



## wwPDB EM Validation Summary Report ⓘ

Sep 15, 2026 – 12:39 AM JST

PDB ID : 8J7B / pdb\_00008j7b  
EMDB ID : EMD-36037  
Title : Coordinates of Cryo-EM structure of the Arabidopsis thaliana PSI in state 2 (PSI-ST2)  
Authors : Chen, S.J.B.; Wu, J.H.; Sui, S.F.; Zhang, L.X.  
Deposited on : 2023-04-27  
Resolution : 3.22 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

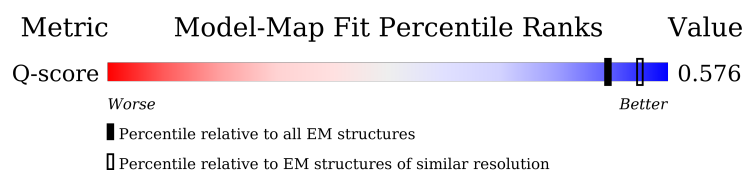
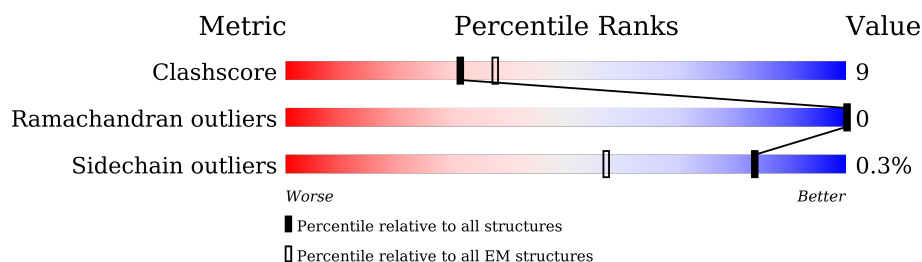
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.22 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                       | 14612 ( 2.72 - 3.72 )                                    |

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   | 1     | 241    |                  |
| 2   | 2     | 257    |                  |
| 3   | 3     | 273    |                  |
| 4   | 4     | 251    |                  |

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| Mol | Chain | Length | Quality of chain                                                                                 |
|-----|-------|--------|--------------------------------------------------------------------------------------------------|
| 5   | A     | 750    |  89% 10% .     |
| 6   | B     | 734    |  89% 11%       |
| 7   | C     | 81     |  91% 7% .      |
| 8   | D     | 204    |  65% 5% 30%    |
| 9   | E     | 143    |  43% . 55%     |
| 10  | F     | 221    |  63% 5% 31%    |
| 11  | G     | 160    |  52% 5% 43%    |
| 12  | H     | 145    |  56% 6% 38%    |
| 13  | I     | 37     |  76% 8% 16%    |
| 14  | J     | 44     |  77% 16% 7%    |
| 15  | K     | 130    |  . 52% 13% 35% |
| 16  | L     | 219    |  66% 7% 27%    |

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 35077 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein 6, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | 1     | 193      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1496  | 975 | 248 | 268 | 5 |         |       |

- Molecule 2 is a protein called Photosystem I chlorophyll a/b-binding protein 2, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | 2     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1566  | 1024 | 256 | 282 | 4 |         |       |

- Molecule 3 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | 3     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1666  | 1088 | 270 | 303 | 5 |         |       |

- Molecule 4 is a protein called Chlorophyll a-b binding protein 4, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | 4     | 196      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1551  | 1013 | 253 | 282 | 3 |         |       |

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | A     | 737      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5807  | 3807 | 986 | 996 | 18 |         |       |

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 6   | B     | 732      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5854  | 3842 | 997 | 1001 | 14 |         |       |

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 7   | C     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 616   | 381 | 107 | 117 | 11 |         |       |

- Molecule 8 is a protein called Photosystem I reaction center subunit II-2, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | D     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1128  | 723 | 195 | 206 | 4 |         |       |

- Molecule 9 is a protein called Photosystem I reaction center subunit IV A, chloroplastic.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | E     | 64       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 517   | 331 | 92 | 94 |   |         |       |

- Molecule 10 is a protein called Photosystem I reaction center subunit III, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | F     | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 789 | 207 | 209 | 3 |         |       |

- Molecule 11 is a protein called Photosystem I reaction center subunit V, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | G     | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 458 | 118 | 132 |   |         |       |

- Molecule 12 is a protein called Photosystem I reaction center subunit VI-2, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | H     | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 693   | 451 | 112 | 130 |   |         |       |

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 13  | I     | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 239   | 162 | 39 | 37 | 1 |         |       |

- Molecule 14 is a protein called Photosystem I reaction center subunit IX.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 14  | J     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 327   | 221 | 50 | 55 | 1 |         |       |

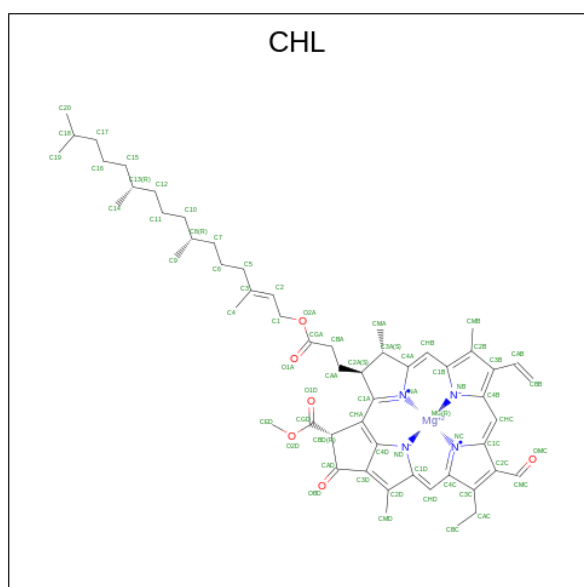
- Molecule 15 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | K     | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 593   | 373 | 104 | 113 | 3 |         |       |

- Molecule 16 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | L     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1207  | 799 | 191 | 215 | 2 |         |       |

- Molecule 17 is CHLOROPHYLL B (CCD ID: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



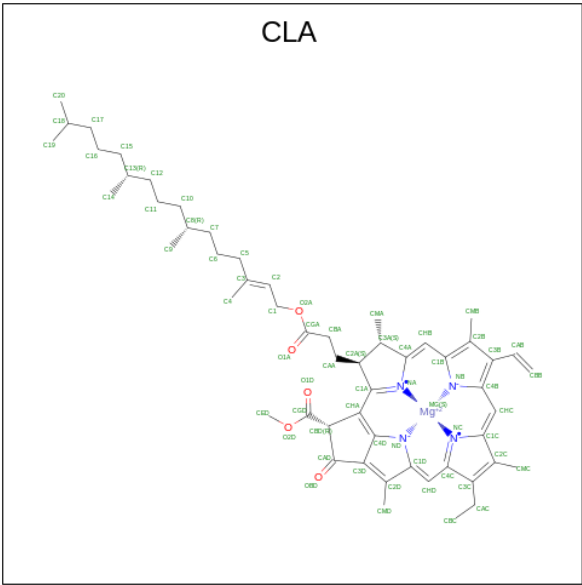
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 17  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 41 | 1  | 4 | 6 |         |
| 17  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 32 | 1  | 4 | 4 |         |
| 17  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 33 | 1  | 4 | 4 |         |
| 17  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 17  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 17  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 17  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 17  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 17  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 17  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 32 | 1  | 4 | 4 |         |
| 17  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 32 | 1  | 4 | 4 |         |
| 17  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (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 |
|-----|-------|----------|-------|----|----|---|---|---------|
| 18  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 18  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 18  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 18  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 18  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 18  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 40    | 32 | 1  | 4 | 3 |         |
| 18  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 18  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 30 | 1  | 4 | 3 |         |
| 18  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 18  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 30 | 1  | 4 | 3 |         |
| 18  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 18  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 18  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 18  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 35 | 1  | 4 | 3 |         |
| 18  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 30 | 1  | 4 | 3 |         |
| 18  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 18  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 18  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 36    | 30 | 1  | 4 | 1 |         |
| 18  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 18  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 18  | 3     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | 3     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 3     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 3     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | 3     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | 3     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 3     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 4     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 4     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 4     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 4     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 4     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 4     | 1        | Total<br>57 | C<br>47 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 4     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | 4     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | 4     | 1        | Total<br>43 | C<br>33 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 4     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 4     | 1        | Total<br>44 | C<br>34 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | A     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 35 | 1  | 4 | 3 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 62    | 52 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 35 | 1  | 4 | 3 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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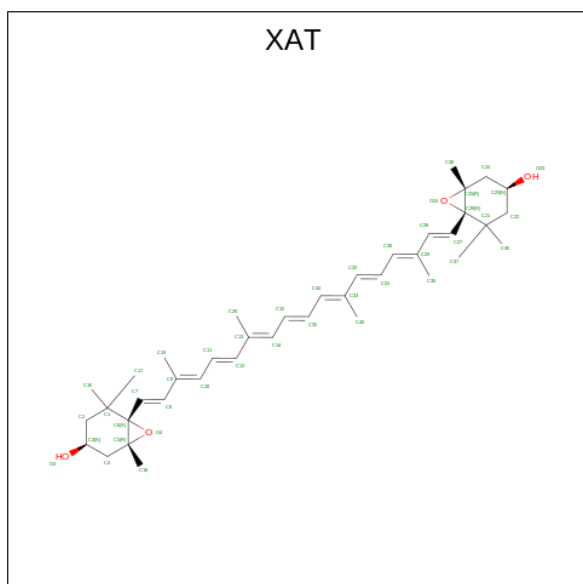
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 18  | B     | 1        | Total<br>43 | C<br>35 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>62 | C<br>52 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>43 | C<br>35 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | B     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | F     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | F     | 1        | Total<br>57 | C<br>47 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | F     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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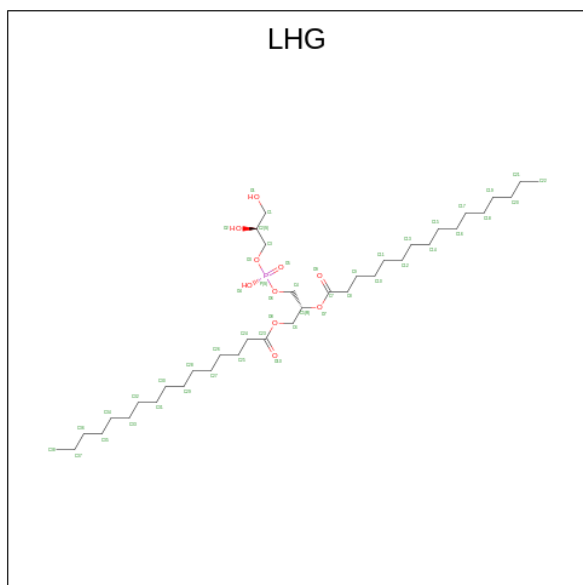
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 18  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 18  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | H     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 18  | J     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 18  | K     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 39    | 31 | 1  | 4 | 3 |         |
| 18  | K     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 37    | 31 | 1  | 4 | 1 |         |
| 18  | K     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 18  | K     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | L     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | L     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | L     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

- Molecule 19 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



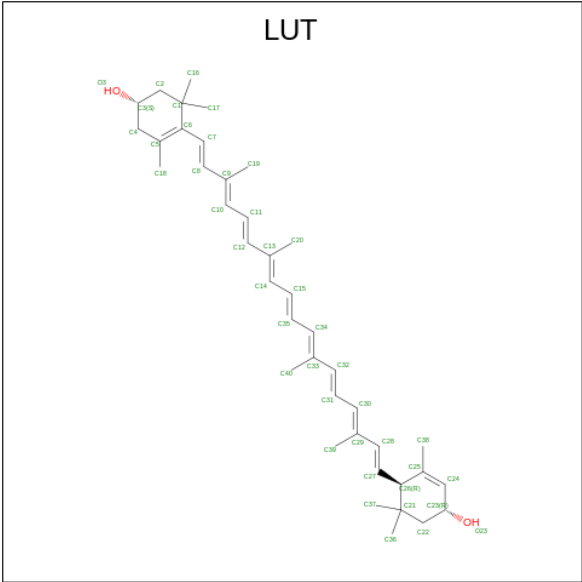
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 19  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 19  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 19  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



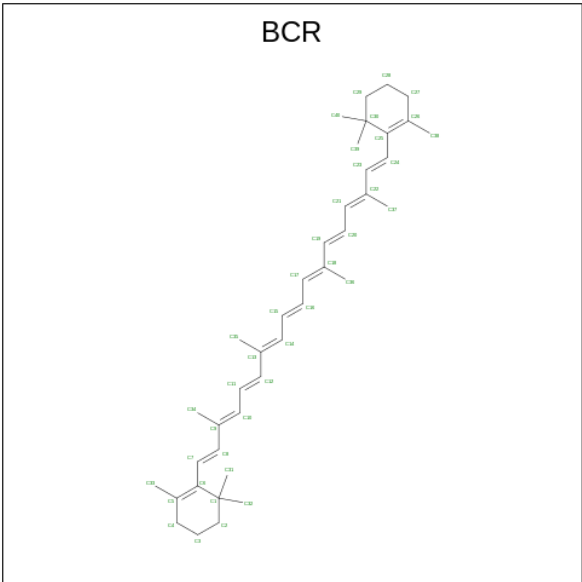
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 20  | 1     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 20  | 2     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |
| 20  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 30    | 19 | 10 | 1 |         |
| 20  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 20  | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 38    | 27 | 10 | 1 |         |
| 20  | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |

- Molecule 21 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula:  $C_{40}H_{56}O_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 21  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 21  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 21  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 21  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 21  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



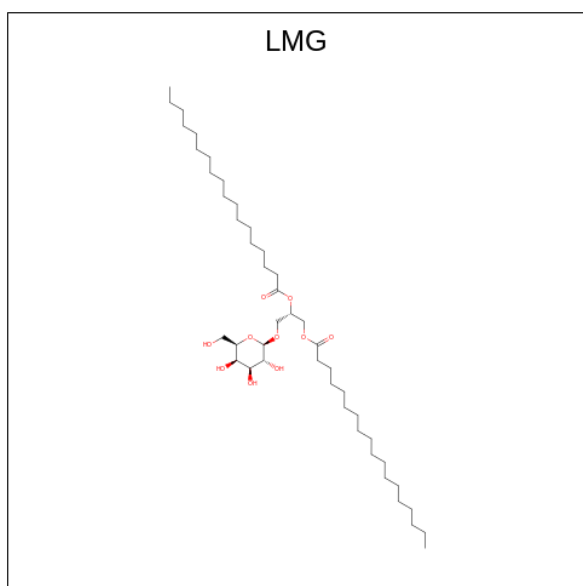
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 22  | 3     | 1        | Total C<br>40 40 | 0       |
| 22  | 4     | 1        | Total C<br>40 40 | 0       |
| 22  | A     | 1        | Total C<br>40 40 | 0       |
| 22  | A     | 1        | Total C<br>40 40 | 0       |
| 22  | A     | 1        | Total C<br>40 40 | 0       |
| 22  | A     | 1        | Total C<br>40 40 | 0       |
| 22  | A     | 1        | Total C<br>40 40 | 0       |
| 22  | A     | 1        | Total C<br>40 40 | 0       |
| 22  | B     | 1        | Total C<br>40 40 | 0       |
| 22  | B     | 1        | Total C<br>40 40 | 0       |
| 22  | B     | 1        | Total C<br>40 40 | 0       |
| 22  | B     | 1        | Total C<br>40 40 | 0       |
| 22  | B     | 1        | Total C<br>40 40 | 0       |
| 22  | B     | 1        | Total C<br>40 40 | 0       |
| 22  | B     | 1        | Total C<br>40 40 | 0       |
| 22  | B     | 1        | Total C<br>40 40 | 0       |
| 22  | F     | 1        | Total C<br>40 40 | 0       |
| 22  | G     | 1        | Total C<br>40 40 | 0       |
| 22  | I     | 1        | Total C<br>40 40 | 0       |
| 22  | J     | 1        | Total C<br>40 40 | 0       |
| 22  | K     | 1        | Total C<br>40 40 | 0       |
| 22  | K     | 1        | Total C<br>40 40 | 0       |

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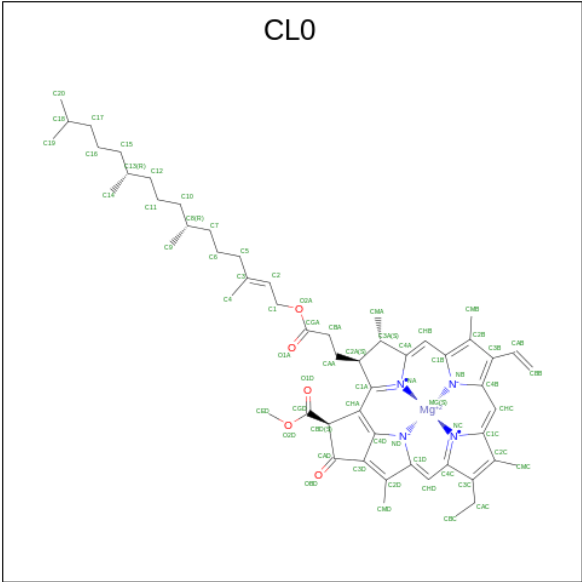
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 22  | L     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 22  | L     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 22  | L     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



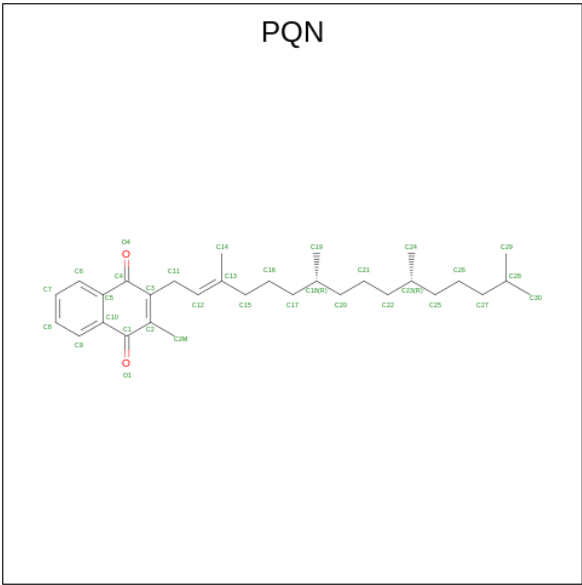
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 23  | 4     | 1        | Total | C  | O  | 0       |
|     |       |          | 39    | 29 | 10 |         |
| 23  | 4     | 1        | Total | C  | O  | 0       |
|     |       |          | 33    | 23 | 10 |         |

- Molecule 24 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



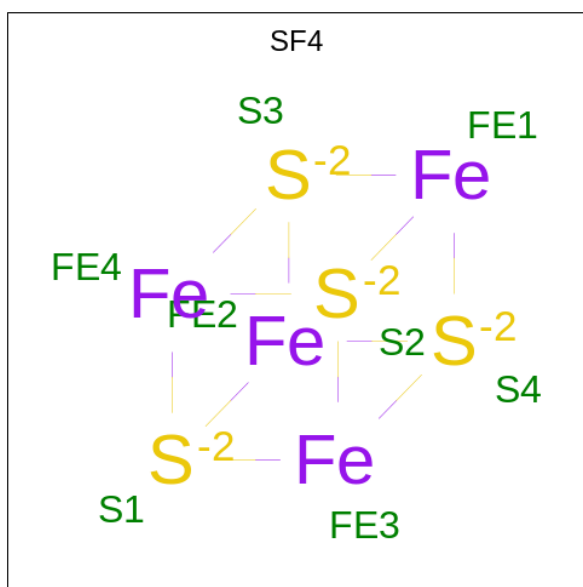
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 24  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 52 | 1  | 4 | 3 |         |

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



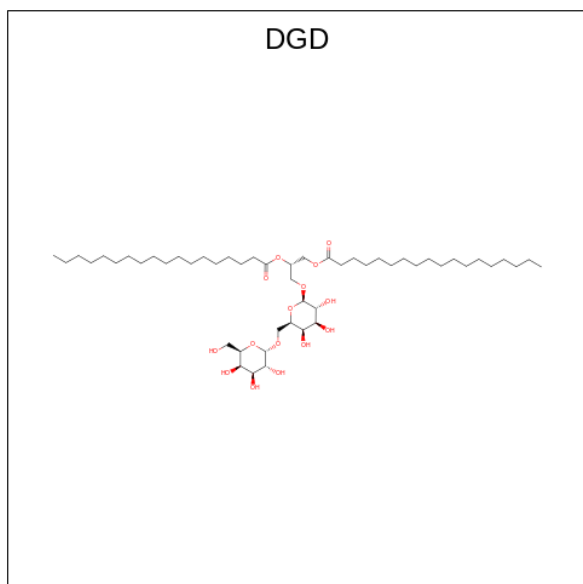
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 25  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 25  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



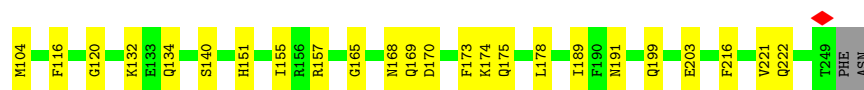
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 26  | A     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 26  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 26  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



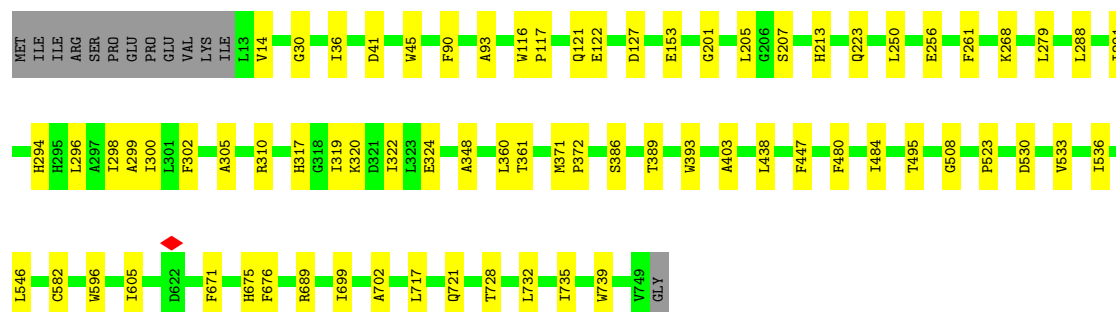
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
|     |       |          | Total | C  | O  |         |
| 27  | B     | 1        | 66    | 51 | 15 | 0       |





- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 89% 10%



- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 89% 11%



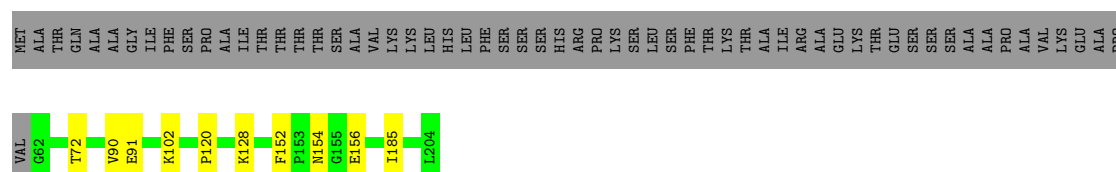
- Molecule 7: Photosystem I iron-sulfur center

Chain C: 91% 7%



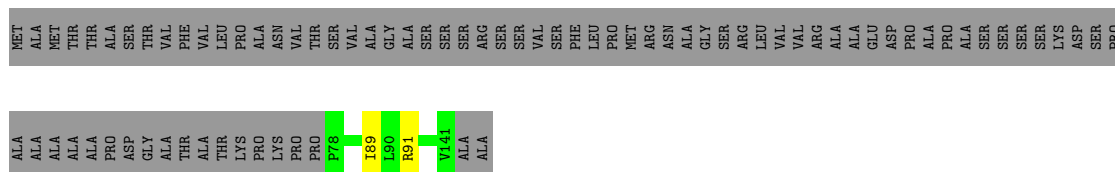
- Molecule 8: Photosystem I reaction center subunit II-2, chloroplastic

Chain D: 65% 5% 30%



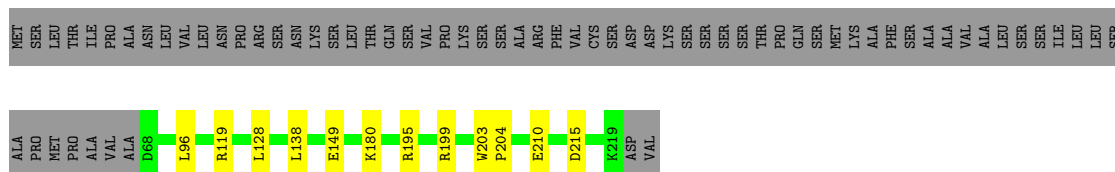
- Molecule 9: Photosystem I reaction center subunit IV A, chloroplastic

Chain E:  43% 55%



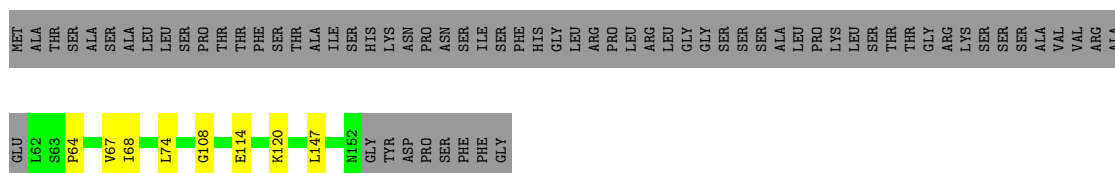
- Molecule 10: Photosystem I reaction center subunit III, chloroplastic

Chain F:  63% 5% 31%



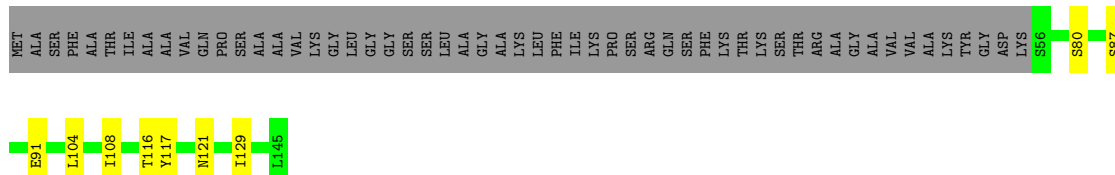
- Molecule 11: Photosystem I reaction center subunit V, chloroplastic

Chain G:  52% 5% 43%



- Molecule 12: Photosystem I reaction center subunit VI-2, chloroplastic

Chain H:  56% 6% 38%



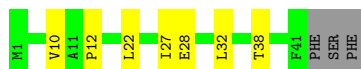
- Molecule 13: Photosystem I reaction center subunit VIII

Chain I:  76% 8% 16%

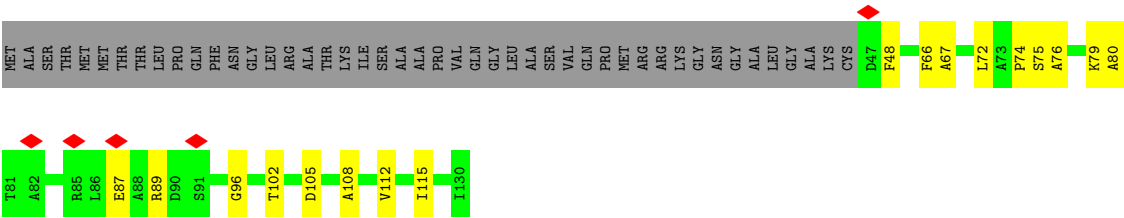


- Molecule 14: Photosystem I reaction center subunit IX

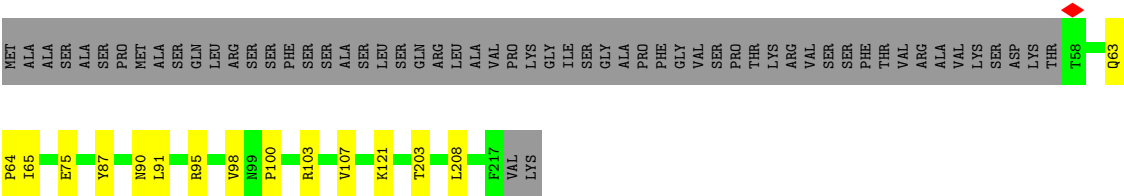
Chain J:  77% 16% 7%



● Molecule 15: Photosystem I reaction center subunit psaK, chloroplastic



● Molecule 16: Photosystem I reaction center subunit XI, chloroplastic



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 137602                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50.5                                    | Depositor |
| Minimum defocus (nm)                 | 1200                                    | Depositor |
| Maximum defocus (nm)                 | 2200                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 35.714                                  | Depositor |
| Minimum map value                    | -22.642                                 | Depositor |
| Average map value                    | 0.012                                   | Depositor |
| Map value standard deviation         | 1.070                                   | Depositor |
| Recommended contour level            | 3.21                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 365.232, 365.232, 365.232               | wwPDB     |
| Map dimensions                       | 336, 336, 336                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.087, 1.087, 1.087                     | Depositor |

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CHL, DGD, PQN, LHG, CL0, CLA, XAT, LMG, LUT, BCR, SF4

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   | 1     | 0.12         | 0/1546  | 0.32        | 0/2110         |
| 2   | 2     | 0.12         | 0/1622  | 0.28        | 0/2219         |
| 3   | 3     | 0.13         | 0/1717  | 0.30        | 0/2336         |
| 4   | 4     | 0.12         | 0/1599  | 0.29        | 0/2178         |
| 5   | A     | 0.10         | 0/6005  | 0.25        | 0/8194         |
| 6   | B     | 0.11         | 0/6065  | 0.28        | 1/8279 (0.0%)  |
| 7   | C     | 0.12         | 0/629   | 0.38        | 0/852          |
| 8   | D     | 0.10         | 0/1157  | 0.30        | 0/1563         |
| 9   | E     | 0.08         | 0/528   | 0.23        | 0/715          |
| 10  | F     | 0.11         | 0/1238  | 0.26        | 0/1670         |
| 11  | G     | 0.08         | 0/724   | 0.25        | 0/981          |
| 12  | H     | 0.10         | 0/713   | 0.27        | 0/968          |
| 13  | I     | 0.12         | 0/245   | 0.29        | 0/333          |
| 14  | J     | 0.10         | 0/336   | 0.25        | 0/458          |
| 15  | K     | 0.16         | 0/599   | 0.50        | 3/809 (0.4%)   |
| 16  | L     | 0.10         | 0/1244  | 0.27        | 0/1700         |
| All | All   | 0.11         | 0/25967 | 0.28        | 4/35365 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 15  | K     | 74  | PRO  | CA-N-CD  | -7.69 | 101.24      | 112.00   |
| 15  | K     | 74  | PRO  | N-CD-CG  | -5.20 | 95.41       | 103.20   |
| 6   | B     | 477 | LEU  | CB-CA-C  | -5.12 | 110.26      | 117.23   |
| 15  | K     | 74  | PRO  | CB-CG-CD | -5.12 | 89.72       | 106.10   |

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   | 1     | 1496  | 0        | 1471     | 30      | 0            |
| 2   | 2     | 1566  | 0        | 1519     | 22      | 0            |
| 3   | 3     | 1666  | 0        | 1627     | 19      | 0            |
| 4   | 4     | 1551  | 0        | 1508     | 24      | 0            |
| 5   | A     | 5807  | 0        | 5659     | 55      | 0            |
| 6   | B     | 5854  | 0        | 5646     | 63      | 0            |
| 7   | C     | 616   | 0        | 600      | 5       | 0            |
| 8   | D     | 1128  | 0        | 1134     | 8       | 0            |
| 9   | E     | 517   | 0        | 526      | 1       | 0            |
| 10  | F     | 1208  | 0        | 1243     | 9       | 0            |
| 11  | G     | 708   | 0        | 700      | 6       | 0            |
| 12  | H     | 693   | 0        | 690      | 6       | 0            |
| 13  | I     | 239   | 0        | 258      | 3       | 0            |
| 14  | J     | 327   | 0        | 342      | 7       | 0            |
| 15  | K     | 593   | 0        | 614      | 13      | 0            |
| 16  | L     | 1207  | 0        | 1209     | 13      | 0            |
| 17  | 1     | 93    | 0        | 62       | 10      | 0            |
| 17  | 2     | 226   | 0        | 150      | 12      | 0            |
| 17  | 3     | 45    | 0        | 30       | 1       | 0            |
| 17  | 4     | 169   | 0        | 100      | 3       | 0            |
| 18  | 1     | 496   | 0        | 354      | 24      | 0            |
| 18  | 2     | 434   | 0        | 352      | 25      | 0            |
| 18  | 3     | 498   | 0        | 377      | 13      | 0            |
| 18  | 4     | 527   | 0        | 412      | 18      | 0            |
| 18  | A     | 2533  | 0        | 2495     | 104     | 0            |
| 18  | B     | 2284  | 0        | 2242     | 93      | 0            |
| 18  | F     | 149   | 0        | 123      | 6       | 0            |
| 18  | G     | 132   | 0        | 97       | 1       | 0            |
| 18  | H     | 60    | 0        | 59       | 2       | 0            |
| 18  | J     | 51    | 0        | 41       | 2       | 0            |
| 18  | K     | 167   | 0        | 116      | 2       | 0            |
| 18  | L     | 155   | 0        | 138      | 7       | 0            |
| 19  | 1     | 44    | 0        | 56       | 18      | 0            |
| 19  | 2     | 44    | 0        | 56       | 7       | 0            |
| 19  | 4     | 44    | 0        | 56       | 5       | 0            |
| 20  | 1     | 49    | 0        | 74       | 13      | 0            |
| 20  | 2     | 37    | 0        | 44       | 3       | 0            |

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*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 20  | A     | 79    | 0        | 104      | 6       | 0            |
| 20  | B     | 87    | 0        | 120      | 5       | 0            |
| 21  | 1     | 42    | 0        | 56       | 3       | 0            |
| 21  | 2     | 84    | 0        | 112      | 10      | 0            |
| 21  | 3     | 42    | 0        | 56       | 6       | 0            |
| 21  | 4     | 42    | 0        | 56       | 4       | 0            |
| 22  | 3     | 40    | 0        | 56       | 4       | 0            |
| 22  | 4     | 40    | 0        | 56       | 4       | 0            |
| 22  | A     | 240   | 0        | 336      | 27      | 0            |
| 22  | B     | 320   | 0        | 448      | 44      | 0            |
| 22  | F     | 40    | 0        | 56       | 2       | 0            |
| 22  | G     | 40    | 0        | 56       | 2       | 0            |
| 22  | I     | 40    | 0        | 56       | 1       | 0            |
| 22  | J     | 40    | 0        | 56       | 6       | 0            |
| 22  | K     | 80    | 0        | 112      | 7       | 0            |
| 22  | L     | 120   | 0        | 168      | 18      | 0            |
| 23  | 4     | 72    | 0        | 84       | 1       | 0            |
| 24  | A     | 60    | 0        | 68       | 5       | 0            |
| 25  | A     | 33    | 0        | 46       | 3       | 0            |
| 25  | B     | 33    | 0        | 46       | 2       | 0            |
| 26  | A     | 8     | 0        | 0        | 0       | 0            |
| 26  | C     | 16    | 0        | 0        | 0       | 0            |
| 27  | B     | 66    | 0        | 96       | 5       | 0            |
| All | All   | 35077 | 0        | 34424    | 610     | 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 9.

The worst 5 of 610 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:B:814:CLA:H3A  | 22:B:845:BCR:H393 | 1.51                     | 0.91              |
| 17:1:601:CHL:HBB1 | 20:1:615:LHG:H252 | 1.57                     | 0.84              |
| 21:2:619:LUT:H8   | 21:2:619:LUT:H181 | 1.60                     | 0.82              |
| 22:B:801:BCR:H12C | 22:B:801:BCR:H341 | 1.63                     | 0.81              |
| 3:3:79:LEU:HD13   | 18:A:813:CLA:H2   | 1.63                     | 0.81              |

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   | 1     | 191/241 (79%)   | 190 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 2   | 2     | 199/257 (77%)   | 198 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 3   | 3     | 216/273 (79%)   | 213 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 4   | 4     | 194/251 (77%)   | 191 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 5   | A     | 735/750 (98%)   | 725 (99%)  | 10 (1%) | 0        | 100         | 100 |
| 6   | B     | 730/734 (100%)  | 716 (98%)  | 14 (2%) | 0        | 100         | 100 |
| 7   | C     | 78/81 (96%)     | 74 (95%)   | 4 (5%)  | 0        | 100         | 100 |
| 8   | D     | 141/204 (69%)   | 137 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 9   | E     | 62/143 (43%)    | 61 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 10  | F     | 150/221 (68%)   | 149 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 11  | G     | 89/160 (56%)    | 88 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 12  | H     | 88/145 (61%)    | 88 (100%)  | 0       | 0        | 100         | 100 |
| 13  | I     | 29/37 (78%)     | 28 (97%)   | 1 (3%)  | 0        | 100         | 100 |
| 14  | J     | 39/44 (89%)     | 38 (97%)   | 1 (3%)  | 0        | 100         | 100 |
| 15  | K     | 82/130 (63%)    | 82 (100%)  | 0       | 0        | 100         | 100 |
| 16  | L     | 158/219 (72%)   | 155 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| All | All   | 3181/3890 (82%) | 3133 (98%) | 48 (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   | 1     | 153/190 (80%)   | 151 (99%)   | 2 (1%)   | 61          | 75  |
| 2   | 2     | 163/205 (80%)   | 163 (100%)  | 0        | 100         | 100 |
| 3   | 3     | 167/211 (79%)   | 166 (99%)   | 1 (1%)   | 78          | 83  |
| 4   | 4     | 163/210 (78%)   | 162 (99%)   | 1 (1%)   | 78          | 83  |
| 5   | A     | 598/610 (98%)   | 597 (100%)  | 1 (0%)   | 87          | 88  |
| 6   | B     | 599/600 (100%)  | 598 (100%)  | 1 (0%)   | 87          | 88  |
| 7   | C     | 70/71 (99%)     | 70 (100%)   | 0        | 100         | 100 |
| 8   | D     | 121/170 (71%)   | 121 (100%)  | 0        | 100         | 100 |
| 9   | E     | 57/114 (50%)    | 57 (100%)   | 0        | 100         | 100 |
| 10  | F     | 125/185 (68%)   | 124 (99%)   | 1 (1%)   | 73          | 80  |
| 11  | G     | 77/133 (58%)    | 77 (100%)   | 0        | 100         | 100 |
| 12  | H     | 75/113 (66%)    | 75 (100%)   | 0        | 100         | 100 |
| 13  | I     | 27/33 (82%)     | 27 (100%)   | 0        | 100         | 100 |
| 14  | J     | 36/39 (92%)     | 36 (100%)   | 0        | 100         | 100 |
| 15  | K     | 61/95 (64%)     | 61 (100%)   | 0        | 100         | 100 |
| 16  | L     | 126/174 (72%)   | 126 (100%)  | 0        | 100         | 100 |
| All | All   | 2618/3153 (83%) | 2611 (100%) | 7 (0%)   | 84          | 87  |

5 of 7 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 4     | 132 | LYS  |
| 5   | A     | 127 | ASP  |
| 10  | F     | 96  | LEU  |
| 6   | B     | 309 | ILE  |
| 3   | 3     | 136 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | A     | 349 | GLN  |
| 11  | G     | 140 | HIS  |
| 6   | B     | 178 | HIS  |
| 8   | D     | 67  | GLN  |
| 6   | B     | 114 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

201 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 18  | CLA  | A     | 843 | -    | 69,73,73     | 1.26 | 6 (8%)      | 83,113,113  | 1.30 | 4 (4%)      |
| 18  | CLA  | A     | 825 | -    | 59,63,73     | 1.37 | 6 (10%)     | 71,101,113  | 1.34 | 6 (8%)      |
| 18  | CLA  | B     | 833 | 6    | 49,53,73     | 1.49 | 6 (12%)     | 59,89,113   | 1.51 | 7 (11%)     |
| 19  | XAT  | 2     | 617 | -    | 39,47,47     | 1.78 | 7 (17%)     | 54,74,74    | 2.05 | 14 (25%)    |
| 18  | CLA  | A     | 810 | 5    | 54,58,73     | 1.42 | 9 (16%)     | 65,95,113   | 1.52 | 11 (16%)    |
| 18  | CLA  | 3     | 601 | -    | 64,68,73     | 1.31 | 8 (12%)     | 77,107,113  | 1.33 | 6 (7%)      |
| 18  | CLA  | G     | 203 | 11   | 49,53,73     | 1.48 | 7 (14%)     | 59,89,113   | 1.45 | 4 (6%)      |
| 18  | CLA  | 2     | 602 | 2    | 69,73,73     | 1.26 | 8 (11%)     | 83,113,113  | 1.29 | 7 (8%)      |
| 17  | CHL  | 4     | 615 | 4    | 44,49,74     | 2.29 | 16 (36%)    | 51,84,114   | 3.28 | 22 (43%)    |
| 21  | LUT  | 3     | 613 | -    | 42,43,43     | 1.71 | 8 (19%)     | 51,60,60    | 1.92 | 14 (27%)    |
| 18  | CLA  | A     | 835 | 5    | 69,73,73     | 1.25 | 7 (10%)     | 83,113,113  | 1.30 | 5 (6%)      |
| 23  | LMG  | 4     | 620 | -    | 33,33,55     | 0.24 | 0           | 41,41,63    | 0.33 | 0           |
| 18  | CLA  | 2     | 612 | 2    | 69,73,73     | 1.25 | 8 (11%)     | 83,113,113  | 1.30 | 6 (7%)      |
| 18  | CLA  | A     | 806 | 5    | 69,73,73     | 1.25 | 8 (11%)     | 83,113,113  | 1.30 | 4 (4%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 18  | CLA  | A     | 812 | -    | 69,73,73     | 1.26 | 8 (11%)  | 83,113,113  | 1.28 | 5 (6%)   |
| 18  | CLA  | B     | 839 | -    | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.29 | 5 (6%)   |
| 18  | CLA  | B     | 836 | 6    | 54,58,73     | 1.42 | 8 (14%)  | 65,95,113   | 3.43 | 11 (16%) |
| 18  | CLA  | 1     | 613 | -    | 41,46,73     | 1.67 | 9 (21%)  | 52,81,113   | 1.61 | 8 (15%)  |
| 18  | CLA  | 4     | 613 | 4    | 49,53,73     | 1.49 | 8 (16%)  | 59,89,113   | 1.58 | 6 (10%)  |
| 18  | CLA  | 4     | 603 | -    | 48,52,73     | 1.57 | 10 (20%) | 61,88,113   | 1.50 | 6 (9%)   |
| 18  | CLA  | B     | 841 | 20   | 69,73,73     | 1.26 | 7 (10%)  | 83,113,113  | 1.30 | 5 (6%)   |
| 18  | CLA  | A     | 826 | -    | 69,73,73     | 1.26 | 6 (8%)   | 83,113,113  | 1.29 | 4 (4%)   |
| 18  | CLA  | B     | 813 | -    | 69,73,73     | 1.26 | 8 (11%)  | 83,113,113  | 1.36 | 8 (9%)   |
| 18  | CLA  | 4     | 602 | 4    | 64,68,73     | 1.30 | 7 (10%)  | 77,107,113  | 1.33 | 7 (9%)   |
| 18  | CLA  | H     | 201 | -    | 64,68,73     | 1.31 | 7 (10%)  | 77,107,113  | 1.32 | 4 (5%)   |
| 26  | SF4  | A     | 854 | -    | 0,12,12      | -    | -        | -           | -    | -        |
| 17  | CHL  | 1     | 601 | 1    | 55,60,74     | 2.21 | 17 (30%) | 61,97,114   | 2.92 | 24 (39%) |
| 18  | CLA  | A     | 820 | 5    | 69,73,73     | 1.26 | 7 (10%)  | 83,113,113  | 1.30 | 8 (9%)   |
| 18  | CLA  | 2     | 609 | -    | 51,55,73     | 1.44 | 8 (15%)  | 61,91,113   | 1.45 | 6 (9%)   |
| 22  | BCR  | B     | 845 | -    | 41,41,41     | 1.80 | 8 (19%)  | 56,56,56    | 1.80 | 14 (25%) |
| 18  | CLA  | A     | 819 | 5    | 63,67,73     | 1.32 | 7 (11%)  | 75,105,113  | 1.36 | 5 (6%)   |
| 18  | CLA  | A     | 830 | -    | 69,73,73     | 1.26 | 7 (10%)  | 83,113,113  | 1.40 | 9 (10%)  |
| 18  | CLA  | B     | 821 | 6    | 51,55,73     | 1.44 | 7 (13%)  | 61,91,113   | 1.56 | 7 (11%)  |
| 18  | CLA  | K     | 206 | 15   | 41,47,73     | 1.61 | 7 (17%)  | 49,81,113   | 1.52 | 6 (12%)  |
| 22  | BCR  | B     | 846 | -    | 41,41,41     | 1.74 | 8 (19%)  | 56,56,56    | 1.70 | 10 (17%) |
| 17  | CHL  | 2     | 601 | 2    | 51,55,74     | 2.30 | 18 (35%) | 57,91,114   | 3.00 | 22 (38%) |
| 17  | CHL  | 2     | 607 | -    | 55,59,74     | 2.21 | 19 (34%) | 62,96,114   | 2.91 | 24 (38%) |
| 18  | CLA  | 3     | 607 | -    | 49,53,73     | 1.51 | 7 (14%)  | 59,89,113   | 1.45 | 6 (10%)  |
| 18  | CLA  | 1     | 604 | -    | 53,57,73     | 1.43 | 7 (13%)  | 62,93,113   | 1.48 | 6 (9%)   |
| 18  | CLA  | B     | 811 | 6    | 58,62,73     | 1.42 | 8 (13%)  | 73,100,113  | 1.45 | 7 (9%)   |
| 18  | CLA  | B     | 831 | 6    | 47,51,73     | 1.49 | 7 (14%)  | 56,86,113   | 1.47 | 5 (8%)   |
| 19  | XAT  | 4     | 617 | -    | 39,47,47     | 1.72 | 8 (20%)  | 54,74,74    | 1.72 | 12 (22%) |
| 22  | BCR  | A     | 853 | -    | 41,41,41     | 1.81 | 8 (19%)  | 56,56,56    | 1.75 | 14 (25%) |
| 17  | CHL  | 3     | 606 | -    | 49,53,74     | 2.29 | 17 (34%) | 59,89,114   | 2.92 | 20 (33%) |
| 18  | CLA  | B     | 818 | 6    | 64,68,73     | 1.30 | 7 (10%)  | 77,107,113  | 1.34 | 6 (7%)   |
| 18  | CLA  | A     | 809 | -    | 69,73,73     | 1.25 | 7 (10%)  | 83,113,113  | 1.30 | 5 (6%)   |
| 18  | CLA  | A     | 829 | 5    | 69,73,73     | 1.25 | 7 (10%)  | 83,113,113  | 1.29 | 5 (6%)   |
| 18  | CLA  | B     | 807 | 6    | 56,60,73     | 1.39 | 7 (12%)  | 67,97,113   | 1.40 | 5 (7%)   |
| 18  | CLA  | B     | 837 | 6    | 69,73,73     | 1.26 | 7 (10%)  | 83,113,113  | 1.32 | 7 (8%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 18  | CLA  | 4     | 612 | 4    | 61,65,73     | 1.33 | 7 (11%)  | 73,103,113  | 1.36 | 6 (8%)   |
| 18  | CLA  | 3     | 611 | -    | 41,44,73     | 1.60 | 8 (19%)  | 49,77,113   | 1.50 | 4 (8%)   |
| 27  | DGD  | B     | 850 | -    | 67,67,67     | 0.84 | 2 (2%)   | 81,81,81    | 0.94 | 4 (4%)   |
| 18  | CLA  | A     | 844 | -    | 69,73,73     | 1.26 | 8 (11%)  | 83,113,113  | 1.31 | 7 (8%)   |
| 18  | CLA  | A     | 815 | 5    | 49,53,73     | 1.47 | 7 (14%)  | 59,89,113   | 1.45 | 4 (6%)   |
| 18  | CLA  | B     | 810 | 6    | 69,73,73     | 1.27 | 7 (10%)  | 83,113,113  | 1.27 | 5 (6%)   |
| 18  | CLA  | A     | 813 | 5    | 58,62,73     | 1.37 | 7 (12%)  | 69,99,113   | 1.41 | 6 (8%)   |
| 22  | BCR  | A     | 851 | -    | 41,41,41     | 1.88 | 8 (19%)  | 56,56,56    | 2.48 | 19 (33%) |
| 18  | CLA  | A     | 823 | 5    | 46,50,73     | 1.50 | 6 (13%)  | 55,85,113   | 1.48 | 4 (7%)   |
| 18  | CLA  | B     | 814 | 6    | 69,73,73     | 1.24 | 6 (8%)   | 83,113,113  | 1.30 | 7 (8%)   |
| 19  | XAT  | 1     | 614 | -    | 39,47,47     | 0.83 | 1 (2%)   | 54,74,74    | 3.20 | 18 (33%) |
| 18  | CLA  | 3     | 610 | 3    | 43,48,73     | 1.57 | 7 (16%)  | 51,83,113   | 1.50 | 5 (9%)   |
| 18  | CLA  | G     | 201 | -    | 49,53,73     | 1.49 | 6 (12%)  | 59,89,113   | 1.44 | 4 (6%)   |
| 22  | BCR  | L     | 301 | -    | 41,41,41     | 1.76 | 8 (19%)  | 56,56,56    | 2.17 | 12 (21%) |
| 18  | CLA  | A     | 804 | 5    | 69,73,73     | 1.26 | 7 (10%)  | 83,113,113  | 1.38 | 7 (8%)   |
| 22  | BCR  | L     | 306 | -    | 41,41,41     | 1.75 | 8 (19%)  | 56,56,56    | 1.91 | 16 (28%) |
| 18  | CLA  | B     | 832 | 6    | 69,73,73     | 1.26 | 6 (8%)   | 83,113,113  | 1.26 | 6 (7%)   |
| 18  | CLA  | B     | 802 | -    | 69,73,73     | 1.27 | 7 (10%)  | 83,113,113  | 1.27 | 5 (6%)   |
| 17  | CHL  | 2     | 606 | -    | 47,51,74     | 2.33 | 17 (36%) | 52,86,114   | 3.11 | 21 (40%) |
| 18  | CLA  | 1     | 605 | -    | 50,54,73     | 1.47 | 7 (14%)  | 60,90,113   | 1.43 | 5 (8%)   |
| 18  | CLA  | 1     | 609 | -    | 46,50,73     | 1.51 | 8 (17%)  | 55,85,113   | 1.51 | 4 (7%)   |
| 22  | BCR  | B     | 847 | -    | 41,41,41     | 1.73 | 8 (19%)  | 56,56,56    | 1.57 | 10 (17%) |
| 18  | CLA  | 1     | 610 | 20   | 41,46,73     | 1.67 | 8 (19%)  | 52,81,113   | 1.60 | 7 (13%)  |
| 20  | LHG  | B     | 852 | -    | 48,48,48     | 0.27 | 0        | 51,54,54    | 0.33 | 0        |
| 17  | CHL  | 4     | 607 | -    | 50,54,74     | 2.27 | 17 (34%) | 56,90,114   | 3.06 | 22 (39%) |
| 18  | CLA  | B     | 812 | 6    | 47,51,73     | 1.51 | 6 (12%)  | 56,86,113   | 1.42 | 5 (8%)   |
| 20  | LHG  | 2     | 618 | 18   | 36,36,48     | 0.31 | 0        | 39,42,54    | 0.53 | 1 (2%)   |
| 18  | CLA  | B     | 820 | 6    | 54,58,73     | 1.41 | 7 (12%)  | 65,95,113   | 1.44 | 6 (9%)   |
| 18  | CLA  | 4     | 614 | 4    | 54,58,73     | 1.42 | 7 (12%)  | 65,95,113   | 1.45 | 6 (9%)   |
| 18  | CLA  | B     | 840 | 6    | 69,73,73     | 1.27 | 8 (11%)  | 83,113,113  | 1.28 | 5 (6%)   |
| 18  | CLA  | B     | 819 | -    | 59,63,73     | 1.36 | 8 (13%)  | 71,101,113  | 1.38 | 6 (8%)   |
| 18  | CLA  | A     | 836 | 5    | 49,53,73     | 1.51 | 7 (14%)  | 59,89,113   | 1.45 | 5 (8%)   |
| 18  | CLA  | B     | 838 | 6    | 51,55,73     | 1.46 | 8 (15%)  | 61,91,113   | 1.41 | 7 (11%)  |
| 18  | CLA  | A     | 805 | 5    | 56,60,73     | 1.39 | 7 (12%)  | 67,97,113   | 1.41 | 4 (5%)   |
| 18  | CLA  | A     | 814 | 5    | 69,73,73     | 1.27 | 6 (8%)   | 83,113,113  | 1.28 | 6 (7%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 18  | CLA  | B     | 822 | 6    | 69,73,73     | 1.26 | 8 (11%)  | 83,113,113  | 1.38 | 9 (10%)  |
| 18  | CLA  | B     | 817 | 6    | 63,67,73     | 1.32 | 8 (12%)  | 75,105,113  | 1.34 | 6 (8%)   |
| 26  | SF4  | C     | 102 | -    | 0,12,12      | -    | -        | -           | -    | -        |
| 25  | PQN  | A     | 855 | -    | 34,34,34     | 0.41 | 0        | 42,45,45    | 0.42 | 0        |
| 18  | CLA  | G     | 202 | 11   | 46,50,73     | 1.51 | 8 (17%)  | 55,85,113   | 1.45 | 4 (7%)   |
| 18  | CLA  | K     | 201 | 15   | 42,45,73     | 1.57 | 8 (19%)  | 50,78,113   | 1.49 | 5 (10%)  |
| 18  | CLA  | A     | 842 | 5    | 69,73,73     | 1.26 | 9 (13%)  | 83,113,113  | 1.37 | 8 (9%)   |
| 18  | CLA  | B     | 803 | -    | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.31 | 5 (6%)   |
| 17  | CHL  | 4     | 606 | -    | 45,49,74     | 2.30 | 15 (33%) | 57,84,114   | 3.07 | 20 (35%) |
| 21  | LUT  | 2     | 616 | -    | 42,43,43     | 1.66 | 8 (19%)  | 51,60,60    | 2.02 | 12 (23%) |
| 18  | CLA  | 1     | 608 | 1    | 44,48,73     | 1.60 | 9 (20%)  | 56,83,113   | 1.58 | 7 (12%)  |
| 18  | CLA  | L     | 304 | -    | 49,53,73     | 1.50 | 6 (12%)  | 59,89,113   | 1.47 | 5 (8%)   |
| 18  | CLA  | A     | 837 | 5    | 49,53,73     | 1.50 | 7 (14%)  | 59,89,113   | 1.44 | 5 (8%)   |
| 18  | CLA  | L     | 302 | -    | 49,53,73     | 1.49 | 8 (16%)  | 59,89,113   | 1.48 | 6 (10%)  |
| 20  | LHG  | 1     | 615 | 18   | 48,48,48     | 0.93 | 2 (4%)   | 51,54,54    | 1.03 | 3 (5%)   |
| 18  | CLA  | 1     | 603 | -    | 58,62,73     | 1.38 | 8 (13%)  | 69,99,113   | 1.39 | 6 (8%)   |
| 21  | LUT  | 4     | 616 | -    | 42,43,43     | 1.64 | 8 (19%)  | 51,60,60    | 1.55 | 11 (21%) |
| 18  | CLA  | A     | 845 | 20   | 54,58,73     | 1.42 | 7 (12%)  | 65,95,113   | 1.41 | 6 (9%)   |
| 18  | CLA  | 3     | 612 | -    | 43,48,73     | 1.54 | 8 (18%)  | 51,83,113   | 1.54 | 5 (9%)   |
| 18  | CLA  | A     | 808 | 5    | 54,58,73     | 1.42 | 7 (12%)  | 65,95,113   | 1.43 | 8 (12%)  |
| 17  | CHL  | 2     | 605 | -    | 46,50,74     | 2.34 | 17 (36%) | 52,85,114   | 3.09 | 21 (40%) |
| 18  | CLA  | 2     | 603 | 2    | 47,52,73     | 1.52 | 7 (14%)  | 56,88,113   | 1.44 | 4 (7%)   |
| 18  | CLA  | B     | 825 | -    | 66,70,73     | 1.27 | 7 (10%)  | 79,109,113  | 1.35 | 10 (12%) |
| 18  | CLA  | A     | 802 | -    | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.34 | 7 (8%)   |
| 18  | CLA  | 3     | 605 | -    | 45,49,73     | 1.58 | 9 (20%)  | 57,84,113   | 1.57 | 6 (10%)  |
| 22  | BCR  | 4     | 618 | -    | 41,41,41     | 1.73 | 8 (19%)  | 56,56,56    | 1.69 | 10 (17%) |
| 21  | LUT  | 1     | 616 | -    | 42,43,43     | 1.69 | 7 (16%)  | 51,60,60    | 2.00 | 12 (23%) |
| 18  | CLA  | A     | 831 | 5    | 69,73,73     | 1.25 | 6 (8%)   | 83,113,113  | 1.30 | 6 (7%)   |
| 17  | CHL  | 2     | 615 | 2    | 47,51,74     | 2.33 | 17 (36%) | 52,86,114   | 3.15 | 23 (44%) |
| 18  | CLA  | A     | 827 | -    | 63,67,73     | 1.31 | 7 (11%)  | 75,105,113  | 1.36 | 6 (8%)   |
| 18  | CLA  | A     | 828 | 5    | 69,73,73     | 1.27 | 8 (11%)  | 83,113,113  | 1.31 | 6 (7%)   |
| 18  | CLA  | B     | 835 | -    | 46,50,73     | 1.52 | 8 (17%)  | 55,85,113   | 1.46 | 6 (10%)  |
| 18  | CLA  | B     | 829 | 6    | 60,64,73     | 1.35 | 9 (15%)  | 72,102,113  | 1.35 | 6 (8%)   |
| 22  | BCR  | B     | 844 | -    | 41,41,41     | 1.74 | 8 (19%)  | 56,56,56    | 1.79 | 12 (21%) |
| 18  | CLA  | 1     | 607 | -    | 47,52,73     | 1.52 | 6 (12%)  | 56,88,113   | 1.44 | 5 (8%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 18  | CLA  | A     | 817 | -    | 49,53,73     | 1.50 | 7 (14%)  | 59,89,113   | 1.44 | 5 (8%)   |
| 18  | CLA  | A     | 821 | 5    | 49,53,73     | 1.50 | 6 (12%)  | 59,89,113   | 1.44 | 5 (8%)   |
| 18  | CLA  | A     | 816 | 5    | 46,50,73     | 1.51 | 8 (17%)  | 55,85,113   | 1.46 | 5 (9%)   |
| 18  | CLA  | A     | 824 | -    | 45,49,73     | 1.53 | 7 (15%)  | 54,84,113   | 1.51 | 7 (12%)  |
| 18  | CLA  | B     | 804 | 6    | 45,49,73     | 1.51 | 7 (15%)  | 54,84,113   | 1.56 | 5 (9%)   |
| 17  | CHL  | 1     | 606 | -    | 44,49,74     | 2.50 | 19 (43%) | 48,84,114   | 3.08 | 21 (43%) |
| 18  | CLA  | F     | 303 | 10   | 45,49,73     | 1.53 | 7 (15%)  | 54,84,113   | 1.52 | 6 (11%)  |
| 18  | CLA  | F     | 302 | -    | 55,59,73     | 1.41 | 7 (12%)  | 66,96,113   | 1.43 | 6 (9%)   |
| 22  | BCR  | L     | 305 | -    | 41,41,41     | 1.76 | 8 (19%)  | 56,56,56    | 1.75 | 14 (25%) |
| 21  | LUT  | 2     | 619 | -    | 42,43,43     | 1.66 | 8 (19%)  | 51,60,60    | 1.88 | 12 (23%) |
| 22  | BCR  | B     | 801 | -    | 41,41,41     | 1.81 | 8 (19%)  | 56,56,56    | 1.77 | 13 (23%) |
| 18  | CLA  | 2     | 611 | -    | 48,52,73     | 1.51 | 8 (16%)  | 58,88,113   | 1.50 | 5 (8%)   |
| 18  | CLA  | B     | 830 | -    | 47,51,73     | 1.49 | 8 (17%)  | 56,86,113   | 1.46 | 5 (8%)   |
| 18  | CLA  | 1     | 612 | 1    | 50,54,73     | 1.46 | 9 (18%)  | 60,90,113   | 1.49 | 5 (8%)   |
| 18  | CLA  | 2     | 604 | -    | 47,51,73     | 1.50 | 8 (17%)  | 55,86,113   | 1.48 | 4 (7%)   |
| 18  | CLA  | 3     | 609 | -    | 57,62,73     | 1.40 | 9 (15%)  | 68,100,113  | 1.34 | 7 (10%)  |
| 18  | CLA  | F     | 301 | -    | 61,65,73     | 1.35 | 7 (11%)  | 73,103,113  | 1.32 | 6 (8%)   |
| 18  | CLA  | 2     | 613 | 2    | 47,51,73     | 1.50 | 8 (17%)  | 56,86,113   | 1.45 | 5 (8%)   |
| 22  | BCR  | A     | 849 | -    | 41,41,41     | 1.79 | 8 (19%)  | 56,56,56    | 1.95 | 13 (23%) |
| 22  | BCR  | J     | 102 | -    | 41,41,41     | 1.75 | 8 (19%)  | 56,56,56    | 1.77 | 14 (25%) |
| 18  | CLA  | 4     | 609 | -    | 58,62,73     | 1.36 | 8 (13%)  | 69,99,113   | 1.38 | 8 (11%)  |
| 18  | CLA  | A     | 818 | 5    | 64,68,73     | 1.29 | 7 (10%)  | 77,107,113  | 4.90 | 7 (9%)   |
| 18  | CLA  | 4     | 611 | -    | 44,49,73     | 1.56 | 8 (18%)  | 52,84,113   | 1.46 | 5 (9%)   |
| 20  | LHG  | A     | 847 | 18   | 29,29,48     | 0.33 | 0        | 32,35,54    | 0.43 | 0        |
| 22  | BCR  | 3     | 614 | -    | 41,41,41     | 1.73 | 8 (19%)  | 56,56,56    | 1.57 | 12 (21%) |
| 18  | CLA  | B     | 808 | -    | 69,73,73     | 1.24 | 8 (11%)  | 83,113,113  | 1.32 | 6 (7%)   |
| 18  | CLA  | J     | 101 | -    | 55,59,73     | 1.42 | 6 (10%)  | 66,96,113   | 1.39 | 7 (10%)  |
| 18  | CLA  | A     | 807 | 5    | 69,73,73     | 1.27 | 7 (10%)  | 83,113,113  | 1.26 | 7 (8%)   |
| 20  | LHG  | A     | 846 | -    | 48,48,48     | 0.27 | 0        | 51,54,54    | 0.33 | 0        |
| 18  | CLA  | B     | 815 | 6    | 47,51,73     | 1.48 | 7 (14%)  | 56,86,113   | 1.46 | 4 (7%)   |
| 18  | CLA  | B     | 823 | 6    | 49,53,73     | 1.49 | 8 (16%)  | 59,89,113   | 1.44 | 5 (8%)   |
| 18  | CLA  | B     | 827 | 6    | 69,73,73     | 1.26 | 7 (10%)  | 83,113,113  | 1.31 | 5 (6%)   |
| 22  | BCR  | F     | 304 | -    | 41,41,41     | 1.84 | 7 (17%)  | 56,56,56    | 2.14 | 16 (28%) |
| 18  | CLA  | A     | 834 | 5    | 69,73,73     | 1.26 | 7 (10%)  | 83,113,113  | 1.30 | 6 (7%)   |
| 18  | CLA  | 2     | 610 | 20   | 41,45,73     | 2.58 | 9 (21%)  | 47,76,113   | 1.35 | 6 (12%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | PQN  | B     | 842 | -    | 34,34,34     | 0.42 | 0        | 42,45,45    | 0.40 | 0        |
| 18  | CLA  | B     | 828 | -    | 69,73,73     | 1.26 | 7 (10%)  | 83,113,113  | 1.27 | 6 (7%)   |
| 22  | BCR  | K     | 202 | -    | 41,41,41     | 1.74 | 8 (19%)  | 56,56,56    | 1.93 | 14 (25%) |
| 18  | CLA  | 3     | 608 | -    | 45,49,73     | 1.50 | 7 (15%)  | 54,84,113   | 1.56 | 7 (12%)  |
| 18  | CLA  | 1     | 602 | 1    | 58,62,73     | 1.36 | 7 (12%)  | 69,99,113   | 1.37 | 5 (7%)   |
| 18  | CLA  | 2     | 608 | -    | 49,53,73     | 1.48 | 6 (12%)  | 59,89,113   | 1.45 | 4 (6%)   |
| 18  | CLA  | B     | 826 | 6    | 66,70,73     | 1.29 | 8 (12%)  | 79,109,113  | 1.32 | 6 (7%)   |
| 18  | CLA  | B     | 816 | 6    | 59,63,73     | 1.35 | 7 (11%)  | 71,101,113  | 1.38 | 7 (9%)   |
| 18  | CLA  | L     | 303 | 16   | 69,73,73     | 1.25 | 6 (8%)   | 83,113,113  | 1.32 | 7 (8%)   |
| 18  | CLA  | B     | 824 | -    | 69,73,73     | 1.25 | 7 (10%)  | 83,113,113  | 1.30 | 5 (6%)   |
| 18  | CLA  | B     | 809 | 6    | 69,73,73     | 1.25 | 7 (10%)  | 83,113,113  | 1.30 | 6 (7%)   |
| 18  | CLA  | A     | 832 | 5    | 54,58,73     | 1.41 | 7 (12%)  | 65,95,113   | 1.44 | 7 (10%)  |
| 23  | LMG  | 4     | 619 | -    | 39,39,55     | 0.22 | 0        | 47,47,63    | 0.24 | 0        |
| 18  | CLA  | A     | 833 | 5    | 60,64,73     | 1.34 | 7 (11%)  | 72,102,113  | 1.36 | 4 (5%)   |
| 18  | CLA  | A     | 841 | 5    | 69,73,73     | 1.26 | 7 (10%)  | 83,113,113  | 1.29 | 7 (8%)   |
| 18  | CLA  | 4     | 601 | 4    | 50,54,73     | 1.45 | 6 (12%)  | 60,90,113   | 1.44 | 4 (6%)   |
| 17  | CHL  | 4     | 605 | -    | 44,49,74     | 2.35 | 16 (36%) | 49,84,114   | 3.11 | 21 (42%) |
| 18  | CLA  | A     | 840 | 5    | 56,60,73     | 1.40 | 7 (12%)  | 67,97,113   | 1.40 | 5 (7%)   |
| 18  | CLA  | 3     | 602 | -    | 59,63,73     | 1.37 | 7 (11%)  | 71,101,113  | 1.33 | 5 (7%)   |
| 18  | CLA  | 1     | 611 | -    | 49,53,73     | 1.50 | 7 (14%)  | 59,89,113   | 1.44 | 4 (6%)   |
| 20  | LHG  | B     | 851 | 18   | 37,37,48     | 0.30 | 0        | 40,43,54    | 0.49 | 0        |
| 22  | BCR  | K     | 205 | -    | 41,41,41     | 1.75 | 8 (19%)  | 56,56,56    | 1.97 | 16 (28%) |
| 18  | CLA  | A     | 838 | 5    | 55,59,73     | 1.41 | 7 (12%)  | 66,96,113   | 1.40 | 8 (12%)  |
| 26  | SF4  | C     | 101 | -    | 0,12,12      | -    | -        | -           | -    | -        |
| 18  | CLA  | K     | 203 | -    | 49,53,73     | 1.49 | 7 (14%)  | 59,89,113   | 1.48 | 6 (10%)  |
| 18  | CLA  | A     | 839 | -    | 59,63,73     | 1.35 | 7 (11%)  | 71,101,113  | 1.37 | 5 (7%)   |
| 22  | BCR  | B     | 849 | -    | 41,41,41     | 1.75 | 8 (19%)  | 56,56,56    | 1.80 | 13 (23%) |
| 22  | BCR  | I     | 101 | -    | 41,41,41     | 1.72 | 8 (19%)  | 56,56,56    | 1.50 | 10 (17%) |
| 18  | CLA  | K     | 204 | 15   | 50,54,73     | 1.48 | 9 (18%)  | 60,90,113   | 1.45 | 5 (8%)   |
| 22  | BCR  | B     | 843 | -    | 41,41,41     | 1.78 | 8 (19%)  | 56,56,56    | 1.92 | 14 (25%) |
| 18  | CLA  | A     | 822 | -    | 69,73,73     | 1.26 | 8 (11%)  | 83,113,113  | 1.28 | 7 (8%)   |
| 18  | CLA  | 4     | 608 | 4    | 49,53,73     | 1.48 | 8 (16%)  | 59,89,113   | 1.46 | 4 (6%)   |
| 18  | CLA  | 3     | 603 | -    | 49,53,73     | 1.49 | 7 (14%)  | 59,89,113   | 1.45 | 6 (10%)  |
| 22  | BCR  | A     | 850 | -    | 41,41,41     | 1.82 | 8 (19%)  | 56,56,56    | 1.90 | 13 (23%) |
| 18  | CLA  | 4     | 610 | -    | 46,50,73     | 1.51 | 7 (15%)  | 55,85,113   | 1.45 | 4 (7%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 18  | CLA  | A     | 803 | -    | 69,73,73     | 1.26 | 7 (10%)  | 83,113,113  | 1.28 | 6 (7%)   |
| 18  | CLA  | B     | 806 | 6    | 69,73,73     | 1.25 | 7 (10%)  | 83,113,113  | 1.29 | 6 (7%)   |
| 18  | CLA  | A     | 811 | -    | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.29 | 5 (6%)   |
| 24  | CL0  | A     | 801 | 5    | 64,67,73     | 2.08 | 20 (31%) | 75,102,113  | 4.21 | 34 (45%) |
| 18  | CLA  | B     | 834 | 6    | 64,68,73     | 1.31 | 7 (10%)  | 77,107,113  | 1.34 | 7 (9%)   |
| 18  | CLA  | 3     | 604 | -    | 44,49,73     | 1.55 | 8 (18%)  | 52,84,113   | 1.44 | 5 (9%)   |
| 18  | CLA  | B     | 805 | 6    | 69,73,73     | 1.27 | 7 (10%)  | 83,113,113  | 1.25 | 7 (8%)   |
| 22  | BCR  | A     | 848 | -    | 41,41,41     | 1.73 | 8 (19%)  | 56,56,56    | 1.61 | 11 (19%) |
| 22  | BCR  | B     | 848 | -    | 41,41,41     | 1.72 | 8 (19%)  | 56,56,56    | 1.58 | 11 (19%) |
| 22  | BCR  | A     | 852 | -    | 41,41,41     | 1.74 | 8 (19%)  | 56,56,56    | 1.90 | 14 (25%) |
| 22  | BCR  | G     | 204 | -    | 41,41,41     | 1.73 | 8 (19%)  | 56,56,56    | 1.64 | 11 (19%) |
| 18  | CLA  | 4     | 604 | -    | 47,51,73     | 1.59 | 9 (19%)  | 60,87,113   | 1.51 | 6 (10%)  |

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   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 18  | CLA  | A     | 843 | -    | -       | 11/39/115/115 | -       |
| 18  | CLA  | A     | 825 | -    | -       | 9/27/103/115  | -       |
| 18  | CLA  | B     | 833 | 6    | -       | 4/15/91/115   | -       |
| 19  | XAT  | 2     | 617 | -    | -       | 16/31/93/93   | 0/4/4/4 |
| 18  | CLA  | A     | 810 | 5    | -       | 5/21/97/115   | -       |
| 18  | CLA  | 3     | 601 | -    | -       | 13/33/109/115 | -       |
| 18  | CLA  | G     | 203 | 11   | -       | 3/15/91/115   | -       |
| 18  | CLA  | 2     | 602 | 2    | -       | 17/39/115/115 | -       |
| 17  | CHL  | 4     | 615 | 4    | -       | 0/10/86/117   | -       |
| 21  | LUT  | 3     | 613 | -    | -       | 6/29/67/67    | 0/2/2/2 |
| 18  | CLA  | A     | 835 | 5    | -       | 18/39/115/115 | -       |
| 23  | LMG  | 4     | 620 | -    | -       | 7/28/48/70    | 0/1/1/1 |
| 18  | CLA  | 2     | 612 | 2    | -       | 17/39/115/115 | -       |
| 18  | CLA  | A     | 806 | 5    | -       | 20/39/115/115 | -       |
| 18  | CLA  | A     | 812 | -    | -       | 19/39/115/115 | -       |
| 18  | CLA  | B     | 839 | -    | -       | 10/39/115/115 | -       |
| 18  | CLA  | B     | 836 | 6    | -       | 7/21/97/115   | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 18  | CLA  | 1     | 613 | -    | -       | 0/4/80/115    | -       |
| 18  | CLA  | 4     | 613 | 4    | -       | 4/15/91/115   | -       |
| 18  | CLA  | 4     | 603 | -    | -       | 6/13/89/115   | -       |
| 18  | CLA  | B     | 841 | 20   | -       | 22/39/115/115 | -       |
| 18  | CLA  | A     | 826 | -    | -       | 9/39/115/115  | -       |
| 18  | CLA  | B     | 813 | -    | -       | 15/39/115/115 | -       |
| 18  | CLA  | 4     | 602 | 4    | -       | 6/33/109/115  | -       |
| 18  | CLA  | H     | 201 | -    | -       | 17/33/109/115 | -       |
| 26  | SF4  | A     | 854 | -    | -       | -             | 0/6/5/5 |
| 17  | CHL  | 1     | 601 | 1    | -       | 10/24/100/117 | -       |
| 18  | CLA  | A     | 820 | 5    | -       | 14/39/115/115 | -       |
| 18  | CLA  | 2     | 609 | -    | -       | 9/18/94/115   | -       |
| 22  | BCR  | B     | 845 | -    | -       | 9/29/63/63    | 0/2/2/2 |
| 18  | CLA  | A     | 819 | 5    | -       | 16/32/108/115 | -       |
| 18  | CLA  | A     | 830 | -    | -       | 13/39/115/115 | -       |
| 18  | CLA  | B     | 821 | 6    | -       | 3/18/94/115   | -       |
| 18  | CLA  | K     | 206 | 15   | -       | 0/8/80/115    | -       |
| 22  | BCR  | B     | 846 | -    | -       | 8/29/63/63    | 0/2/2/2 |
| 17  | CHL  | 2     | 601 | 2    | -       | 7/19/95/117   | -       |
| 17  | CHL  | 2     | 607 | -    | -       | 7/23/99/117   | -       |
| 18  | CLA  | 3     | 607 | -    | -       | 4/15/91/115   | -       |
| 18  | CLA  | 1     | 604 | -    | -       | 9/20/96/115   | -       |
| 18  | CLA  | B     | 811 | 6    | -       | 11/25/101/115 | -       |
| 18  | CLA  | B     | 831 | 6    | -       | 0/13/89/115   | -       |
| 19  | XAT  | 4     | 617 | -    | -       | 3/31/93/93    | 0/4/4/4 |
| 22  | BCR  | A     | 853 | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 17  | CHL  | 3     | 606 | -    | -       | 5/15/91/117   | -       |
| 18  | CLA  | B     | 818 | 6    | -       | 7/33/109/115  | -       |
| 18  | CLA  | A     | 809 | -    | -       | 14/39/115/115 | -       |
| 18  | CLA  | A     | 829 | 5    | -       | 17/39/115/115 | -       |
| 18  | CLA  | B     | 807 | 6    | -       | 7/24/100/115  | -       |
| 18  | CLA  | B     | 837 | 6    | -       | 13/39/115/115 | -       |
| 18  | CLA  | 4     | 612 | 4    | -       | 13/30/106/115 | -       |
| 18  | CLA  | 3     | 611 | -    | -       | 2/2/74/115    | -       |
| 27  | DGD  | B     | 850 | -    | -       | 11/55/95/95   | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 18  | CLA  | A     | 844 | -    | -       | 12/39/115/115 | -       |
| 18  | CLA  | A     | 815 | 5    | -       | 6/15/91/115   | -       |
| 18  | CLA  | B     | 810 | 6    | -       | 12/39/115/115 | -       |
| 18  | CLA  | A     | 813 | 5    | -       | 11/26/102/115 | -       |
| 22  | BCR  | A     | 851 | -    | -       | 7/29/63/63    | 0/2/2/2 |
| 18  | CLA  | A     | 823 | 5    | -       | 4/12/88/115   | -       |
| 18  | CLA  | B     | 814 | 6    | -       | 15/39/115/115 | -       |
| 19  | XAT  | 1     | 614 | -    | -       | 8/31/93/93    | 0/4/4/4 |
| 18  | CLA  | 3     | 610 | 3    | -       | 3/8/84/115    | -       |
| 18  | CLA  | G     | 201 | -    | -       | 9/15/91/115   | -       |
| 22  | BCR  | L     | 301 | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 18  | CLA  | A     | 804 | 5    | -       | 19/39/115/115 | -       |
| 22  | BCR  | L     | 306 | -    | -       | 5/29/63/63    | 0/2/2/2 |
| 18  | CLA  | B     | 832 | 6    | -       | 15/39/115/115 | -       |
| 18  | CLA  | B     | 802 | -    | -       | 15/39/115/115 | -       |
| 17  | CHL  | 2     | 606 | -    | -       | 2/14/90/117   | -       |
| 18  | CLA  | 1     | 605 | -    | -       | 8/17/93/115   | -       |
| 18  | CLA  | 1     | 609 | -    | -       | 4/11/87/115   | -       |
| 22  | BCR  | B     | 847 | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 18  | CLA  | 1     | 610 | 20   | -       | 1/4/80/115    | -       |
| 20  | LHG  | B     | 852 | -    | -       | 14/53/53/53   | -       |
| 17  | CHL  | 4     | 607 | -    | -       | 5/17/93/117   | -       |
| 18  | CLA  | B     | 812 | 6    | -       | 1/13/89/115   | -       |
| 20  | LHG  | 2     | 618 | 18   | -       | 11/41/41/53   | -       |
| 18  | CLA  | B     | 820 | 6    | -       | 5/21/97/115   | -       |
| 18  | CLA  | 4     | 614 | 4    | -       | 10/21/97/115  | -       |
| 18  | CLA  | B     | 840 | 6    | -       | 19/39/115/115 | -       |
| 18  | CLA  | B     | 819 | -    | -       | 11/27/103/115 | -       |
| 18  | CLA  | A     | 836 | 5    | -       | 8/15/91/115   | -       |
| 18  | CLA  | B     | 838 | 6    | -       | 1/18/94/115   | -       |
| 18  | CLA  | A     | 805 | 5    | -       | 5/24/100/115  | -       |
| 18  | CLA  | A     | 814 | 5    | -       | 10/39/115/115 | -       |
| 18  | CLA  | B     | 822 | 6    | -       | 16/39/115/115 | -       |
| 18  | CLA  | B     | 817 | 6    | -       | 11/32/108/115 | -       |
| 26  | SF4  | C     | 102 | -    | -       | -             | 0/6/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 25  | PQN  | A     | 855 | -    | -       | 1/23/43/43    | 0/2/2/2 |
| 18  | CLA  | G     | 202 | 11   | -       | 5/12/88/115   | -       |
| 18  | CLA  | K     | 201 | 15   | -       | 2/4/76/115    | -       |
| 18  | CLA  | A     | 842 | 5    | -       | 17/39/115/115 | -       |
| 18  | CLA  | B     | 803 | -    | -       | 11/39/115/115 | -       |
| 17  | CHL  | 4     | 606 | -    | -       | 2/10/86/117   | -       |
| 21  | LUT  | 2     | 616 | -    | -       | 4/29/67/67    | 0/2/2/2 |
| 18  | CLA  | 1     | 608 | 1    | -       | 2/8/84/115    | -       |
| 18  | CLA  | L     | 304 | -    | -       | 3/15/91/115   | -       |
| 18  | CLA  | A     | 837 | 5    | -       | 5/15/91/115   | -       |
| 18  | CLA  | L     | 302 | -    | -       | 3/15/91/115   | -       |
| 20  | LHG  | 1     | 615 | 18   | -       | 34/53/53/53   | -       |
| 18  | CLA  | 1     | 603 | -    | -       | 8/26/102/115  | -       |
| 21  | LUT  | 4     | 616 | -    | -       | 2/29/67/67    | 0/2/2/2 |
| 18  | CLA  | A     | 845 | 20   | -       | 8/21/97/115   | -       |
| 18  | CLA  | 3     | 612 | -    | -       | 2/8/84/115    | -       |
| 18  | CLA  | A     | 808 | 5    | -       | 4/21/97/115   | -       |
| 17  | CHL  | 2     | 605 | -    | -       | 4/12/88/117   | -       |
| 18  | CLA  | 2     | 603 | 2    | -       | 3/13/89/115   | -       |
| 18  | CLA  | B     | 825 | -    | -       | 10/36/112/115 | -       |
| 18  | CLA  | A     | 802 | -    | -       | 17/39/115/115 | -       |
| 18  | CLA  | 3     | 605 | -    | -       | 6/10/86/115   | -       |
| 22  | BCR  | 4     | 618 | -    | -       | 6/29/63/63    | 0/2/2/2 |
| 21  | LUT  | 1     | 616 | -    | -       | 1/29/67/67    | 0/2/2/2 |
| 18  | CLA  | A     | 831 | 5    | -       | 11/39/115/115 | -       |
| 17  | CHL  | 2     | 615 | 2    | -       | 2/14/90/117   | -       |
| 18  | CLA  | A     | 827 | -    | -       | 3/32/108/115  | -       |
| 18  | CLA  | A     | 828 | 5    | -       | 8/39/115/115  | -       |
| 18  | CLA  | B     | 835 | -    | -       | 6/12/88/115   | -       |
| 18  | CLA  | B     | 829 | 6    | -       | 4/29/105/115  | -       |
| 22  | BCR  | B     | 844 | -    | -       | 11/29/63/63   | 0/2/2/2 |
| 18  | CLA  | 1     | 607 | -    | -       | 8/13/89/115   | -       |
| 18  | CLA  | A     | 817 | -    | -       | 5/15/91/115   | -       |
| 18  | CLA  | A     | 821 | 5    | -       | 1/15/91/115   | -       |
| 18  | CLA  | A     | 816 | 5    | -       | 4/12/88/115   | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 18  | CLA  | A     | 824 | -    | -       | 4/10/86/115   | -       |
| 18  | CLA  | B     | 804 | 6    | -       | 2/10/86/115   | -       |
| 17  | CHL  | 1     | 606 | -    | -       | 0/10/86/117   | -       |
| 18  | CLA  | F     | 303 | 10   | -       | 2/10/86/115   | -       |
| 18  | CLA  | F     | 302 | -    | -       | 5/23/99/115   | -       |
| 22  | BCR  | L     | 305 | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 21  | LUT  | 2     | 619 | -    | -       | 5/29/67/67    | 0/2/2/2 |
| 22  | BCR  | B     | 801 | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 18  | CLA  | 2     | 611 | -    | -       | 5/13/89/115   | -       |
| 18  | CLA  | B     | 830 | -    | -       | 2/13/89/115   | -       |
| 18  | CLA  | 1     | 612 | 1    | -       | 6/17/93/115   | -       |
| 18  | CLA  | 2     | 604 | -    | -       | 8/11/88/115   | -       |
| 18  | CLA  | 3     | 609 | -    | -       | 9/25/101/115  | -       |
| 18  | CLA  | F     | 301 | -    | -       | 16/30/106/115 | -       |
| 18  | CLA  | 2     | 613 | 2    | -       | 6/13/89/115   | -       |
| 22  | BCR  | A     | 849 | -    | -       | 6/29/63/63    | 0/2/2/2 |
| 22  | BCR  | J     | 102 | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 18  | CLA  | 4     | 609 | -    | -       | 8/26/102/115  | -       |
| 18  | CLA  | A     | 818 | 5    | -       | 13/33/109/115 | -       |
| 18  | CLA  | 4     | 611 | -    | -       | 6/10/86/115   | -       |
| 20  | LHG  | A     | 847 | 18   | -       | 2/34/34/53    | -       |
| 22  | BCR  | 3     | 614 | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 18  | CLA  | B     | 808 | -    | -       | 18/39/115/115 | -       |
| 18  | CLA  | J     | 101 | -    | -       | 9/23/99/115   | -       |
| 18  | CLA  | A     | 807 | 5    | -       | 13/39/115/115 | -       |
| 20  | LHG  | A     | 846 | -    | -       | 5/53/53/53    | -       |
| 18  | CLA  | B     | 815 | 6    | -       | 2/13/89/115   | -       |
| 18  | CLA  | B     | 823 | 6    | -       | 8/15/91/115   | -       |
| 18  | CLA  | B     | 827 | 6    | -       | 22/39/115/115 | -       |
| 22  | BCR  | F     | 304 | -    | -       | 12/29/63/63   | 0/2/2/2 |
| 18  | CLA  | A     | 834 | 5    | -       | 9/39/115/115  | -       |
| 18  | CLA  | 2     | 610 | 20   | -       | 5/10/70/115   | -       |
| 25  | PQN  | B     | 842 | -    | -       | 6/23/43/43    | 0/2/2/2 |
| 18  | CLA  | B     | 828 | -    | -       | 19/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 22  | BCR  | K     | 202 | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 18  | CLA  | 3     | 608 | -    | -       | 3/10/86/115   | -       |
| 18  | CLA  | 1     | 602 | 1    | -       | 6/26/102/115  | -       |
| 18  | CLA  | 2     | 608 | -    | -       | 7/15/91/115   | -       |
| 18  | CLA  | B     | 826 | 6    | -       | 6/36/112/115  | -       |
| 18  | CLA  | B     | 816 | 6    | -       | 6/27/103/115  | -       |
| 18  | CLA  | L     | 303 | 16   | -       | 11/39/115/115 | -       |
| 18  | CLA  | B     | 824 | -    | -       | 14/39/115/115 | -       |
| 18  | CLA  | B     | 809 | 6    | -       | 18/39/115/115 | -       |
| 18  | CLA  | A     | 832 | 5    | -       | 6/21/97/115   | -       |
| 23  | LMG  | 4     | 619 | -    | -       | 5/34/54/70    | 0/1/1/1 |
| 18  | CLA  | A     | 833 | 5    | -       | 7/29/105/115  | -       |
| 18  | CLA  | A     | 841 | 5    | -       | 14/39/115/115 | -       |
| 18  | CLA  | 4     | 601 | 4    | -       | 7/17/93/115   | -       |
| 17  | CHL  | 4     | 605 | -    | -       | 2/10/86/117   | -       |
| 18  | CLA  | A     | 840 | 5    | -       | 8/24/100/115  | -       |
| 18  | CLA  | 3     | 602 | -    | -       | 11/27/103/115 | -       |
| 18  | CLA  | 1     | 611 | -    | -       | 6/15/91/115   | -       |
| 20  | LHG  | B     | 851 | 18   | -       | 5/42/42/53    | -       |
| 22  | BCR  | K     | 205 | -    | -       | 9/29/63/63    | 0/2/2/2 |
| 18  | CLA  | A     | 838 | 5    | -       | 6/23/99/115   | -       |
| 26  | SF4  | C     | 101 | -    | -       | -             | 0/6/5/5 |
| 18  | CLA  | K     | 203 | -    | -       | 6/15/91/115   | -       |
| 18  | CLA  | A     | 839 | -    | -       | 11/27/103/115 | -       |
| 22  | BCR  | B     | 849 | -    | -       | 7/29/63/63    | 0/2/2/2 |
| 22  | BCR  | I     | 101 | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 18  | CLA  | K     | 204 | 15   | -       | 12/17/93/115  | -       |
| 22  | BCR  | B     | 843 | -    | -       | 1/29/63/63    | 0/2/2/2 |
| 18  | CLA  | A     | 822 | -    | -       | 13/39/115/115 | -       |
| 18  | CLA  | 4     | 608 | 4    | -       | 6/15/91/115   | -       |
| 18  | CLA  | 3     | 603 | -    | -       | 8/15/91/115   | -       |
| 22  | BCR  | A     | 850 | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 18  | CLA  | 4     | 610 | -    | -       | 4/12/88/115   | -       |
| 18  | CLA  | A     | 803 | -    | -       | 21/39/115/115 | -       |
| 18  | CLA  | B     | 806 | 6    | -       | 12/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 18  | CLA  | A     | 811 | -    | -       | 10/39/115/115 | -       |
| 24  | CL0  | A     | 801 | 5    | -       | 8/35/95/115   | -       |
| 18  | CLA  | B     | 834 | 6    | -       | 9/33/109/115  | -       |
| 18  | CLA  | 3     | 604 | -    | -       | 2/10/86/115   | -       |
| 18  | CLA  | B     | 805 | 6    | -       | 16/39/115/115 | -       |
| 22  | BCR  | A     | 848 | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 22  | BCR  | B     | 848 | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 22  | BCR  | A     | 852 | -    | -       | 13/29/63/63   | 0/2/2/2 |
| 22  | BCR  | G     | 204 | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 18  | CLA  | 4     | 604 | -    | -       | 6/11/87/115   | -       |

The worst 5 of 1520 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | 2     | 610 | CLA  | C1A-NA  | 12.67 | 1.40        | 1.29     |
| 24  | A     | 801 | CL0  | C1D-ND  | 8.48  | 1.48        | 1.37     |
| 24  | A     | 801 | CL0  | C3D-C4D | -6.44 | 1.34        | 1.46     |
| 17  | 2     | 606 | CHL  | O2D-CGD | 5.18  | 1.45        | 1.33     |
| 17  | 4     | 606 | CHL  | O2D-CGD | 5.17  | 1.45        | 1.33     |

The worst 5 of 1557 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 18  | A     | 818 | CLA  | O2D-CGD-CBD | 26.04  | 157.54      | 111.27   |
| 18  | A     | 818 | CLA  | O2D-CGD-O1D | -25.22 | 74.53       | 123.84   |
| 18  | A     | 818 | CLA  | O1D-CGD-CBD | -20.27 | 83.01       | 124.48   |
| 18  | B     | 836 | CLA  | C5-C3-C4    | -16.66 | 77.79       | 114.60   |
| 24  | A     | 801 | CL0  | C2B-C1B-NB  | 15.14  | 120.38      | 110.23   |

There are no chirality outliers.

