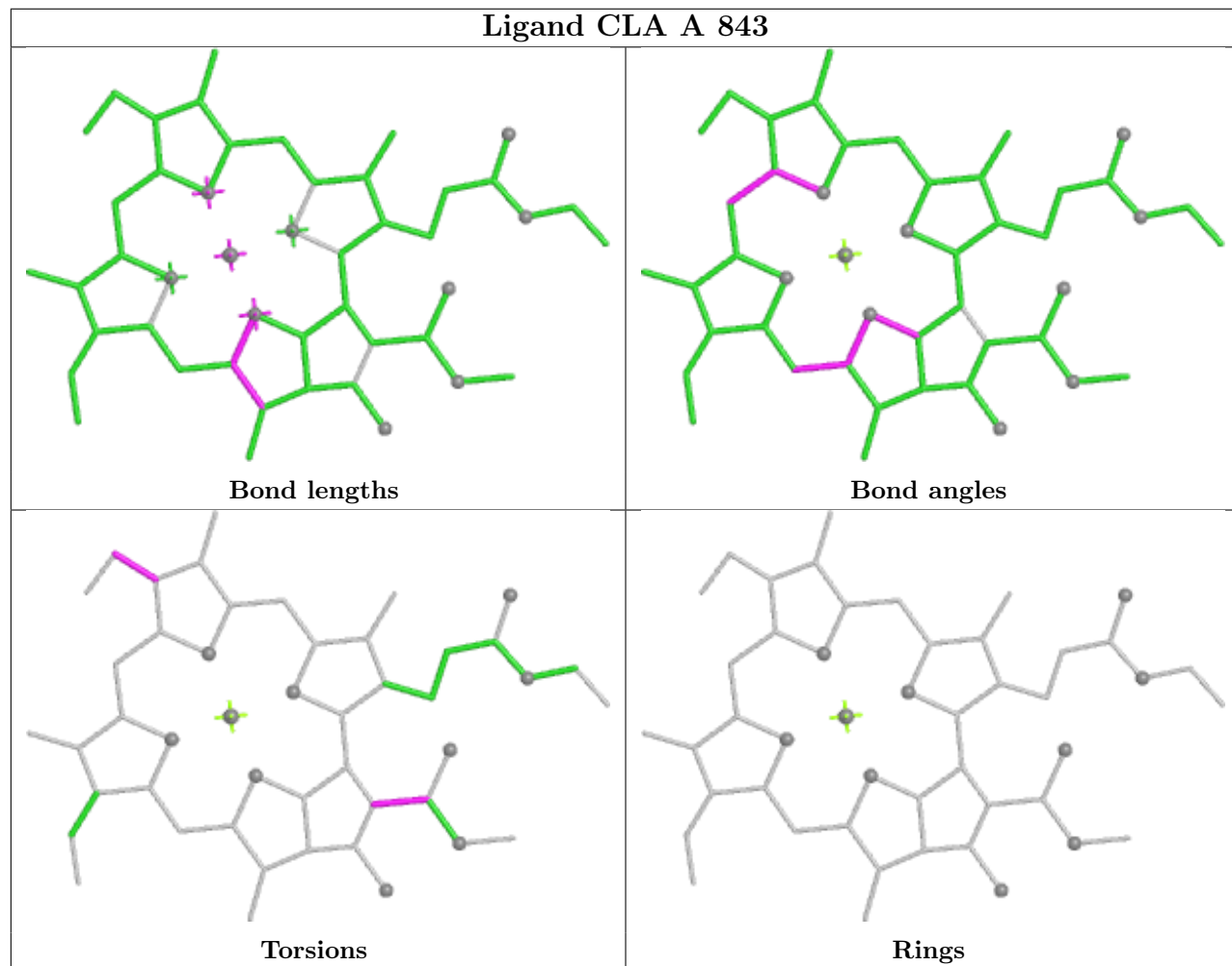
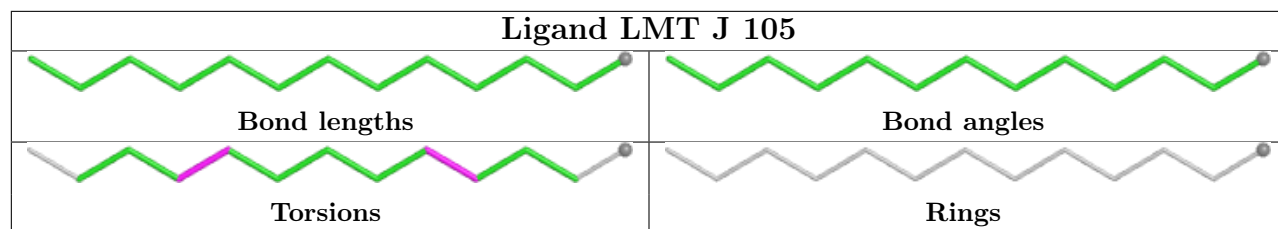


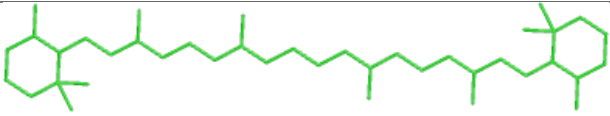
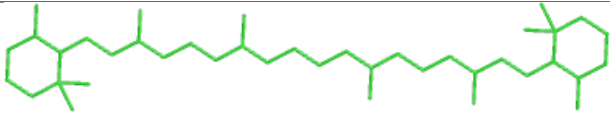
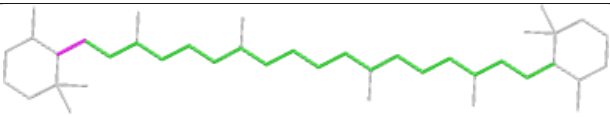
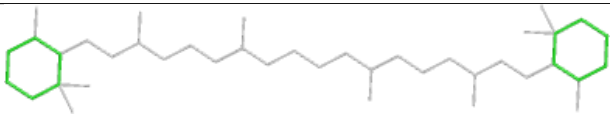
## Ligand CLA A 840



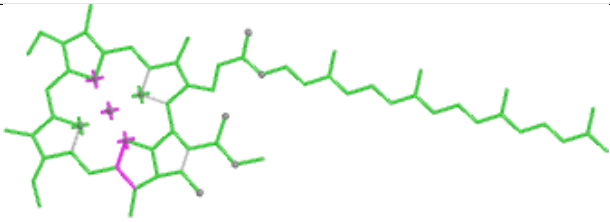
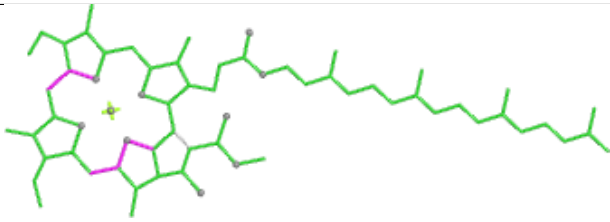
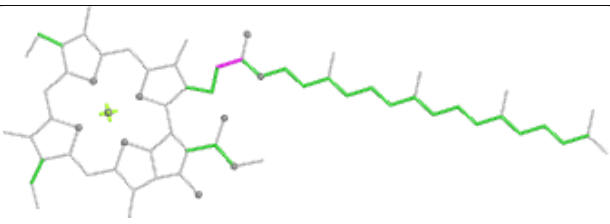
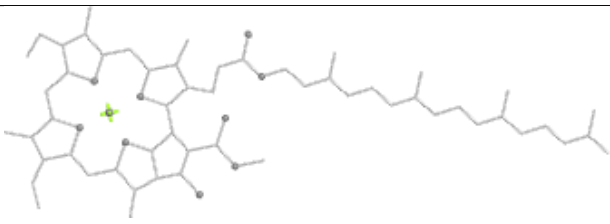




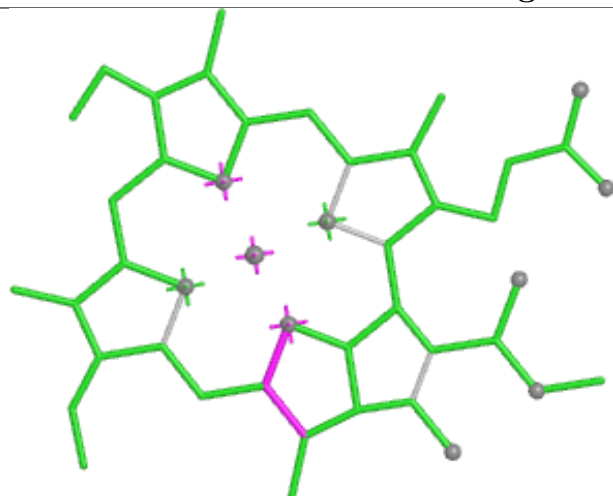


| Ligand BCR J 103                                                                  |                                                                                    |  |  |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|--|--|
|  |  |  |  |
| Bond lengths                                                                      | Bond angles                                                                        |  |  |
|  |  |  |  |
| Torsions                                                                          | Rings                                                                              |  |  |

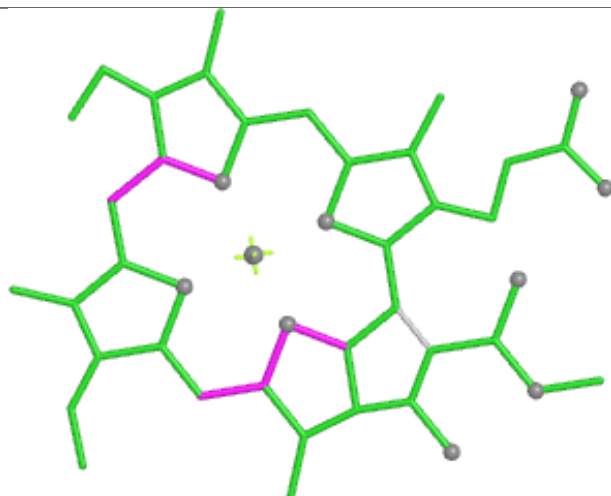
  

| Ligand CLA A 811                                                                   |                                                                                     |  |  |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|--|--|
|   |   |  |  |
| Bond lengths                                                                       | Bond angles                                                                         |  |  |
|  |  |  |  |
| Torsions                                                                           | Rings                                                                               |  |  |

