



## wwPDB EM Validation Summary Report ⓘ

Sep 14, 2026 – 12:32 PM JST

PDB ID : 7DZ8 / pdb\_00007dz8  
EMDB ID : EMD-30926  
Title : State transition supercomplex PSI-LHCI-LHCII from the LhcbM1 lacking mutant of *Chlamydomonas reinhardtii*  
Authors : Pan, X.W.; Li, A.J.; Liu, Z.F.; Li, M.  
Deposited on : 2021-01-23  
Resolution : 3.16 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

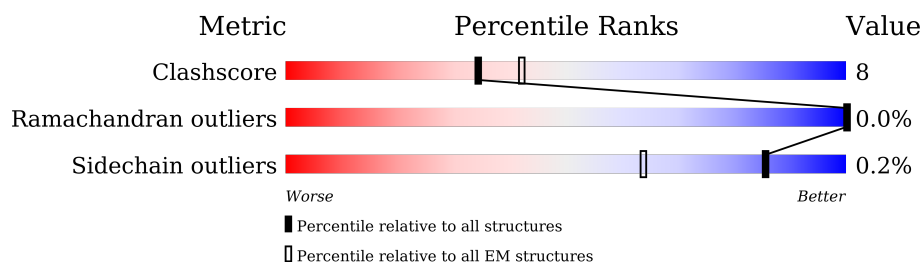
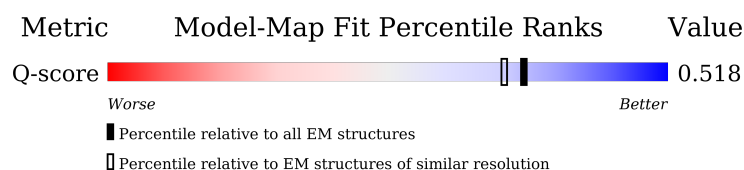
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.16 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.



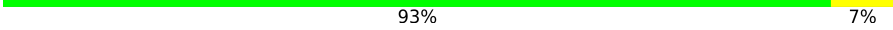
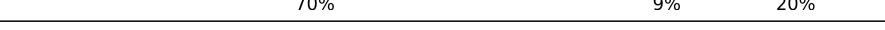
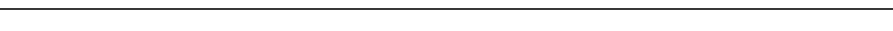
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14474 ( 2.66 - 3.66 )                                    |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|-------------------|
| 1   | A     | 751    | <br>84% 15% .     |
| 2   | B     | 735    | <br>82% 18%       |
| 3   | C     | 81     | <br>78% 19% ...   |
| 4   | D     | 196    | <br>62% 10% . 27% |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 5   | E     | 97     |    |
| 6   | F     | 227    |    |
| 7   | G     | 126    |    |
| 8   | H     | 130    |    |
| 9   | I     | 106    |    |
| 10  | J     | 41     |    |
| 11  | K     | 113    |    |
| 12  | L     | 196    |    |
| 13  | O     | 126    |    |
| 14  | 1     | 228    |    |
| 14  | a     | 228    |    |
| 15  | 2     | 246    |   |
| 16  | 3     | 298    |  |
| 17  | 4     | 264    |  |
| 18  | 5     | 257    |  |
| 19  | 6     | 257    |  |
| 20  | 7     | 241    |  |
| 21  | 8     | 243    |  |
| 22  | 9     | 213    |  |
| 23  | W     | 249    |  |
| 23  | X     | 249    |  |
| 24  | U     | 257    |  |
| 24  | Y     | 257    |  |
| 24  | Z     | 257    |  |
| 25  | V     | 268    |  |

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 69460 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 Photosystem I P700 chlorophyll a apoprotein A1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 741      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5819  | 3805 | 993 | 999 | 22 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 2   | B     | 733      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5824  | 3825 | 977 | 1004 | 18 |         |       |

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | C     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 600   | 369 | 103 | 116 | 12 |         |       |

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1124  | 719 | 199 | 199 | 7 |         |       |

- Molecule 5 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 5   | E     | 63       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 496   | 316 | 87 | 93 |         |       |

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 165      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1265  | 817 | 213 | 232 | 3 |         |       |



- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 7   | G     | 94       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 699   | 449 | 118 | 132 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 776   | 482 | 138 | 154 | 2 |         |       |

- Molecule 9 is a protein called Photosystem I reaction center subunit VIII.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | I     | 42       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 316   | 217 | 45 | 53 | 1 |         |       |

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10  | J     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 337   | 231 | 47 | 58 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | K     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 582   | 370 | 100 | 110 | 2 |         |       |

- Molecule 12 is a protein called PSI subunit V.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | L     | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1161  | 757 | 189 | 212 | 3 |         |       |

- Molecule 13 is a protein called Photosystem I subunit O.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 13  | O     | 97       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 758   | 503 | 123 | 132 |         |       |

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | 1     | 194      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1444  | 941 | 240 | 260 | 3 |         |       |
| 14  | a     | 194      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1444  | 941 | 240 | 260 | 3 |         |       |

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | 2     | 217      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1682  | 1094 | 274 | 304 | 10 |         |       |

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | 3     | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1678  | 1097 | 270 | 303 | 8 |         |       |

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | 4     | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1631  | 1071 | 263 | 292 | 5 |         |       |

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 18  | 5     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1774  | 1154 | 297 | 315 | 8 |         |       |

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 19  | 6     | 230      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1771  | 1167 | 293 | 305 | 6 |         |       |

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20  | 7     | 213      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1649  | 1072 | 274 | 297 | 6 |         |       |

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21  | 8     | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1641  | 1067 | 279 | 291 | 4 |         |       |

- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | 9     | 183      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1403  | 909 | 235 | 252 | 7 |         |       |

- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 23  | X     | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1680  | 1091 | 274 | 310 | 5 |         |       |
| 23  | W     | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1671  | 1085 | 273 | 308 | 5 |         |       |

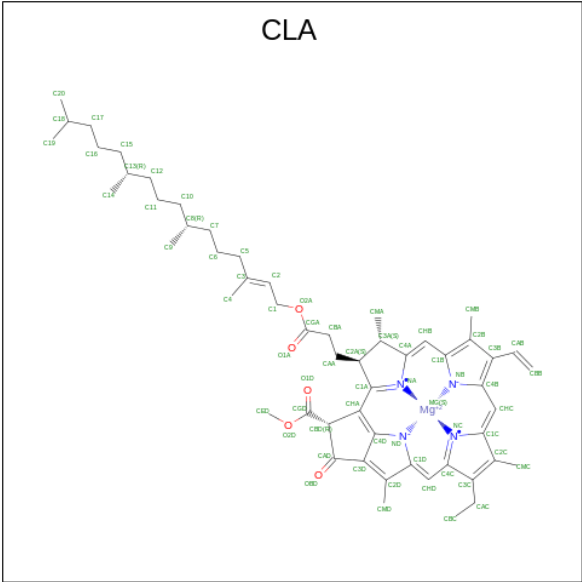
- Molecule 24 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 24  | Y     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1675  | 1084 | 272 | 314 | 5 |         |       |
| 24  | Z     | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1684  | 1089 | 274 | 316 | 5 |         |       |
| 24  | U     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1669  | 1080 | 272 | 312 | 5 |         |       |

- Molecule 25 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 25  | V     | 238      | Total | C    | N   | O   | P S | 0       | 0     |
|     |       |          | 1815  | 1176 | 300 | 333 | 1 5 |         |       |

- Molecule 26 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 |
|-----|-------|----------|-------|----|----|---|---|---------|
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 53    | 43 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 64    | 55 | 1  | 4 | 4 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 26  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | A     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | A     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>64 | C<br>55 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 26  | B     | 1        | Total<br>52 | C<br>43 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 26  | B     | 1        | Total<br>43 | C<br>35 | Mg<br>1 | N<br>4 | O<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 26  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>43 | C<br>35 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | B     | 1        | Total<br>54 | C<br>45 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 26  | B     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>43 | C<br>33 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>62 | C<br>52 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>62 | C<br>52 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>43 | C<br>35 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 26  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | F     | 1        | Total<br>57 | C<br>47 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | F     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | F     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | G     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | G     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | H     | 1        | Total<br>39 | C<br>31 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | H     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | J     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | K     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | K     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | K     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | K     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | L     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 26  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | L     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | L     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | L     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | O     | 1        | Total<br>38 | C<br>30 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | O     | 1        | Total<br>38 | C<br>30 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | O     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 1     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 1     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 1     | 1        | Total<br>53 | C<br>44 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 26  | 1     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 1     | 1        | Total<br>39 | C<br>32 | Mg<br>1 | N<br>4 | O<br>2 | 0       |
| 26  | 1     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 1     | 1        | Total<br>44 | C<br>34 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 1     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 1     | 1        | Total<br>39 | C<br>31 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 1     | 1        | Total<br>57 | C<br>47 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 1     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 1     | 1        | Total<br>37 | C<br>29 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 1     | 1        | Total<br>43 | C<br>33 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 26  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 26  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 26  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 45 | 1  | 4 | 4 |         |
| 26  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 26  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 35 | 1  | 4 | 4 |         |
| 26  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 26  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 26  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 64    | 54 | 1  | 4 | 5 |         |
| 26  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 26  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 30 | 1  | 4 | 3 |         |
| 26  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 26  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 26  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 26  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 26  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 63    | 54 | 1  | 3 | 5 |         |
| 26  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 26  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 26  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 35 | 1  | 4 | 3 |         |
| 26  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 26  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 26  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 26  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 26  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 26  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 26  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 33 | 1  | 4 | 5 |         |
| 26  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 26  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 26  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 26  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 26  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 26  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 26  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 30 | 1  | 4 | 3 |         |
| 26  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 35 | 1  | 4 | 3 |         |
| 26  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 53    | 44 | 1  | 4 | 4 |         |
| 26  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 40    | 32 | 1  | 4 | 3 |         |
| 26  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 40    | 32 | 1  | 4 | 3 |         |
| 26  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 40    | 32 | 1  | 4 | 3 |         |
| 26  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 26  | 4     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 4     | 1        | Total<br>44 | C<br>34 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 4     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 4     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 4     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 4     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 4     | 1        | Total<br>57 | C<br>47 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 4     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 4     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 4     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 4     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 4     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 4     | 1        | Total<br>43 | C<br>33 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 4     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 5     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 5     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 5     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 5     | 1        | Total<br>63 | C<br>53 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 5     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 5     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 5     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 26  | 5     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 5     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 5     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 5     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 5     | 1        | Total<br>64 | C<br>55 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 26  | 5     | 1        | Total<br>44 | C<br>34 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 5     | 1        | Total<br>42 | C<br>33 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 26  | 5     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 5     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 5     | 1        | Total<br>43 | C<br>33 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 6     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 6     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 6     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 6     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 6     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 6     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 6     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 6     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 6     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 6     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 6     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 26  | 6     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 6     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 6     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 6     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 6     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 6     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 7     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 7     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 7     | 1        | Total<br>44 | C<br>34 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 7     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 7     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 7     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 7     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 7     | 1        | Total<br>44 | C<br>35 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 26  | 7     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 7     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 7     | 1        | Total<br>44 | C<br>34 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 7     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 7     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 7     | 1        | Total<br>42 | C<br>33 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 26  | 7     | 1        | Total<br>43 | C<br>33 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 26  | 8     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 8     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 8     | 1        | Total<br>44 | C<br>34 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 8     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 8     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 8     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 8     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 8     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 8     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 8     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 8     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 8     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 8     | 1        | Total<br>53 | C<br>43 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 8     | 1        | Total<br>43 | C<br>33 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 9     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 9     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 9     | 1        | Total<br>44 | C<br>34 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 9     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 9     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 9     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 9     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 26  | 9     | 1        | Total<br>57 | C<br>47 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 9     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 9     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | 9     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | 9     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | X     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | X     | 1        | Total<br>62 | C<br>52 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | X     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | X     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | X     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | X     | 1        | Total<br>43 | C<br>35 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | X     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | X     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | Y     | 1        | Total<br>58 | C<br>48 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | Y     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | Y     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | Y     | 1        | Total<br>43 | C<br>35 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 26  | Y     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 26  | Y     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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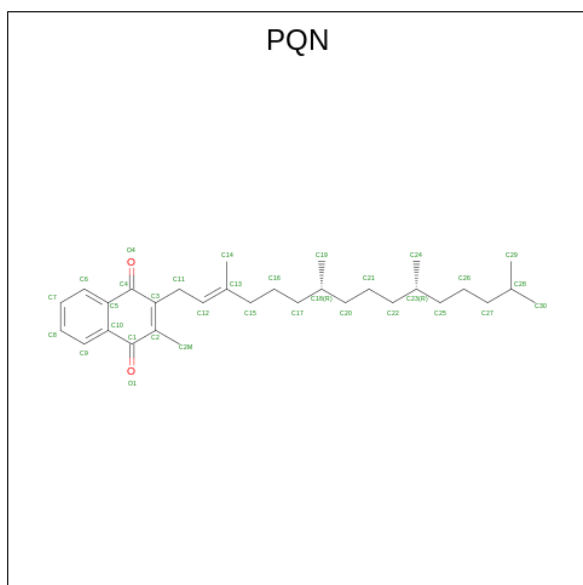
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 26  | Z     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |
| 26  | Z     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 26  | Z     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 40 | 1  | 4 | 4 |         |
| 26  | Z     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | Z     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 26  | Z     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 26  | Z     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | Z     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 38 | 1  | 4 | 5 |         |
| 26  | U     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 26  | U     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 26  | U     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 39 | 1  | 4 | 4 |         |
| 26  | U     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 26  | U     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 26  | U     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 26  | U     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 26  | U     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 26  | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 26  | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 26  | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 26  | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 62    | 52 | 1  | 4 | 5 |         |
| 26  | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 35 | 1  | 4 | 3 |         |

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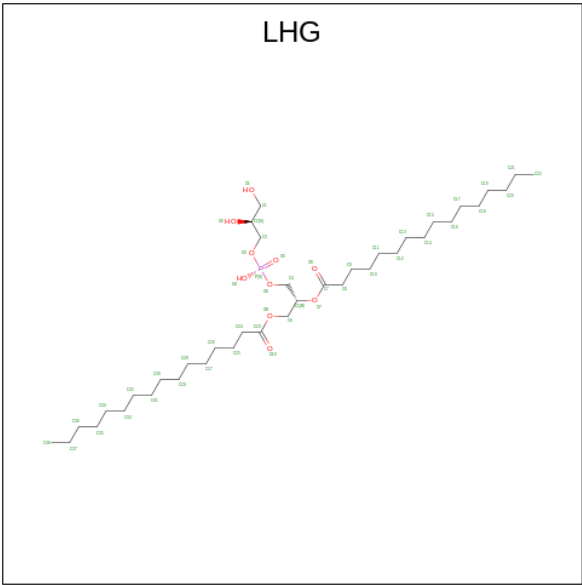
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 26  | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 26  | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 26  | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 26  | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 26  | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 26  | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 26  | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 57    | 47 | 1  | 4 | 5 |         |
| 26  | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 26  | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 26  | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

- Molecule 27 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 27  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 27  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



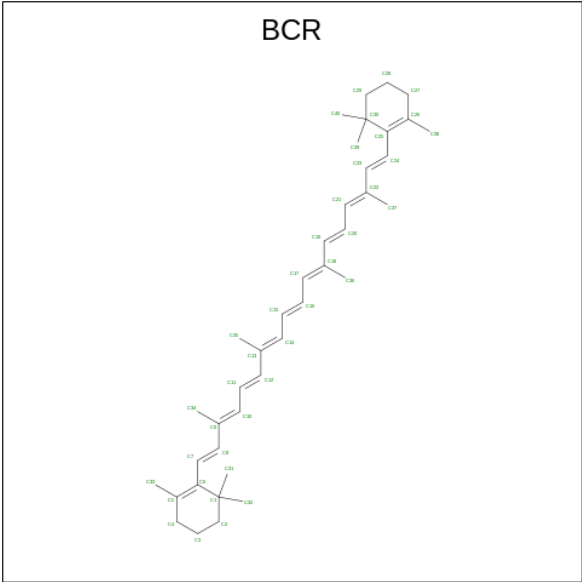
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 28  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 30    | 19 | 10 | 1 |         |
| 28  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 38    | 27 | 10 | 1 |         |
| 28  | H     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | O     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 36    | 25 | 10 | 1 |         |
| 28  | 1     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |
| 28  | 2     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 36    | 25 | 10 | 1 |         |

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| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 28  | 3     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 45    | 34 | 10 | 1 |         |
| 28  | 3     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | 4     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | 5     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | 5     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | 6     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 48    | 37 | 10 | 1 |         |
| 28  | 7     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |
| 28  | 8     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | 8     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 40    | 29 | 10 | 1 |         |
| 28  | 9     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 30    | 19 | 10 | 1 |         |
| 28  | 9     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | 9     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | X     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | Y     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | Z     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | U     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | V     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 36    | 25 | 10 | 1 |         |
| 28  | W     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 34    | 23 | 10 | 1 |         |

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 29  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 29  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 29  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 29  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 29  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 29  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 29  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 29  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 29  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 29  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 29  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 29  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 29  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

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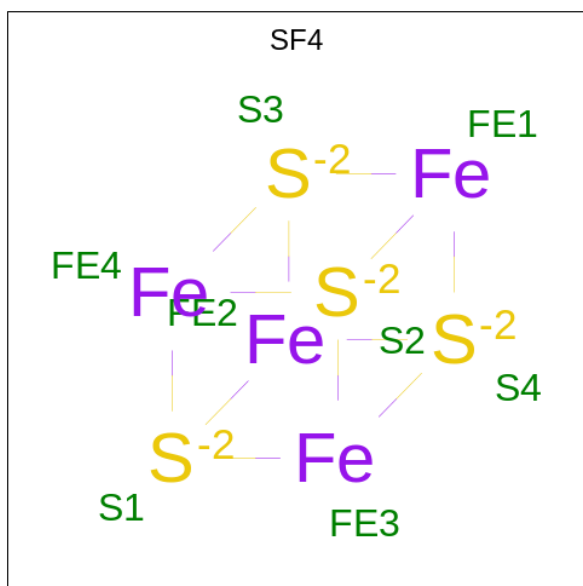
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 29  | B     | 1        | Total C<br>40 40 | 0       |
| 29  | B     | 1        | Total C<br>40 40 | 0       |
| 29  | F     | 1        | Total C<br>40 40 | 0       |
| 29  | G     | 1        | Total C<br>40 40 | 0       |
| 29  | J     | 1        | Total C<br>40 40 | 0       |
| 29  | K     | 1        | Total C<br>40 40 | 0       |
| 29  | K     | 1        | Total C<br>40 40 | 0       |
| 29  | L     | 1        | Total C<br>40 40 | 0       |
| 29  | L     | 1        | Total C<br>40 40 | 0       |
| 29  | L     | 1        | Total C<br>40 40 | 0       |
| 29  | L     | 1        | Total C<br>40 40 | 0       |
| 29  | O     | 1        | Total C<br>40 40 | 0       |
| 29  | O     | 1        | Total C<br>40 40 | 0       |
| 29  | 1     | 1        | Total C<br>40 40 | 0       |
| 29  | a     | 1        | Total C<br>40 40 | 0       |
| 29  | 2     | 1        | Total C<br>40 40 | 0       |
| 29  | 3     | 1        | Total C<br>40 40 | 0       |
| 29  | 3     | 1        | Total C<br>40 40 | 0       |
| 29  | 3     | 1        | Total C<br>40 40 | 0       |
| 29  | 4     | 1        | Total C<br>40 40 | 0       |
| 29  | 5     | 1        | Total C<br>40 40 | 0       |

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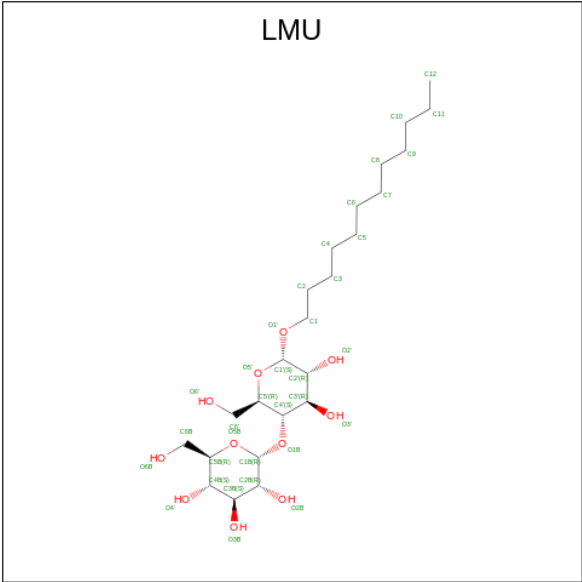
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 29  | 6     | 1        | Total C<br>40 40 | 0       |
| 29  | 7     | 1        | Total C<br>40 40 | 0       |
| 29  | 7     | 1        | Total C<br>40 40 | 0       |
| 29  | 8     | 1        | Total C<br>40 40 | 0       |
| 29  | 9     | 1        | Total C<br>40 40 | 0       |

- Molecule 30 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



| Mol | Chain | Residues | Atoms               | AltConf |
|-----|-------|----------|---------------------|---------|
| 30  | A     | 1        | Total Fe S<br>8 4 4 | 0       |
| 30  | C     | 1        | Total Fe S<br>8 4 4 | 0       |
| 30  | C     | 1        | Total Fe S<br>8 4 4 | 0       |

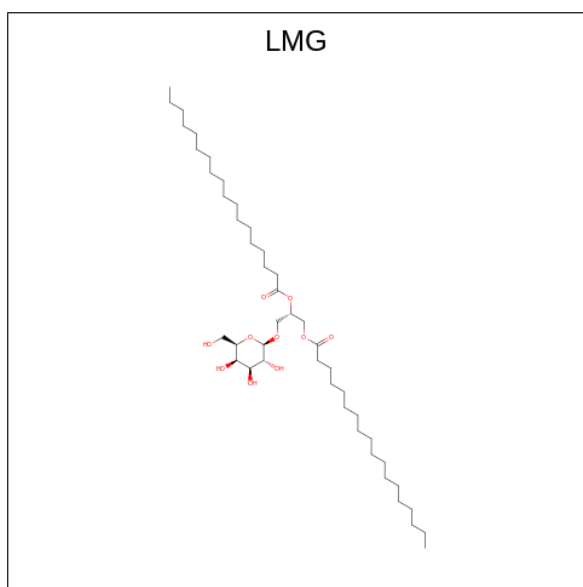
- Molecule 31 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula:  $\text{C}_{24}\text{H}_{46}\text{O}_{11}$ ).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 31  | A     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 31  | A     | 1        | Total | C  | O  | 0       |
|     |       |          | 34    | 24 | 10 |         |
| 31  | K     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 31  | 1     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 31  | 5     | 1        | Total | C  | O  | 0       |
|     |       |          | 33    | 22 | 11 |         |
| 31  | 5     | 1        | Total | C  | O  | 0       |
|     |       |          | 32    | 21 | 11 |         |
| 31  | 8     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

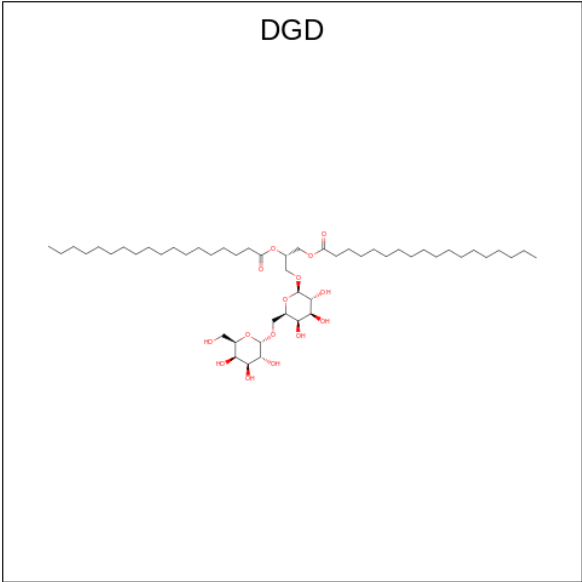
- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).





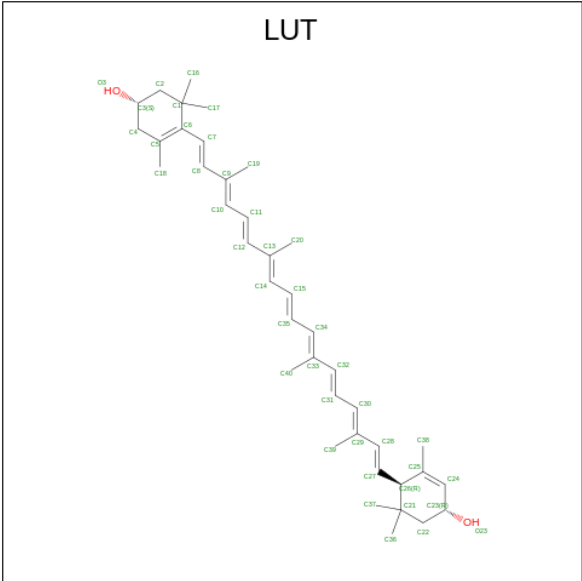
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 32  | A     | 1        | Total | C  | O  | 0       |
|     |       |          | 40    | 30 | 10 |         |
| 32  | H     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |
| 32  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 42    | 32 | 10 |         |
| 32  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 40    | 30 | 10 |         |
| 32  | L     | 1        | Total | C  | O  | 0       |
|     |       |          | 37    | 27 | 10 |         |
| 32  | 4     | 1        | Total | C  | O  | 0       |
|     |       |          | 40    | 30 | 10 |         |
| 32  | 4     | 1        | Total | C  | O  | 0       |
|     |       |          | 40    | 30 | 10 |         |
| 32  | 5     | 1        | Total | C  | O  | 0       |
|     |       |          | 40    | 30 | 10 |         |
| 32  | 8     | 1        | Total | C  | O  | 0       |
|     |       |          | 46    | 36 | 10 |         |
| 32  | 9     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |
| 32  | V     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 33  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 15 |         |

- Molecule 34 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



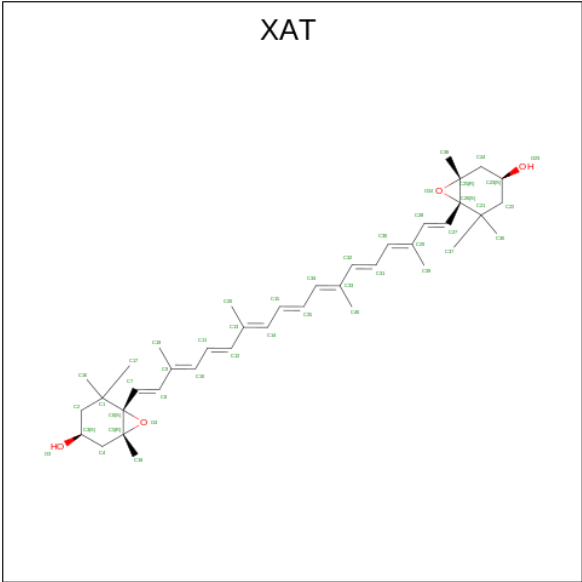
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 34  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 34  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

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| Mol | Chain | Residues | Atoms       |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|
| 34  | 2     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | 3     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | 4     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | 5     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | 6     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | 7     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | 8     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | 9     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | X     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | X     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | Y     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | Y     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | Z     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | Z     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | U     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | U     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | V     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | V     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | W     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |
| 34  | W     | 1        | Total<br>42 | C<br>40 | O<br>2 | 0       |

- Molecule 35 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>).



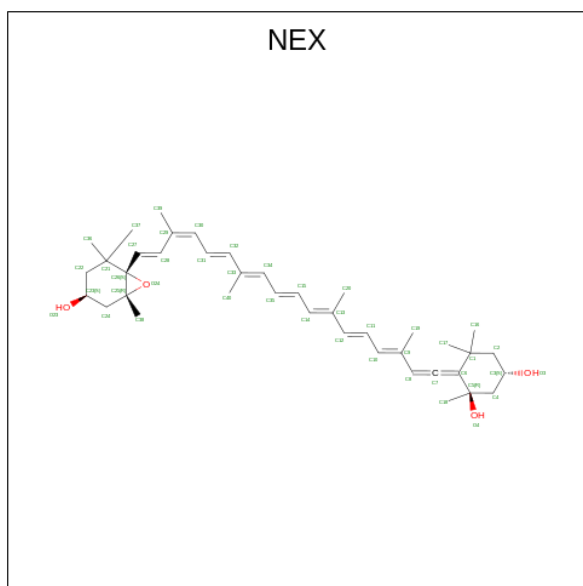
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 35  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 35  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 35  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 35  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 35  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 35  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 35  | 6     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 35  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 35  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 35  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 35  | X     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 35  | Y     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 35  | Z     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 35  | U     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

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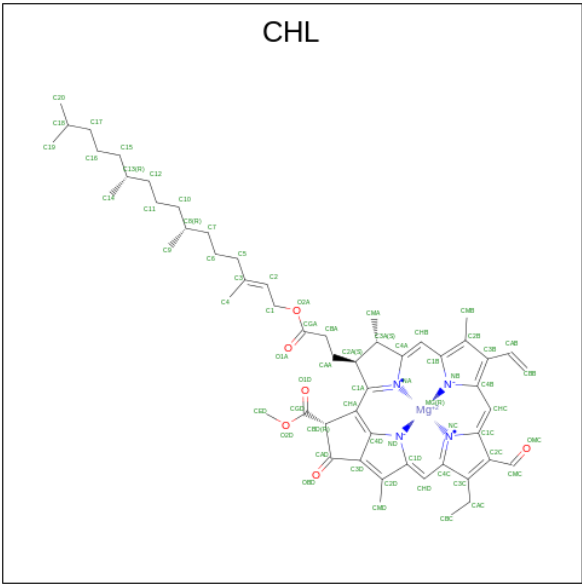
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 35  | V     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 35  | W     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

- Molecule 36 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 36  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 36  | 6     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 36  | X     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 36  | Y     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 36  | Z     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 36  | U     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 36  | V     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 36  | W     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

- Molecule 37 is CHLOROPHYLL B (CCD ID: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 37  | X     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 37  | X     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 37  | X     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 35 | 1  | 4 | 4 |         |
| 37  | X     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 37  | X     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 37  | X     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 37  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 37  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 33 | 1  | 4 | 4 |         |
| 37  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 37  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 37  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 38 | 1  | 4 | 6 |         |
| 37  | Y     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 37  | Z     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 37  | Z     | 1        | Total<br>42 | C<br>33 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 37  | Z     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 37  | Z     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 37  | Z     | 1        | Total<br>49 | C<br>38 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 37  | Z     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 37  | U     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 37  | U     | 1        | Total<br>43 | C<br>34 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 37  | U     | 1        | Total<br>44 | C<br>35 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 37  | U     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 37  | U     | 1        | Total<br>44 | C<br>35 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 37  | U     | 1        | Total<br>60 | C<br>49 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 37  | V     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 37  | V     | 1        | Total<br>44 | C<br>35 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 37  | V     | 1        | Total<br>44 | C<br>35 | Mg<br>1 | N<br>4 | O<br>4 | 0       |
| 37  | V     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 37  | V     | 1        | Total<br>48 | C<br>37 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 37  | V     | 1        | Total<br>61 | C<br>50 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 37  | W     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 37  | W     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 37  | W     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |

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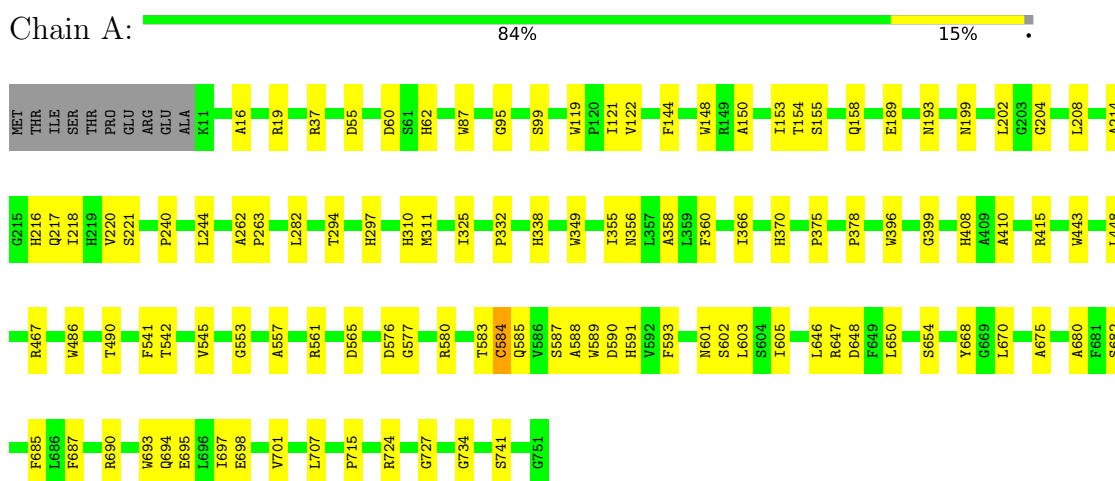
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 37  | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 54 | 1  | 4 | 6 |         |
| 37  | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 37  | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |



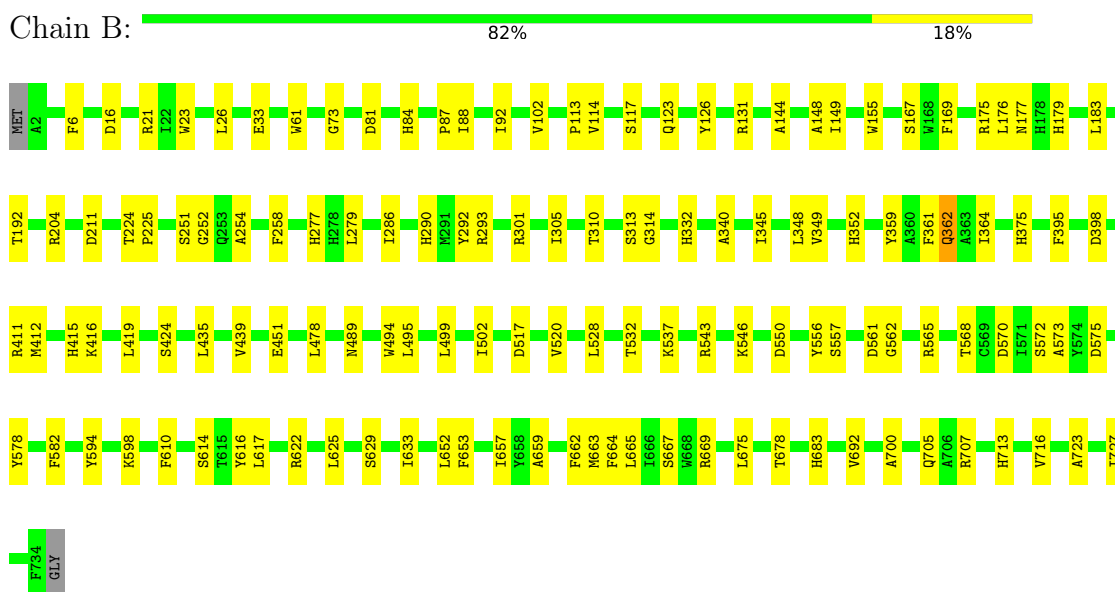
### 3 Residue-property plots

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center

| MET | A2 | C14 | T15 | P22 | G33 | C34 | K35 | A36 | S37 | Q38 | N39 | E55 | C58 | D61 | F62 | L63 | R66 | S71 | E72 | S73 | T74 | Y91 |
|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- Chain D:  62% 10% 27%

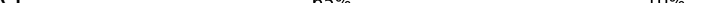
[illegible]

- Chain E:  60% 5% 35%

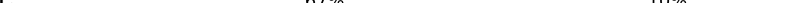
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | GLN | ALA | LEU | SER | SER | ARG | VAL | ASN | ILE | ALA | ALA | LYS | PRO | GLN | ARG | ALA | GLN | ARG | LEU | VAL | VAL | ARG | GLU | GLU | VAL | LYS | ALA | ALA | PRO | PRO | LYS | LYS | E34 | S50 | V67 | P70 | N86 | A89 | A96 | LYS |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- Chain F:  65% 7% 27%

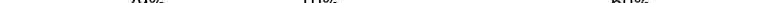
[illegible]

- Chain G:  65% 10% 25%

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|
| MET | GLN | THR | LEU | LEU | SER | ARG | PRO | SER | LEU | ARG | ALA | ALA | SER | ALA | ARG | VAL | ALA | ALA | PRO | ARG | ARG | ALA | ALA | PRO | PRO | VAL | ALA | ALA | LYS | THR | VAL | VAL | ALA | ALA | L32 | Q57 | R58 | R59 | E50 | A61 | S65 | T66 | V67 | G68 | T71 | T72 | G73 | A74 | T75 | T76 | T77 | D78 | Q81 | G94 | L125 | SER |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|

- Chain H:  67% 10% 23%

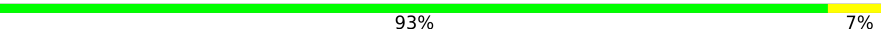
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|
| MET | ALA | LEU | VAL | ALA | ARG | PRO | VAL | VAL | SER | SER | ALA | ARG | VAL | ALA | ALA | ALA | ALA | ARG | LYS | VAL | VAL | VAL | SER | SER | ALA | K31 | Y32 | G33 | E34 | E45 | R61 | Y62 | Q66 | I77 | S82 | L83 | R84 | G89 | T117 | N120 | L130 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|

- Chain I:  29% 10% 60%

MET ALA ALA LEU ARG ALA VAL SER ALA LYS SER ALA VAL ARG PRO THR VAL ALA ALA LEU LYS PRO GLN LYS MET MET ALA ALA ALA ALA ALA SER VAL ALA LEU LEU ALA ALA SER SER SER SER ALA GLU ALA ALA GLN VAL THR ALA VAL

ALA SER A63 Y67 P68 F69 A75 P76 S77 V80 P81 F96 I99 F103 SER

- Molecule 10: Photosystem I reaction center subunit IX

Chain J:  93% 7%

M1 Y7 T10 F41

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

Chain K:  65% 11% 24%

MET GLN ALA LEU MET THR ARG PRO SER SER ALA ILE ARG PRO THR LYS ALA ALA ARG ARG SER SER VAL VAL VAL ARG ALA ASP G28 M38 T56 V57 T62 A63 G64 L65 K66 D69 N72 S73 A74 G75 V76 I86 V89 L113

- Molecule 12: PSI subunit V

Chain L:  72% 9% 19%

MET ALA VAL ALA MET ARG SER THR SER THR LEU ARG ALA THR ALA ALA ARG ARG GLN MET PRO LEU GLY VAL GLY ARG VAL SER THR VAL ARG VAL THR K38 V42 D49 T57 P58 V59 T60 N71 A74 V79 A80 R84 E87 L90

L128 S137 K149 G177 W184 S196

- Molecule 13: Photosystem I subunit O

Chain O:  64% 13% 23%

MET ALA VAL ALA MET ARG SER SER ALA MET PRO ARG THR LEU ALA SER ARG ARG ARG VAL VAL VAL VAL E30 A31 S32 N33 D39 P45 P48 V49 L50 I57 P58 A59 V63 Q77 E81 T112 G120 G124 W126

- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

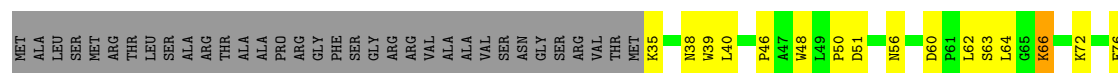
Chain 1:  65% 19% 15%

MET ALA LEU SER MET ARG THR LEU ALA THR ALA PRO ARG GLY PHE SER GLY ARG ARG VAL ALA VAL VAL SER ASN GLY SER VAL MET K35 N38 W39 L40 P41 W48 L49 P50 D51 N56 D60 P61 L62 S63 L64 K72 E76 V79

V89 A90 G91 V95 D105 A106 P107 K115 E122 D126 L127 L131 A137 E142 R145 G146 D147 G150 V151 V152 Y153 L161 K169 S170 L173 K174 I178 F191 F218 S224 V225 P226 F227 F228

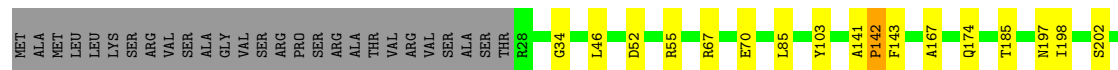
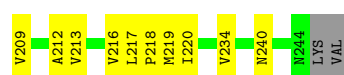
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain a:  68% 16% 15%



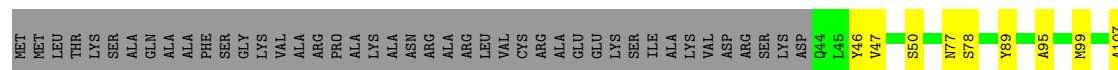
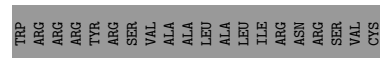
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 2: 77% 11% 12%



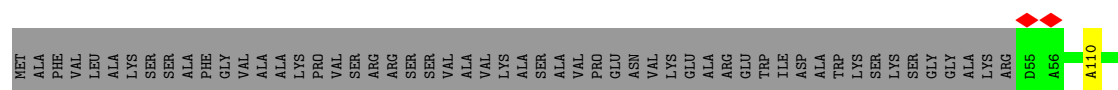
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 3: 63% 11% 26%



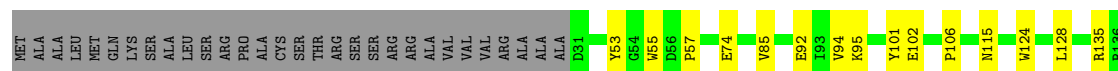
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 4: 70% 9% 20%



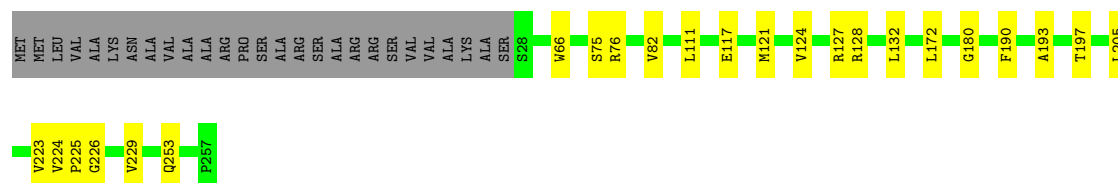
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 5: 74% 14% 12%



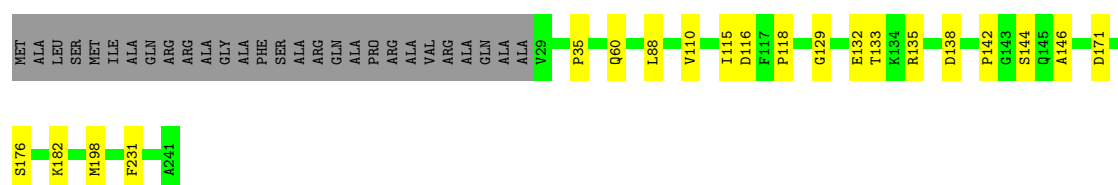
- Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 6:  81% 9% 11%



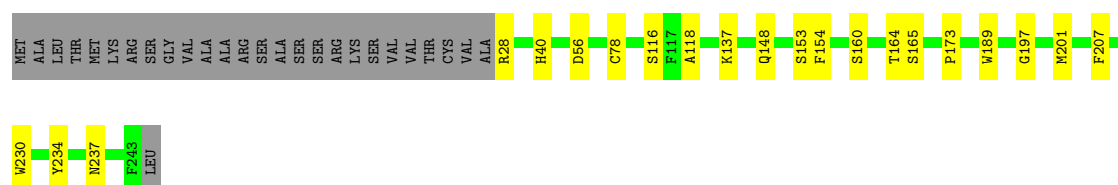
- Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 7:  80% 8% 12%



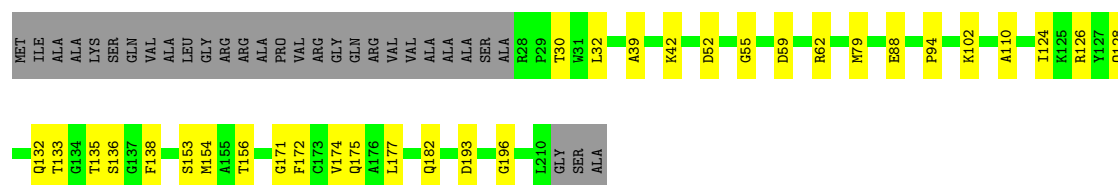
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain 8:  80% 9% 11%



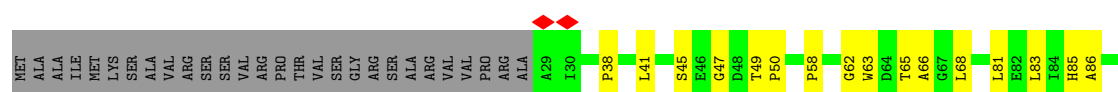
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

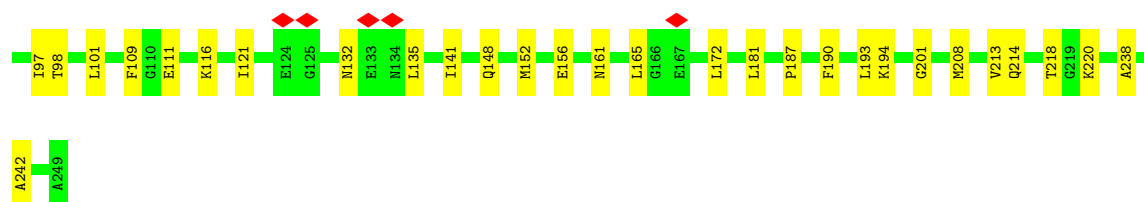
Chain 9:  71% 15% 14%



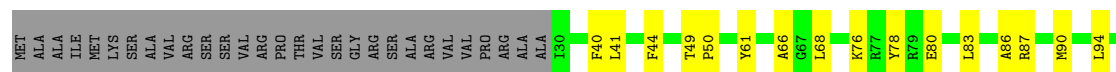
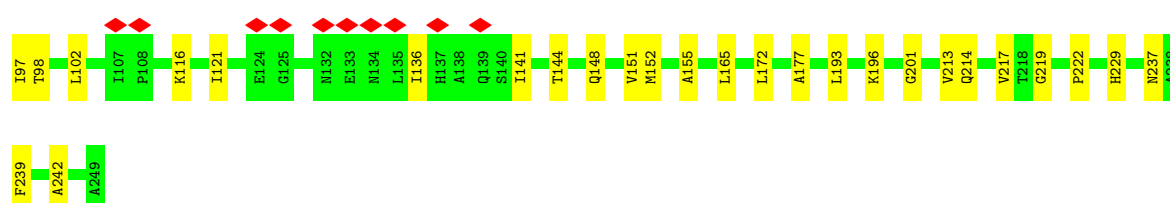
- Molecule 23: Chlorophyll a-b binding protein, chloroplastic

Chain X:  70% 18% 11%

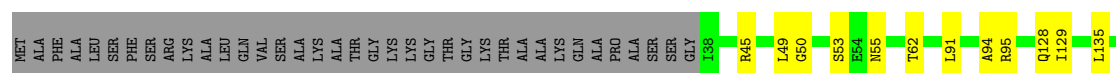




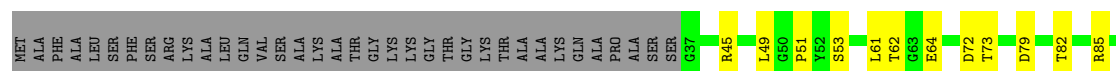
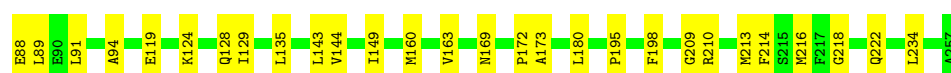
- Molecule 23: Chlorophyll a-b binding protein, chloroplastic



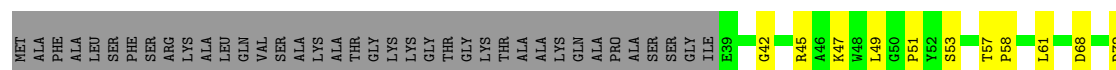
- Molecule 24: Chlorophyll a-b binding protein, chloroplastic

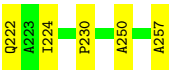


- Molecule 24: Chlorophyll a-b binding protein, chloroplastic

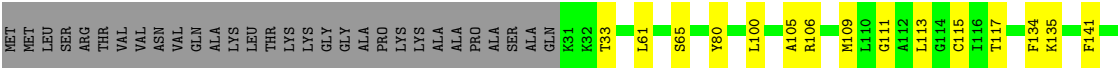


- Molecule 24: Chlorophyll a-b binding protein, chloroplastic





● Molecule 25: Chlorophyll a-b binding protein, chloroplastic



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 123997                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TALOS ARCTICA                       | Depositor |
| Voltage (kV)                         | 200                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 1.5625                                  | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.116                                   | Depositor |
| Minimum map value                    | -0.049                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.003                                   | Depositor |
| Recommended contour level            | 0.005                                   | Depositor |
| Map size (Å)                         | 360.0, 360.0, 360.0                     | wwPDB     |
| Map dimensions                       | 360, 360, 360                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.0, 1.0, 1.0                           | Depositor |



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.53         | 0/6015  | 0.39        | 0/8201         |
| 2   | B     | 0.52         | 0/6036  | 0.45        | 5/8242 (0.1%)  |
| 3   | C     | 0.51         | 0/610   | 0.62        | 1/826 (0.1%)   |
| 4   | D     | 0.44         | 0/1152  | 0.46        | 1/1556 (0.1%)  |
| 5   | E     | 0.41         | 0/506   | 0.34        | 0/689          |
| 6   | F     | 0.39         | 0/1291  | 0.37        | 0/1747         |
| 7   | G     | 0.27         | 0/714   | 0.34        | 0/972          |
| 8   | H     | 0.39         | 0/788   | 0.37        | 0/1059         |
| 9   | I     | 0.52         | 0/329   | 0.46        | 0/456          |
| 10  | J     | 0.45         | 0/349   | 0.33        | 0/478          |
| 11  | K     | 0.38         | 0/587   | 0.42        | 0/795          |
| 12  | L     | 0.47         | 0/1190  | 0.41        | 0/1628         |
| 13  | O     | 0.40         | 0/784   | 0.39        | 0/1069         |
| 14  | 1     | 0.37         | 0/1490  | 0.46        | 0/2028         |
| 14  | a     | 0.37         | 0/1490  | 0.46        | 0/2028         |
| 15  | 2     | 0.38         | 0/1730  | 0.43        | 0/2353         |
| 16  | 3     | 0.43         | 0/1726  | 0.38        | 0/2342         |
| 17  | 4     | 0.29         | 0/1686  | 0.34        | 0/2300         |
| 18  | 5     | 0.37         | 0/1829  | 0.40        | 0/2492         |
| 19  | 6     | 0.34         | 0/1833  | 0.38        | 0/2505         |
| 20  | 7     | 0.44         | 0/1701  | 0.38        | 0/2310         |
| 21  | 8     | 0.40         | 0/1692  | 0.37        | 0/2304         |
| 22  | 9     | 0.36         | 0/1444  | 0.43        | 0/1964         |
| 23  | W     | 0.22         | 0/1721  | 0.54        | 0/2341         |
| 23  | X     | 0.24         | 0/1730  | 0.54        | 0/2355         |
| 24  | U     | 0.23         | 0/1717  | 0.55        | 1/2336 (0.0%)  |
| 24  | Y     | 0.25         | 0/1723  | 0.53        | 0/2345         |
| 24  | Z     | 0.23         | 0/1732  | 0.53        | 0/2357         |
| 25  | V     | 0.22         | 0/1856  | 0.46        | 0/2518         |
| All | All   | 0.41         | 0/47451 | 0.44        | 8/64596 (0.0%) |

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | D     | 150 | LEU  | N-CA-C | 7.75  | 122.50      | 112.12   |
| 24  | U     | 116 | GLN  | N-CA-C | 6.74  | 118.62      | 111.28   |
| 2   | B     | 495 | LEU  | N-CA-C | 5.71  | 121.31      | 113.77   |
| 2   | B     | 362 | GLN  | N-CA-C | -5.51 | 101.81      | 110.36   |
| 2   | B     | 310 | THR  | CA-C-N | -5.44 | 114.78      | 120.38   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5819  | 0        | 5670     | 87      | 0            |
| 2   | B     | 5824  | 0        | 5579     | 104     | 0            |
| 3   | C     | 600   | 0        | 581      | 15      | 0            |
| 4   | D     | 1124  | 0        | 1139     | 16      | 0            |
| 5   | E     | 496   | 0        | 491      | 5       | 0            |
| 6   | F     | 1265  | 0        | 1301     | 19      | 0            |
| 7   | G     | 699   | 0        | 681      | 11      | 0            |
| 8   | H     | 776   | 0        | 765      | 10      | 0            |
| 9   | I     | 316   | 0        | 321      | 9       | 0            |
| 10  | J     | 337   | 0        | 336      | 2       | 0            |
| 11  | K     | 582   | 0        | 620      | 10      | 0            |
| 12  | L     | 1161  | 0        | 1184     | 15      | 0            |
| 13  | O     | 758   | 0        | 740      | 13      | 0            |
| 14  | 1     | 1444  | 0        | 1396     | 34      | 0            |
| 14  | a     | 1444  | 0        | 1396     | 27      | 0            |
| 15  | 2     | 1682  | 0        | 1665     | 22      | 0            |
| 16  | 3     | 1678  | 0        | 1637     | 25      | 0            |
| 17  | 4     | 1631  | 0        | 1587     | 18      | 0            |
| 18  | 5     | 1774  | 0        | 1746     | 42      | 0            |
| 19  | 6     | 1771  | 0        | 1770     | 21      | 0            |
| 20  | 7     | 1649  | 0        | 1589     | 15      | 0            |
| 21  | 8     | 1641  | 0        | 1618     | 23      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | 9     | 1403  | 0        | 1381     | 21      | 0            |
| 23  | W     | 1671  | 0        | 1604     | 30      | 0            |
| 23  | X     | 1680  | 0        | 1622     | 32      | 0            |
| 24  | U     | 1669  | 0        | 1603     | 40      | 0            |
| 24  | Y     | 1675  | 0        | 1617     | 26      | 0            |
| 24  | Z     | 1684  | 0        | 1625     | 29      | 0            |
| 25  | V     | 1815  | 0        | 1766     | 50      | 0            |
| 26  | 1     | 666   | 0        | 522      | 6       | 0            |
| 26  | 2     | 637   | 0        | 530      | 4       | 0            |
| 26  | 3     | 724   | 0        | 628      | 5       | 0            |
| 26  | 4     | 778   | 0        | 678      | 7       | 0            |
| 26  | 5     | 878   | 0        | 758      | 17      | 0            |
| 26  | 6     | 903   | 0        | 831      | 11      | 0            |
| 26  | 7     | 756   | 0        | 635      | 13      | 0            |
| 26  | 8     | 724   | 0        | 629      | 8       | 0            |
| 26  | 9     | 595   | 0        | 491      | 4       | 0            |
| 26  | A     | 2669  | 0        | 2693     | 56      | 0            |
| 26  | B     | 2284  | 0        | 2237     | 33      | 0            |
| 26  | F     | 140   | 0        | 113      | 6       | 0            |
| 26  | G     | 87    | 0        | 64       | 0       | 0            |
| 26  | H     | 104   | 0        | 93       | 0       | 0            |
| 26  | J     | 42    | 0        | 31       | 0       | 0            |
| 26  | K     | 191   | 0        | 150      | 3       | 0            |
| 26  | L     | 235   | 0        | 184      | 7       | 0            |
| 26  | O     | 116   | 0        | 61       | 0       | 0            |
| 26  | U     | 400   | 0        | 342      | 11      | 0            |
| 26  | V     | 415   | 0        | 365      | 11      | 0            |
| 26  | W     | 426   | 0        | 377      | 12      | 0            |
| 26  | X     | 436   | 0        | 415      | 16      | 0            |
| 26  | Y     | 429   | 0        | 389      | 10      | 0            |
| 26  | Z     | 427   | 0        | 386      | 17      | 0            |
| 26  | a     | 710   | 0        | 591      | 8       | 0            |
| 27  | A     | 33    | 0        | 46       | 2       | 0            |
| 27  | B     | 33    | 0        | 46       | 3       | 0            |
| 28  | 1     | 49    | 0        | 74       | 0       | 0            |
| 28  | 2     | 36    | 0        | 42       | 0       | 0            |
| 28  | 3     | 94    | 0        | 137      | 3       | 0            |
| 28  | 4     | 49    | 0        | 74       | 0       | 0            |
| 28  | 5     | 98    | 0        | 148      | 6       | 0            |
| 28  | 6     | 48    | 0        | 69       | 0       | 0            |
| 28  | 7     | 37    | 0        | 44       | 0       | 0            |
| 28  | 8     | 89    | 0        | 124      | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28  | 9     | 128   | 0        | 178      | 1       | 0            |
| 28  | A     | 128   | 0        | 178      | 0       | 0            |
| 28  | B     | 38    | 0        | 46       | 0       | 0            |
| 28  | H     | 49    | 0        | 74       | 0       | 0            |
| 28  | O     | 36    | 0        | 42       | 1       | 0            |
| 28  | U     | 49    | 0        | 74       | 1       | 0            |
| 28  | V     | 36    | 0        | 42       | 3       | 0            |
| 28  | W     | 34    | 0        | 38       | 1       | 0            |
| 28  | X     | 49    | 0        | 74       | 6       | 0            |
| 28  | Y     | 49    | 0        | 74       | 6       | 0            |
| 28  | Z     | 49    | 0        | 74       | 9       | 0            |
| 28  | a     | 43    | 0        | 59       | 1       | 0            |
| 29  | 1     | 40    | 0        | 56       | 2       | 0            |
| 29  | 2     | 40    | 0        | 56       | 5       | 0            |
| 29  | 3     | 120   | 0        | 168      | 19      | 0            |
| 29  | 4     | 40    | 0        | 56       | 5       | 0            |
| 29  | 5     | 40    | 0        | 56       | 2       | 0            |
| 29  | 6     | 40    | 0        | 56       | 1       | 0            |
| 29  | 7     | 80    | 0        | 112      | 8       | 0            |
| 29  | 8     | 40    | 0        | 56       | 3       | 0            |
| 29  | 9     | 40    | 0        | 56       | 7       | 0            |
| 29  | A     | 240   | 0        | 336      | 42      | 0            |
| 29  | B     | 400   | 0        | 560      | 44      | 0            |
| 29  | F     | 40    | 0        | 56       | 7       | 0            |
| 29  | G     | 40    | 0        | 56       | 4       | 0            |
| 29  | J     | 40    | 0        | 56       | 8       | 0            |
| 29  | K     | 80    | 0        | 112      | 8       | 0            |
| 29  | L     | 160   | 0        | 224      | 29      | 0            |
| 29  | O     | 80    | 0        | 112      | 9       | 0            |
| 29  | a     | 40    | 0        | 56       | 3       | 0            |
| 30  | A     | 8     | 0        | 0        | 0       | 0            |
| 30  | C     | 16    | 0        | 0        | 1       | 0            |
| 31  | 1     | 35    | 0        | 46       | 0       | 0            |
| 31  | 5     | 65    | 0        | 76       | 0       | 0            |
| 31  | 8     | 35    | 0        | 46       | 0       | 0            |
| 31  | A     | 69    | 0        | 90       | 1       | 0            |
| 31  | K     | 35    | 0        | 46       | 0       | 0            |
| 32  | 4     | 80    | 0        | 100      | 0       | 0            |
| 32  | 5     | 40    | 0        | 50       | 1       | 0            |
| 32  | 8     | 46    | 0        | 65       | 3       | 0            |
| 32  | 9     | 55    | 0        | 86       | 2       | 0            |
| 32  | A     | 40    | 0        | 50       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 32  | H     | 55    | 0        | 86       | 0       | 0            |
| 32  | J     | 82    | 0        | 107      | 0       | 0            |
| 32  | L     | 37    | 0        | 44       | 0       | 0            |
| 32  | V     | 55    | 0        | 86       | 2       | 0            |
| 33  | B     | 62    | 0        | 85       | 1       | 0            |
| 34  | 1     | 42    | 0        | 56       | 6       | 0            |
| 34  | 2     | 42    | 0        | 56       | 7       | 0            |
| 34  | 3     | 42    | 0        | 56       | 7       | 0            |
| 34  | 4     | 42    | 0        | 56       | 3       | 0            |
| 34  | 5     | 42    | 0        | 56       | 4       | 0            |
| 34  | 6     | 42    | 0        | 56       | 5       | 0            |
| 34  | 7     | 42    | 0        | 56       | 3       | 0            |
| 34  | 8     | 42    | 0        | 56       | 6       | 0            |
| 34  | 9     | 42    | 0        | 56       | 5       | 0            |
| 34  | U     | 84    | 0        | 112      | 8       | 0            |
| 34  | V     | 84    | 0        | 112      | 10      | 0            |
| 34  | W     | 84    | 0        | 112      | 8       | 0            |
| 34  | X     | 84    | 0        | 112      | 12      | 0            |
| 34  | Y     | 84    | 0        | 112      | 9       | 0            |
| 34  | Z     | 84    | 0        | 112      | 10      | 0            |
| 34  | a     | 42    | 0        | 56       | 5       | 0            |
| 35  | 1     | 44    | 0        | 56       | 3       | 0            |
| 35  | 2     | 44    | 0        | 56       | 1       | 0            |
| 35  | 3     | 44    | 0        | 56       | 2       | 0            |
| 35  | 4     | 44    | 0        | 56       | 3       | 0            |
| 35  | 5     | 44    | 0        | 56       | 2       | 0            |
| 35  | 6     | 44    | 0        | 56       | 1       | 0            |
| 35  | 7     | 44    | 0        | 56       | 1       | 0            |
| 35  | 8     | 44    | 0        | 56       | 1       | 0            |
| 35  | 9     | 44    | 0        | 56       | 0       | 0            |
| 35  | U     | 44    | 0        | 56       | 5       | 0            |
| 35  | V     | 44    | 0        | 56       | 6       | 0            |
| 35  | W     | 44    | 0        | 56       | 3       | 0            |
| 35  | X     | 44    | 0        | 56       | 3       | 0            |
| 35  | Y     | 44    | 0        | 56       | 3       | 0            |
| 35  | Z     | 44    | 0        | 56       | 5       | 0            |
| 35  | a     | 44    | 0        | 56       | 3       | 0            |
| 36  | 5     | 44    | 0        | 56       | 1       | 0            |
| 36  | 6     | 44    | 0        | 56       | 6       | 0            |
| 36  | U     | 44    | 0        | 56       | 0       | 0            |
| 36  | V     | 44    | 0        | 56       | 11      | 0            |
| 36  | W     | 44    | 0        | 56       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 36  | X     | 44    | 0        | 56       | 2       | 0            |
| 36  | Y     | 44    | 0        | 56       | 2       | 0            |
| 36  | Z     | 44    | 0        | 56       | 3       | 0            |
| 37  | U     | 303   | 0        | 248      | 14      | 0            |
| 37  | V     | 309   | 0        | 253      | 15      | 0            |
| 37  | W     | 336   | 0        | 298      | 9       | 0            |
| 37  | X     | 353   | 0        | 342      | 15      | 0            |
| 37  | Y     | 335   | 0        | 302      | 16      | 0            |
| 37  | Z     | 335   | 0        | 302      | 14      | 0            |
| All | All   | 69460 | 0        | 68604    | 1115    | 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 8.

The worst 5 of 1115 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:8:78:CYS:SG    | 21:8:201:MET:HE2   | 1.64                     | 1.34              |
| 25:V:174:ILE:CG2  | 36:V:1623:NEX:H15  | 1.78                     | 1.14              |
| 21:8:78:CYS:SG    | 21:8:201:MET:CE    | 2.44                     | 1.06              |
| 18:5:192:LEU:CD1  | 26:5:611:CLA:HMD1  | 1.87                     | 1.04              |
| 25:V:174:ILE:HG22 | 36:V:1623:NEX:H201 | 1.42                     | 1.00              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 739/751 (98%)  | 713 (96%) | 26 (4%) | 0        | 100         | 100 |
| 2   | B     | 731/735 (100%) | 701 (96%) | 30 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 3   | C     | 78/81 (96%)     | 67 (86%)   | 11 (14%) | 0        | 100         | 100 |
| 4   | D     | 141/196 (72%)   | 135 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 5   | E     | 61/97 (63%)     | 57 (93%)   | 4 (7%)   | 0        | 100         | 100 |
| 6   | F     | 163/227 (72%)   | 156 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 7   | G     | 92/126 (73%)    | 86 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 8   | H     | 98/130 (75%)    | 94 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 9   | I     | 40/106 (38%)    | 35 (88%)   | 5 (12%)  | 0        | 100         | 100 |
| 10  | J     | 39/41 (95%)     | 38 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 11  | K     | 84/113 (74%)    | 78 (93%)   | 6 (7%)   | 0        | 100         | 100 |
| 12  | L     | 157/196 (80%)   | 146 (93%)  | 11 (7%)  | 0        | 100         | 100 |
| 13  | O     | 95/126 (75%)    | 87 (92%)   | 8 (8%)   | 0        | 100         | 100 |
| 14  | 1     | 192/228 (84%)   | 186 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 14  | a     | 192/228 (84%)   | 186 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 15  | 2     | 215/246 (87%)   | 203 (94%)  | 10 (5%)  | 2 (1%)   | 14          | 43  |
| 16  | 3     | 218/298 (73%)   | 211 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 17  | 4     | 208/264 (79%)   | 202 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 18  | 5     | 225/257 (88%)   | 211 (94%)  | 14 (6%)  | 0        | 100         | 100 |
| 19  | 6     | 228/257 (89%)   | 210 (92%)  | 18 (8%)  | 0        | 100         | 100 |
| 20  | 7     | 211/241 (88%)   | 197 (93%)  | 14 (7%)  | 0        | 100         | 100 |
| 21  | 8     | 214/243 (88%)   | 210 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 22  | 9     | 181/213 (85%)   | 165 (91%)  | 16 (9%)  | 0        | 100         | 100 |
| 23  | W     | 218/249 (88%)   | 202 (93%)  | 16 (7%)  | 0        | 100         | 100 |
| 23  | X     | 219/249 (88%)   | 194 (89%)  | 25 (11%) | 0        | 100         | 100 |
| 24  | U     | 217/257 (84%)   | 196 (90%)  | 21 (10%) | 0        | 100         | 100 |
| 24  | Y     | 217/257 (84%)   | 198 (91%)  | 19 (9%)  | 0        | 100         | 100 |
| 24  | Z     | 219/257 (85%)   | 204 (93%)  | 15 (7%)  | 0        | 100         | 100 |
| 25  | V     | 235/268 (88%)   | 222 (94%)  | 13 (6%)  | 0        | 100         | 100 |
| All | All   | 5927/6937 (85%) | 5590 (94%) | 335 (6%) | 2 (0%)   | 100         | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | 2     | 142 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | 2     | 143 | PHE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | A     | 601/610 (98%)  | 600 (100%) | 1 (0%)   | 87          | 87  |
| 2   | B     | 596/597 (100%) | 596 (100%) | 0        | 100         | 100 |
| 3   | C     | 69/70 (99%)    | 67 (97%)   | 2 (3%)   | 37          | 63  |
| 4   | D     | 120/152 (79%)  | 120 (100%) | 0        | 100         | 100 |
| 5   | E     | 54/81 (67%)    | 54 (100%)  | 0        | 100         | 100 |
| 6   | F     | 127/169 (75%)  | 127 (100%) | 0        | 100         | 100 |
| 7   | G     | 70/94 (74%)    | 70 (100%)  | 0        | 100         | 100 |
| 8   | H     | 81/102 (79%)   | 81 (100%)  | 0        | 100         | 100 |
| 9   | I     | 33/76 (43%)    | 33 (100%)  | 0        | 100         | 100 |
| 10  | J     | 37/37 (100%)   | 37 (100%)  | 0        | 100         | 100 |
| 11  | K     | 59/80 (74%)    | 59 (100%)  | 0        | 100         | 100 |
| 12  | L     | 121/148 (82%)  | 121 (100%) | 0        | 100         | 100 |
| 13  | O     | 78/101 (77%)   | 78 (100%)  | 0        | 100         | 100 |
| 14  | 1     | 137/162 (85%)  | 135 (98%)  | 2 (2%)   | 57          | 72  |
| 14  | a     | 137/162 (85%)  | 135 (98%)  | 2 (2%)   | 57          | 72  |
| 15  | 2     | 173/198 (87%)  | 173 (100%) | 0        | 100         | 100 |
| 16  | 3     | 167/230 (73%)  | 167 (100%) | 0        | 100         | 100 |
| 17  | 4     | 165/205 (80%)  | 164 (99%)  | 1 (1%)   | 78          | 81  |
| 18  | 5     | 184/206 (89%)  | 184 (100%) | 0        | 100         | 100 |
| 19  | 6     | 184/203 (91%)  | 184 (100%) | 0        | 100         | 100 |
| 20  | 7     | 164/181 (91%)  | 164 (100%) | 0        | 100         | 100 |
| 21  | 8     | 162/183 (88%)  | 162 (100%) | 0        | 100         | 100 |
| 22  | 9     | 140/159 (88%)  | 140 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 23  | W     | 164/187 (88%)   | 164 (100%)  | 0        | 100         | 100 |
| 23  | X     | 165/187 (88%)   | 164 (99%)   | 1 (1%)   | 78          | 81  |
| 24  | U     | 168/194 (87%)   | 168 (100%)  | 0        | 100         | 100 |
| 24  | Y     | 170/194 (88%)   | 170 (100%)  | 0        | 100         | 100 |
| 24  | Z     | 170/194 (88%)   | 170 (100%)  | 0        | 100         | 100 |
| 25  | V     | 178/201 (89%)   | 178 (100%)  | 0        | 100         | 100 |
| All | All   | 4674/5363 (87%) | 4665 (100%) | 9 (0%)   | 85          | 87  |

5 of 9 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | 4     | 177 | ASP  |
| 23  | X     | 165 | LEU  |
| 14  | 1     | 72  | LYS  |
| 14  | 1     | 227 | PHE  |
| 14  | a     | 66  | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | O     | 82  | ASN  |
| 24  | U     | 147 | GLN  |
| 15  | 2     | 196 | ASN  |
| 23  | W     | 161 | ASN  |
| 23  | X     | 161 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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 | $\# Z  > 2$ |
| 25  | TPO  | V     | 33  | 25   | 8,10,11      | 1.56 | 1 (12%)     | 10,14,16    | 1.95 | 2 (20%)     |

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 |
|-----|------|-------|-----|------|---------|-----------|-------|
| 25  | TPO  | V     | 33  | 25   | -       | 3/9/11/13 | -     |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 25  | V     | 33  | TPO  | P-O1P | 3.28 | 1.61        | 1.50     |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 25  | V     | 33  | TPO  | P-OG1-CB  | -5.21 | 107.48      | 123.21   |
| 25  | V     | 33  | TPO  | CG2-CB-CA | -2.55 | 108.14      | 113.16   |

There are no chirality outliers.

All (3) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 25  | V     | 33  | TPO  | N-CA-CB-CG2 |
| 25  | V     | 33  | TPO  | N-CA-CB-OG1 |
| 25  | V     | 33  | TPO  | C-CA-CB-CG2 |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