5 of 1560 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | 2     | 605 | CHL  | C3C-C2C-CMC-OMC |
| 17  | 2     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 17  | 2     | 601 | CHL  | C3A-C2A-CAA-CBA |
| 17  | 2     | 601 | CHL  | CHA-CBD-CGD-O1D |
| 17  | 2     | 601 | CHL  | CHA-CBD-CGD-O2D |

There are no ring outliers.

164 monomers are involved in 464 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 18  | A     | 843 | CLA  | 2       | 0            |
| 18  | A     | 825 | CLA  | 3       | 0            |
| 18  | B     | 833 | CLA  | 1       | 0            |
| 19  | 2     | 617 | XAT  | 7       | 0            |
| 18  | A     | 810 | CLA  | 1       | 0            |
| 18  | 3     | 601 | CLA  | 4       | 0            |
| 18  | 2     | 602 | CLA  | 8       | 0            |
| 17  | 4     | 615 | CHL  | 1       | 0            |
| 21  | 3     | 613 | LUT  | 6       | 0            |
| 18  | A     | 835 | CLA  | 5       | 0            |
| 23  | 4     | 620 | LMG  | 1       | 0            |
| 18  | 2     | 612 | CLA  | 4       | 0            |
| 18  | A     | 806 | CLA  | 3       | 0            |
| 18  | A     | 812 | CLA  | 6       | 0            |
| 18  | B     | 836 | CLA  | 2       | 0            |
| 18  | 4     | 613 | CLA  | 2       | 0            |
| 18  | 4     | 603 | CLA  | 1       | 0            |
| 18  | B     | 841 | CLA  | 2       | 0            |
| 18  | A     | 826 | CLA  | 2       | 0            |
| 18  | B     | 813 | CLA  | 4       | 0            |
| 18  | 4     | 602 | CLA  | 5       | 0            |
| 18  | H     | 201 | CLA  | 2       | 0            |
| 17  | 1     | 601 | CHL  | 10      | 0            |
| 18  | A     | 820 | CLA  | 4       | 0            |
| 18  | 2     | 609 | CLA  | 5       | 0            |
| 22  | B     | 845 | BCR  | 8       | 0            |
| 18  | A     | 819 | CLA  | 4       | 0            |
| 18  | A     | 830 | CLA  | 4       | 0            |
| 18  | B     | 821 | CLA  | 1       | 0            |
| 22  | B     | 846 | BCR  | 7       | 0            |
| 17  | 2     | 601 | CHL  | 1       | 0            |
| 17  | 2     | 607 | CHL  | 2       | 0            |
| 18  | 3     | 607 | CLA  | 3       | 0            |
| 18  | 1     | 604 | CLA  | 3       | 0            |
| 18  | B     | 831 | CLA  | 1       | 0            |
| 19  | 4     | 617 | XAT  | 5       | 0            |
| 22  | A     | 853 | BCR  | 7       | 0            |
| 17  | 3     | 606 | CHL  | 1       | 0            |
| 18  | B     | 818 | CLA  | 4       | 0            |
| 18  | A     | 809 | CLA  | 9       | 0            |
| 18  | A     | 829 | CLA  | 6       | 0            |
| 18  | B     | 837 | CLA  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 18  | 4     | 612 | CLA  | 2       | 0            |
| 27  | B     | 850 | DGD  | 5       | 0            |
| 18  | A     | 844 | CLA  | 4       | 0            |
| 18  | A     | 815 | CLA  | 1       | 0            |
| 18  | A     | 813 | CLA  | 4       | 0            |
| 22  | A     | 851 | BCR  | 8       | 0            |
| 18  | A     | 823 | CLA  | 1       | 0            |
| 18  | B     | 814 | CLA  | 3       | 0            |
| 19  | 1     | 614 | XAT  | 18      | 0            |
| 18  | G     | 201 | CLA  | 1       | 0            |
| 22  | L     | 301 | BCR  | 4       | 0            |
| 18  | A     | 804 | CLA  | 6       | 0            |
| 22  | L     | 306 | BCR  | 5       | 0            |
| 18  | B     | 832 | CLA  | 6       | 0            |
| 18  | B     | 802 | CLA  | 4       | 0            |
| 17  | 2     | 606 | CHL  | 1       | 0            |
| 18  | 1     | 605 | CLA  | 1       | 0            |
| 18  | 1     | 609 | CLA  | 7       | 0            |
| 22  | B     | 847 | BCR  | 4       | 0            |
| 20  | B     | 852 | LHG  | 3       | 0            |
| 17  | 4     | 607 | CHL  | 2       | 0            |
| 18  | B     | 812 | CLA  | 1       | 0            |
| 20  | 2     | 618 | LHG  | 3       | 0            |
| 18  | B     | 820 | CLA  | 2       | 0            |
| 18  | 4     | 614 | CLA  | 2       | 0            |
| 18  | B     | 840 | CLA  | 6       | 0            |
| 18  | B     | 819 | CLA  | 1       | 0            |
| 18  | A     | 836 | CLA  | 1       | 0            |
| 18  | B     | 838 | CLA  | 2       | 0            |
| 18  | A     | 805 | CLA  | 3       | 0            |
| 18  | A     | 814 | CLA  | 2       | 0            |
| 18  | B     | 822 | CLA  | 8       | 0            |
| 18  | B     | 817 | CLA  | 3       | 0            |
| 25  | A     | 855 | PQN  | 3       | 0            |
| 18  | K     | 201 | CLA  | 1       | 0            |
| 18  | A     | 842 | CLA  | 5       | 0            |
| 18  | B     | 803 | CLA  | 4       | 0            |
| 21  | 2     | 616 | LUT  | 4       | 0            |
| 18  | 1     | 608 | CLA  | 1       | 0            |
| 18  | L     | 302 | CLA  | 2       | 0            |
| 20  | 1     | 615 | LHG  | 13      | 0            |
| 18  | 1     | 603 | CLA  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 21  | 4     | 616 | LUT  | 4       | 0            |
| 18  | A     | 845 | CLA  | 1       | 0            |
| 18  | 3     | 612 | CLA  | 1       | 0            |
| 18  | A     | 808 | CLA  | 2       | 0            |
| 17  | 2     | 605 | CHL  | 3       | 0            |
| 18  | B     | 825 | CLA  | 2       | 0            |
| 18  | A     | 802 | CLA  | 3       | 0            |
| 18  | 3     | 605 | CLA  | 1       | 0            |
| 22  | 4     | 618 | BCR  | 4       | 0            |
| 21  | 1     | 616 | LUT  | 3       | 0            |
| 18  | A     | 831 | CLA  | 1       | 0            |
| 17  | 2     | 615 | CHL  | 5       | 0            |
| 18  | A     | 827 | CLA  | 1       | 0            |
| 18  | A     | 828 | CLA  | 1       | 0            |
| 22  | B     | 844 | BCR  | 2       | 0            |
| 18  | 1     | 607 | CLA  | 1       | 0            |
| 18  | A     | 817 | CLA  | 1       | 0            |
| 18  | A     | 821 | CLA  | 2       | 0            |
| 18  | B     | 804 | CLA  | 1       | 0            |
| 18  | F     | 302 | CLA  | 5       | 0            |
| 22  | L     | 305 | BCR  | 9       | 0            |
| 21  | 2     | 619 | LUT  | 6       | 0            |
| 22  | B     | 801 | BCR  | 10      | 0            |
| 18  | B     | 830 | CLA  | 1       | 0            |
| 18  | 1     | 612 | CLA  | 1       | 0            |
| 18  | 2     | 604 | CLA  | 5       | 0            |
| 18  | 3     | 609 | CLA  | 1       | 0            |
| 18  | F     | 301 | CLA  | 1       | 0            |
| 18  | 2     | 613 | CLA  | 1       | 0            |
| 22  | A     | 849 | BCR  | 2       | 0            |
| 22  | J     | 102 | BCR  | 6       | 0            |
| 18  | 4     | 609 | CLA  | 4       | 0            |
| 18  | A     | 818 | CLA  | 1       | 0            |
| 22  | 3     | 614 | BCR  | 4       | 0            |
| 18  | B     | 808 | CLA  | 5       | 0            |
| 18  | J     | 101 | CLA  | 2       | 0            |
| 18  | A     | 807 | CLA  | 3       | 0            |
| 20  | A     | 846 | LHG  | 6       | 0            |
| 18  | B     | 823 | CLA  | 2       | 0            |
| 18  | B     | 827 | CLA  | 5       | 0            |
| 22  | F     | 304 | BCR  | 2       | 0            |
| 18  | A     | 834 | CLA  | 3       | 0            |

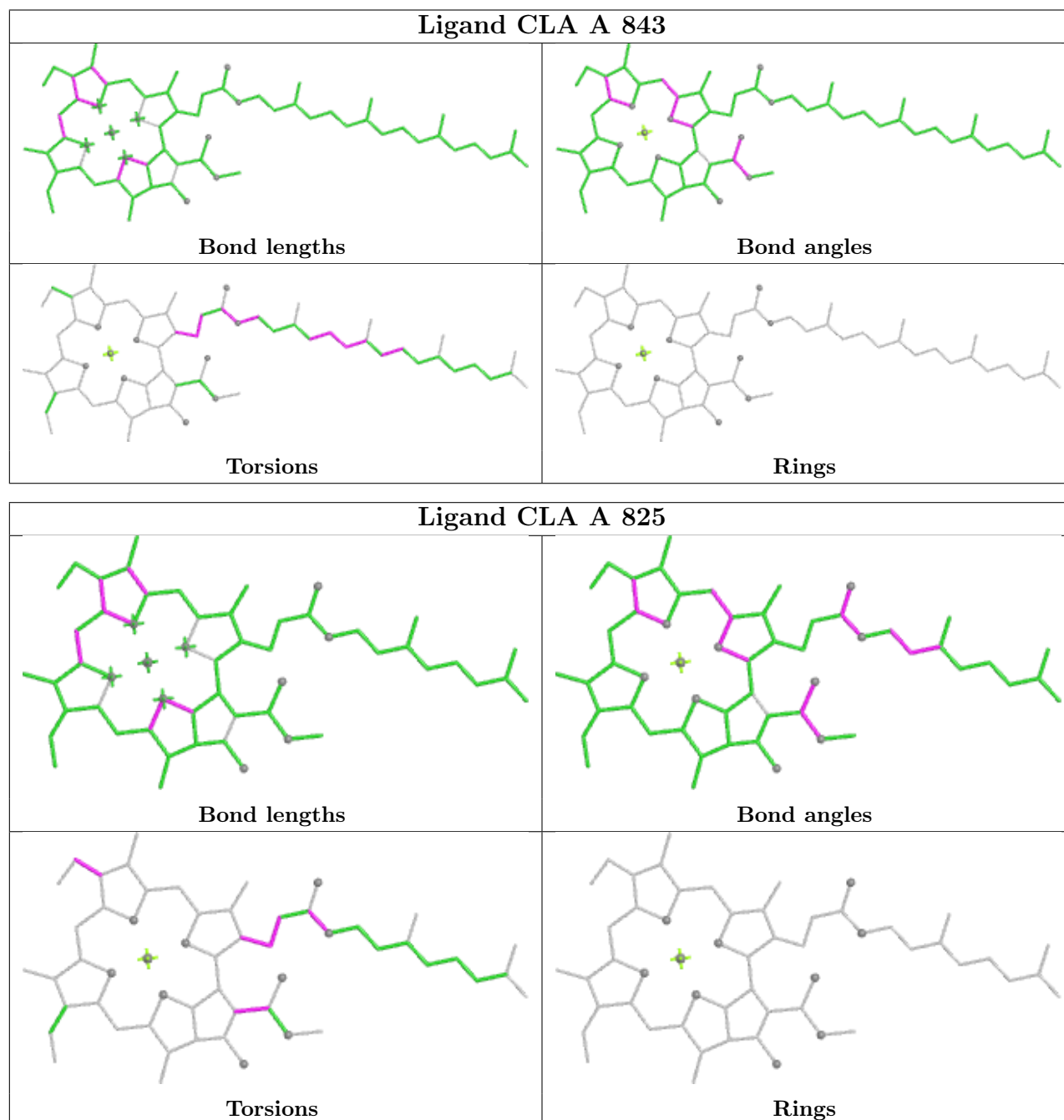
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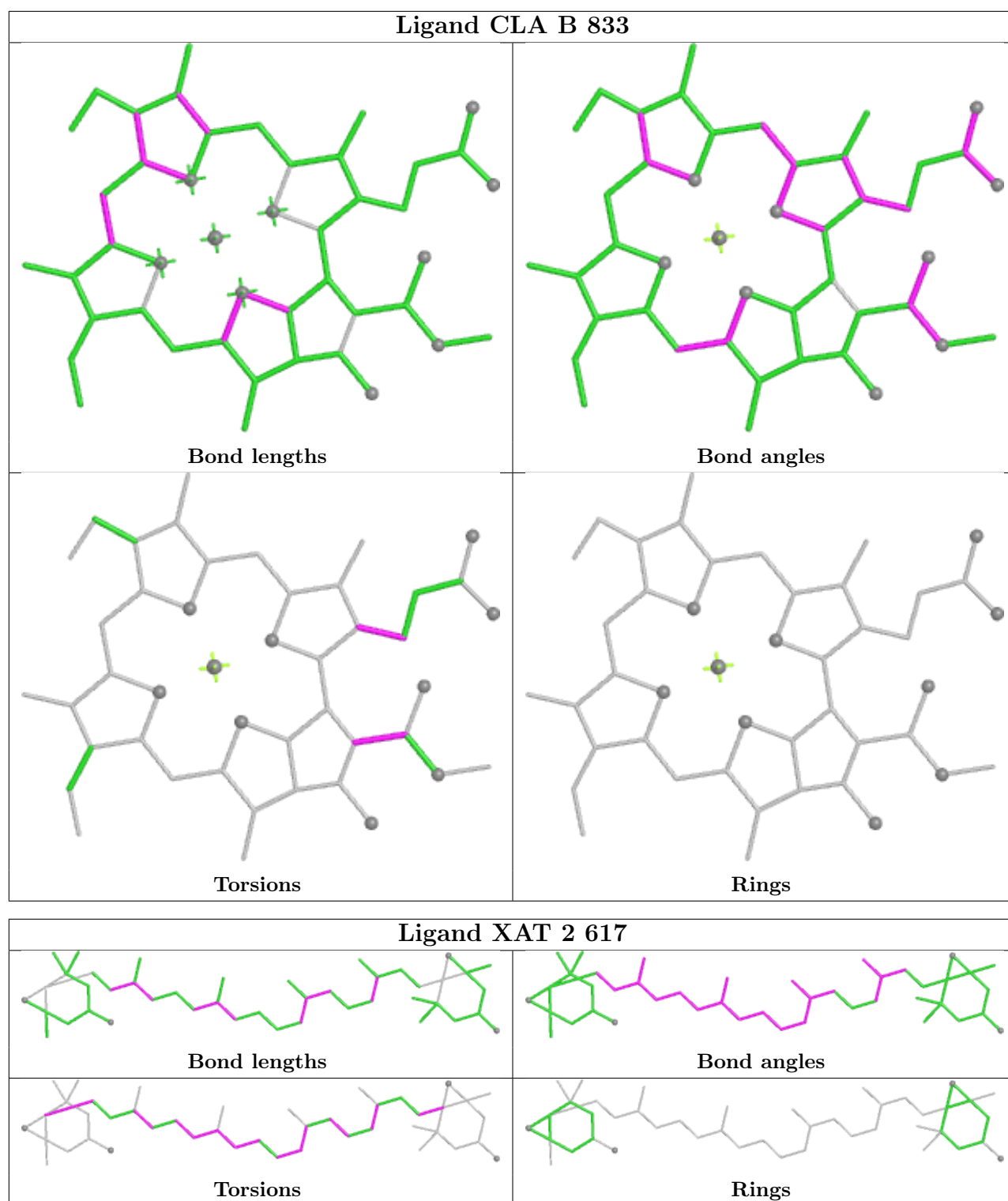
*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | B     | 842 | PQN  | 2       | 0            |
| 18  | B     | 828 | CLA  | 6       | 0            |
| 22  | K     | 202 | BCR  | 3       | 0            |
| 18  | 1     | 602 | CLA  | 8       | 0            |
| 18  | 2     | 608 | CLA  | 2       | 0            |
| 18  | B     | 826 | CLA  | 3       | 0            |
| 18  | L     | 303 | CLA  | 5       | 0            |
| 18  | B     | 824 | CLA  | 6       | 0            |
| 18  | B     | 809 | CLA  | 4       | 0            |
| 18  | A     | 832 | CLA  | 1       | 0            |
| 18  | A     | 833 | CLA  | 3       | 0            |
| 18  | A     | 841 | CLA  | 6       | 0            |
| 17  | 4     | 605 | CHL  | 1       | 0            |
| 18  | A     | 840 | CLA  | 1       | 0            |
| 18  | 3     | 602 | CLA  | 2       | 0            |
| 18  | 1     | 611 | CLA  | 1       | 0            |
| 20  | B     | 851 | LHG  | 2       | 0            |
| 22  | K     | 205 | BCR  | 4       | 0            |
| 18  | A     | 839 | CLA  | 1       | 0            |
| 22  | B     | 849 | BCR  | 4       | 0            |
| 22  | I     | 101 | BCR  | 1       | 0            |
| 18  | K     | 204 | CLA  | 1       | 0            |
| 22  | B     | 843 | BCR  | 4       | 0            |
| 18  | A     | 822 | CLA  | 4       | 0            |
| 18  | 4     | 608 | CLA  | 2       | 0            |
| 18  | 3     | 603 | CLA  | 2       | 0            |
| 22  | A     | 850 | BCR  | 5       | 0            |
| 18  | 4     | 610 | CLA  | 1       | 0            |
| 18  | A     | 803 | CLA  | 3       | 0            |
| 18  | B     | 806 | CLA  | 3       | 0            |
| 18  | A     | 811 | CLA  | 3       | 0            |
| 24  | A     | 801 | CL0  | 5       | 0            |
| 18  | B     | 834 | CLA  | 1       | 0            |
| 18  | B     | 805 | CLA  | 6       | 0            |
| 22  | A     | 848 | BCR  | 3       | 0            |
| 22  | B     | 848 | BCR  | 5       | 0            |
| 22  | A     | 852 | BCR  | 2       | 0            |
| 22  | G     | 204 | BCR  | 2       | 0            |

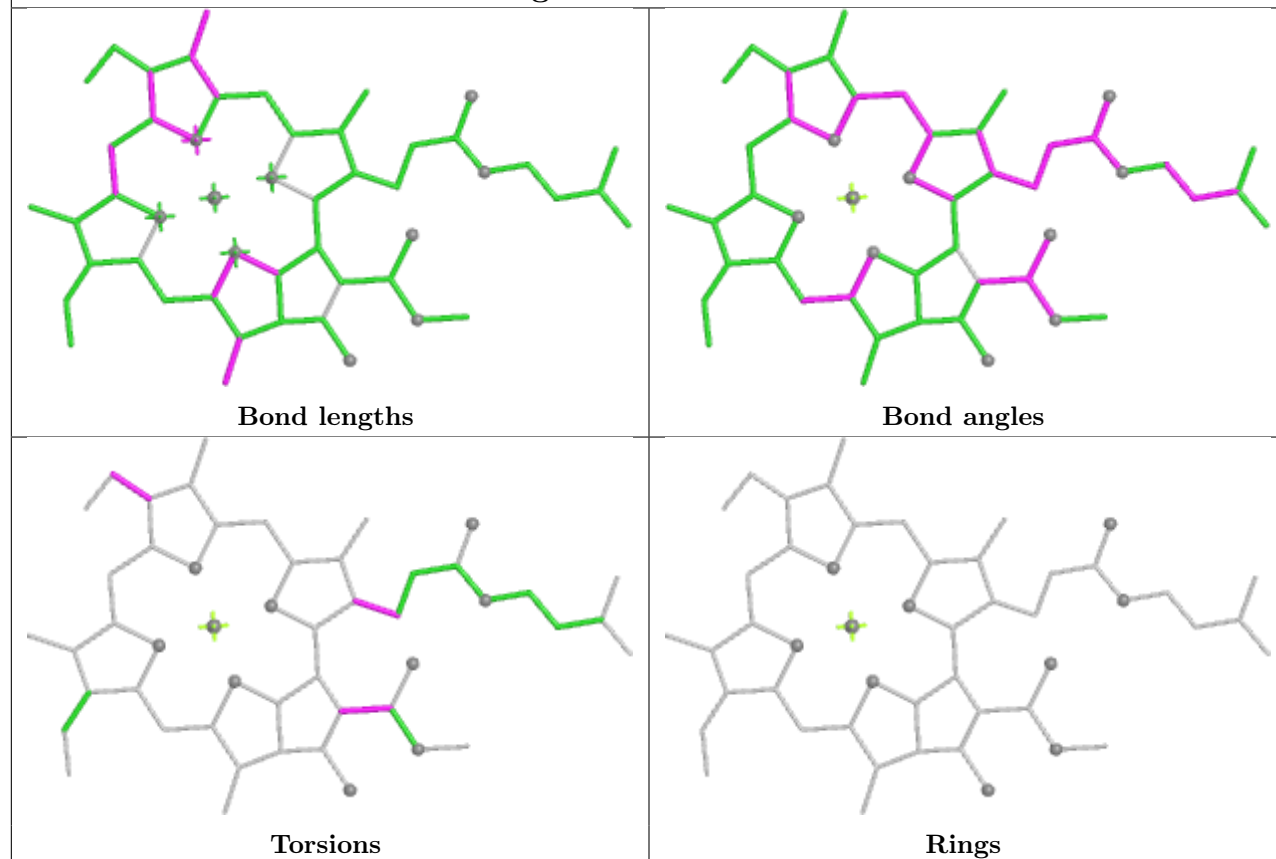
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

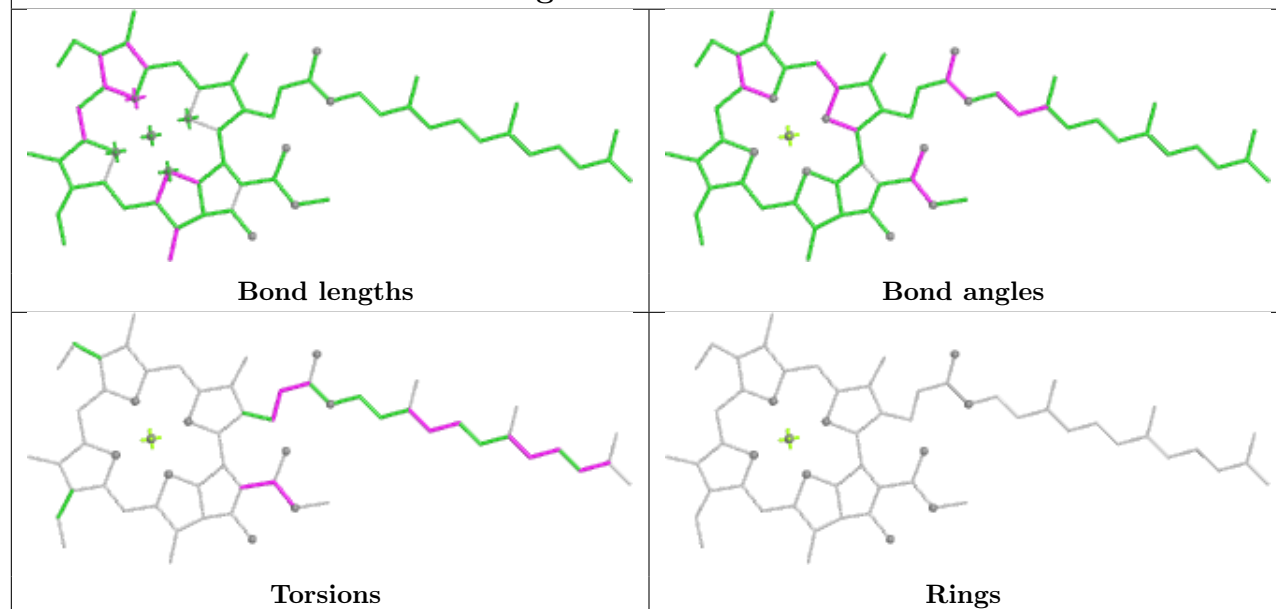


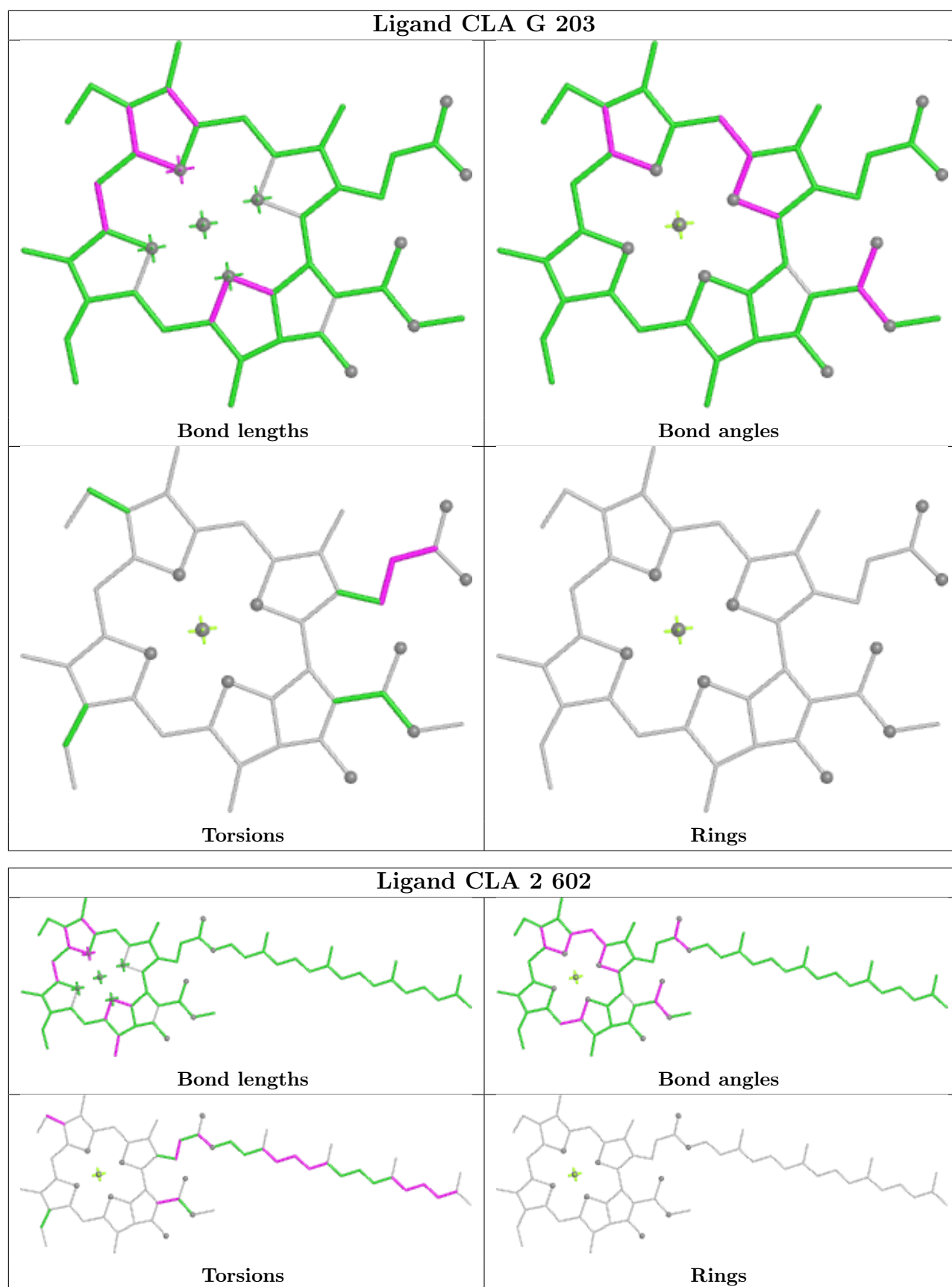


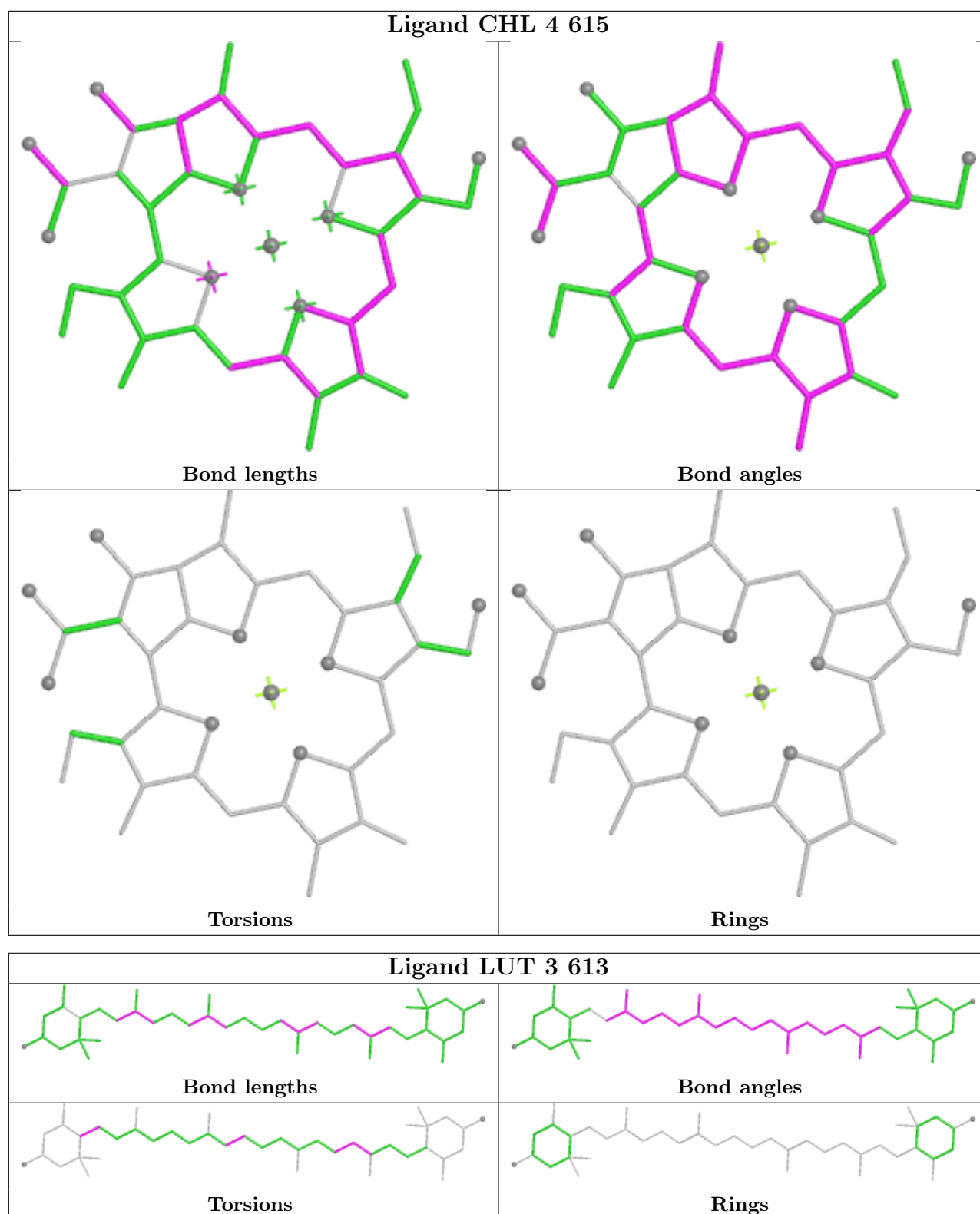
## Ligand CLA A 810

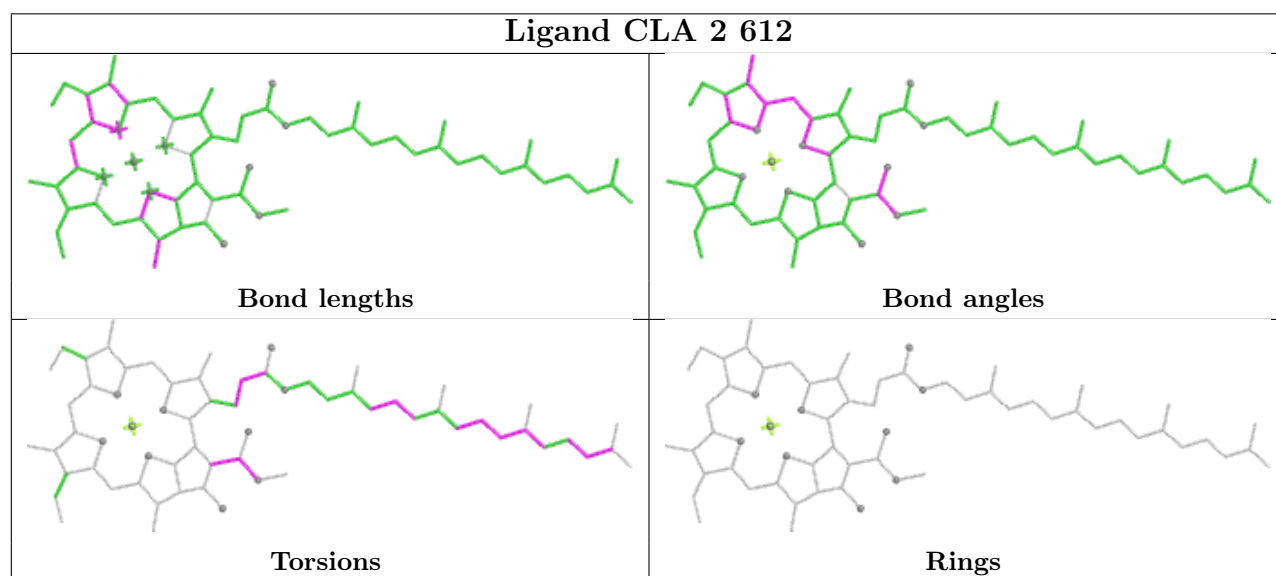
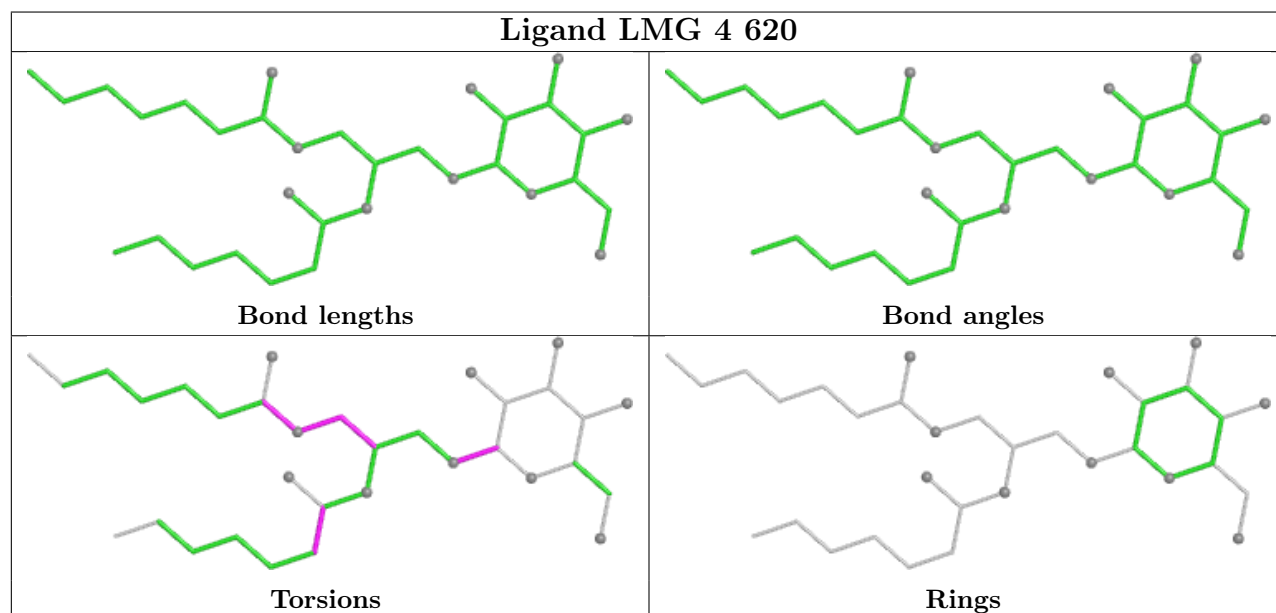
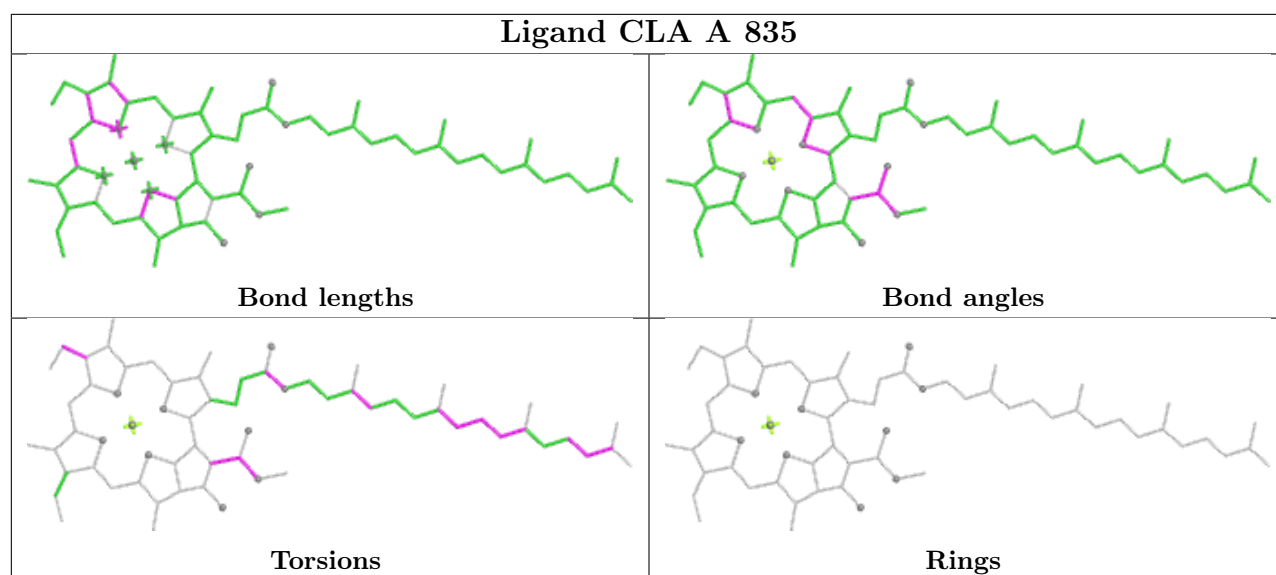


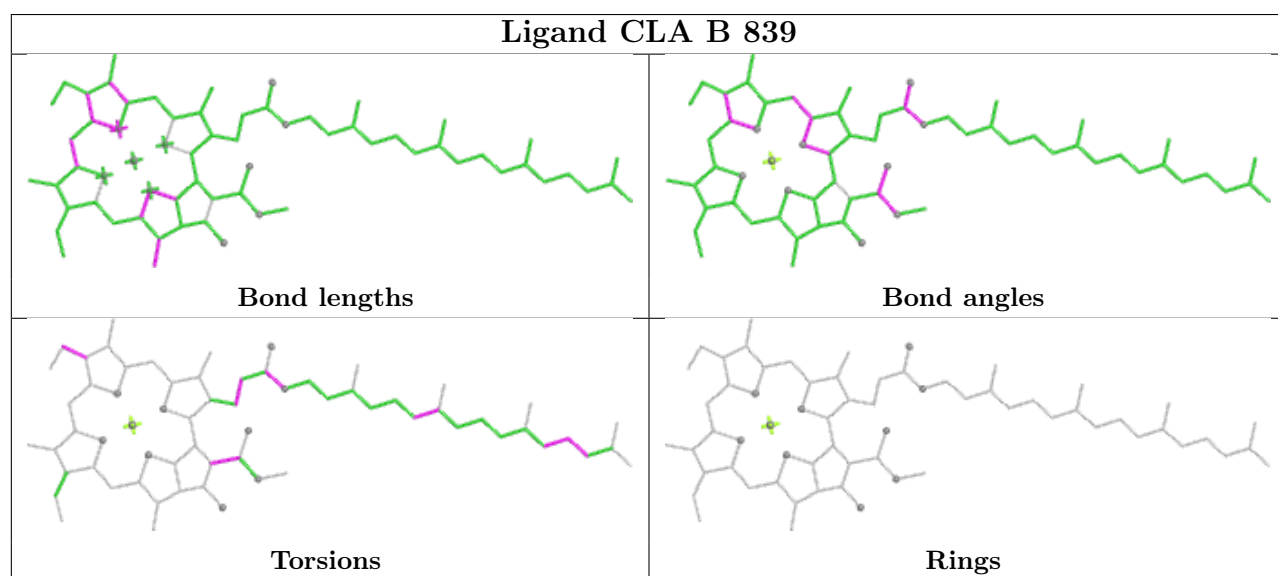
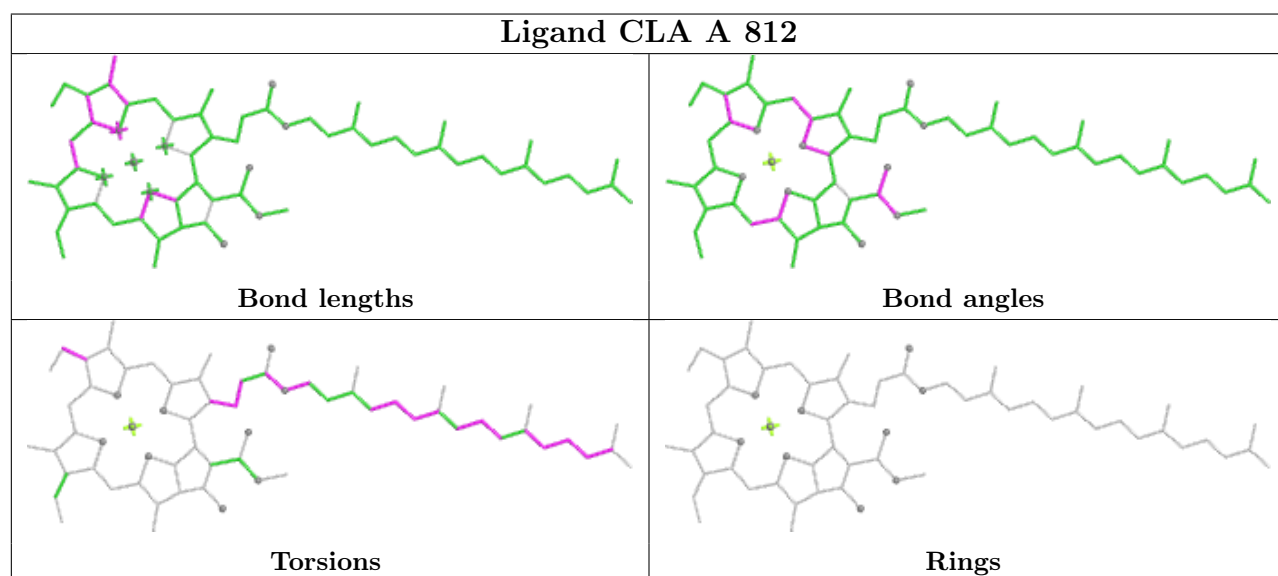
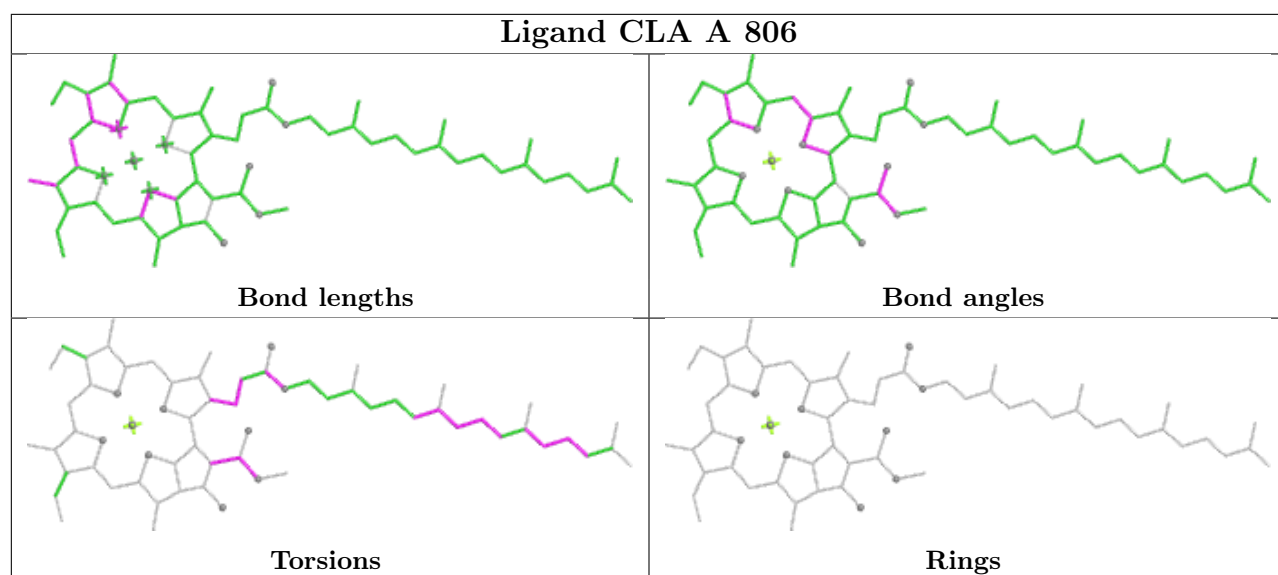
## Ligand CLA 3 601

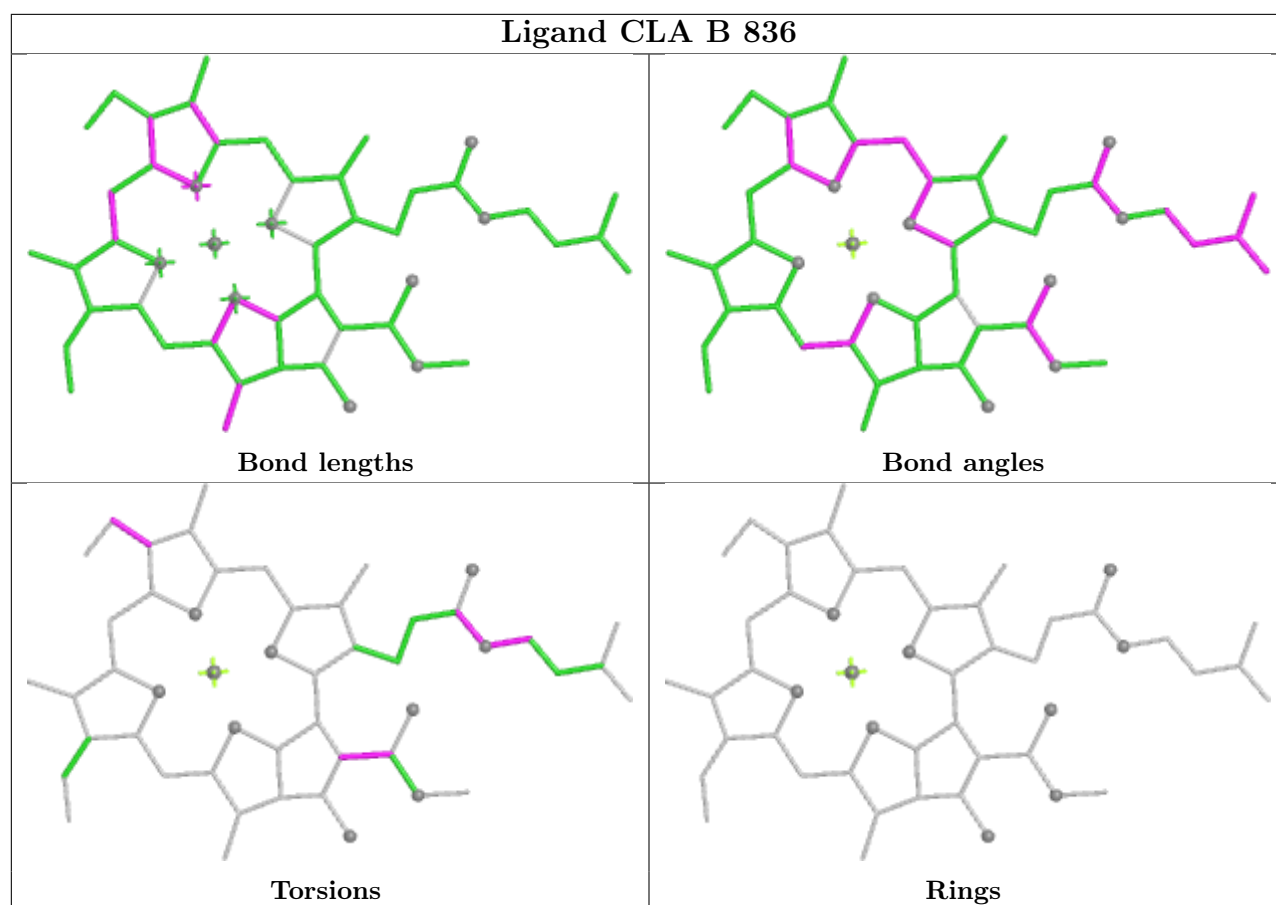




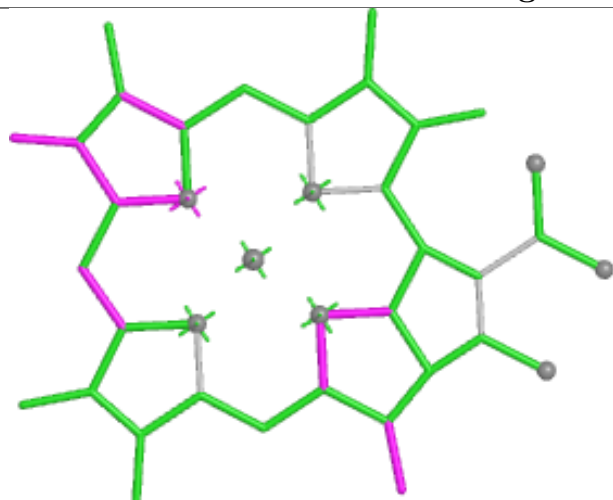




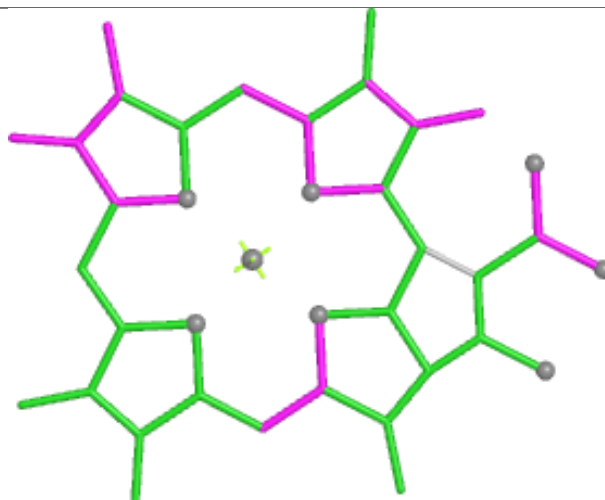




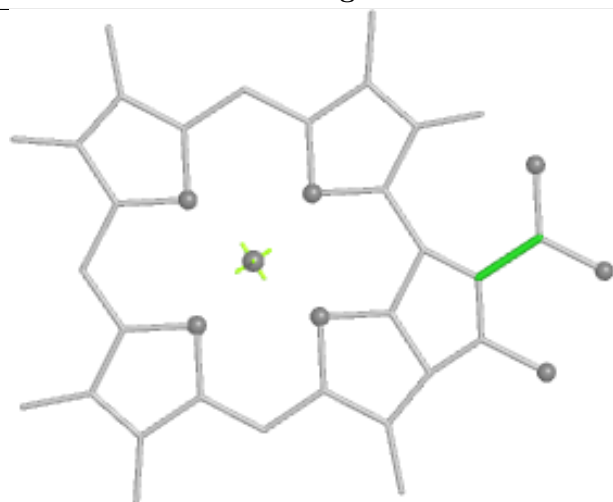
## Ligand CLA 1 613



Bond lengths



Bond angles

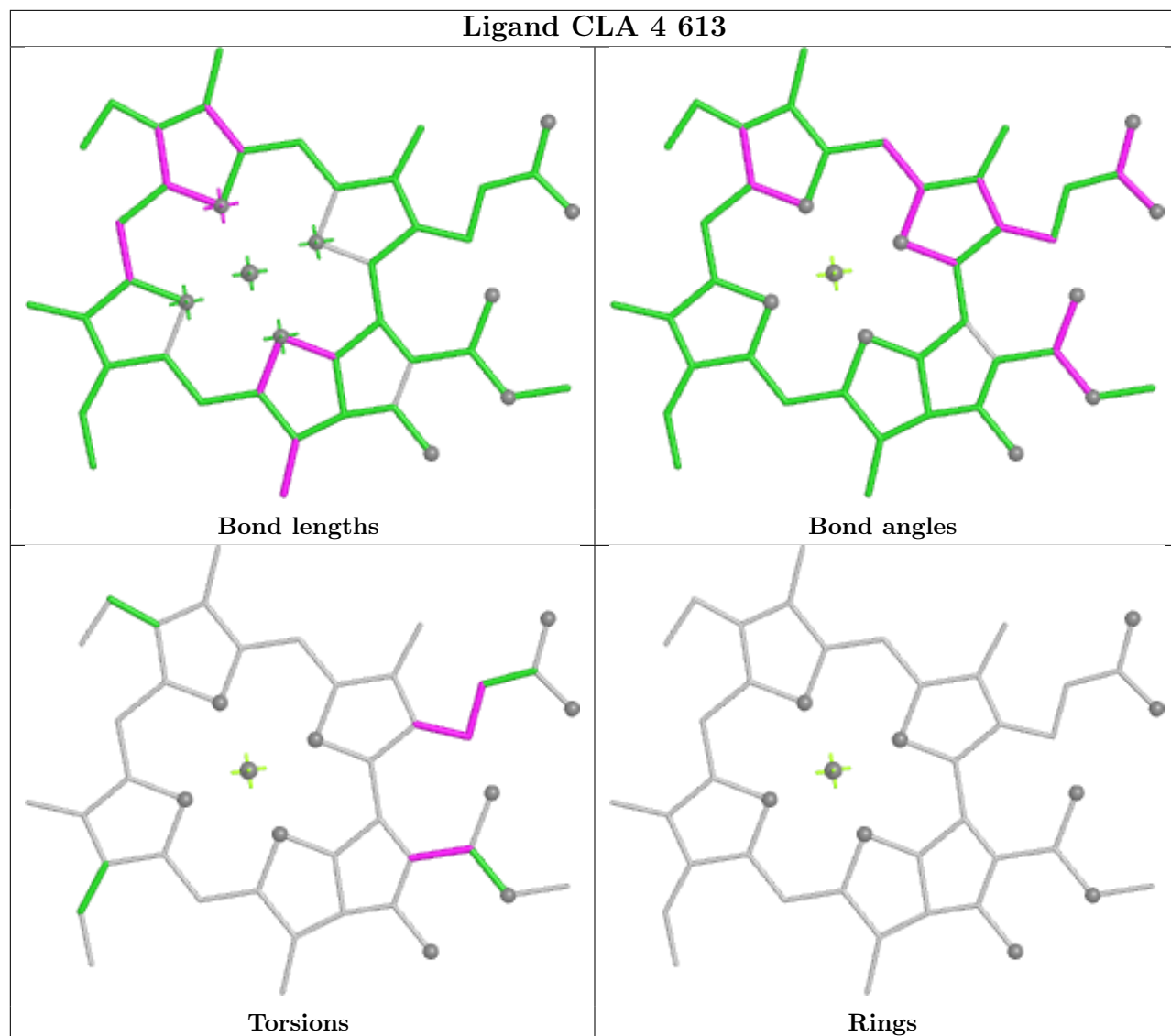


Torsions

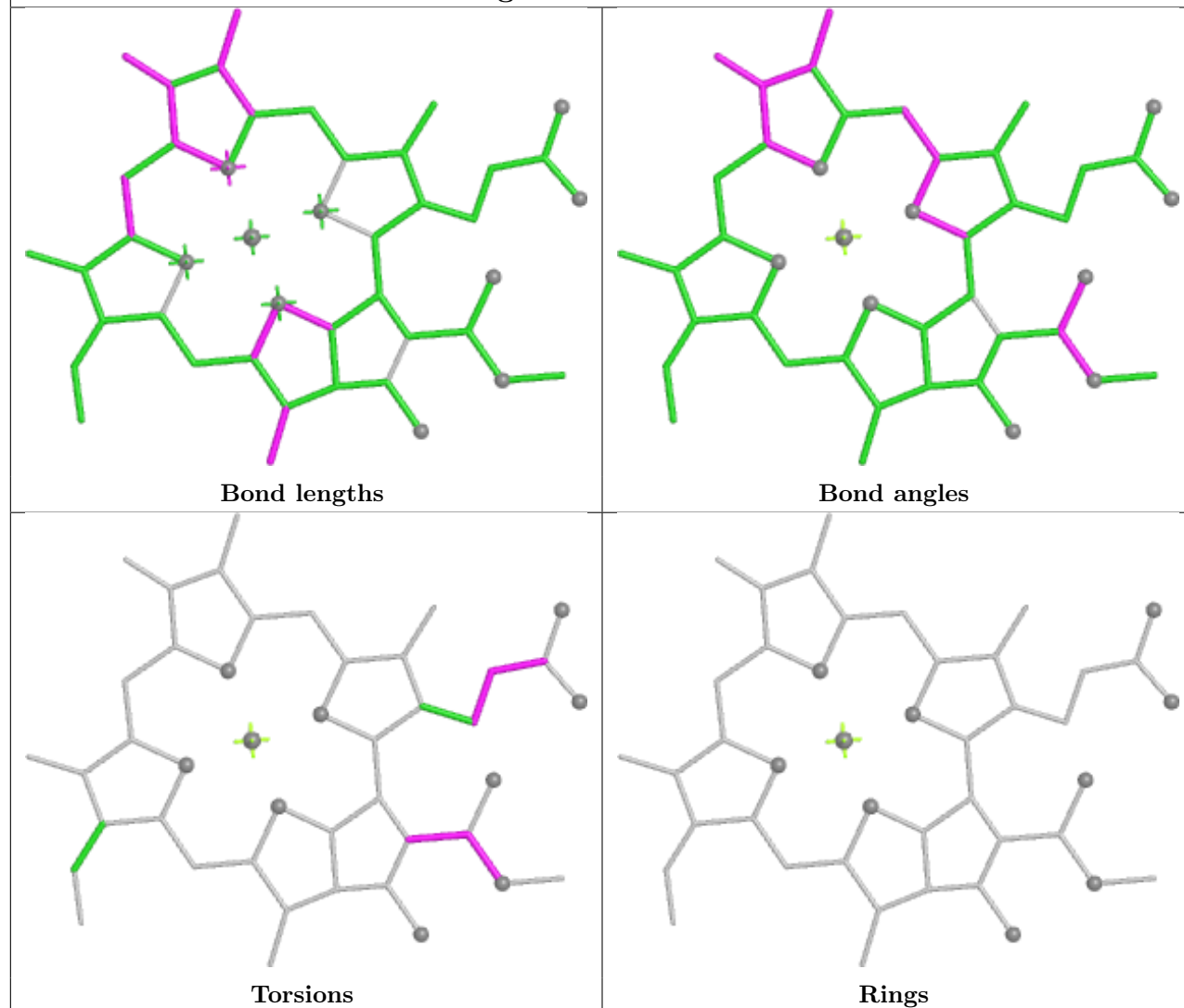


Rings

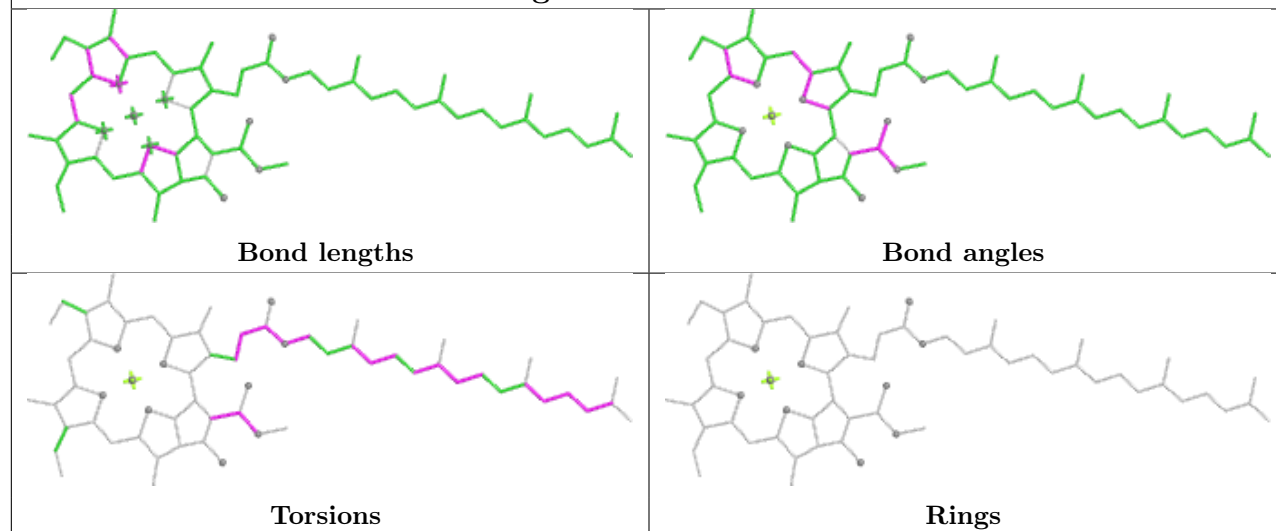
## Ligand CLA 4 613

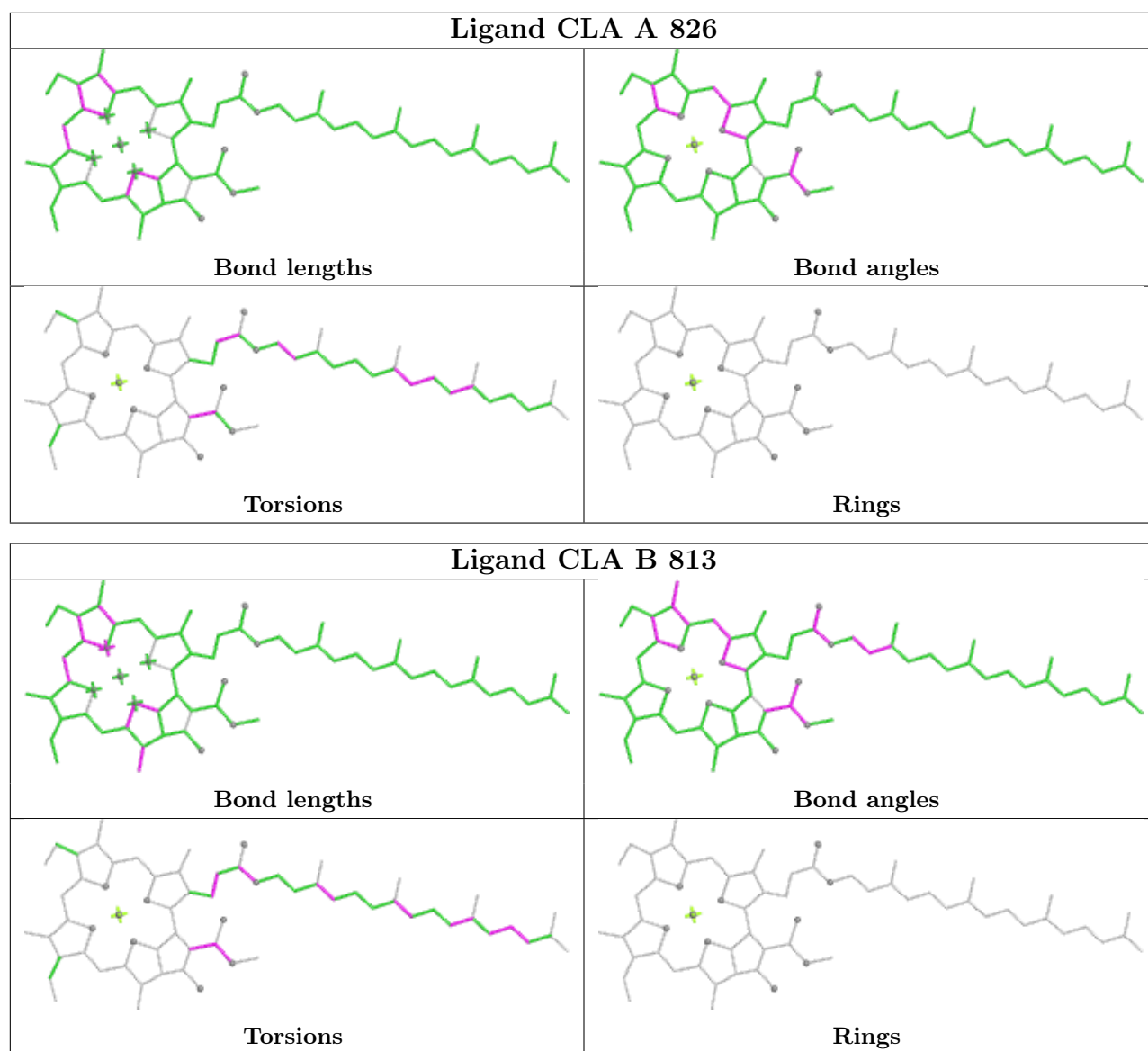


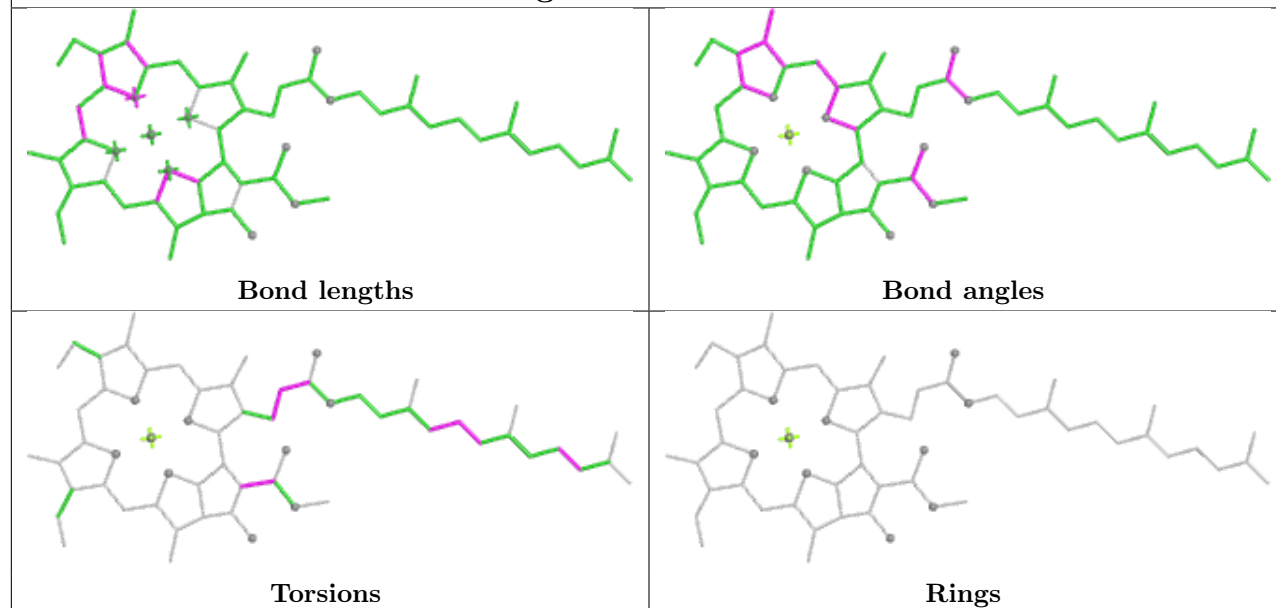
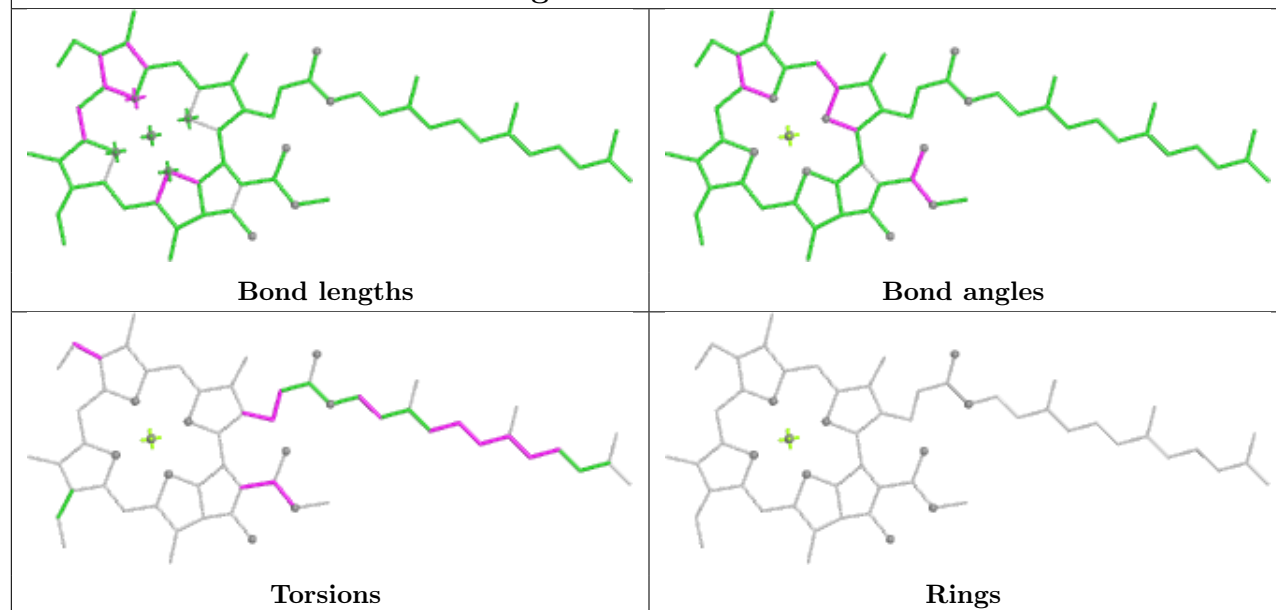
## Ligand CLA 4 603