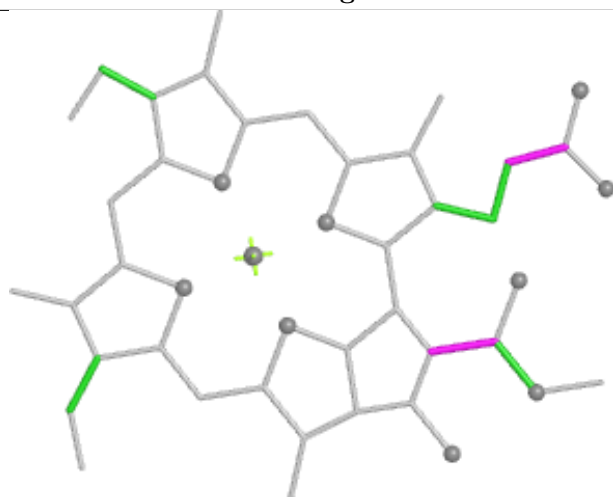
## Ligand CLA J 102



Bond lengths



Bond angles

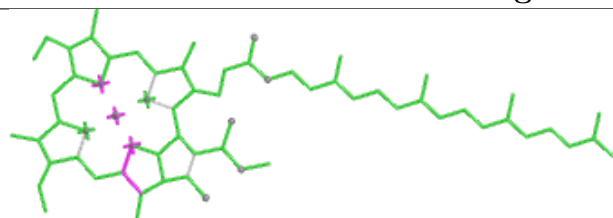


Torsions

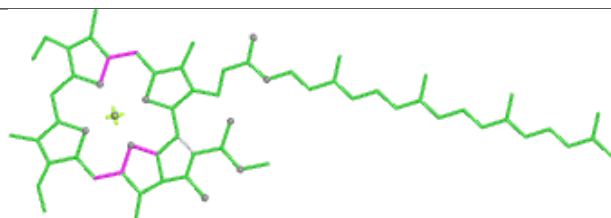


Rings

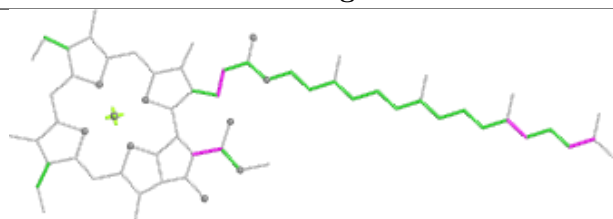
## Ligand CLA B 802



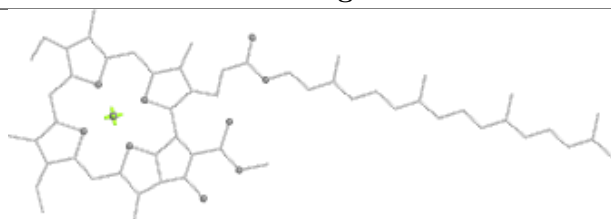
Bond lengths



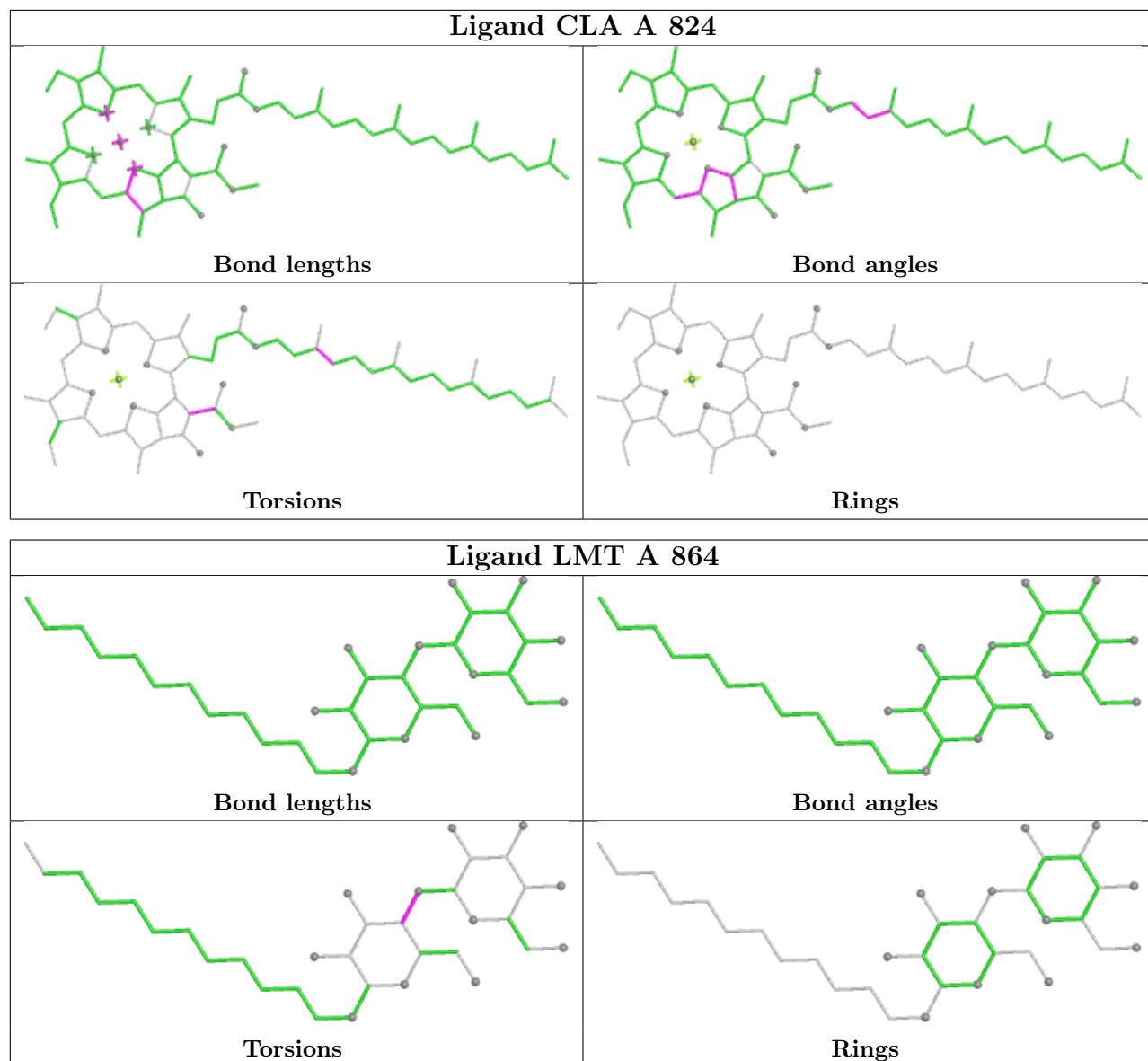
Bond angles



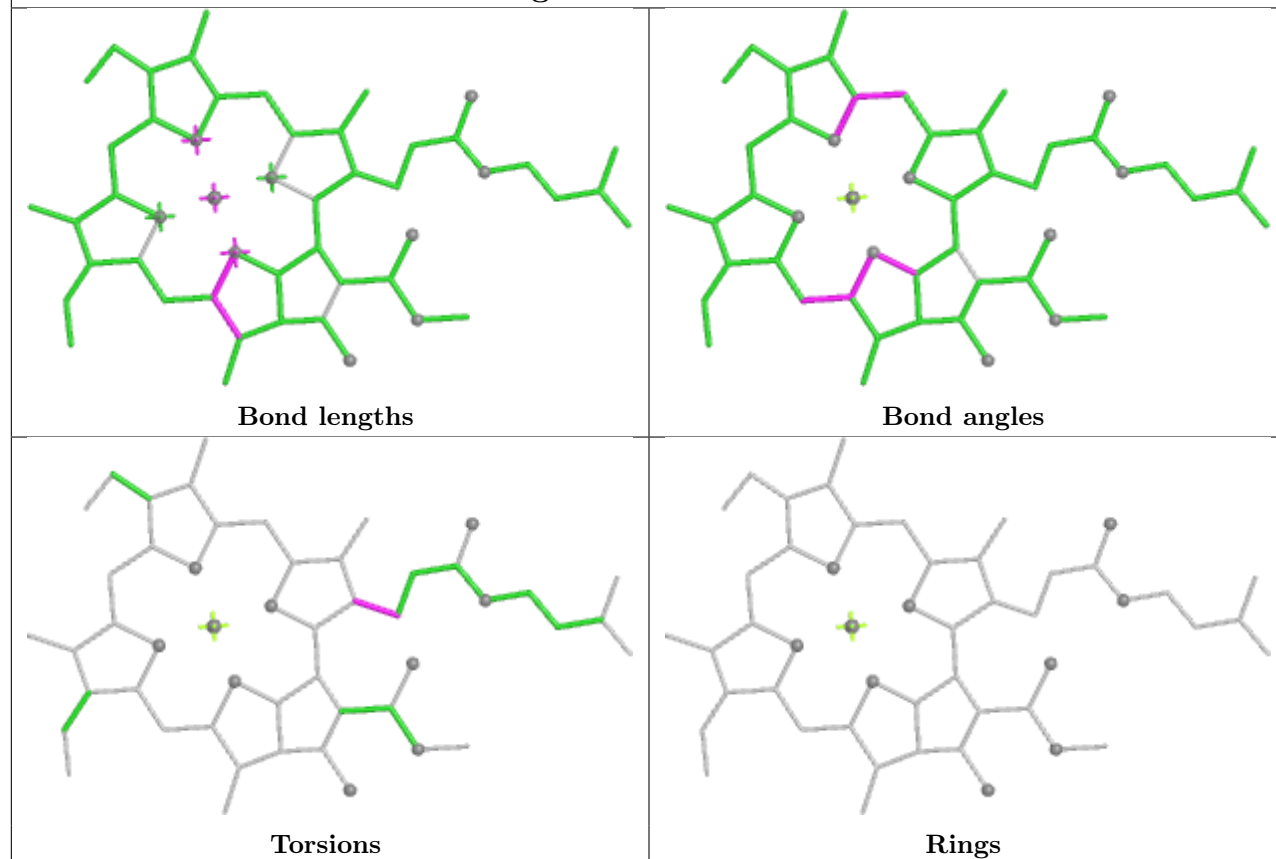
Torsions



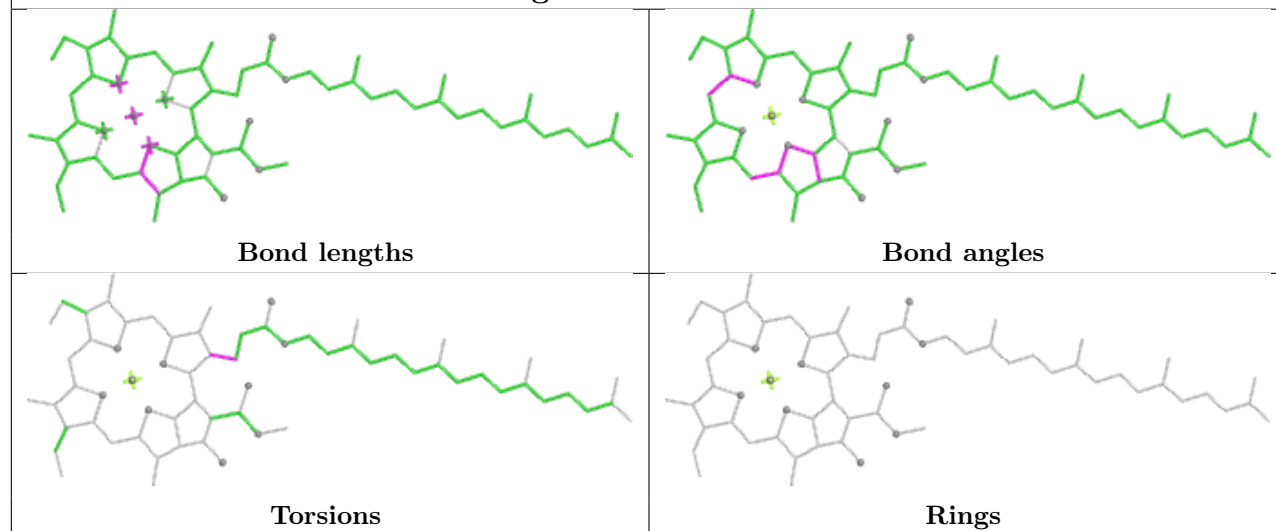
Rings



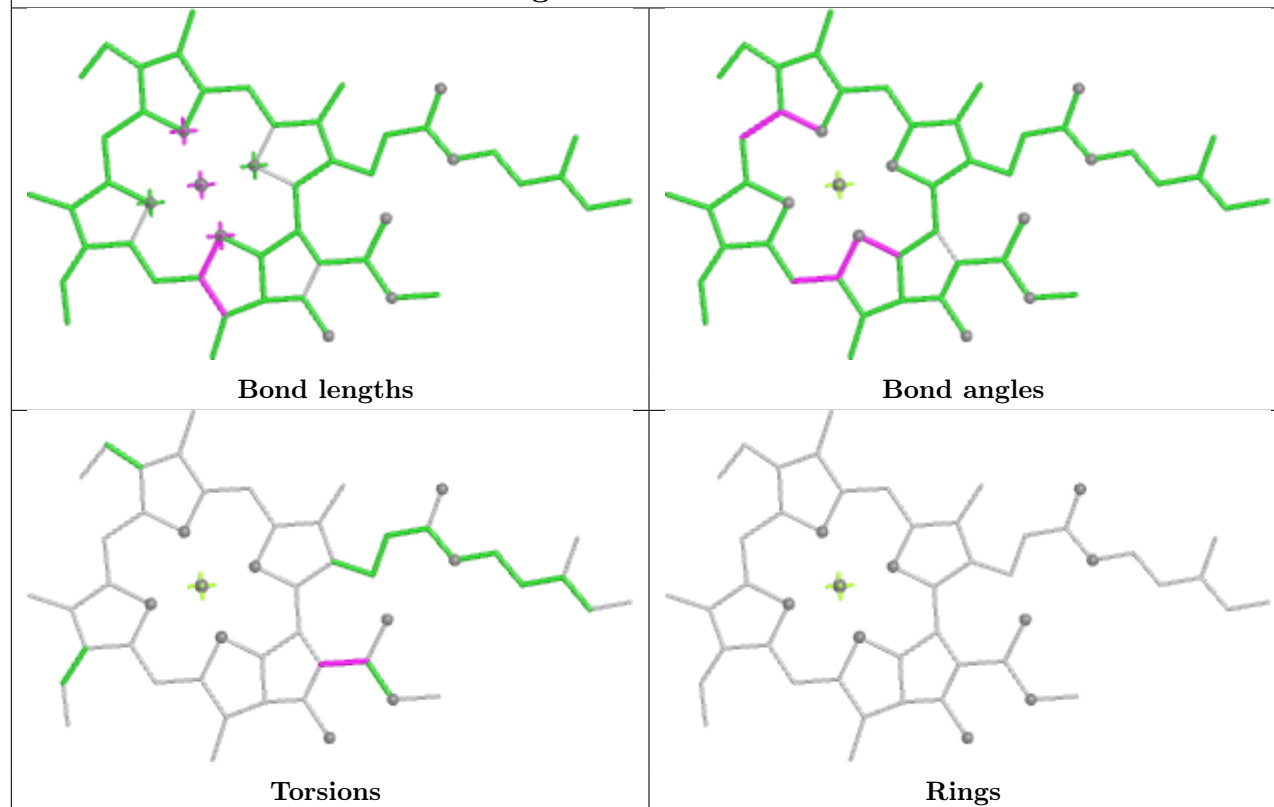
## Ligand CLA A 814



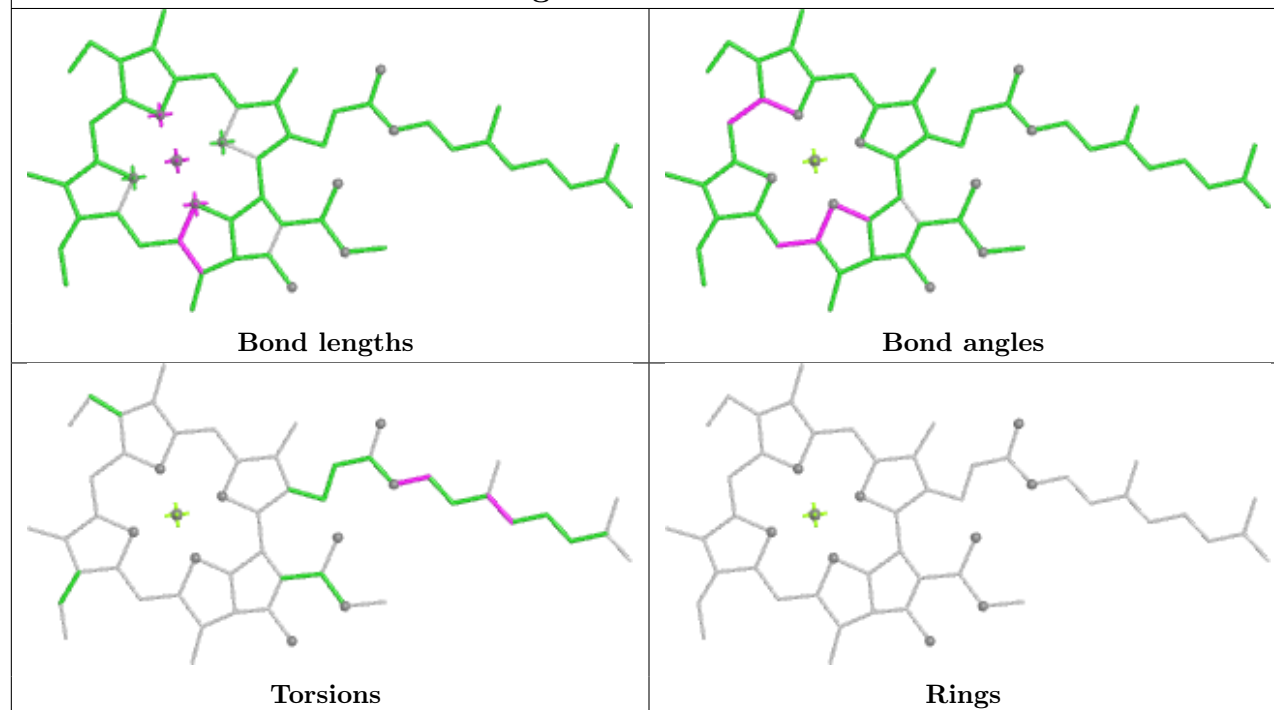
## Ligand CLA A 808

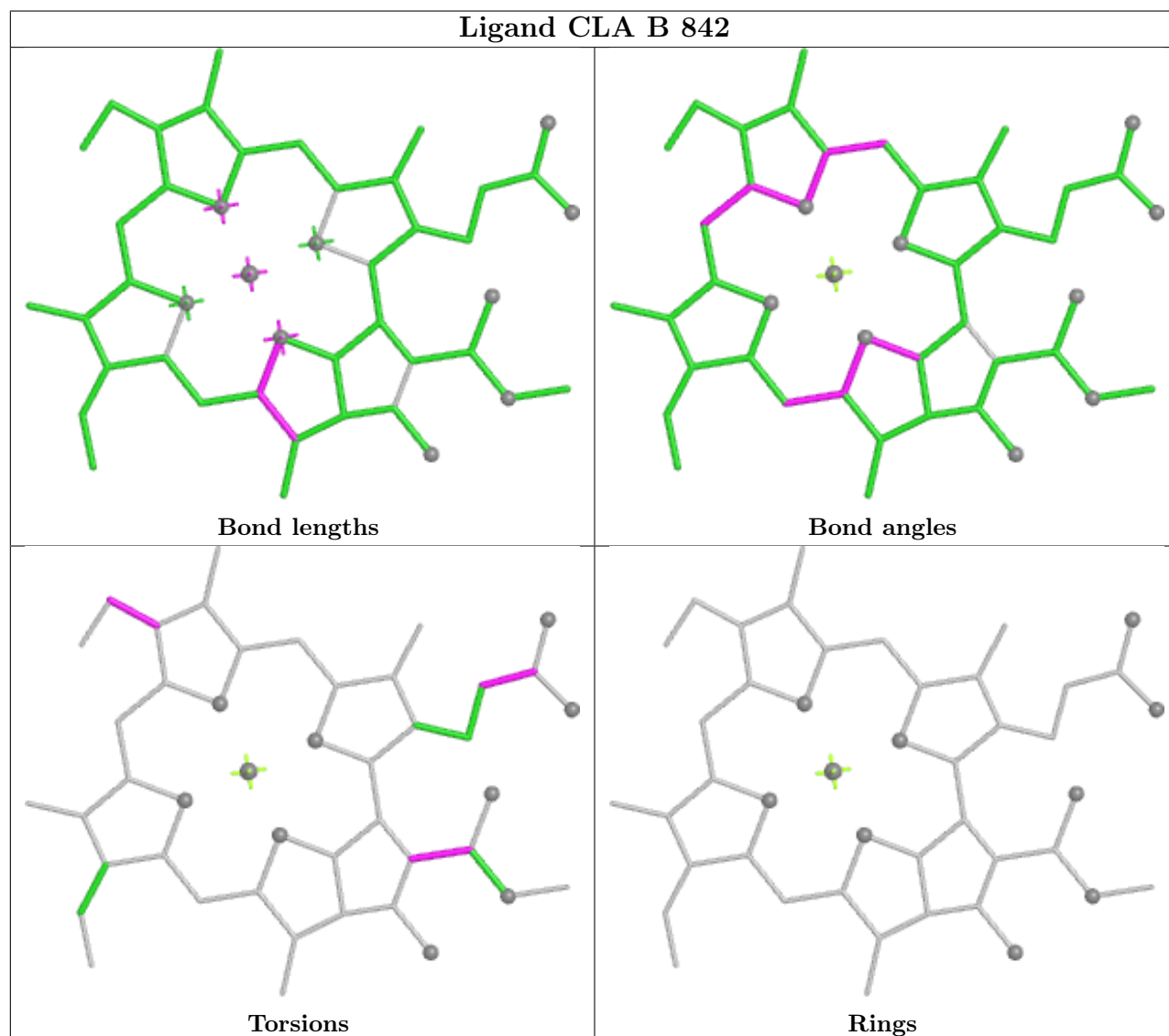
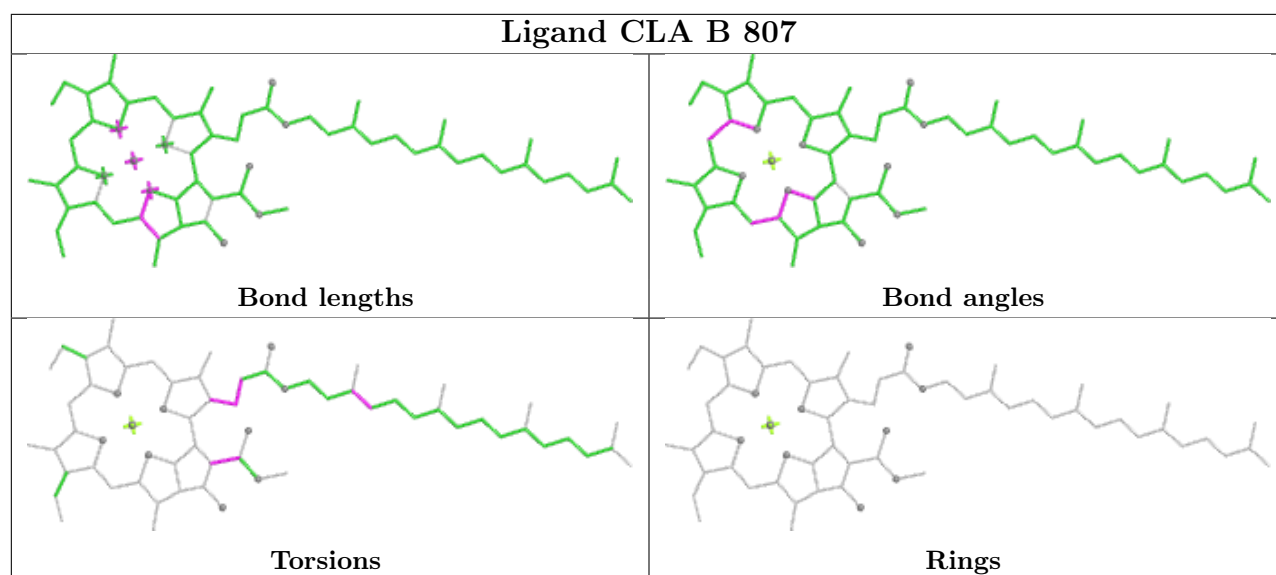