471 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$ |
| 26  | CLA  | 3     | 612  | 16   | 47,51,73     | 1.51 | 9 (19%)     | 56,86,113   | 1.24 | 6 (10%)     |
| 26  | CLA  | U     | 614  | 24   | 46,50,73     | 1.49 | 7 (15%)     | 55,85,113   | 1.36 | 5 (9%)      |
| 26  | CLA  | a     | 609  | 14   | 67,72,73     | 1.26 | 8 (11%)     | 80,112,113  | 1.19 | 6 (7%)      |
| 34  | LUT  | U     | 1621 | -    | 42,43,43     | 0.75 | 0           | 51,60,60    | 1.55 | 9 (17%)     |
| 26  | CLA  | B     | 841  | 28   | 69,73,73     | 1.25 | 9 (13%)     | 83,113,113  | 1.23 | 7 (8%)      |
| 26  | CLA  | B     | 832  | 2    | 64,68,73     | 1.34 | 9 (14%)     | 77,107,113  | 1.32 | 8 (10%)     |
| 35  | XAT  | 9     | 620  | -    | 39,47,47     | 0.99 | 2 (5%)      | 54,74,74    | 2.51 | 19 (35%)    |
| 28  | LHG  | W     | 2630 | 26   | 33,33,48     | 1.13 | 2 (6%)      | 36,39,54    | 1.17 | 3 (8%)      |
| 29  | BCR  | L     | 301  | -    | 41,41,41     | 0.80 | 0           | 56,56,56    | 2.26 | 24 (42%)    |
| 37  | CHL  | Z     | 605  | 24   | 46,50,74     | 2.34 | 18 (39%)    | 51,85,114   | 3.55 | 24 (47%)    |
| 37  | CHL  | U     | 607  | -    | 50,54,74     | 2.27 | 19 (38%)    | 56,90,114   | 3.35 | 22 (39%)    |
| 26  | CLA  | 5     | 607  | -    | 69,73,73     | 1.26 | 10 (14%)    | 83,113,113  | 1.23 | 8 (9%)      |
| 26  | CLA  | B     | 837  | 2    | 69,73,73     | 1.29 | 11 (15%)    | 83,113,113  | 1.32 | 10 (12%)    |
| 26  | CLA  | F     | 301  | -    | 61,65,73     | 1.35 | 9 (14%)     | 73,103,113  | 1.18 | 6 (8%)      |
| 28  | LHG  | Z     | 2630 | 26   | 48,48,48     | 0.92 | 2 (4%)      | 51,54,54    | 0.97 | 2 (3%)      |
| 26  | CLA  | B     | 819  | -    | 59,63,73     | 1.37 | 8 (13%)     | 71,101,113  | 1.22 | 9 (12%)     |
| 28  | LHG  | 9     | 624  | -    | 48,48,48     | 0.93 | 2 (4%)      | 51,54,54    | 0.87 | 2 (3%)      |
| 28  | LHG  | A     | 861  | -    | 48,48,48     | 0.94 | 2 (4%)      | 51,54,54    | 1.00 | 2 (3%)      |
| 35  | XAT  | 8     | 620  | -    | 39,47,47     | 1.02 | 2 (5%)      | 54,74,74    | 2.45 | 24 (44%)    |
| 26  | CLA  | 5     | 608  | -    | 54,58,73     | 1.43 | 9 (16%)     | 65,95,113   | 1.22 | 6 (9%)      |
| 27  | PQN  | A     | 844  | -    | 34,34,34     | 3.31 | 9 (26%)     | 42,45,45    | 2.07 | 4 (9%)      |
| 29  | BCR  | 7     | 621  | -    | 41,41,41     | 0.80 | 1 (2%)      | 56,56,56    | 2.28 | 22 (39%)    |
| 26  | CLA  | a     | 607  | -    | 49,53,73     | 1.52 | 10 (20%)    | 59,89,113   | 1.21 | 5 (8%)      |
| 26  | CLA  | 6     | 618  | 19   | 43,48,73     | 1.60 | 9 (20%)     | 54,83,113   | 1.43 | 7 (12%)     |
| 29  | BCR  | a     | 619  | -    | 41,41,41     | 0.84 | 0           | 56,56,56    | 2.38 | 22 (39%)    |
| 26  | CLA  | 5     | 610  | 18   | 58,62,73     | 1.36 | 9 (15%)     | 69,99,113   | 1.22 | 6 (8%)      |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | CLA  | V     | 612  | 25   | 49,53,73     | 1.47 | 8 (16%)  | 59,89,113   | 1.35 | 5 (8%)   |
| 26  | CLA  | A     | 801  | 1    | 69,73,73     | 1.27 | 11 (15%) | 83,113,113  | 1.28 | 7 (8%)   |
| 26  | CLA  | U     | 610  | 24   | 60,64,73     | 1.32 | 7 (11%)  | 72,102,113  | 1.27 | 5 (6%)   |
| 26  | CLA  | 5     | 618  | 18   | 43,48,73     | 1.61 | 10 (23%) | 54,83,113   | 1.36 | 7 (12%)  |
| 29  | BCR  | F     | 305  | -    | 41,41,41     | 0.89 | 1 (2%)   | 56,56,56    | 2.34 | 20 (35%) |
| 37  | CHL  | W     | 605  | 23   | 50,54,74     | 2.28 | 20 (40%) | 56,90,114   | 3.38 | 22 (39%) |
| 26  | CLA  | 4     | 606  | -    | 43,48,73     | 1.55 | 9 (20%)  | 51,83,113   | 1.28 | 6 (11%)  |
| 26  | CLA  | 9     | 609  | 22   | 65,69,73     | 1.30 | 9 (13%)  | 78,108,113  | 1.23 | 5 (6%)   |
| 36  | NEX  | U     | 1623 | -    | 38,46,46     | 0.93 | 1 (2%)   | 50,70,70    | 2.60 | 20 (40%) |
| 26  | CLA  | A     | 804  | 1    | 69,73,73     | 1.25 | 10 (14%) | 83,113,113  | 1.29 | 7 (8%)   |
| 29  | BCR  | K     | 202  | -    | 41,41,41     | 0.94 | 2 (4%)   | 56,56,56    | 2.28 | 21 (37%) |
| 26  | CLA  | 9     | 604  | -    | 54,58,73     | 1.48 | 9 (16%)  | 68,95,113   | 1.30 | 8 (11%)  |
| 26  | CLA  | 3     | 610  | 16   | 69,73,73     | 1.28 | 8 (11%)  | 83,113,113  | 1.16 | 6 (7%)   |
| 26  | CLA  | Z     | 610  | 24   | 69,73,73     | 1.23 | 9 (13%)  | 83,113,113  | 1.19 | 8 (9%)   |
| 26  | CLA  | A     | 835  | 1    | 65,69,73     | 1.30 | 10 (15%) | 78,108,113  | 1.28 | 8 (10%)  |
| 26  | CLA  | 6     | 620  | -    | 68,72,73     | 1.25 | 8 (11%)  | 81,111,113  | 1.20 | 5 (6%)   |
| 26  | CLA  | 6     | 607  | -    | 45,49,73     | 1.58 | 9 (20%)  | 57,84,113   | 1.35 | 6 (10%)  |
| 26  | CLA  | 7     | 604  | -    | 54,58,73     | 1.40 | 9 (16%)  | 65,95,113   | 1.23 | 6 (9%)   |
| 26  | CLA  | a     | 614  | 14   | 58,62,73     | 1.37 | 8 (13%)  | 67,99,113   | 1.34 | 6 (8%)   |
| 26  | CLA  | 5     | 604  | -    | 67,71,73     | 1.36 | 9 (13%)  | 84,111,113  | 1.20 | 9 (10%)  |
| 32  | LMG  | 4     | 623  | -    | 40,40,55     | 1.07 | 2 (5%)   | 48,48,63    | 1.15 | 5 (10%)  |
| 26  | CLA  | W     | 612  | 23   | 49,53,73     | 1.48 | 8 (16%)  | 59,89,113   | 1.40 | 6 (10%)  |
| 26  | CLA  | 8     | 608  | -    | 55,59,73     | 1.41 | 10 (18%) | 66,96,113   | 1.40 | 9 (13%)  |
| 32  | LMG  | J     | 103  | -    | 42,42,55     | 0.98 | 2 (4%)   | 50,50,63    | 1.22 | 6 (12%)  |
| 29  | BCR  | A     | 848  | -    | 41,41,41     | 1.01 | 3 (7%)   | 56,56,56    | 2.24 | 14 (25%) |
| 34  | LUT  | Y     | 1620 | -    | 42,43,43     | 0.80 | 0        | 51,60,60    | 3.18 | 18 (35%) |
| 26  | CLA  | A     | 830  | 1    | 69,73,73     | 1.27 | 10 (14%) | 83,113,113  | 1.24 | 7 (8%)   |
| 28  | LHG  | 5     | 625  | -    | 48,48,48     | 0.91 | 2 (4%)   | 51,54,54    | 1.02 | 3 (5%)   |
| 29  | BCR  | 9     | 621  | -    | 41,41,41     | 0.76 | 1 (2%)   | 56,56,56    | 2.90 | 18 (32%) |
| 28  | LHG  | 3     | 623  | -    | 44,44,48     | 0.93 | 2 (4%)   | 47,50,54    | 1.00 | 3 (6%)   |
| 26  | CLA  | a     | 602  | 14   | 65,69,73     | 1.34 | 11 (16%) | 78,108,113  | 1.24 | 8 (10%)  |
| 26  | CLA  | 8     | 616  | 21   | 47,51,73     | 1.58 | 7 (14%)  | 60,87,113   | 1.38 | 9 (15%)  |
| 26  | CLA  | 3     | 602  | 16   | 64,68,73     | 1.31 | 8 (12%)  | 77,107,113  | 1.20 | 8 (10%)  |
| 35  | XAT  | W     | 1622 | -    | 39,47,47     | 0.92 | 1 (2%)   | 54,74,74    | 4.26 | 25 (46%) |
| 35  | XAT  | V     | 1622 | -    | 39,47,47     | 0.87 | 0        | 54,74,74    | 2.68 | 20 (37%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | CLA  | B     | 803  | -    | 69,73,73     | 1.25 | 11 (15%) | 83,113,113  | 1.26 | 6 (7%)   |
| 37  | CHL  | V     | 605  | 25   | 48,52,74     | 2.30 | 18 (37%) | 53,87,114   | 3.30 | 20 (37%) |
| 26  | CLA  | 8     | 611  | 28   | 46,50,73     | 1.50 | 8 (17%)  | 55,85,113   | 1.29 | 5 (9%)   |
| 28  | LHG  | Y     | 2630 | 26   | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.01 | 2 (3%)   |
| 26  | CLA  | B     | 804  | 2    | 45,49,73     | 1.48 | 9 (20%)  | 54,84,113   | 1.36 | 4 (7%)   |
| 26  | CLA  | 2     | 607  | -    | 47,52,73     | 1.48 | 9 (19%)  | 56,88,113   | 1.38 | 7 (12%)  |
| 28  | LHG  | 6     | 623  | 26   | 47,47,48     | 0.91 | 2 (4%)   | 50,53,54    | 0.96 | 3 (6%)   |
| 26  | CLA  | 4     | 603  | 17   | 48,52,73     | 1.56 | 10 (20%) | 61,88,113   | 1.40 | 9 (14%)  |
| 28  | LHG  | H     | 204  | -    | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 0.94 | 2 (3%)   |
| 26  | CLA  | H     | 203  | -    | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.23 | 5 (6%)   |
| 26  | CLA  | a     | 616  | 14   | 49,53,73     | 1.47 | 6 (12%)  | 59,89,113   | 1.39 | 8 (13%)  |
| 26  | CLA  | A     | 827  | -    | 62,66,73     | 1.34 | 9 (14%)  | 74,104,113  | 1.20 | 6 (8%)   |
| 37  | CHL  | Z     | 608  | -    | 53,57,74     | 2.22 | 19 (35%) | 59,93,114   | 3.23 | 22 (37%) |
| 26  | CLA  | A     | 816  | 1    | 69,73,73     | 1.26 | 11 (15%) | 83,113,113  | 1.29 | 7 (8%)   |
| 26  | CLA  | 8     | 609  | 21   | 49,53,73     | 1.48 | 8 (16%)  | 59,89,113   | 1.33 | 5 (8%)   |
| 26  | CLA  | B     | 827  | 2    | 66,70,73     | 1.27 | 10 (15%) | 79,109,113  | 1.34 | 9 (11%)  |
| 32  | LMG  | 9     | 625  | -    | 55,55,55     | 0.88 | 2 (3%)   | 63,63,63    | 1.03 | 6 (9%)   |
| 36  | NEX  | 5     | 624  | -    | 38,46,46     | 1.08 | 1 (2%)   | 50,70,70    | 2.27 | 18 (36%) |
| 26  | CLA  | B     | 834  | 2    | 64,68,73     | 1.30 | 10 (15%) | 77,107,113  | 1.24 | 7 (9%)   |
| 35  | XAT  | U     | 1622 | -    | 39,47,47     | 0.92 | 1 (2%)   | 54,74,74    | 4.40 | 22 (40%) |
| 29  | BCR  | O     | 2004 | -    | 41,41,41     | 0.82 | 0        | 56,56,56    | 1.96 | 14 (25%) |
| 37  | CHL  | X     | 609  | 23   | 70,74,74     | 1.94 | 19 (27%) | 80,114,114  | 2.83 | 25 (31%) |
| 26  | CLA  | W     | 604  | -    | 51,55,73     | 1.47 | 8 (15%)  | 61,91,113   | 1.28 | 7 (11%)  |
| 34  | LUT  | V     | 1621 | -    | 42,43,43     | 0.79 | 0        | 51,60,60    | 1.99 | 16 (31%) |
| 26  | CLA  | 3     | 617  | 16   | 43,48,73     | 1.52 | 9 (20%)  | 51,83,113   | 1.40 | 6 (11%)  |
| 26  | CLA  | 7     | 603  | 20   | 47,52,73     | 1.52 | 10 (21%) | 56,88,113   | 1.50 | 7 (12%)  |
| 28  | LHG  | 8     | 622  | 26   | 48,48,48     | 0.91 | 2 (4%)   | 51,54,54    | 0.86 | 2 (3%)   |
| 34  | LUT  | X     | 1620 | -    | 42,43,43     | 0.73 | 0        | 51,60,60    | 1.54 | 9 (17%)  |
| 28  | LHG  | 8     | 623  | -    | 39,39,48     | 1.03 | 2 (5%)   | 42,45,54    | 1.07 | 2 (4%)   |
| 26  | CLA  | A     | 829  | 1    | 69,73,73     | 1.27 | 8 (11%)  | 83,113,113  | 1.35 | 9 (10%)  |
| 26  | CLA  | 6     | 610  | 19   | 69,73,73     | 1.28 | 8 (11%)  | 83,113,113  | 1.18 | 7 (8%)   |
| 26  | CLA  | V     | 603  | 25   | 49,53,73     | 1.47 | 7 (14%)  | 59,89,113   | 1.46 | 4 (6%)   |
| 26  | CLA  | Y     | 614  | 24   | 52,56,73     | 1.42 | 6 (11%)  | 62,92,113   | 1.29 | 8 (12%)  |
| 29  | BCR  | 7     | 623  | -    | 41,41,41     | 0.87 | 0        | 56,56,56    | 2.01 | 17 (30%) |
| 26  | CLA  | K     | 203  | -    | 60,64,73     | 1.35 | 10 (16%) | 72,102,113  | 1.38 | 10 (13%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | LMU  | 8     | 625  | -    | 36,36,36     | 1.10 | 2 (5%)   | 47,47,47    | 1.24 | 3 (6%)   |
| 29  | BCR  | B     | 801  | -    | 41,41,41     | 0.94 | 1 (2%)   | 56,56,56    | 2.10 | 18 (32%) |
| 36  | NEX  | Y     | 1623 | -    | 38,46,46     | 0.98 | 1 (2%)   | 50,70,70    | 2.52 | 16 (32%) |
| 36  | NEX  | Z     | 1623 | -    | 38,46,46     | 1.02 | 1 (2%)   | 50,70,70    | 2.64 | 19 (38%) |
| 29  | BCR  | 5     | 622  | -    | 41,41,41     | 0.87 | 2 (4%)   | 56,56,56    | 2.31 | 19 (33%) |
| 26  | CLA  | 5     | 619  | -    | 47,51,73     | 1.60 | 9 (19%)  | 60,87,113   | 1.42 | 8 (13%)  |
| 37  | CHL  | U     | 609  | 24   | 64,68,74     | 2.01 | 17 (26%) | 72,106,114  | 2.95 | 25 (34%) |
| 26  | CLA  | 3     | 603  | 16   | 59,63,73     | 1.36 | 11 (18%) | 71,101,113  | 1.39 | 6 (8%)   |
| 34  | LUT  | 1     | 617  | -    | 42,43,43     | 0.80 | 1 (2%)   | 51,60,60    | 1.89 | 16 (31%) |
| 26  | CLA  | A     | 813  | 1    | 58,62,73     | 1.39 | 9 (15%)  | 69,99,113   | 1.32 | 8 (11%)  |
| 37  | CHL  | W     | 606  | -    | 50,54,74     | 2.20 | 19 (38%) | 56,90,114   | 3.24 | 24 (42%) |
| 29  | BCR  | B     | 849  | -    | 41,41,41     | 0.93 | 2 (4%)   | 56,56,56    | 2.53 | 19 (33%) |
| 26  | CLA  | B     | 838  | 2    | 50,54,73     | 1.47 | 10 (20%) | 60,90,113   | 1.38 | 7 (11%)  |
| 37  | CHL  | V     | 601  | 25   | 70,74,74     | 1.95 | 19 (27%) | 80,114,114  | 2.80 | 24 (30%) |
| 26  | CLA  | W     | 611  | 28   | 61,65,73     | 1.33 | 6 (9%)   | 73,103,113  | 1.15 | 7 (9%)   |
| 26  | CLA  | G     | 204  | 7    | 49,53,73     | 1.50 | 9 (18%)  | 59,89,113   | 1.33 | 7 (11%)  |
| 29  | BCR  | L     | 305  | -    | 41,41,41     | 0.89 | 0        | 56,56,56    | 2.52 | 25 (44%) |
| 26  | CLA  | A     | 819  | 1    | 63,67,73     | 1.34 | 12 (19%) | 75,105,113  | 1.36 | 7 (9%)   |
| 26  | CLA  | 4     | 608  | -    | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.19 | 8 (9%)   |
| 26  | CLA  | B     | 817  | 2    | 63,67,73     | 1.32 | 9 (14%)  | 75,105,113  | 1.31 | 6 (8%)   |
| 29  | BCR  | 3     | 622  | -    | 41,41,41     | 0.89 | 1 (2%)   | 56,56,56    | 2.23 | 18 (32%) |
| 37  | CHL  | W     | 609  | 23   | 70,74,74     | 1.98 | 18 (25%) | 80,114,114  | 2.78 | 22 (27%) |
| 34  | LUT  | 6     | 619  | -    | 42,43,43     | 0.77 | 1 (2%)   | 51,60,60    | 2.07 | 18 (35%) |
| 26  | CLA  | 2     | 602  | 15   | 61,69,73     | 1.33 | 8 (13%)  | 70,102,113  | 0.96 | 3 (4%)   |
| 26  | CLA  | 6     | 617  | 19   | 49,53,73     | 1.46 | 8 (16%)  | 59,89,113   | 1.30 | 7 (11%)  |
| 26  | CLA  | B     | 825  | -    | 53,57,73     | 1.42 | 8 (15%)  | 62,93,113   | 1.35 | 8 (12%)  |
| 26  | CLA  | 5     | 612  | 18   | 44,49,73     | 1.52 | 7 (15%)  | 52,84,113   | 1.28 | 4 (7%)   |
| 26  | CLA  | B     | 831  | 2    | 69,73,73     | 1.25 | 9 (13%)  | 83,113,113  | 1.19 | 6 (7%)   |
| 26  | CLA  | A     | 831  | 1    | 69,73,73     | 1.29 | 11 (15%) | 83,113,113  | 1.22 | 7 (8%)   |
| 26  | CLA  | L     | 307  | 8    | 43,48,73     | 1.52 | 9 (20%)  | 51,83,113   | 1.42 | 5 (9%)   |
| 26  | CLA  | 6     | 614  | 19   | 64,68,73     | 1.31 | 8 (12%)  | 77,107,113  | 1.21 | 8 (10%)  |
| 26  | CLA  | 7     | 615  | -    | 45,50,73     | 1.60 | 10 (22%) | 56,85,113   | 1.33 | 5 (8%)   |
| 26  | CLA  | O     | 2002 | -    | 41,46,73     | 1.64 | 9 (21%)  | 52,81,113   | 1.36 | 7 (13%)  |
| 37  | CHL  | X     | 606  | -    | 48,52,74     | 2.28 | 16 (33%) | 53,87,114   | 3.31 | 21 (39%) |
| 26  | CLA  | Z     | 603  | 24   | 59,63,73     | 1.35 | 7 (11%)  | 71,101,113  | 1.41 | 8 (11%)  |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | CLA  | X     | 611  | 28   | 49,53,73     | 1.48 | 7 (14%)  | 59,89,113   | 1.29 | 5 (8%)   |
| 27  | PQN  | B     | 842  | -    | 34,34,34     | 3.33 | 8 (23%)  | 42,45,45    | 2.02 | 7 (16%)  |
| 26  | CLA  | A     | 837  | 1    | 49,53,73     | 1.51 | 11 (22%) | 59,89,113   | 1.50 | 8 (13%)  |
| 26  | CLA  | V     | 602  | 25   | 64,68,73     | 1.29 | 8 (12%)  | 77,107,113  | 1.23 | 8 (10%)  |
| 26  | CLA  | 2     | 610  | 15   | 59,63,73     | 1.37 | 9 (15%)  | 71,101,113  | 1.23 | 7 (9%)   |
| 37  | CHL  | Y     | 601  | 24   | 70,74,74     | 1.95 | 19 (27%) | 80,114,114  | 2.86 | 24 (30%) |
| 26  | CLA  | 1     | 608  | -    | 47,52,73     | 1.50 | 9 (19%)  | 56,88,113   | 1.30 | 7 (12%)  |
| 28  | LHG  | B     | 851  | 26   | 37,37,48     | 1.04 | 2 (5%)   | 40,43,54    | 1.14 | 4 (10%)  |
| 26  | CLA  | B     | 840  | 2    | 69,73,73     | 1.33 | 10 (14%) | 83,113,113  | 1.26 | 5 (6%)   |
| 26  | CLA  | B     | 802  | 2    | 69,73,73     | 1.25 | 10 (14%) | 83,113,113  | 1.24 | 7 (8%)   |
| 26  | CLA  | 4     | 611  | 28   | 46,50,73     | 1.46 | 7 (15%)  | 55,85,113   | 1.35 | 8 (14%)  |
| 28  | LHG  | O     | 2631 | -    | 35,35,48     | 1.07 | 2 (5%)   | 38,41,54    | 1.12 | 3 (7%)   |
| 26  | CLA  | 4     | 604  | -    | 58,62,73     | 1.42 | 9 (15%)  | 73,100,113  | 1.31 | 8 (10%)  |
| 34  | LUT  | 9     | 619  | -    | 42,43,43     | 0.87 | 1 (2%)   | 51,60,60    | 1.90 | 14 (27%) |
| 26  | CLA  | 6     | 601  | 19   | 69,73,73     | 1.24 | 8 (11%)  | 83,113,113  | 1.13 | 6 (7%)   |
| 34  | LUT  | Z     | 1621 | -    | 42,43,43     | 0.79 | 0        | 51,60,60    | 1.41 | 8 (15%)  |
| 26  | CLA  | A     | 843  | -    | 68,72,73     | 1.29 | 10 (14%) | 81,111,113  | 1.25 | 9 (11%)  |
| 29  | BCR  | B     | 853  | -    | 41,41,41     | 0.87 | 3 (7%)   | 56,56,56    | 1.81 | 14 (25%) |
| 37  | CHL  | Y     | 605  | 24   | 46,50,74     | 2.47 | 20 (43%) | 51,85,114   | 3.36 | 23 (45%) |
| 26  | CLA  | A     | 818  | 1    | 64,68,73     | 1.30 | 10 (15%) | 77,107,113  | 1.28 | 8 (10%)  |
| 34  | LUT  | 7     | 619  | -    | 42,43,43     | 0.91 | 2 (4%)   | 51,60,60    | 1.99 | 14 (27%) |
| 36  | NEX  | X     | 1623 | -    | 38,46,46     | 0.90 | 1 (2%)   | 50,70,70    | 4.33 | 20 (40%) |
| 31  | LMU  | A     | 858  | -    | 34,35,36     | 1.26 | 4 (11%)  | 42,45,47    | 0.99 | 2 (4%)   |
| 26  | CLA  | 7     | 614  | 20   | 46,50,73     | 1.50 | 9 (19%)  | 55,85,113   | 1.31 | 6 (10%)  |
| 26  | CLA  | 1     | 606  | -    | 41,47,73     | 1.59 | 9 (21%)  | 48,80,113   | 1.38 | 6 (12%)  |
| 26  | CLA  | Y     | 611  | 28   | 47,51,73     | 1.48 | 7 (14%)  | 56,86,113   | 1.27 | 4 (7%)   |
| 26  | CLA  | Z     | 611  | 28   | 46,50,73     | 1.55 | 9 (19%)  | 58,85,113   | 1.38 | 7 (12%)  |
| 26  | CLA  | Y     | 604  | -    | 54,58,73     | 1.43 | 8 (14%)  | 65,95,113   | 1.23 | 4 (6%)   |
| 28  | LHG  | 5     | 623  | 26   | 48,48,48     | 0.93 | 2 (4%)   | 51,54,54    | 0.87 | 2 (3%)   |
| 37  | CHL  | V     | 606  | -    | 48,52,74     | 2.16 | 18 (37%) | 53,87,114   | 3.32 | 23 (43%) |
| 26  | CLA  | 3     | 607  | 16   | 60,64,73     | 1.38 | 8 (13%)  | 75,102,113  | 1.23 | 7 (9%)   |
| 26  | CLA  | 1     | 611  | 28   | 61,65,73     | 1.33 | 8 (13%)  | 73,103,113  | 1.20 | 8 (10%)  |
| 26  | CLA  | A     | 811  | 1    | 69,73,73     | 1.28 | 9 (13%)  | 83,113,113  | 1.24 | 5 (6%)   |
| 37  | CHL  | V     | 607  | -    | 50,54,74     | 2.27 | 19 (38%) | 56,90,114   | 3.25 | 23 (41%) |
| 28  | LHG  | a     | 620  | 26   | 42,42,48     | 0.98 | 2 (4%)   | 45,48,54    | 0.82 | 2 (4%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | CLA  | A     | 828  | 1    | 69,73,73     | 1.27 | 11 (15%) | 83,113,113  | 1.31 | 10 (12%) |
| 29  | BCR  | L     | 309  | -    | 41,41,41     | 0.78 | 0        | 56,56,56    | 2.40 | 25 (44%) |
| 26  | CLA  | 2     | 612  | 15   | 48,52,73     | 1.49 | 8 (16%)  | 58,88,113   | 1.29 | 3 (5%)   |
| 26  | CLA  | B     | 839  | -    | 69,73,73     | 1.28 | 12 (17%) | 83,113,113  | 1.17 | 6 (7%)   |
| 26  | CLA  | L     | 302  | 12   | 49,53,73     | 1.53 | 8 (16%)  | 59,89,113   | 1.33 | 6 (10%)  |
| 26  | CLA  | X     | 604  | -    | 53,57,73     | 1.44 | 6 (11%)  | 62,93,113   | 1.24 | 5 (8%)   |
| 26  | CLA  | 8     | 612  | 21   | 44,49,73     | 1.51 | 8 (18%)  | 52,84,113   | 1.37 | 4 (7%)   |
| 26  | CLA  | B     | 812  | 2    | 47,51,73     | 1.48 | 8 (17%)  | 56,86,113   | 1.27 | 5 (8%)   |
| 26  | CLA  | A     | 834  | 1    | 69,73,73     | 1.30 | 11 (15%) | 83,113,113  | 1.34 | 9 (10%)  |
| 26  | CLA  | Z     | 602  | 24   | 62,66,73     | 1.32 | 8 (12%)  | 74,104,113  | 1.22 | 6 (8%)   |
| 26  | CLA  | A     | 832  | 1    | 54,58,73     | 1.45 | 10 (18%) | 65,95,113   | 1.46 | 11 (16%) |
| 26  | CLA  | a     | 608  | -    | 47,52,73     | 1.50 | 8 (17%)  | 56,88,113   | 1.31 | 7 (12%)  |
| 26  | CLA  | 8     | 614  | 21   | 57,61,73     | 1.39 | 10 (17%) | 68,98,113   | 1.31 | 7 (10%)  |
| 36  | NEX  | V     | 1623 | -    | 38,46,46     | 0.94 | 2 (5%)   | 50,70,70    | 2.30 | 18 (36%) |
| 26  | CLA  | 9     | 607  | -    | 49,53,73     | 1.45 | 9 (18%)  | 59,89,113   | 1.28 | 6 (10%)  |
| 28  | LHG  | 7     | 622  | 26   | 36,36,48     | 1.05 | 2 (5%)   | 39,42,54    | 1.02 | 3 (7%)   |
| 26  | CLA  | V     | 610  | 25   | 66,70,73     | 1.26 | 7 (10%)  | 79,109,113  | 1.20 | 8 (10%)  |
| 26  | CLA  | A     | 817  | -    | 49,53,73     | 1.50 | 9 (18%)  | 59,89,113   | 1.41 | 6 (10%)  |
| 26  | CLA  | B     | 808  | 2    | 69,73,73     | 1.27 | 9 (13%)  | 83,113,113  | 1.23 | 9 (10%)  |
| 26  | CLA  | 3     | 614  | 16   | 43,48,73     | 1.55 | 9 (20%)  | 51,83,113   | 1.36 | 6 (11%)  |
| 28  | LHG  | 4     | 622  | 26   | 48,48,48     | 0.91 | 2 (4%)   | 51,54,54    | 0.82 | 2 (3%)   |
| 26  | CLA  | A     | 838  | 1    | 54,58,73     | 1.42 | 12 (22%) | 65,95,113   | 1.36 | 6 (9%)   |
| 34  | LUT  | V     | 1620 | -    | 42,43,43     | 0.75 | 0        | 51,60,60    | 1.65 | 10 (19%) |
| 34  | LUT  | X     | 1621 | -    | 42,43,43     | 0.81 | 0        | 51,60,60    | 1.74 | 15 (29%) |
| 37  | CHL  | Y     | 607  | -    | 70,74,74     | 1.87 | 17 (24%) | 80,114,114  | 2.89 | 23 (28%) |
| 26  | CLA  | 6     | 611  | 28   | 46,50,73     | 1.49 | 8 (17%)  | 55,85,113   | 1.30 | 5 (9%)   |
| 26  | CLA  | 7     | 608  | -    | 54,58,73     | 1.42 | 11 (20%) | 65,95,113   | 1.34 | 8 (12%)  |
| 26  | CLA  | 6     | 604  | -    | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.11 | 7 (8%)   |
| 26  | CLA  | A     | 822  | -    | 69,73,73     | 1.31 | 9 (13%)  | 83,113,113  | 1.28 | 11 (13%) |
| 29  | BCR  | B     | 845  | -    | 41,41,41     | 0.93 | 1 (2%)   | 56,56,56    | 2.50 | 23 (41%) |
| 37  | CHL  | Y     | 609  | 24   | 70,74,74     | 1.93 | 20 (28%) | 80,114,114  | 2.85 | 25 (31%) |
| 26  | CLA  | B     | 815  | 2    | 47,51,73     | 1.48 | 9 (19%)  | 56,86,113   | 1.26 | 4 (7%)   |
| 29  | BCR  | B     | 844  | -    | 41,41,41     | 1.08 | 4 (9%)   | 56,56,56    | 2.60 | 26 (46%) |
| 31  | LMU  | A     | 857  | -    | 36,36,36     | 1.09 | 2 (5%)   | 47,47,47    | 1.37 | 8 (17%)  |
| 29  | BCR  | A     | 856  | -    | 41,41,41     | 0.91 | 2 (4%)   | 56,56,56    | 1.97 | 17 (30%) |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | CLA  | L     | 306  | -    | 43,48,73     | 1.53 | 8 (18%)  | 51,83,113   | 1.35 | 3 (5%)   |
| 26  | CLA  | B     | 807  | 2    | 56,60,73     | 1.44 | 12 (21%) | 67,97,113   | 1.39 | 9 (13%)  |
| 26  | CLA  | A     | 805  | 1    | 56,60,73     | 1.41 | 10 (17%) | 67,97,113   | 1.49 | 11 (16%) |
| 26  | CLA  | 3     | 606  | -    | 57,62,73     | 1.35 | 9 (15%)  | 68,100,113  | 1.36 | 8 (11%)  |
| 26  | CLA  | 4     | 616  | 17   | 47,51,73     | 1.58 | 9 (19%)  | 60,87,113   | 1.30 | 5 (8%)   |
| 26  | CLA  | 9     | 614  | 22   | 49,53,73     | 1.48 | 9 (18%)  | 59,89,113   | 1.24 | 7 (11%)  |
| 37  | CHL  | U     | 608  | -    | 48,52,74     | 2.21 | 16 (33%) | 53,87,114   | 3.48 | 22 (41%) |
| 26  | CLA  | 5     | 602  | 18   | 69,73,73     | 1.27 | 9 (13%)  | 83,113,113  | 1.19 | 7 (8%)   |
| 26  | CLA  | 5     | 609  | 18   | 69,73,73     | 1.29 | 9 (13%)  | 83,113,113  | 1.22 | 8 (9%)   |
| 30  | SF4  | A     | 853  | 2,1  | 0,12,12      | -    | -        | -           | -    | -        |
| 26  | CLA  | A     | 808  | 1    | 54,58,73     | 1.41 | 8 (14%)  | 65,95,113   | 1.35 | 7 (10%)  |
| 26  | CLA  | 3     | 604  | -    | 69,73,73     | 1.27 | 9 (13%)  | 83,113,113  | 1.19 | 8 (9%)   |
| 34  | LUT  | W     | 1621 | -    | 42,43,43     | 0.69 | 0        | 51,60,60    | 1.78 | 13 (25%) |
| 26  | CLA  | 1     | 603  | 14   | 56,61,73     | 1.36 | 8 (14%)  | 66,98,113   | 1.34 | 4 (6%)   |
| 26  | CLA  | 7     | 616  | 20   | 47,51,73     | 1.59 | 10 (21%) | 60,87,113   | 1.37 | 7 (11%)  |
| 35  | XAT  | a     | 618  | -    | 39,47,47     | 0.90 | 0        | 54,74,74    | 2.47 | 21 (38%) |
| 26  | CLA  | A     | 854  | -    | 69,73,73     | 1.30 | 10 (14%) | 83,113,113  | 1.31 | 8 (9%)   |
| 29  | BCR  | 3     | 621  | -    | 41,41,41     | 0.83 | 1 (2%)   | 56,56,56    | 1.84 | 15 (26%) |
| 36  | NEX  | 6     | 624  | -    | 38,46,46     | 1.13 | 3 (7%)   | 50,70,70    | 2.40 | 18 (36%) |
| 26  | CLA  | 3     | 609  | 16   | 64,68,73     | 1.33 | 9 (14%)  | 77,107,113  | 1.26 | 7 (9%)   |
| 26  | CLA  | 7     | 611  | 28   | 63,67,73     | 1.31 | 9 (14%)  | 75,105,113  | 1.21 | 7 (9%)   |
| 37  | CHL  | W     | 607  | -    | 69,73,74     | 2.00 | 19 (27%) | 80,113,114  | 2.71 | 24 (30%) |
| 26  | CLA  | 7     | 613  | 20   | 69,73,73     | 1.27 | 9 (13%)  | 83,113,113  | 1.24 | 6 (7%)   |
| 37  | CHL  | U     | 606  | -    | 48,52,74     | 2.18 | 18 (37%) | 53,87,114   | 3.36 | 21 (39%) |
| 26  | CLA  | B     | 818  | 2    | 64,68,73     | 1.32 | 11 (17%) | 77,107,113  | 1.36 | 8 (10%)  |
| 26  | CLA  | 7     | 612  | 20   | 48,52,73     | 1.50 | 8 (16%)  | 58,88,113   | 1.29 | 4 (6%)   |
| 28  | LHG  | V     | 2630 | 26   | 35,35,48     | 1.07 | 2 (5%)   | 38,41,54    | 1.08 | 2 (5%)   |
| 26  | CLA  | 9     | 602  | 22   | 64,68,73     | 1.31 | 9 (14%)  | 77,107,113  | 1.27 | 8 (10%)  |
| 26  | CLA  | B     | 814  | 2    | 68,72,73     | 1.25 | 9 (13%)  | 81,111,113  | 1.29 | 6 (7%)   |
| 26  | CLA  | 1     | 601  | 14   | 57,62,73     | 1.36 | 9 (15%)  | 68,100,113  | 1.23 | 8 (11%)  |
| 26  | CLA  | B     | 822  | 2    | 46,50,73     | 1.48 | 9 (19%)  | 55,85,113   | 1.29 | 6 (10%)  |
| 26  | CLA  | A     | 823  | 1    | 46,50,73     | 1.49 | 9 (19%)  | 55,85,113   | 1.36 | 4 (7%)   |
| 26  | CLA  | 5     | 603  | 18   | 58,62,73     | 1.43 | 11 (18%) | 73,100,113  | 1.35 | 6 (8%)   |
| 26  | CLA  | V     | 611  | 28   | 47,51,73     | 1.50 | 7 (14%)  | 56,86,113   | 1.25 | 3 (5%)   |
| 26  | CLA  | U     | 603  | 24   | 56,60,73     | 1.38 | 7 (12%)  | 67,97,113   | 1.36 | 7 (10%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | CLA  | 7     | 609  | 20   | 47,52,73     | 1.50 | 9 (19%)  | 55,87,113   | 1.24 | 5 (9%)   |
| 26  | CLA  | X     | 614  | 23   | 46,50,73     | 1.52 | 8 (17%)  | 55,85,113   | 1.30 | 5 (9%)   |
| 37  | CHL  | X     | 607  | -    | 70,74,74     | 1.86 | 18 (25%) | 80,114,114  | 2.97 | 24 (30%) |
| 26  | CLA  | A     | 824  | 1    | 69,73,73     | 1.26 | 10 (14%) | 83,113,113  | 1.30 | 6 (7%)   |
| 26  | CLA  | 4     | 601  | 17   | 69,73,73     | 1.24 | 9 (13%)  | 83,113,113  | 1.23 | 5 (6%)   |
| 26  | CLA  | A     | 841  | 1    | 69,73,73     | 1.26 | 9 (13%)  | 83,113,113  | 1.20 | 6 (7%)   |
| 37  | CHL  | V     | 609  | 25   | 65,69,74     | 2.00 | 18 (27%) | 74,108,114  | 3.01 | 25 (33%) |
| 26  | CLA  | 3     | 611  | 28   | 41,46,73     | 1.62 | 7 (17%)  | 52,81,113   | 1.31 | 4 (7%)   |
| 26  | CLA  | 5     | 601  | 18   | 60,64,73     | 1.33 | 7 (11%)  | 72,102,113  | 1.30 | 5 (6%)   |
| 26  | CLA  | B     | 830  | 2    | 47,51,73     | 1.50 | 8 (17%)  | 56,86,113   | 1.37 | 8 (14%)  |
| 26  | CLA  | 8     | 601  | 21   | 69,73,73     | 1.30 | 8 (11%)  | 83,113,113  | 1.18 | 6 (7%)   |
| 29  | BCR  | A     | 850  | -    | 41,41,41     | 0.93 | 1 (2%)   | 56,56,56    | 2.02 | 14 (25%) |
| 26  | CLA  | F     | 303  | -    | 46,50,73     | 1.53 | 10 (21%) | 55,85,113   | 1.38 | 7 (12%)  |
| 29  | BCR  | A     | 852  | -    | 41,41,41     | 0.97 | 1 (2%)   | 56,56,56    | 2.56 | 26 (46%) |
| 28  | LHG  | 2     | 622  | 26   | 35,35,48     | 1.05 | 2 (5%)   | 38,41,54    | 1.16 | 3 (7%)   |
| 26  | CLA  | B     | 809  | 2    | 69,73,73     | 1.29 | 10 (14%) | 83,113,113  | 1.29 | 8 (9%)   |
| 29  | BCR  | A     | 851  | -    | 41,41,41     | 0.91 | 1 (2%)   | 56,56,56    | 2.29 | 24 (42%) |
| 34  | LUT  | a     | 617  | -    | 42,43,43     | 0.80 | 1 (2%)   | 51,60,60    | 1.90 | 16 (31%) |
| 37  | CHL  | Y     | 606  | -    | 50,54,74     | 2.24 | 17 (34%) | 56,90,114   | 3.23 | 22 (39%) |
| 26  | CLA  | 1     | 604  | -    | 53,57,73     | 1.42 | 8 (15%)  | 62,93,113   | 1.28 | 5 (8%)   |
| 26  | CLA  | X     | 603  | 23   | 66,70,73     | 1.29 | 6 (9%)   | 79,109,113  | 1.29 | 5 (6%)   |
| 34  | LUT  | 2     | 619  | -    | 42,43,43     | 0.91 | 2 (4%)   | 51,60,60    | 1.95 | 14 (27%) |
| 28  | LHG  | 1     | 620  | 26   | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 0.79 | 2 (3%)   |
| 26  | CLA  | B     | 821  | 2    | 47,51,73     | 1.61 | 9 (19%)  | 55,86,113   | 1.34 | 6 (10%)  |
| 26  | CLA  | A     | 839  | 1    | 59,63,73     | 1.40 | 10 (16%) | 71,101,113  | 1.34 | 9 (12%)  |
| 35  | XAT  | 2     | 620  | -    | 39,47,47     | 1.05 | 2 (5%)   | 54,74,74    | 2.48 | 26 (48%) |
| 34  | LUT  | W     | 1620 | -    | 42,43,43     | 0.72 | 0        | 51,60,60    | 1.59 | 11 (21%) |
| 26  | CLA  | A     | 802  | 2    | 69,73,73     | 1.28 | 10 (14%) | 83,113,113  | 1.39 | 10 (12%) |
| 28  | LHG  | X     | 2630 | 26   | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.02 | 3 (5%)   |
| 37  | CHL  | Z     | 609  | 24   | 70,74,74     | 1.95 | 19 (27%) | 80,114,114  | 2.84 | 25 (31%) |
| 37  | CHL  | X     | 601  | 23   | 70,74,74     | 1.91 | 19 (27%) | 80,114,114  | 2.85 | 28 (35%) |
| 29  | BCR  | B     | 848  | -    | 41,41,41     | 0.84 | 1 (2%)   | 56,56,56    | 2.53 | 14 (25%) |
| 26  | CLA  | 3     | 615  | -    | 43,48,73     | 1.53 | 8 (18%)  | 51,83,113   | 1.31 | 6 (11%)  |
| 26  | CLA  | 6     | 616  | 19   | 69,73,73     | 1.26 | 10 (14%) | 83,113,113  | 1.29 | 10 (12%) |
| 29  | BCR  | B     | 843  | -    | 41,41,41     | 1.04 | 4 (9%)   | 56,56,56    | 1.94 | 18 (32%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 29  | BCR  | 2     | 623  | -    | 41,41,41     | 0.86 | 1 (2%)   | 56,56,56    | 2.36 | 20 (35%) |
| 26  | CLA  | A     | 806  | 1    | 69,73,73     | 1.31 | 11 (15%) | 83,113,113  | 1.40 | 12 (14%) |
| 32  | LMG  | A     | 860  | -    | 40,40,55     | 1.00 | 2 (5%)   | 48,48,63    | 1.09 | 4 (8%)   |
| 26  | CLA  | G     | 203  | 7    | 46,50,73     | 1.49 | 8 (17%)  | 55,85,113   | 1.38 | 6 (10%)  |
| 26  | CLA  | 8     | 604  | -    | 54,58,73     | 1.41 | 8 (14%)  | 65,95,113   | 1.39 | 9 (13%)  |
| 26  | CLA  | 2     | 613  | 15   | 69,73,73     | 1.24 | 7 (10%)  | 83,113,113  | 1.12 | 5 (6%)   |
| 31  | LMU  | K     | 208  | -    | 36,36,36     | 1.14 | 2 (5%)   | 47,47,47    | 1.00 | 3 (6%)   |
| 37  | CHL  | U     | 601  | 24   | 70,74,74     | 1.97 | 20 (28%) | 80,114,114  | 2.75 | 23 (28%) |
| 26  | CLA  | 6     | 613  | -    | 67,72,73     | 1.30 | 9 (13%)  | 80,112,113  | 1.22 | 8 (10%)  |
| 26  | CLA  | 1     | 610  | 14   | 42,47,73     | 1.56 | 8 (19%)  | 51,81,113   | 1.39 | 7 (13%)  |
| 29  | BCR  | 8     | 621  | -    | 41,41,41     | 0.75 | 0        | 56,56,56    | 2.77 | 21 (37%) |
| 26  | CLA  | 7     | 602  | 20   | 69,73,73     | 1.30 | 10 (14%) | 83,113,113  | 1.22 | 7 (8%)   |
| 26  | CLA  | B     | 836  | 2    | 54,58,73     | 1.43 | 11 (20%) | 65,95,113   | 1.46 | 8 (12%)  |
| 26  | CLA  | K     | 204  | 11   | 49,53,73     | 1.49 | 9 (18%)  | 59,89,113   | 1.45 | 5 (8%)   |
| 26  | CLA  | 4     | 610  | 17   | 65,69,73     | 1.27 | 7 (10%)  | 78,108,113  | 1.21 | 6 (7%)   |
| 35  | XAT  | 6     | 621  | -    | 39,47,47     | 0.98 | 3 (7%)   | 54,74,74    | 2.42 | 23 (42%) |
| 26  | CLA  | H     | 202  | -    | 42,47,73     | 1.57 | 7 (16%)  | 50,82,113   | 1.25 | 3 (6%)   |
| 26  | CLA  | 4     | 618  | 17   | 43,48,73     | 1.60 | 8 (18%)  | 54,83,113   | 1.33 | 5 (9%)   |
| 26  | CLA  | a     | 611  | 28   | 41,46,73     | 1.64 | 10 (24%) | 52,81,113   | 1.40 | 10 (19%) |
| 26  | CLA  | W     | 614  | 23   | 49,53,73     | 1.46 | 6 (12%)  | 59,89,113   | 1.38 | 3 (5%)   |
| 26  | CLA  | A     | 803  | -    | 69,73,73     | 1.32 | 12 (17%) | 83,113,113  | 1.21 | 4 (4%)   |
| 32  | LMG  | H     | 205  | -    | 55,55,55     | 0.86 | 2 (3%)   | 63,63,63    | 1.11 | 6 (9%)   |
| 32  | LMG  | V     | 2631 | -    | 55,55,55     | 0.87 | 2 (3%)   | 63,63,63    | 1.11 | 5 (7%)   |
| 26  | CLA  | 1     | 609  | 14   | 44,48,73     | 1.57 | 9 (20%)  | 56,83,113   | 1.48 | 9 (16%)  |
| 26  | CLA  | U     | 612  | 24   | 46,50,73     | 1.50 | 5 (10%)  | 55,85,113   | 1.45 | 6 (10%)  |
| 26  | CLA  | 8     | 610  | 21   | 64,68,73     | 1.28 | 8 (12%)  | 77,107,113  | 1.31 | 8 (10%)  |
| 26  | CLA  | B     | 816  | 2    | 58,62,73     | 1.35 | 9 (15%)  | 69,99,113   | 1.30 | 8 (11%)  |
| 26  | CLA  | X     | 613  | 23   | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.14 | 6 (7%)   |
| 26  | CLA  | 6     | 608  | -    | 49,53,73     | 1.48 | 8 (16%)  | 59,89,113   | 1.35 | 8 (13%)  |
| 26  | CLA  | X     | 612  | 23   | 47,51,73     | 1.49 | 7 (14%)  | 56,86,113   | 1.38 | 7 (12%)  |
| 26  | CLA  | a     | 612  | 14   | 49,53,73     | 1.48 | 9 (18%)  | 59,89,113   | 1.38 | 5 (8%)   |
| 32  | LMG  | 5     | 627  | -    | 40,40,55     | 1.03 | 2 (5%)   | 48,48,63    | 1.02 | 3 (6%)   |
| 26  | CLA  | B     | 806  | 2    | 69,73,73     | 1.30 | 13 (18%) | 83,113,113  | 1.38 | 8 (9%)   |
| 28  | LHG  | A     | 846  | -    | 48,48,48     | 0.91 | 2 (4%)   | 51,54,54    | 0.87 | 2 (3%)   |
| 26  | CLA  | A     | 807  | 1    | 69,73,73     | 1.29 | 11 (15%) | 83,113,113  | 1.27 | 6 (7%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | CLA  | W     | 602  | 23   | 64,68,73     | 1.31 | 9 (14%)  | 77,107,113  | 1.17 | 8 (10%)  |
| 29  | BCR  | G     | 205  | -    | 41,41,41     | 0.80 | 1 (2%)   | 56,56,56    | 1.97 | 15 (26%) |
| 26  | CLA  | B     | 813  | 2    | 69,73,73     | 1.30 | 11 (15%) | 83,113,113  | 1.21 | 7 (8%)   |
| 29  | BCR  | 6     | 622  | -    | 41,41,41     | 0.75 | 0        | 56,56,56    | 2.46 | 25 (44%) |
| 26  | CLA  | 2     | 603  | 15   | 47,52,73     | 1.51 | 9 (19%)  | 56,88,113   | 1.31 | 7 (12%)  |
| 29  | BCR  | J     | 102  | -    | 41,41,41     | 0.93 | 2 (4%)   | 56,56,56    | 2.40 | 22 (39%) |
| 29  | BCR  | K     | 207  | -    | 41,41,41     | 0.85 | 1 (2%)   | 56,56,56    | 2.72 | 21 (37%) |
| 26  | CLA  | Y     | 613  | 24   | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.20 | 6 (7%)   |
| 26  | CLA  | a     | 610  | 14   | 63,67,73     | 1.31 | 8 (12%)  | 76,106,113  | 1.15 | 6 (7%)   |
| 26  | CLA  | A     | 842  | 1    | 69,73,73     | 1.31 | 10 (14%) | 83,113,113  | 1.35 | 11 (13%) |
| 26  | CLA  | F     | 304  | 6    | 45,49,73     | 1.52 | 8 (17%)  | 54,84,113   | 1.37 | 6 (11%)  |
| 26  | CLA  | L     | 304  | -    | 49,53,73     | 1.46 | 8 (16%)  | 59,89,113   | 1.30 | 6 (10%)  |
| 26  | CLA  | 2     | 614  | 15   | 45,50,73     | 1.53 | 9 (20%)  | 53,85,113   | 1.36 | 8 (15%)  |
| 26  | CLA  | 9     | 611  | 28   | 46,50,73     | 1.50 | 7 (15%)  | 55,85,113   | 1.23 | 2 (3%)   |
| 35  | XAT  | 1     | 618  | -    | 39,47,47     | 0.91 | 0        | 54,74,74    | 2.46 | 21 (38%) |
| 26  | CLA  | 3     | 608  | -    | 59,63,73     | 1.38 | 11 (18%) | 71,101,113  | 1.18 | 4 (5%)   |
| 36  | NEX  | W     | 1623 | -    | 38,46,46     | 0.90 | 2 (5%)   | 50,70,70    | 2.54 | 12 (24%) |
| 28  | LHG  | A     | 847  | 26   | 29,29,48     | 1.16 | 2 (6%)   | 32,35,54    | 1.04 | 3 (9%)   |
| 26  | CLA  | B     | 833  | 2    | 69,73,73     | 1.26 | 9 (13%)  | 83,113,113  | 1.15 | 5 (6%)   |
| 34  | LUT  | Y     | 1621 | -    | 42,43,43     | 0.87 | 1 (2%)   | 51,60,60    | 1.87 | 14 (27%) |
| 26  | CLA  | V     | 614  | 25   | 49,53,73     | 1.46 | 8 (16%)  | 59,89,113   | 1.33 | 6 (10%)  |
| 37  | CHL  | Z     | 607  | -    | 70,74,74     | 1.92 | 18 (25%) | 80,114,114  | 2.90 | 21 (26%) |
| 26  | CLA  | B     | 826  | 2    | 66,70,73     | 1.29 | 9 (13%)  | 79,109,113  | 1.45 | 6 (7%)   |
| 26  | CLA  | 1     | 616  | 14   | 47,51,73     | 1.56 | 8 (17%)  | 60,87,113   | 1.46 | 9 (15%)  |
| 26  | CLA  | A     | 814  | 1    | 69,73,73     | 1.26 | 11 (15%) | 83,113,113  | 1.40 | 10 (12%) |
| 26  | CLA  | W     | 613  | 23   | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.14 | 3 (3%)   |
| 26  | CLA  | 2     | 601  | 15   | 69,73,73     | 1.23 | 10 (14%) | 83,113,113  | 1.34 | 8 (9%)   |
| 26  | CLA  | O     | 2001 | 13   | 40,46,73     | 1.60 | 9 (22%)  | 48,80,113   | 1.35 | 5 (10%)  |
| 26  | CLA  | A     | 809  | 1    | 69,73,73     | 1.27 | 11 (15%) | 83,113,113  | 1.31 | 7 (8%)   |
| 35  | XAT  | Y     | 1622 | -    | 39,47,47     | 0.92 | 0        | 54,74,74    | 2.75 | 22 (40%) |
| 26  | CLA  | X     | 602  | 23   | 69,73,73     | 1.25 | 9 (13%)  | 83,113,113  | 1.20 | 6 (7%)   |
| 26  | CLA  | U     | 611  | 28   | 46,50,73     | 1.51 | 6 (13%)  | 55,85,113   | 1.33 | 4 (7%)   |
| 26  | CLA  | 9     | 613  | 22   | 69,73,73     | 1.27 | 9 (13%)  | 83,113,113  | 1.24 | 6 (7%)   |
| 28  | LHG  | U     | 2630 | 26   | 48,48,48     | 0.94 | 2 (4%)   | 51,54,54    | 1.08 | 4 (7%)   |
| 26  | CLA  | 8     | 606  | -    | 68,72,73     | 1.29 | 9 (13%)  | 82,112,113  | 1.13 | 7 (8%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 35  | XAT  | Z     | 1622 | -    | 39,47,47     | 0.93 | 0        | 54,74,74    | 2.87 | 21 (38%) |
| 26  | CLA  | 4     | 609  | 17   | 61,65,73     | 1.33 | 7 (11%)  | 73,103,113  | 1.18 | 5 (6%)   |
| 37  | CHL  | W     | 608  | -    | 51,55,74     | 2.25 | 18 (35%) | 57,91,114   | 3.26 | 21 (36%) |
| 26  | CLA  | 8     | 602  | 21   | 64,68,73     | 1.34 | 9 (14%)  | 77,107,113  | 1.31 | 10 (12%) |
| 26  | CLA  | 9     | 612  | 22   | 44,49,73     | 1.53 | 6 (13%)  | 52,84,113   | 1.21 | 3 (5%)   |
| 37  | CHL  | X     | 608  | -    | 70,73,74     | 1.99 | 16 (22%) | 75,112,114  | 2.82 | 21 (28%) |
| 26  | CLA  | W     | 603  | 23   | 56,60,73     | 1.37 | 6 (10%)  | 67,97,113   | 1.40 | 8 (11%)  |
| 29  | BCR  | 3     | 620  | -    | 41,41,41     | 0.80 | 0        | 56,56,56    | 2.38 | 23 (41%) |
| 26  | CLA  | W     | 610  | 23   | 59,63,73     | 1.34 | 6 (10%)  | 71,101,113  | 1.26 | 9 (12%)  |
| 28  | LHG  | 3     | 624  | 26   | 48,48,48     | 0.91 | 2 (4%)   | 51,54,54    | 0.97 | 3 (5%)   |
| 35  | XAT  | 7     | 620  | -    | 39,47,47     | 0.99 | 2 (5%)   | 54,74,74    | 2.50 | 18 (33%) |
| 26  | CLA  | 4     | 607  | -    | 49,53,73     | 1.49 | 8 (16%)  | 59,89,113   | 1.27 | 6 (10%)  |
| 26  | CLA  | V     | 604  | -    | 54,58,73     | 1.40 | 8 (14%)  | 65,95,113   | 1.31 | 7 (10%)  |
| 26  | CLA  | 1     | 602  | 14   | 65,69,73     | 1.33 | 10 (15%) | 78,108,113  | 1.25 | 8 (10%)  |
| 37  | CHL  | X     | 605  | -    | 50,54,74     | 2.42 | 19 (38%) | 56,90,114   | 3.08 | 21 (37%) |
| 26  | CLA  | 5     | 616  | 18   | 45,50,73     | 1.60 | 11 (24%) | 56,85,113   | 1.30 | 4 (7%)   |
| 26  | CLA  | A     | 820  | 1    | 69,73,73     | 1.26 | 11 (15%) | 83,113,113  | 1.28 | 9 (10%)  |
| 26  | CLA  | a     | 606  | -    | 47,52,73     | 1.52 | 9 (19%)  | 55,87,113   | 1.26 | 4 (7%)   |
| 26  | CLA  | 7     | 607  | -    | 46,50,73     | 1.49 | 8 (17%)  | 55,85,113   | 1.20 | 4 (7%)   |
| 37  | CHL  | V     | 608  | -    | 52,56,74     | 2.17 | 17 (32%) | 58,92,114   | 3.35 | 23 (39%) |
| 26  | CLA  | 5     | 611  | 28   | 46,50,73     | 1.48 | 7 (15%)  | 55,85,113   | 1.27 | 7 (12%)  |
| 26  | CLA  | 4     | 602  | 17   | 64,68,73     | 1.34 | 9 (14%)  | 77,107,113  | 1.22 | 7 (9%)   |
| 34  | LUT  | Z     | 1620 | -    | 42,43,43     | 0.78 | 0        | 51,60,60    | 1.80 | 12 (23%) |
| 26  | CLA  | 2     | 611  | 28   | 46,50,73     | 1.48 | 8 (17%)  | 55,85,113   | 1.35 | 6 (10%)  |
| 26  | CLA  | U     | 602  | 24   | 63,67,73     | 1.31 | 8 (12%)  | 75,105,113  | 1.20 | 6 (8%)   |
| 29  | BCR  | 4     | 621  | -    | 41,41,41     | 0.83 | 1 (2%)   | 56,56,56    | 2.03 | 18 (32%) |
| 26  | CLA  | Z     | 614  | 24   | 52,56,73     | 1.45 | 7 (13%)  | 62,92,113   | 1.28 | 6 (9%)   |
| 26  | CLA  | B     | 828  | 2    | 69,73,73     | 1.28 | 9 (13%)  | 83,113,113  | 1.18 | 7 (8%)   |
| 26  | CLA  | 8     | 607  | -    | 45,49,73     | 1.60 | 11 (24%) | 57,84,113   | 1.33 | 6 (10%)  |
| 26  | CLA  | 6     | 603  | 19   | 55,59,73     | 1.46 | 10 (18%) | 69,96,113   | 1.40 | 7 (10%)  |
| 26  | CLA  | J     | 101  | 10   | 46,50,73     | 1.50 | 8 (17%)  | 55,85,113   | 1.29 | 6 (10%)  |
| 26  | CLA  | 2     | 616  | -    | 47,51,73     | 1.57 | 9 (19%)  | 60,87,113   | 1.33 | 6 (10%)  |
| 26  | CLA  | A     | 810  | 1    | 54,58,73     | 1.45 | 8 (14%)  | 65,95,113   | 1.38 | 8 (12%)  |
| 34  | LUT  | 4     | 619  | -    | 42,43,43     | 0.80 | 1 (2%)   | 51,60,60    | 2.02 | 18 (35%) |
| 26  | CLA  | 2     | 604  | -    | 46,50,73     | 1.50 | 8 (17%)  | 55,85,113   | 1.33 | 8 (14%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | CLA  | 5     | 606  | -    | 43,48,73     | 1.55 | 8 (18%)  | 51,83,113   | 1.31 | 6 (11%)  |
| 29  | BCR  | B     | 846  | -    | 41,41,41     | 0.81 | 1 (2%)   | 56,56,56    | 2.34 | 21 (37%) |
| 26  | CLA  | V     | 613  | 25   | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.17 | 5 (6%)   |
| 35  | XAT  | 5     | 621  | -    | 39,47,47     | 0.95 | 2 (5%)   | 54,74,74    | 2.52 | 18 (33%) |
| 26  | CLA  | O     | 2003 | -    | 43,48,73     | 1.54 | 9 (20%)  | 51,83,113   | 1.28 | 3 (5%)   |
| 26  | CLA  | A     | 826  | -    | 68,72,73     | 1.28 | 11 (16%) | 81,111,113  | 1.25 | 7 (8%)   |
| 26  | CLA  | B     | 835  | -    | 49,53,73     | 1.49 | 10 (20%) | 59,89,113   | 1.33 | 7 (11%)  |
| 26  | CLA  | X     | 610  | 23   | 69,73,73     | 1.26 | 8 (11%)  | 83,113,113  | 1.17 | 7 (8%)   |
| 35  | XAT  | X     | 1622 | -    | 39,47,47     | 0.87 | 0        | 54,74,74    | 2.63 | 20 (37%) |
| 26  | CLA  | A     | 840  | 1    | 56,60,73     | 1.39 | 11 (19%) | 67,97,113   | 1.41 | 9 (13%)  |
| 31  | LMU  | 5     | 629  | -    | 33,33,36     | 1.21 | 2 (6%)   | 44,44,47    | 1.27 | 6 (13%)  |
| 26  | CLA  | 2     | 609  | 15   | 49,53,73     | 1.52 | 9 (18%)  | 59,89,113   | 1.27 | 7 (11%)  |
| 26  | CLA  | 7     | 601  | 20   | 64,68,73     | 1.33 | 11 (17%) | 77,107,113  | 1.31 | 9 (11%)  |
| 26  | CLA  | 6     | 609  | 19   | 49,53,73     | 1.50 | 9 (18%)  | 59,89,113   | 1.31 | 6 (10%)  |
| 32  | LMG  | 8     | 626  | -    | 46,46,55     | 0.97 | 2 (4%)   | 54,54,63    | 1.10 | 4 (7%)   |
| 26  | CLA  | Z     | 604  | -    | 54,57,73     | 1.50 | 9 (16%)  | 60,93,113   | 1.33 | 8 (13%)  |
| 26  | CLA  | 5     | 617  | 18   | 54,58,73     | 1.41 | 11 (20%) | 65,95,113   | 1.26 | 6 (9%)   |
| 26  | CLA  | Z     | 612  | 24   | 49,53,73     | 1.48 | 7 (14%)  | 59,89,113   | 1.32 | 7 (11%)  |
| 34  | LUT  | 8     | 619  | -    | 42,43,43     | 0.86 | 1 (2%)   | 51,60,60    | 1.87 | 11 (21%) |
| 26  | CLA  | 9     | 606  | -    | 43,48,73     | 1.56 | 10 (23%) | 51,83,113   | 1.32 | 4 (7%)   |
| 29  | BCR  | O     | 2005 | -    | 41,41,41     | 0.88 | 1 (2%)   | 56,56,56    | 3.05 | 23 (41%) |
| 26  | CLA  | L     | 303  | 12   | 69,73,73     | 1.26 | 9 (13%)  | 83,113,113  | 1.27 | 8 (9%)   |
| 26  | CLA  | B     | 829  | 2    | 69,73,73     | 1.31 | 11 (15%) | 83,113,113  | 1.31 | 10 (12%) |
| 26  | CLA  | 4     | 613  | 17   | 69,73,73     | 1.29 | 10 (14%) | 83,113,113  | 1.27 | 9 (10%)  |
| 37  | CHL  | W     | 601  | 23   | 70,74,74     | 1.98 | 19 (27%) | 80,114,114  | 2.76 | 24 (30%) |
| 26  | CLA  | A     | 836  | 1    | 69,73,73     | 1.25 | 10 (14%) | 83,113,113  | 1.26 | 7 (8%)   |
| 26  | CLA  | 4     | 612  | 17   | 44,49,73     | 1.53 | 7 (15%)  | 52,84,113   | 1.26 | 3 (5%)   |
| 26  | CLA  | 6     | 606  | -    | 43,48,73     | 1.55 | 8 (18%)  | 51,83,113   | 1.25 | 5 (9%)   |
| 37  | CHL  | Z     | 601  | 24   | 70,74,74     | 1.91 | 18 (25%) | 80,114,114  | 2.87 | 23 (28%) |
| 37  | CHL  | Z     | 606  | -    | 50,54,74     | 2.29 | 19 (38%) | 56,90,114   | 3.30 | 25 (44%) |
| 29  | BCR  | L     | 308  | -    | 41,41,41     | 0.81 | 0        | 56,56,56    | 2.33 | 23 (41%) |
| 26  | CLA  | 6     | 602  | 19   | 69,73,73     | 1.28 | 9 (13%)  | 83,113,113  | 1.18 | 8 (9%)   |
| 26  | CLA  | a     | 601  | 14   | 57,62,73     | 1.36 | 9 (15%)  | 68,100,113  | 1.24 | 8 (11%)  |
| 26  | CLA  | Z     | 613  | 24   | 69,73,73     | 1.26 | 9 (13%)  | 83,113,113  | 1.22 | 5 (6%)   |
| 26  | CLA  | B     | 810  | 2    | 68,72,73     | 1.26 | 11 (16%) | 81,111,113  | 1.38 | 9 (11%)  |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | CLA  | 1     | 607  | -    | 43,48,73     | 1.59 | 10 (23%) | 51,83,113   | 1.24 | 5 (9%)   |
| 26  | CLA  | 1     | 613  | -    | 69,73,73     | 1.28 | 10 (14%) | 83,113,113  | 1.15 | 6 (7%)   |
| 26  | CLA  | Y     | 603  | 24   | 59,63,73     | 1.35 | 7 (11%)  | 71,101,113  | 1.39 | 7 (9%)   |
| 26  | CLA  | 8     | 603  | 21   | 48,52,73     | 1.58 | 9 (18%)  | 61,88,113   | 1.51 | 8 (13%)  |
| 26  | CLA  | Y     | 612  | 24   | 49,53,73     | 1.48 | 7 (14%)  | 59,89,113   | 1.32 | 4 (6%)   |
| 35  | XAT  | 4     | 620  | -    | 39,47,47     | 0.94 | 2 (5%)   | 54,74,74    | 2.49 | 24 (44%) |
| 29  | BCR  | A     | 849  | -    | 41,41,41     | 0.85 | 0        | 56,56,56    | 2.22 | 21 (37%) |
| 26  | CLA  | Y     | 610  | 24   | 69,73,73     | 1.26 | 9 (13%)  | 83,113,113  | 1.14 | 7 (8%)   |
| 26  | CLA  | B     | 805  | 2    | 69,73,73     | 1.27 | 10 (14%) | 83,113,113  | 1.25 | 10 (12%) |
| 33  | DGD  | B     | 850  | -    | 63,63,67     | 0.83 | 2 (3%)   | 77,77,81    | 1.24 | 7 (9%)   |
| 26  | CLA  | 1     | 612  | 14   | 49,53,73     | 1.46 | 9 (18%)  | 59,89,113   | 1.37 | 5 (8%)   |
| 30  | SF4  | C     | 101  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 28  | LHG  | 9     | 622  | 26   | 29,29,48     | 1.18 | 2 (6%)   | 32,35,54    | 1.02 | 1 (3%)   |
| 31  | LMU  | 1     | 621  | -    | 36,36,36     | 1.15 | 2 (5%)   | 47,47,47    | 1.00 | 1 (2%)   |
| 26  | CLA  | B     | 823  | 2    | 49,53,73     | 1.49 | 10 (20%) | 59,89,113   | 1.36 | 7 (11%)  |
| 26  | CLA  | B     | 811  | 2    | 57,60,73     | 1.50 | 11 (19%) | 68,97,113   | 1.35 | 8 (11%)  |
| 26  | CLA  | A     | 833  | 1    | 49,53,73     | 1.49 | 10 (20%) | 59,89,113   | 1.50 | 11 (18%) |
| 26  | CLA  | A     | 821  | 1    | 57,61,73     | 1.37 | 8 (14%)  | 68,98,113   | 1.30 | 7 (10%)  |
| 26  | CLA  | 7     | 606  | -    | 45,49,73     | 1.54 | 11 (24%) | 54,84,113   | 1.28 | 4 (7%)   |
| 26  | CLA  | A     | 825  | 1    | 69,73,73     | 1.27 | 9 (13%)  | 83,113,113  | 1.20 | 6 (7%)   |
| 30  | SF4  | C     | 102  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 34  | LUT  | 5     | 620  | -    | 42,43,43     | 0.84 | 1 (2%)   | 51,60,60    | 1.91 | 15 (29%) |
| 26  | CLA  | A     | 845  | 28   | 54,58,73     | 1.44 | 10 (18%) | 65,95,113   | 1.36 | 7 (10%)  |
| 34  | LUT  | U     | 1620 | -    | 42,43,43     | 0.74 | 0        | 51,60,60    | 1.60 | 10 (19%) |
| 26  | CLA  | B     | 820  | 2    | 54,58,73     | 1.40 | 10 (18%) | 65,95,113   | 1.37 | 6 (9%)   |
| 26  | CLA  | A     | 815  | 1    | 54,58,73     | 1.43 | 9 (16%)  | 65,95,113   | 1.34 | 5 (7%)   |
| 26  | CLA  | K     | 206  | 11   | 49,53,73     | 1.50 | 8 (16%)  | 59,89,113   | 1.26 | 4 (6%)   |
| 32  | LMG  | L     | 2631 | -    | 37,37,55     | 1.08 | 2 (5%)   | 45,45,63    | 1.18 | 4 (8%)   |
| 26  | CLA  | a     | 603  | 14   | 58,62,73     | 1.34 | 8 (13%)  | 69,99,113   | 1.33 | 4 (5%)   |
| 26  | CLA  | 1     | 614  | 14   | 40,45,73     | 1.67 | 9 (22%)  | 50,79,113   | 1.53 | 9 (18%)  |
| 37  | CHL  | U     | 605  | 24   | 47,51,74     | 2.39 | 18 (38%) | 52,86,114   | 3.23 | 21 (40%) |
| 26  | CLA  | B     | 824  | -    | 69,73,73     | 1.27 | 10 (14%) | 83,113,113  | 1.16 | 5 (6%)   |
| 31  | LMU  | 5     | 628  | -    | 34,34,36     | 1.19 | 2 (5%)   | 45,45,47    | 1.14 | 5 (11%)  |
| 26  | CLA  | 2     | 606  | -    | 47,51,73     | 1.49 | 10 (21%) | 56,86,113   | 1.32 | 5 (8%)   |
| 26  | CLA  | 9     | 603  | 22   | 48,52,73     | 1.60 | 13 (27%) | 61,88,113   | 1.40 | 6 (9%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 32  | LMG  | 4     | 624 | -    | 40,40,55     | 1.03 | 2 (5%)   | 48,48,63    | 1.15 | 5 (10%)  |
| 26  | CLA  | 8     | 613 | 21   | 69,73,73     | 1.27 | 9 (13%)  | 83,113,113  | 1.16 | 6 (7%)   |
| 26  | CLA  | 9     | 610 | 22   | 61,65,73     | 1.36 | 9 (14%)  | 73,103,113  | 1.27 | 8 (10%)  |
| 35  | XAT  | 3     | 619 | -    | 39,47,47     | 0.98 | 2 (5%)   | 54,74,74    | 2.60 | 19 (35%) |
| 29  | BCR  | 1     | 619 | -    | 41,41,41     | 0.83 | 0        | 56,56,56    | 2.38 | 22 (39%) |
| 26  | CLA  | U     | 604 | -    | 53,56,73     | 1.52 | 10 (18%) | 57,91,113   | 1.38 | 8 (14%)  |
| 26  | CLA  | 4     | 614 | 17   | 60,64,73     | 1.34 | 8 (13%)  | 72,102,113  | 1.25 | 7 (9%)   |
| 26  | CLA  | A     | 812 | 1    | 69,73,73     | 1.26 | 9 (13%)  | 83,113,113  | 1.19 | 5 (6%)   |
| 26  | CLA  | 6     | 612 | 19   | 44,49,73     | 1.52 | 8 (18%)  | 52,84,113   | 1.26 | 5 (9%)   |
| 26  | CLA  | 5     | 613 | 18   | 68,72,73     | 1.23 | 9 (13%)  | 81,111,113  | 1.28 | 8 (9%)   |
| 29  | BCR  | B     | 852 | -    | 41,41,41     | 0.82 | 0        | 56,56,56    | 4.21 | 30 (53%) |
| 26  | CLA  | Y     | 602 | 24   | 62,66,73     | 1.32 | 8 (12%)  | 74,104,113  | 1.23 | 8 (10%)  |
| 26  | CLA  | U     | 613 | 24   | 63,67,73     | 1.33 | 8 (12%)  | 75,105,113  | 1.20 | 7 (9%)   |
| 26  | CLA  | 5     | 614 | 18   | 48,52,73     | 1.49 | 9 (18%)  | 55,87,113   | 1.32 | 5 (9%)   |
| 26  | CLA  | a     | 604 | -    | 53,57,73     | 1.42 | 8 (15%)  | 62,93,113   | 1.27 | 4 (6%)   |
| 37  | CHL  | Y     | 608 | -    | 53,57,74     | 2.18 | 18 (33%) | 59,93,114   | 3.31 | 24 (40%) |
| 26  | CLA  | K     | 201 | 11   | 49,53,73     | 1.46 | 7 (14%)  | 59,89,113   | 1.24 | 4 (6%)   |
| 26  | CLA  | 3     | 613 | 16   | 56,61,73     | 1.39 | 9 (16%)  | 66,98,113   | 1.17 | 5 (7%)   |
| 26  | CLA  | 7     | 610 | 20   | 69,73,73     | 1.29 | 9 (13%)  | 83,113,113  | 1.11 | 6 (7%)   |
| 26  | CLA  | 9     | 601 | 22   | 49,53,73     | 1.48 | 8 (16%)  | 59,89,113   | 1.31 | 5 (8%)   |
| 32  | LMG  | J     | 104 | -    | 40,40,55     | 1.02 | 2 (5%)   | 48,48,63    | 1.30 | 6 (12%)  |
| 34  | LUT  | 3     | 618 | -    | 42,43,43     | 0.83 | 1 (2%)   | 51,60,60    | 2.01 | 12 (23%) |
| 26  | CLA  | a     | 613 | -    | 58,62,73     | 1.40 | 10 (17%) | 69,99,113   | 1.23 | 6 (8%)   |
| 29  | BCR  | B     | 847 | -    | 41,41,41     | 0.92 | 2 (4%)   | 56,56,56    | 2.20 | 16 (28%) |
| 28  | LHG  | 9     | 623 | -    | 48,48,48     | 0.91 | 2 (4%)   | 51,54,54    | 0.96 | 2 (3%)   |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 26  | CLA  | 3     | 612  | 16   | -       | 5/13/89/115   | -       |
| 26  | CLA  | U     | 614  | 24   | -       | 5/12/88/115   | -       |
| 26  | CLA  | a     | 609  | 14   | -       | 15/37/113/115 | -       |
| 34  | LUT  | U     | 1621 | -    | -       | 5/29/67/67    | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 26  | CLA  | B     | 841  | 28   | -       | 15/39/115/115 | -       |
| 26  | CLA  | B     | 832  | 2    | -       | 12/33/109/115 | -       |
| 35  | XAT  | 9     | 620  | -    | -       | 0/31/93/93    | 0/4/4/4 |
| 28  | LHG  | W     | 2630 | 26   | -       | 13/38/38/53   | -       |
| 29  | BCR  | L     | 301  | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 37  | CHL  | Z     | 605  | 24   | -       | 6/12/88/117   | -       |
| 37  | CHL  | U     | 607  | -    | -       | 11/17/93/117  | -       |
| 26  | CLA  | 5     | 607  | -    | -       | 15/39/115/115 | -       |
| 26  | CLA  | B     | 837  | 2    | -       | 10/39/115/115 | -       |
| 26  | CLA  | F     | 301  | -    | -       | 14/30/106/115 | -       |
| 28  | LHG  | Z     | 2630 | 26   | -       | 19/53/53/53   | -       |
| 26  | CLA  | B     | 819  | -    | -       | 8/27/103/115  | -       |
| 28  | LHG  | 9     | 624  | -    | -       | 17/53/53/53   | -       |
| 28  | LHG  | A     | 861  | -    | -       | 18/53/53/53   | -       |
| 35  | XAT  | 8     | 620  | -    | -       | 0/31/93/93    | 0/4/4/4 |
| 26  | CLA  | 5     | 608  | -    | -       | 6/21/97/115   | -       |
| 27  | PQN  | A     | 844  | -    | -       | 6/23/43/43    | 0/2/2/2 |
| 29  | BCR  | 7     | 621  | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 26  | CLA  | a     | 607  | -    | -       | 6/15/91/115   | -       |
| 26  | CLA  | 6     | 618  | 19   | -       | 1/8/84/115    | -       |
| 29  | BCR  | a     | 619  | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 26  | CLA  | 5     | 610  | 18   | -       | 6/26/102/115  | -       |
| 26  | CLA  | V     | 612  | 25   | -       | 7/15/91/115   | -       |
| 26  | CLA  | A     | 801  | 1    | -       | 10/39/115/115 | -       |
| 26  | CLA  | U     | 610  | 24   | -       | 4/29/105/115  | -       |
| 26  | CLA  | 5     | 618  | 18   | -       | 3/8/84/115    | -       |
| 29  | BCR  | F     | 305  | -    | -       | 6/29/63/63    | 0/2/2/2 |
| 37  | CHL  | W     | 605  | 23   | -       | 12/17/93/117  | -       |
| 26  | CLA  | 4     | 606  | -    | -       | 4/8/84/115    | -       |
| 26  | CLA  | 9     | 609  | 22   | -       | 4/35/111/115  | -       |
| 36  | NEX  | U     | 1623 | -    | -       | 6/27/83/83    | 0/3/3/3 |
| 26  | CLA  | A     | 804  | 1    | -       | 16/39/115/115 | -       |
| 29  | BCR  | K     | 202  | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 26  | CLA  | 9     | 604  | -    | -       | 8/20/96/115   | -       |
| 26  | CLA  | 3     | 610  | 16   | -       | 14/39/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 26  | CLA  | Z     | 610  | 24   | -       | 9/39/115/115  | -       |
| 26  | CLA  | A     | 835  | 1    | -       | 14/35/111/115 | -       |
| 26  | CLA  | 6     | 620  | -    | -       | 12/37/113/115 | -       |
| 26  | CLA  | 6     | 607  | -    | -       | 2/10/86/115   | -       |
| 26  | CLA  | 7     | 604  | -    | -       | 8/21/97/115   | -       |
| 26  | CLA  | a     | 614  | 14   | -       | 9/27/99/115   | -       |
| 26  | CLA  | 5     | 604  | -    | -       | 12/35/111/115 | -       |
| 32  | LMG  | 4     | 623  | -    | -       | 6/35/55/70    | 0/1/1/1 |
| 26  | CLA  | W     | 612  | 23   | -       | 7/15/91/115   | -       |
| 26  | CLA  | 8     | 608  | -    | -       | 7/23/99/115   | -       |
| 32  | LMG  | J     | 103  | -    | -       | 10/37/57/70   | 0/1/1/1 |
| 29  | BCR  | A     | 848  | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 34  | LUT  | Y     | 1620 | -    | -       | 5/29/67/67    | 0/2/2/2 |
| 26  | CLA  | A     | 830  | 1    | -       | 13/39/115/115 | -       |
| 28  | LHG  | 5     | 625  | -    | -       | 14/53/53/53   | -       |
| 29  | BCR  | 9     | 621  | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 28  | LHG  | 3     | 623  | -    | -       | 15/49/49/53   | -       |
| 26  | CLA  | a     | 602  | 14   | -       | 5/35/111/115  | -       |
| 26  | CLA  | 8     | 616  | 21   | -       | 5/11/87/115   | -       |
| 26  | CLA  | 3     | 602  | 16   | -       | 3/33/109/115  | -       |
| 35  | XAT  | W     | 1622 | -    | -       | 2/31/93/93    | 0/4/4/4 |
| 35  | XAT  | V     | 1622 | -    | -       | 2/31/93/93    | 0/4/4/4 |
| 26  | CLA  | B     | 803  | -    | -       | 12/39/115/115 | -       |
| 37  | CHL  | V     | 605  | 25   | -       | 7/15/91/117   | -       |
| 26  | CLA  | 8     | 611  | 28   | -       | 6/12/88/115   | -       |
| 28  | LHG  | Y     | 2630 | 26   | -       | 13/53/53/53   | -       |
| 26  | CLA  | B     | 804  | 2    | -       | 3/10/86/115   | -       |
| 26  | CLA  | 2     | 607  | -    | -       | 2/13/89/115   | -       |
| 28  | LHG  | 6     | 623  | 26   | -       | 19/52/52/53   | -       |
| 26  | CLA  | 4     | 603  | 17   | -       | 5/13/89/115   | -       |
| 28  | LHG  | H     | 204  | -    | -       | 15/53/53/53   | -       |
| 26  | CLA  | H     | 203  | -    | -       | 17/39/115/115 | -       |
| 26  | CLA  | a     | 616  | 14   | -       | 7/15/91/115   | -       |
| 26  | CLA  | A     | 827  | -    | -       | 7/31/107/115  | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 37  | CHL  | Z     | 608  | -    | -       | 8/21/97/117   | -       |
| 26  | CLA  | A     | 816  | 1    | -       | 15/39/115/115 | -       |
| 26  | CLA  | 8     | 609  | 21   | -       | 2/15/91/115   | -       |
| 26  | CLA  | B     | 827  | 2    | -       | 12/36/112/115 | -       |
| 32  | LMG  | 9     | 625  | -    | -       | 11/50/70/70   | 0/1/1/1 |
| 36  | NEX  | 5     | 624  | -    | -       | 2/27/83/83    | 0/3/3/3 |
| 26  | CLA  | B     | 834  | 2    | -       | 5/33/109/115  | -       |
| 35  | XAT  | U     | 1622 | -    | -       | 4/31/93/93    | 0/4/4/4 |
| 29  | BCR  | O     | 2004 | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 37  | CHL  | X     | 609  | 23   | -       | 26/41/117/117 | -       |
| 26  | CLA  | W     | 604  | -    | -       | 6/18/94/115   | -       |
| 34  | LUT  | V     | 1621 | -    | -       | 3/29/67/67    | 0/2/2/2 |
| 26  | CLA  | 3     | 617  | 16   | -       | 1/8/84/115    | -       |
| 26  | CLA  | 7     | 603  | 20   | -       | 7/13/89/115   | -       |
| 28  | LHG  | 8     | 622  | 26   | -       | 13/53/53/53   | -       |
| 34  | LUT  | X     | 1620 | -    | -       | 4/29/67/67    | 0/2/2/2 |
| 28  | LHG  | 8     | 623  | -    | -       | 12/44/44/53   | -       |
| 26  | CLA  | A     | 829  | 1    | -       | 10/39/115/115 | -       |
| 26  | CLA  | 6     | 610  | 19   | -       | 12/39/115/115 | -       |
| 26  | CLA  | V     | 603  | 25   | -       | 6/15/91/115   | -       |
| 26  | CLA  | Y     | 614  | 24   | -       | 10/19/95/115  | -       |
| 29  | BCR  | 7     | 623  | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 26  | CLA  | K     | 203  | -    | -       | 10/29/105/115 | -       |
| 31  | LMU  | 8     | 625  | -    | -       | 12/21/61/61   | 0/2/2/2 |
| 29  | BCR  | B     | 801  | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 36  | NEX  | Y     | 1623 | -    | -       | 6/27/83/83    | 0/3/3/3 |
| 36  | NEX  | Z     | 1623 | -    | -       | 6/27/83/83    | 0/3/3/3 |
| 29  | BCR  | 5     | 622  | -    | -       | 1/29/63/63    | 0/2/2/2 |
| 26  | CLA  | 5     | 619  | -    | -       | 10/11/87/115  | -       |
| 37  | CHL  | U     | 609  | 24   | -       | 14/34/110/117 | -       |
| 26  | CLA  | 3     | 603  | 16   | -       | 10/27/103/115 | -       |
| 34  | LUT  | 1     | 617  | -    | -       | 4/29/67/67    | 0/2/2/2 |
| 26  | CLA  | A     | 813  | 1    | -       | 7/26/102/115  | -       |
| 37  | CHL  | W     | 606  | -    | -       | 4/17/93/117   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 29  | BCR  | B     | 849  | -    | -       | 5/29/63/63    | 0/2/2/2 |
| 26  | CLA  | B     | 838  | 2    | -       | 3/17/93/115   | -       |
| 37  | CHL  | V     | 601  | 25   | -       | 13/41/117/117 | -       |
| 26  | CLA  | W     | 611  | 28   | -       | 9/30/106/115  | -       |
| 26  | CLA  | G     | 204  | 7    | -       | 7/15/91/115   | -       |
| 29  | BCR  | L     | 305  | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 26  | CLA  | A     | 819  | 1    | -       | 5/32/108/115  | -       |
| 26  | CLA  | 4     | 608  | -    | -       | 11/39/115/115 | -       |
| 26  | CLA  | B     | 817  | 2    | -       | 10/32/108/115 | -       |
| 29  | BCR  | 3     | 622  | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 37  | CHL  | W     | 609  | 23   | -       | 13/41/117/117 | -       |
| 34  | LUT  | 6     | 619  | -    | -       | 4/29/67/67    | 0/2/2/2 |
| 26  | CLA  | 2     | 602  | 15   | -       | 18/49/99/115  | -       |
| 26  | CLA  | 6     | 617  | 19   | -       | 9/15/91/115   | -       |
| 26  | CLA  | B     | 825  | -    | -       | 4/20/96/115   | -       |
| 26  | CLA  | 5     | 612  | 18   | -       | 2/10/86/115   | -       |
| 26  | CLA  | B     | 831  | 2    | -       | 12/39/115/115 | -       |
| 26  | CLA  | A     | 831  | 1    | -       | 16/39/115/115 | -       |
| 26  | CLA  | L     | 307  | 8    | -       | 2/8/84/115    | -       |
| 26  | CLA  | 6     | 614  | 19   | -       | 9/33/109/115  | -       |
| 26  | CLA  | 7     | 615  | -    | -       | 6/8/84/115    | -       |
| 26  | CLA  | O     | 2002 | -    | -       | 0/4/80/115    | -       |
| 37  | CHL  | X     | 606  | -    | -       | 6/15/91/117   | -       |
| 26  | CLA  | Z     | 603  | 24   | -       | 11/27/103/115 | -       |
| 26  | CLA  | X     | 611  | 28   | -       | 6/15/91/115   | -       |
| 27  | PQN  | B     | 842  | -    | -       | 7/23/43/43    | 0/2/2/2 |
| 26  | CLA  | A     | 837  | 1    | -       | 9/15/91/115   | -       |
| 26  | CLA  | V     | 602  | 25   | -       | 8/33/109/115  | -       |
| 26  | CLA  | 2     | 610  | 15   | -       | 5/27/103/115  | -       |
| 37  | CHL  | Y     | 601  | 24   | -       | 21/41/117/117 | -       |
| 26  | CLA  | 1     | 608  | -    | -       | 4/13/89/115   | -       |
| 28  | LHG  | B     | 851  | 26   | -       | 14/42/42/53   | -       |
| 26  | CLA  | B     | 840  | 2    | -       | 9/39/115/115  | -       |
| 26  | CLA  | B     | 802  | 2    | -       | 18/39/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 26  | CLA  | 4     | 611  | 28   | -       | 9/12/88/115   | -       |
| 28  | LHG  | O     | 2631 | -    | -       | 13/40/40/53   | -       |
| 26  | CLA  | 4     | 604  | -    | -       | 9/25/101/115  | -       |
| 34  | LUT  | 9     | 619  | -    | -       | 4/29/67/67    | 0/2/2/2 |
| 26  | CLA  | 6     | 601  | 19   | -       | 17/39/115/115 | -       |
| 34  | LUT  | Z     | 1621 | -    | -       | 3/29/67/67    | 0/2/2/2 |
| 26  | CLA  | A     | 843  | -    | -       | 14/37/113/115 | -       |
| 29  | BCR  | B     | 853  | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 37  | CHL  | Y     | 605  | 24   | -       | 6/12/88/117   | -       |
| 26  | CLA  | A     | 818  | 1    | -       | 15/33/109/115 | -       |
| 34  | LUT  | 7     | 619  | -    | -       | 2/29/67/67    | 0/2/2/2 |
| 36  | NEX  | X     | 1623 | -    | -       | 5/27/83/83    | 0/3/3/3 |
| 31  | LMU  | A     | 858  | -    | -       | 10/21/57/61   | 0/2/2/2 |
| 26  | CLA  | 7     | 614  | 20   | -       | 3/12/88/115   | -       |
| 26  | CLA  | 1     | 606  | -    | -       | 3/7/79/115    | -       |
| 26  | CLA  | Y     | 611  | 28   | -       | 9/13/89/115   | -       |
| 26  | CLA  | Z     | 611  | 28   | -       | 5/11/87/115   | -       |
| 26  | CLA  | Y     | 604  | -    | -       | 8/21/97/115   | -       |
| 28  | LHG  | 5     | 623  | 26   | -       | 15/53/53/53   | -       |
| 37  | CHL  | V     | 606  | -    | -       | 6/15/91/117   | -       |
| 26  | CLA  | 3     | 607  | 16   | -       | 6/28/104/115  | -       |
| 26  | CLA  | 1     | 611  | 28   | -       | 7/30/106/115  | -       |
| 26  | CLA  | A     | 811  | 1    | -       | 15/39/115/115 | -       |
| 37  | CHL  | V     | 607  | -    | -       | 12/17/93/117  | -       |
| 28  | LHG  | a     | 620  | 26   | -       | 7/47/47/53    | -       |
| 26  | CLA  | A     | 828  | 1    | -       | 16/39/115/115 | -       |
| 29  | BCR  | L     | 309  | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 26  | CLA  | 2     | 612  | 15   | -       | 7/13/89/115   | -       |
| 26  | CLA  | B     | 839  | -    | -       | 14/39/115/115 | -       |
| 26  | CLA  | L     | 302  | 12   | -       | 8/15/91/115   | -       |
| 26  | CLA  | X     | 604  | -    | -       | 11/20/96/115  | -       |
| 26  | CLA  | 8     | 612  | 21   | -       | 2/10/86/115   | -       |
| 26  | CLA  | B     | 812  | 2    | -       | 5/13/89/115   | -       |
| 26  | CLA  | A     | 834  | 1    | -       | 12/39/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 26  | CLA  | Z     | 602  | 24   | -       | 7/31/107/115  | -       |
| 26  | CLA  | A     | 832  | 1    | -       | 11/21/97/115  | -       |
| 26  | CLA  | a     | 608  | -    | -       | 4/13/89/115   | -       |
| 26  | CLA  | 8     | 614  | 21   | -       | 8/25/101/115  | -       |
| 36  | NEX  | V     | 1623 | -    | -       | 7/27/83/83    | 0/3/3/3 |
| 26  | CLA  | 9     | 607  | -    | -       | 11/15/91/115  | -       |
| 28  | LHG  | 7     | 622  | 26   | -       | 19/41/41/53   | -       |
| 26  | CLA  | V     | 610  | 25   | -       | 9/36/112/115  | -       |
| 26  | CLA  | A     | 817  | -    | -       | 2/15/91/115   | -       |
| 26  | CLA  | B     | 808  | 2    | -       | 13/39/115/115 | -       |
| 26  | CLA  | 3     | 614  | 16   | -       | 2/8/84/115    | -       |
| 28  | LHG  | 4     | 622  | 26   | -       | 8/53/53/53    | -       |
| 26  | CLA  | A     | 838  | 1    | -       | 8/21/97/115   | -       |
| 34  | LUT  | V     | 1620 | -    | -       | 4/29/67/67    | 0/2/2/2 |
| 34  | LUT  | X     | 1621 | -    | -       | 3/29/67/67    | 0/2/2/2 |
| 37  | CHL  | Y     | 607  | -    | -       | 21/41/117/117 | -       |
| 26  | CLA  | 6     | 611  | 28   | -       | 5/12/88/115   | -       |
| 26  | CLA  | 7     | 608  | -    | -       | 4/21/97/115   | -       |
| 26  | CLA  | 6     | 604  | -    | -       | 18/39/115/115 | -       |
| 26  | CLA  | A     | 822  | -    | -       | 6/39/115/115  | -       |
| 29  | BCR  | B     | 845  | -    | -       | 9/29/63/63    | 0/2/2/2 |
| 37  | CHL  | Y     | 609  | 24   | -       | 17/41/117/117 | -       |
| 26  | CLA  | B     | 815  | 2    | -       | 2/13/89/115   | -       |
| 29  | BCR  | B     | 844  | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 31  | LMU  | A     | 857  | -    | -       | 9/21/61/61    | 0/2/2/2 |
| 29  | BCR  | A     | 856  | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 26  | CLA  | L     | 306  | -    | -       | 1/8/84/115    | -       |
| 26  | CLA  | B     | 807  | 2    | -       | 4/24/100/115  | -       |
| 26  | CLA  | A     | 805  | 1    | -       | 7/24/100/115  | -       |
| 26  | CLA  | 3     | 606  | -    | -       | 4/25/101/115  | -       |
| 26  | CLA  | 4     | 616  | 17   | -       | 7/11/87/115   | -       |
| 26  | CLA  | 9     | 614  | 22   | -       | 5/15/91/115   | -       |
| 37  | CHL  | U     | 608  | -    | -       | 7/15/91/117   | -       |
| 26  | CLA  | 5     | 602  | 18   | -       | 10/39/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 26  | CLA  | 5     | 609  | 18   | -       | 12/39/115/115 | -       |
| 30  | SF4  | A     | 853  | 2,1  | -       | -             | 0/6/5/5 |
| 26  | CLA  | A     | 808  | 1    | -       | 3/21/97/115   | -       |
| 26  | CLA  | 3     | 604  | -    | -       | 7/39/115/115  | -       |
| 34  | LUT  | W     | 1621 | -    | -       | 5/29/67/67    | 0/2/2/2 |
| 26  | CLA  | 1     | 603  | 14   | -       | 7/23/99/115   | -       |
| 26  | CLA  | 7     | 616  | 20   | -       | 8/11/87/115   | -       |
| 35  | XAT  | a     | 618  | -    | -       | 0/31/93/93    | 0/4/4/4 |
| 26  | CLA  | A     | 854  | -    | -       | 9/39/115/115  | -       |
| 29  | BCR  | 3     | 621  | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 36  | NEX  | 6     | 624  | -    | -       | 3/27/83/83    | 0/3/3/3 |
| 26  | CLA  | 3     | 609  | 16   | -       | 14/33/109/115 | -       |
| 26  | CLA  | 7     | 611  | 28   | -       | 6/31/107/115  | -       |
| 37  | CHL  | W     | 607  | -    | -       | 21/39/115/117 | -       |
| 26  | CLA  | 7     | 613  | 20   | -       | 18/39/115/115 | -       |
| 37  | CHL  | U     | 606  | -    | -       | 8/15/91/117   | -       |
| 26  | CLA  | B     | 818  | 2    | -       | 11/33/109/115 | -       |
| 26  | CLA  | 7     | 612  | 20   | -       | 4/13/89/115   | -       |
| 28  | LHG  | V     | 2630 | 26   | -       | 6/40/40/53    | -       |
| 26  | CLA  | 9     | 602  | 22   | -       | 7/33/109/115  | -       |
| 26  | CLA  | B     | 814  | 2    | -       | 15/38/114/115 | -       |
| 26  | CLA  | 1     | 601  | 14   | -       | 4/25/101/115  | -       |
| 26  | CLA  | B     | 822  | 2    | -       | 7/12/88/115   | -       |
| 26  | CLA  | A     | 823  | 1    | -       | 1/12/88/115   | -       |
| 26  | CLA  | 5     | 603  | 18   | -       | 5/25/101/115  | -       |
| 26  | CLA  | V     | 611  | 28   | -       | 7/13/89/115   | -       |
| 26  | CLA  | U     | 603  | 24   | -       | 10/24/100/115 | -       |
| 26  | CLA  | 7     | 609  | 20   | -       | 6/12/88/115   | -       |
| 26  | CLA  | X     | 614  | 23   | -       | 3/12/88/115   | -       |
| 37  | CHL  | X     | 607  | -    | -       | 27/41/117/117 | -       |
| 26  | CLA  | A     | 824  | 1    | -       | 11/39/115/115 | -       |
| 26  | CLA  | 4     | 601  | 17   | -       | 16/39/115/115 | -       |
| 26  | CLA  | A     | 841  | 1    | -       | 18/39/115/115 | -       |
| 37  | CHL  | V     | 609  | 25   | -       | 13/35/111/117 | -       |
| 26  | CLA  | 3     | 611  | 28   | -       | 3/4/80/115    | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 26  | CLA  | 5     | 601  | 18   | -       | 3/29/105/115  | -       |
| 26  | CLA  | B     | 830  | 2    | -       | 4/13/89/115   | -       |
| 26  | CLA  | 8     | 601  | 21   | -       | 16/39/115/115 | -       |
| 29  | BCR  | A     | 850  | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 26  | CLA  | F     | 303  | -    | -       | 7/12/88/115   | -       |
| 29  | BCR  | A     | 852  | -    | -       | 8/29/63/63    | 0/2/2/2 |
| 28  | LHG  | 2     | 622  | 26   | -       | 9/40/40/53    | -       |
| 26  | CLA  | B     | 809  | 2    | -       | 11/39/115/115 | -       |
| 29  | BCR  | A     | 851  | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 34  | LUT  | a     | 617  | -    | -       | 4/29/67/67    | 0/2/2/2 |
| 37  | CHL  | Y     | 606  | -    | -       | 8/17/93/117   | -       |
| 26  | CLA  | 1     | 604  | -    | -       | 8/20/96/115   | -       |
| 26  | CLA  | X     | 603  | 23   | -       | 15/36/112/115 | -       |
| 34  | LUT  | 2     | 619  | -    | -       | 2/29/67/67    | 0/2/2/2 |
| 28  | LHG  | 1     | 620  | 26   | -       | 9/53/53/53    | -       |
| 26  | CLA  | B     | 821  | 2    | -       | 5/13/89/115   | -       |
| 26  | CLA  | A     | 839  | 1    | -       | 10/27/103/115 | -       |
| 35  | XAT  | 2     | 620  | -    | -       | 0/31/93/93    | 0/4/4/4 |
| 34  | LUT  | W     | 1620 | -    | -       | 6/29/67/67    | 0/2/2/2 |
| 26  | CLA  | A     | 802  | 2    | -       | 12/39/115/115 | -       |
| 28  | LHG  | X     | 2630 | 26   | -       | 13/53/53/53   | -       |
| 37  | CHL  | Z     | 609  | 24   | -       | 18/41/117/117 | -       |
| 37  | CHL  | X     | 601  | 23   | -       | 21/41/117/117 | -       |
| 29  | BCR  | B     | 848  | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 26  | CLA  | 3     | 615  | -    | -       | 3/8/84/115    | -       |
| 26  | CLA  | 6     | 616  | 19   | -       | 18/39/115/115 | -       |
| 29  | BCR  | B     | 843  | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 29  | BCR  | 2     | 623  | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 26  | CLA  | A     | 806  | 1    | -       | 13/39/115/115 | -       |
| 32  | LMG  | A     | 860  | -    | -       | 9/35/55/70    | 0/1/1/1 |
| 26  | CLA  | G     | 203  | 7    | -       | 5/12/88/115   | -       |
| 26  | CLA  | 8     | 604  | -    | -       | 6/21/97/115   | -       |
| 26  | CLA  | 2     | 613  | 15   | -       | 10/39/115/115 | -       |
| 31  | LMU  | K     | 208  | -    | -       | 10/21/61/61   | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 37  | CHL  | U     | 601  | 24   | -       | 19/41/117/117 | -       |
| 26  | CLA  | 6     | 613  | -    | -       | 15/37/113/115 | -       |
| 26  | CLA  | 1     | 610  | 14   | -       | 2/8/80/115    | -       |
| 29  | BCR  | 8     | 621  | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 26  | CLA  | 7     | 602  | 20   | -       | 11/39/115/115 | -       |
| 26  | CLA  | B     | 836  | 2    | -       | 5/21/97/115   | -       |
| 26  | CLA  | K     | 204  | 11   | -       | 5/15/91/115   | -       |
| 26  | CLA  | 4     | 610  | 17   | -       | 8/35/111/115  | -       |
| 35  | XAT  | 6     | 621  | -    | -       | 0/31/93/93    | 0/4/4/4 |
| 26  | CLA  | H     | 202  | -    | -       | 4/6/82/115    | -       |
| 26  | CLA  | 4     | 618  | 17   | -       | 2/8/84/115    | -       |
| 26  | CLA  | a     | 611  | 28   | -       | 0/4/80/115    | -       |
| 26  | CLA  | W     | 614  | 23   | -       | 8/15/91/115   | -       |
| 26  | CLA  | A     | 803  | -    | -       | 9/39/115/115  | -       |
| 32  | LMG  | H     | 205  | -    | -       | 14/50/70/70   | 0/1/1/1 |
| 32  | LMG  | V     | 2631 | -    | -       | 12/50/70/70   | 0/1/1/1 |
| 26  | CLA  | 1     | 609  | 14   | -       | 3/8/84/115    | -       |
| 26  | CLA  | U     | 612  | 24   | -       | 5/12/88/115   | -       |
| 26  | CLA  | 8     | 610  | 21   | -       | 9/33/109/115  | -       |
| 26  | CLA  | B     | 816  | 2    | -       | 10/25/101/115 | -       |
| 26  | CLA  | X     | 613  | 23   | -       | 14/39/115/115 | -       |
| 26  | CLA  | 6     | 608  | -    | -       | 8/15/91/115   | -       |
| 26  | CLA  | X     | 612  | 23   | -       | 8/13/89/115   | -       |
| 26  | CLA  | a     | 612  | 14   | -       | 6/15/91/115   | -       |
| 32  | LMG  | 5     | 627  | -    | -       | 7/35/55/70    | 0/1/1/1 |
| 26  | CLA  | B     | 806  | 2    | -       | 19/39/115/115 | -       |
| 28  | LHG  | A     | 846  | -    | -       | 15/53/53/53   | -       |
| 26  | CLA  | A     | 807  | 1    | -       | 20/39/115/115 | -       |
| 26  | CLA  | W     | 602  | 23   | -       | 12/33/109/115 | -       |
| 29  | BCR  | G     | 205  | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 26  | CLA  | B     | 813  | 2    | -       | 20/39/115/115 | -       |
| 29  | BCR  | 6     | 622  | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 26  | CLA  | 2     | 603  | 15   | -       | 7/13/89/115   | -       |
| 29  | BCR  | J     | 102  | -    | -       | 2/29/63/63    | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 29  | BCR  | K     | 207  | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 26  | CLA  | Y     | 613  | 24   | -       | 16/39/115/115 | -       |
| 26  | CLA  | a     | 610  | 14   | -       | 7/31/107/115  | -       |
| 26  | CLA  | A     | 842  | 1    | -       | 18/39/115/115 | -       |
| 26  | CLA  | F     | 304  | 6    | -       | 5/10/86/115   | -       |
| 26  | CLA  | L     | 304  | -    | -       | 3/15/91/115   | -       |
| 26  | CLA  | 2     | 614  | 15   | -       | 0/11/87/115   | -       |
| 26  | CLA  | 9     | 611  | 28   | -       | 5/12/88/115   | -       |
| 35  | XAT  | 1     | 618  | -    | -       | 0/31/93/93    | 0/4/4/4 |
| 26  | CLA  | 3     | 608  | -    | -       | 10/27/103/115 | -       |
| 36  | NEX  | W     | 1623 | -    | -       | 6/27/83/83    | 0/3/3/3 |
| 28  | LHG  | A     | 847  | 26   | -       | 6/34/34/53    | -       |
| 26  | CLA  | B     | 833  | 2    | -       | 13/39/115/115 | -       |
| 34  | LUT  | Y     | 1621 | -    | -       | 3/29/67/67    | 0/2/2/2 |
| 26  | CLA  | V     | 614  | 25   | -       | 6/15/91/115   | -       |
| 37  | CHL  | Z     | 607  | -    | -       | 22/41/117/117 | -       |
| 26  | CLA  | B     | 826  | 2    | -       | 14/36/112/115 | -       |
| 26  | CLA  | 1     | 616  | 14   | -       | 7/11/87/115   | -       |
| 26  | CLA  | A     | 814  | 1    | -       | 18/39/115/115 | -       |
| 26  | CLA  | W     | 613  | 23   | -       | 22/39/115/115 | -       |
| 26  | CLA  | 2     | 601  | 15   | -       | 8/39/115/115  | -       |
| 26  | CLA  | O     | 2001 | 13   | -       | 2/6/78/115    | -       |
| 26  | CLA  | A     | 809  | 1    | -       | 11/39/115/115 | -       |
| 35  | XAT  | Y     | 1622 | -    | -       | 3/31/93/93    | 0/4/4/4 |
| 26  | CLA  | X     | 602  | 23   | -       | 13/39/115/115 | -       |
| 26  | CLA  | U     | 611  | 28   | -       | 4/12/88/115   | -       |
| 26  | CLA  | 9     | 613  | 22   | -       | 14/39/115/115 | -       |
| 28  | LHG  | U     | 2630 | 26   | -       | 21/53/53/53   | -       |
| 26  | CLA  | 8     | 606  | -    | -       | 8/37/113/115  | -       |
| 35  | XAT  | Z     | 1622 | -    | -       | 4/31/93/93    | 0/4/4/4 |
| 26  | CLA  | 4     | 609  | 17   | -       | 5/30/106/115  | -       |
| 37  | CHL  | W     | 608  | -    | -       | 11/19/95/117  | -       |
| 26  | CLA  | 8     | 602  | 21   | -       | 14/33/109/115 | -       |
| 26  | CLA  | 9     | 612  | 22   | -       | 2/10/86/115   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 37  | CHL  | X     | 608  | -    | -       | 21/41/113/117 | -       |
| 26  | CLA  | W     | 603  | 23   | -       | 9/24/100/115  | -       |
| 29  | BCR  | 3     | 620  | -    | -       | 4/29/63/63    | 0/2/2/2 |
| 26  | CLA  | W     | 610  | 23   | -       | 7/27/103/115  | -       |
| 28  | LHG  | 3     | 624  | 26   | -       | 14/53/53/53   | -       |
| 35  | XAT  | 7     | 620  | -    | -       | 0/31/93/93    | 0/4/4/4 |
| 26  | CLA  | 4     | 607  | -    | -       | 5/15/91/115   | -       |
| 26  | CLA  | V     | 604  | -    | -       | 8/21/97/115   | -       |
| 26  | CLA  | 1     | 602  | 14   | -       | 5/35/111/115  | -       |
| 37  | CHL  | X     | 605  | -    | -       | 9/17/93/117   | -       |
| 26  | CLA  | 5     | 616  | 18   | -       | 4/8/84/115    | -       |
| 26  | CLA  | A     | 820  | 1    | -       | 8/39/115/115  | -       |
| 26  | CLA  | a     | 606  | -    | -       | 8/12/88/115   | -       |
| 26  | CLA  | 7     | 607  | -    | -       | 1/12/88/115   | -       |
| 37  | CHL  | V     | 608  | -    | -       | 7/20/96/117   | -       |
| 26  | CLA  | 5     | 611  | 28   | -       | 2/12/88/115   | -       |
| 26  | CLA  | 4     | 602  | 17   | -       | 8/33/109/115  | -       |
| 34  | LUT  | Z     | 1620 | -    | -       | 5/29/67/67    | 0/2/2/2 |
| 26  | CLA  | 2     | 611  | 28   | -       | 4/12/88/115   | -       |
| 26  | CLA  | U     | 602  | 24   | -       | 18/32/108/115 | -       |
| 29  | BCR  | 4     | 621  | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 26  | CLA  | Z     | 614  | 24   | -       | 9/19/95/115   | -       |
| 26  | CLA  | B     | 828  | 2    | -       | 17/39/115/115 | -       |
| 26  | CLA  | 8     | 607  | -    | -       | 2/10/86/115   | -       |
| 26  | CLA  | 6     | 603  | 19   | -       | 5/22/98/115   | -       |
| 26  | CLA  | J     | 101  | 10   | -       | 7/12/88/115   | -       |
| 26  | CLA  | 2     | 616  | -    | -       | 3/11/87/115   | -       |
| 26  | CLA  | A     | 810  | 1    | -       | 7/21/97/115   | -       |
| 34  | LUT  | 4     | 619  | -    | -       | 4/29/67/67    | 0/2/2/2 |
| 26  | CLA  | 2     | 604  | -    | -       | 3/11/87/115   | -       |
| 26  | CLA  | 5     | 606  | -    | -       | 3/8/84/115    | -       |
| 29  | BCR  | B     | 846  | -    | -       | 0/29/63/63    | 0/2/2/2 |
| 26  | CLA  | V     | 613  | 25   | -       | 20/39/115/115 | -       |
| 35  | XAT  | 5     | 621  | -    | -       | 0/31/93/93    | 0/4/4/4 |
| 26  | CLA  | O     | 2003 | -    | -       | 6/8/84/115    | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 26  | CLA  | A     | 826  | -    | -       | 8/37/113/115  | -       |
| 26  | CLA  | B     | 835  | -    | -       | 2/15/91/115   | -       |
| 26  | CLA  | X     | 610  | 23   | -       | 13/39/115/115 | -       |
| 35  | XAT  | X     | 1622 | -    | -       | 3/31/93/93    | 0/4/4/4 |
| 26  | CLA  | A     | 840  | 1    | -       | 5/24/100/115  | -       |
| 31  | LMU  | 5     | 629  | -    | -       | 11/18/58/61   | 0/2/2/2 |
| 26  | CLA  | 2     | 609  | 15   | -       | 5/15/91/115   | -       |
| 26  | CLA  | 7     | 601  | 20   | -       | 8/33/109/115  | -       |
| 26  | CLA  | 6     | 609  | 19   | -       | 7/15/91/115   | -       |
| 32  | LMG  | 8     | 626  | -    | -       | 16/41/61/70   | 0/1/1/1 |
| 26  | CLA  | Z     | 604  | -    | -       | 5/21/93/115   | -       |
| 26  | CLA  | 5     | 617  | 18   | -       | 12/21/97/115  | -       |
| 26  | CLA  | Z     | 612  | 24   | -       | 8/15/91/115   | -       |
| 34  | LUT  | 8     | 619  | -    | -       | 4/29/67/67    | 0/2/2/2 |
| 26  | CLA  | 9     | 606  | -    | -       | 2/8/84/115    | -       |
| 29  | BCR  | O     | 2005 | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 26  | CLA  | L     | 303  | 12   | -       | 14/39/115/115 | -       |
| 26  | CLA  | B     | 829  | 2    | -       | 8/39/115/115  | -       |
| 26  | CLA  | 4     | 613  | 17   | -       | 13/39/115/115 | -       |
| 37  | CHL  | W     | 601  | 23   | -       | 19/41/117/117 | -       |
| 26  | CLA  | A     | 836  | 1    | -       | 9/39/115/115  | -       |
| 26  | CLA  | 4     | 612  | 17   | -       | 4/10/86/115   | -       |
| 26  | CLA  | 6     | 606  | -    | -       | 2/8/84/115    | -       |
| 37  | CHL  | Z     | 601  | 24   | -       | 16/41/117/117 | -       |
| 37  | CHL  | Z     | 606  | -    | -       | 8/17/93/117   | -       |
| 29  | BCR  | L     | 308  | -    | -       | 6/29/63/63    | 0/2/2/2 |
| 26  | CLA  | 6     | 602  | 19   | -       | 9/39/115/115  | -       |
| 26  | CLA  | a     | 601  | 14   | -       | 4/25/101/115  | -       |
| 26  | CLA  | Z     | 613  | 24   | -       | 8/39/115/115  | -       |
| 26  | CLA  | B     | 810  | 2    | -       | 20/37/113/115 | -       |
| 26  | CLA  | 1     | 607  | -    | -       | 2/8/84/115    | -       |
| 26  | CLA  | 1     | 613  | -    | -       | 17/39/115/115 | -       |
| 26  | CLA  | Y     | 603  | 24   | -       | 12/27/103/115 | -       |
| 26  | CLA  | 8     | 603  | 21   | -       | 4/13/89/115   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 26  | CLA  | Y     | 612  | 24   | -       | 7/15/91/115   | -       |
| 35  | XAT  | 4     | 620  | -    | -       | 2/31/93/93    | 0/4/4/4 |
| 29  | BCR  | A     | 849  | -    | -       | 5/29/63/63    | 0/2/2/2 |
| 26  | CLA  | Y     | 610  | 24   | -       | 10/39/115/115 | -       |
| 26  | CLA  | B     | 805  | 2    | -       | 11/39/115/115 | -       |
| 33  | DGD  | B     | 850  | -    | -       | 15/51/91/95   | 0/2/2/2 |
| 26  | CLA  | 1     | 612  | 14   | -       | 6/15/91/115   | -       |
| 30  | SF4  | C     | 101  | 3    | -       | -             | 0/6/5/5 |
| 28  | LHG  | 9     | 622  | 26   | -       | 10/34/34/53   | -       |
| 31  | LMU  | 1     | 621  | -    | -       | 7/21/61/61    | 0/2/2/2 |
| 26  | CLA  | B     | 823  | 2    | -       | 7/15/91/115   | -       |
| 26  | CLA  | B     | 811  | 2    | -       | 11/23/95/115  | -       |
| 26  | CLA  | A     | 833  | 1    | -       | 5/15/91/115   | -       |
| 26  | CLA  | A     | 821  | 1    | -       | 14/25/101/115 | -       |
| 26  | CLA  | 7     | 606  | -    | -       | 2/10/86/115   | -       |
| 26  | CLA  | A     | 825  | 1    | -       | 17/39/115/115 | -       |
| 30  | SF4  | C     | 102  | 3    | -       | -             | 0/6/5/5 |
| 34  | LUT  | 5     | 620  | -    | -       | 0/29/67/67    | 0/2/2/2 |
| 26  | CLA  | A     | 845  | 28   | -       | 7/21/97/115   | -       |
| 34  | LUT  | U     | 1620 | -    | -       | 7/29/67/67    | 0/2/2/2 |
| 26  | CLA  | B     | 820  | 2    | -       | 3/21/97/115   | -       |
| 26  | CLA  | A     | 815  | 1    | -       | 12/21/97/115  | -       |
| 26  | CLA  | K     | 206  | 11   | -       | 6/15/91/115   | -       |
| 32  | LMG  | L     | 2631 | -    | -       | 4/32/52/70    | 0/1/1/1 |
| 26  | CLA  | a     | 603  | 14   | -       | 10/25/101/115 | -       |
| 26  | CLA  | 1     | 614  | 14   | -       | 0/4/76/115    | -       |
| 37  | CHL  | U     | 605  | 24   | -       | 6/14/90/117   | -       |
| 26  | CLA  | B     | 824  | -    | -       | 10/39/115/115 | -       |
| 31  | LMU  | 5     | 628  | -    | -       | 10/19/59/61   | 0/2/2/2 |
| 26  | CLA  | 2     | 606  | -    | -       | 3/13/89/115   | -       |
| 26  | CLA  | 9     | 603  | 22   | -       | 5/13/89/115   | -       |
| 32  | LMG  | 4     | 624  | -    | -       | 5/35/55/70    | 0/1/1/1 |
| 26  | CLA  | 8     | 613  | 21   | -       | 18/39/115/115 | -       |
| 26  | CLA  | 9     | 610  | 22   | -       | 5/30/106/115  | -       |
| 35  | XAT  | 3     | 619  | -    | -       | 0/31/93/93    | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 29  | BCR  | 1     | 619 | -    | -       | 3/29/63/63    | 0/2/2/2 |
| 26  | CLA  | U     | 604 | -    | -       | 7/20/92/115   | -       |
| 26  | CLA  | 4     | 614 | 17   | -       | 9/29/105/115  | -       |
| 26  | CLA  | A     | 812 | 1    | -       | 9/39/115/115  | -       |
| 26  | CLA  | 6     | 612 | 19   | -       | 3/10/86/115   | -       |
| 26  | CLA  | 5     | 613 | 18   | -       | 16/37/113/115 | -       |
| 29  | BCR  | B     | 852 | -    | -       | 6/29/63/63    | 0/2/2/2 |
| 26  | CLA  | Y     | 602 | 24   | -       | 14/31/107/115 | -       |
| 26  | CLA  | U     | 613 | 24   | -       | 13/32/108/115 | -       |
| 26  | CLA  | 5     | 614 | 18   | -       | 9/15/87/115   | -       |
| 26  | CLA  | a     | 604 | -    | -       | 8/20/96/115   | -       |
| 37  | CHL  | Y     | 608 | -    | -       | 8/21/97/117   | -       |
| 26  | CLA  | K     | 201 | 11   | -       | 7/15/91/115   | -       |
| 26  | CLA  | 3     | 613 | 16   | -       | 7/23/99/115   | -       |
| 26  | CLA  | 7     | 610 | 20   | -       | 7/39/115/115  | -       |
| 26  | CLA  | 9     | 601 | 22   | -       | 8/15/91/115   | -       |
| 32  | LMG  | J     | 104 | -    | -       | 12/35/55/70   | 0/1/1/1 |
| 34  | LUT  | 3     | 618 | -    | -       | 4/29/67/67    | 0/2/2/2 |
| 26  | CLA  | a     | 613 | -    | -       | 9/26/102/115  | -       |
| 29  | BCR  | B     | 847 | -    | -       | 2/29/63/63    | 0/2/2/2 |
| 28  | LHG  | 9     | 623 | -    | -       | 20/53/53/53   | -       |

The worst 5 of 3510 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 27  | B     | 842 | PQN  | C12-C13 | 9.58 | 1.56        | 1.33     |
| 27  | A     | 844 | PQN  | C12-C13 | 9.30 | 1.55        | 1.33     |
| 27  | B     | 842 | PQN  | O4-C4   | 7.74 | 1.39        | 1.23     |
| 27  | A     | 844 | PQN  | O4-C4   | 7.72 | 1.39        | 1.23     |
| 27  | A     | 844 | PQN  | O1-C1   | 7.56 | 1.39        | 1.23     |

The worst 5 of 4551 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 36  | X     | 1623 | NEX  | C17-C1-C6   | -20.23 | 92.37       | 110.47   |
| 35  | U     | 1622 | XAT  | C37-C21-C36 | -17.41 | 81.69       | 107.37   |
| 35  | W     | 1622 | XAT  | C37-C21-C36 | -17.39 | 81.72       | 107.37   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 29  | B     | 852  | BCR  | C32-C1-C6   | -16.31 | 83.85       | 110.30   |
| 35  | U     | 1622 | XAT  | C37-C21-C22 | -15.46 | 82.13       | 108.98   |

There are no chirality outliers.

5 of 3788 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | A     | 801 | CLA  | CBD-CGD-O2D-CED |
| 26  | A     | 801 | CLA  | O1D-CGD-O2D-CED |
| 26  | A     | 804 | CLA  | C1A-C2A-CAA-CBA |
| 26  | A     | 804 | CLA  | C3A-C2A-CAA-CBA |
| 26  | A     | 804 | CLA  | CHA-CBD-CGD-O1D |

There are no ring outliers.

290 monomers are involved in 664 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 26  | 3     | 612  | CLA  | 1       | 0            |
| 34  | U     | 1621 | LUT  | 2       | 0            |
| 28  | W     | 2630 | LHG  | 1       | 0            |
| 29  | L     | 301  | BCR  | 10      | 0            |
| 37  | U     | 607  | CHL  | 2       | 0            |
| 26  | 5     | 607  | CLA  | 2       | 0            |
| 26  | B     | 837  | CLA  | 2       | 0            |
| 26  | F     | 301  | CLA  | 1       | 0            |
| 28  | Z     | 2630 | LHG  | 9       | 0            |
| 26  | B     | 819  | CLA  | 1       | 0            |
| 35  | 8     | 620  | XAT  | 1       | 0            |
| 27  | A     | 844  | PQN  | 2       | 0            |
| 29  | 7     | 621  | BCR  | 3       | 0            |
| 26  | a     | 607  | CLA  | 1       | 0            |
| 29  | a     | 619  | BCR  | 3       | 0            |
| 26  | 5     | 610  | CLA  | 1       | 0            |
| 26  | V     | 612  | CLA  | 2       | 0            |
| 26  | U     | 610  | CLA  | 4       | 0            |
| 29  | F     | 305  | BCR  | 7       | 0            |
| 37  | W     | 605  | CHL  | 2       | 0            |
| 26  | 4     | 606  | CLA  | 1       | 0            |
| 26  | 9     | 609  | CLA  | 1       | 0            |
| 29  | K     | 202  | BCR  | 5       | 0            |
| 26  | 3     | 610  | CLA  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 26  | Z     | 610  | CLA  | 5       | 0            |
| 26  | A     | 835  | CLA  | 2       | 0            |
| 26  | 6     | 607  | CLA  | 1       | 0            |
| 26  | 7     | 604  | CLA  | 1       | 0            |
| 26  | W     | 612  | CLA  | 1       | 0            |
| 29  | A     | 848  | BCR  | 3       | 0            |
| 34  | Y     | 1620 | LUT  | 5       | 0            |
| 26  | A     | 830  | CLA  | 1       | 0            |
| 29  | 9     | 621  | BCR  | 7       | 0            |
| 28  | 3     | 623  | LHG  | 1       | 0            |
| 35  | W     | 1622 | XAT  | 3       | 0            |
| 35  | V     | 1622 | XAT  | 6       | 0            |
| 26  | B     | 803  | CLA  | 2       | 0            |
| 37  | V     | 605  | CHL  | 1       | 0            |
| 26  | 8     | 611  | CLA  | 2       | 0            |
| 28  | Y     | 2630 | LHG  | 6       | 0            |
| 26  | A     | 827  | CLA  | 1       | 0            |
| 37  | Z     | 608  | CHL  | 2       | 0            |
| 26  | A     | 816  | CLA  | 1       | 0            |
| 26  | B     | 827  | CLA  | 1       | 0            |
| 32  | 9     | 625  | LMG  | 2       | 0            |
| 36  | 5     | 624  | NEX  | 1       | 0            |
| 26  | B     | 834  | CLA  | 3       | 0            |
| 35  | U     | 1622 | XAT  | 5       | 0            |
| 29  | O     | 2004 | BCR  | 3       | 0            |
| 37  | X     | 609  | CHL  | 4       | 0            |
| 34  | V     | 1621 | LUT  | 5       | 0            |
| 34  | X     | 1620 | LUT  | 6       | 0            |
| 26  | A     | 829  | CLA  | 5       | 0            |
| 26  | 6     | 610  | CLA  | 3       | 0            |
| 29  | 7     | 623  | BCR  | 5       | 0            |
| 26  | K     | 203  | CLA  | 1       | 0            |
| 29  | B     | 801  | BCR  | 7       | 0            |
| 36  | Y     | 1623 | NEX  | 2       | 0            |
| 36  | Z     | 1623 | NEX  | 3       | 0            |
| 29  | 5     | 622  | BCR  | 2       | 0            |
| 26  | 5     | 619  | CLA  | 3       | 0            |
| 37  | U     | 609  | CHL  | 3       | 0            |
| 34  | 1     | 617  | LUT  | 6       | 0            |
| 37  | W     | 606  | CHL  | 1       | 0            |
| 29  | B     | 849  | BCR  | 2       | 0            |
| 37  | V     | 601  | CHL  | 4       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 29  | L     | 305  | BCR  | 8       | 0            |
| 26  | A     | 819  | CLA  | 2       | 0            |
| 26  | B     | 817  | CLA  | 1       | 0            |
| 29  | 3     | 622  | BCR  | 7       | 0            |
| 37  | W     | 609  | CHL  | 1       | 0            |
| 34  | 6     | 619  | LUT  | 5       | 0            |
| 26  | B     | 825  | CLA  | 2       | 0            |
| 26  | A     | 831  | CLA  | 1       | 0            |
| 26  | L     | 307  | CLA  | 2       | 0            |
| 26  | 6     | 614  | CLA  | 2       | 0            |
| 26  | 7     | 615  | CLA  | 1       | 0            |
| 26  | Z     | 603  | CLA  | 1       | 0            |
| 26  | X     | 611  | CLA  | 2       | 0            |
| 27  | B     | 842  | PQN  | 3       | 0            |
| 26  | A     | 837  | CLA  | 1       | 0            |
| 26  | V     | 602  | CLA  | 3       | 0            |
| 37  | Y     | 601  | CHL  | 6       | 0            |
| 26  | B     | 840  | CLA  | 1       | 0            |
| 26  | B     | 802  | CLA  | 1       | 0            |
| 26  | 4     | 611  | CLA  | 1       | 0            |
| 28  | O     | 2631 | LHG  | 1       | 0            |
| 34  | 9     | 619  | LUT  | 5       | 0            |
| 26  | 6     | 601  | CLA  | 1       | 0            |
| 34  | Z     | 1621 | LUT  | 4       | 0            |
| 26  | A     | 843  | CLA  | 2       | 0            |
| 29  | B     | 853  | BCR  | 3       | 0            |
| 37  | Y     | 605  | CHL  | 1       | 0            |
| 26  | A     | 818  | CLA  | 1       | 0            |
| 34  | 7     | 619  | LUT  | 3       | 0            |
| 36  | X     | 1623 | NEX  | 2       | 0            |
| 26  | 7     | 614  | CLA  | 2       | 0            |
| 26  | 1     | 606  | CLA  | 1       | 0            |
| 26  | Z     | 611  | CLA  | 3       | 0            |
| 28  | 5     | 623  | LHG  | 6       | 0            |
| 37  | V     | 606  | CHL  | 2       | 0            |
| 26  | 1     | 611  | CLA  | 1       | 0            |
| 37  | V     | 607  | CHL  | 4       | 0            |
| 28  | a     | 620  | LHG  | 1       | 0            |
| 29  | L     | 309  | BCR  | 4       | 0            |
| 26  | B     | 839  | CLA  | 1       | 0            |
| 26  | L     | 302  | CLA  | 3       | 0            |
| 26  | X     | 604  | CLA  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 26  | 8     | 612  | CLA  | 2       | 0            |
| 26  | A     | 834  | CLA  | 2       | 0            |
| 26  | Z     | 602  | CLA  | 4       | 0            |
| 36  | V     | 1623 | NEX  | 11      | 0            |
| 26  | V     | 610  | CLA  | 3       | 0            |
| 26  | B     | 808  | CLA  | 3       | 0            |
| 34  | V     | 1620 | LUT  | 5       | 0            |
| 34  | X     | 1621 | LUT  | 6       | 0            |
| 37  | Y     | 607  | CHL  | 3       | 0            |
| 26  | A     | 822  | CLA  | 4       | 0            |
| 29  | B     | 845  | BCR  | 3       | 0            |
| 37  | Y     | 609  | CHL  | 3       | 0            |
| 29  | B     | 844  | BCR  | 6       | 0            |
| 31  | A     | 857  | LMU  | 1       | 0            |
| 29  | A     | 856  | BCR  | 10      | 0            |
| 26  | A     | 805  | CLA  | 1       | 0            |
| 26  | 3     | 606  | CLA  | 1       | 0            |
| 26  | 4     | 616  | CLA  | 1       | 0            |
| 37  | U     | 608  | CHL  | 3       | 0            |
| 26  | 5     | 602  | CLA  | 2       | 0            |
| 26  | A     | 808  | CLA  | 2       | 0            |
| 34  | W     | 1621 | LUT  | 4       | 0            |
| 26  | 7     | 616  | CLA  | 1       | 0            |
| 35  | a     | 618  | XAT  | 3       | 0            |
| 26  | A     | 854  | CLA  | 5       | 0            |
| 29  | 3     | 621  | BCR  | 4       | 0            |
| 36  | 6     | 624  | NEX  | 6       | 0            |
| 26  | 7     | 611  | CLA  | 4       | 0            |
| 37  | W     | 607  | CHL  | 3       | 0            |
| 26  | 7     | 613  | CLA  | 2       | 0            |
| 37  | U     | 606  | CHL  | 2       | 0            |
| 26  | B     | 818  | CLA  | 1       | 0            |
| 28  | V     | 2630 | LHG  | 3       | 0            |
| 26  | 1     | 601  | CLA  | 2       | 0            |
| 26  | B     | 822  | CLA  | 1       | 0            |
| 26  | 5     | 603  | CLA  | 1       | 0            |
| 26  | 7     | 609  | CLA  | 1       | 0            |
| 26  | X     | 614  | CLA  | 1       | 0            |
| 37  | X     | 607  | CHL  | 2       | 0            |
| 26  | A     | 824  | CLA  | 2       | 0            |
| 26  | 4     | 601  | CLA  | 1       | 0            |
| 26  | A     | 841  | CLA  | 4       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 37  | V     | 609  | CHL  | 3       | 0            |
| 26  | B     | 830  | CLA  | 1       | 0            |
| 29  | A     | 850  | BCR  | 8       | 0            |
| 26  | F     | 303  | CLA  | 4       | 0            |
| 29  | A     | 852  | BCR  | 10      | 0            |
| 29  | A     | 851  | BCR  | 6       | 0            |
| 34  | a     | 617  | LUT  | 5       | 0            |
| 37  | Y     | 606  | CHL  | 2       | 0            |
| 26  | 1     | 604  | CLA  | 1       | 0            |
| 26  | X     | 603  | CLA  | 1       | 0            |
| 34  | 2     | 619  | LUT  | 7       | 0            |
| 26  | B     | 821  | CLA  | 3       | 0            |
| 35  | 2     | 620  | XAT  | 1       | 0            |
| 34  | W     | 1620 | LUT  | 4       | 0            |
| 26  | A     | 802  | CLA  | 3       | 0            |
| 28  | X     | 2630 | LHG  | 6       | 0            |
| 37  | Z     | 609  | CHL  | 3       | 0            |
| 37  | X     | 601  | CHL  | 7       | 0            |
| 29  | B     | 848  | BCR  | 2       | 0            |
| 26  | 6     | 616  | CLA  | 1       | 0            |
| 29  | B     | 843  | BCR  | 9       | 0            |
| 29  | 2     | 623  | BCR  | 5       | 0            |
| 26  | A     | 806  | CLA  | 2       | 0            |
| 32  | A     | 860  | LMG  | 1       | 0            |
| 26  | 8     | 604  | CLA  | 1       | 0            |
| 26  | 2     | 613  | CLA  | 3       | 0            |
| 37  | U     | 601  | CHL  | 4       | 0            |
| 29  | 8     | 621  | BCR  | 3       | 0            |
| 26  | 7     | 602  | CLA  | 1       | 0            |
| 26  | K     | 204  | CLA  | 2       | 0            |
| 35  | 6     | 621  | XAT  | 1       | 0            |
| 26  | 4     | 618  | CLA  | 1       | 0            |
| 26  | a     | 611  | CLA  | 1       | 0            |
| 26  | W     | 614  | CLA  | 4       | 0            |
| 26  | A     | 803  | CLA  | 3       | 0            |
| 32  | V     | 2631 | LMG  | 2       | 0            |
| 26  | 8     | 610  | CLA  | 1       | 0            |
| 26  | B     | 816  | CLA  | 1       | 0            |
| 26  | X     | 613  | CLA  | 4       | 0            |
| 26  | 6     | 608  | CLA  | 1       | 0            |
| 26  | X     | 612  | CLA  | 1       | 0            |
| 32  | 5     | 627  | LMG  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 26  | A     | 807  | CLA  | 3       | 0            |
| 26  | W     | 602  | CLA  | 2       | 0            |
| 29  | G     | 205  | BCR  | 4       | 0            |
| 26  | B     | 813  | CLA  | 2       | 0            |
| 29  | 6     | 622  | BCR  | 1       | 0            |
| 29  | J     | 102  | BCR  | 8       | 0            |
| 29  | K     | 207  | BCR  | 3       | 0            |
| 26  | Y     | 613  | CLA  | 4       | 0            |
| 26  | F     | 304  | CLA  | 1       | 0            |
| 35  | 1     | 618  | XAT  | 3       | 0            |
| 26  | 3     | 608  | CLA  | 1       | 0            |
| 36  | W     | 1623 | NEX  | 2       | 0            |
| 26  | B     | 833  | CLA  | 2       | 0            |
| 34  | Y     | 1621 | LUT  | 4       | 0            |
| 26  | V     | 614  | CLA  | 1       | 0            |
| 37  | Z     | 607  | CHL  | 3       | 0            |
| 26  | W     | 613  | CLA  | 4       | 0            |
| 26  | A     | 809  | CLA  | 1       | 0            |
| 35  | Y     | 1622 | XAT  | 3       | 0            |
| 26  | X     | 602  | CLA  | 4       | 0            |
| 26  | 9     | 613  | CLA  | 2       | 0            |
| 28  | U     | 2630 | LHG  | 1       | 0            |
| 26  | 8     | 606  | CLA  | 1       | 0            |
| 35  | Z     | 1622 | XAT  | 5       | 0            |
| 26  | 4     | 609  | CLA  | 1       | 0            |
| 37  | X     | 608  | CHL  | 3       | 0            |
| 26  | W     | 603  | CLA  | 2       | 0            |
| 29  | 3     | 620  | BCR  | 8       | 0            |
| 26  | W     | 610  | CLA  | 1       | 0            |
| 28  | 3     | 624  | LHG  | 2       | 0            |
| 35  | 7     | 620  | XAT  | 1       | 0            |
| 26  | 4     | 607  | CLA  | 1       | 0            |
| 26  | A     | 820  | CLA  | 2       | 0            |
| 26  | a     | 606  | CLA  | 1       | 0            |
| 37  | V     | 608  | CHL  | 2       | 0            |
| 26  | 5     | 611  | CLA  | 7       | 0            |
| 34  | Z     | 1620 | LUT  | 6       | 0            |
| 26  | U     | 602  | CLA  | 1       | 0            |
| 29  | 4     | 621  | BCR  | 5       | 0            |
| 26  | Z     | 614  | CLA  | 1       | 0            |
| 26  | B     | 828  | CLA  | 2       | 0            |
| 34  | 4     | 619  | LUT  | 3       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 29  | B     | 846  | BCR  | 3       | 0            |
| 26  | V     | 613  | CLA  | 4       | 0            |
| 35  | 5     | 621  | XAT  | 2       | 0            |
| 26  | B     | 835  | CLA  | 1       | 0            |
| 26  | X     | 610  | CLA  | 3       | 0            |
| 35  | X     | 1622 | XAT  | 3       | 0            |
| 26  | A     | 840  | CLA  | 1       | 0            |
| 26  | 7     | 601  | CLA  | 1       | 0            |
| 26  | 6     | 609  | CLA  | 1       | 0            |
| 32  | 8     | 626  | LMG  | 3       | 0            |
| 26  | Z     | 612  | CLA  | 1       | 0            |
| 34  | 8     | 619  | LUT  | 6       | 0            |
| 29  | O     | 2005 | BCR  | 6       | 0            |
| 26  | L     | 303  | CLA  | 2       | 0            |
| 37  | W     | 601  | CHL  | 3       | 0            |
| 26  | 6     | 606  | CLA  | 1       | 0            |
| 37  | Z     | 601  | CHL  | 4       | 0            |
| 37  | Z     | 606  | CHL  | 3       | 0            |
| 29  | L     | 308  | BCR  | 7       | 0            |
| 26  | 6     | 602  | CLA  | 1       | 0            |
| 26  | a     | 601  | CLA  | 3       | 0            |
| 26  | Z     | 613  | CLA  | 4       | 0            |
| 26  | 1     | 607  | CLA  | 1       | 0            |
| 26  | 1     | 613  | CLA  | 1       | 0            |
| 26  | Y     | 603  | CLA  | 3       | 0            |
| 35  | 4     | 620  | XAT  | 3       | 0            |
| 29  | A     | 849  | BCR  | 5       | 0            |
| 26  | Y     | 610  | CLA  | 2       | 0            |
| 33  | B     | 850  | DGD  | 1       | 0            |
| 28  | 9     | 622  | LHG  | 1       | 0            |
| 26  | A     | 821  | CLA  | 1       | 0            |
| 26  | A     | 825  | CLA  | 3       | 0            |
| 30  | C     | 102  | SF4  | 1       | 0            |
| 34  | 5     | 620  | LUT  | 4       | 0            |
| 34  | U     | 1620 | LUT  | 6       | 0            |
| 26  | A     | 815  | CLA  | 2       | 0            |
| 26  | a     | 603  | CLA  | 1       | 0            |
| 37  | U     | 605  | CHL  | 1       | 0            |
| 26  | B     | 824  | CLA  | 1       | 0            |
| 26  | 2     | 606  | CLA  | 1       | 0            |
| 26  | 8     | 613  | CLA  | 2       | 0            |
| 26  | 9     | 610  | CLA  | 1       | 0            |

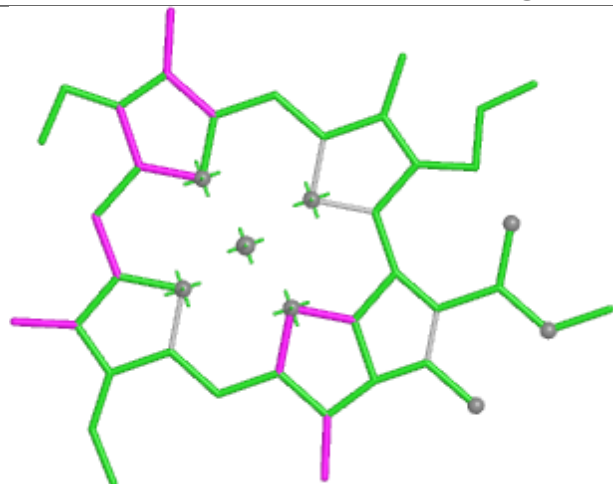
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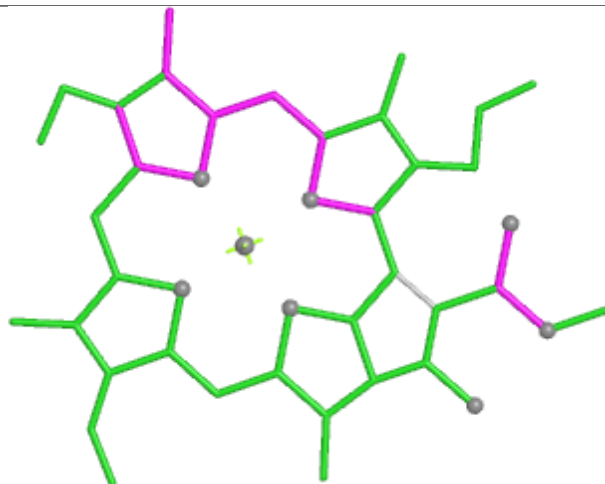
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 35  | 3     | 619 | XAT  | 2       | 0            |
| 29  | 1     | 619 | BCR  | 2       | 0            |
| 26  | U     | 604 | CLA  | 3       | 0            |
| 26  | A     | 812 | CLA  | 1       | 0            |
| 26  | 5     | 613 | CLA  | 1       | 0            |
| 29  | B     | 852 | BCR  | 6       | 0            |
| 26  | Y     | 602 | CLA  | 2       | 0            |
| 26  | U     | 613 | CLA  | 3       | 0            |
| 26  | a     | 604 | CLA  | 1       | 0            |
| 37  | Y     | 608 | CHL  | 2       | 0            |
| 26  | 3     | 613 | CLA  | 1       | 0            |
| 34  | 3     | 618 | LUT  | 7       | 0            |
| 26  | a     | 613 | CLA  | 1       | 0            |
| 29  | B     | 847 | BCR  | 4       | 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.

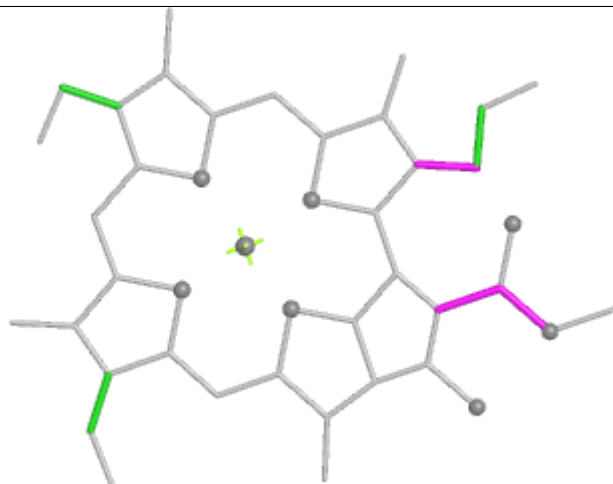
## Ligand CLA 3 612



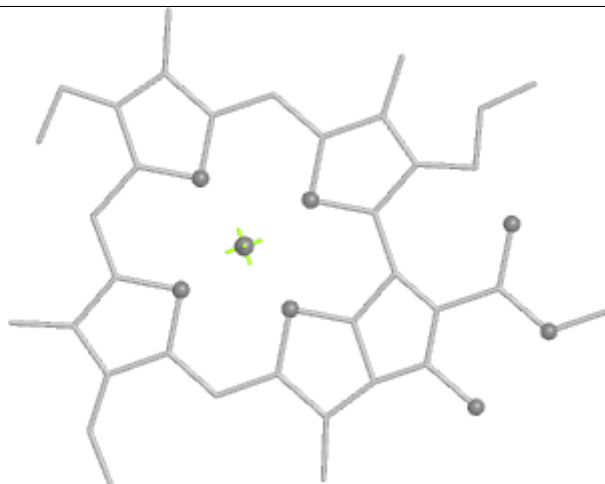
Bond lengths



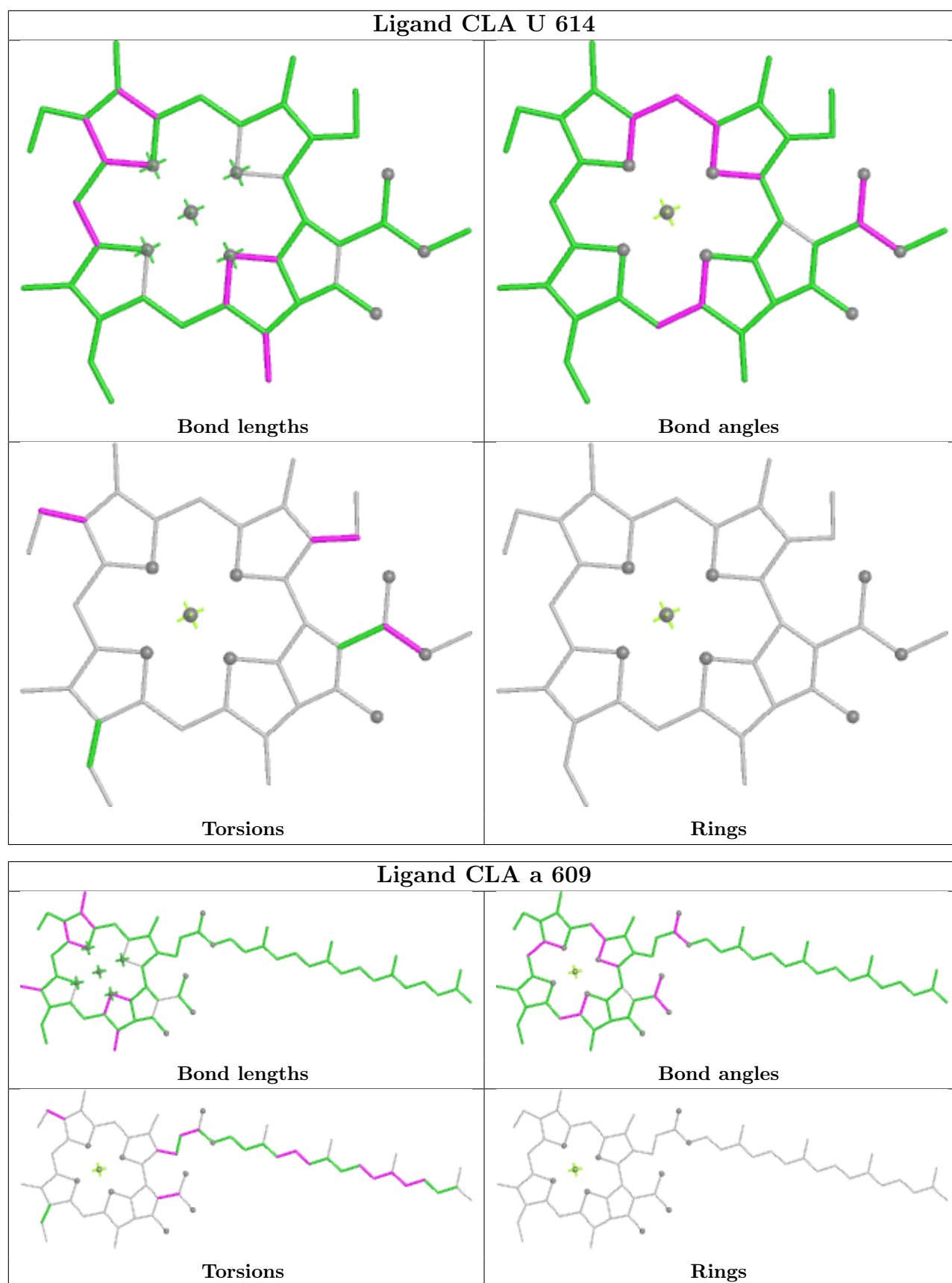
Bond angles



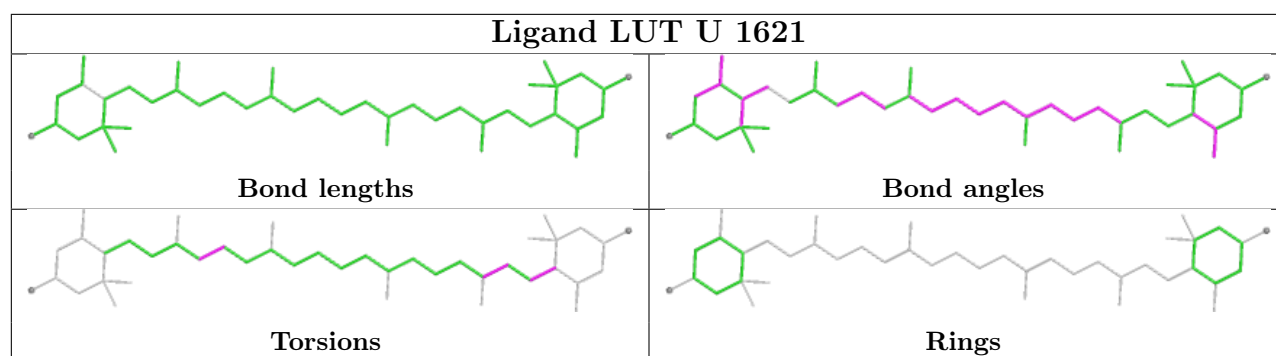
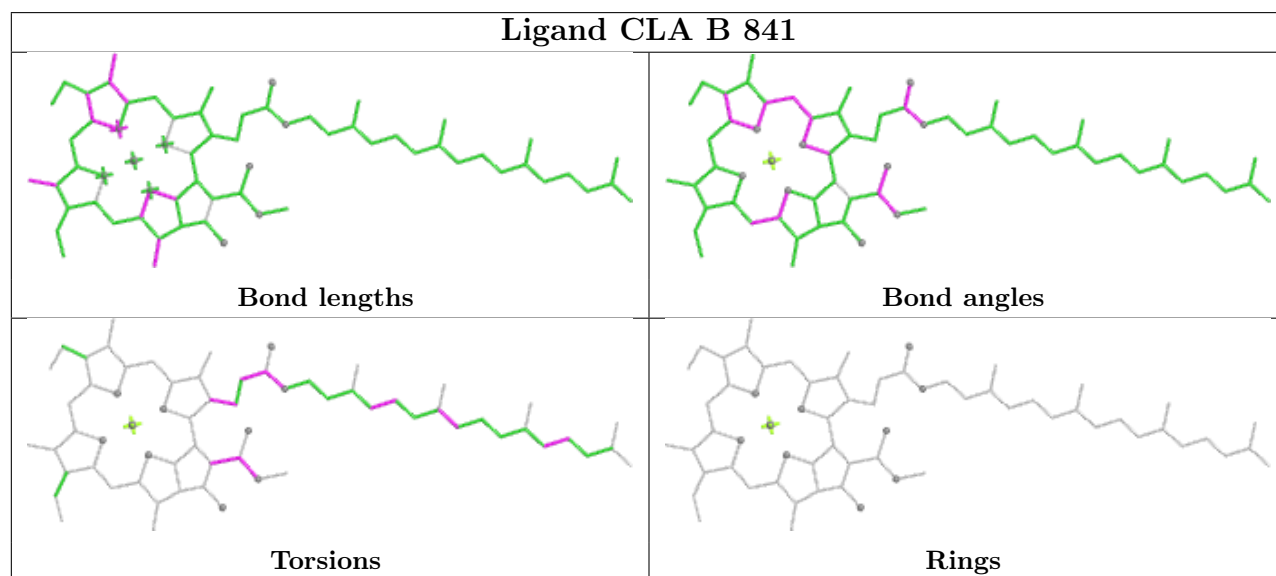
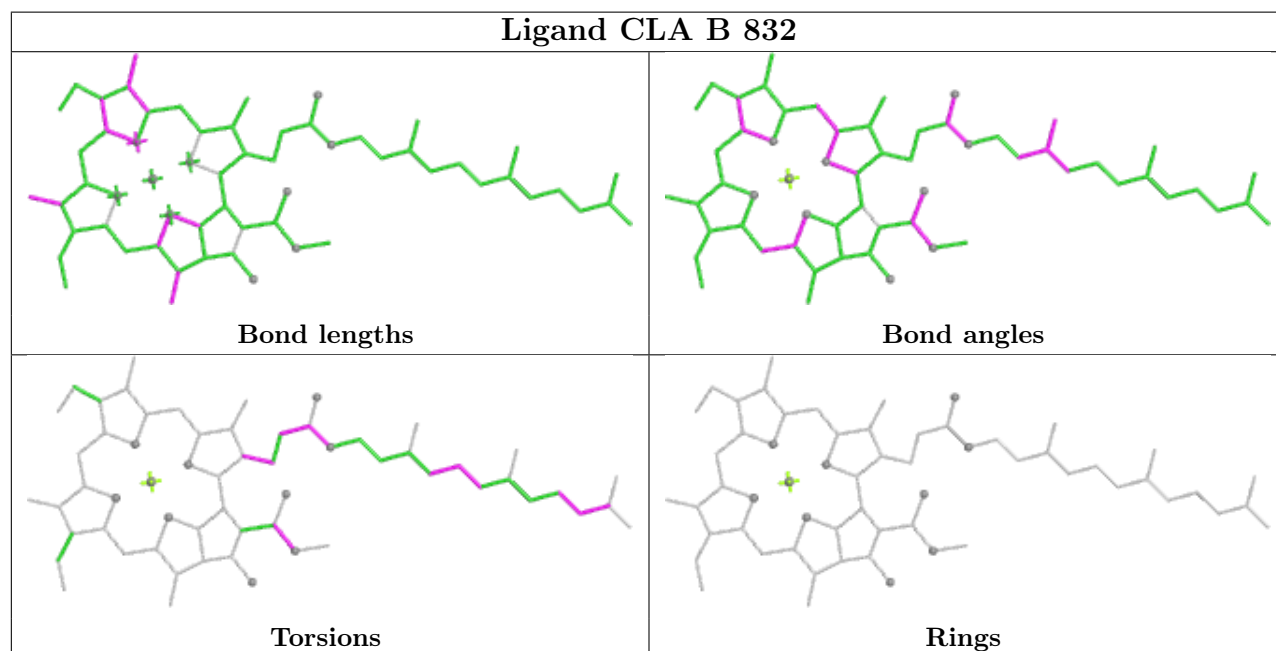
Torsions

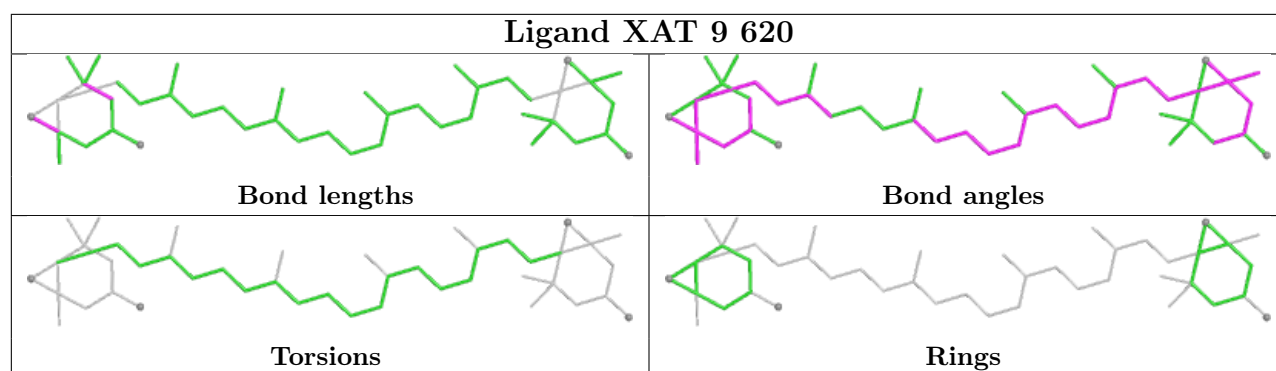
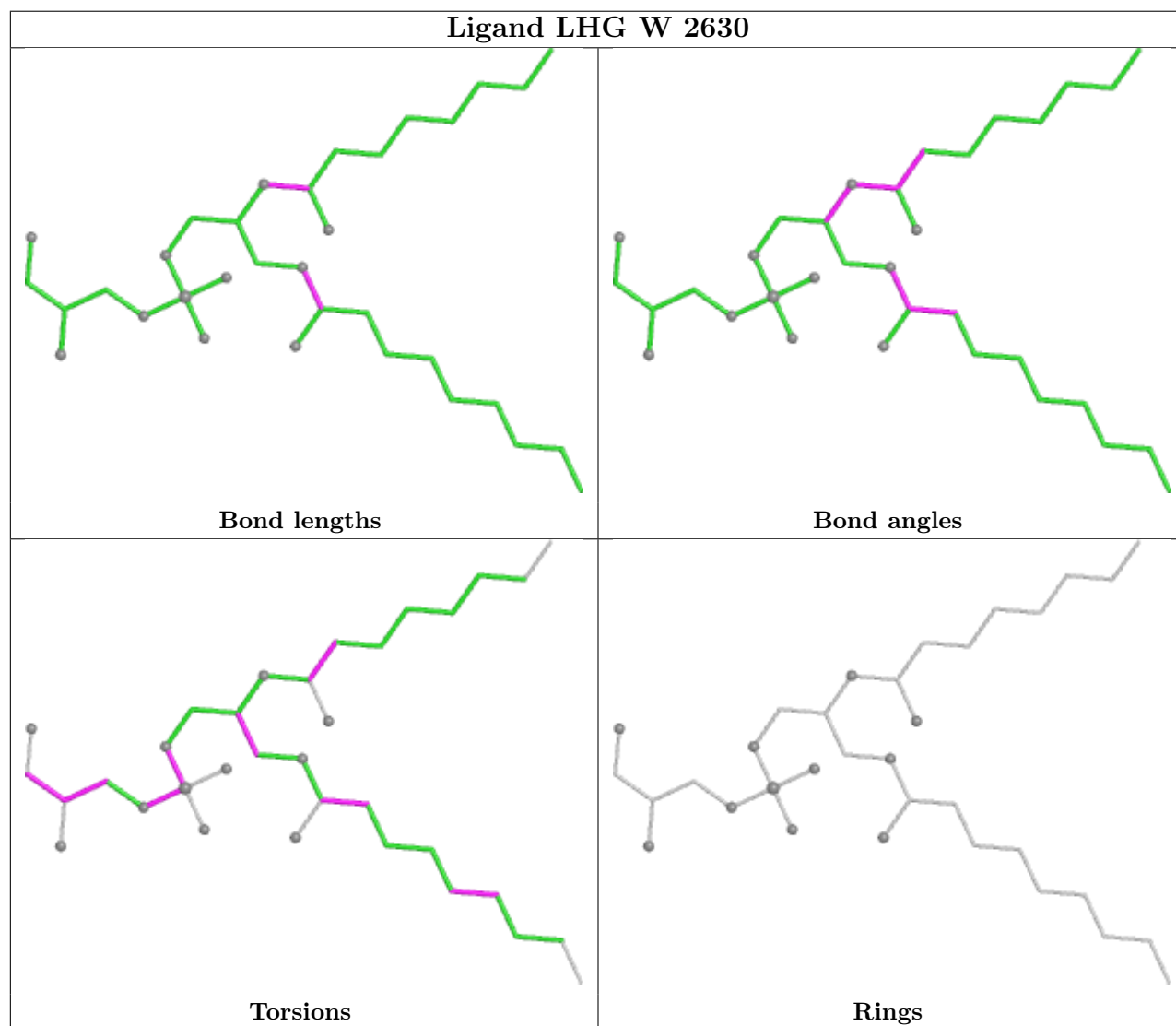


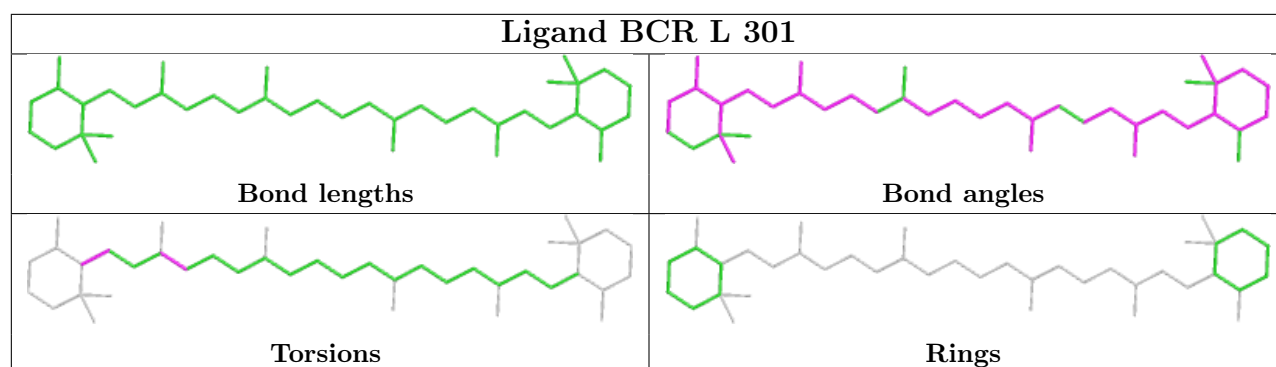
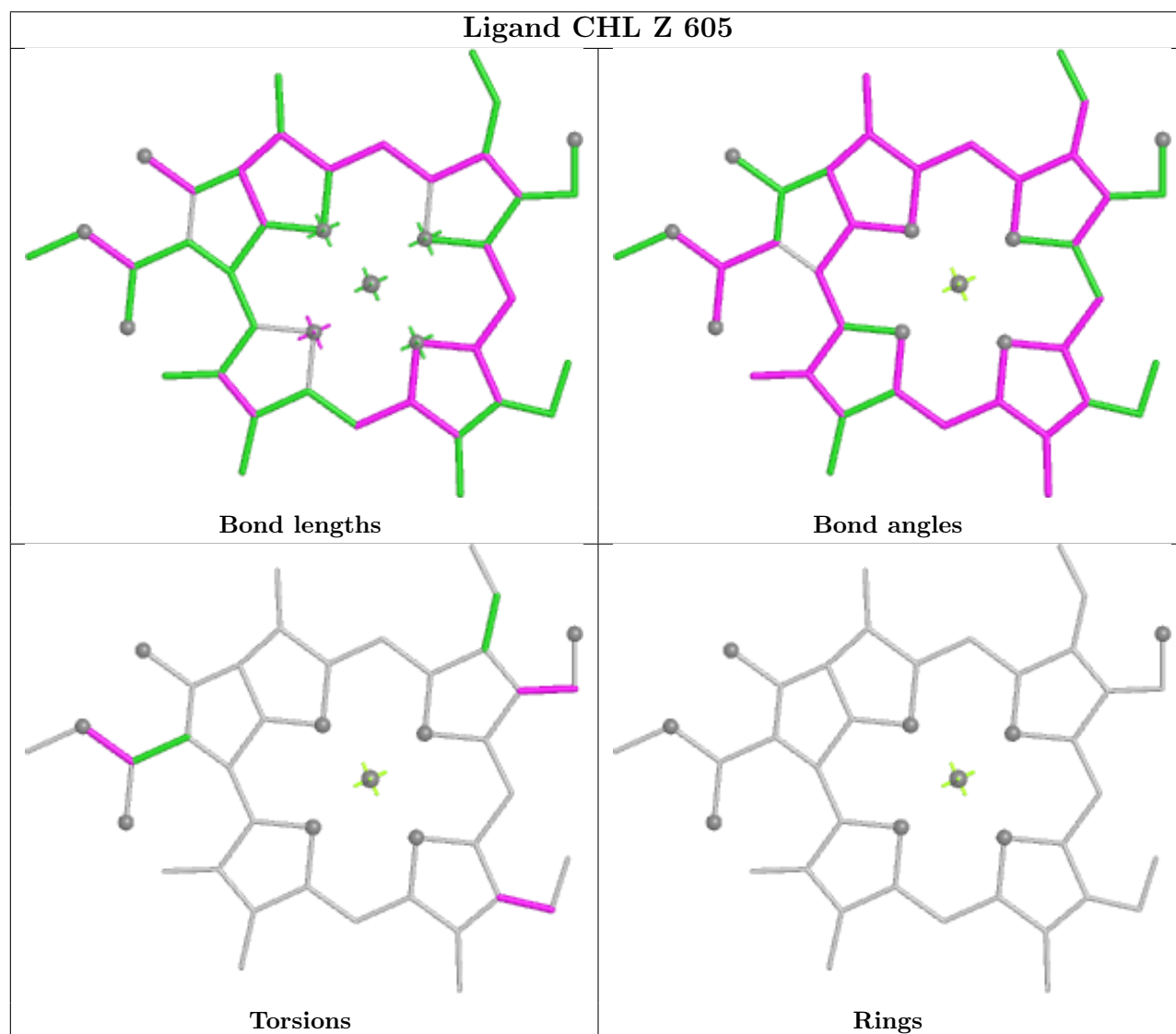
Rings