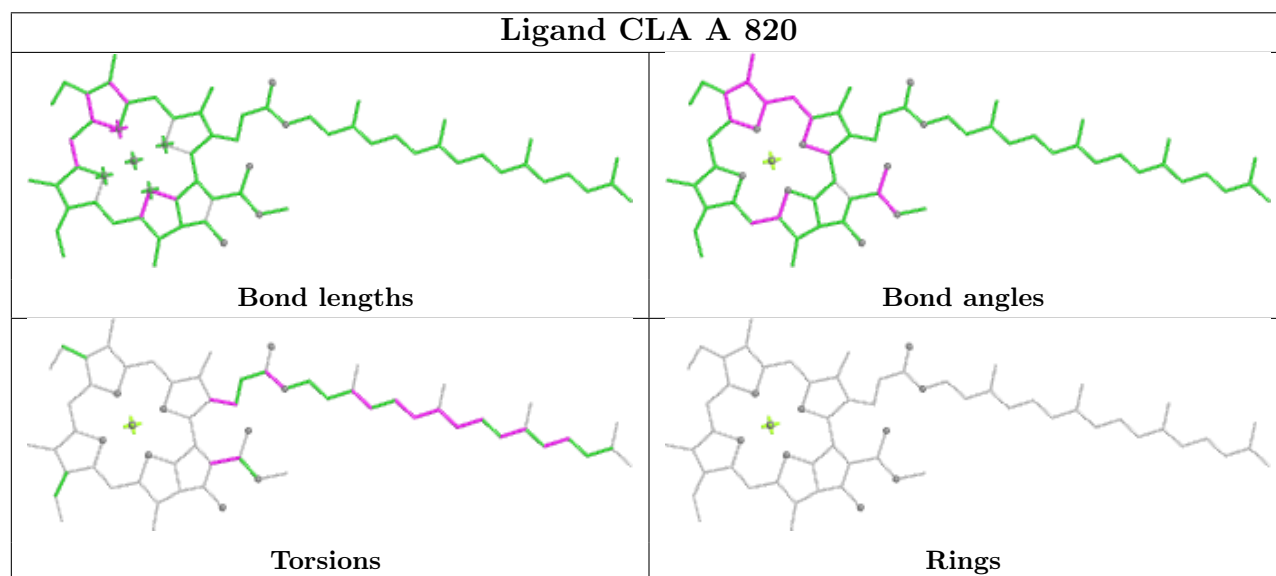
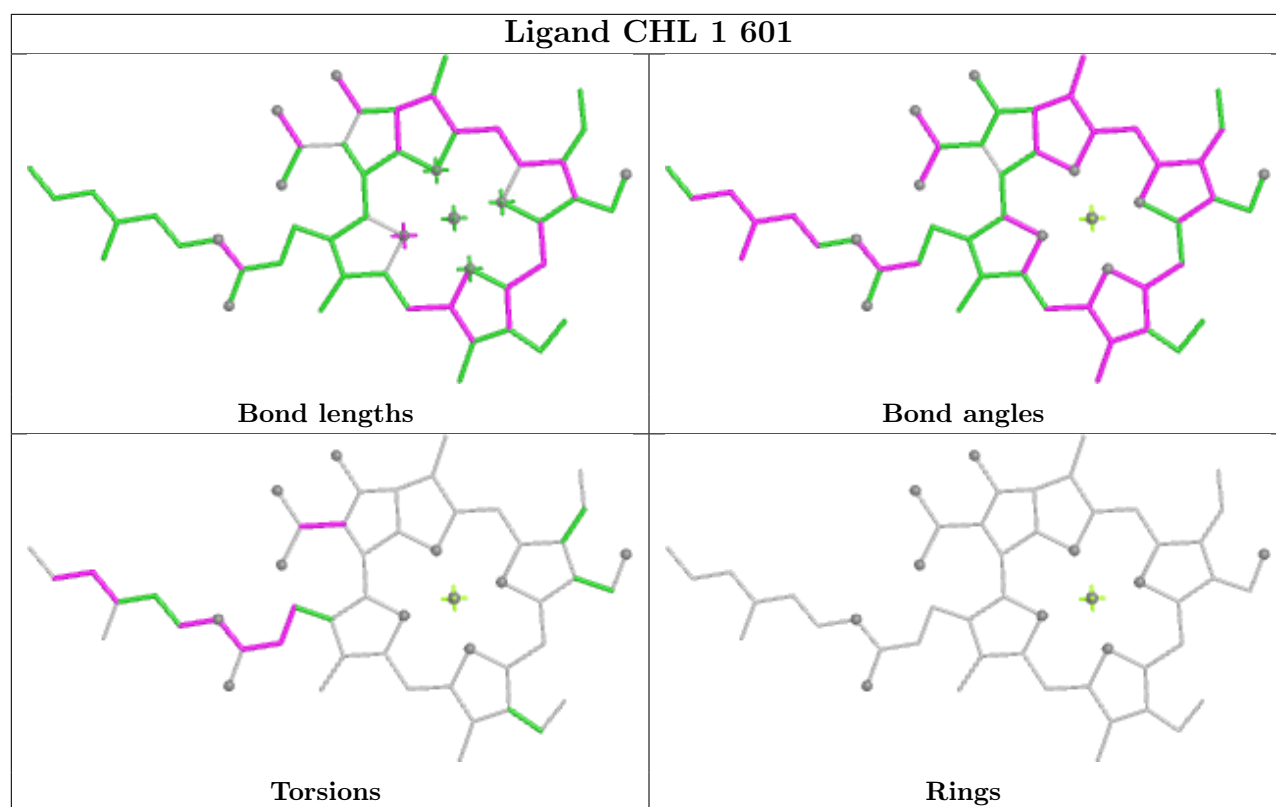


## Ligand CLA B 841

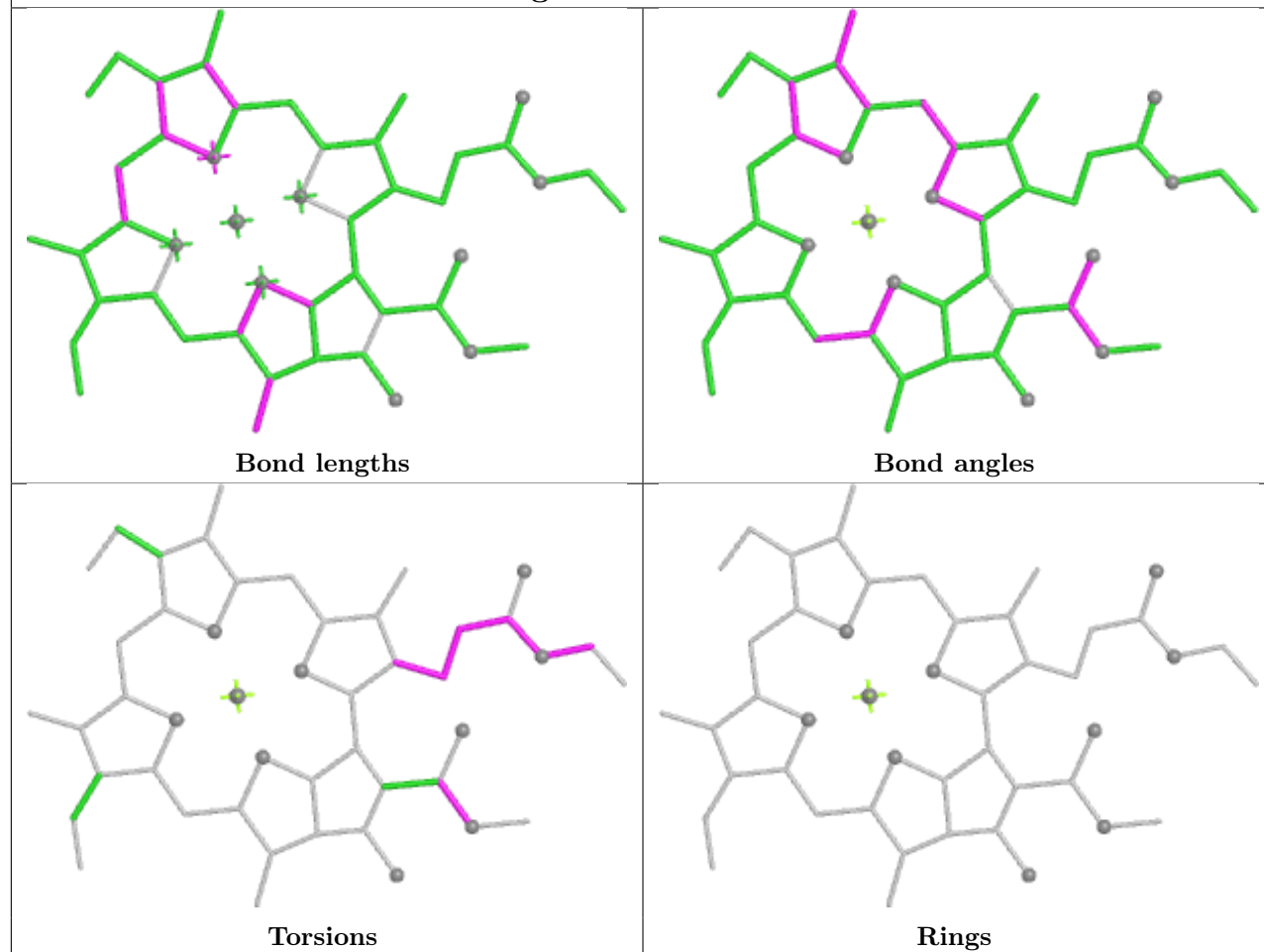




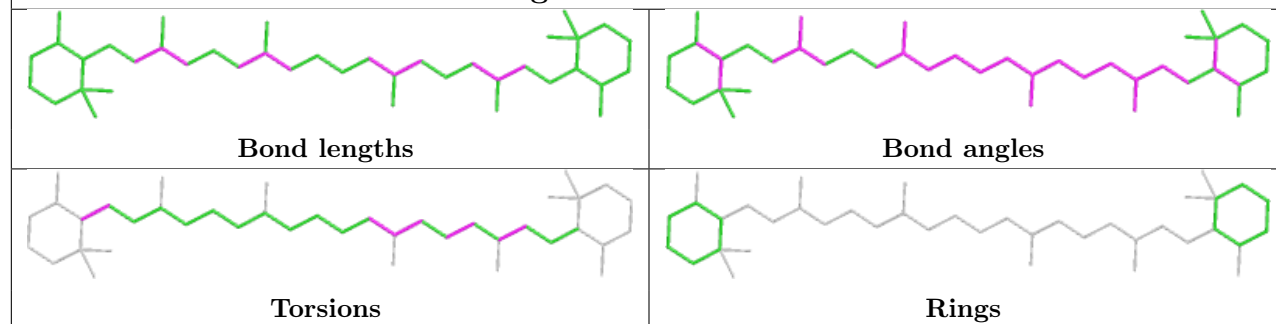
**Ligand CLA 4 602****Ligand CLA H 201**



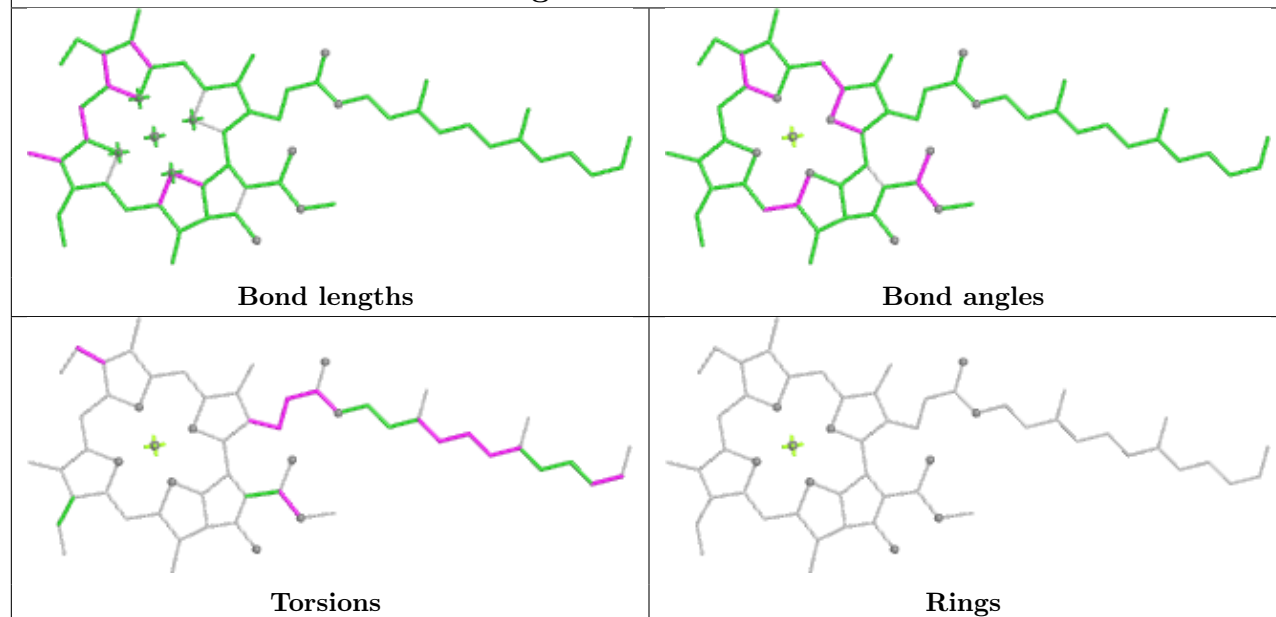
## Ligand CLA 2 609



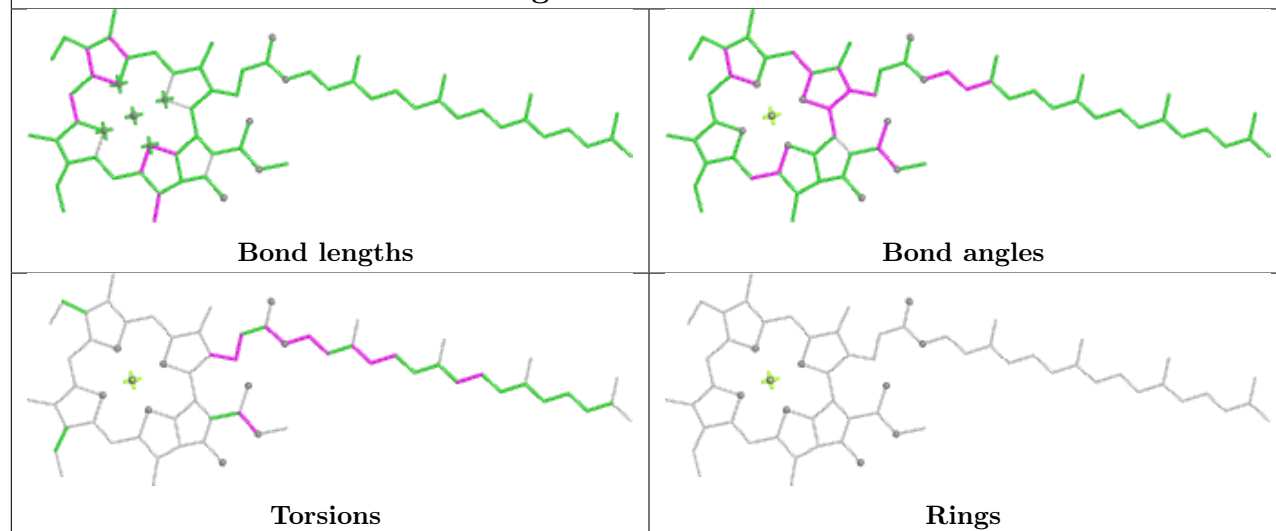
## Ligand BCR B 845



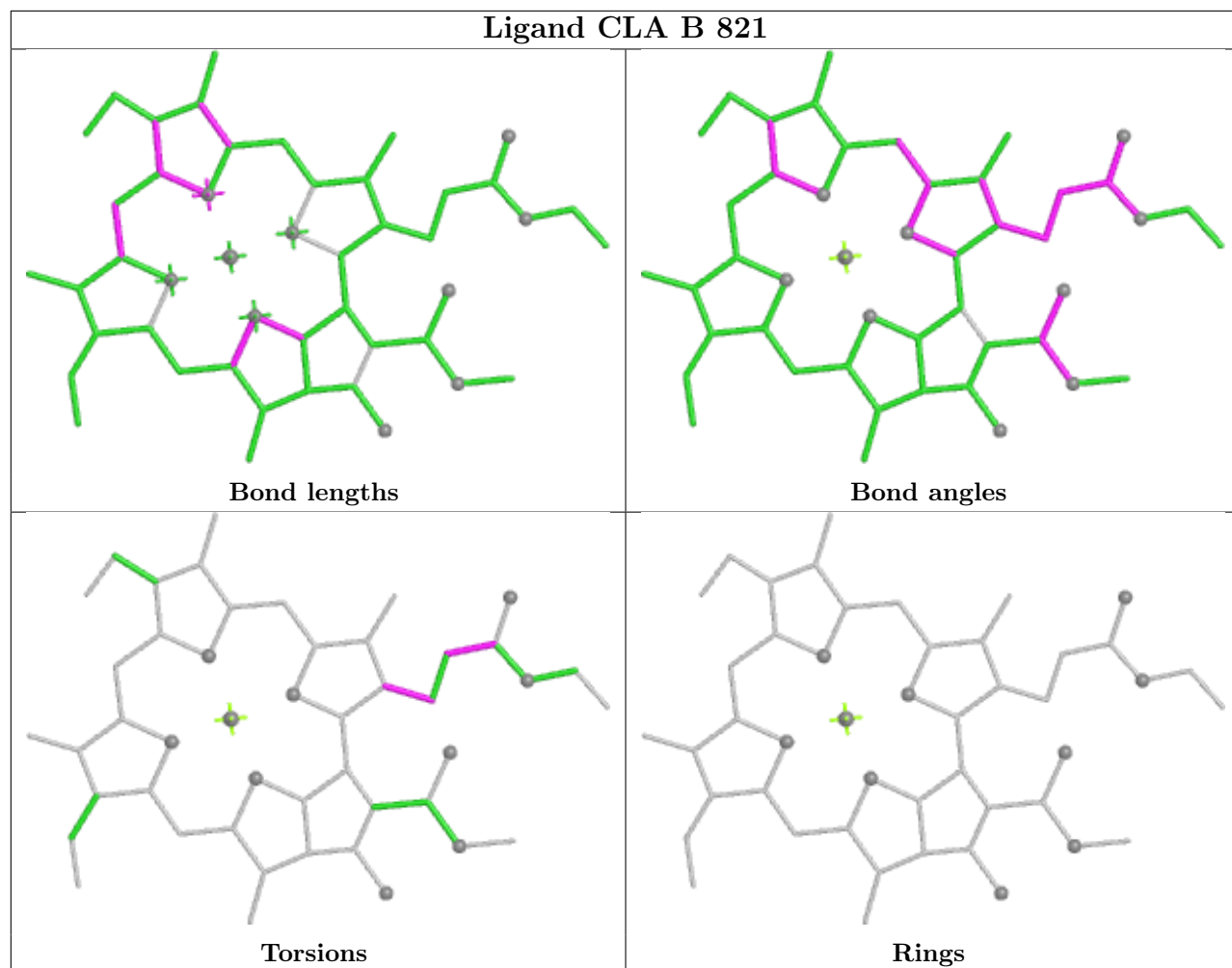
## Ligand CLA A 819

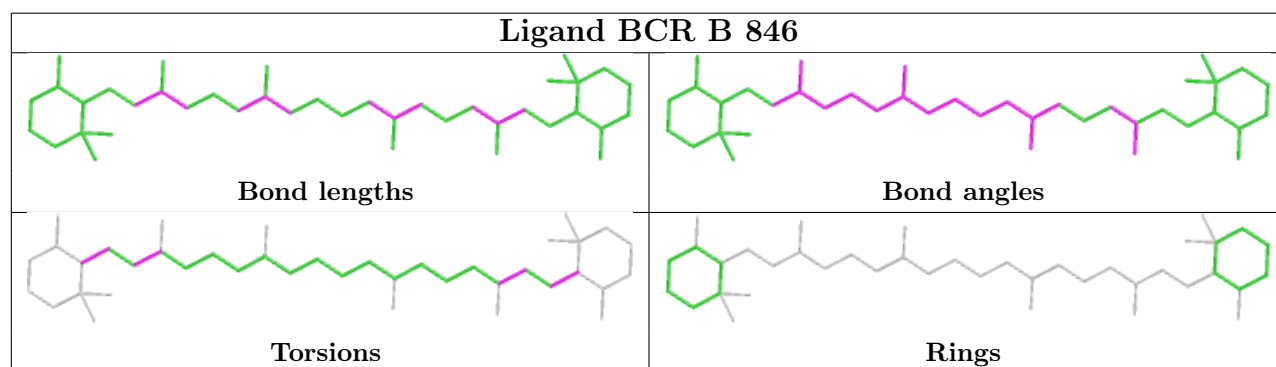
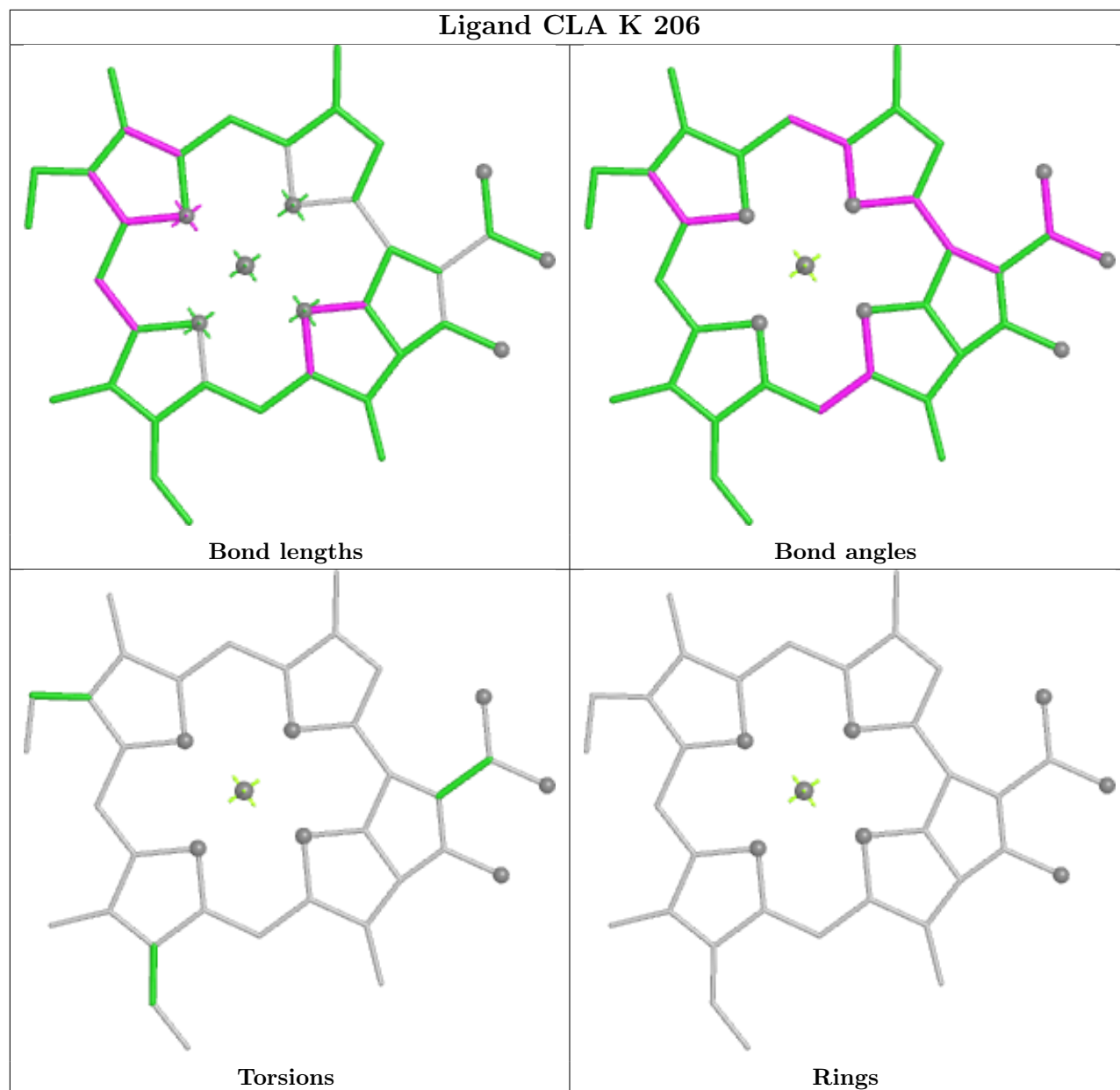


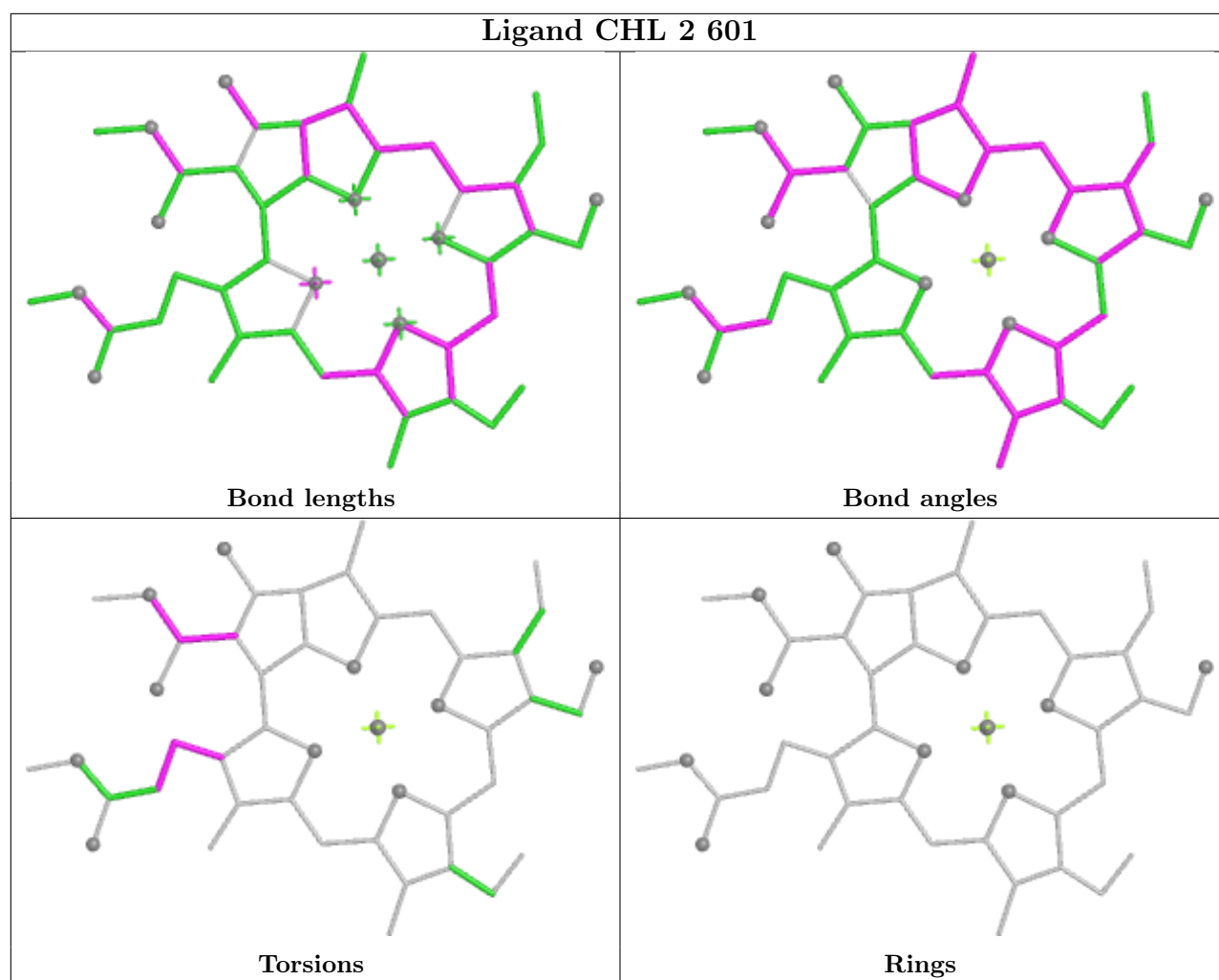
## Ligand CLA A 830

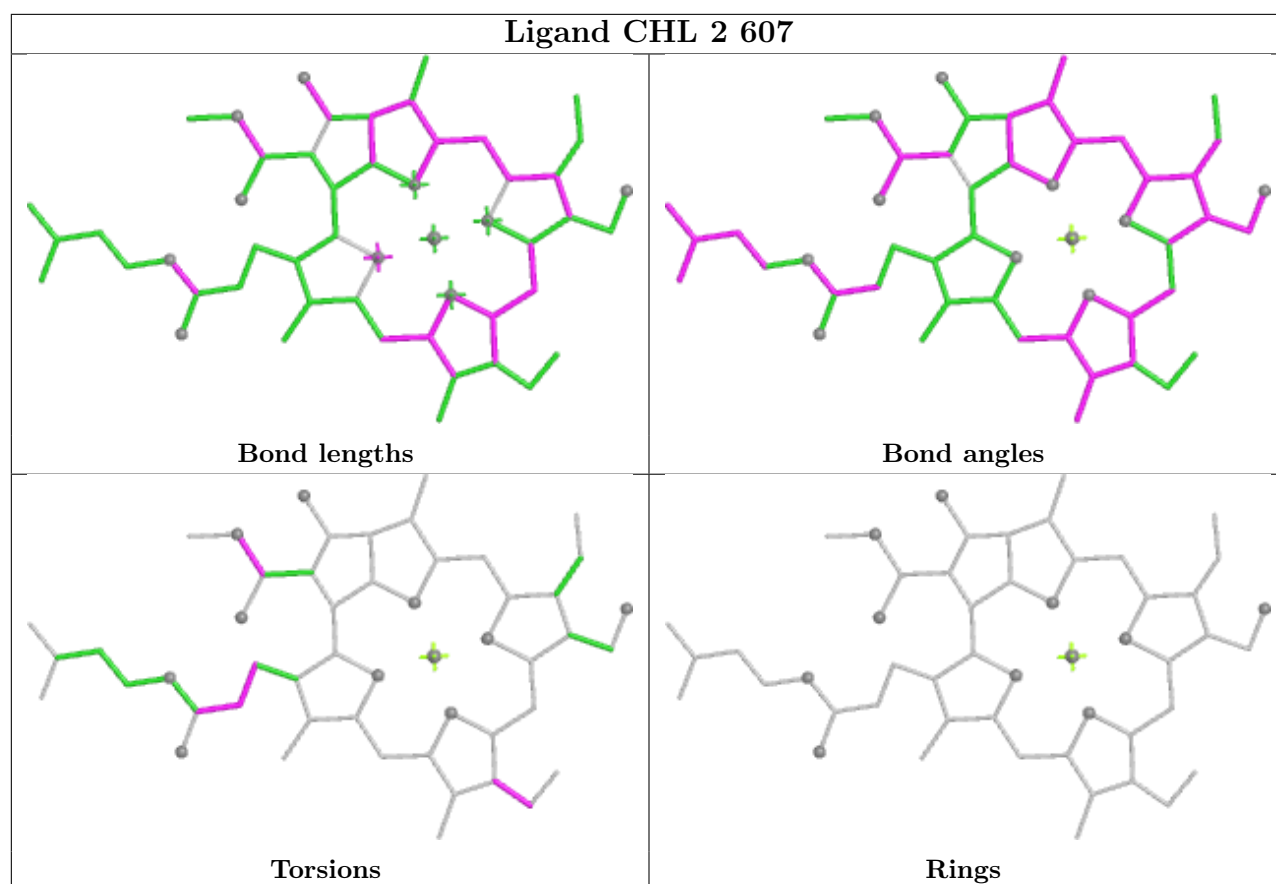


## Ligand CLA B 821

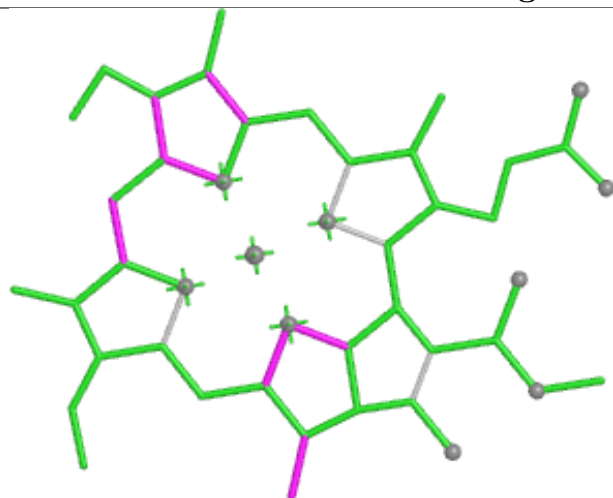




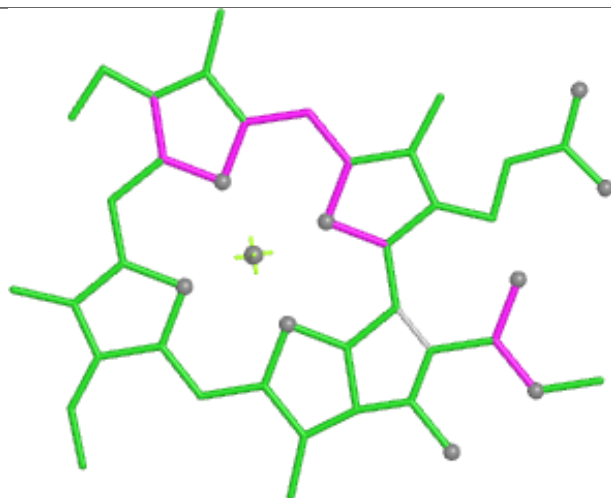




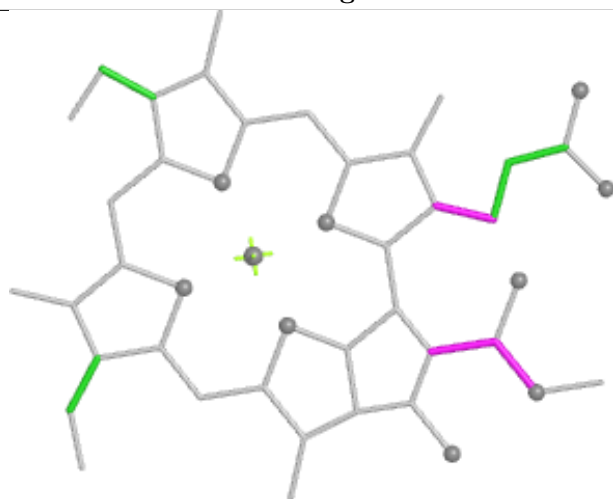
## Ligand CLA 3 607



Bond lengths



Bond angles

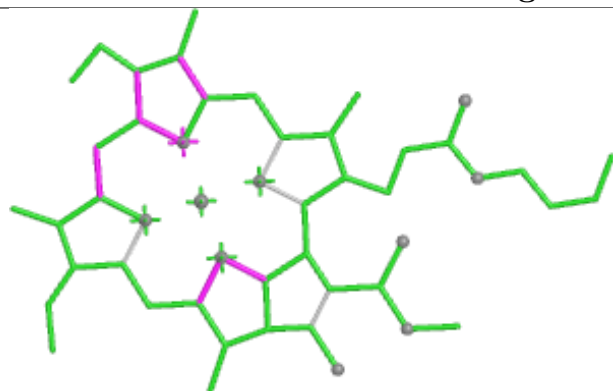


Torsions

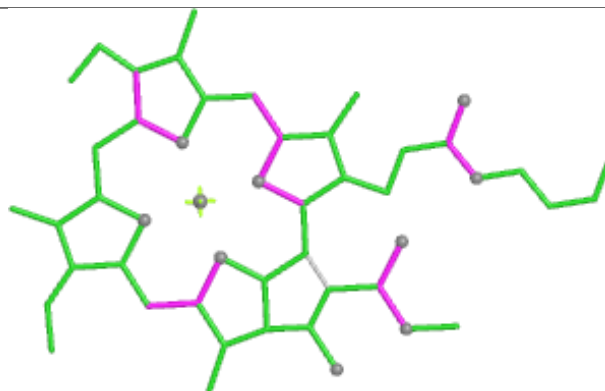


Rings

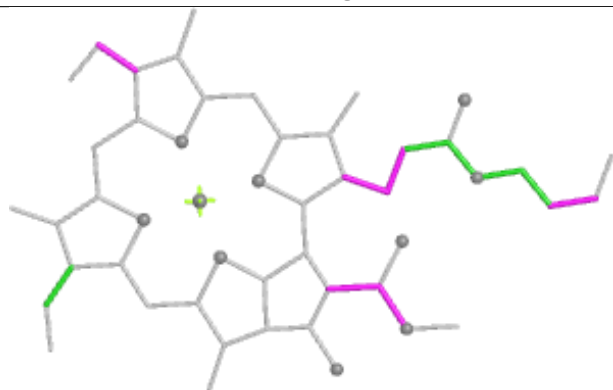
## Ligand CLA 1 604



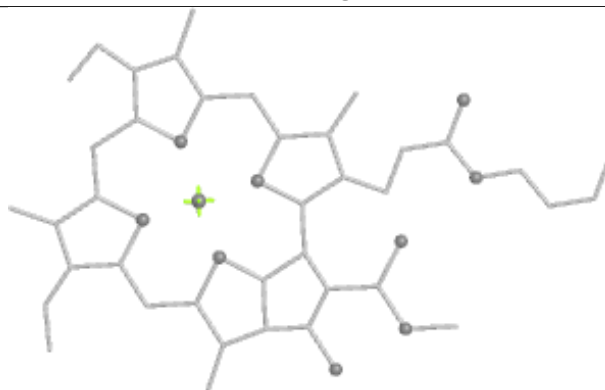
Bond lengths



Bond angles

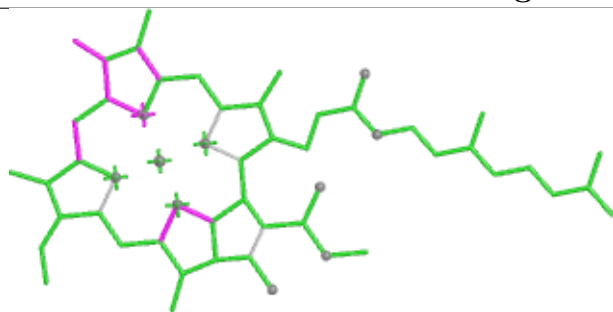


Torsions

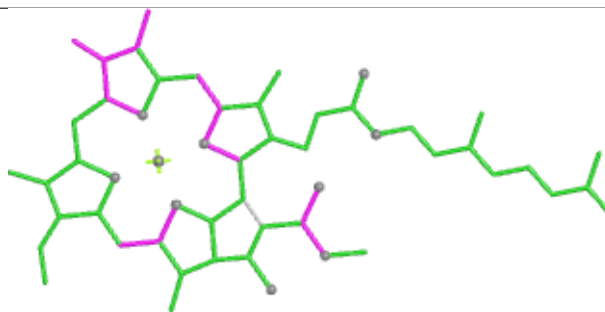


Rings

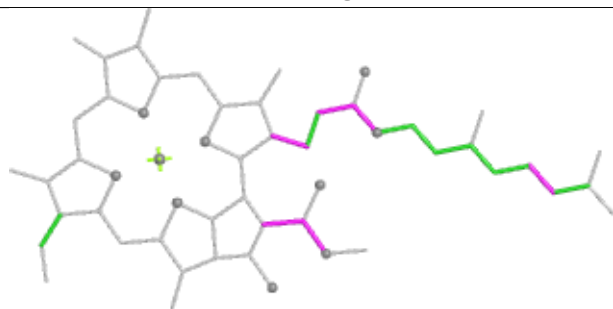
## Ligand CLA B 811



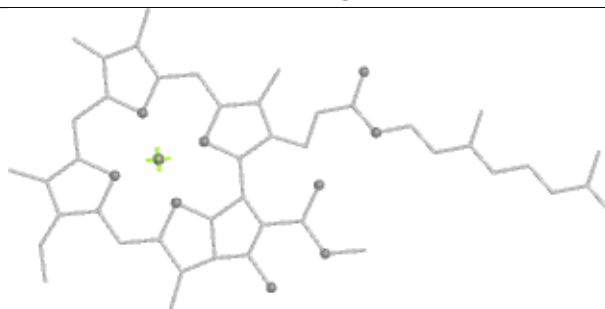
Bond lengths



Bond angles

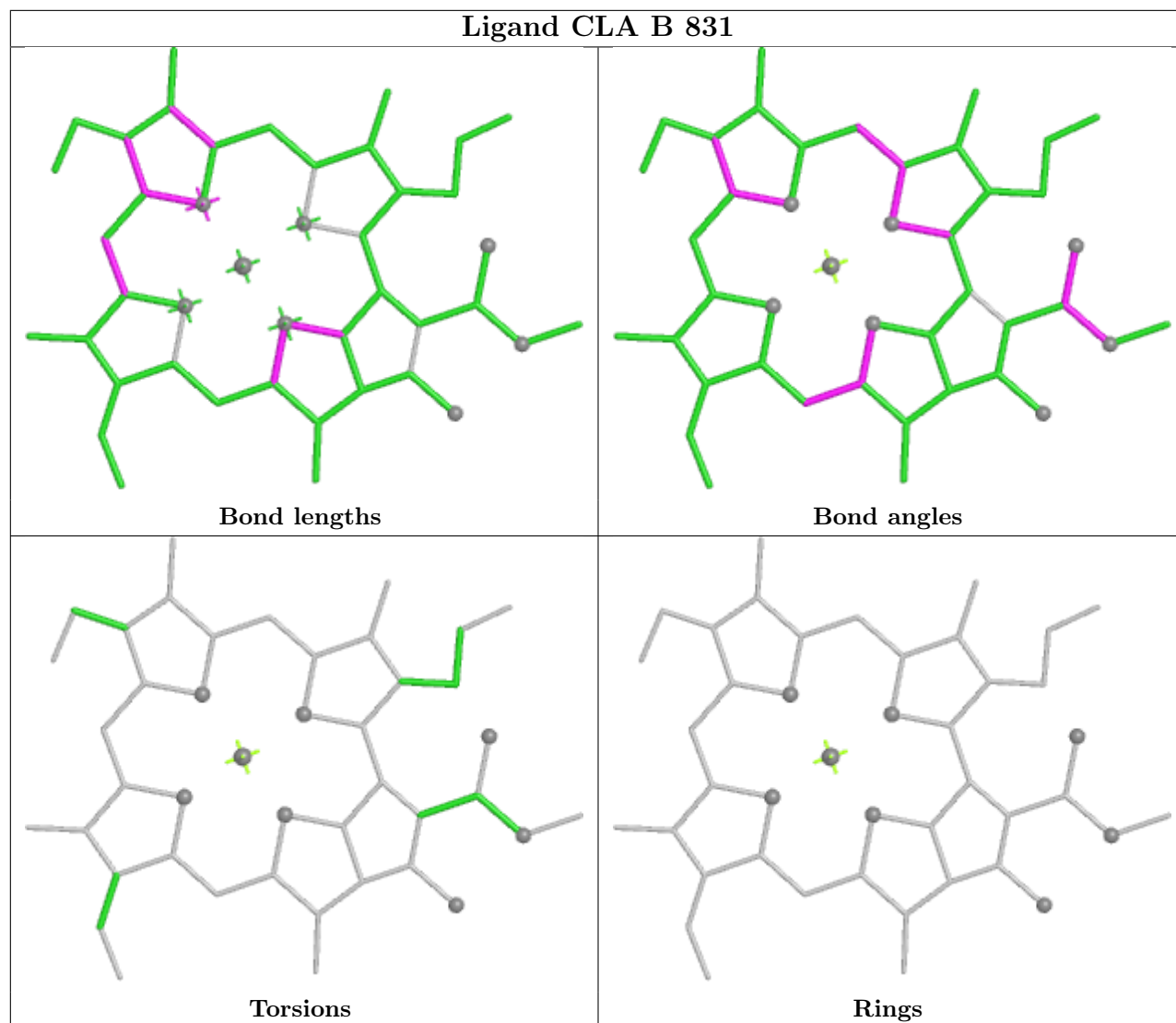


Torsions

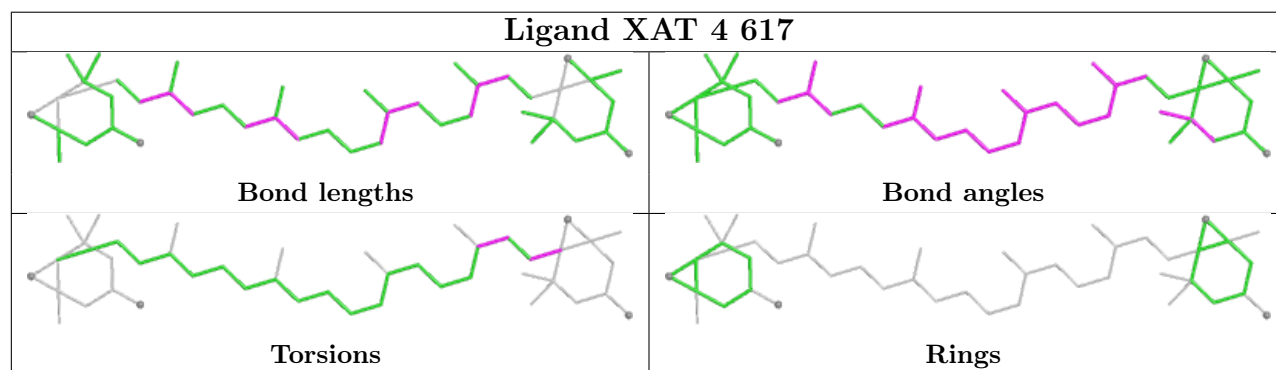


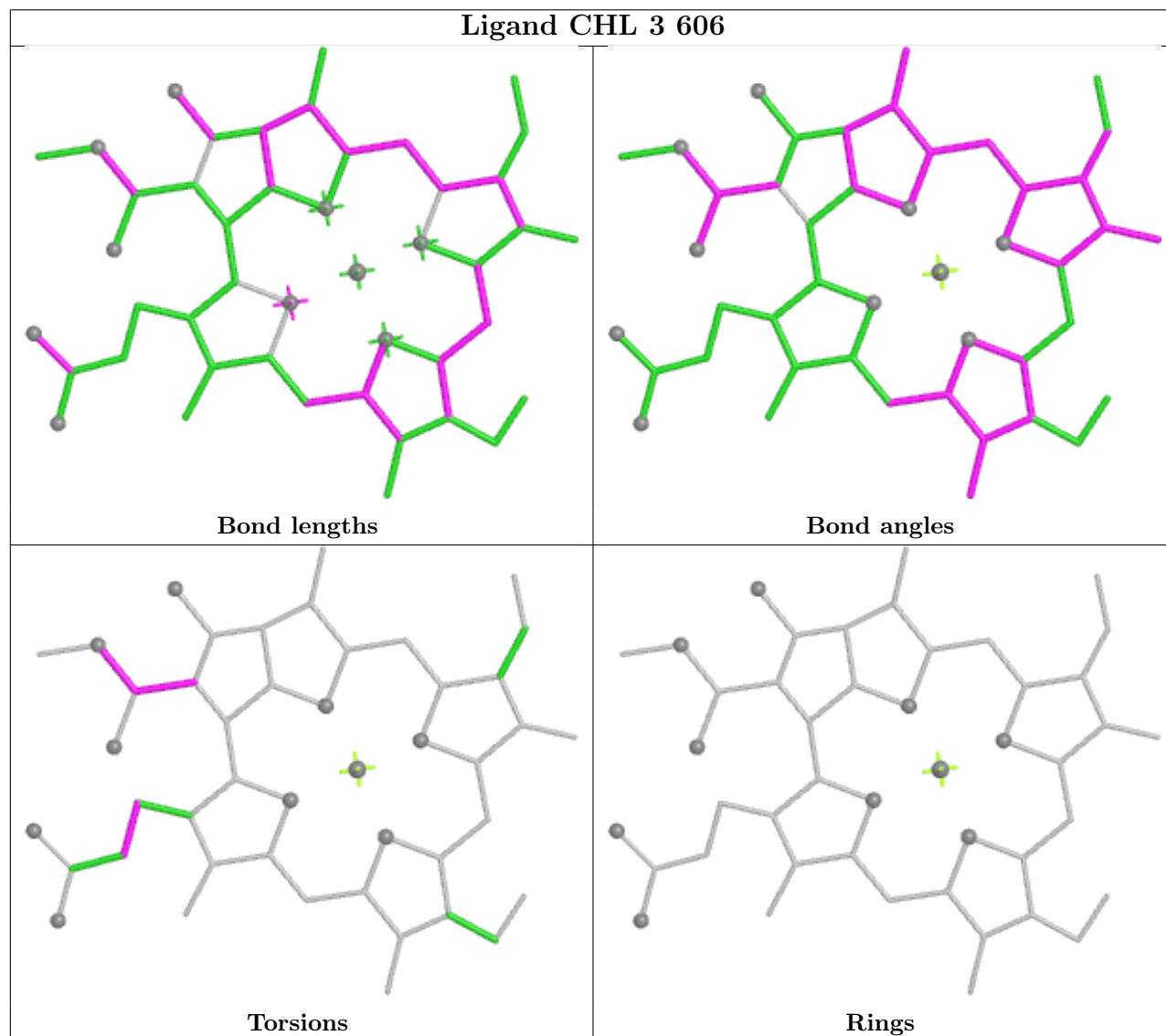
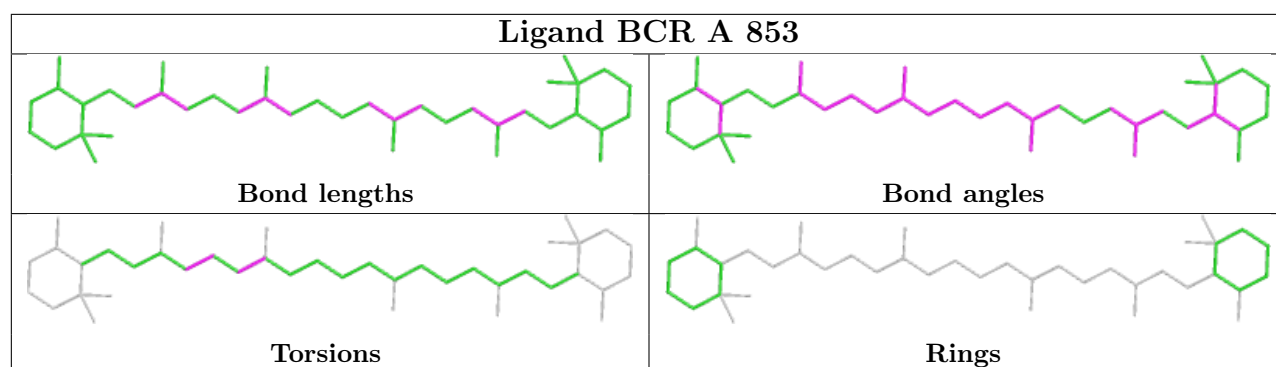
Rings

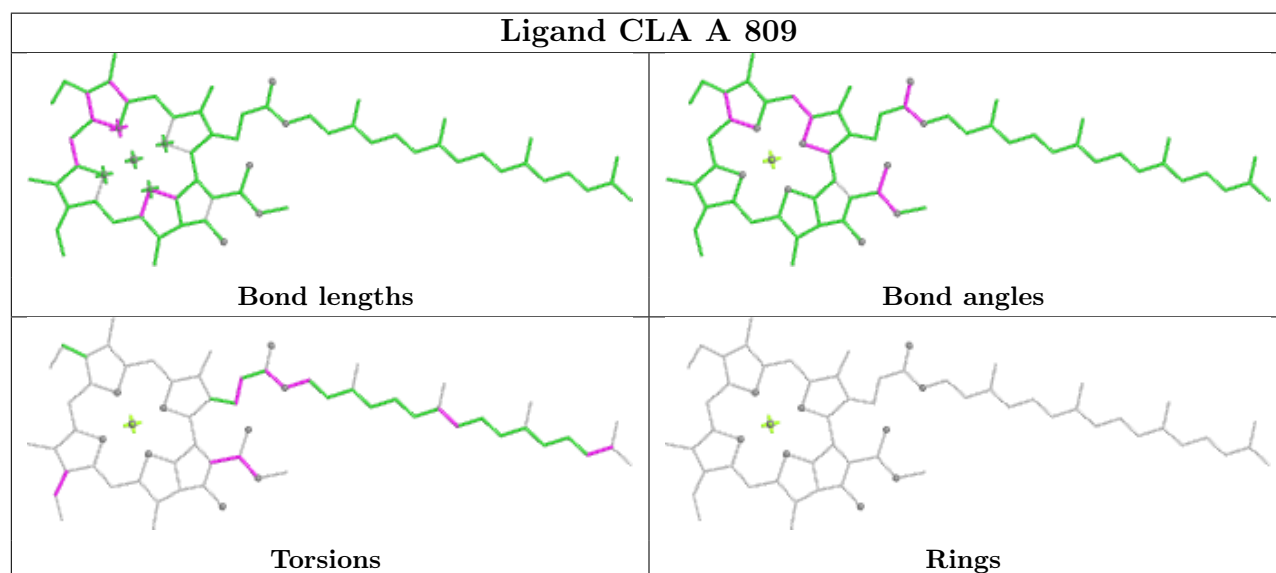
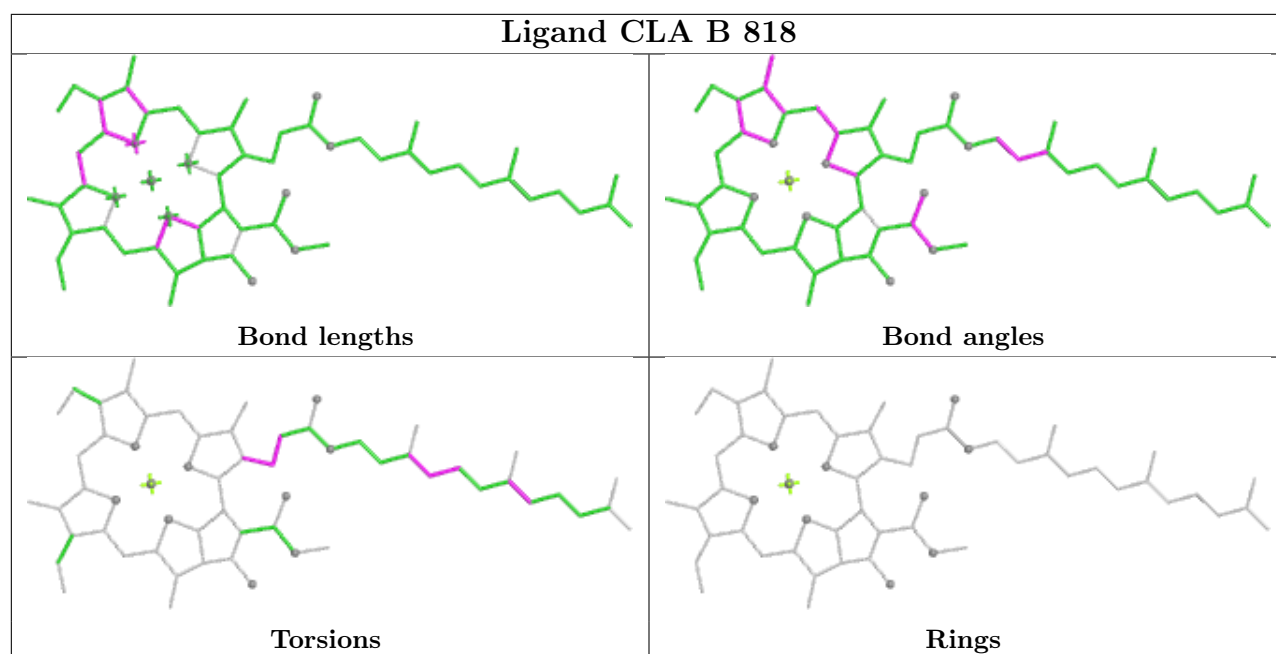
## Ligand CLA B 831

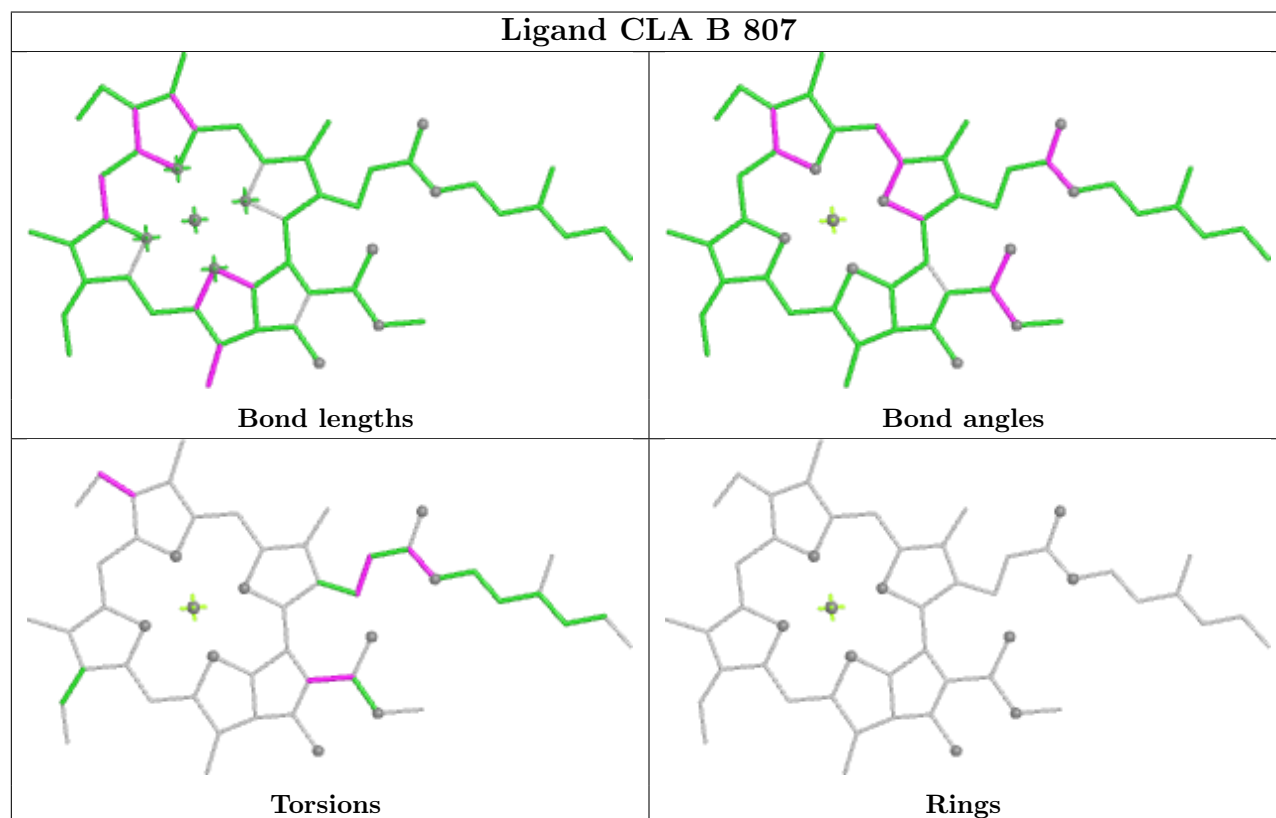
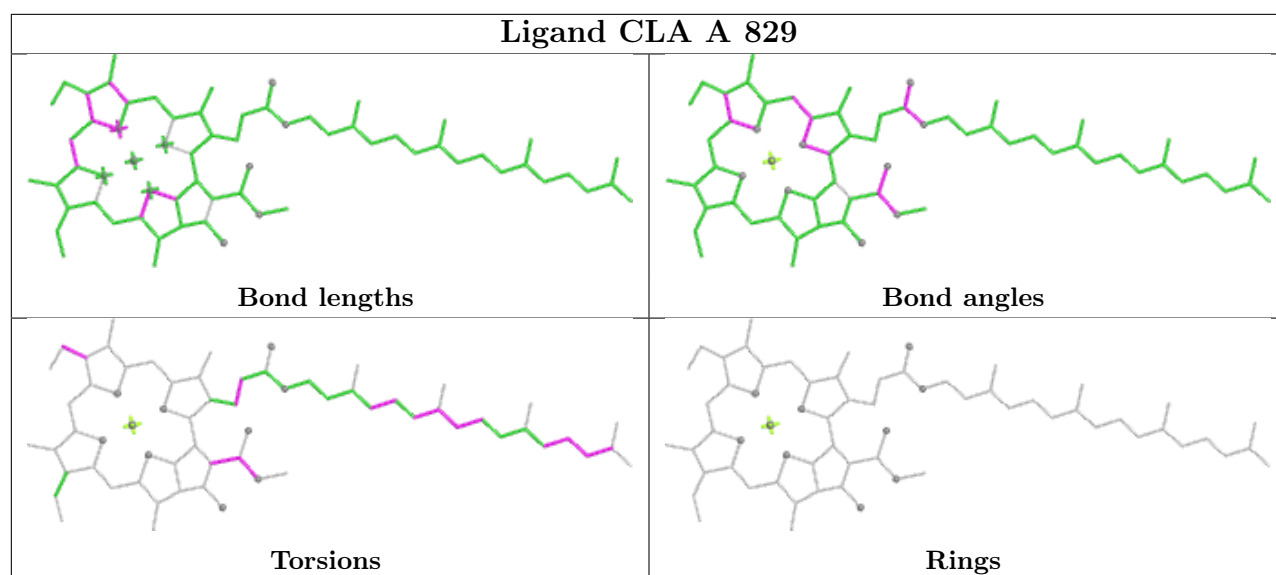


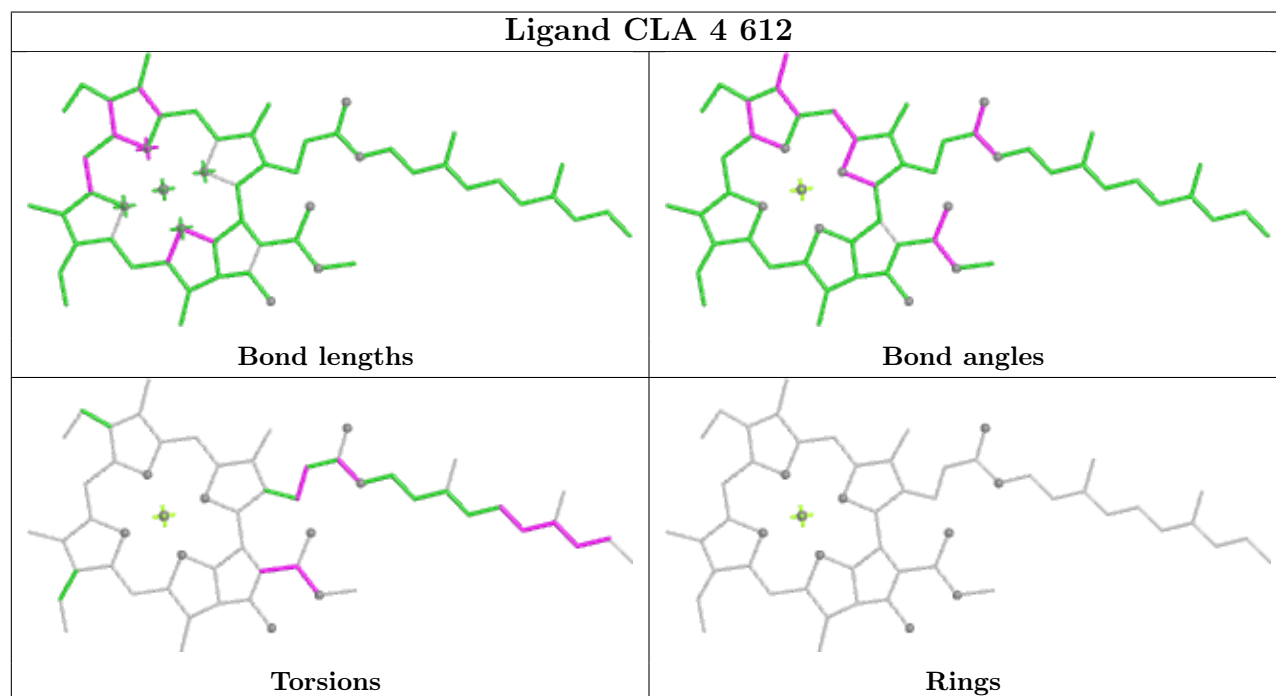
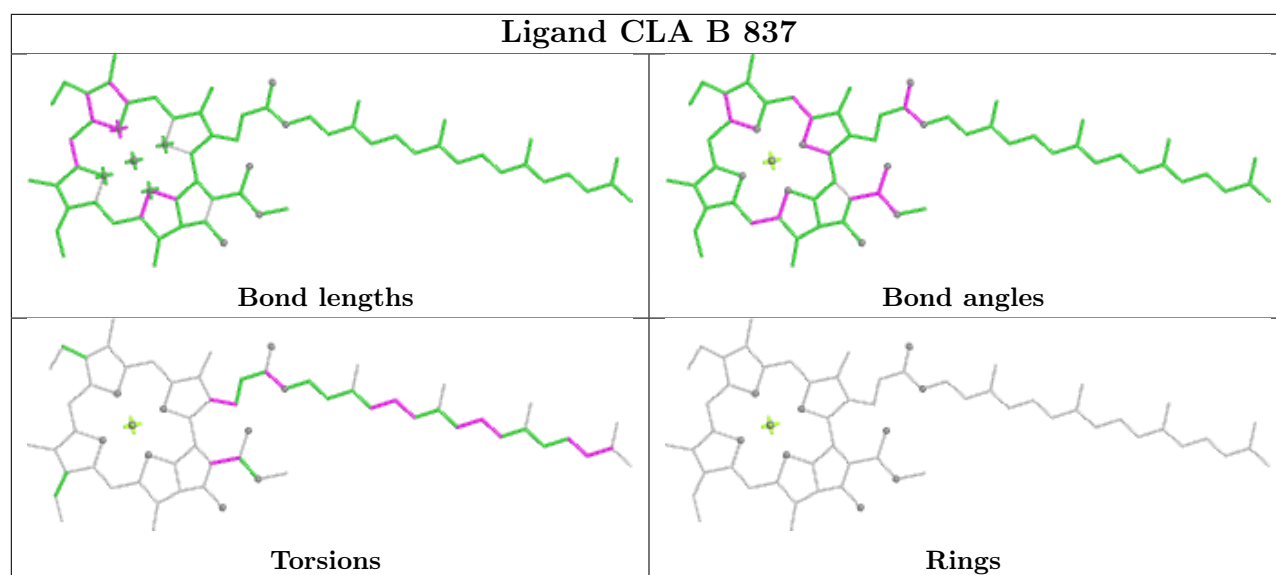
## Ligand XAT 4 617







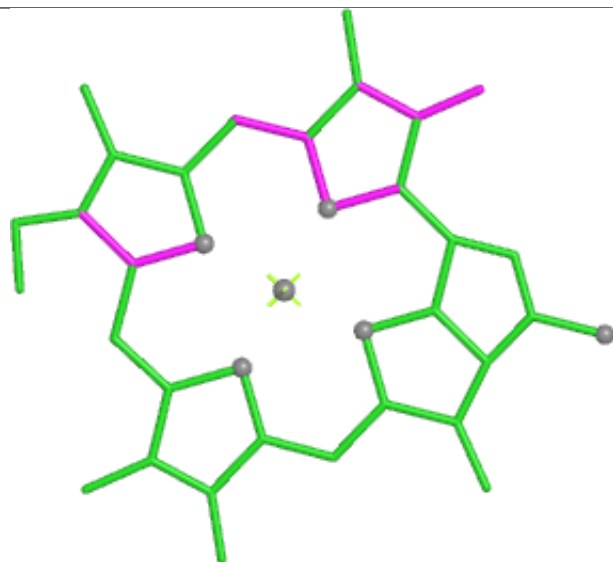




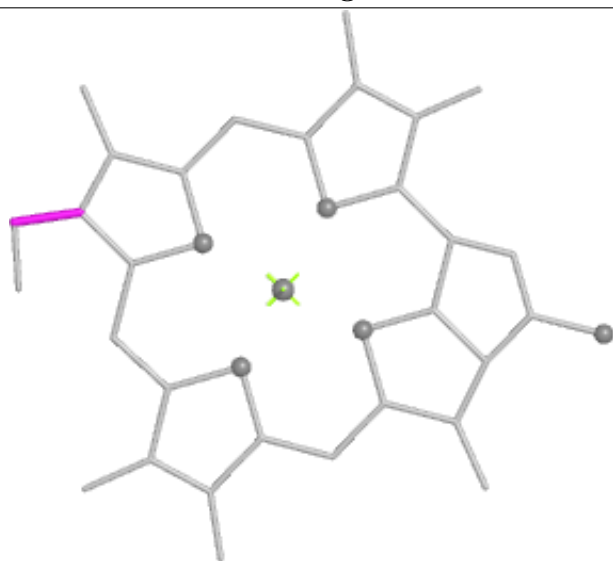
## Ligand CLA 3 611



Bond lengths



Bond angles

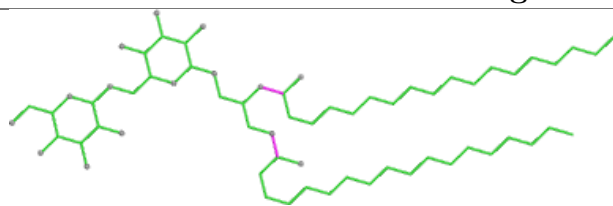


Torsions

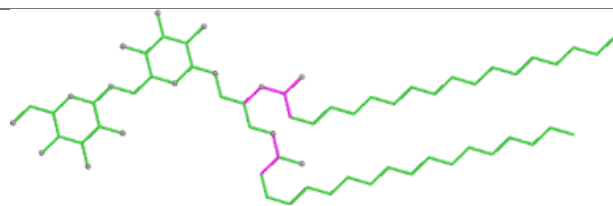


Rings

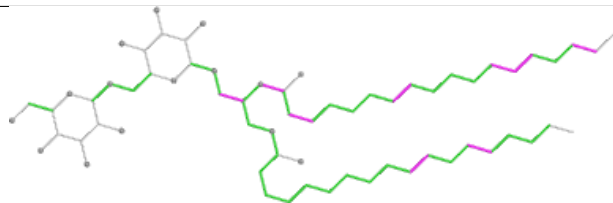
## Ligand DGD B 850



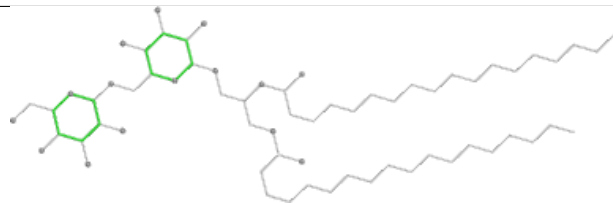
Bond lengths



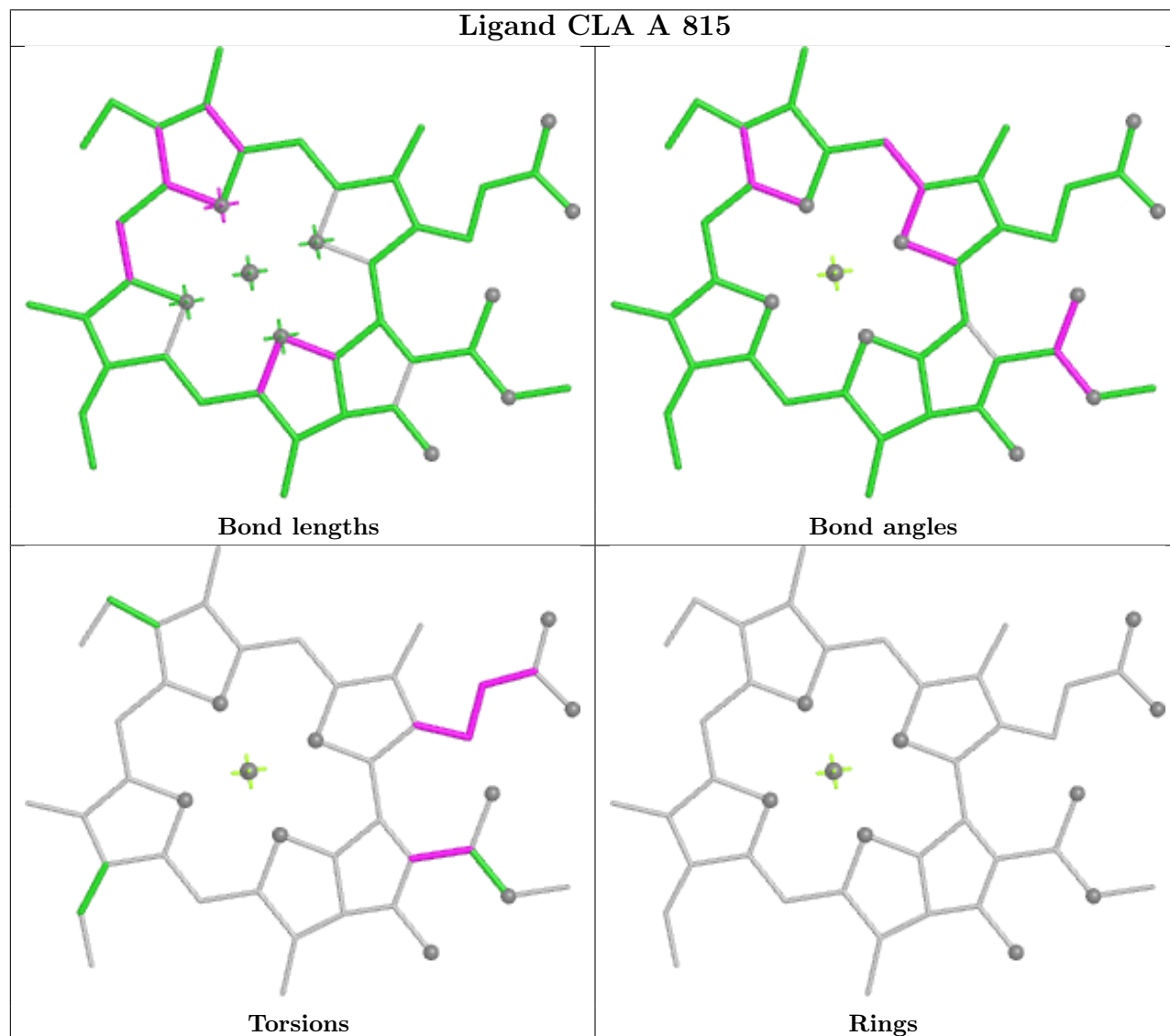
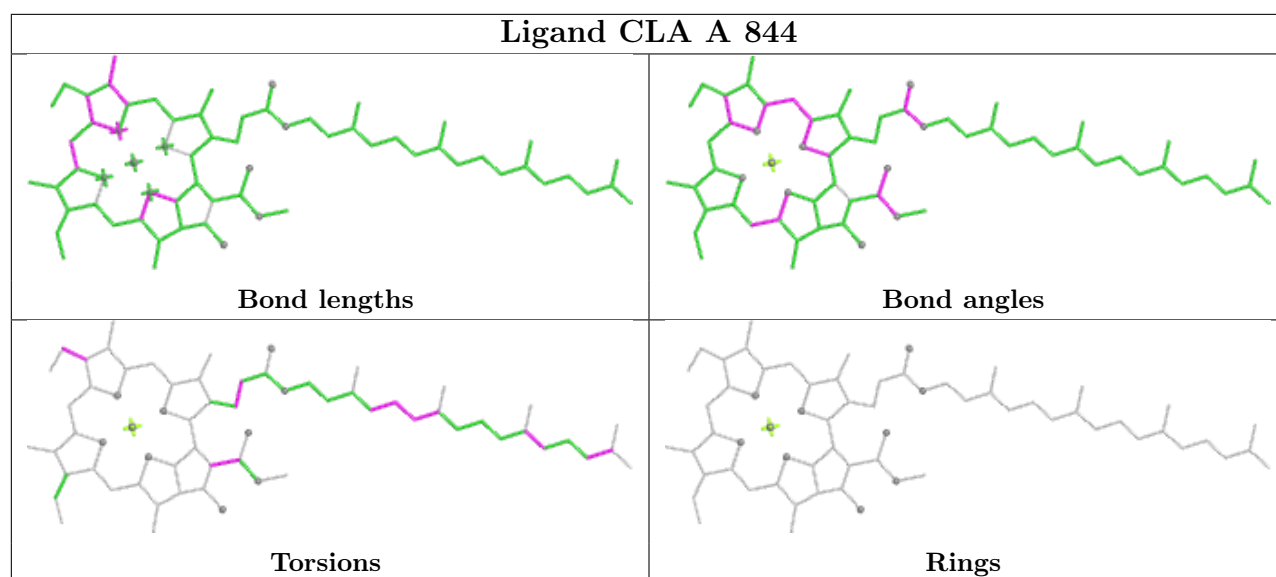
Bond angles

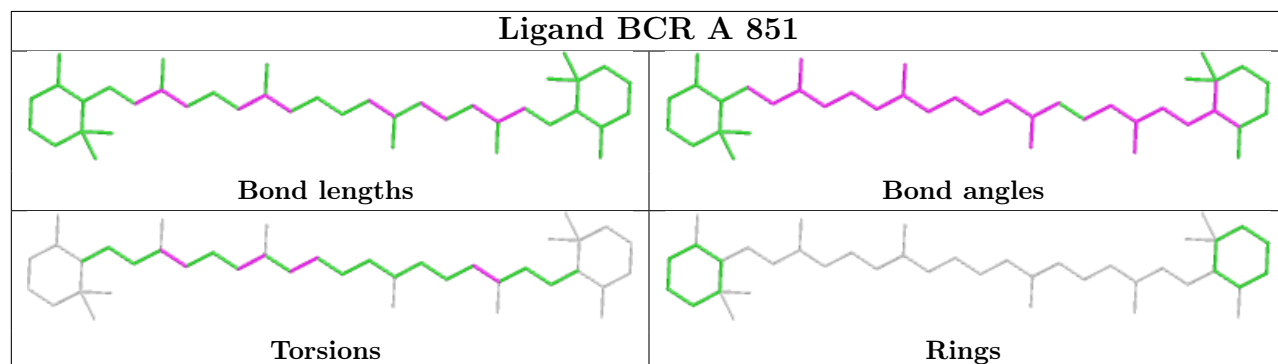
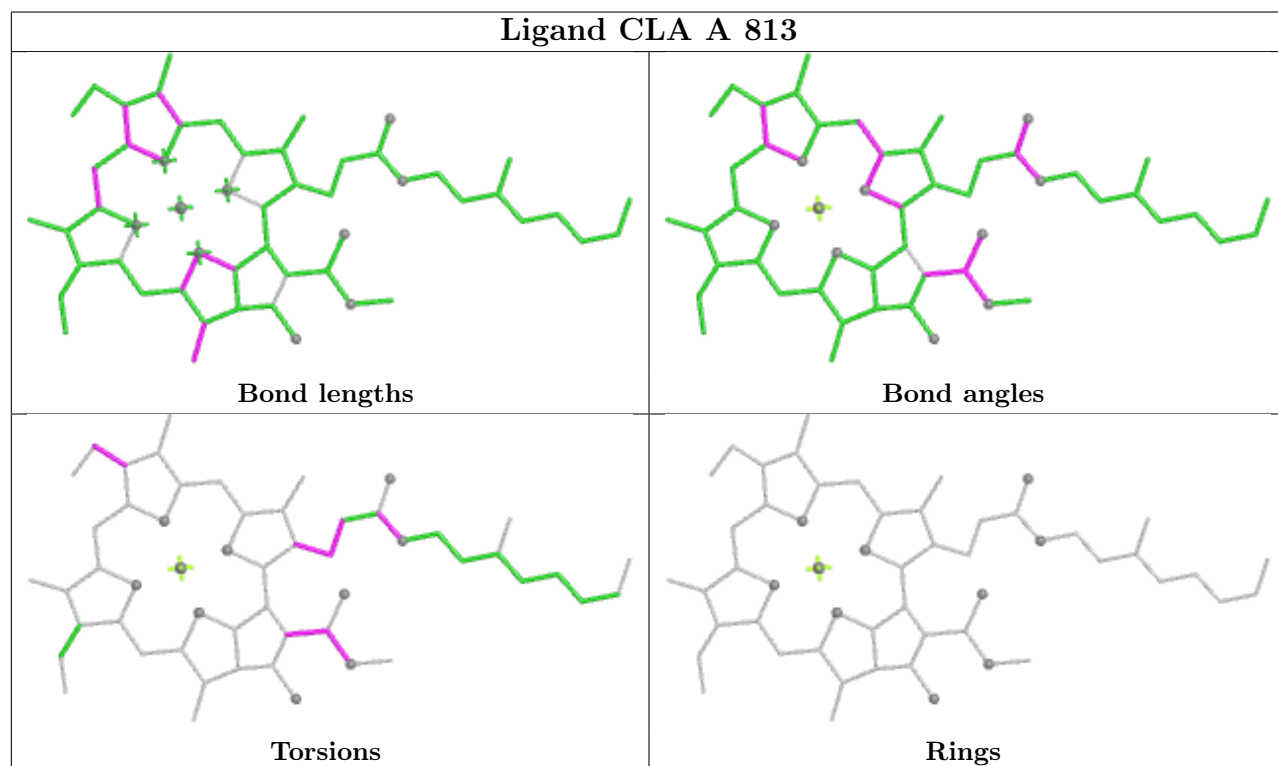
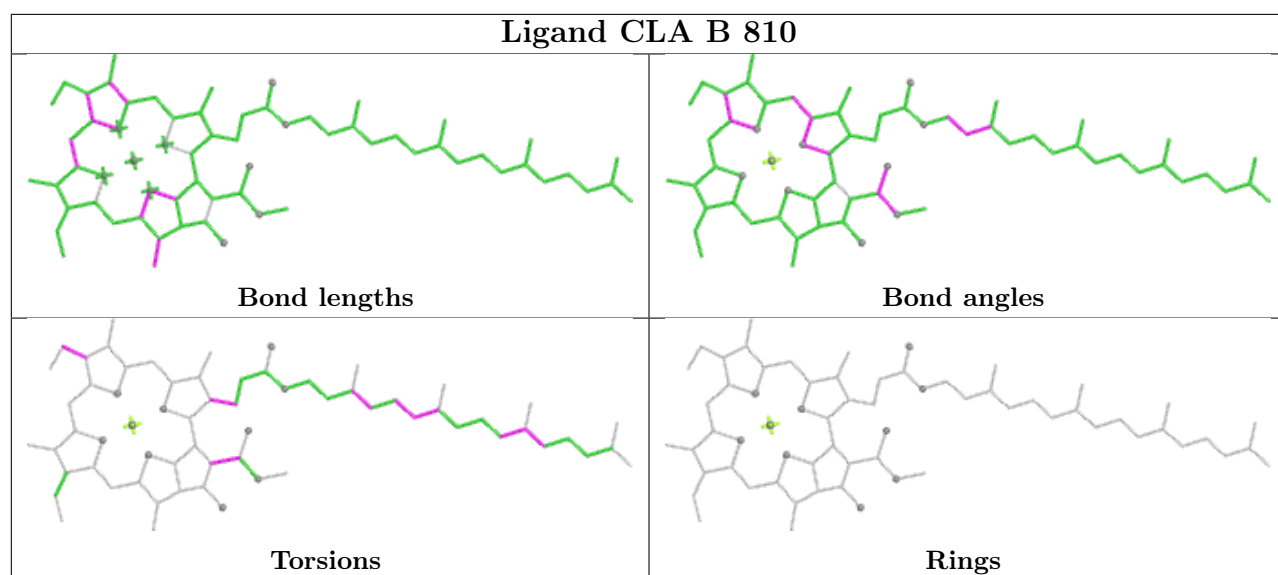