## Ligand CLA A 841

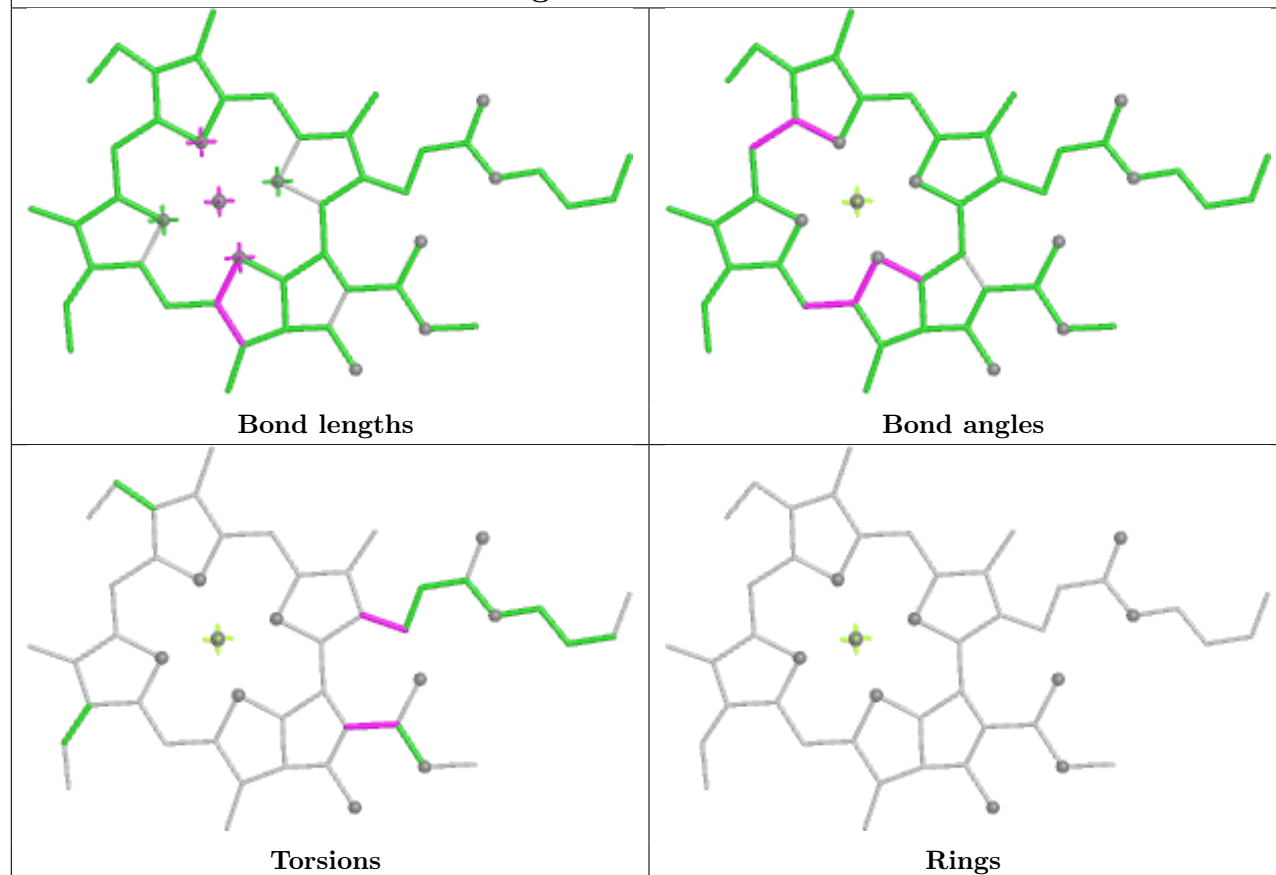


## Ligand CLA B 833

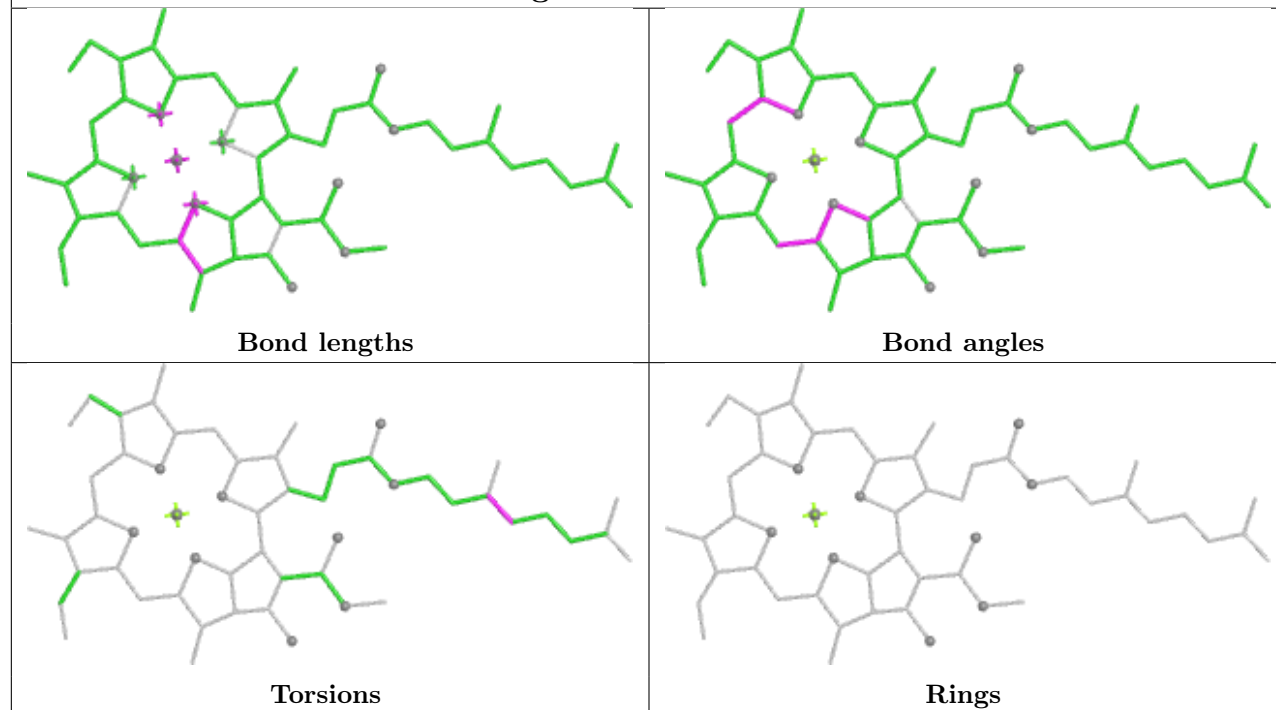


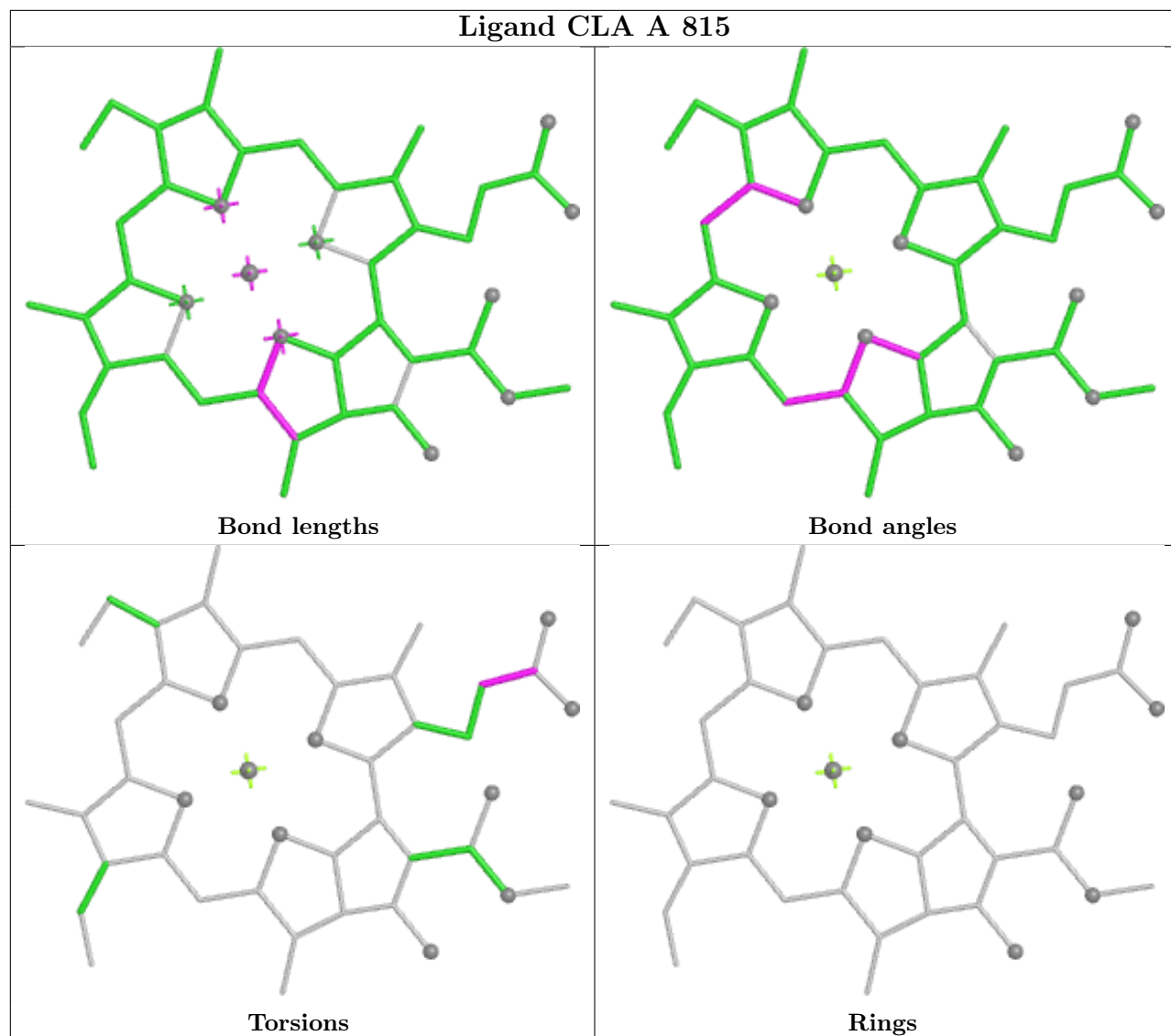


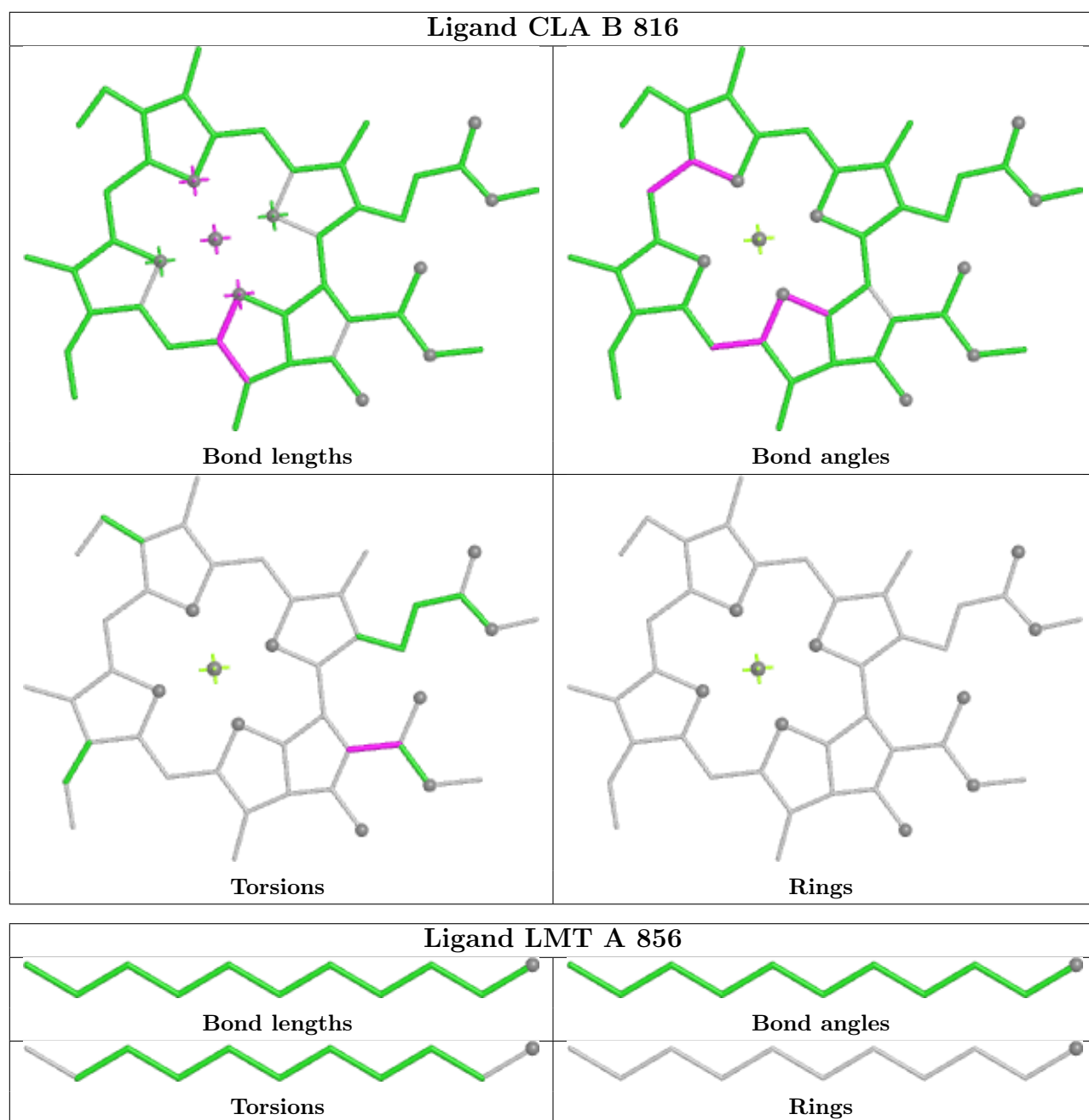
## Ligand CLA A 827

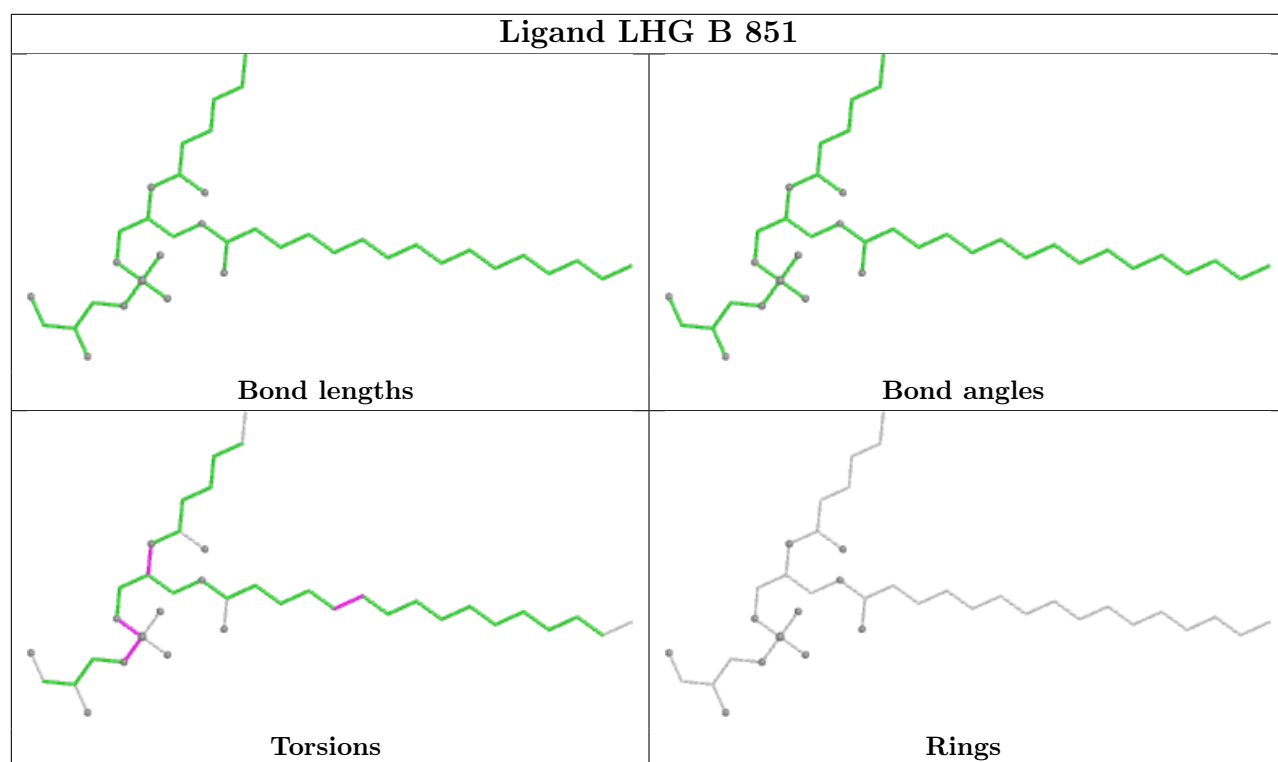


## Ligand CLA A 842

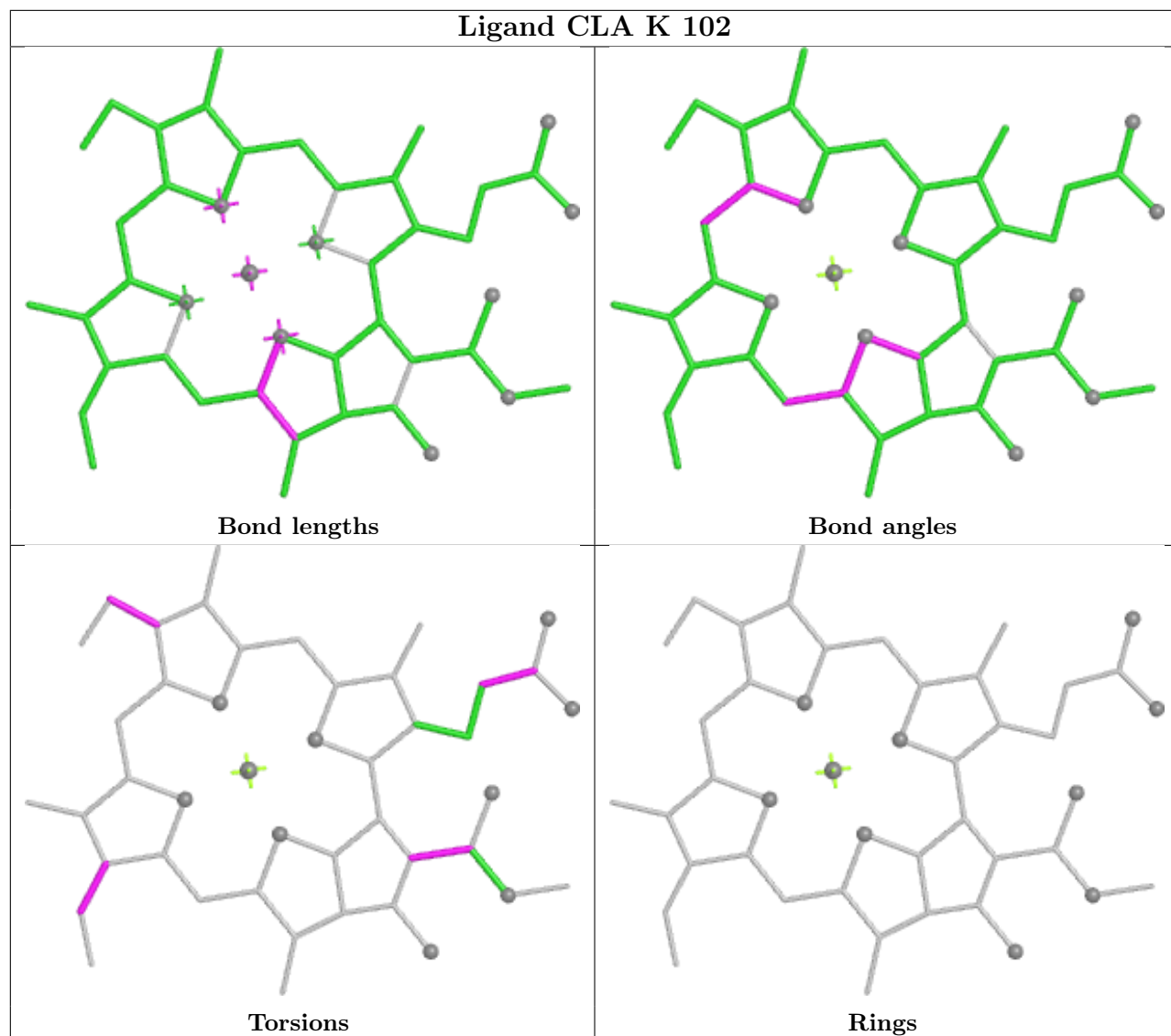




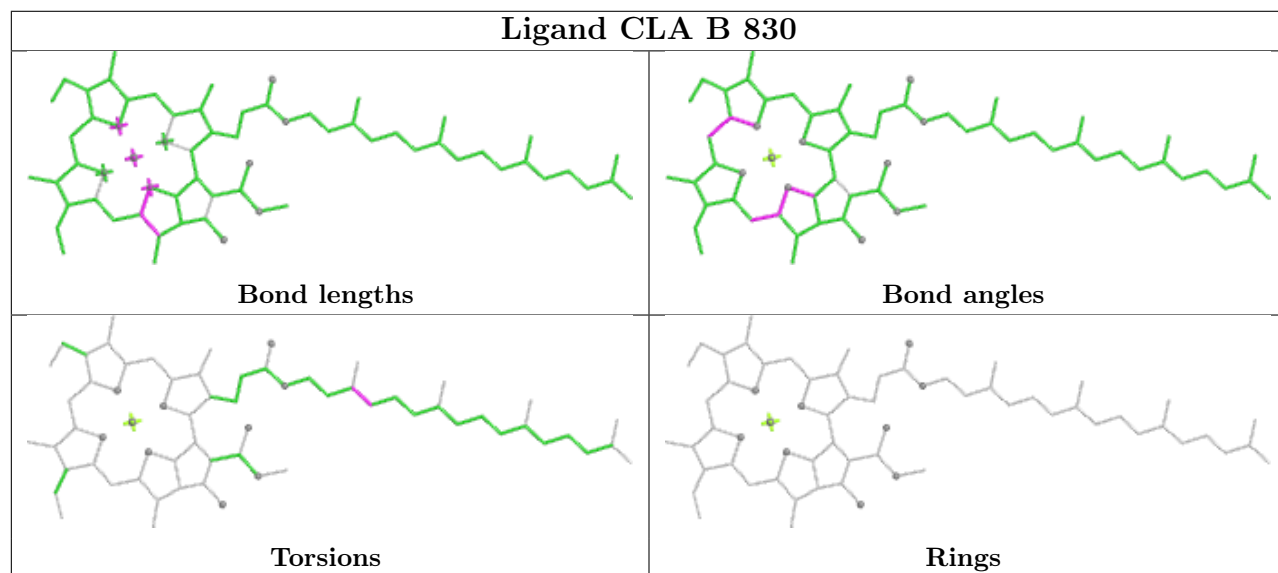