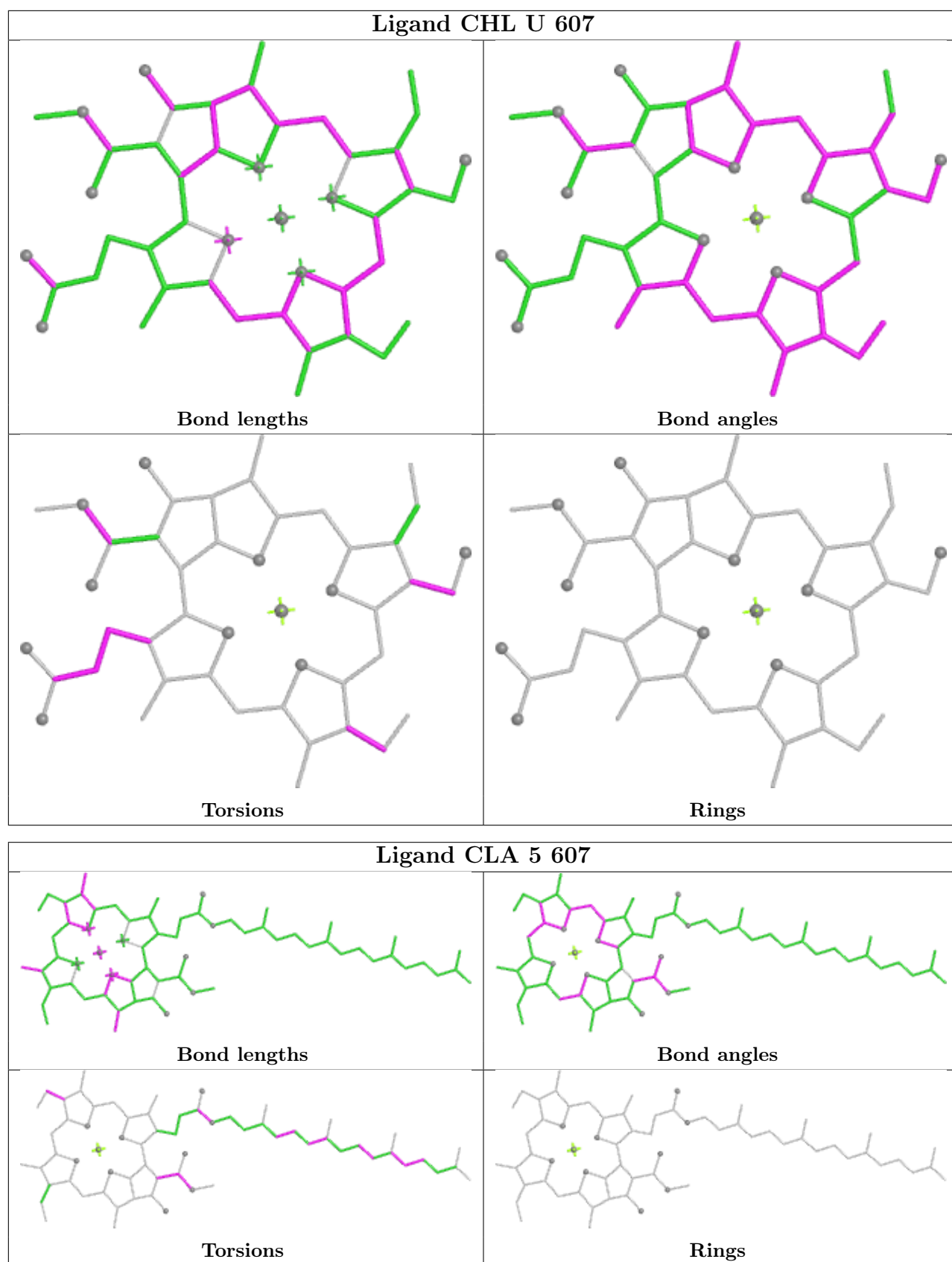


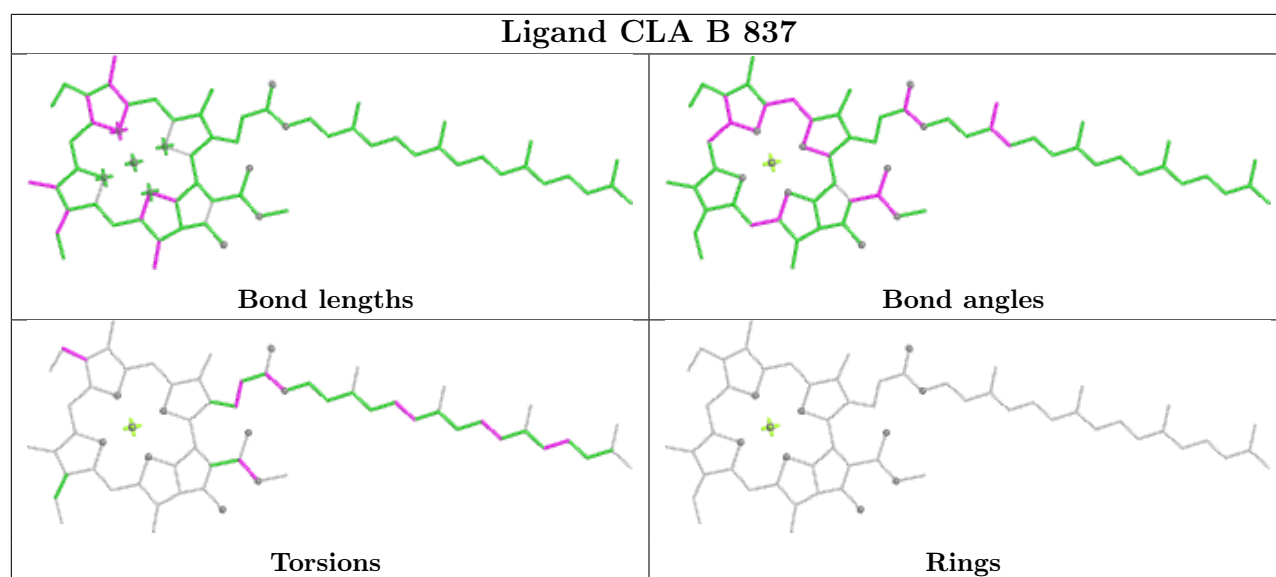
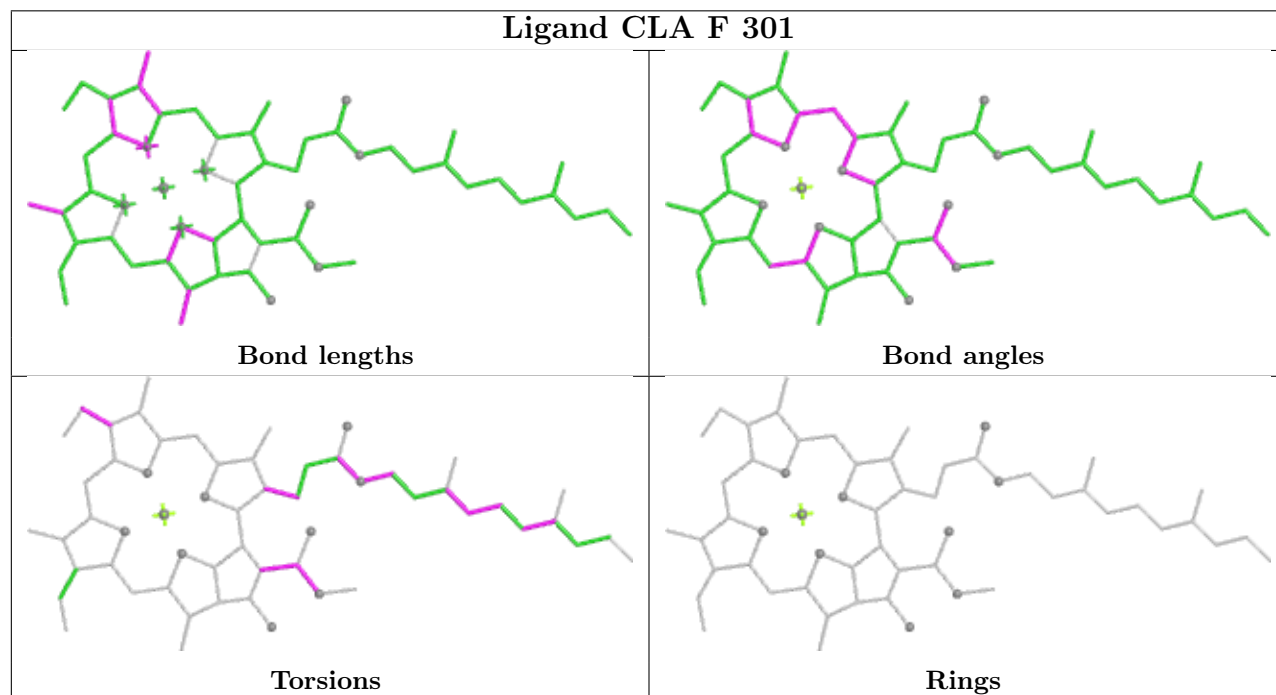


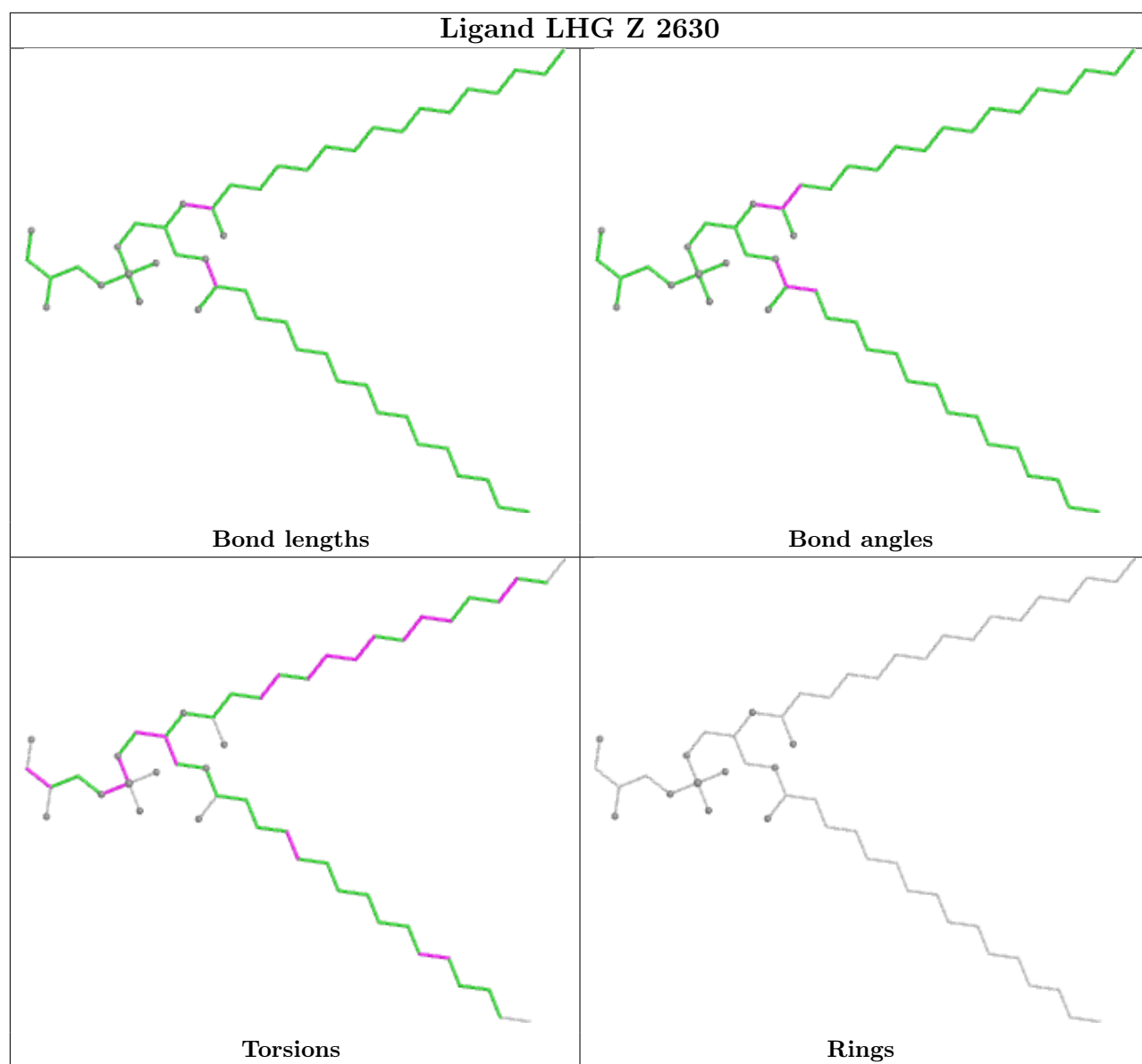


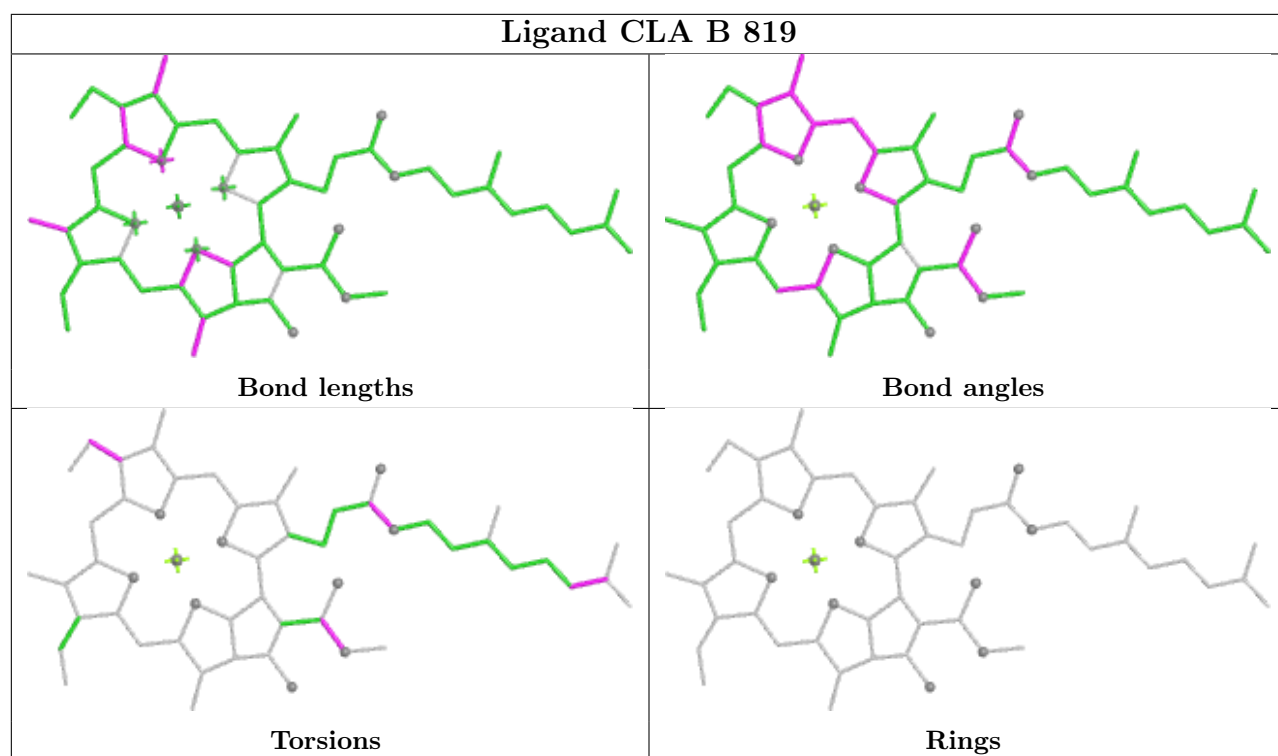


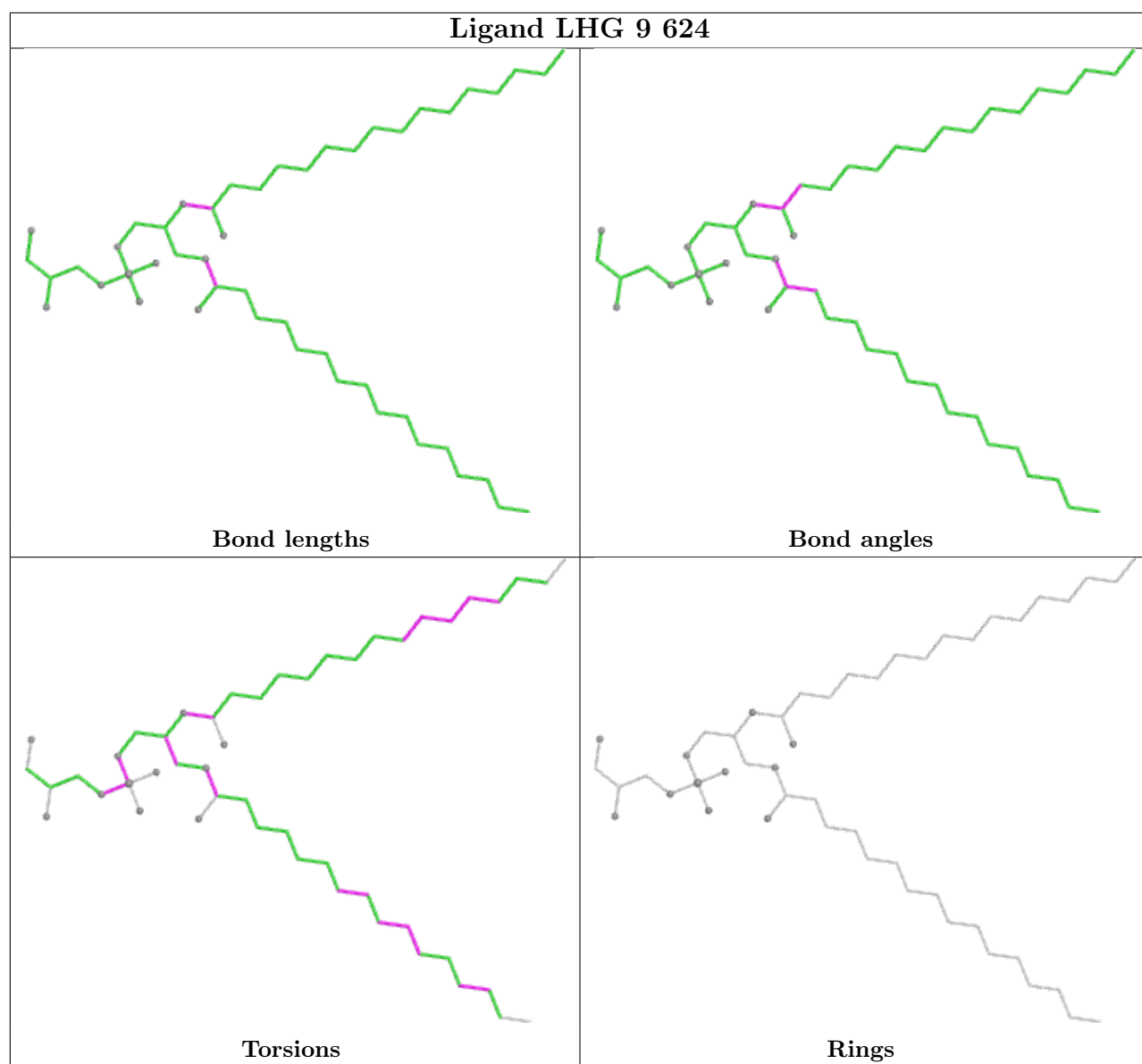




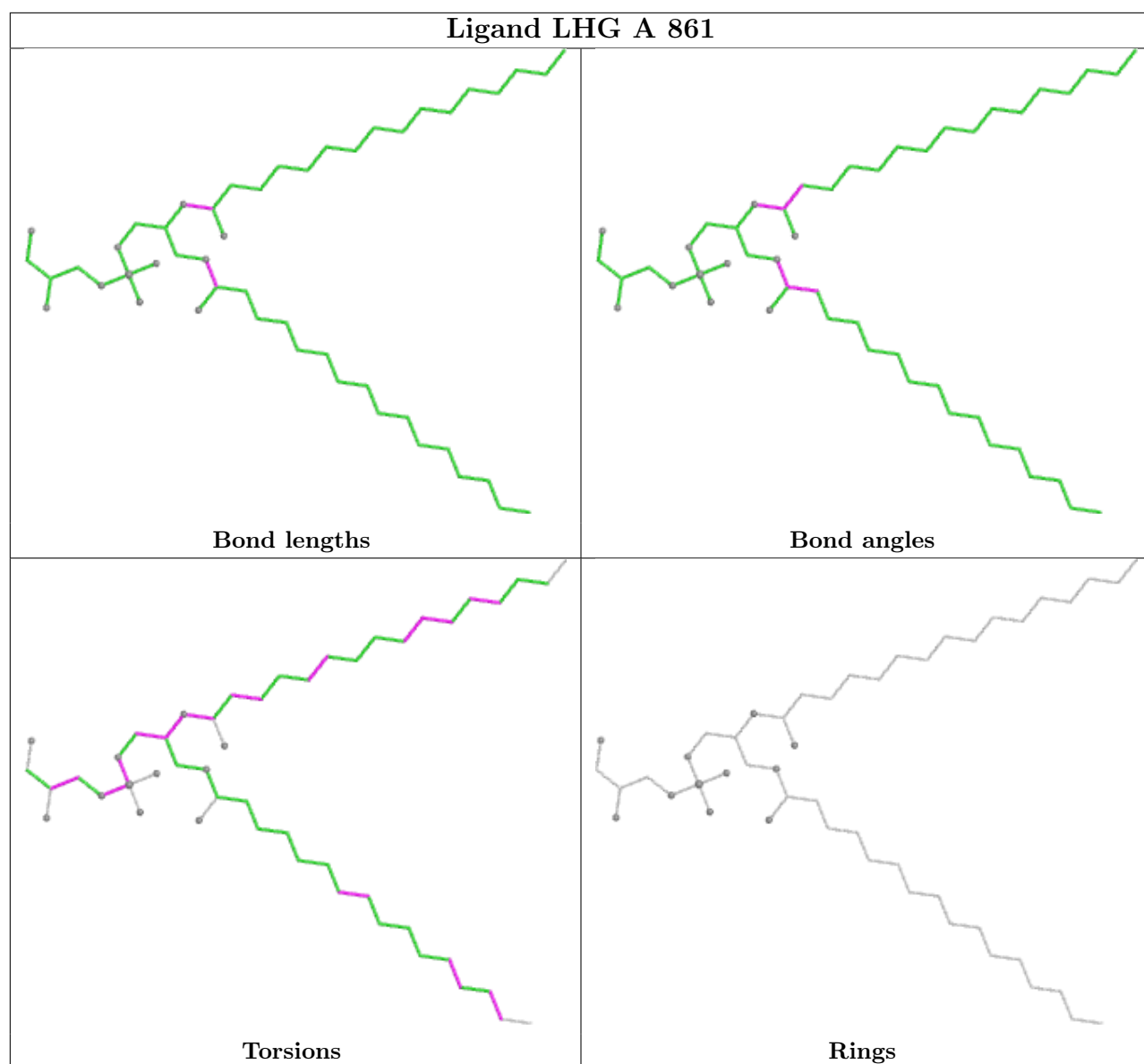
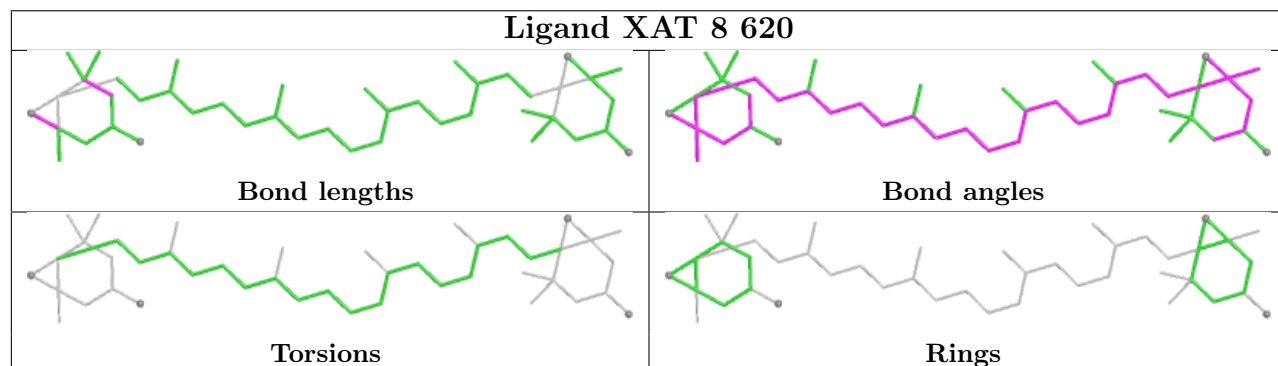


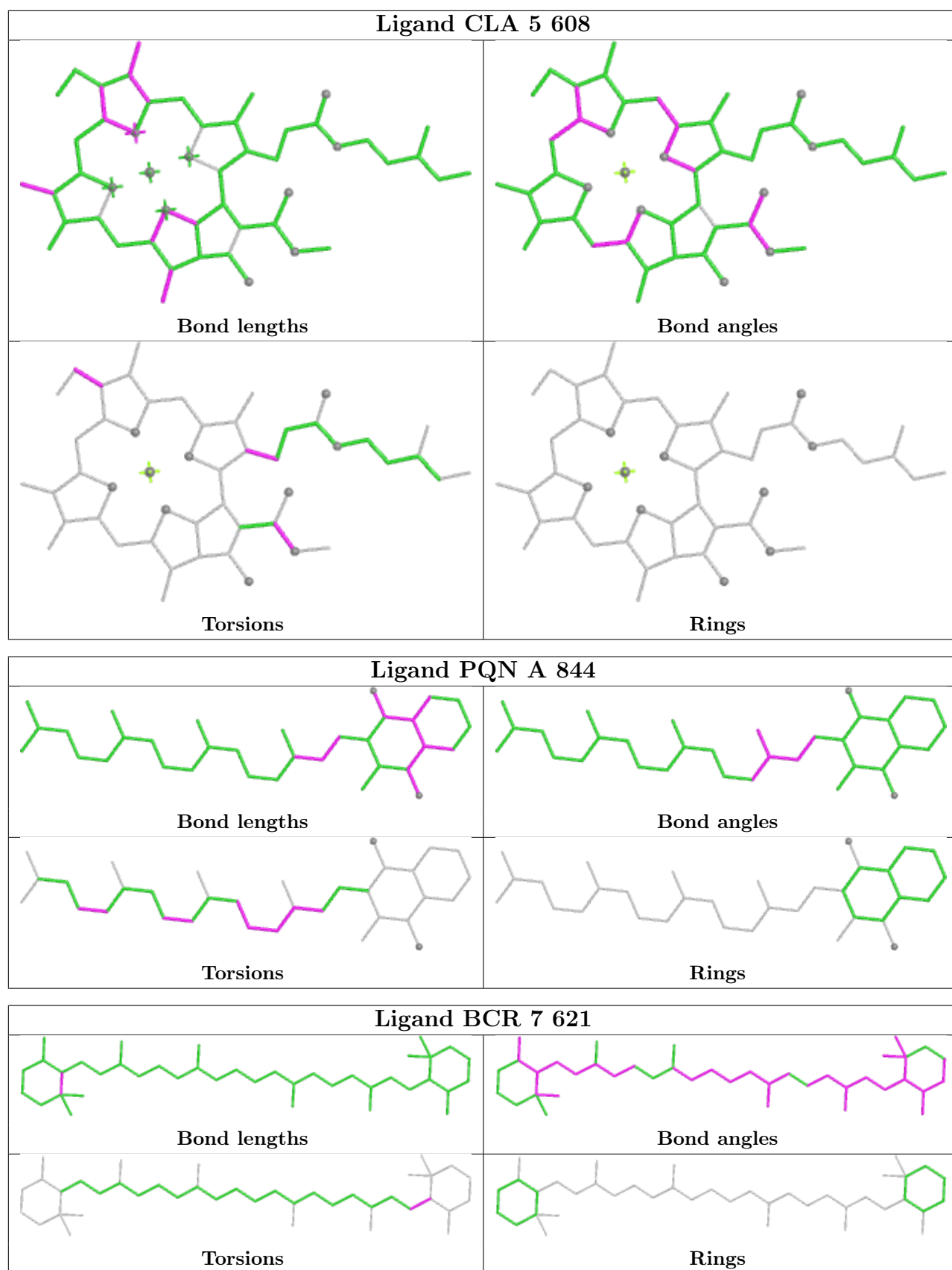




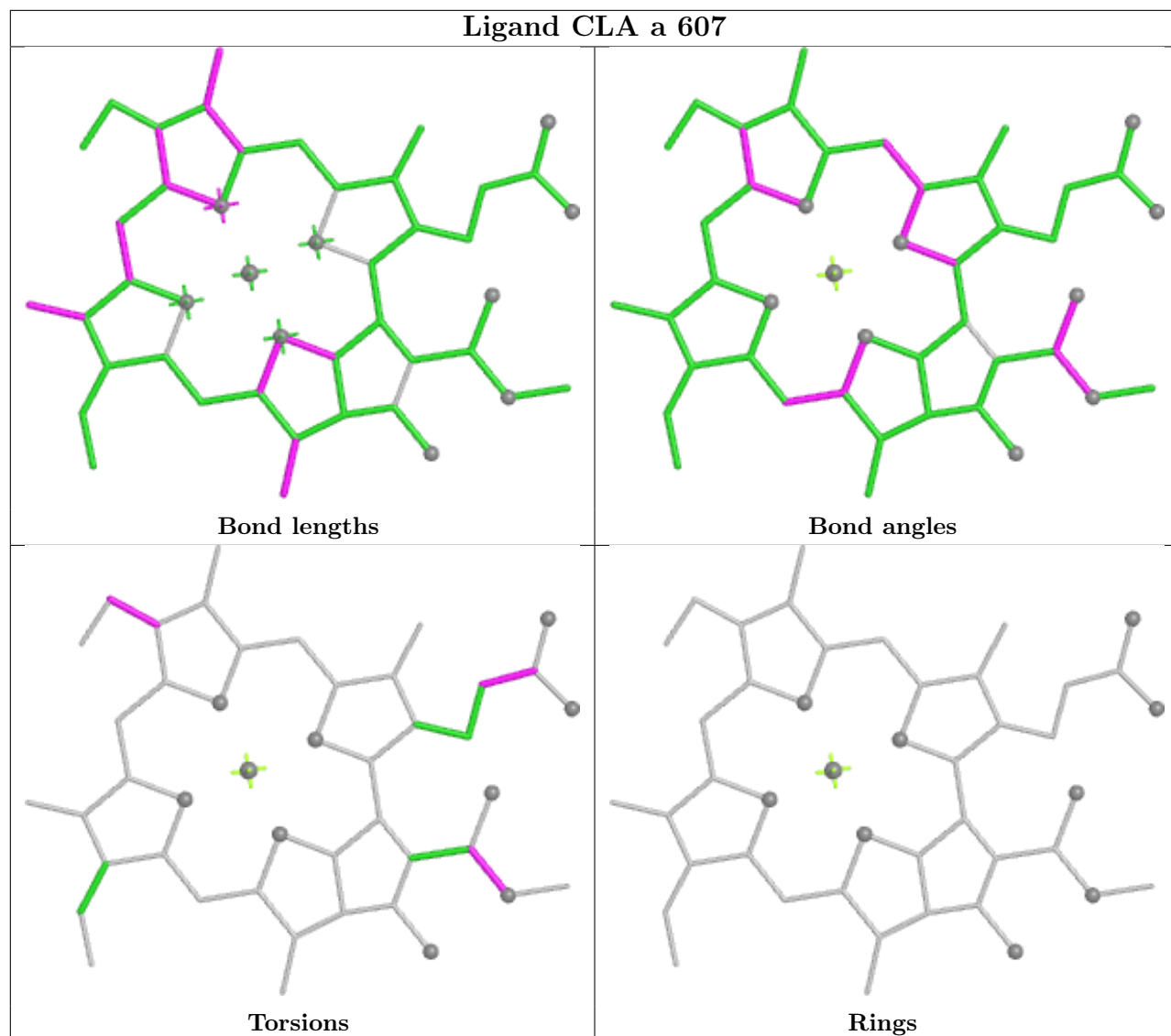




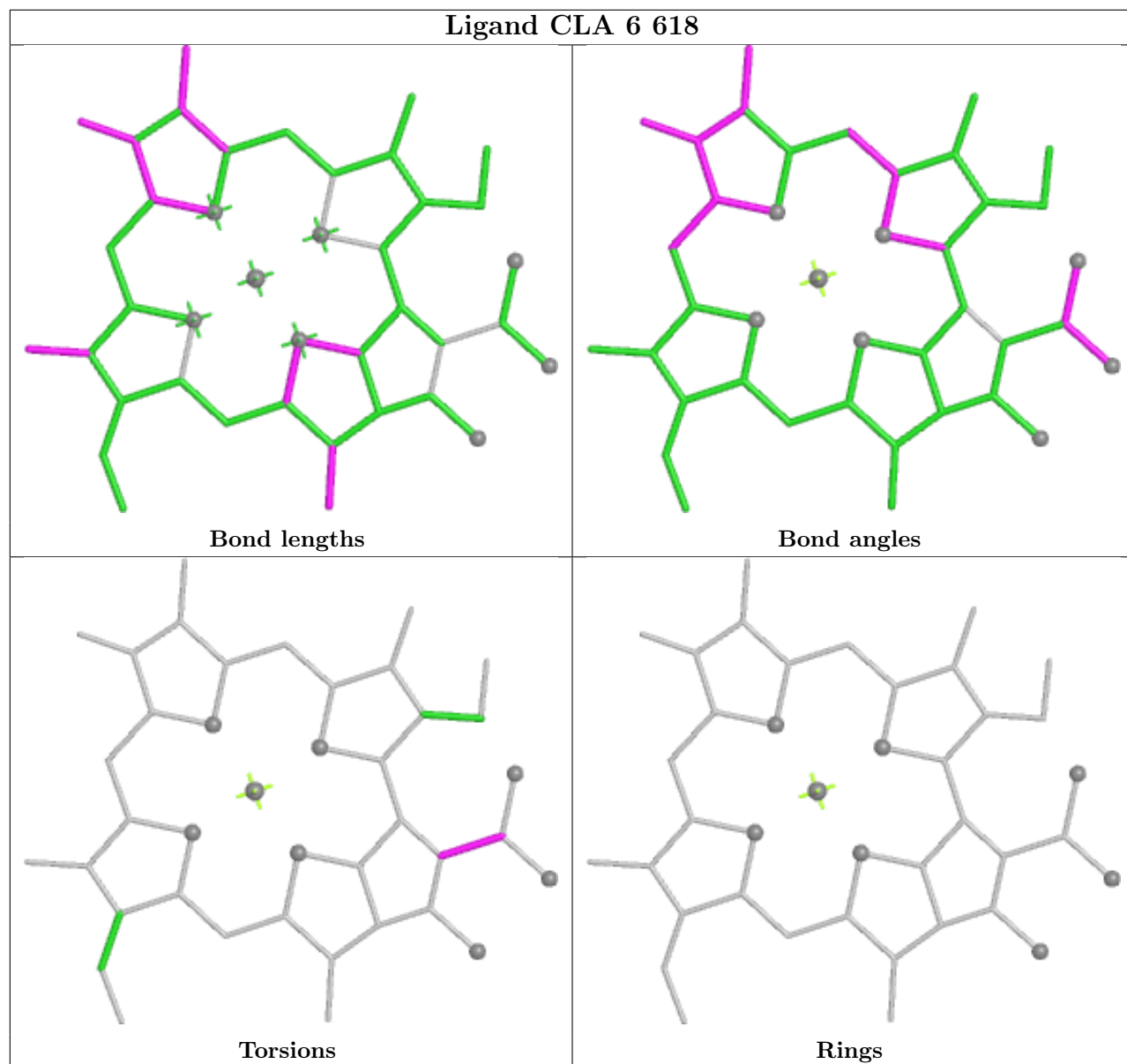




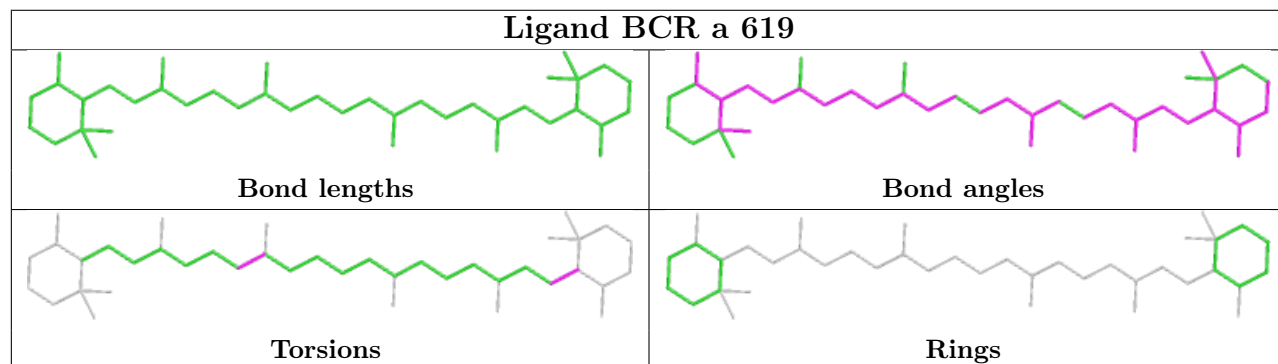
## Ligand CLA a 607

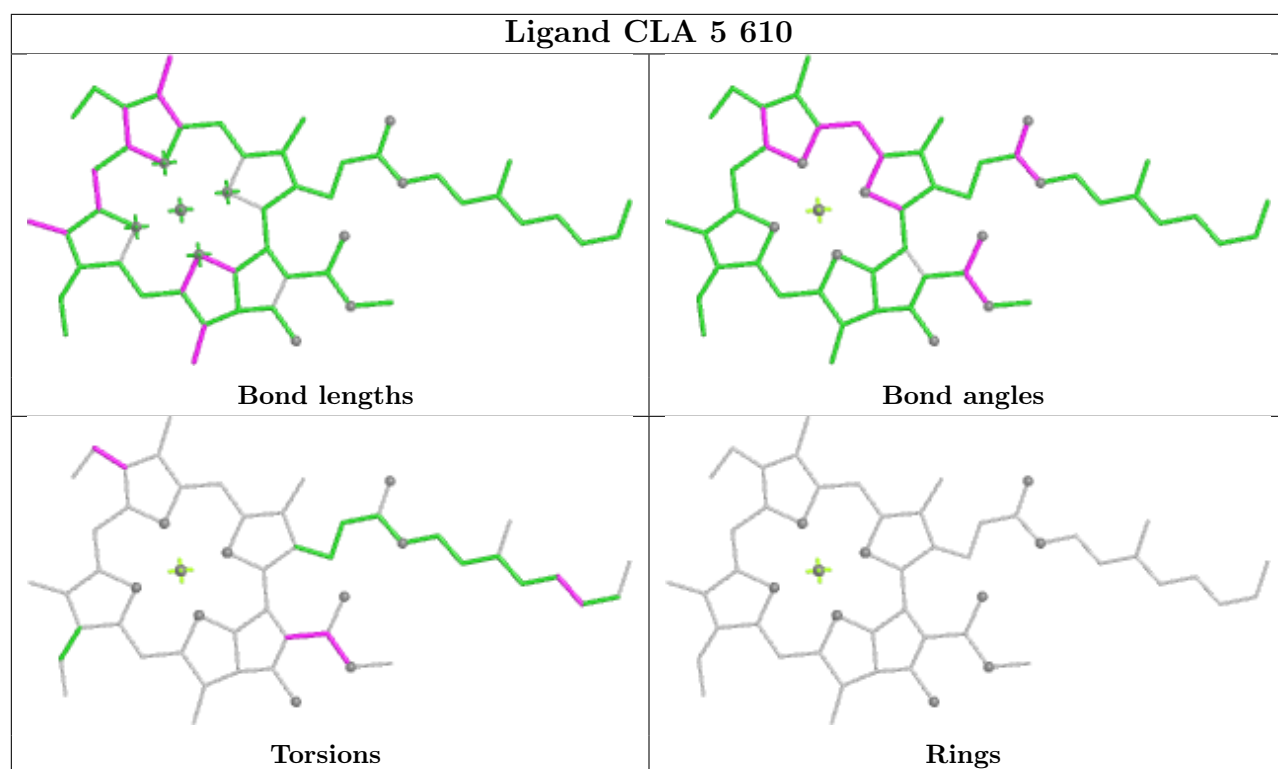


## Ligand CLA 6 618

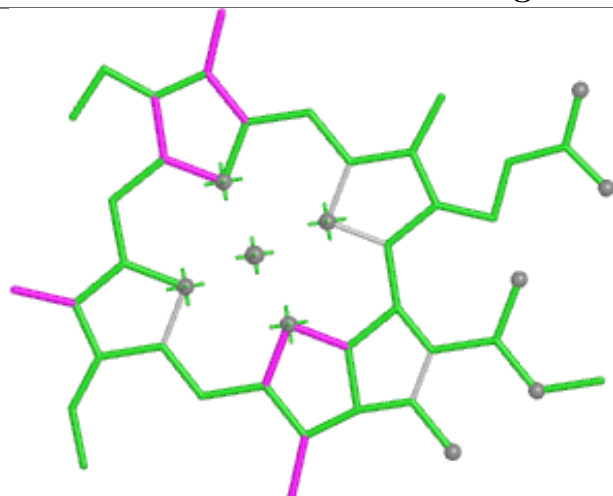


## Ligand BCR a 619

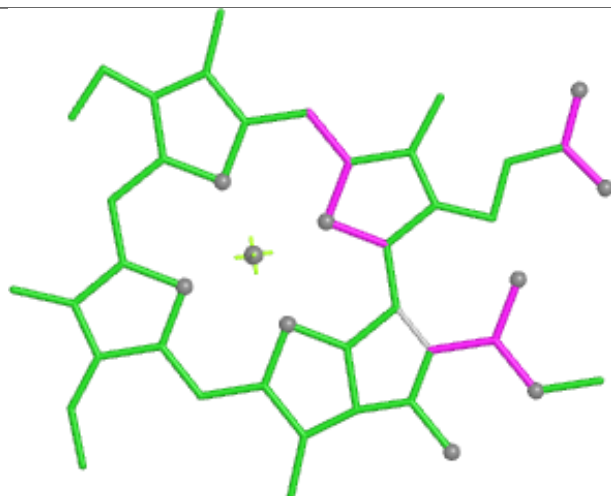




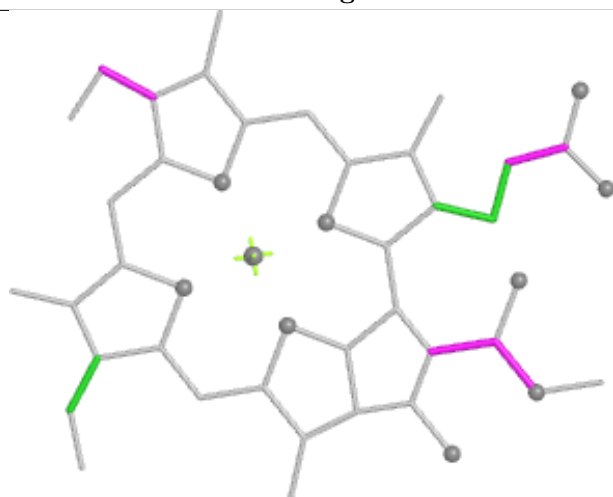
## Ligand CLA V 612



Bond lengths



Bond angles

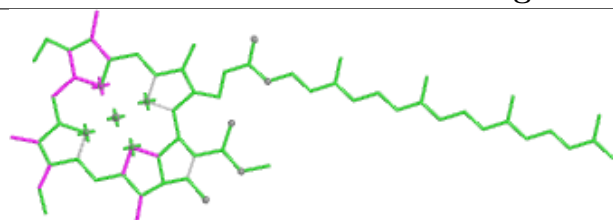


Torsions

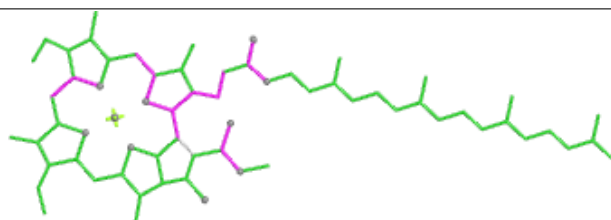


Rings

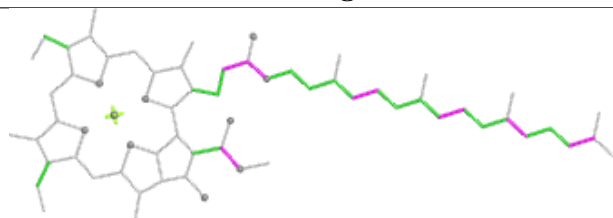
## Ligand CLA A 801



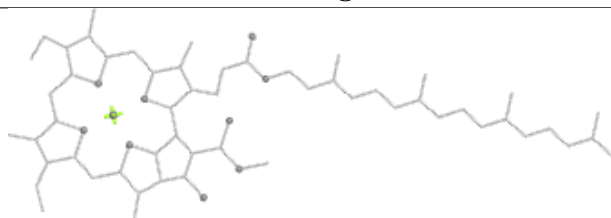
Bond lengths



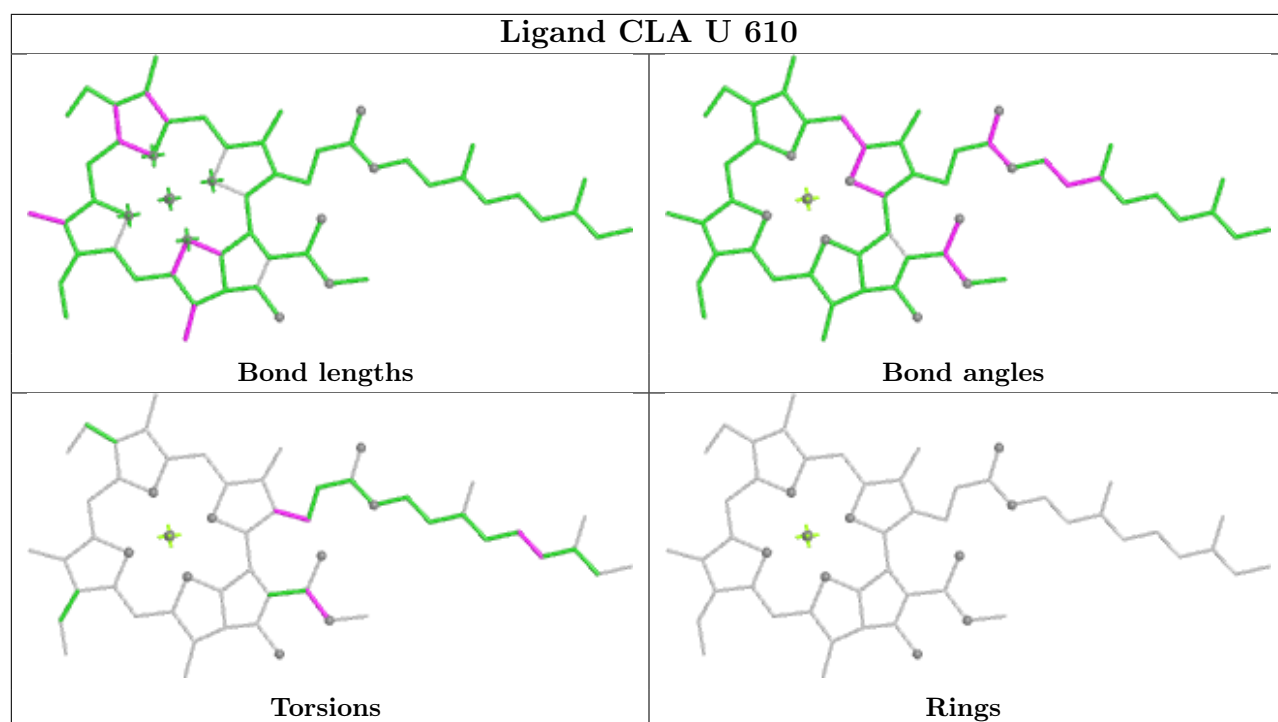
Bond angles



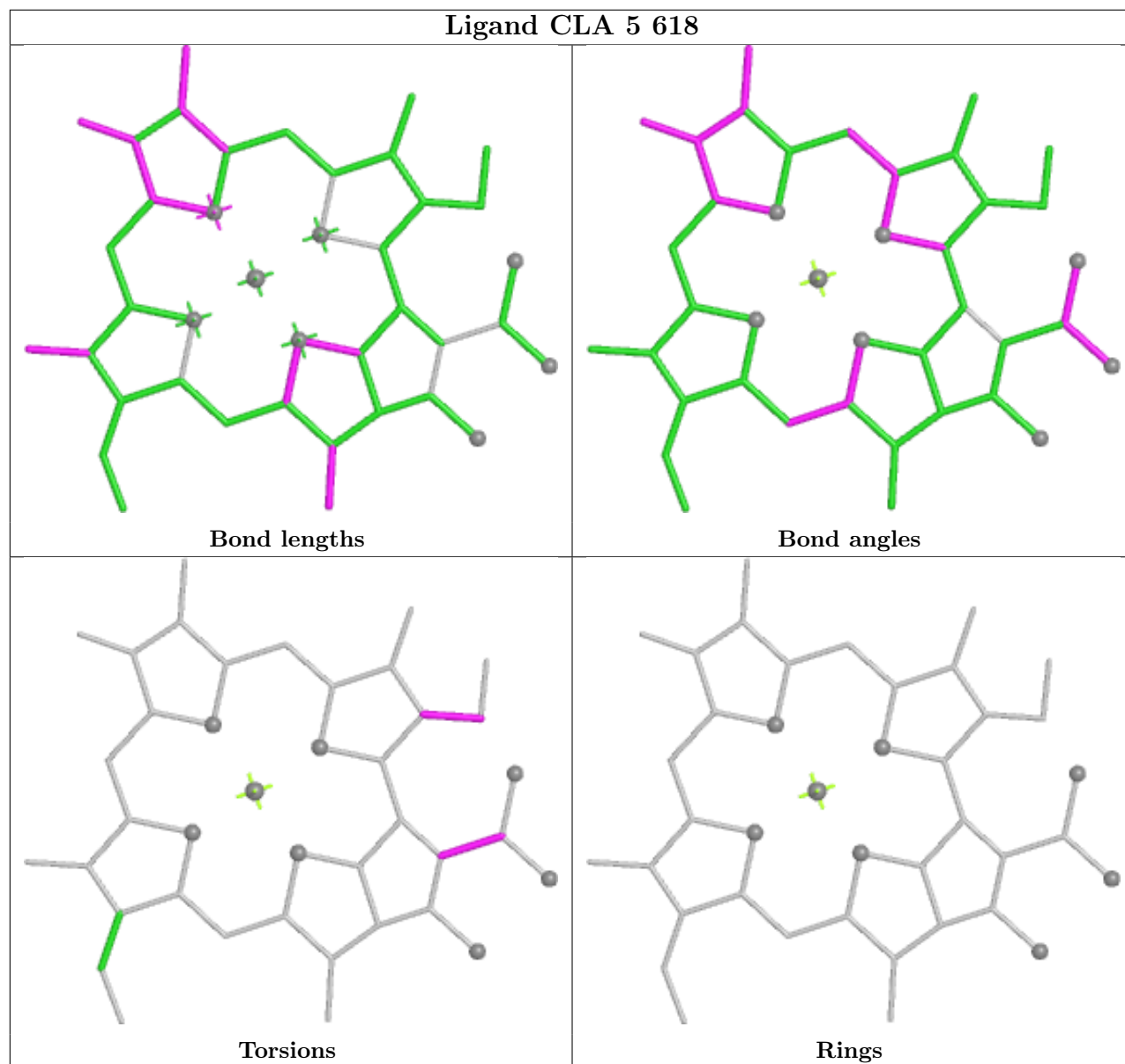
Torsions



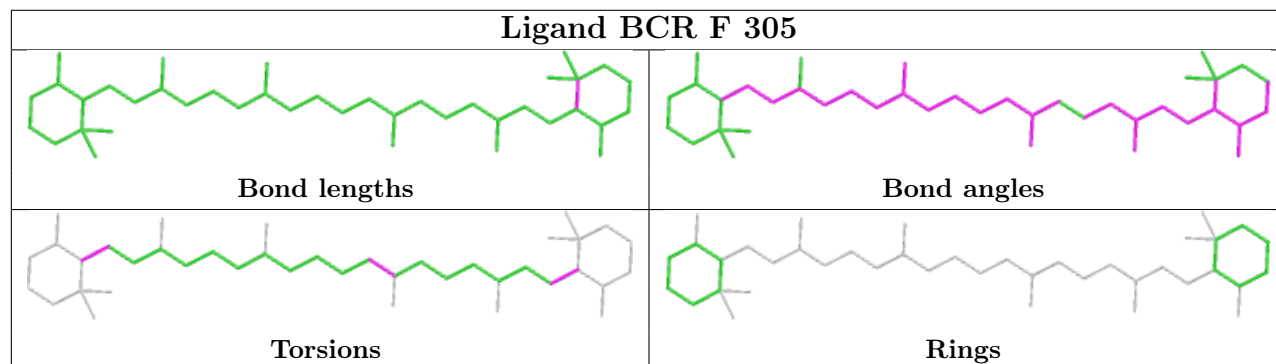
Rings



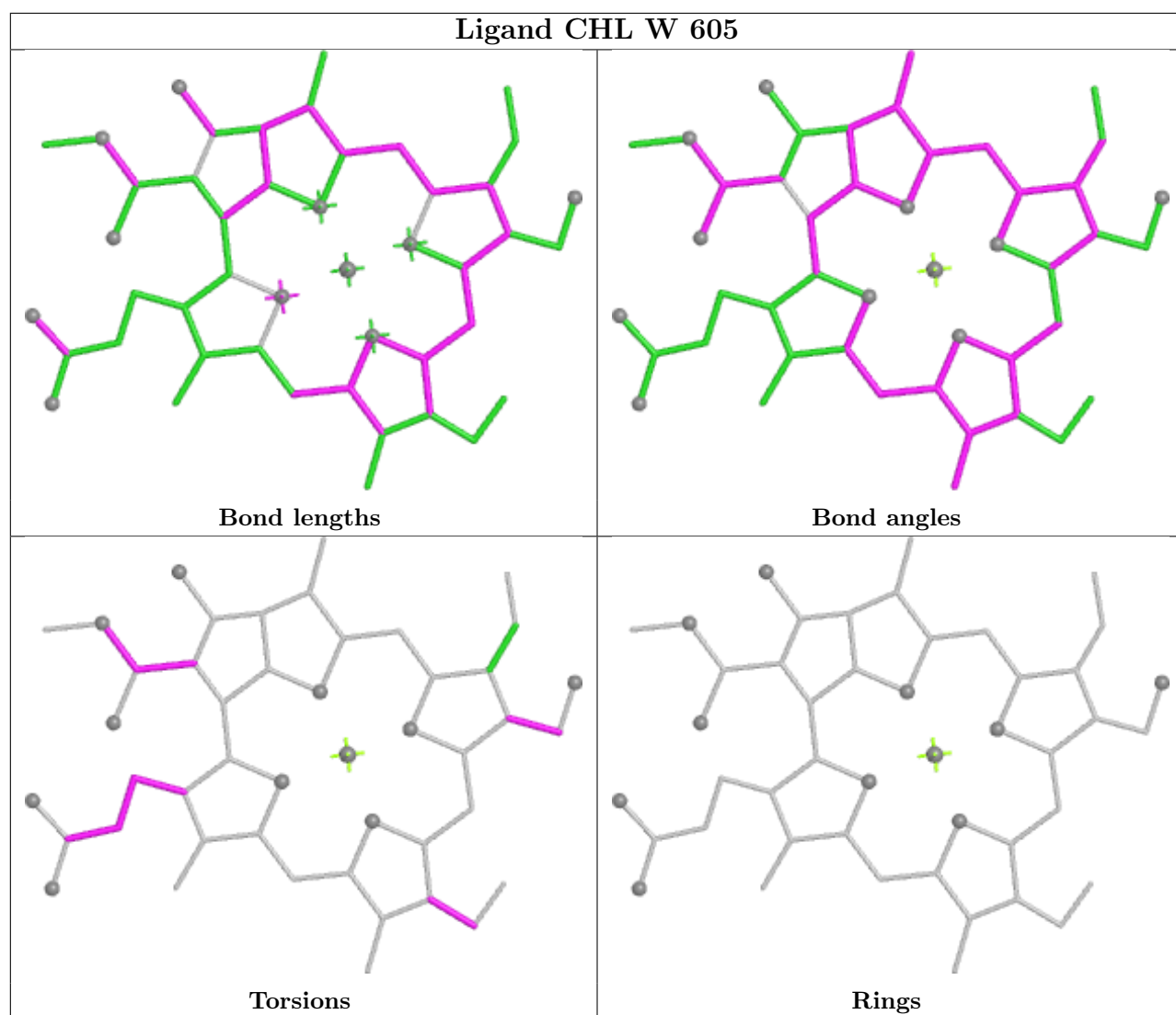
## Ligand CLA 5 618



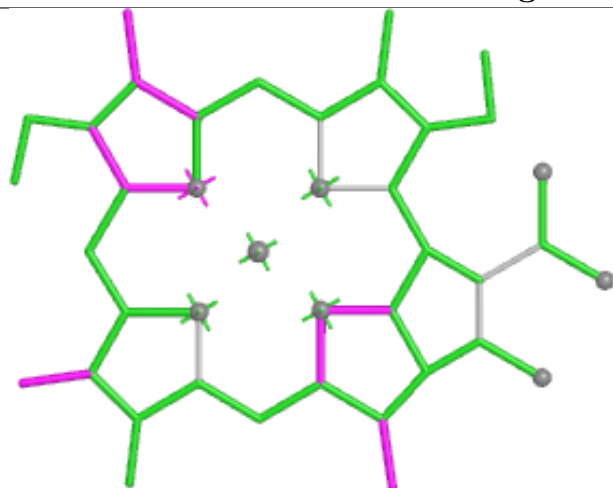
## Ligand BCR F 305



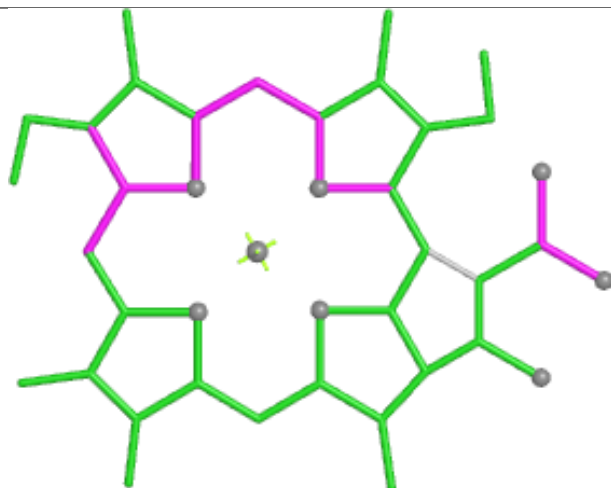




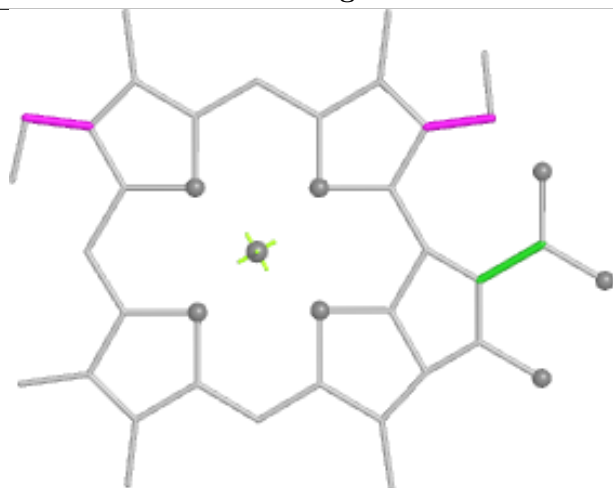
## Ligand CLA 4 606



Bond lengths



Bond angles

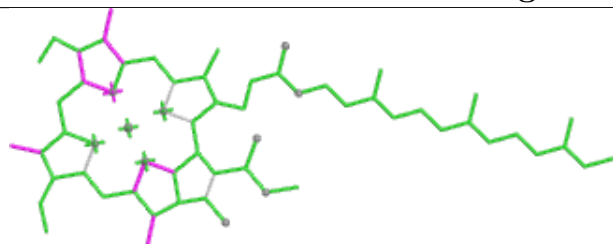


Torsions

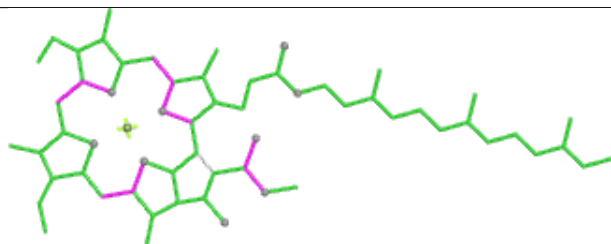


Rings

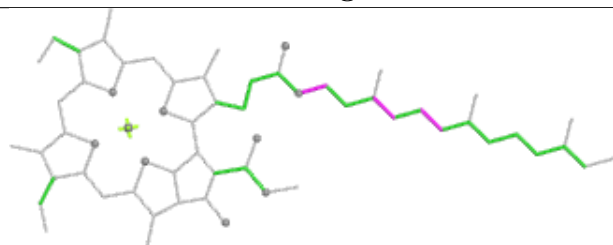
## Ligand CLA 9 609



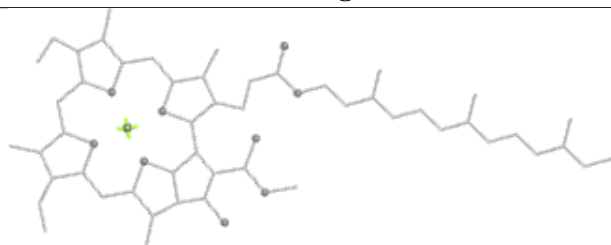
Bond lengths



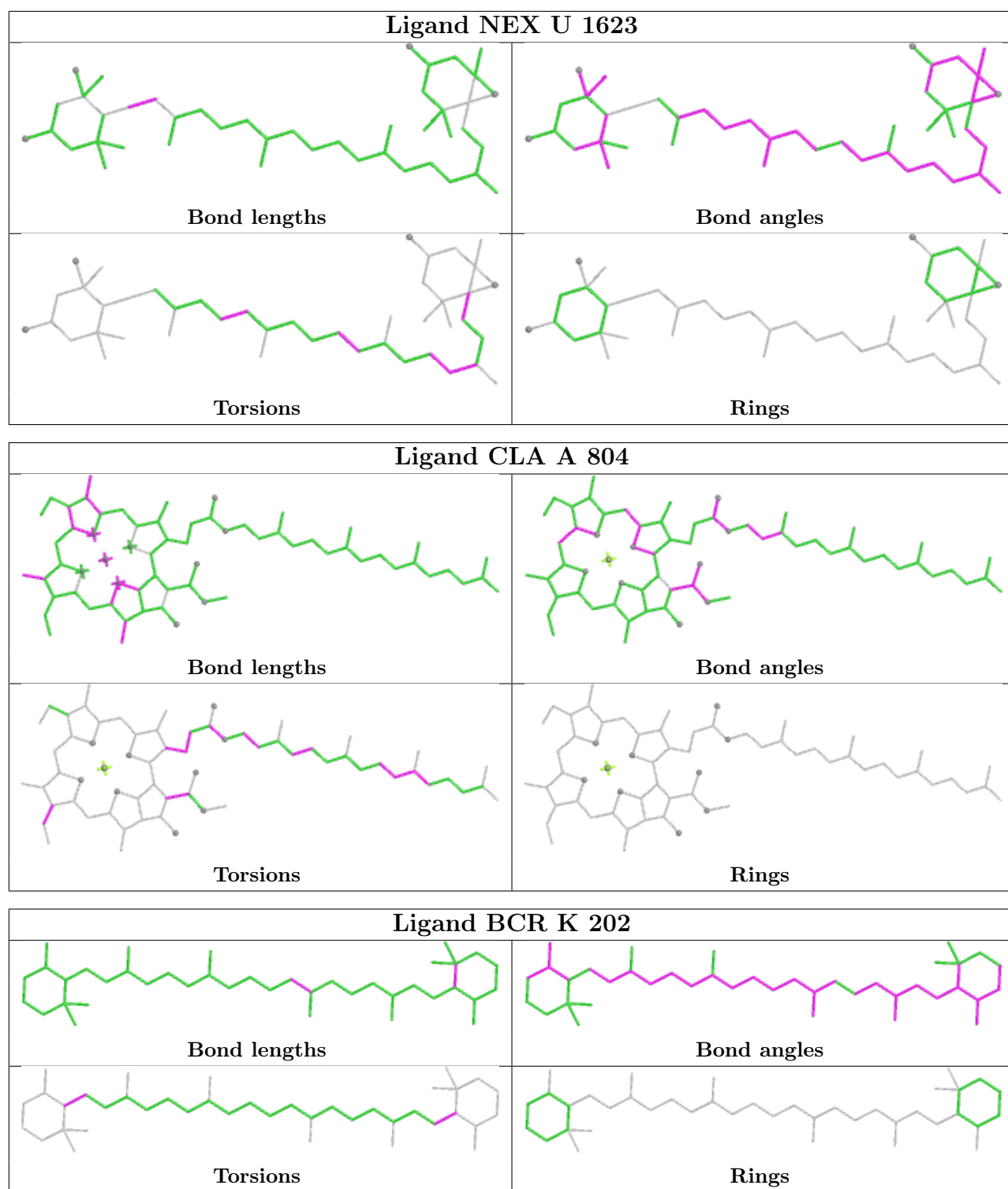
Bond angles



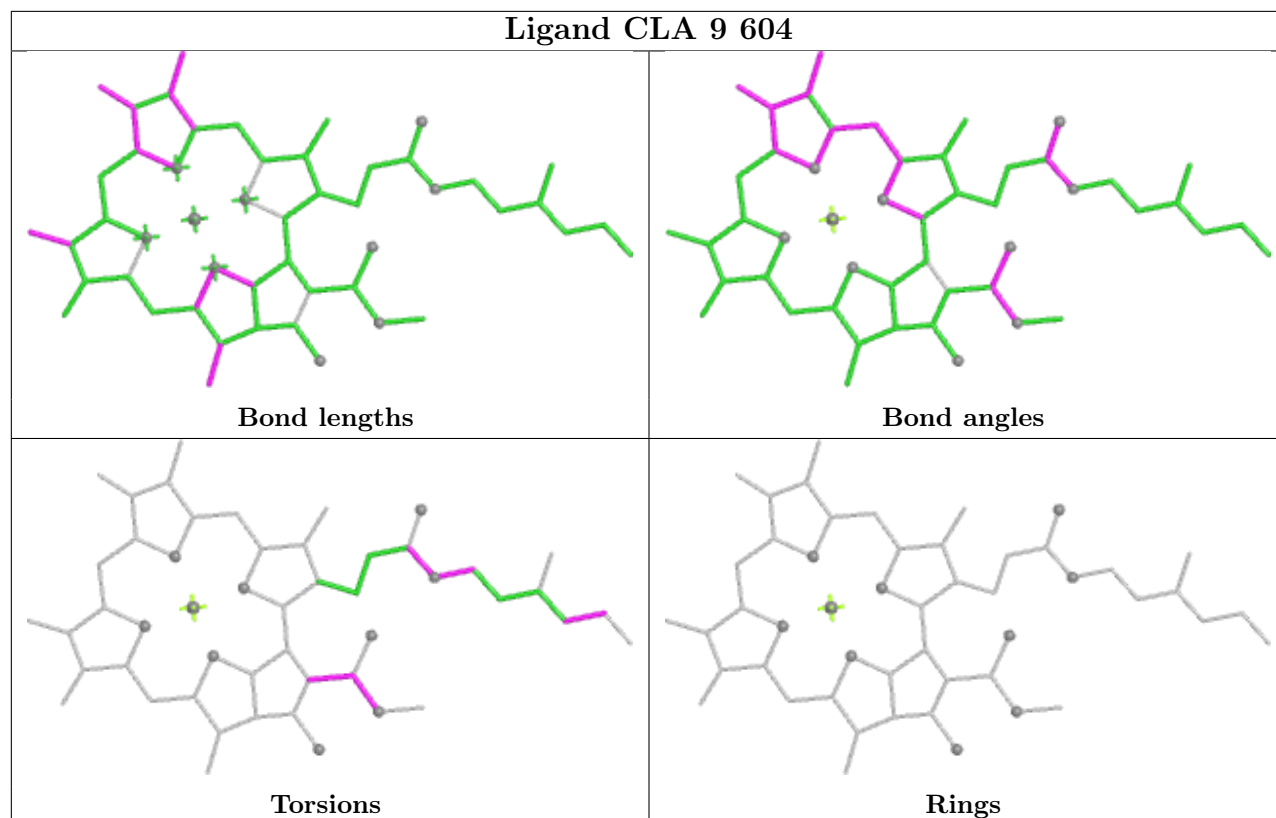
Torsions



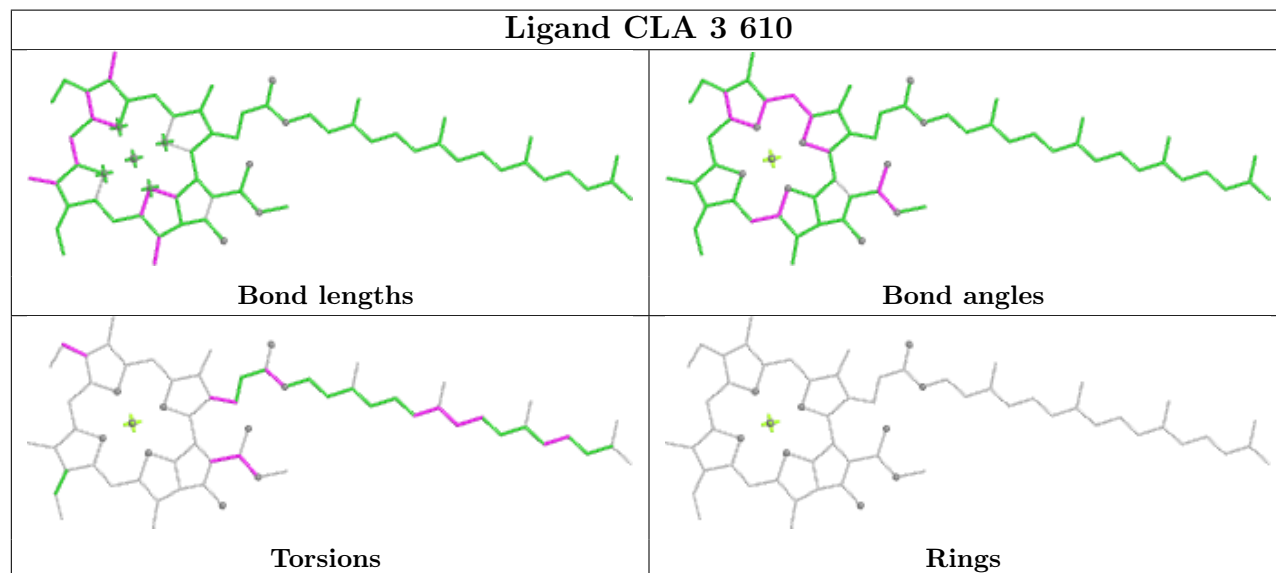
Rings



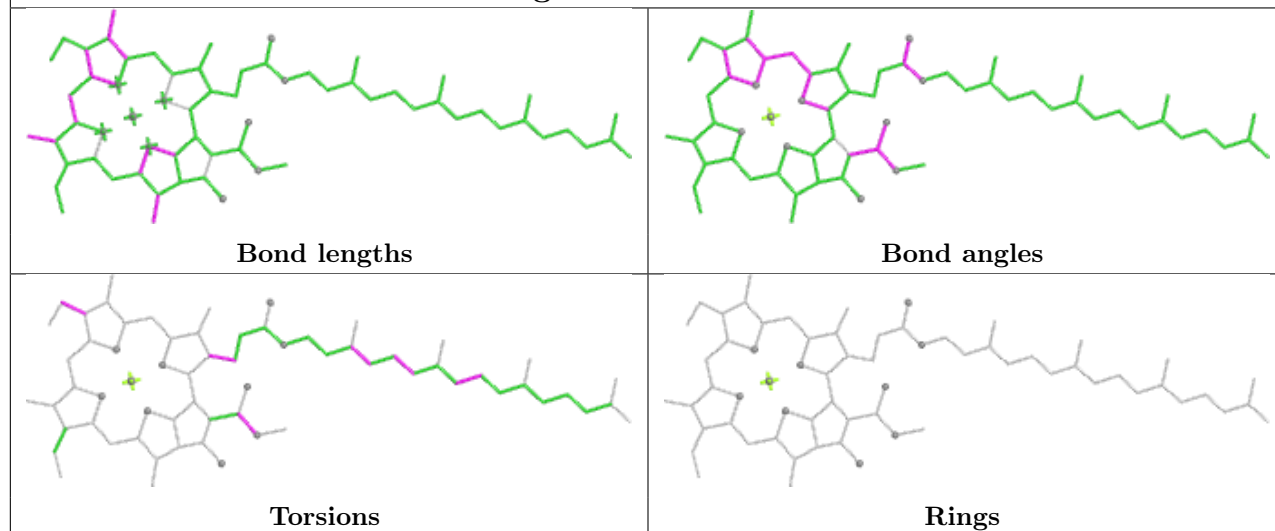
## Ligand CLA 9 604



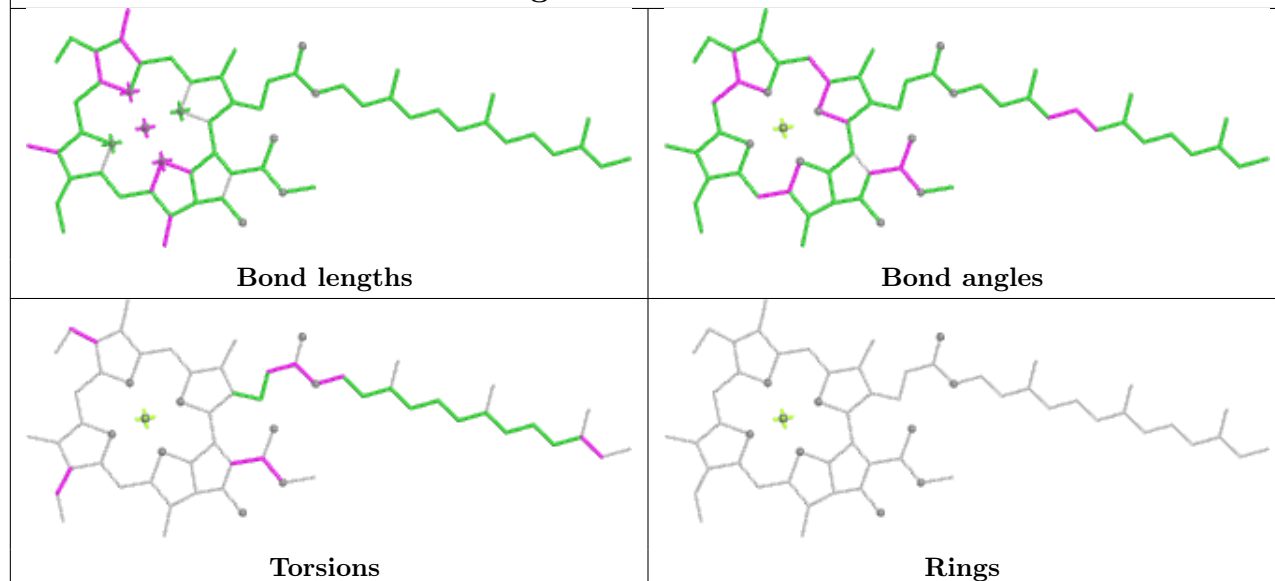
## Ligand CLA 3 610



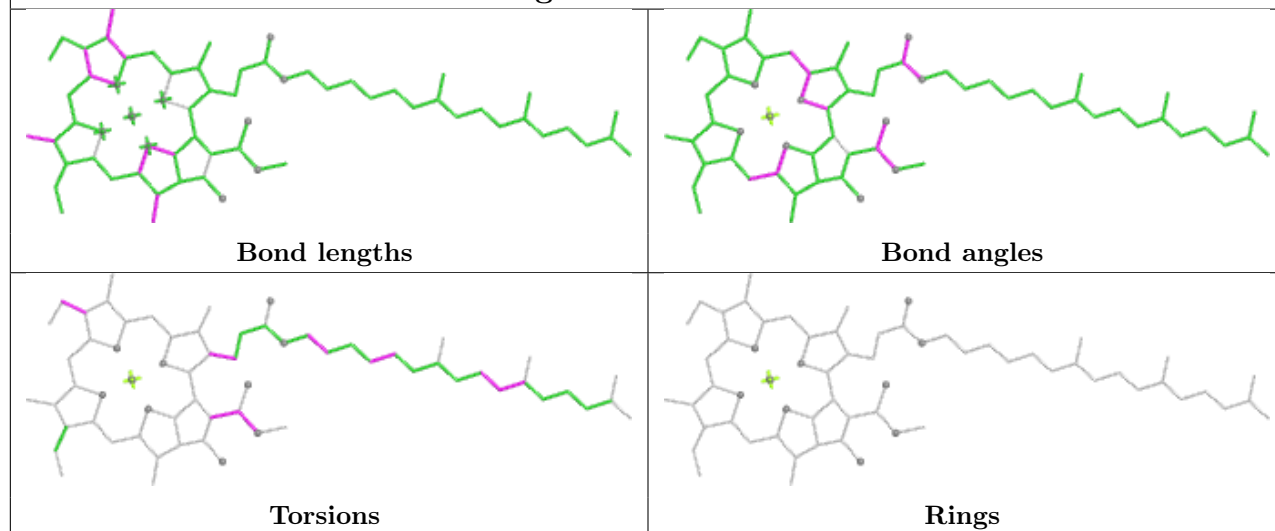
## Ligand CLA Z 610



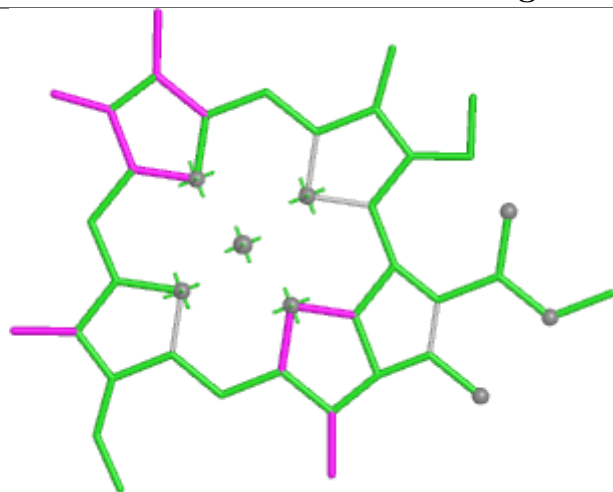
## Ligand CLA A 835



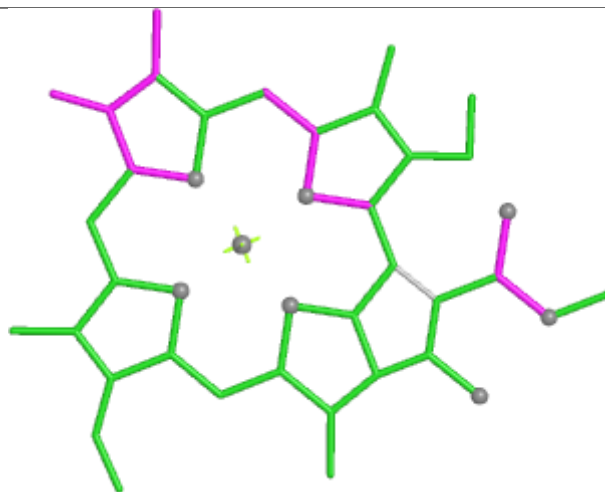
## Ligand CLA 6 620



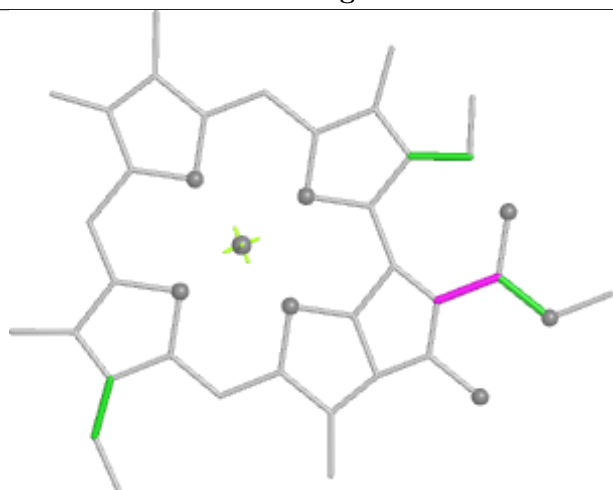
## Ligand CLA 6 607



Bond lengths



Bond angles

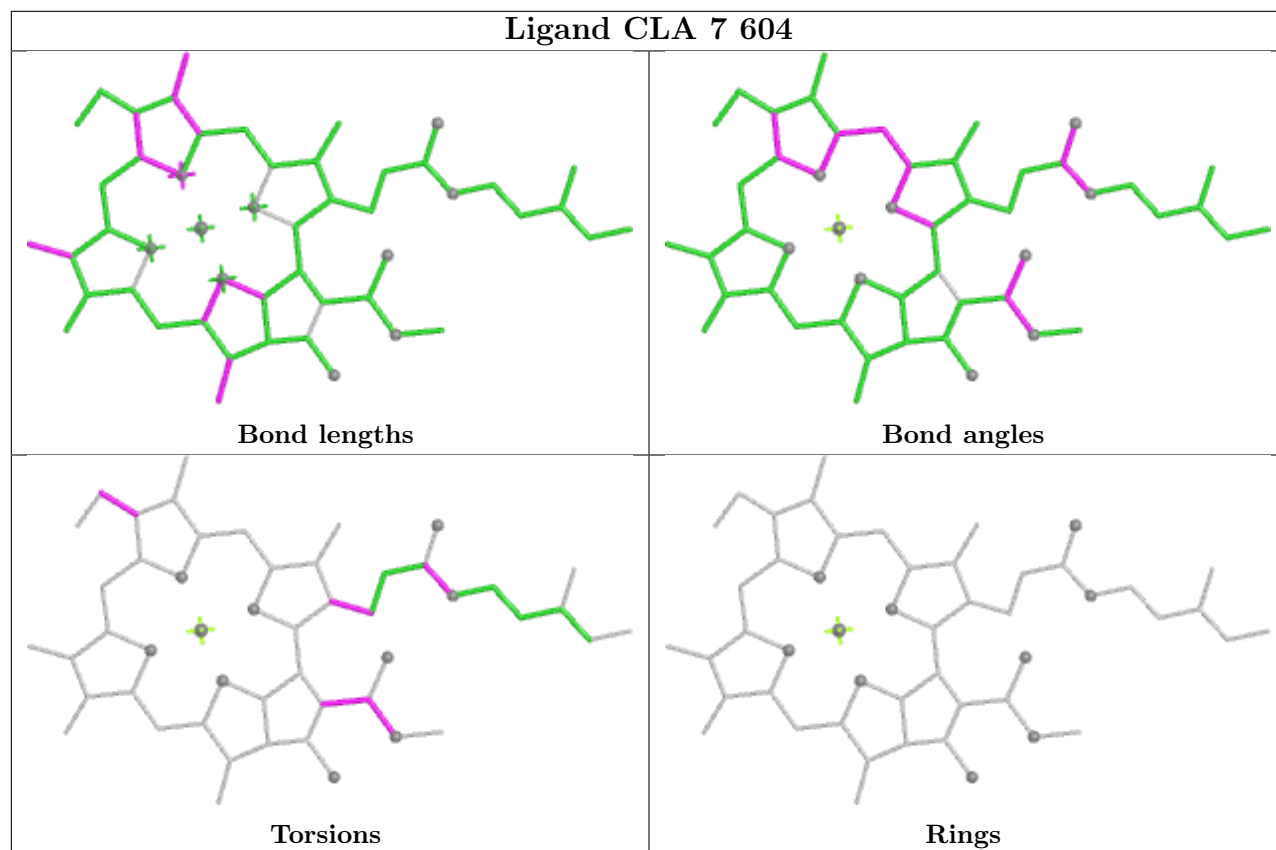


Torsions

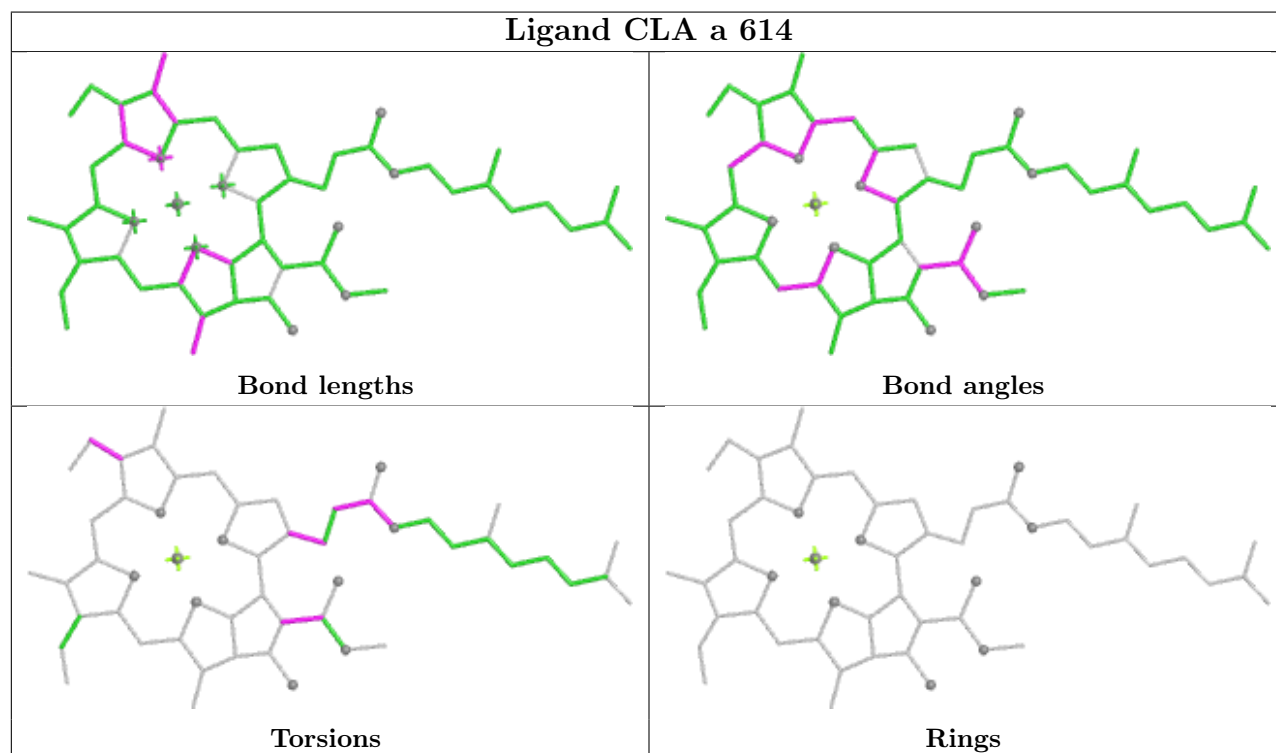


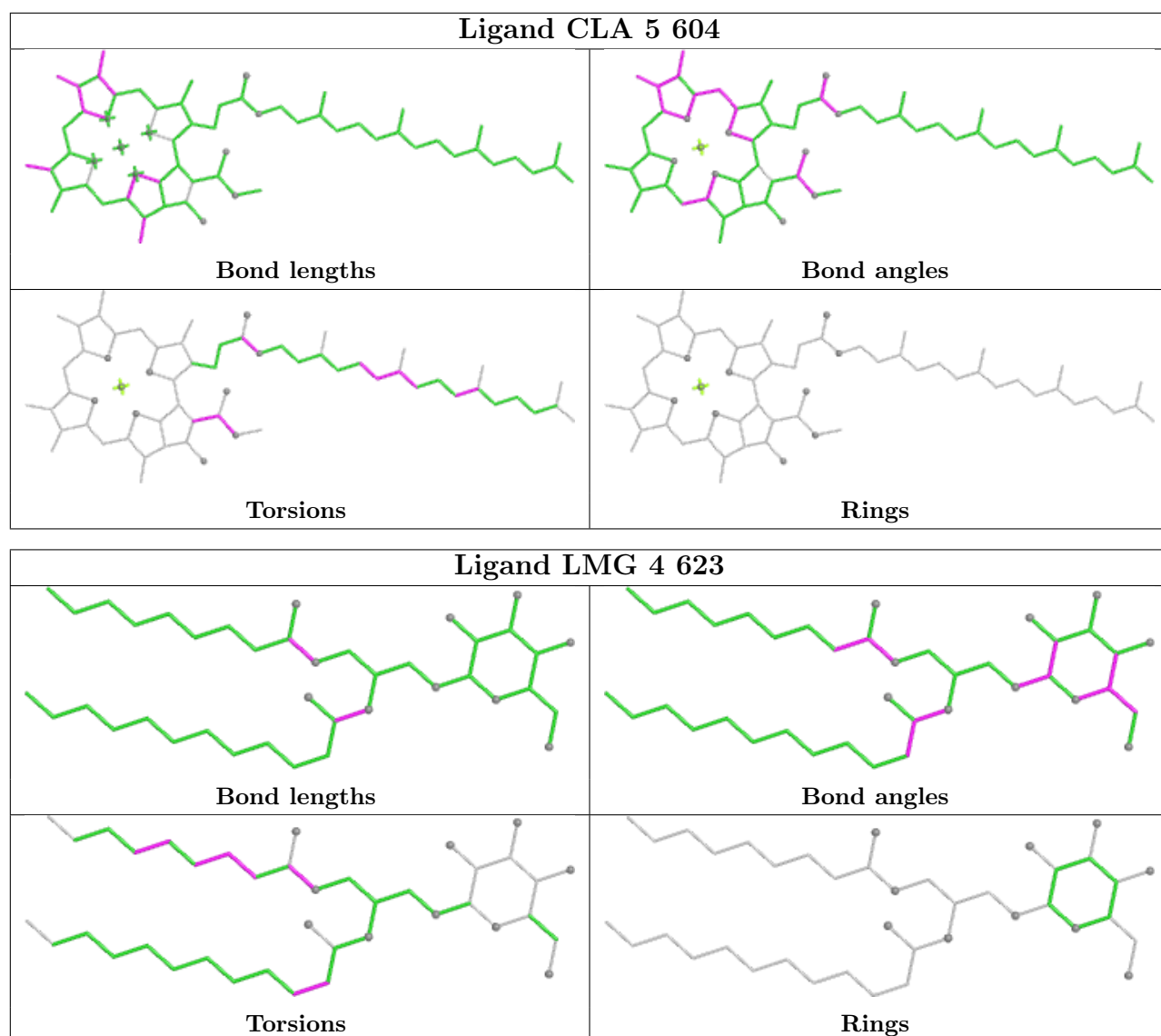
Rings

## Ligand CLA 7 604

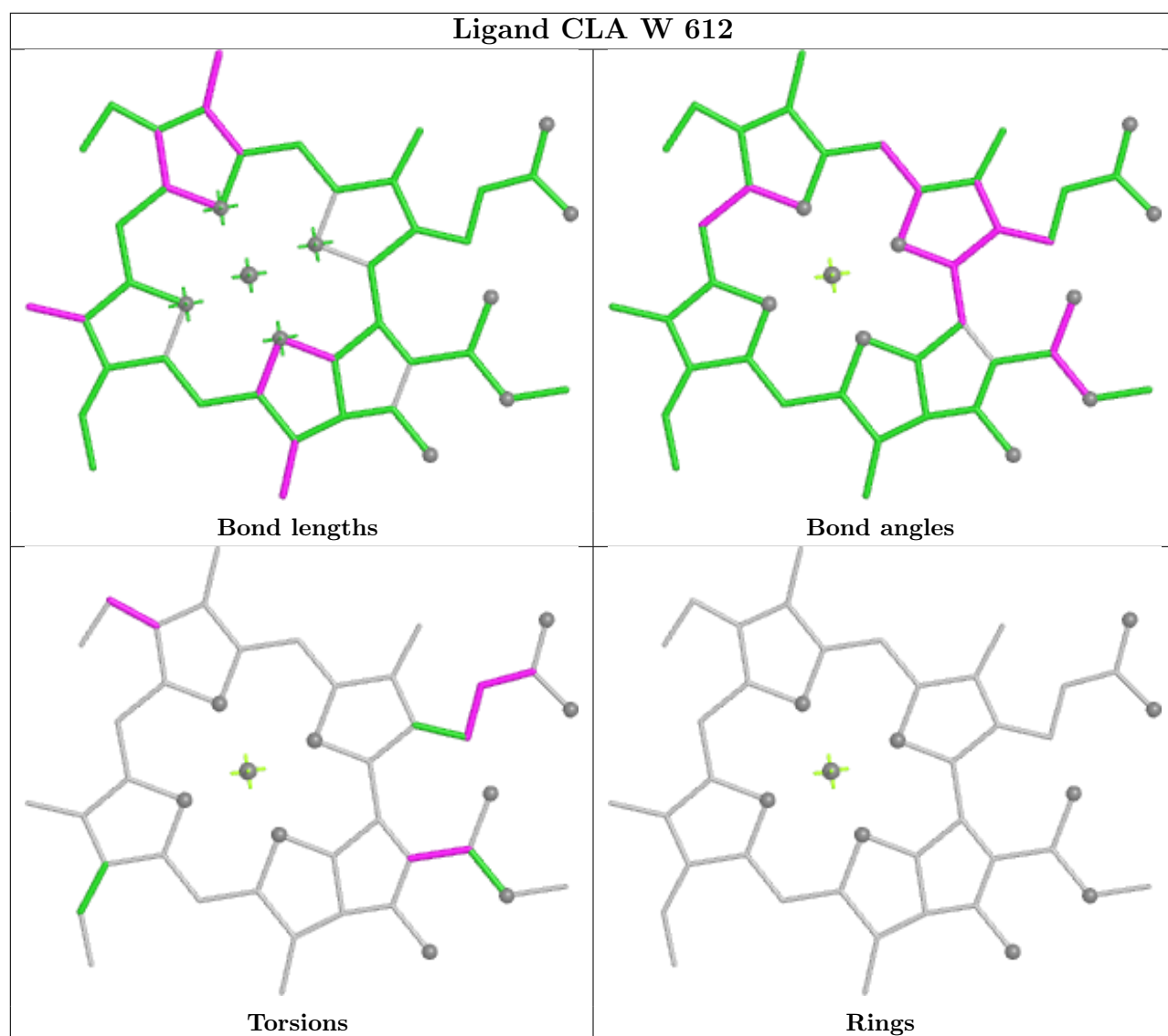


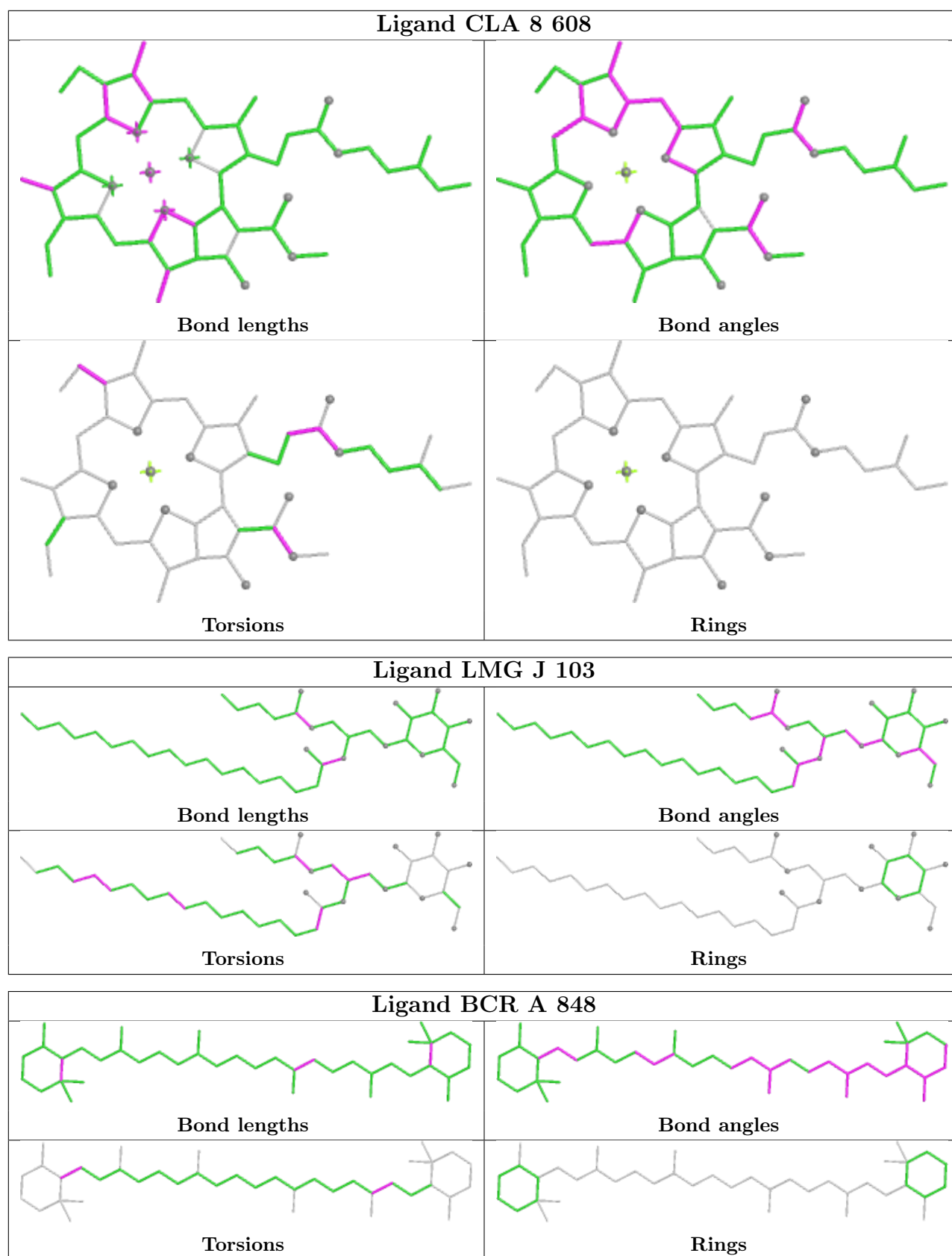
## Ligand CLA a 614

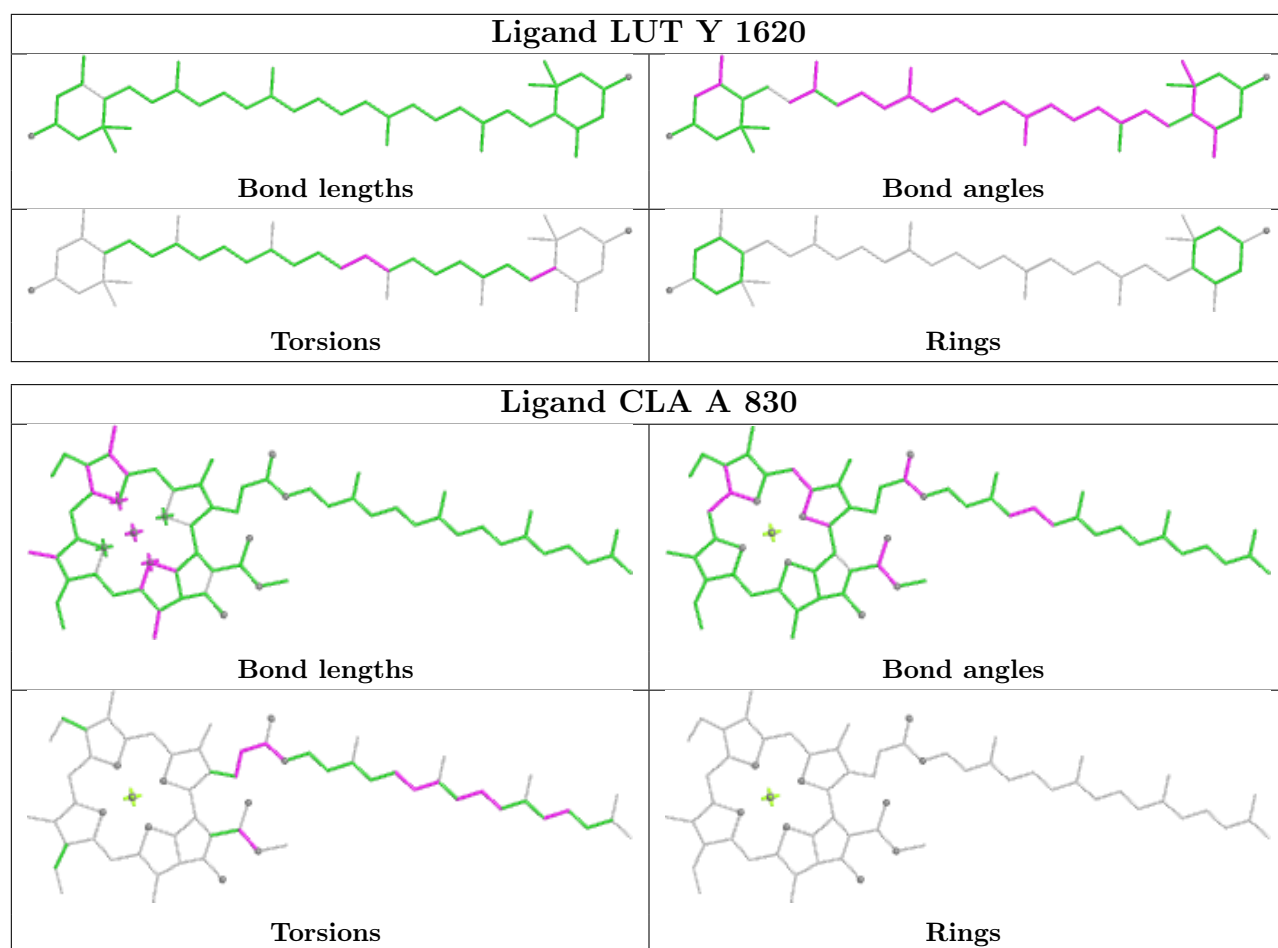


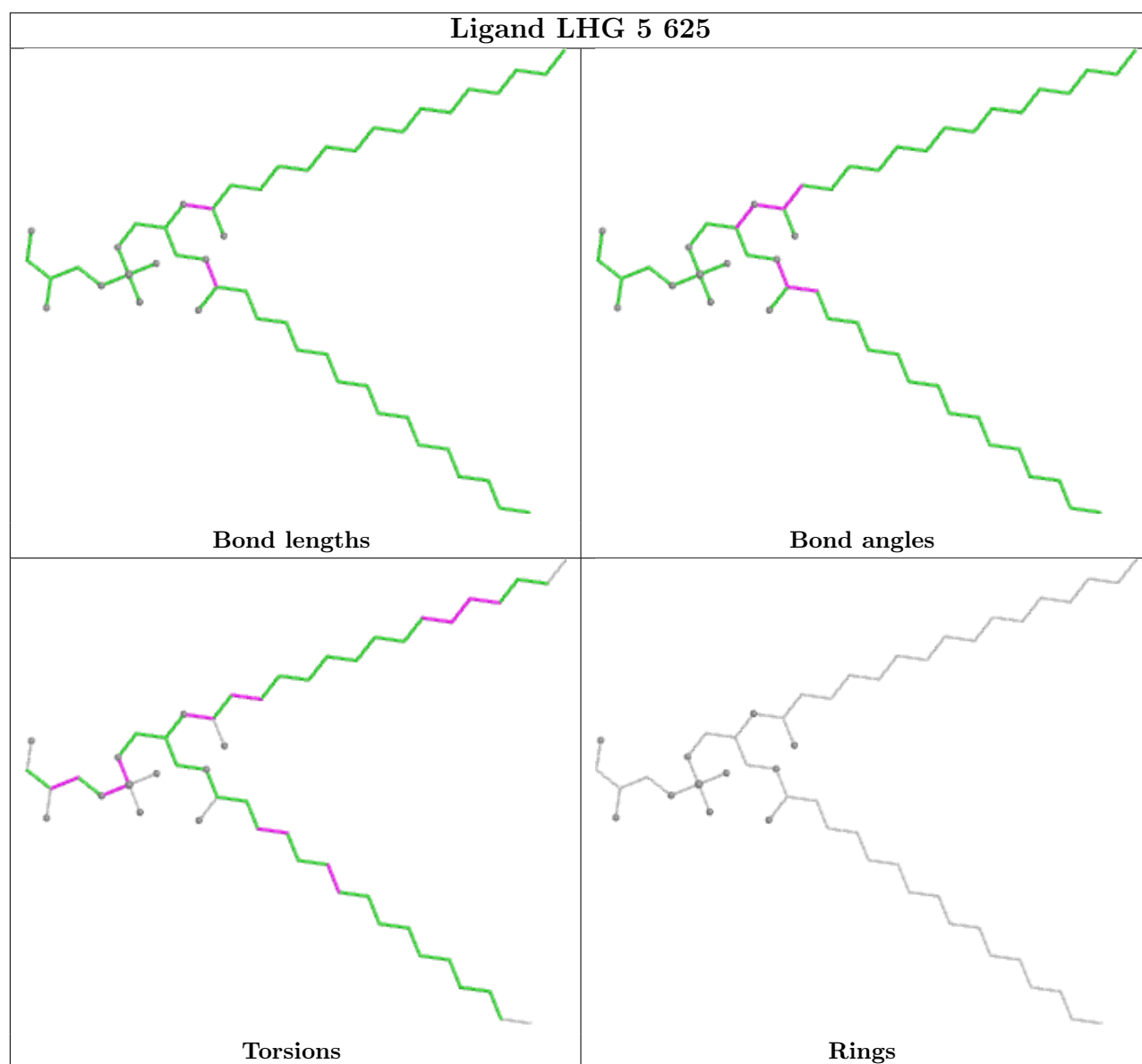
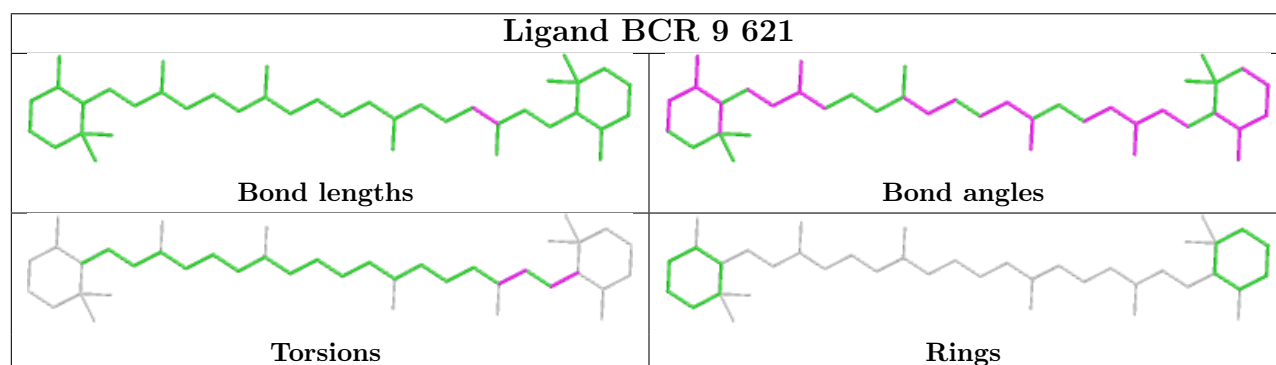


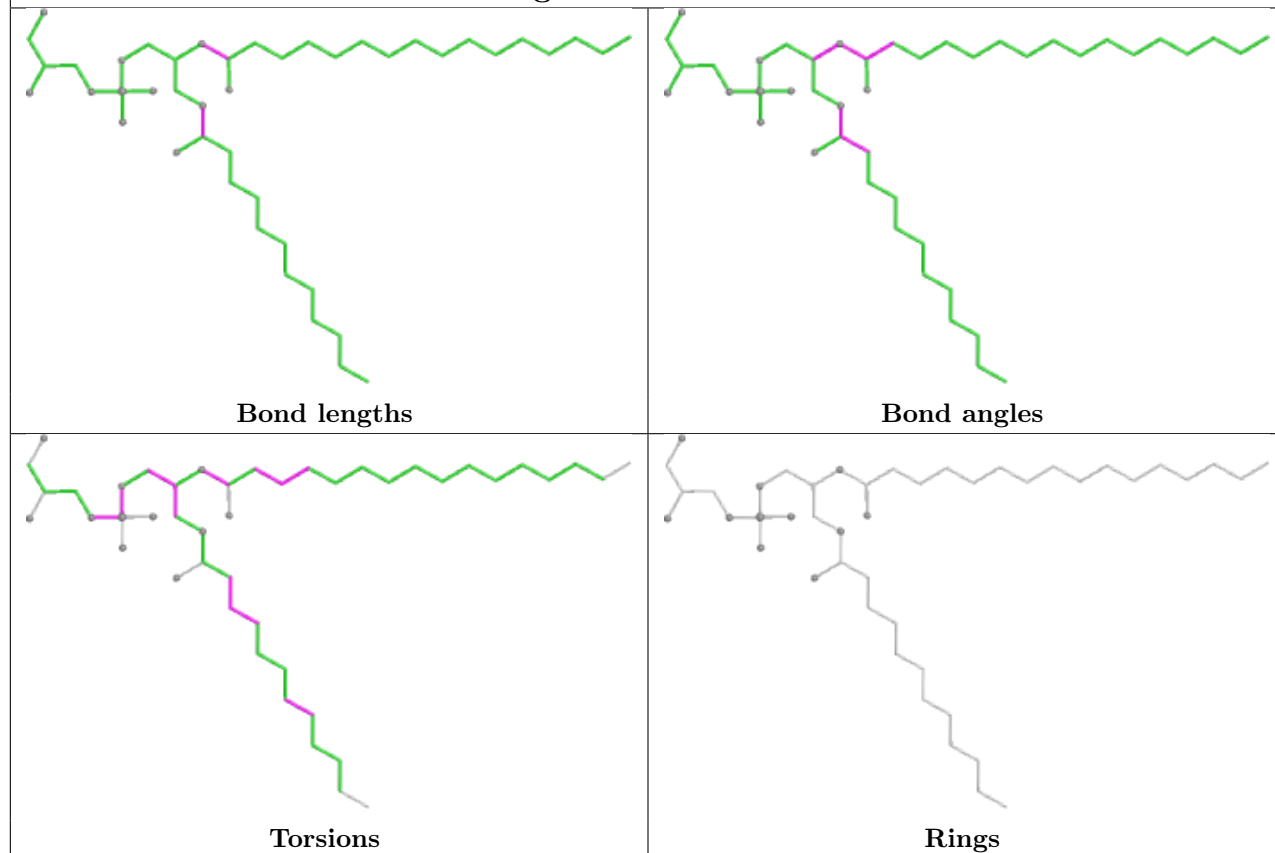
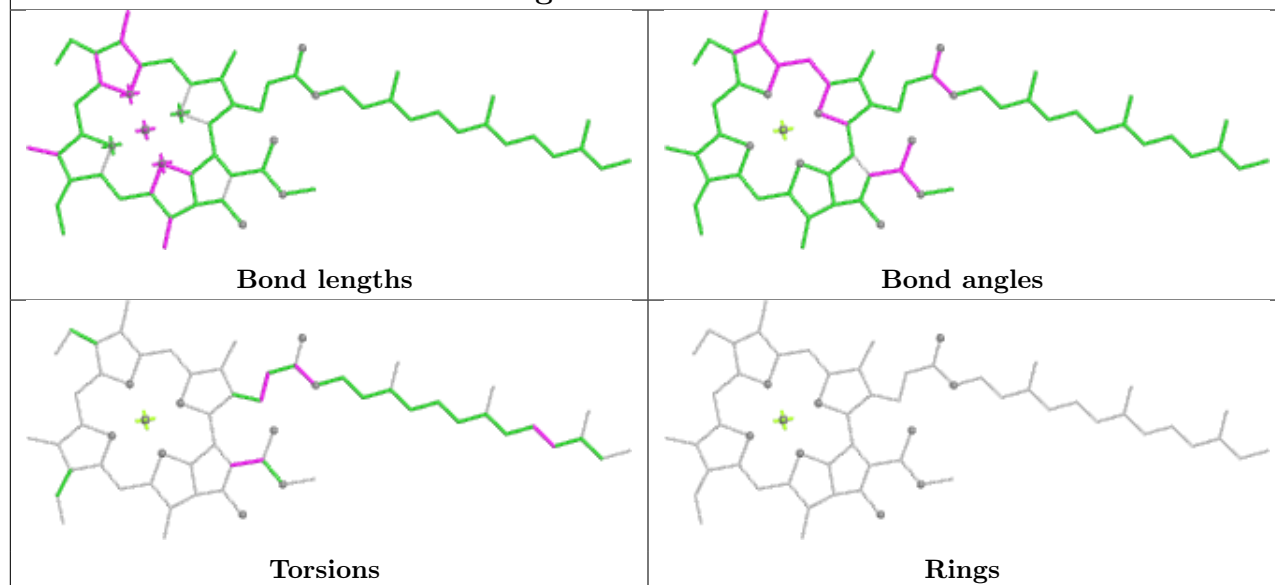