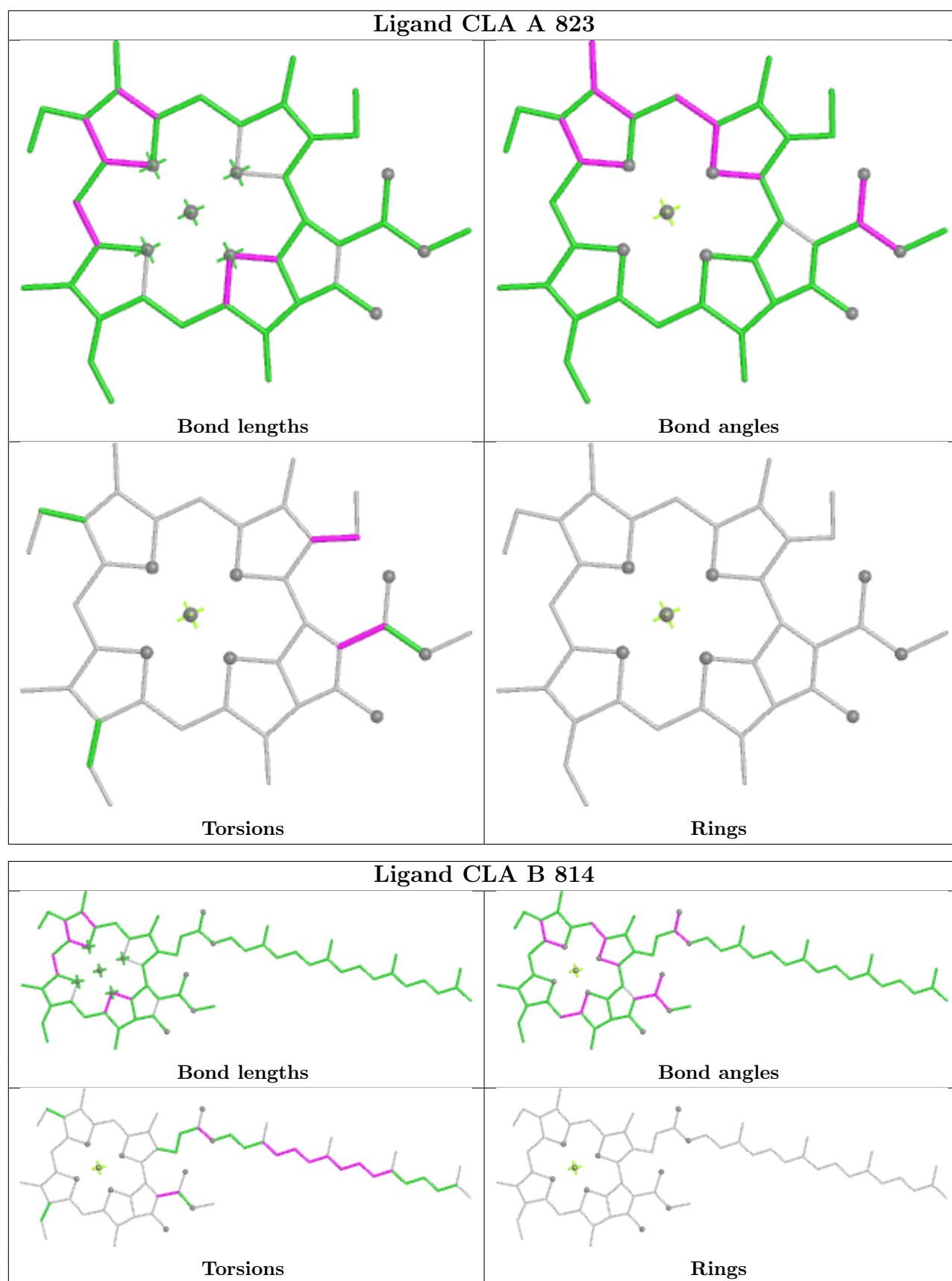
Torsions

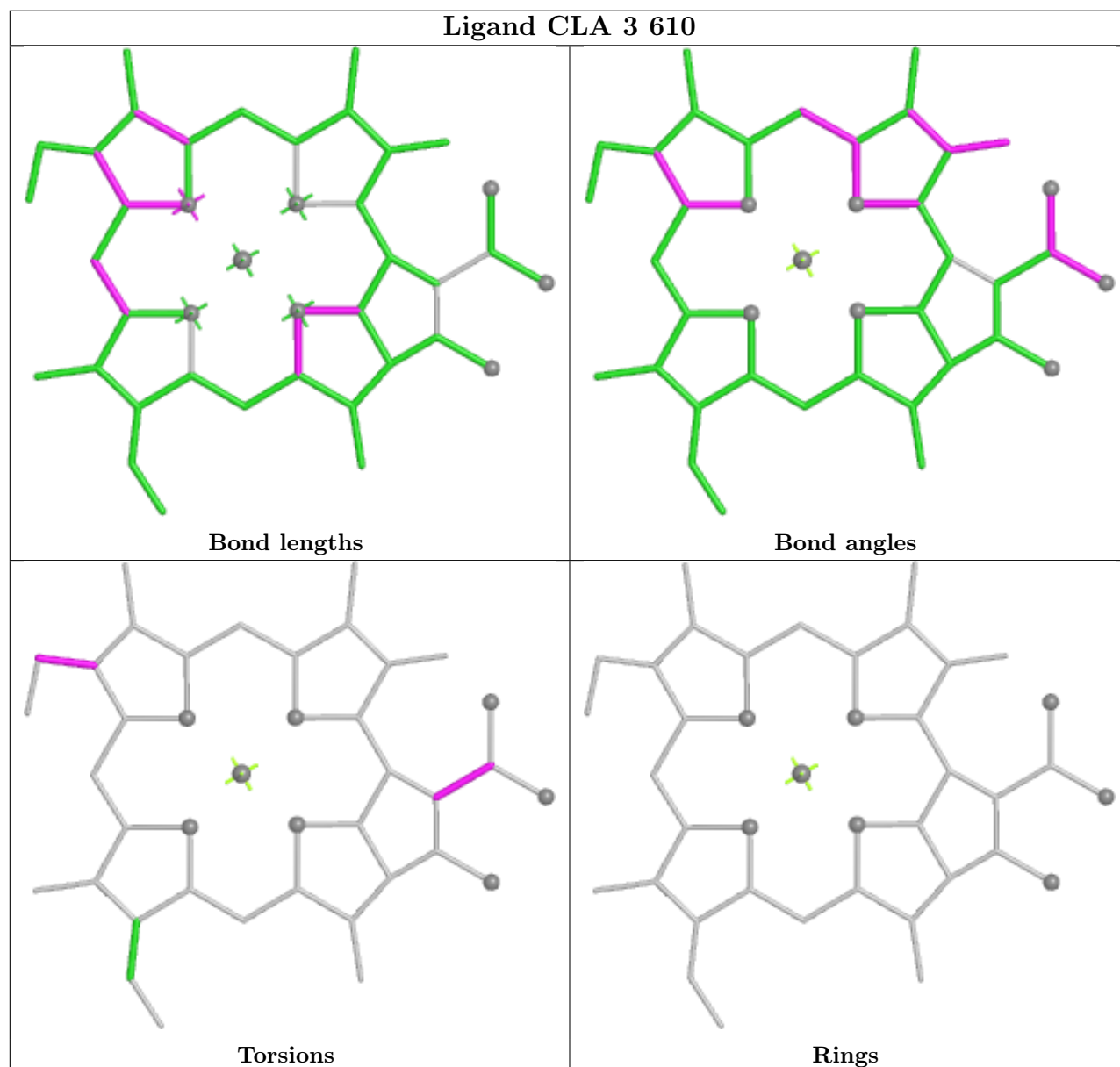
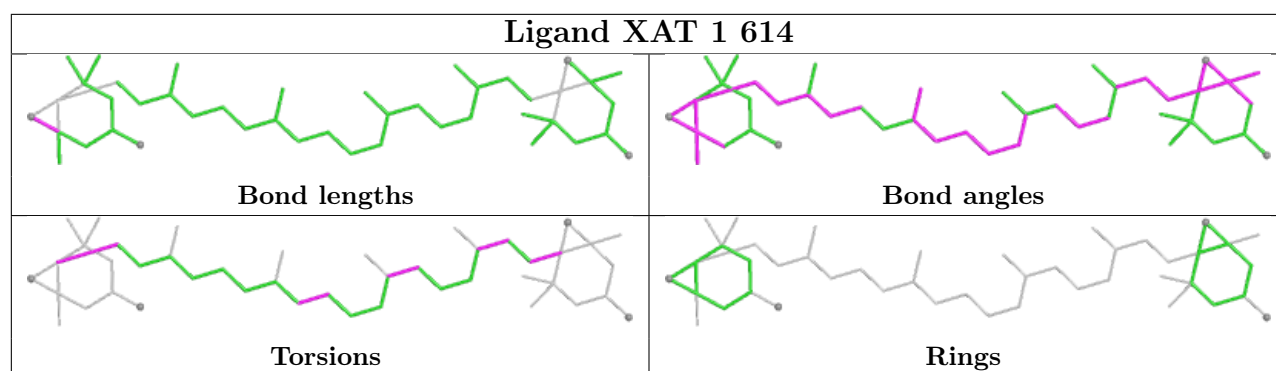


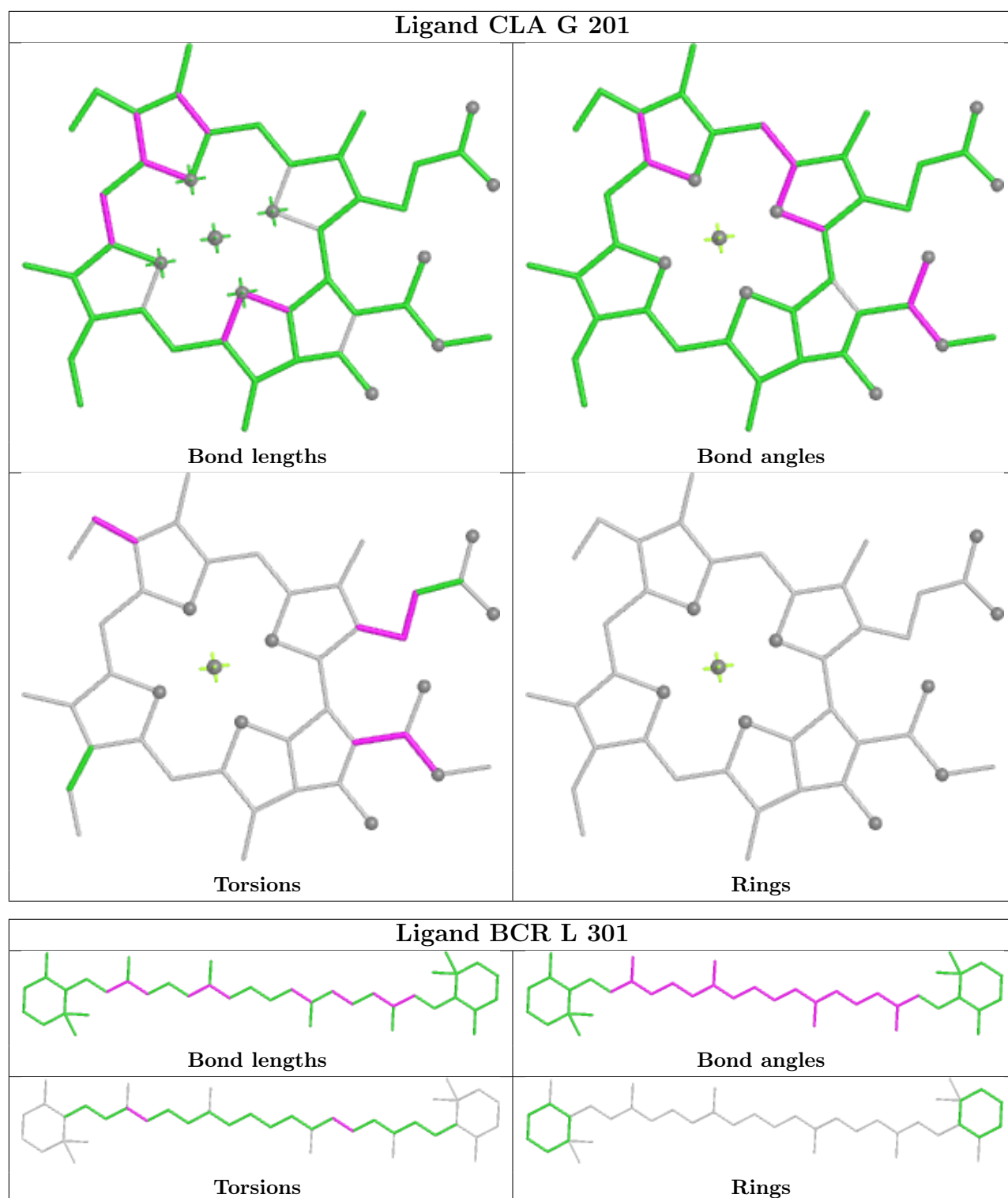
Rings

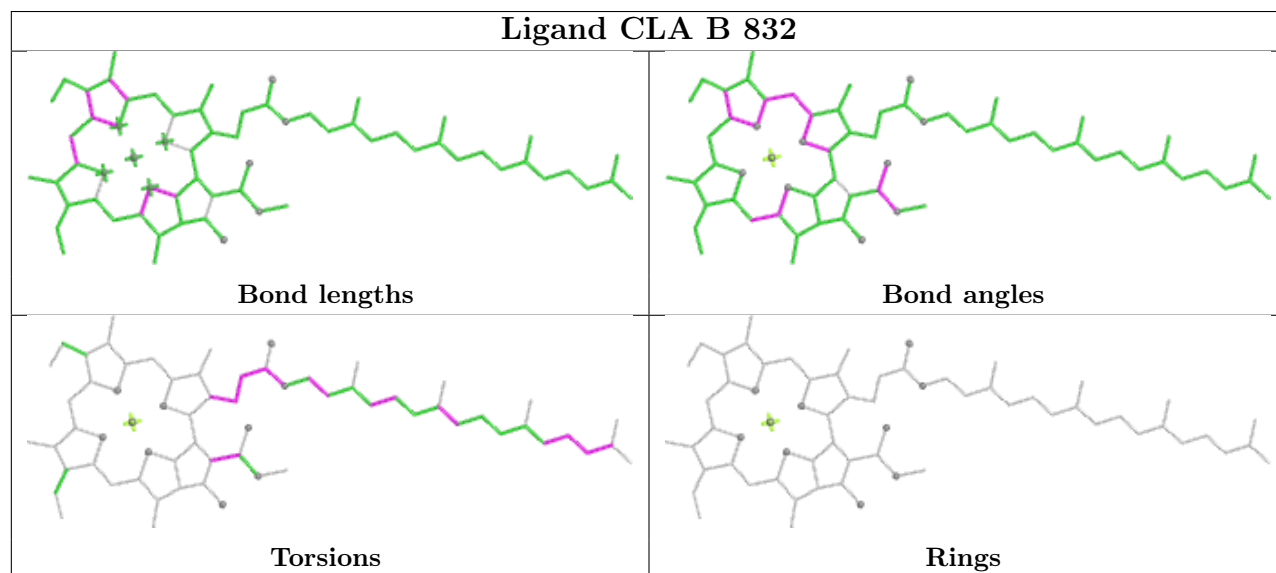
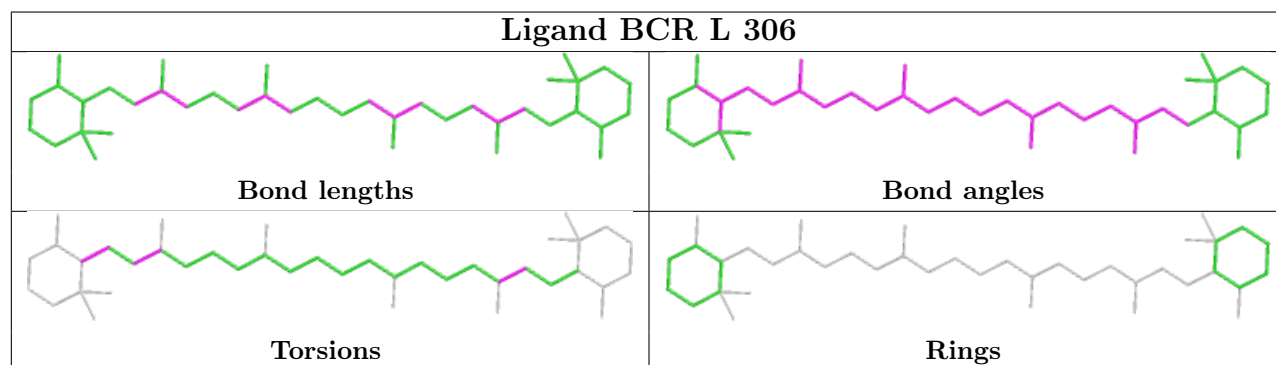
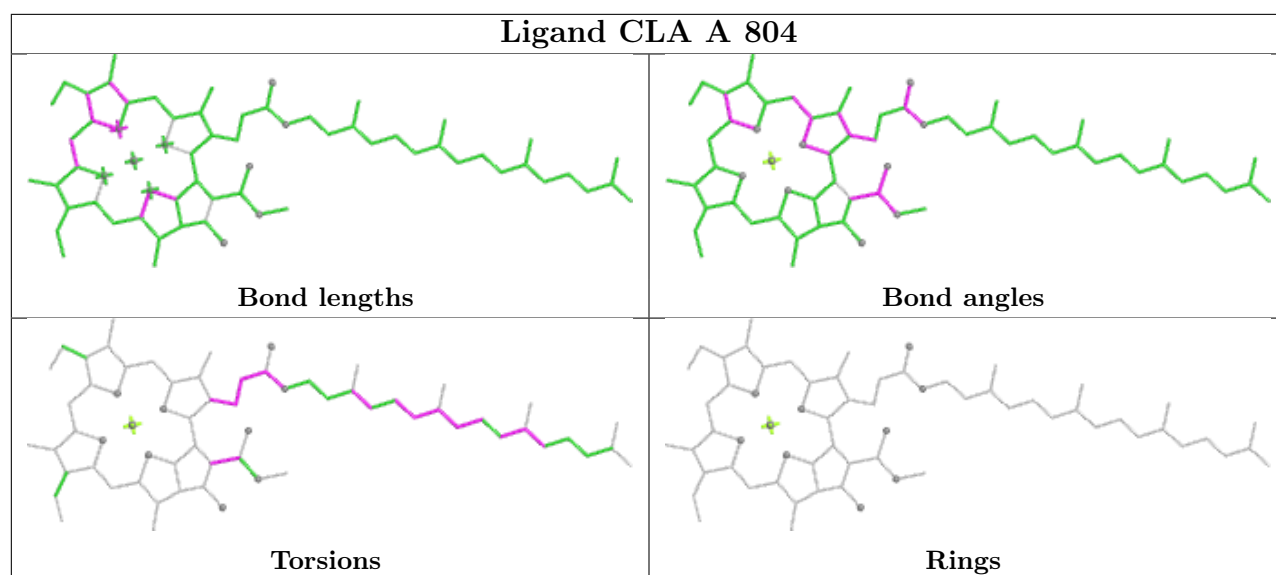


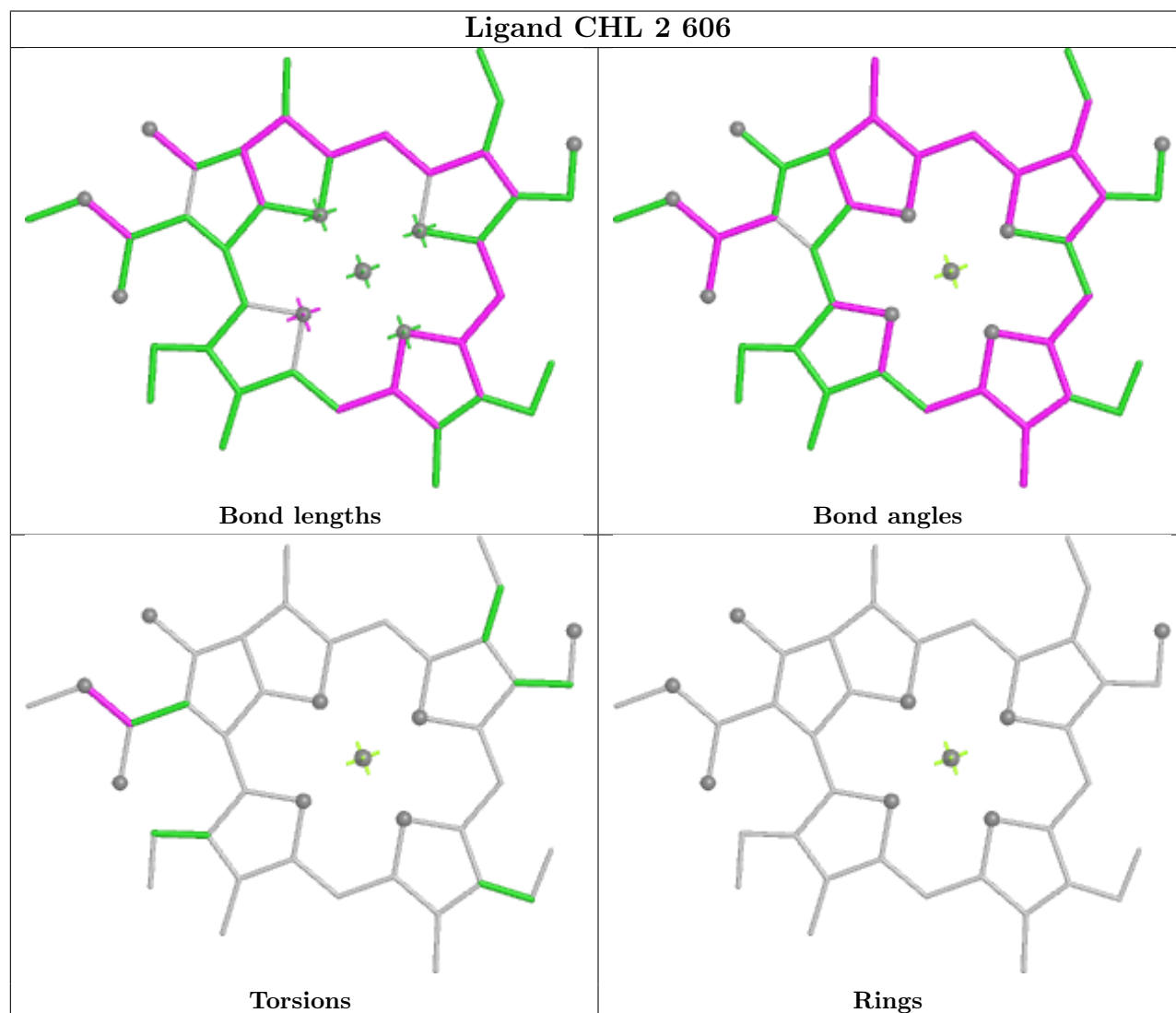
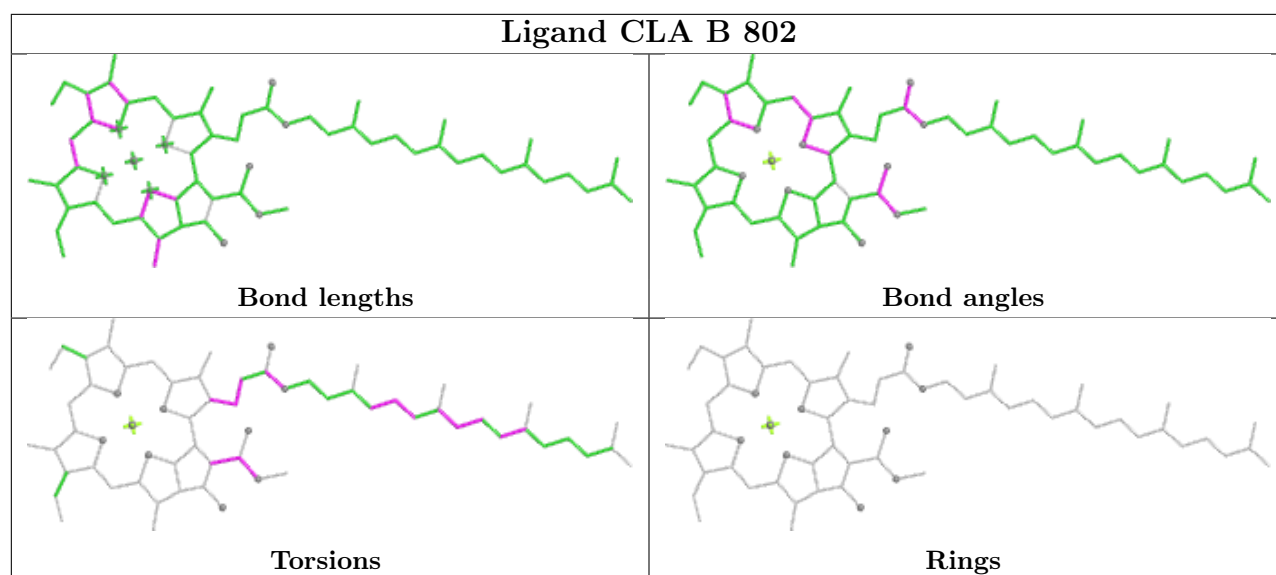




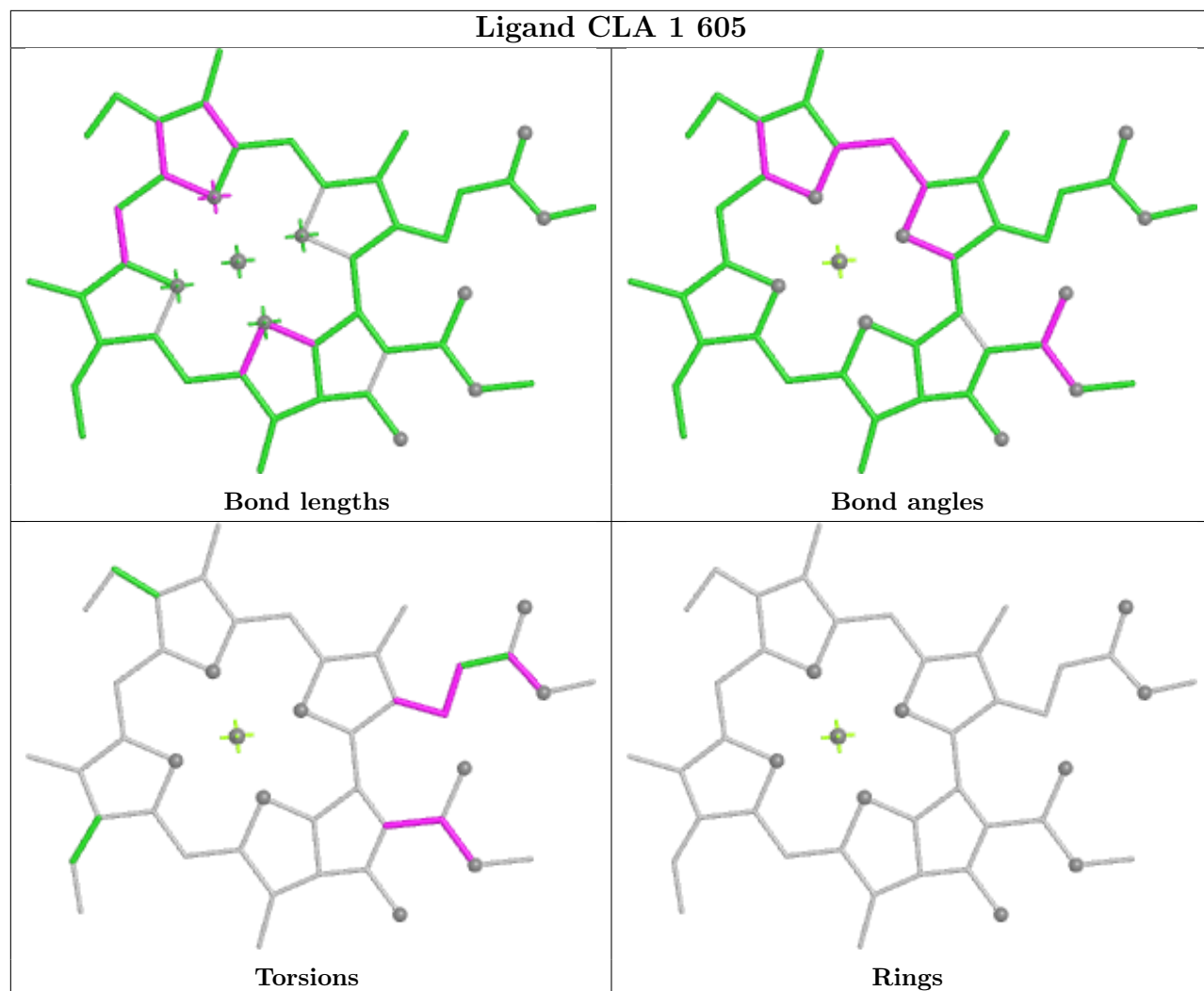




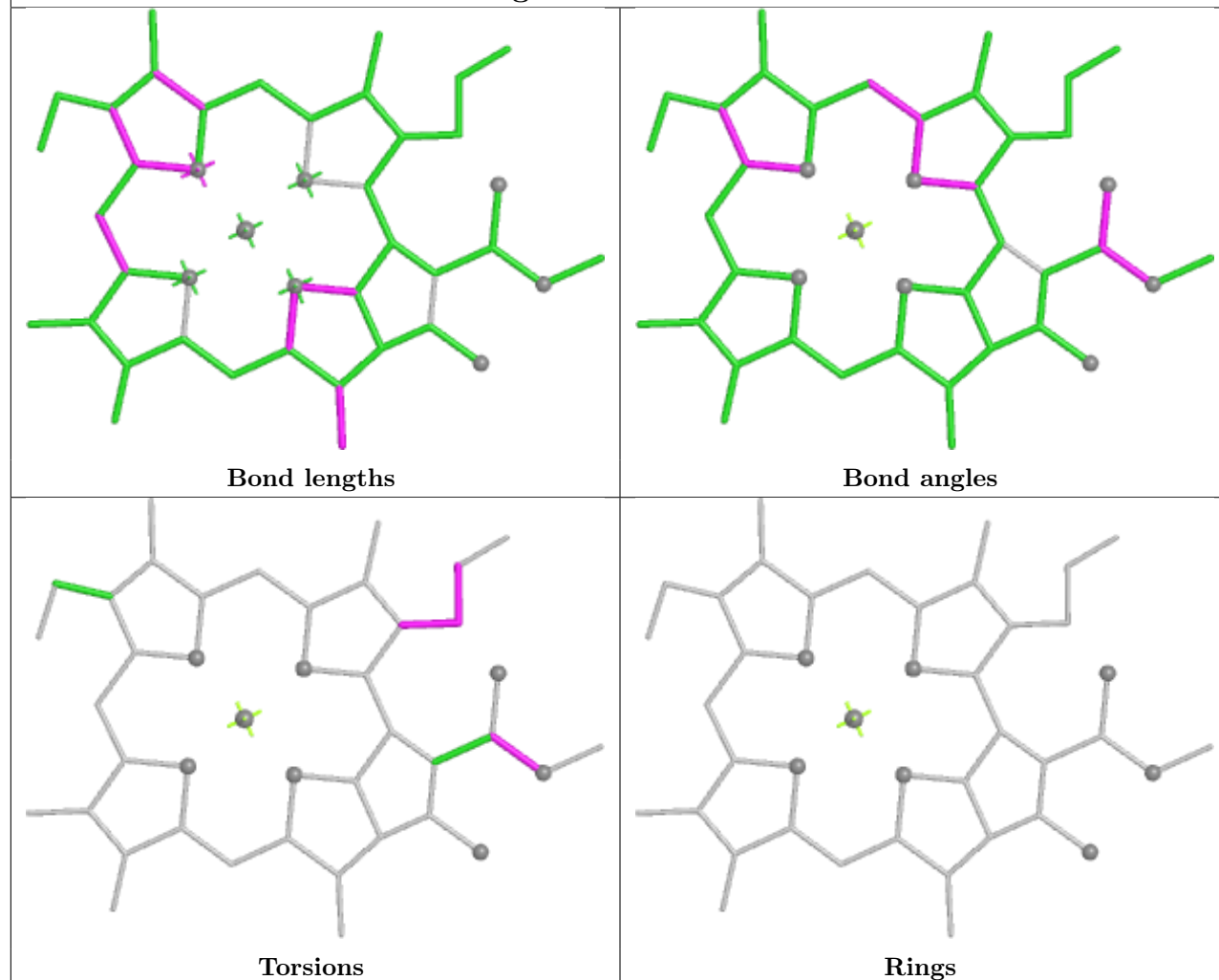




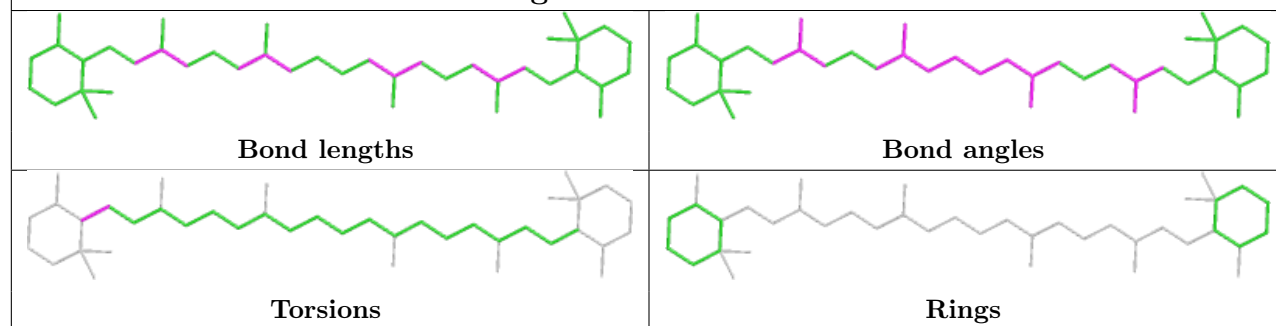
## Ligand CLA 1 605



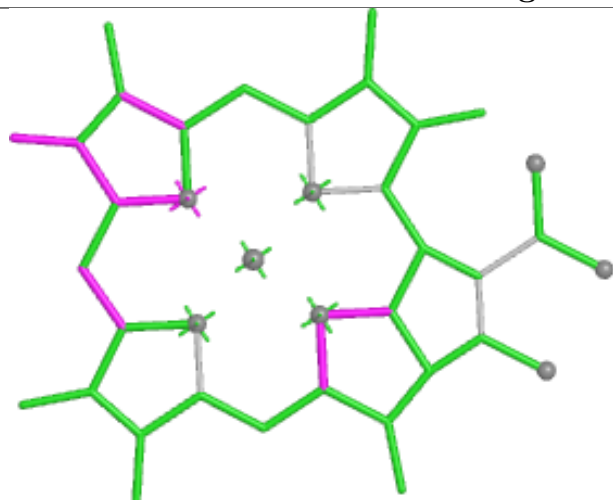
## Ligand CLA 1 609



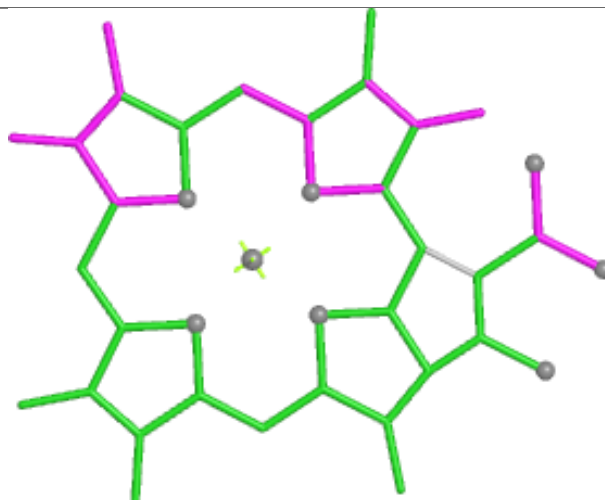
## Ligand BCR B 847



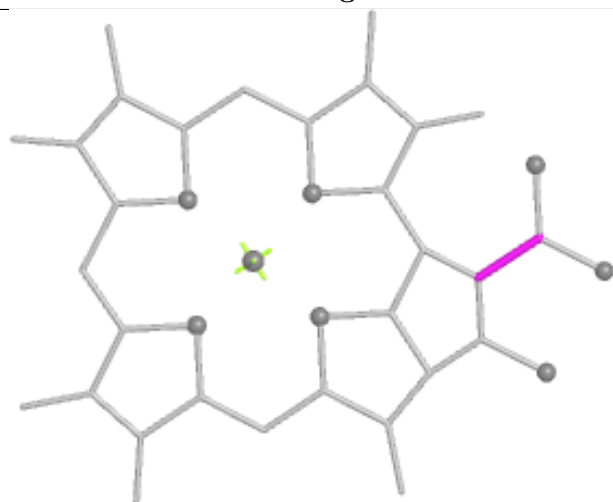
## Ligand CLA 1 610



Bond lengths



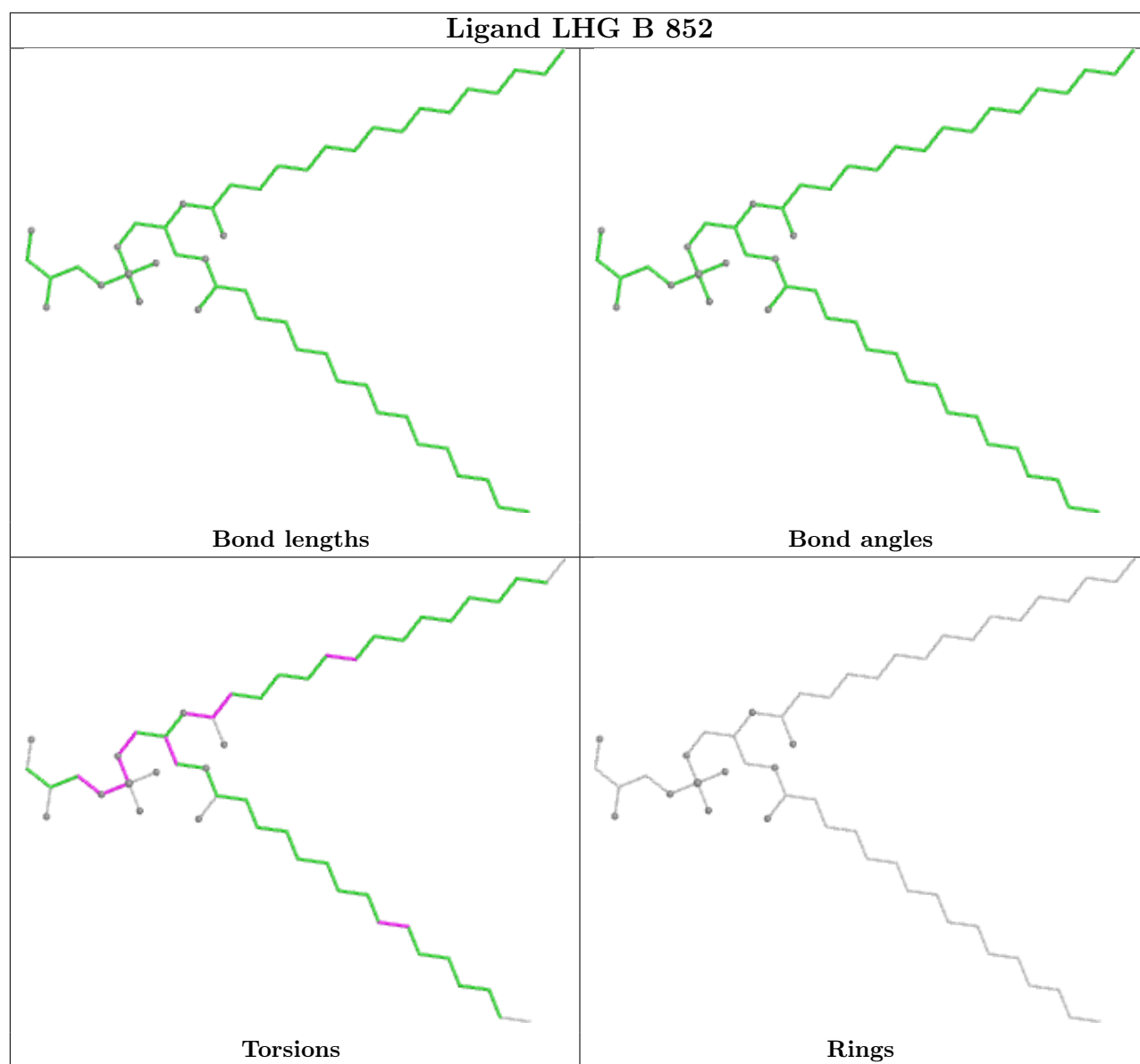
Bond angles



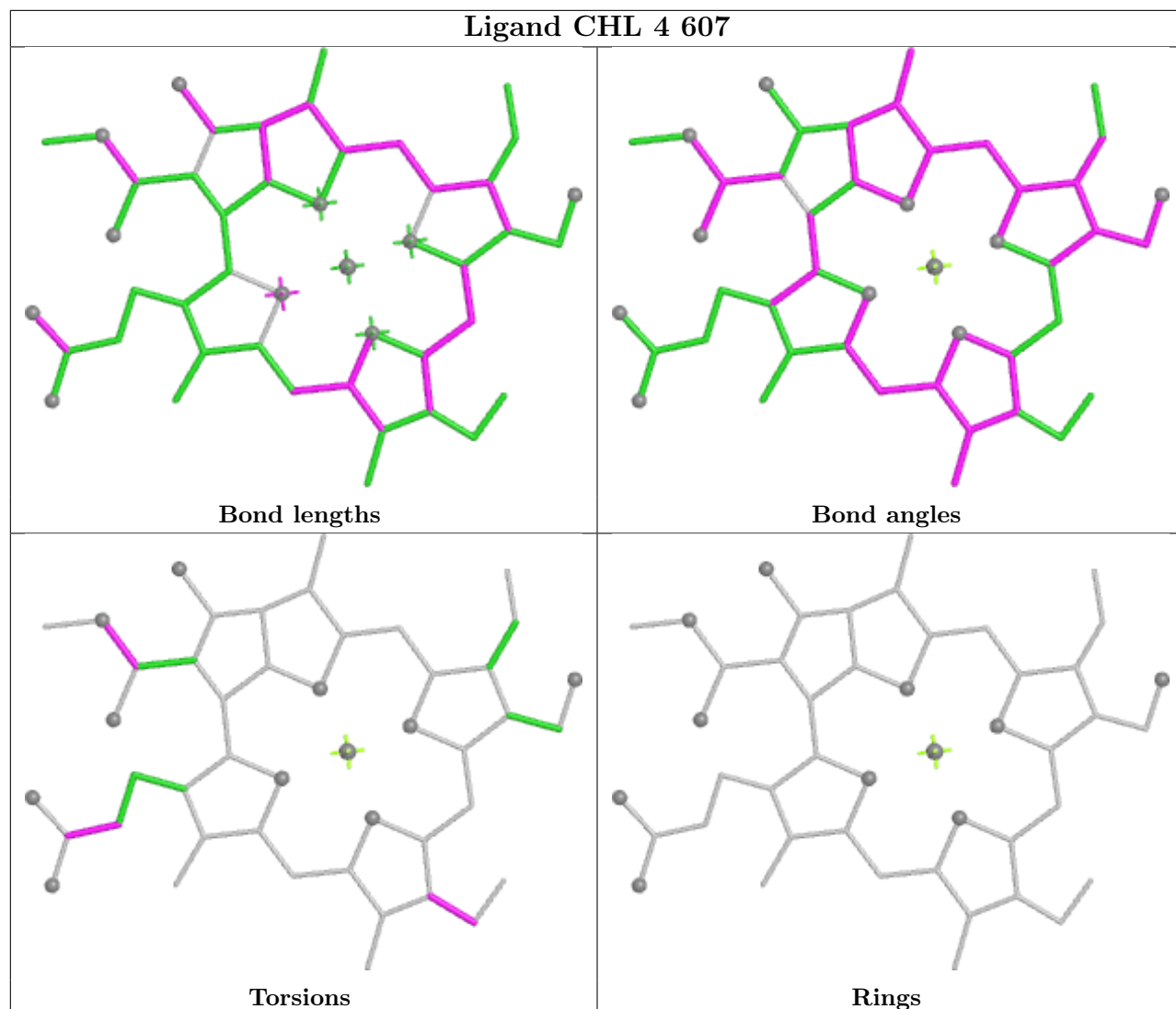
Torsions



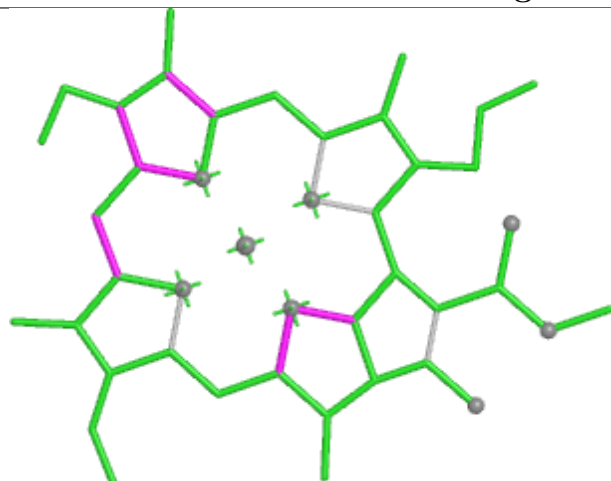
Rings



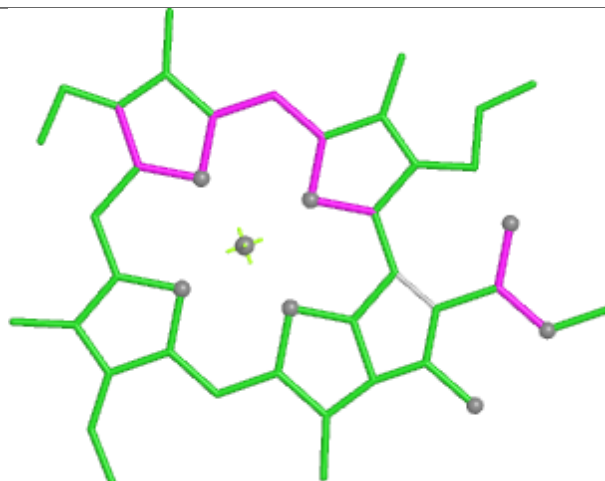
## Ligand CHL 4 607



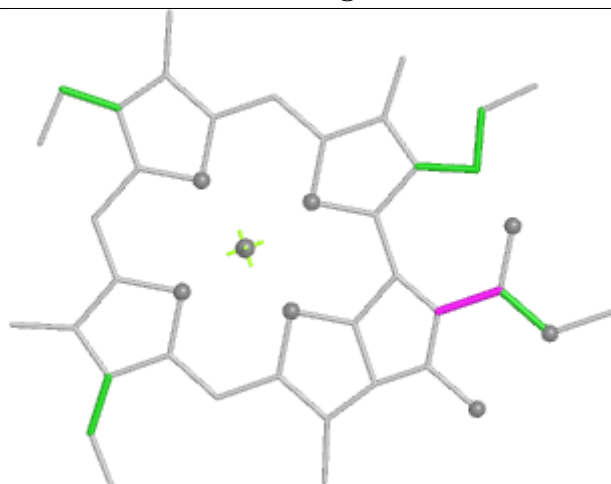
## Ligand CLA B 812



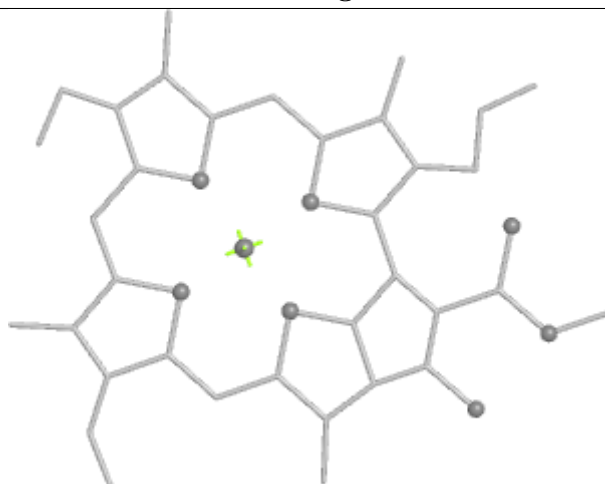
Bond lengths



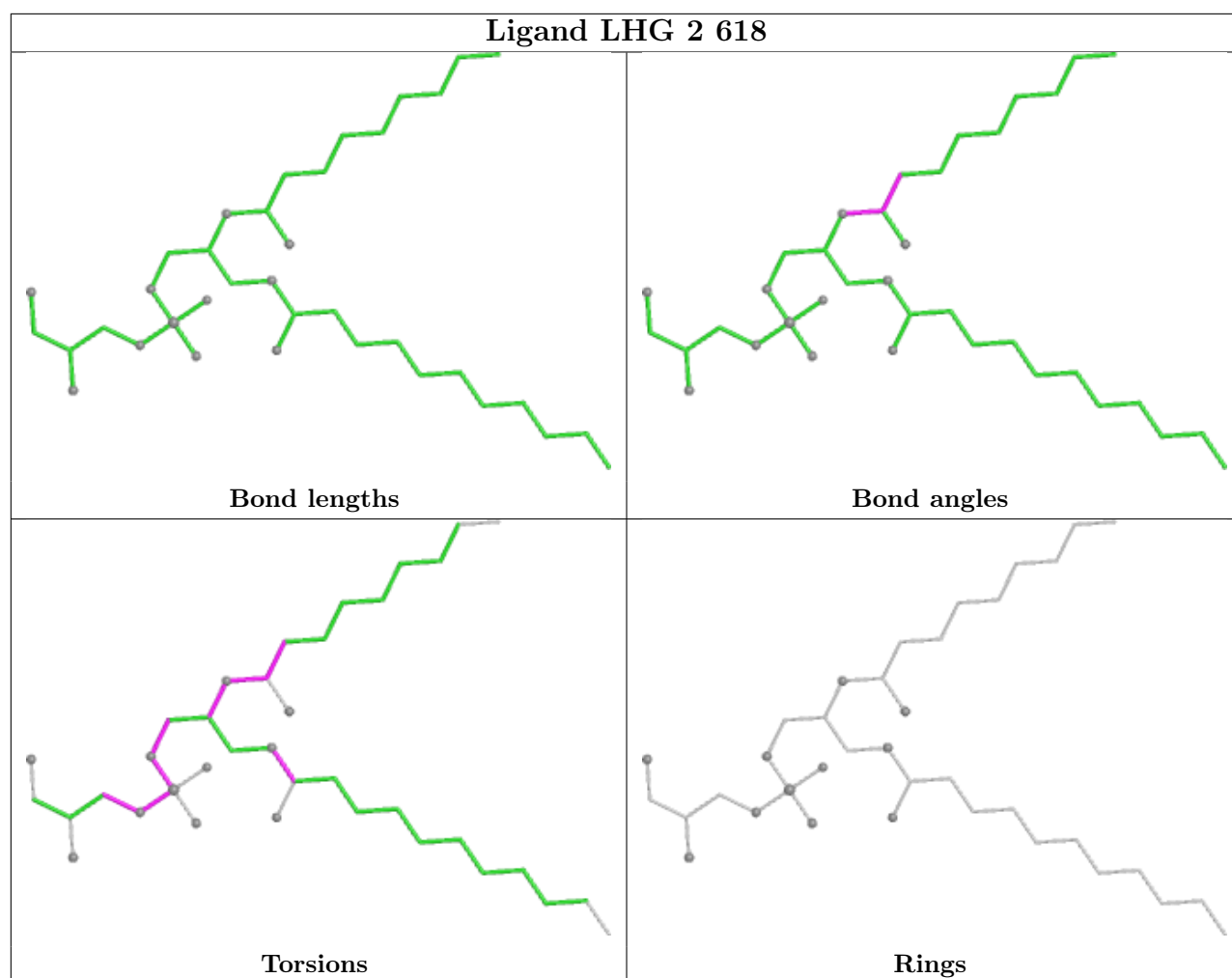
Bond angles

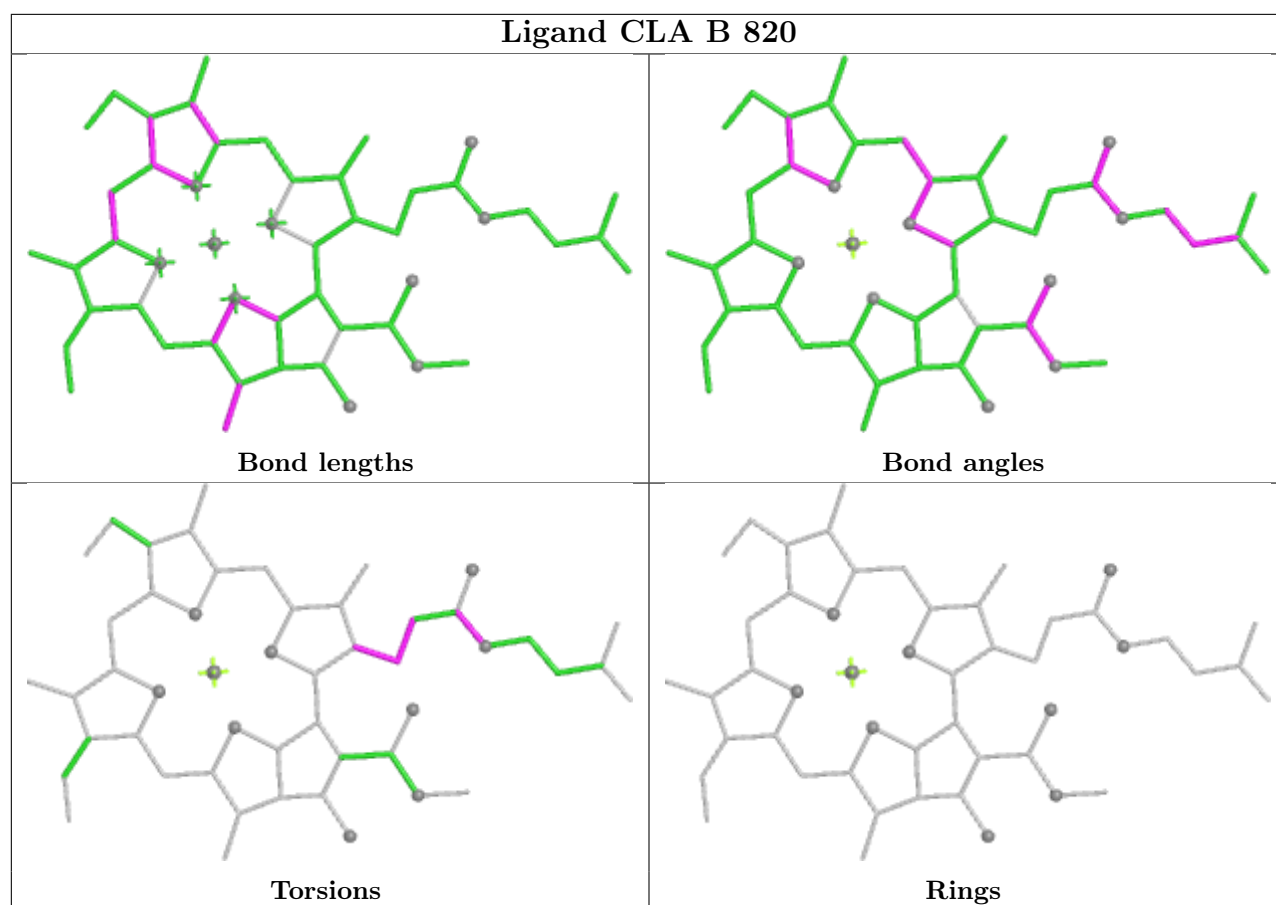


Torsions

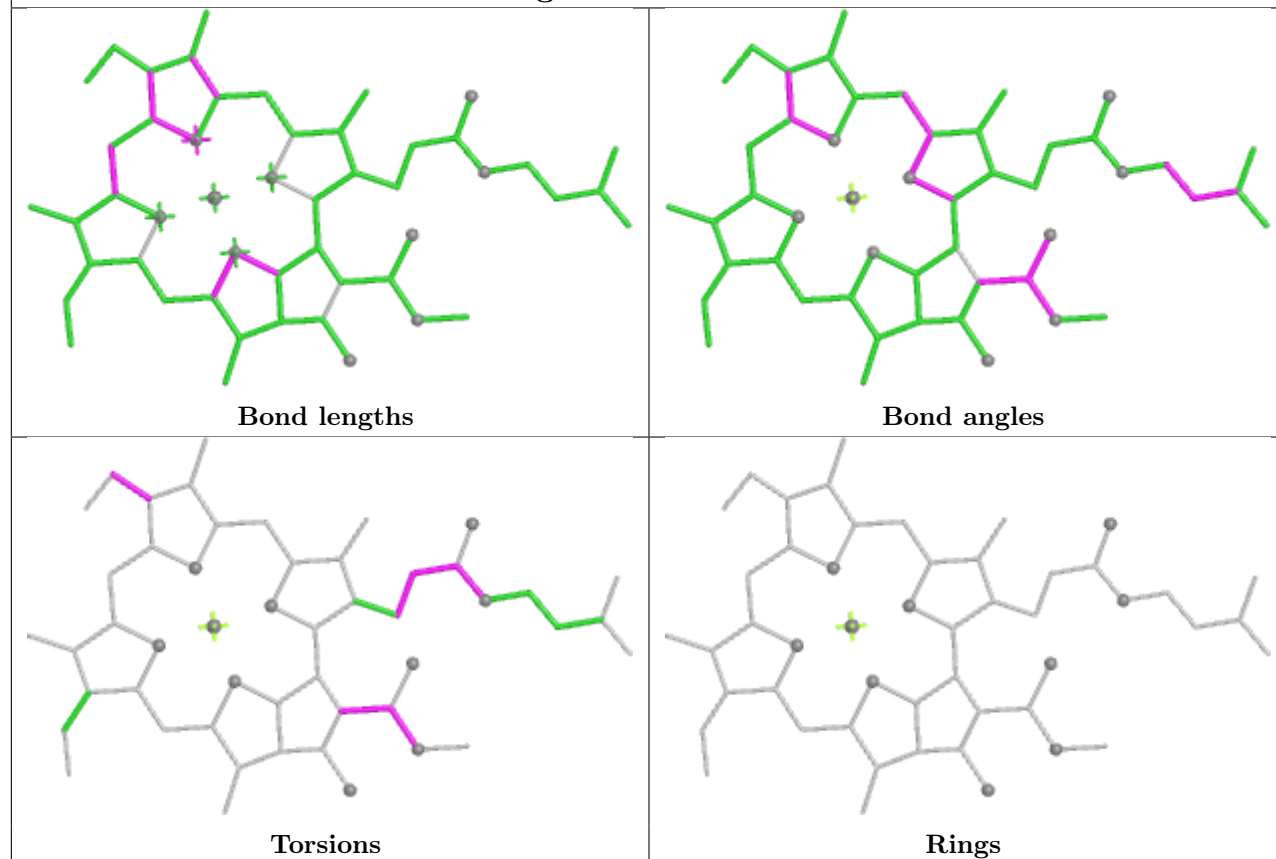


Rings

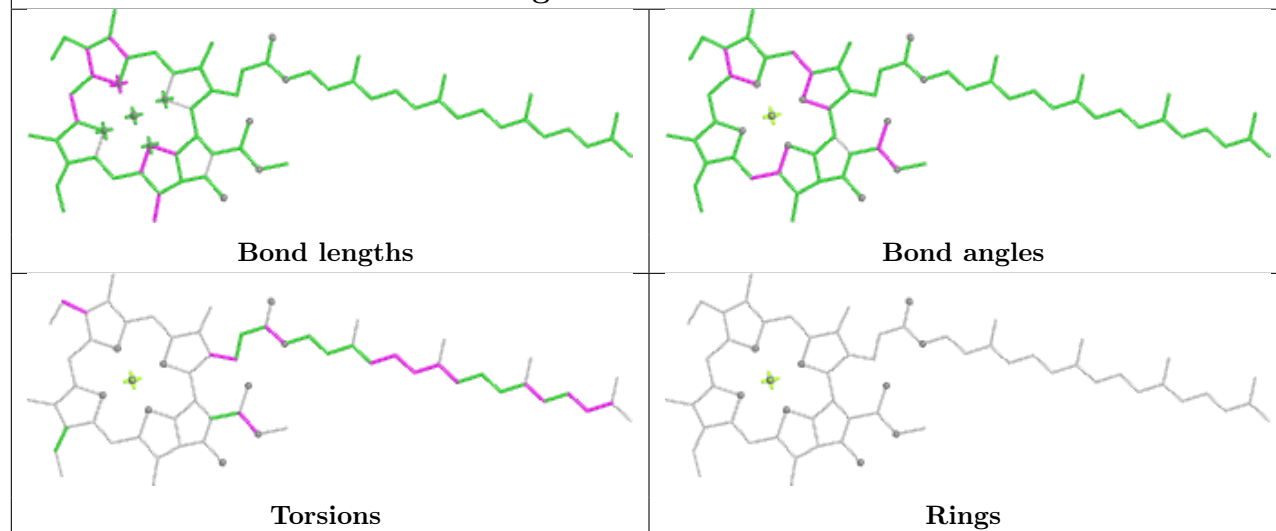


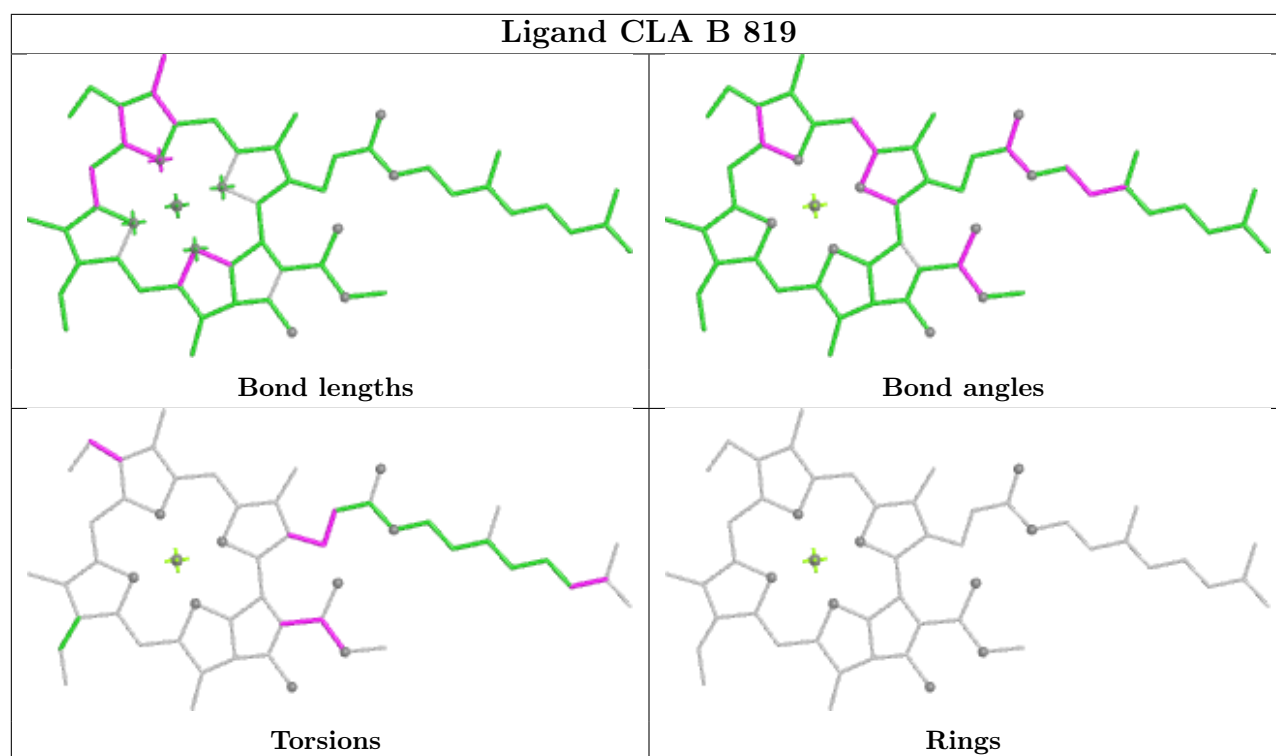


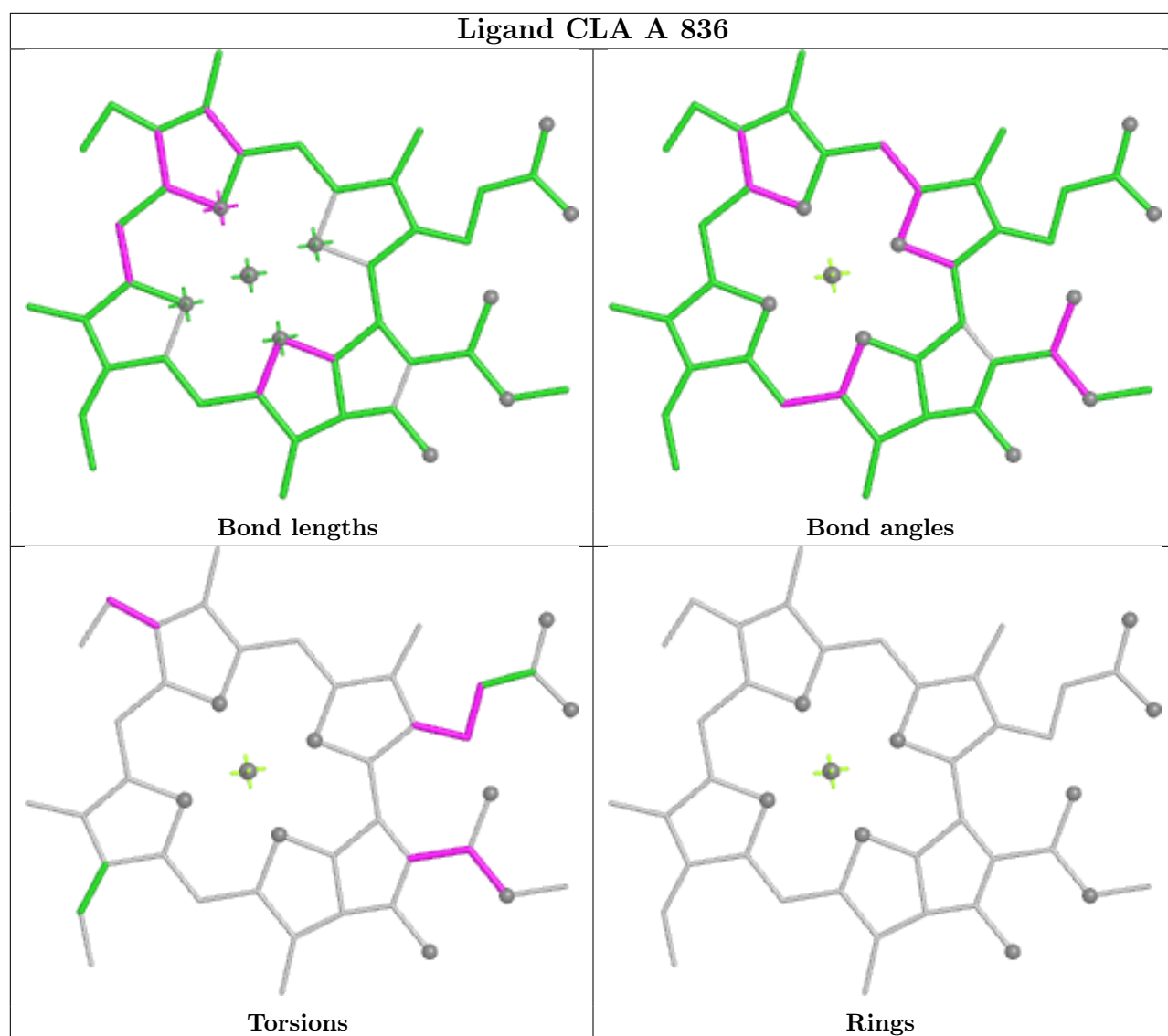
## Ligand CLA 4 614



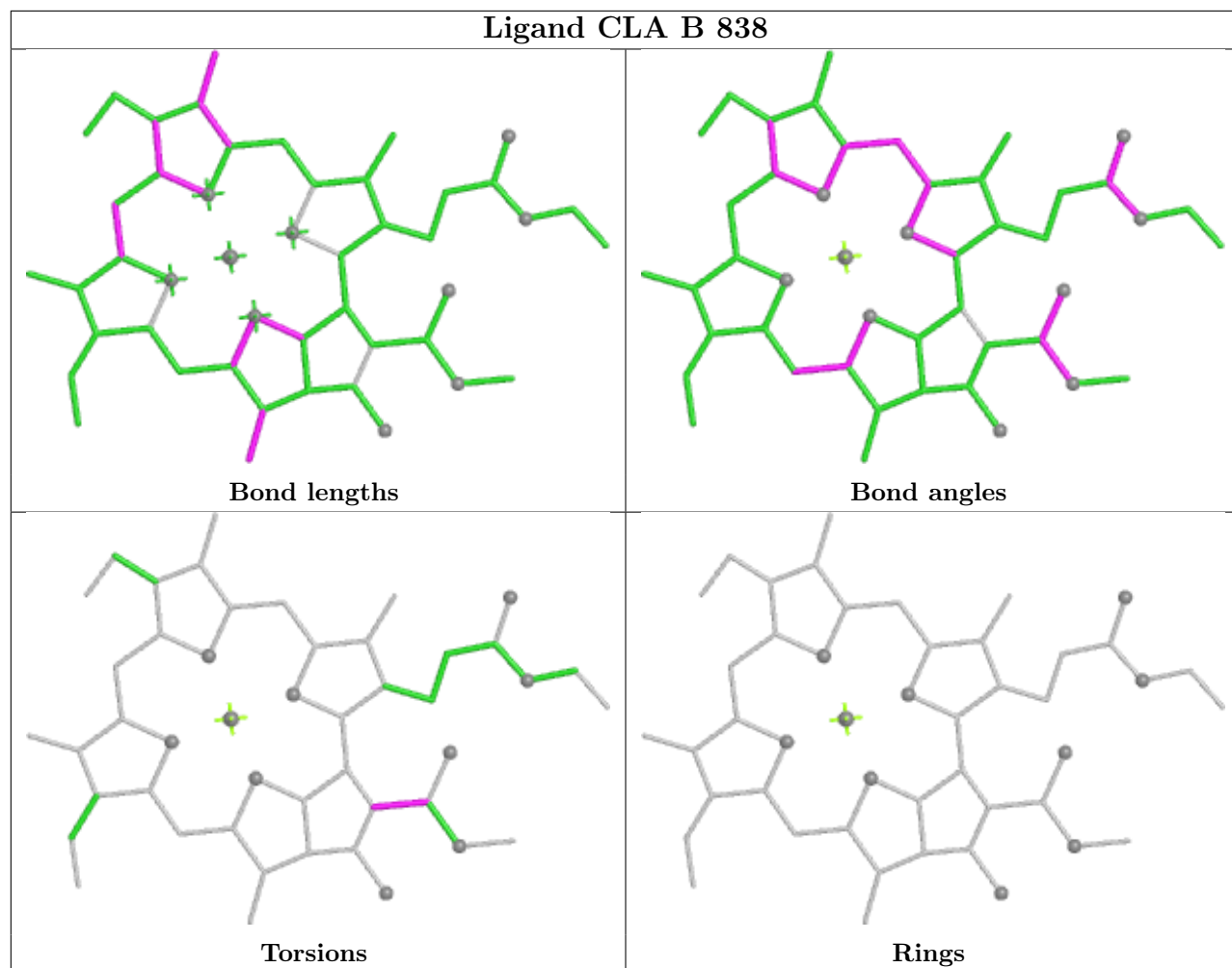
## Ligand CLA B 840

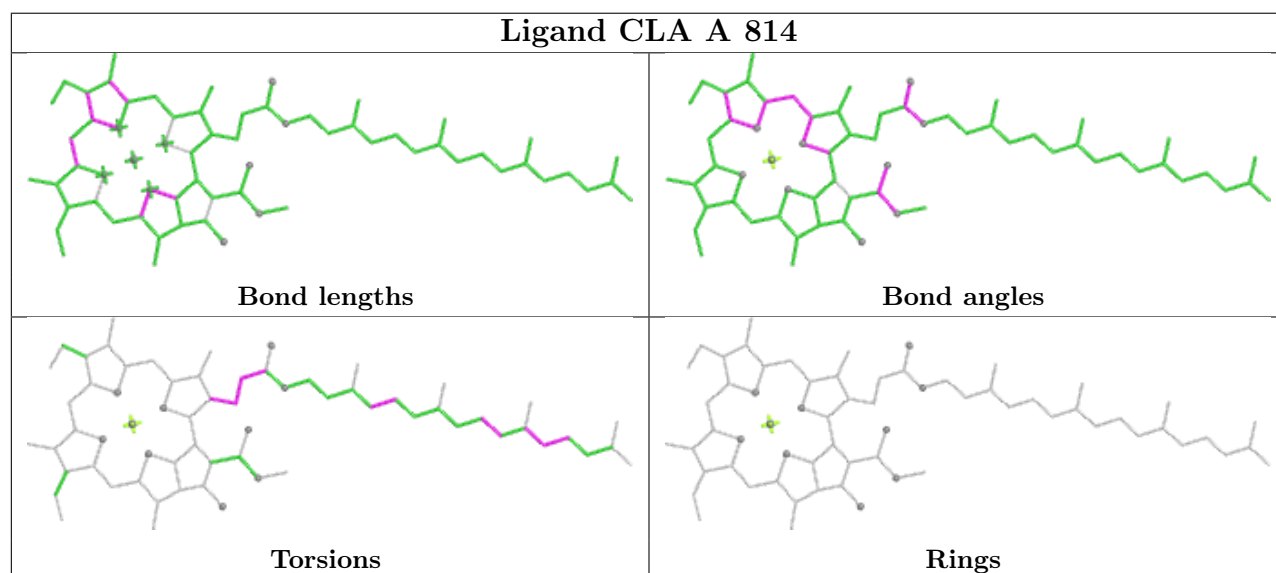
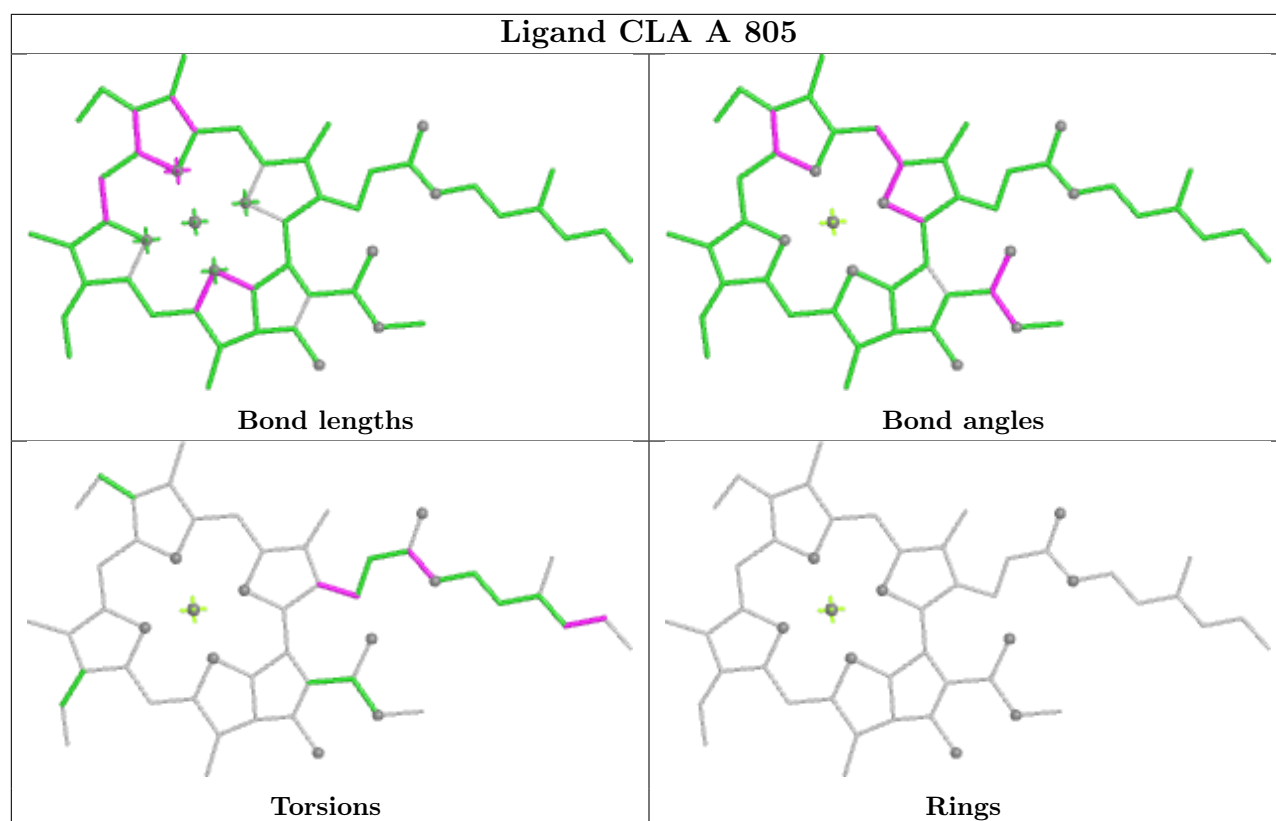