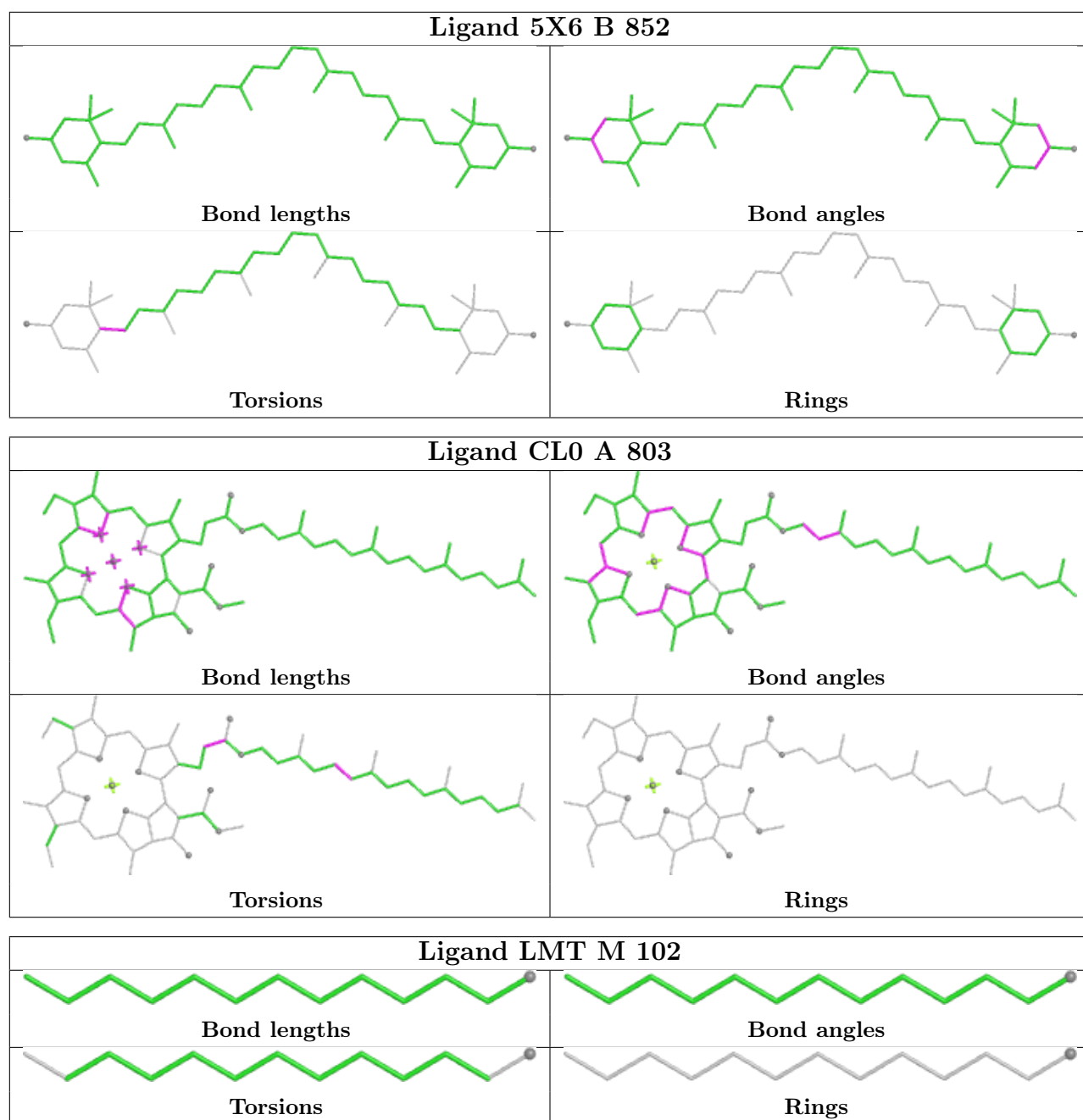


## Ligand CLA K 102

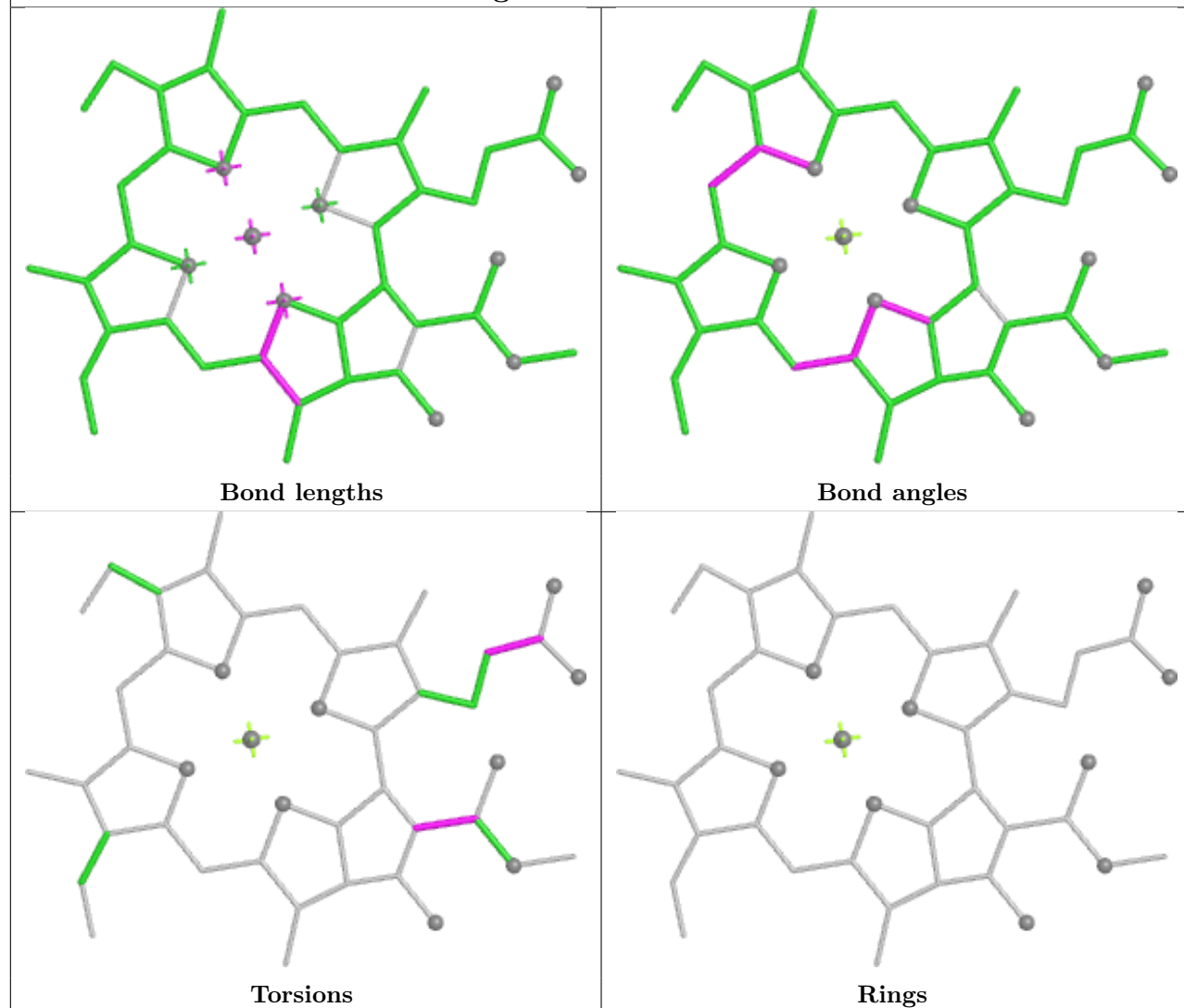


## Ligand CLA B 830

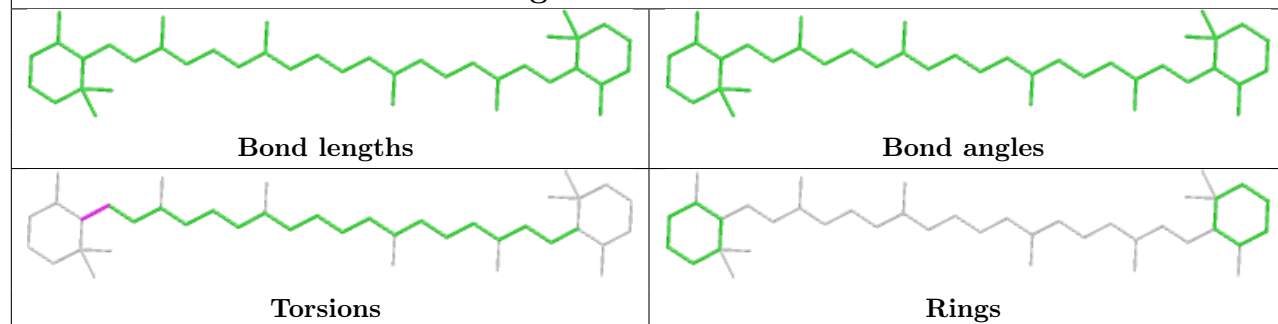


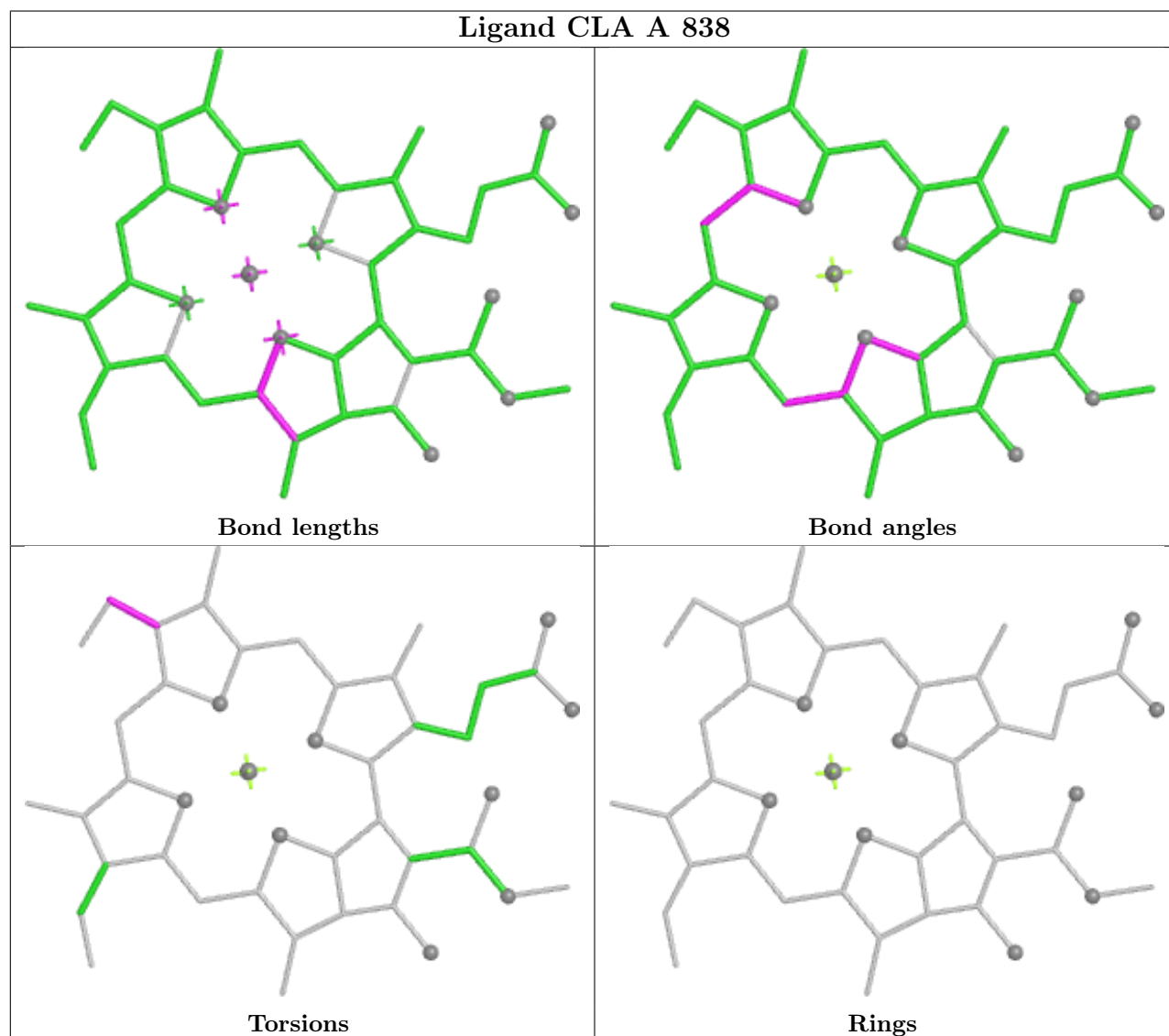
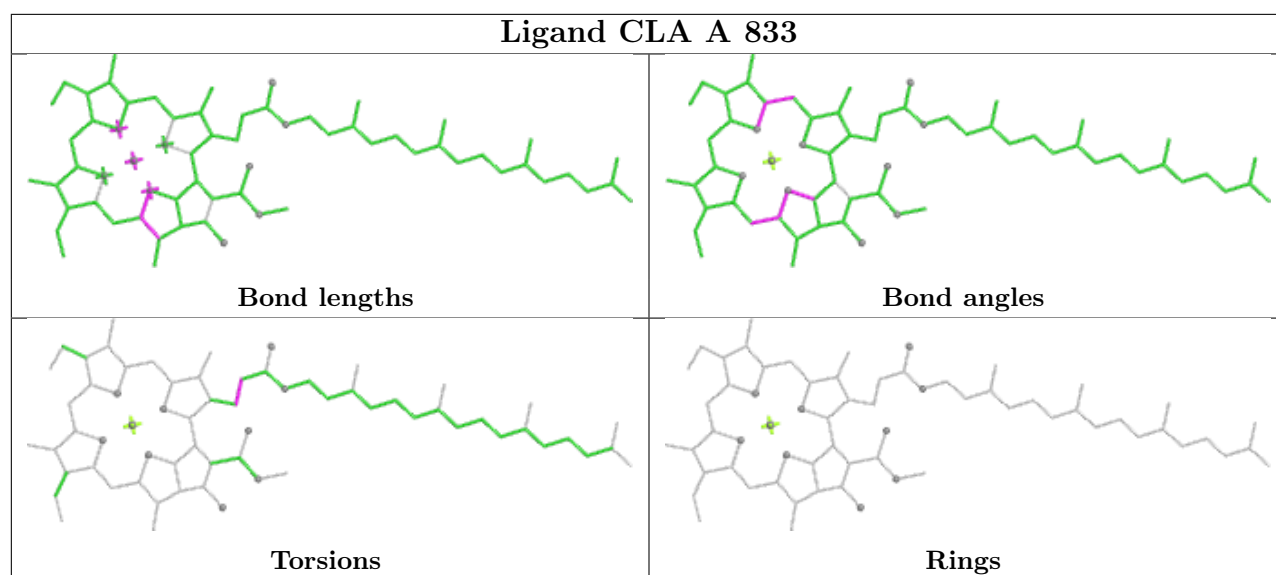


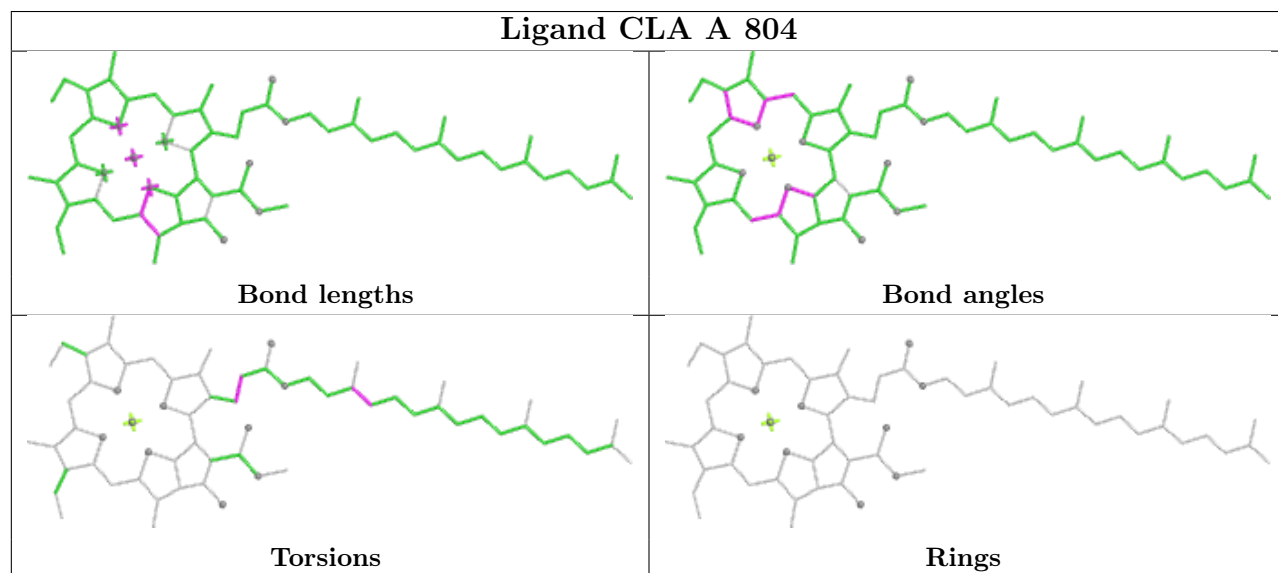
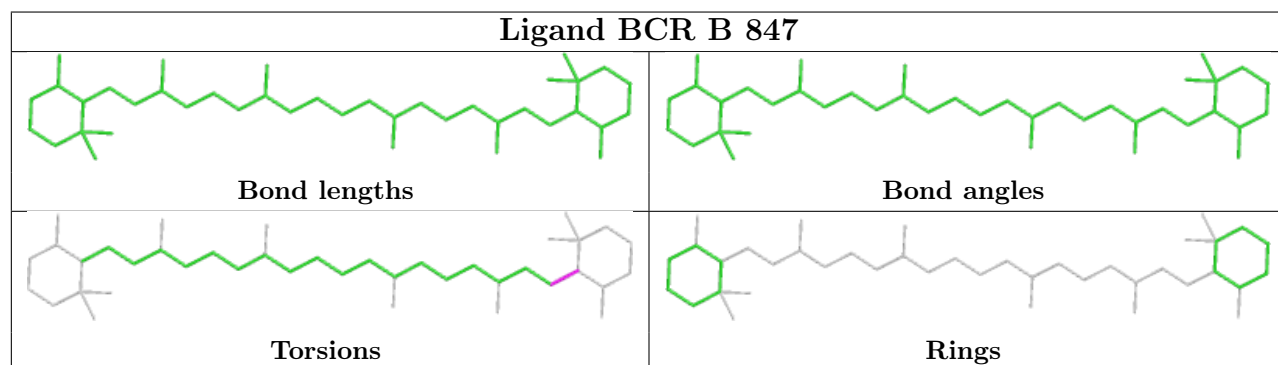
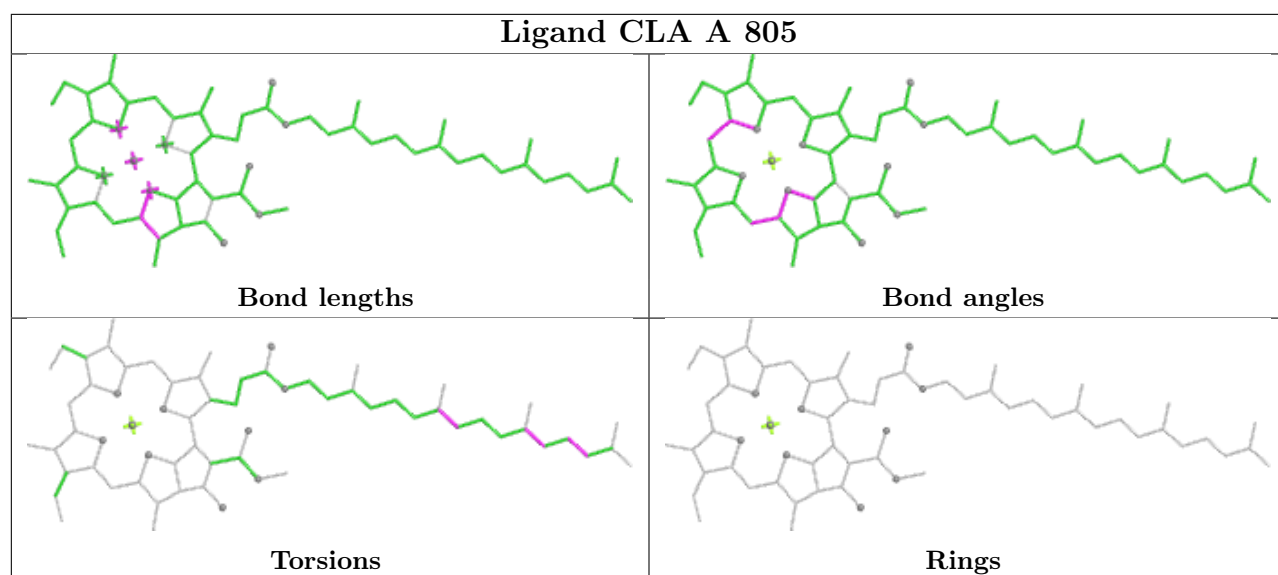
## Ligand CLA B 814