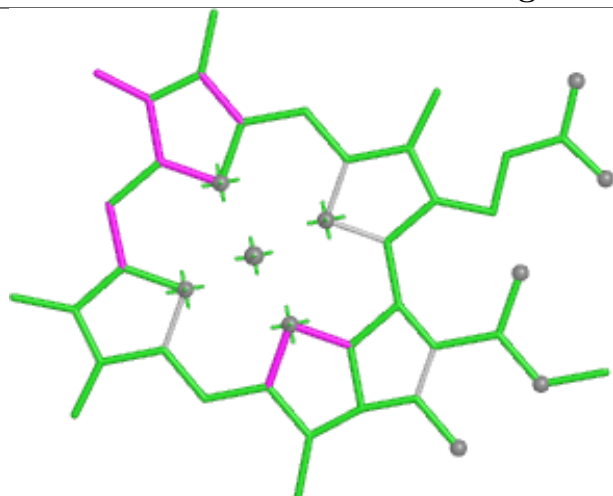




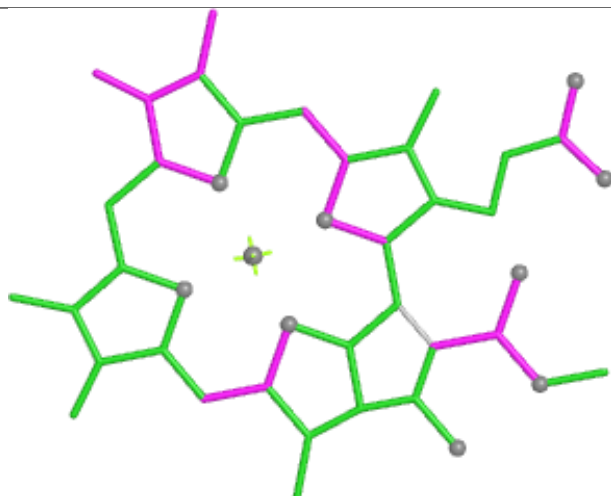


**Ligand LHG 3 623****Ligand CLA a 602**

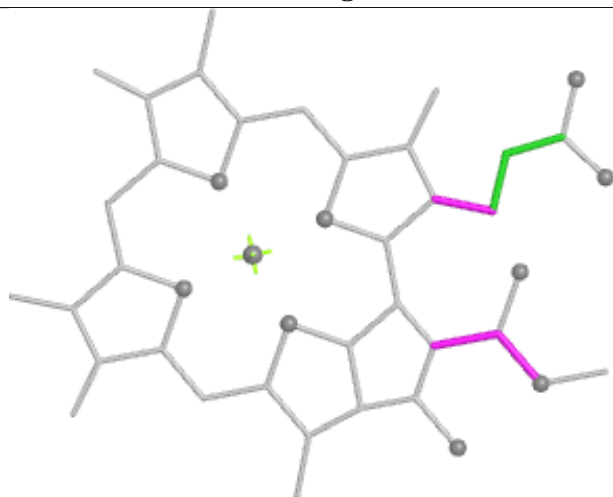
## Ligand CLA 8 616



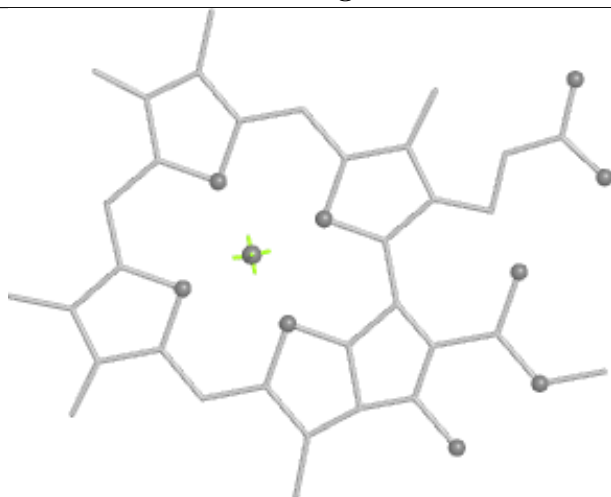
Bond lengths



Bond angles

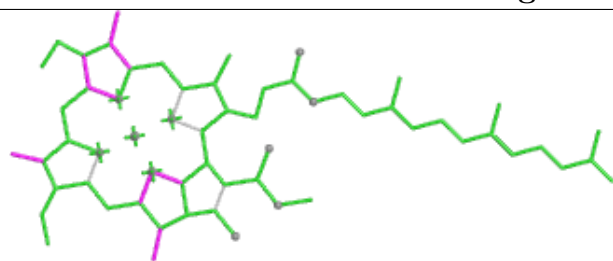


Torsions

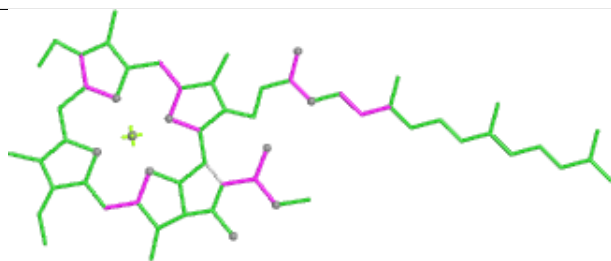


Rings

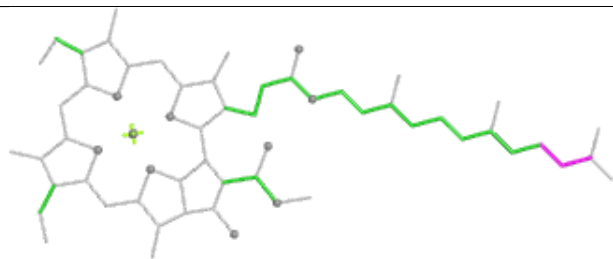
## Ligand CLA 3 602



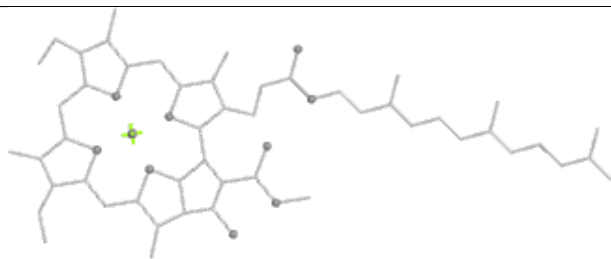
Bond lengths



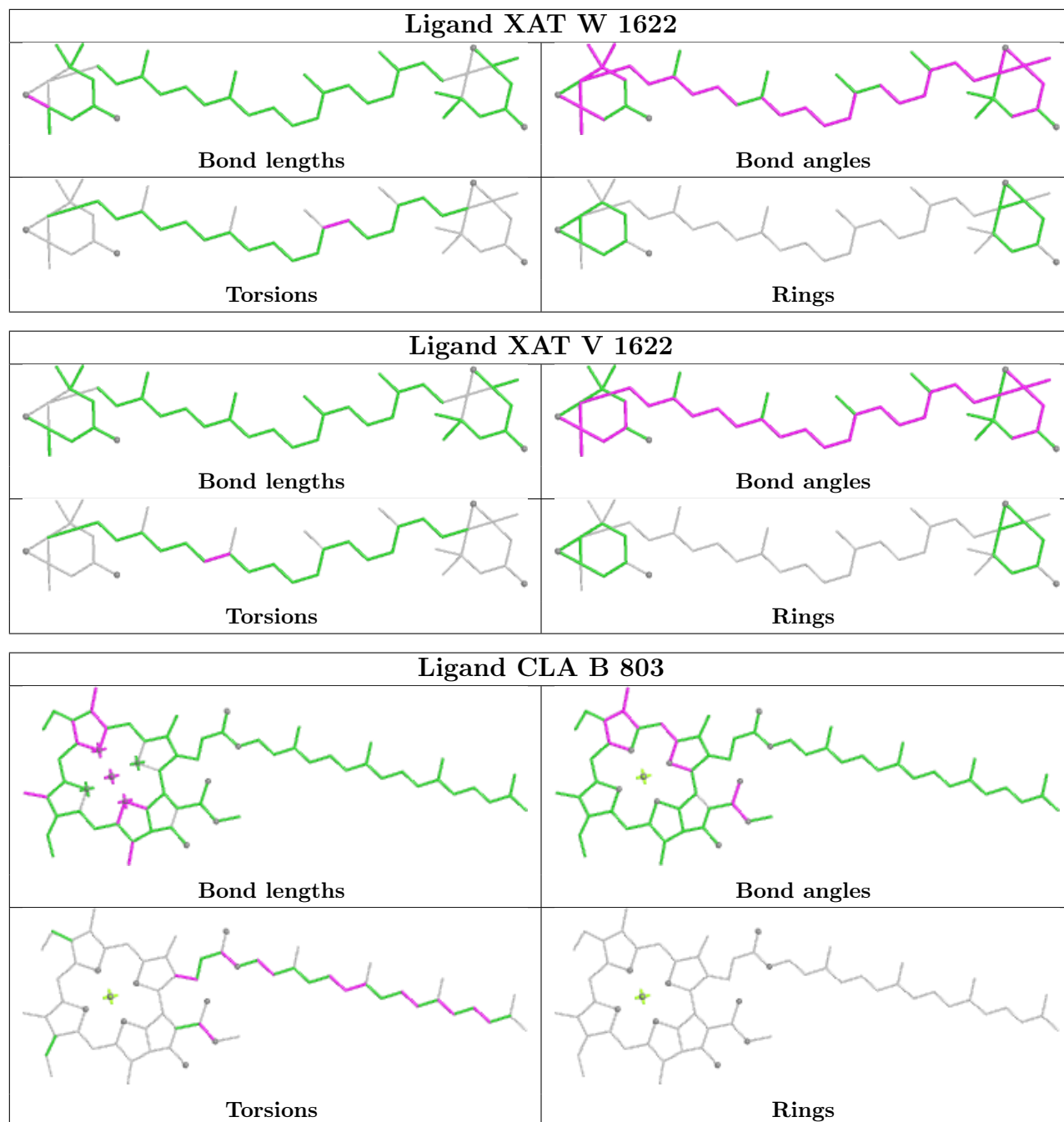
Bond angles

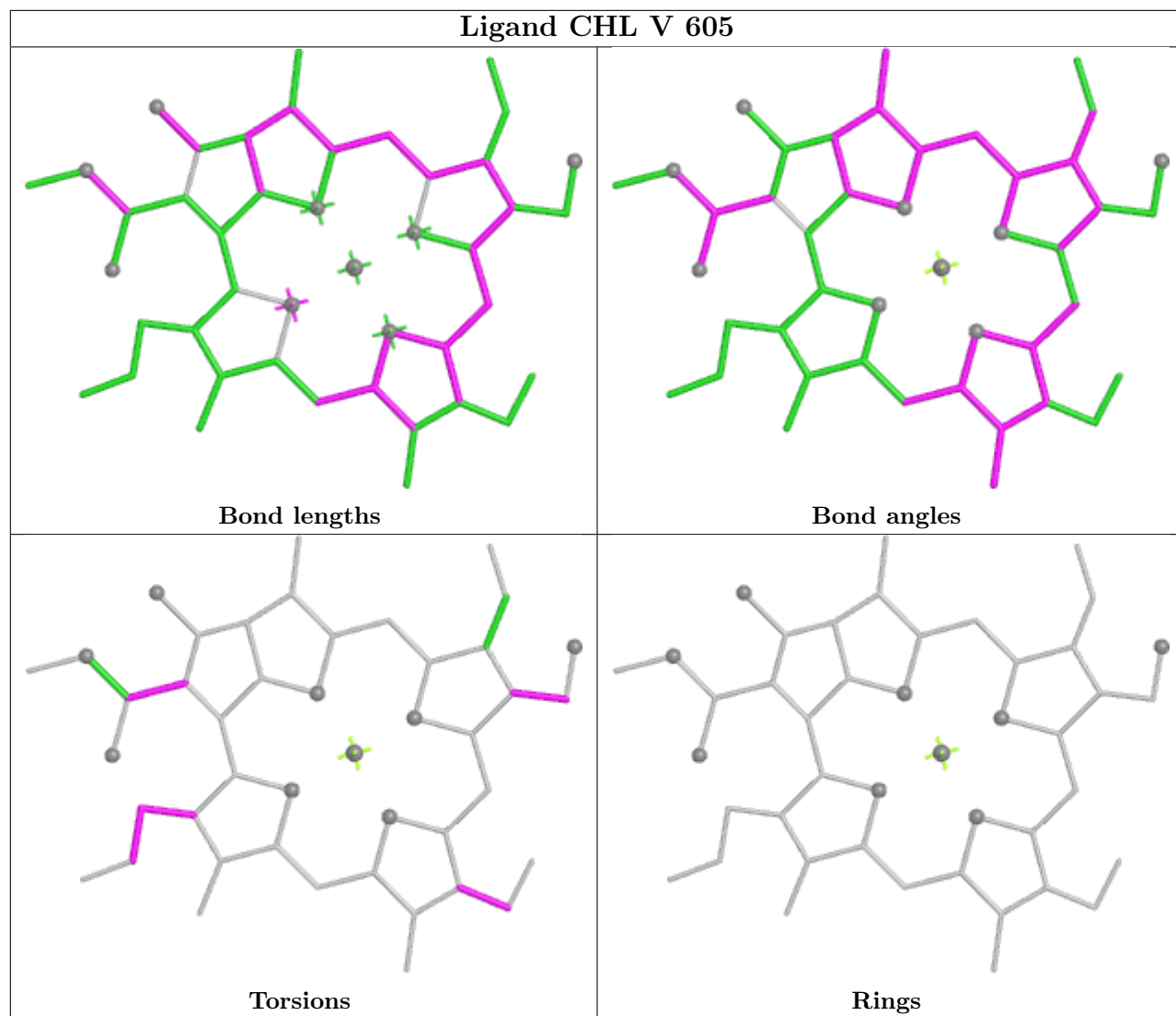


Torsions



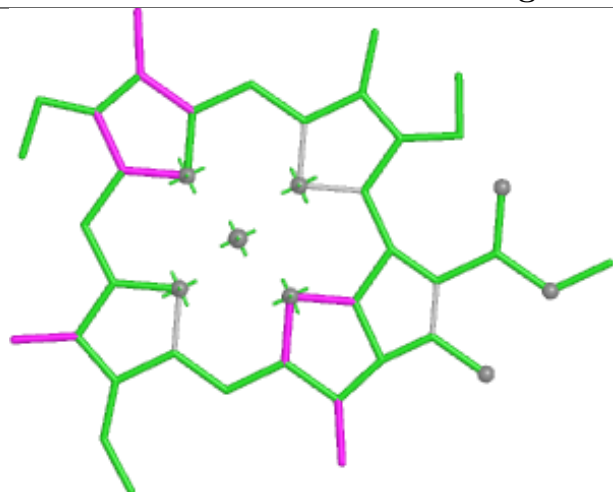
Rings



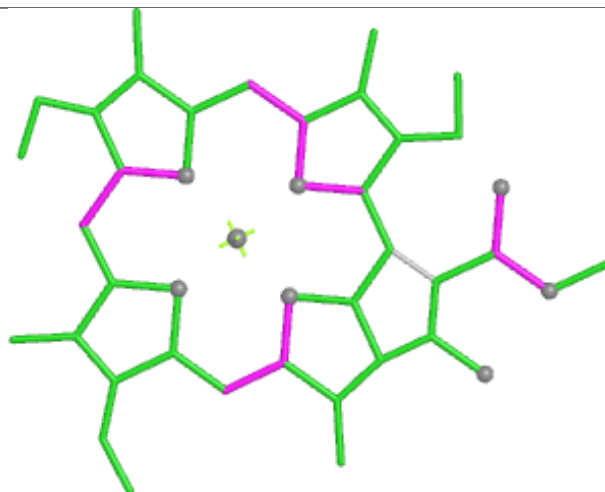




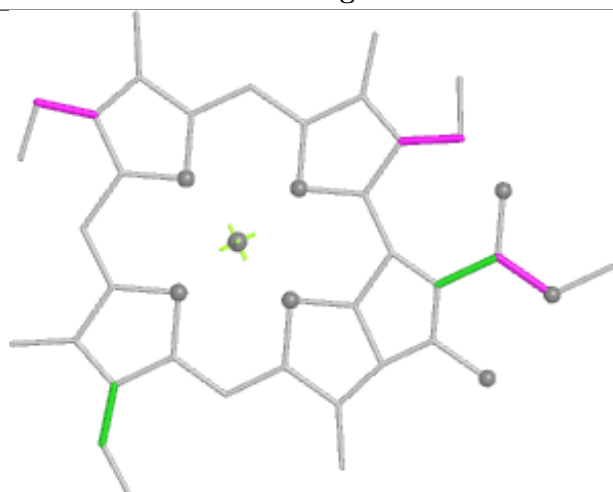
## Ligand CLA 8 611



Bond lengths



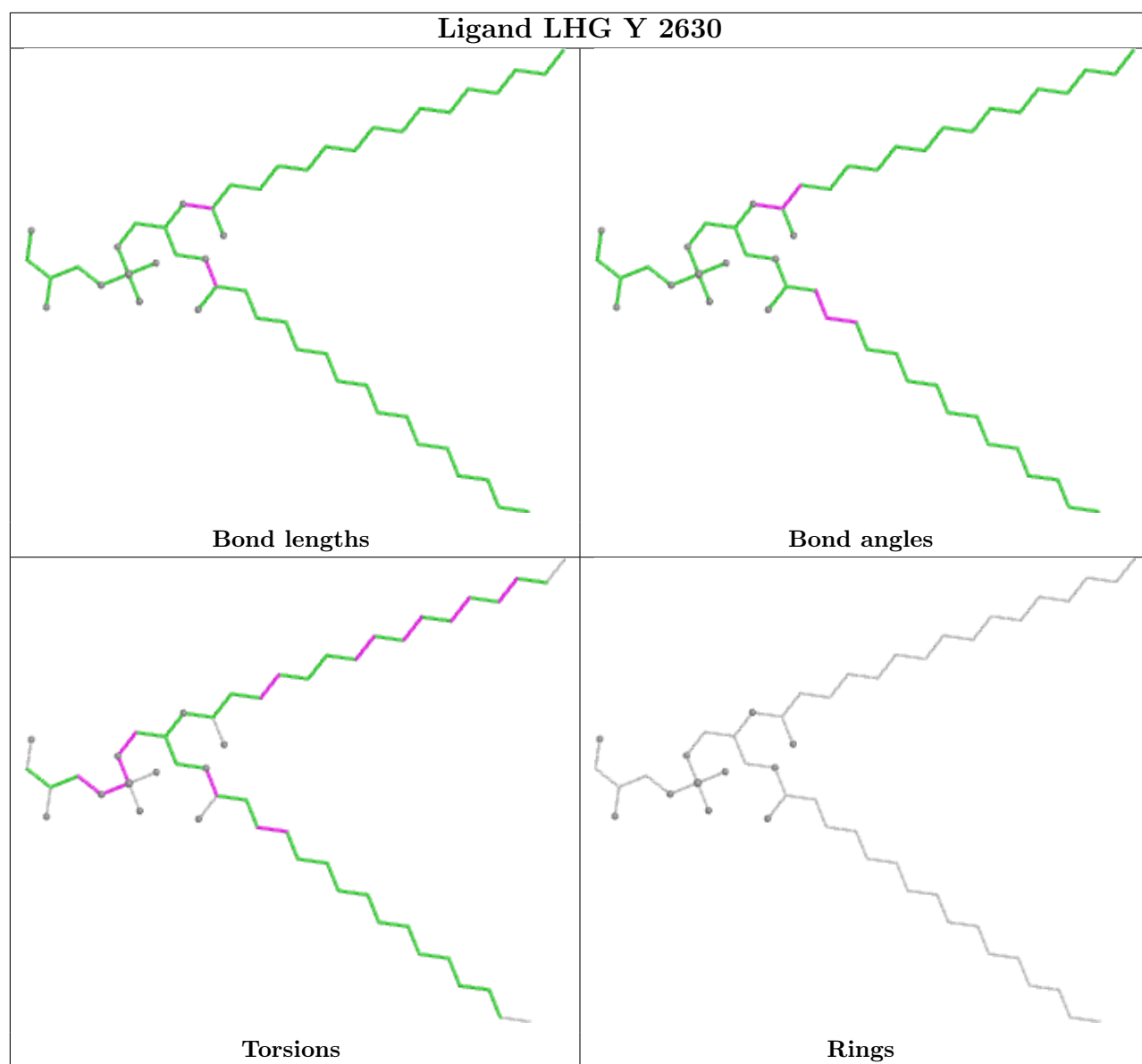
Bond angles



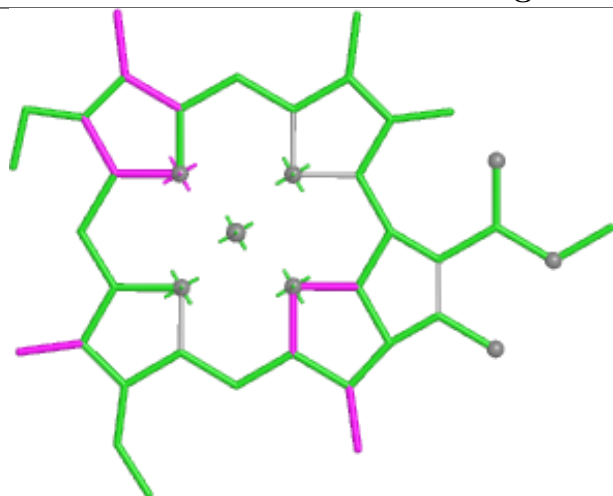
Torsions



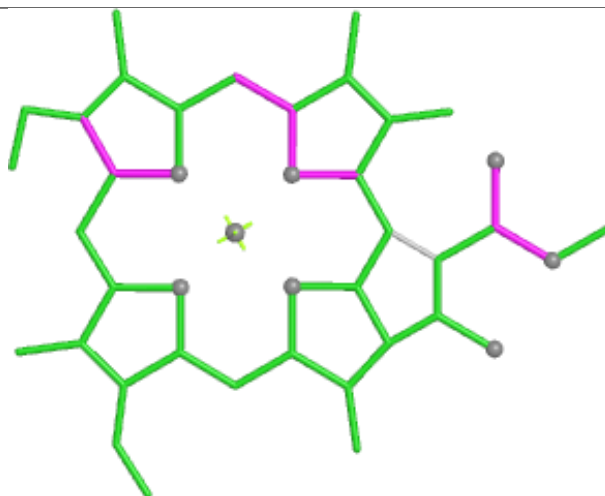
Rings



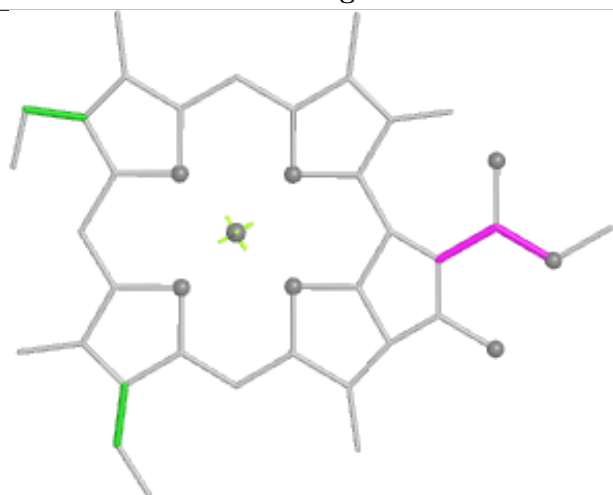
## Ligand CLA B 804



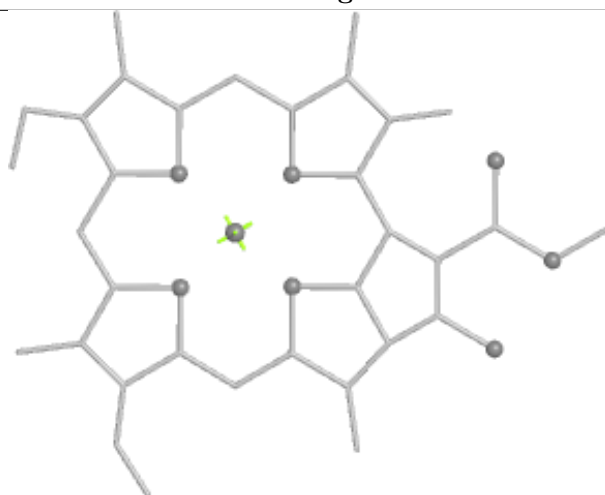
Bond lengths



Bond angles

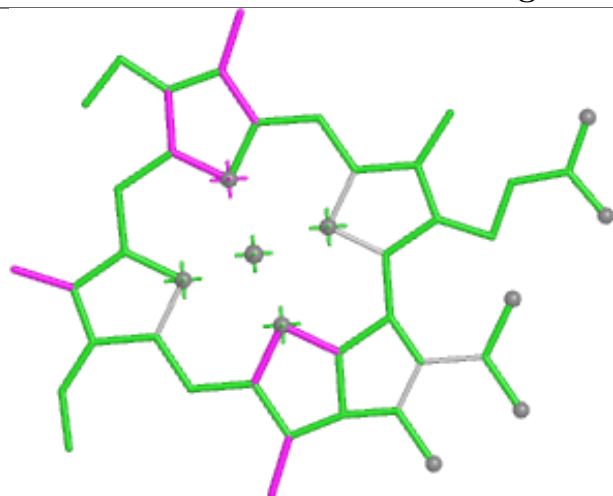


Torsions

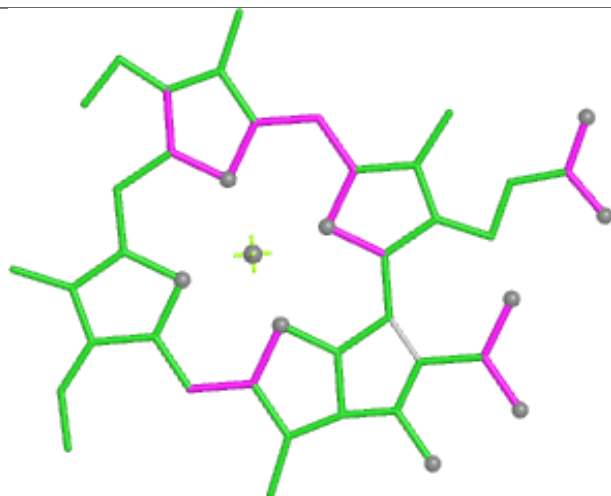


Rings

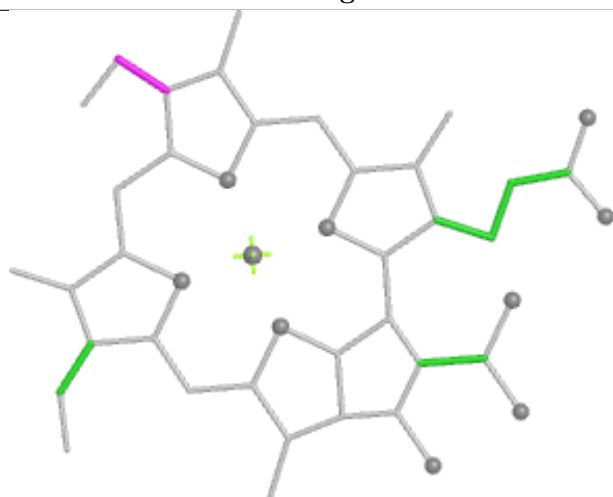
## Ligand CLA 2 607



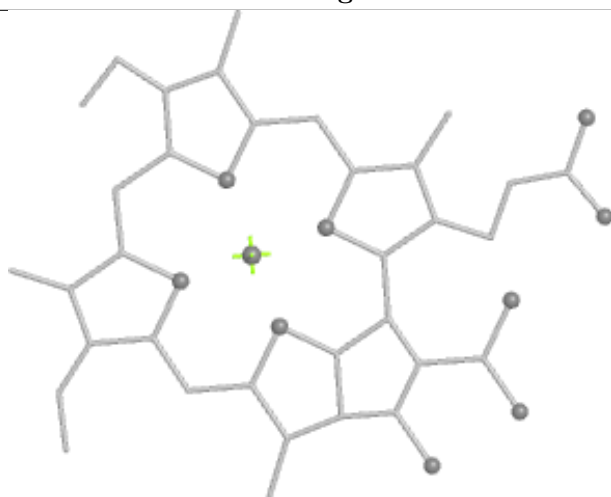
Bond lengths



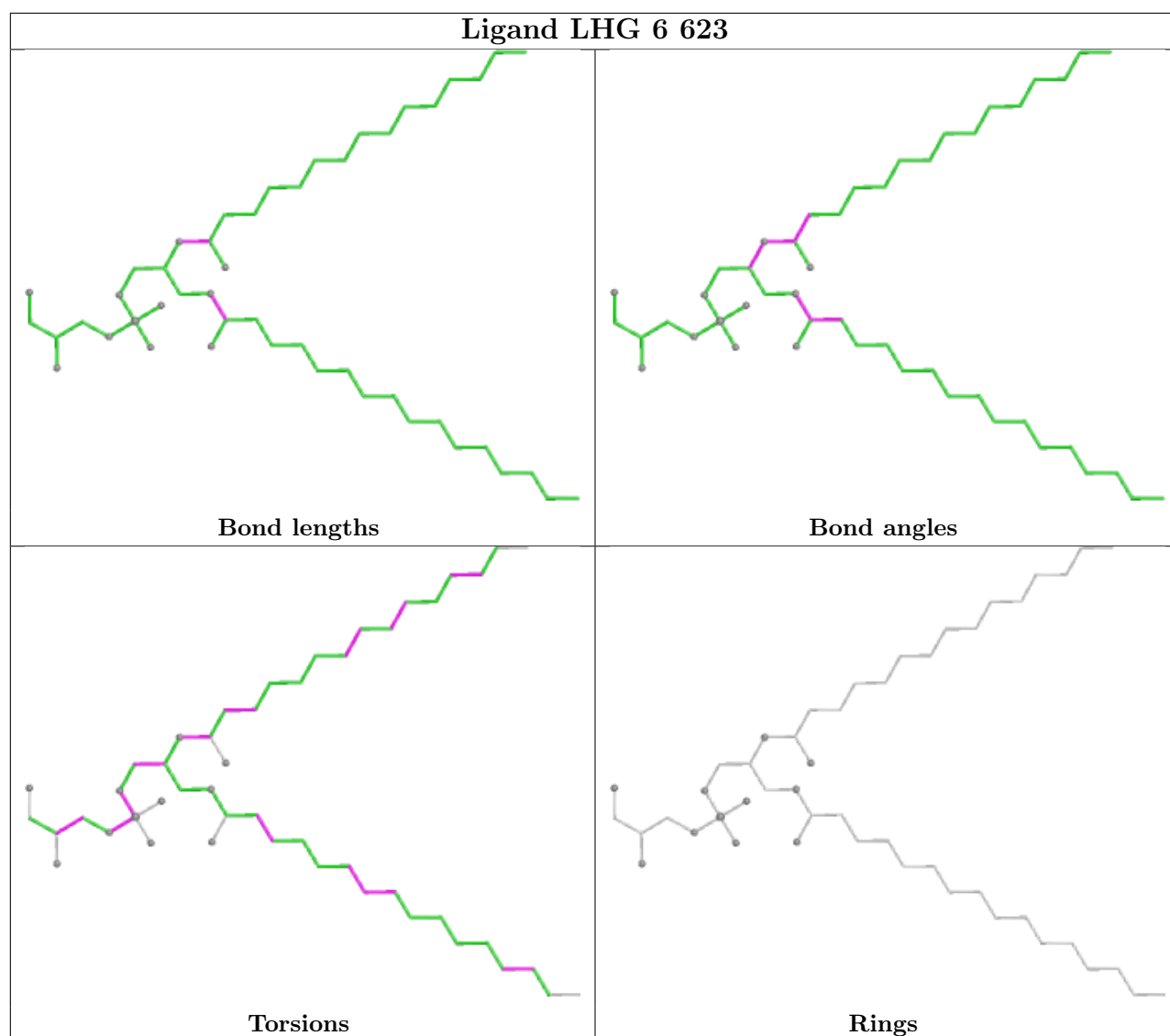
Bond angles



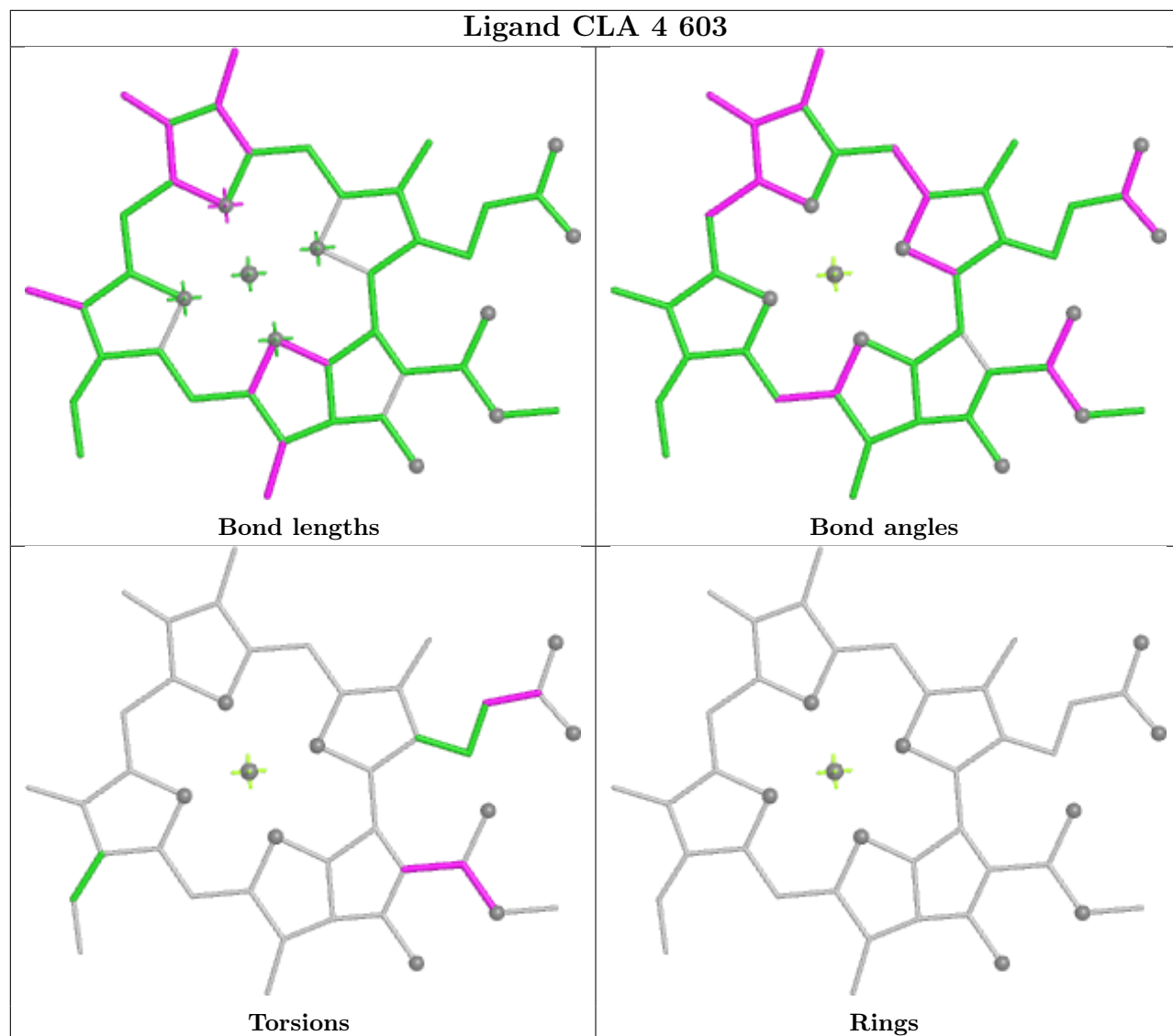
Torsions

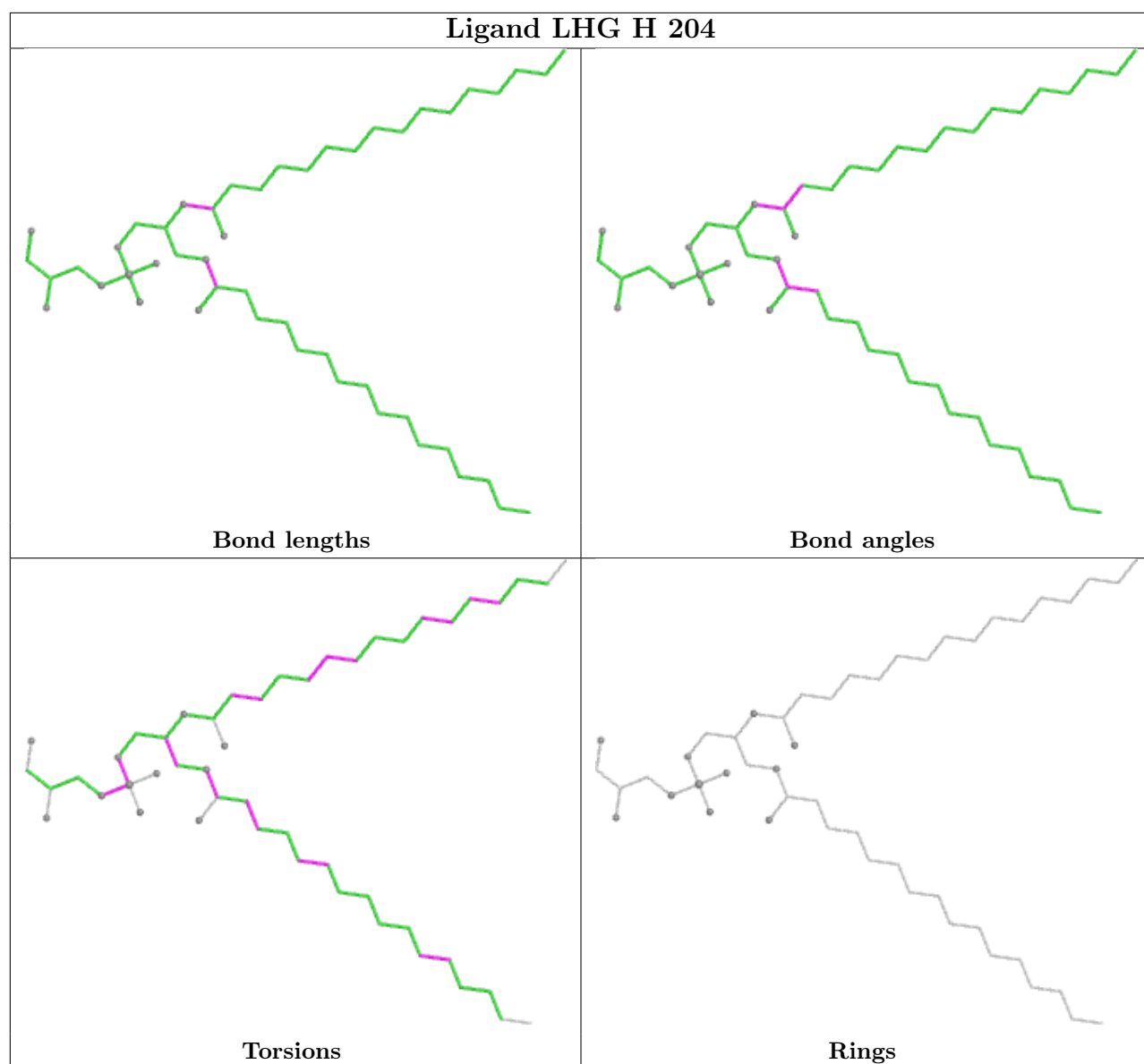
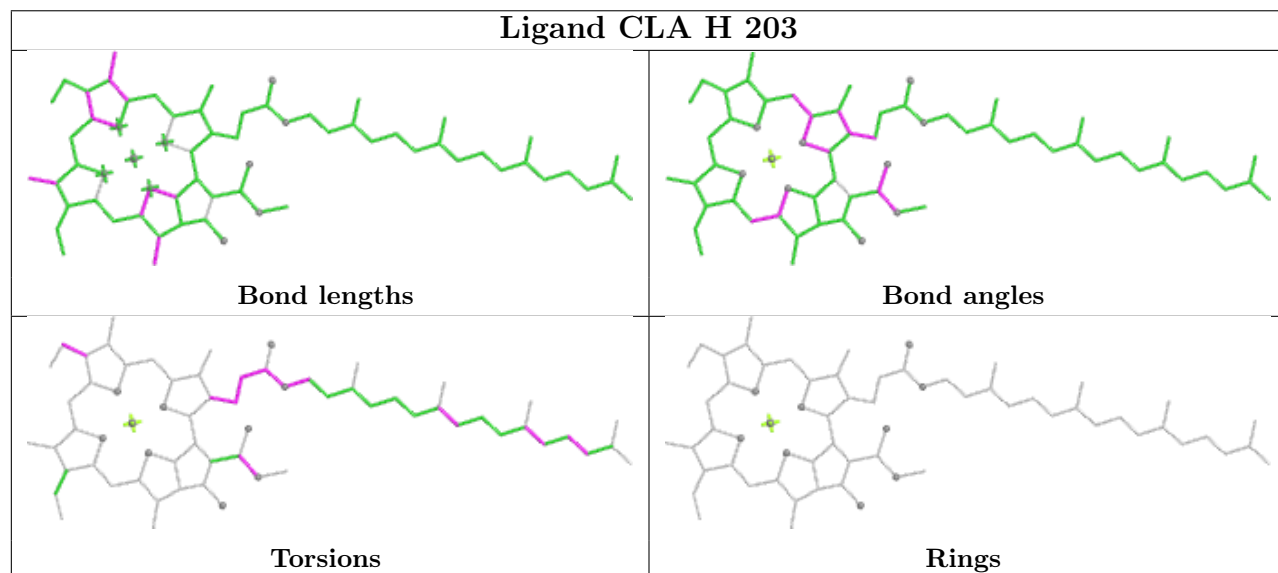


Rings

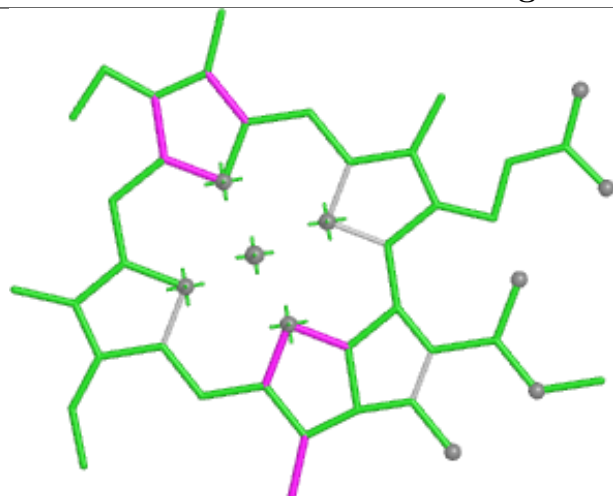


## Ligand CLA 4 603

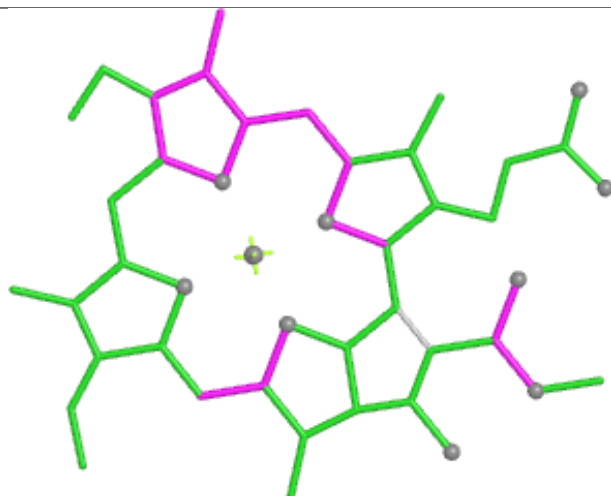




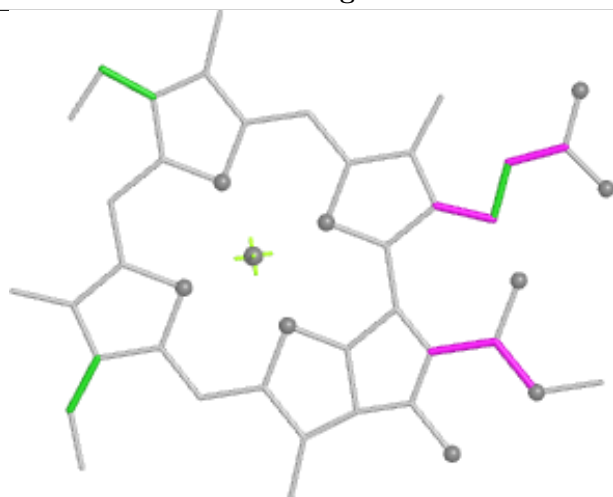
## Ligand CLA a 616



Bond lengths



Bond angles

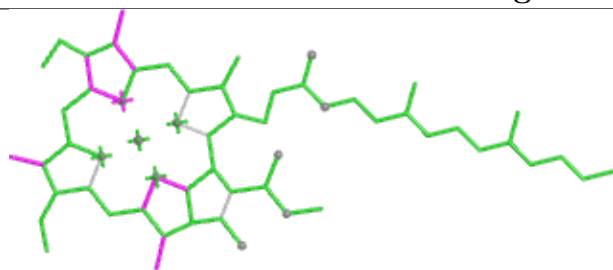


Torsions

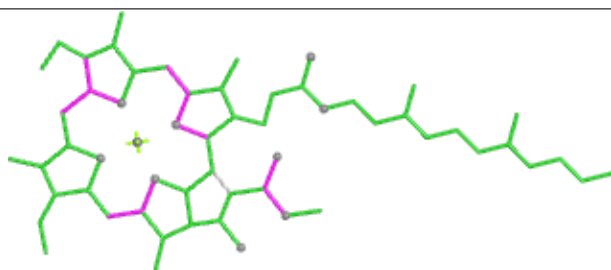


Rings

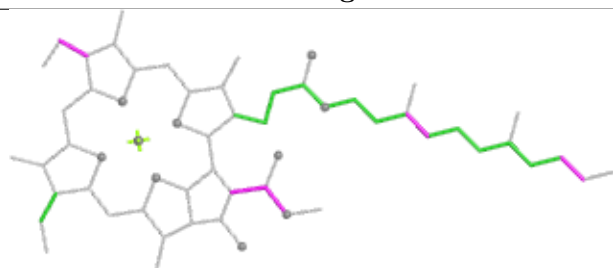
## Ligand CLA A 827



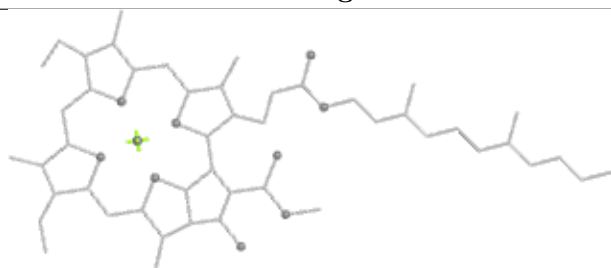
Bond lengths



Bond angles



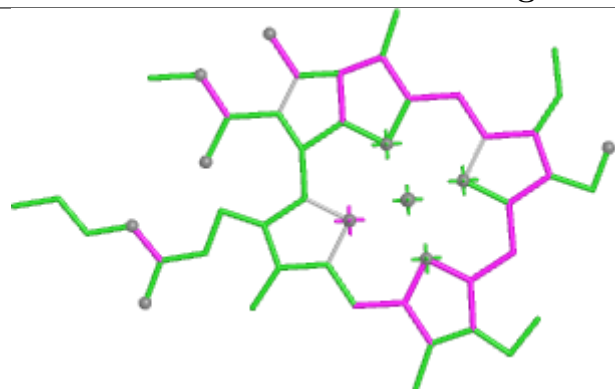
Torsions



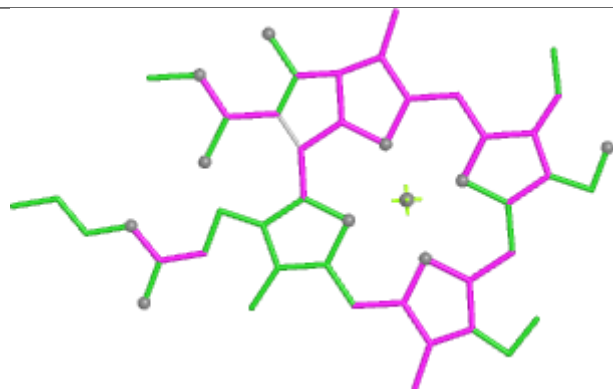
Rings



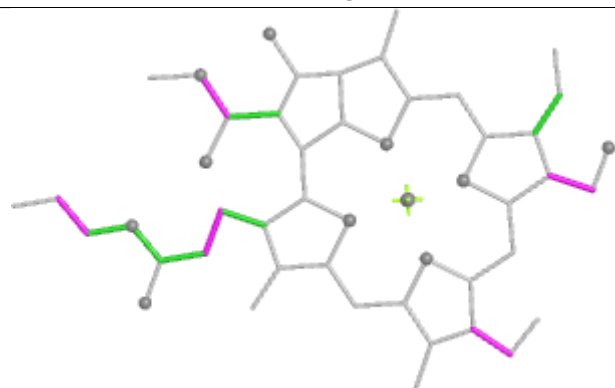
## Ligand CHL Z 608



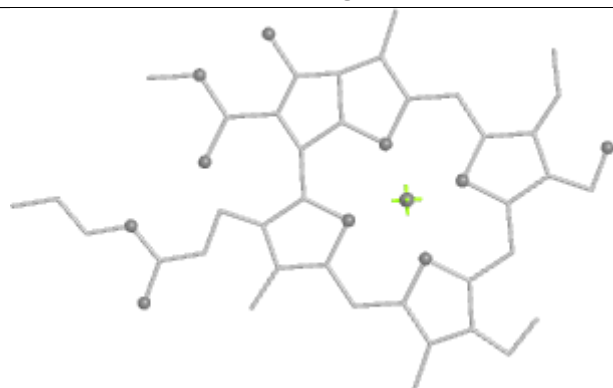
Bond lengths



Bond angles

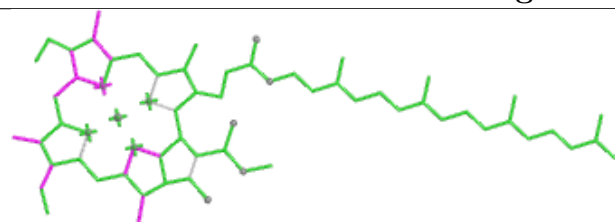


Torsions

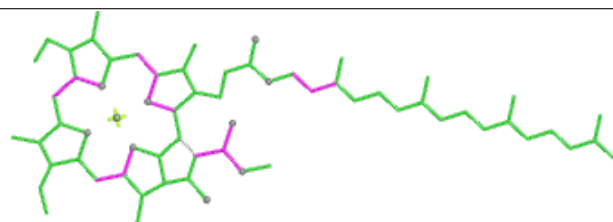


Rings

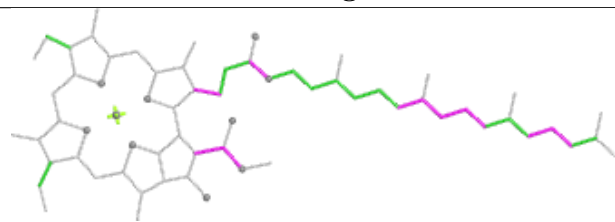
## Ligand CLA A 816



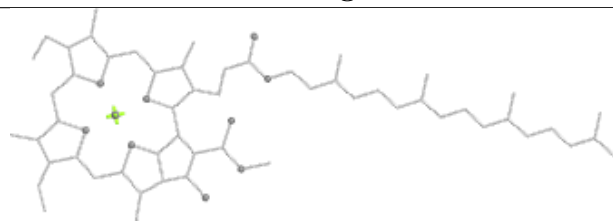
Bond lengths



Bond angles

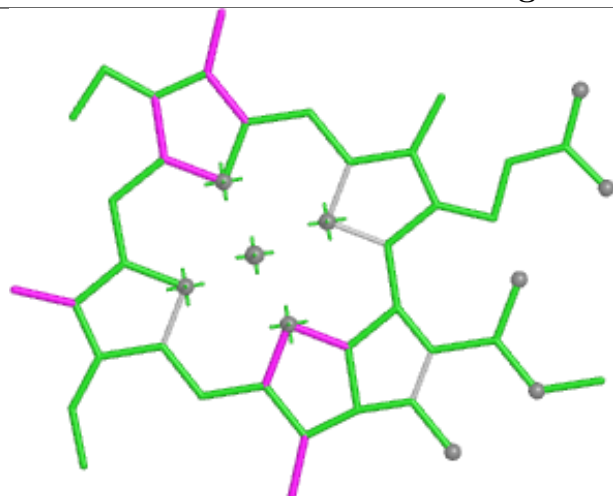


Torsions

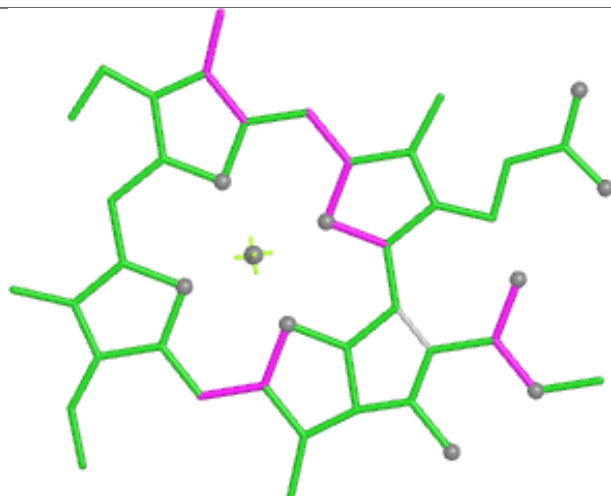


Rings

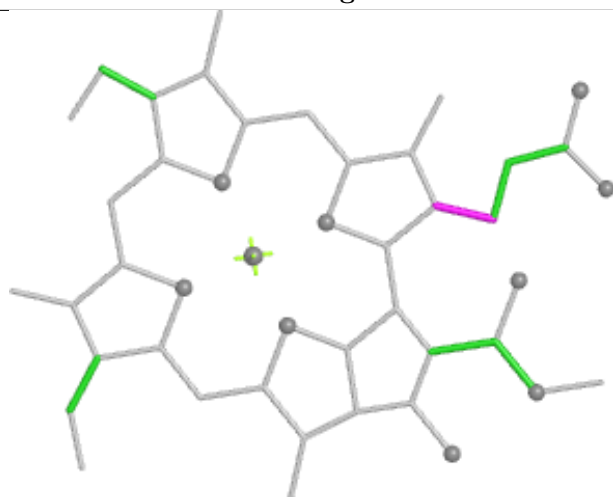
## Ligand CLA 8 609



Bond lengths



Bond angles

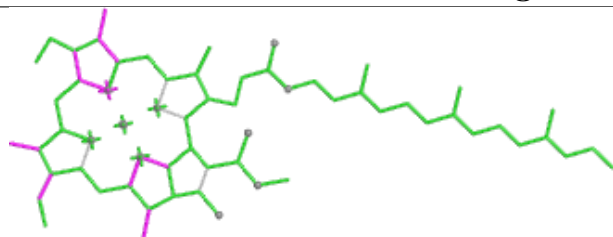


Torsions

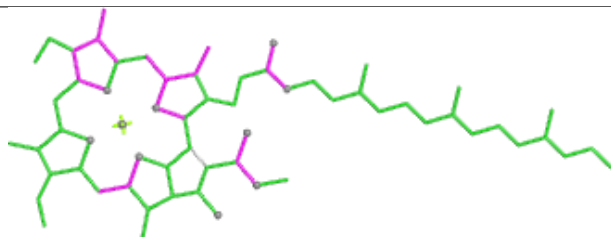


Rings

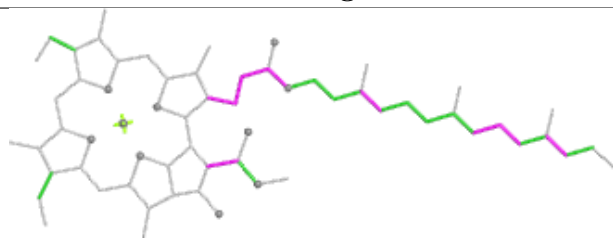
## Ligand CLA B 827



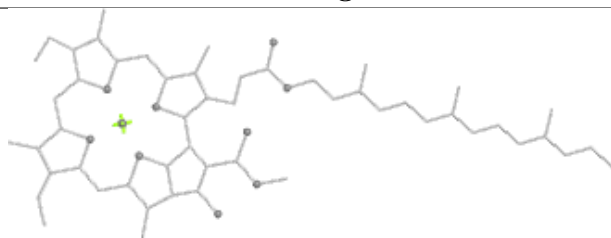
Bond lengths



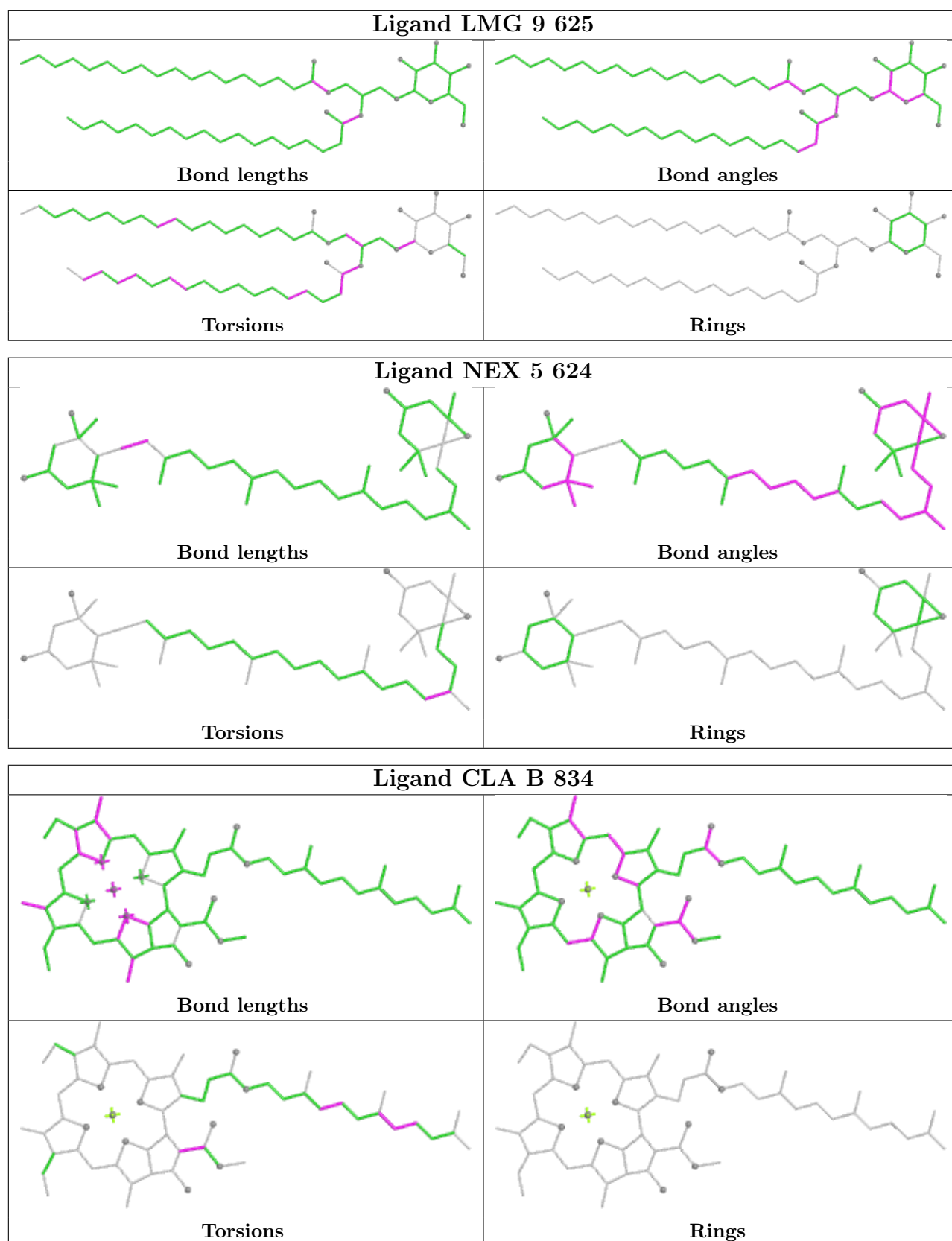
Bond angles

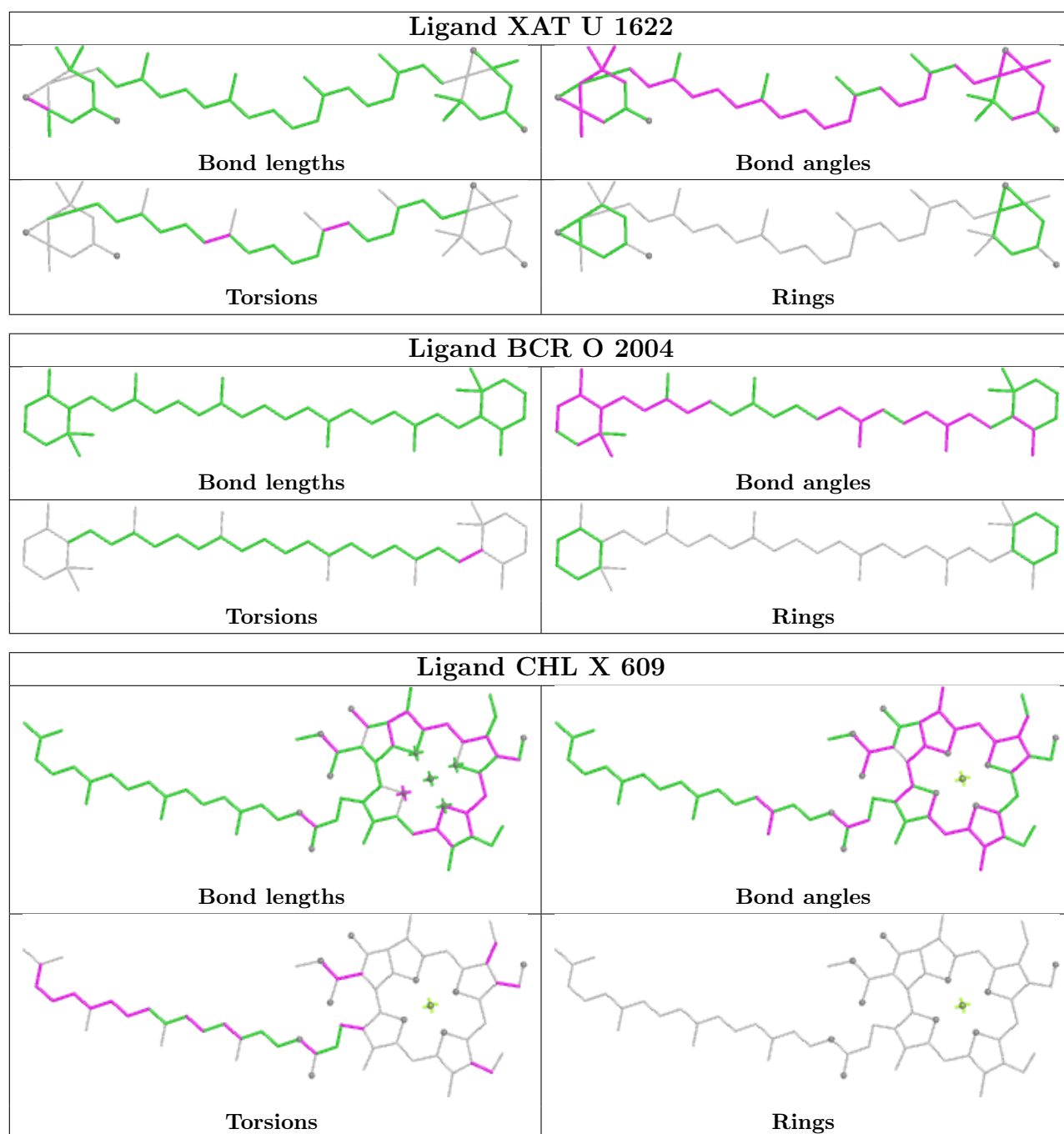


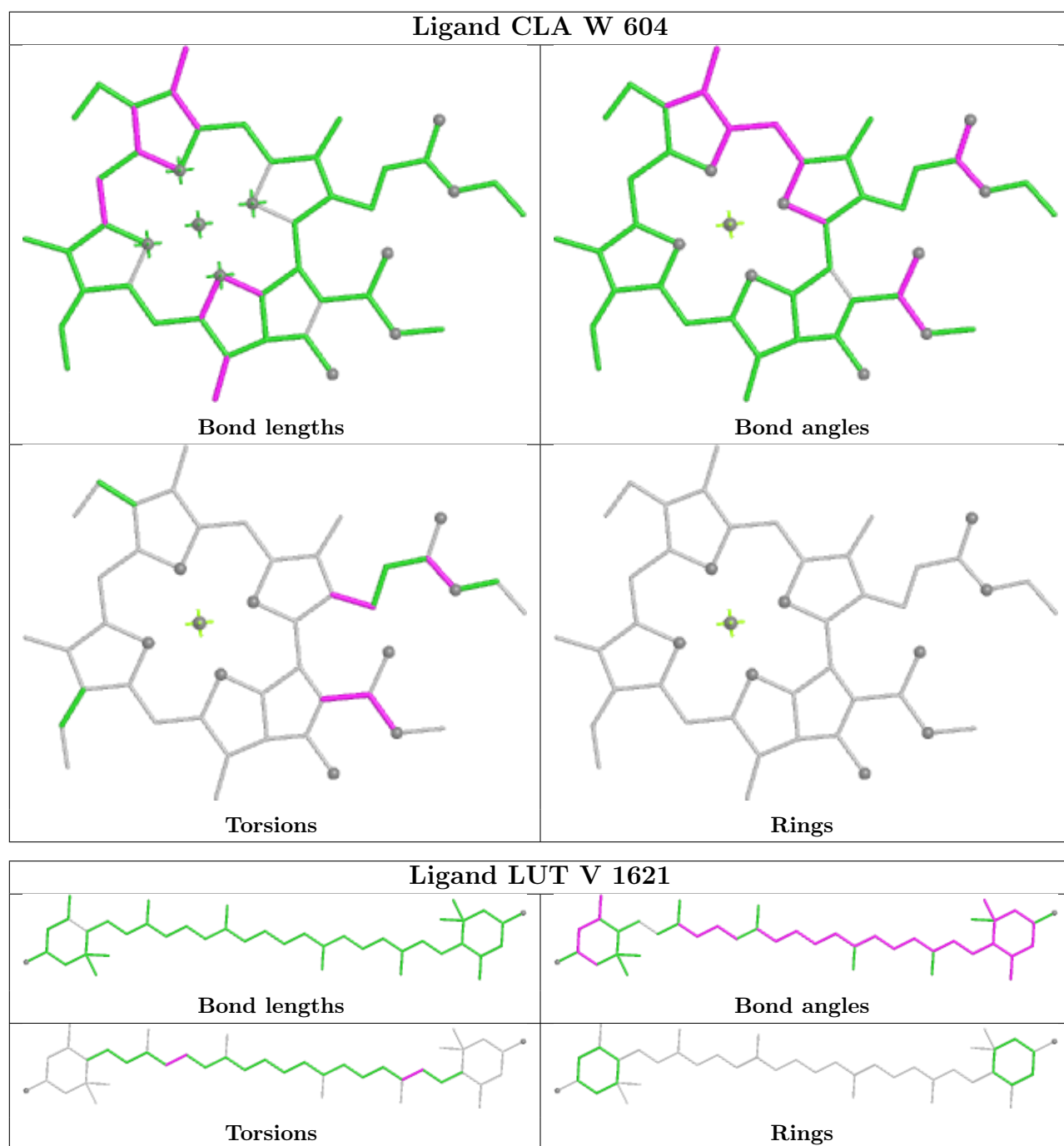
Torsions



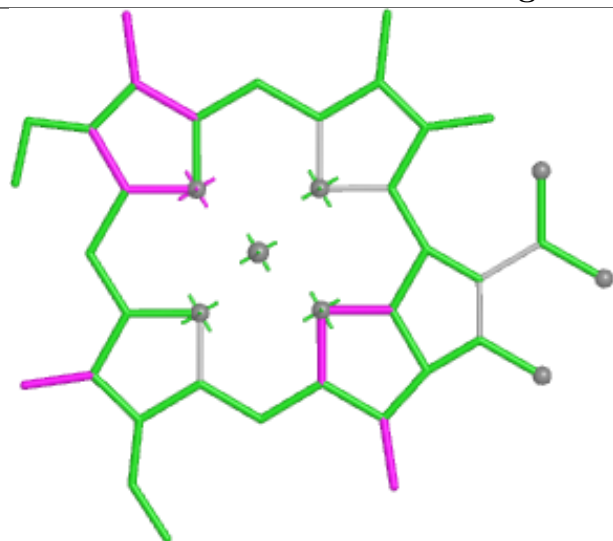
Rings



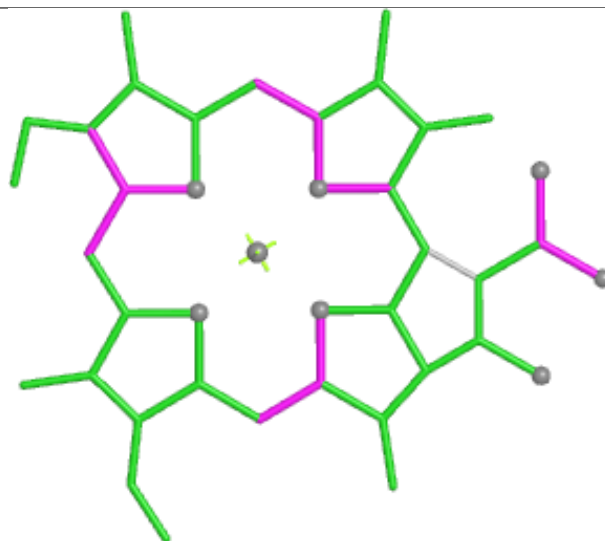




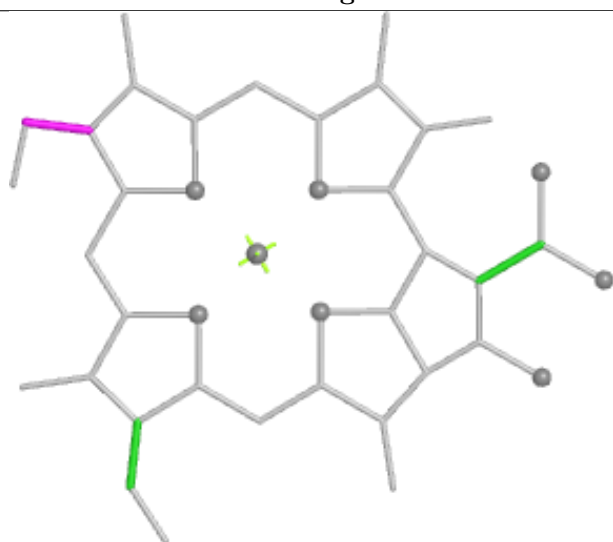
## Ligand CLA 3 617



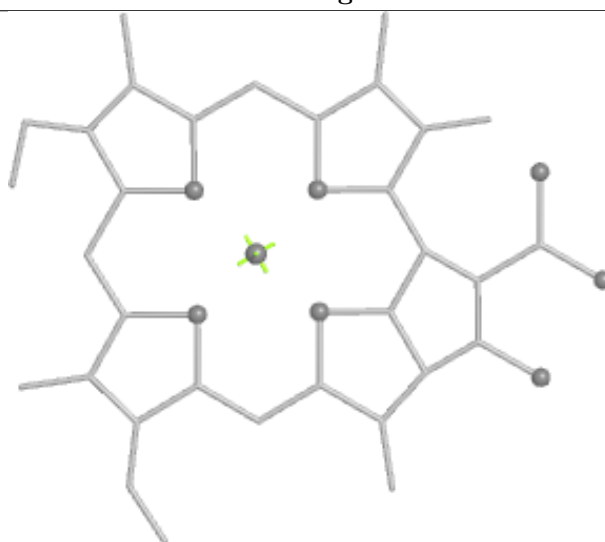
Bond lengths



Bond angles

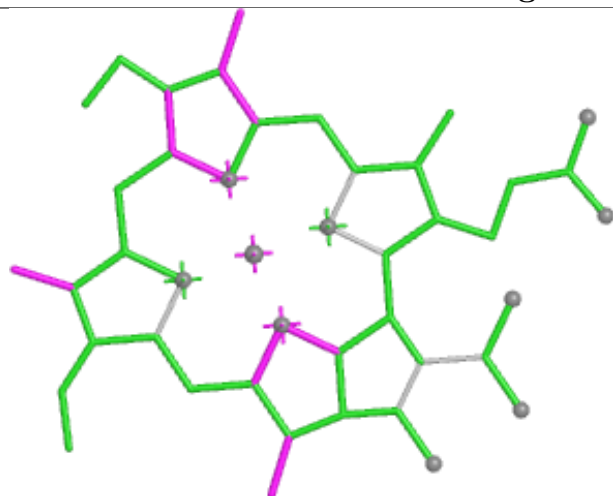


Torsions

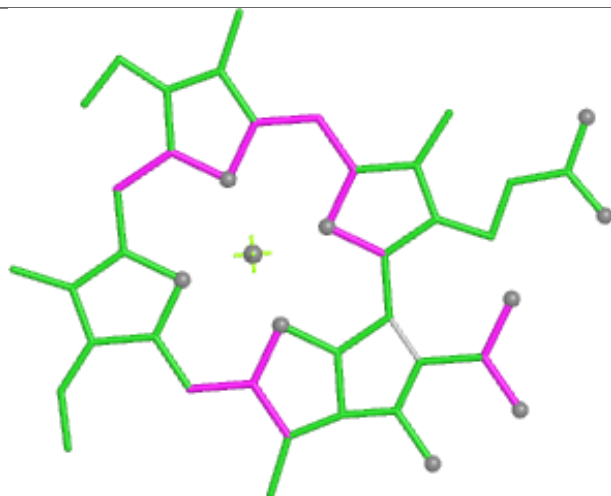


Rings

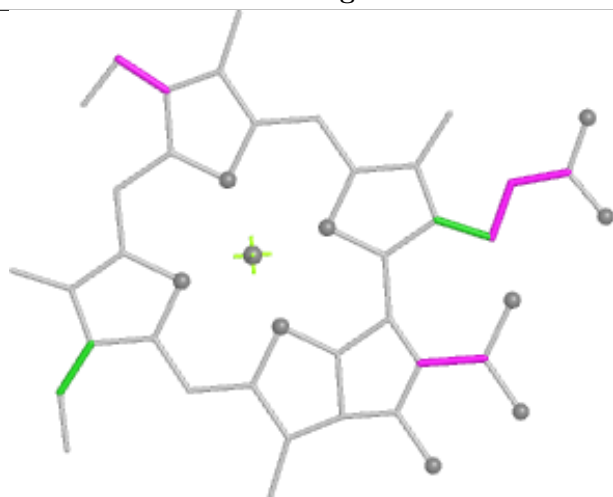
## Ligand CLA 7 603



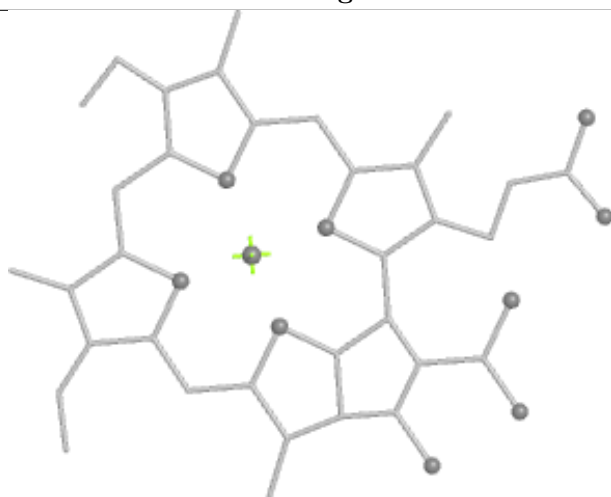
Bond lengths



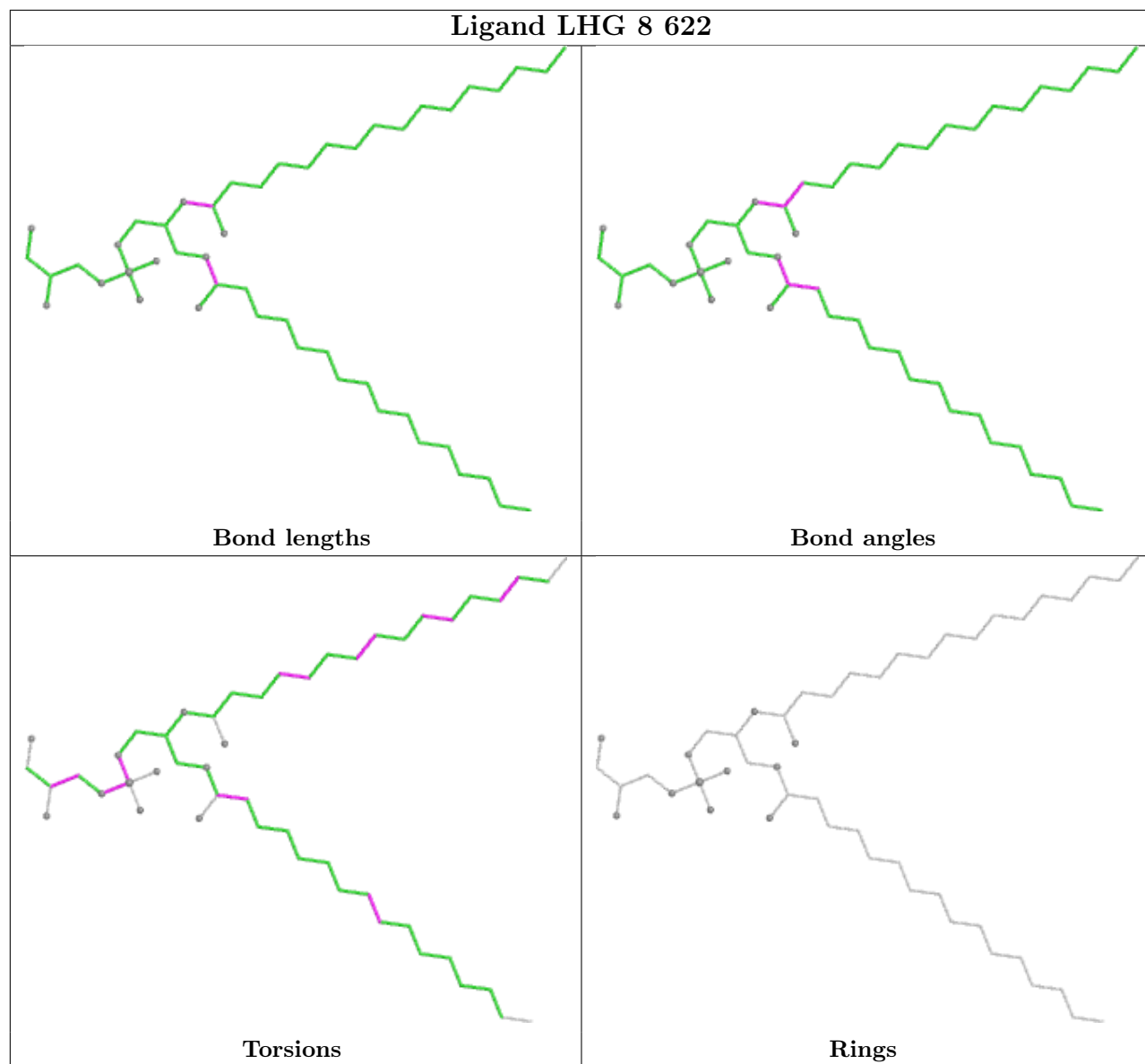
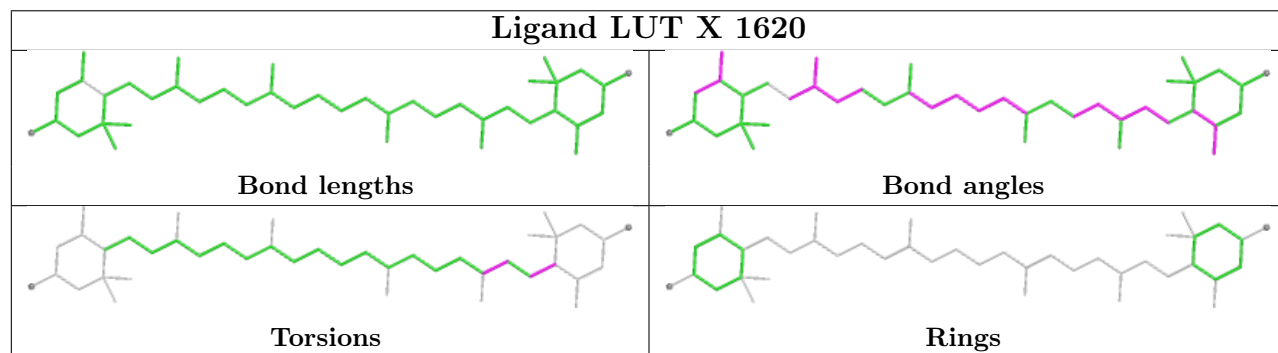
Bond angles



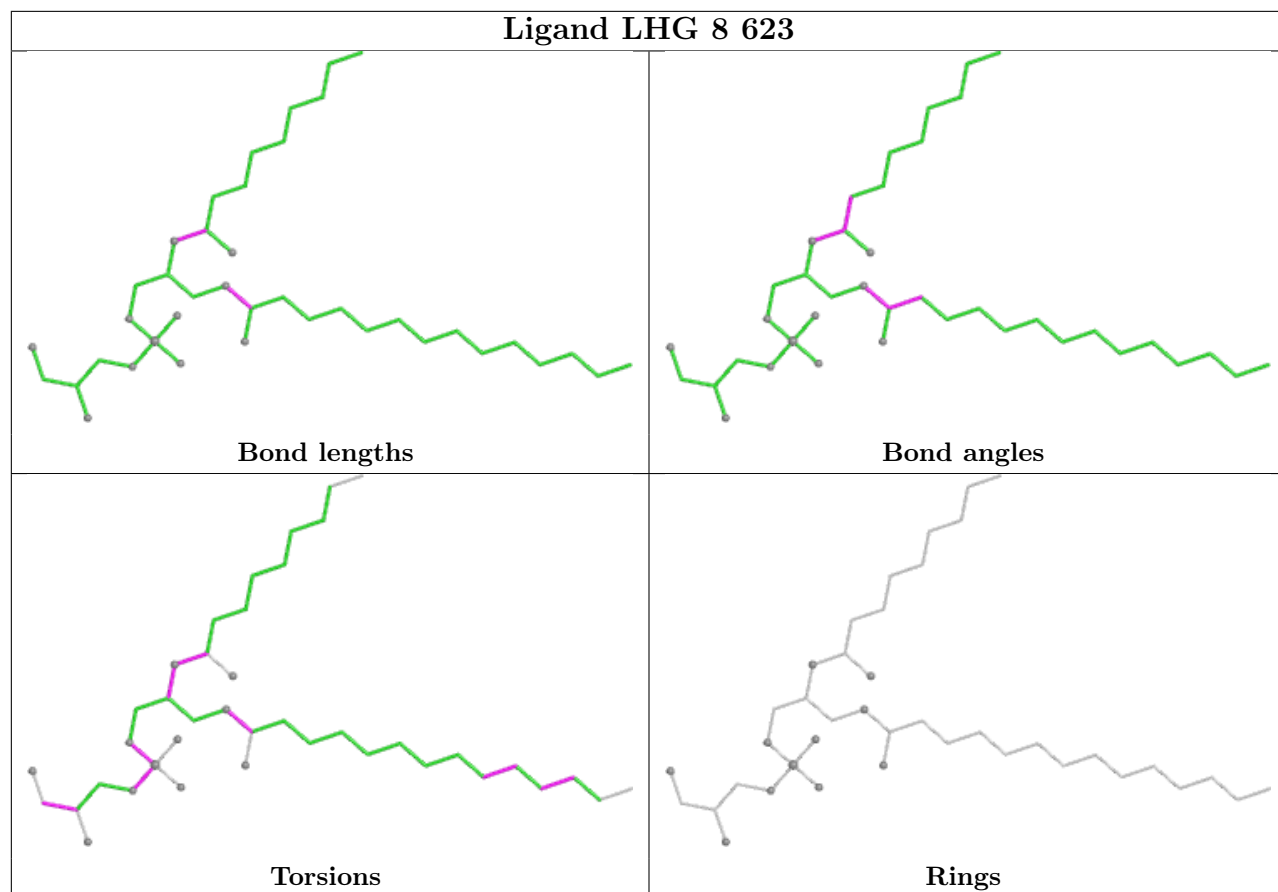
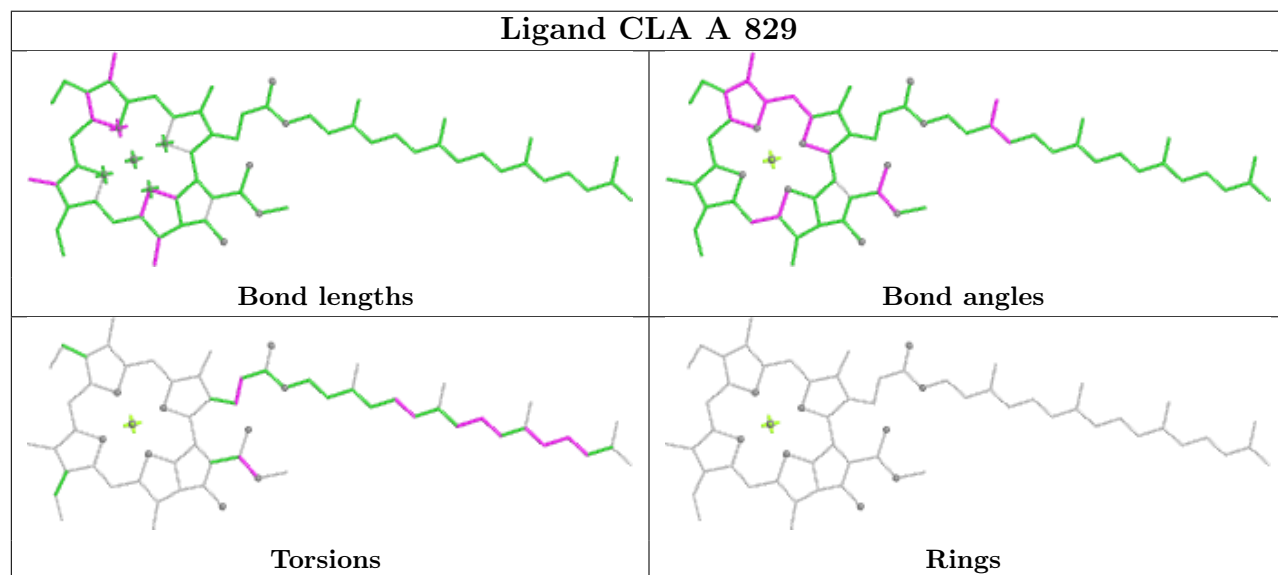
Torsions



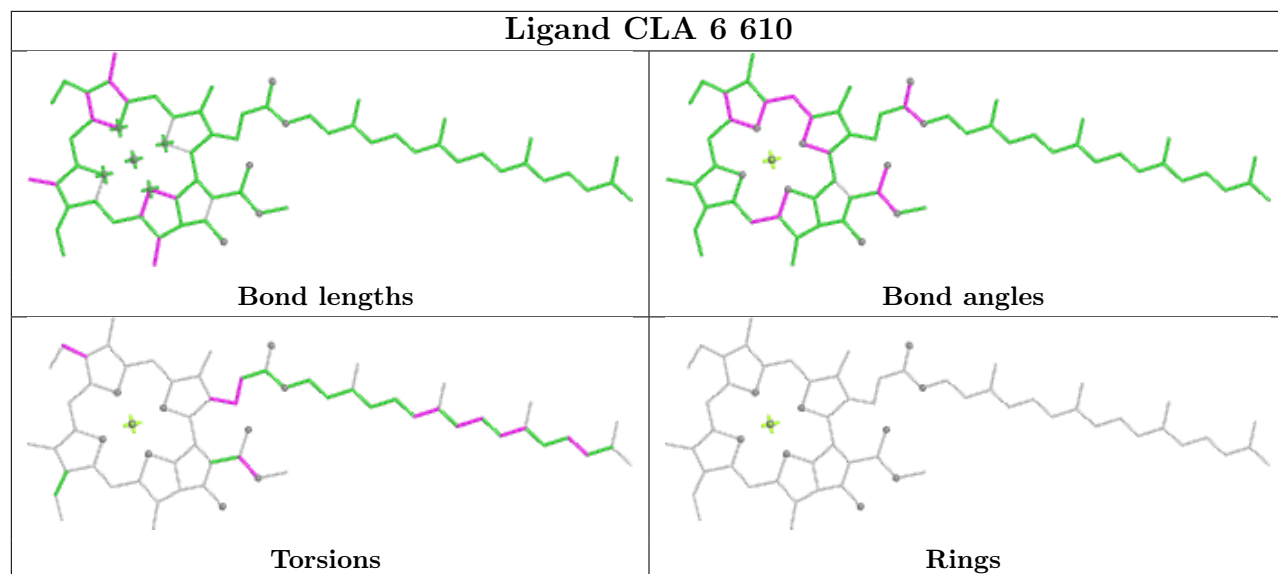
Rings



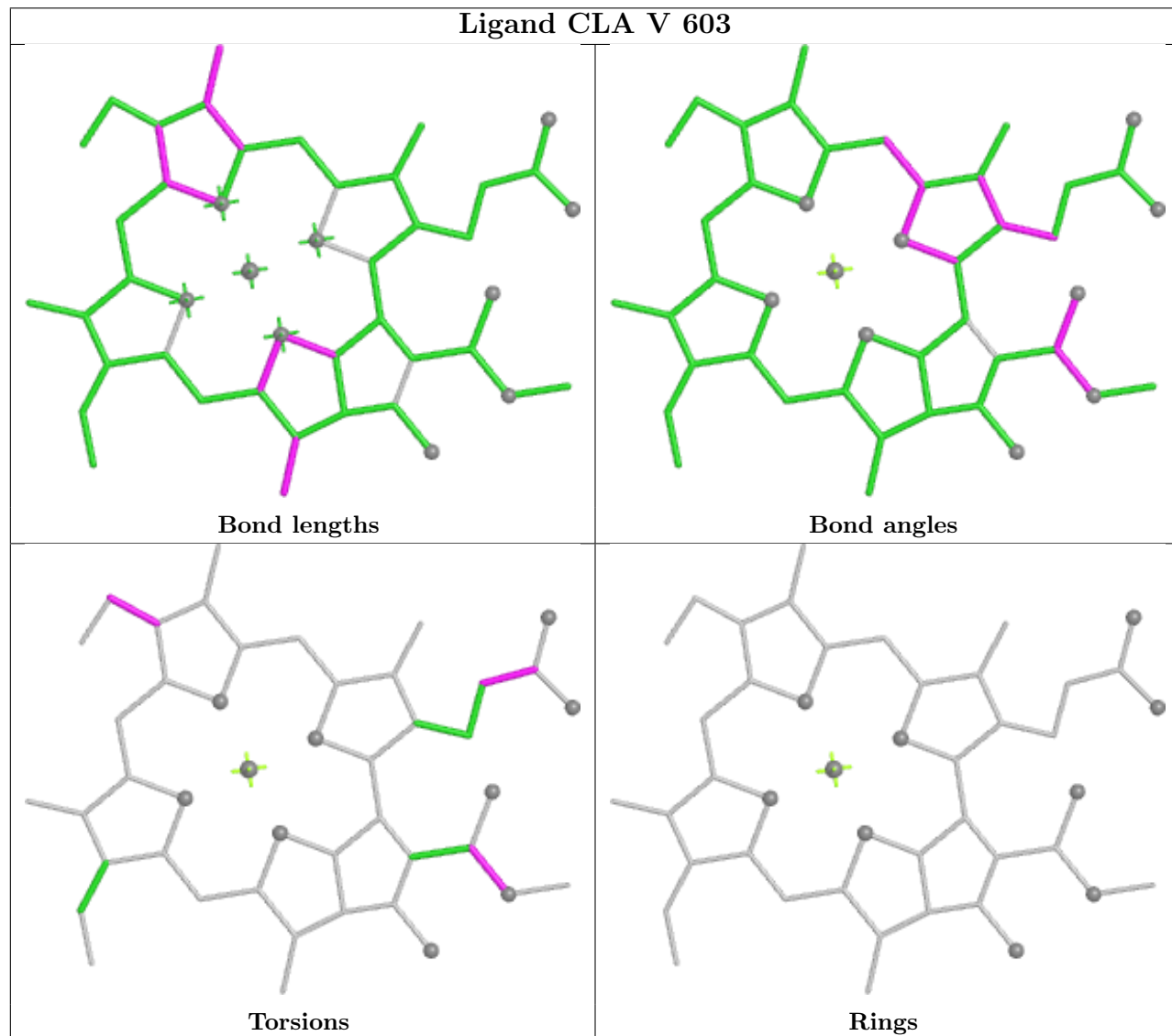




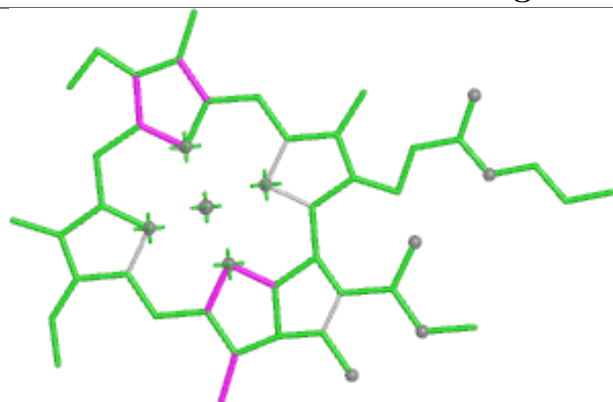
## Ligand CLA 6 610



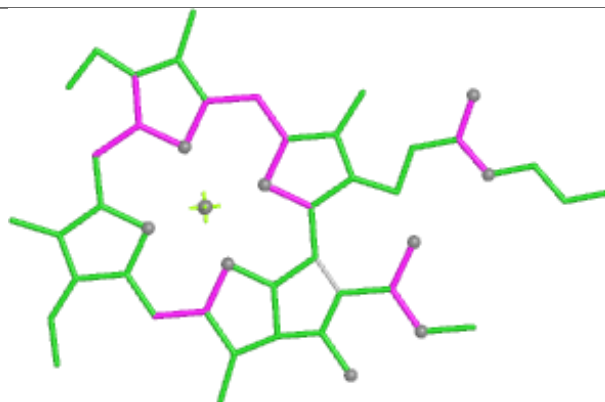
## Ligand CLA V 603



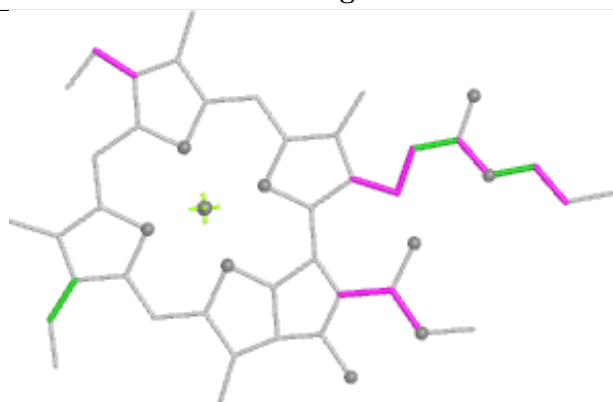
## Ligand CLA Y 614



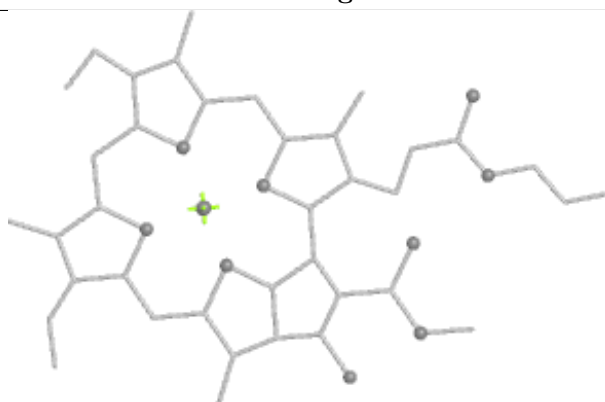
Bond lengths



Bond angles

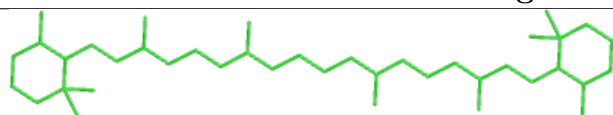


Torsions

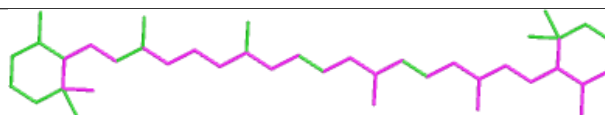


Rings

## Ligand BCR 7 623



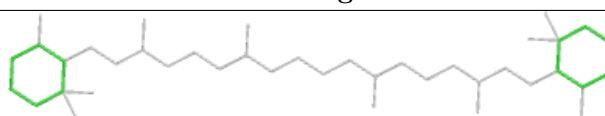
Bond lengths



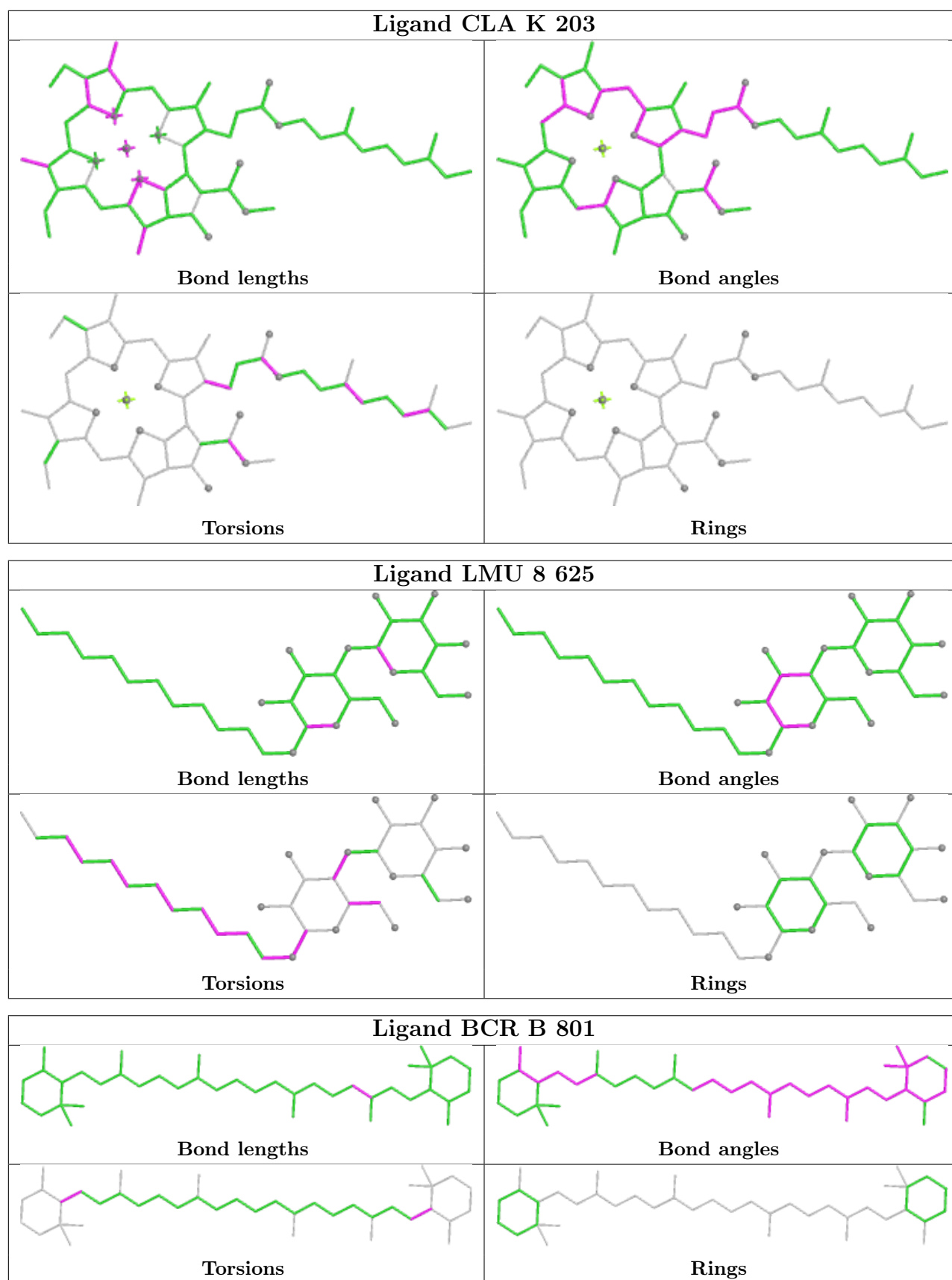
Bond angles

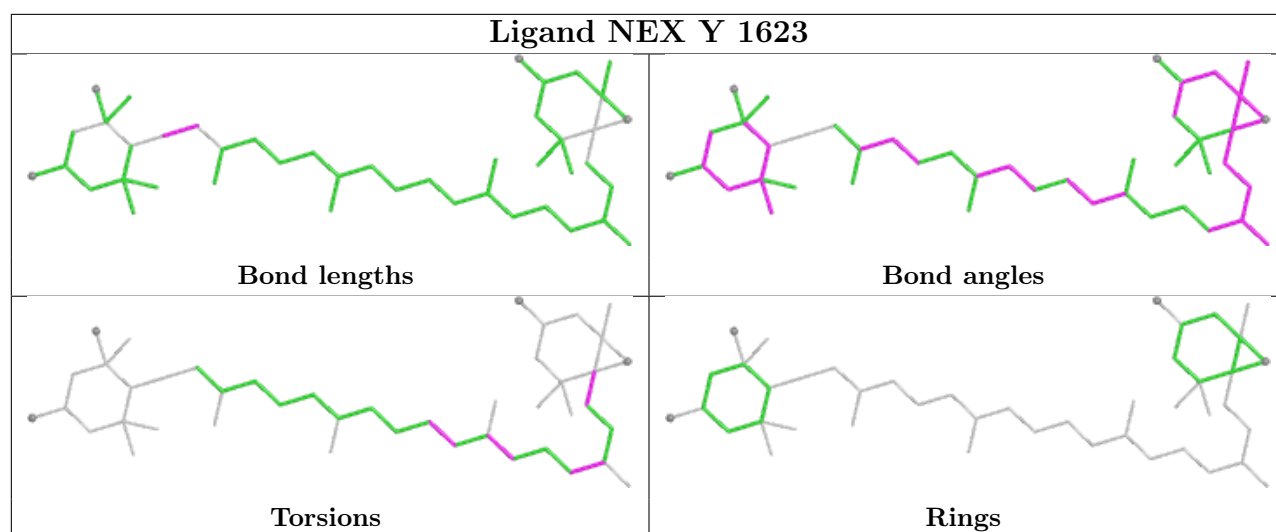
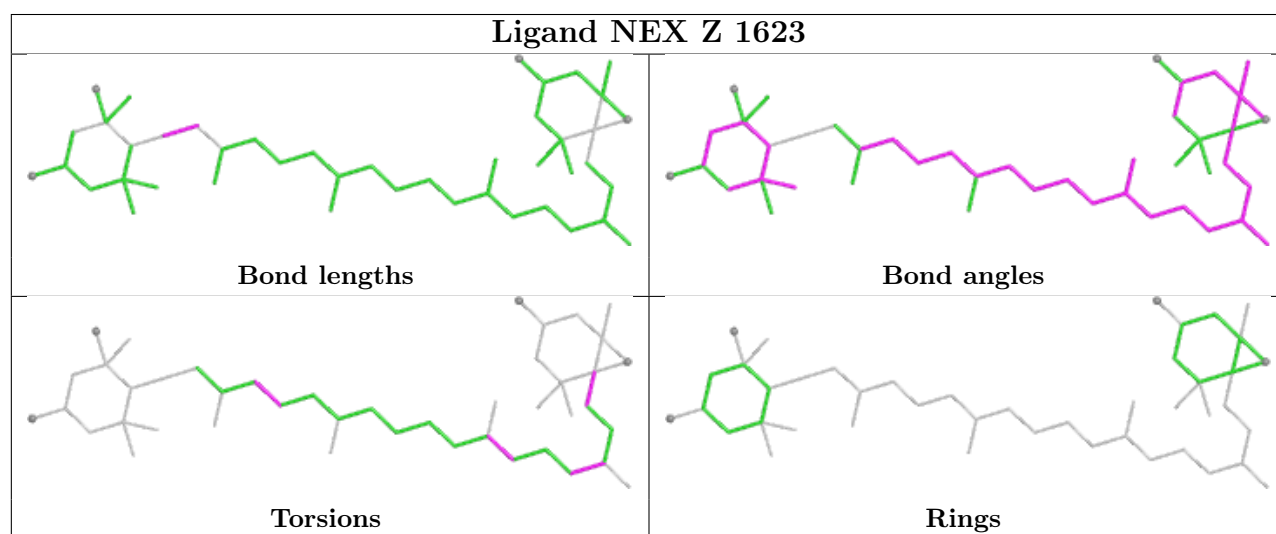
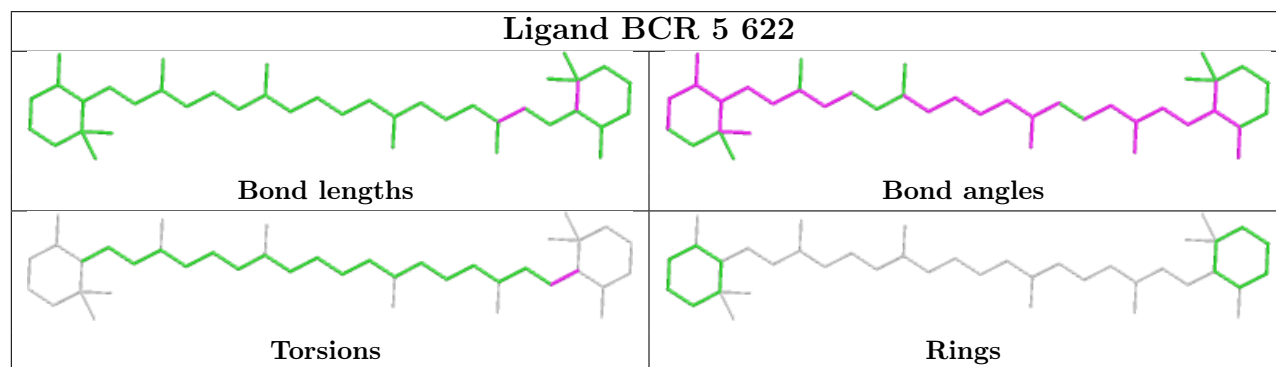