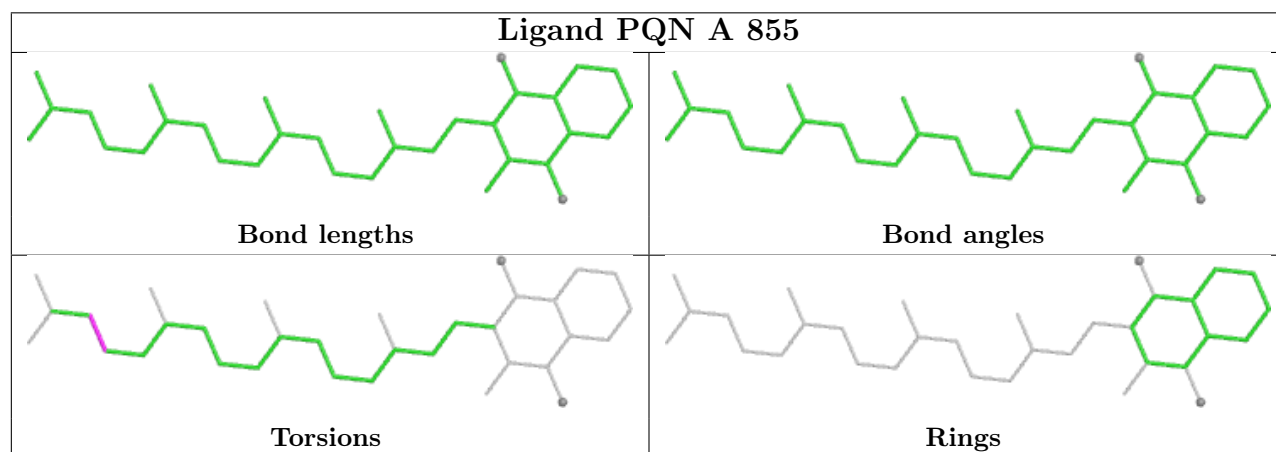
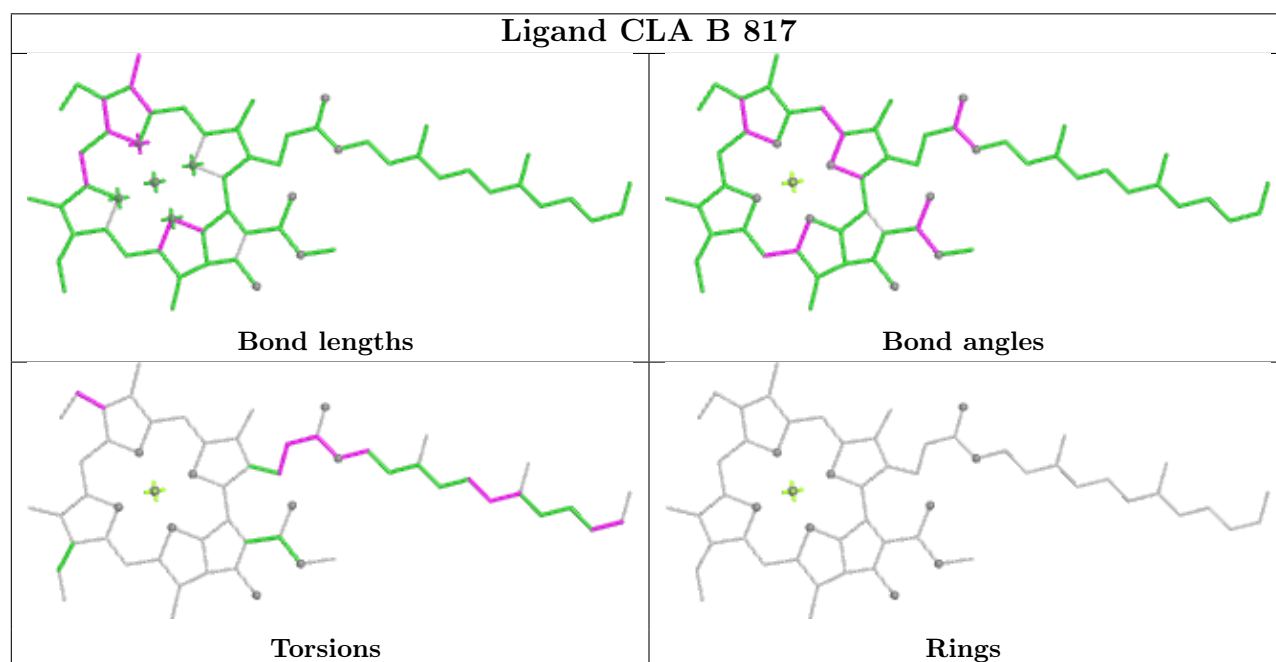
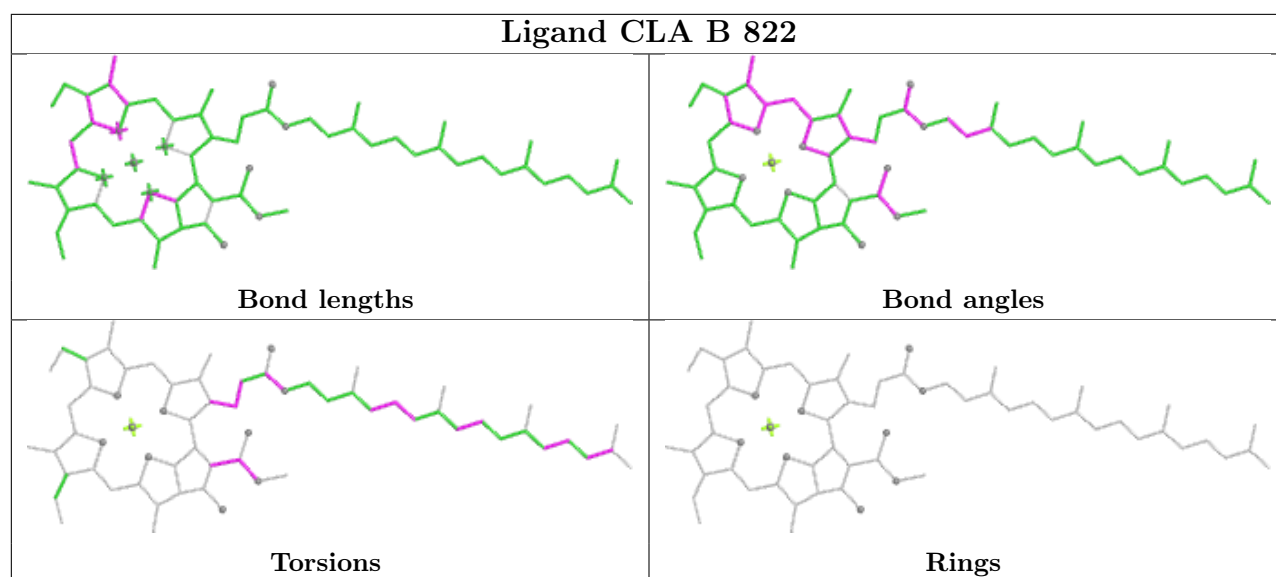




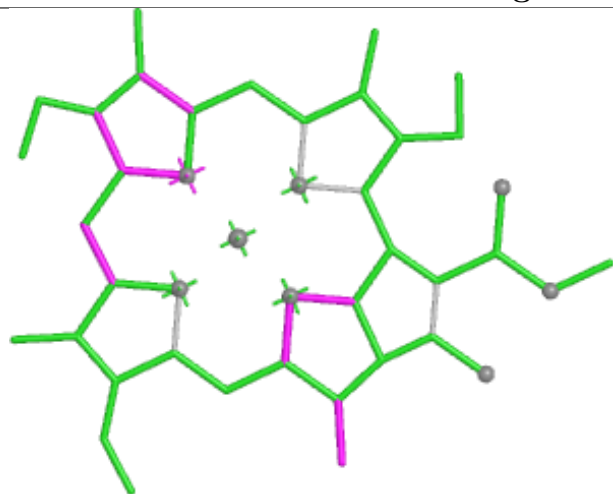
## Ligand CLA B 838



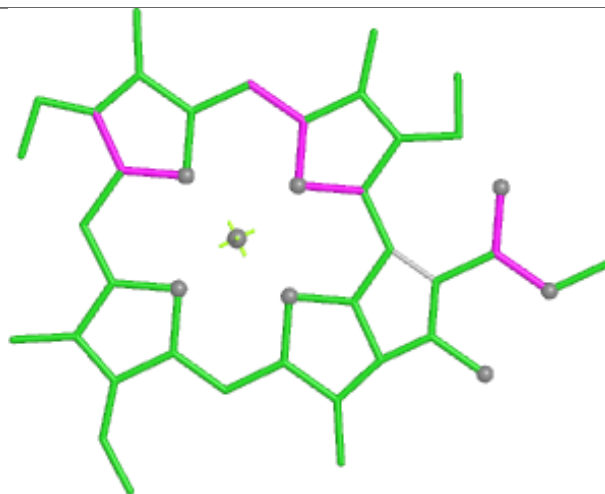




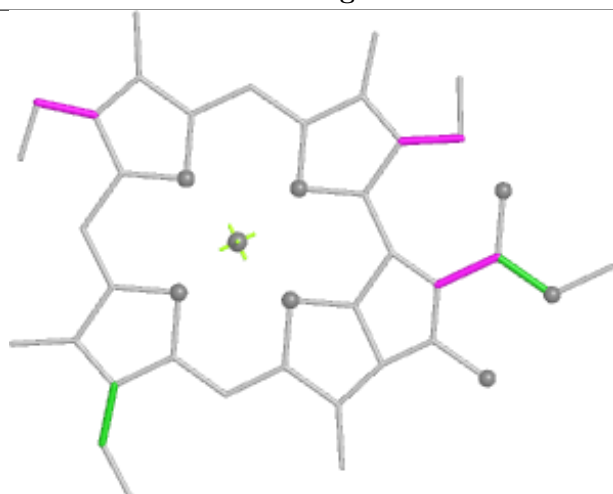
## Ligand CLA G 202



Bond lengths



Bond angles

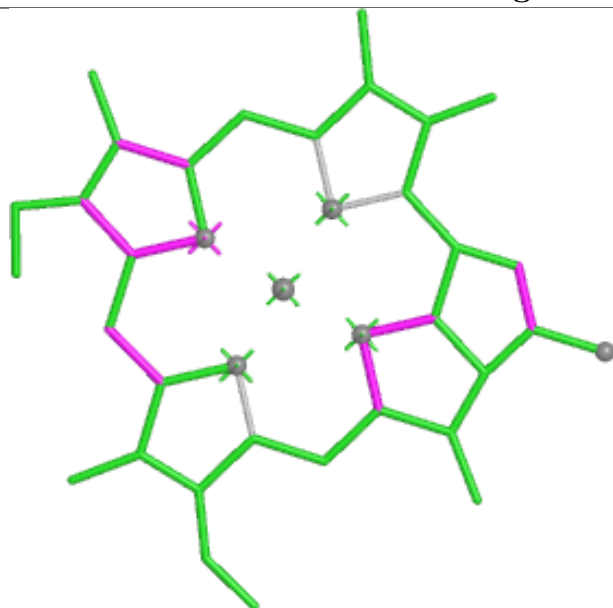


Torsions

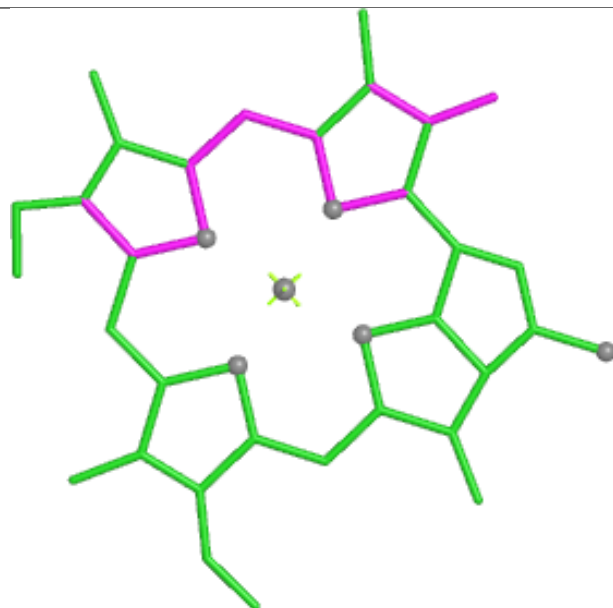


Rings

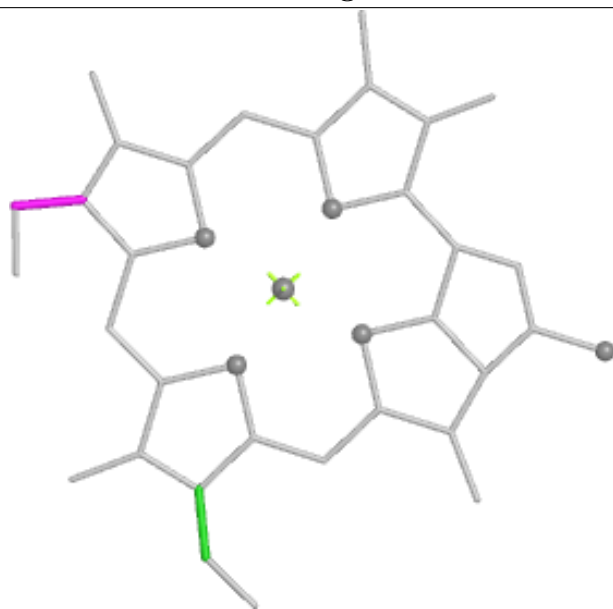
## Ligand CLA K 201



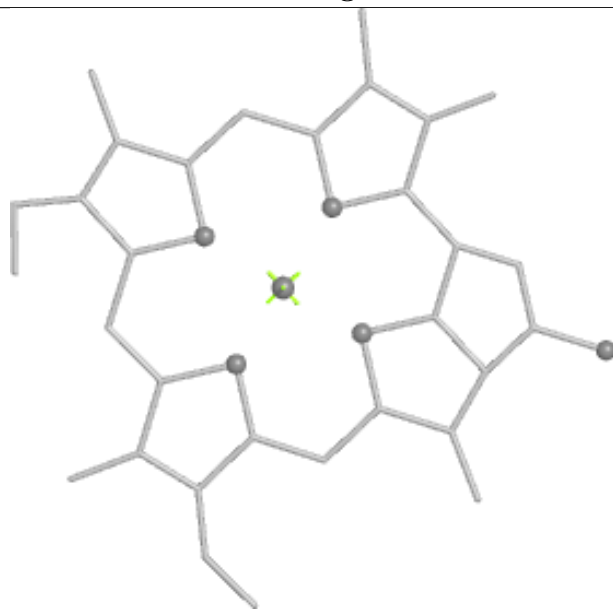
Bond lengths



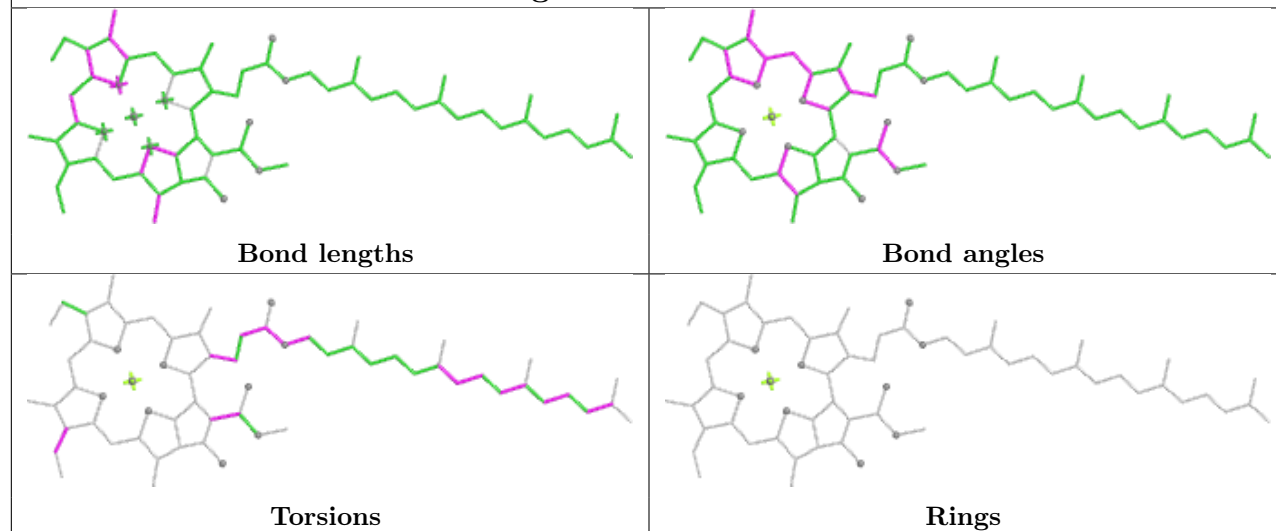
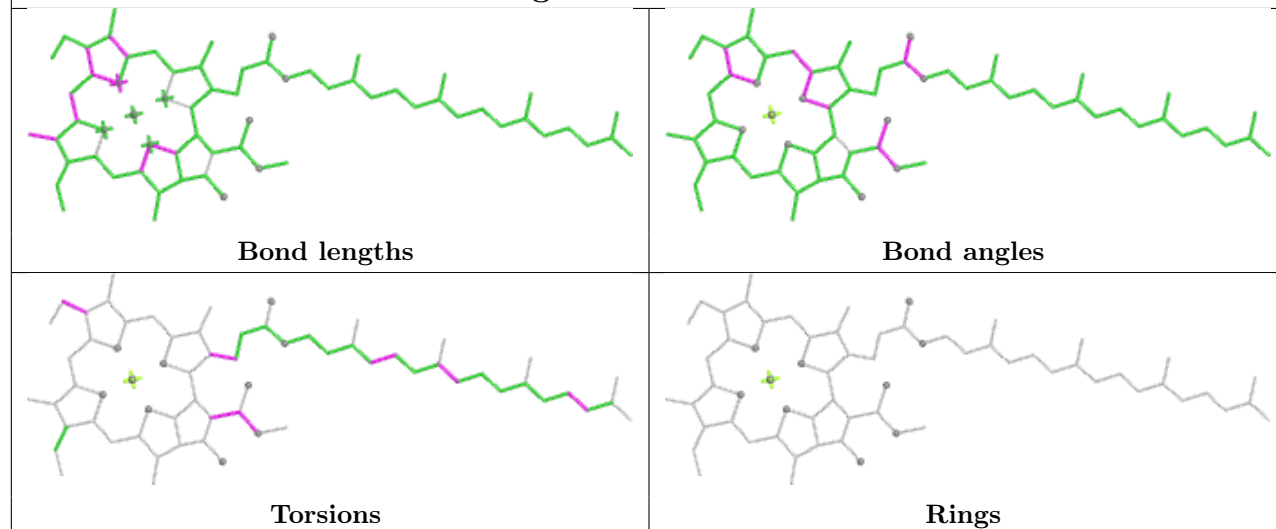
Bond angles



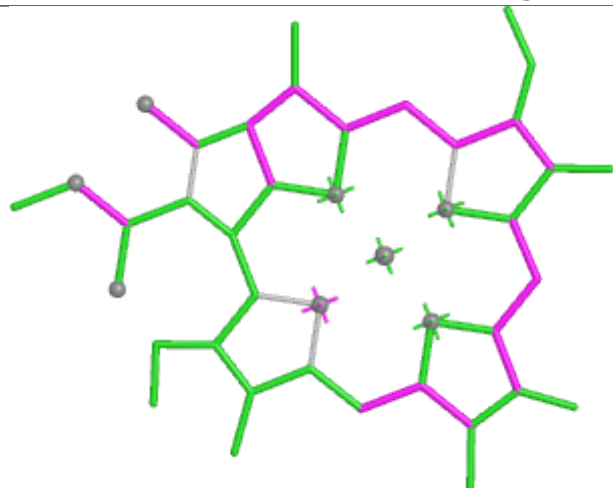
Torsions



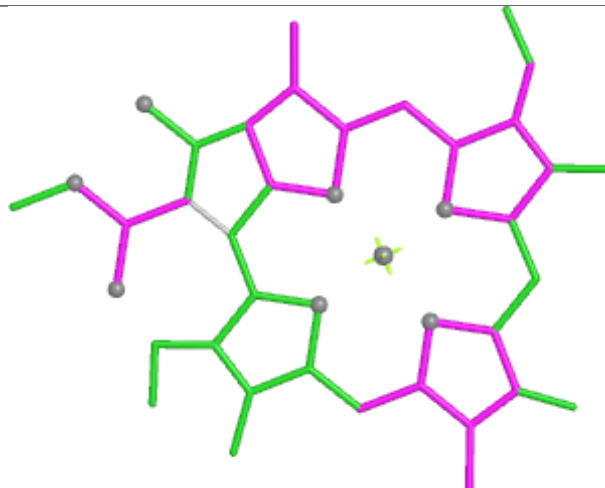
Rings

**Ligand CLA A 842****Ligand CLA B 803**

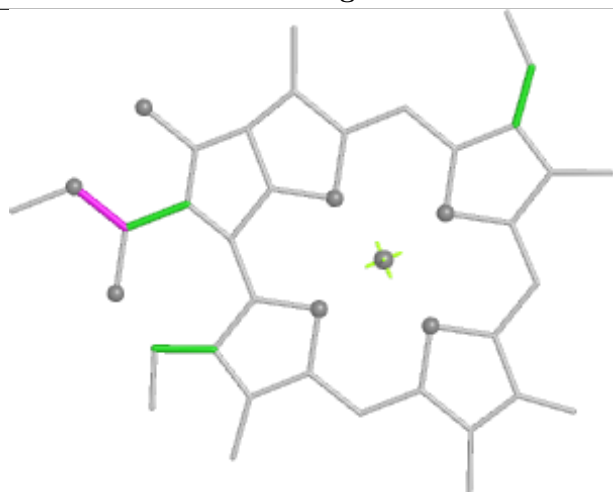
## Ligand CHL 4 606



Bond lengths



Bond angles

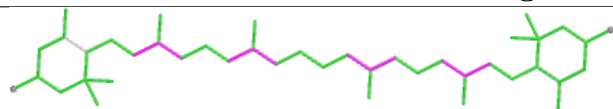


Torsions

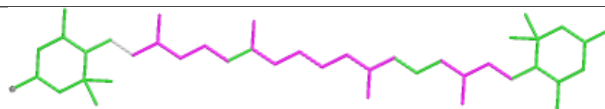


Rings

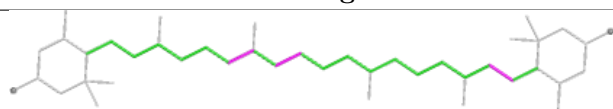
## Ligand LUT 2 616



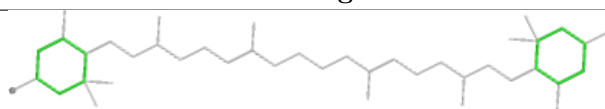
Bond lengths



Bond angles

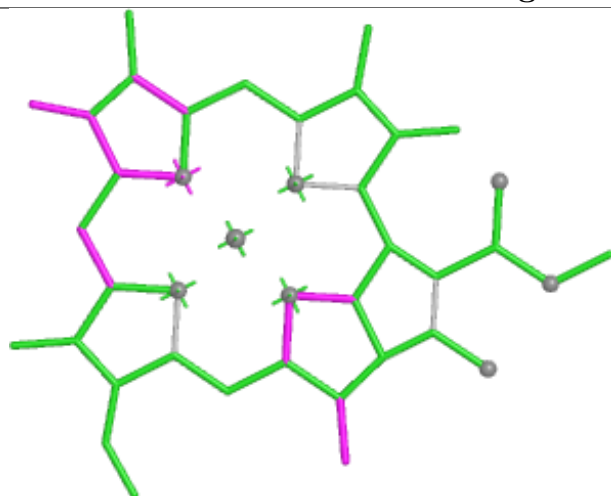


Torsions

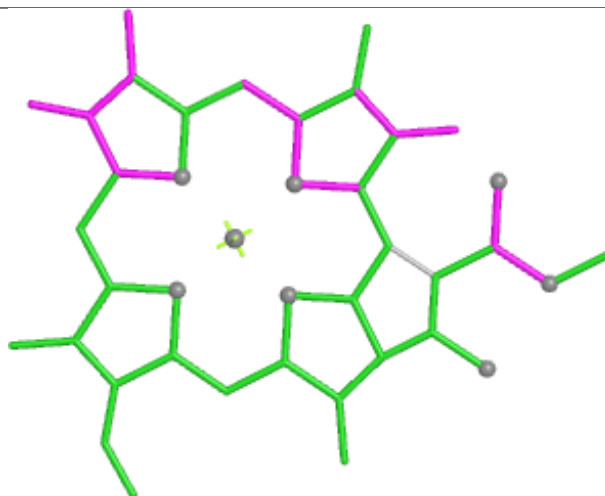


Rings

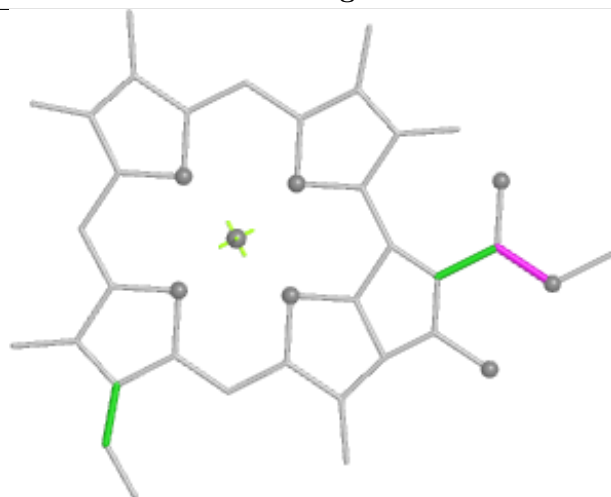
## Ligand CLA 1 608



Bond lengths



Bond angles

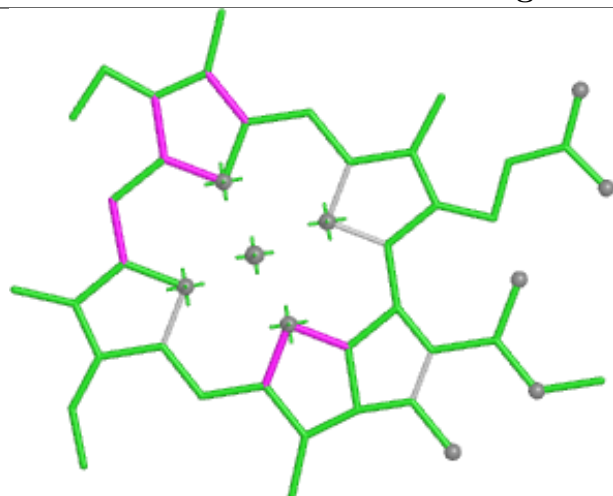


Torsions

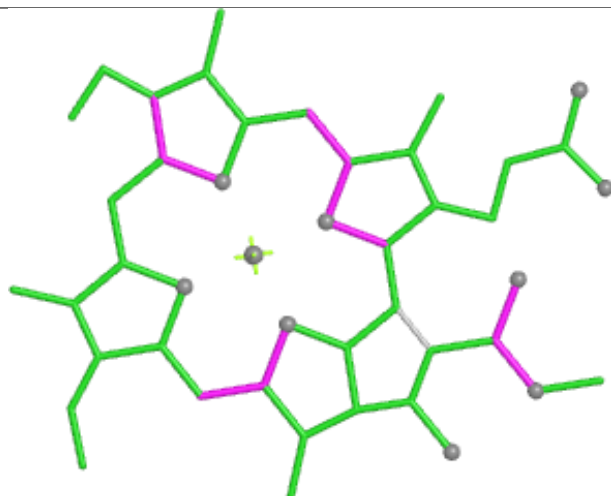


Rings

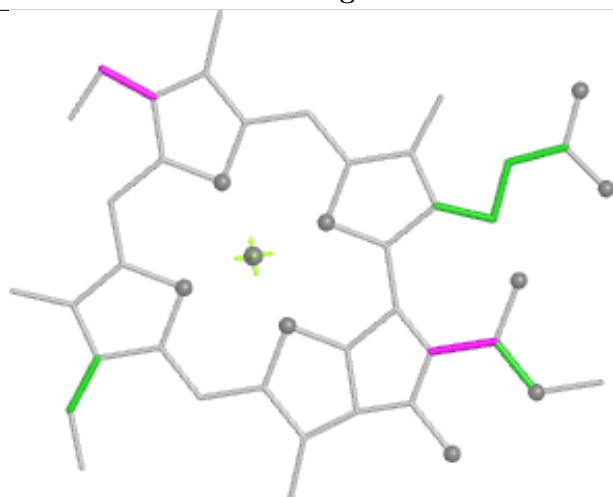
## Ligand CLA L 304



Bond lengths



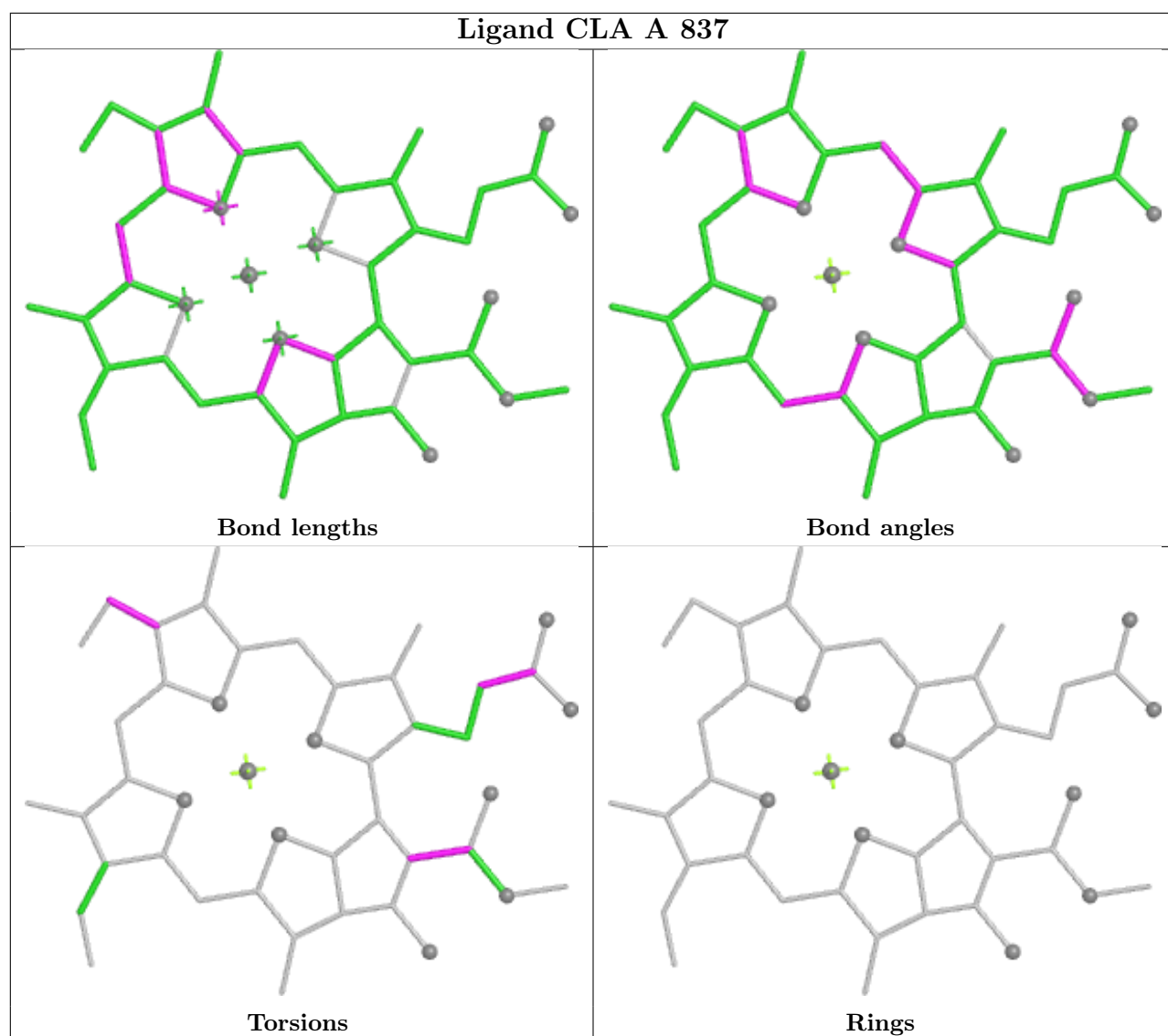
Bond angles



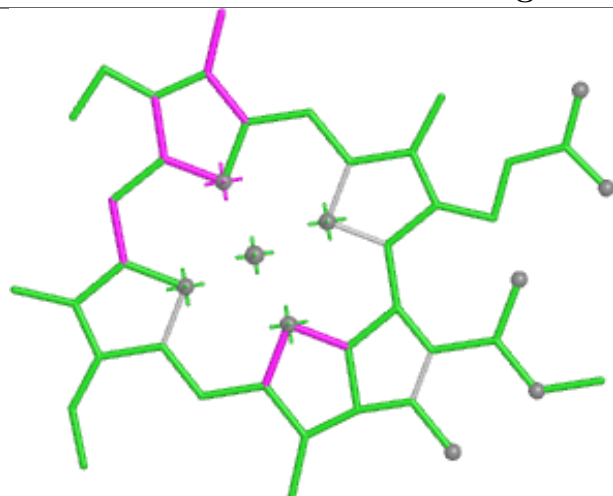
Torsions



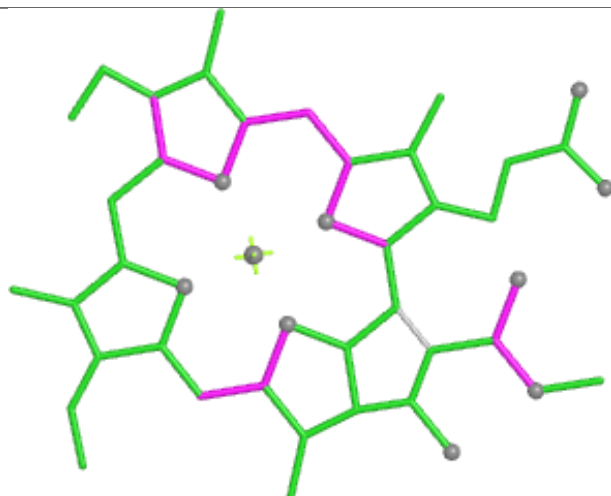
Rings



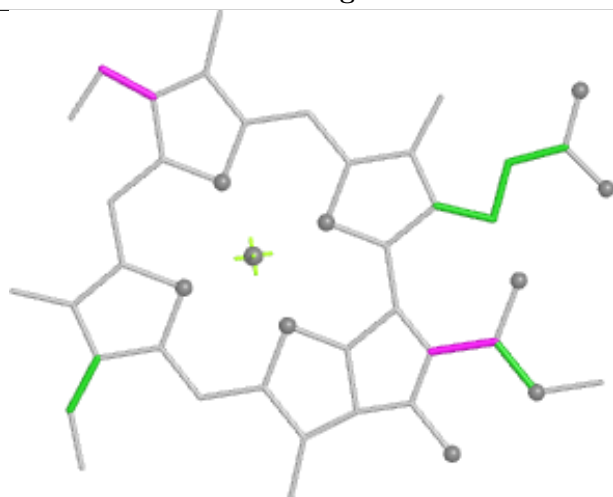
## Ligand CLA L 302



Bond lengths



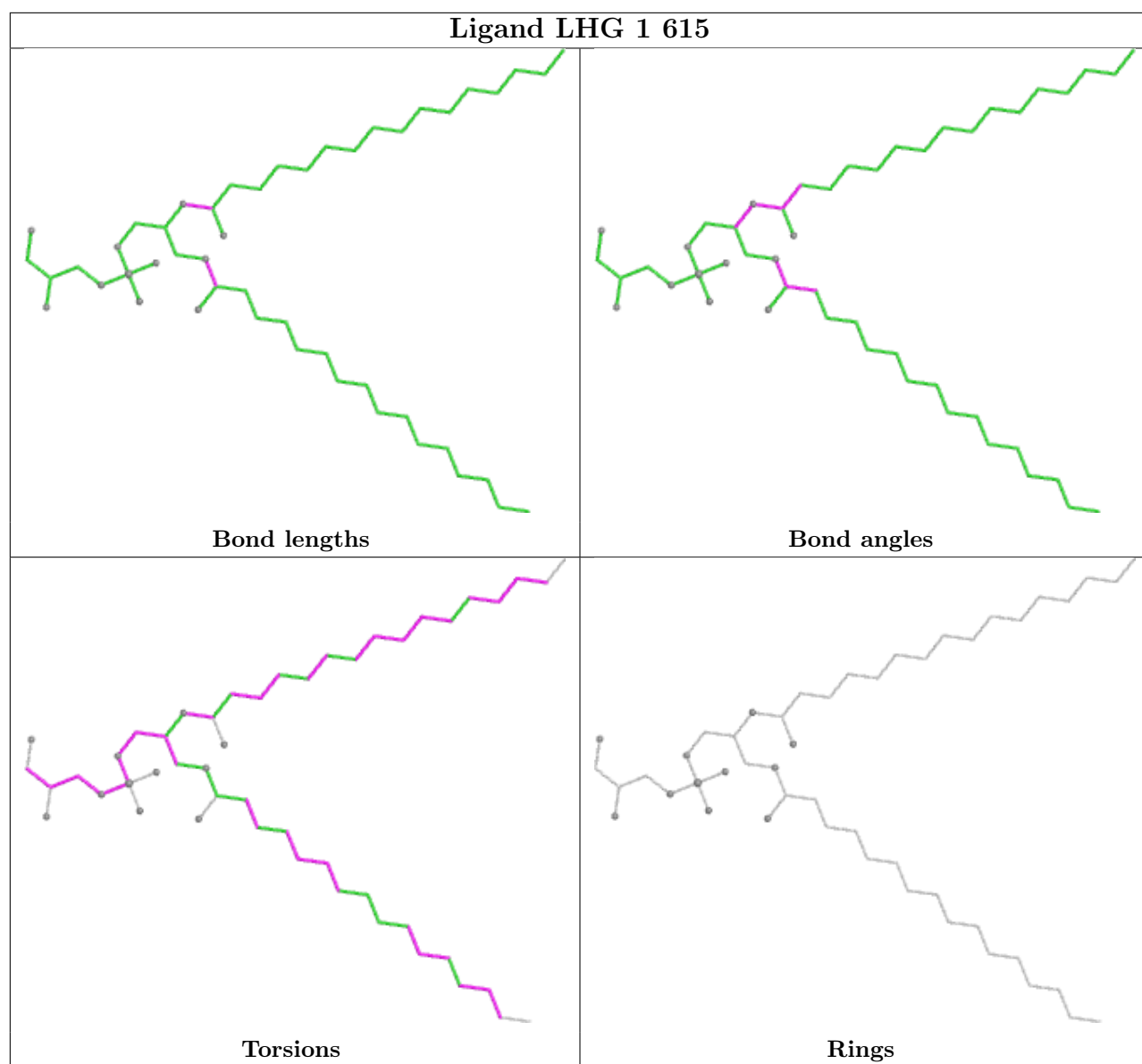
Bond angles

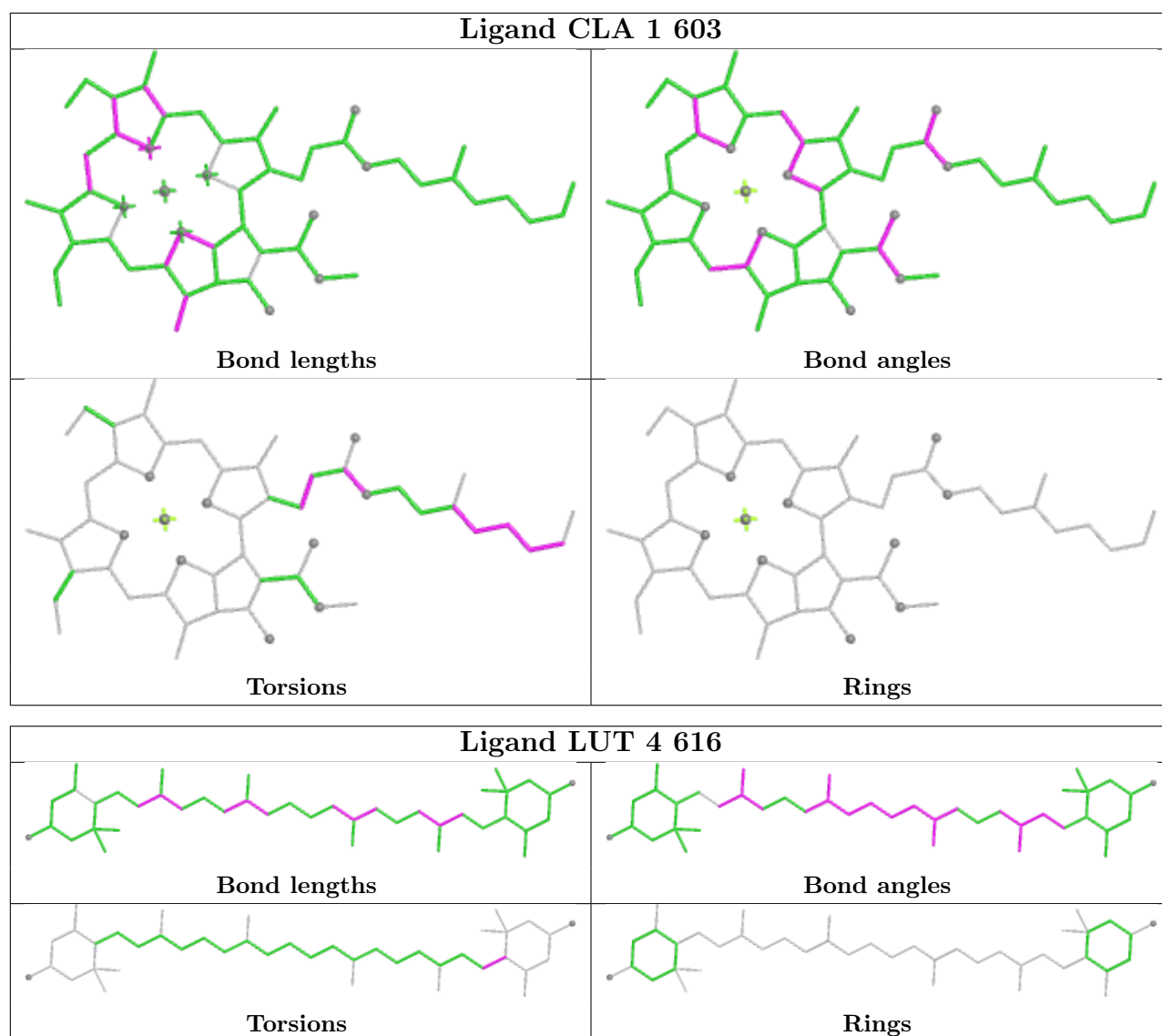


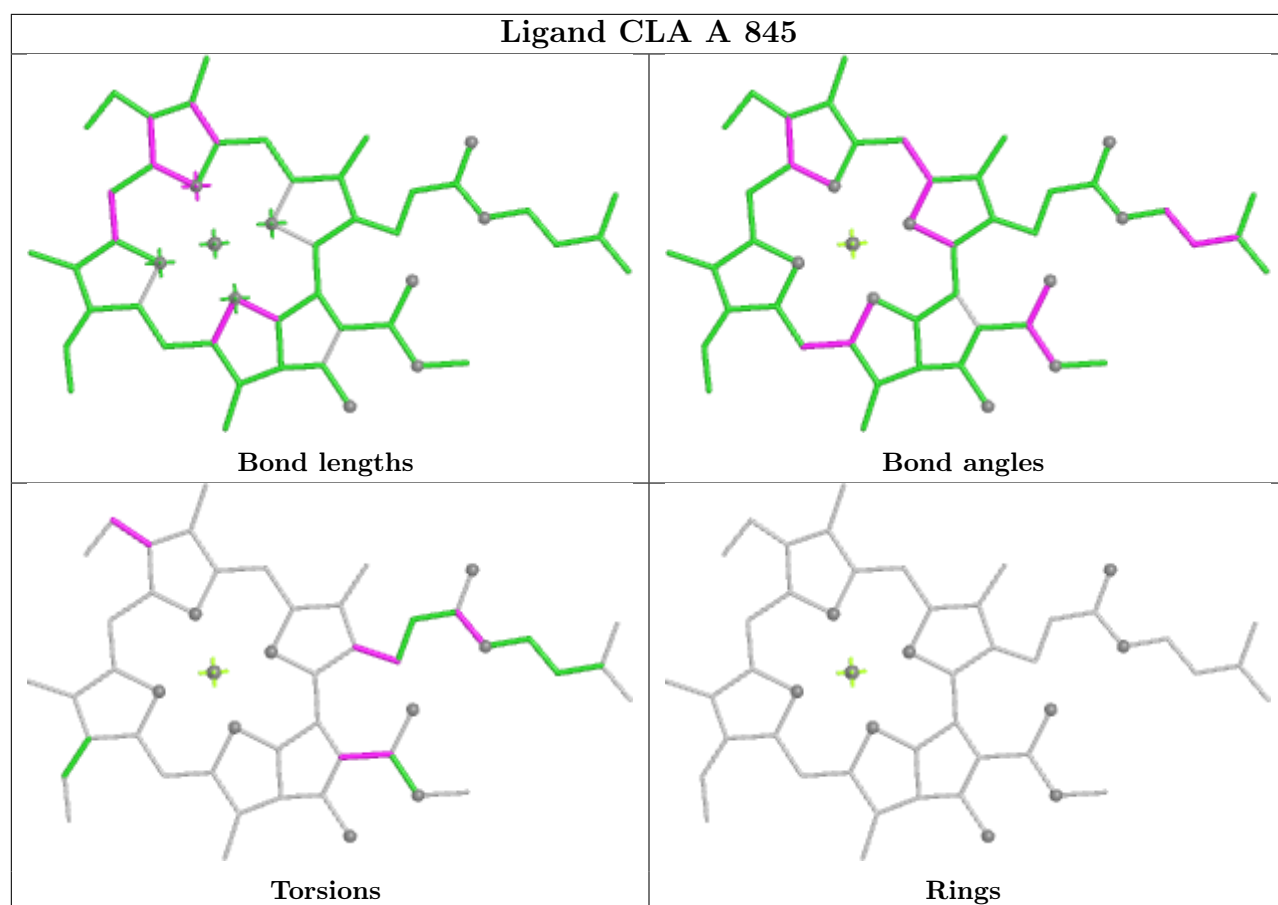
Torsions



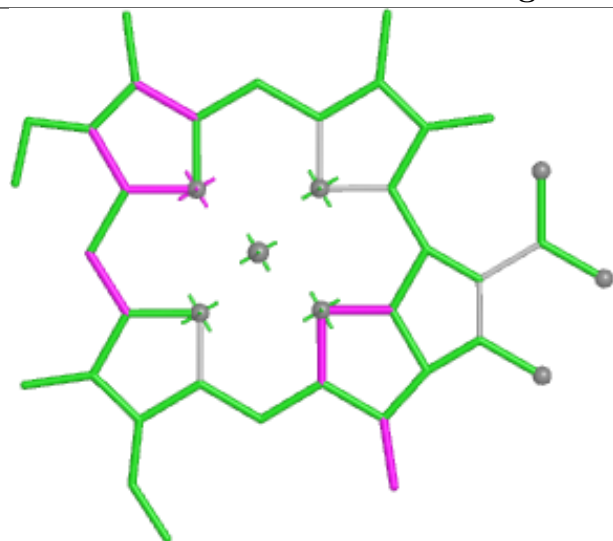
Rings



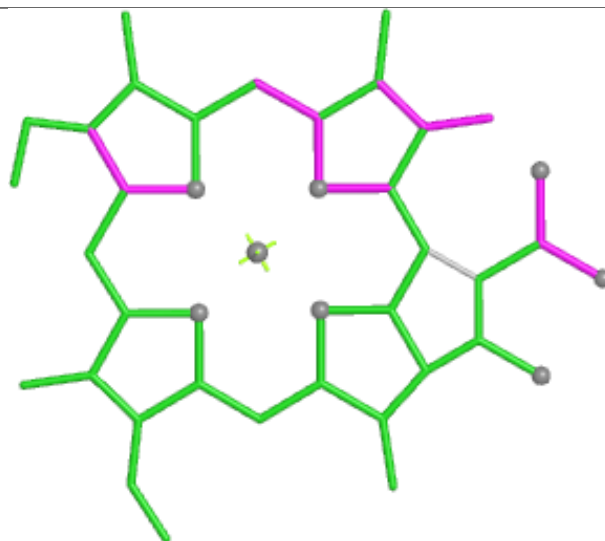




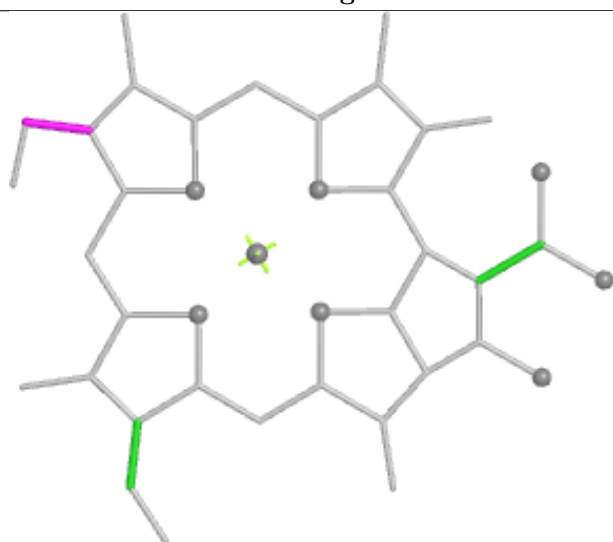
## Ligand CLA 3 612



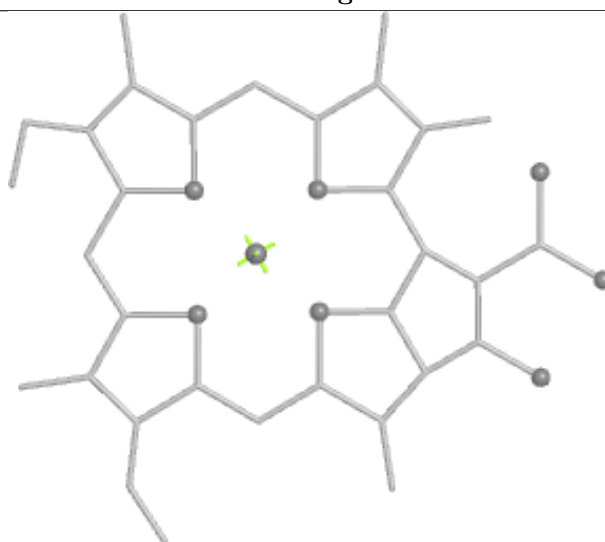
Bond lengths



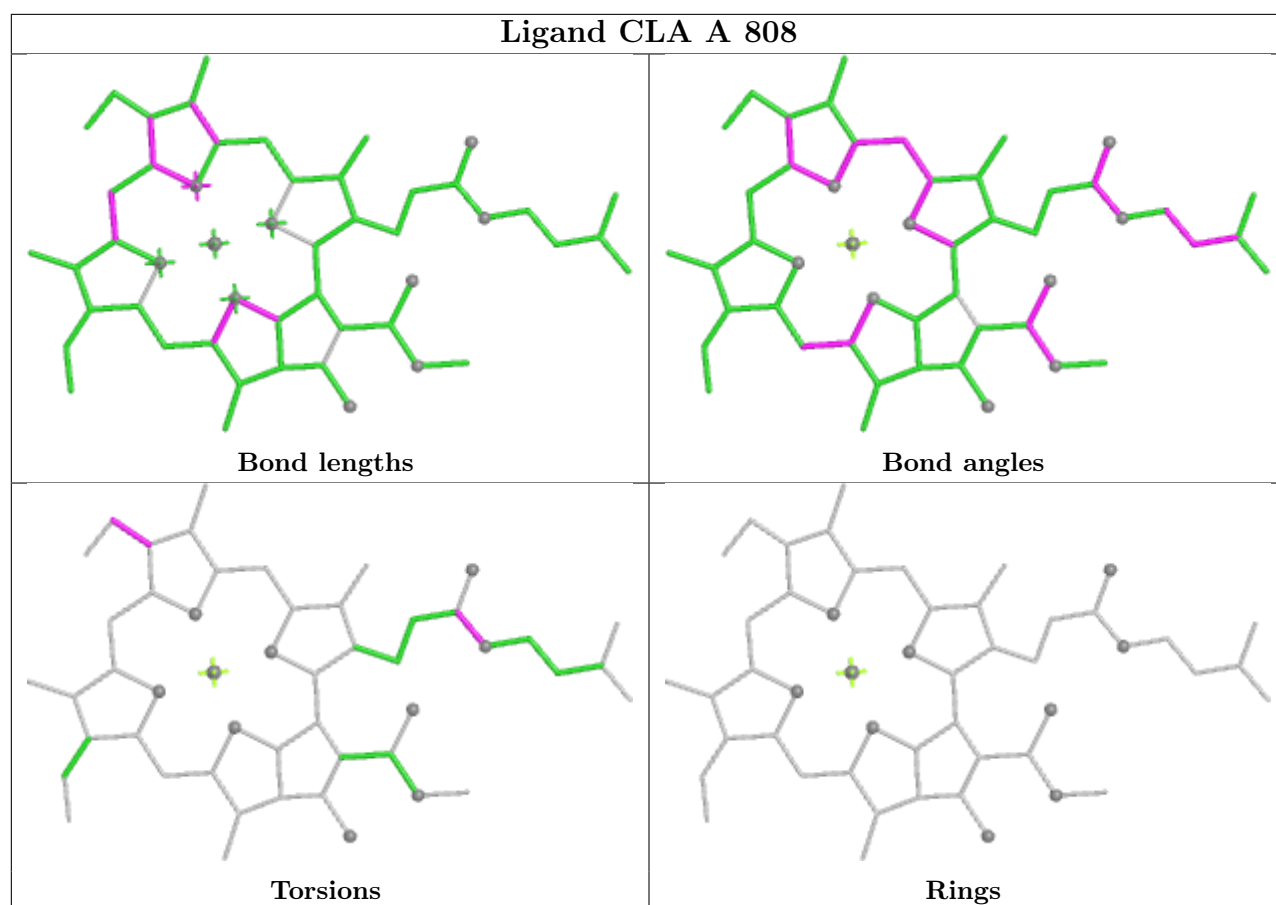
Bond angles



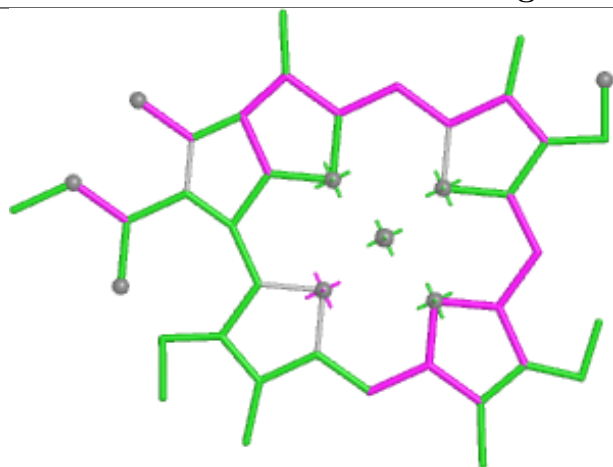
Torsions



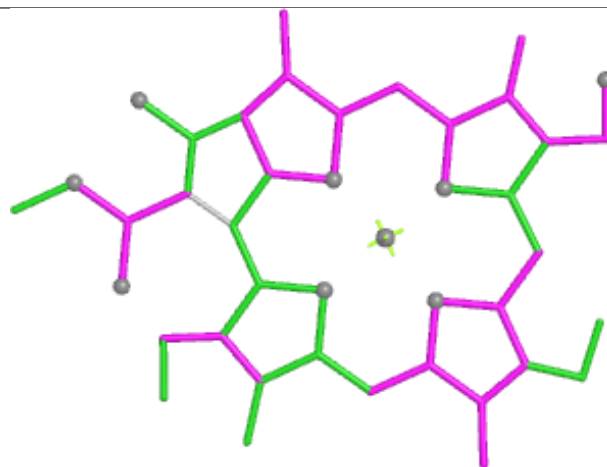
Rings



## Ligand CHL 2 605



Bond lengths



Bond angles

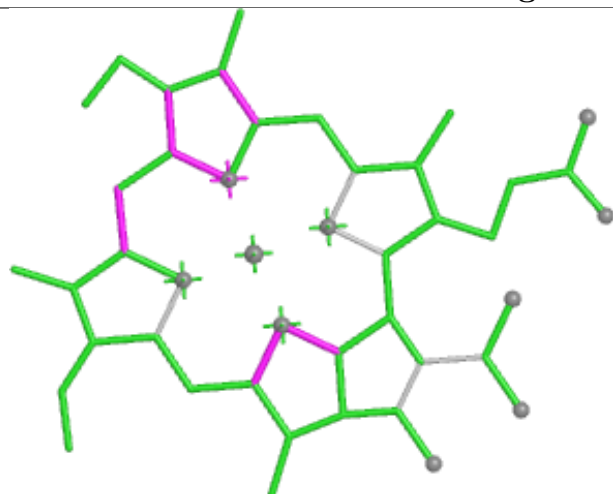


Torsions

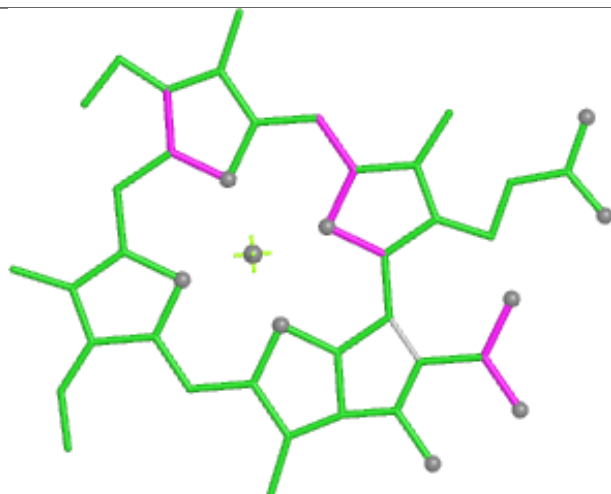


Rings

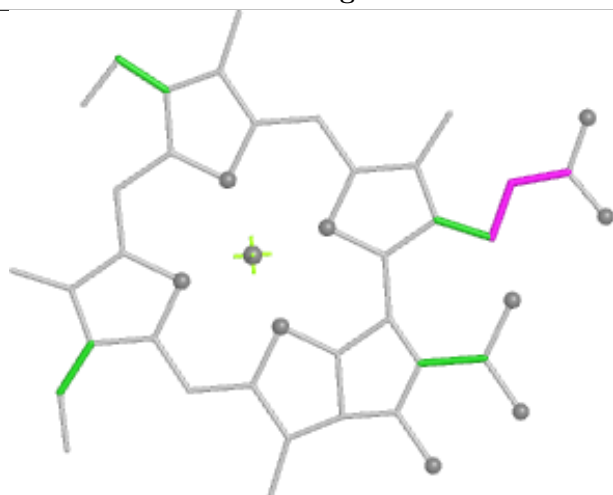
## Ligand CLA 2 603



Bond lengths



Bond angles

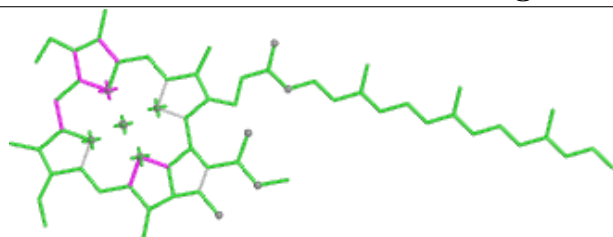


Torsions

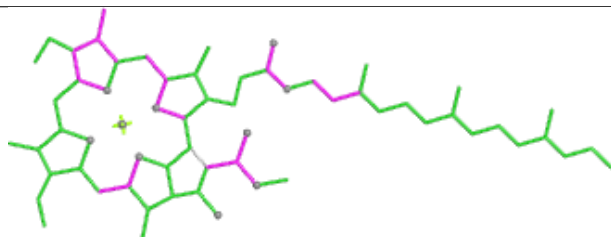


Rings

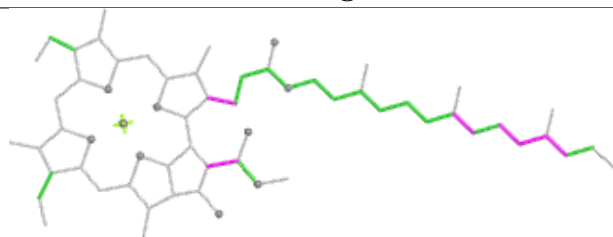
## Ligand CLA B 825



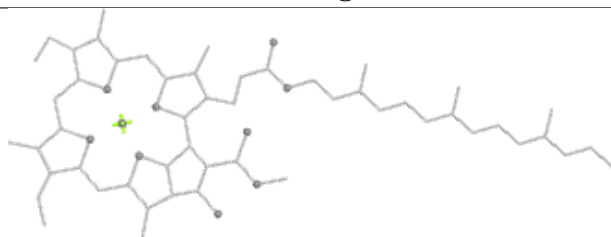
Bond lengths



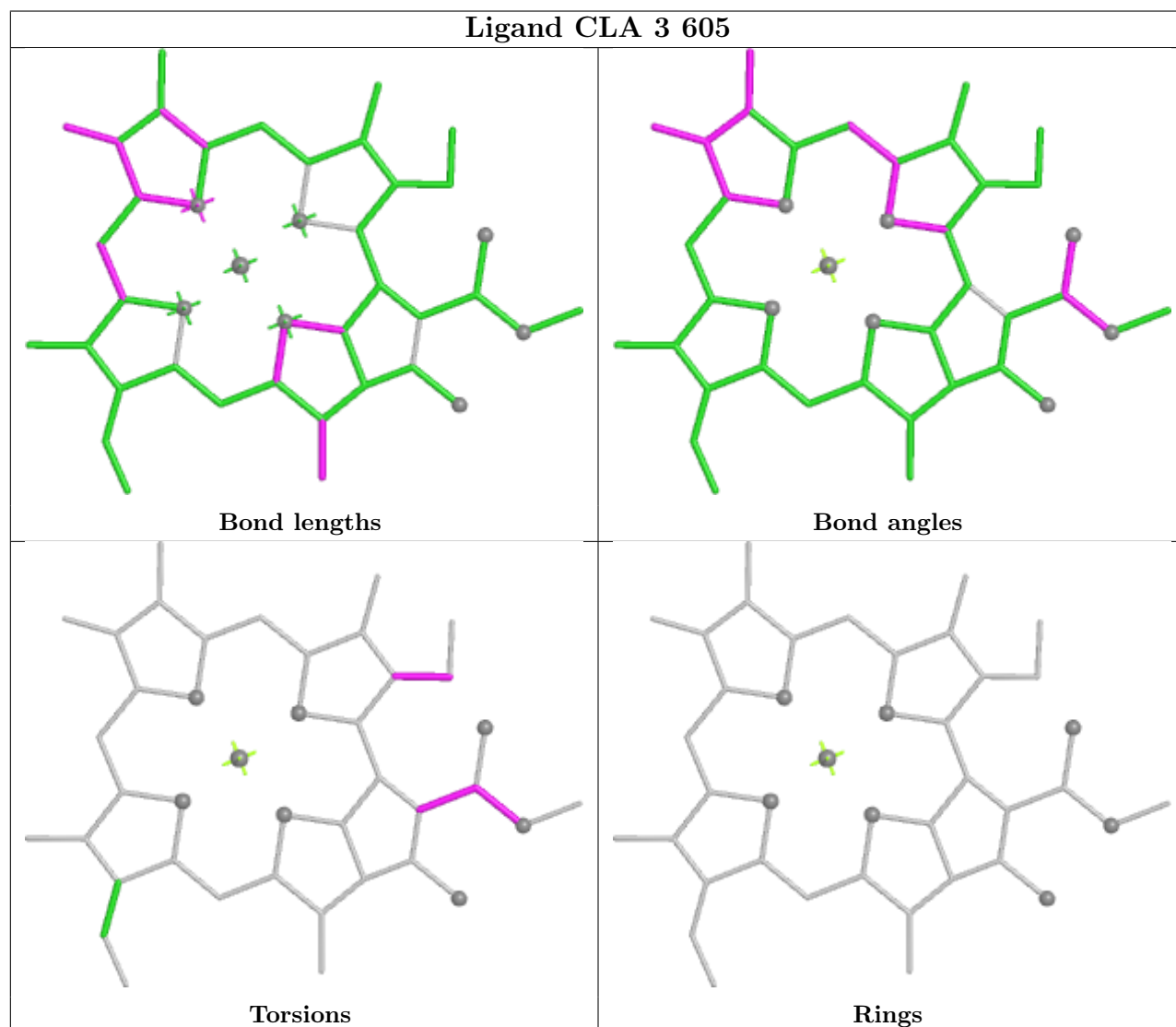
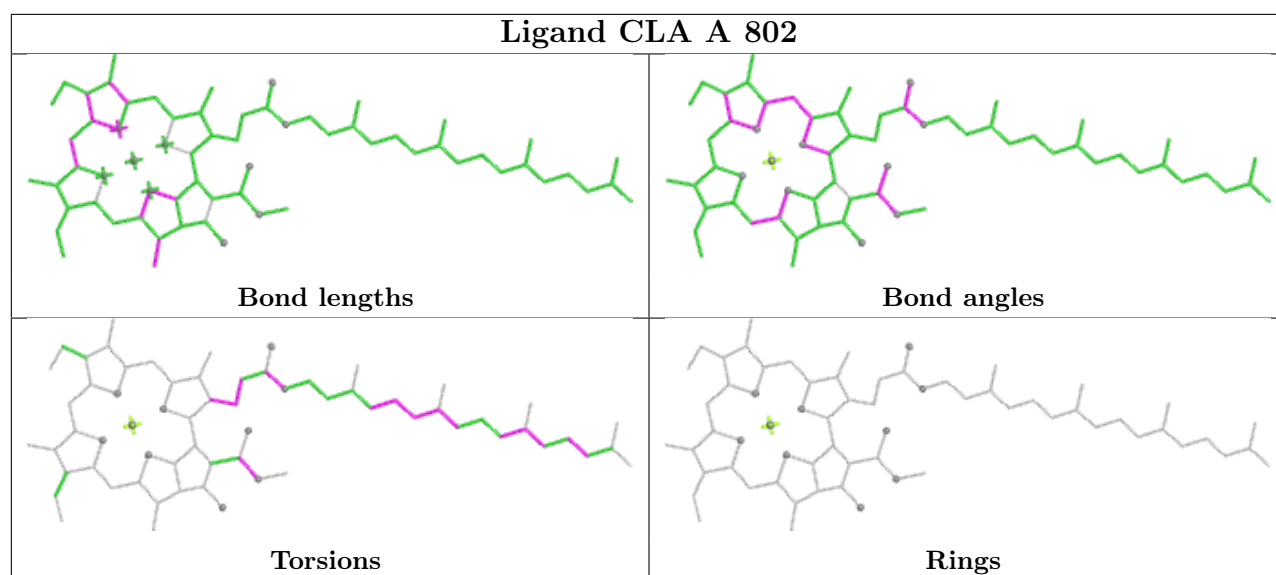
Bond angles

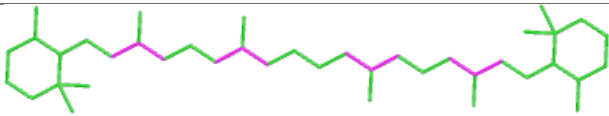
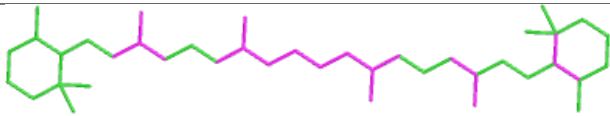
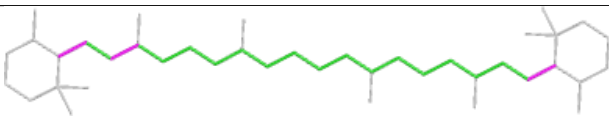
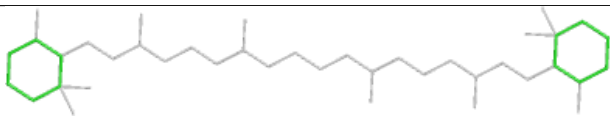


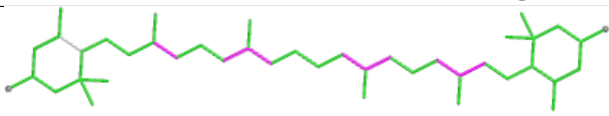
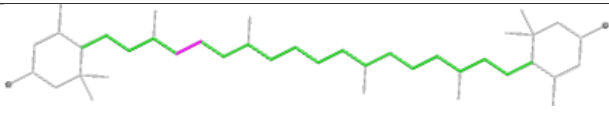
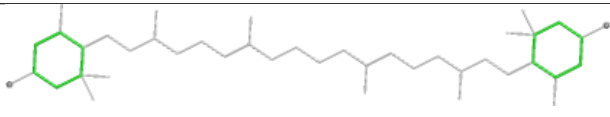
Torsions

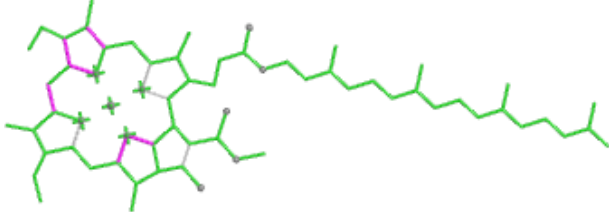
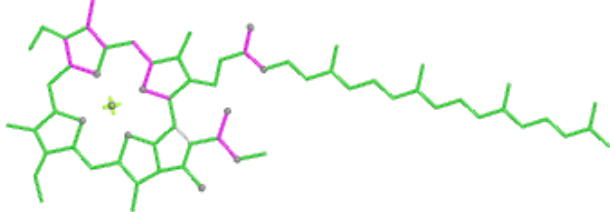
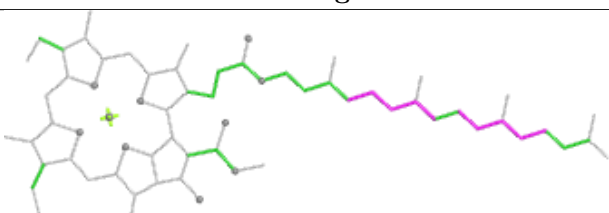
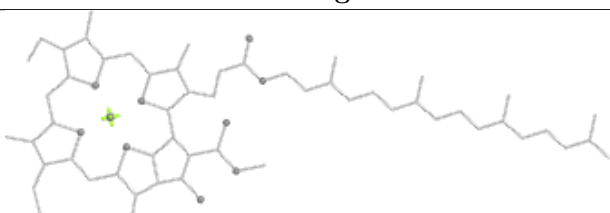


Rings

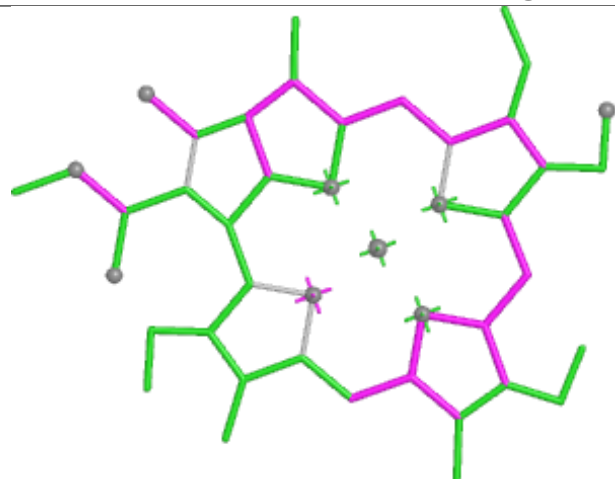


| Ligand BCR 4 618                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

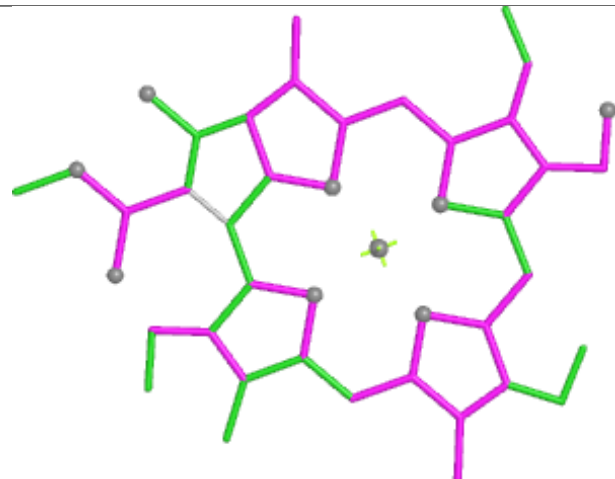
| Ligand LUT 1 616                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