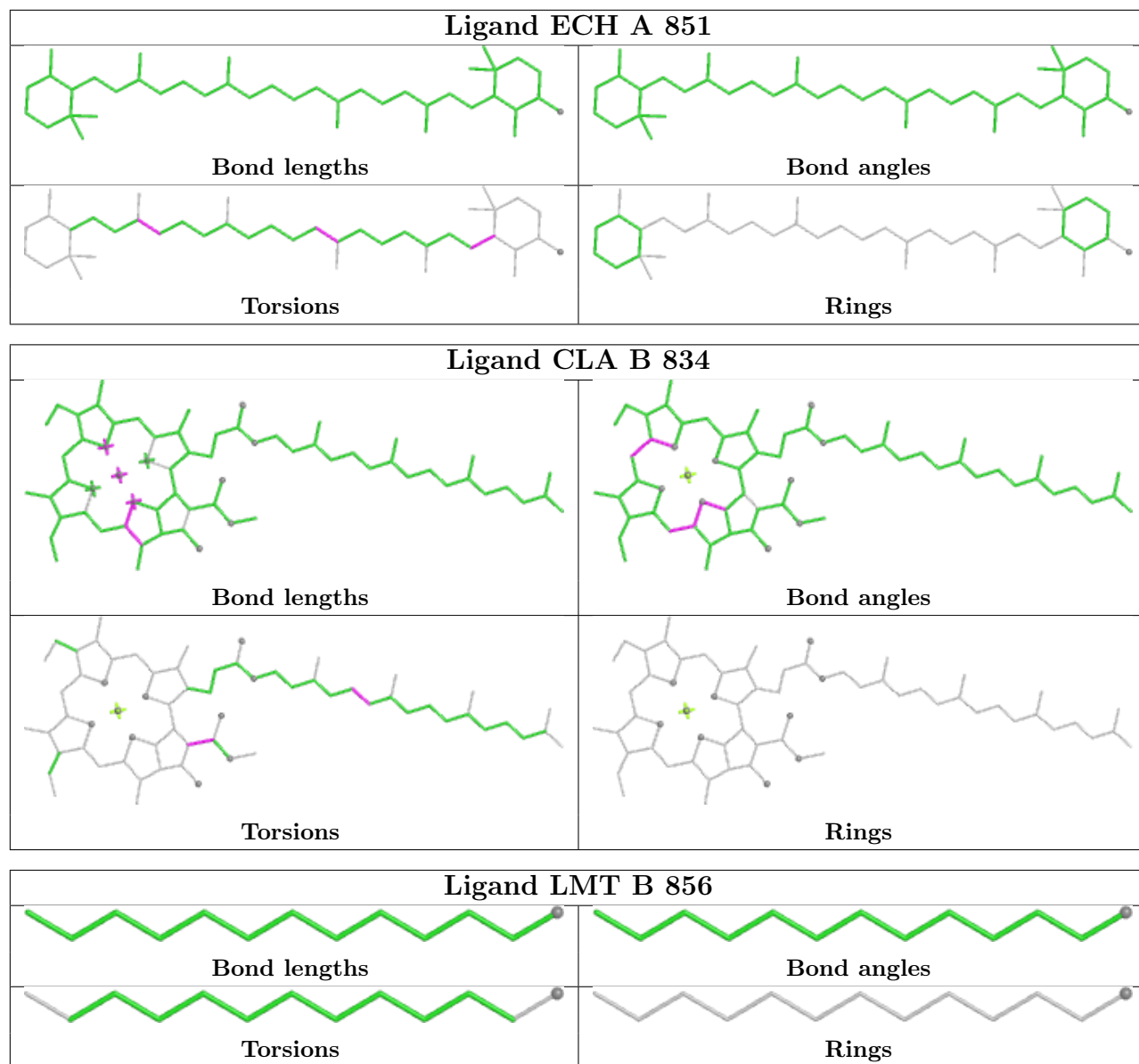


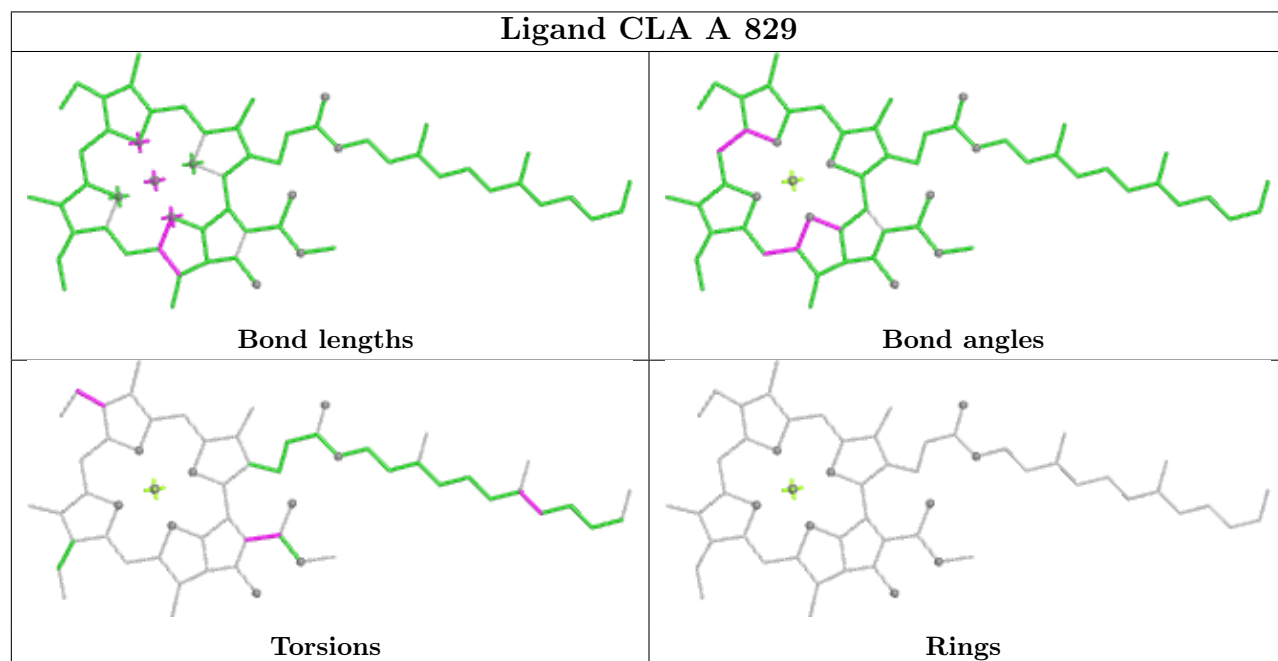
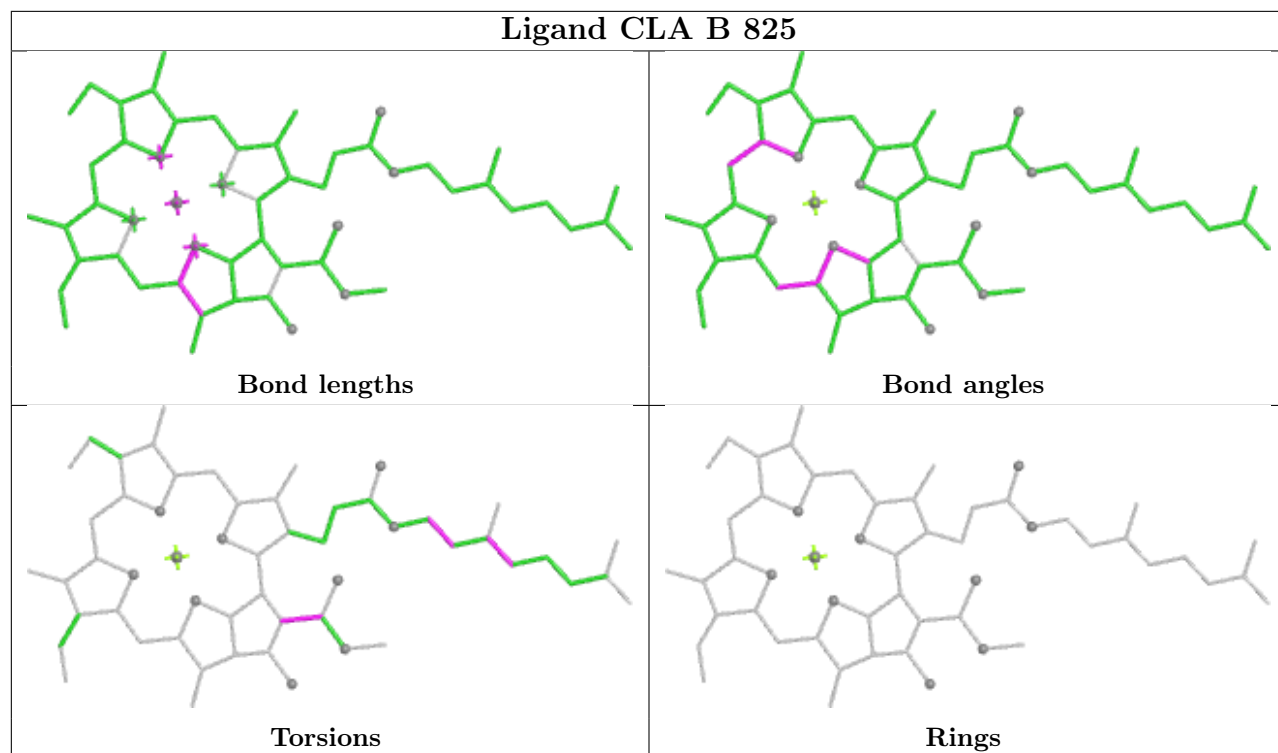
## Ligand BCR A 848