Torsions

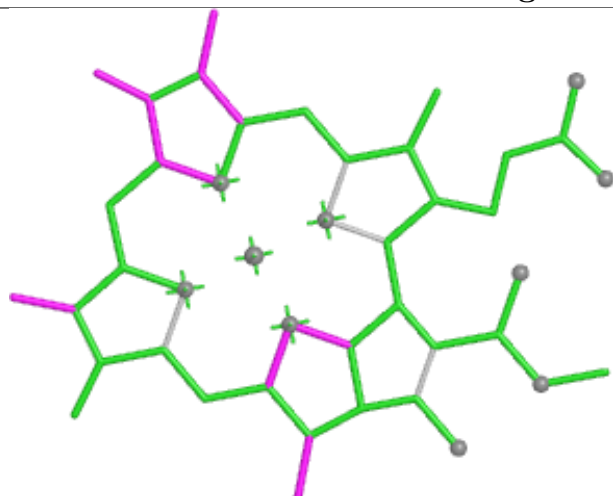


Rings

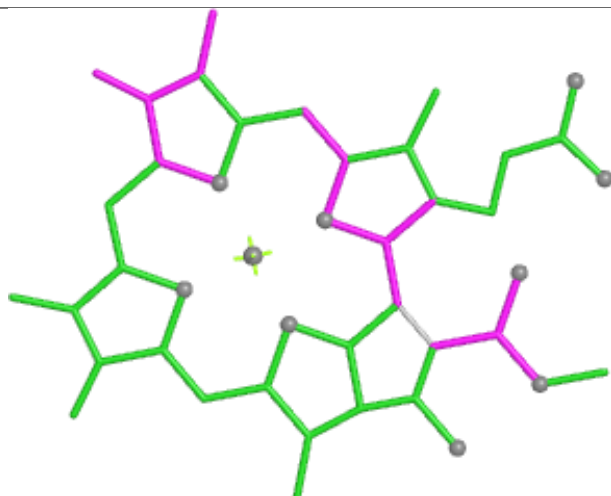




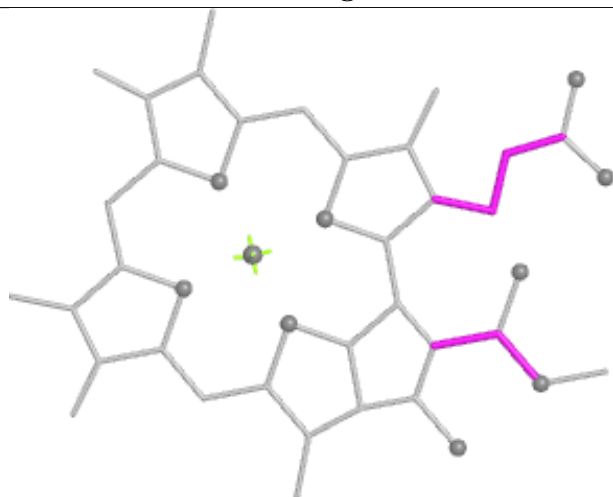
## Ligand CLA 5 619



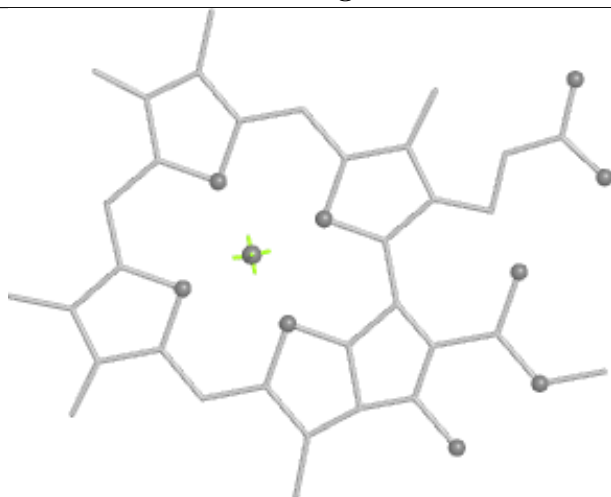
Bond lengths



Bond angles

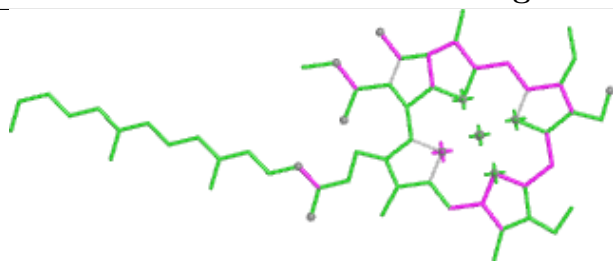


Torsions

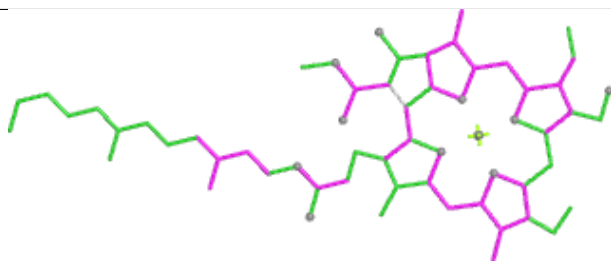


Rings

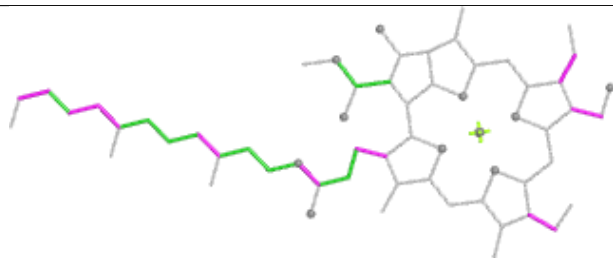
## Ligand CHL U 609



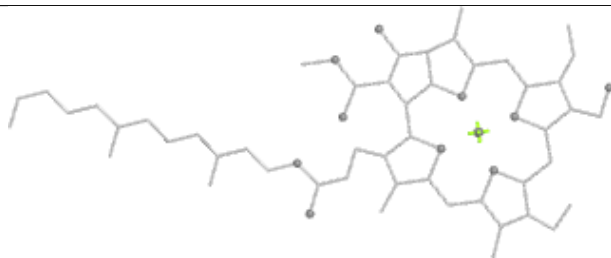
Bond lengths



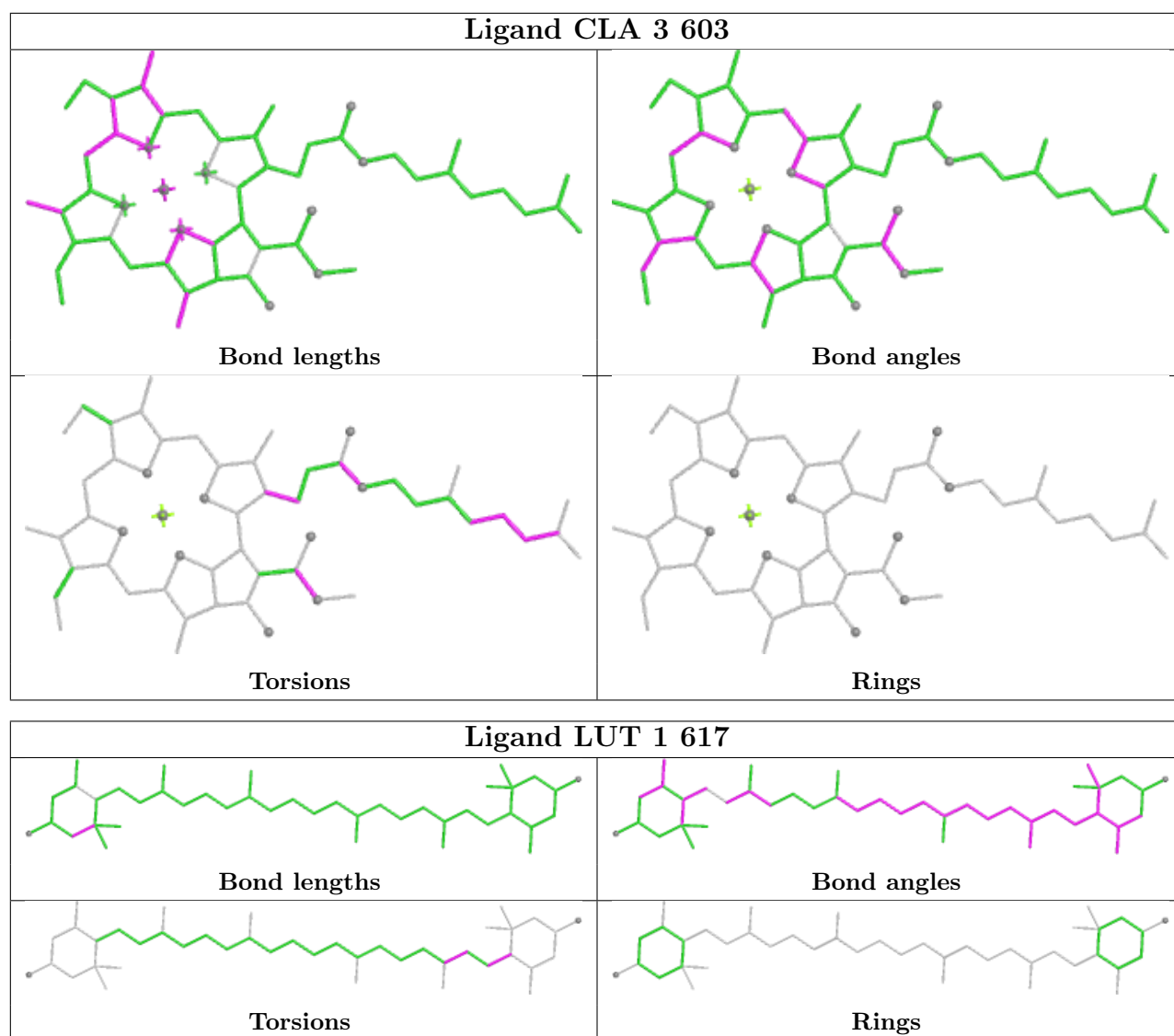
Bond angles

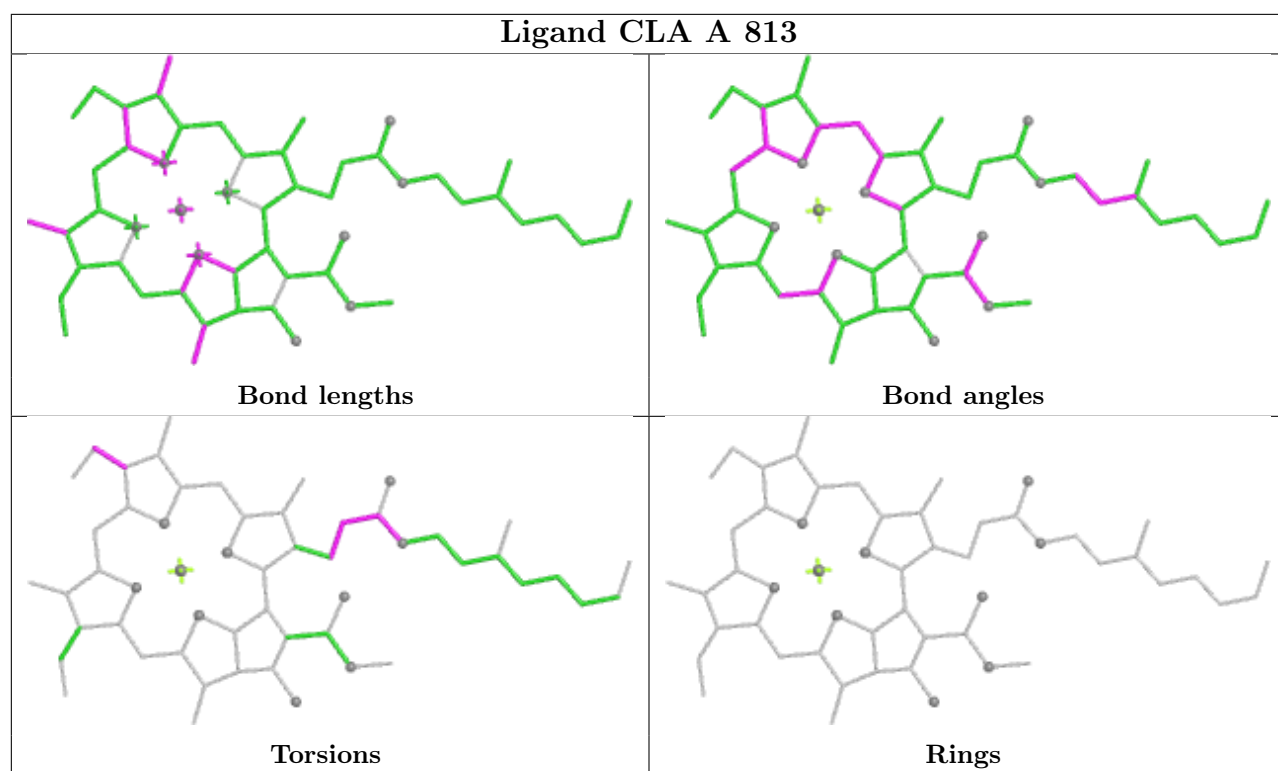


Torsions

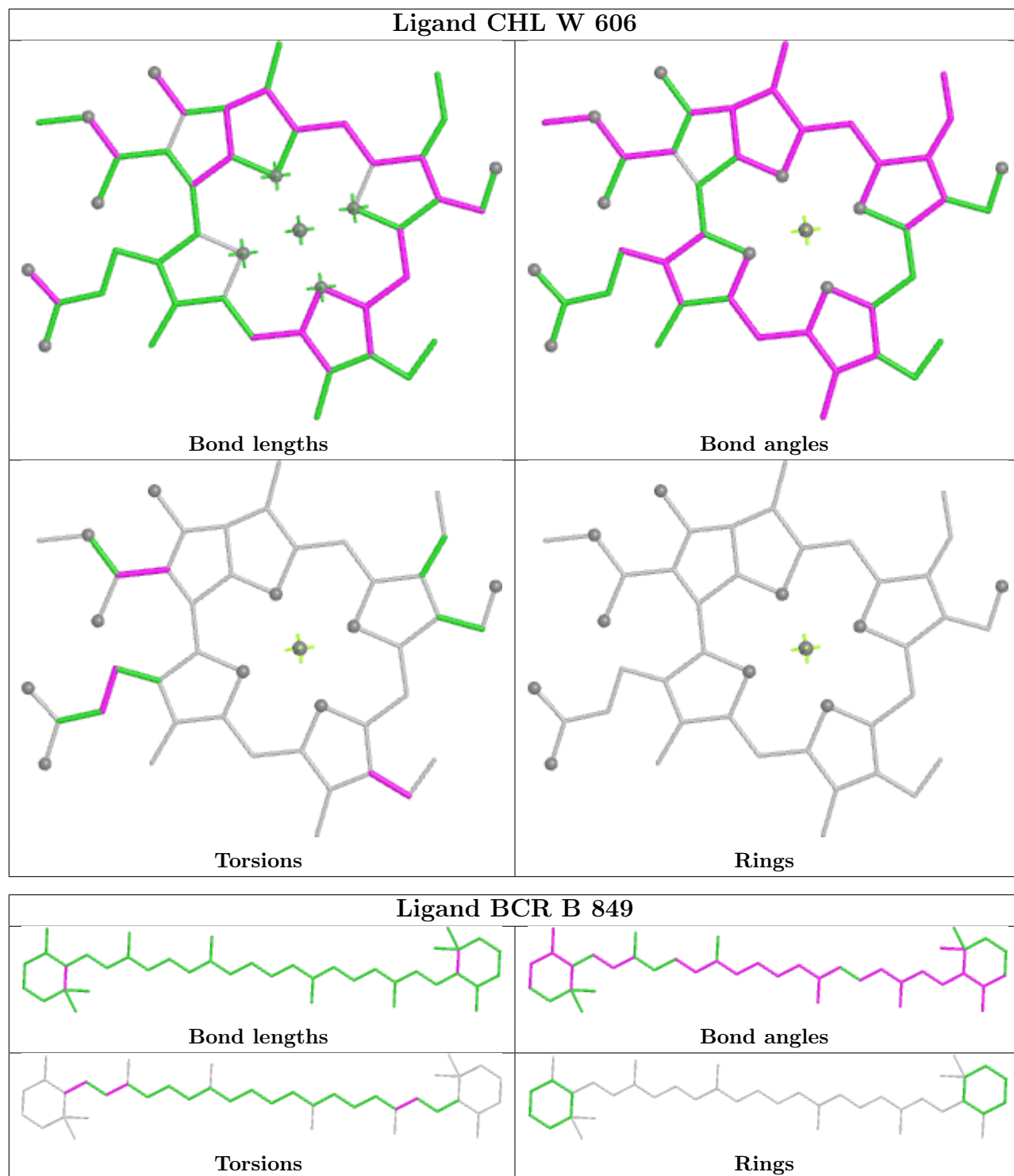


Rings

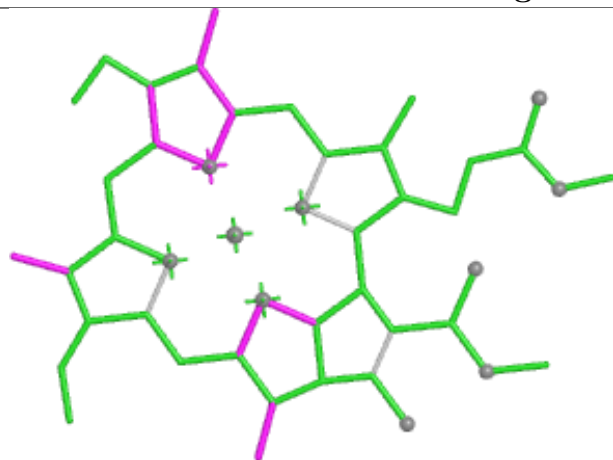




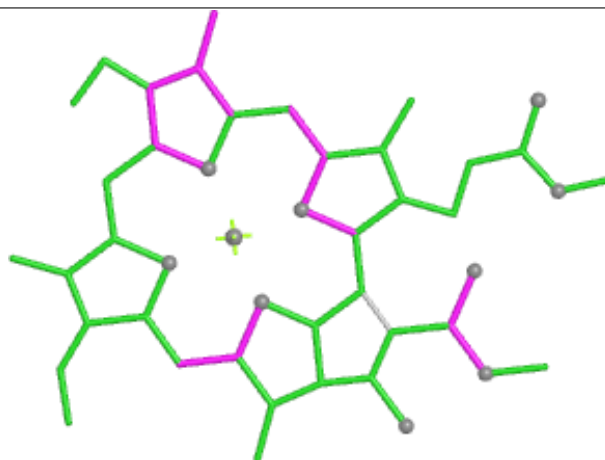




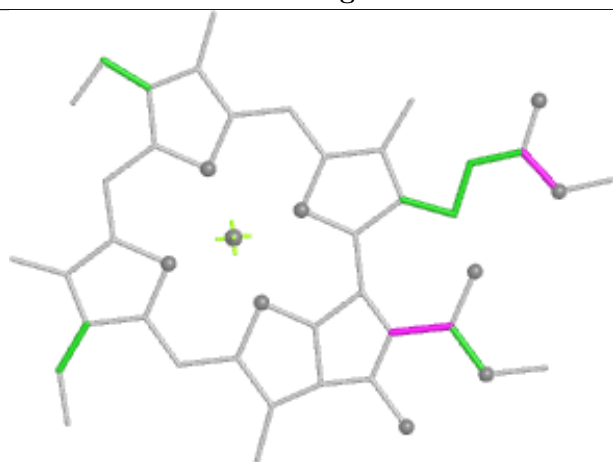
## Ligand CLA B 838



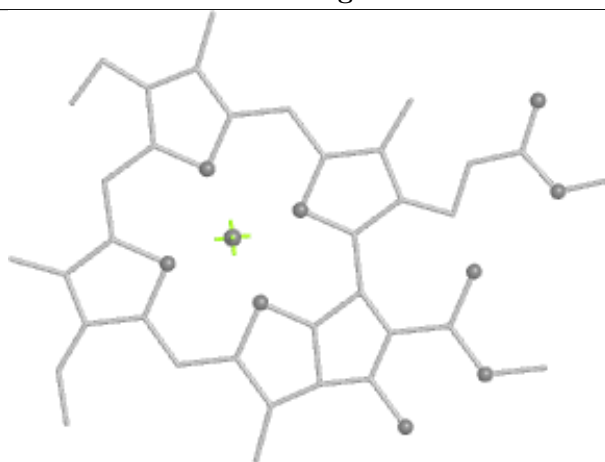
Bond lengths



Bond angles

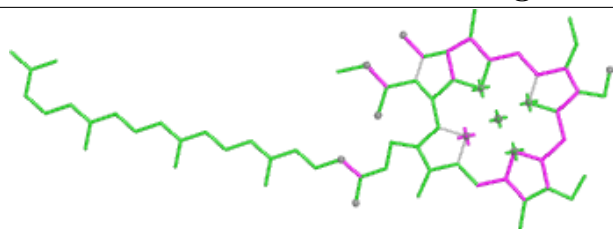


Torsions

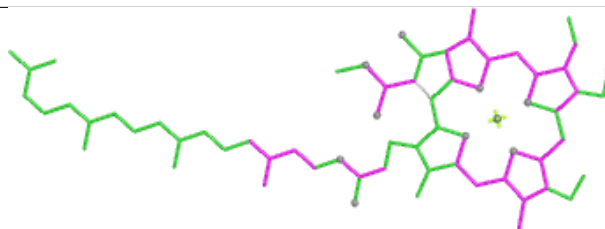


Rings

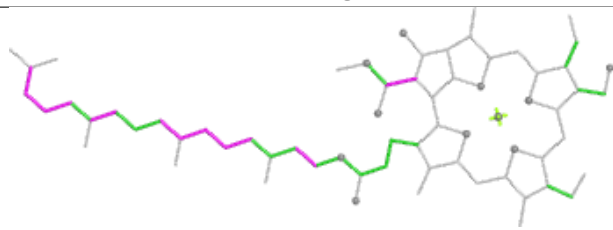
## Ligand CHL V 601



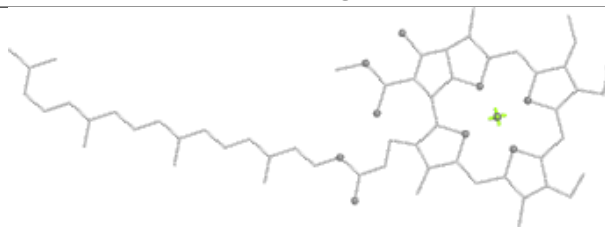
Bond lengths



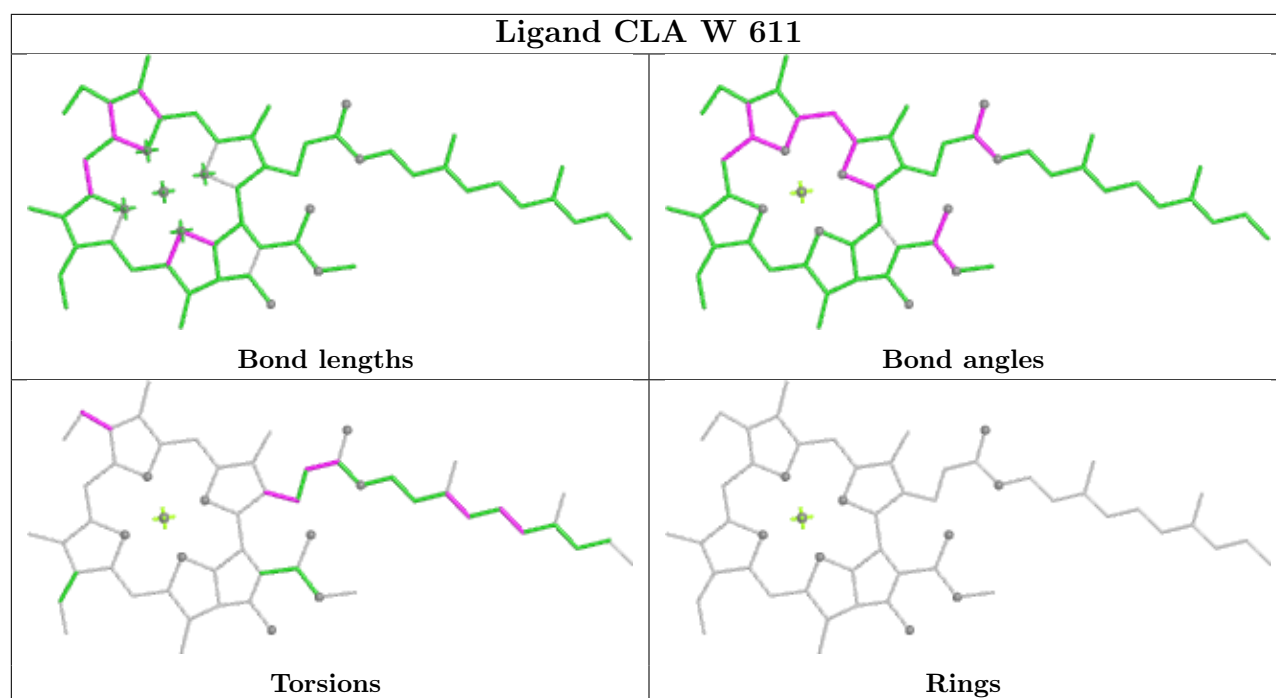
Bond angles

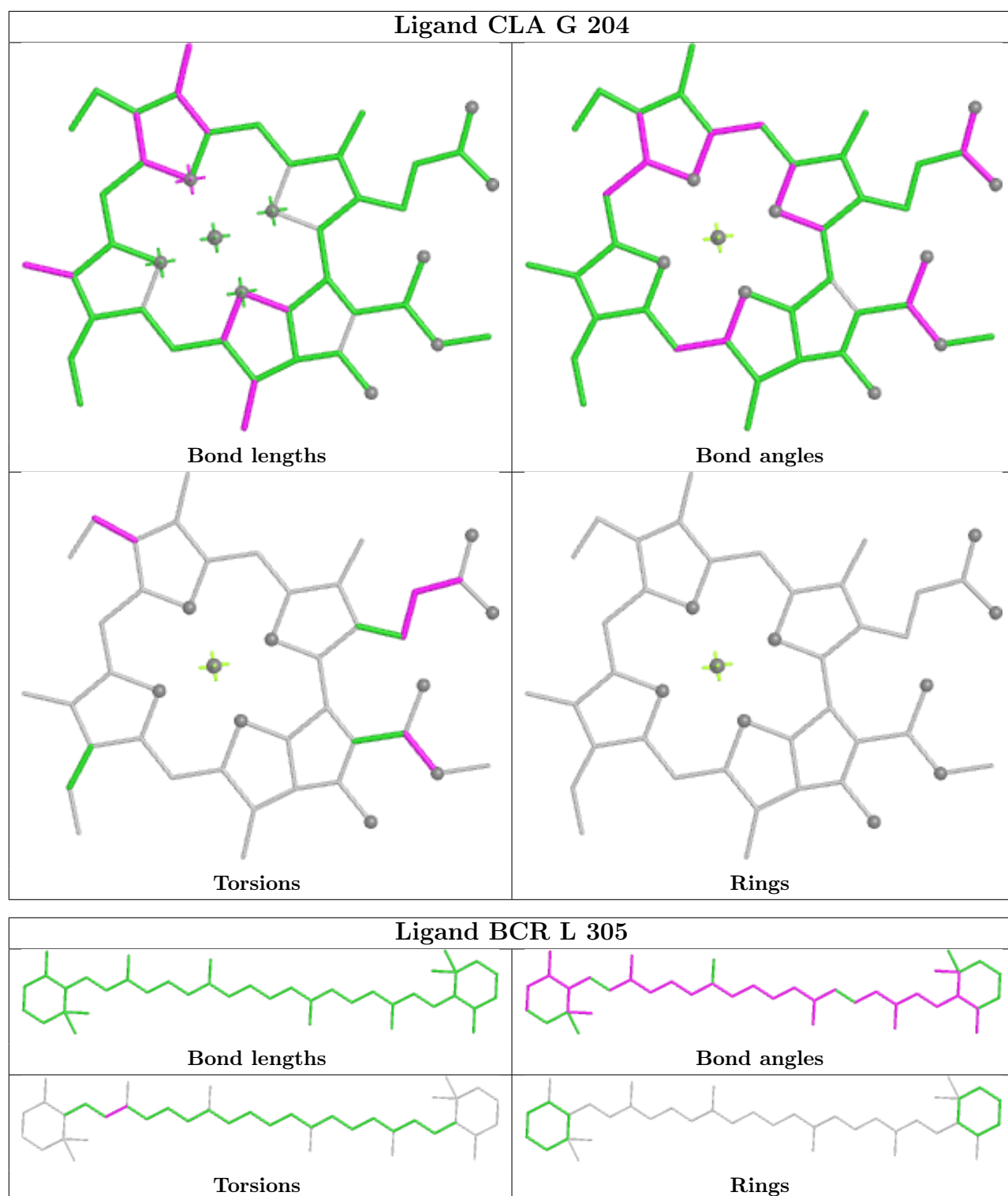


Torsions

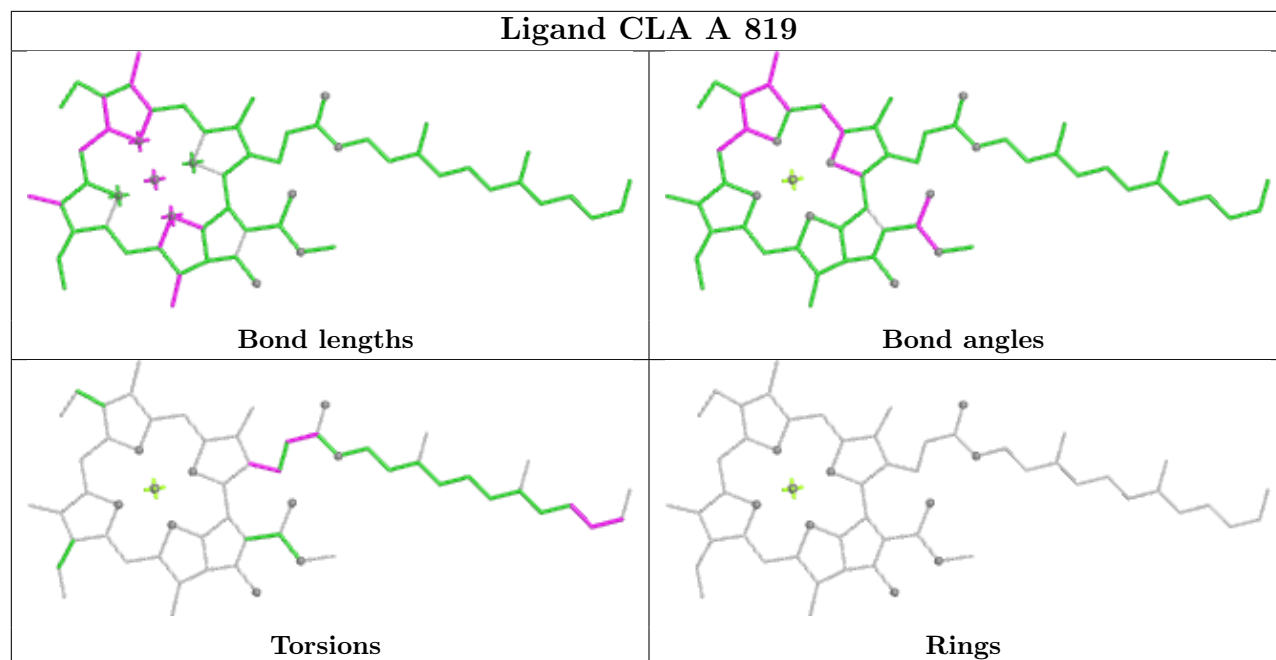


Rings

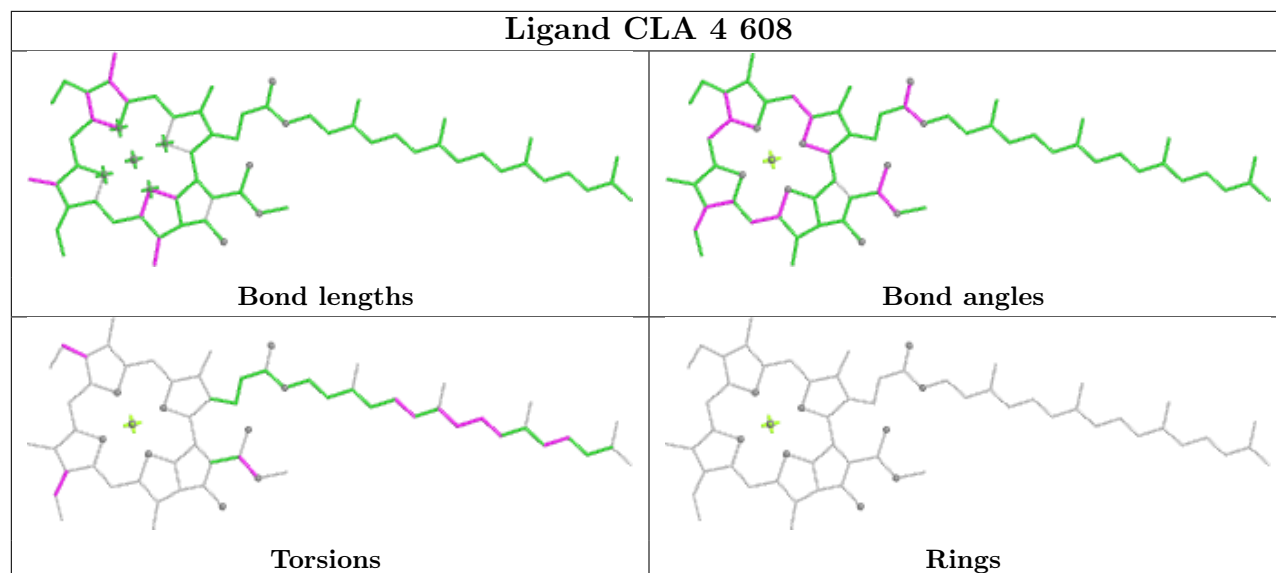


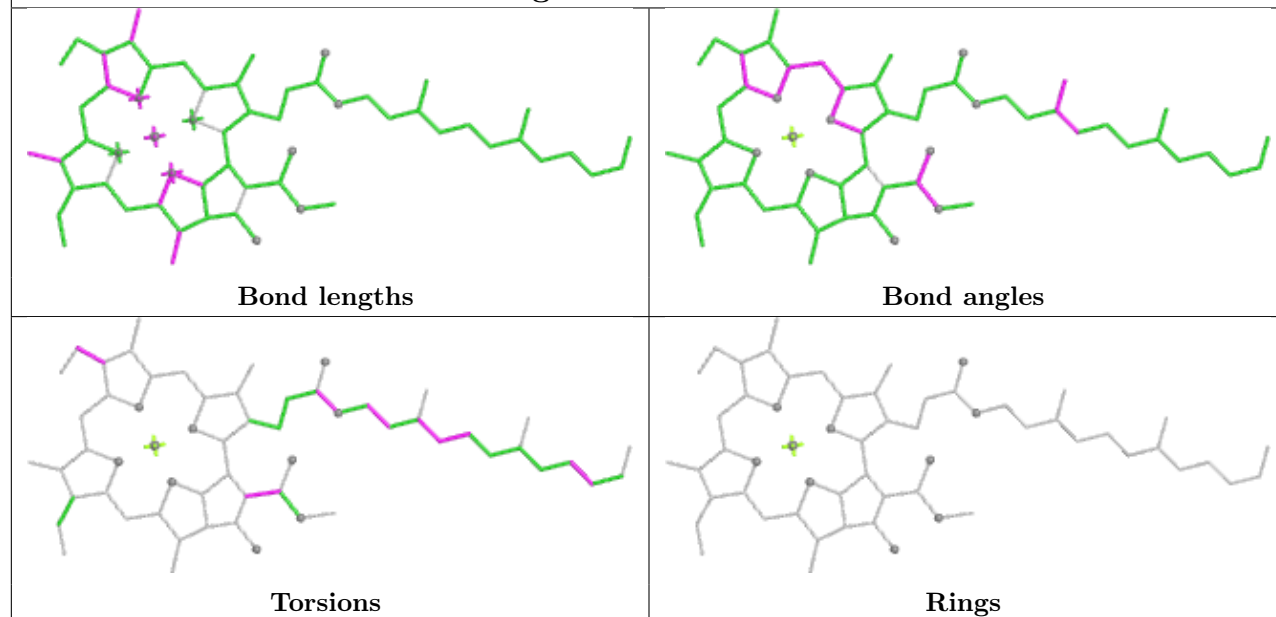
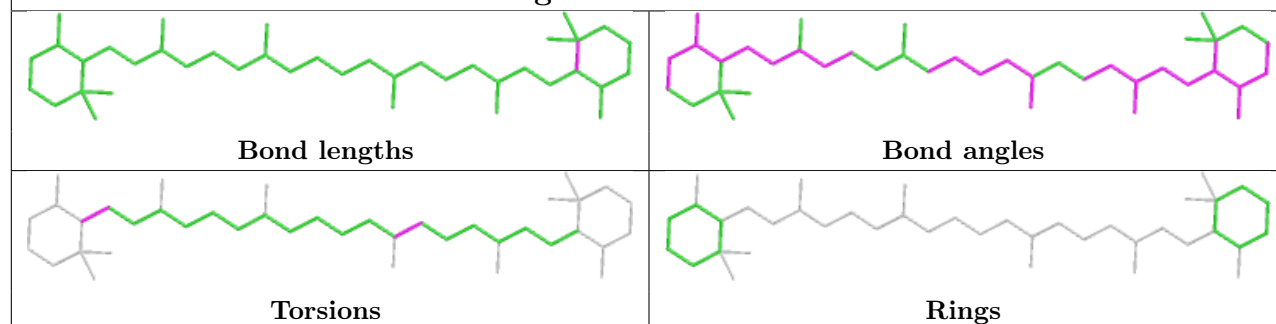
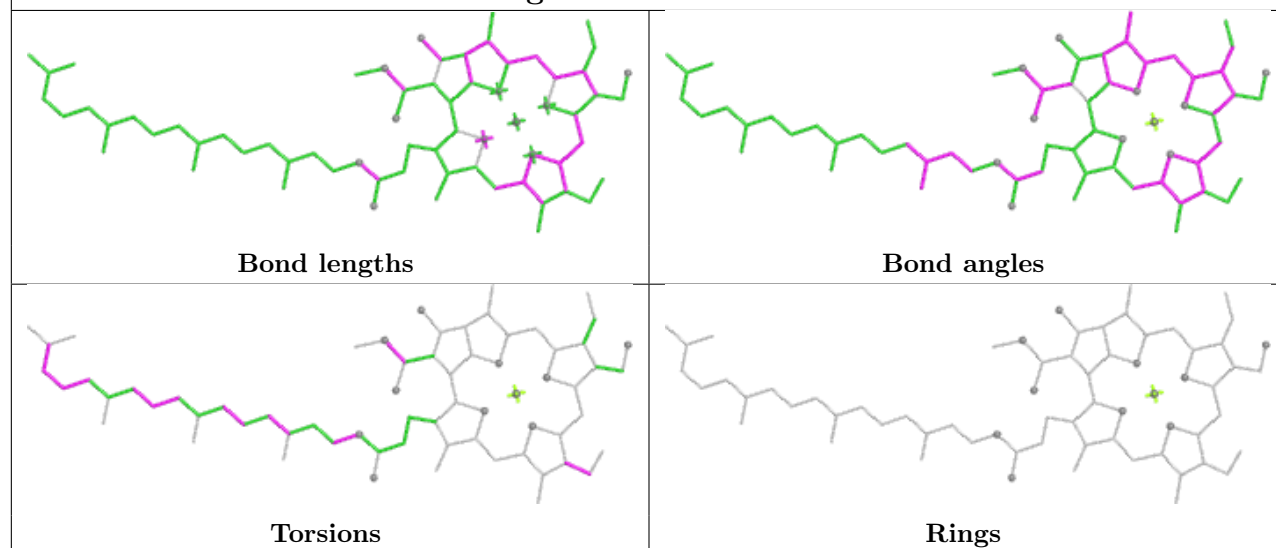


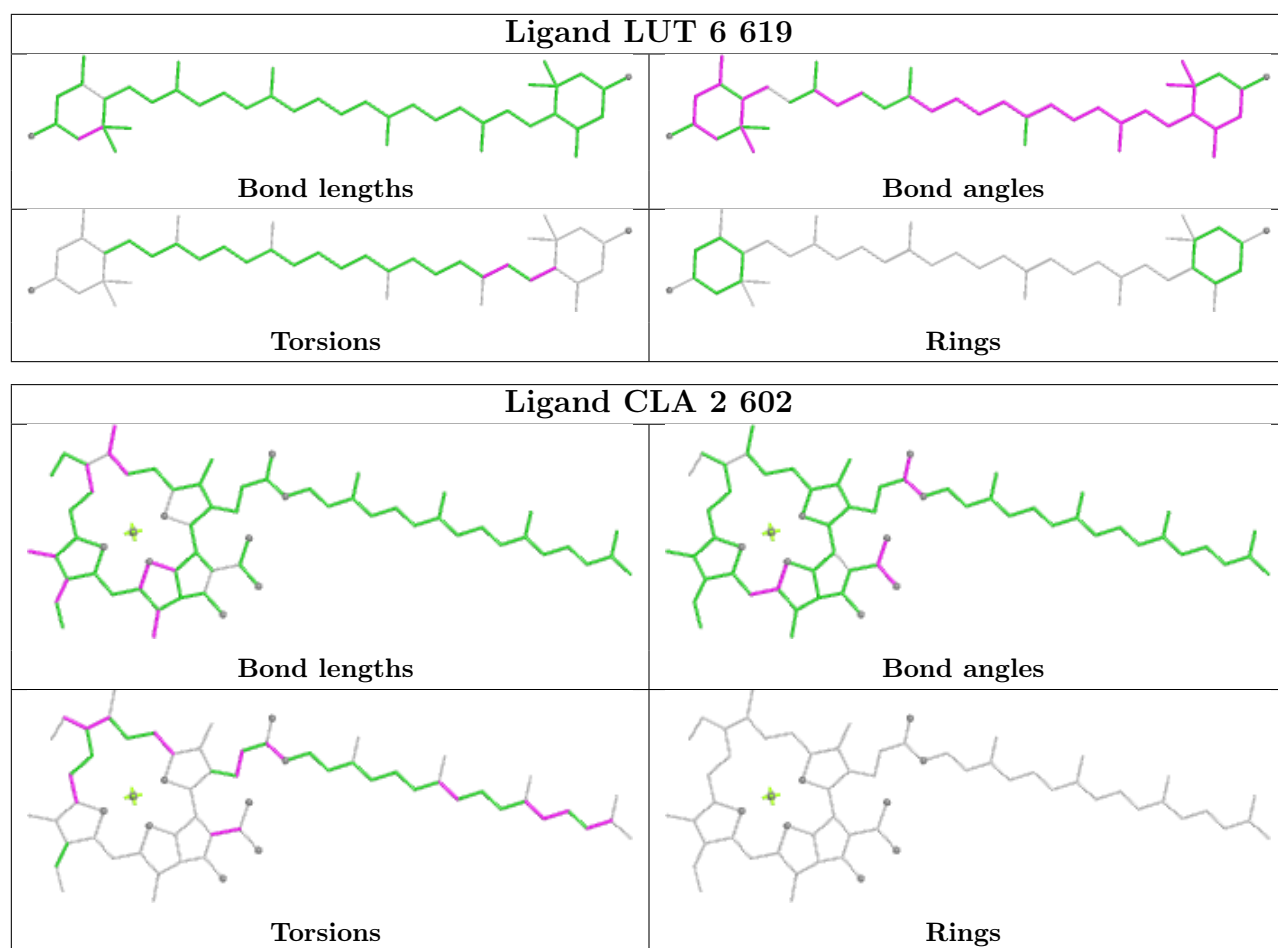
## Ligand CLA A 819



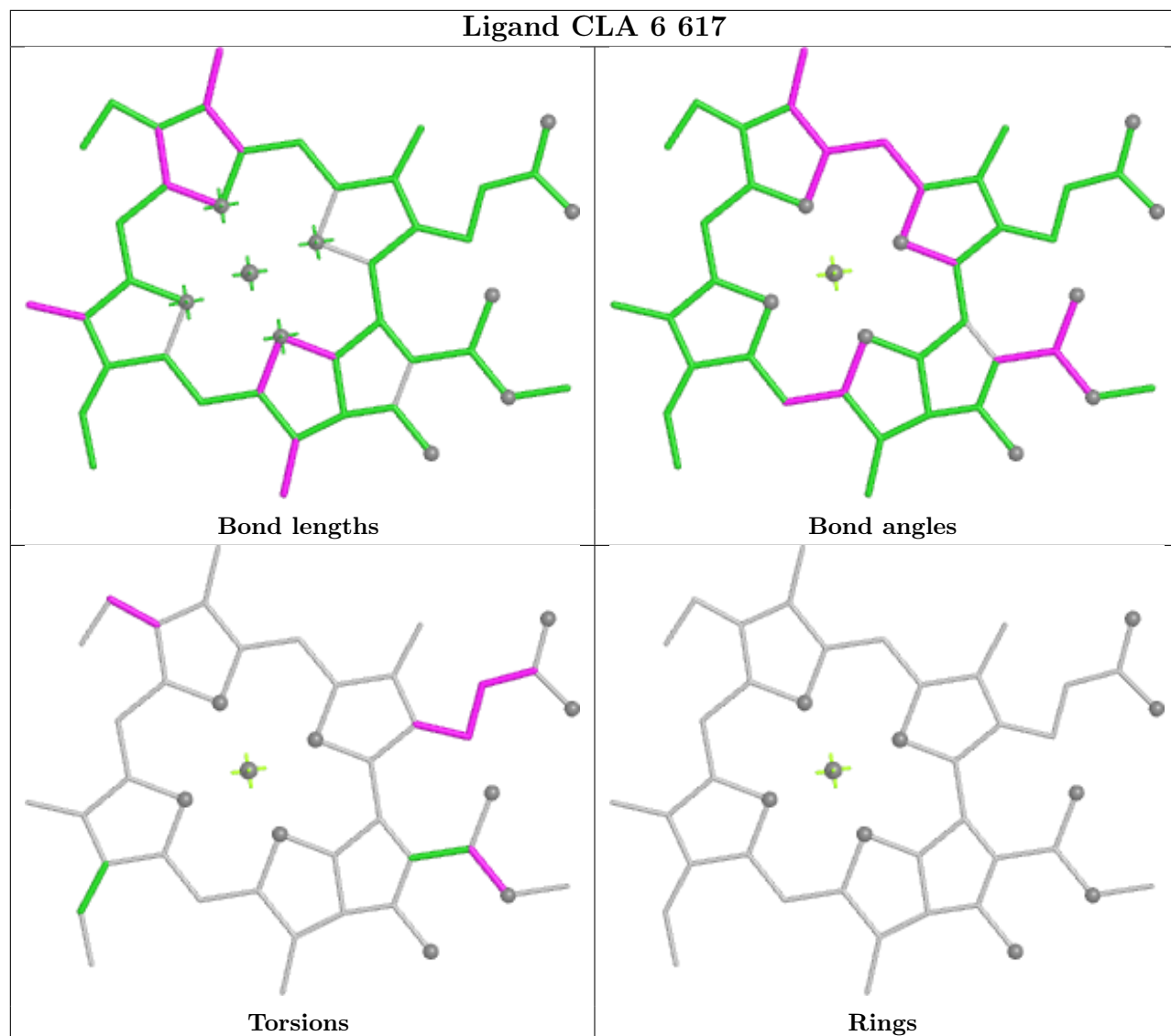
## Ligand CLA 4 608



**Ligand CLA B 817****Ligand BCR 3 622****Ligand CHL W 609**

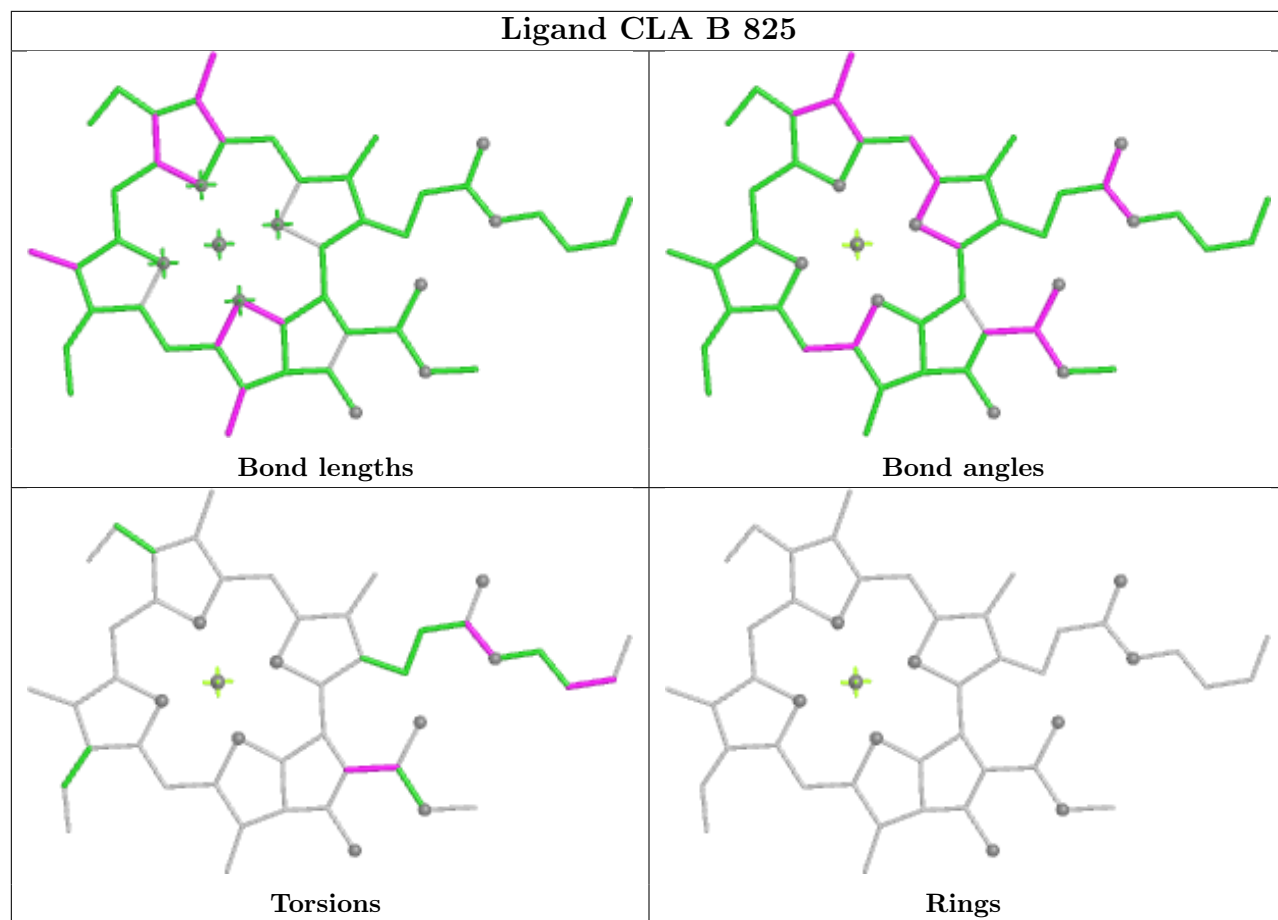


## Ligand CLA 6 617

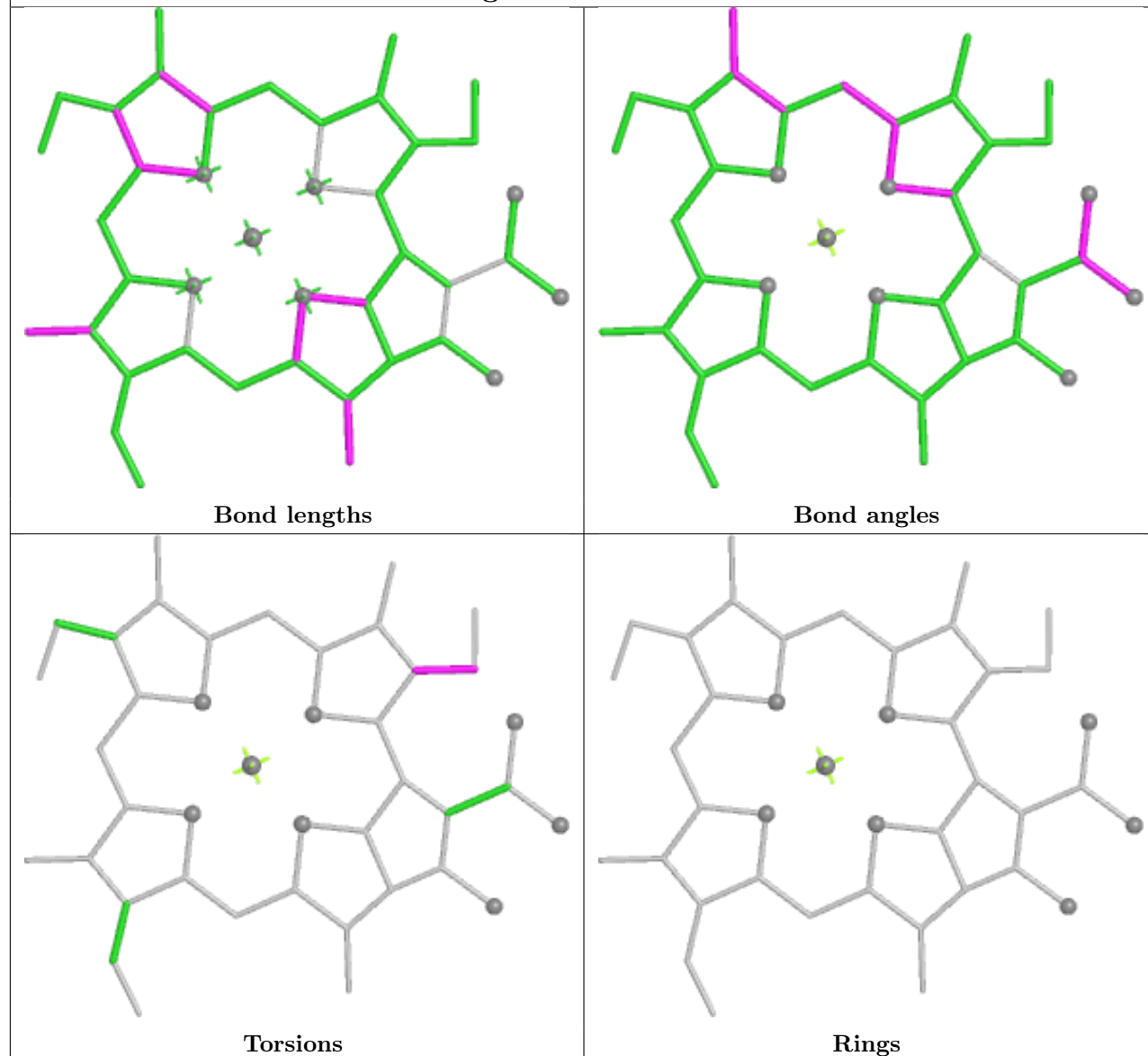




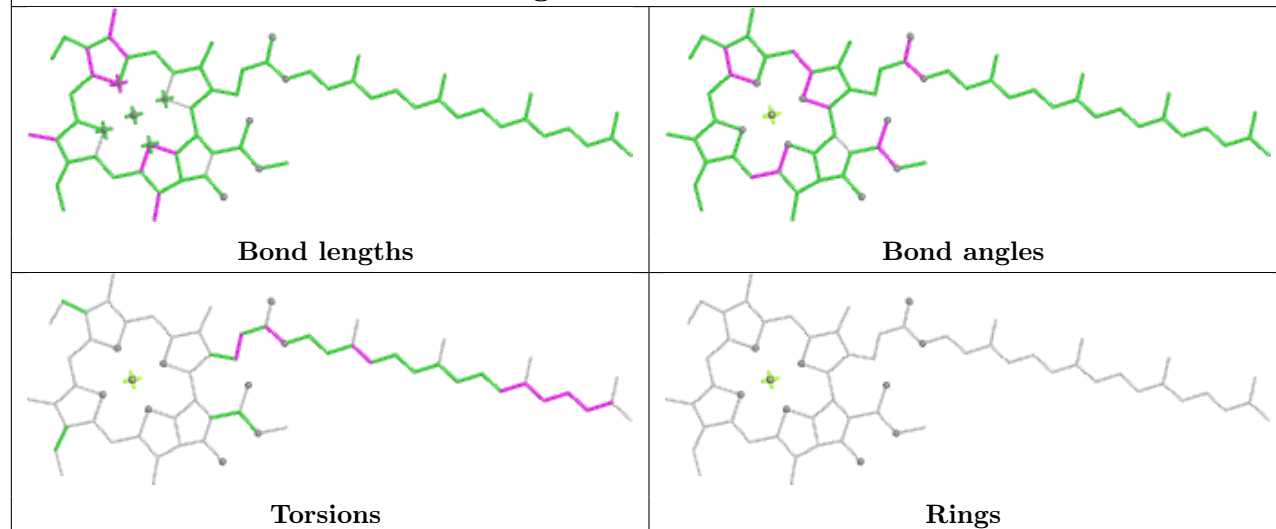
## Ligand CLA B 825



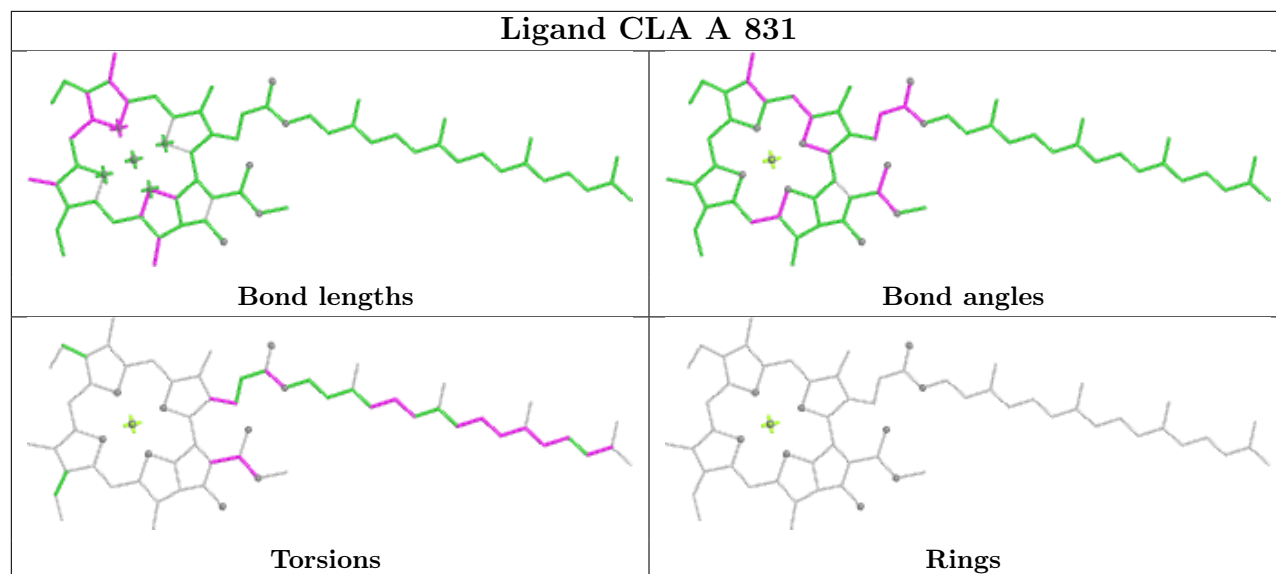
## Ligand CLA 5 612



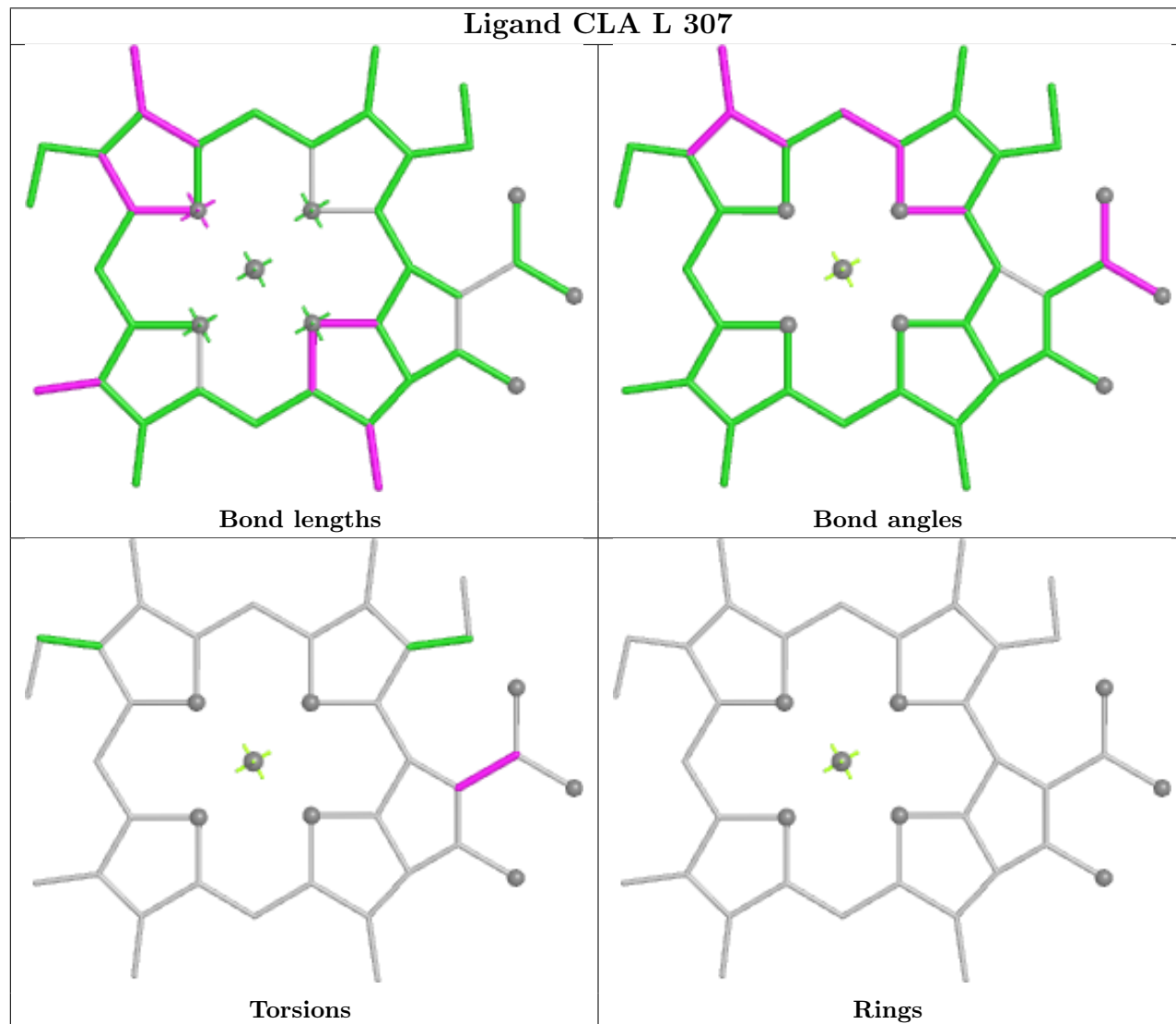
## Ligand CLA B 831



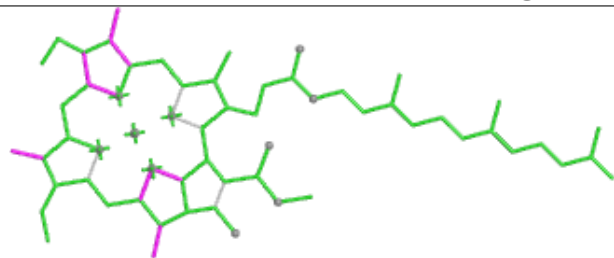
## Ligand CLA A 831



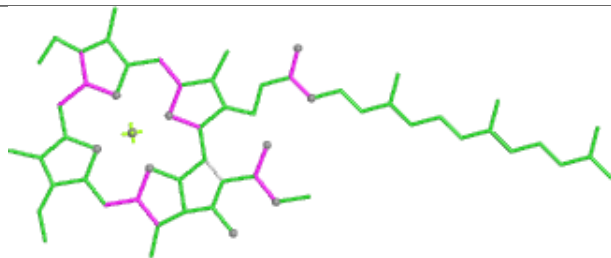
## Ligand CLA L 307



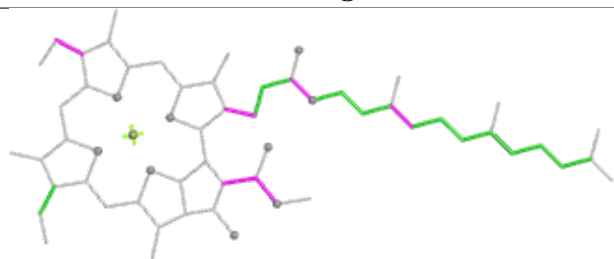
## Ligand CLA 6 614



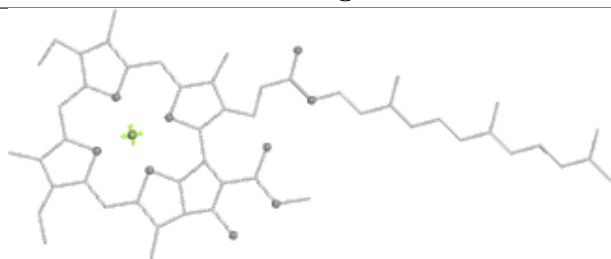
Bond lengths



Bond angles

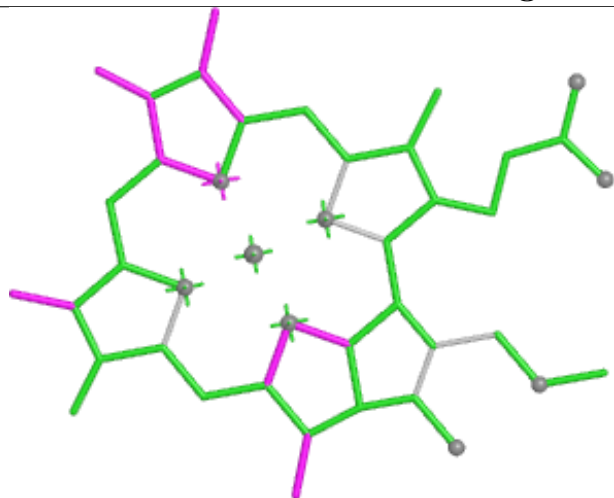


Torsions

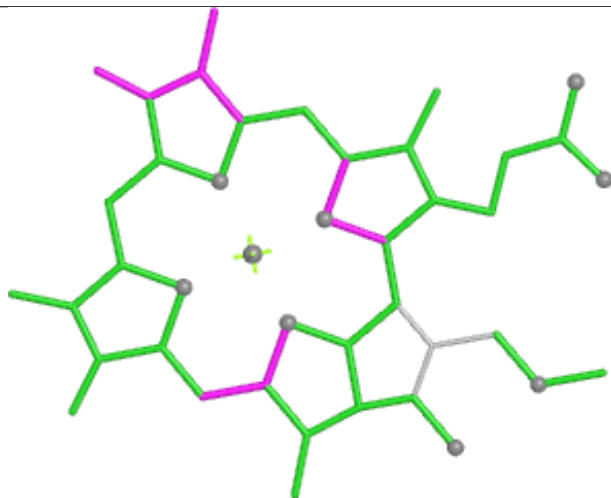


Rings

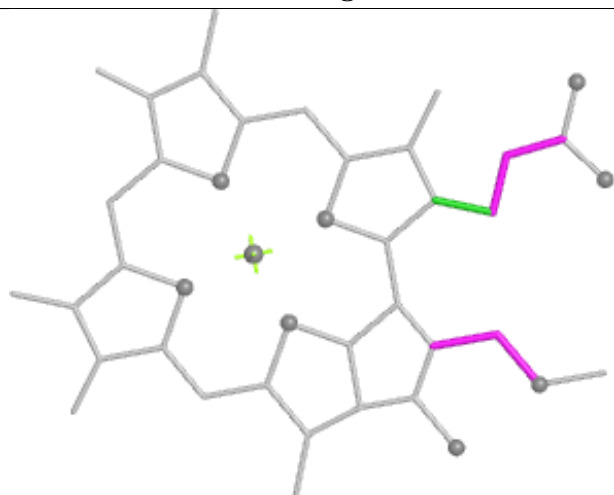
## Ligand CLA 7 615



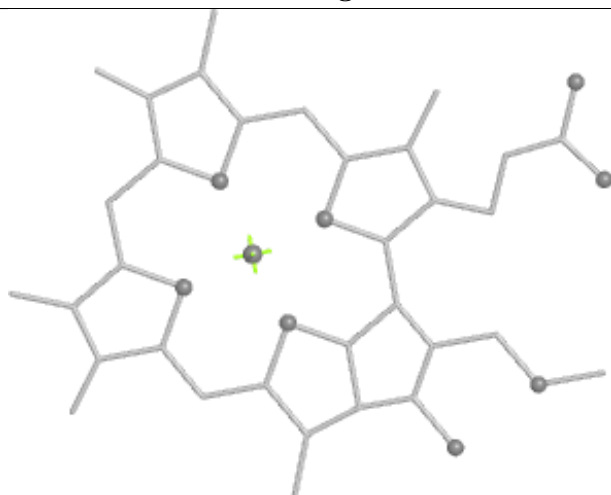
Bond lengths



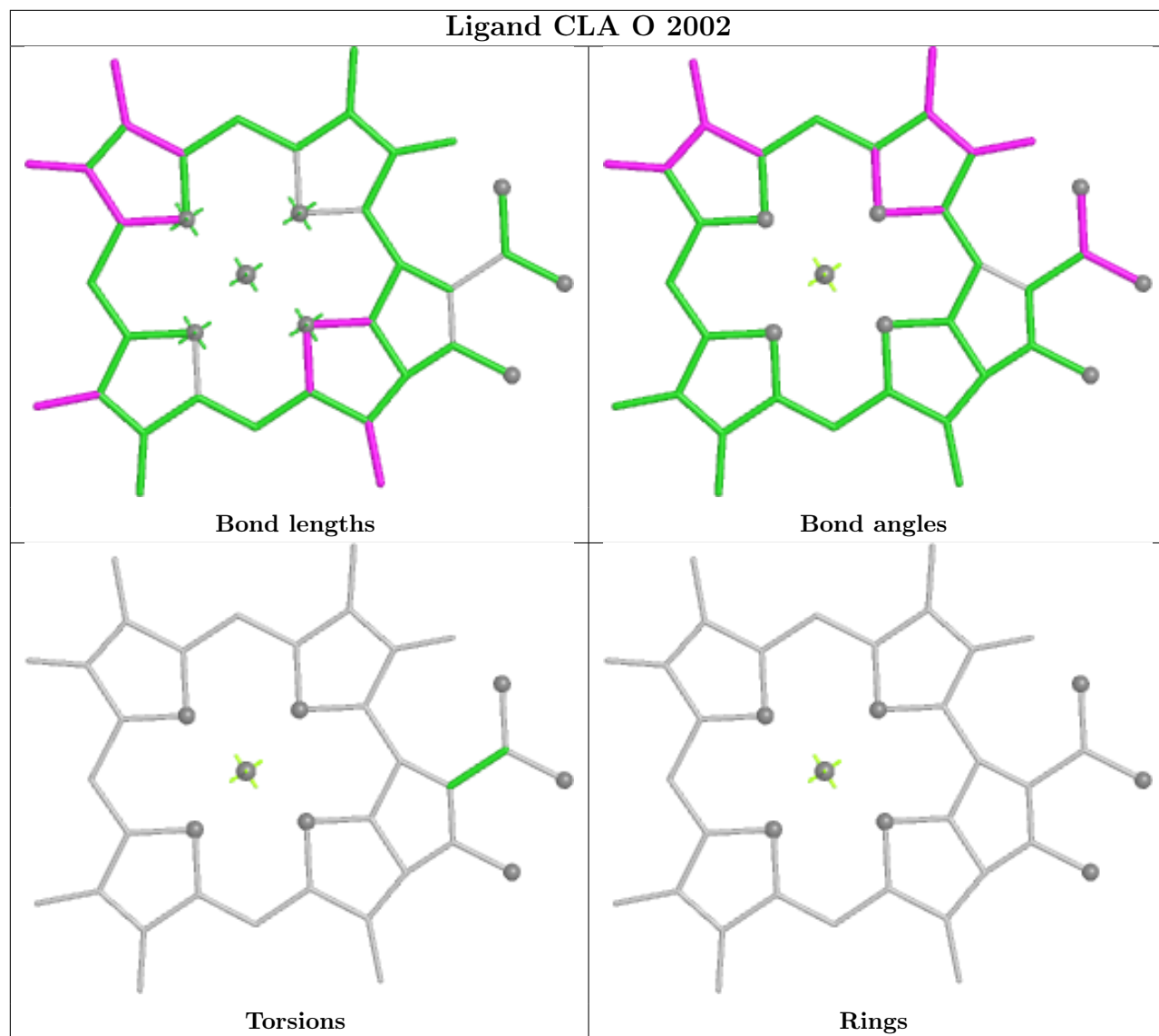
Bond angles

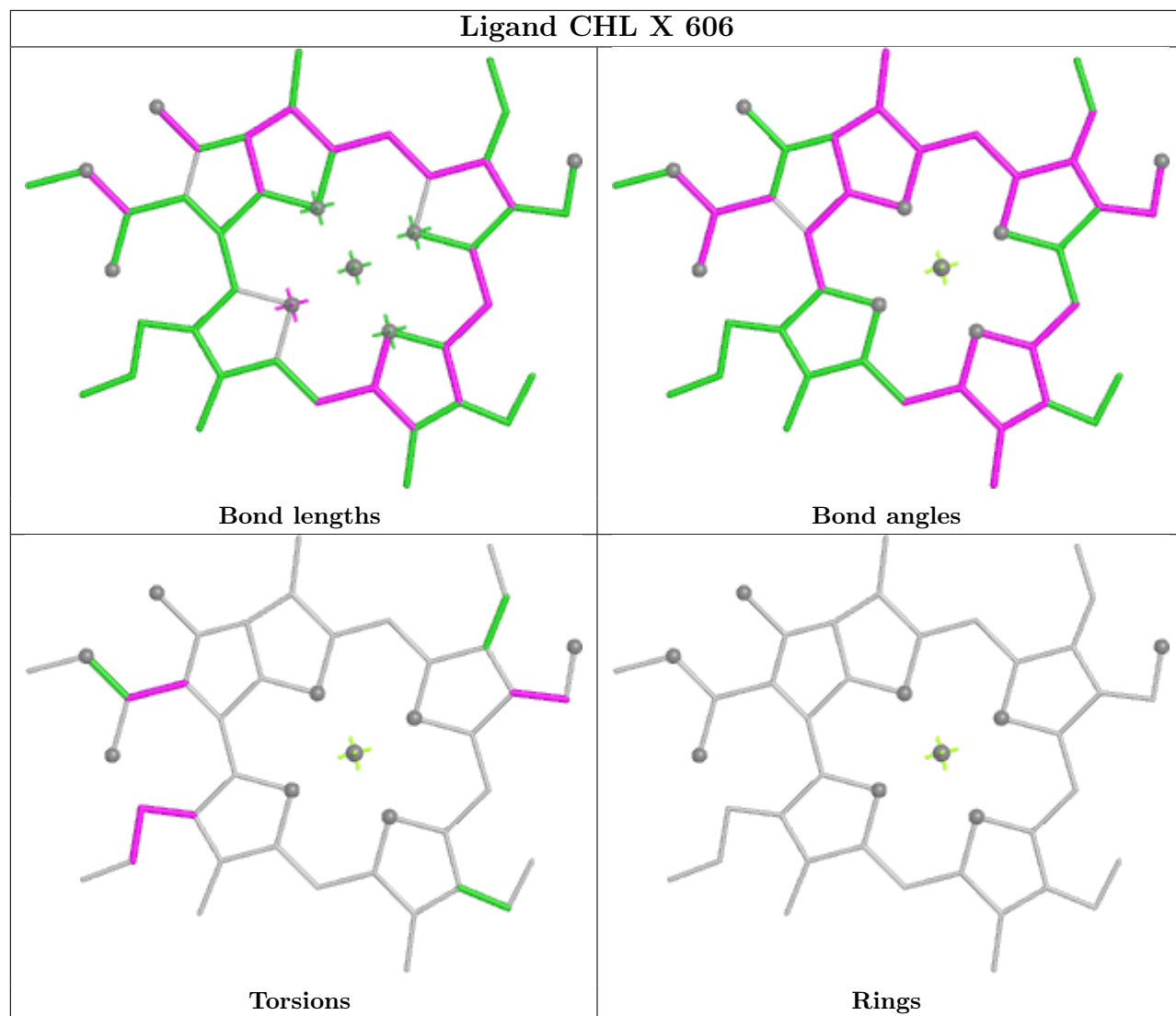


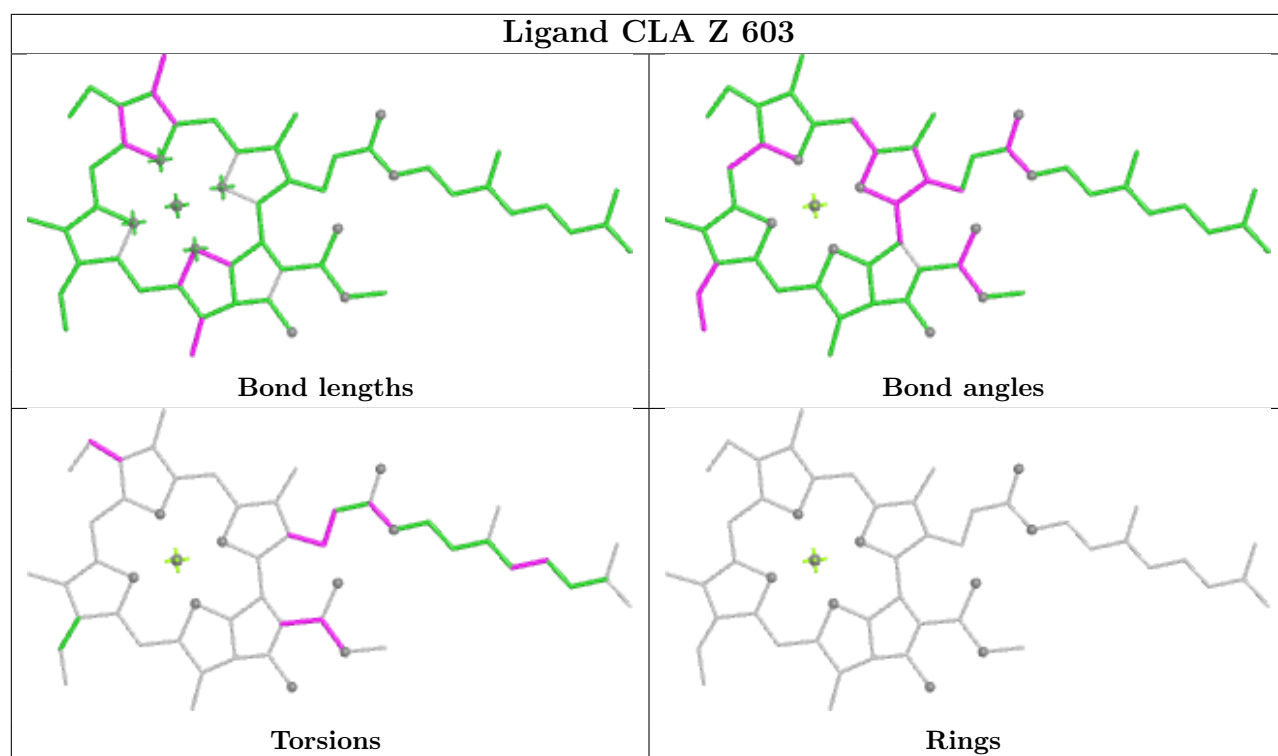
Torsions



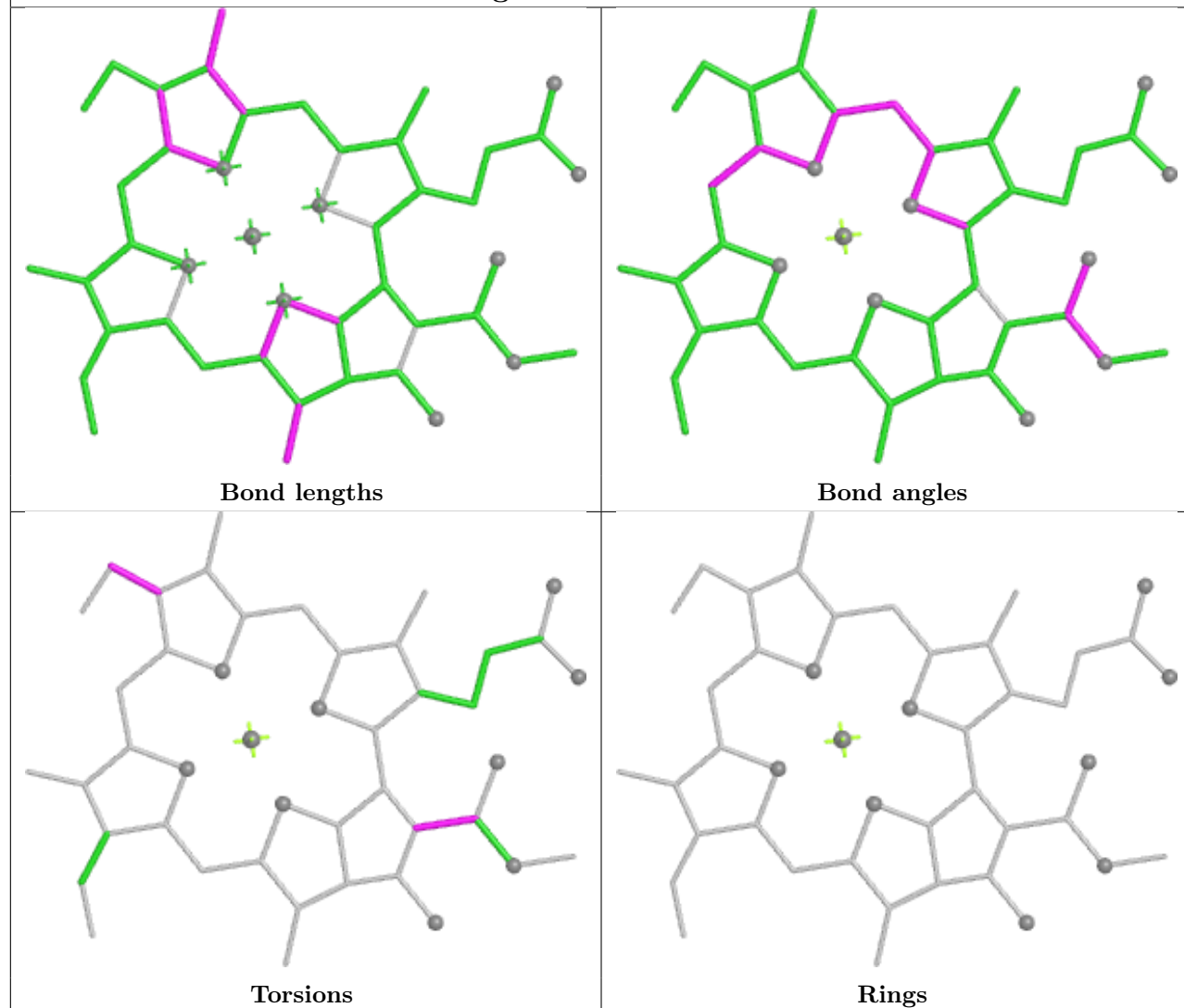
Rings



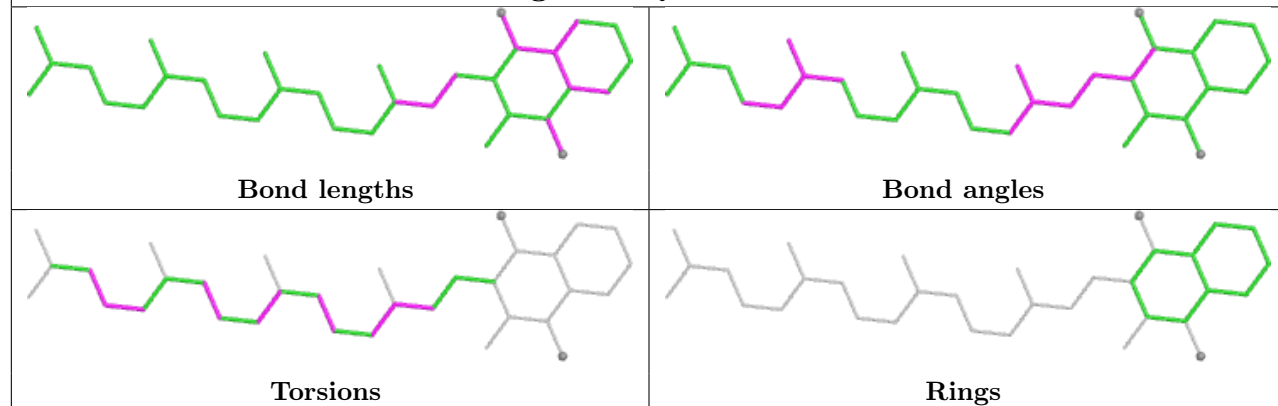




## Ligand CLA X 611

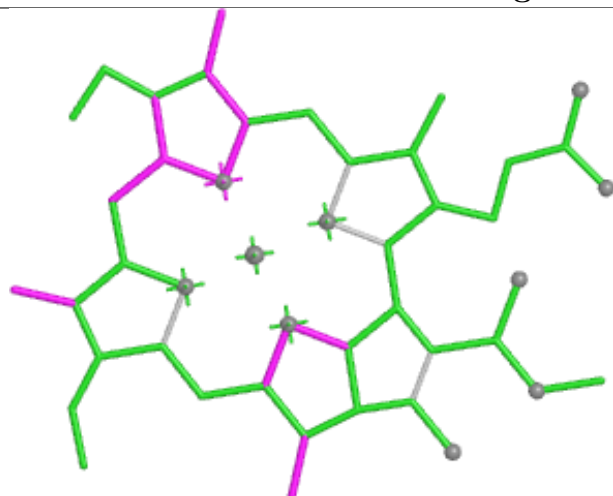


## Ligand PQN B 842

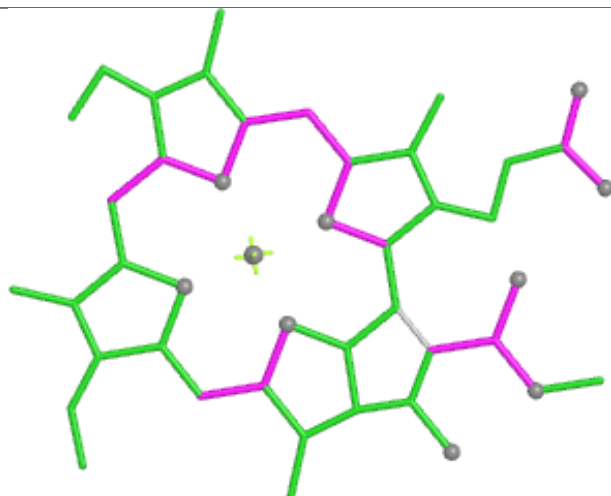




## Ligand CLA A 837



Bond lengths



Bond angles

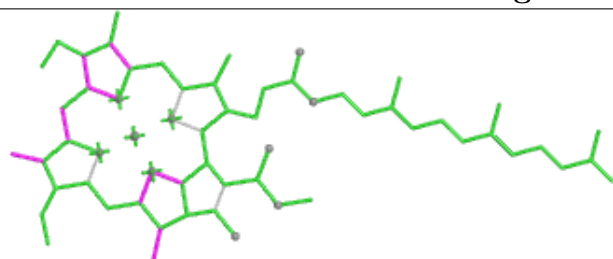


Torsions

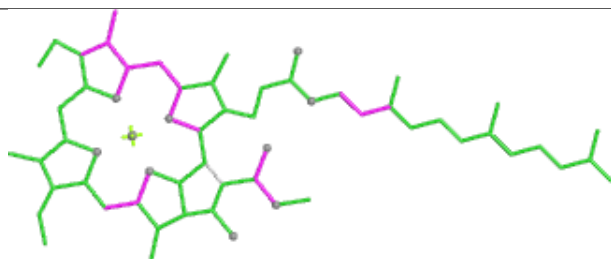


Rings

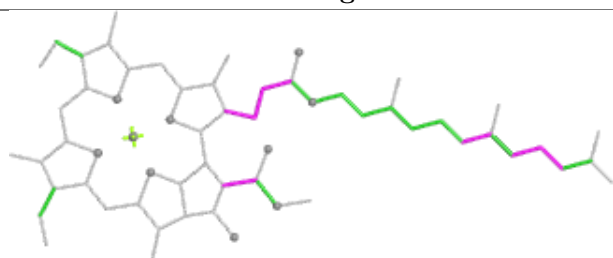
## Ligand CLA V 602



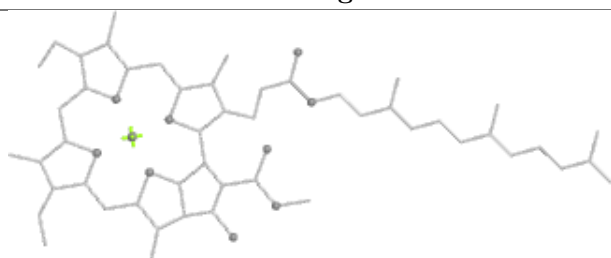
Bond lengths



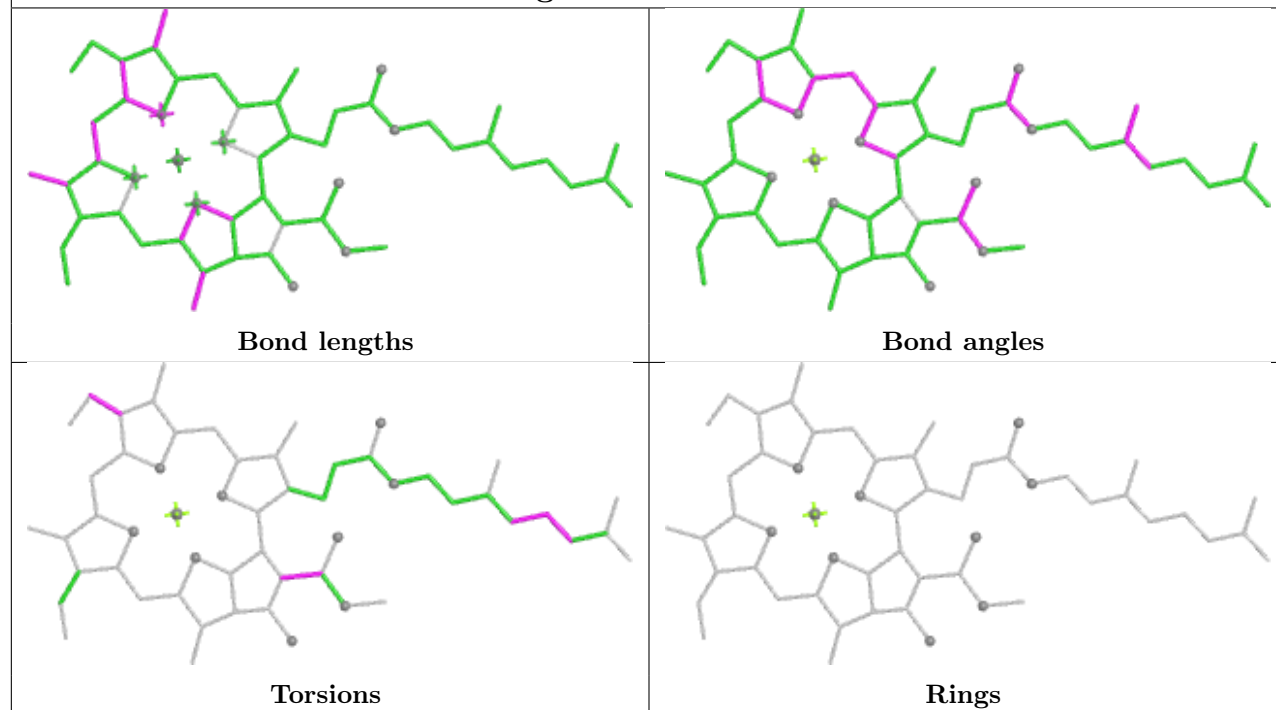
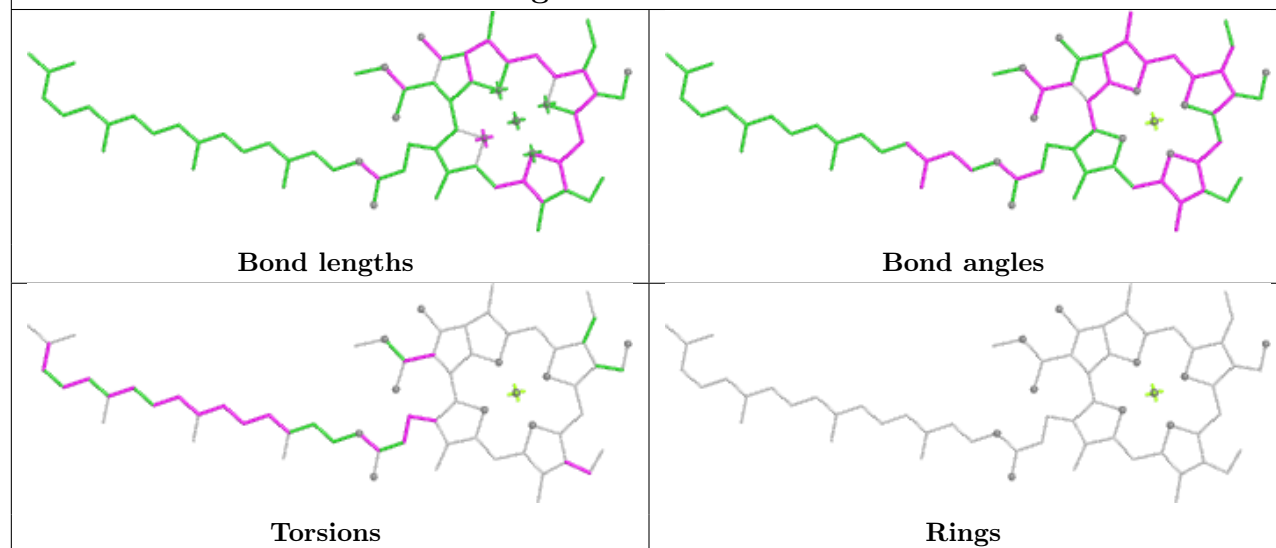
Bond angles



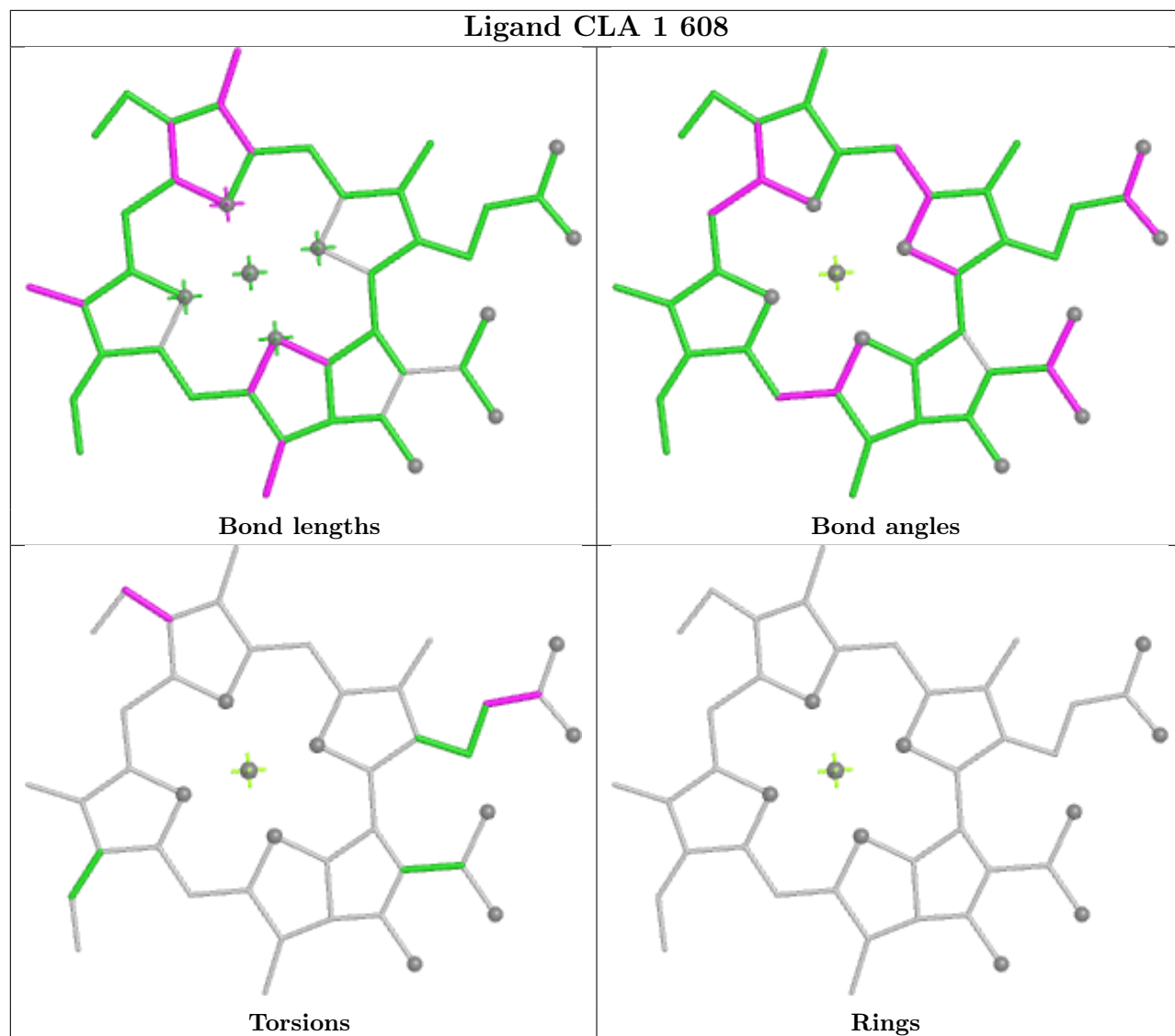
Torsions

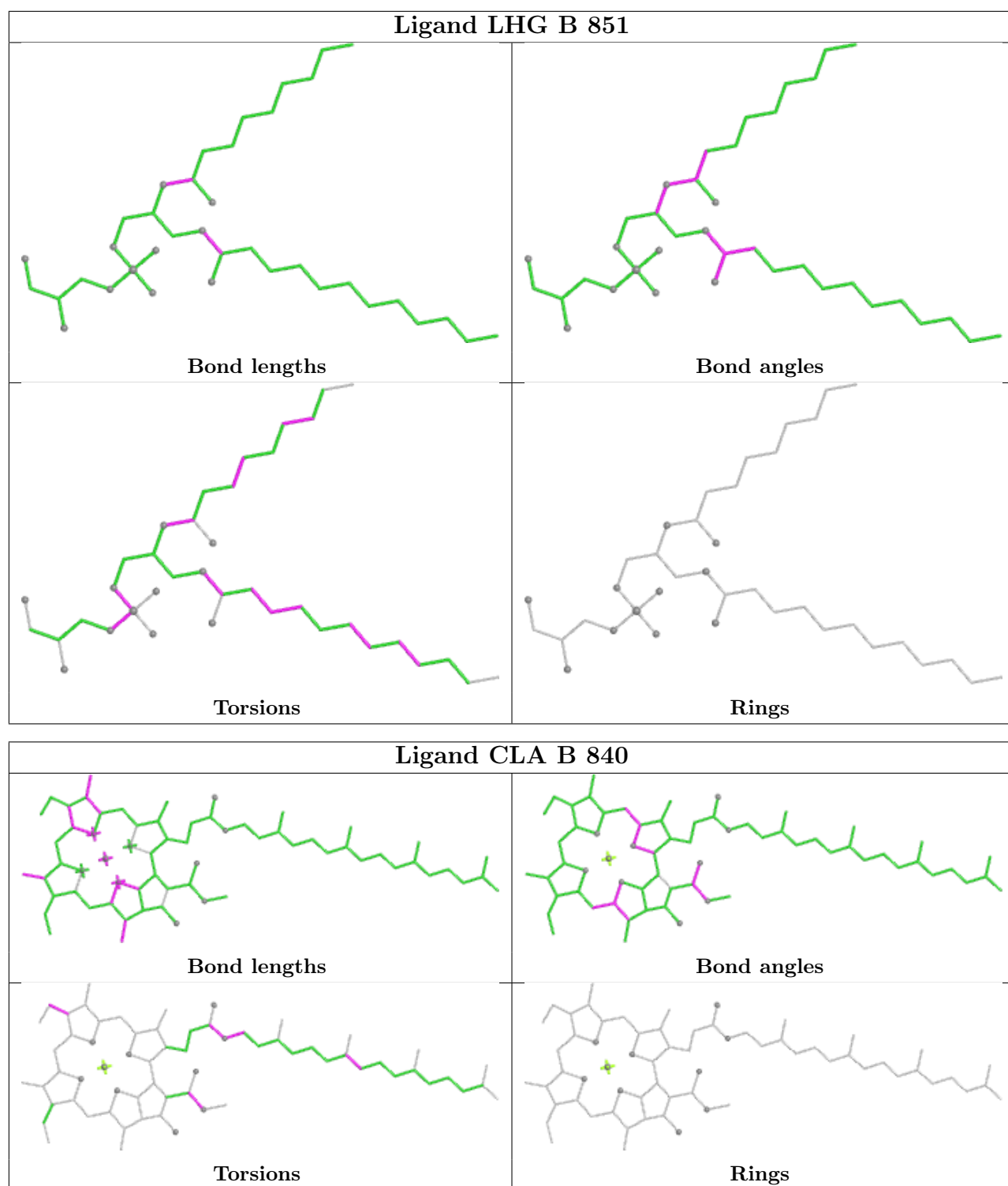


Rings

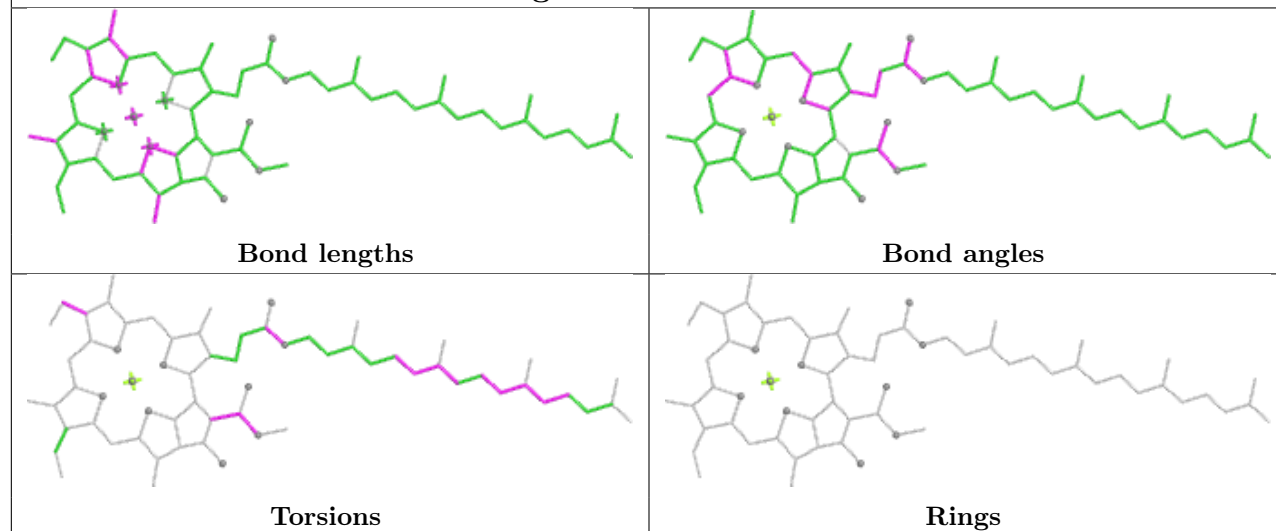
**Ligand CLA 2 610****Ligand CHL Y 601**

## Ligand CLA 1 608

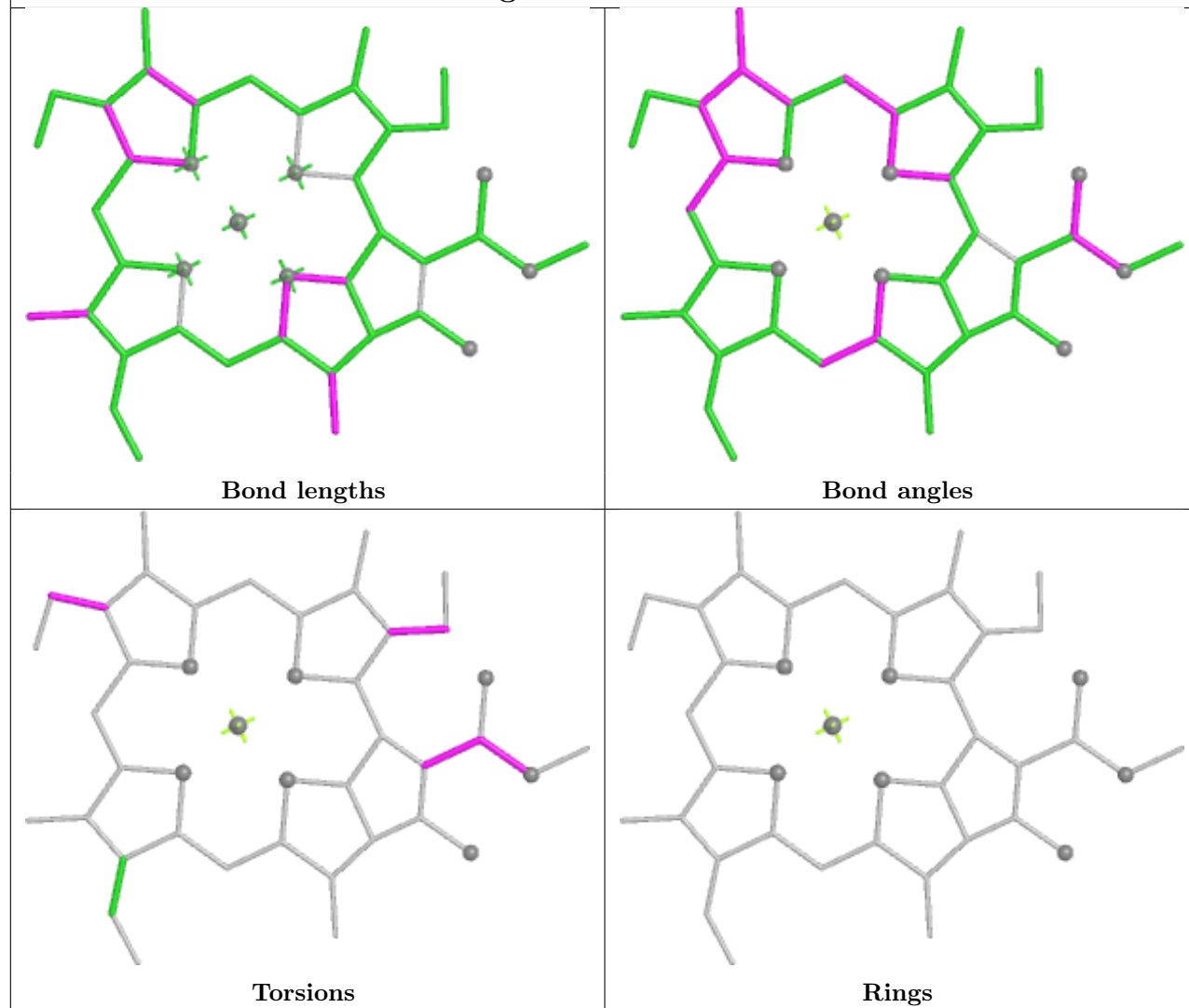


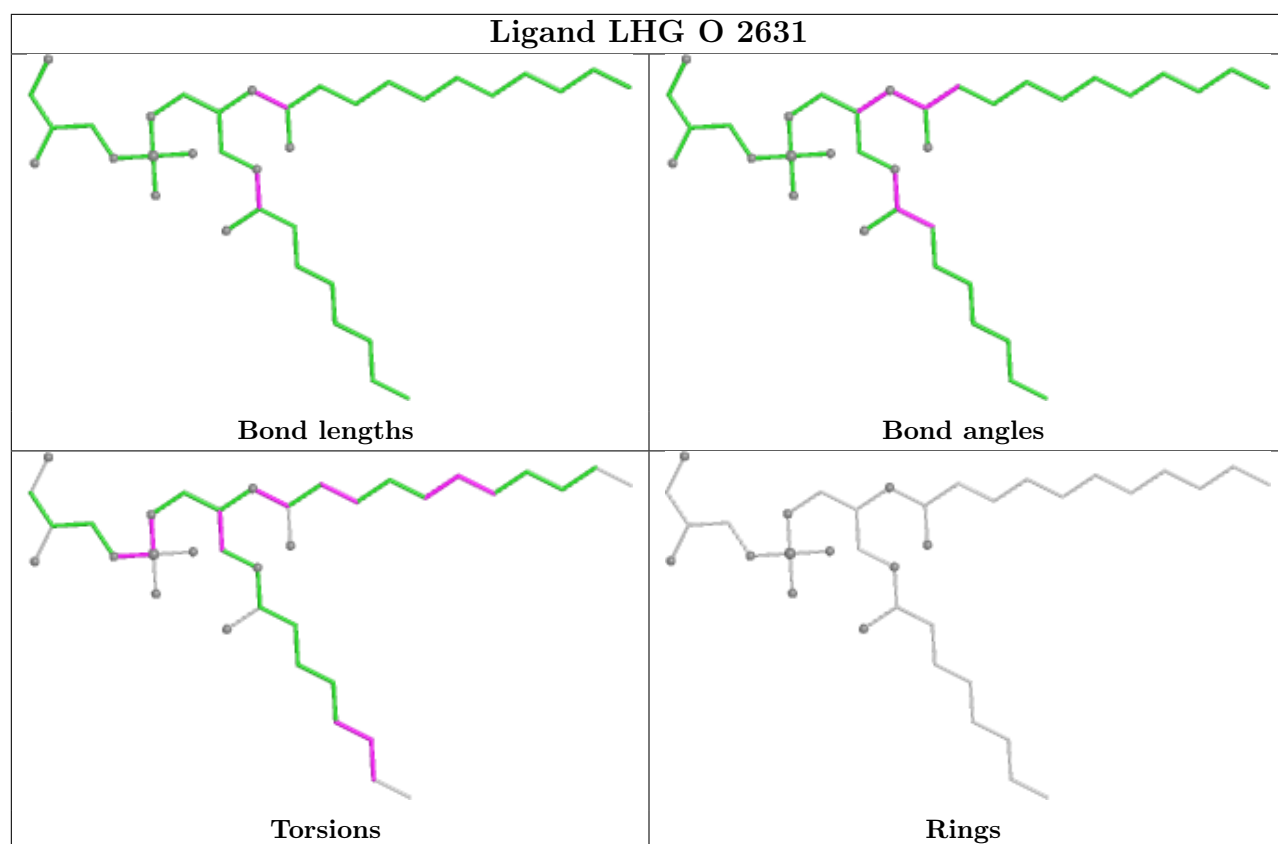
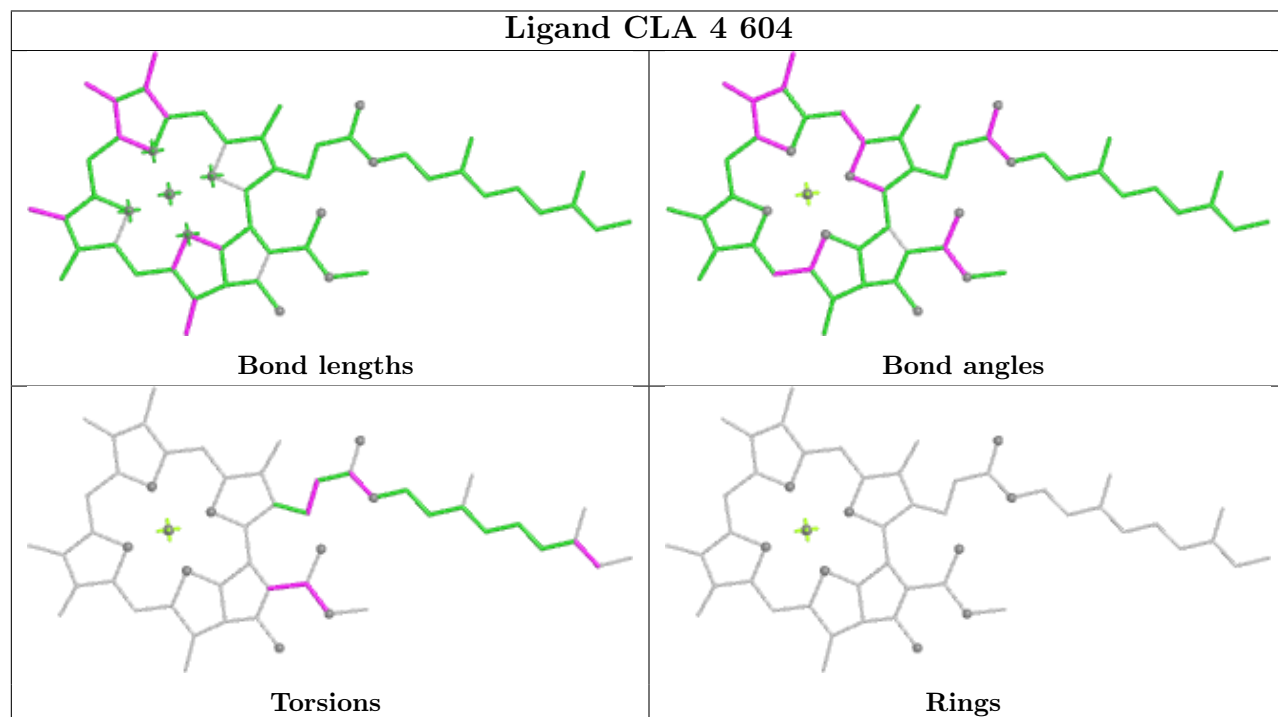


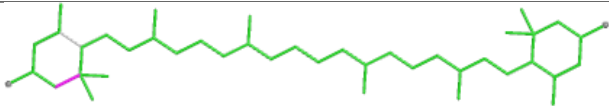
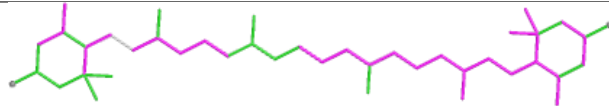
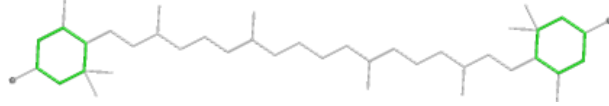
## Ligand CLA B 802

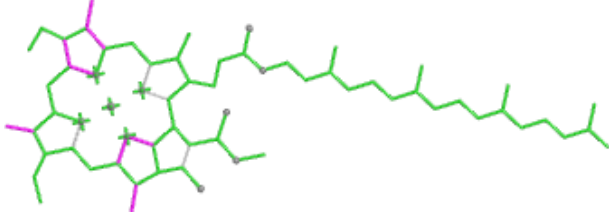
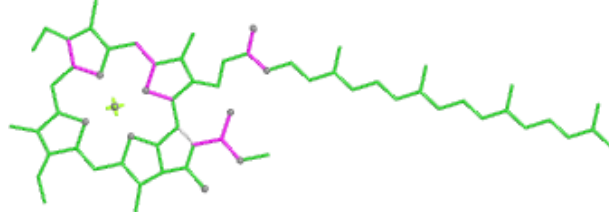
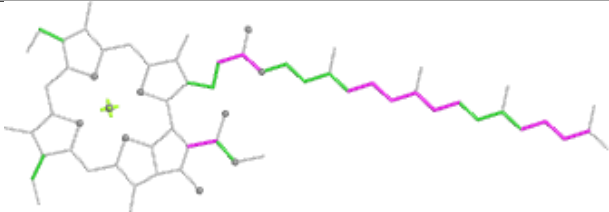
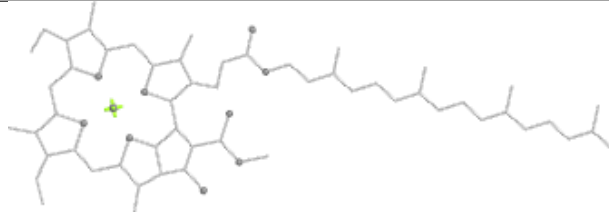


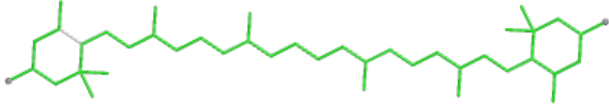
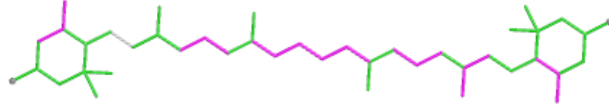
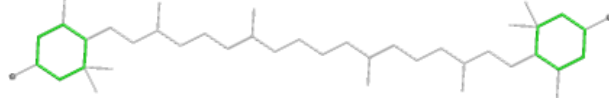
## Ligand CLA 4 611

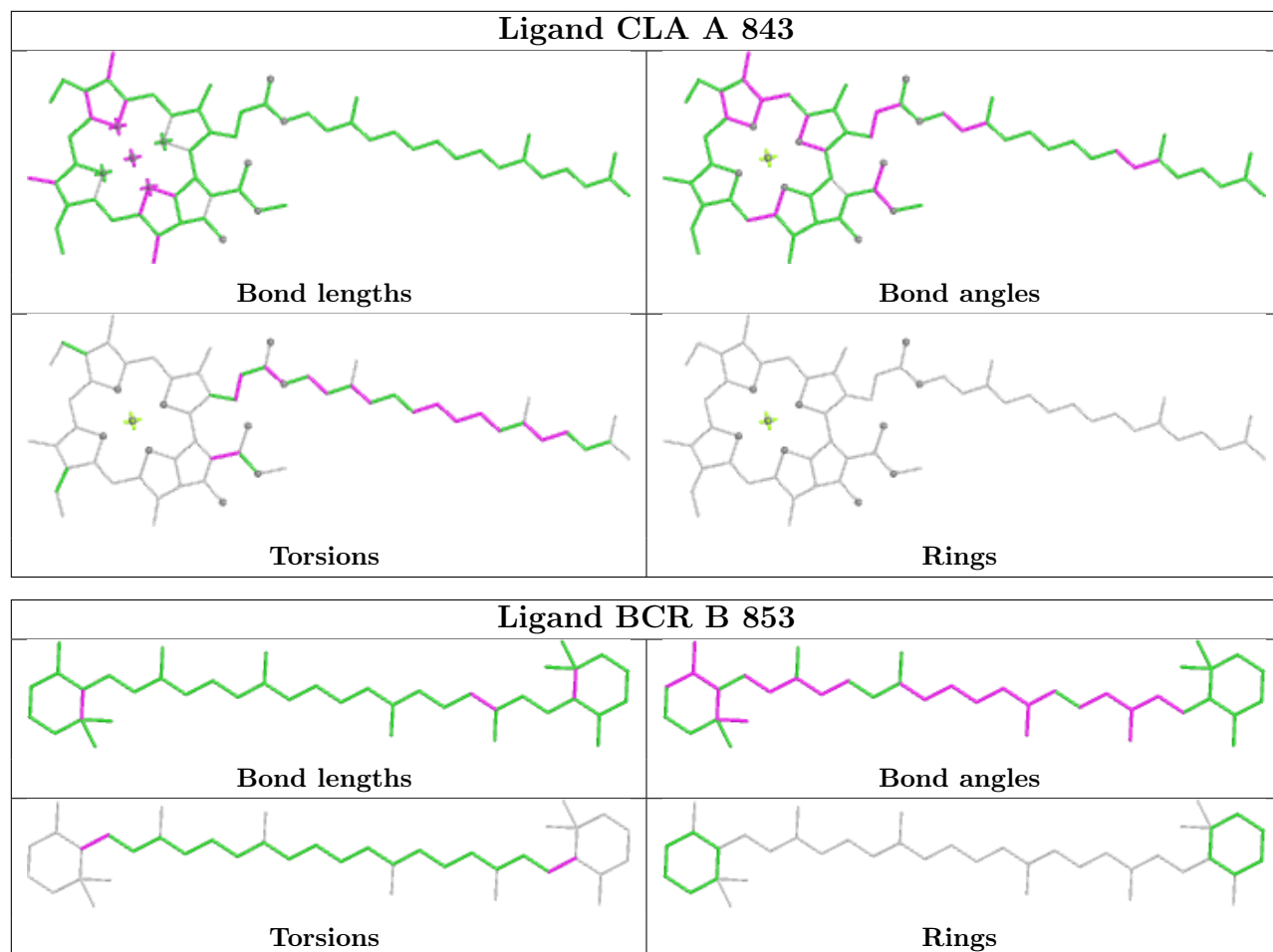




| Ligand LUT 9 619                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

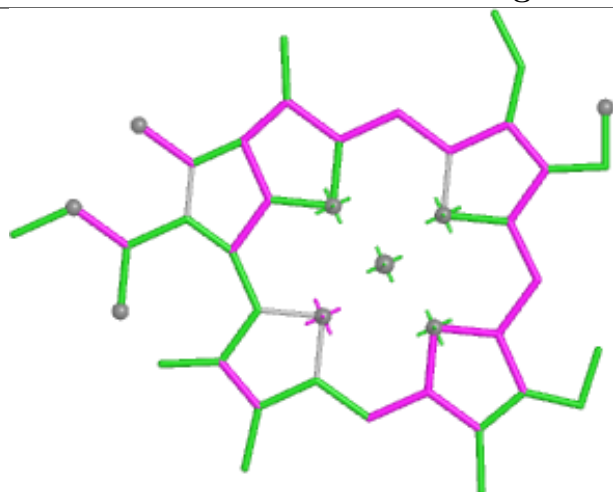
| Ligand CLA 6 601                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

| Ligand LUT Z 1621                                                                   |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