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

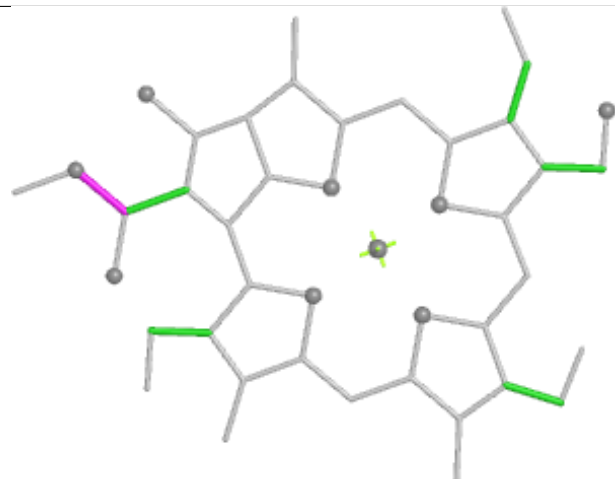
## Ligand CHL 2 615



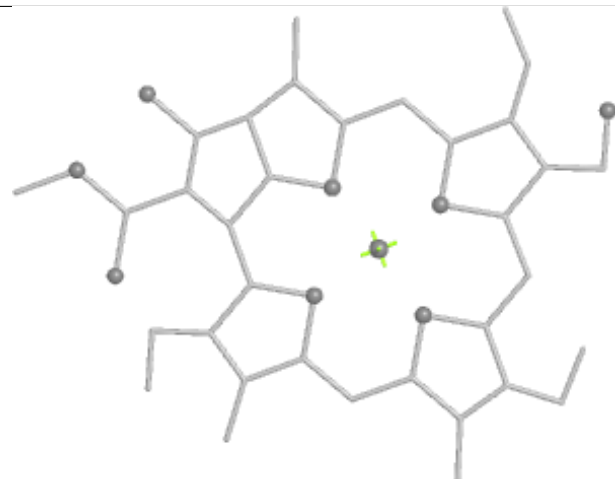
Bond lengths



Bond angles

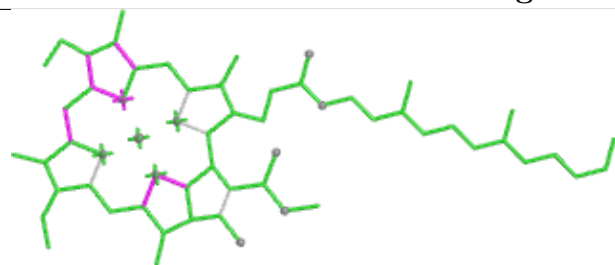


Torsions

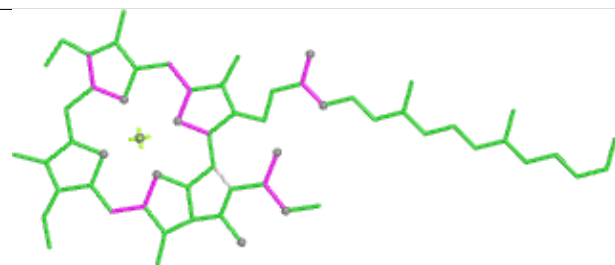


Rings

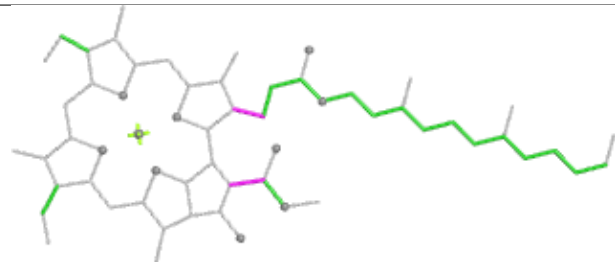
## Ligand CLA A 827



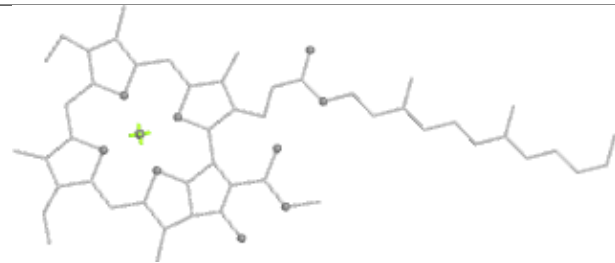
Bond lengths



Bond angles

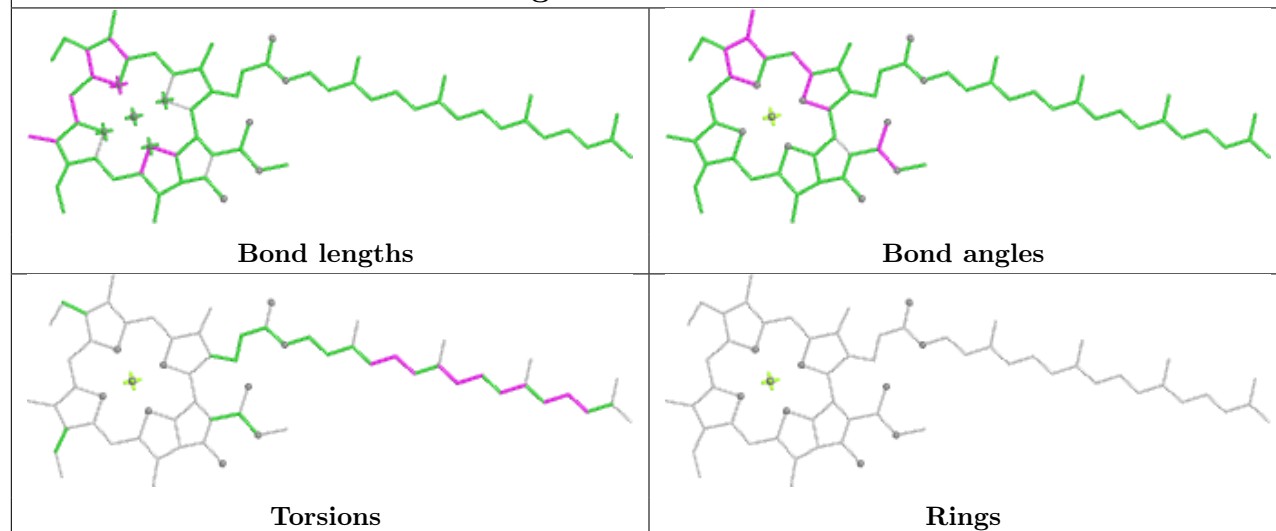


Torsions

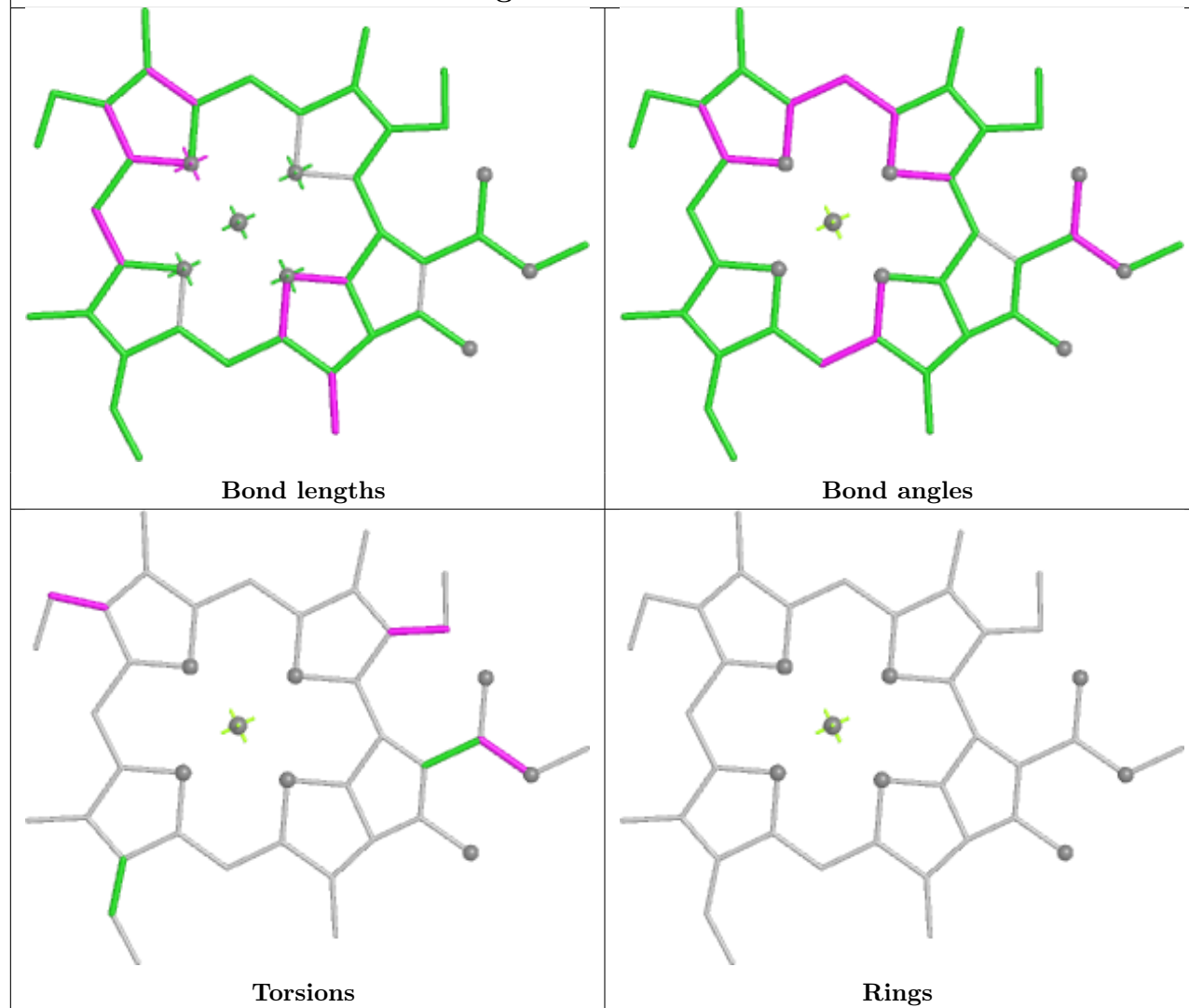


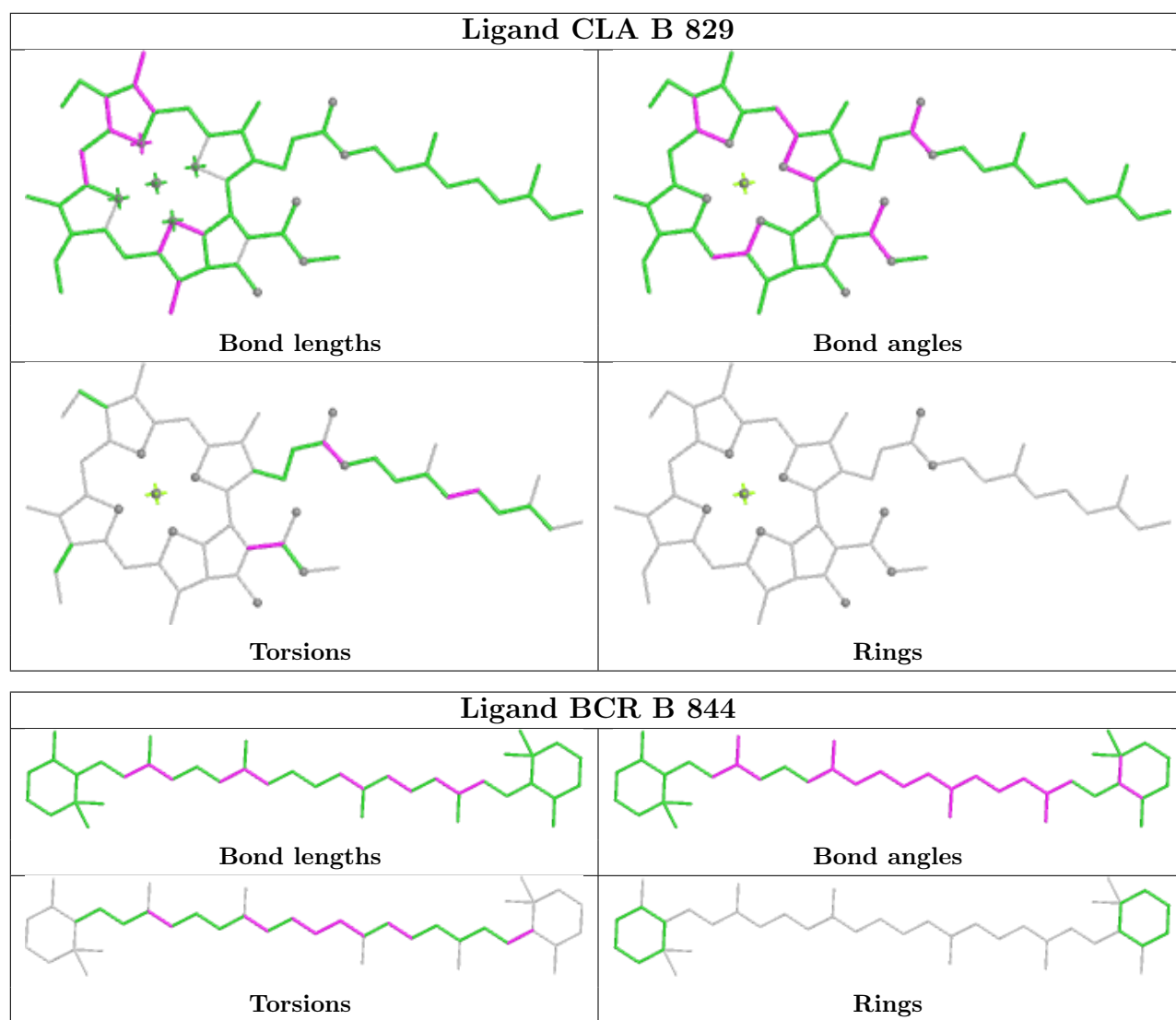
Rings

## Ligand CLA A 828

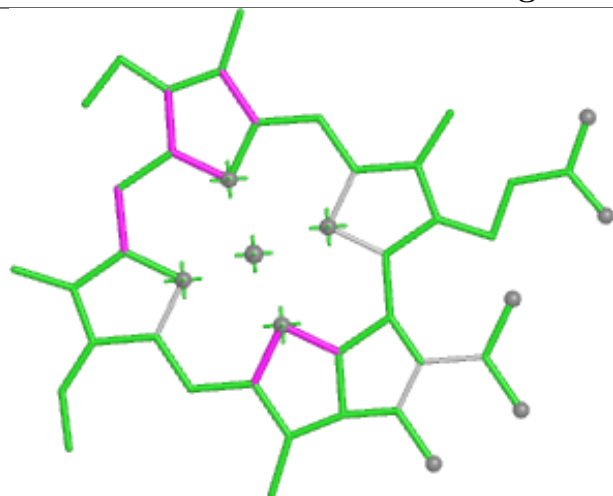


## Ligand CLA B 835

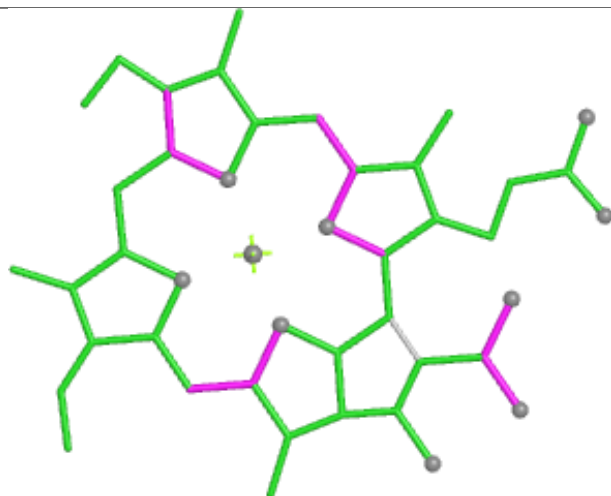




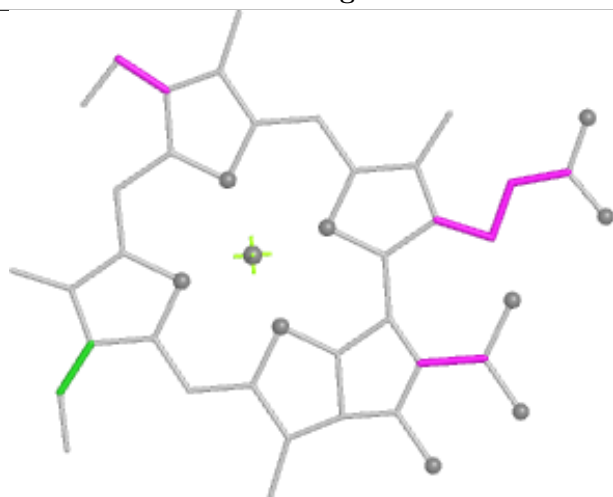
## Ligand CLA 1 607



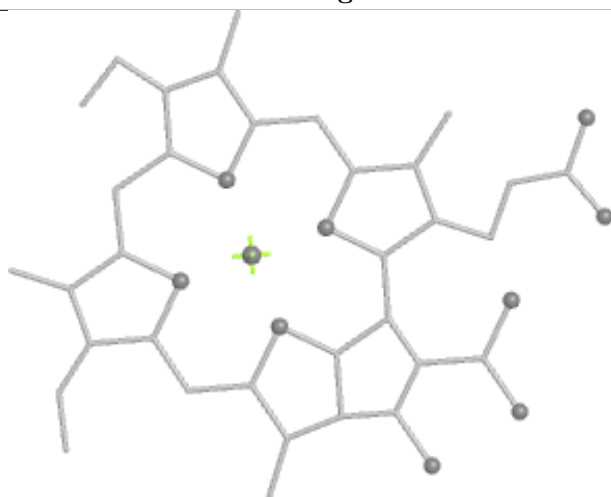
Bond lengths



Bond angles

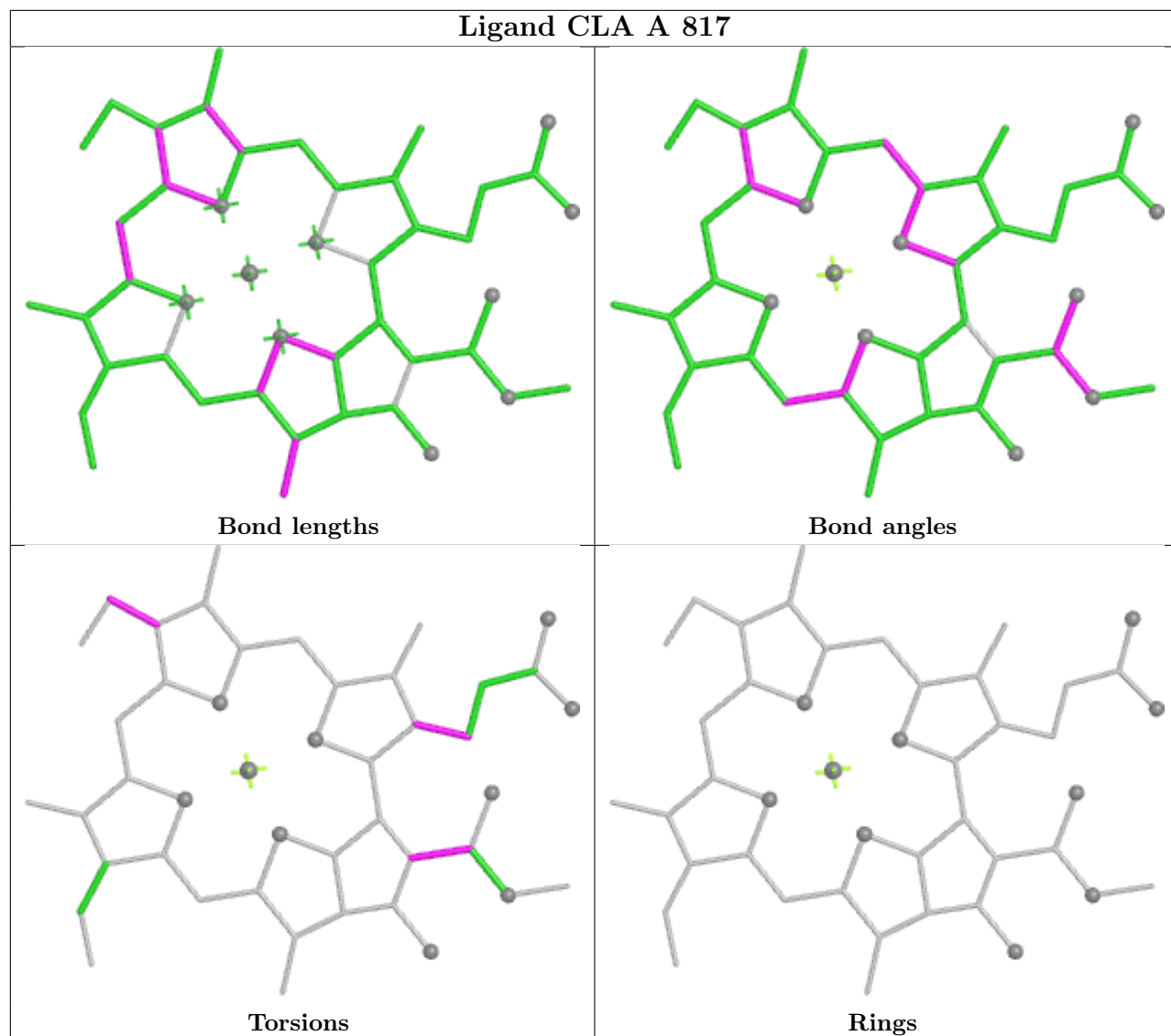


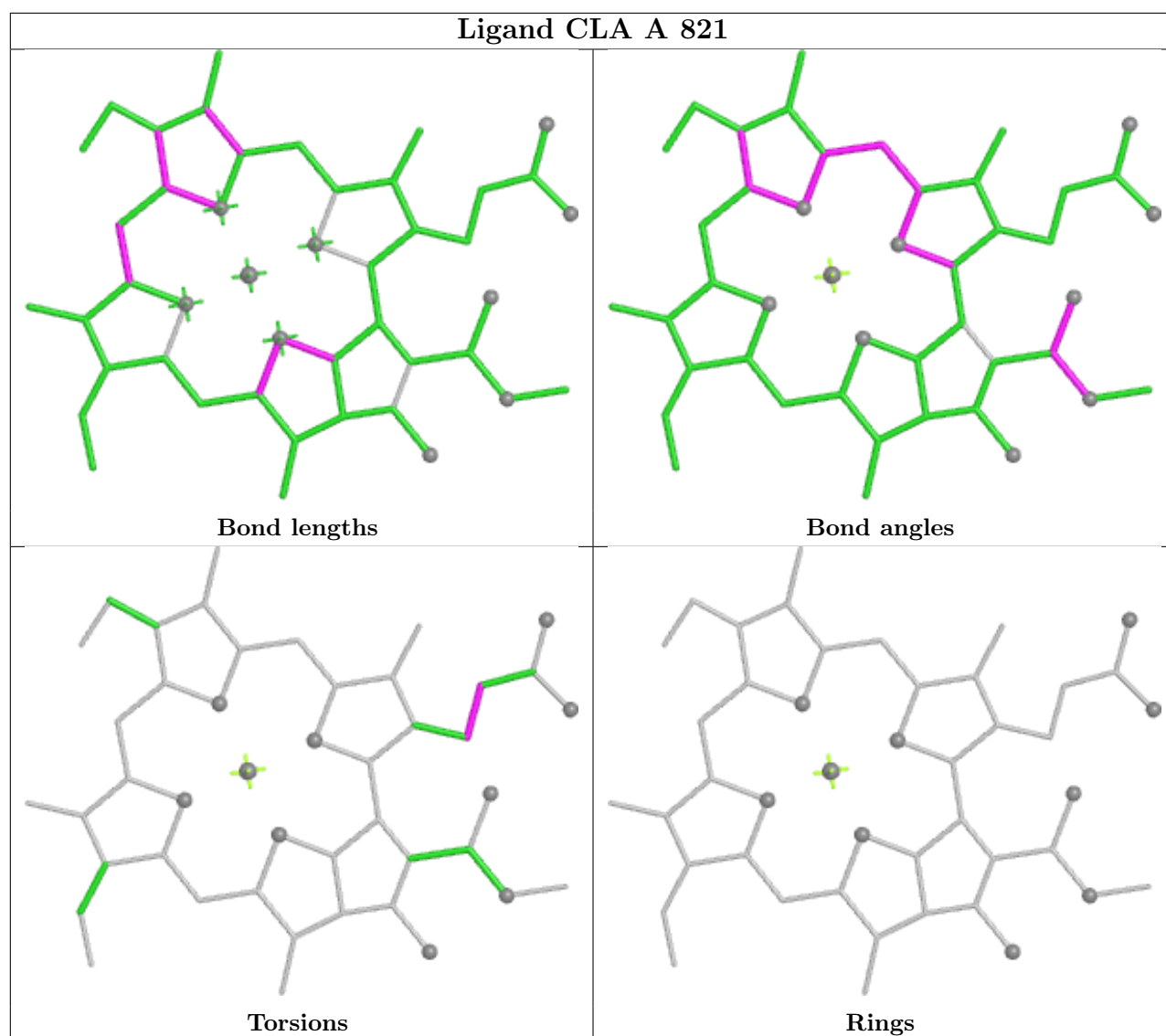
Torsions



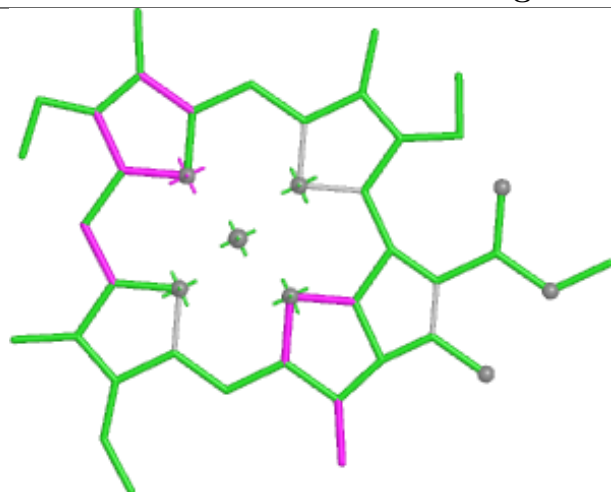
Rings

## Ligand CLA A 817

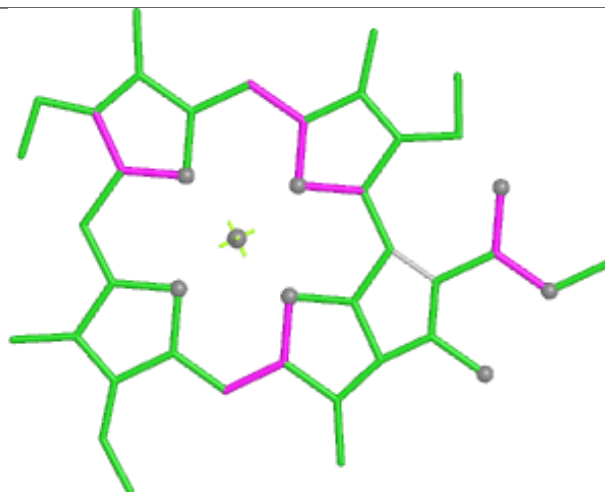




## Ligand CLA A 816



Bond lengths



Bond angles

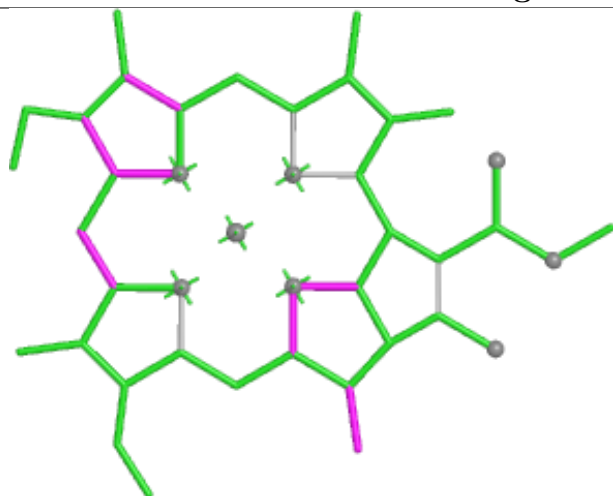


Torsions

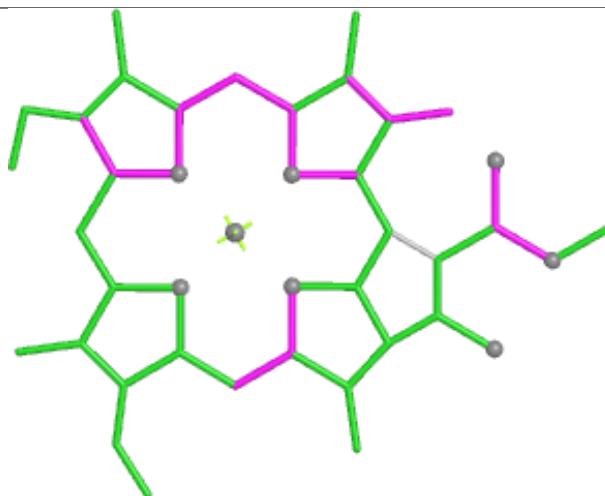


Rings

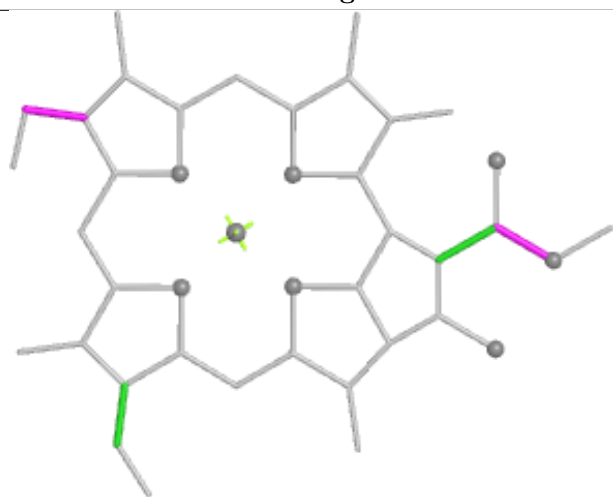
## Ligand CLA A 824



Bond lengths



Bond angles

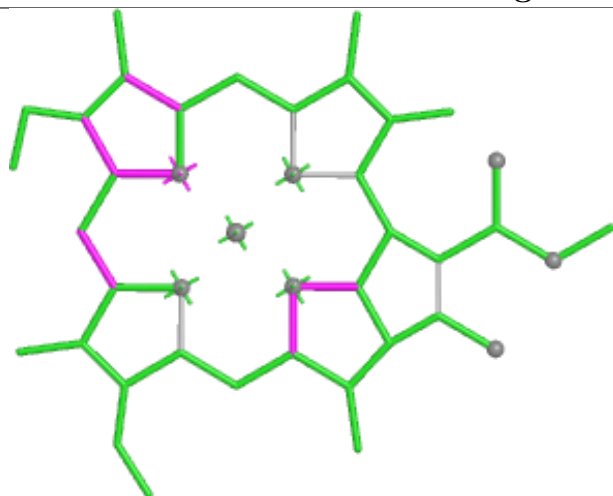


Torsions

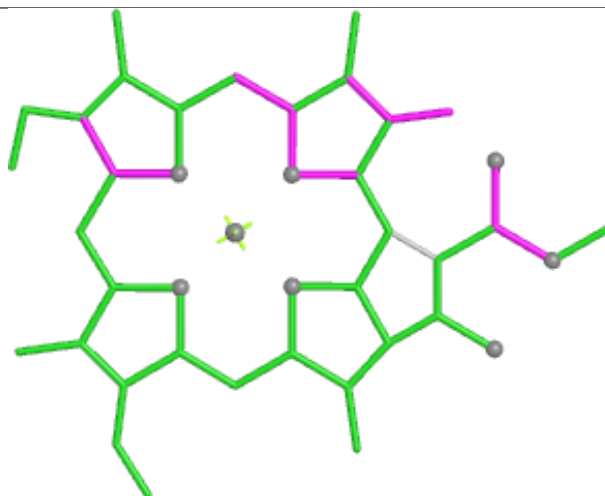


Rings

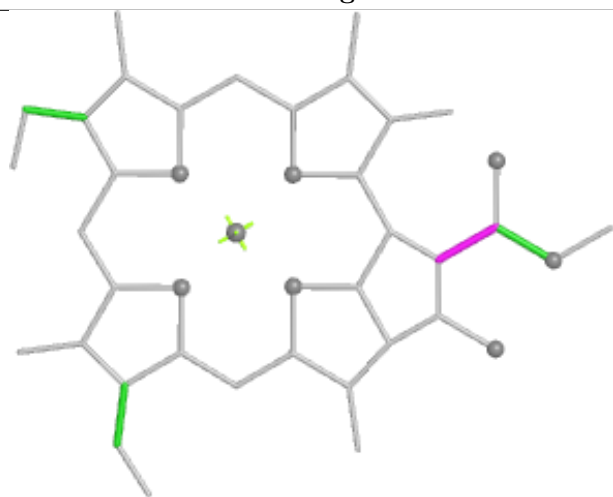
## Ligand CLA B 804



Bond lengths



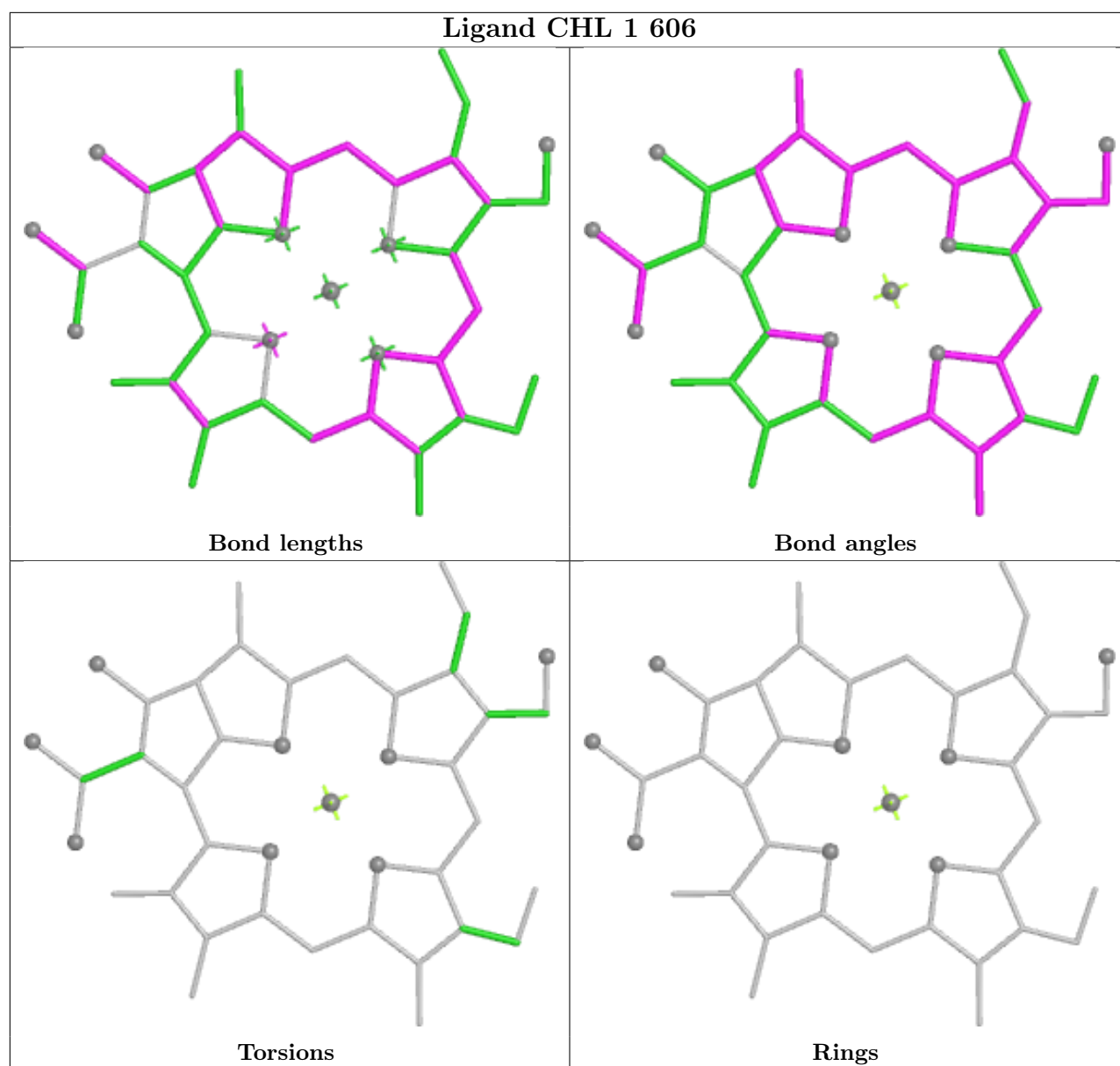
Bond angles



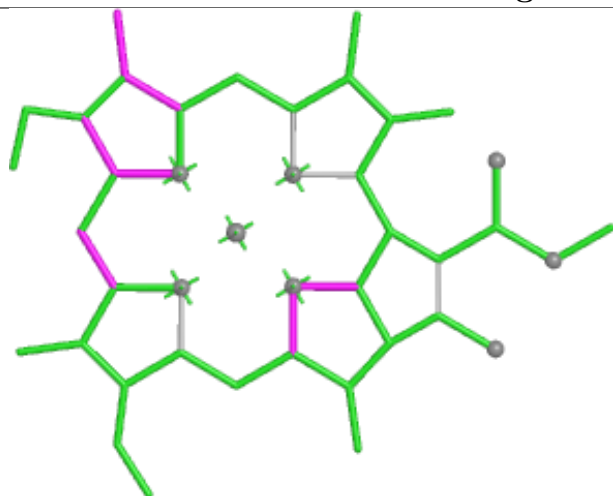
Torsions



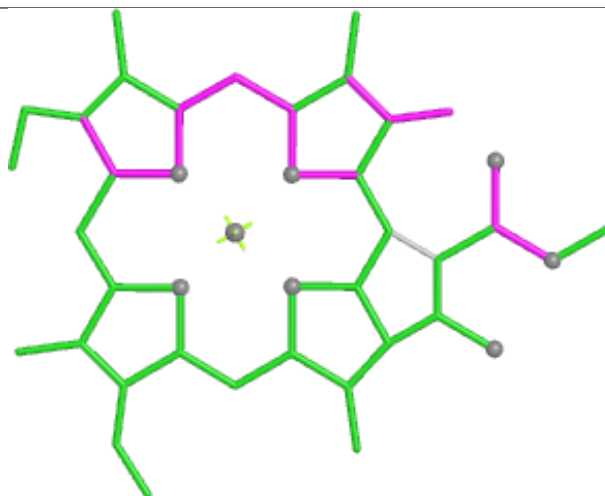
Rings



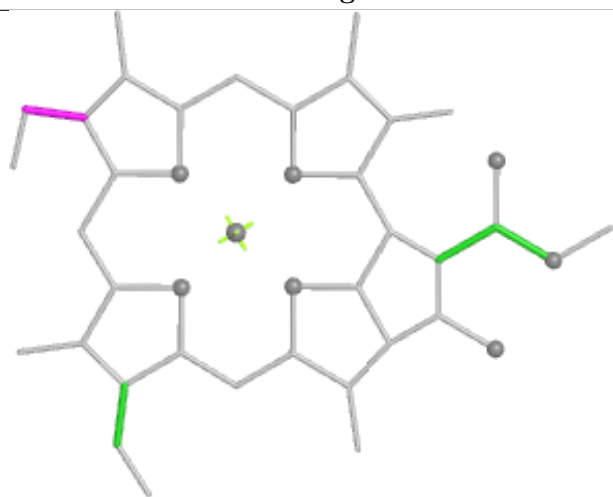
## Ligand CLA F 303



Bond lengths



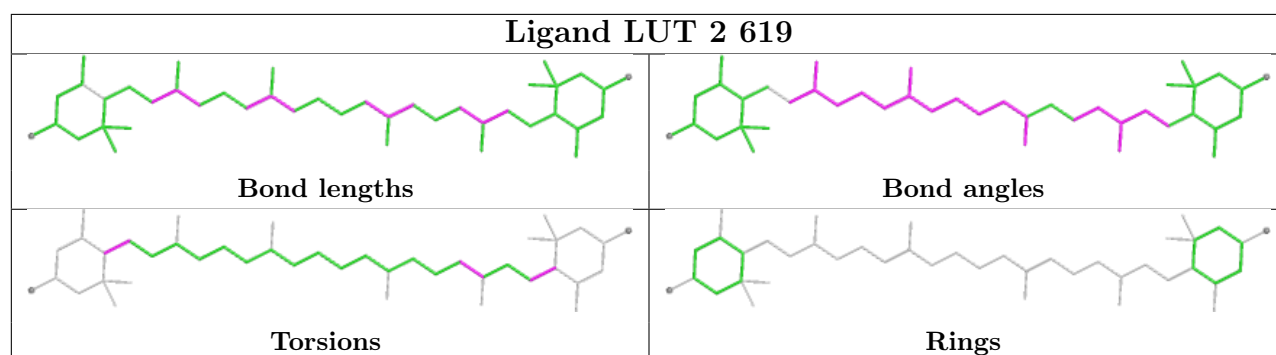
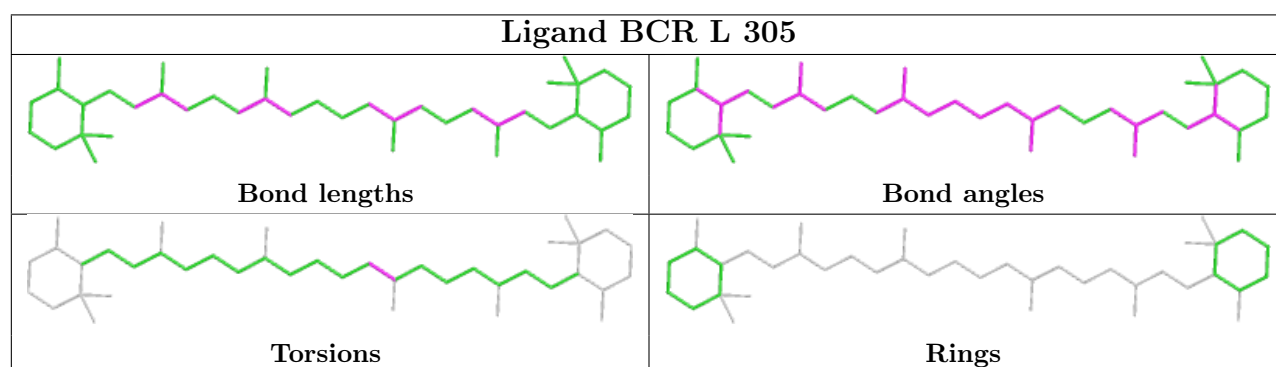
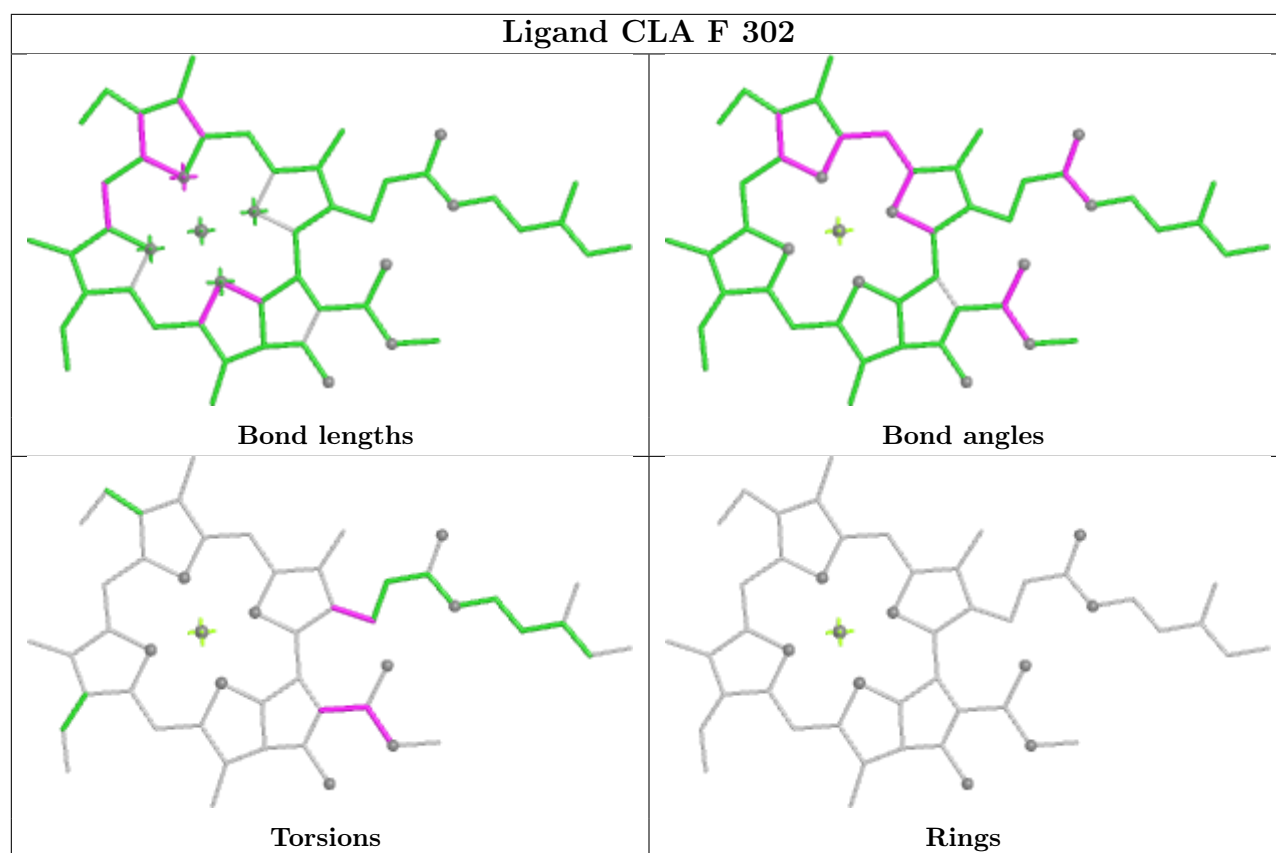
Bond angles

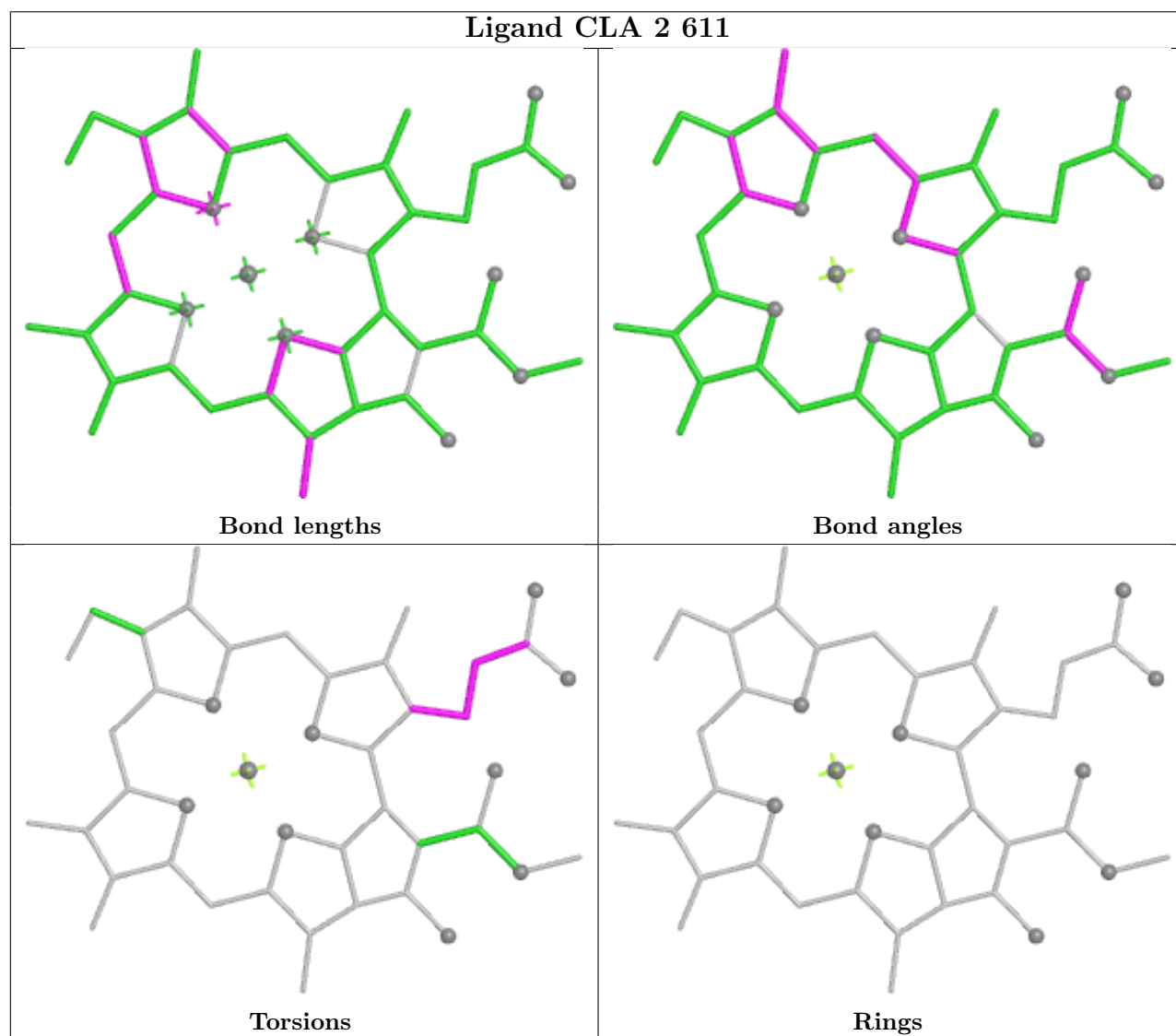
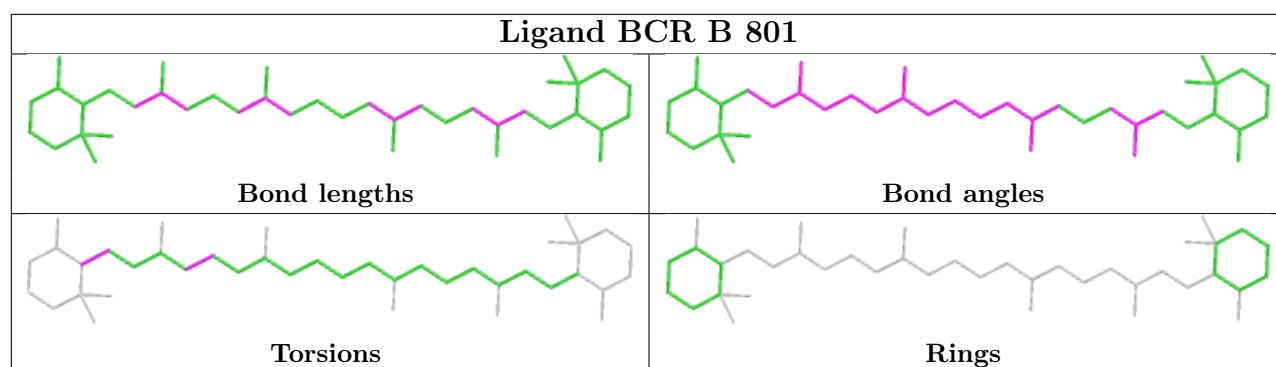


Torsions

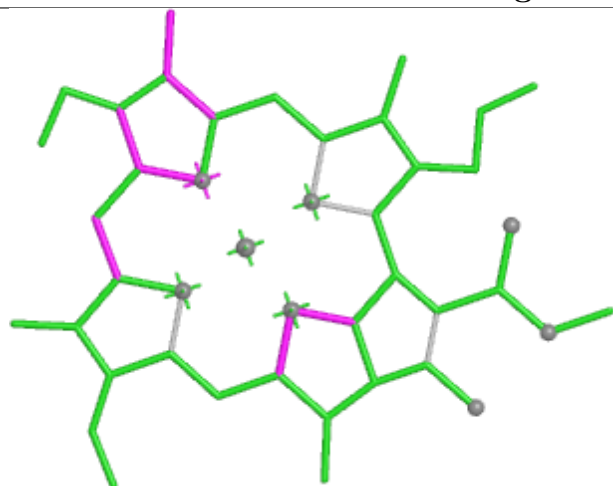


Rings

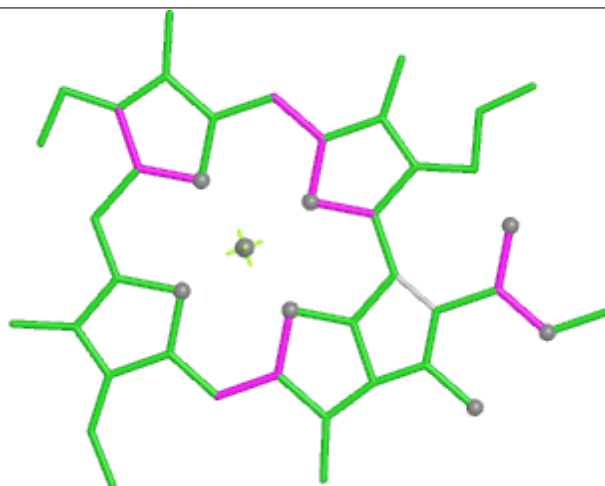




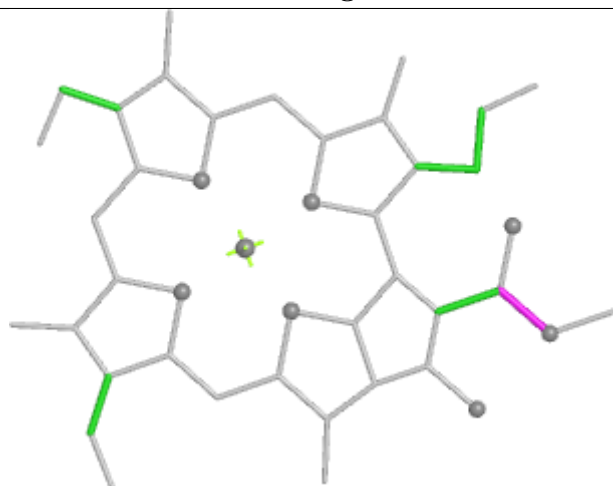
## Ligand CLA B 830



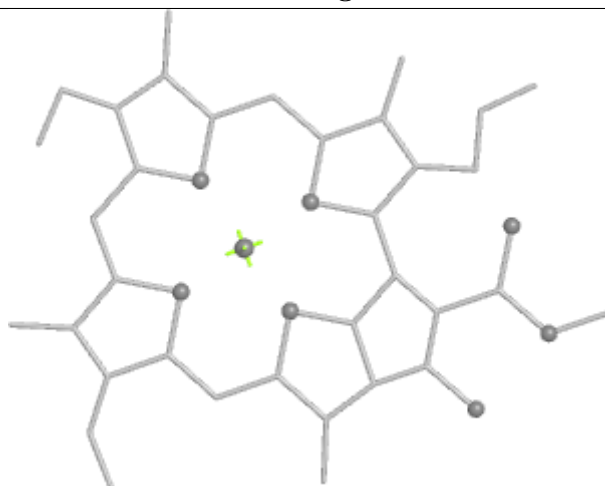
Bond lengths



Bond angles

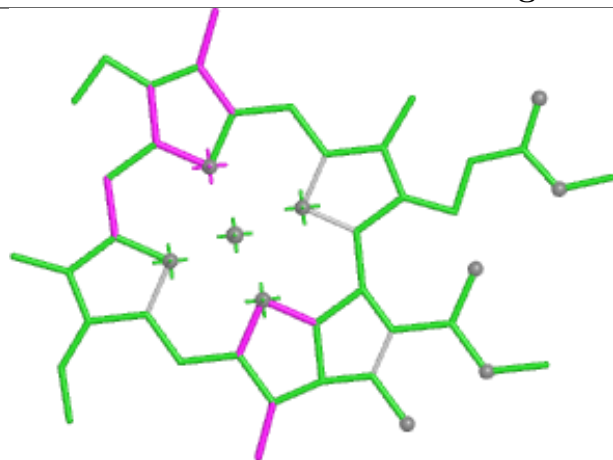


Torsions

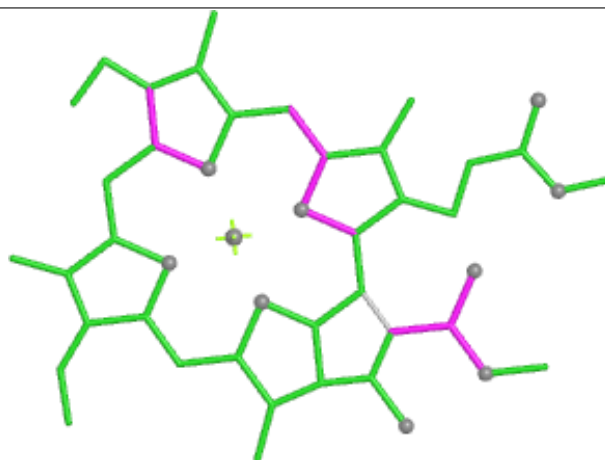


Rings

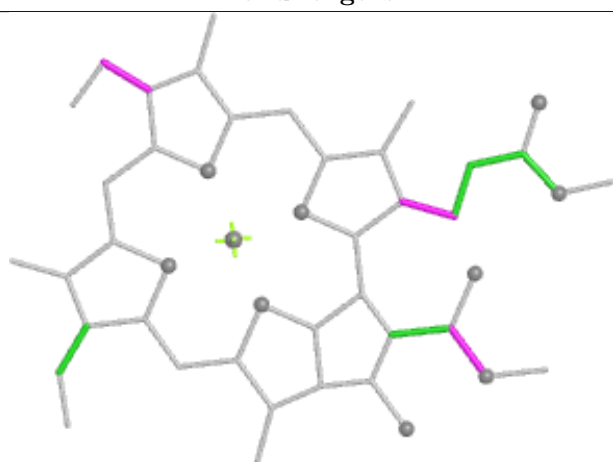
## Ligand CLA 1 612



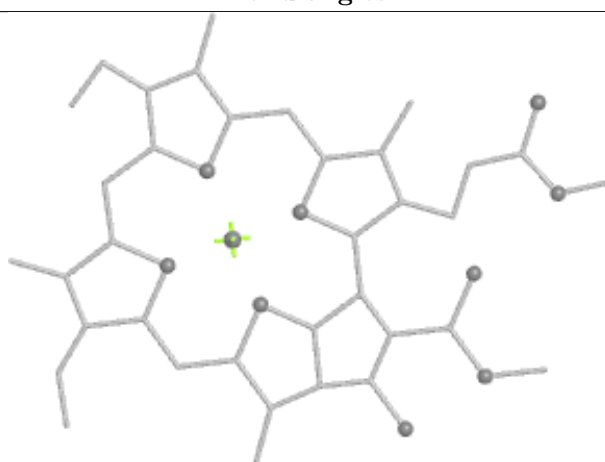
Bond lengths



Bond angles

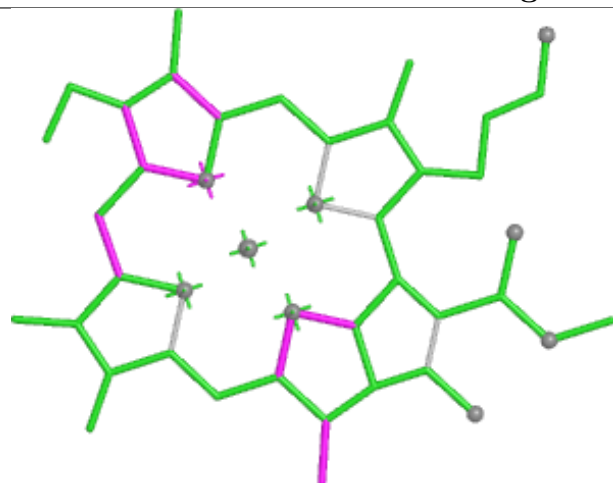


Torsions

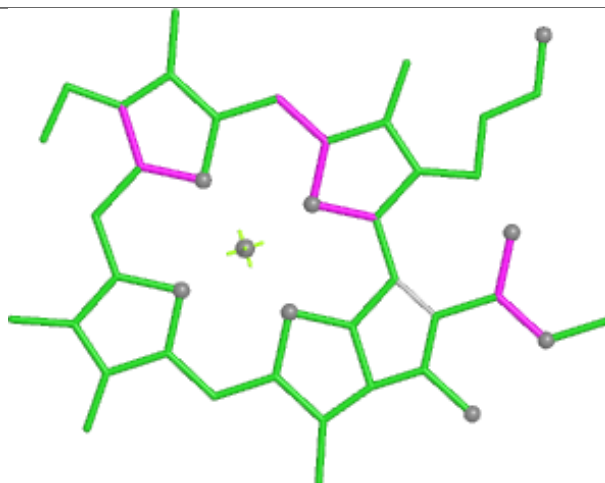


Rings

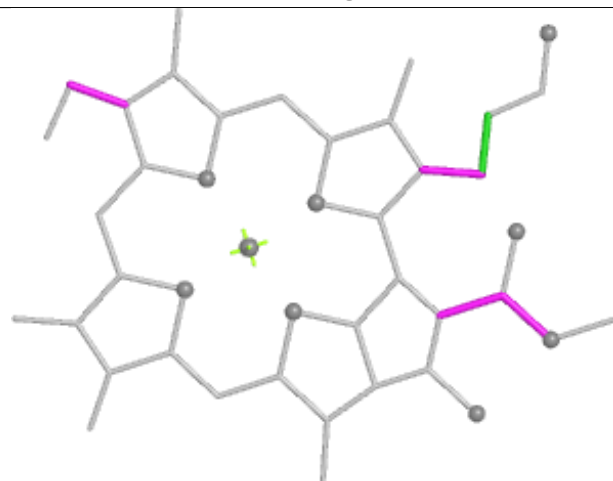
## Ligand CLA 2 604



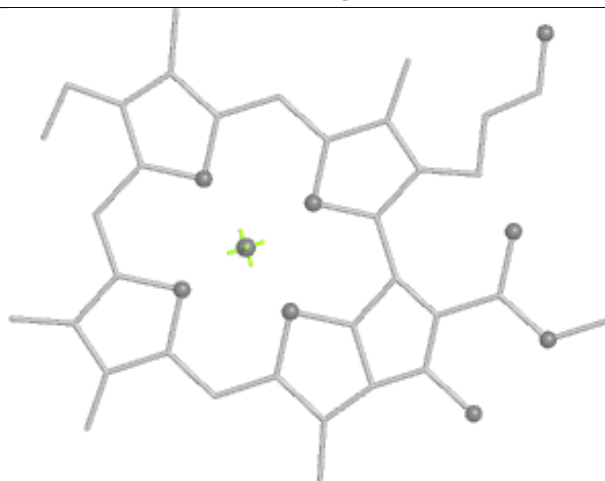
Bond lengths



Bond angles

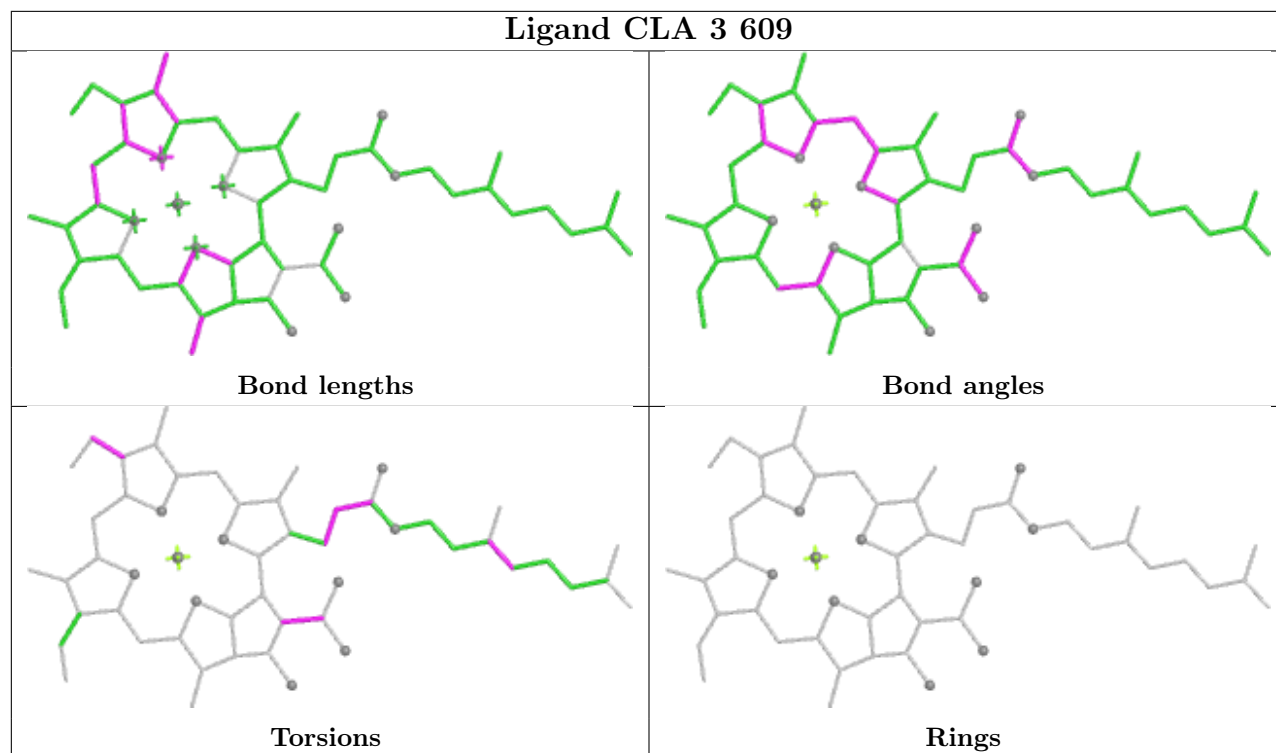


Torsions

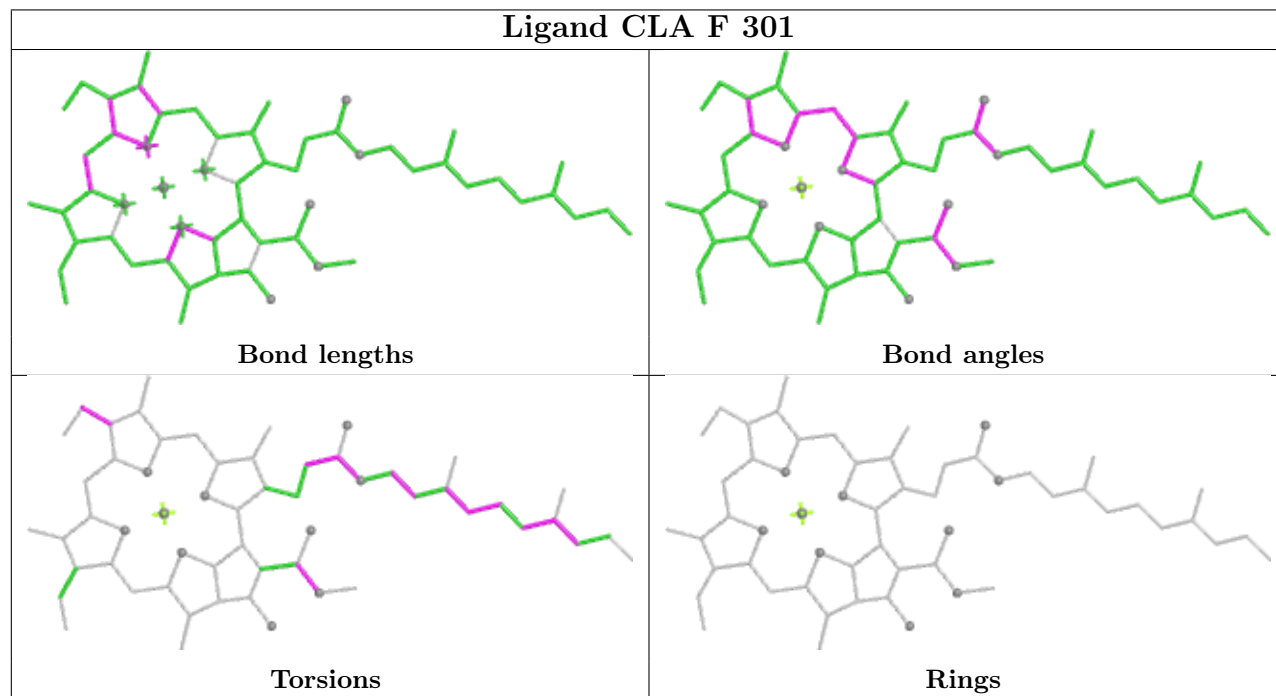


Rings

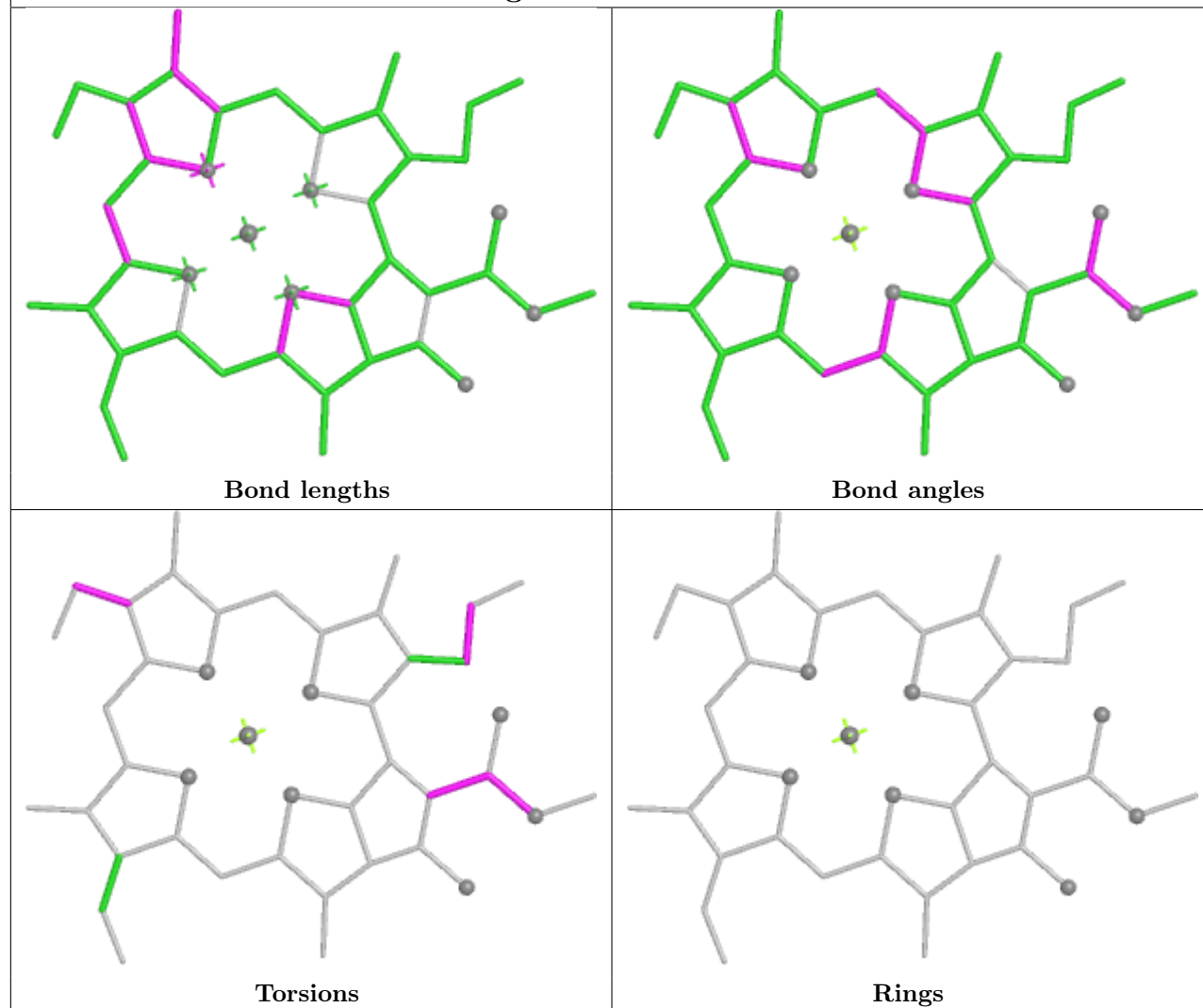
## Ligand CLA 3 609



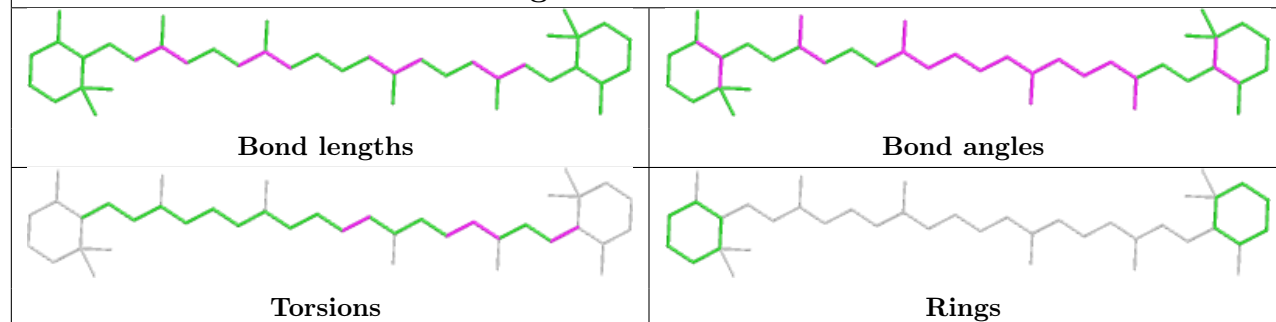
## Ligand CLA F 301

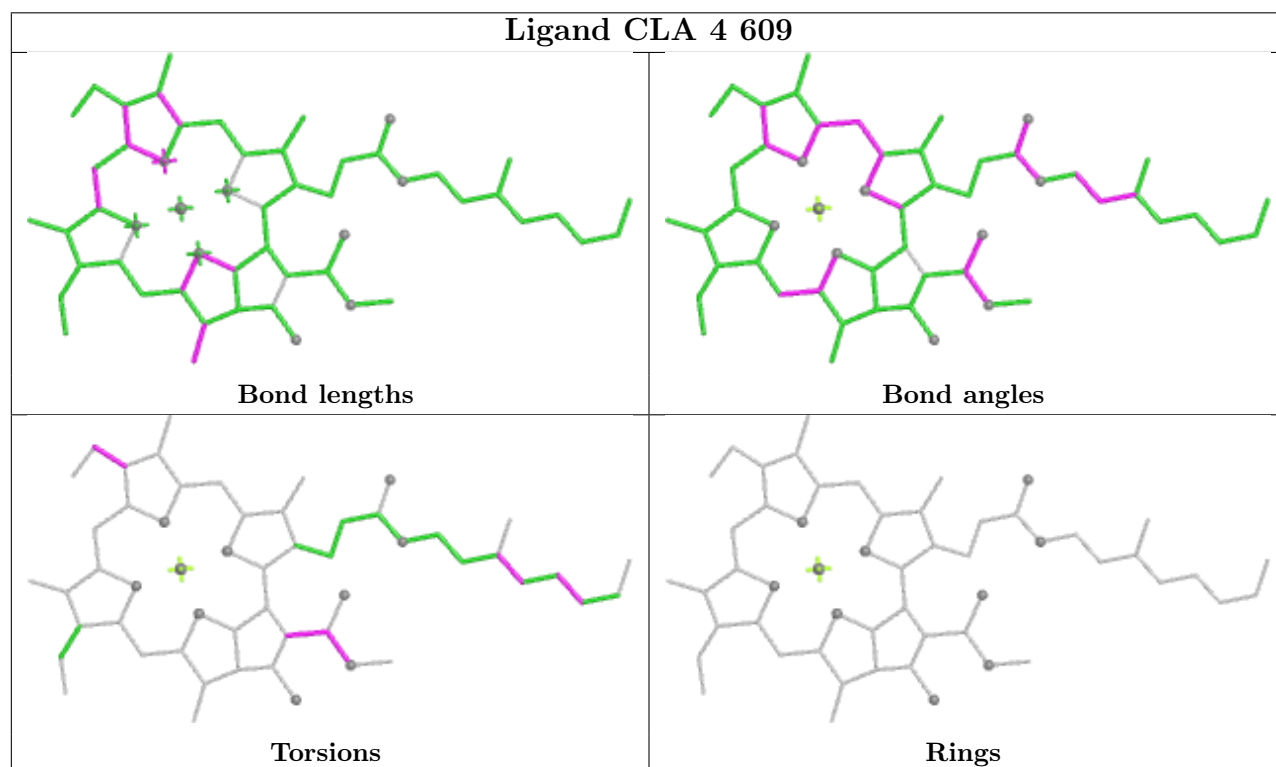
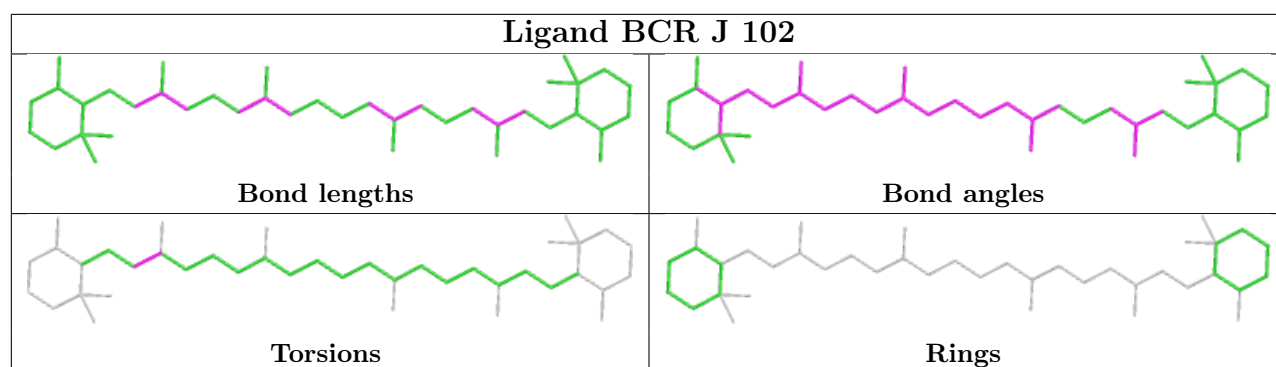


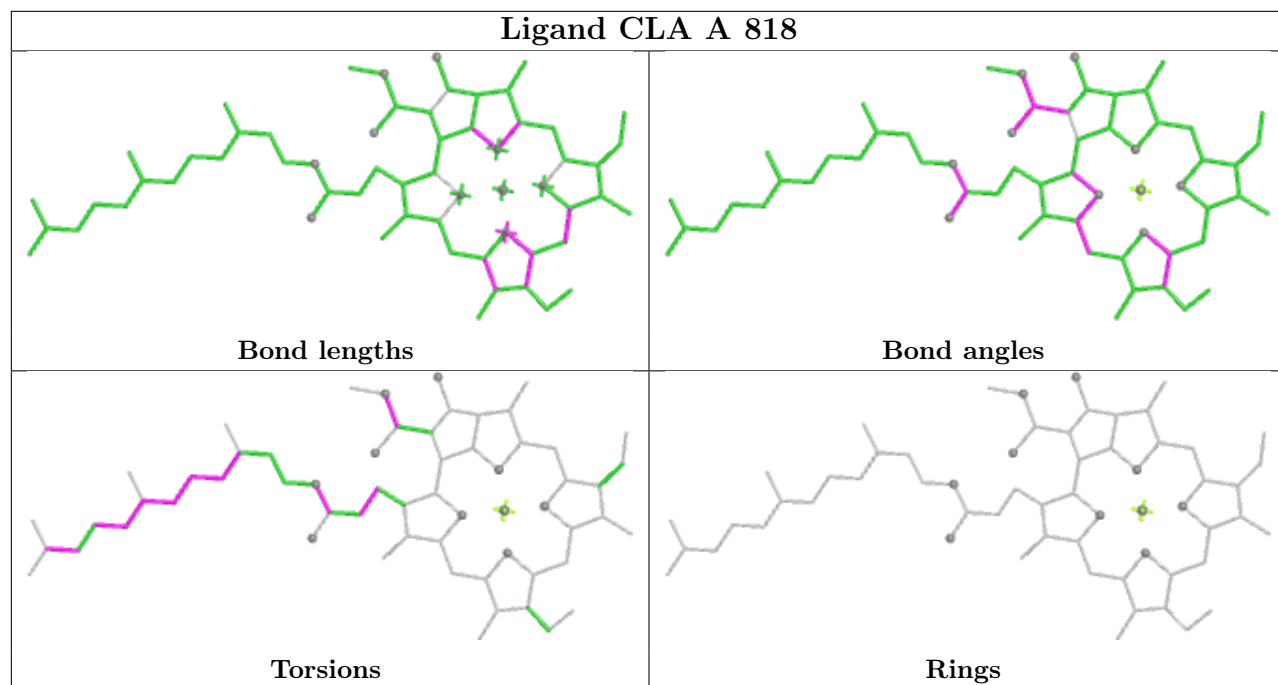
## Ligand CLA 2 613



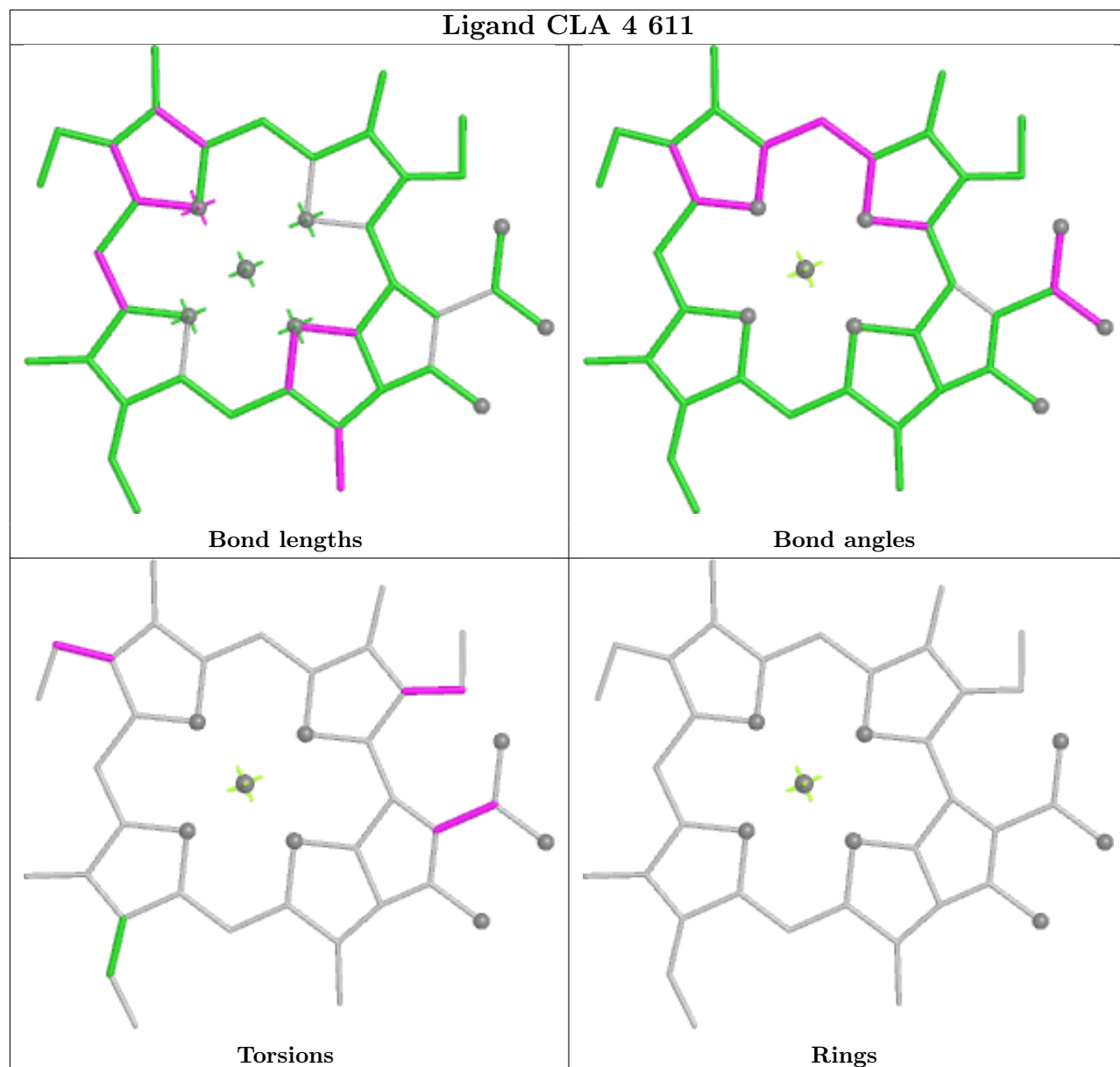
## Ligand BCR A 849

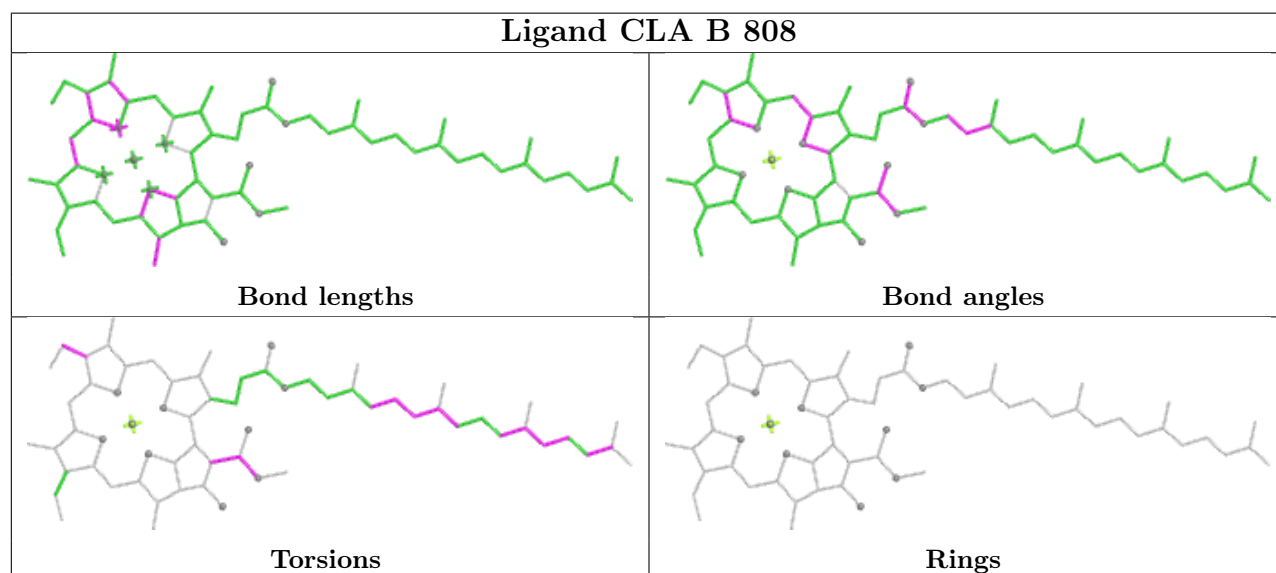
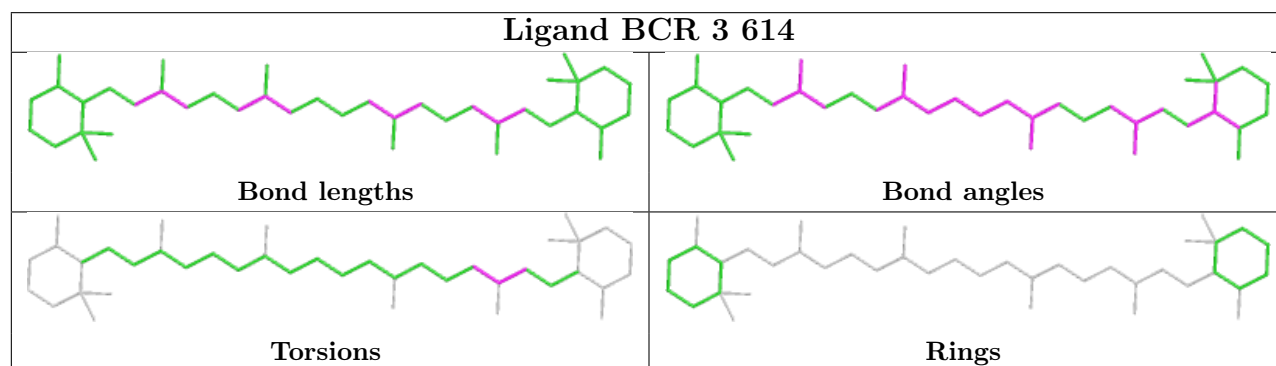
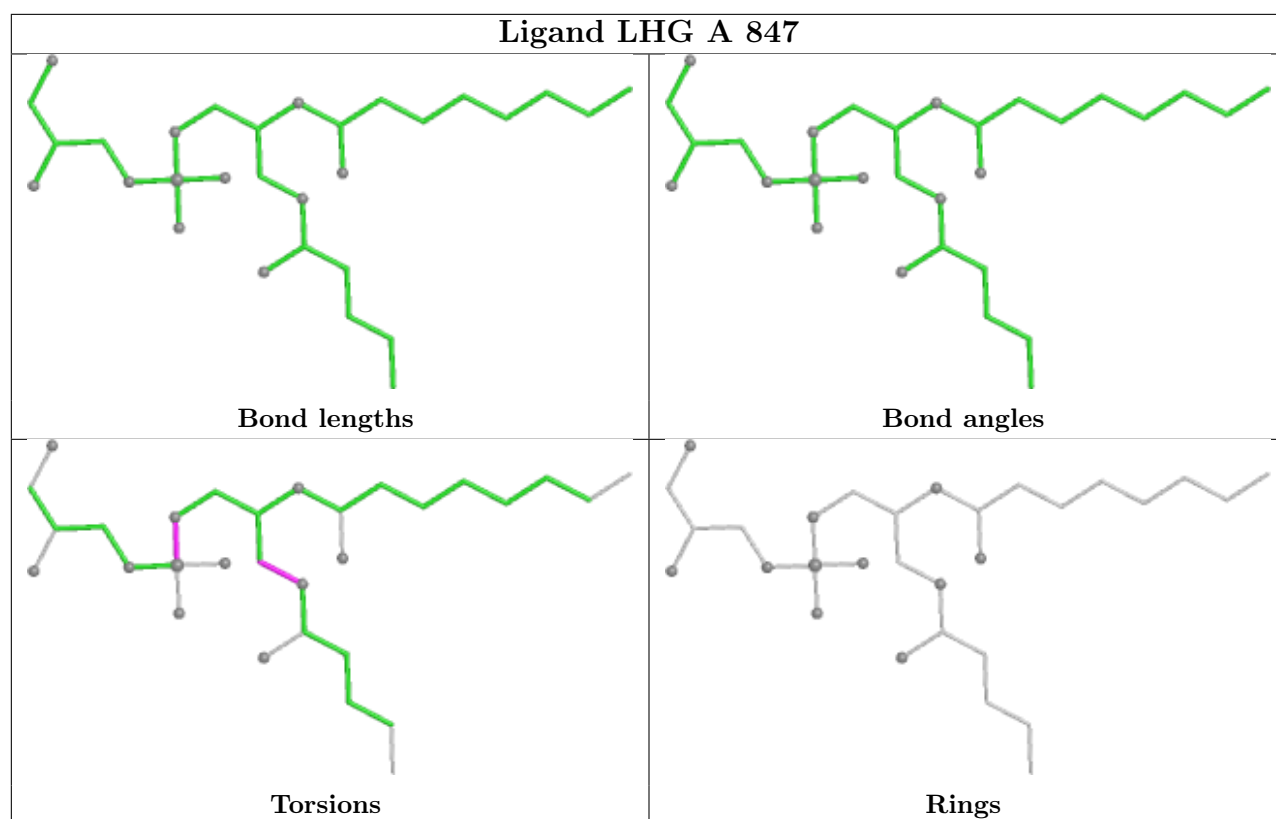