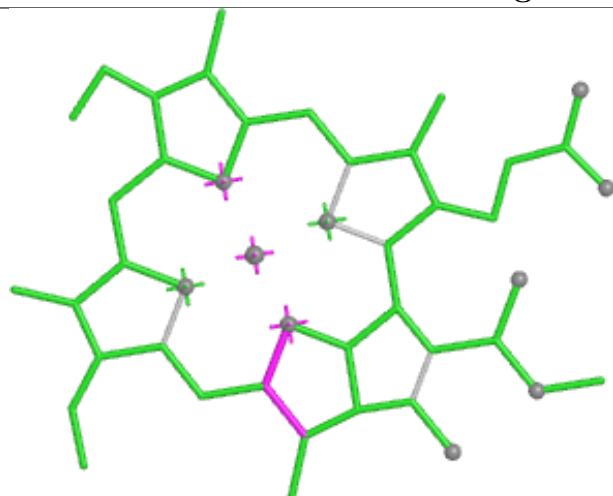




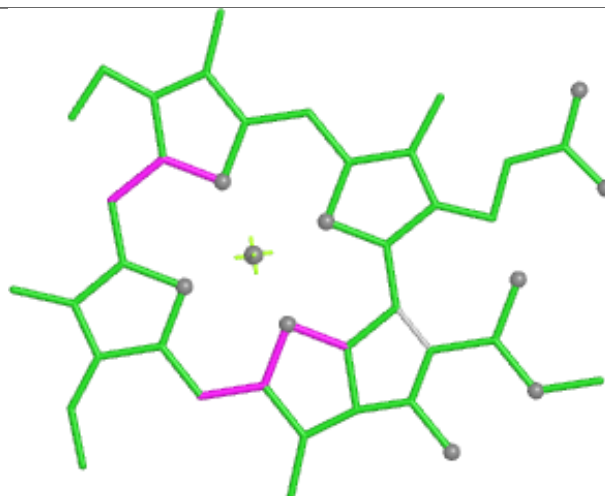




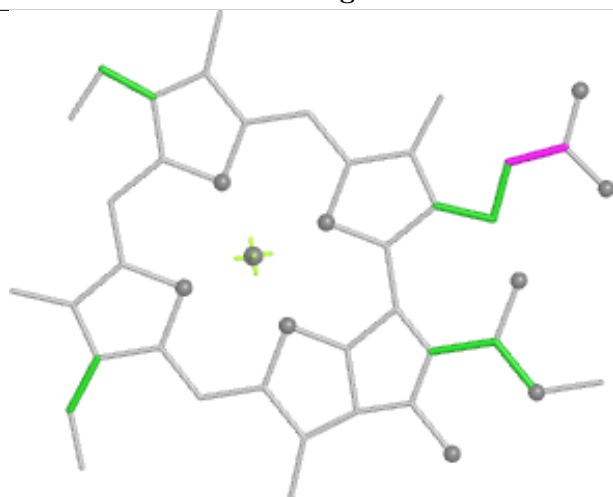
## Ligand CLA B 837



Bond lengths



Bond angles

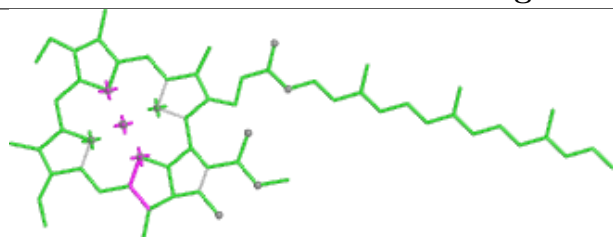


Torsions

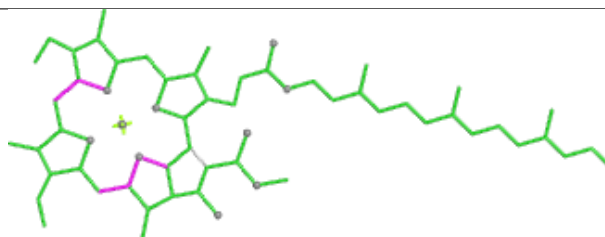


Rings

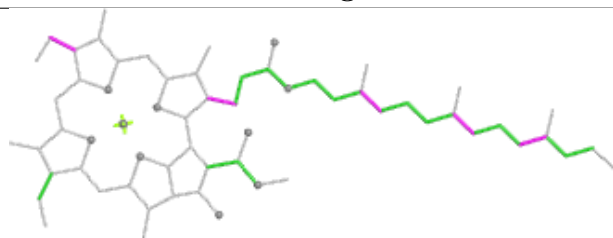
## Ligand CLA B 822



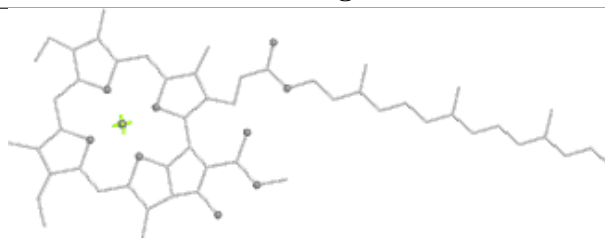
Bond lengths



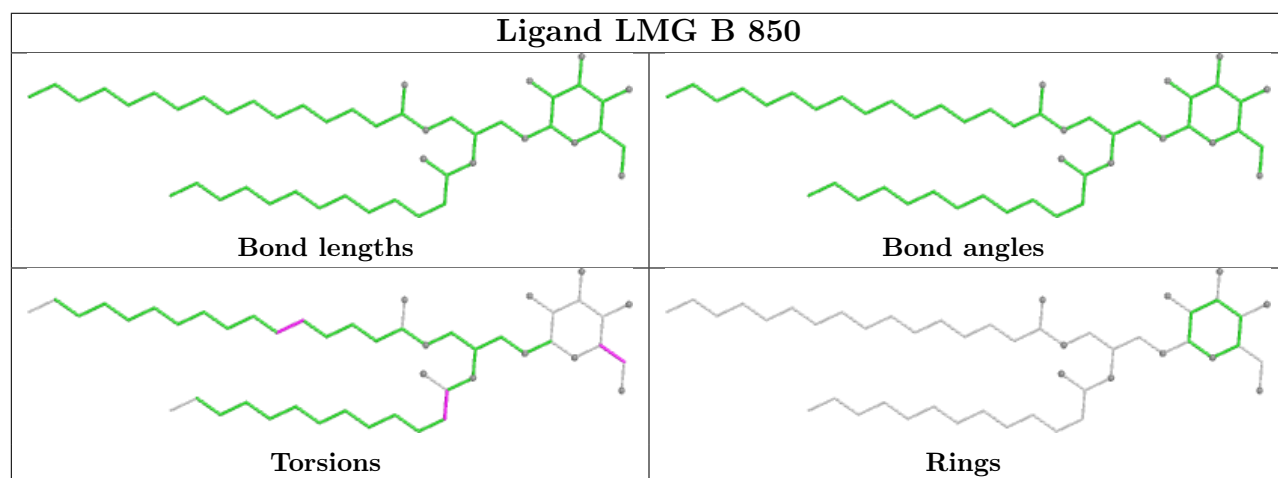
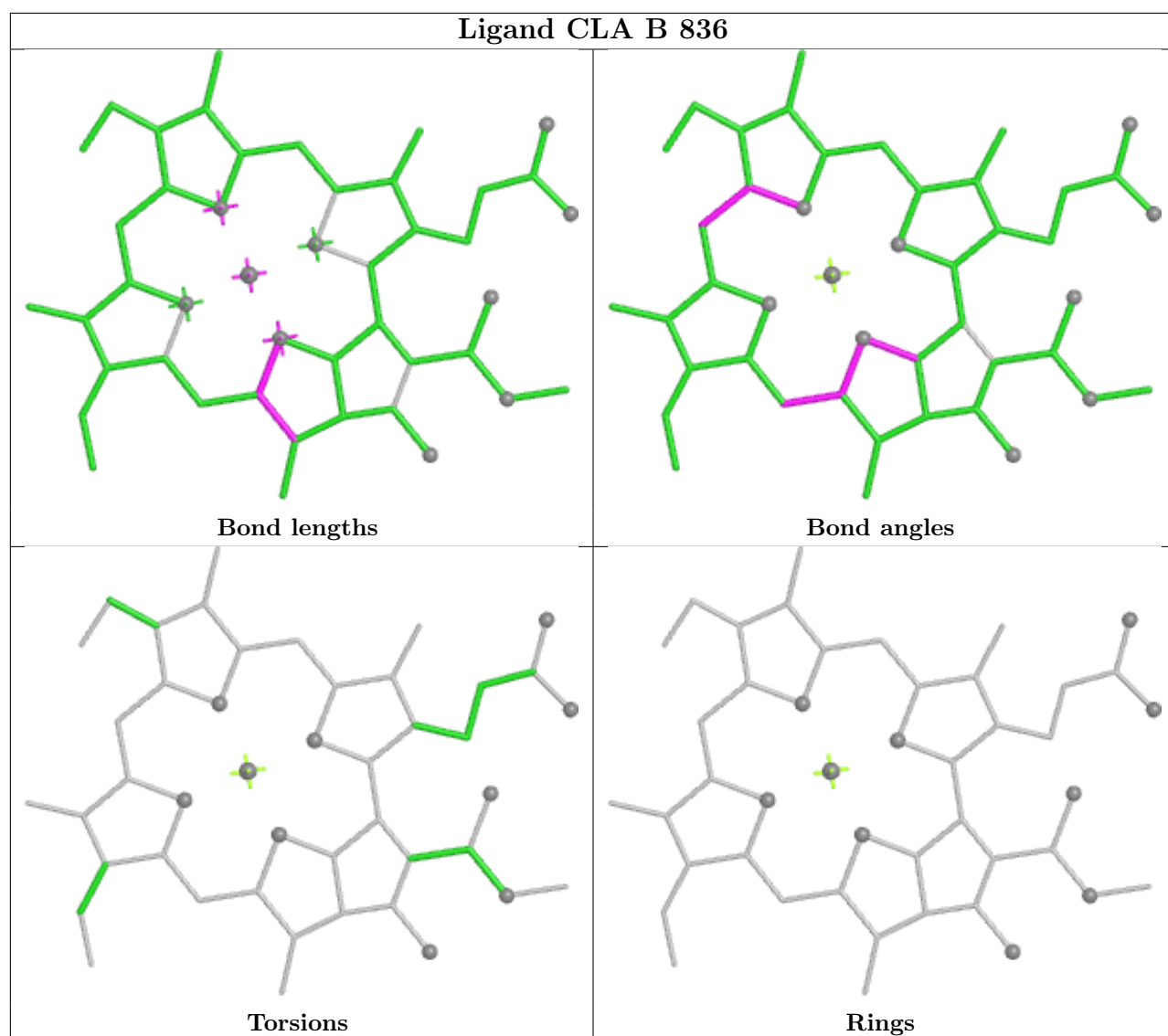
Bond angles

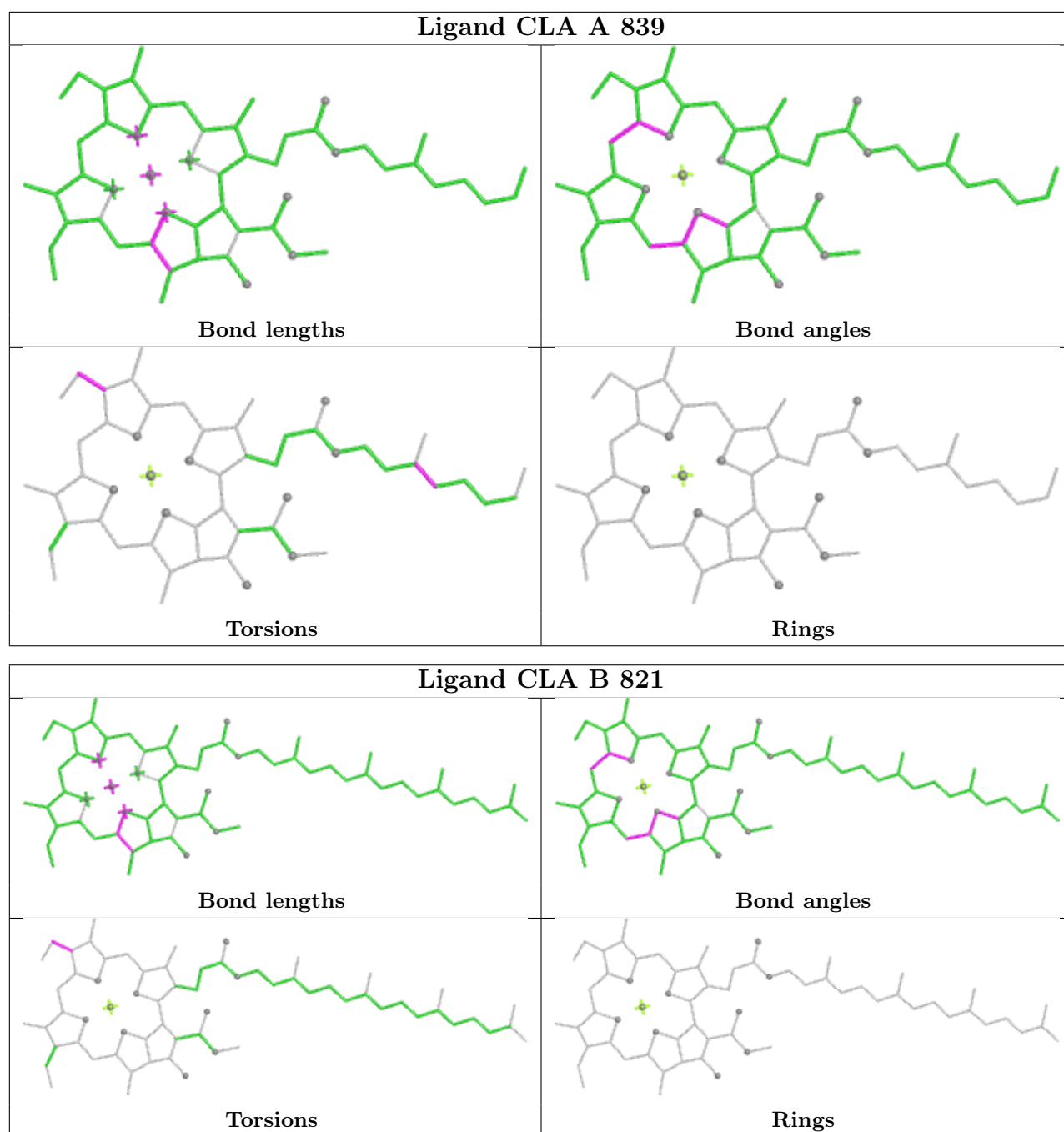


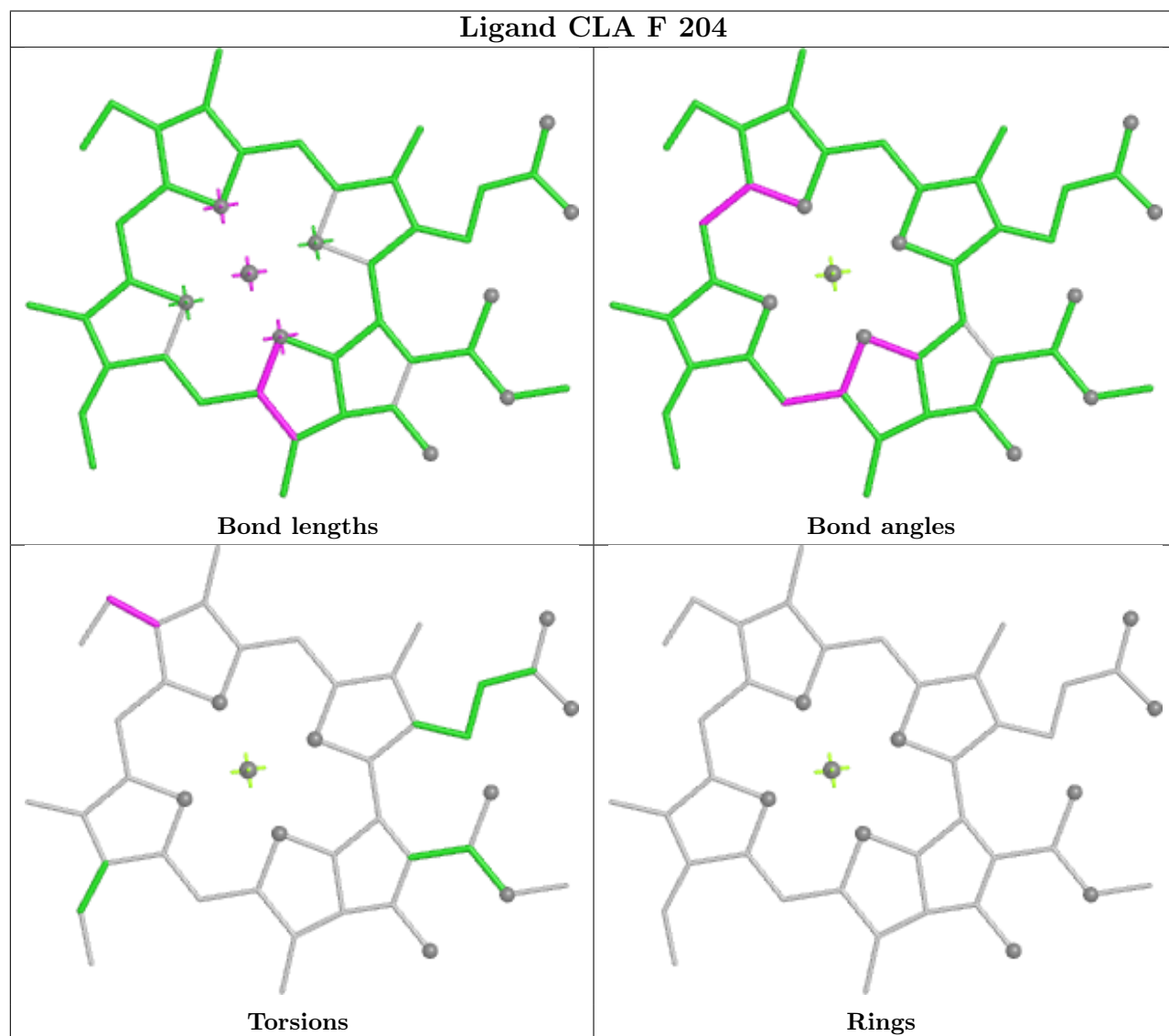
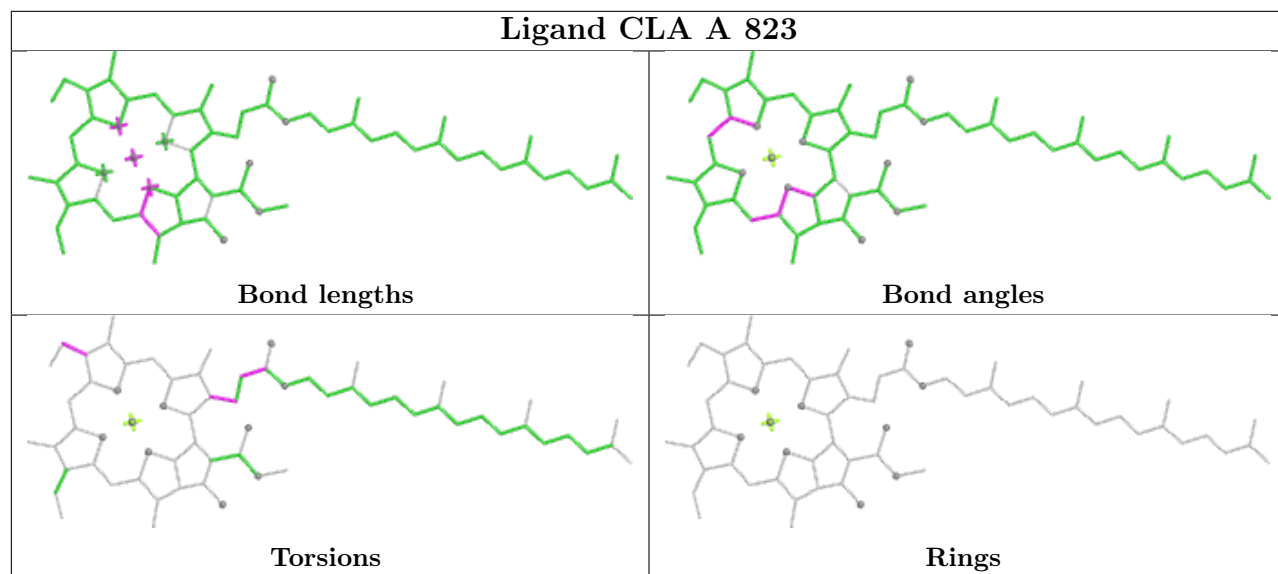
Torsions

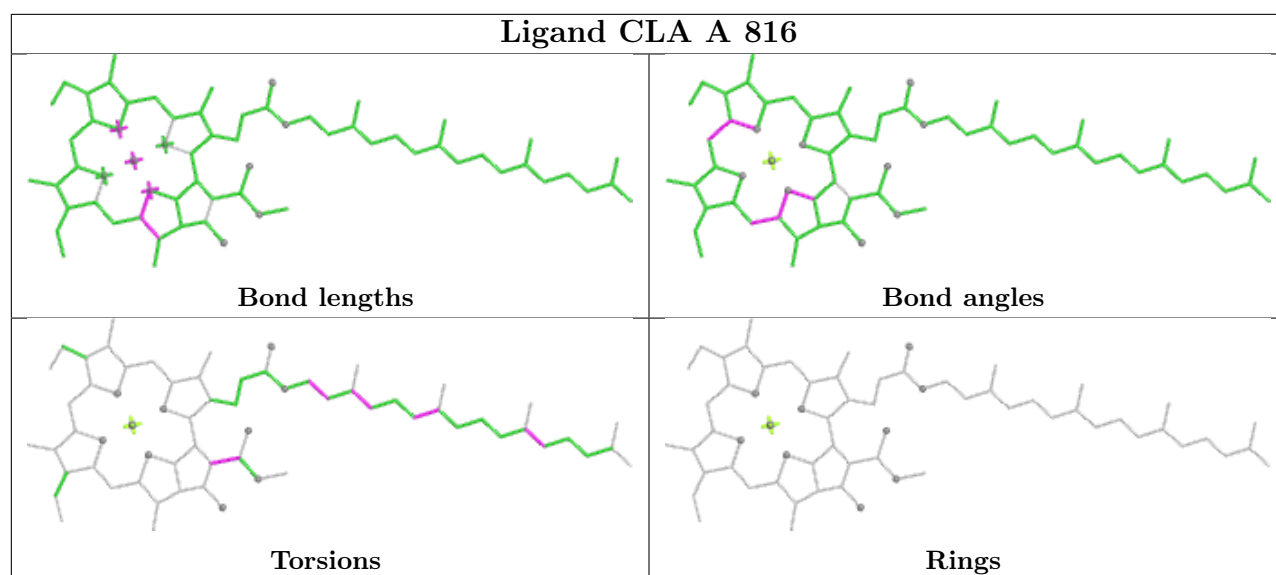


Rings









## 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.

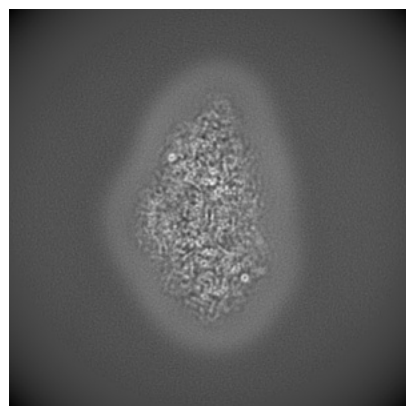
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60522. These allow visual inspection of the internal detail of the map and identification of artifacts.

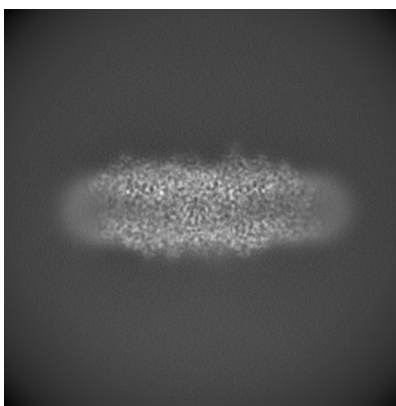
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

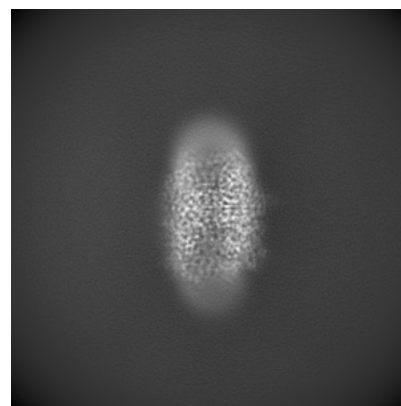
#### 6.1.1 Primary map



X

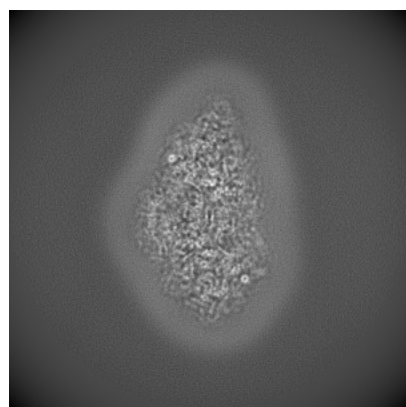


Y

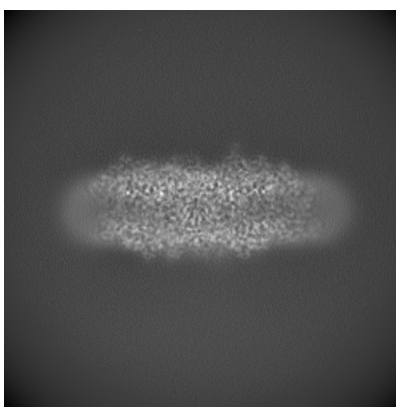


Z

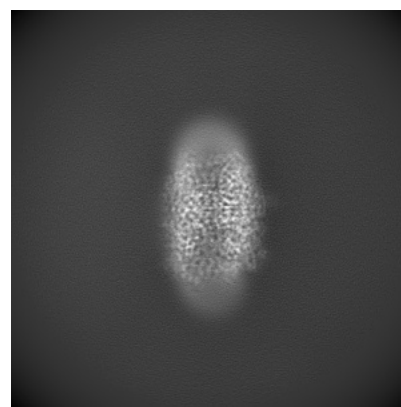
#### 6.1.2 Raw map



X



Y

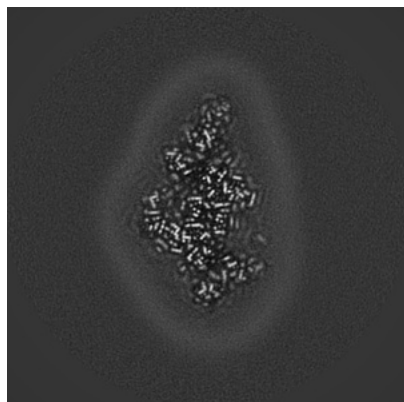


Z

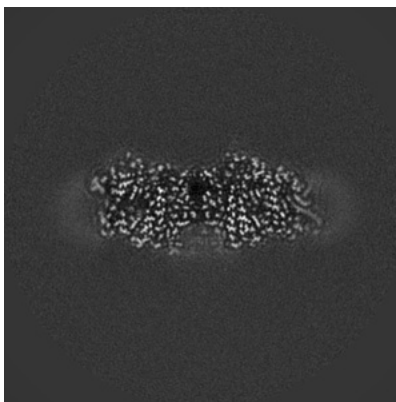
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