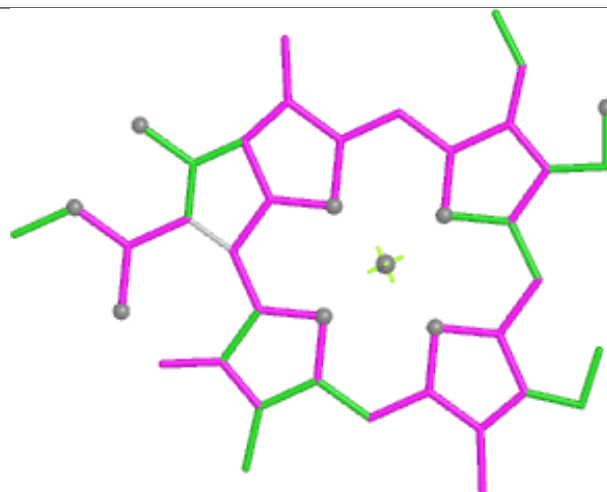




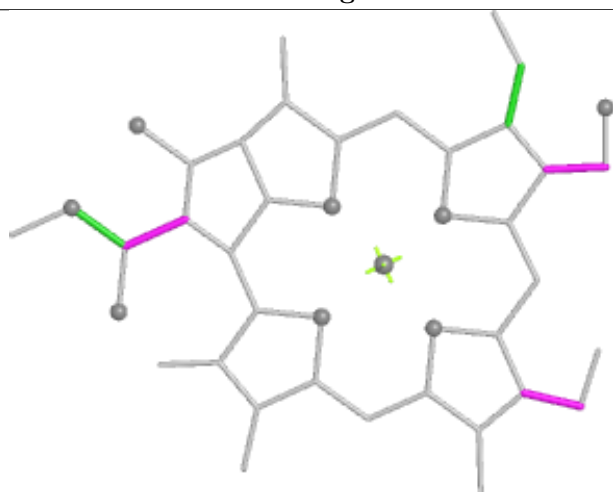
## Ligand CHL Y 605



Bond lengths



Bond angles

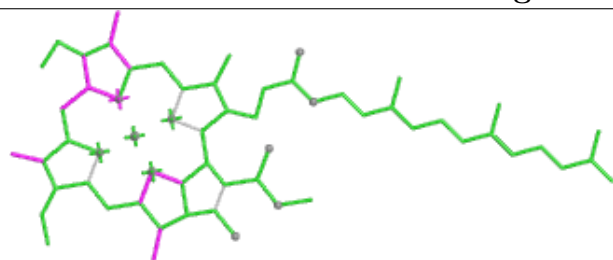


Torsions

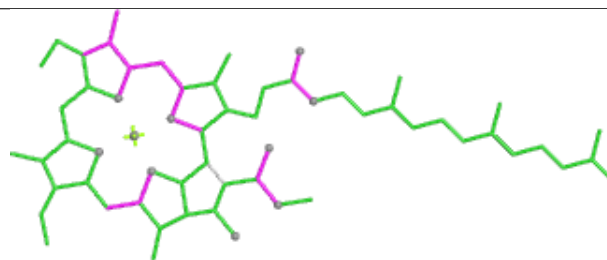


Rings

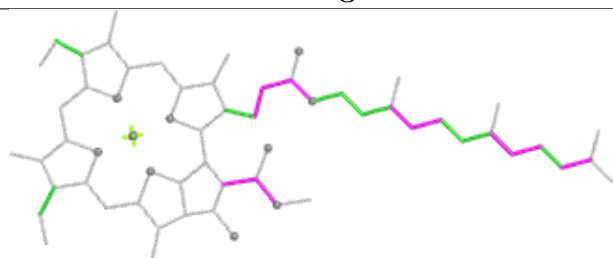
## Ligand CLA A 818



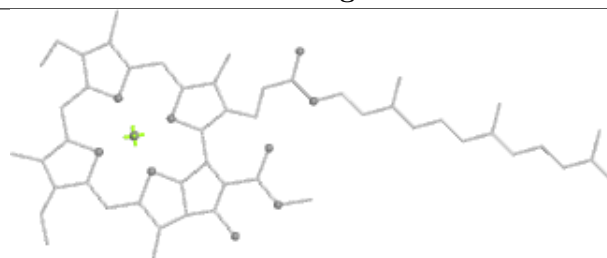
Bond lengths



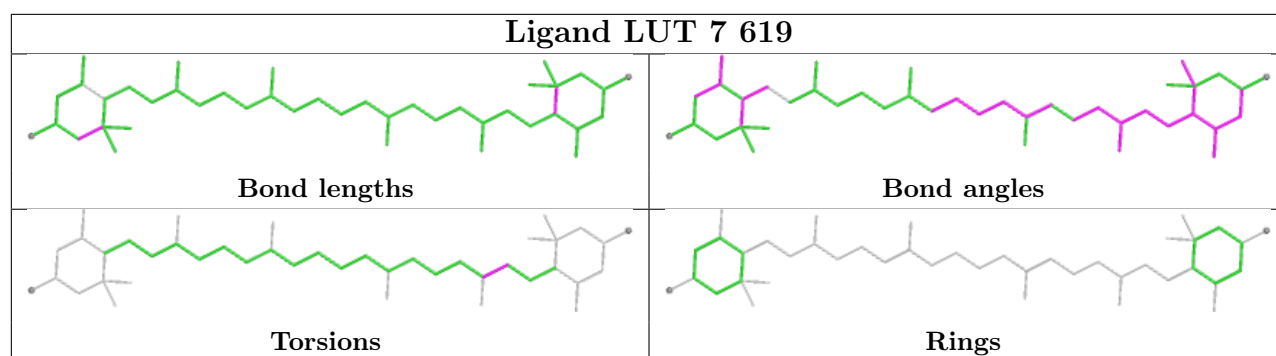
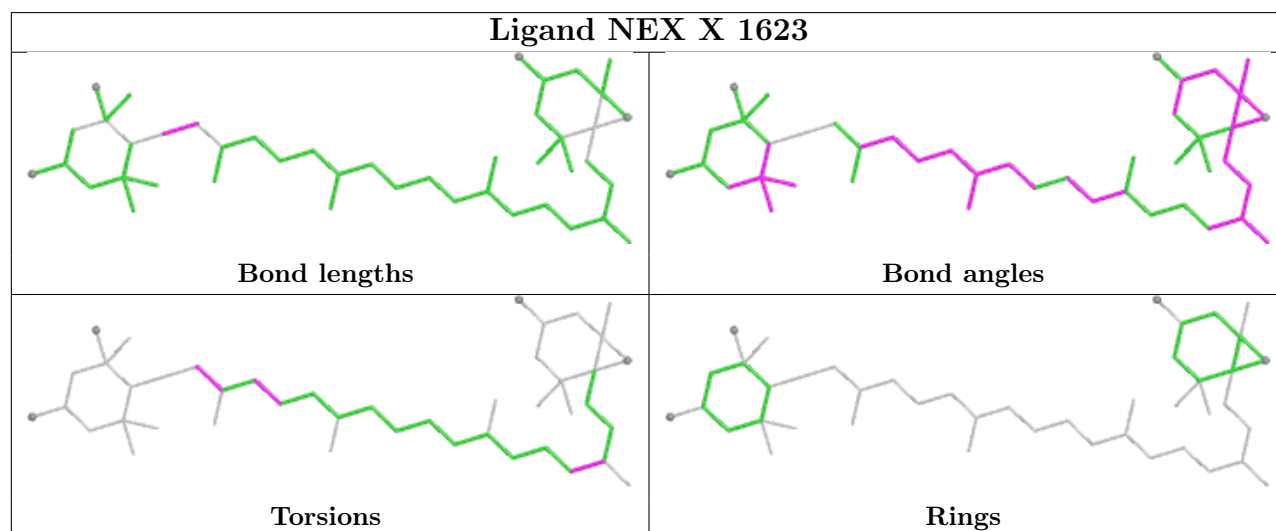
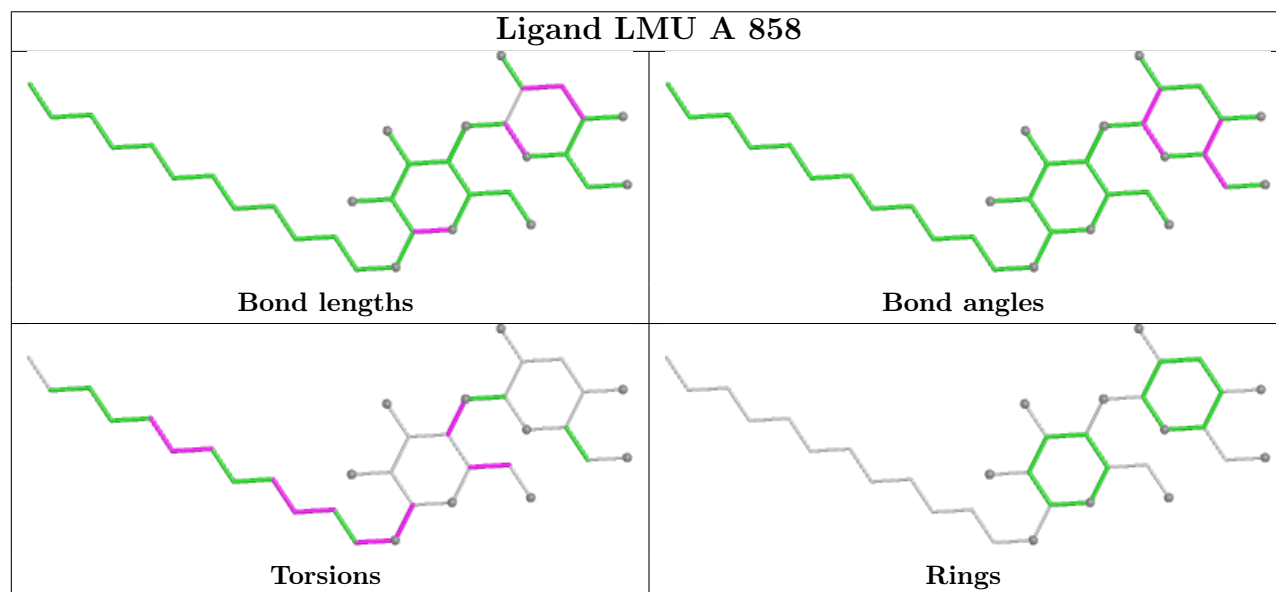
Bond angles



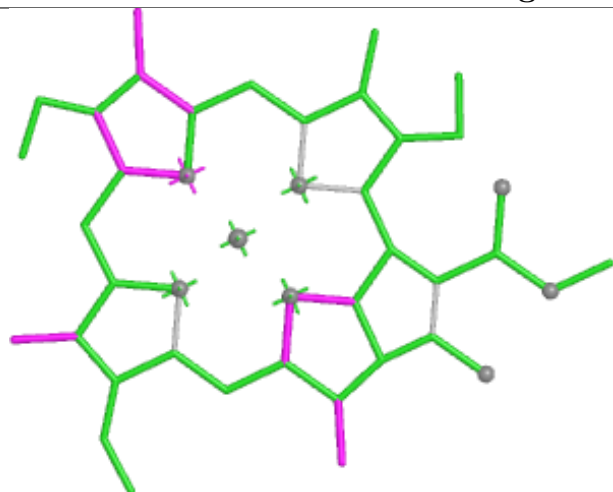
Torsions



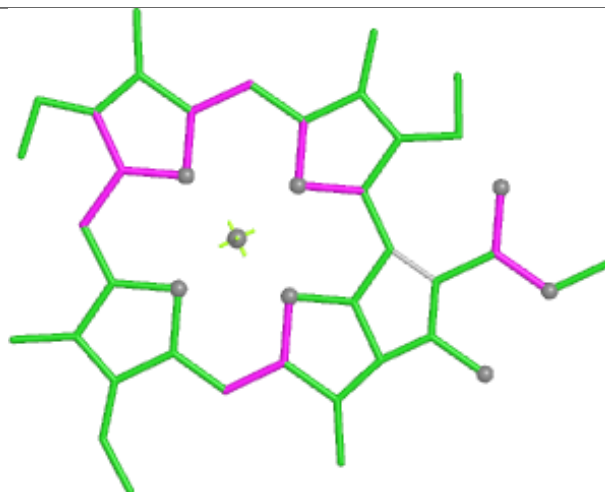
Rings



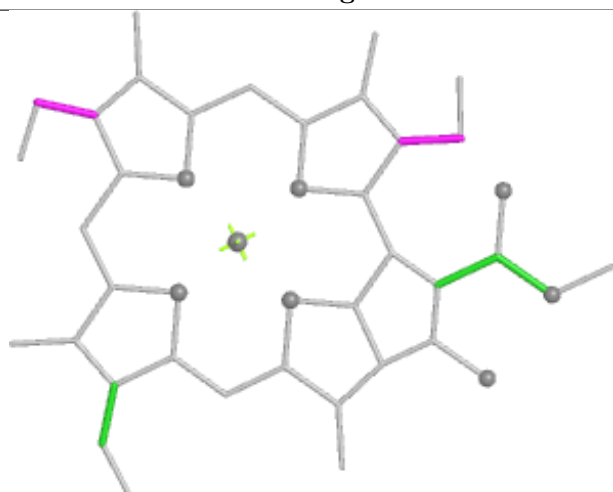
## Ligand CLA 7 614



Bond lengths



Bond angles

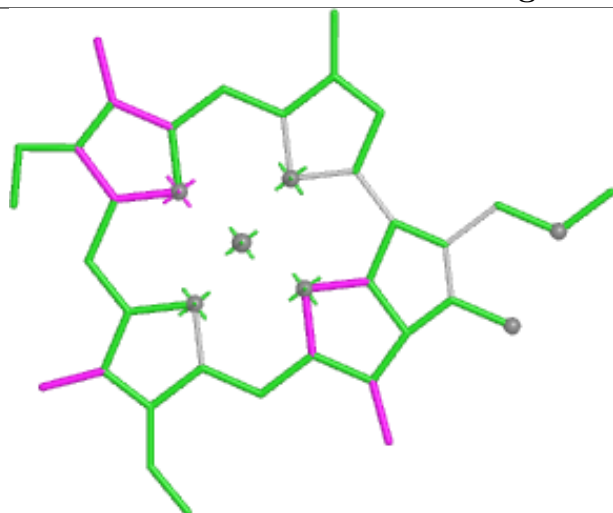


Torsions



Rings

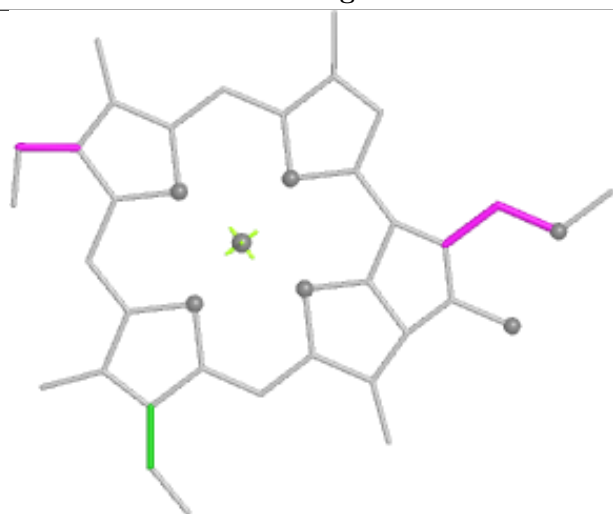
## Ligand CLA 1 606



Bond lengths



Bond angles

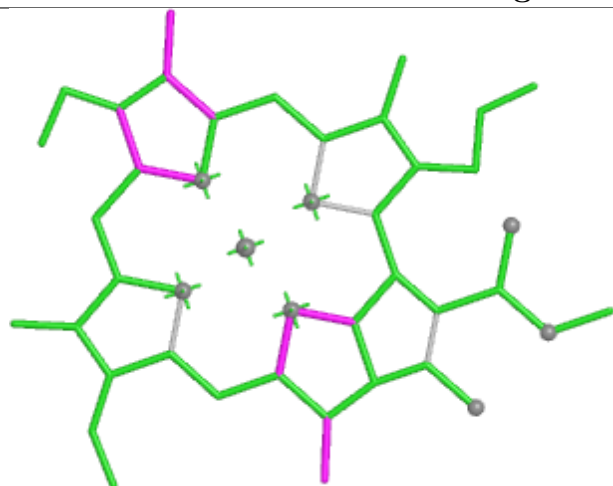


Torsions

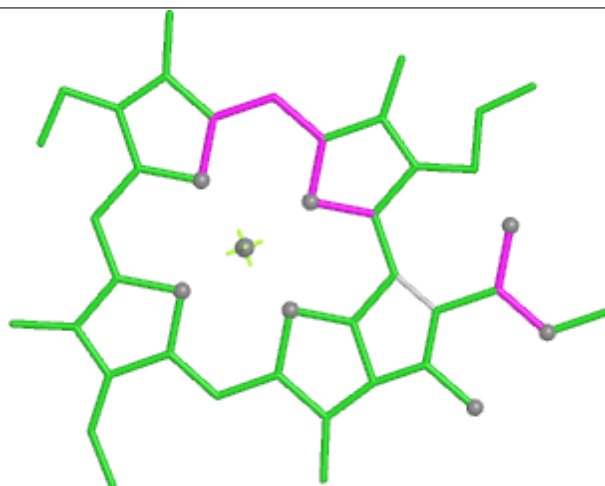


Rings

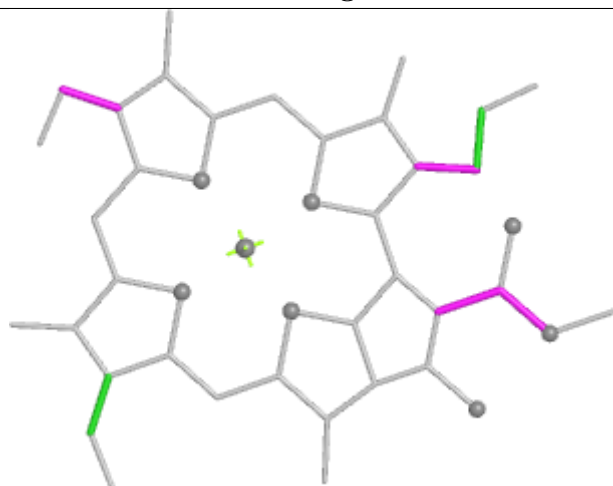
## Ligand CLA Y 611



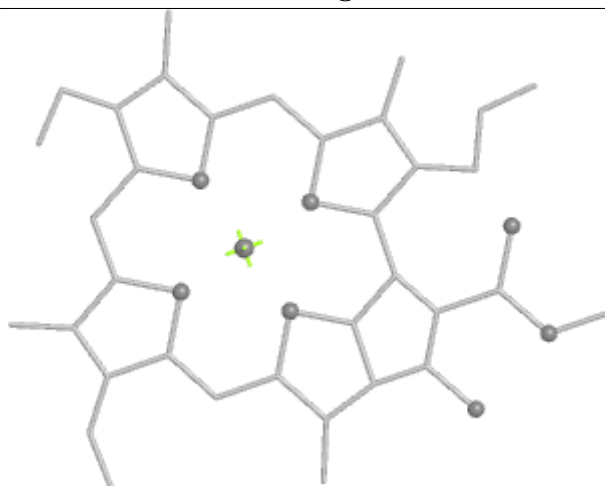
Bond lengths



Bond angles

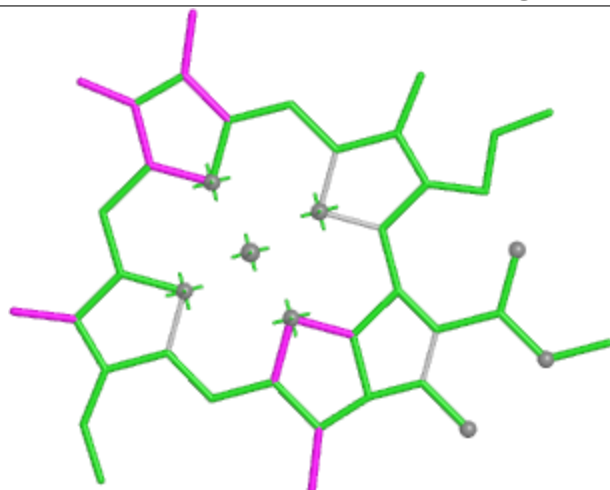


Torsions

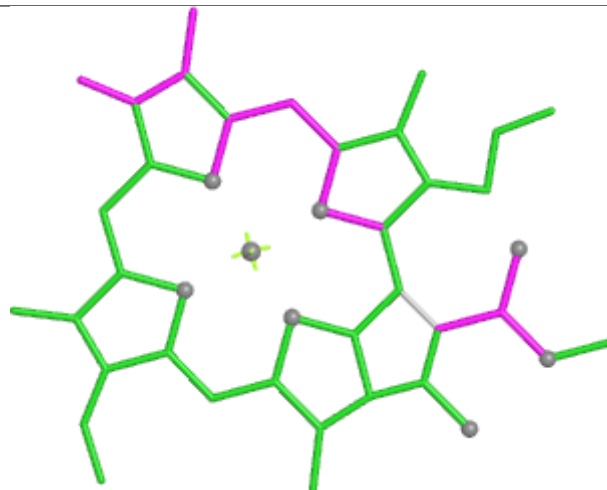


Rings

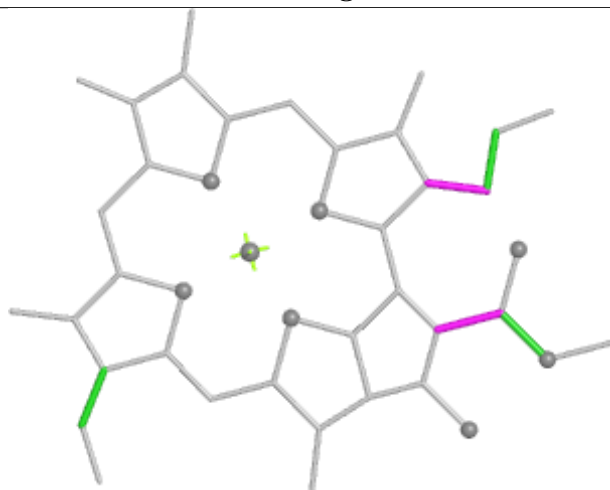
## Ligand CLA Z 611



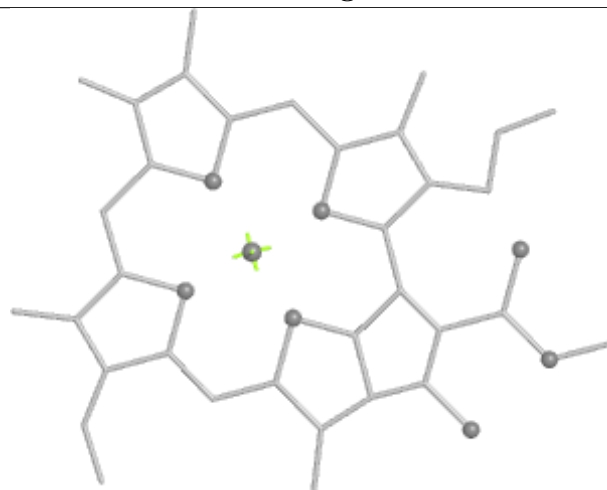
Bond lengths



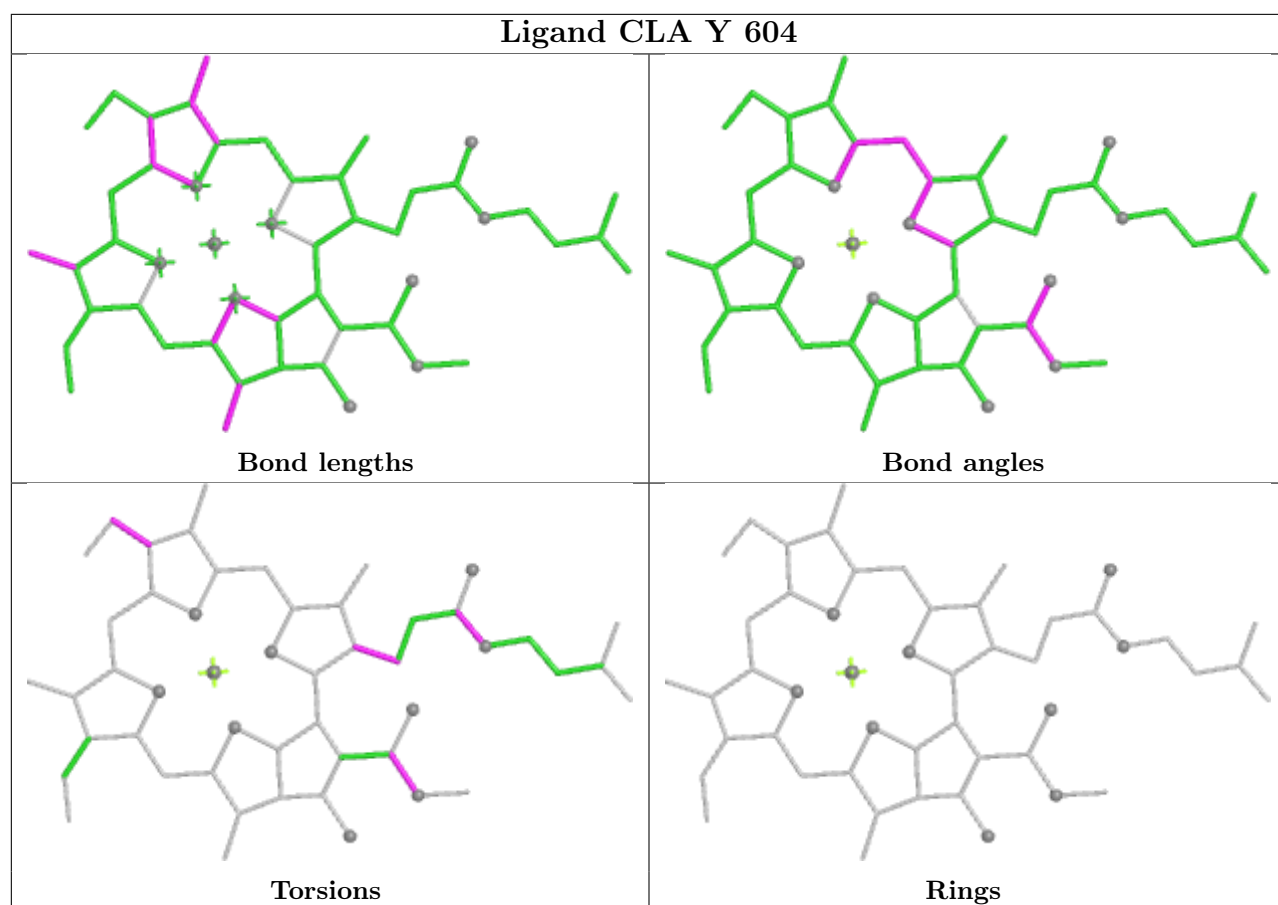
Bond angles

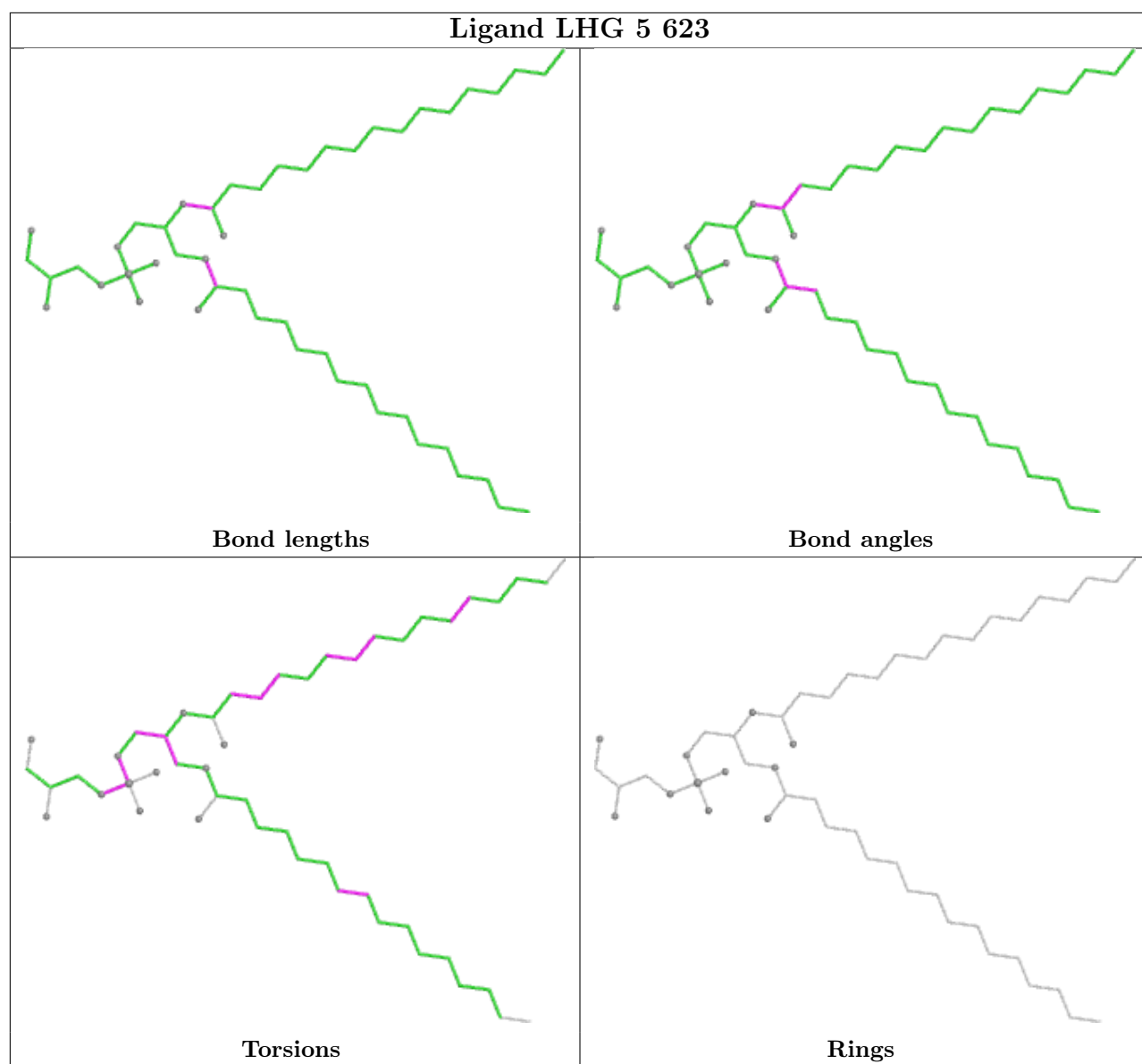


Torsions

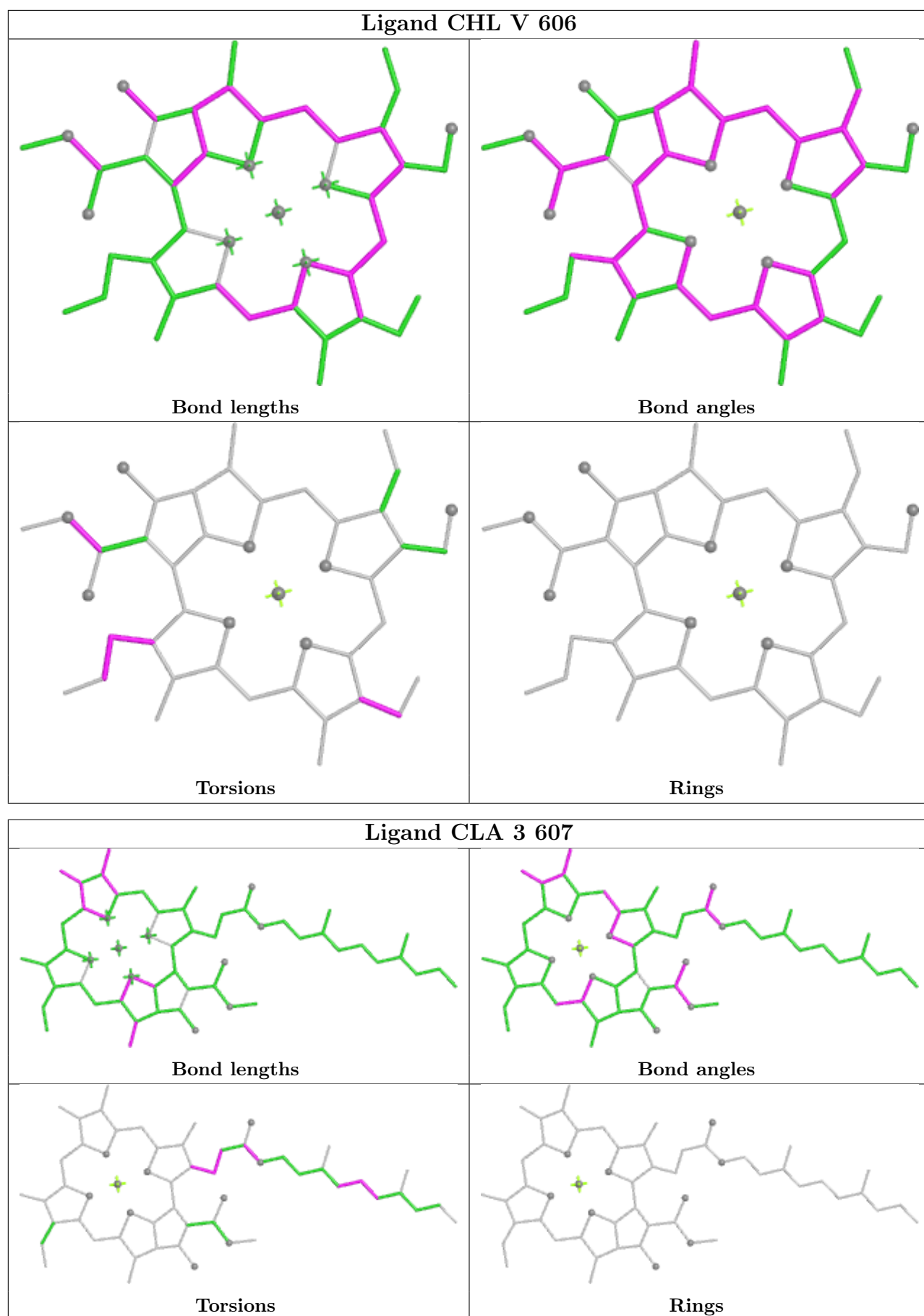


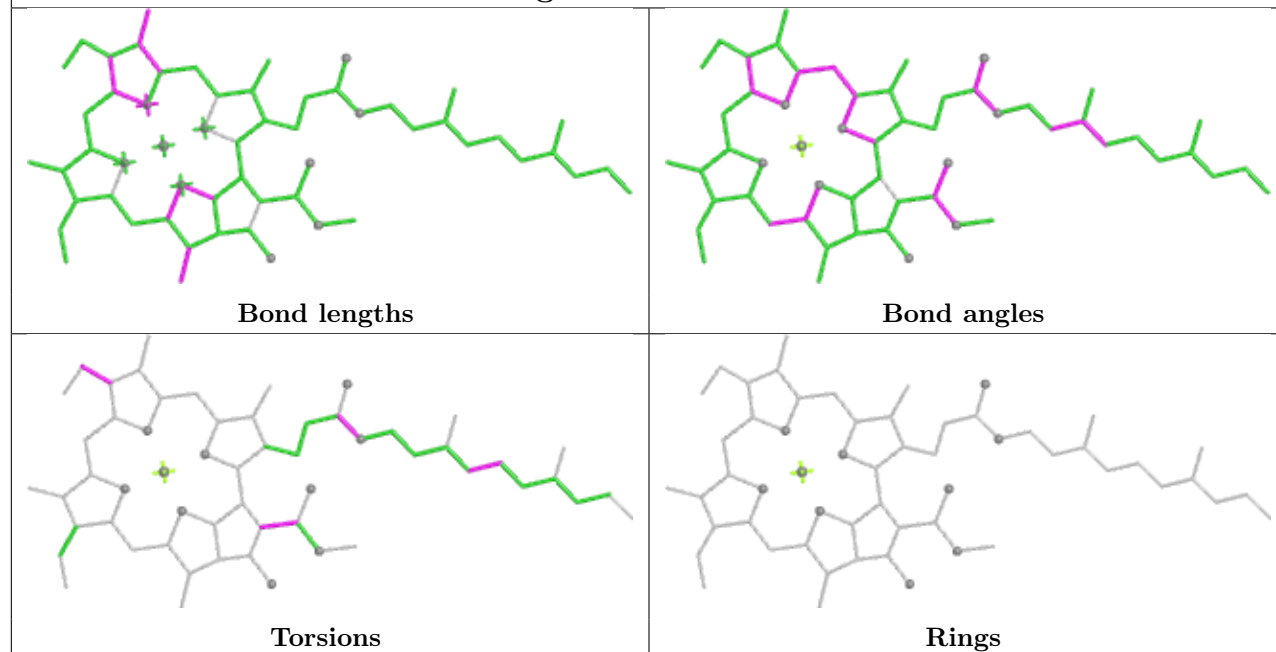
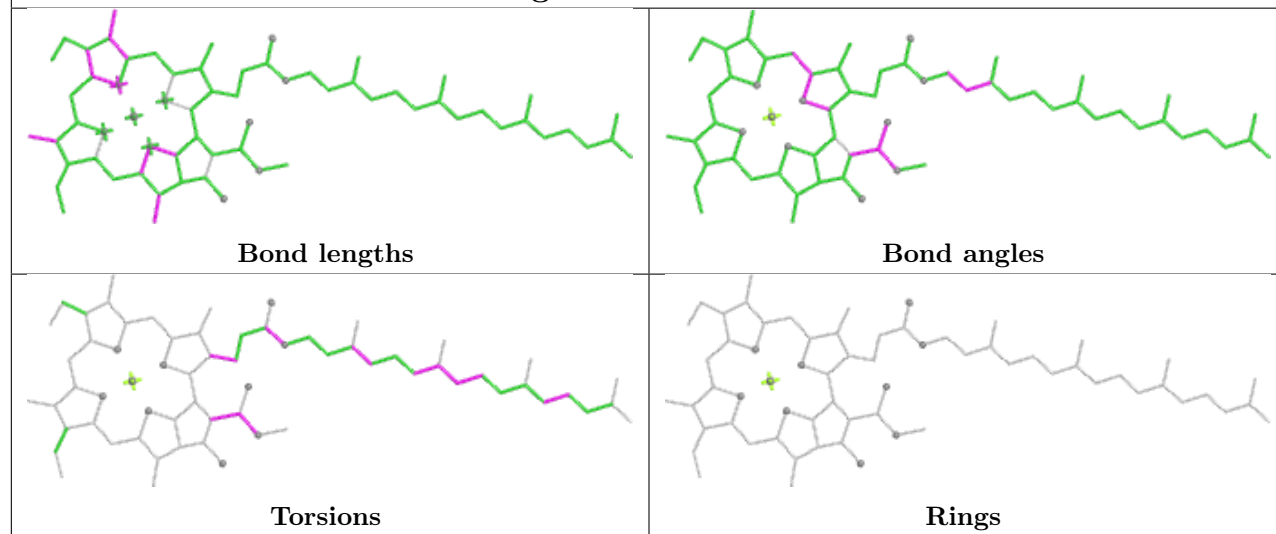
Rings

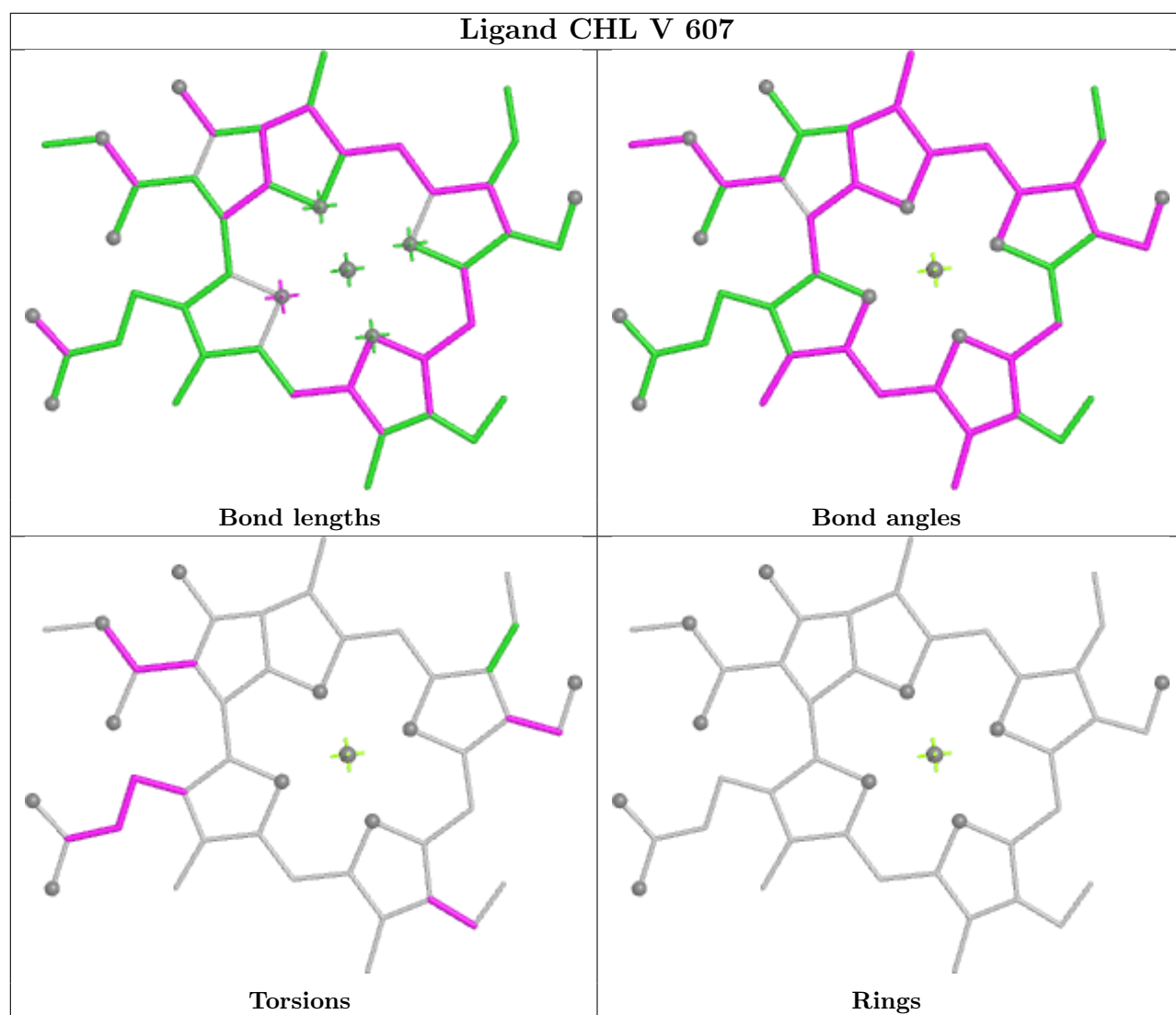


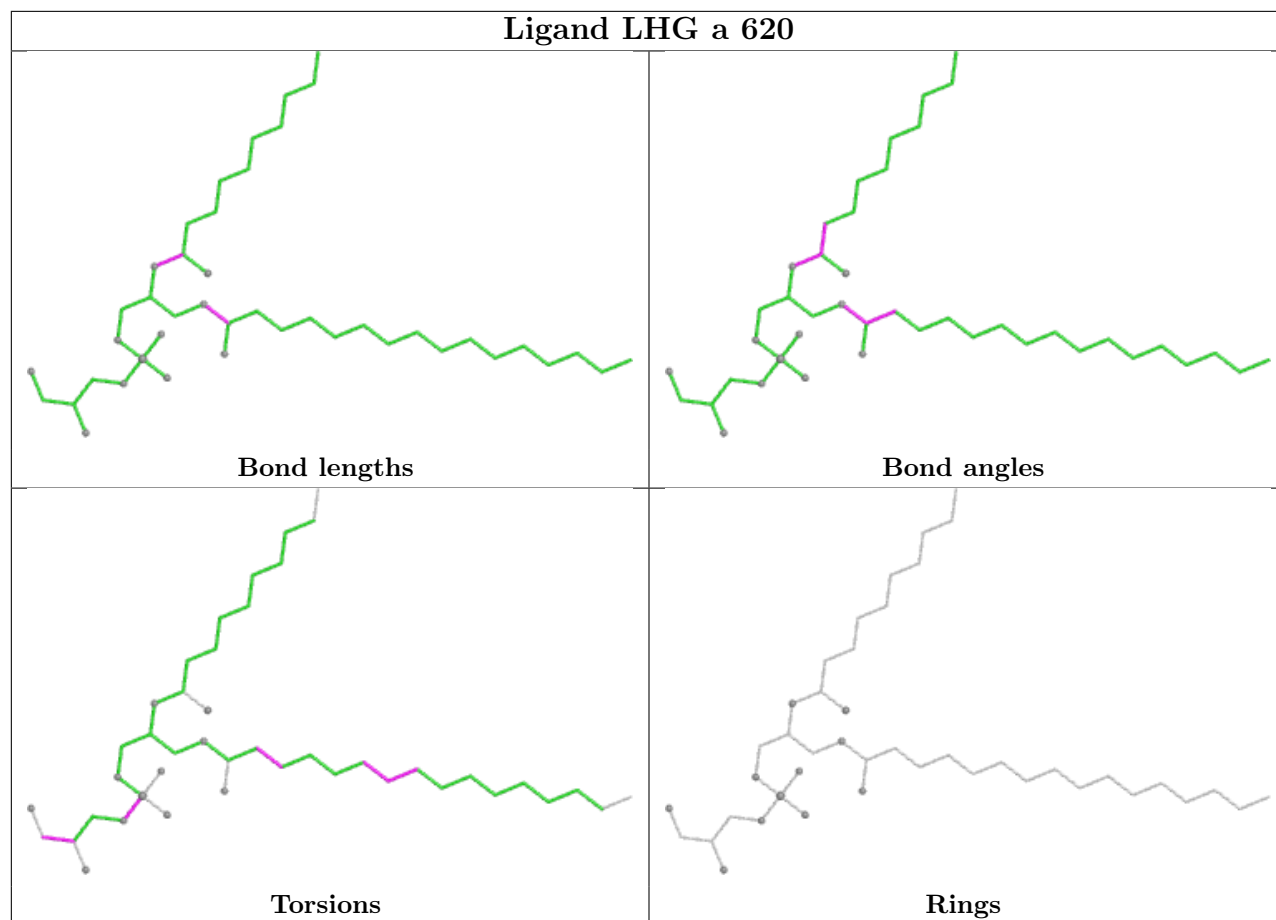
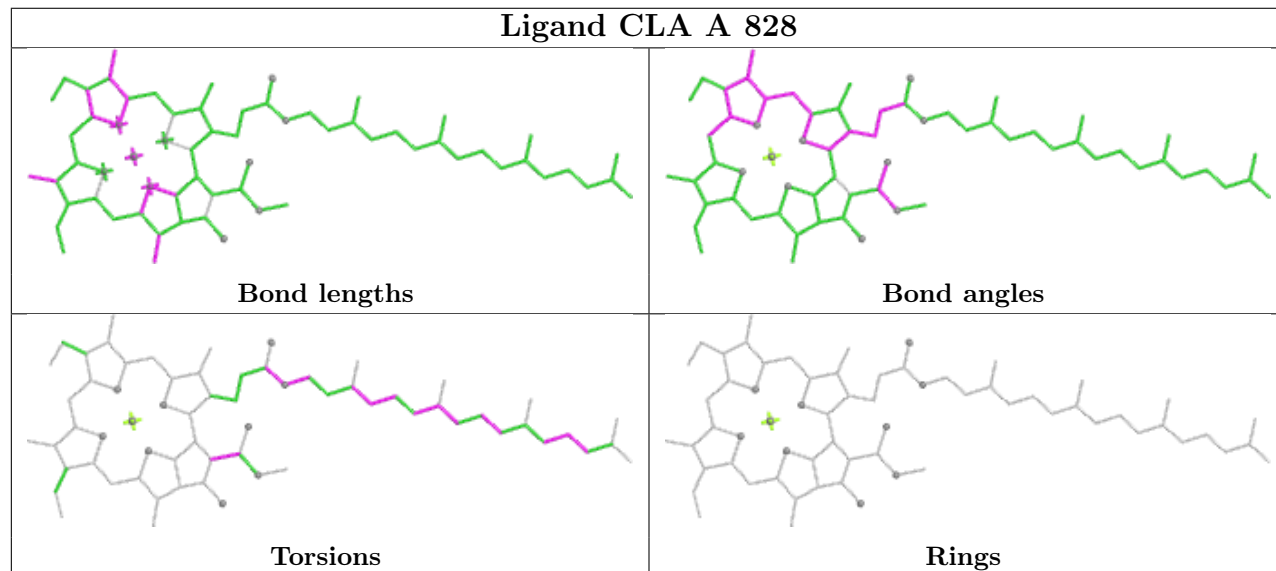


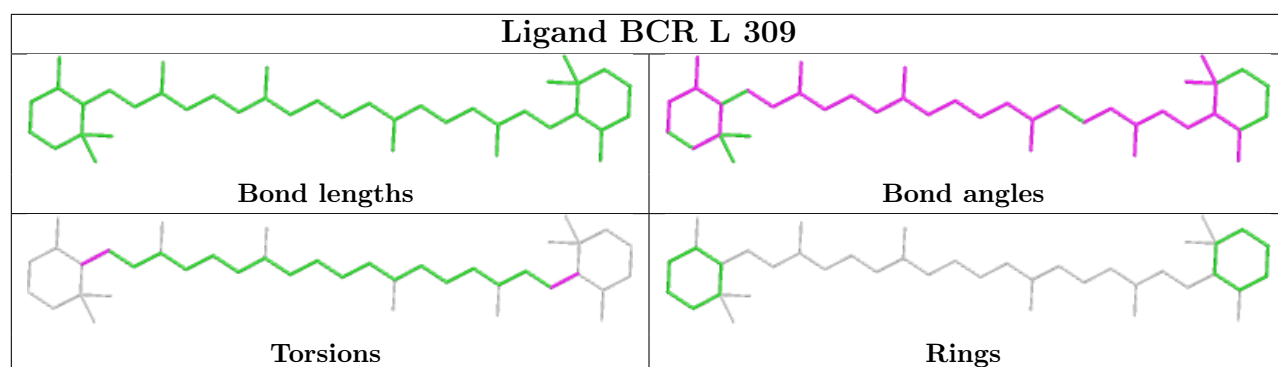
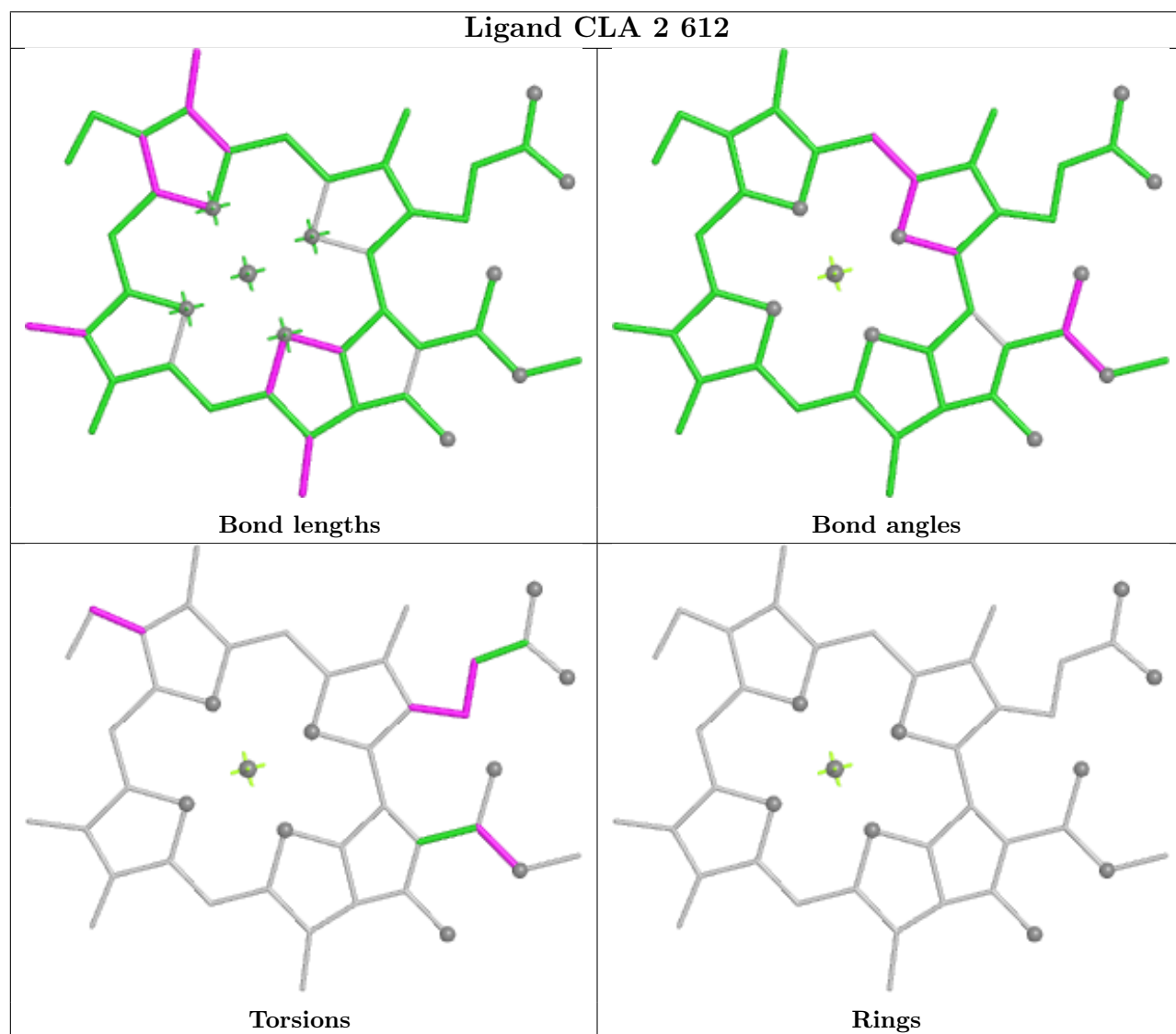




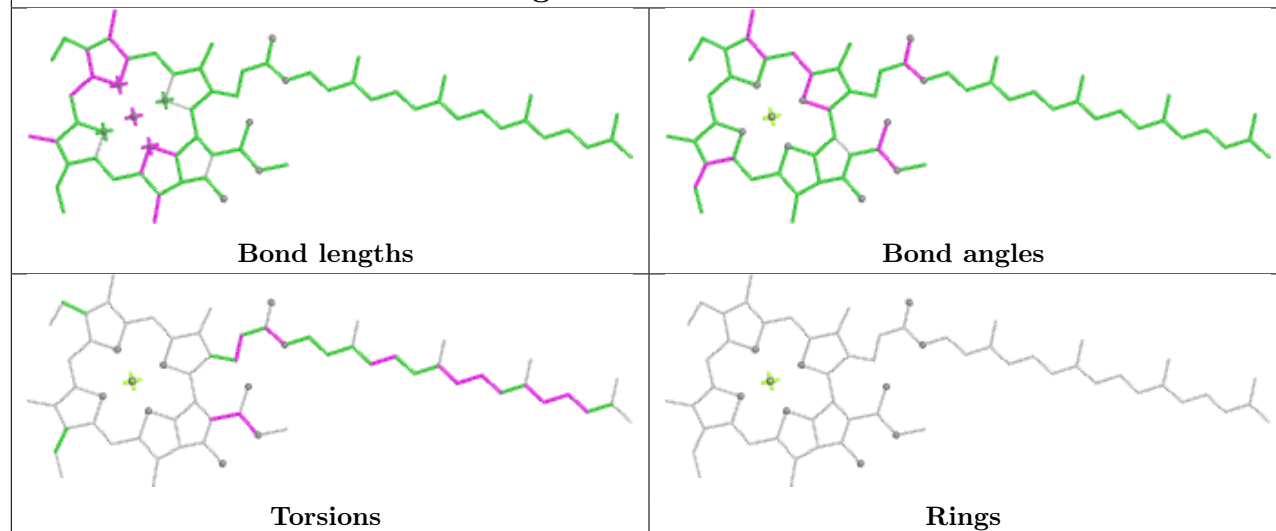
**Ligand CLA 1 611****Ligand CLA A 811**



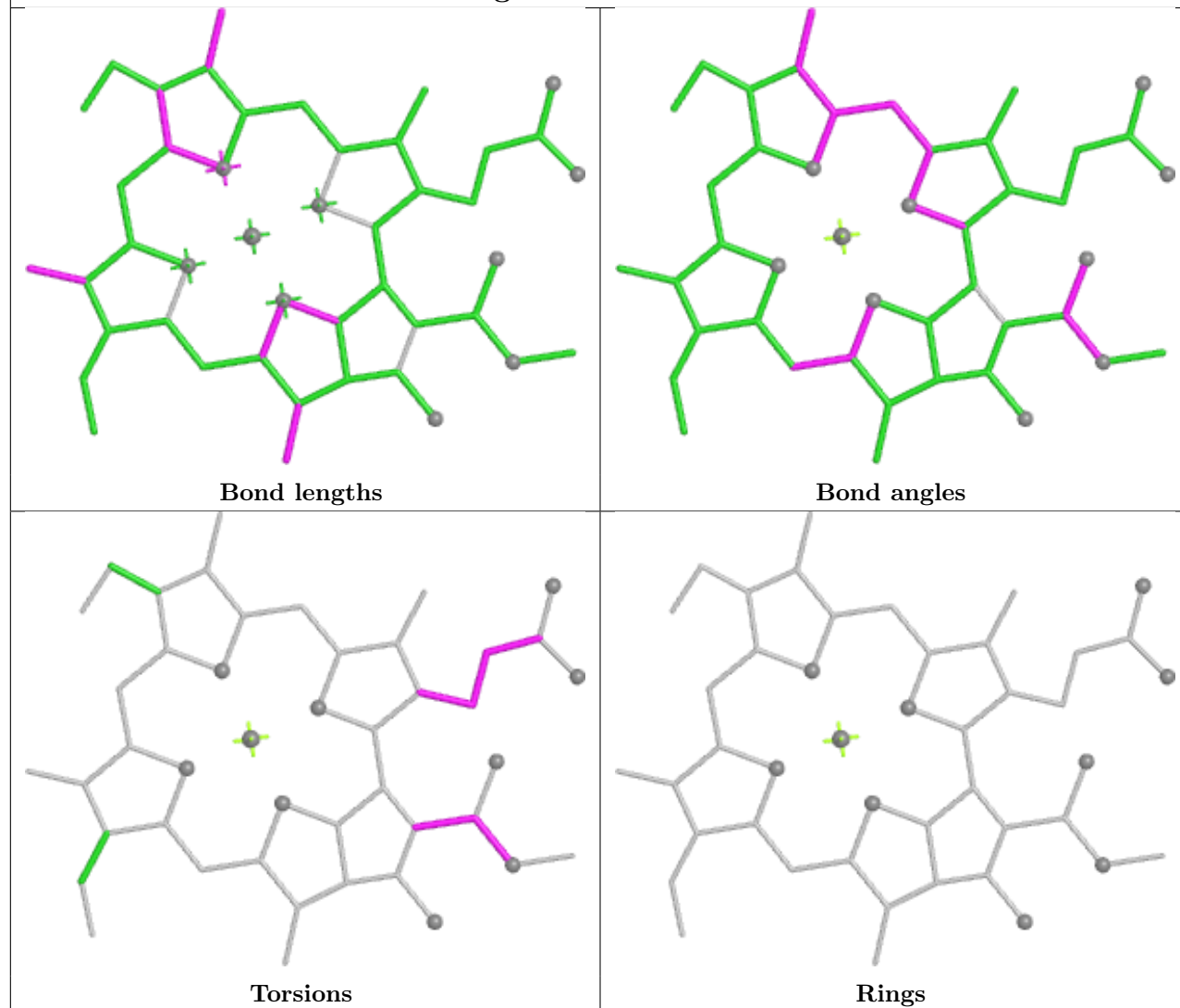
**Ligand LHG a 620****Ligand CLA A 828**

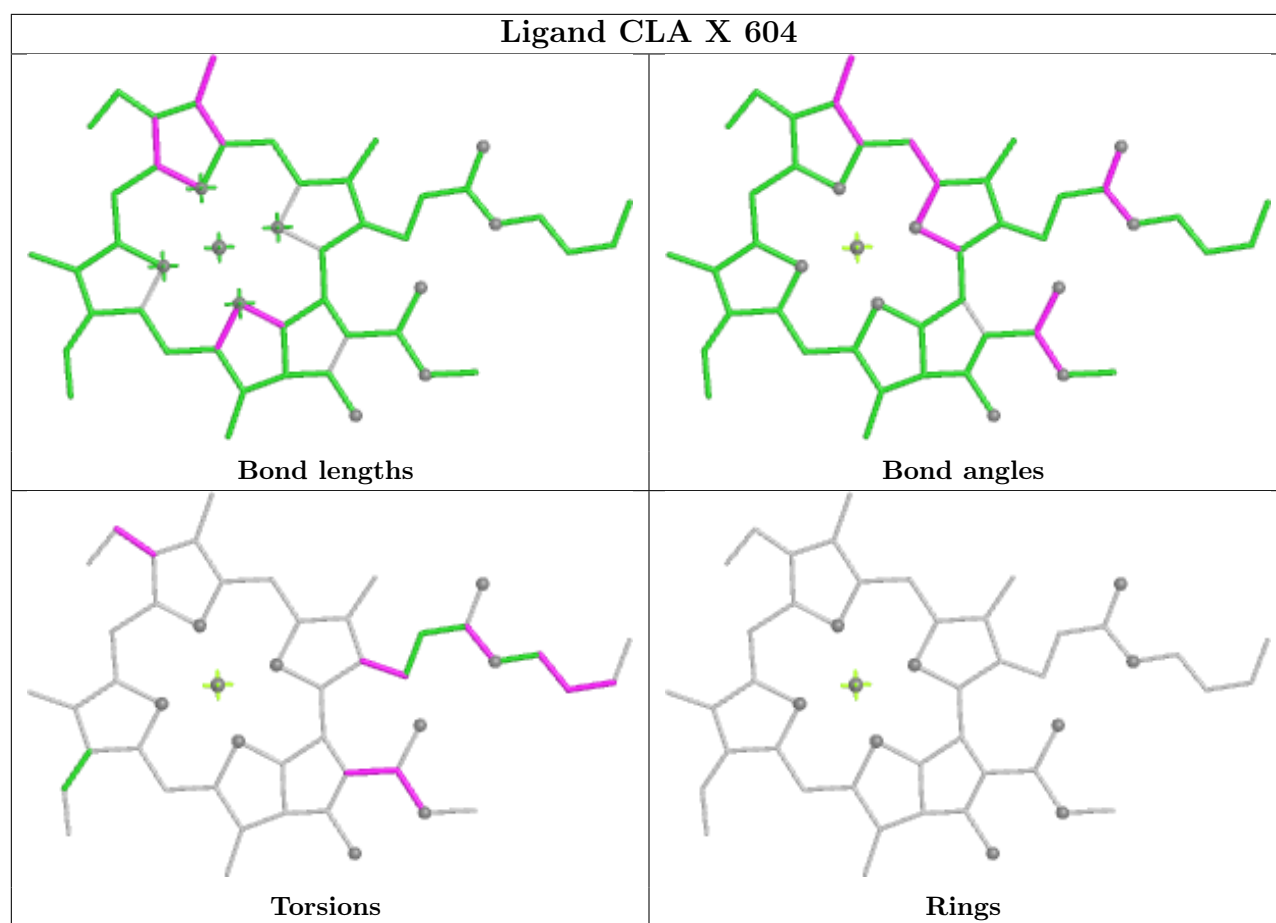


## Ligand CLA B 839

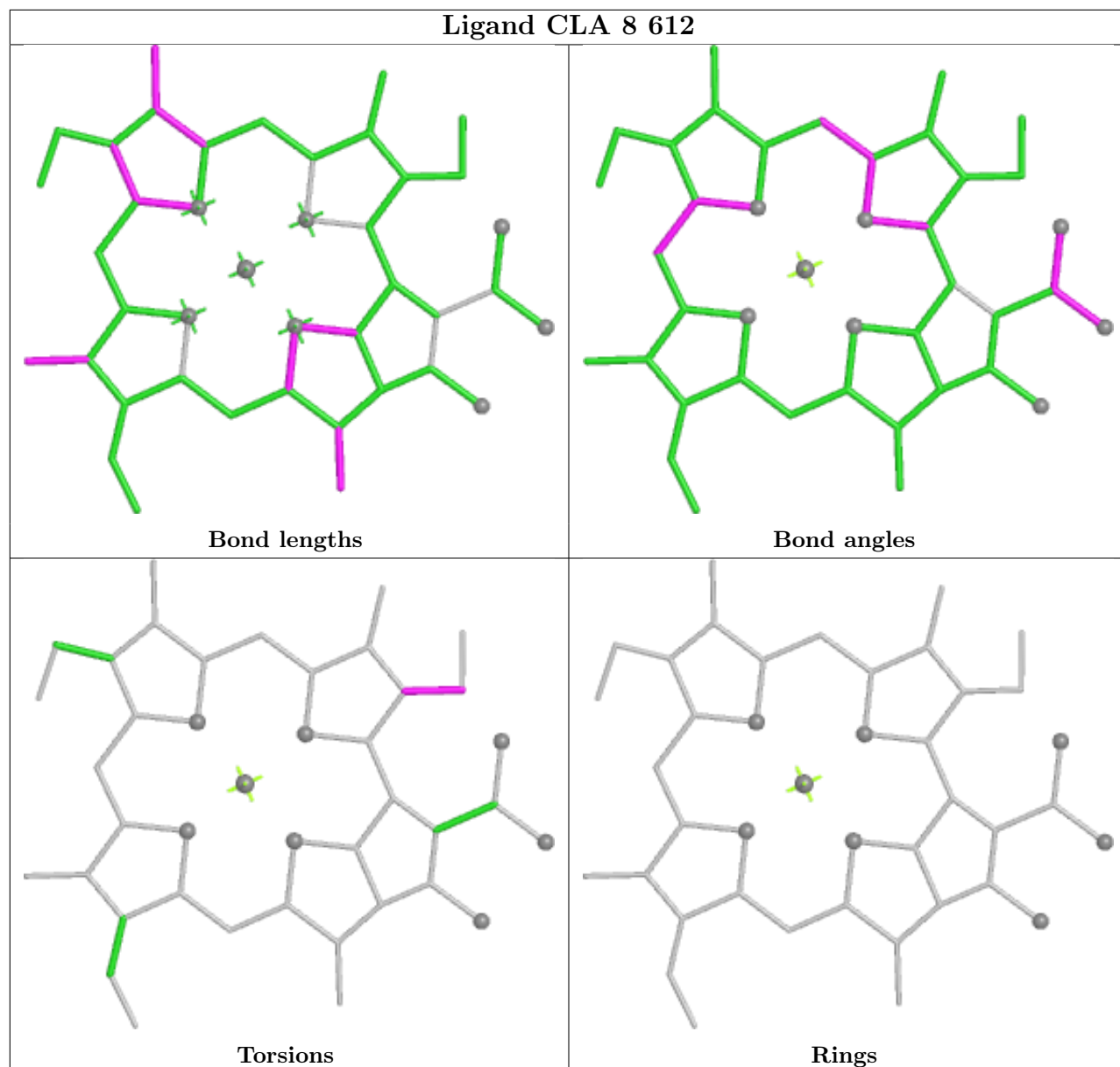


## Ligand CLA L 302



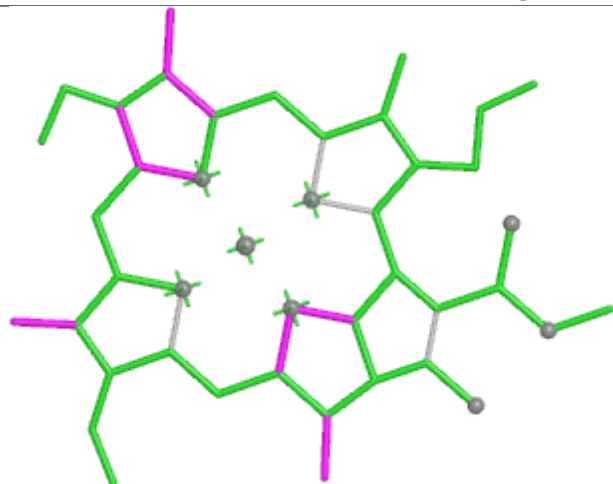


## Ligand CLA 8 612

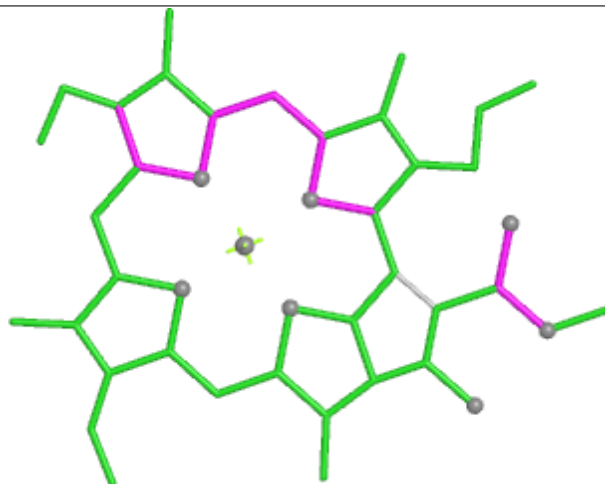




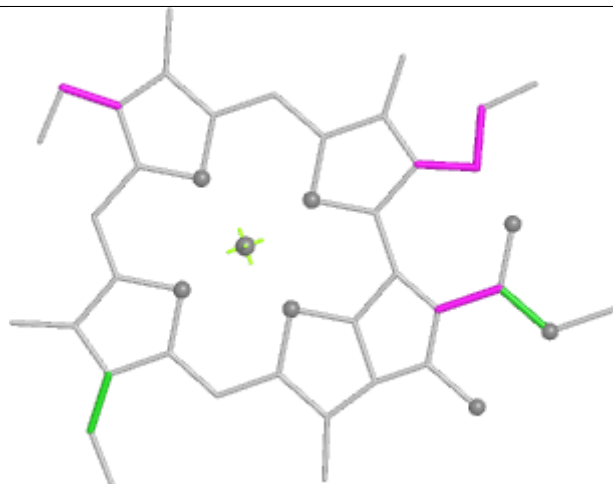
## Ligand CLA B 812



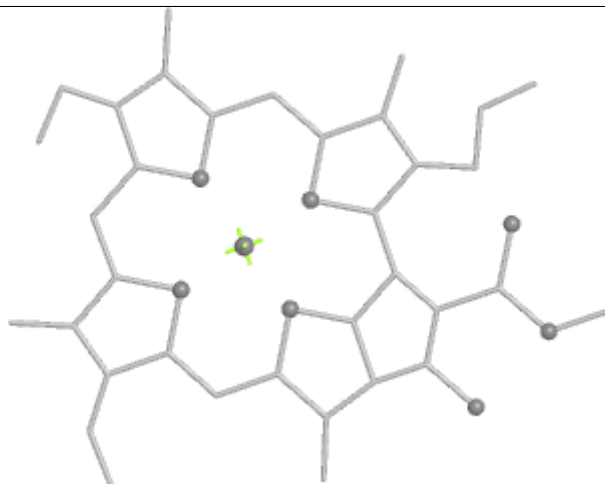
Bond lengths



Bond angles

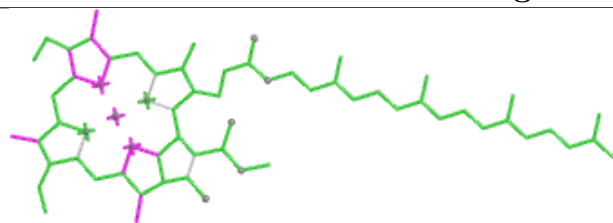


Torsions

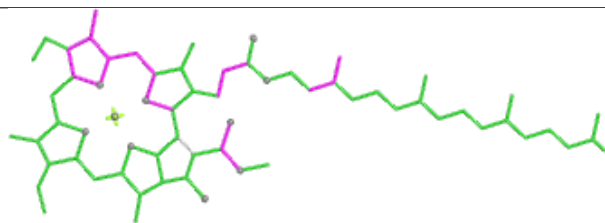


Rings

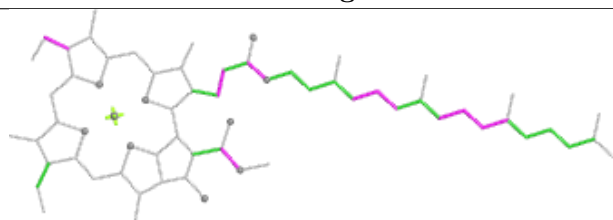
## Ligand CLA A 834



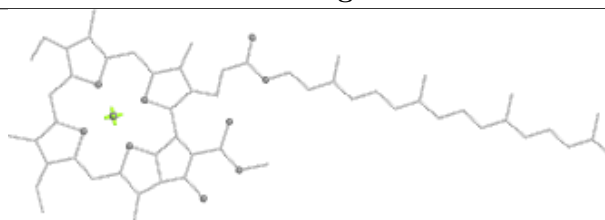
Bond lengths



Bond angles

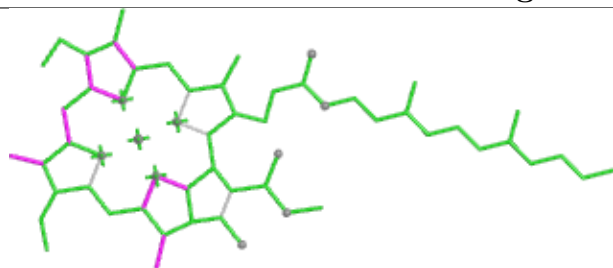


Torsions

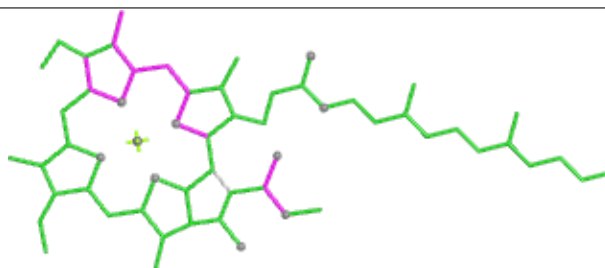


Rings

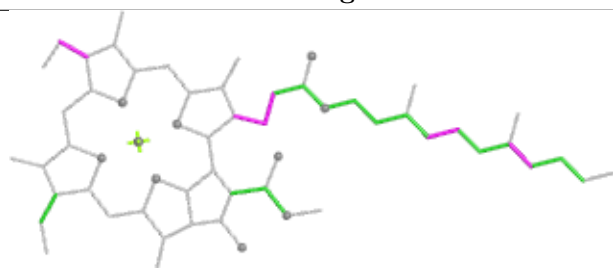
## Ligand CLA Z 602



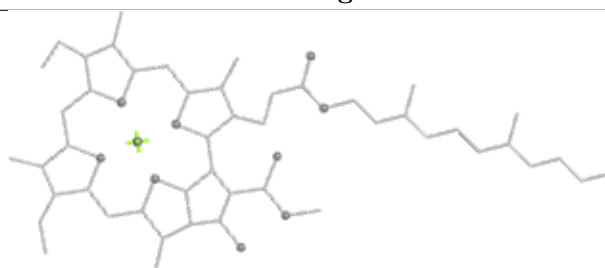
Bond lengths



Bond angles

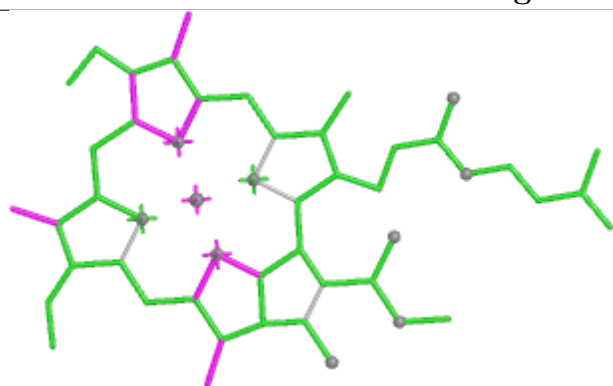


Torsions

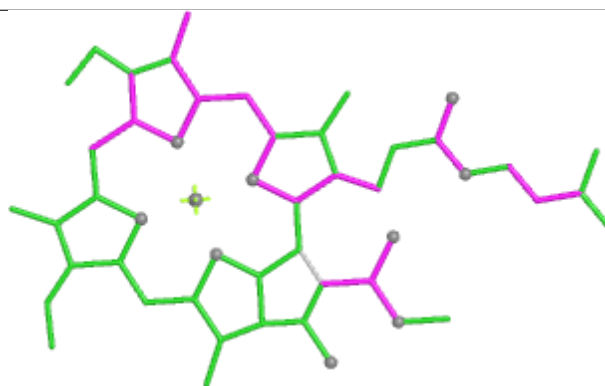


Rings

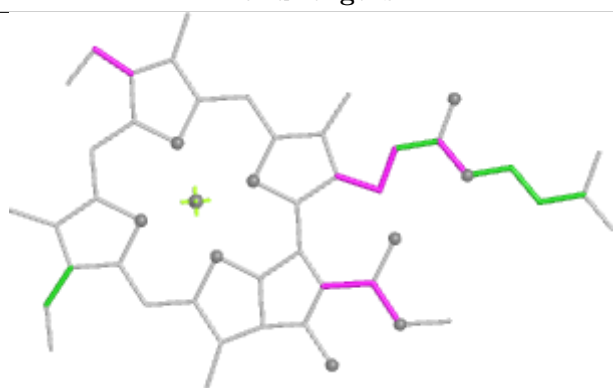
## Ligand CLA A 832



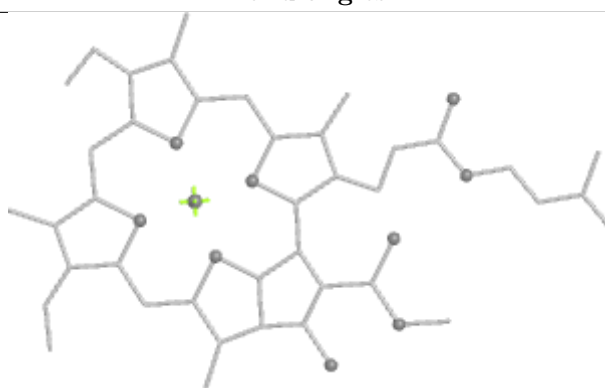
Bond lengths



Bond angles

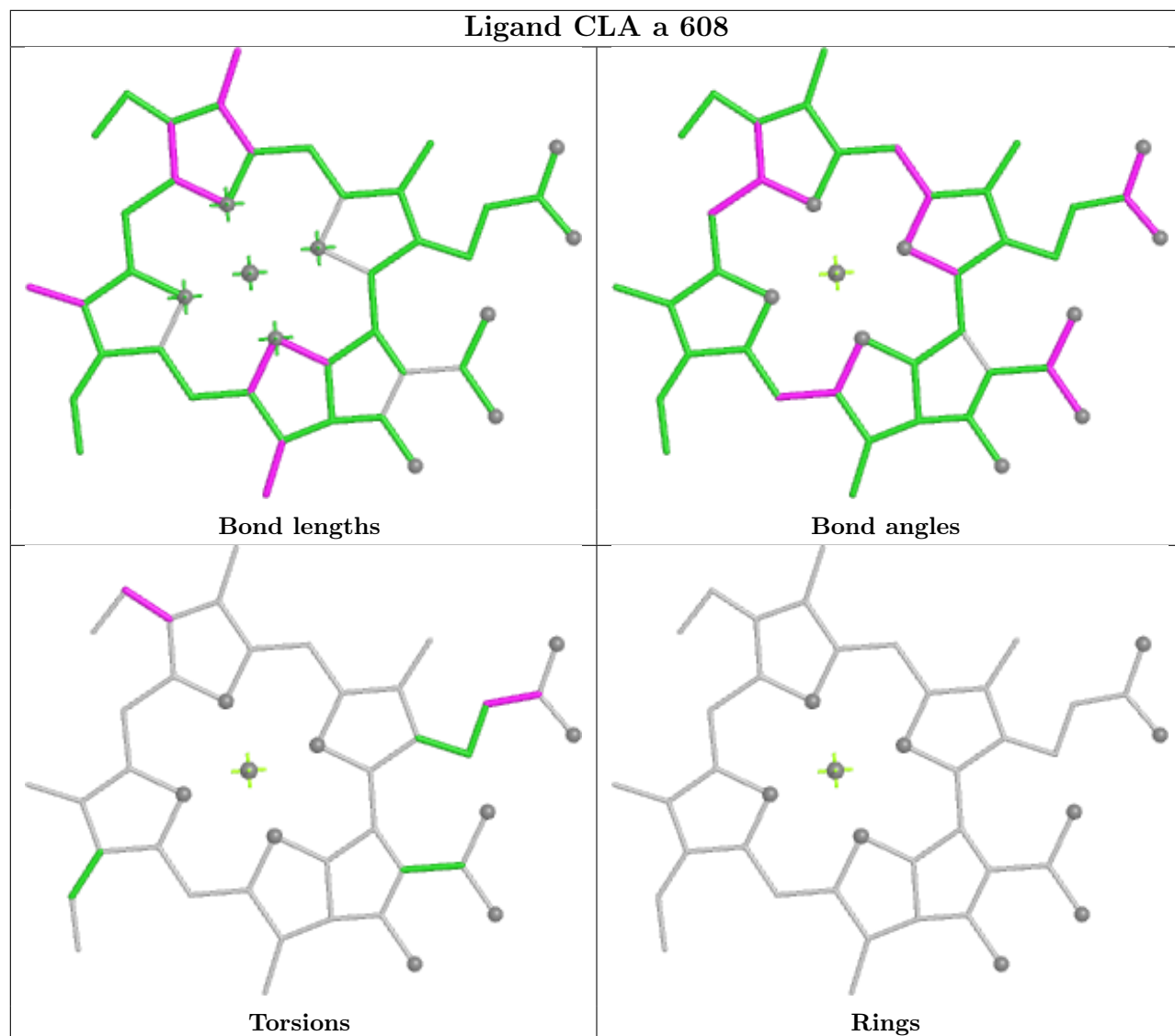


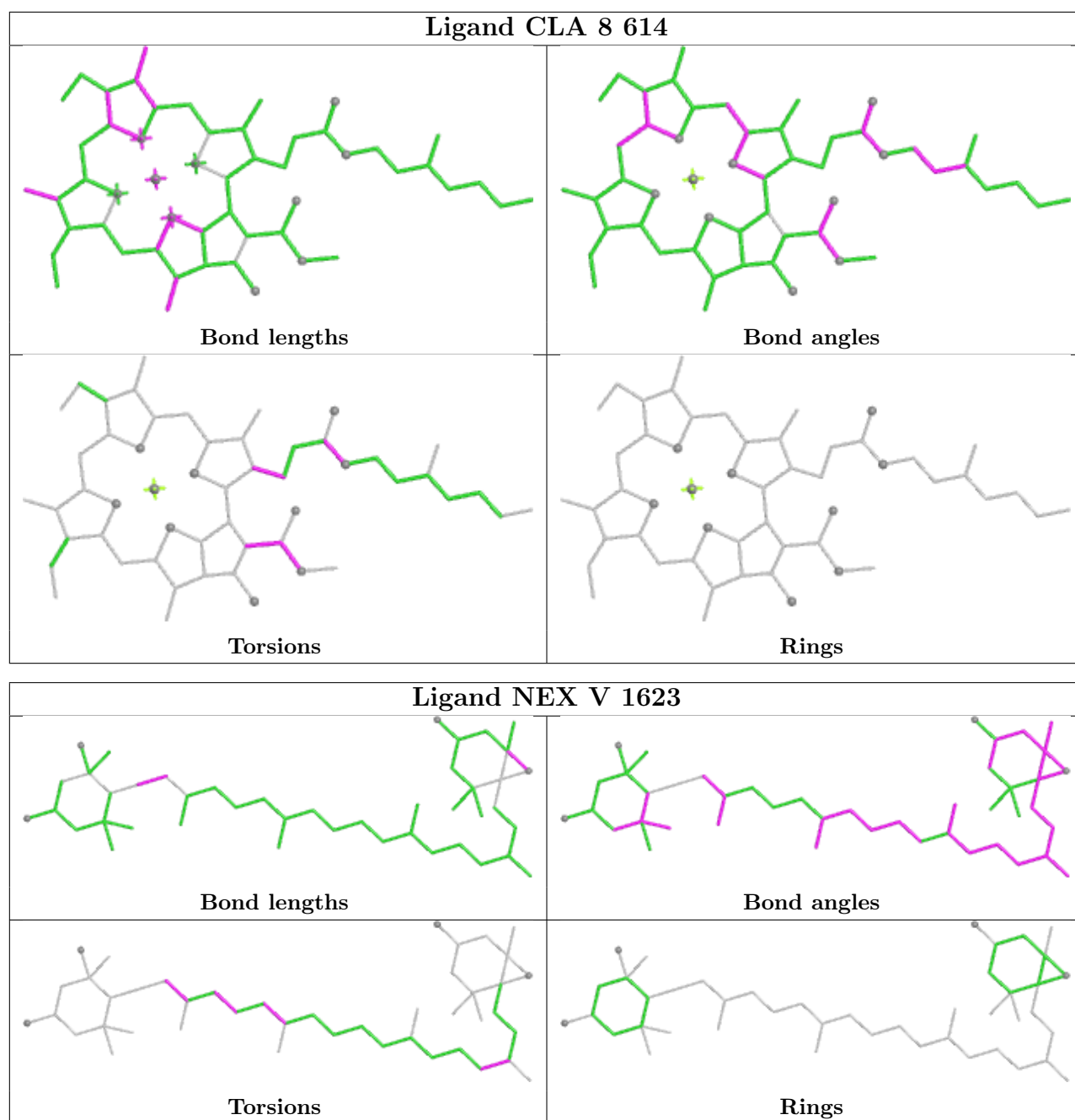
Torsions



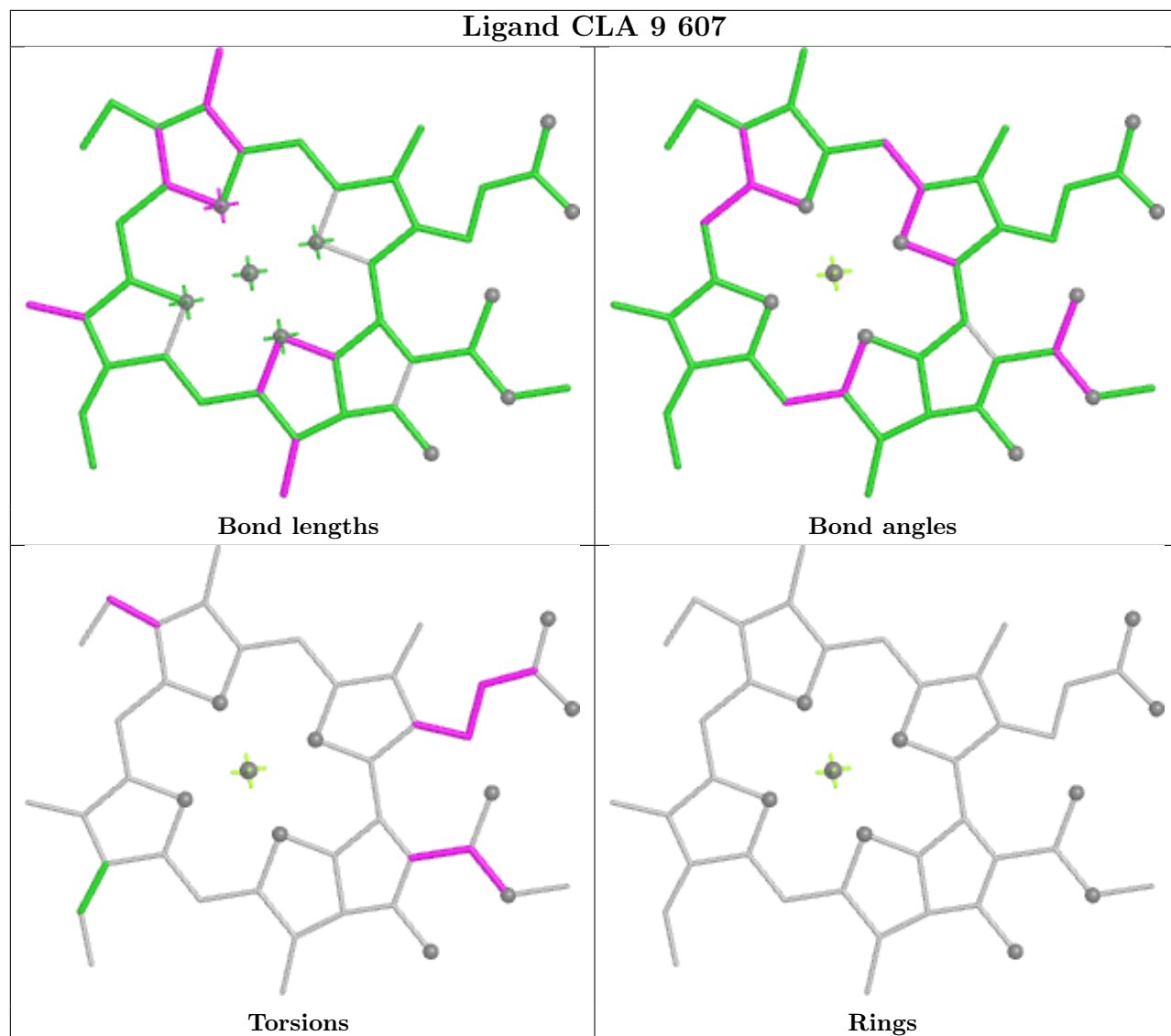
Rings

## Ligand CLA a 608

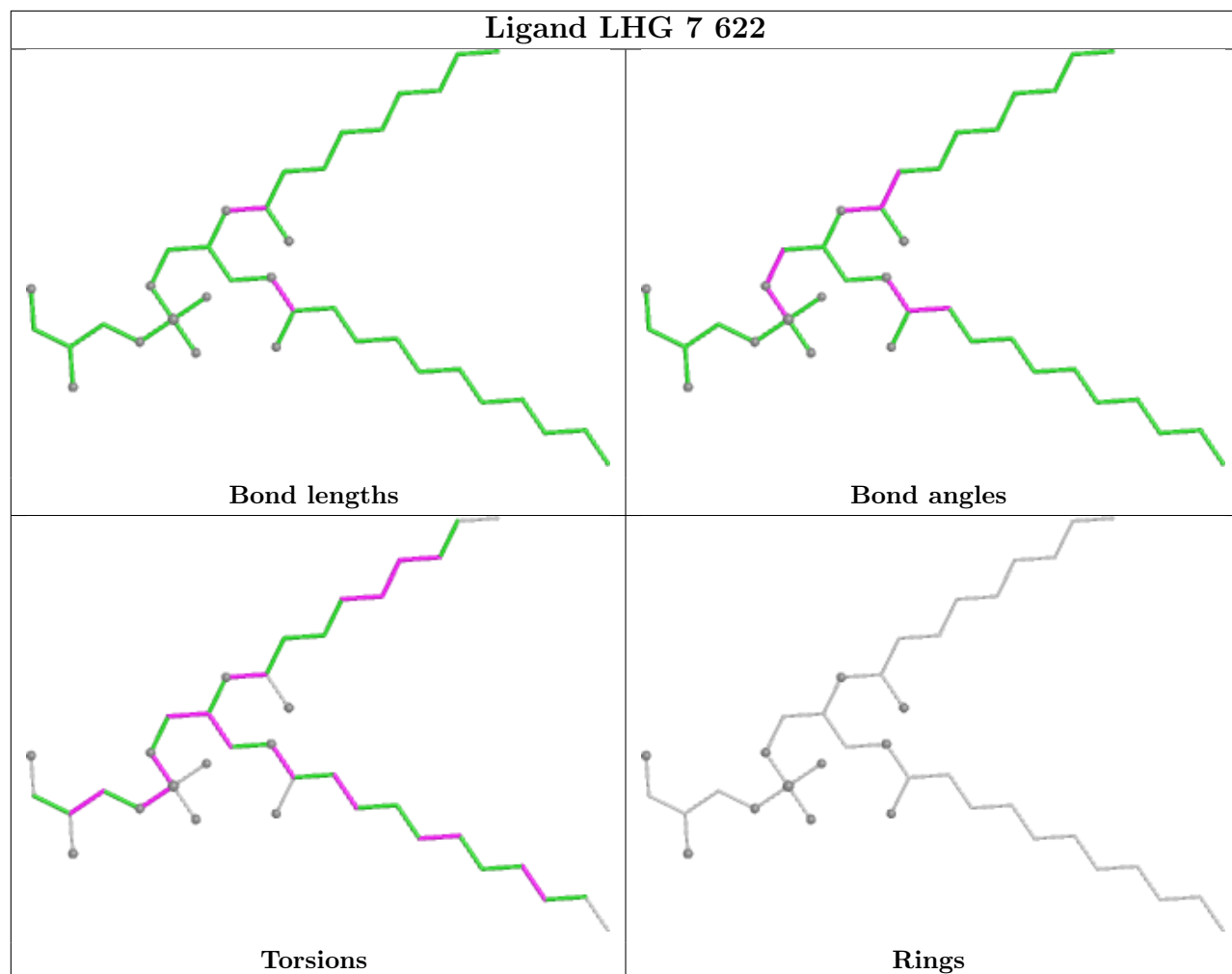




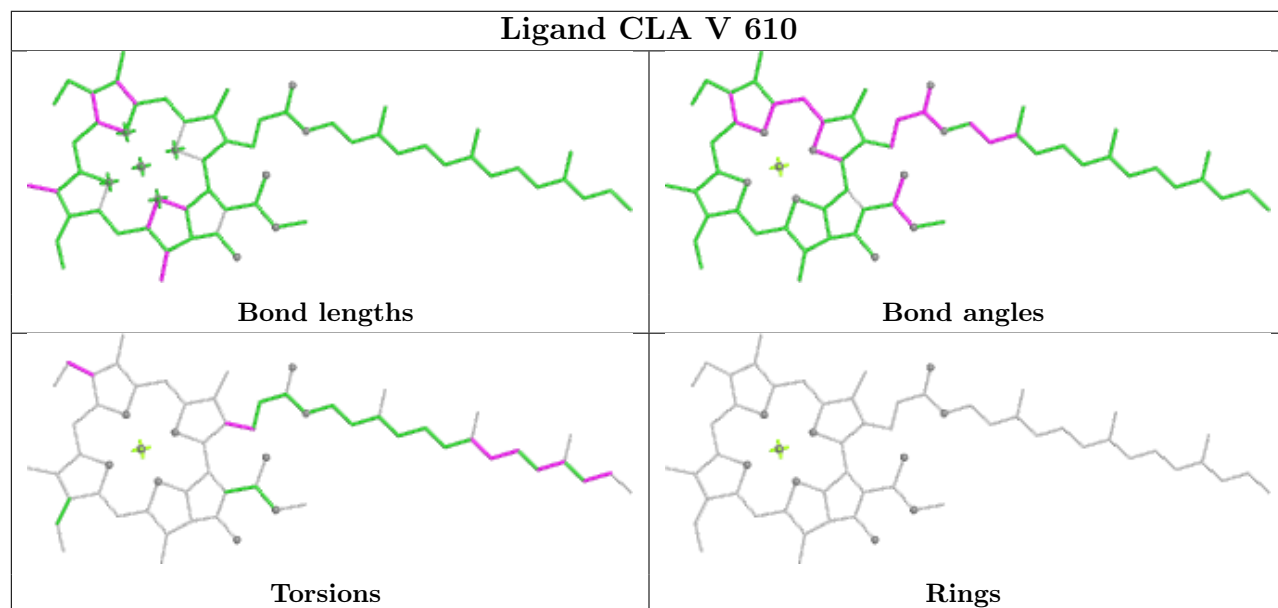
## Ligand CLA 9 607



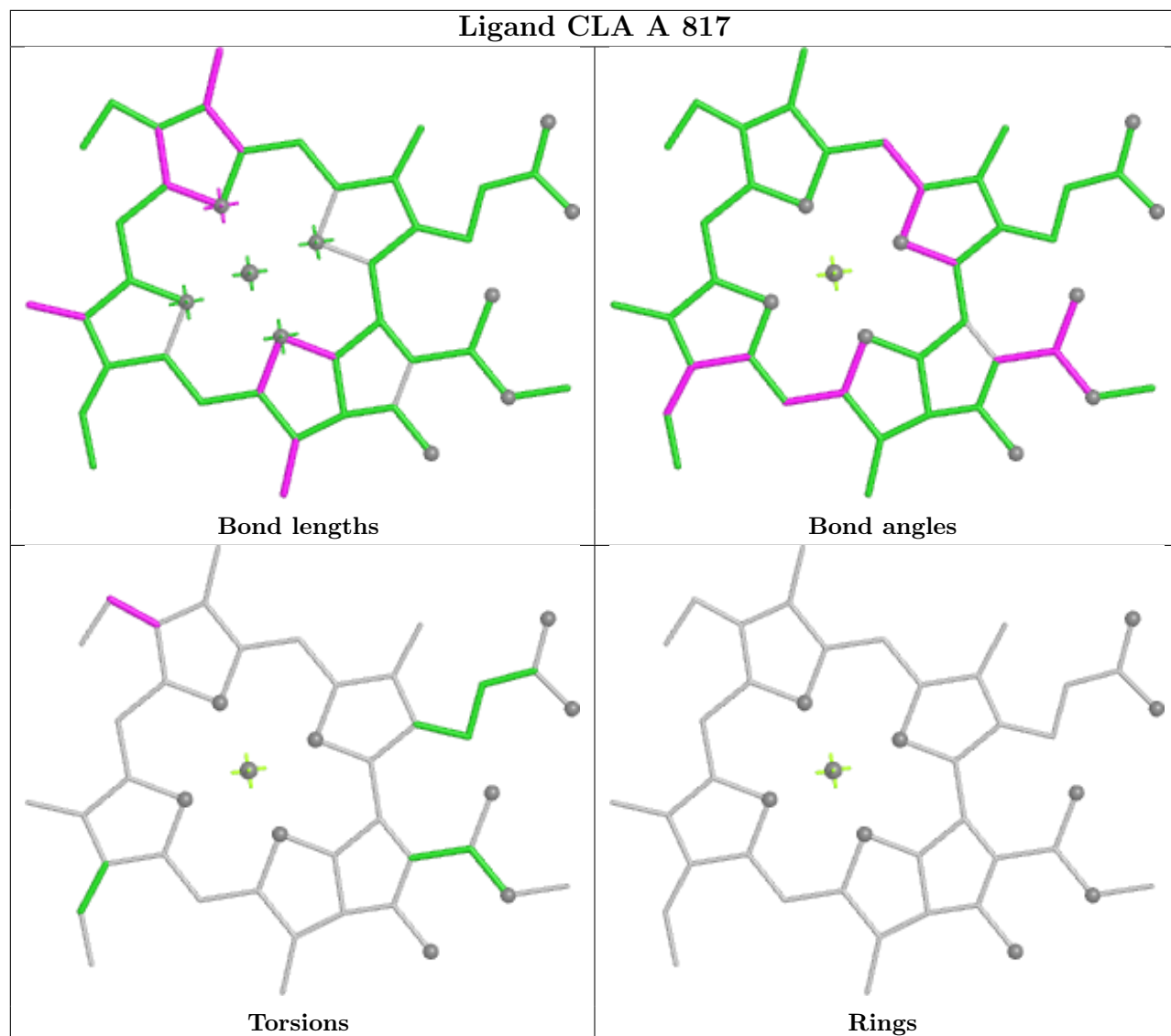
## Ligand LHG 7 622



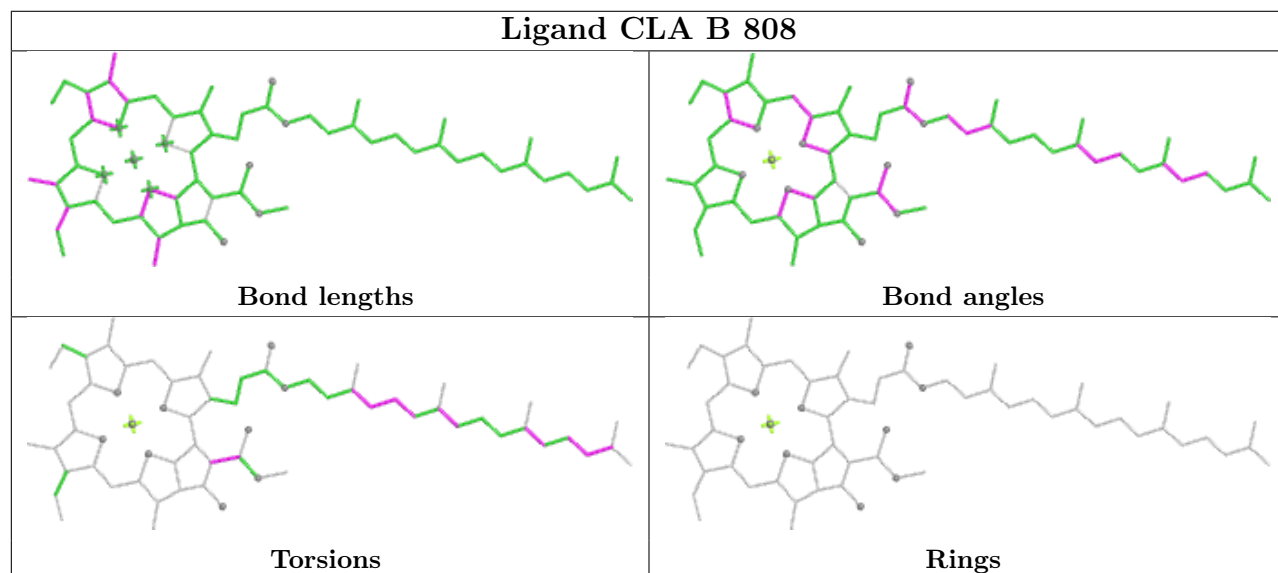
## Ligand CLA V 610



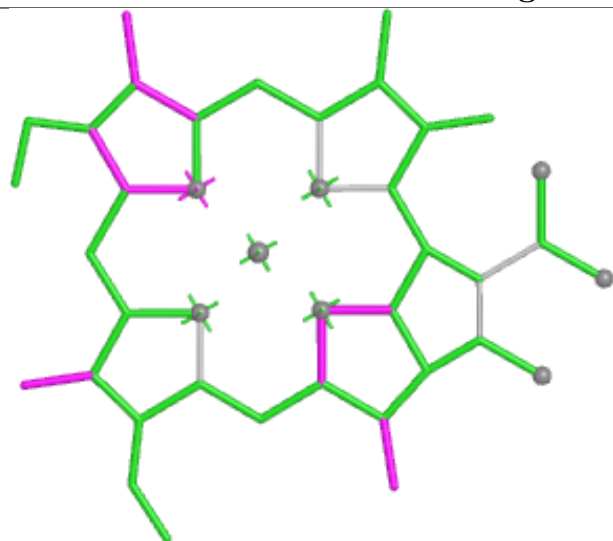
## Ligand CLA A 817



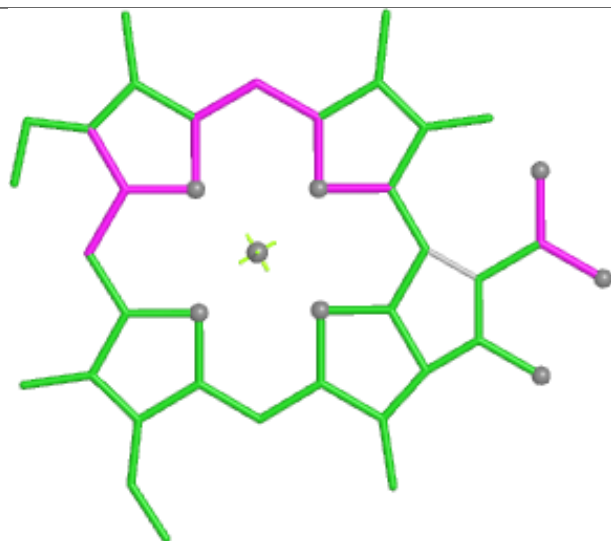
## Ligand CLA B 808



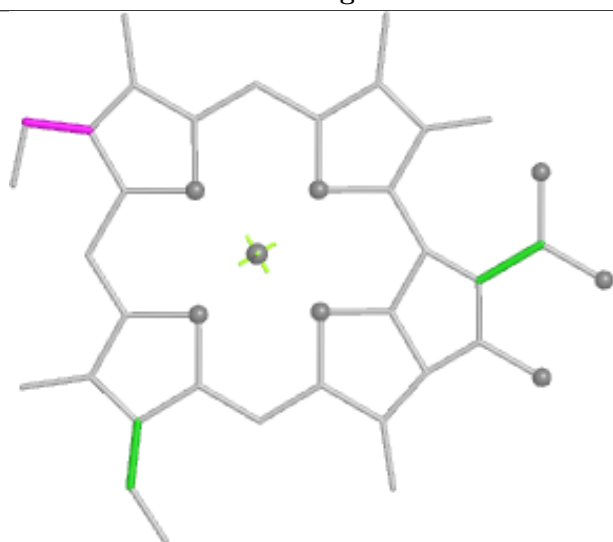
## Ligand CLA 3 614



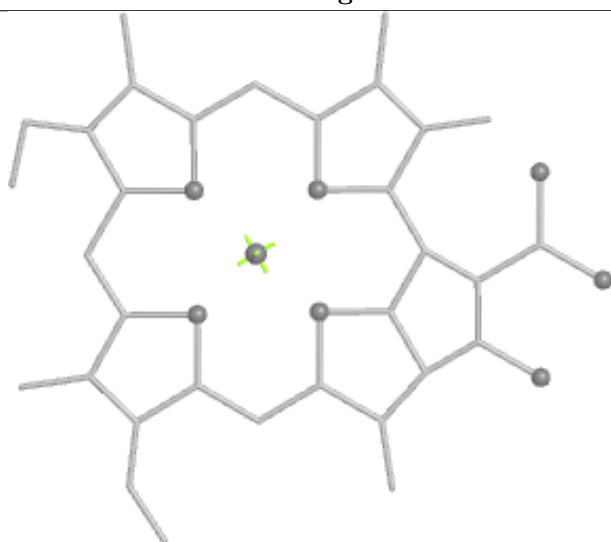
Bond lengths



Bond angles

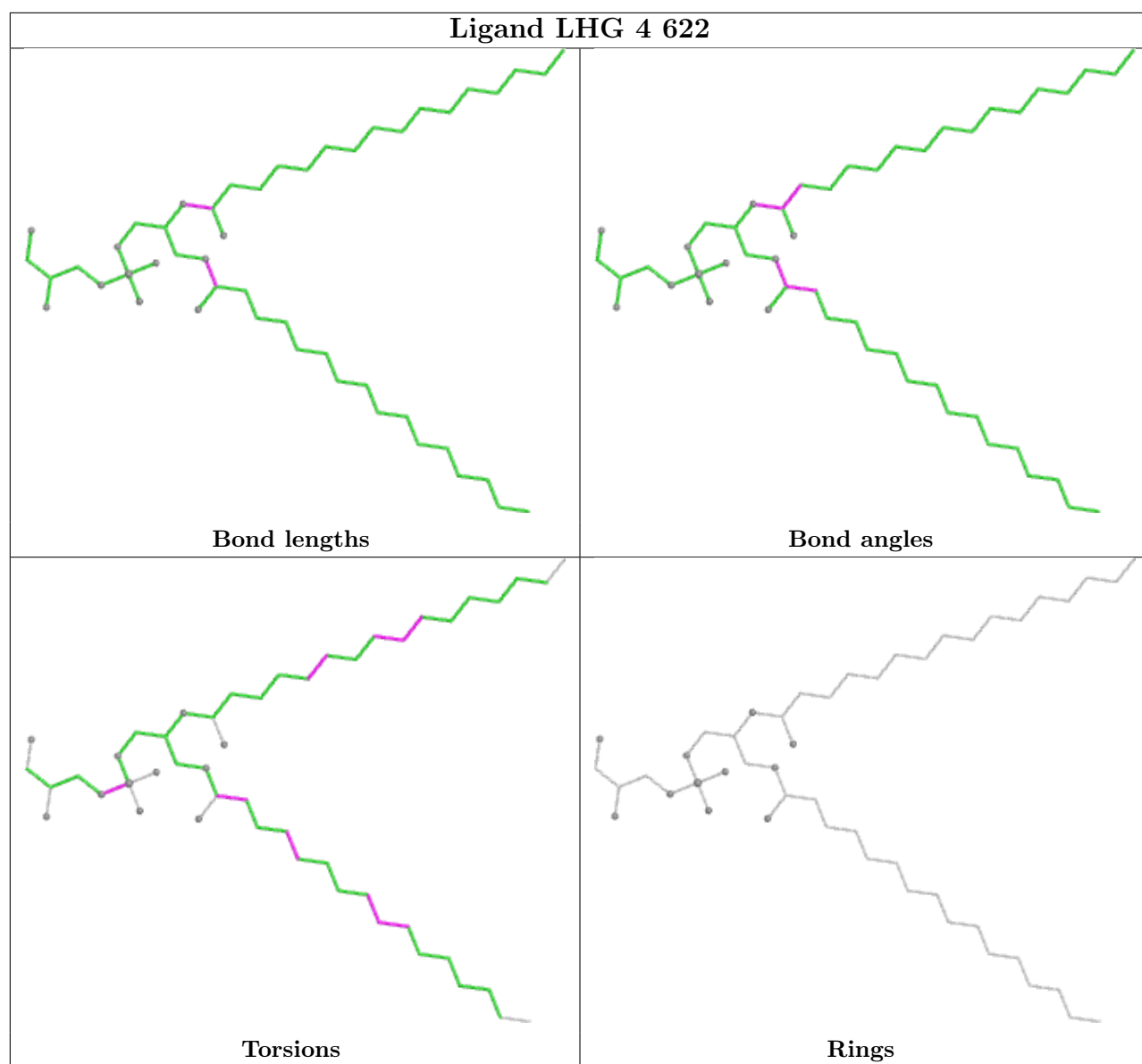


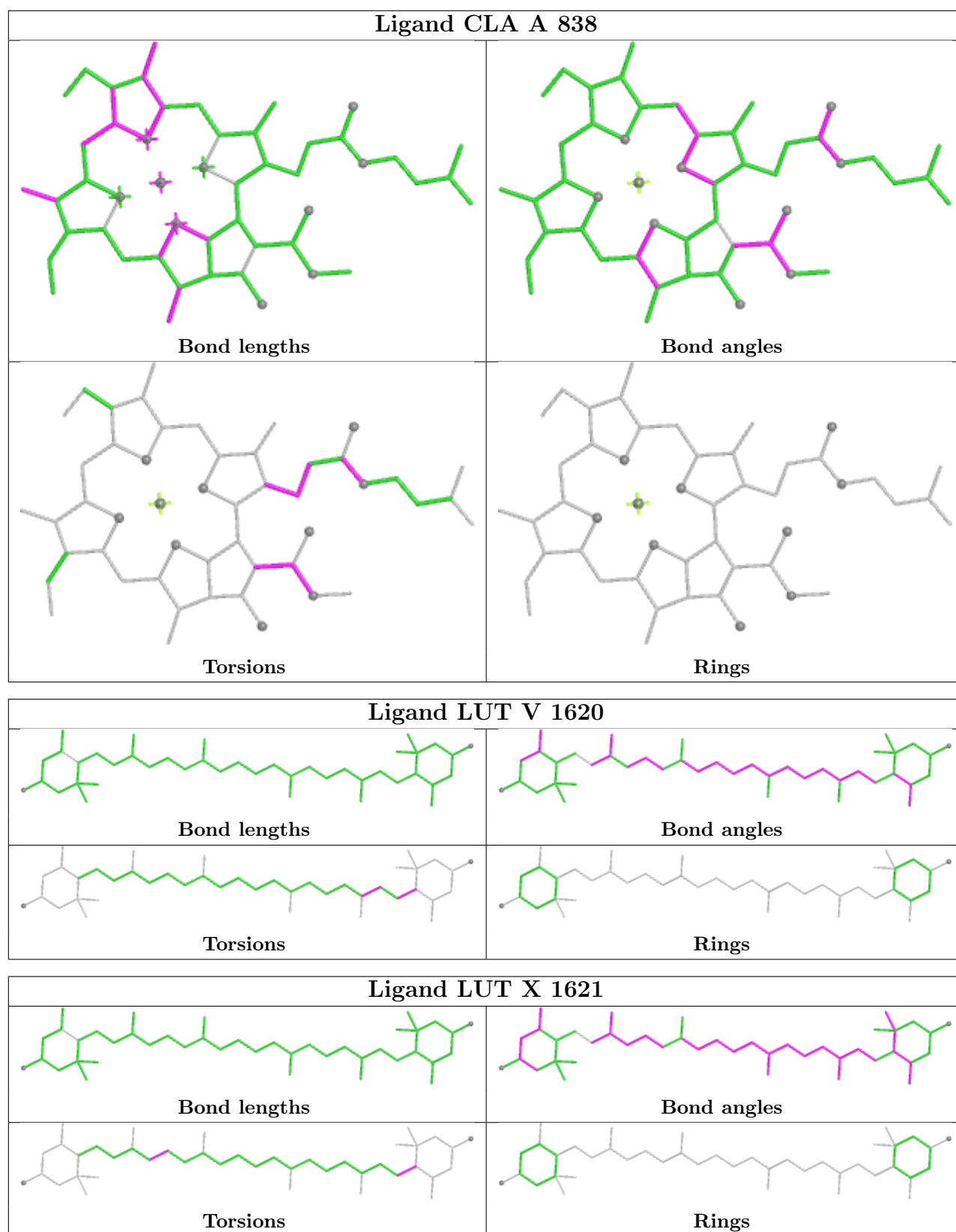
Torsions

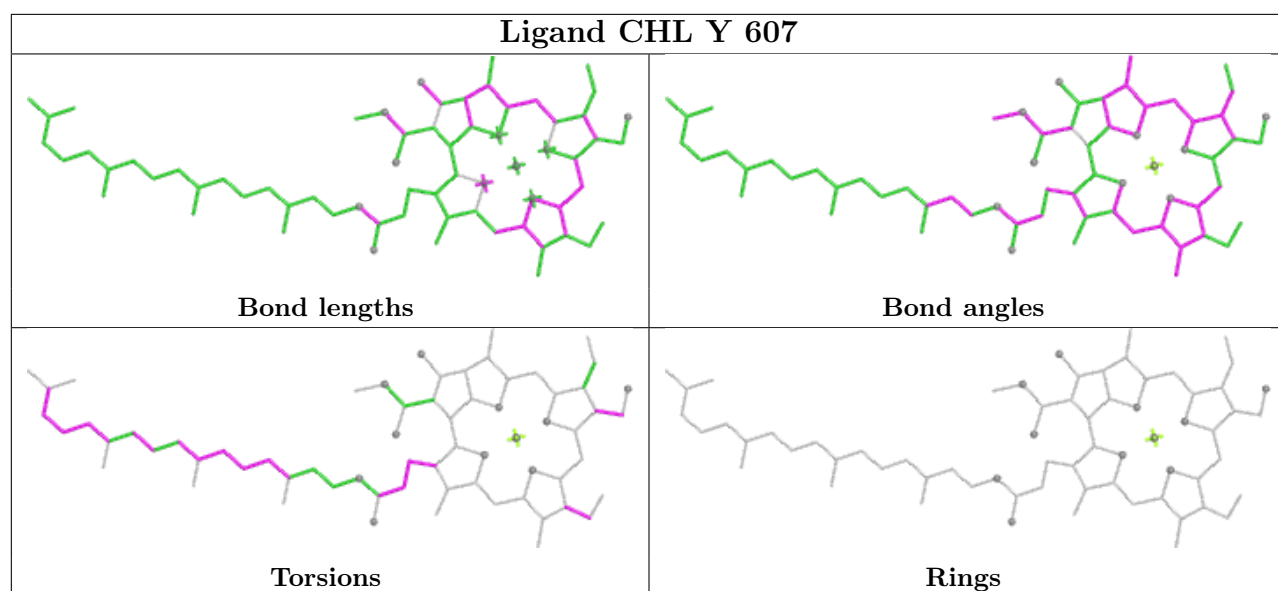
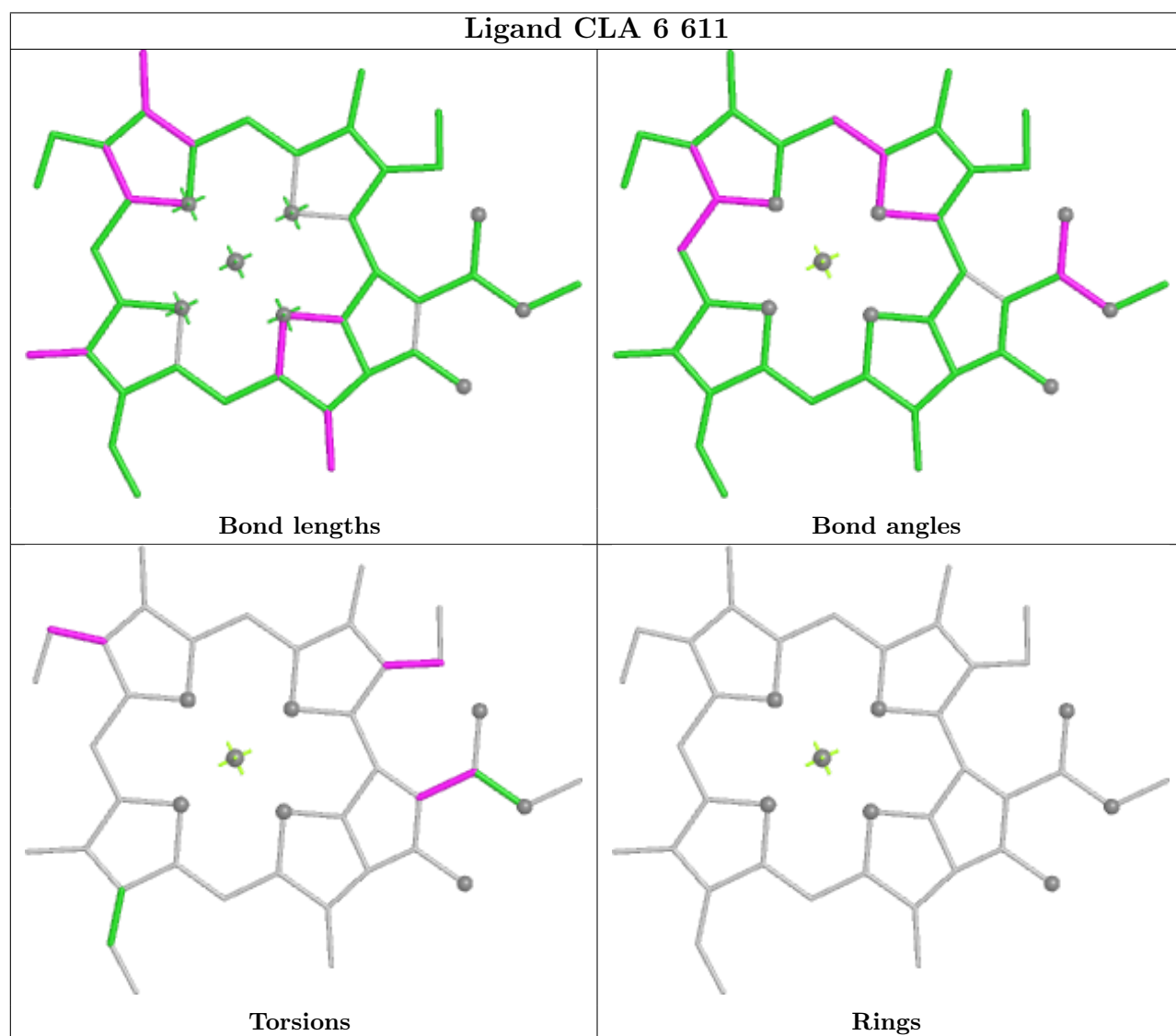