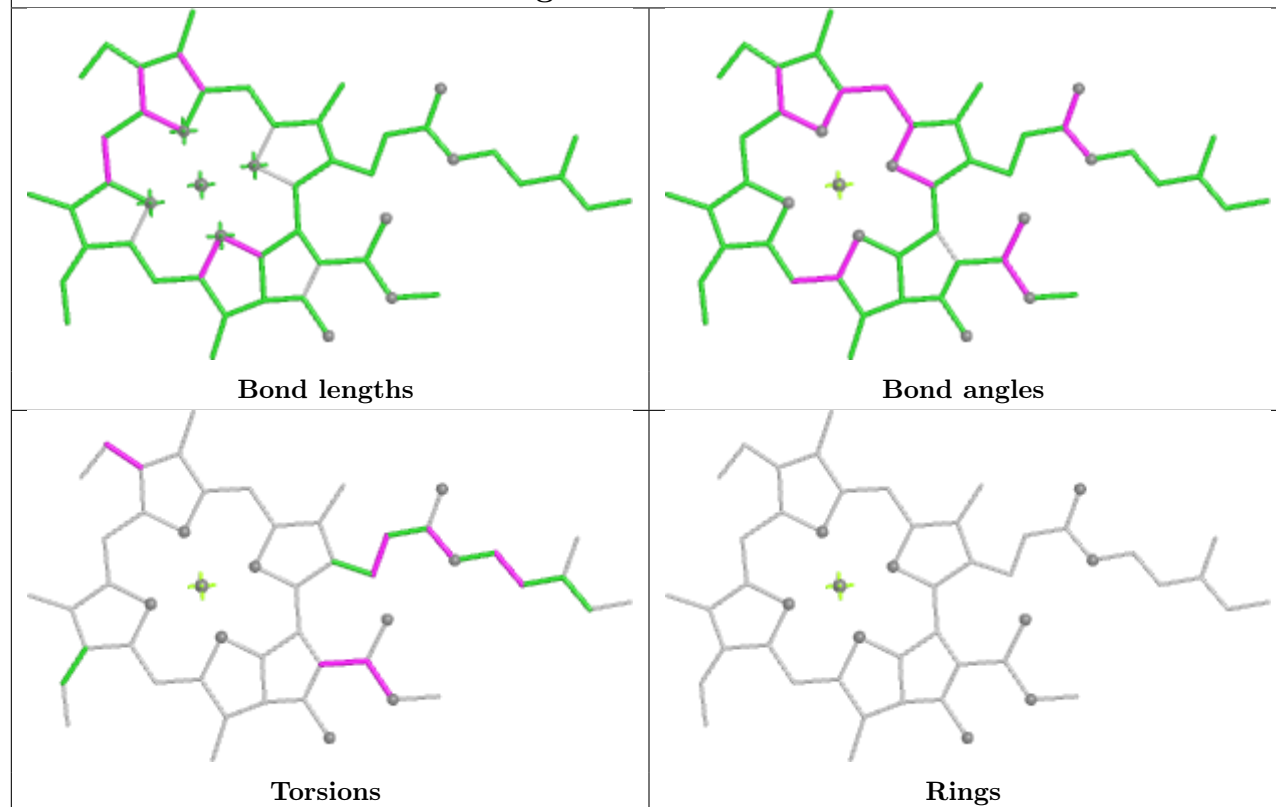


## Ligand CLA 4 611

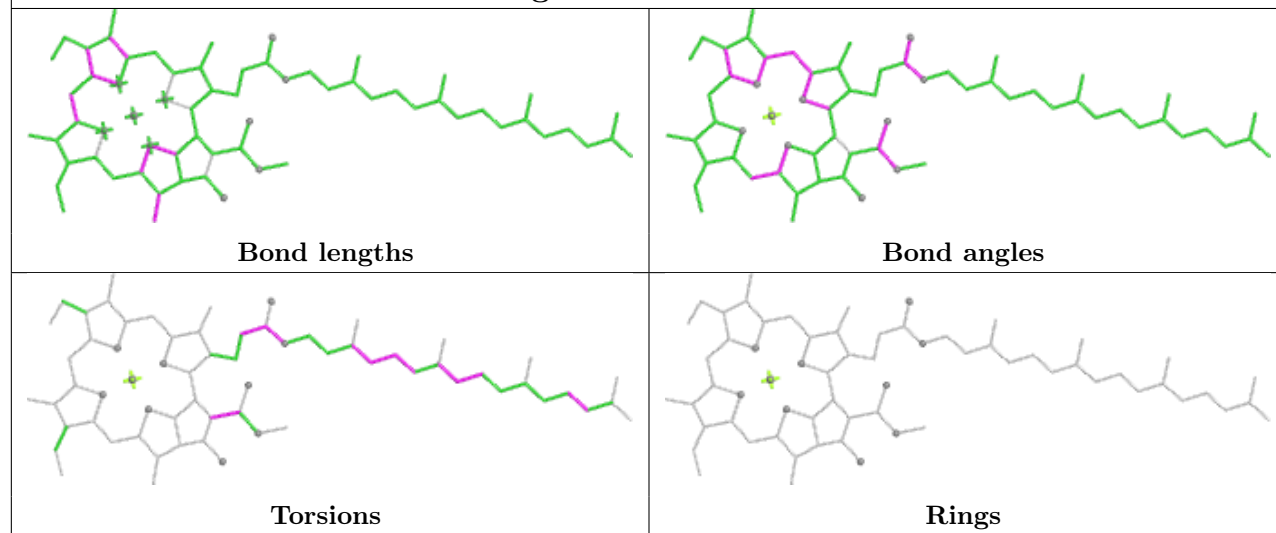


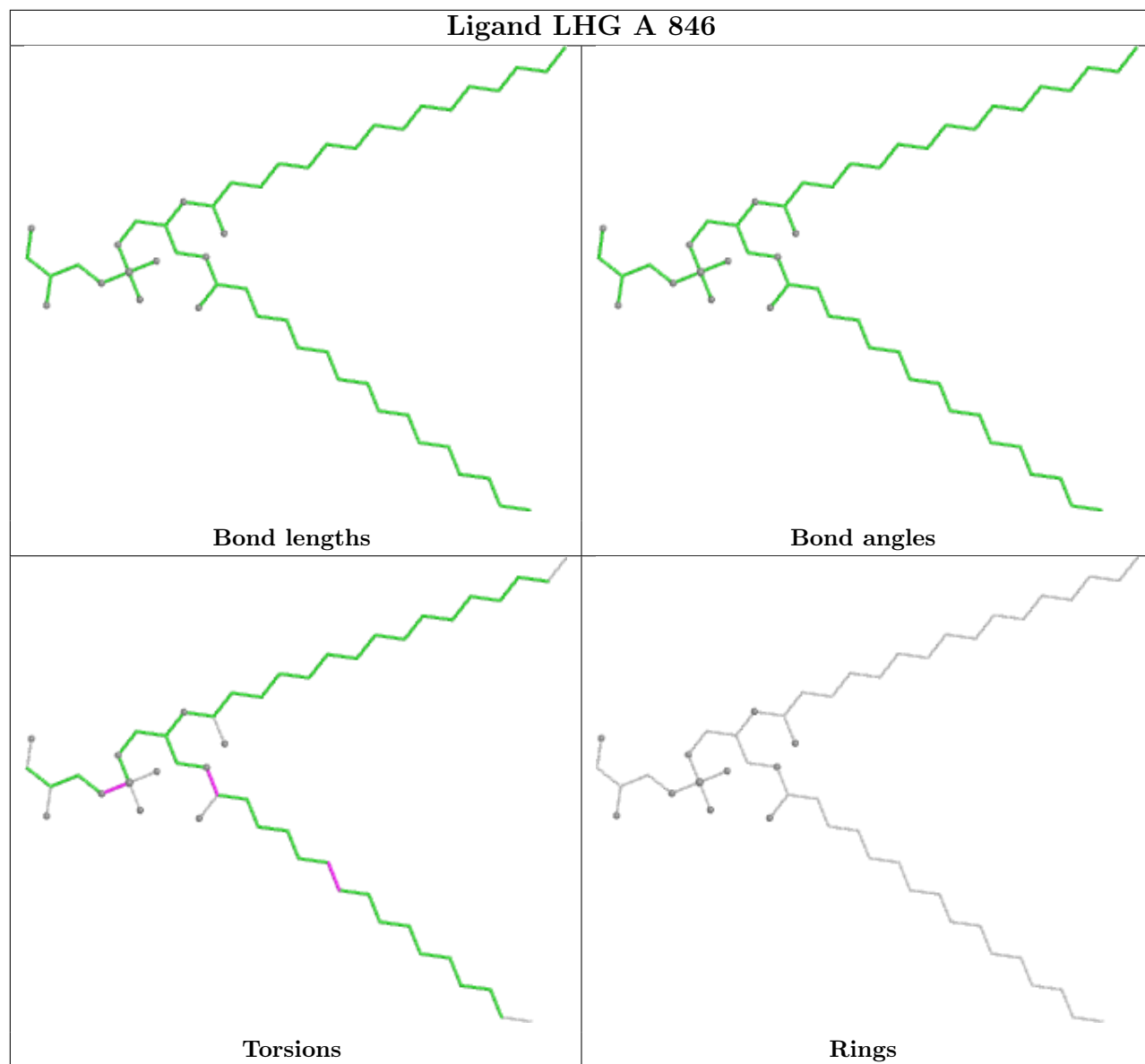


## Ligand CLA J 101

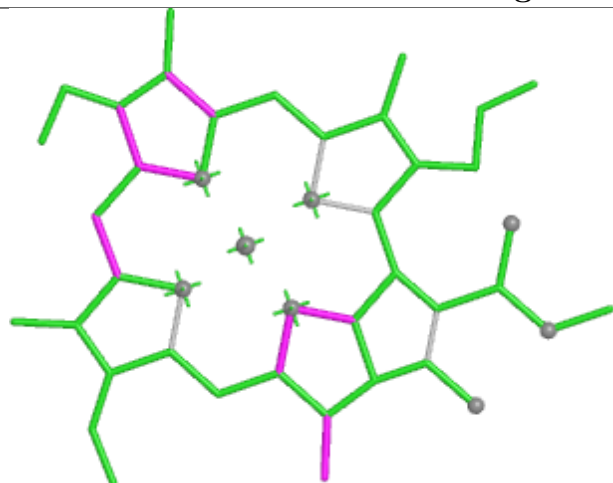


## Ligand CLA A 807

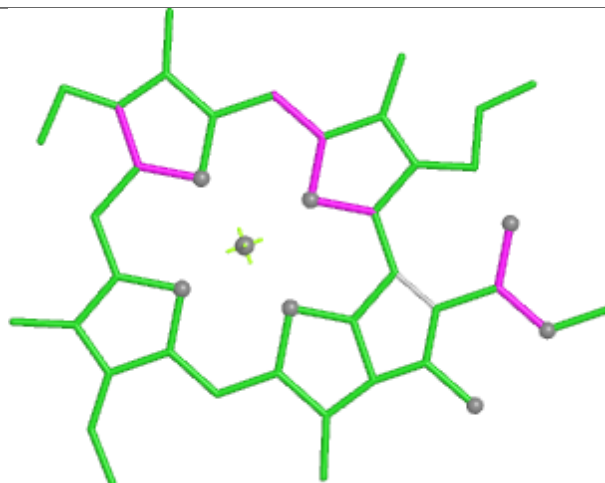




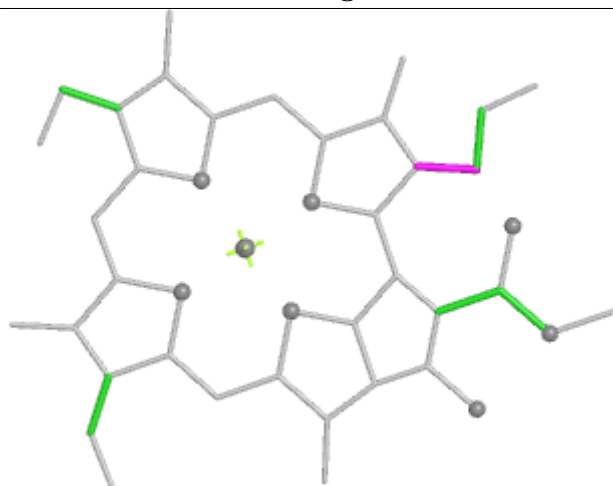
## Ligand CLA B 815



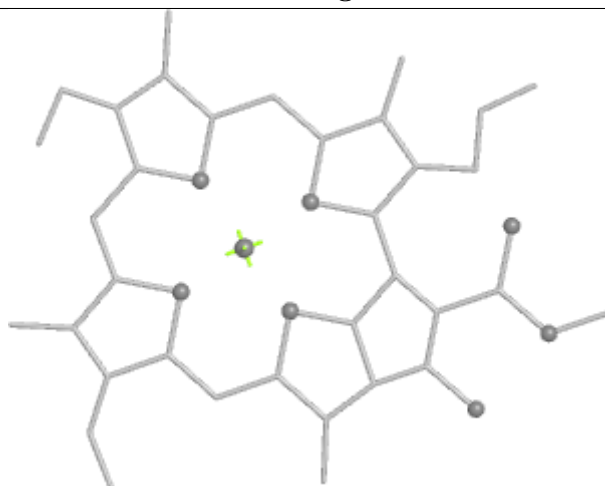
Bond lengths



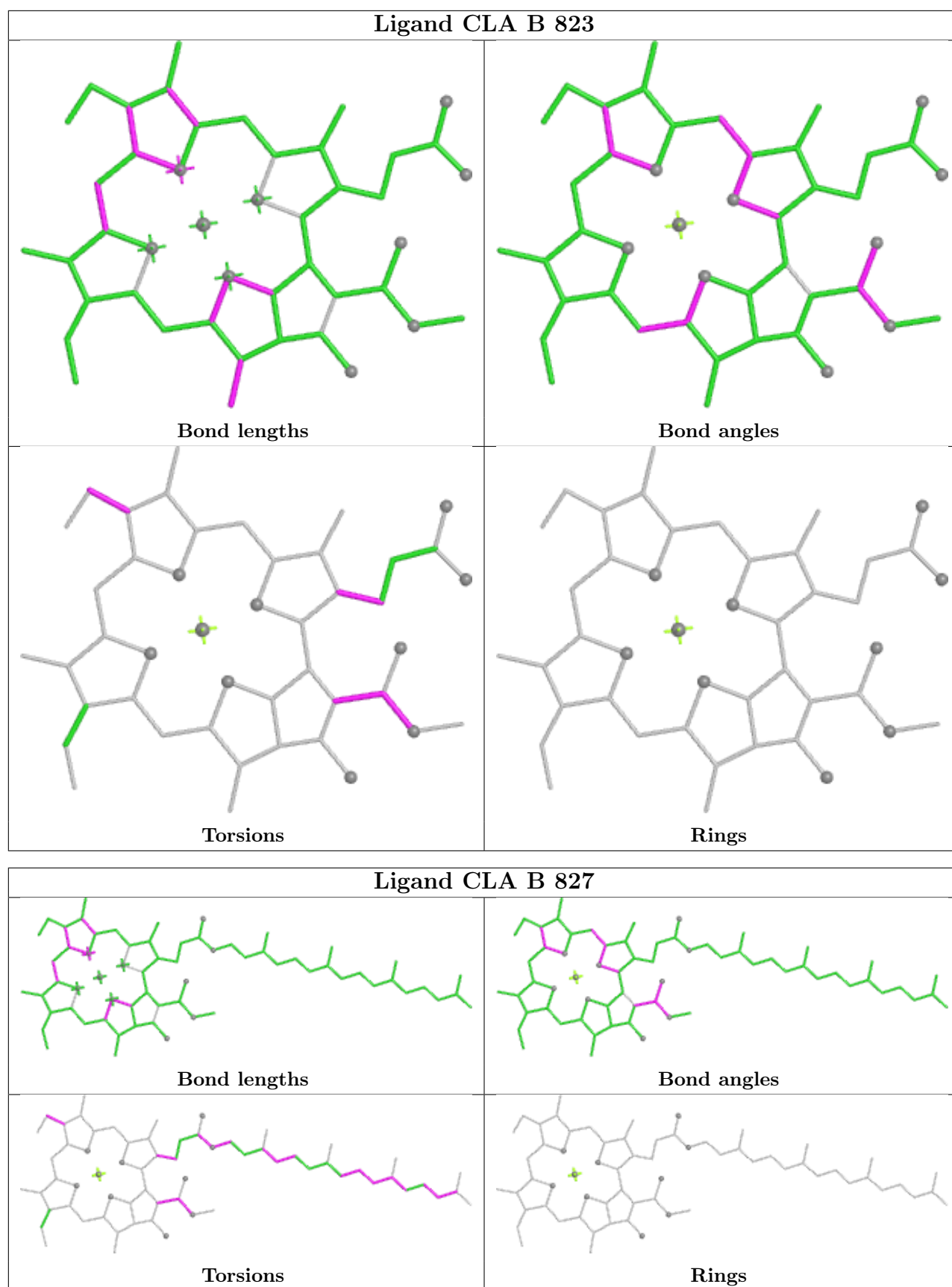
Bond angles

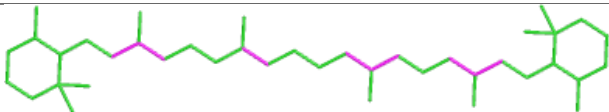
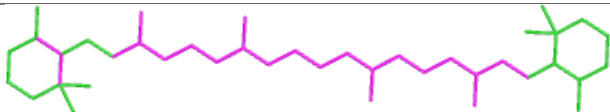
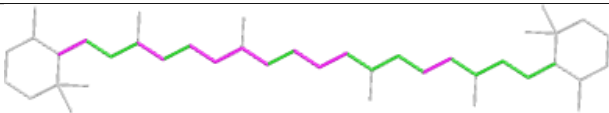
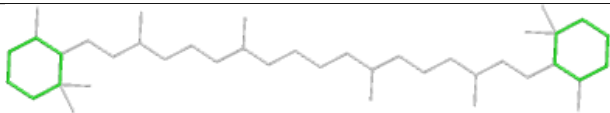
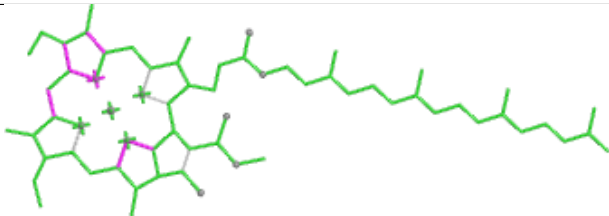
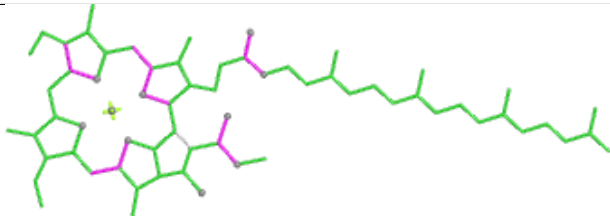
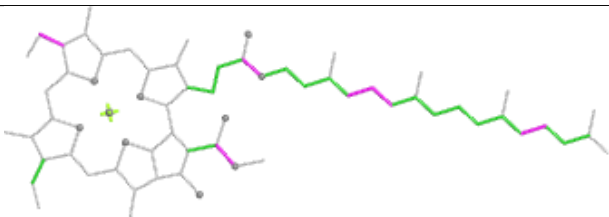
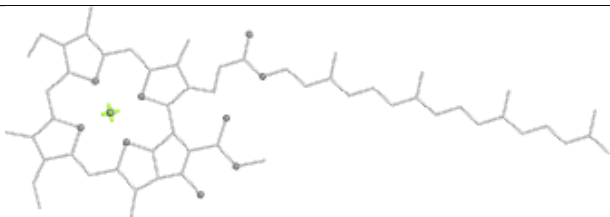


Torsions

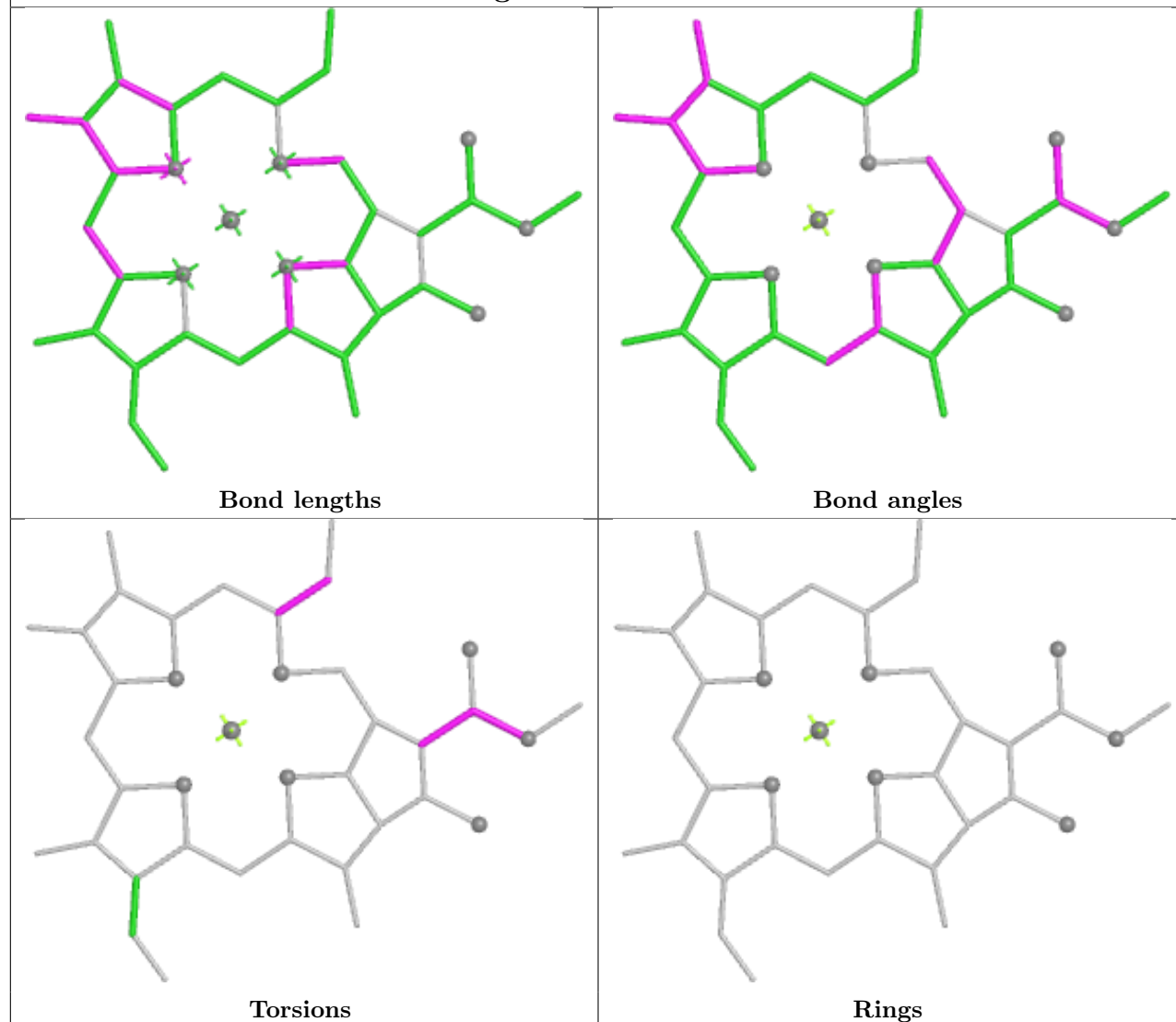


Rings

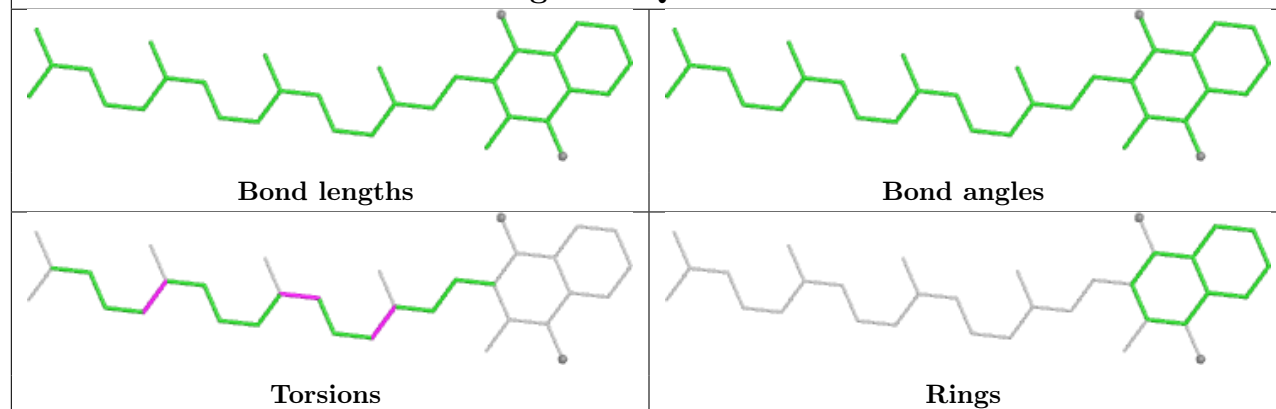


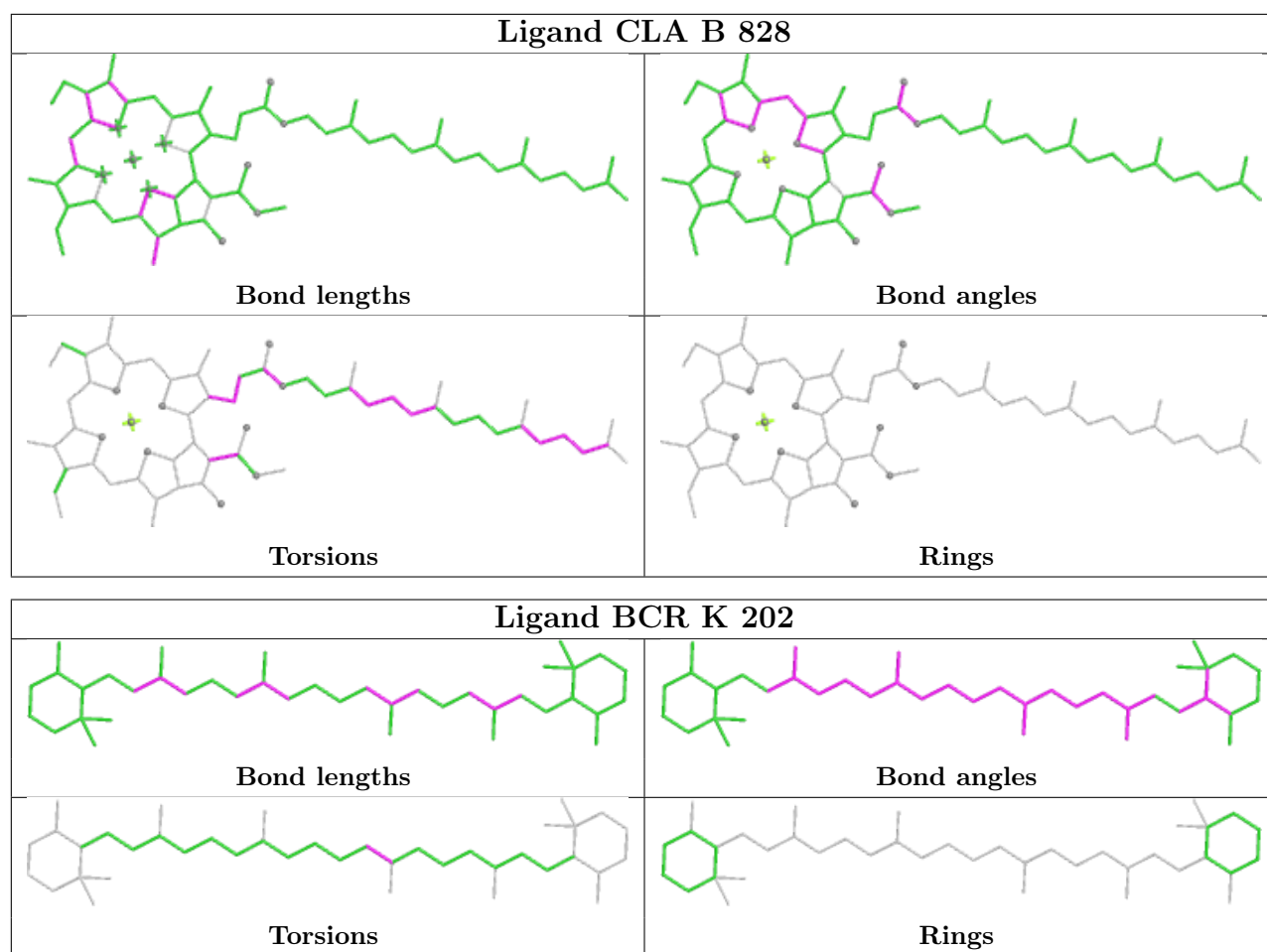
| Ligand BCR F 304                                                                                      |                                                                                                       |
|-------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand CLA A 834                                                                                      |                                                                                                       |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>    |  <p>Rings</p>      |

## Ligand CLA 2 610

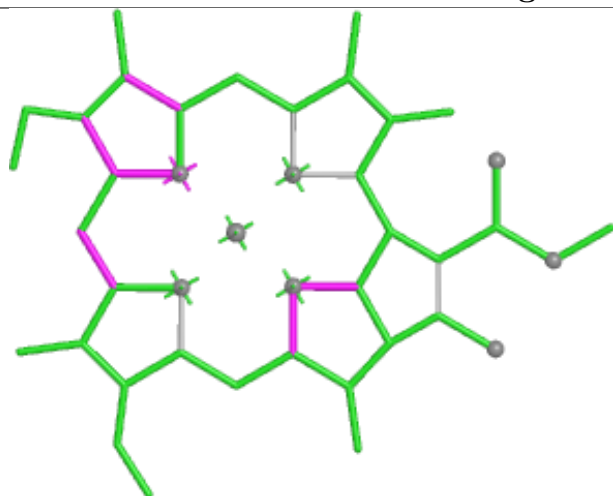


## Ligand PQN B 842





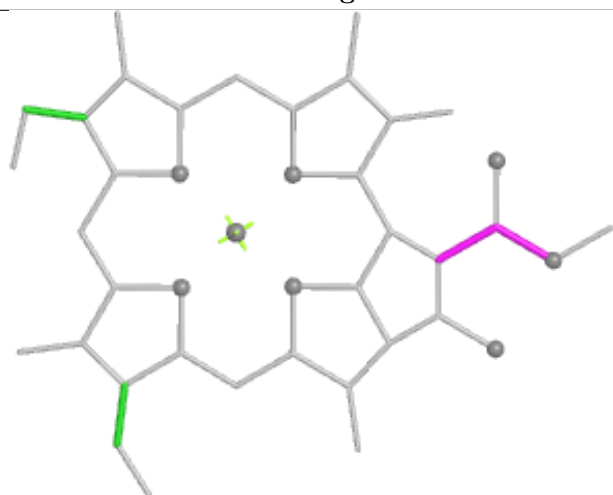
## Ligand CLA 3 608



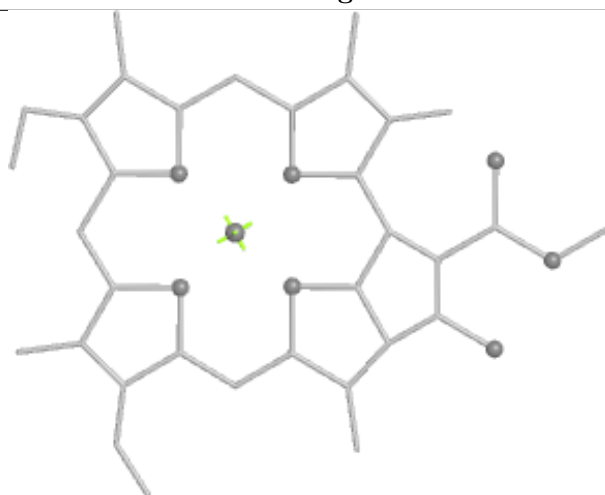
Bond lengths



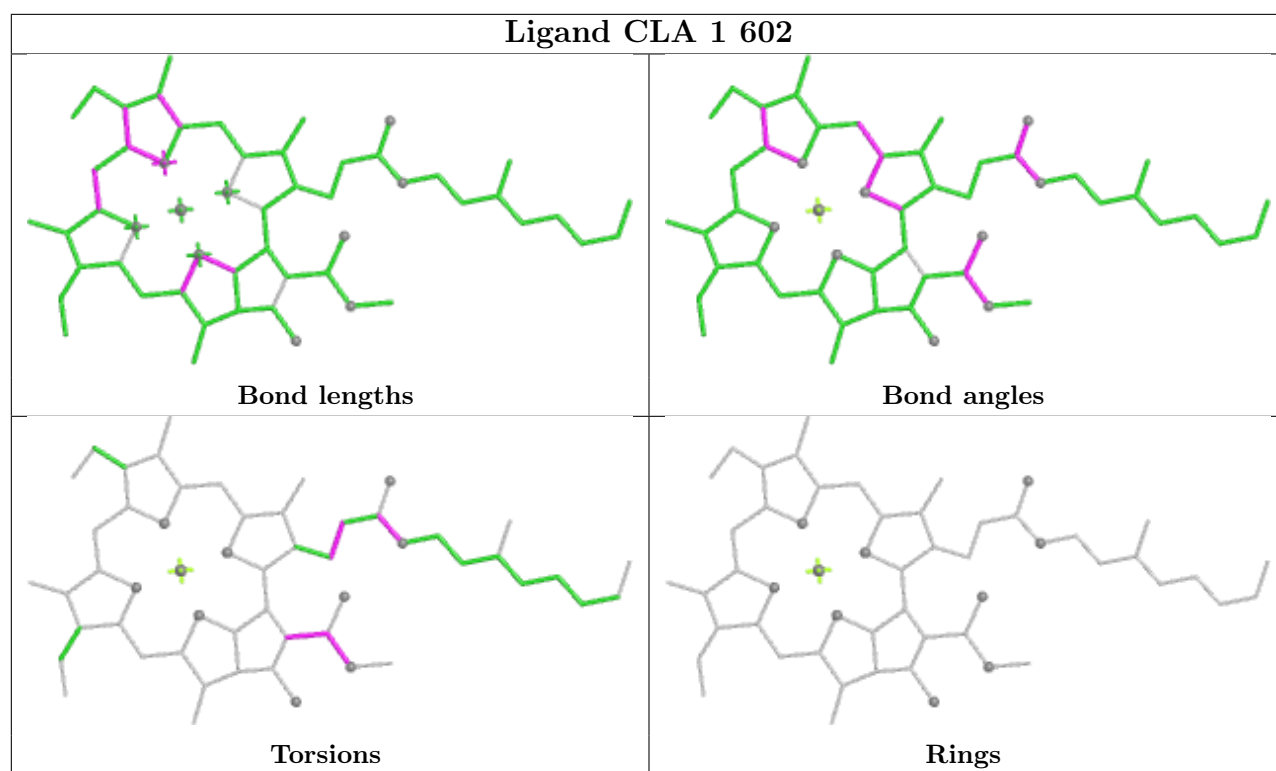
Bond angles



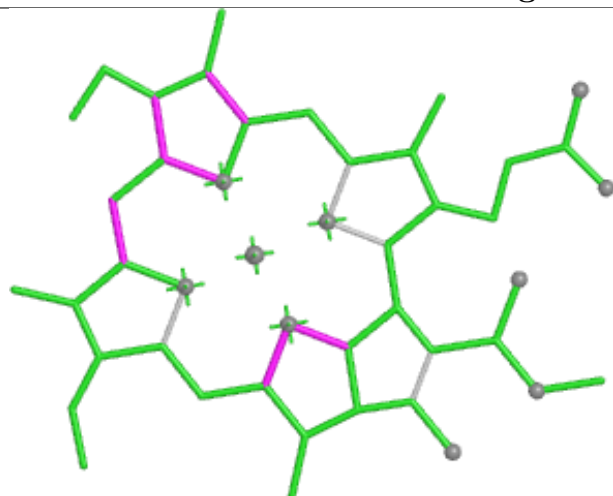
Torsions



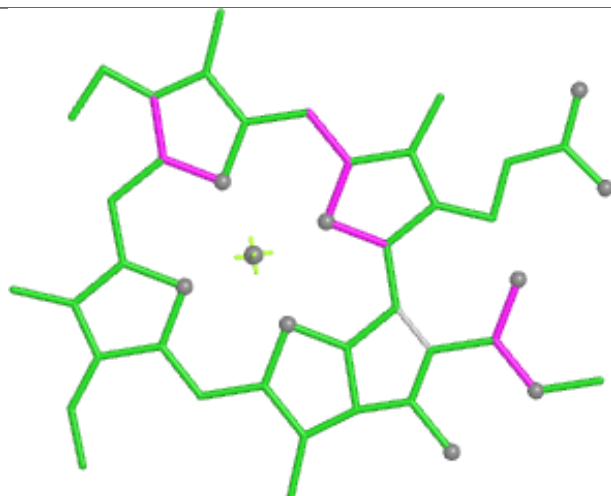
Rings



## Ligand CLA 2 608



Bond lengths



Bond angles

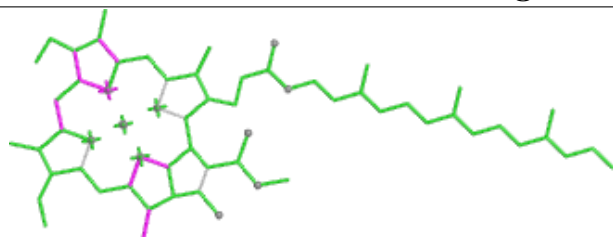


Torsions

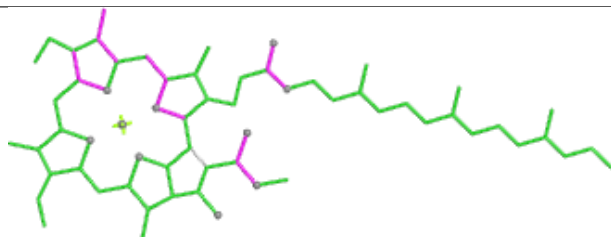


Rings

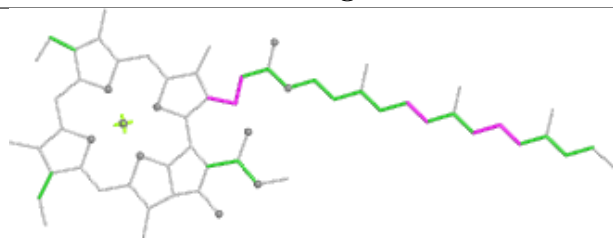
## Ligand CLA B 826



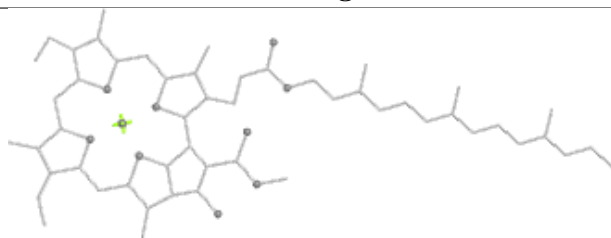
Bond lengths



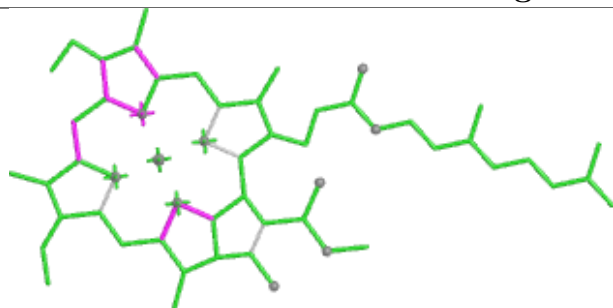
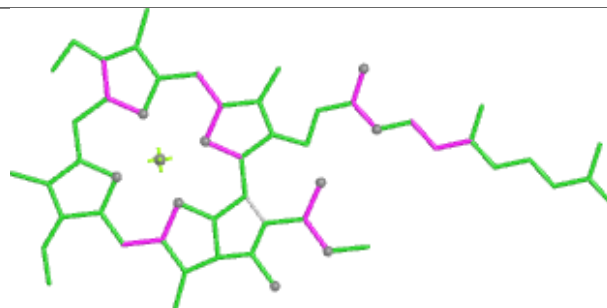
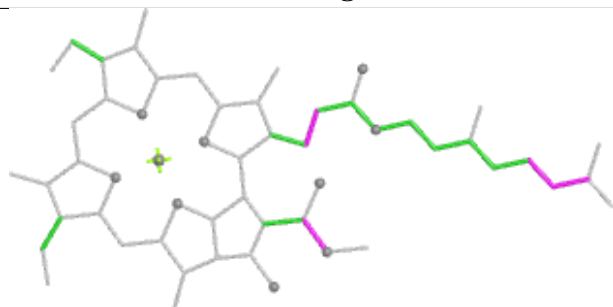
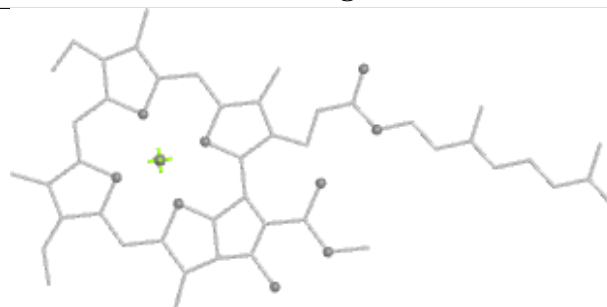
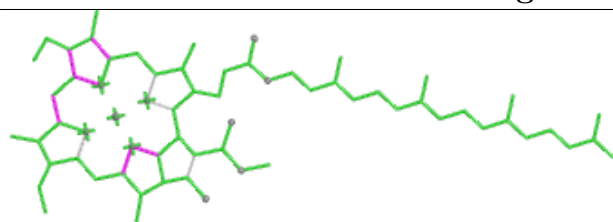
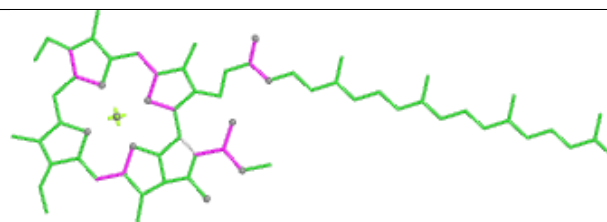
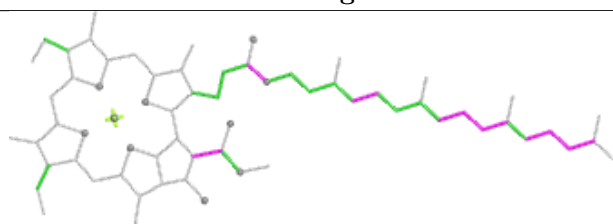
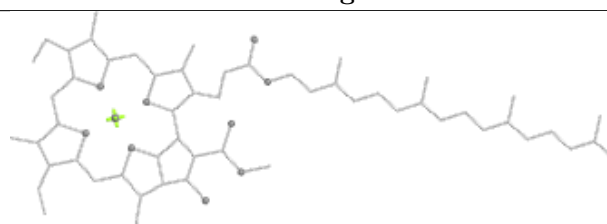
Bond angles

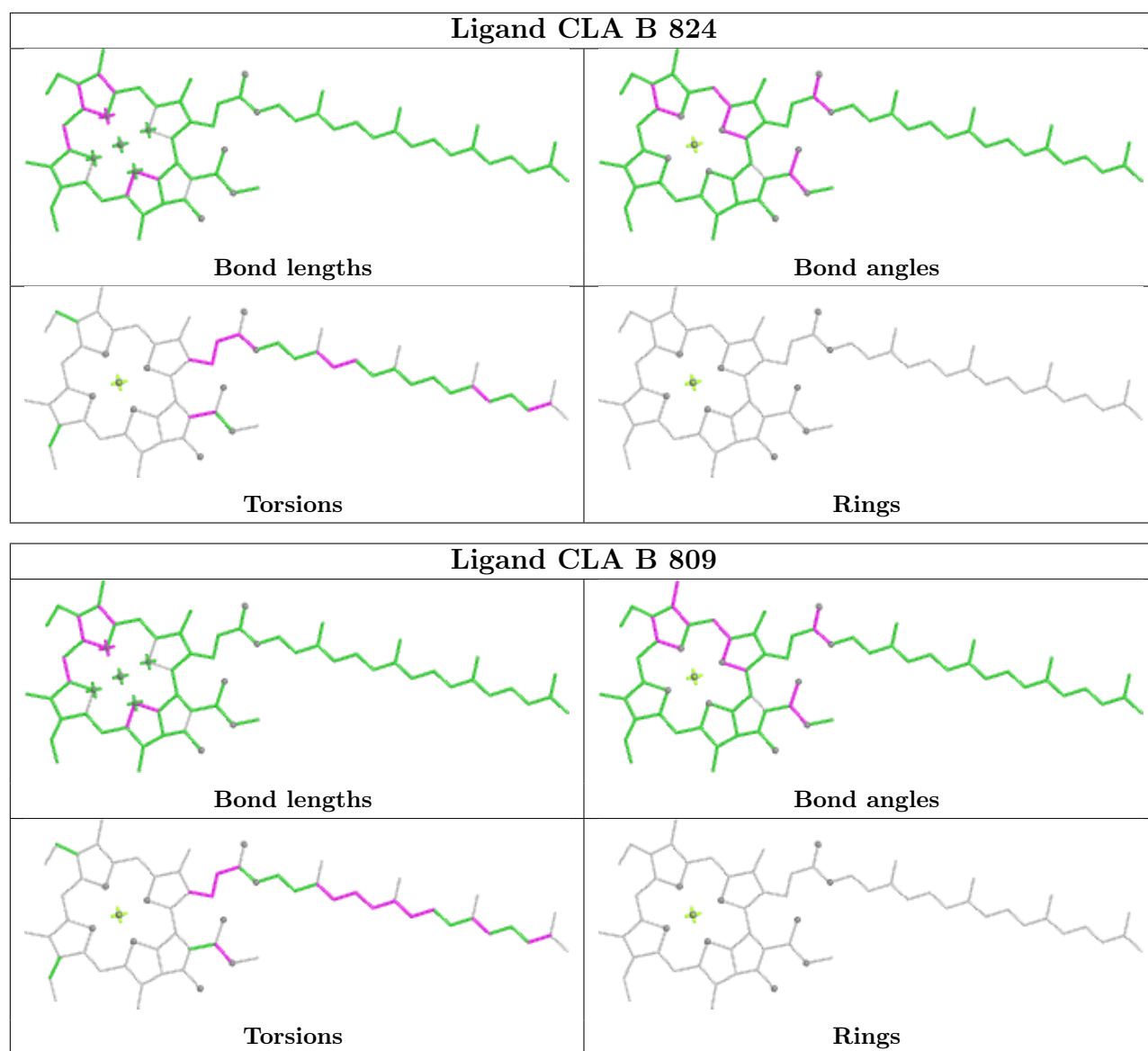


Torsions

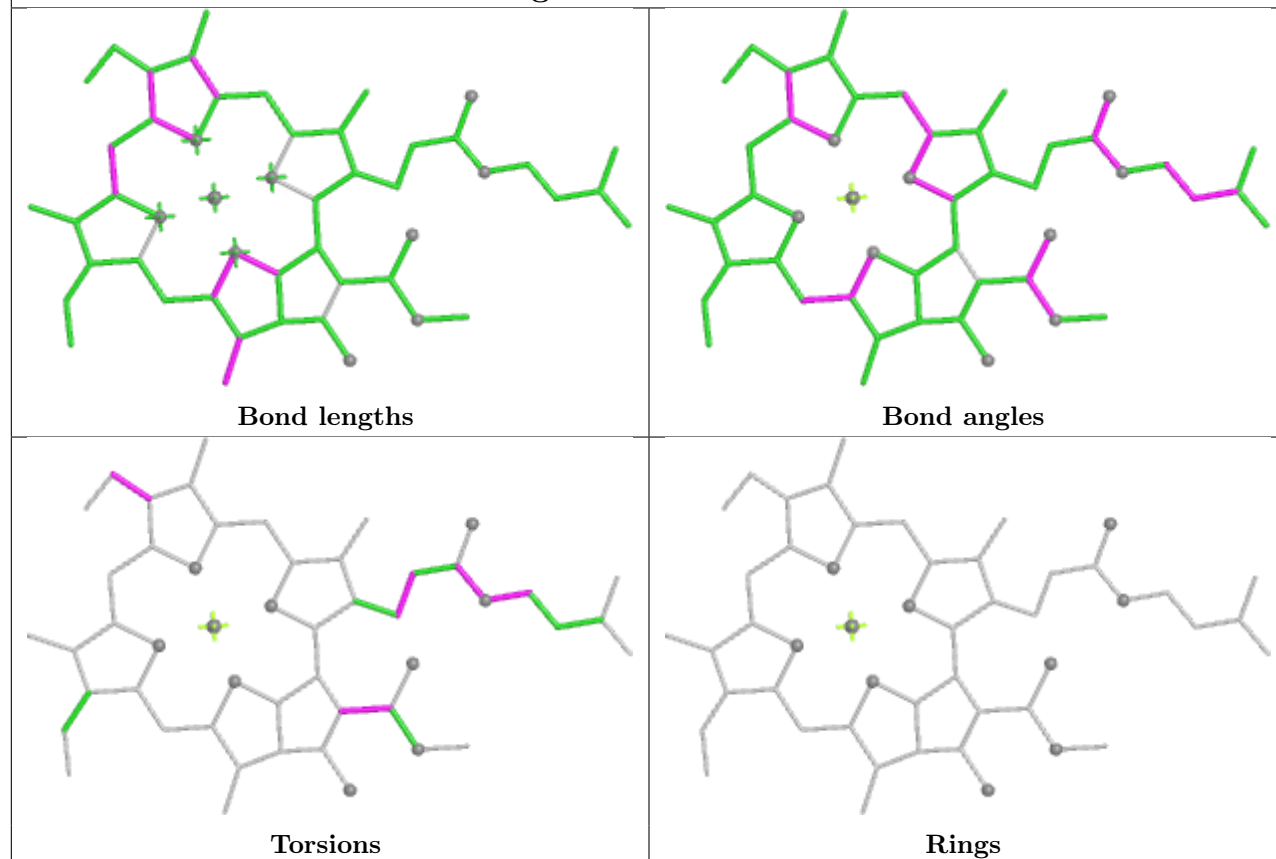


Rings

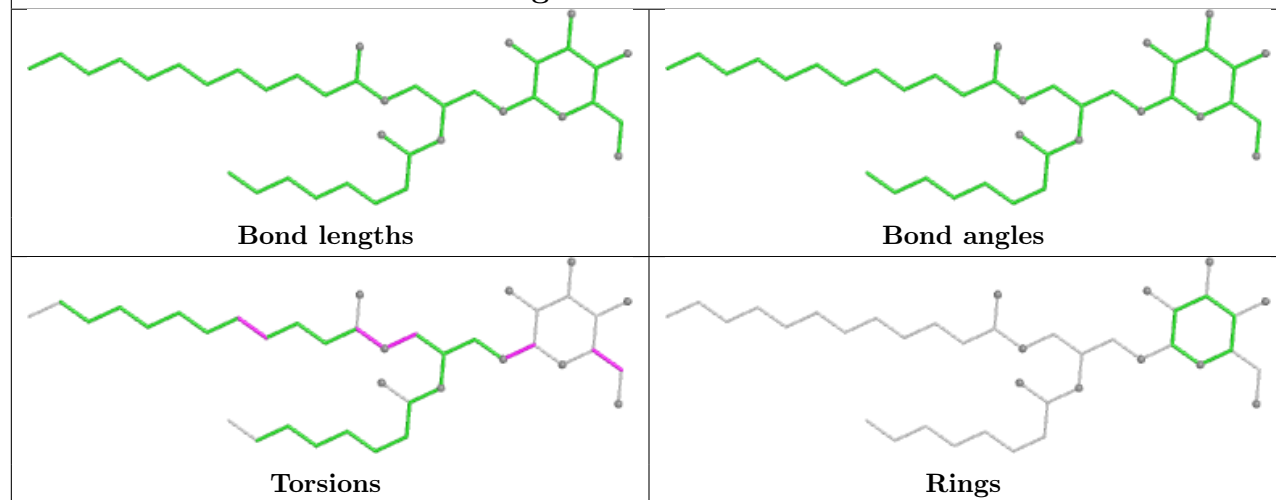
**Ligand CLA B 816****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA L 303****Bond lengths****Bond angles****Torsions****Rings**

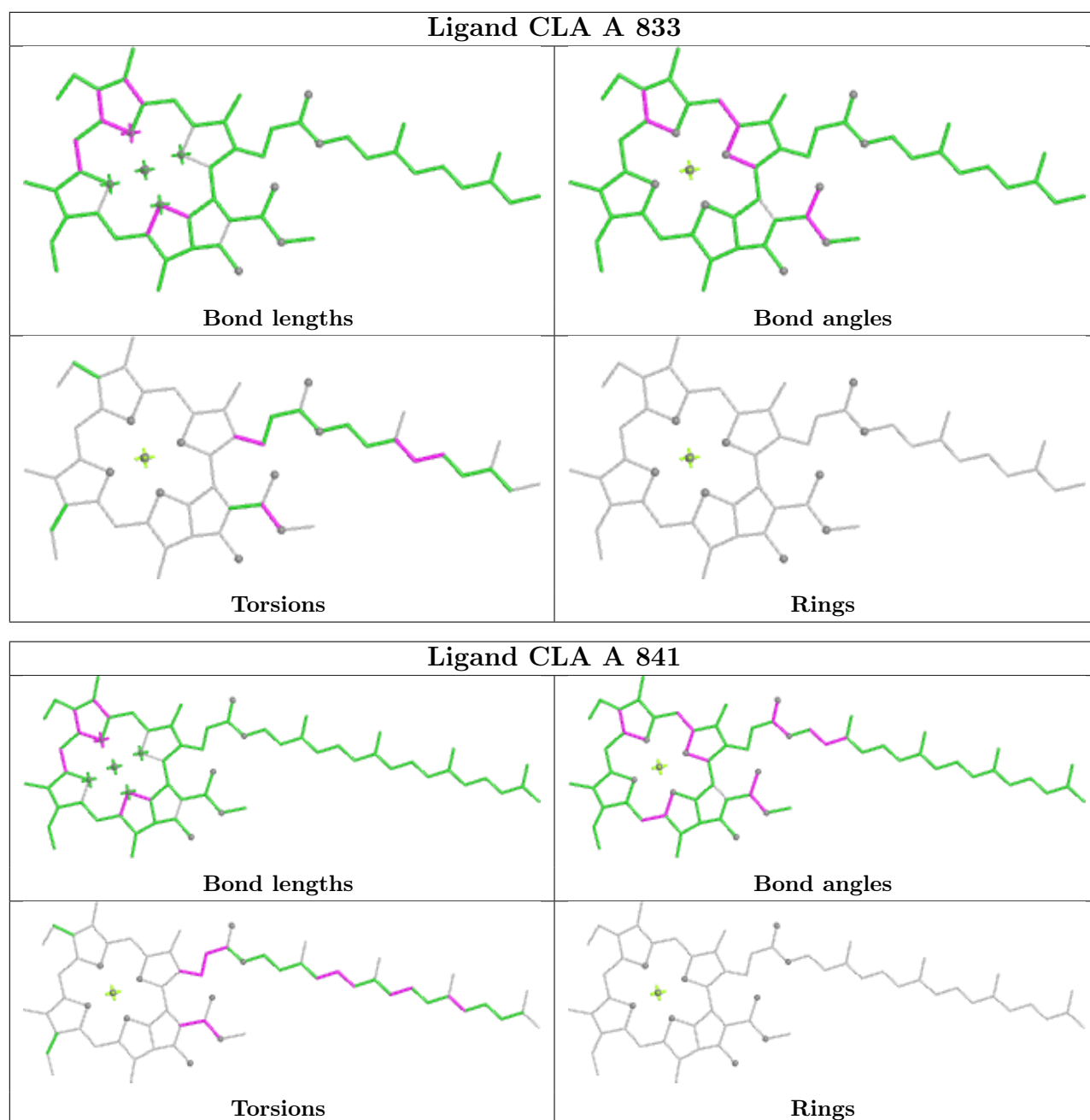


## Ligand CLA A 832

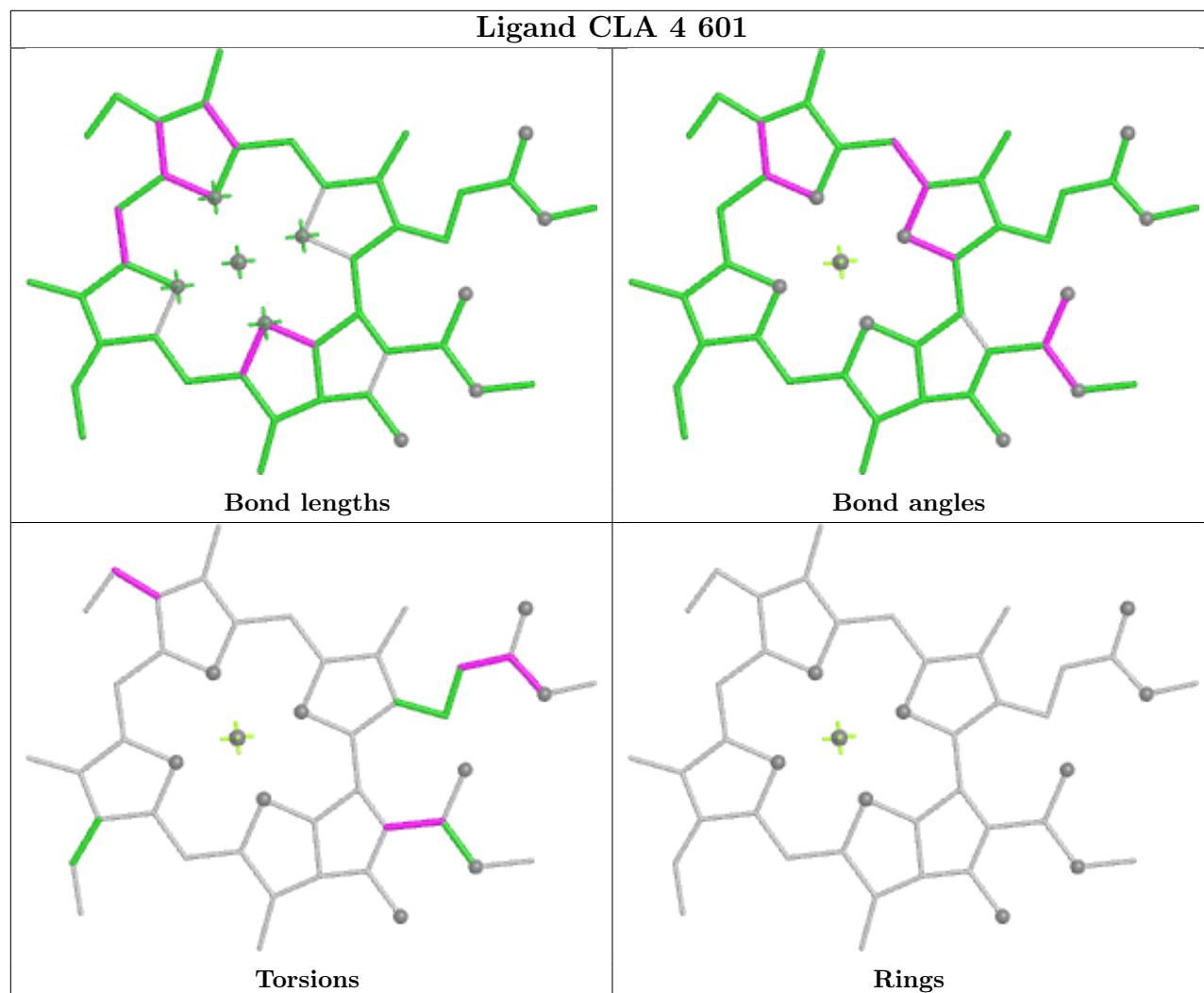


## Ligand LMG 4 619

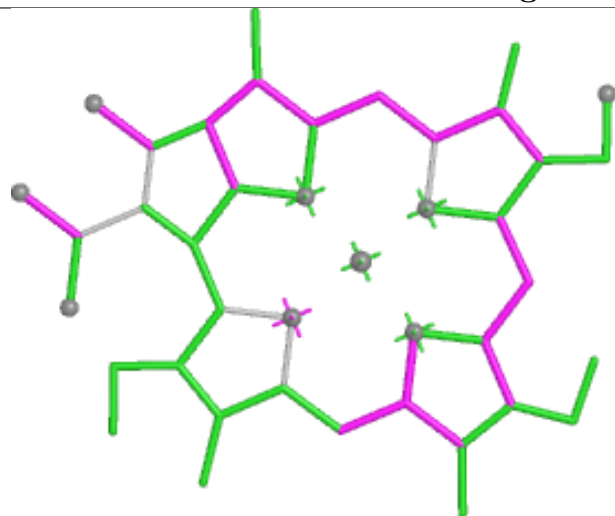




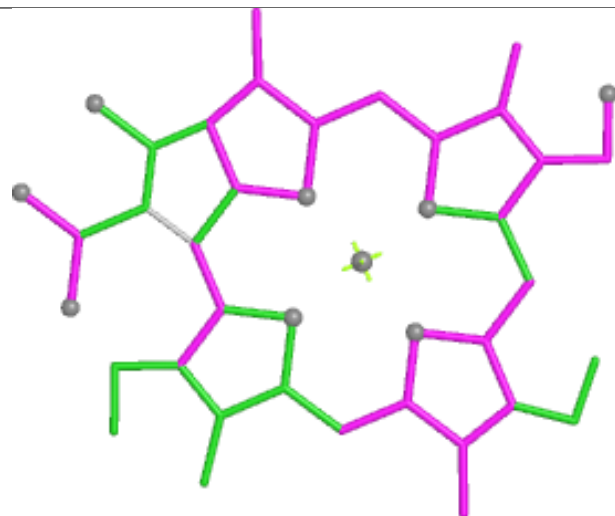
## Ligand CLA 4 601



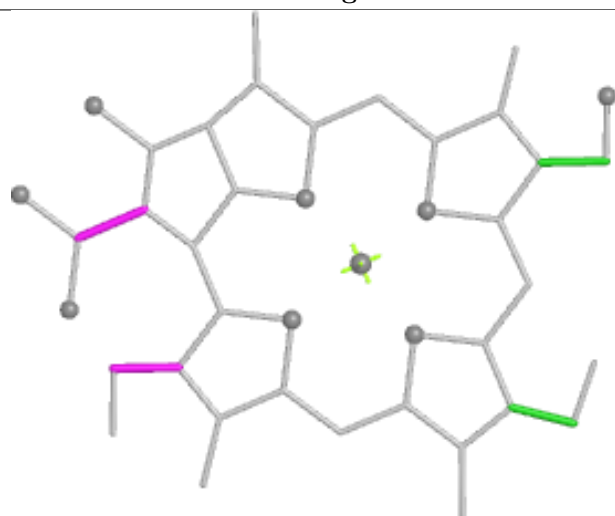
## Ligand CHL 4 605



Bond lengths



Bond angles

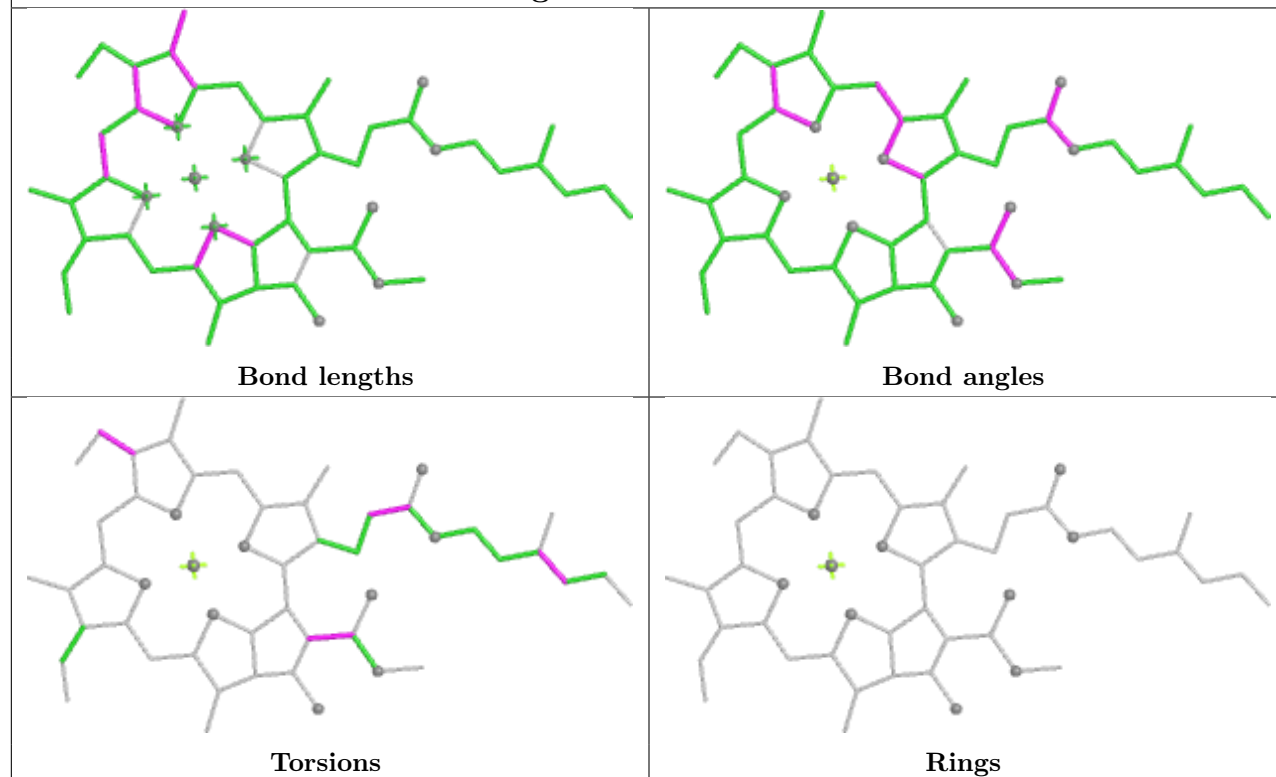


Torsions

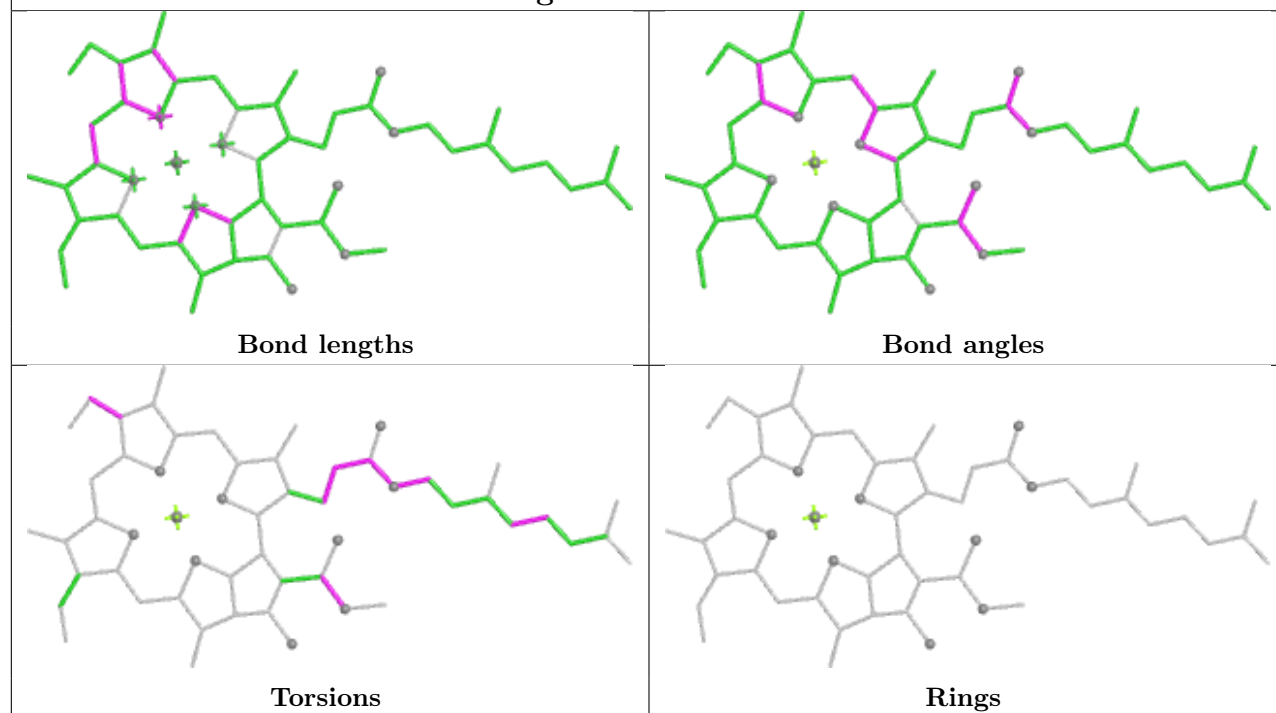


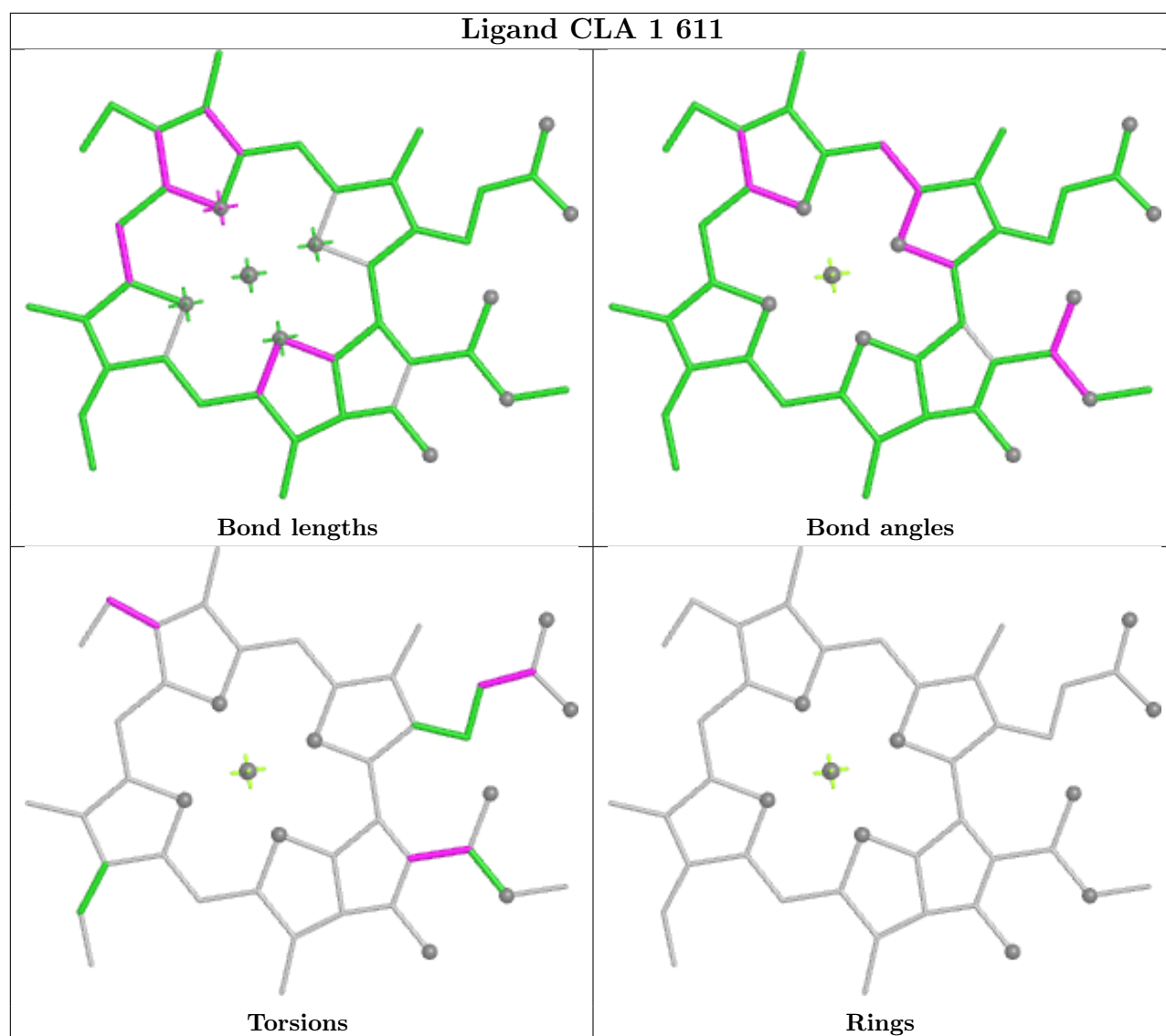
Rings

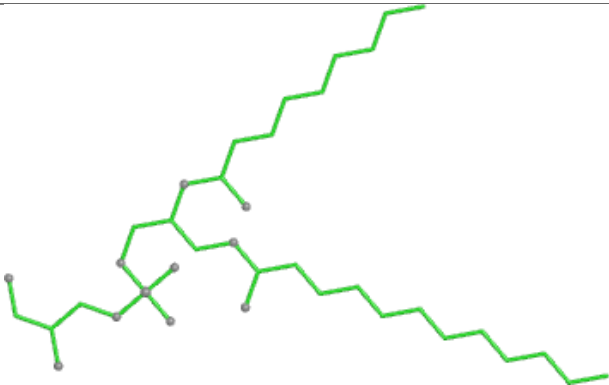
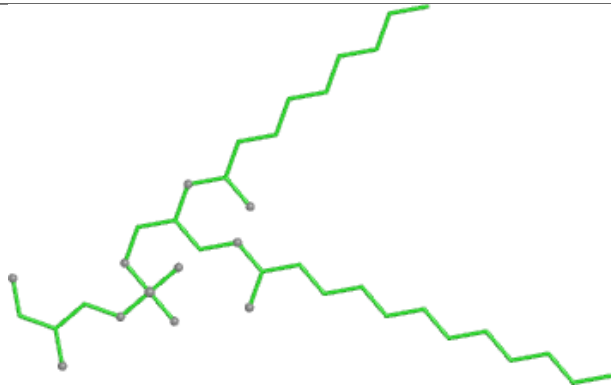
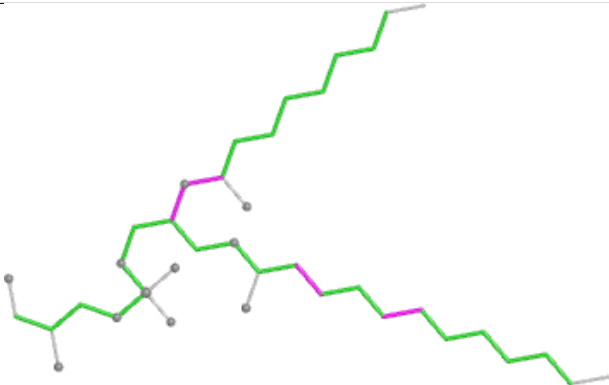
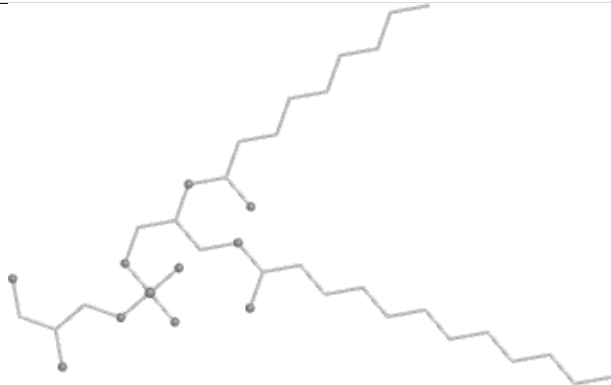
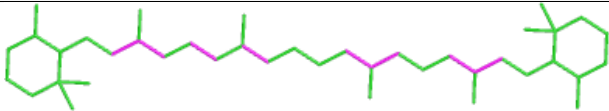
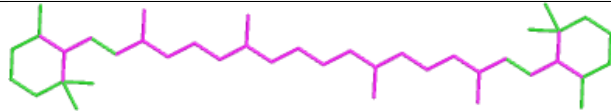
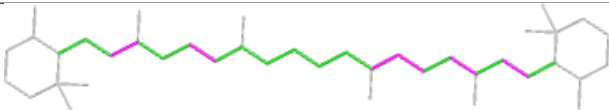
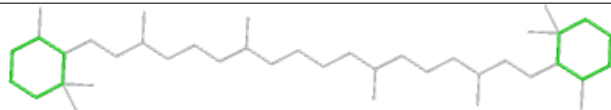
## Ligand CLA A 840