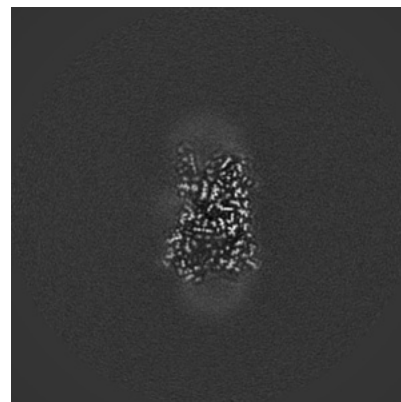
### 6.2.1 Primary map



X Index: 175

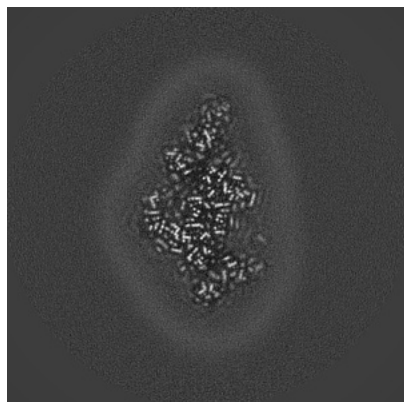


Y Index: 175

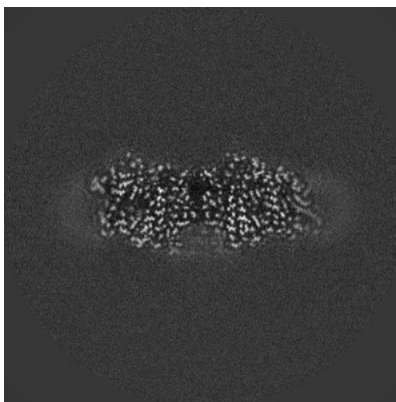


Z Index: 175

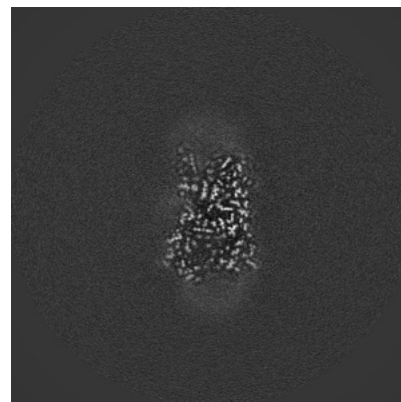
### 6.2.2 Raw map



X Index: 175



Y Index: 175

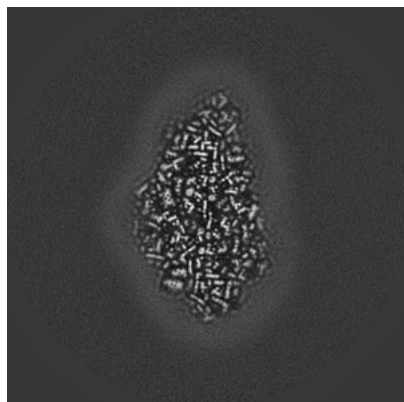


Z Index: 175

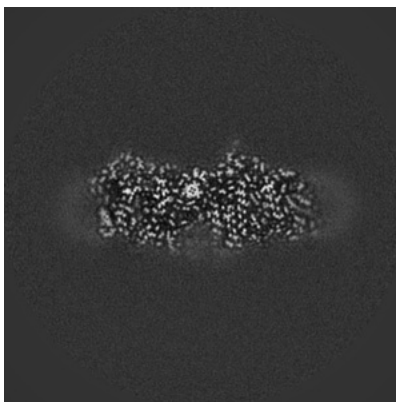
The images above show central slices of the map in three orthogonal directions.

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

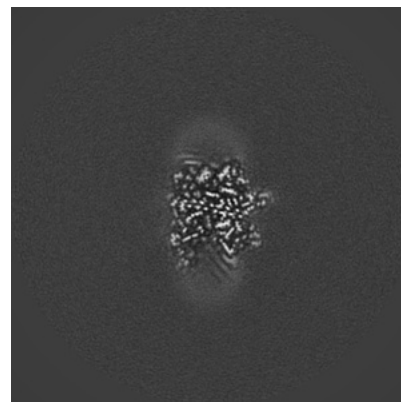
### 6.3.1 Primary map



X Index: 190

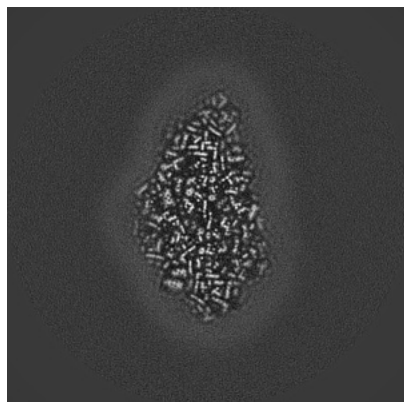


Y Index: 177

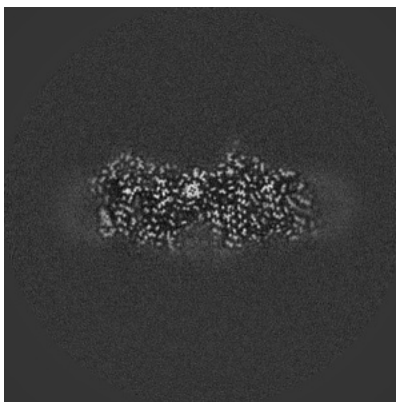


Z Index: 198

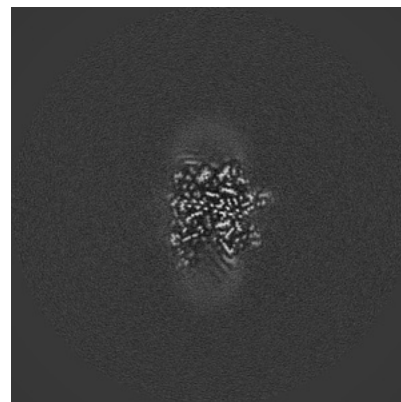
### 6.3.2 Raw map



X Index: 190



Y Index: 177

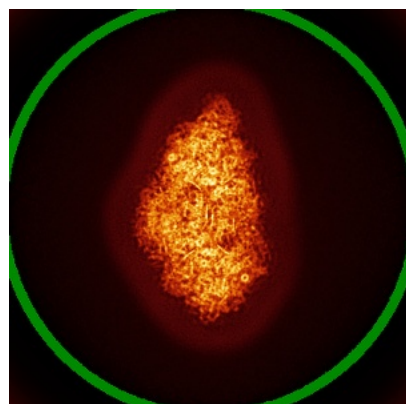


Z Index: 198

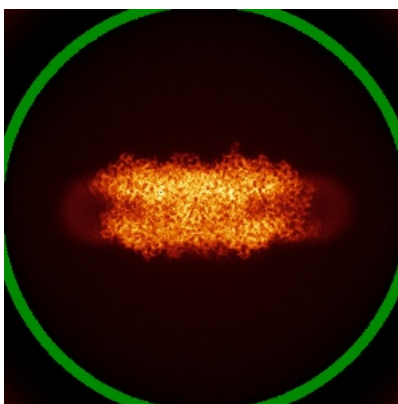
The images above show the largest variance slices of the map in three orthogonal directions.

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

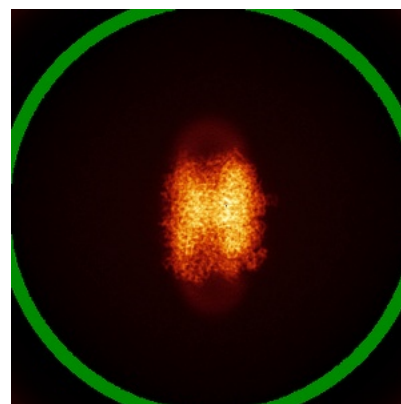
### 6.4.1 Primary map



X

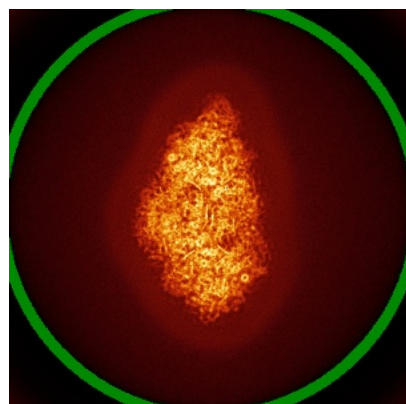


Y

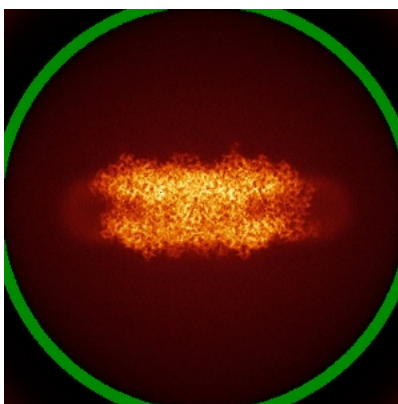


Z

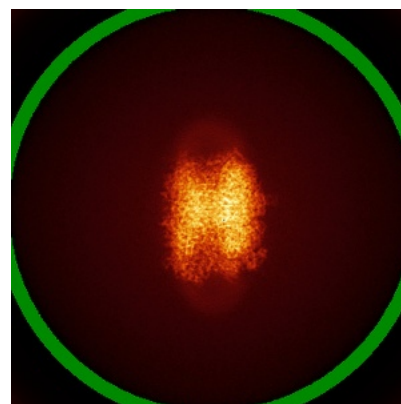
### 6.4.2 Raw map



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.

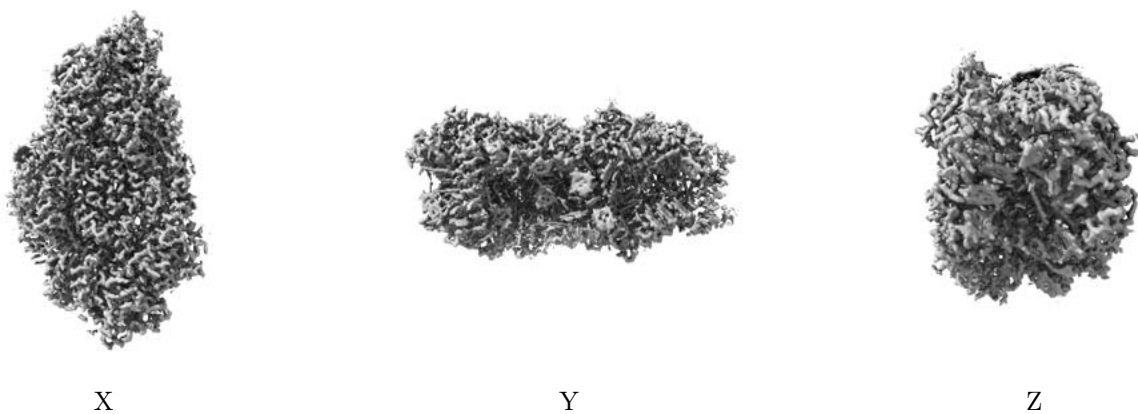
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

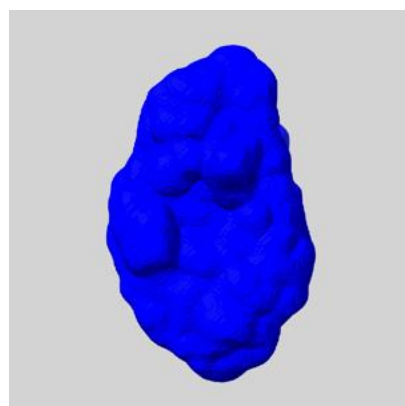
## 6.6 Mask visualisation [i](#)

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

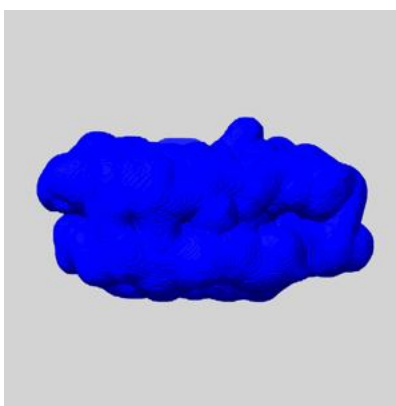
A mask typically either:

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

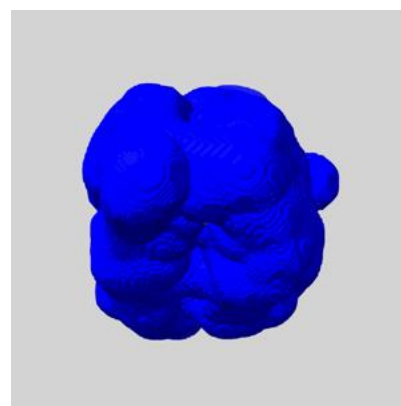
### 6.6.1 emd\_60522\_msk\_1.map [i](#)



X



Y

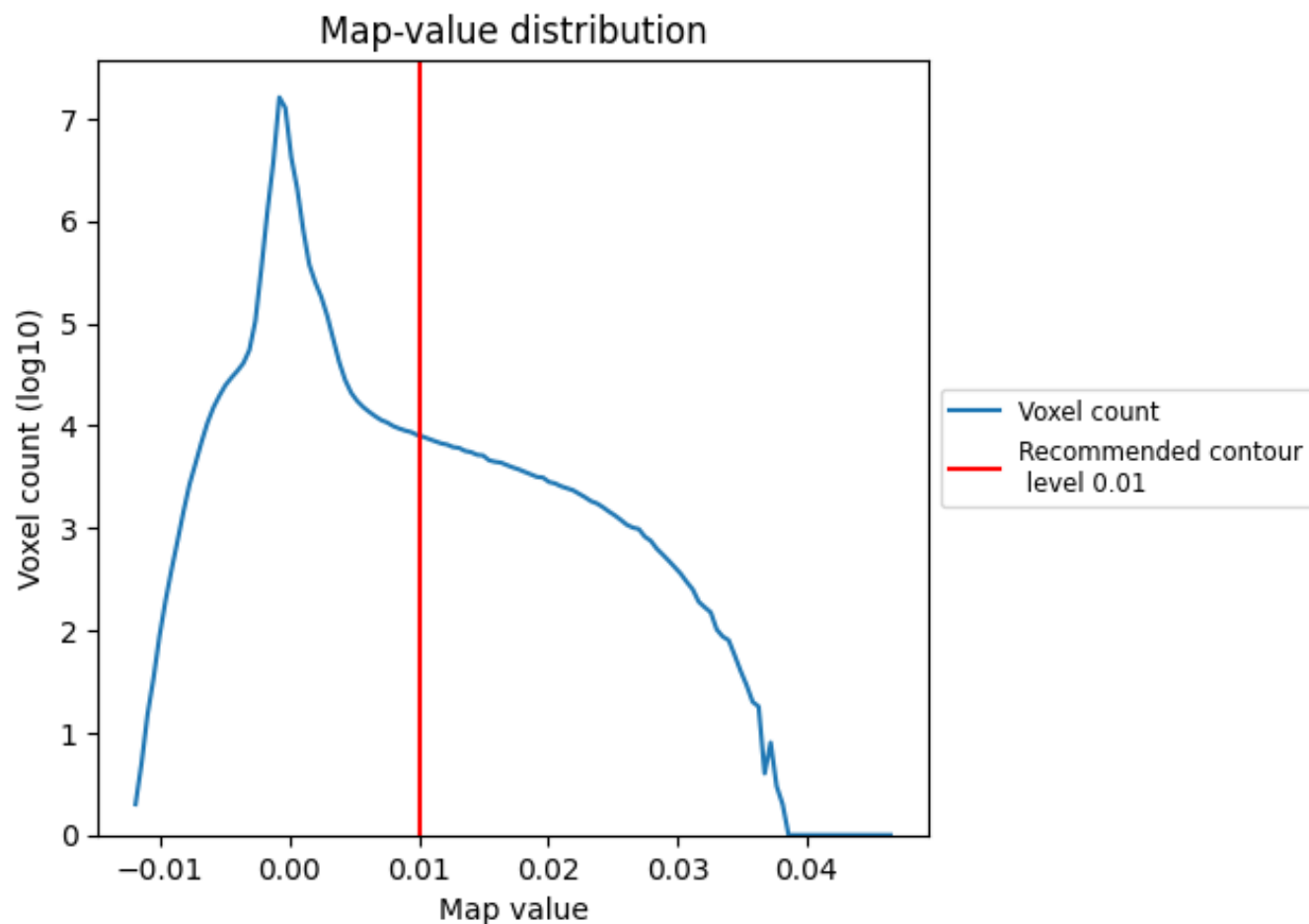


Z

## 7 Map analysis [i](#)

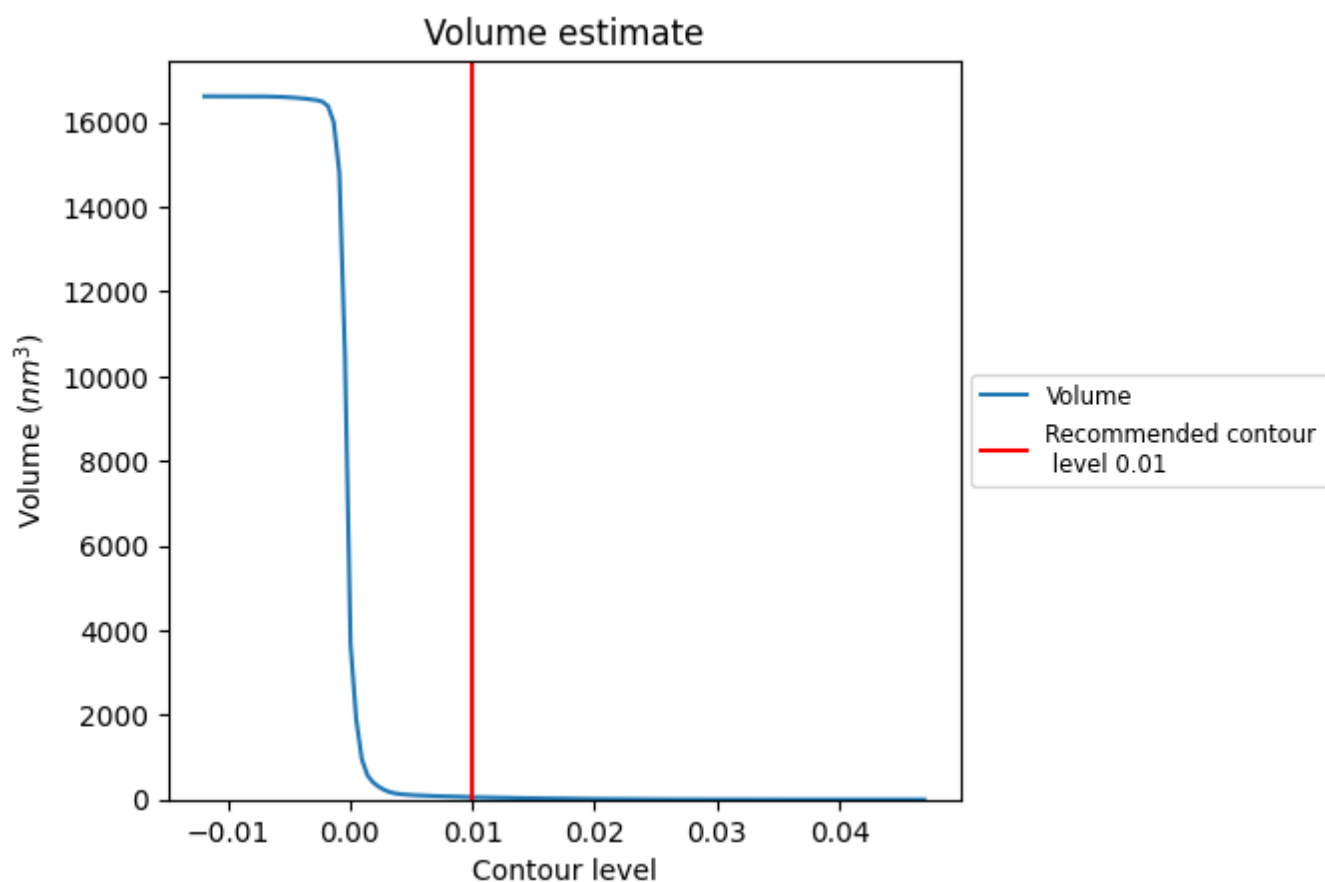
This section contains the results of statistical analysis of the map.