Rings

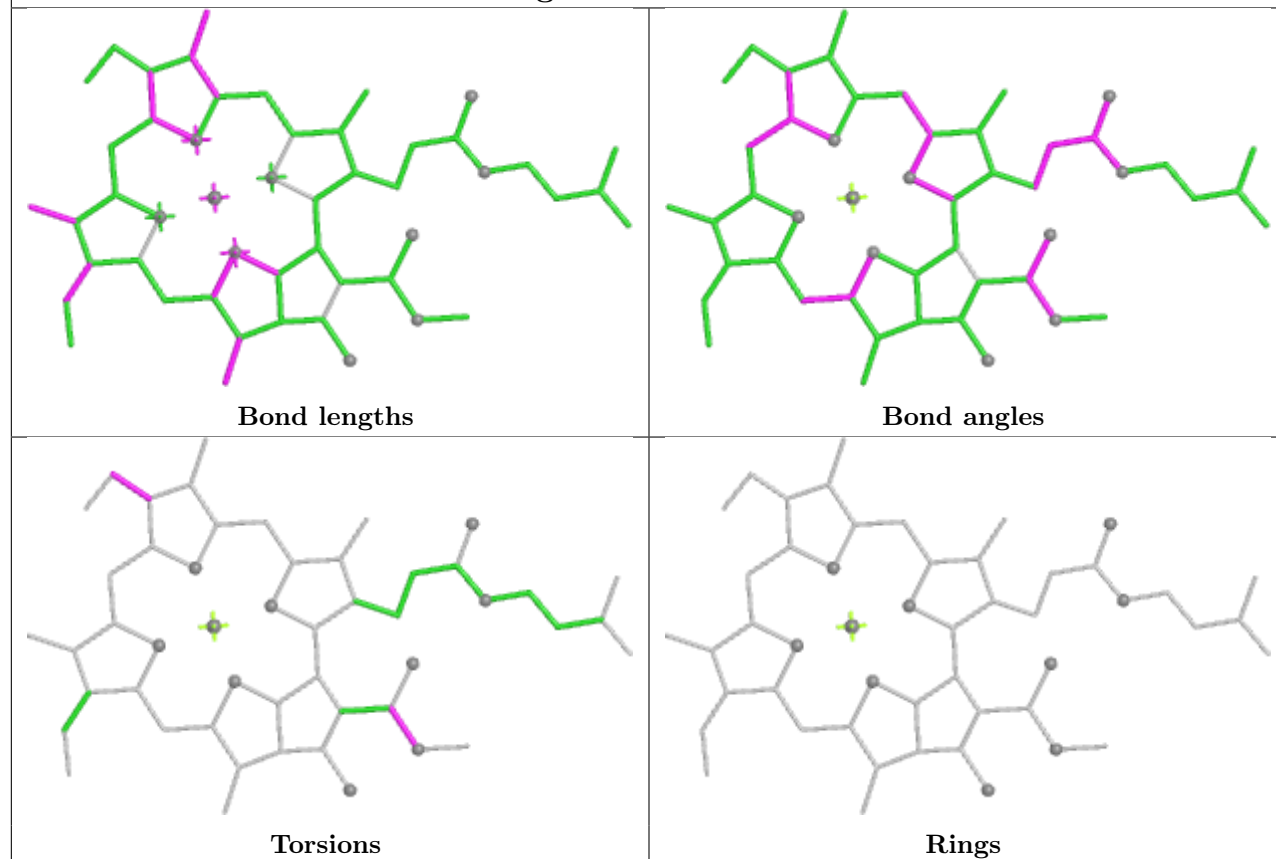




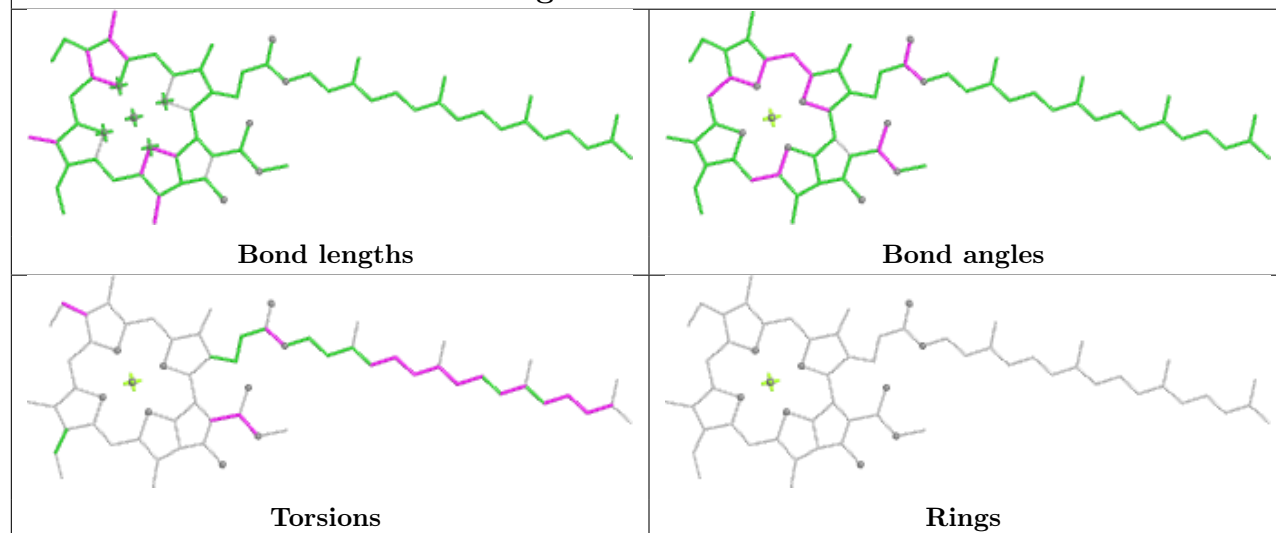


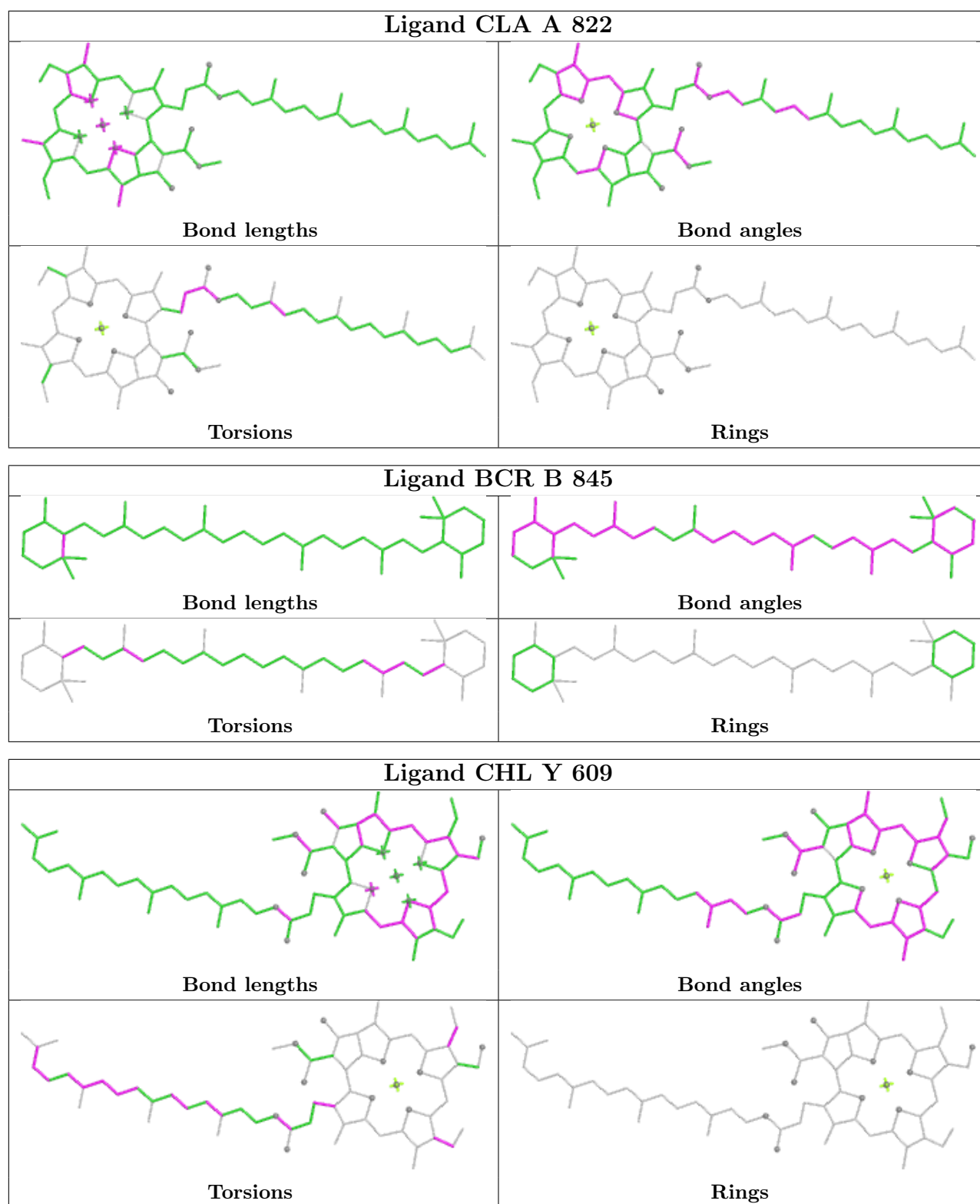


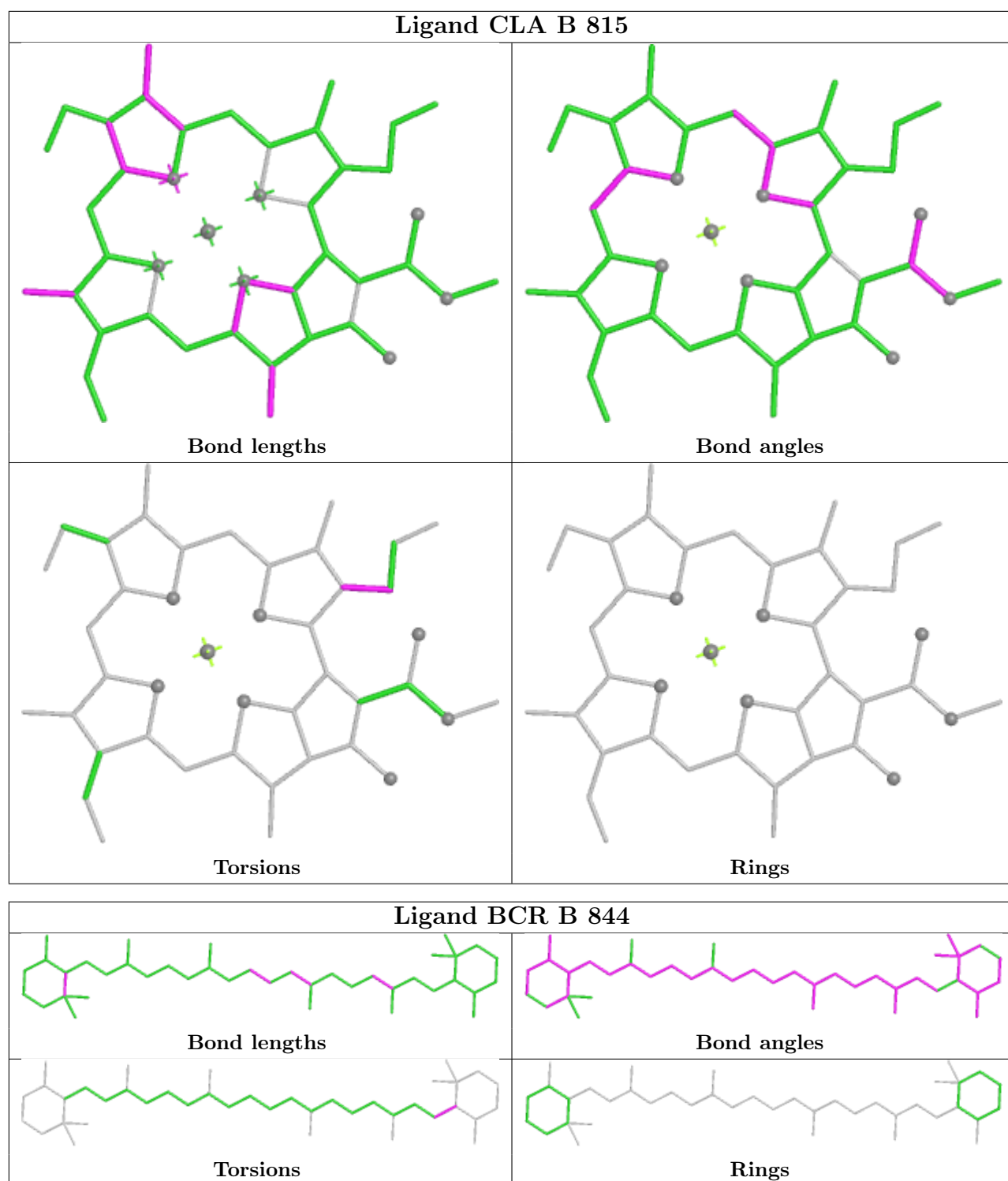
## Ligand CLA 7 608

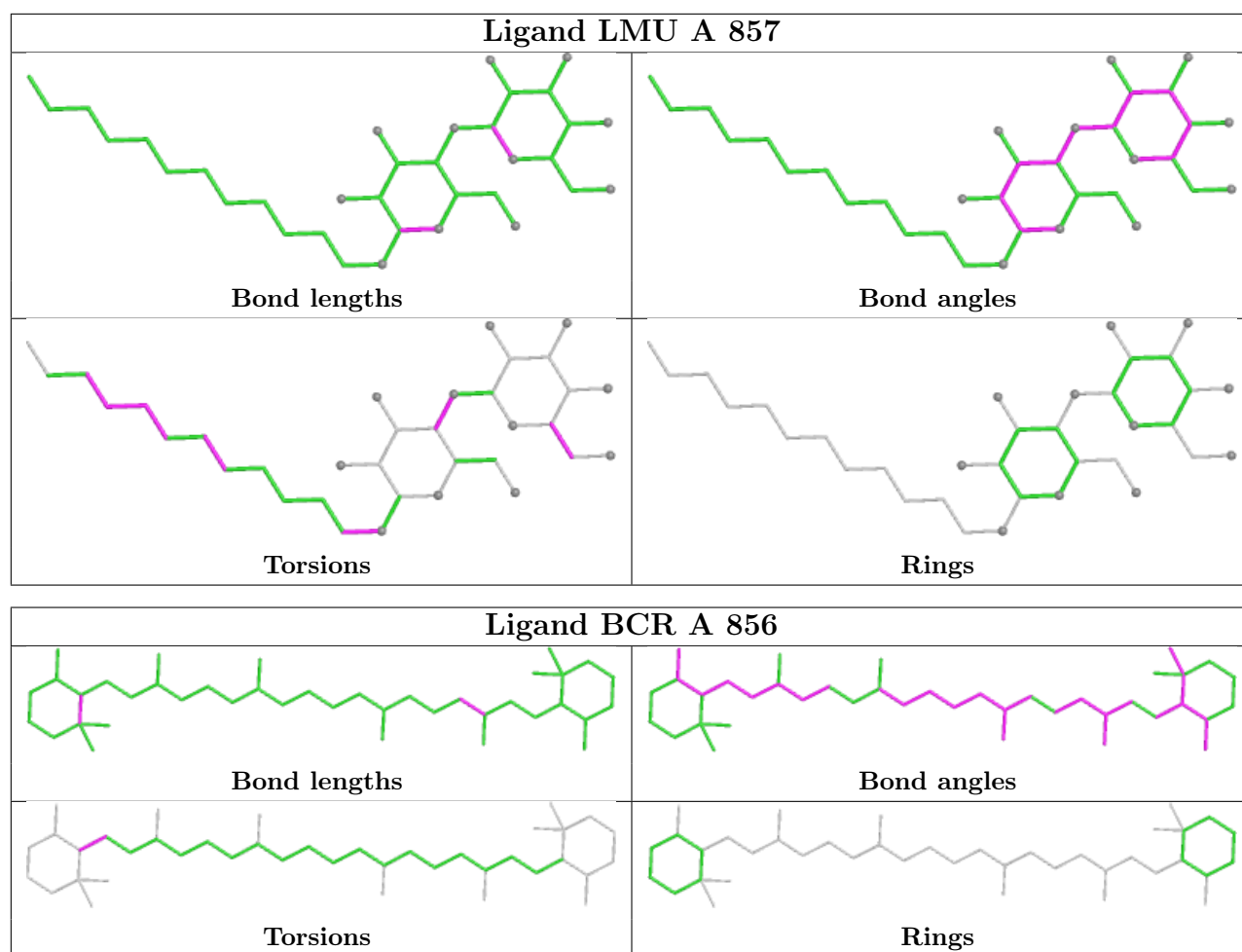


## Ligand CLA 6 604

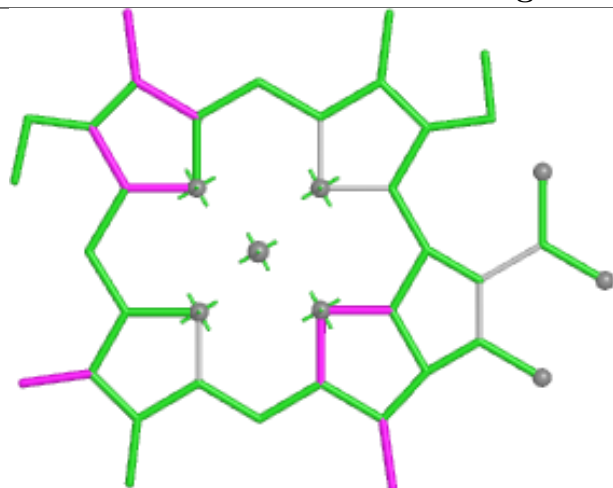




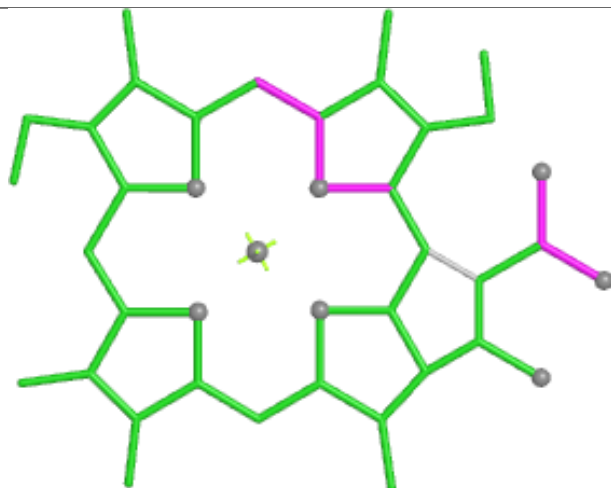




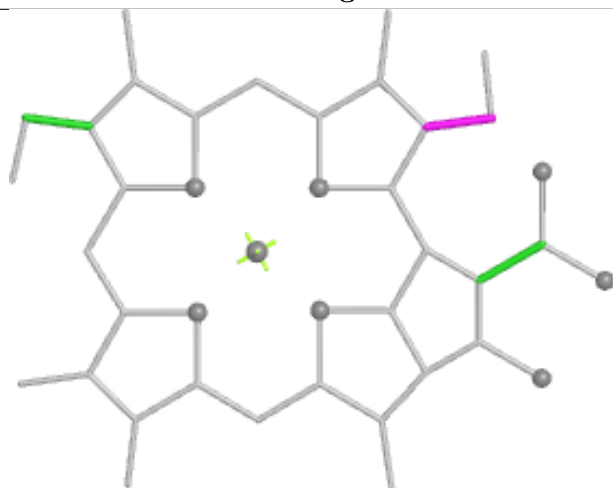
## Ligand CLA L 306



Bond lengths



Bond angles



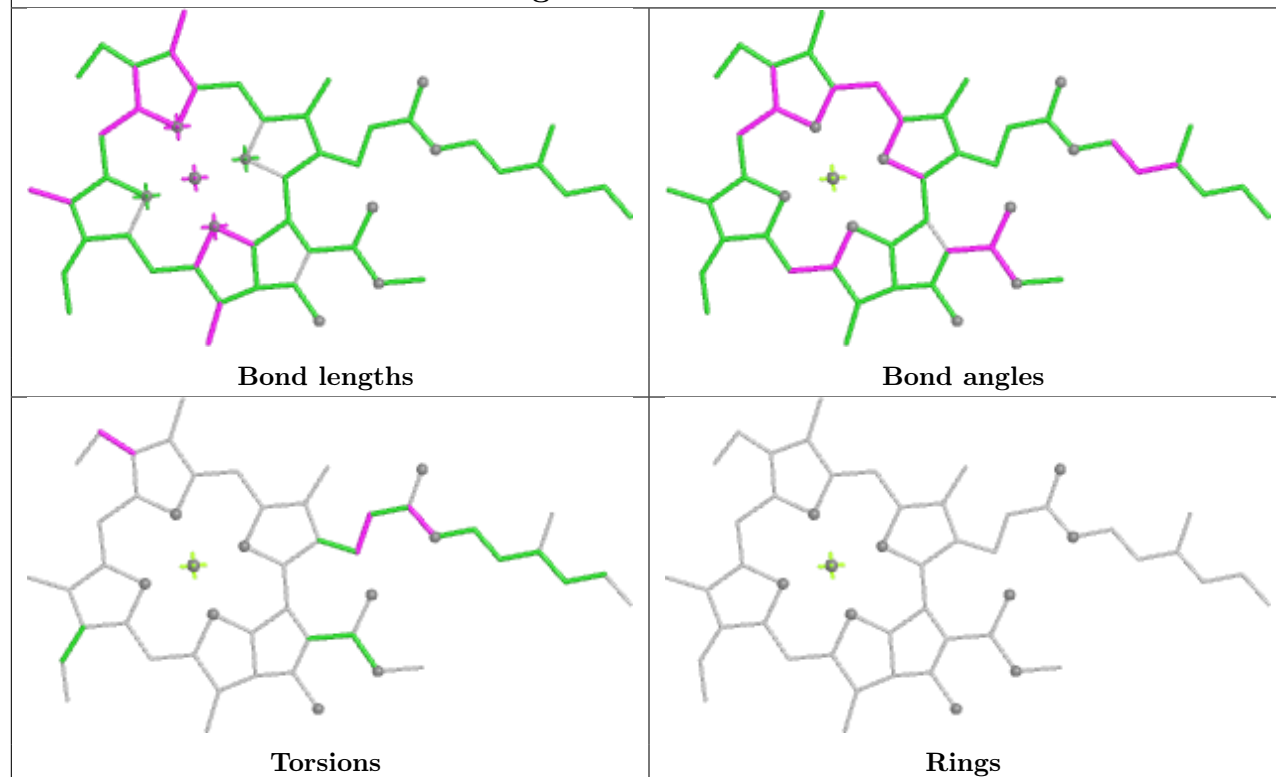
Torsions



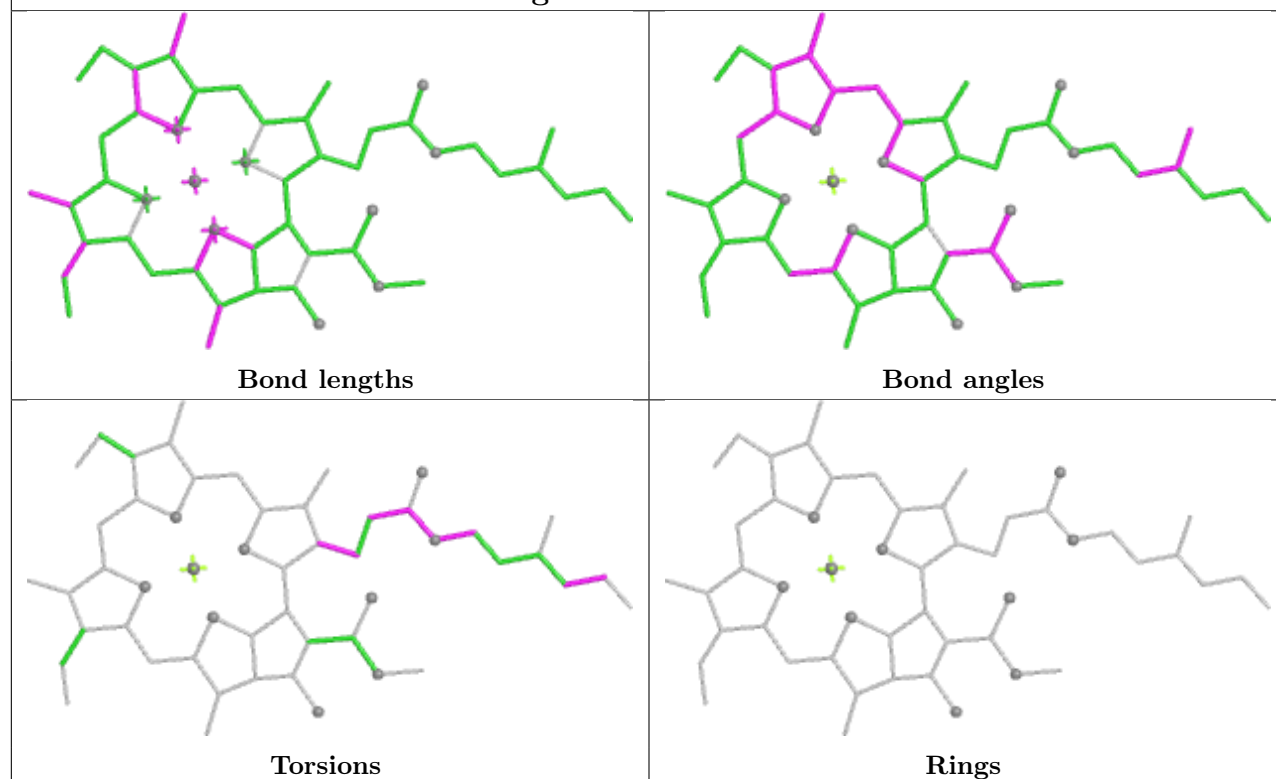
Rings

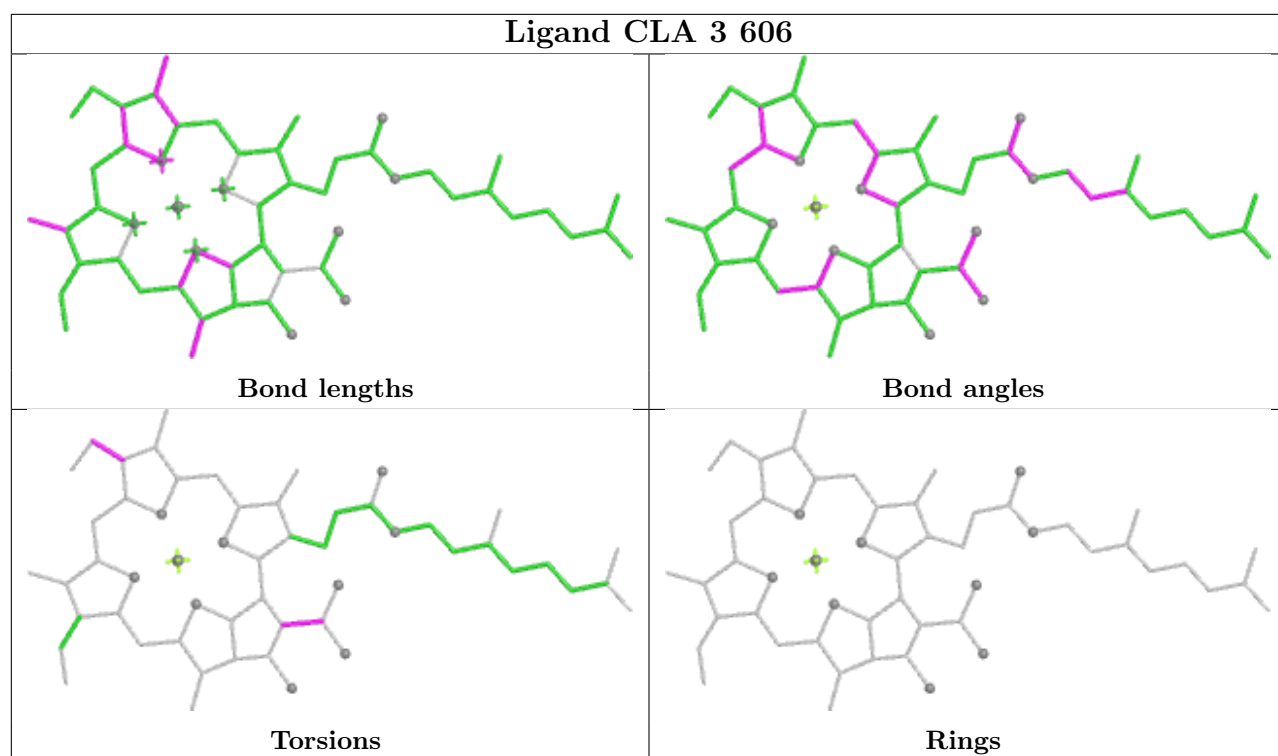


## Ligand CLA B 807

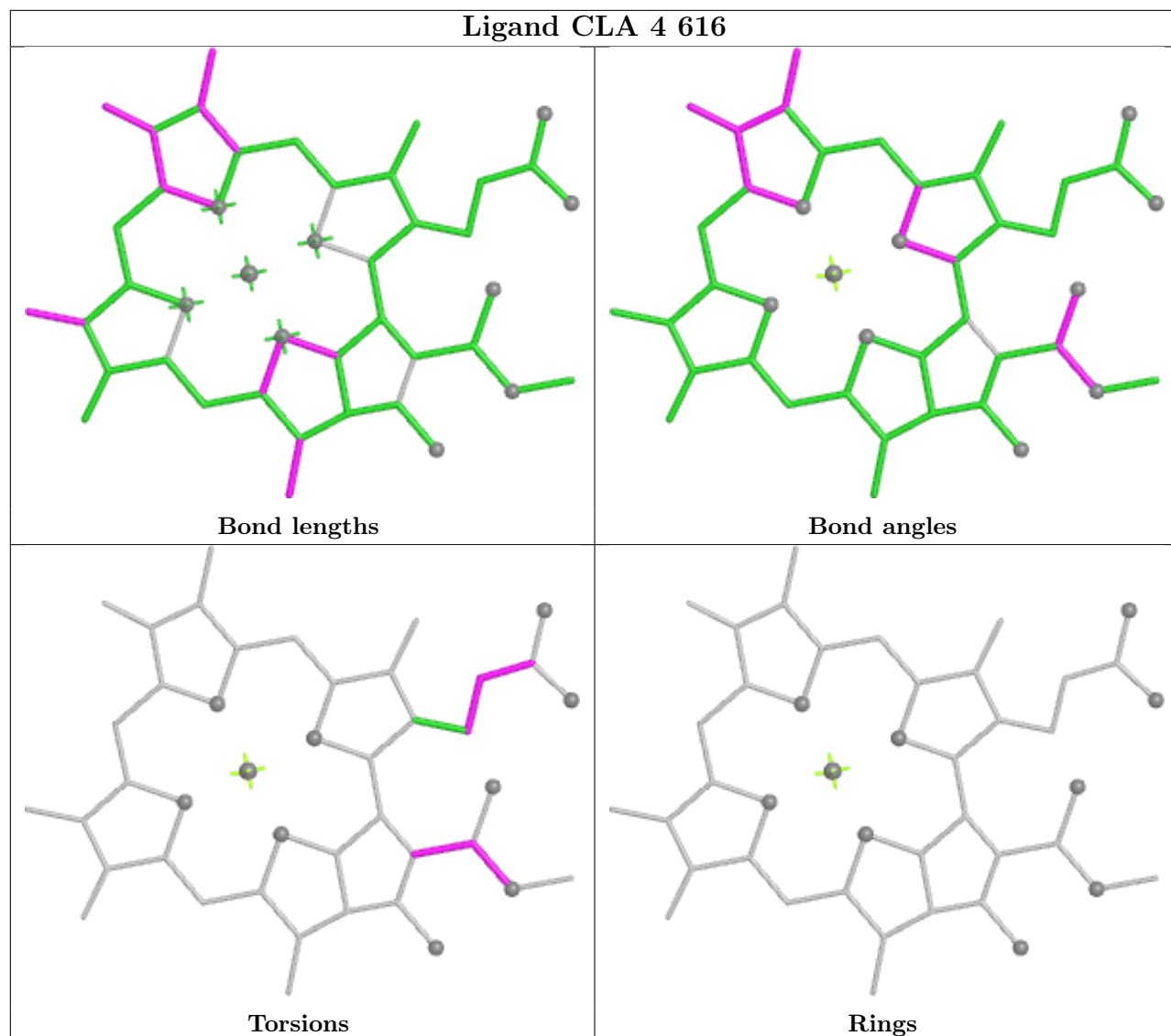


## Ligand CLA A 805

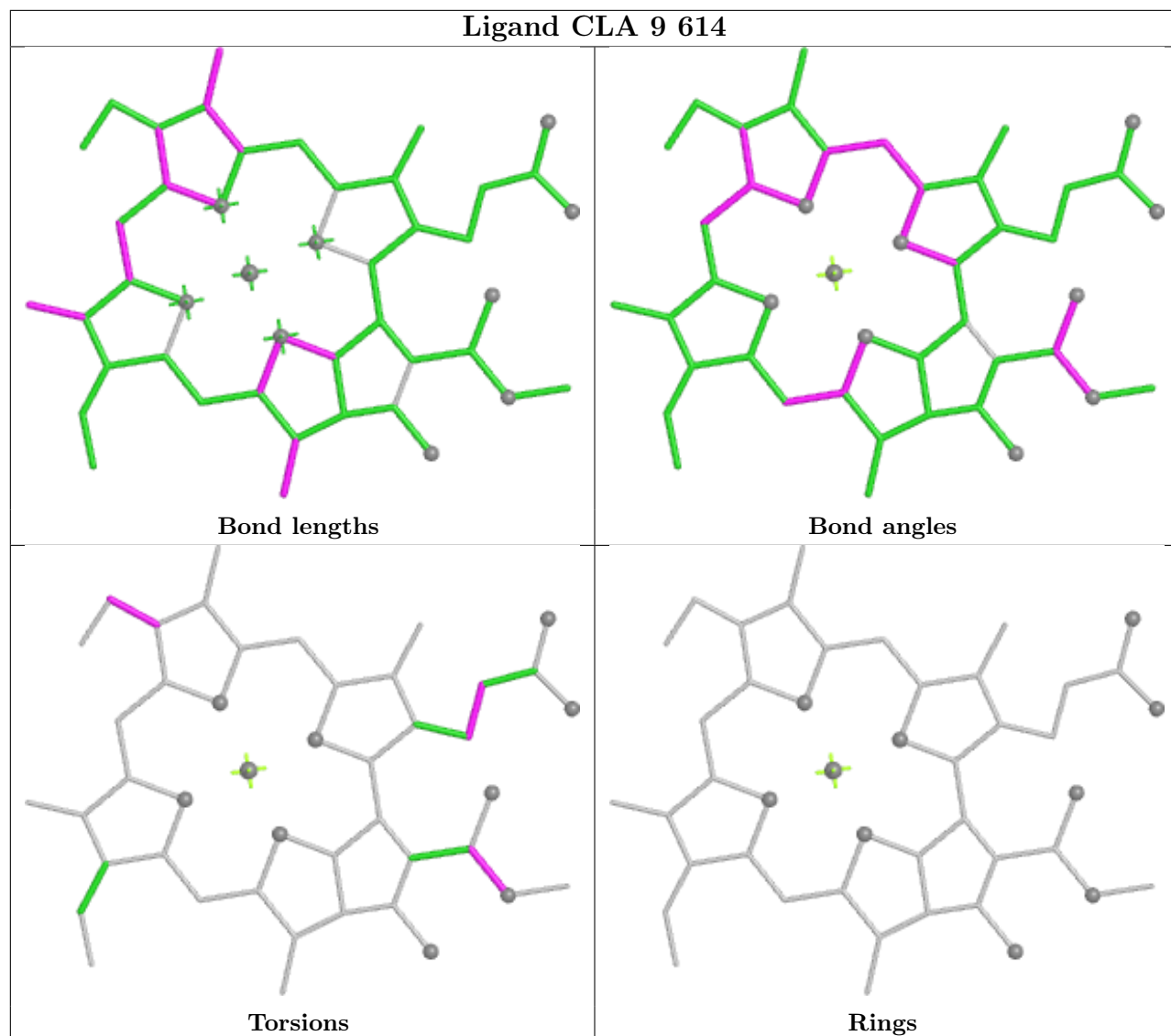


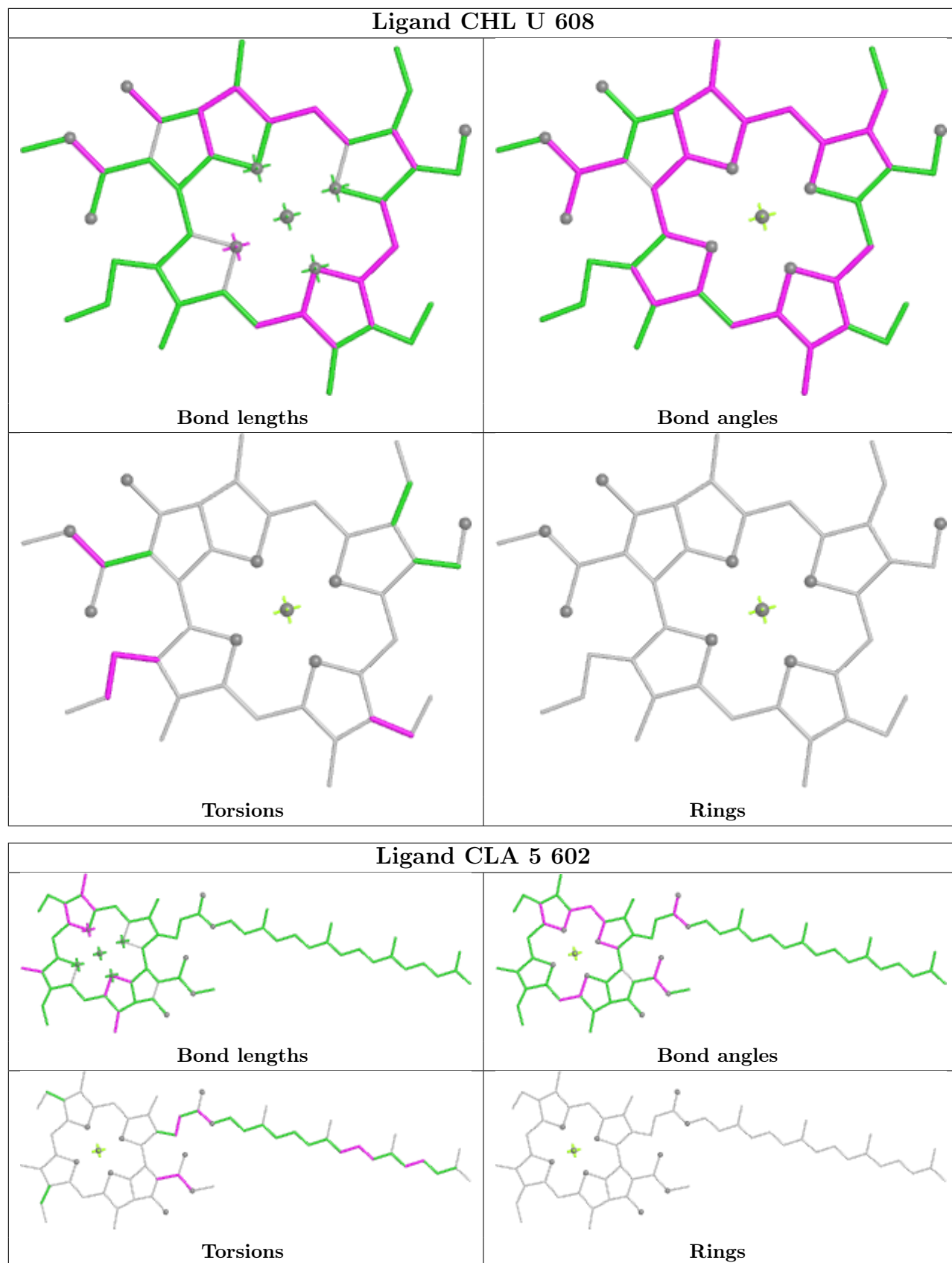


## Ligand CLA 4 616

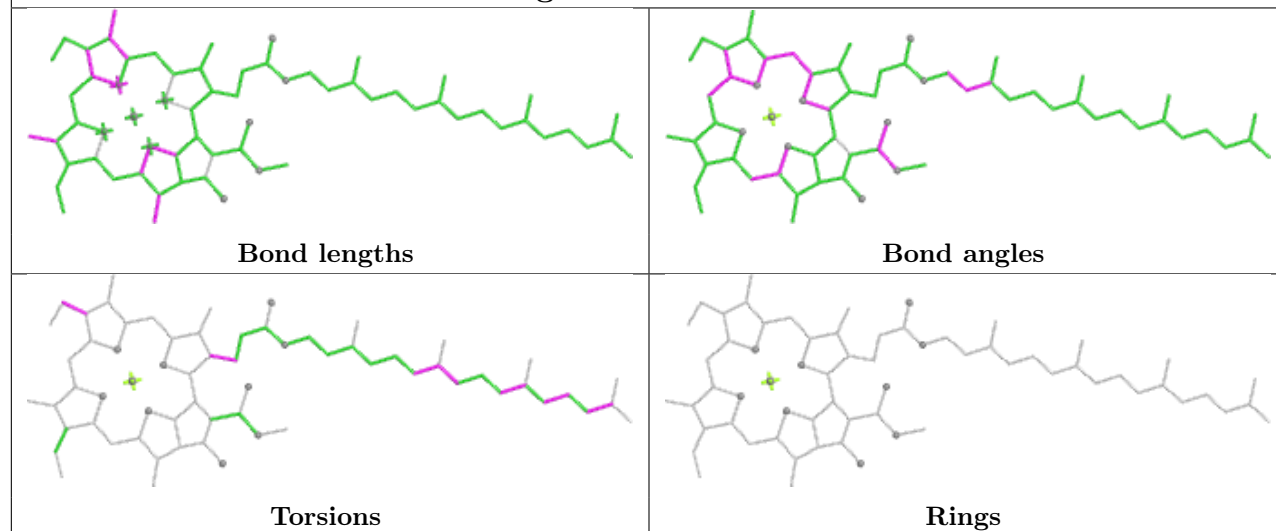


## Ligand CLA 9 614

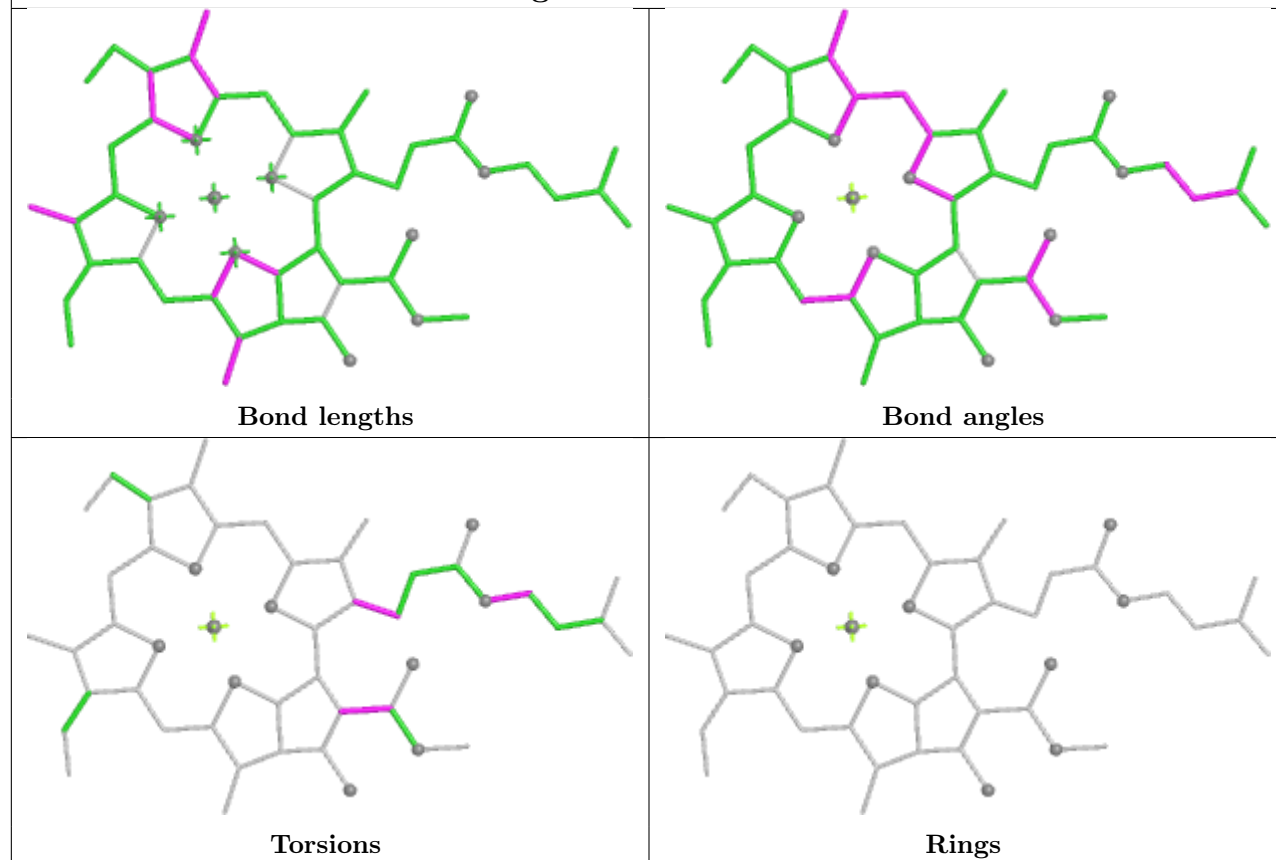


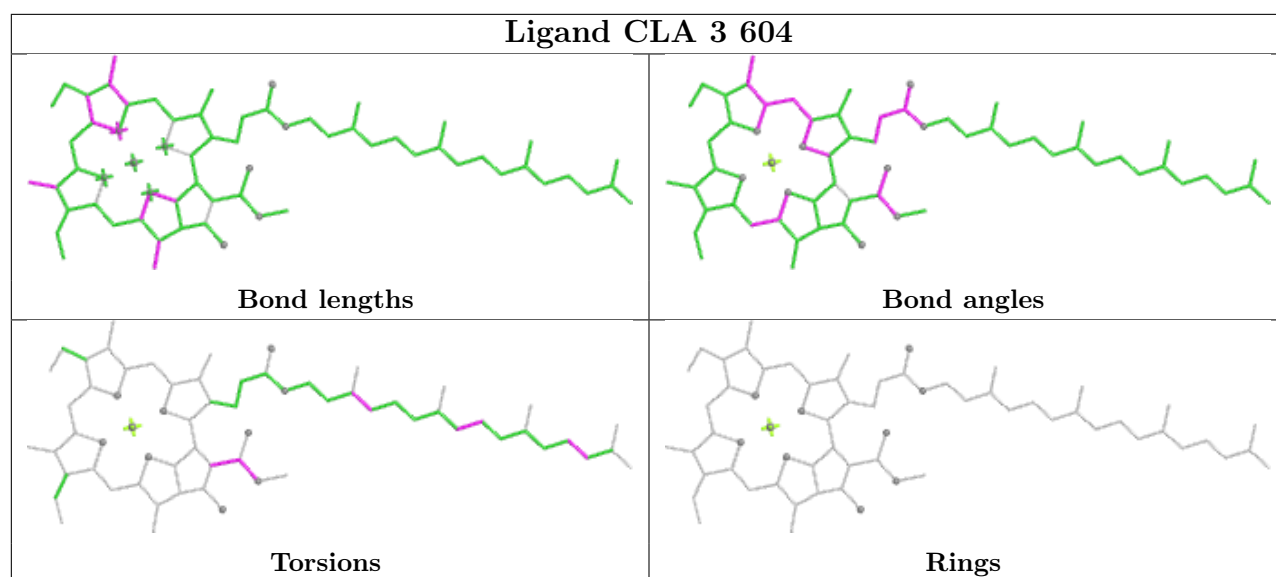
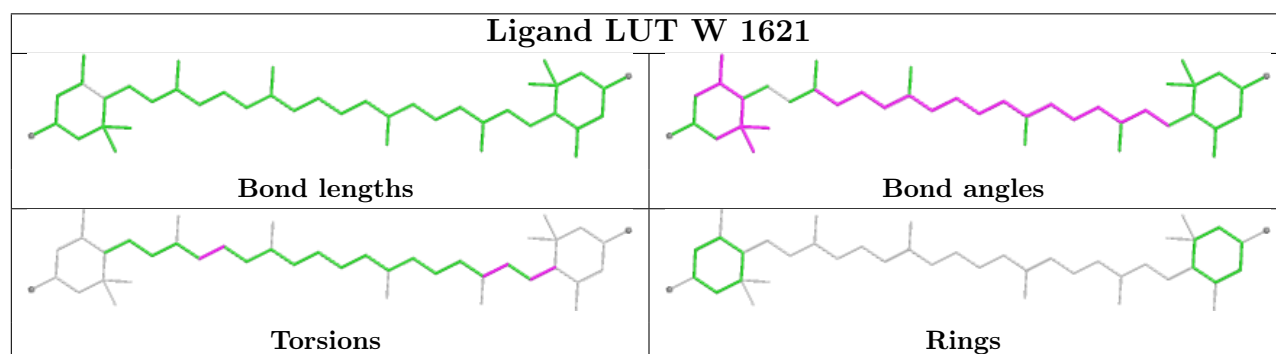
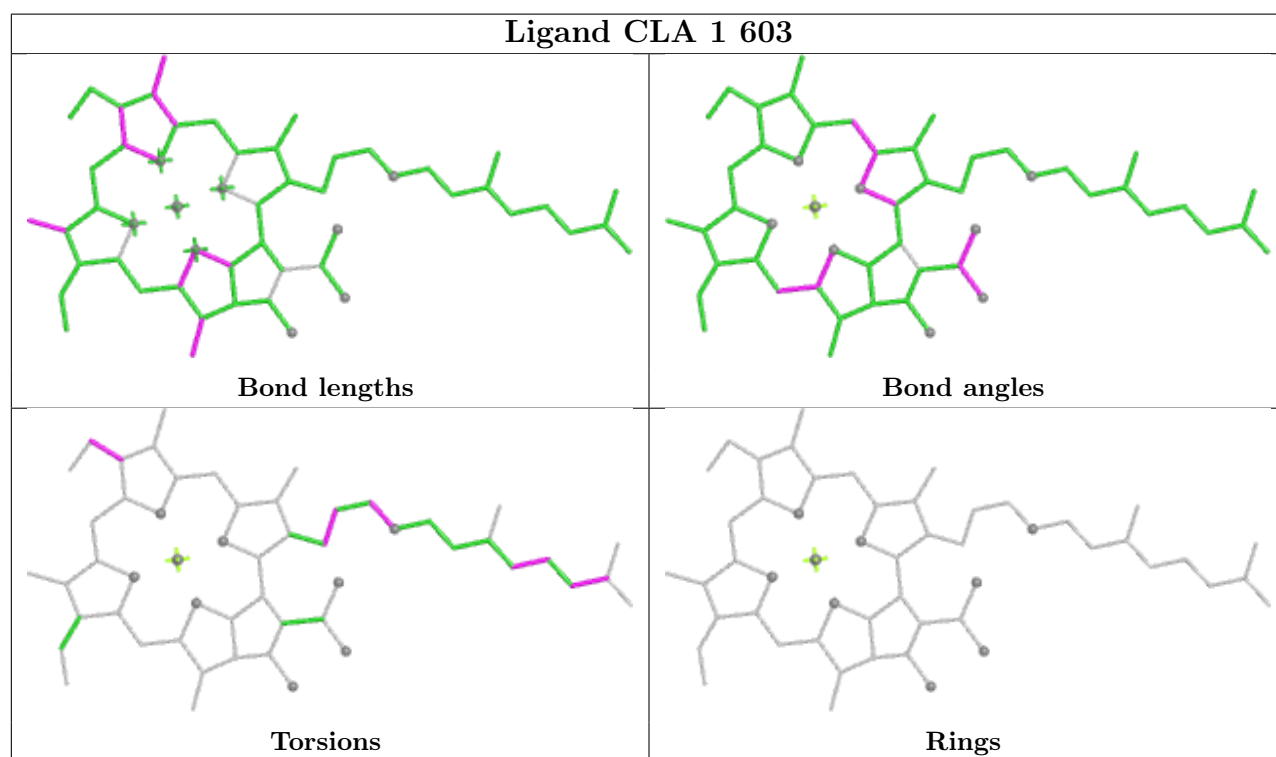


## Ligand CLA 5 609

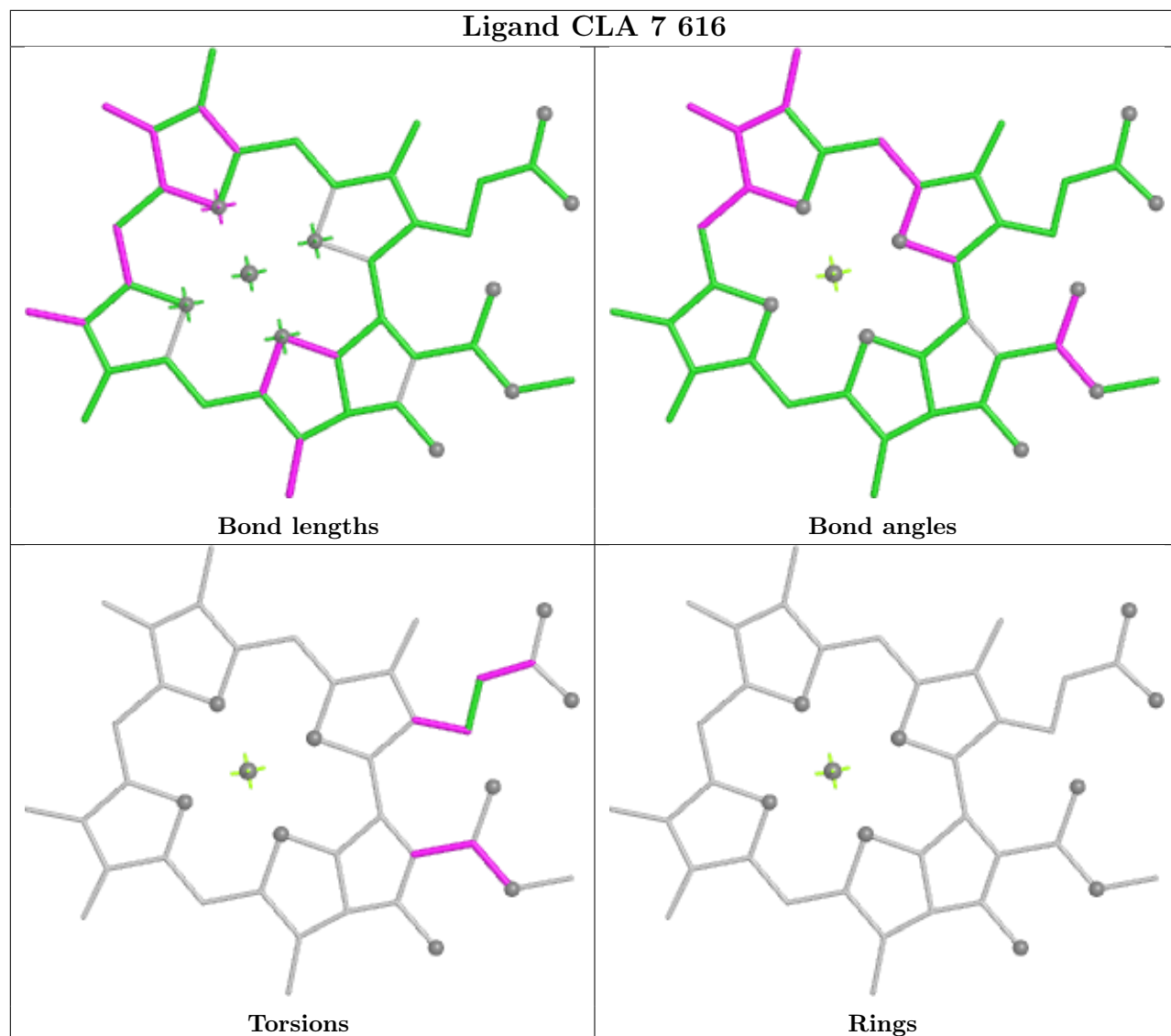


## Ligand CLA A 808

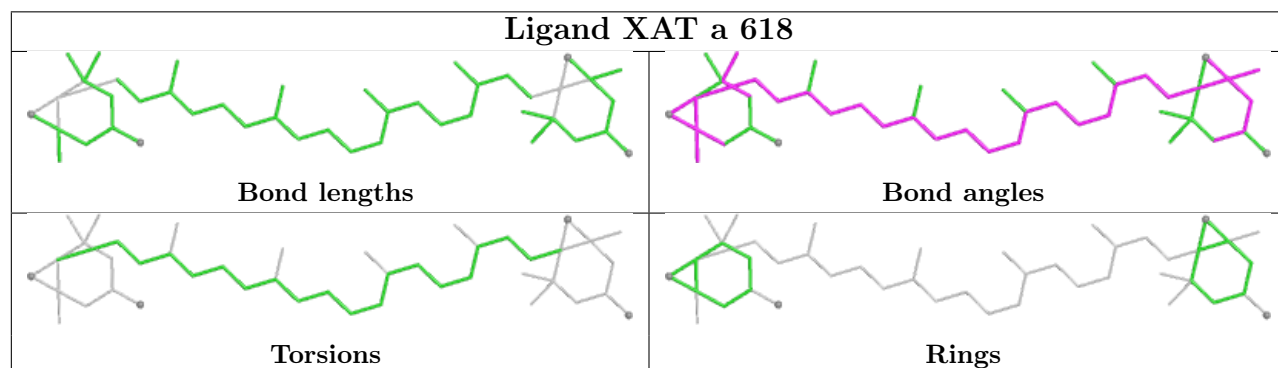




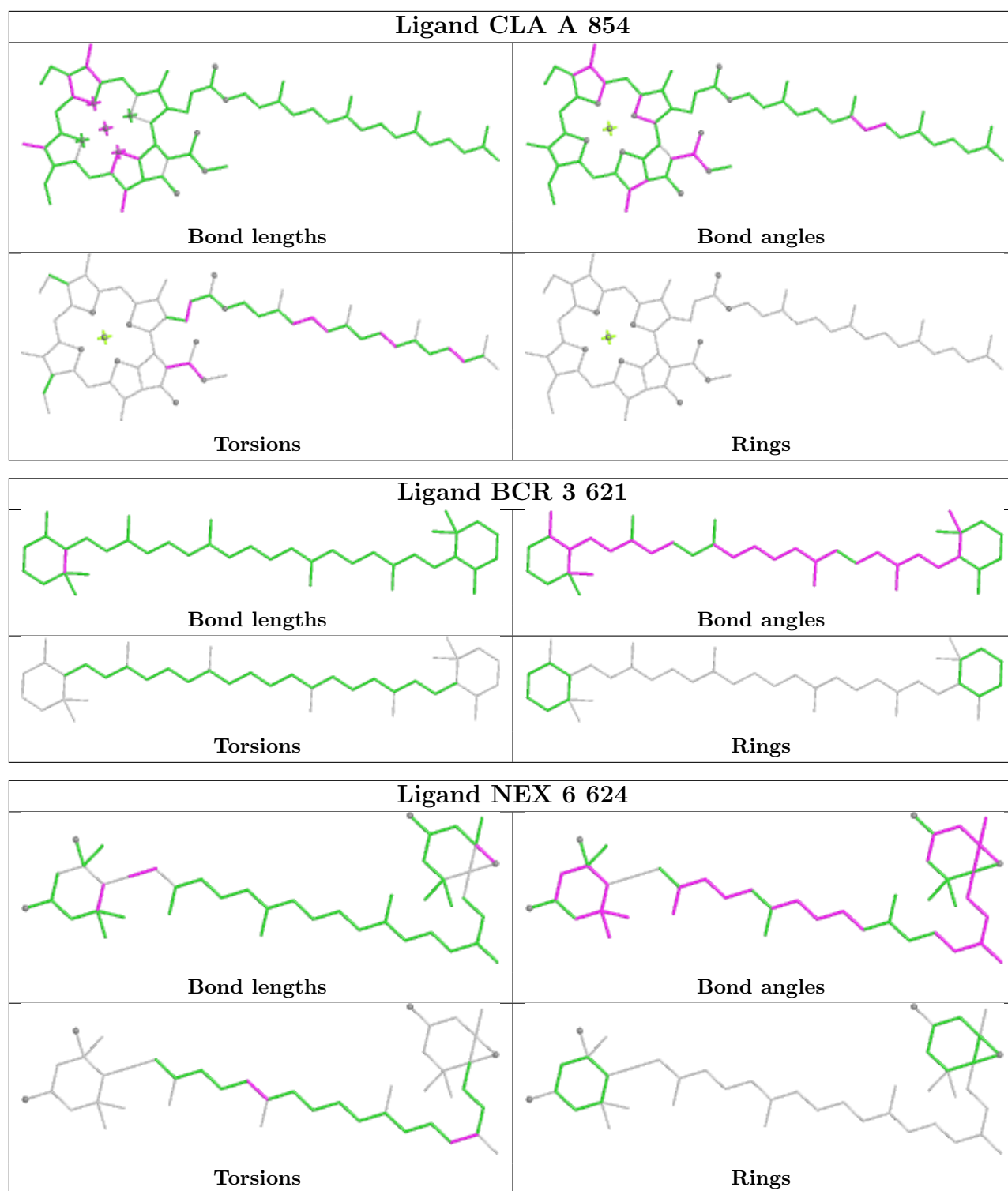
## Ligand CLA 7 616

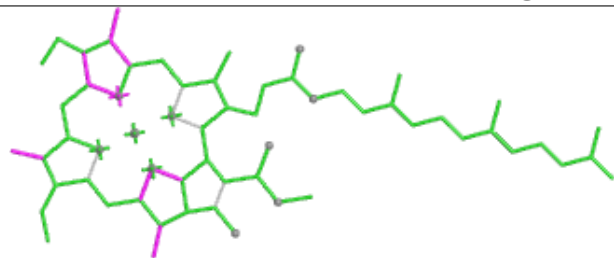
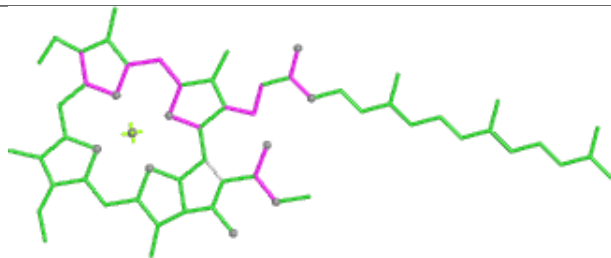
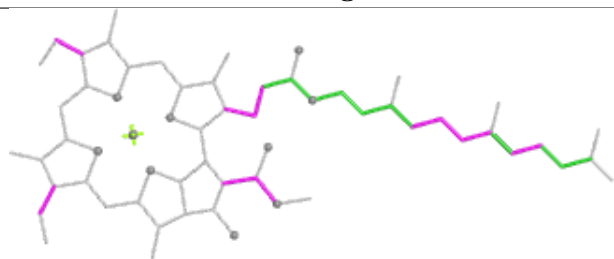
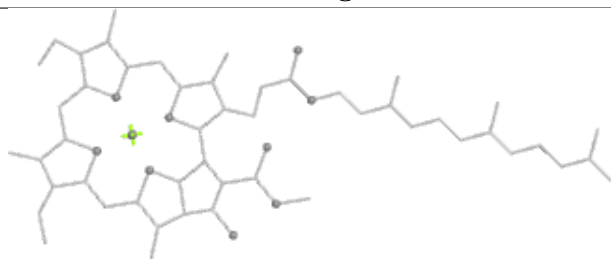
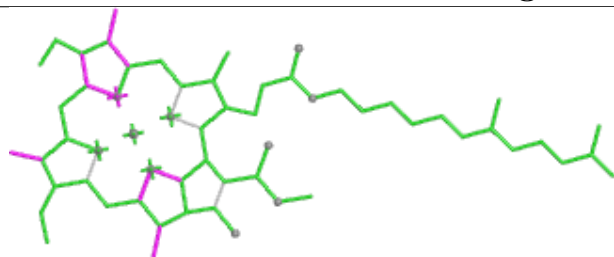
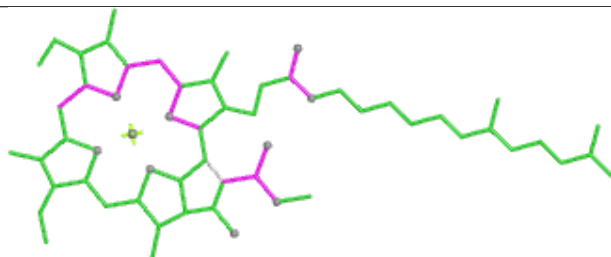
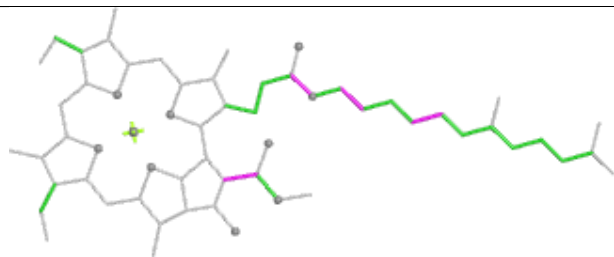
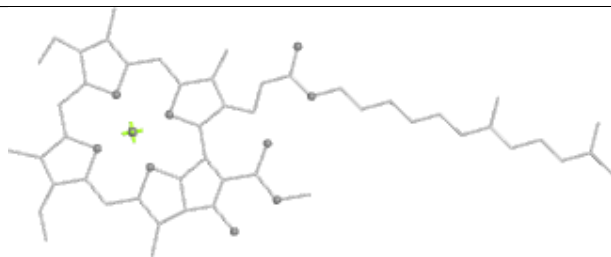


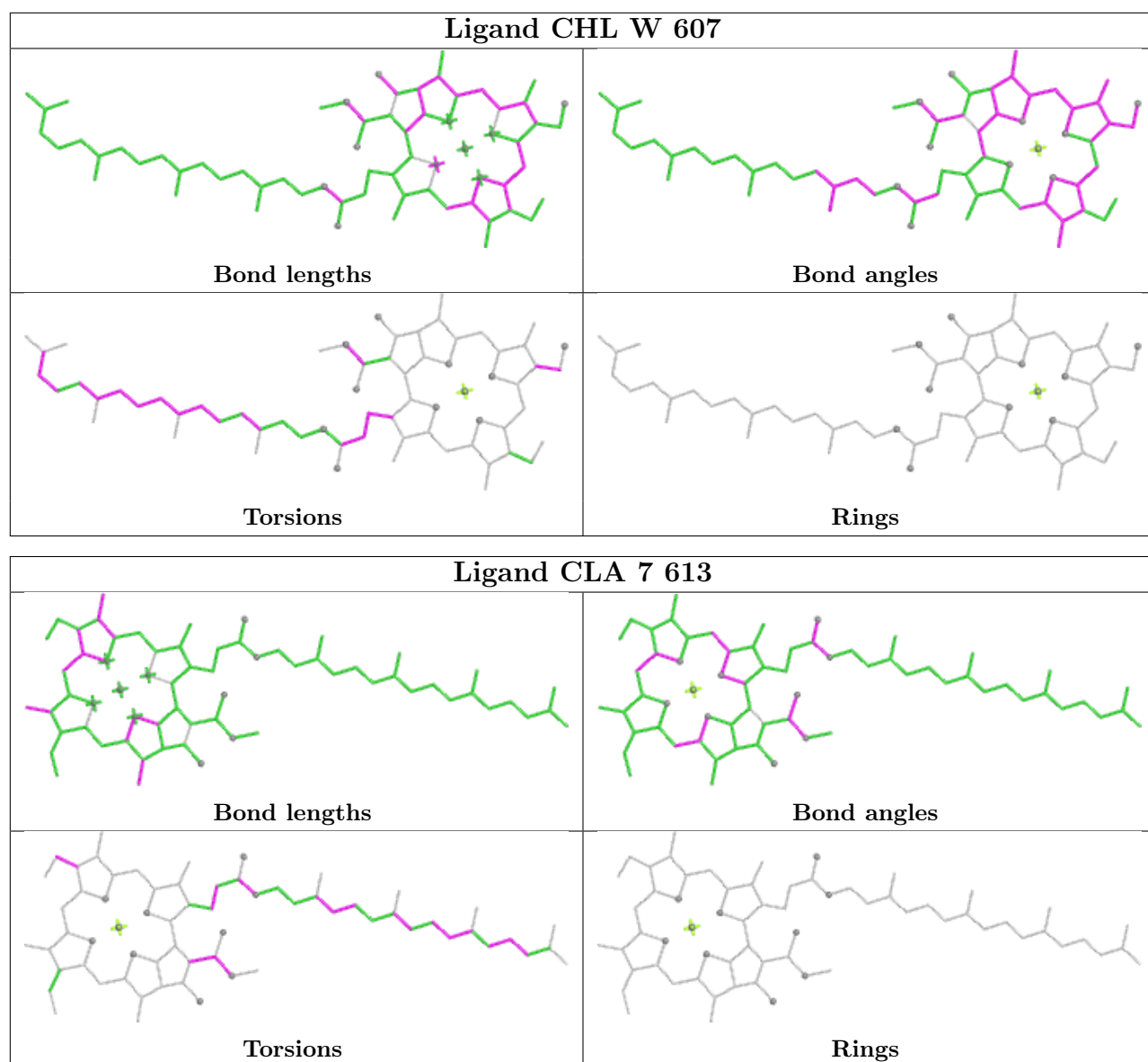
## Ligand XAT a 618

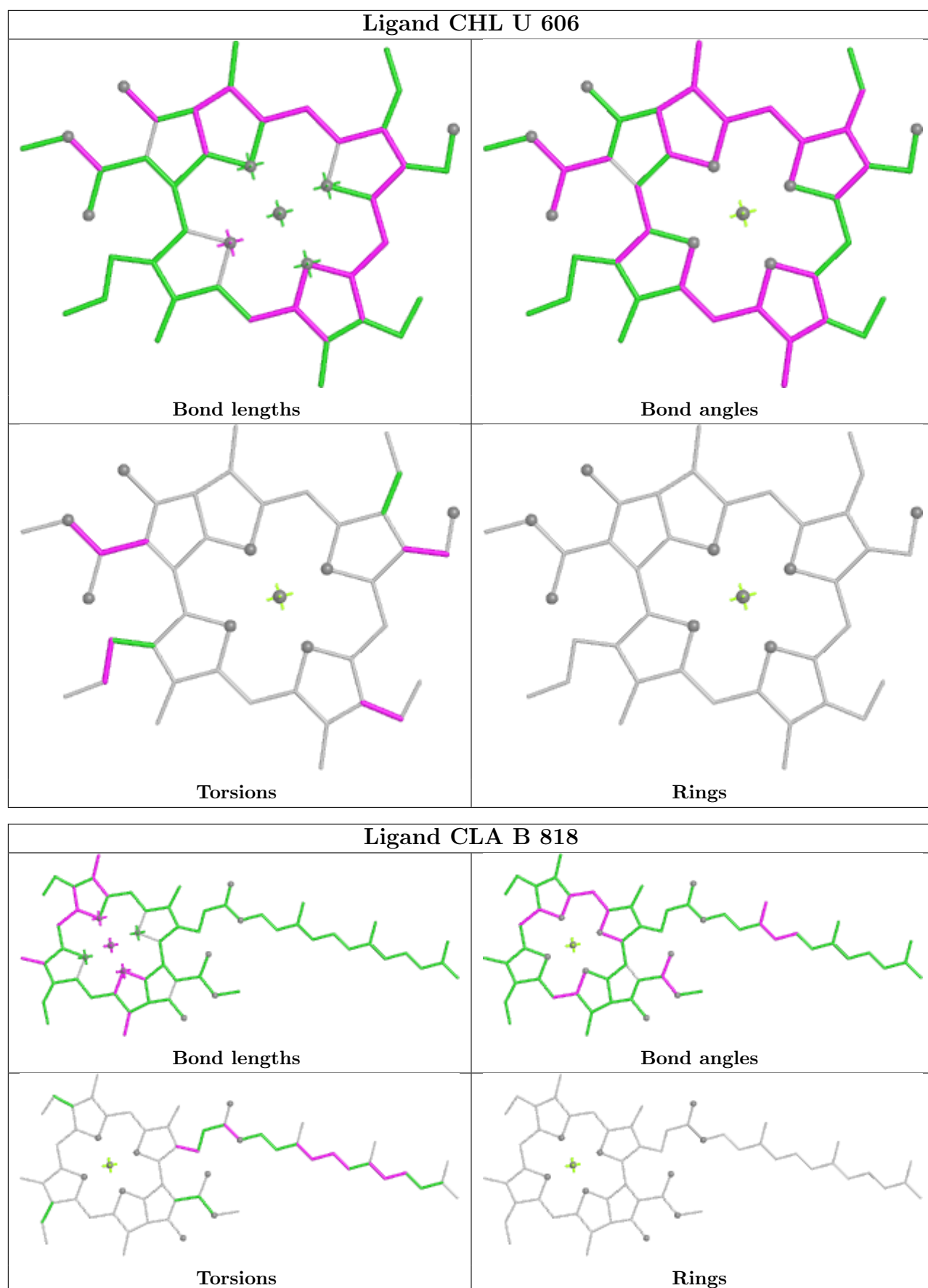




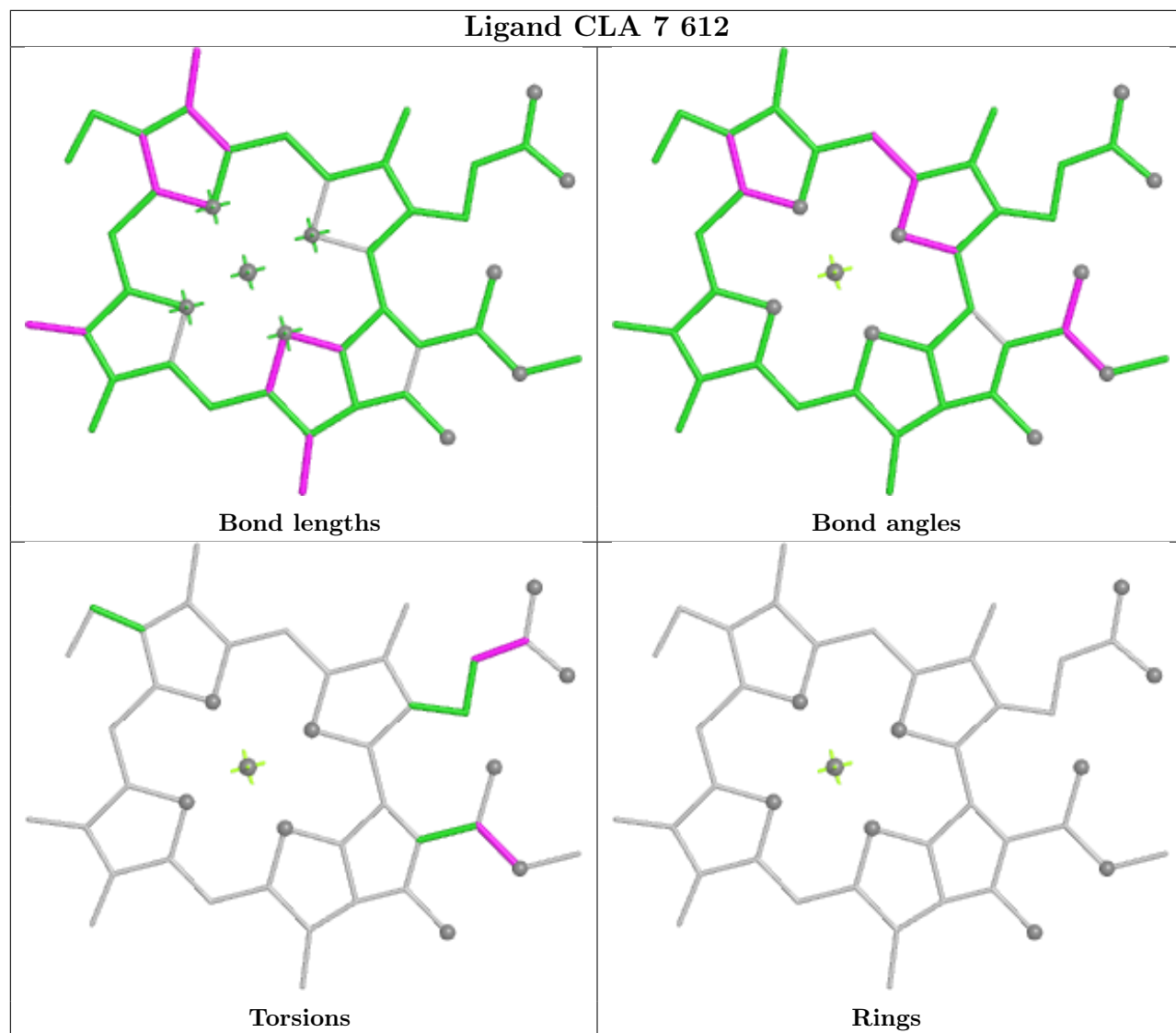


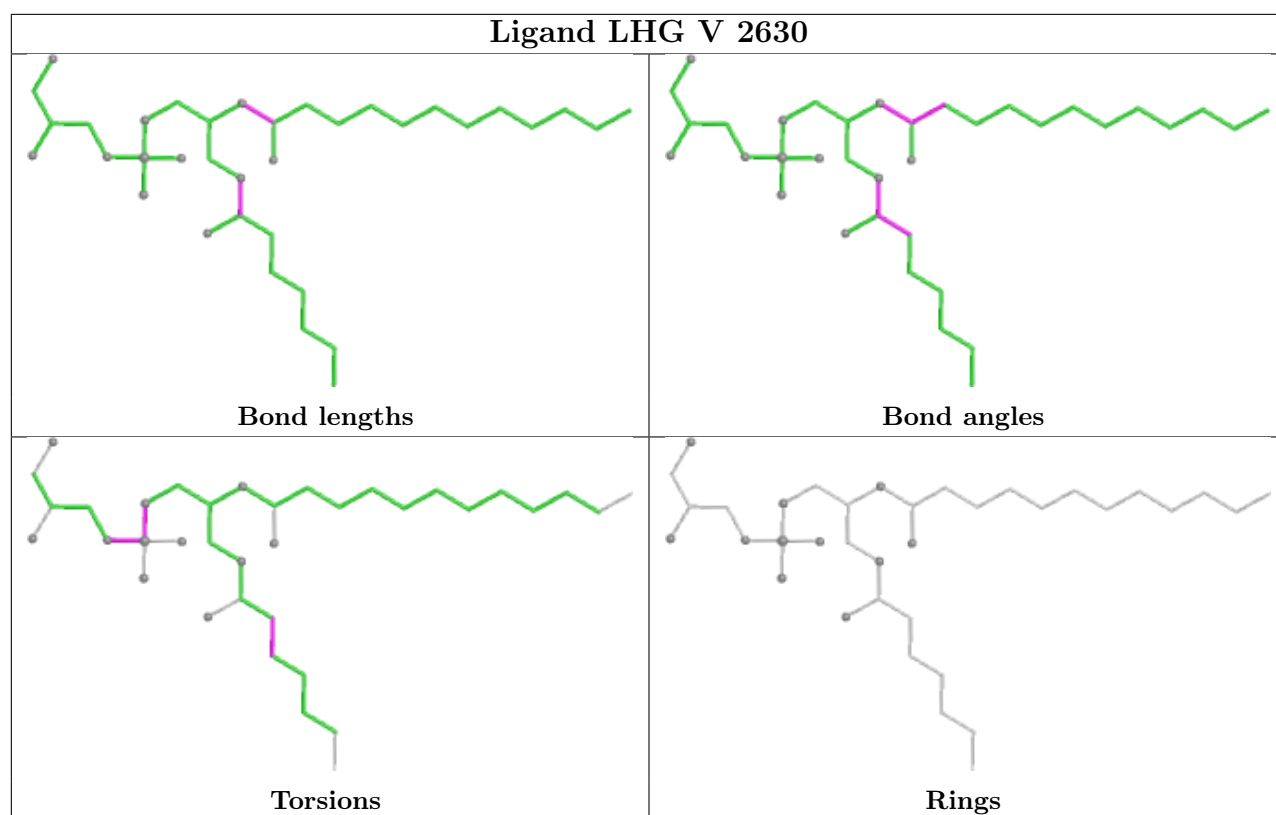
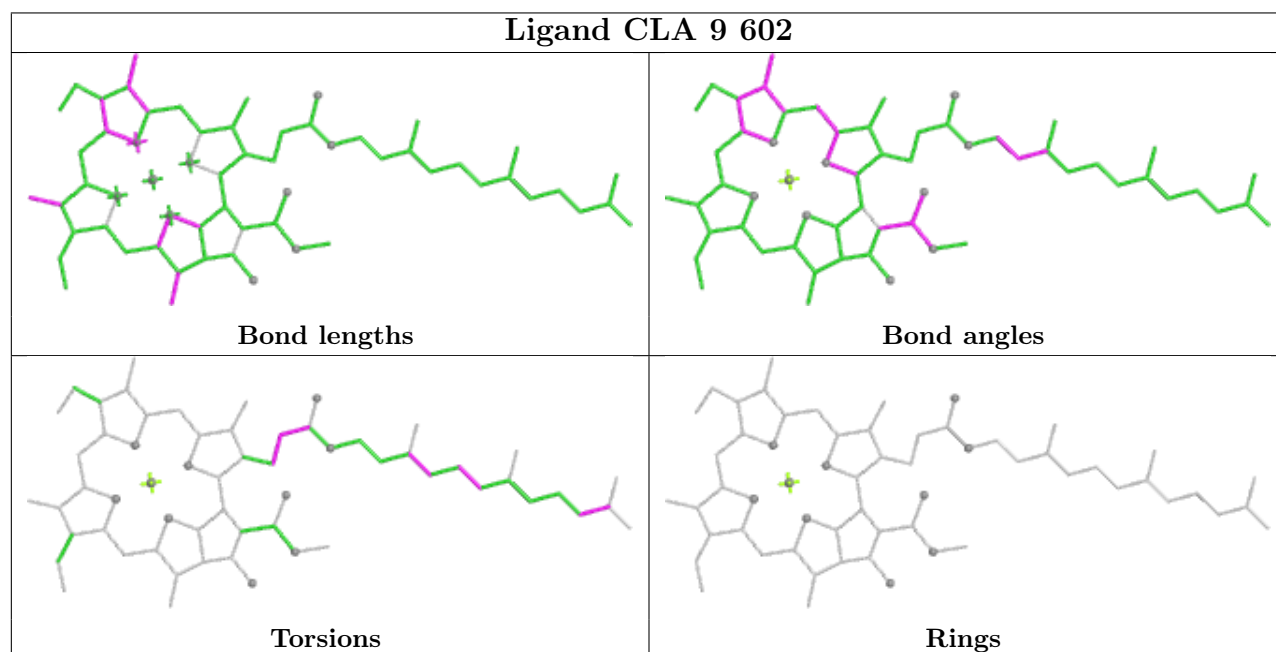
**Ligand CLA 3 609****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 7 611****Bond lengths****Bond angles****Torsions****Rings**

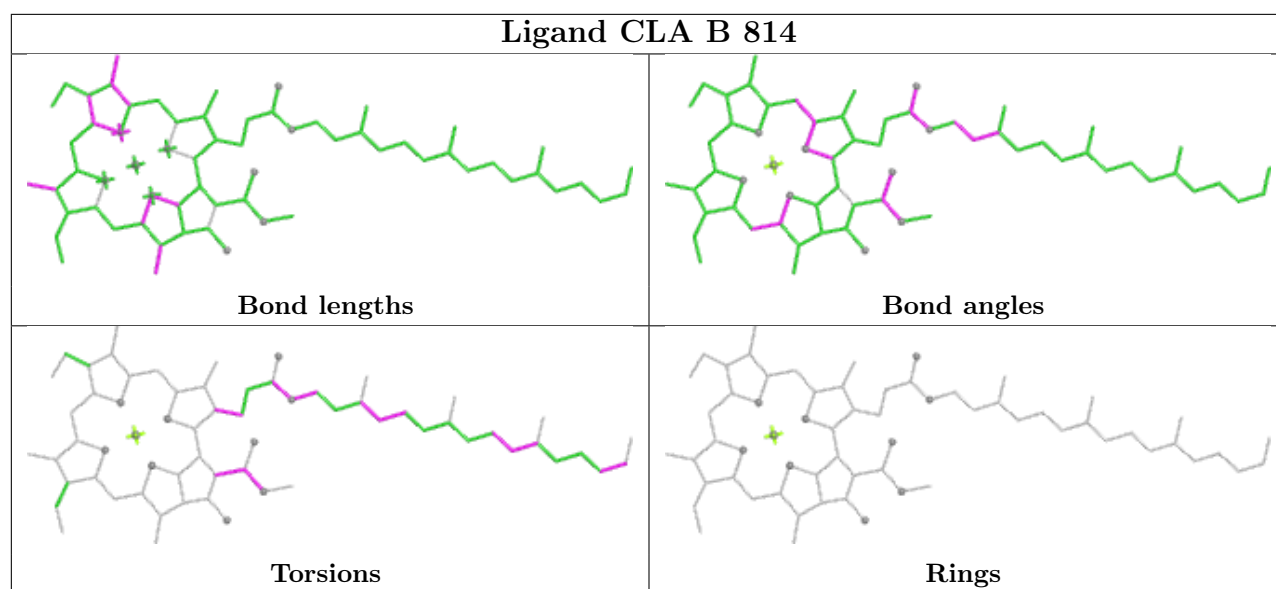
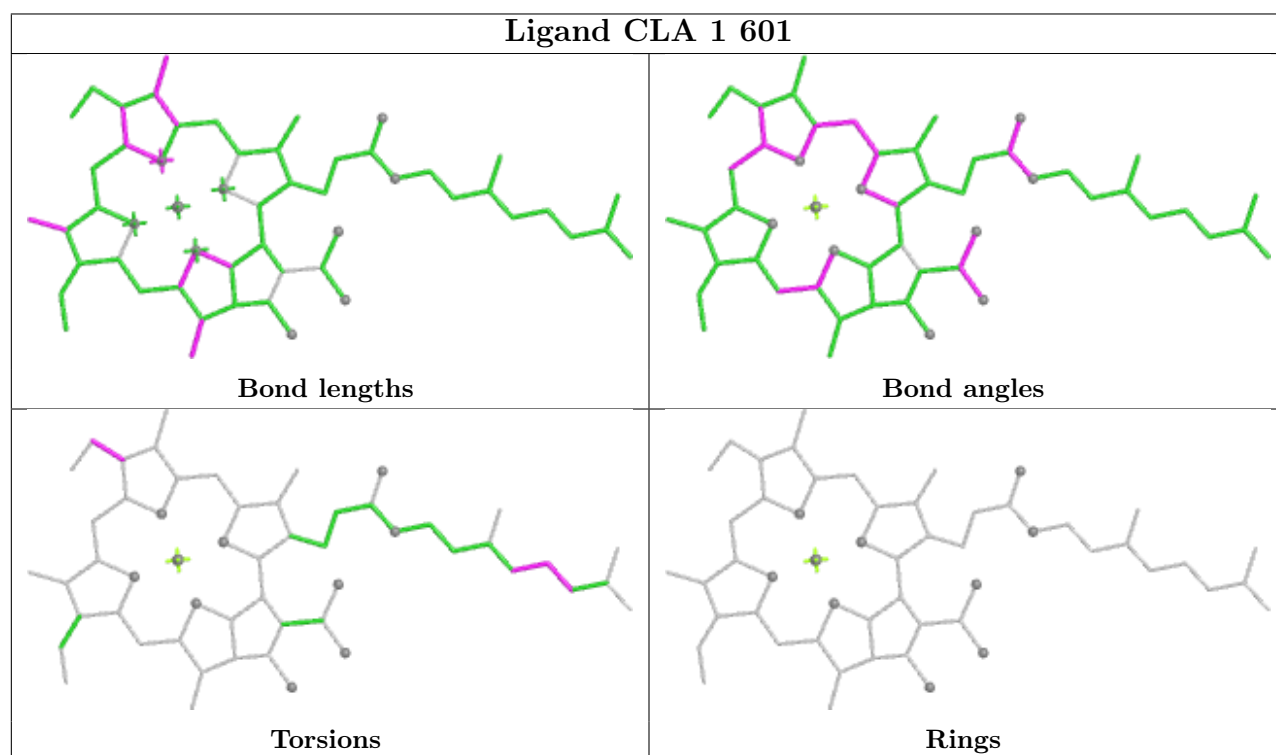




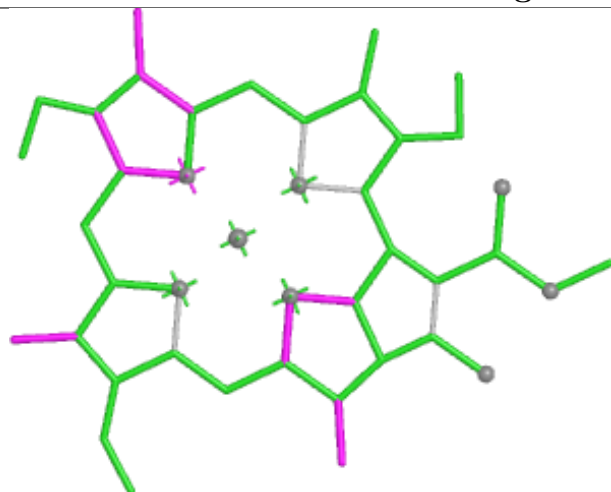
## Ligand CLA 7 612



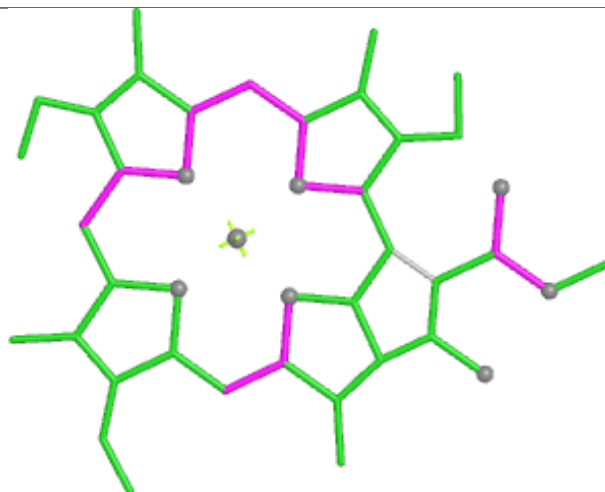




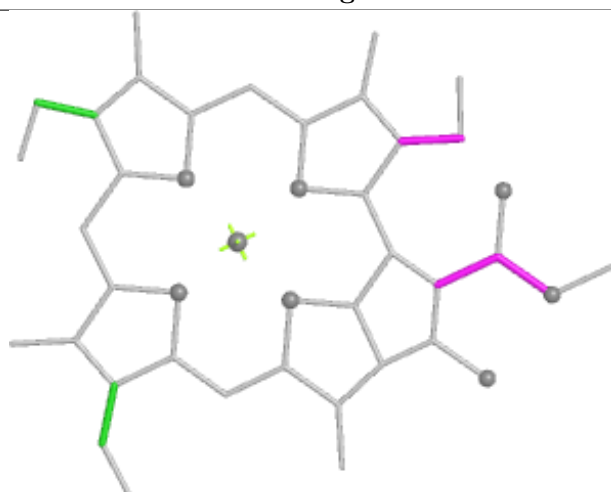
## Ligand CLA B 822



Bond lengths



Bond angles



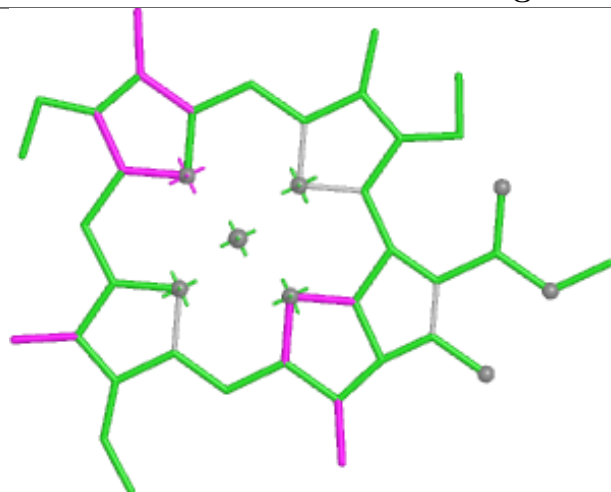
Torsions



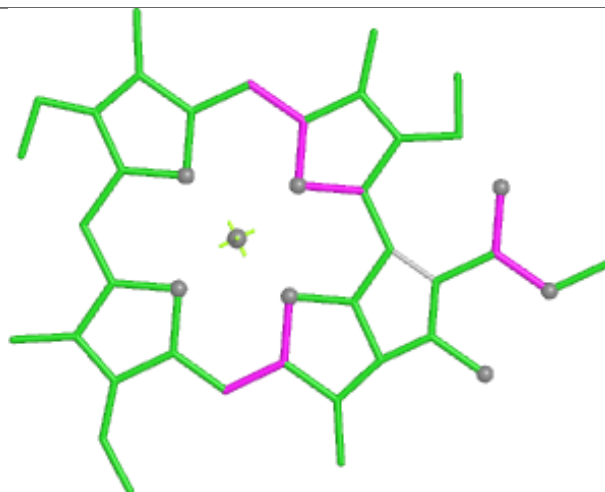
Rings



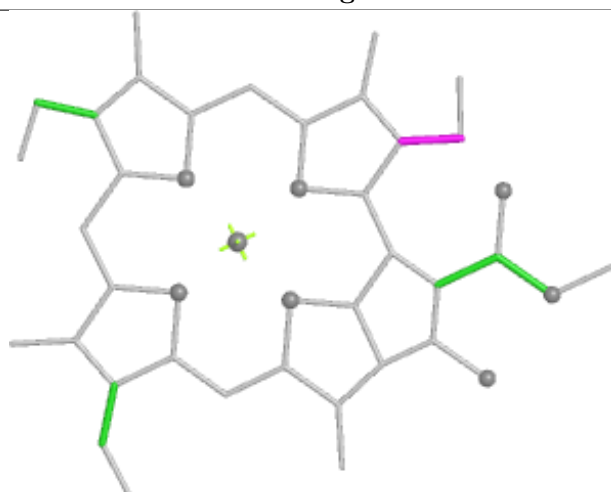
## Ligand CLA A 823



Bond lengths



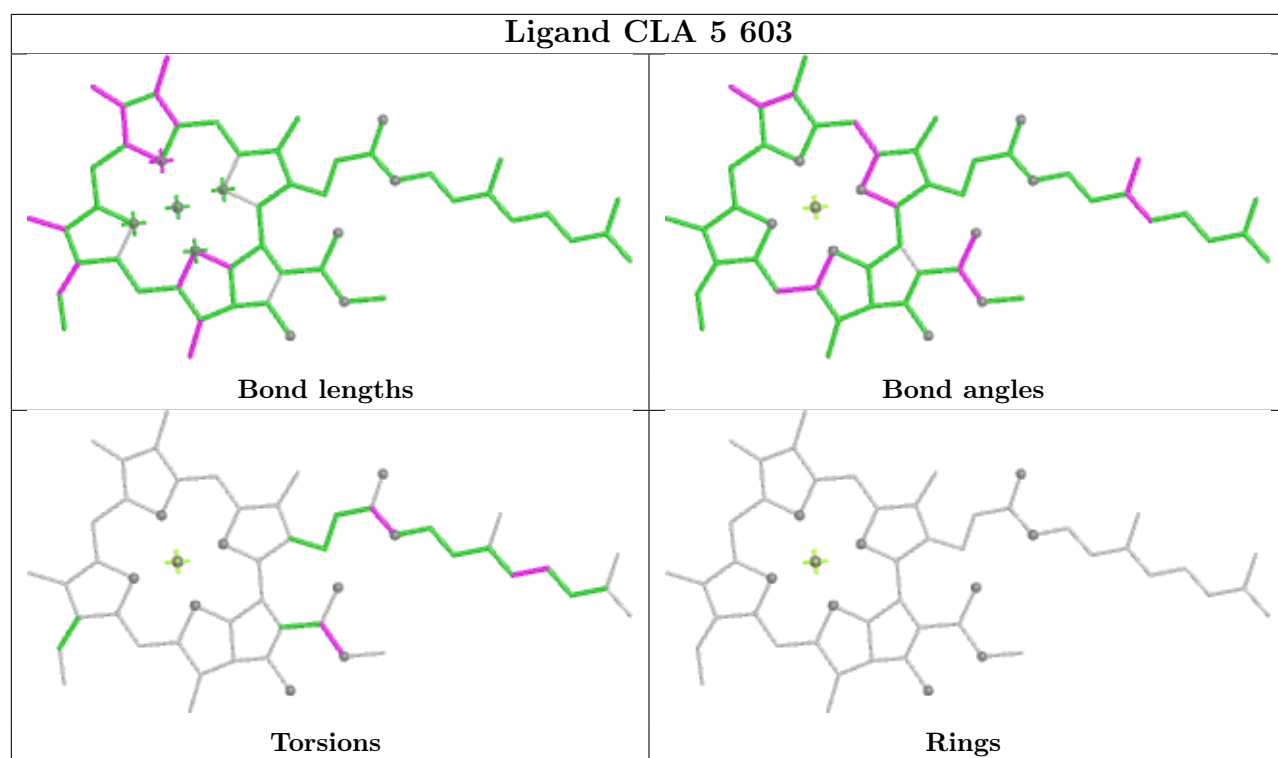
Bond angles



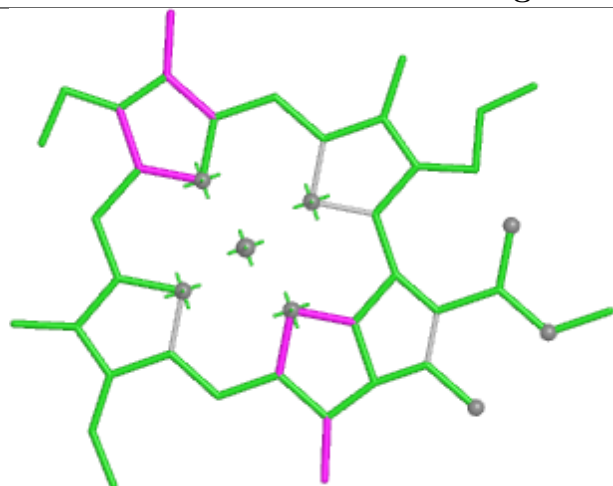
Torsions



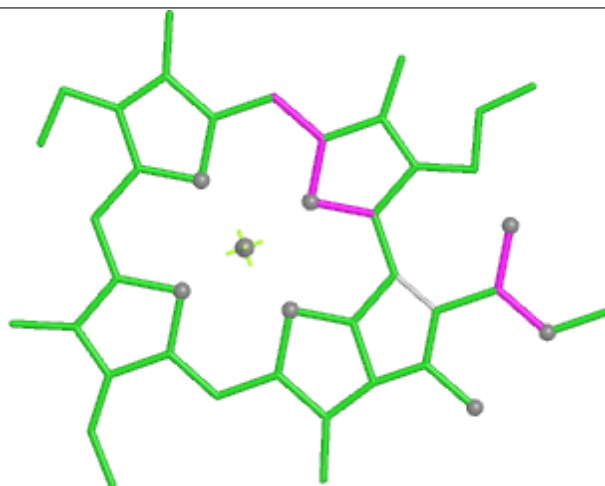
Rings



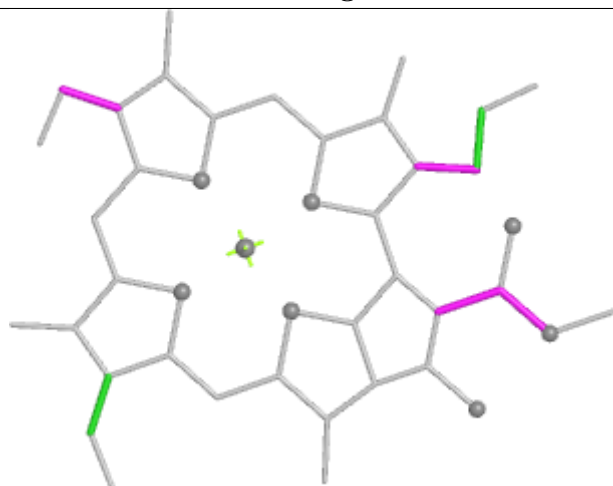
## Ligand CLA V 611



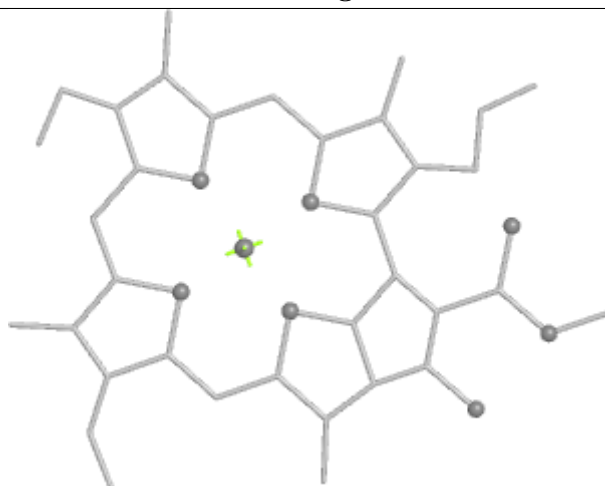
Bond lengths



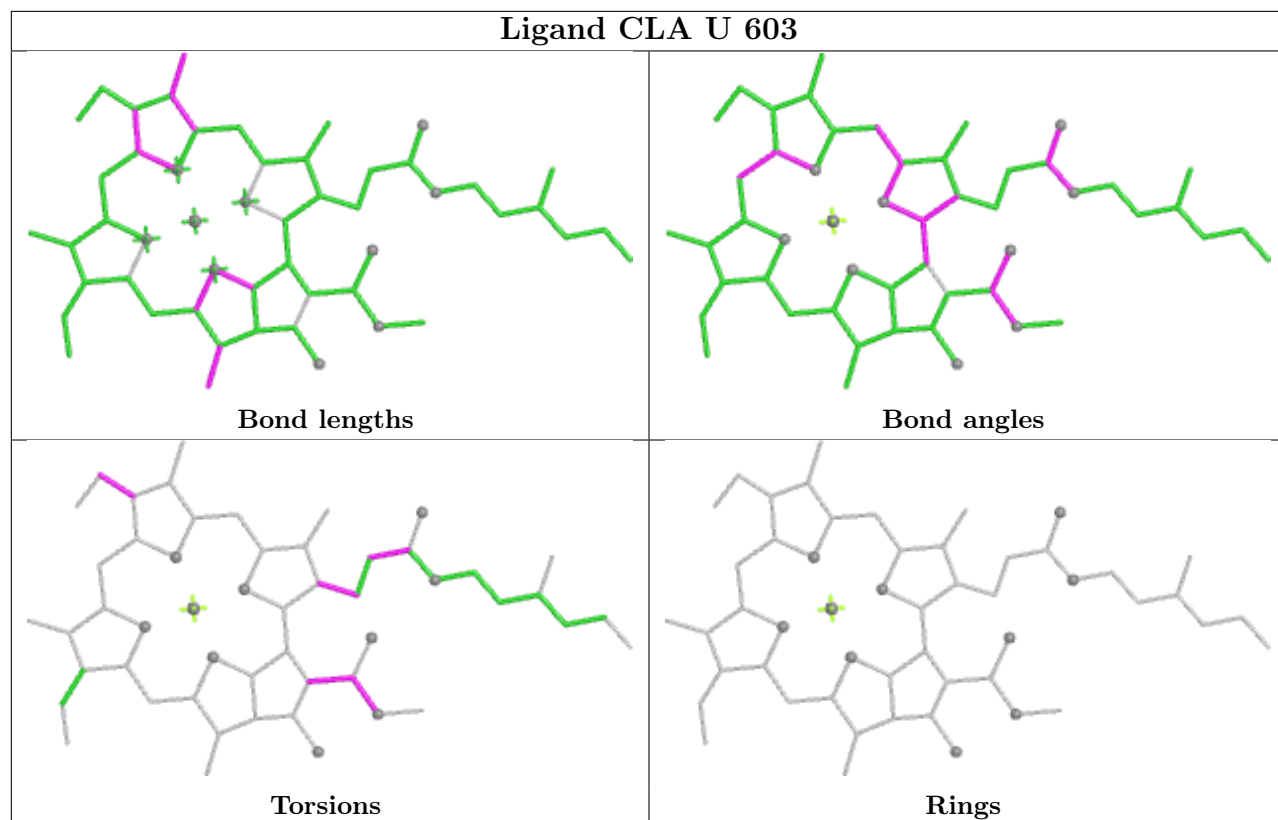
Bond angles



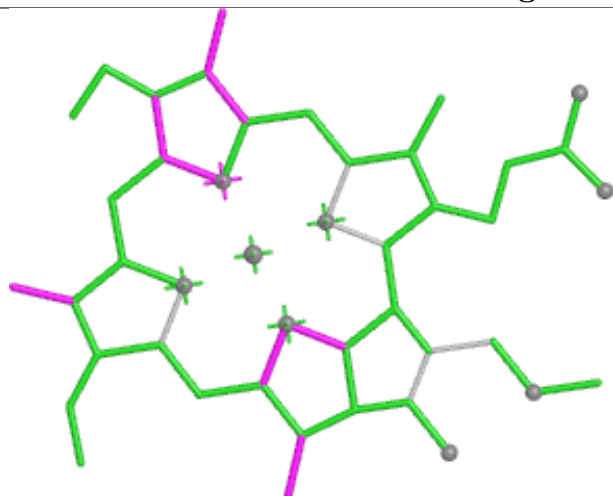
Torsions



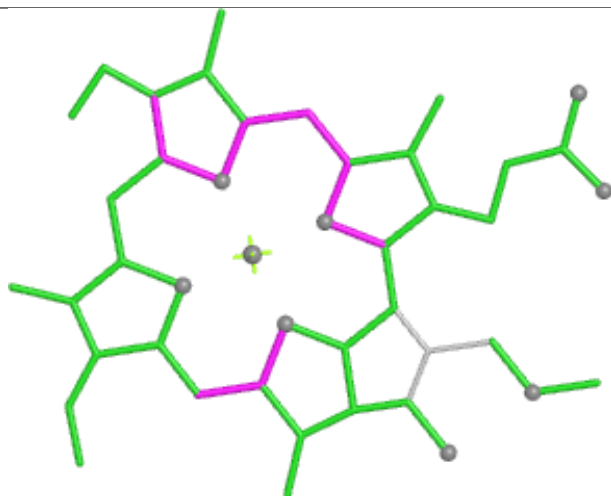
Rings



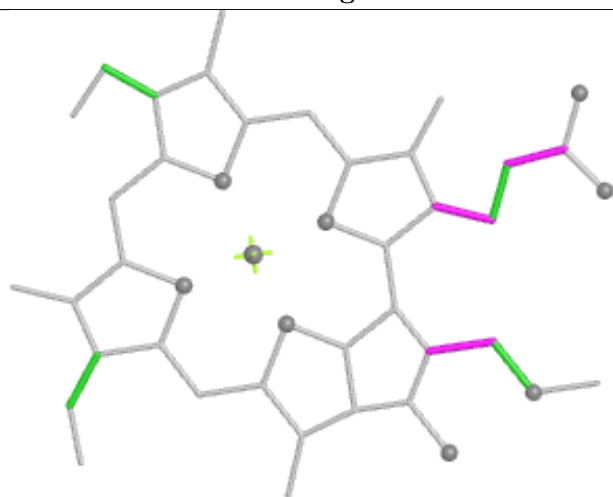
## Ligand CLA 7 609



Bond lengths



Bond angles

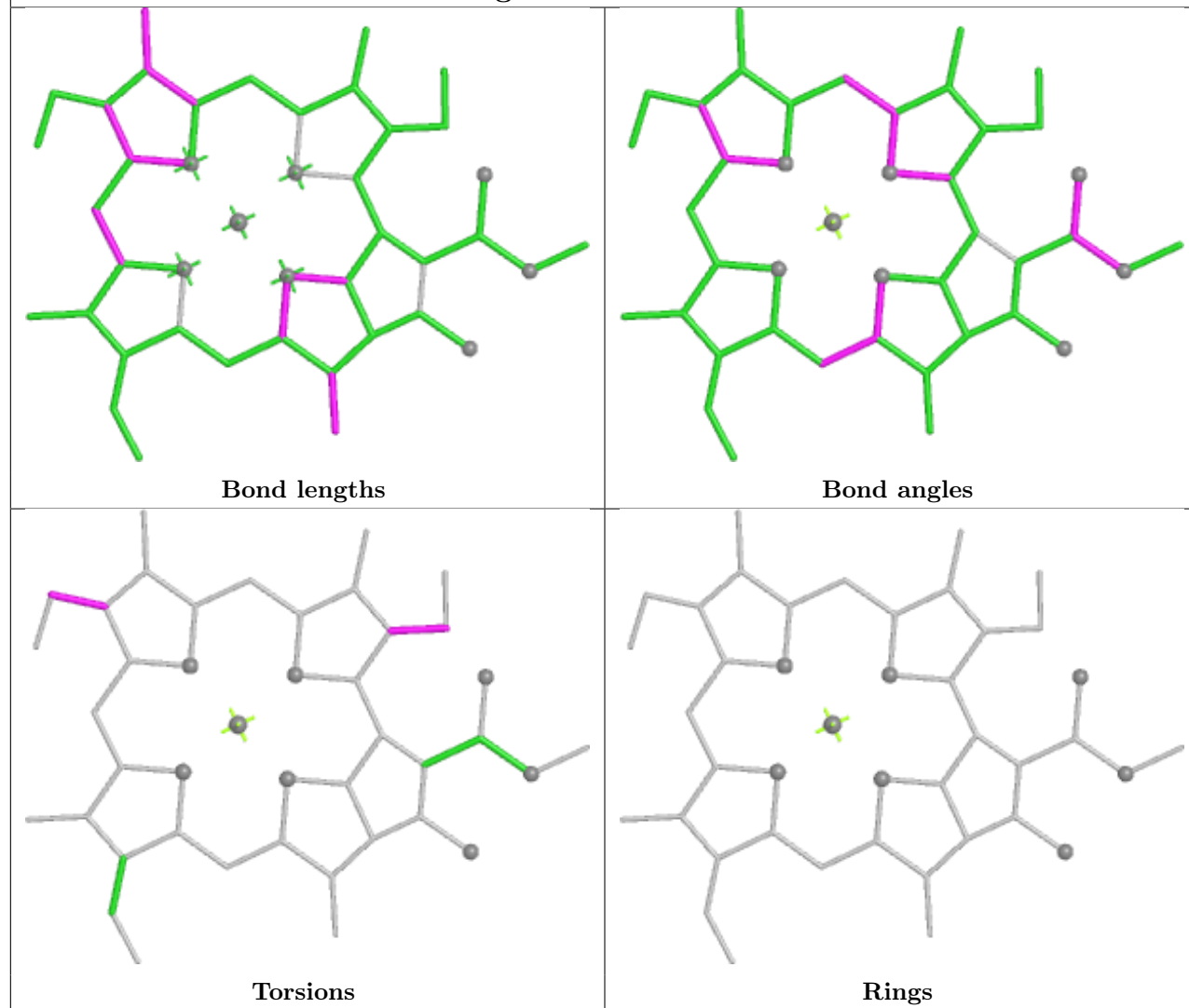


Torsions

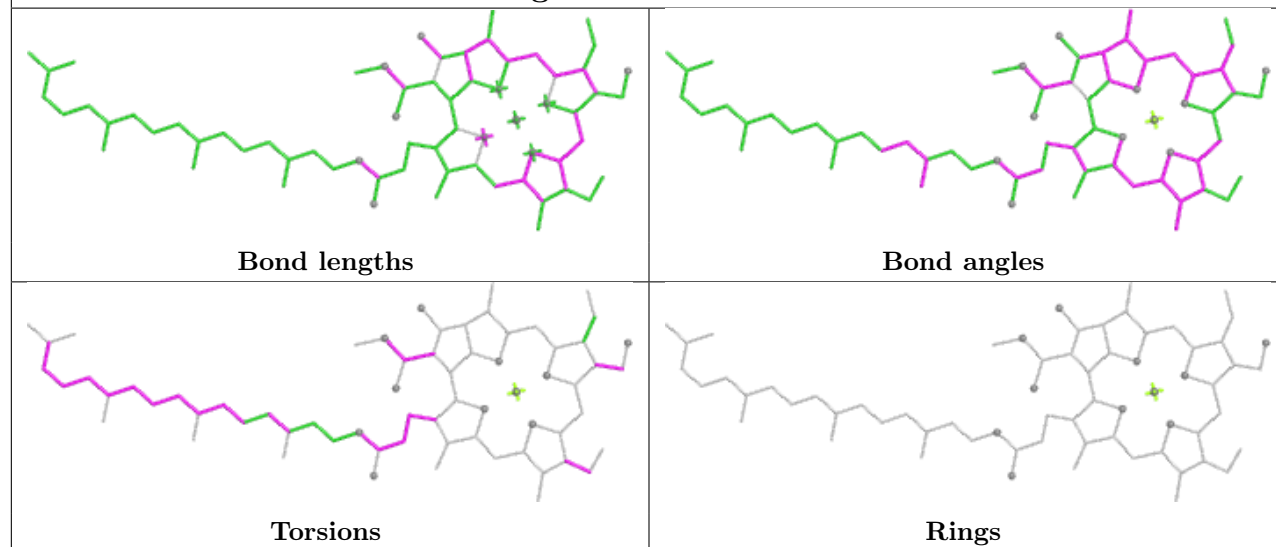


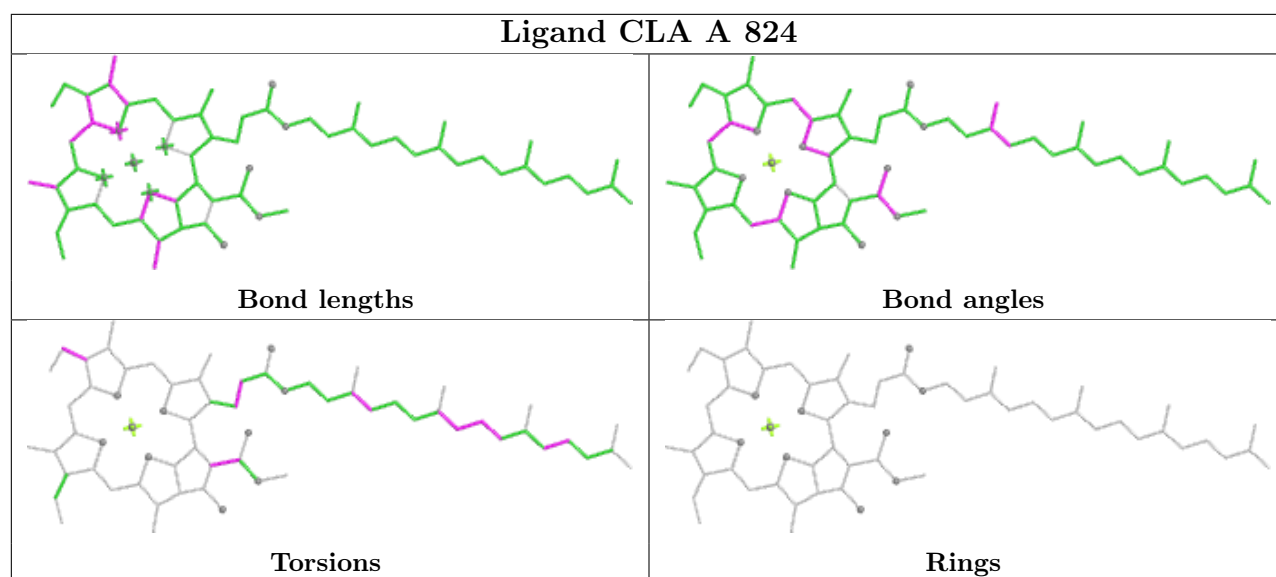
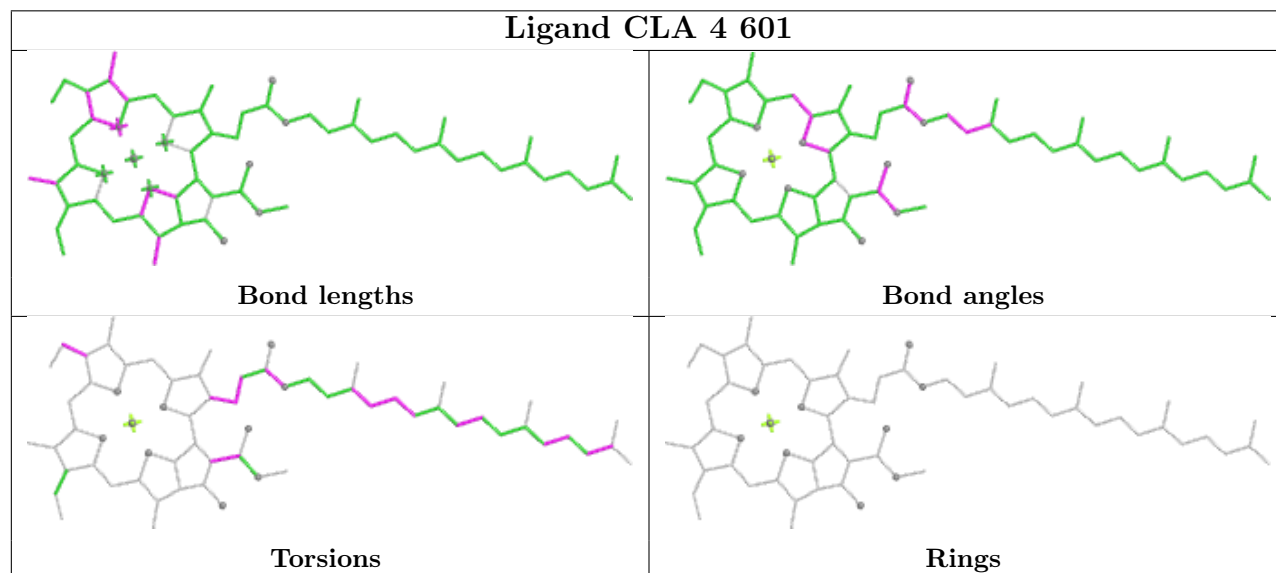
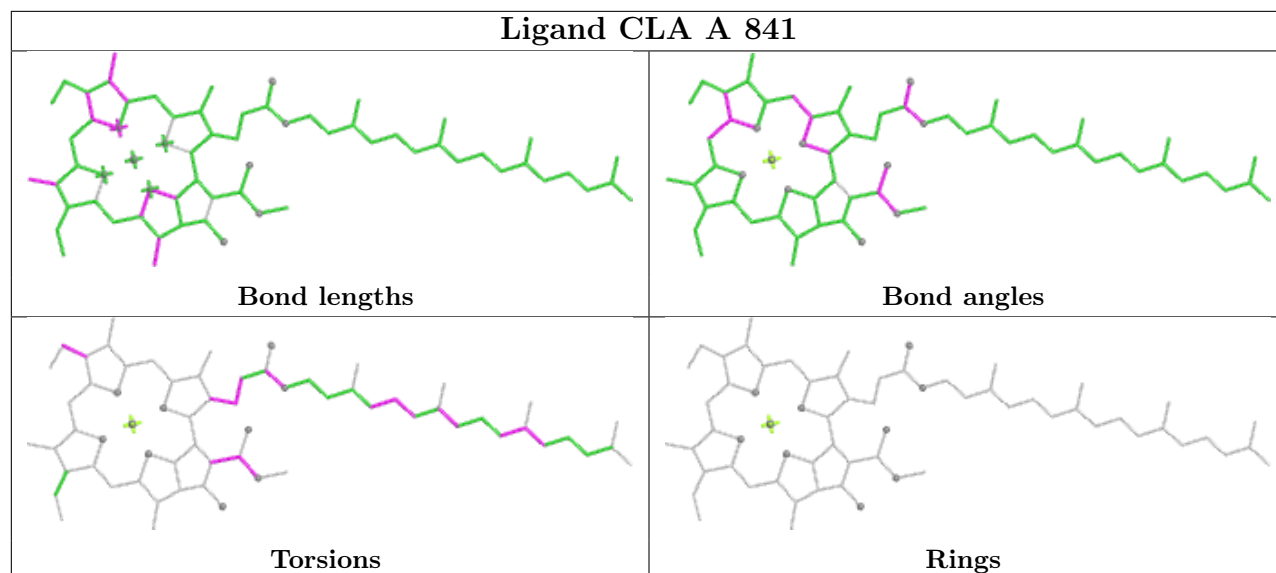
Rings