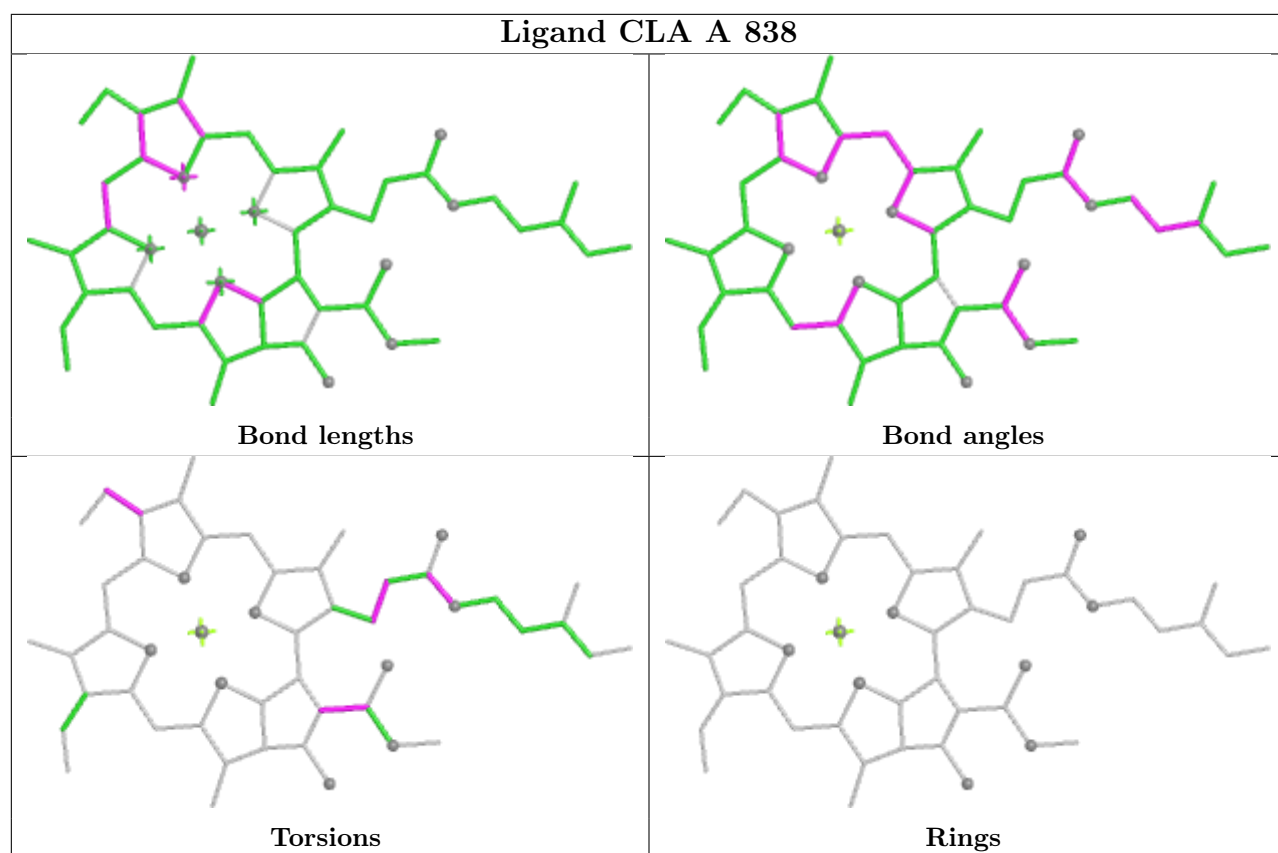


## Ligand CLA 3 602

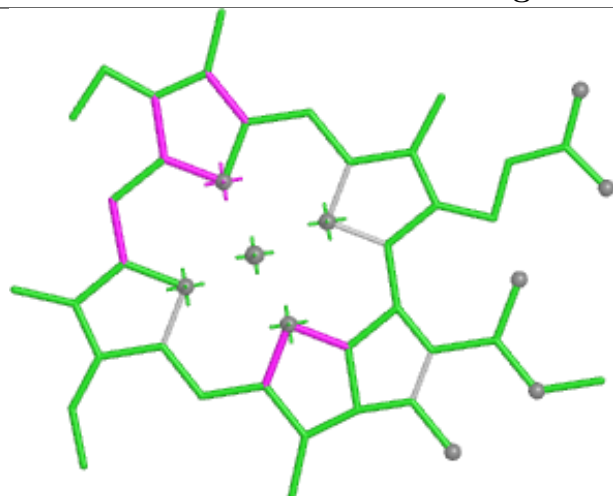




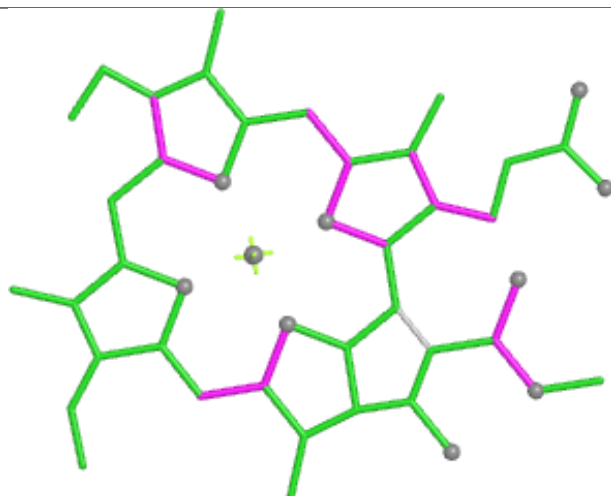
| Ligand LHG B 851                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|   |   |
| Torsions                                                                            | Rings                                                                                |
| Ligand BCR K 205                                                                    |                                                                                      |
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



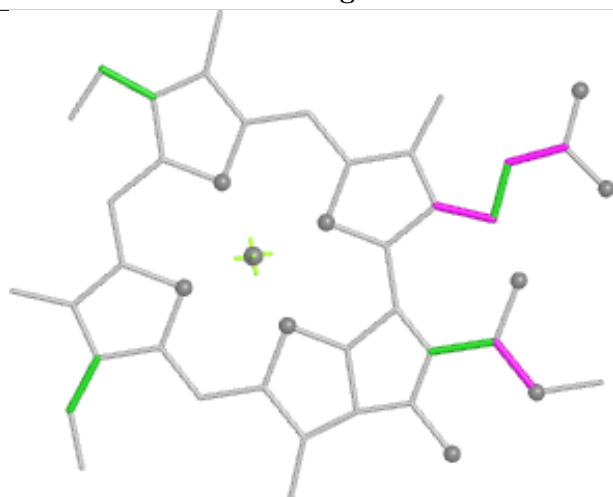
## Ligand CLA K 203



Bond lengths



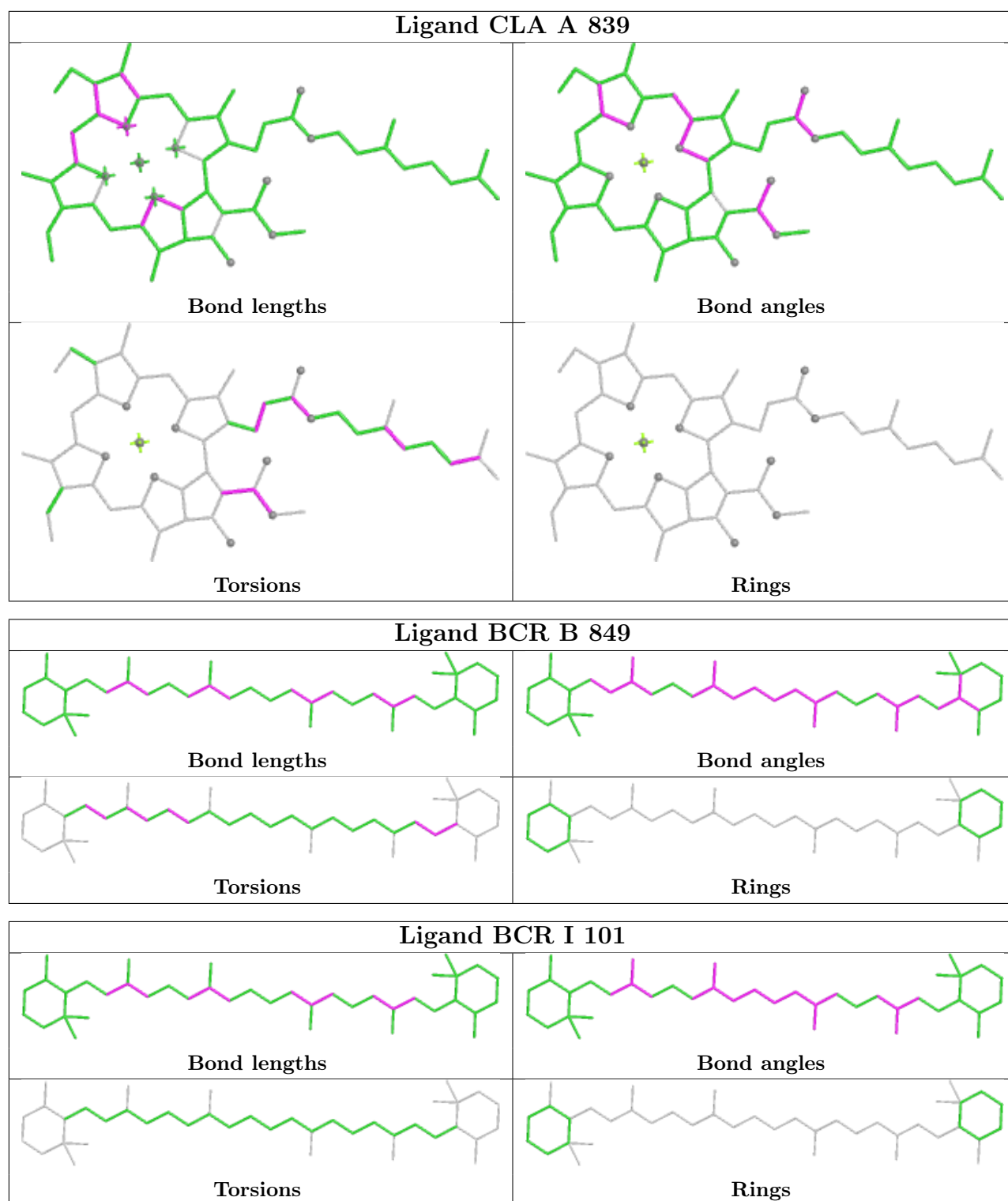
Bond angles

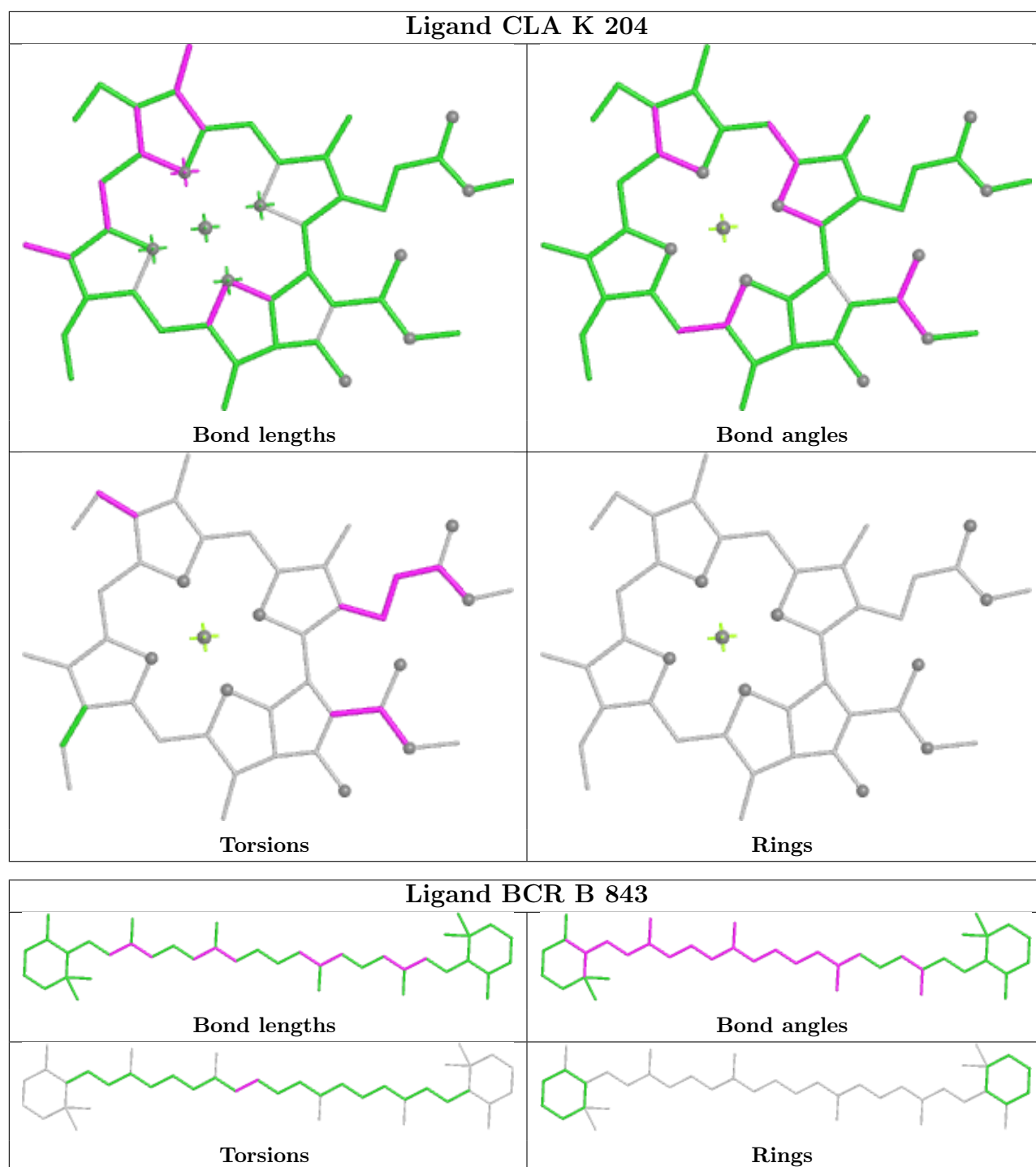


Torsions

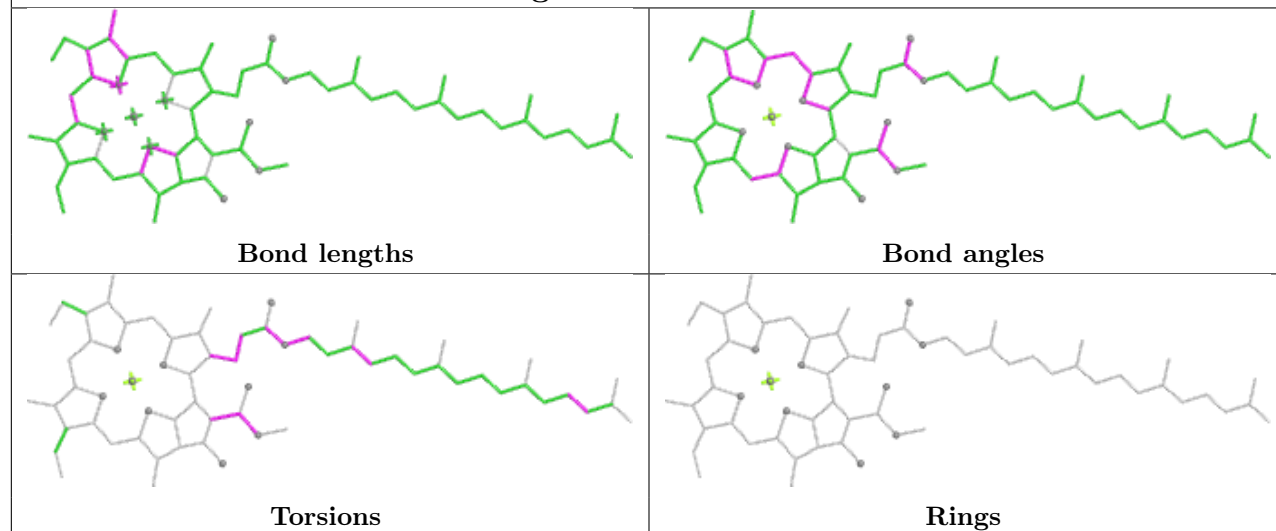


Rings

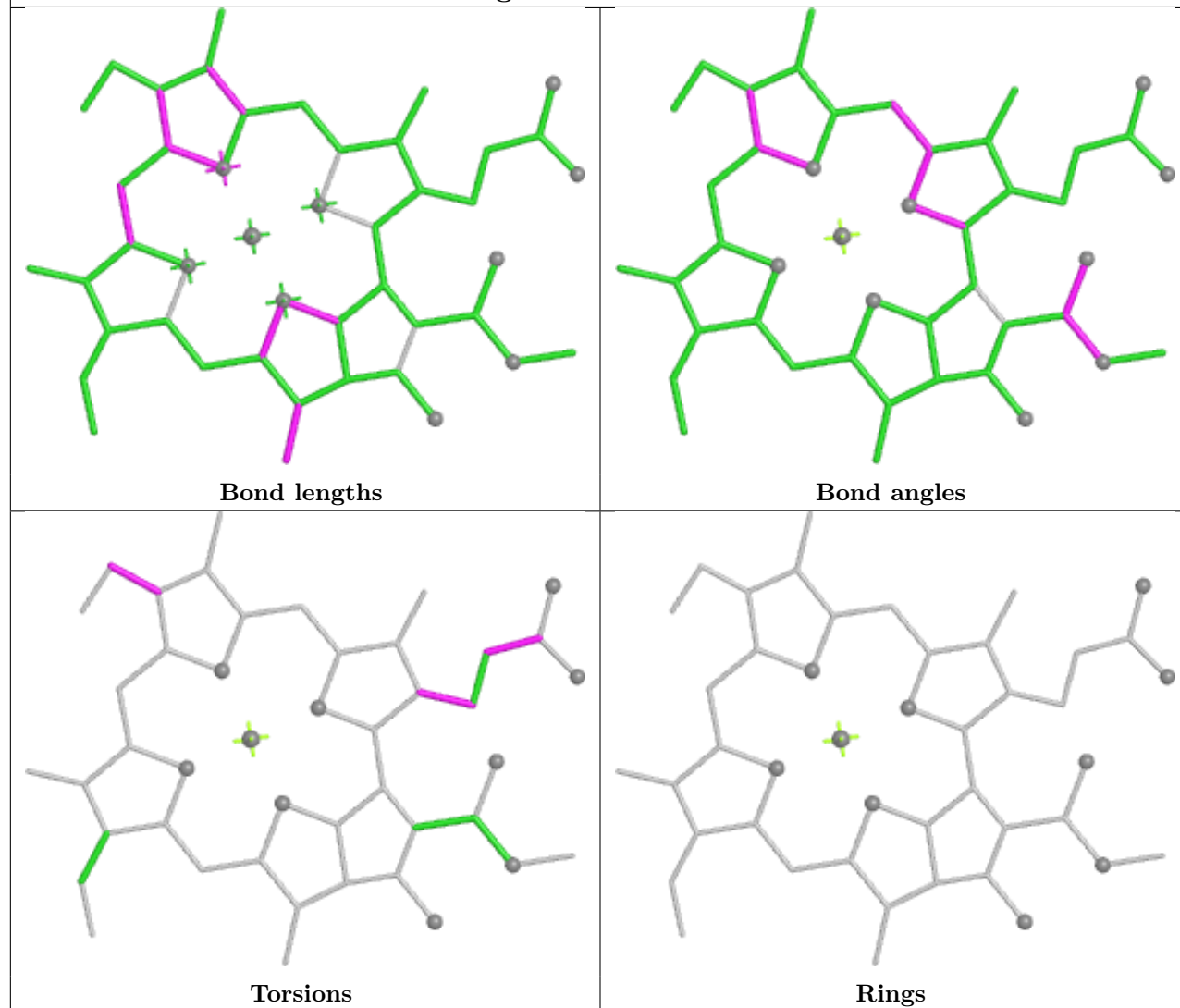




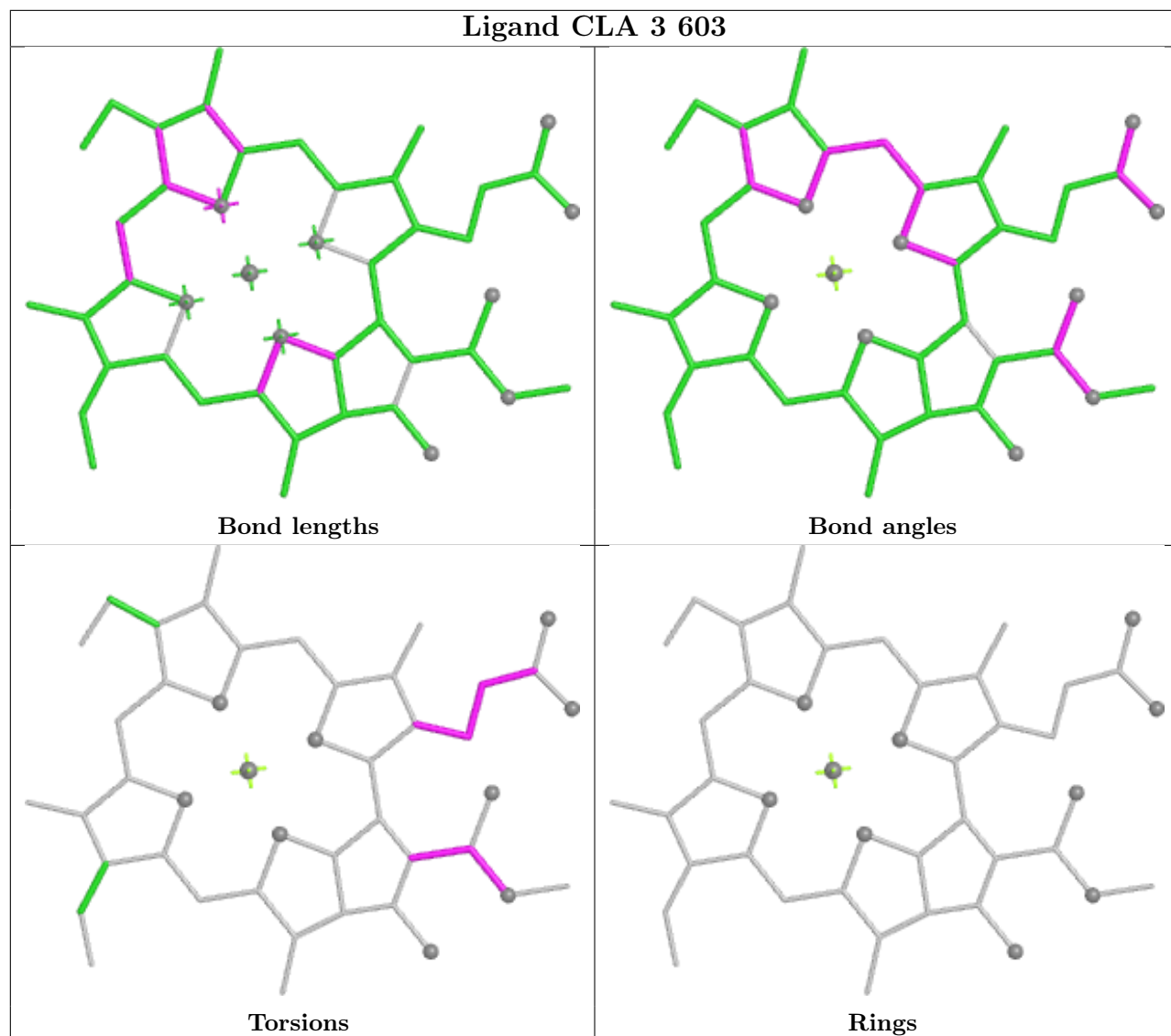
## Ligand CLA A 822



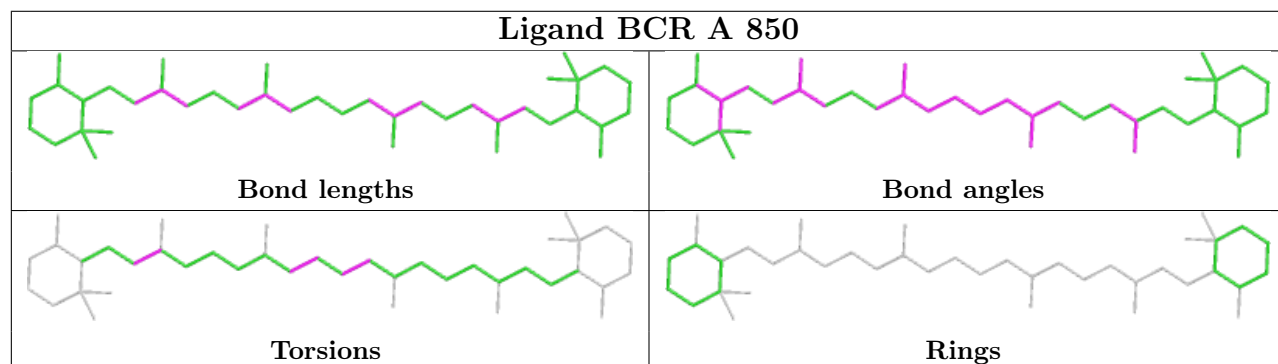
## Ligand CLA 4 608



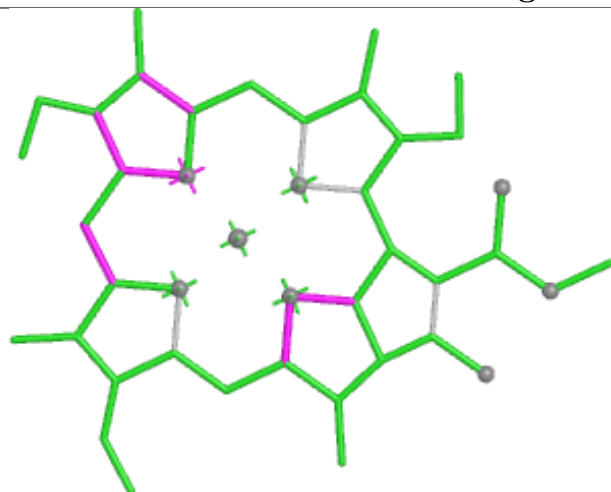
## Ligand CLA 3 603



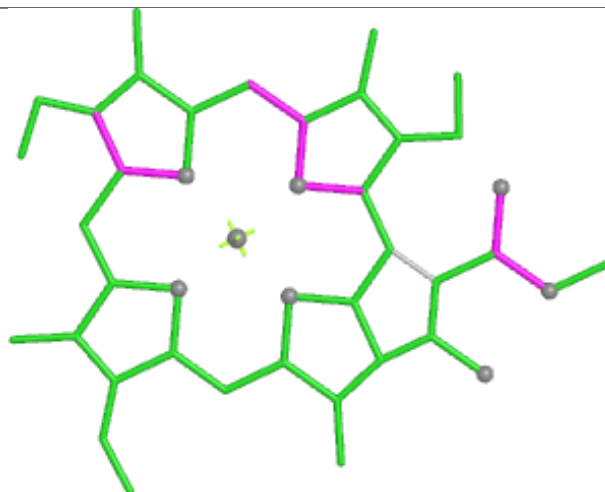
## Ligand BCR A 850



## Ligand CLA 4 610



Bond lengths



Bond angles

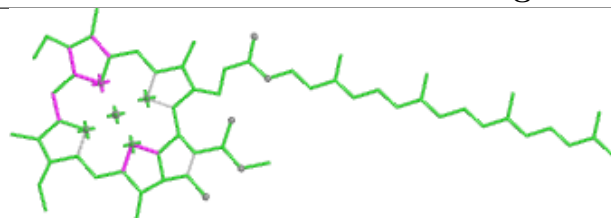


Torsions

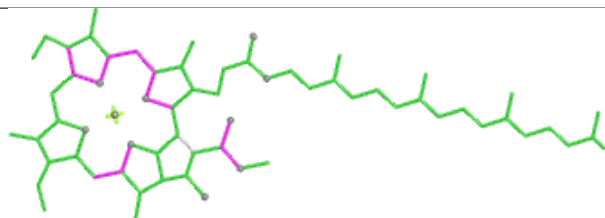


Rings

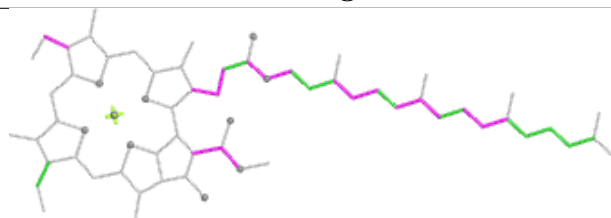
## Ligand CLA A 803



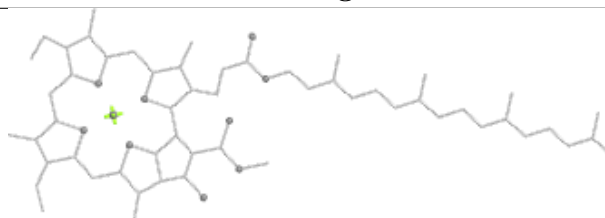
Bond lengths



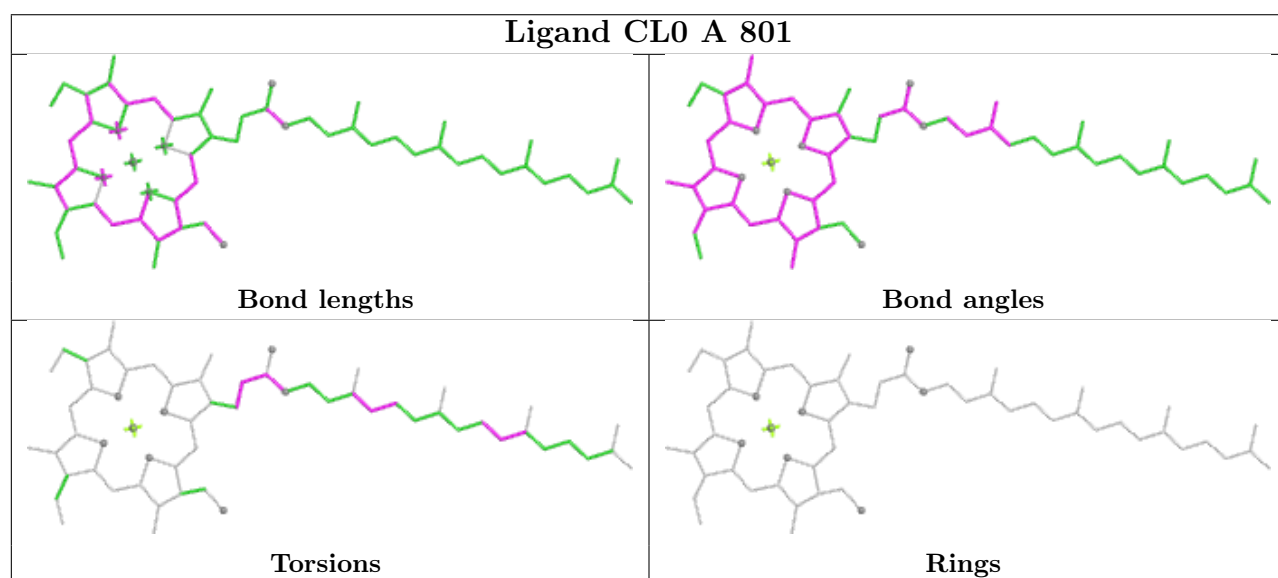
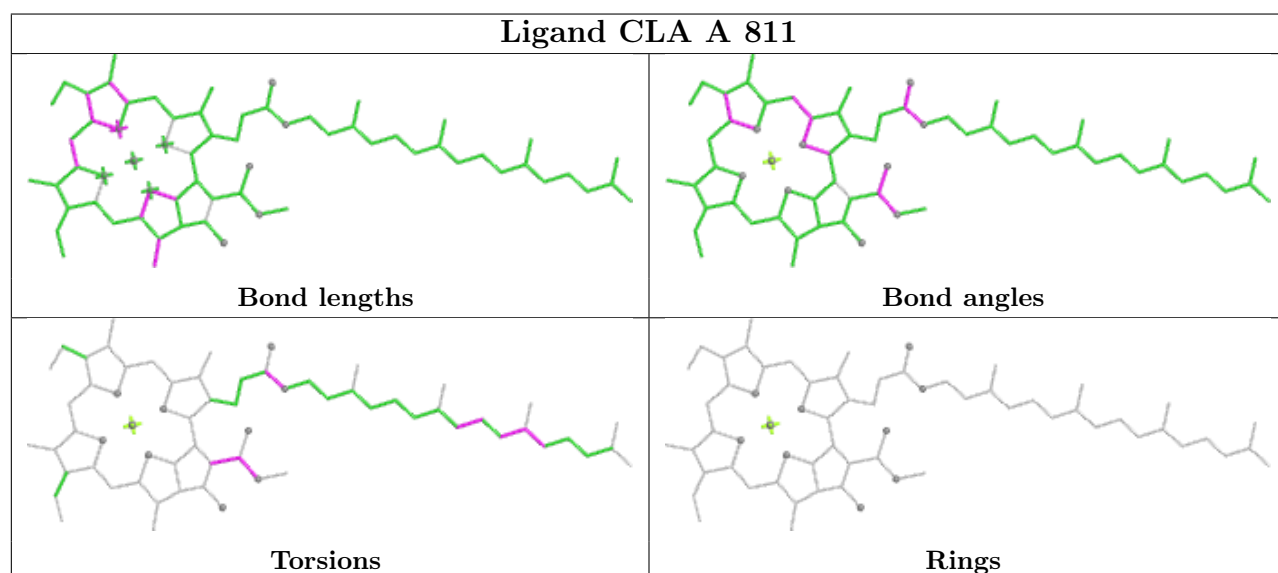
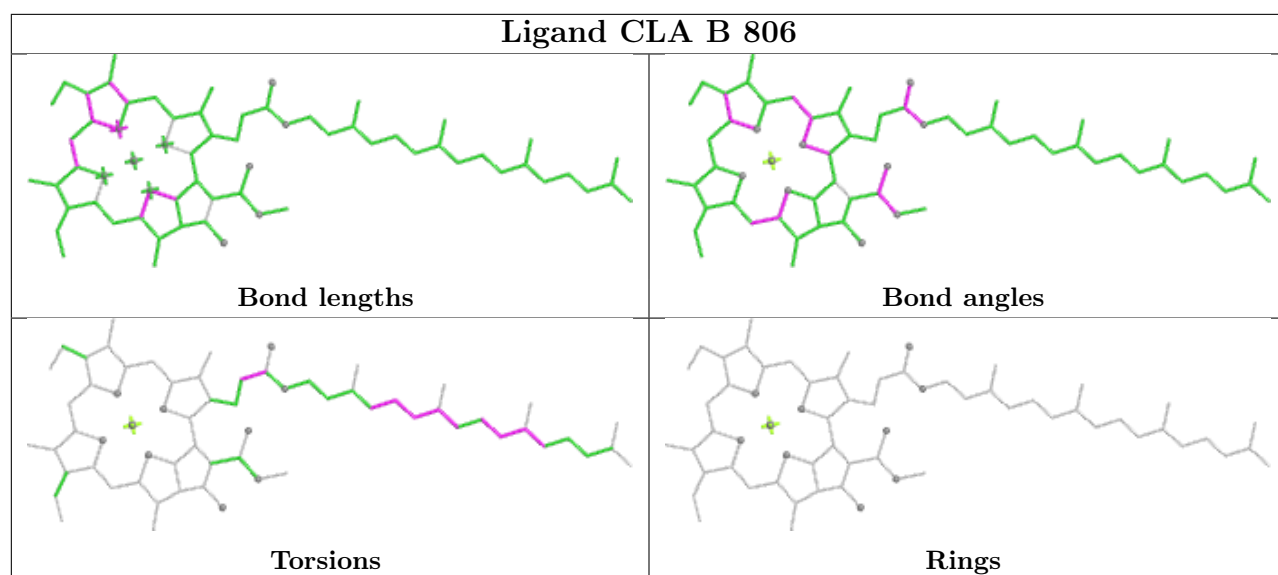
Bond angles

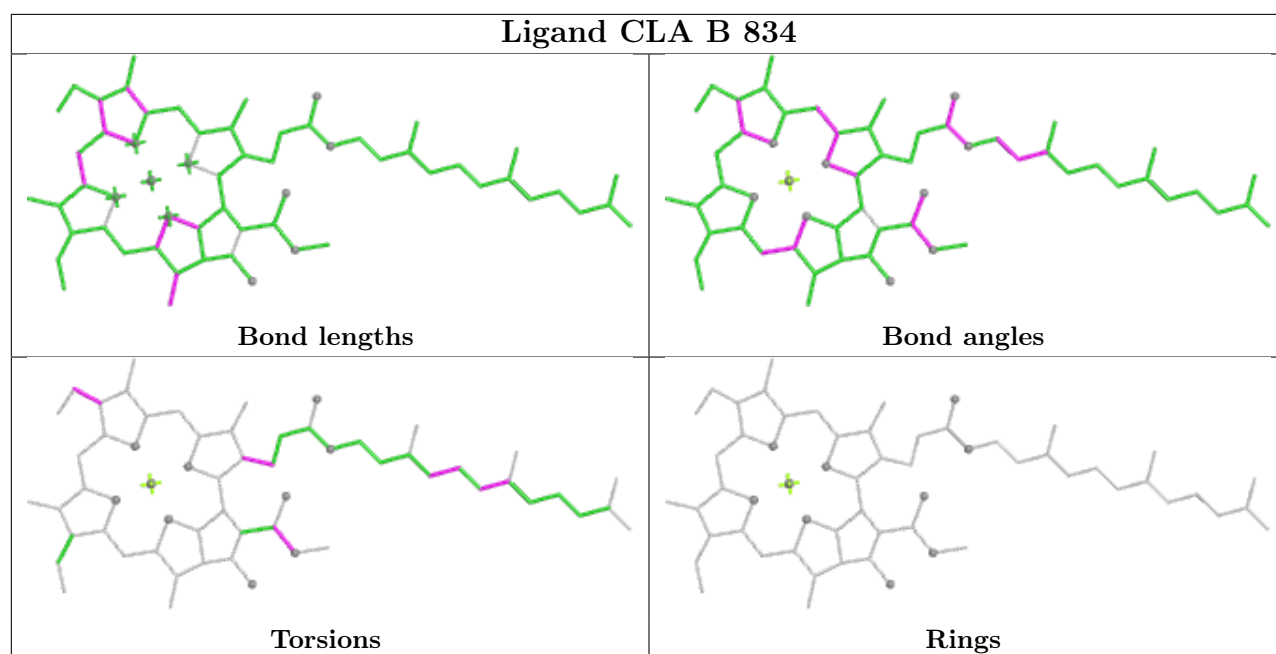


Torsions

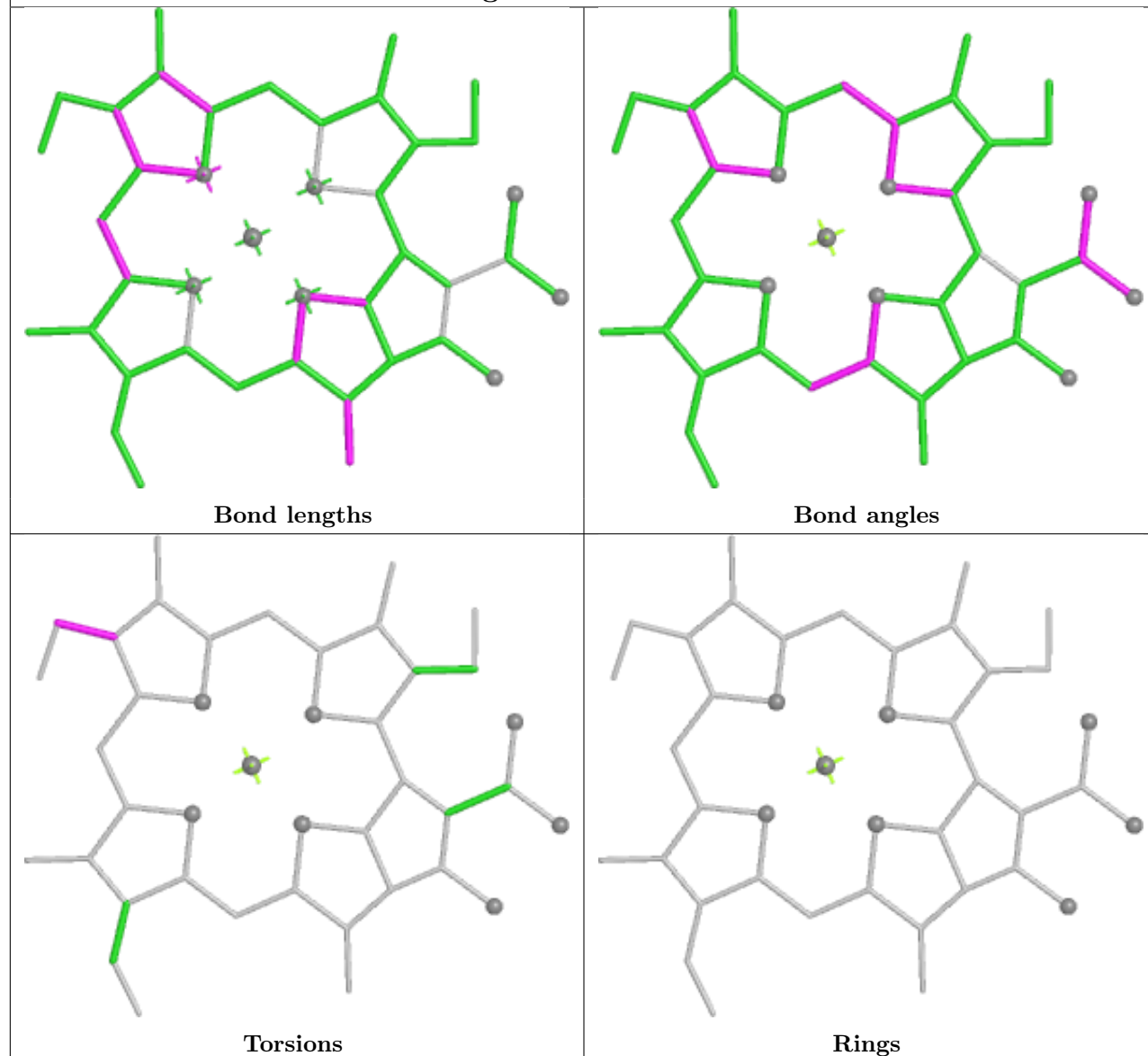


Rings

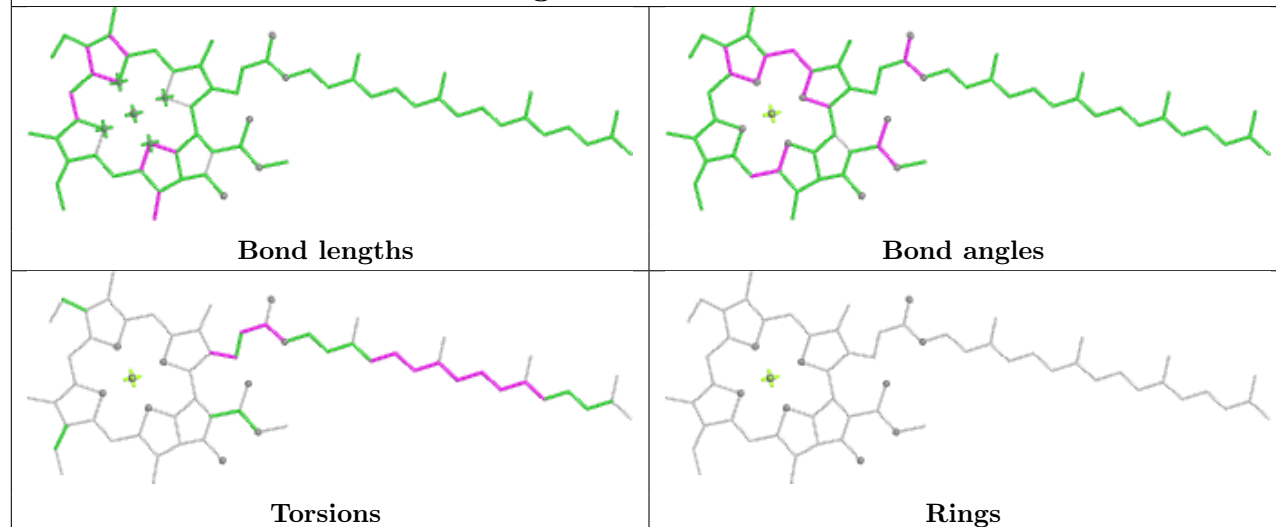


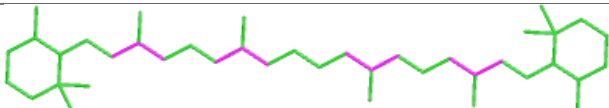
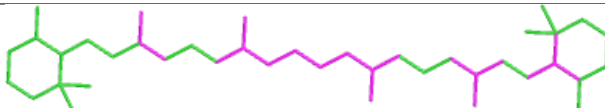
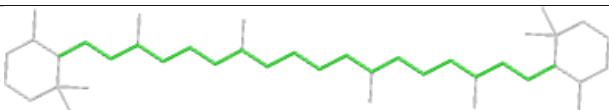
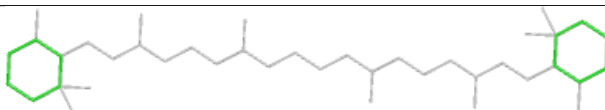


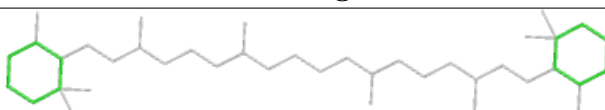
## Ligand CLA 3 604

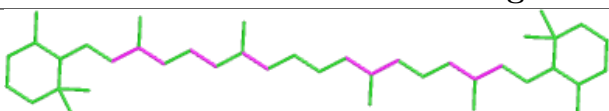
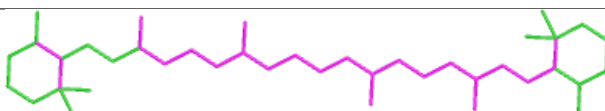
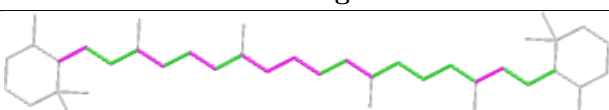
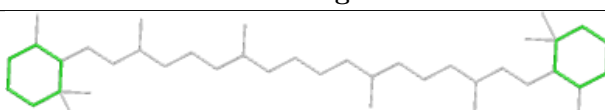


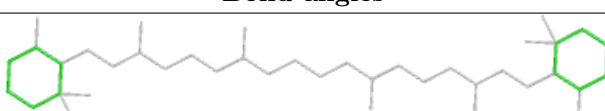
## Ligand CLA B 805

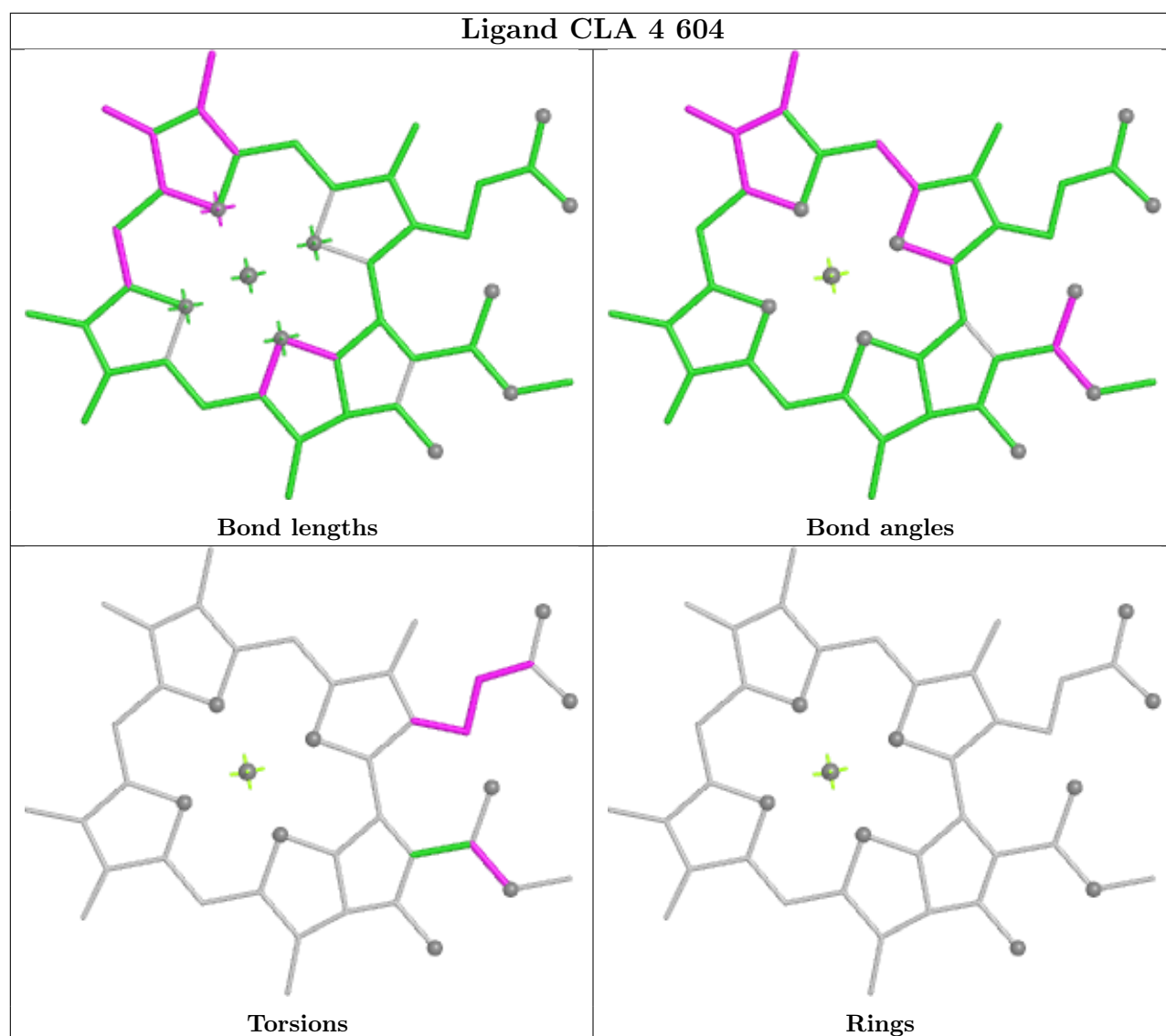


| Ligand BCR A 848                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand BCR B 848                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand BCR A 852                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

| Ligand BCR G 204                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| 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.

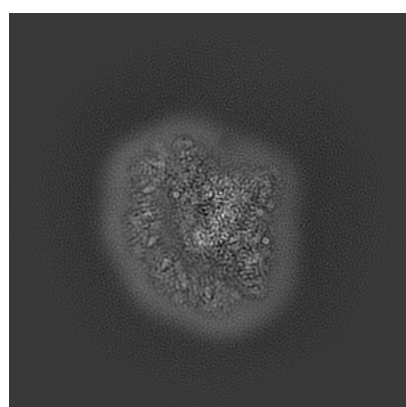
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36037. These allow visual inspection of the internal detail of the map and identification of artifacts.

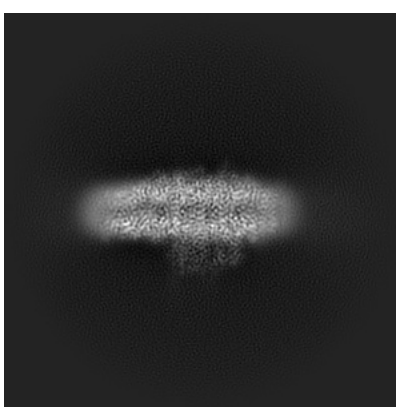
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

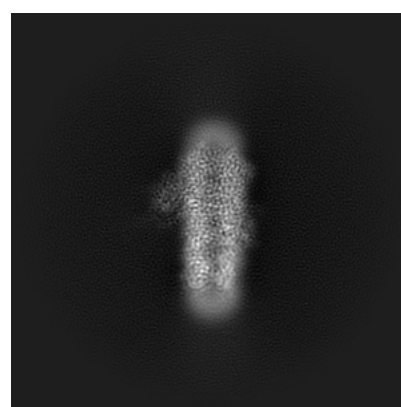
#### 6.1.1 Primary map



X



Y

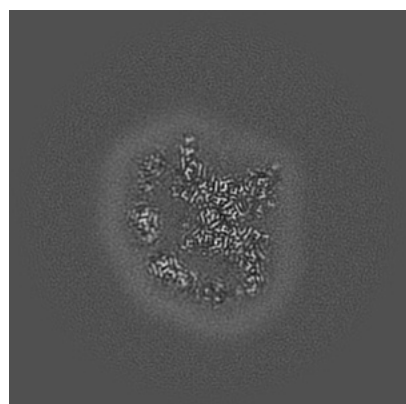


Z

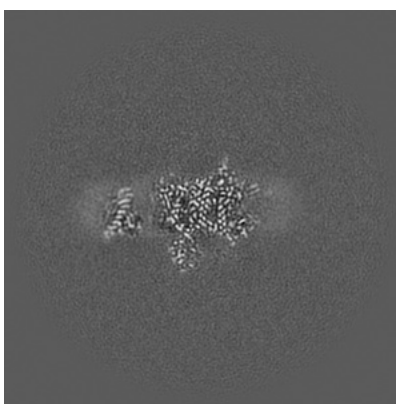
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

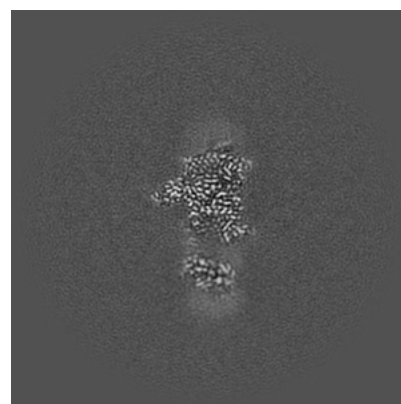
#### 6.2.1 Primary map



X Index: 168



Y Index: 168

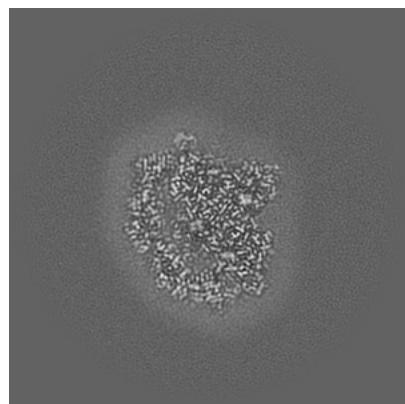


Z Index: 168

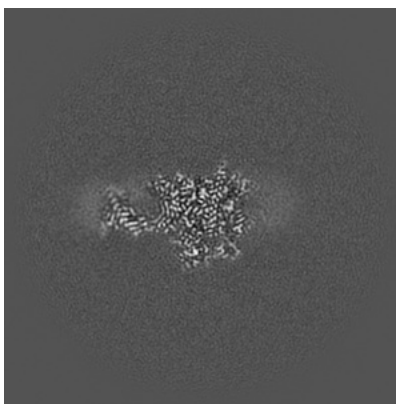
The images above show central slices of the map in three orthogonal directions.

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

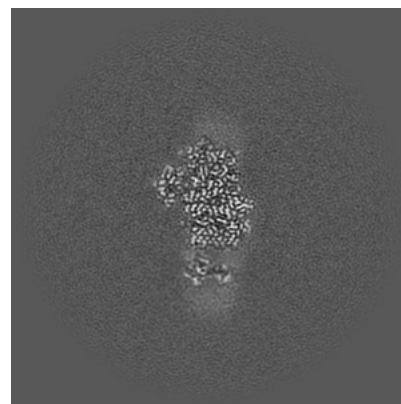
### 6.3.1 Primary map



X Index: 157



Y Index: 174

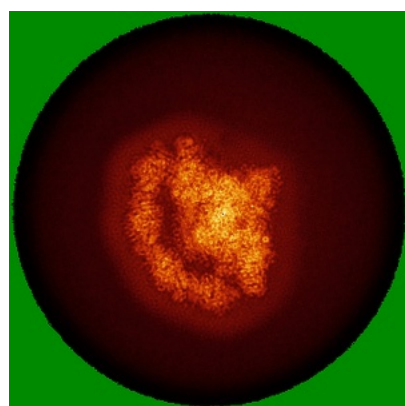


Z Index: 182

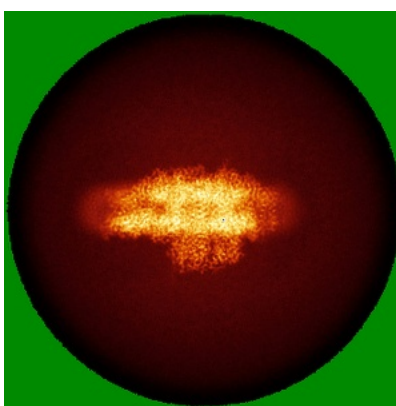
The images above show the largest variance slices of the map in three orthogonal directions.

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

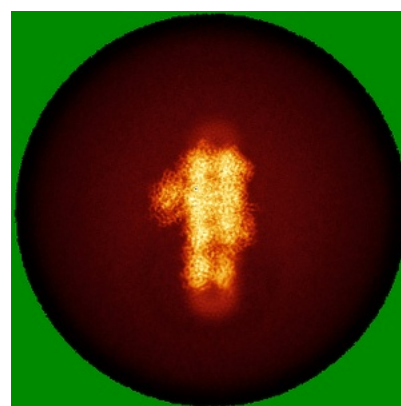
### 6.4.1 Primary map



X



Y

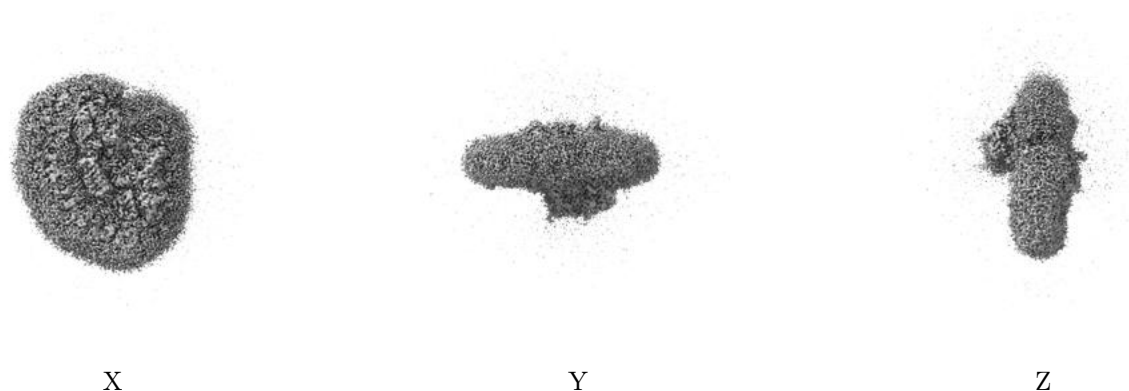


Z

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 3.21. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

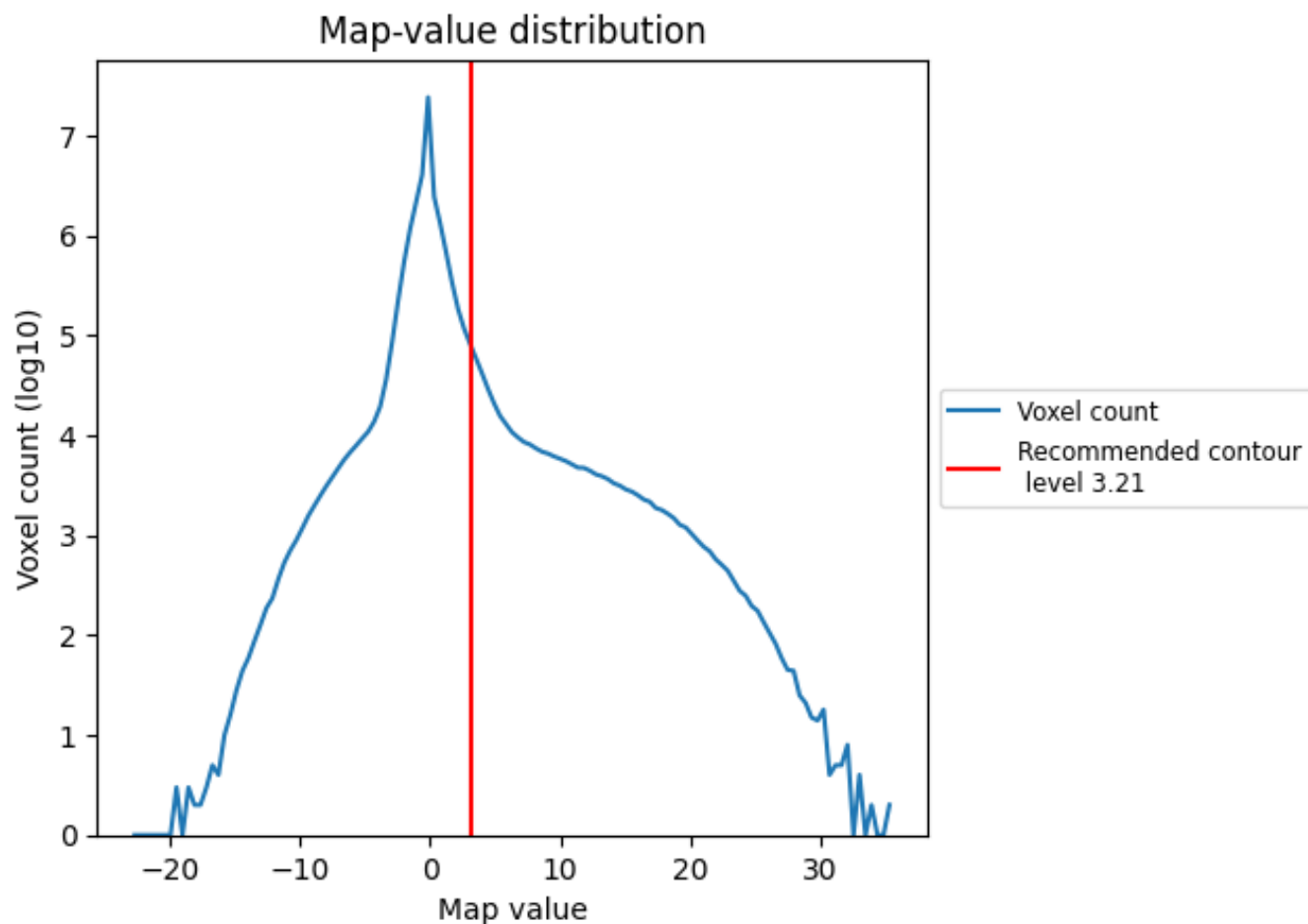
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

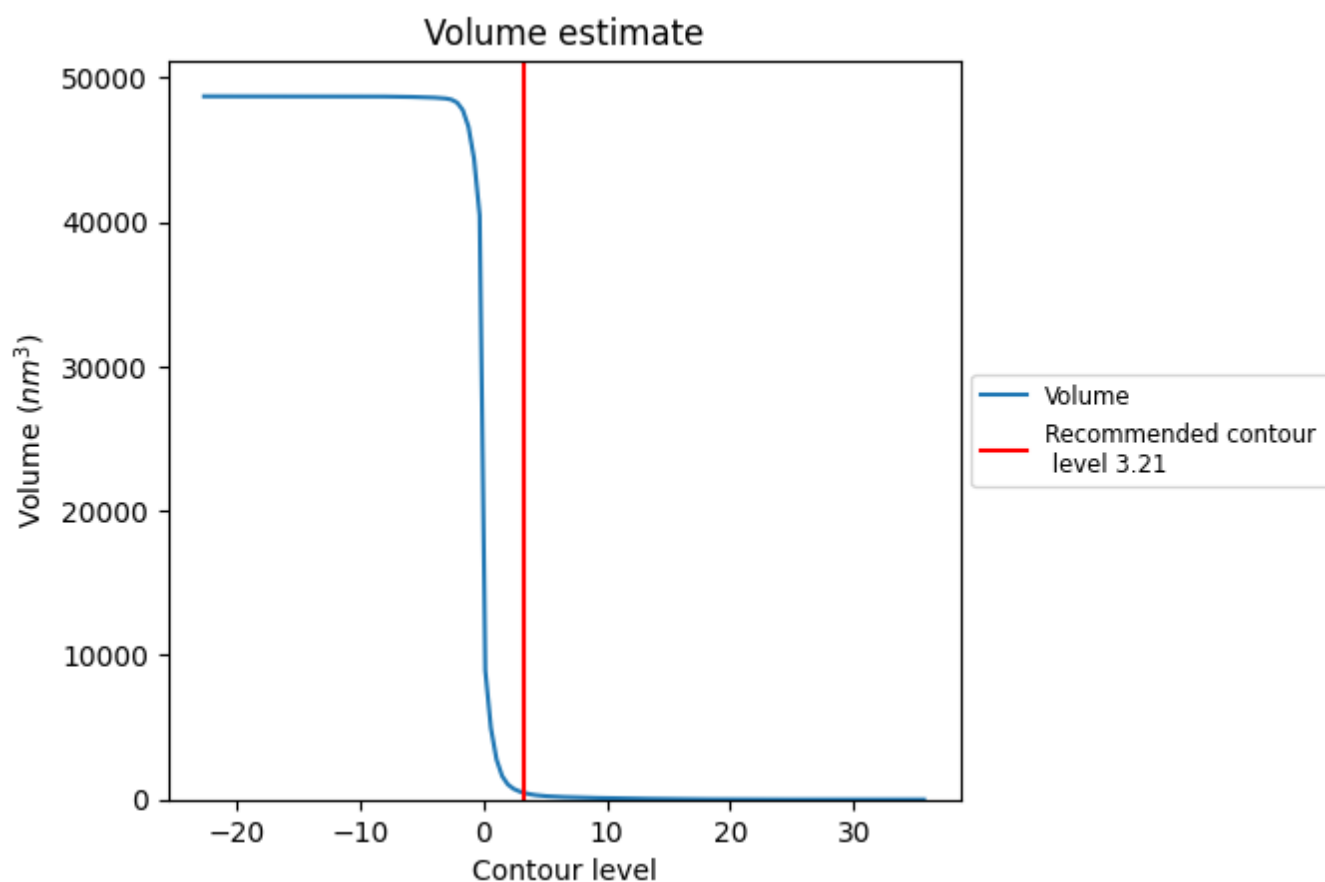
This section contains the results of statistical analysis of the map.

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



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

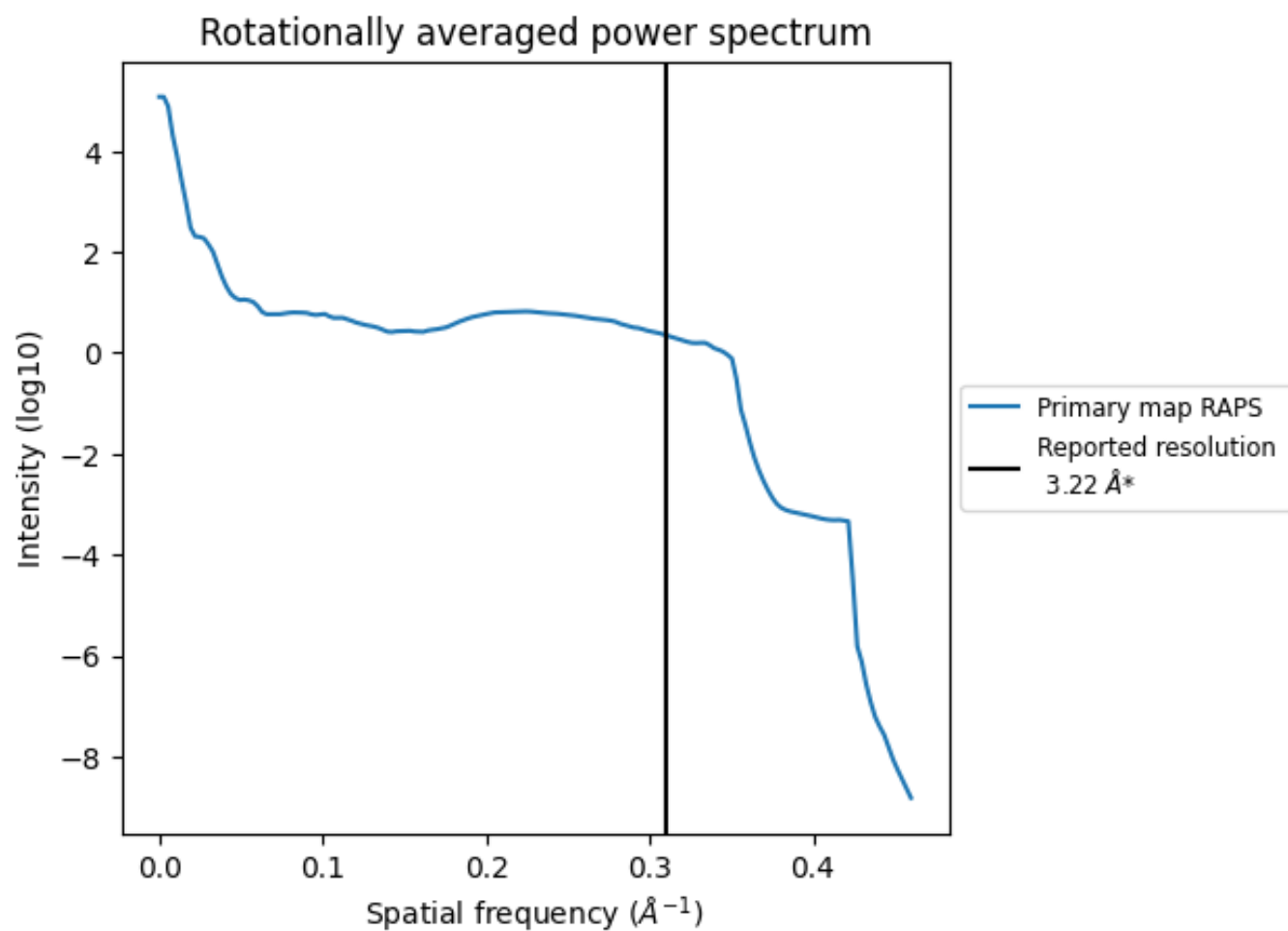
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 489 nm<sup>3</sup>; this corresponds to an approximate mass of 442 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 0.311 Å<sup>-1</sup>

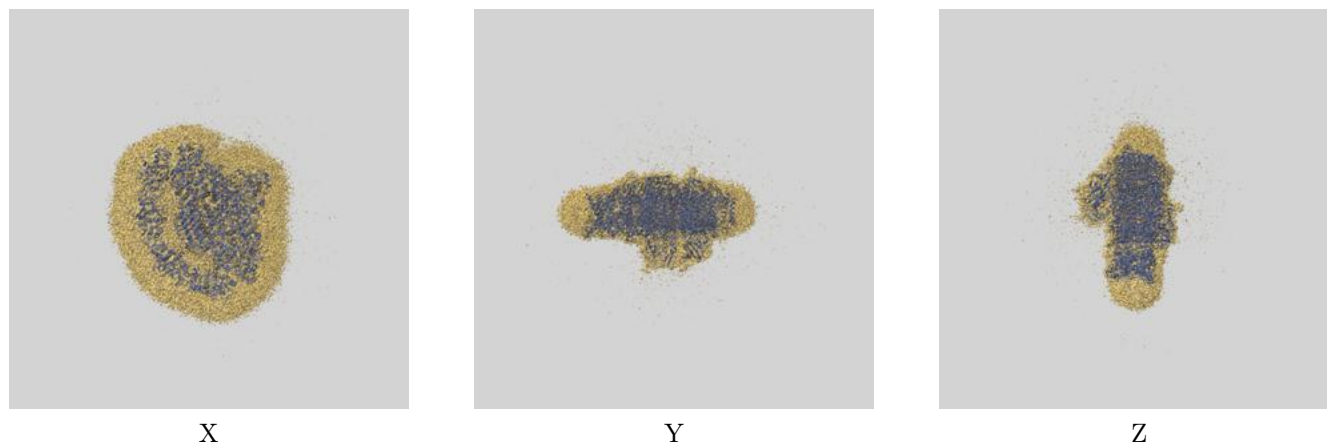
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

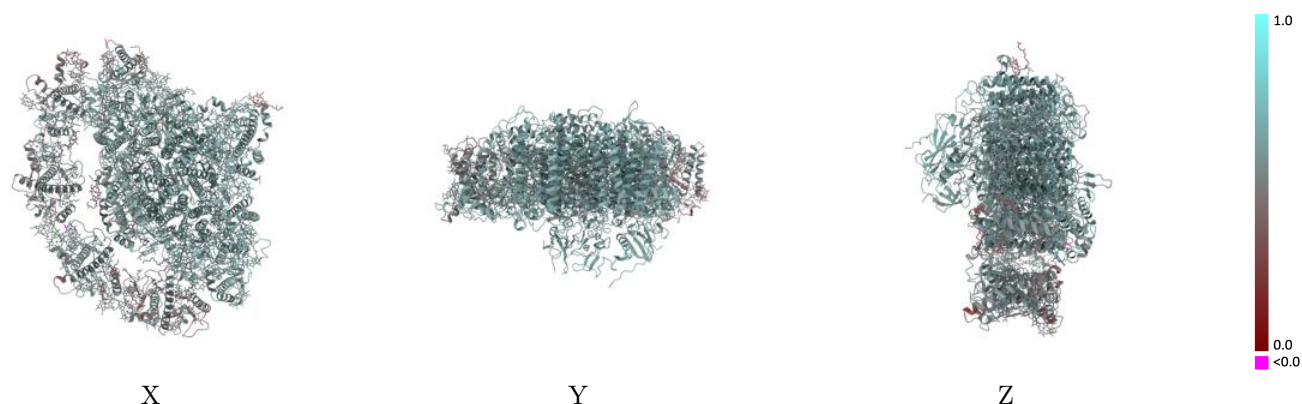
This section contains information regarding the fit between EMDB map EMD-36037 and PDB model 8J7B. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

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



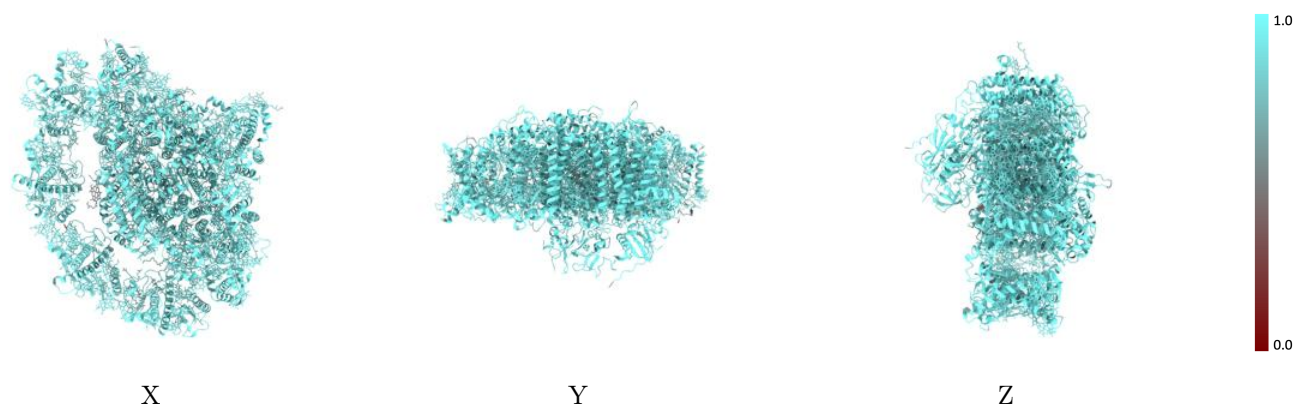
The images above show the 3D surface view of the map at the recommended contour level 3.21 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



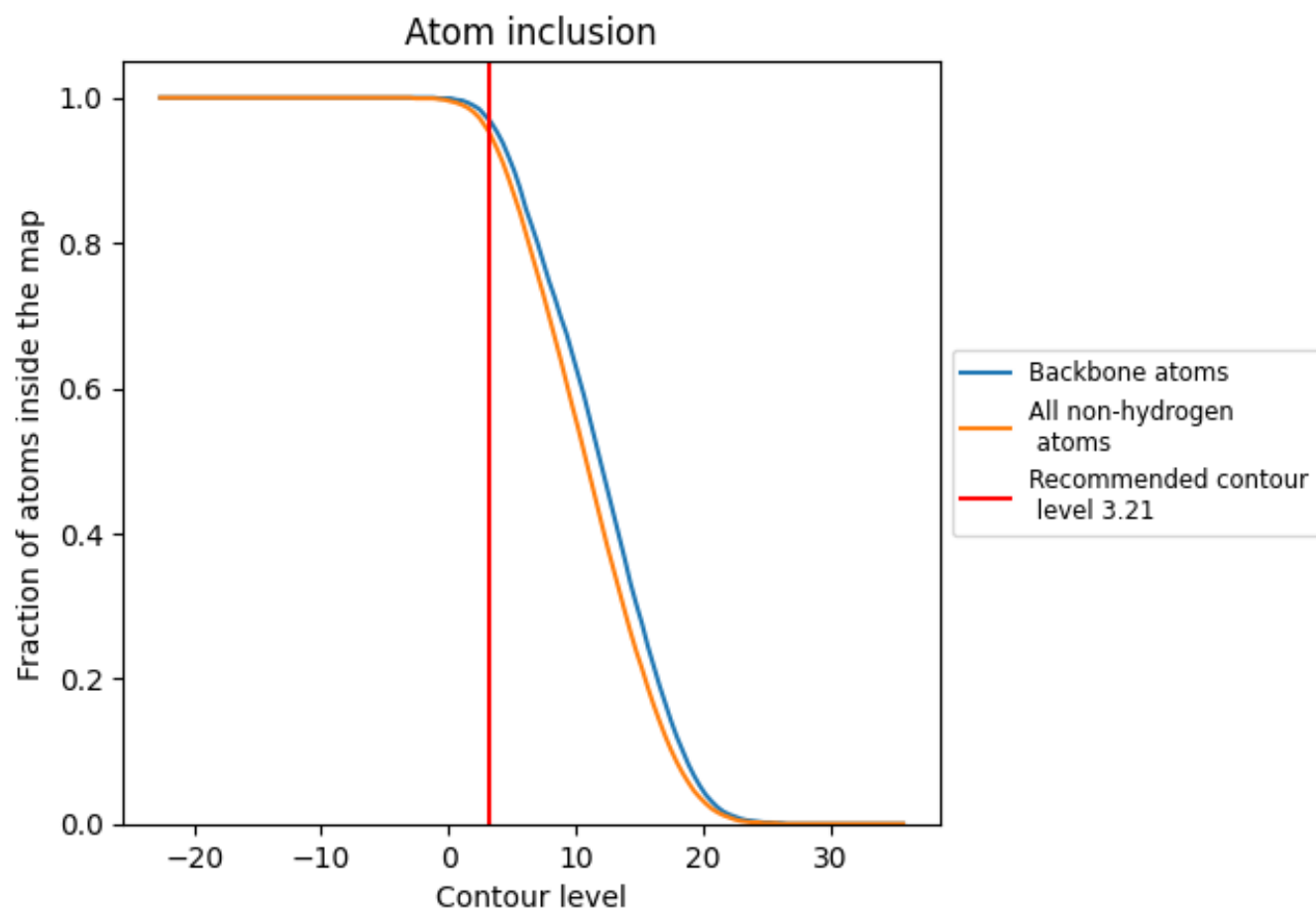
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.21).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (3.21) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.9520 | <div><div></div></div> 0.5760 |
| 1     | <div><div></div></div> 0.9220 | <div><div></div></div> 0.4980 |
| 2     | <div><div></div></div> 0.9450 | <div><div></div></div> 0.5180 |
| 3     | <div><div></div></div> 0.9450 | <div><div></div></div> 0.5120 |
| 4     | <div><div></div></div> 0.9520 | <div><div></div></div> 0.5350 |
| A     | <div><div></div></div> 0.9570 | <div><div></div></div> 0.6050 |
| B     | <div><div></div></div> 0.9670 | <div><div></div></div> 0.6150 |
| C     | <div><div></div></div> 0.9810 | <div><div></div></div> 0.6130 |
| D     | <div><div></div></div> 0.9770 | <div><div></div></div> 0.6080 |
| E     | <div><div></div></div> 0.9760 | <div><div></div></div> 0.6050 |
| F     | <div><div></div></div> 0.9210 | <div><div></div></div> 0.5690 |
| G     | <div><div></div></div> 0.9520 | <div><div></div></div> 0.5730 |
| H     | <div><div></div></div> 0.9350 | <div><div></div></div> 0.5650 |
| I     | <div><div></div></div> 0.9790 | <div><div></div></div> 0.6000 |
| J     | <div><div></div></div> 0.8600 | <div><div></div></div> 0.5340 |
| K     | <div><div></div></div> 0.8620 | <div><div></div></div> 0.4680 |
| L     | <div><div></div></div> 0.9610 | <div><div></div></div> 0.5960 |

1.0

0.0

<0.0