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



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

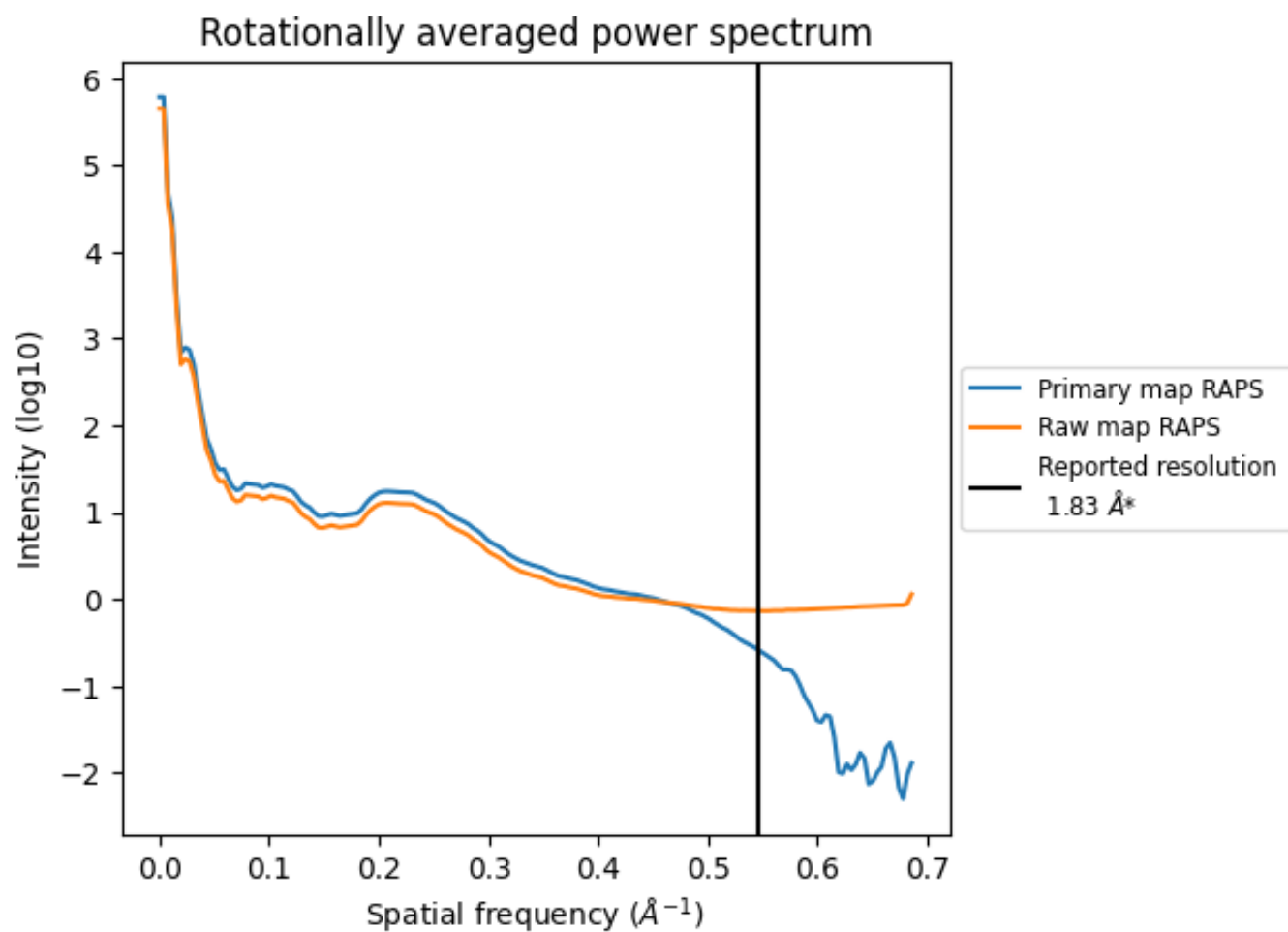
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 57  $\text{nm}^3$ ; this corresponds to an approximate mass of 52 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 ⓘ

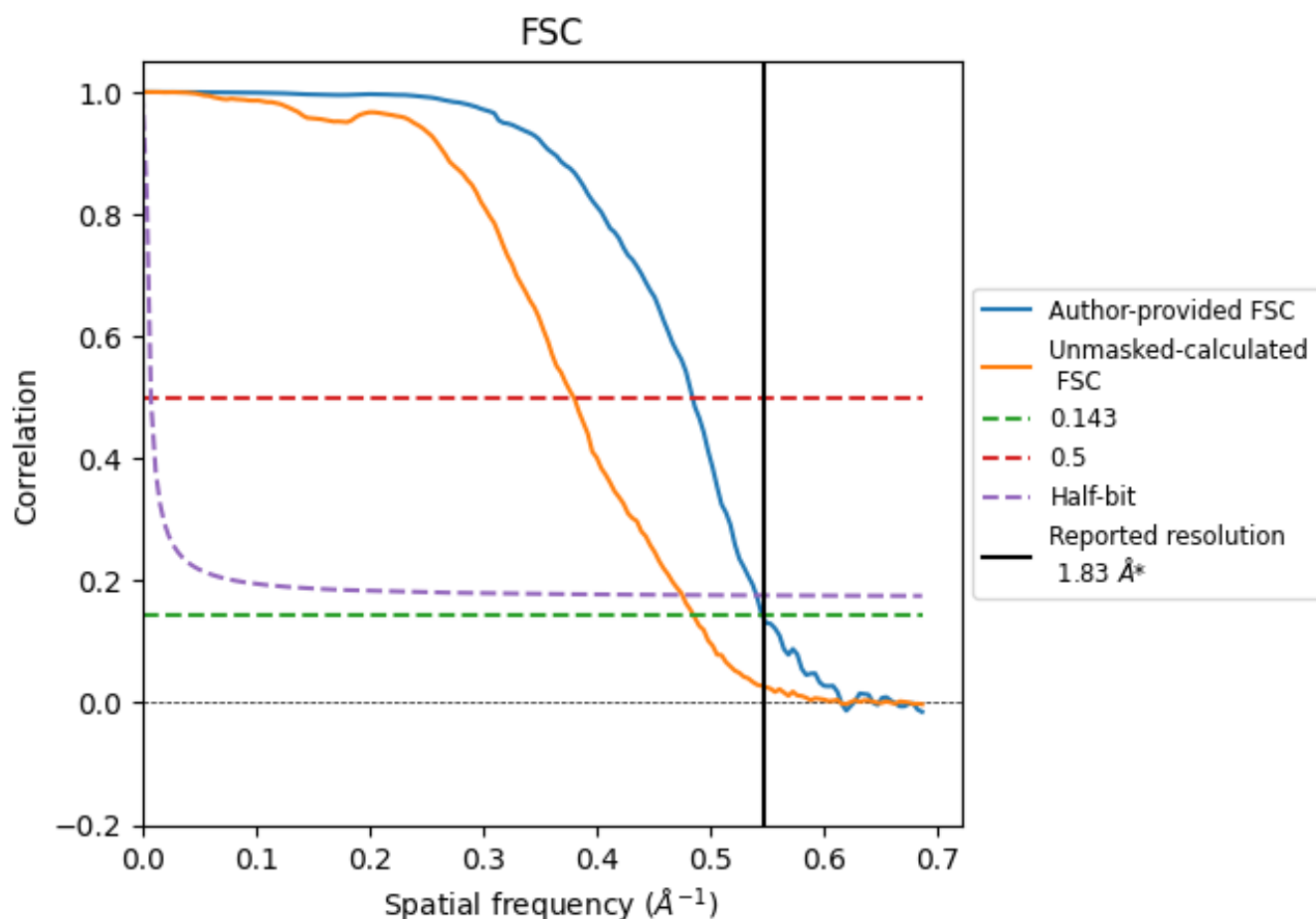


\*Reported resolution corresponds to spatial frequency of 0.546 Å<sup>-1</sup>

## 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 0.546  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

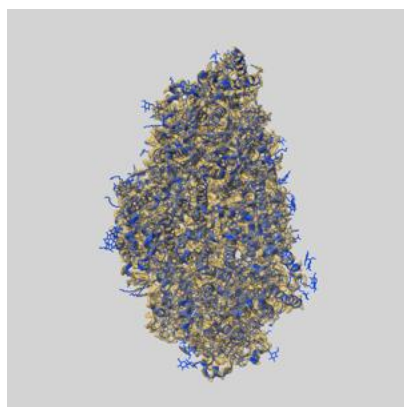
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 1.83                               | -    | -        |
| Author-provided FSC curve | 1.83                               | 2.07 | 1.85     |
| Unmasked-calculated*      | 2.06                               | 2.64 | 2.11     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.06 differs from the reported value 1.83 by more than 10 %

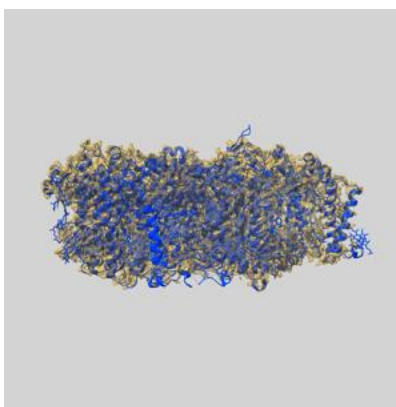
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60522 and PDB model 8ZWB. Per-residue inclusion information can be found in section [3](#) on page [18](#).

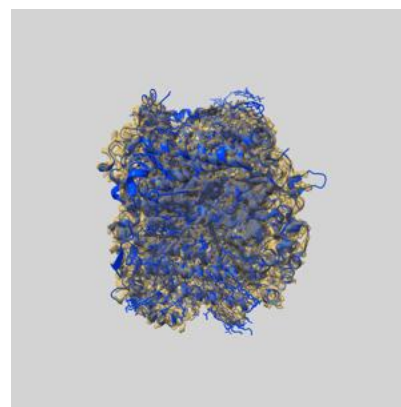
### 9.1 Map-model overlay [i](#)



X



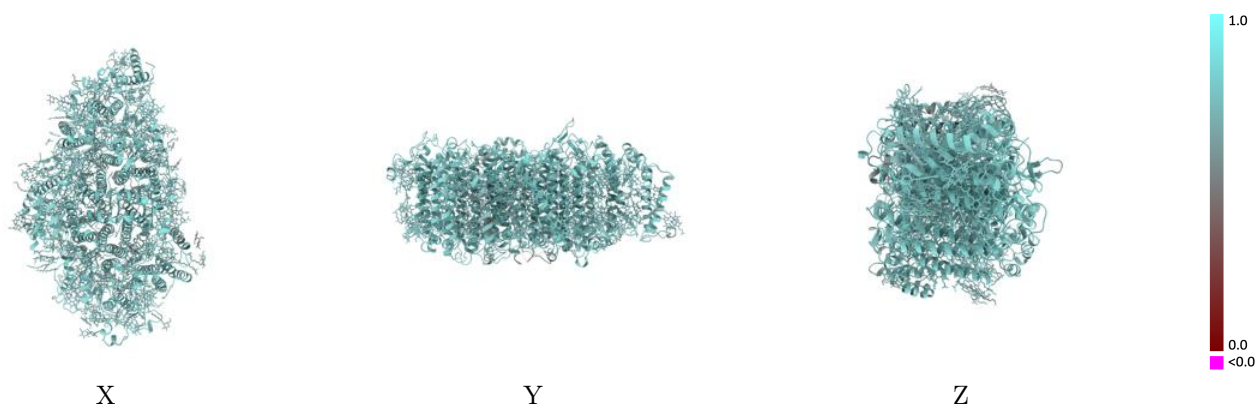
Y



Z

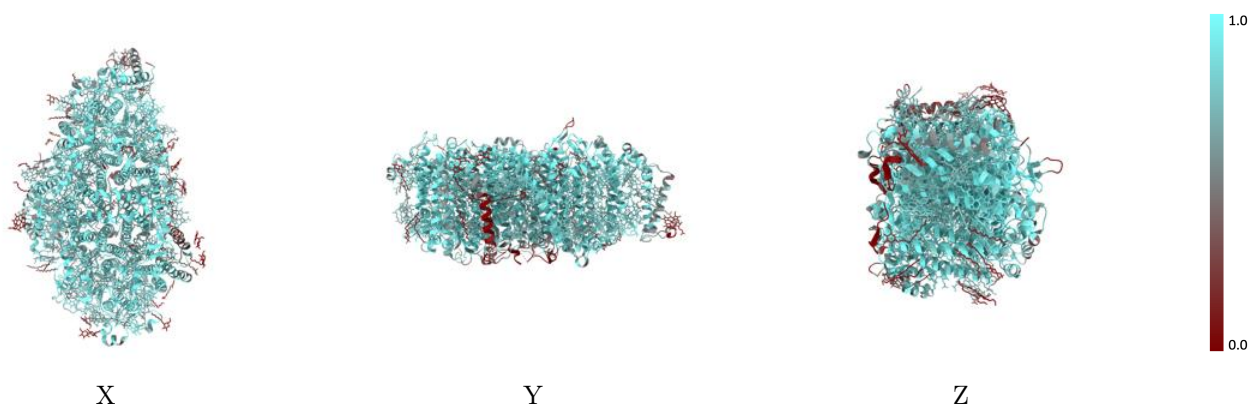
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



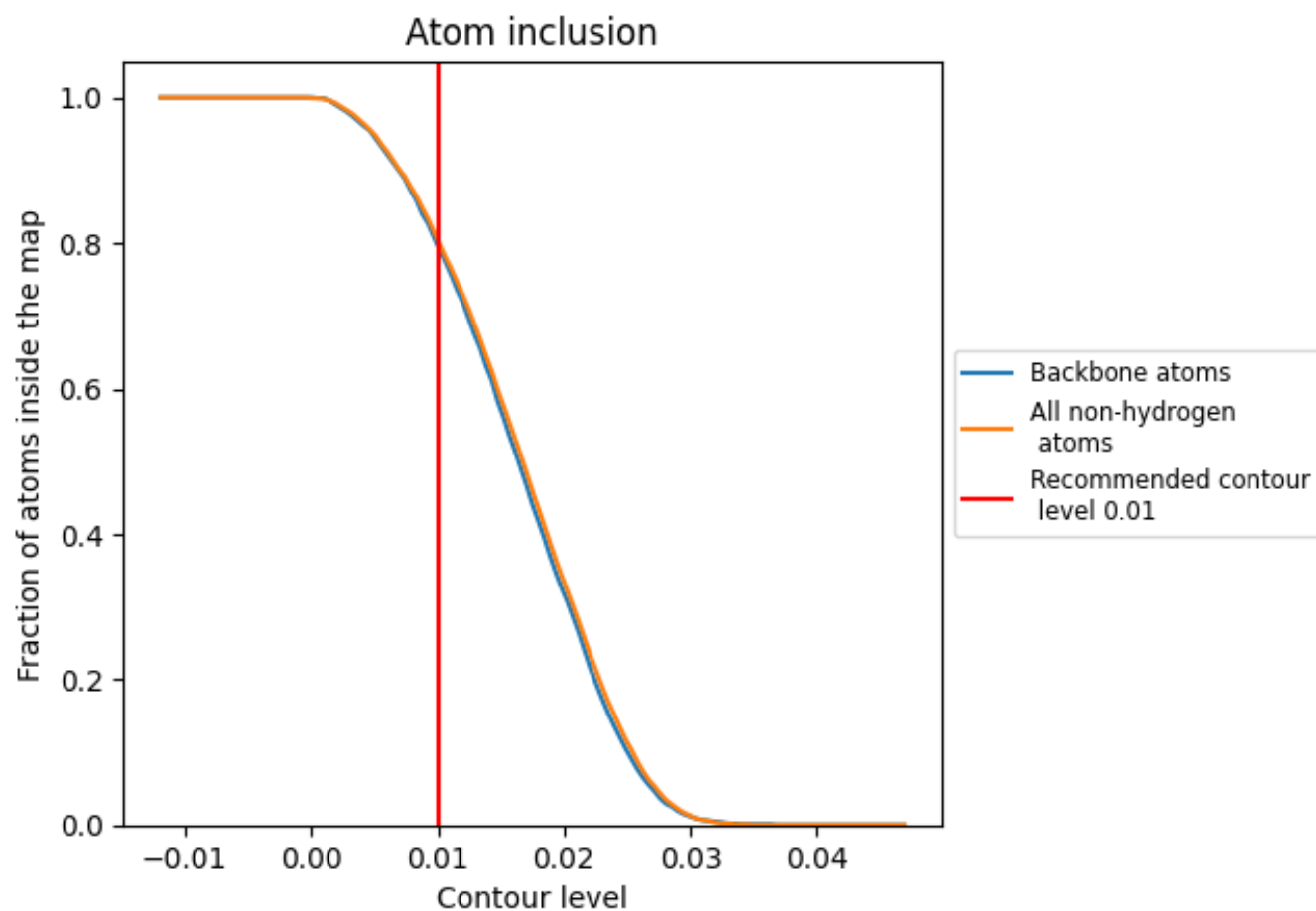
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.01) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion               | Q-score                      |
|-------|------------------------------|------------------------------|
| All   | <div><div></div>0.8050</div> | <div><div></div>0.7450</div> |
| A     | <div><div></div>0.8480</div> | <div><div></div>0.7550</div> |
| B     | <div><div></div>0.8240</div> | <div><div></div>0.7490</div> |
| F     | <div><div></div>0.7400</div> | <div><div></div>0.7330</div> |
| I     | <div><div></div>0.2070</div> | <div><div></div>0.6250</div> |
| J     | <div><div></div>0.7130</div> | <div><div></div>0.7220</div> |
| K     | <div><div></div>0.5660</div> | <div><div></div>0.7020</div> |
| M     | <div><div></div>0.5810</div> | <div><div></div>0.7170</div> |

1.0

0.0

<0.0