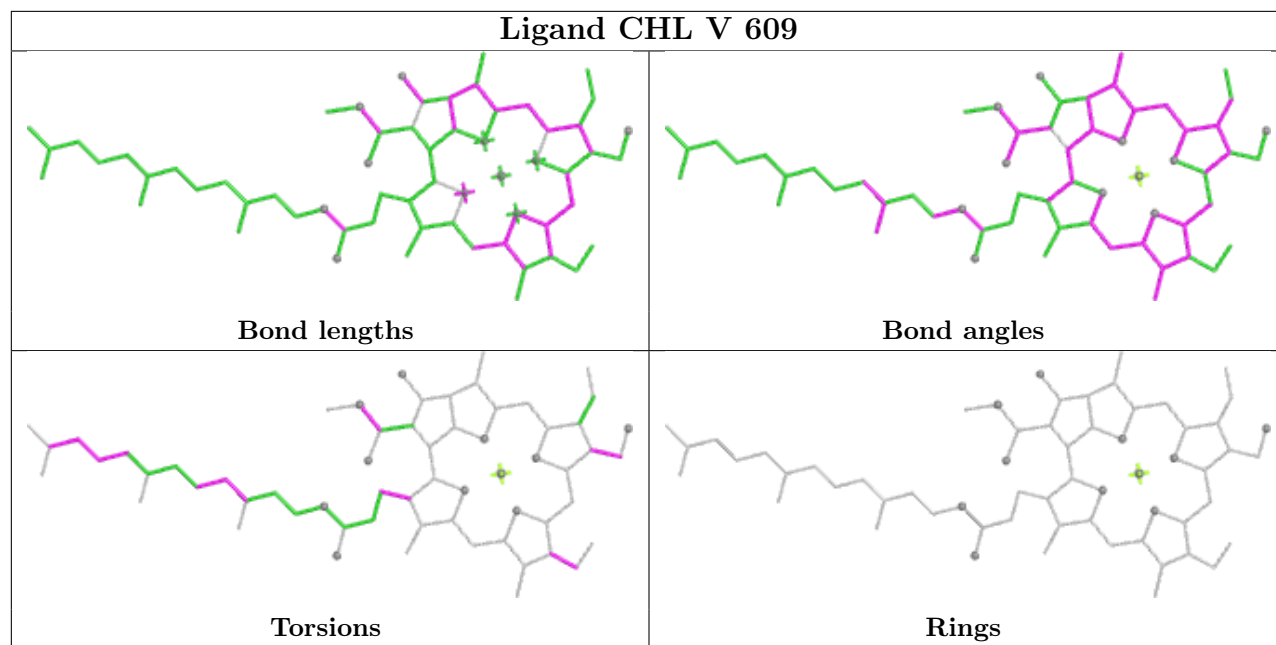
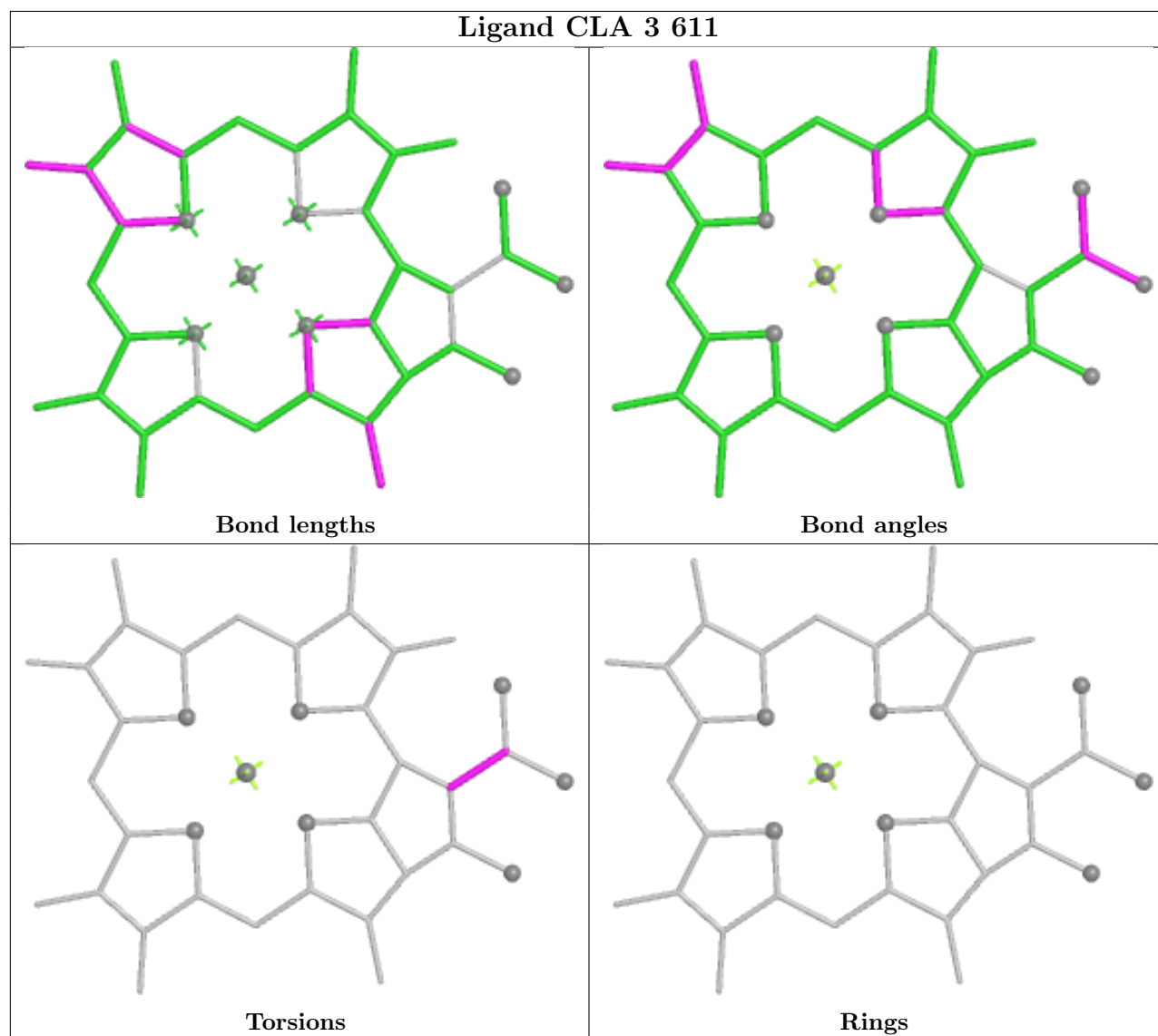
## Ligand CLA X 614



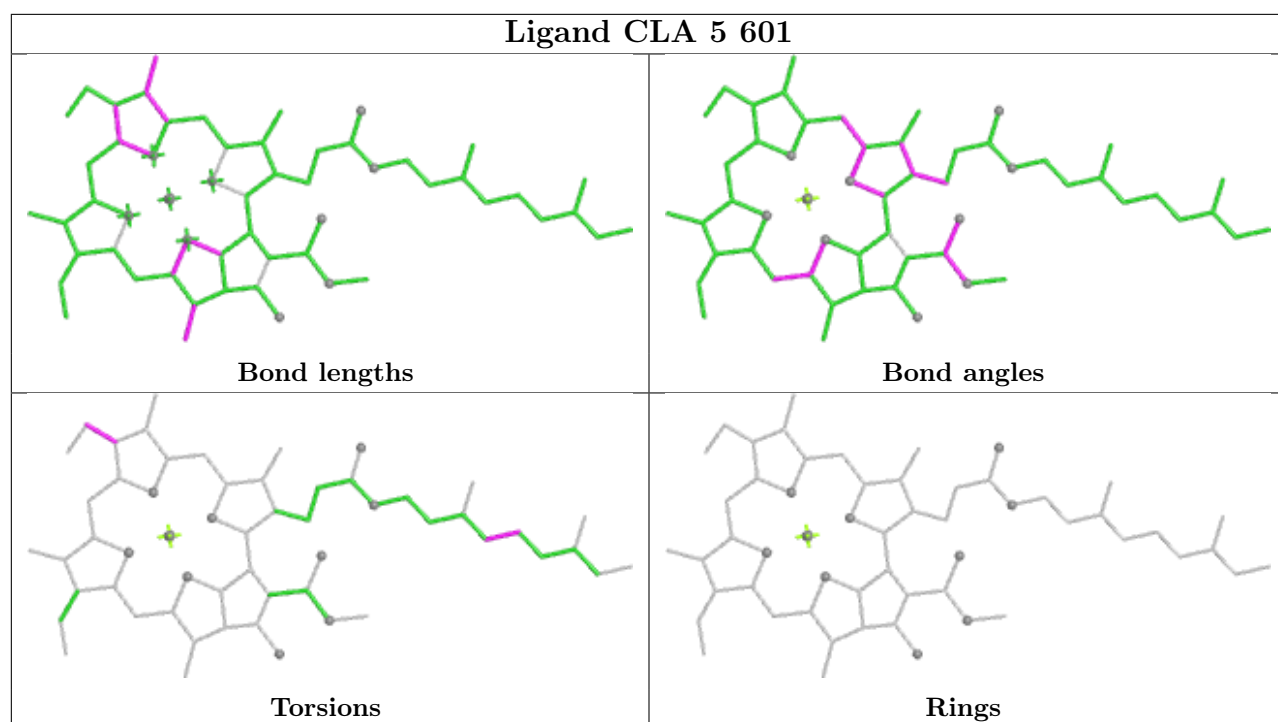
## Ligand CHL X 607



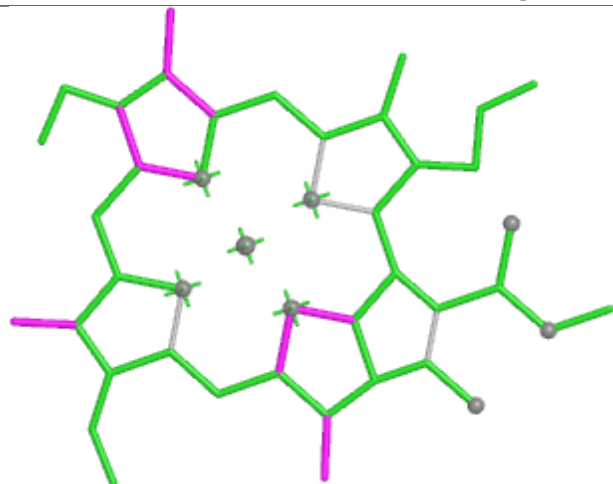




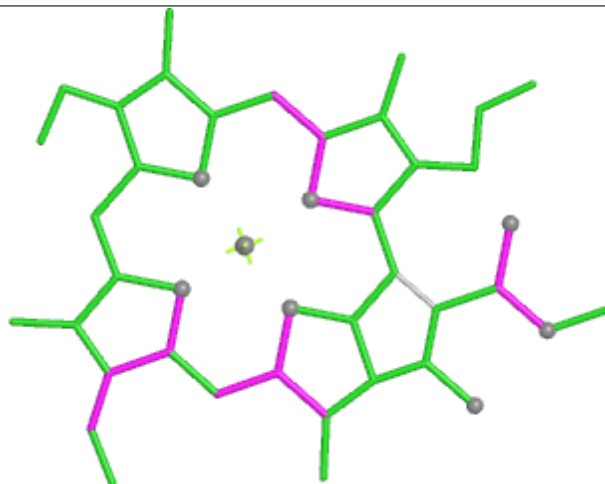




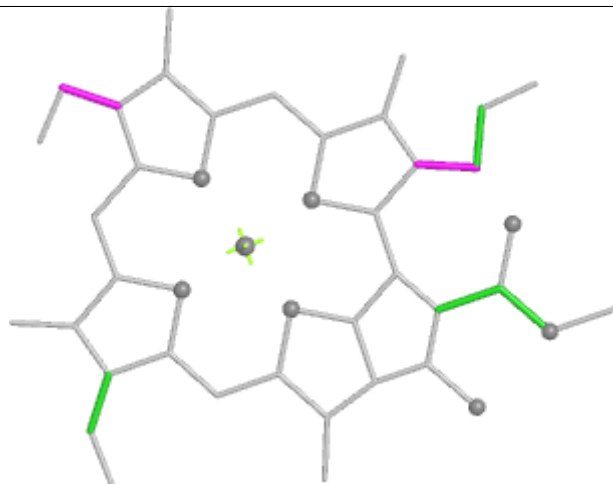
## Ligand CLA B 830



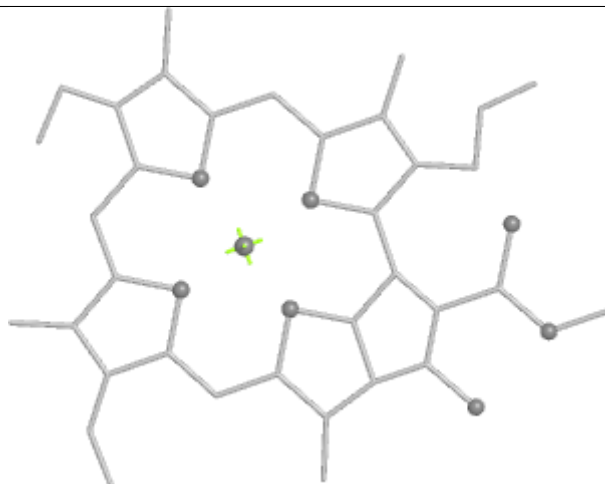
Bond lengths



Bond angles

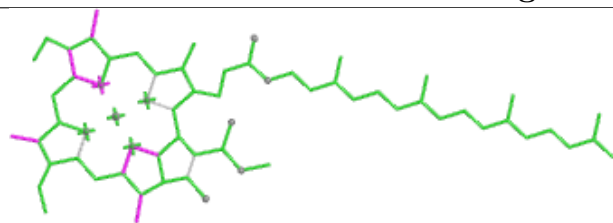


Torsions

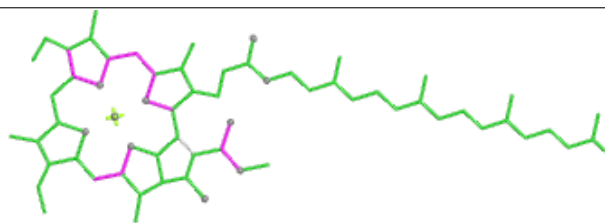


Rings

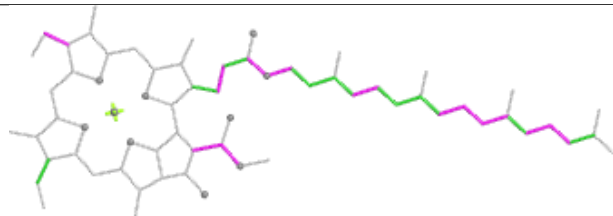
## Ligand CLA 8 601



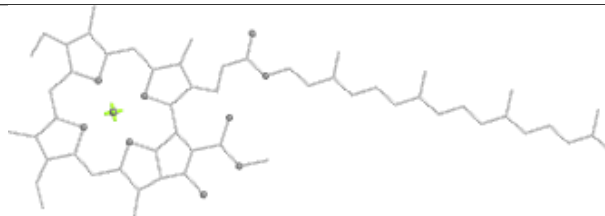
Bond lengths



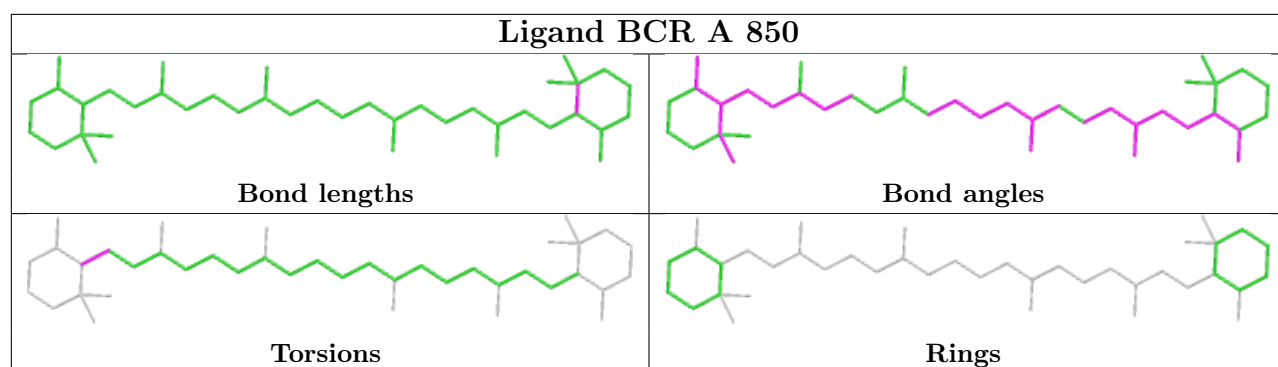
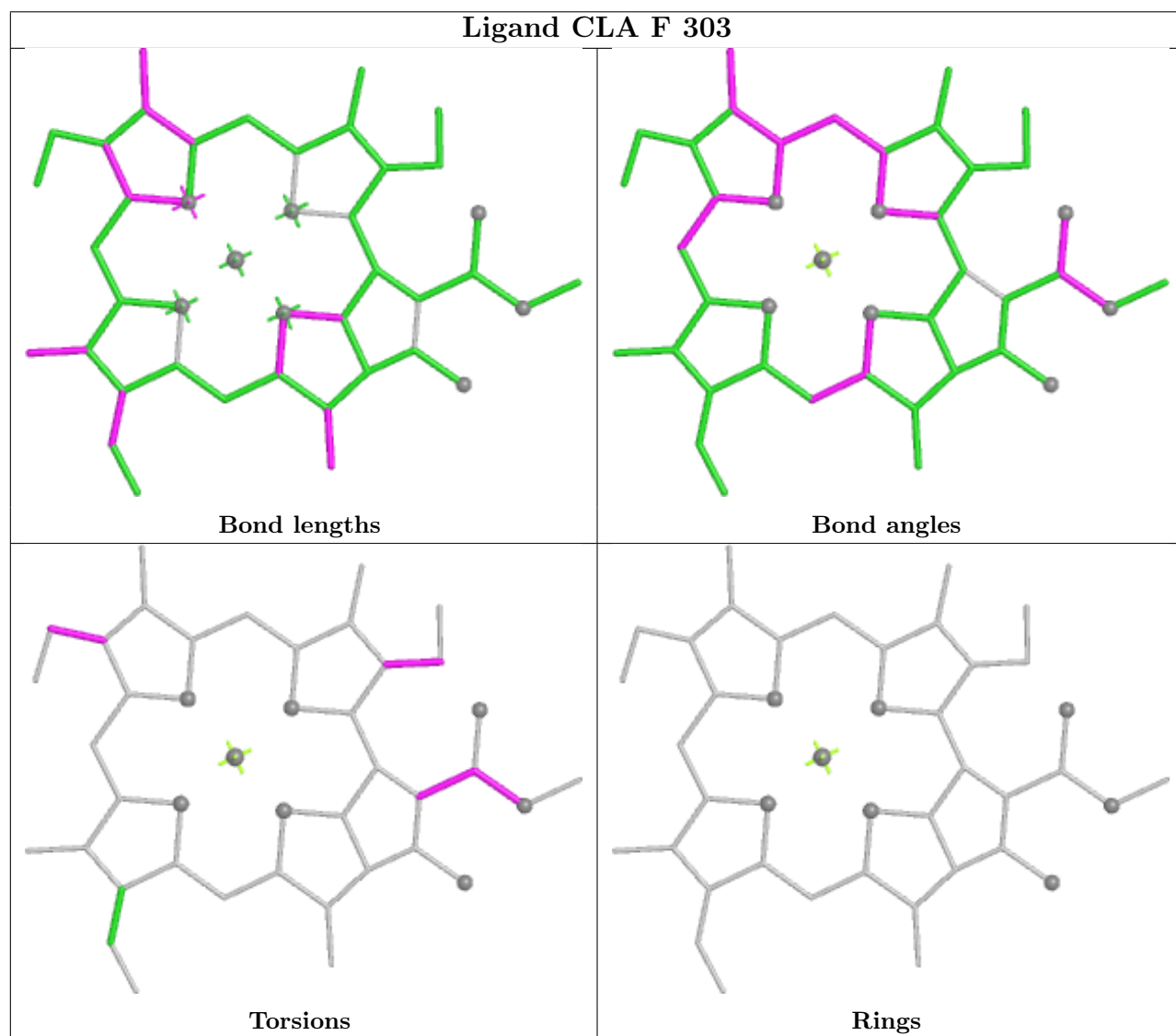
Bond angles

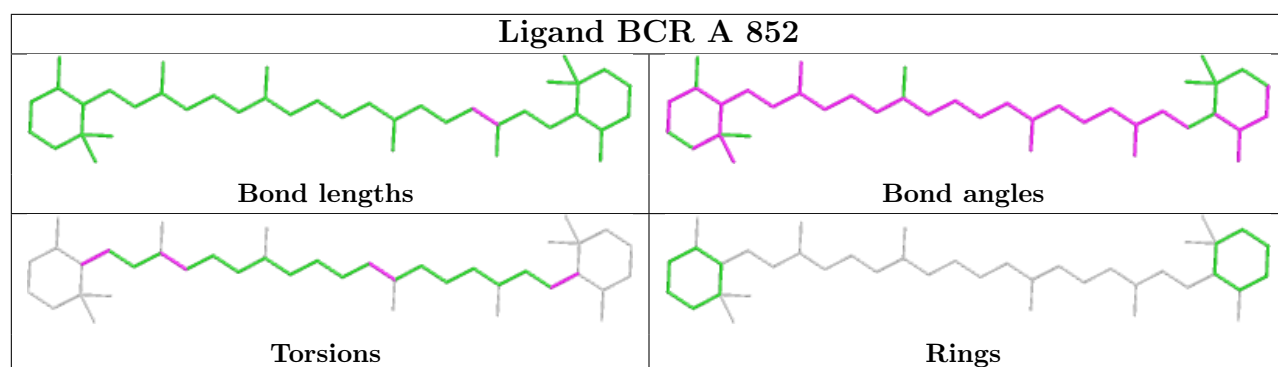
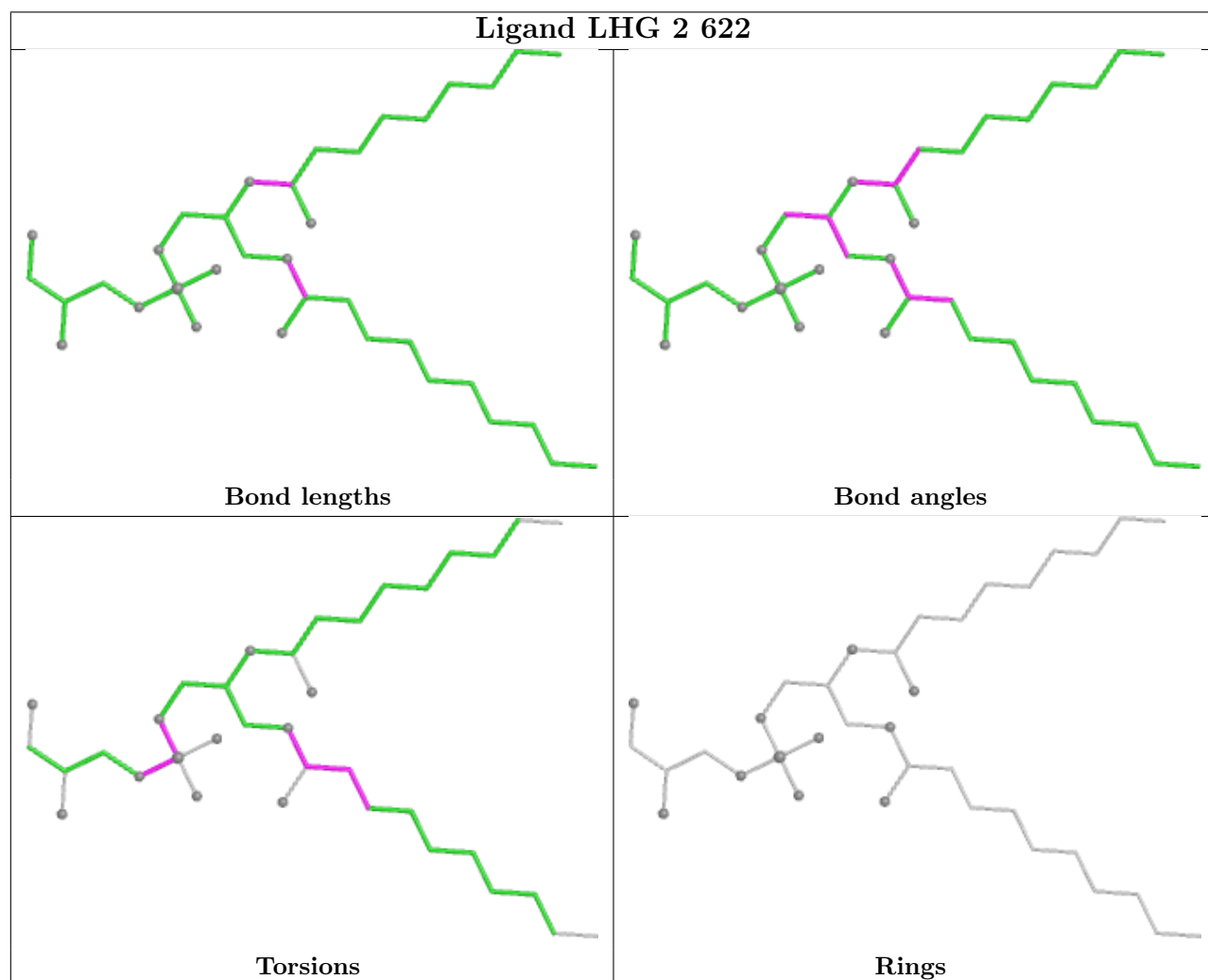


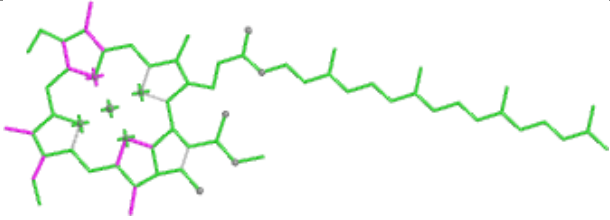
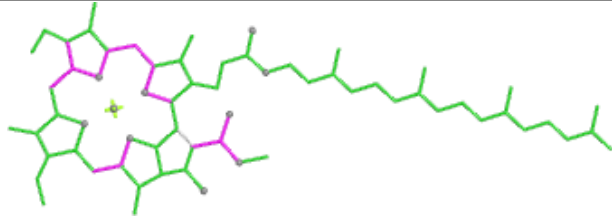
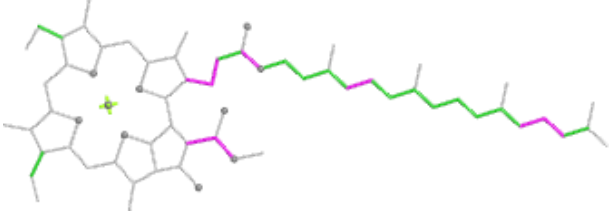
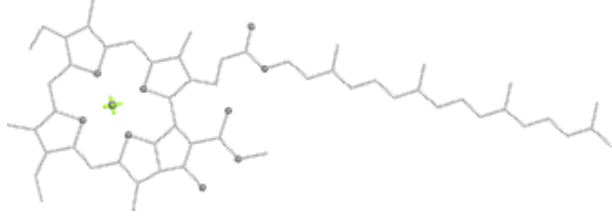
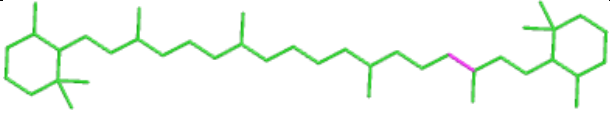
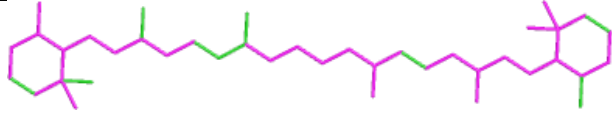
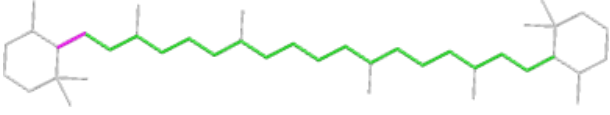
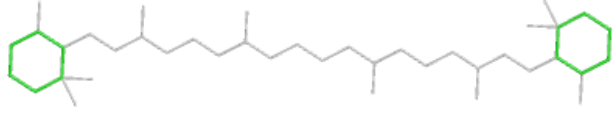
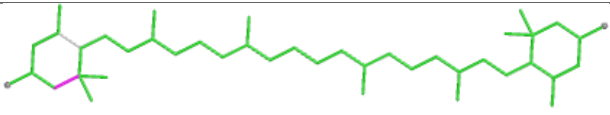
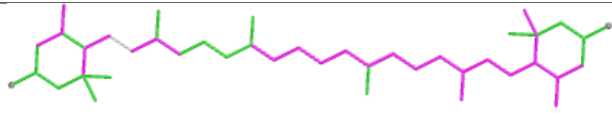
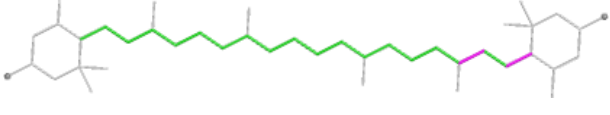
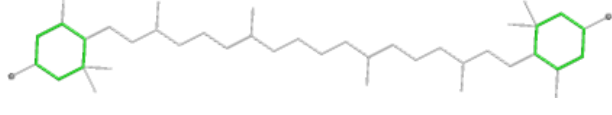
Torsions

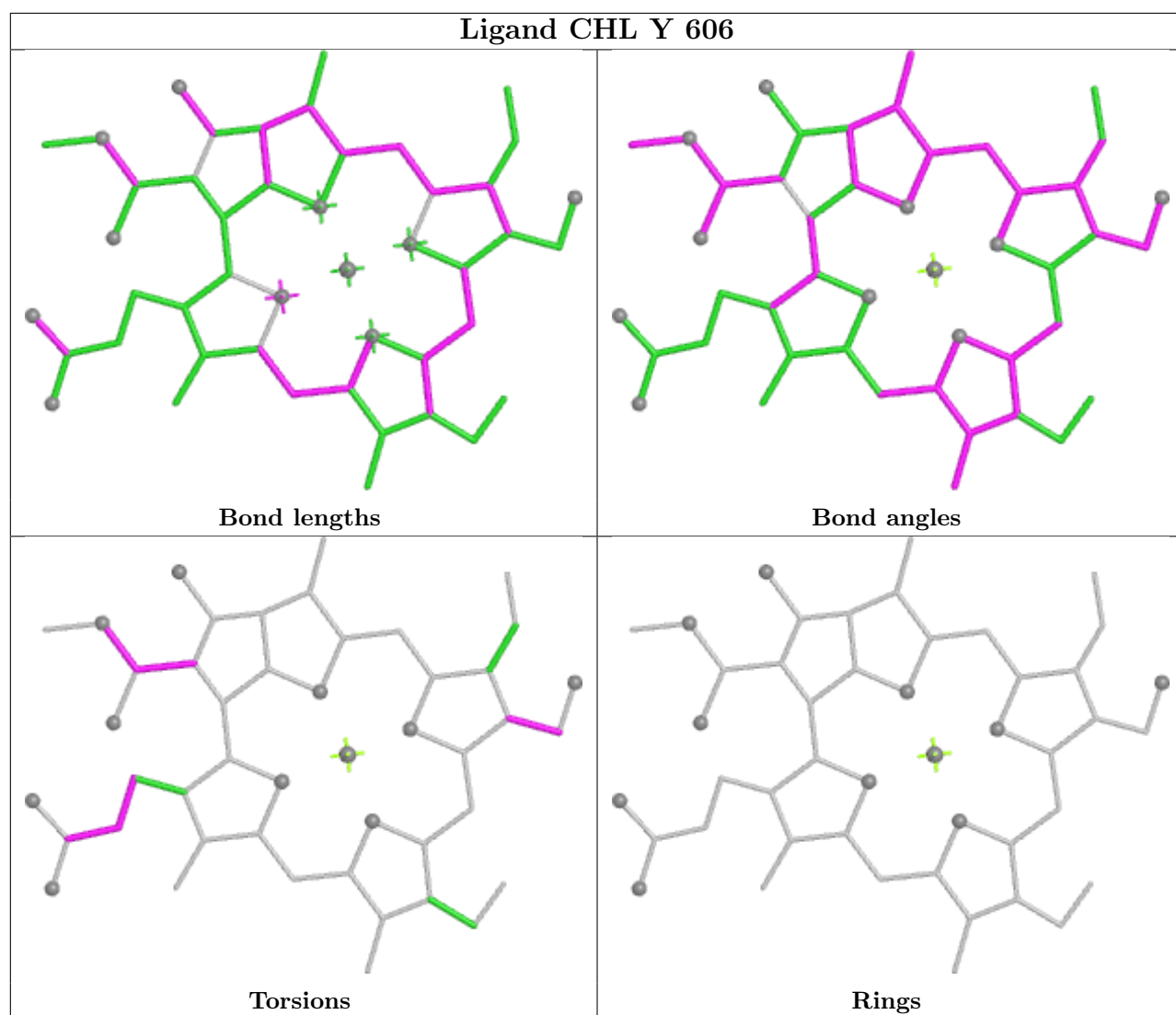


Rings

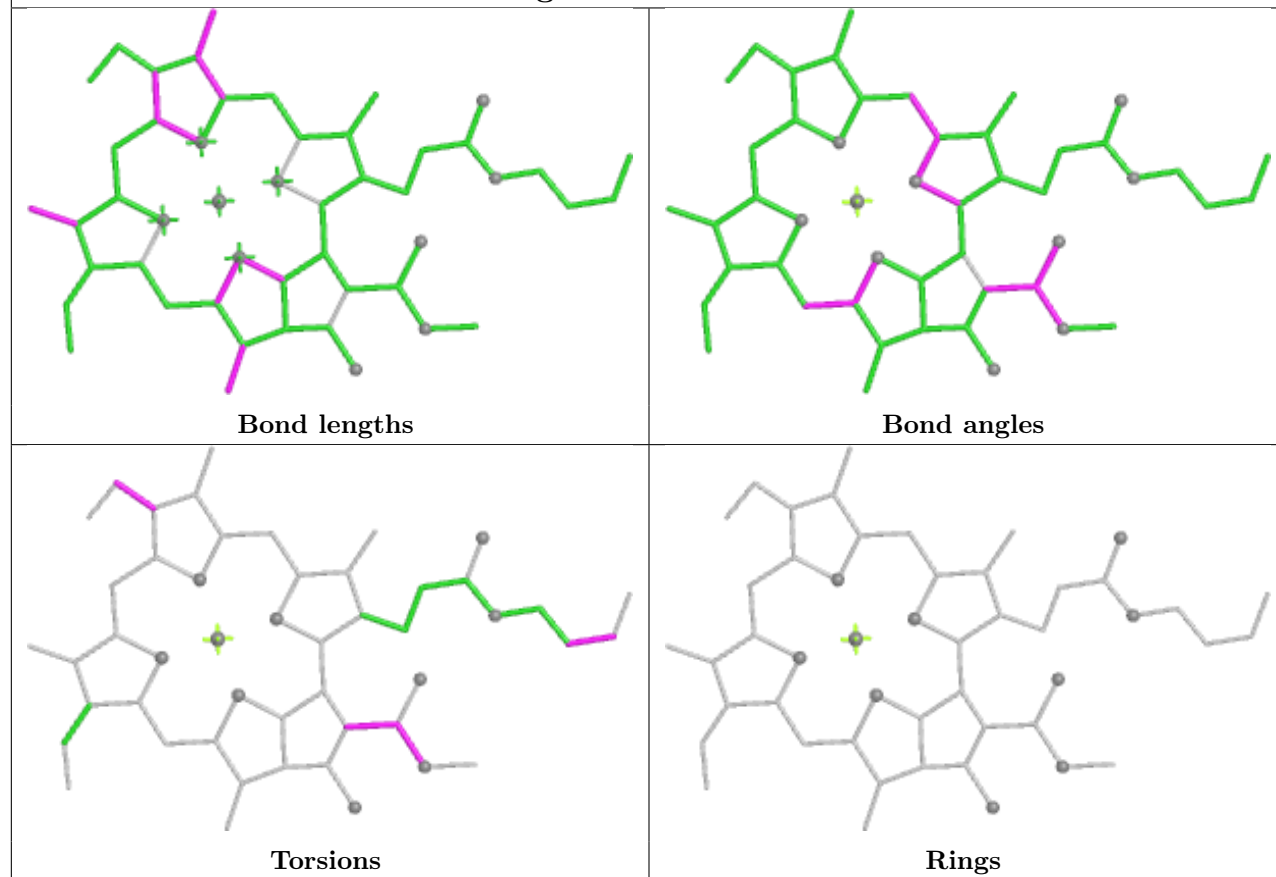




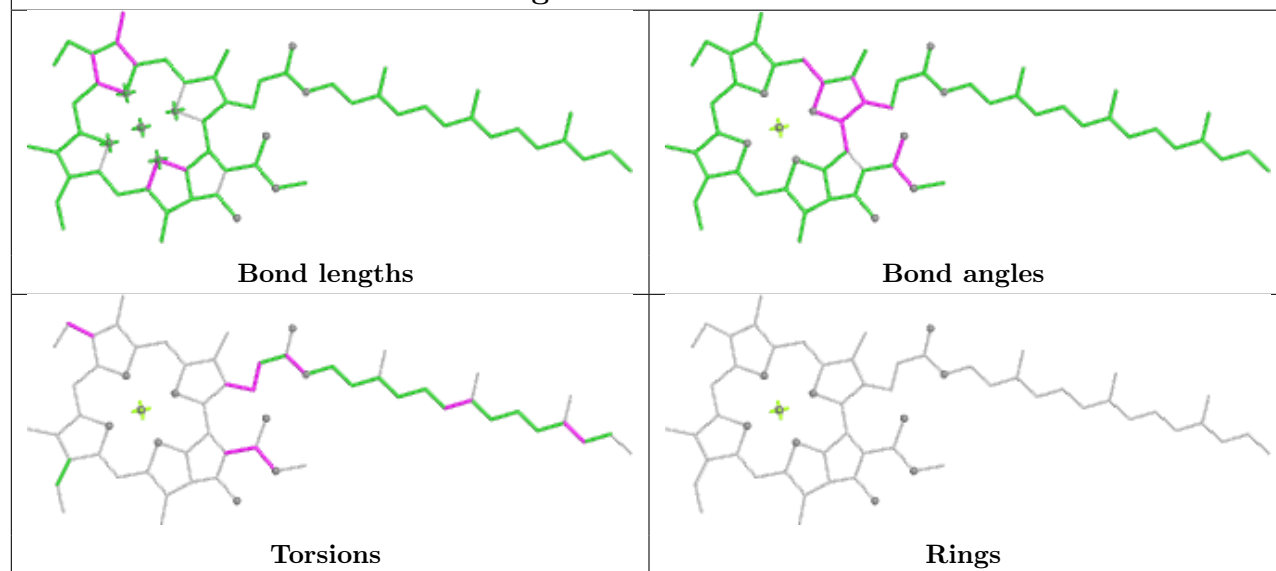
| Ligand CLA B 809                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand BCR A 851                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand LUT a 617                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

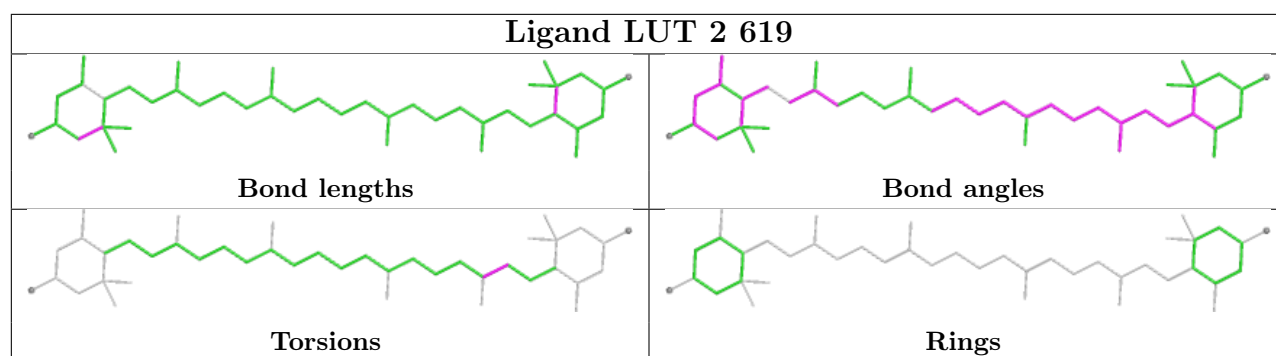
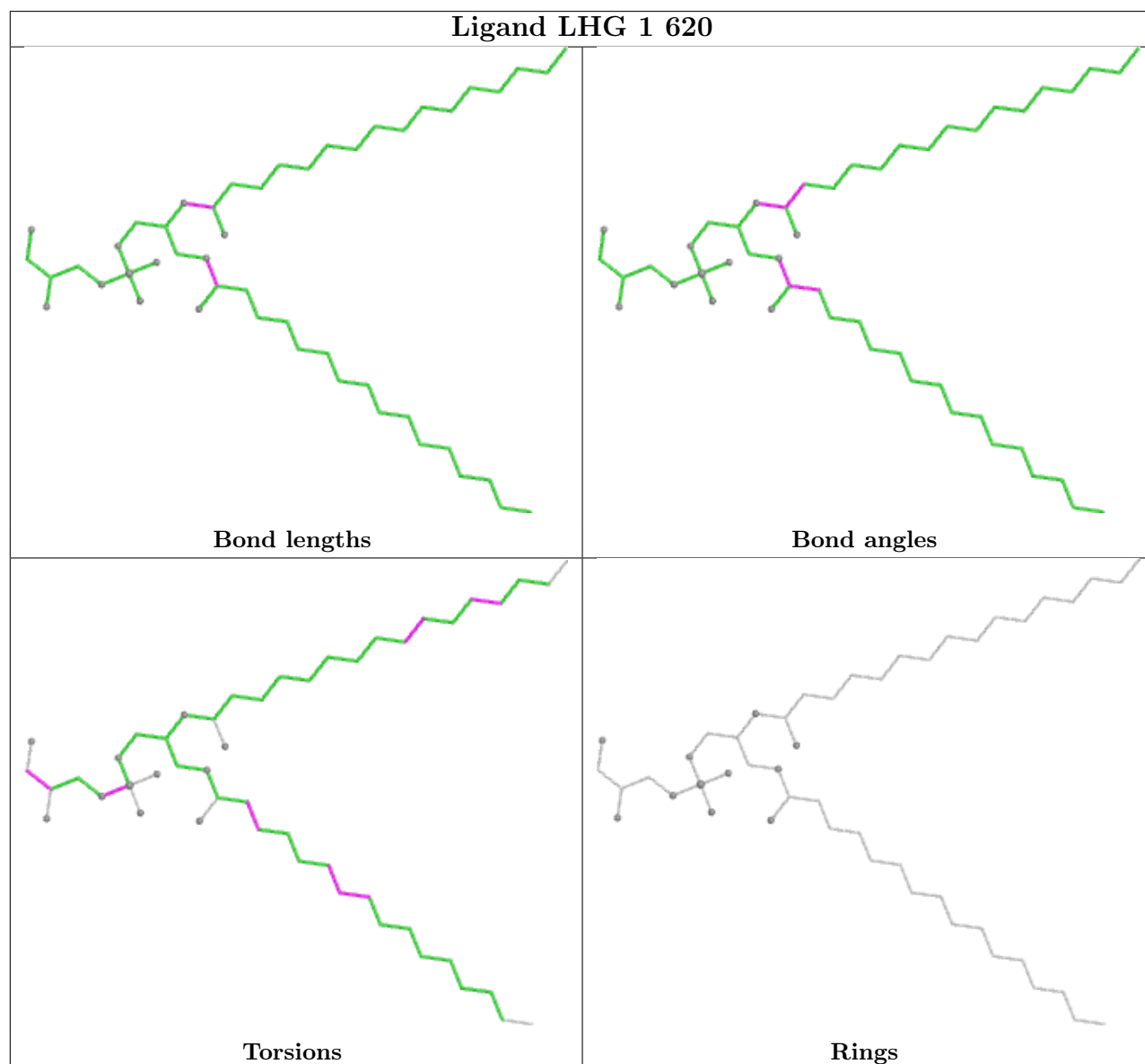


## Ligand CLA 1 604



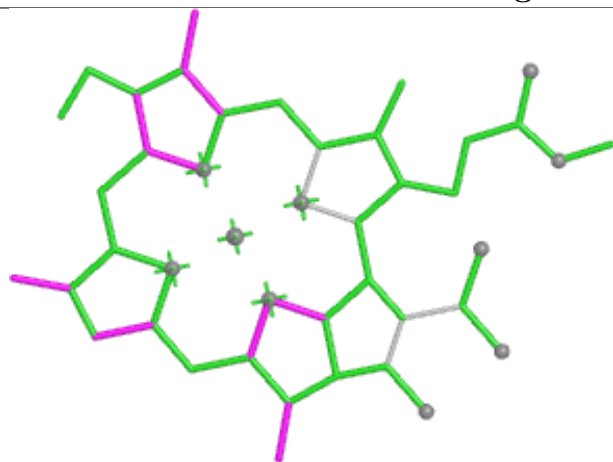
## Ligand CLA X 603



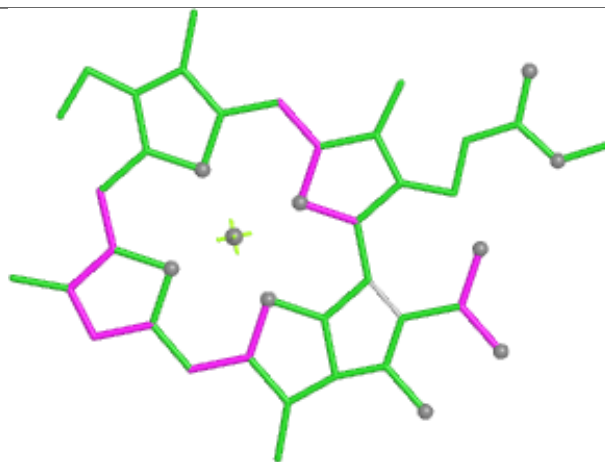




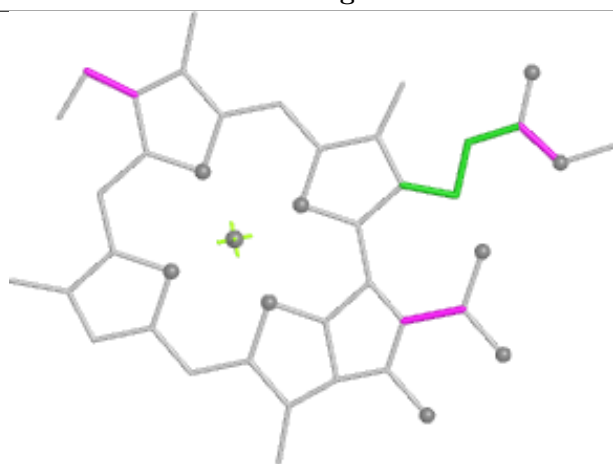
## Ligand CLA B 821



Bond lengths



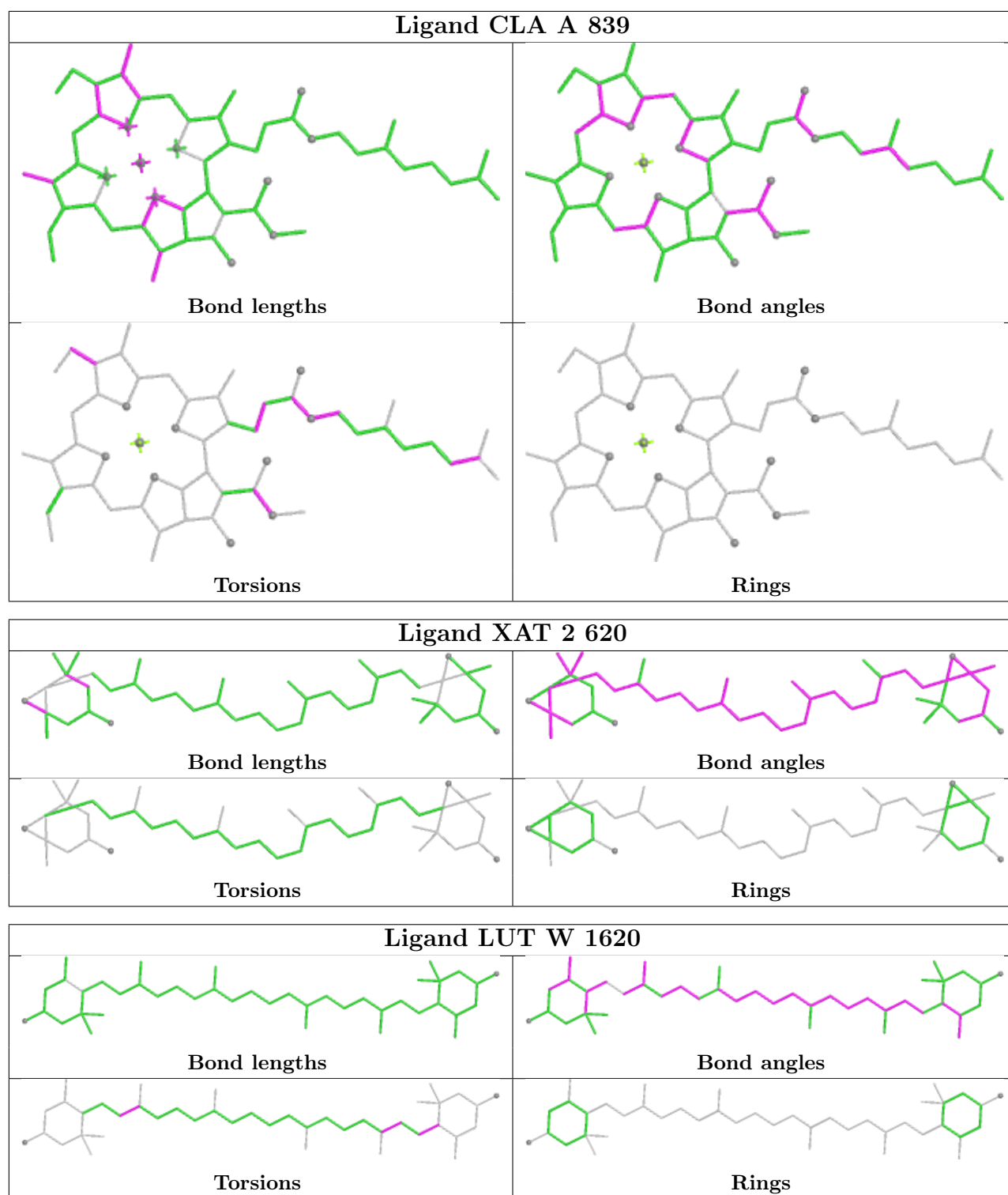
Bond angles

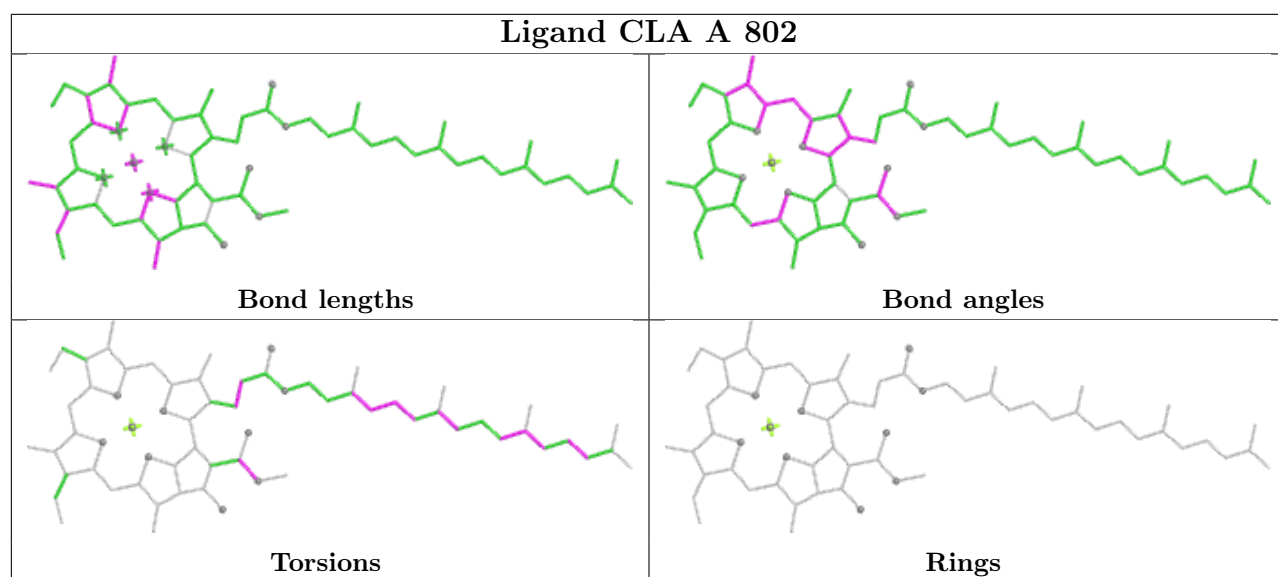
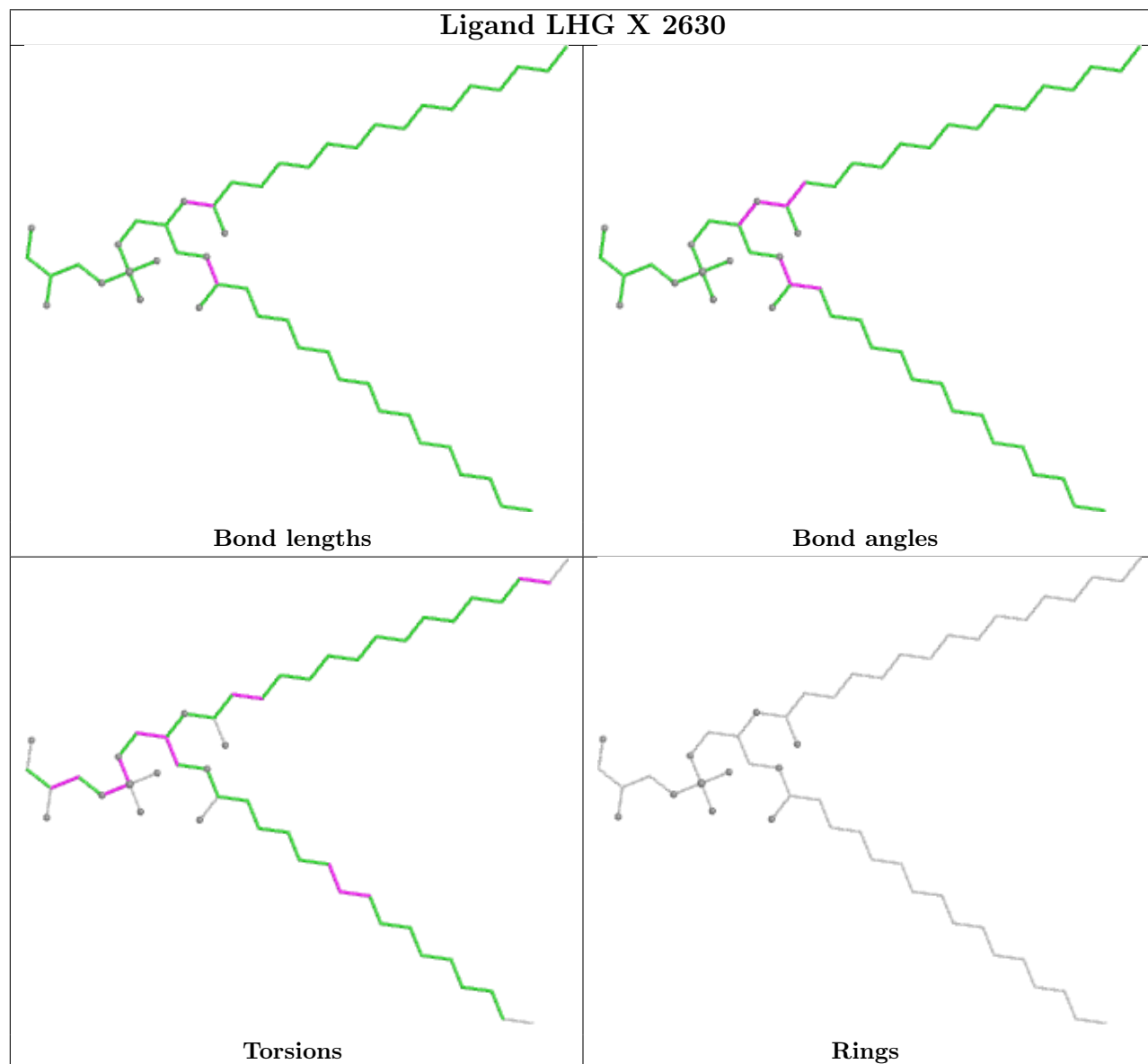


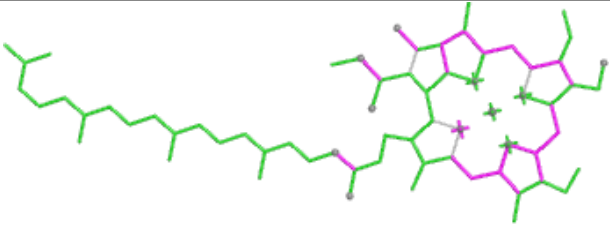
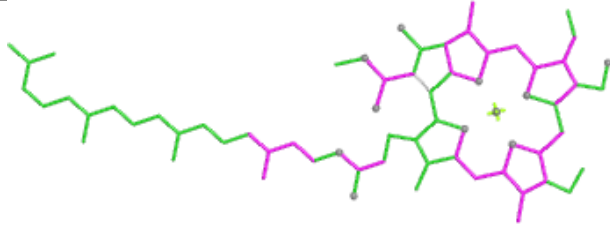
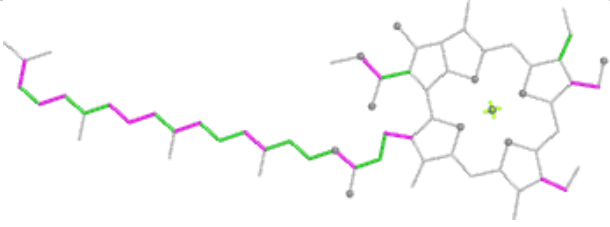
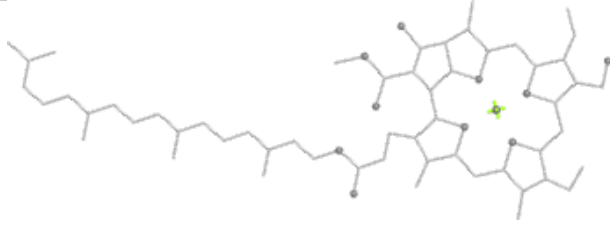
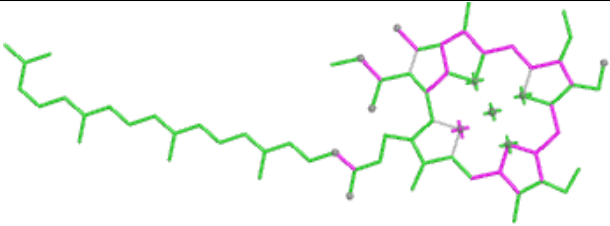
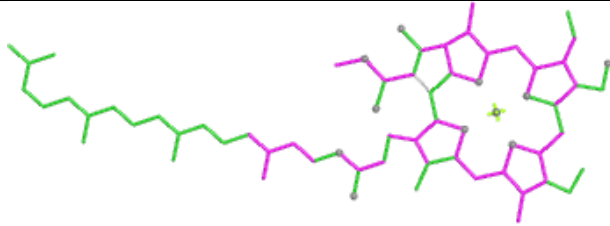
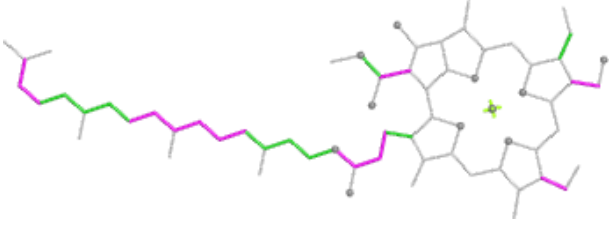
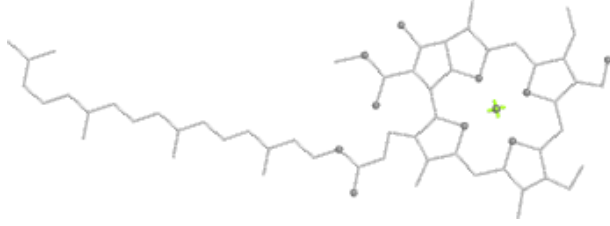
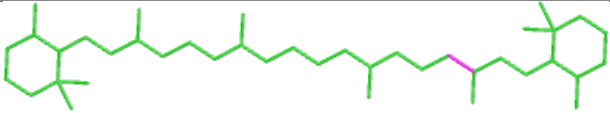
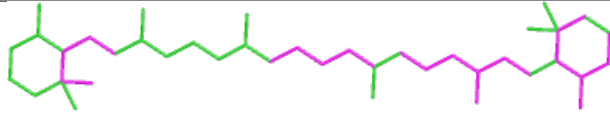
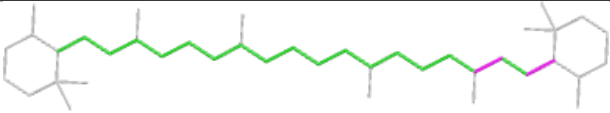
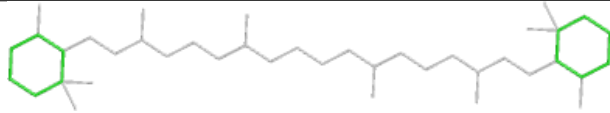
Torsions



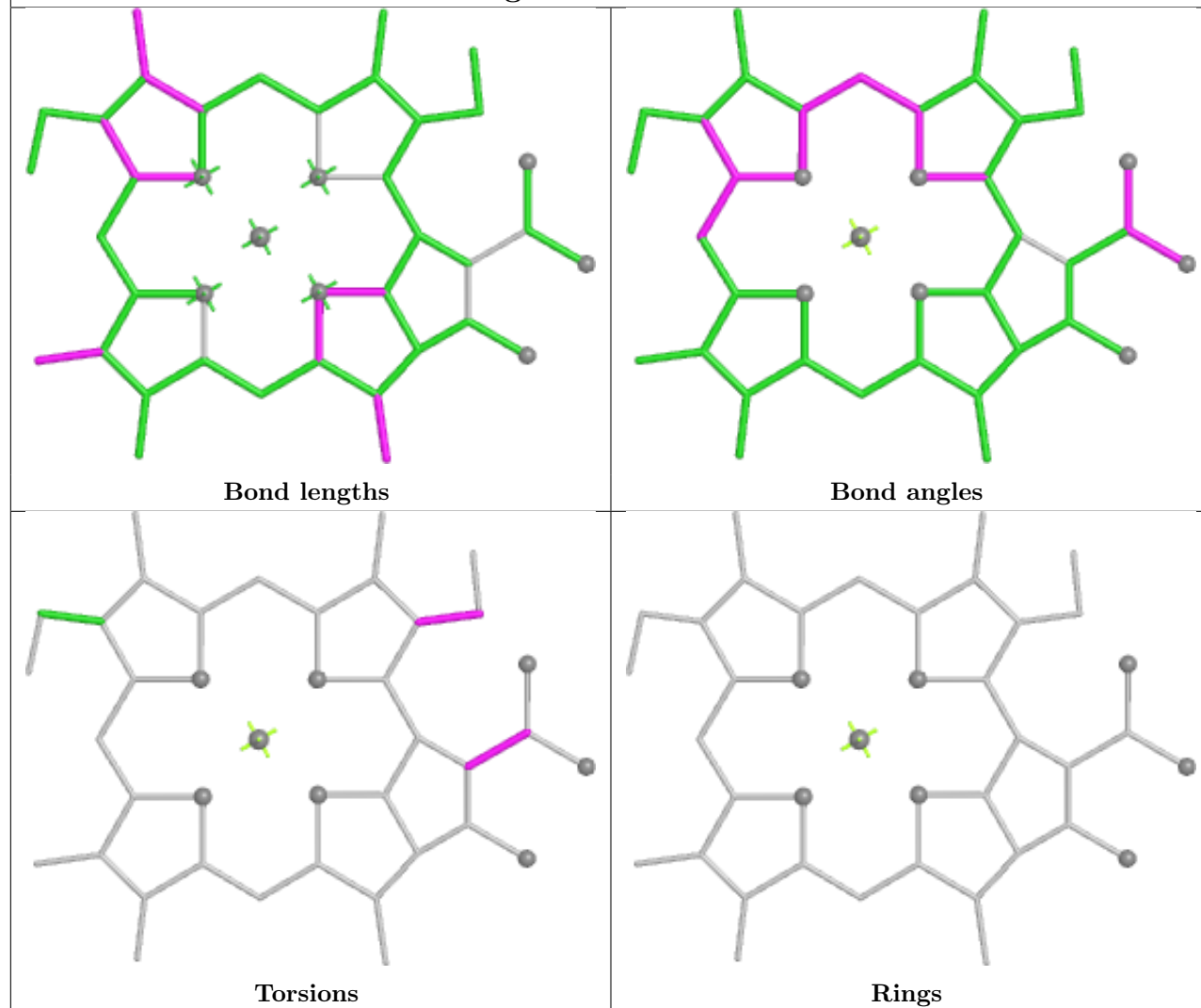
Rings



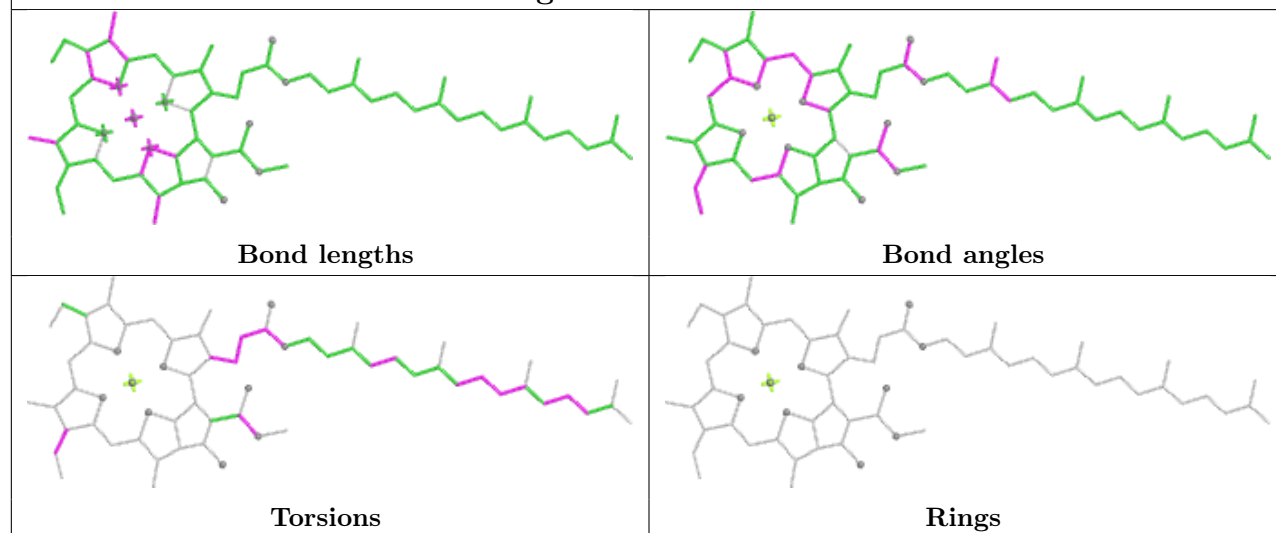


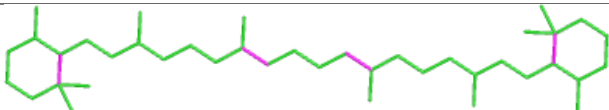
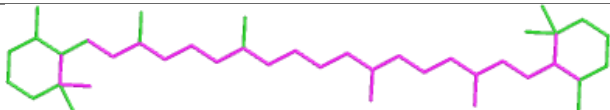
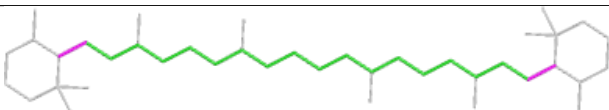
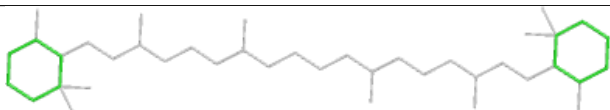
| Ligand CHL Z 609                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand CHL X 601                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>  |  <p>Bond angles</p>  |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand BCR B 848                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

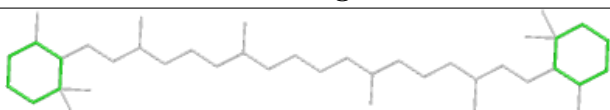
## Ligand CLA 3 615

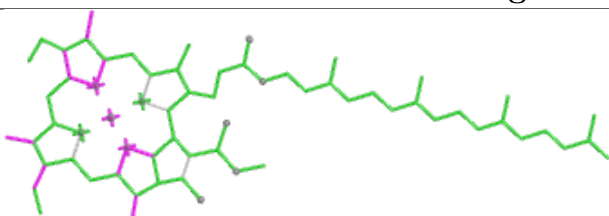
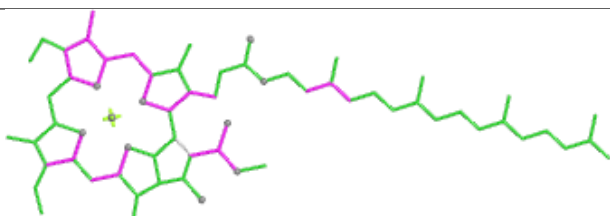
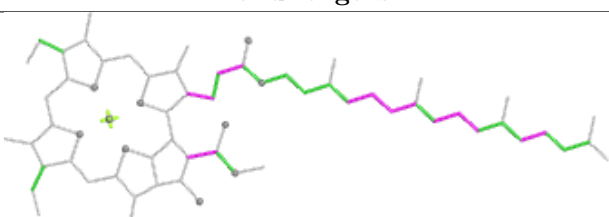
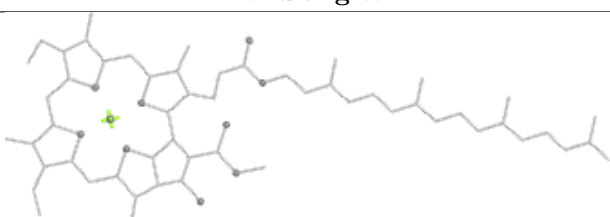


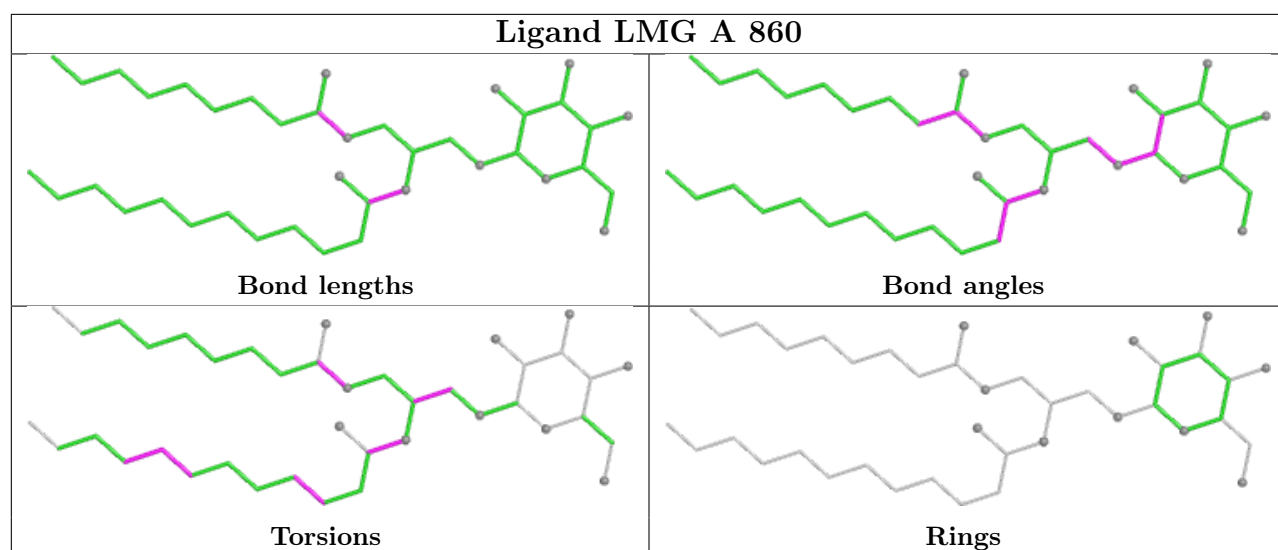
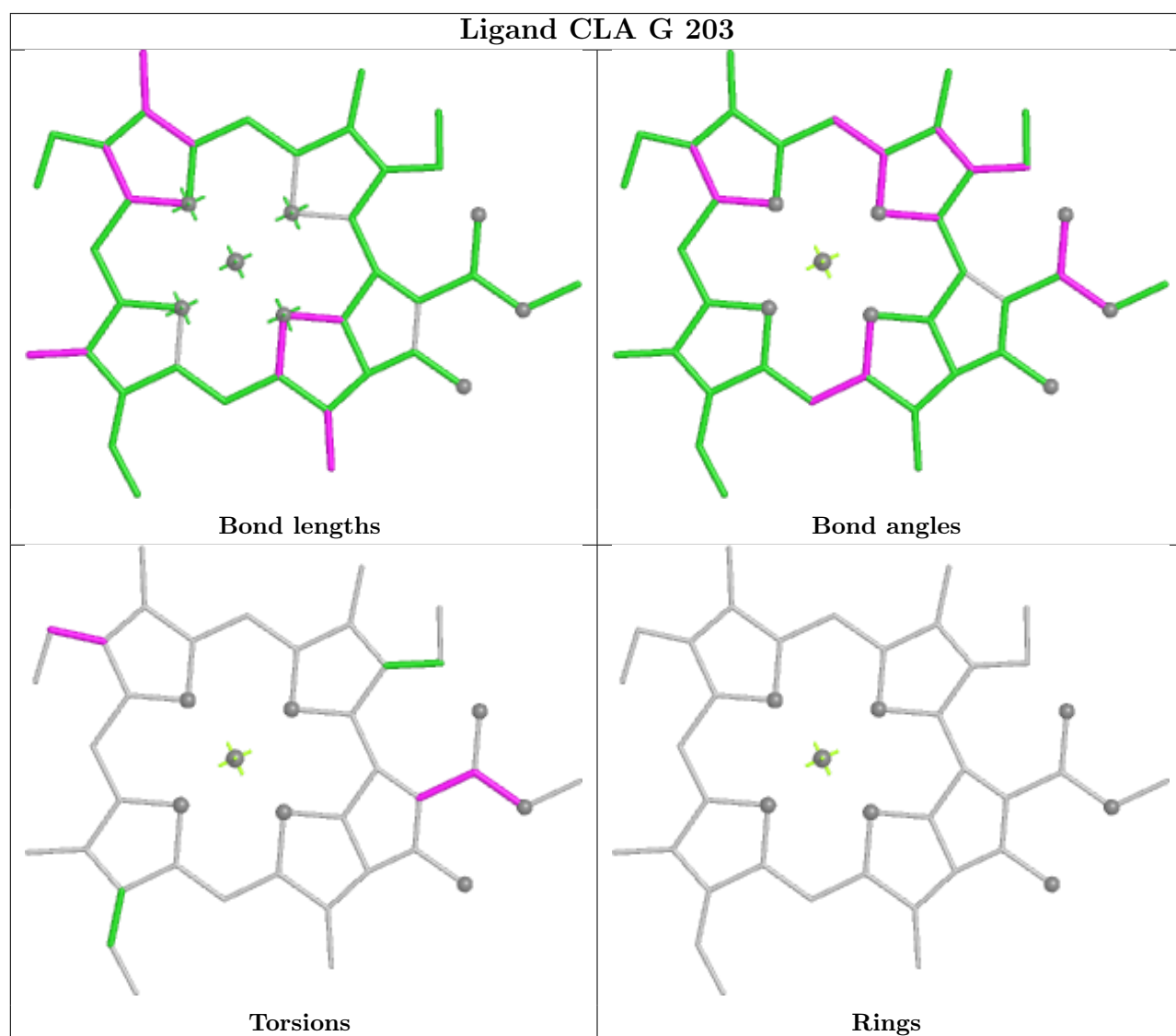
## Ligand CLA 6 616



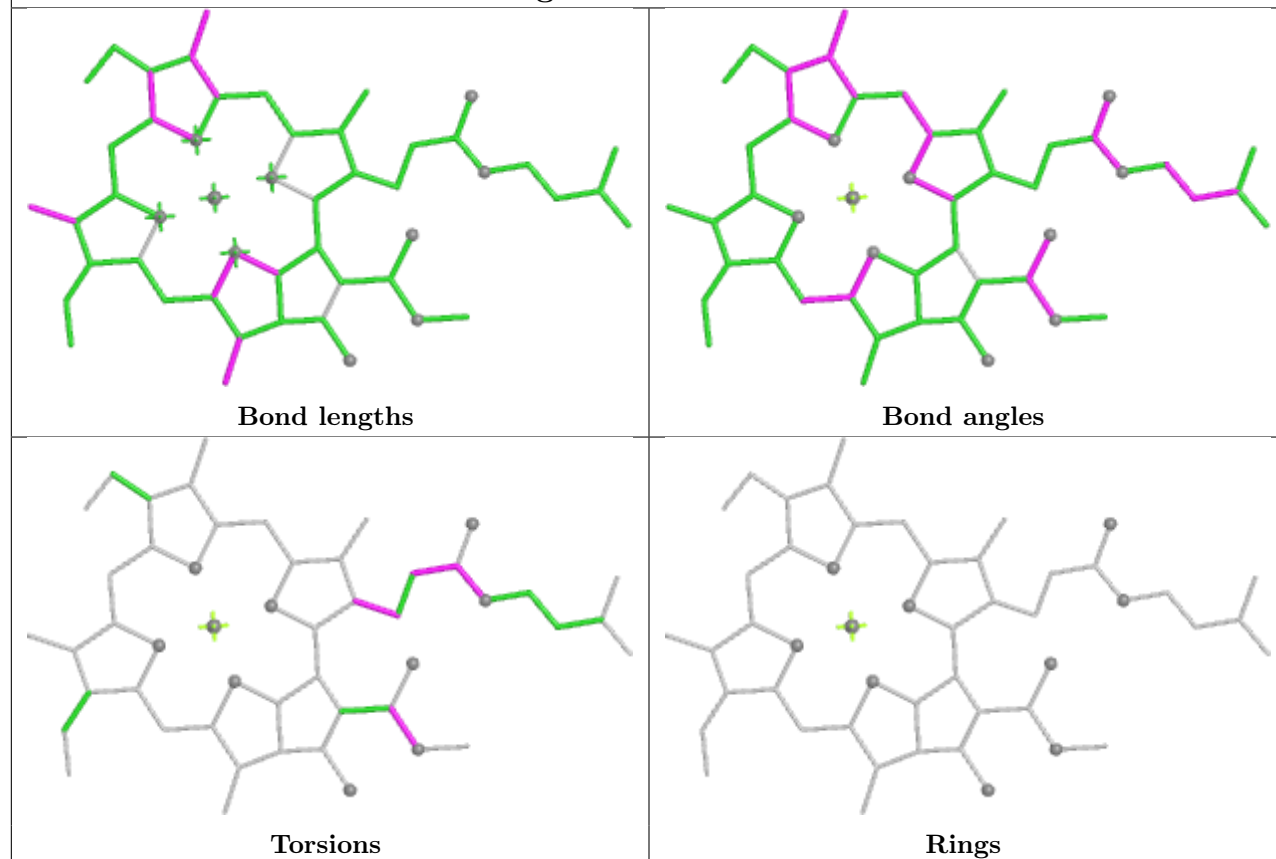
| Ligand BCR B 843                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand BCR 2 623                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

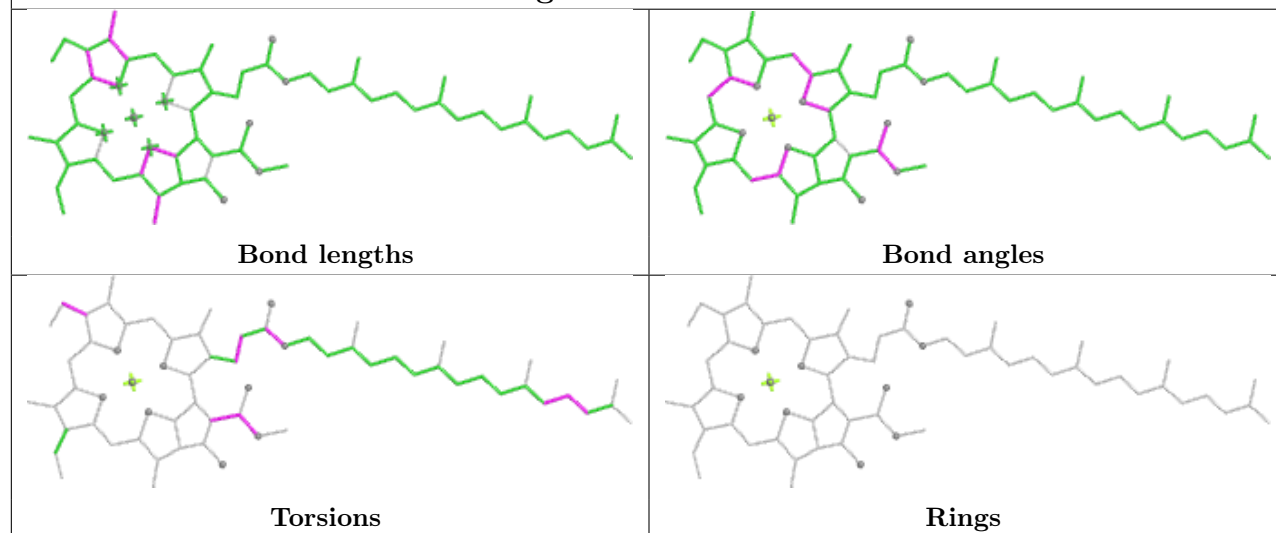
| Ligand CLA A 806                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



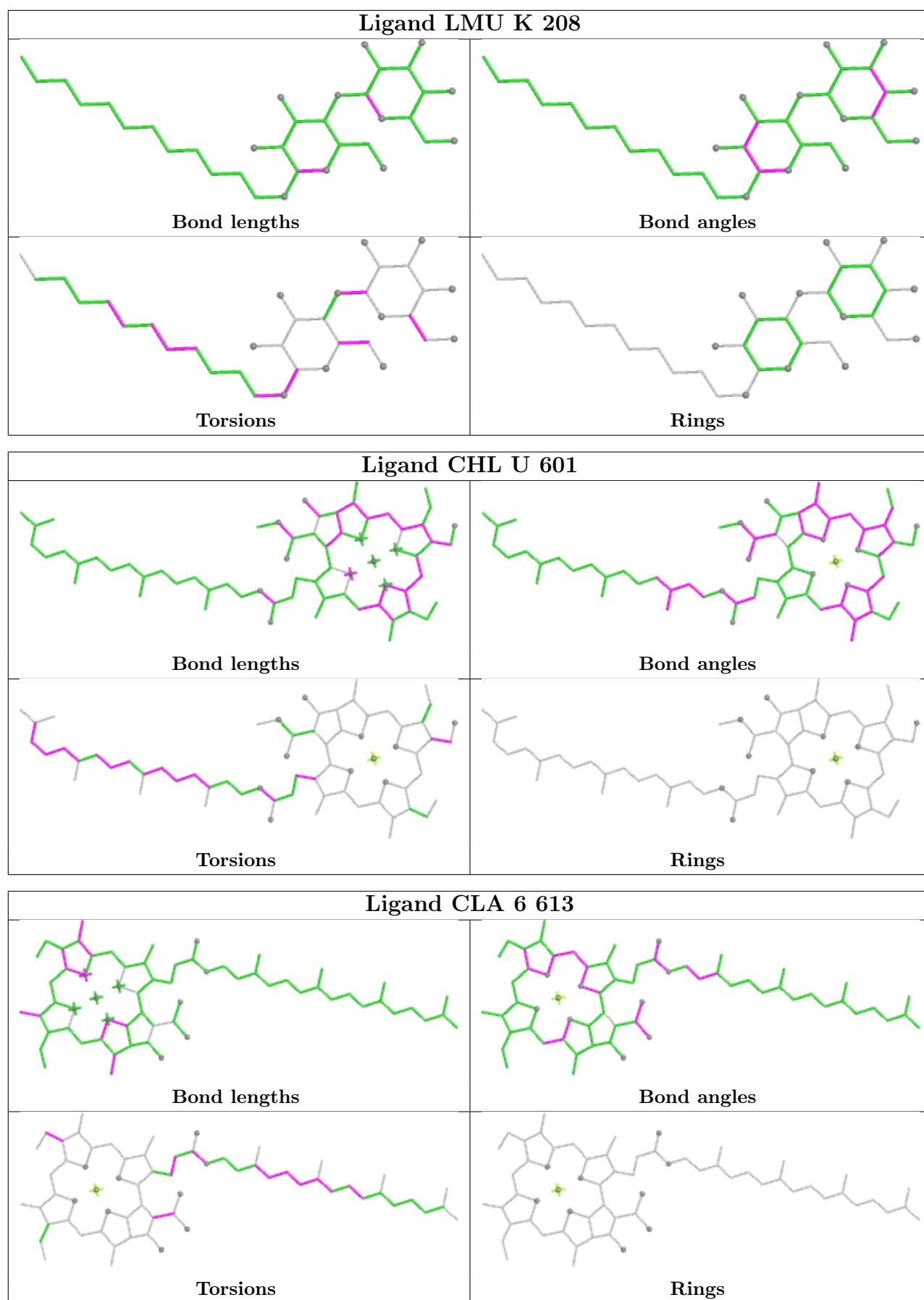
## Ligand CLA 8 604



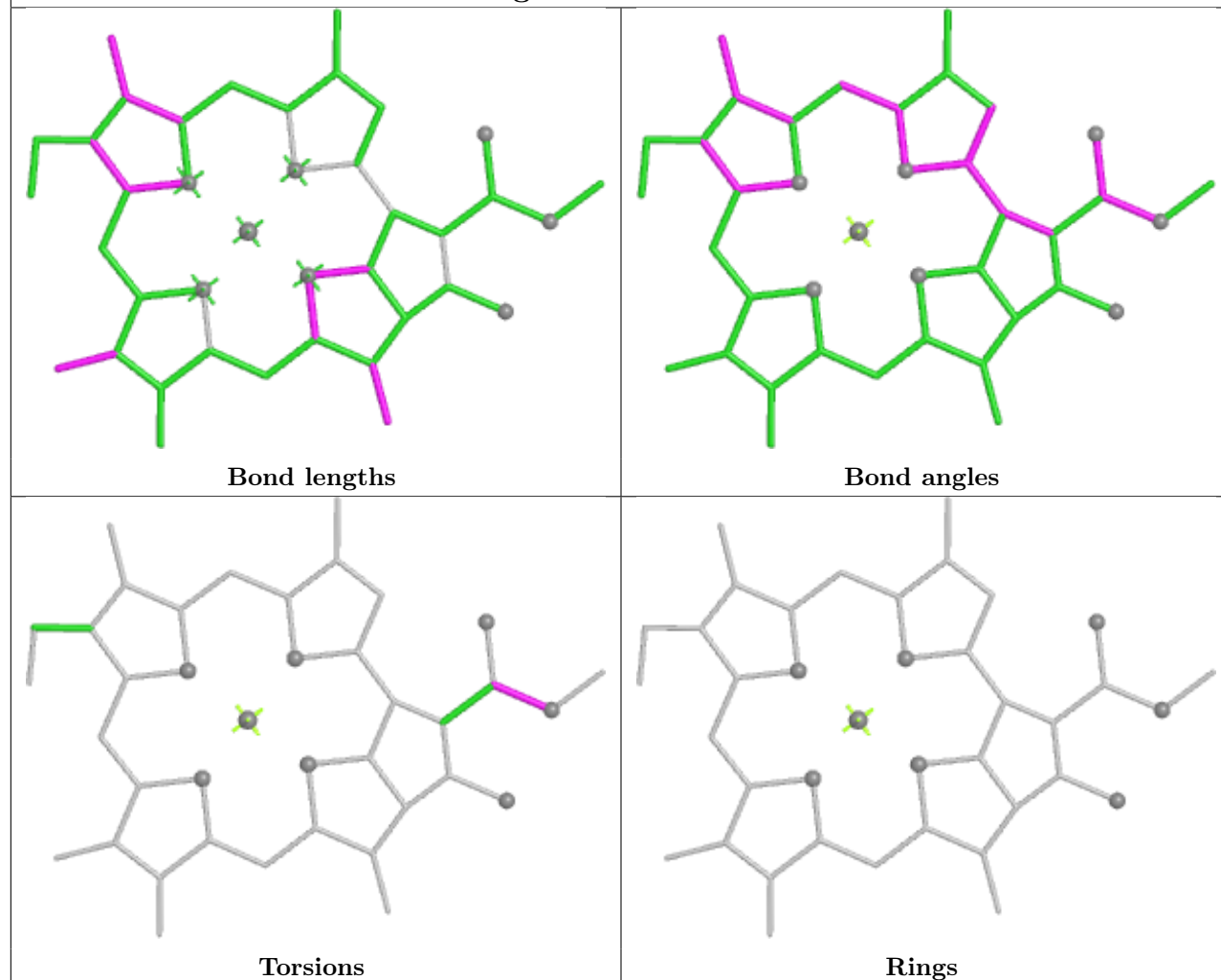
## Ligand CLA 2 613



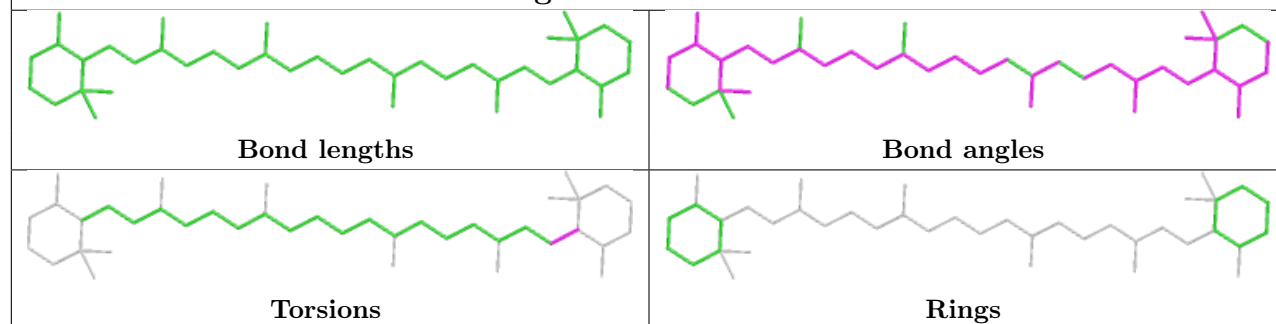




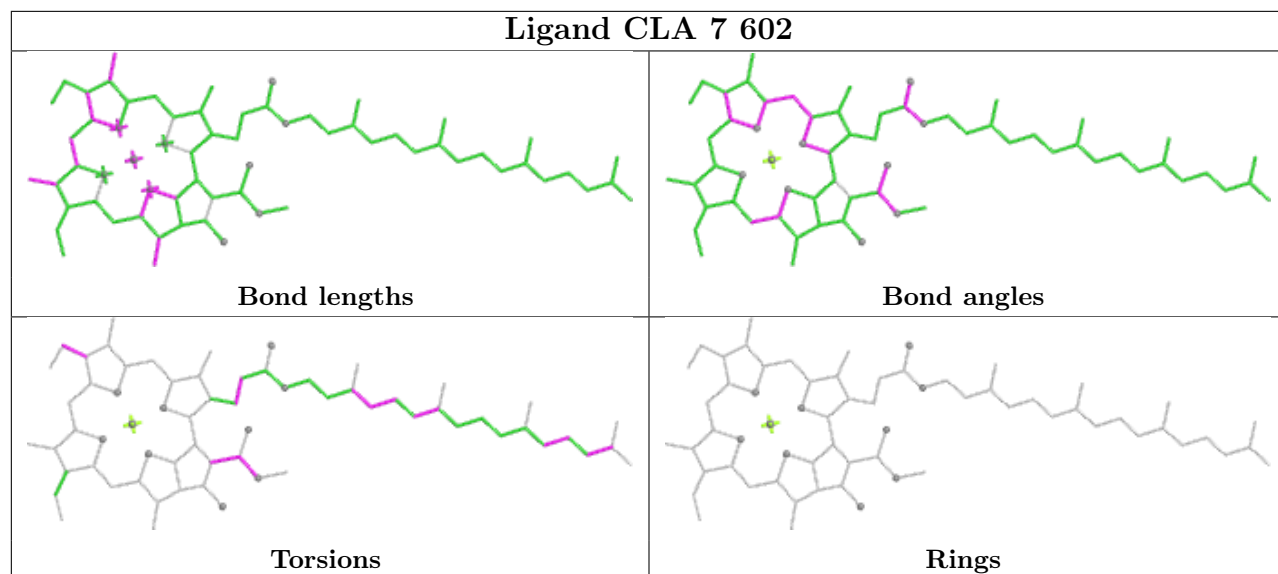
## Ligand CLA 1 610



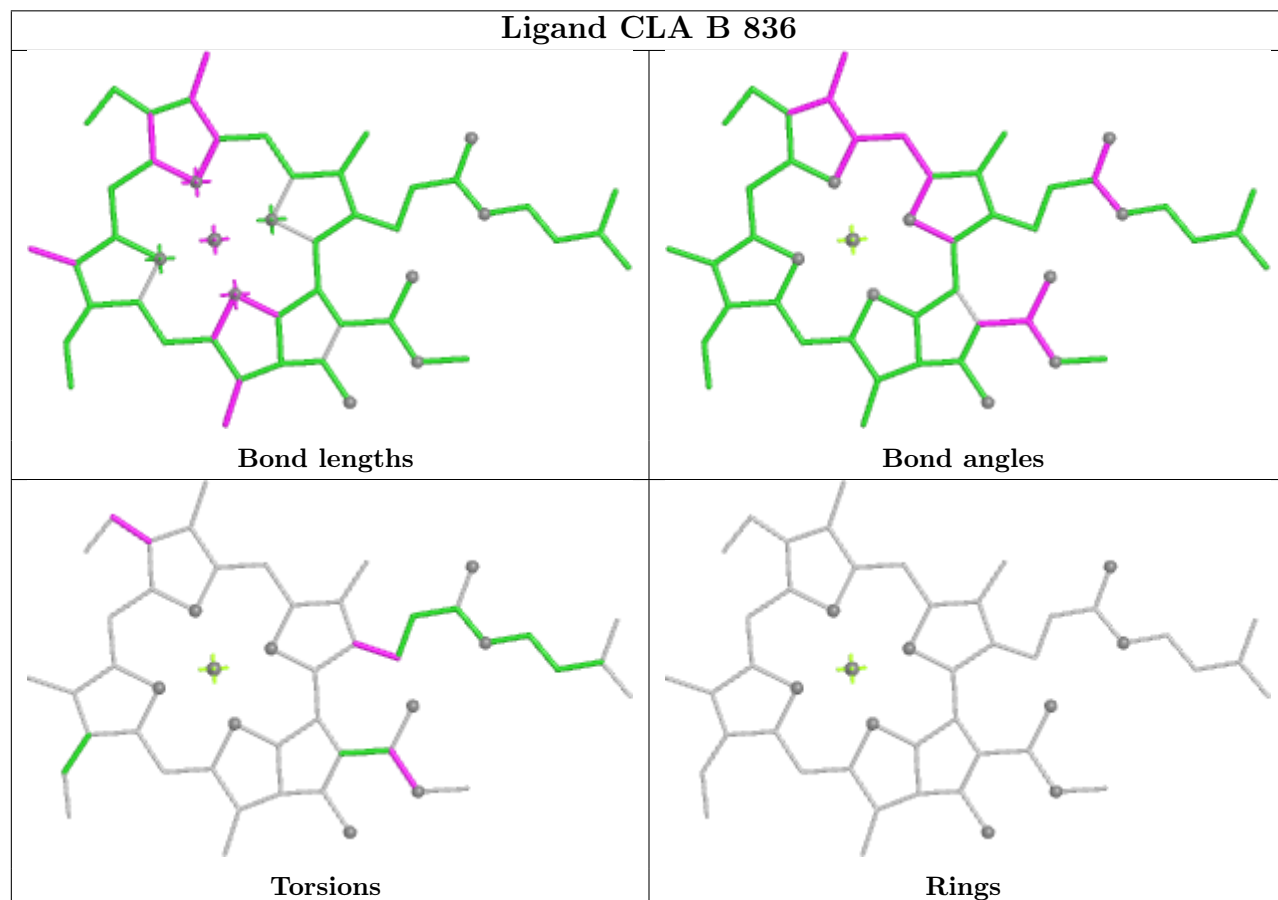
## Ligand BCR 8 621



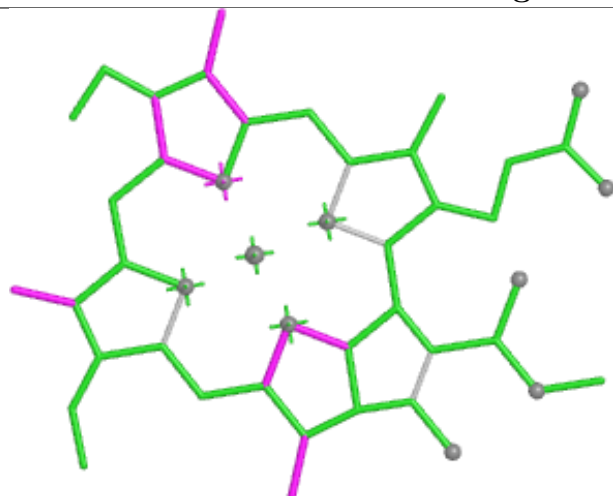
## Ligand CLA 7 602



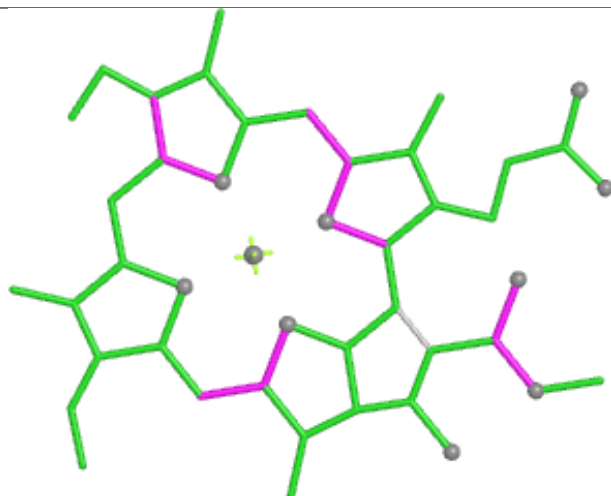
## Ligand CLA B 836



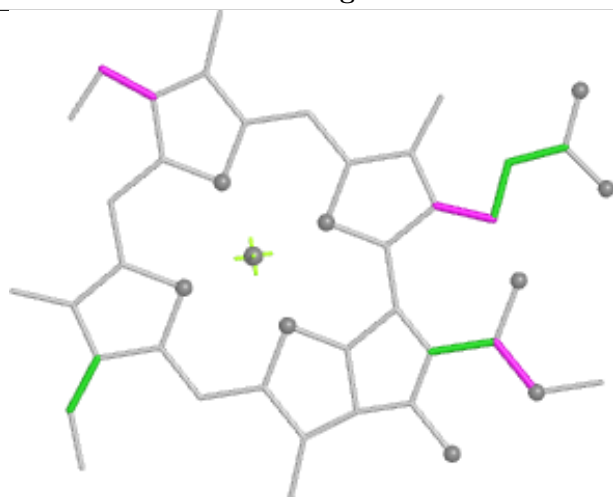
## Ligand CLA K 204



Bond lengths



Bond angles

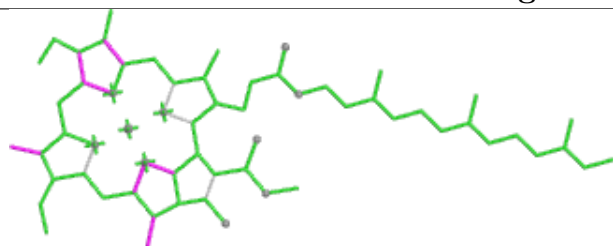


Torsions

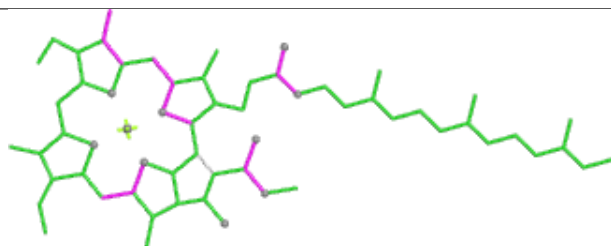


Rings

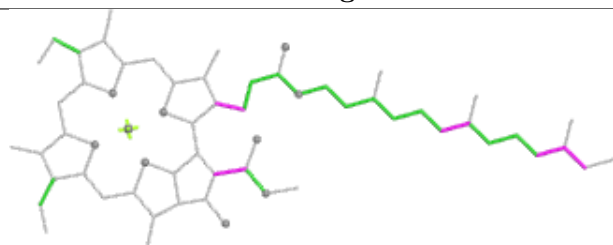
## Ligand CLA 4 610



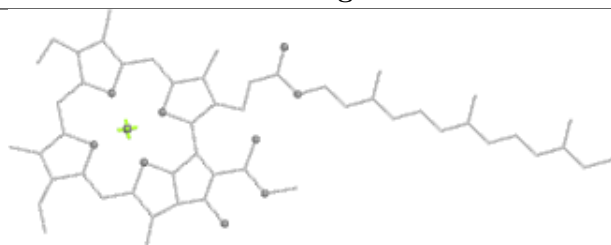
Bond lengths



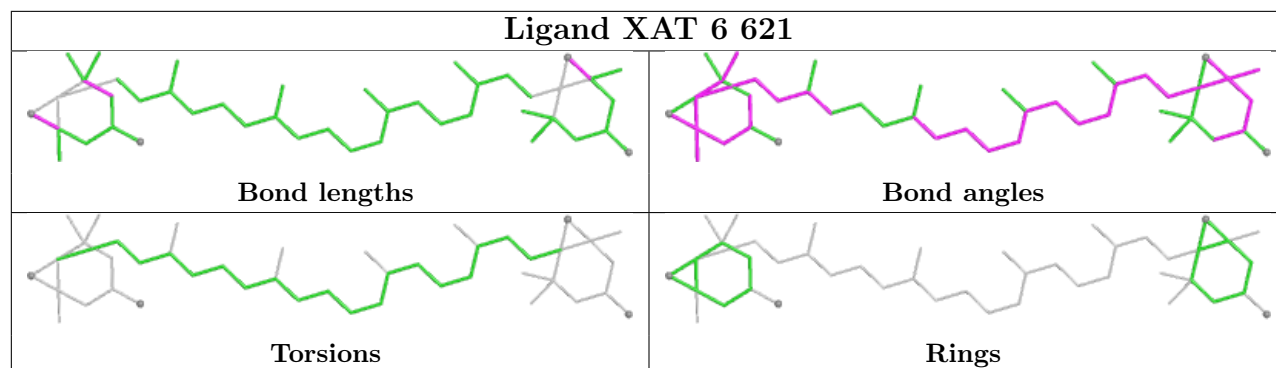
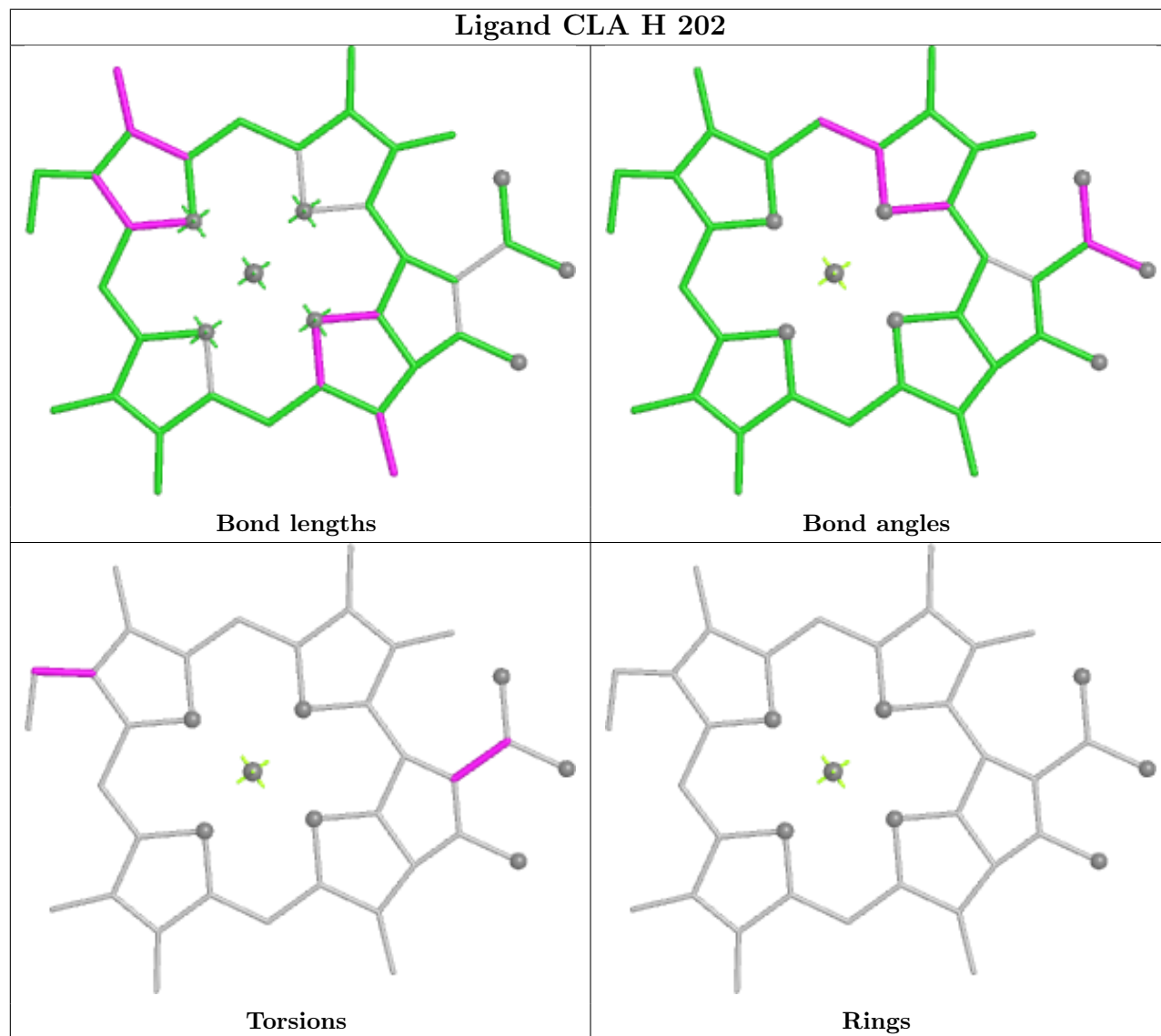
Bond angles



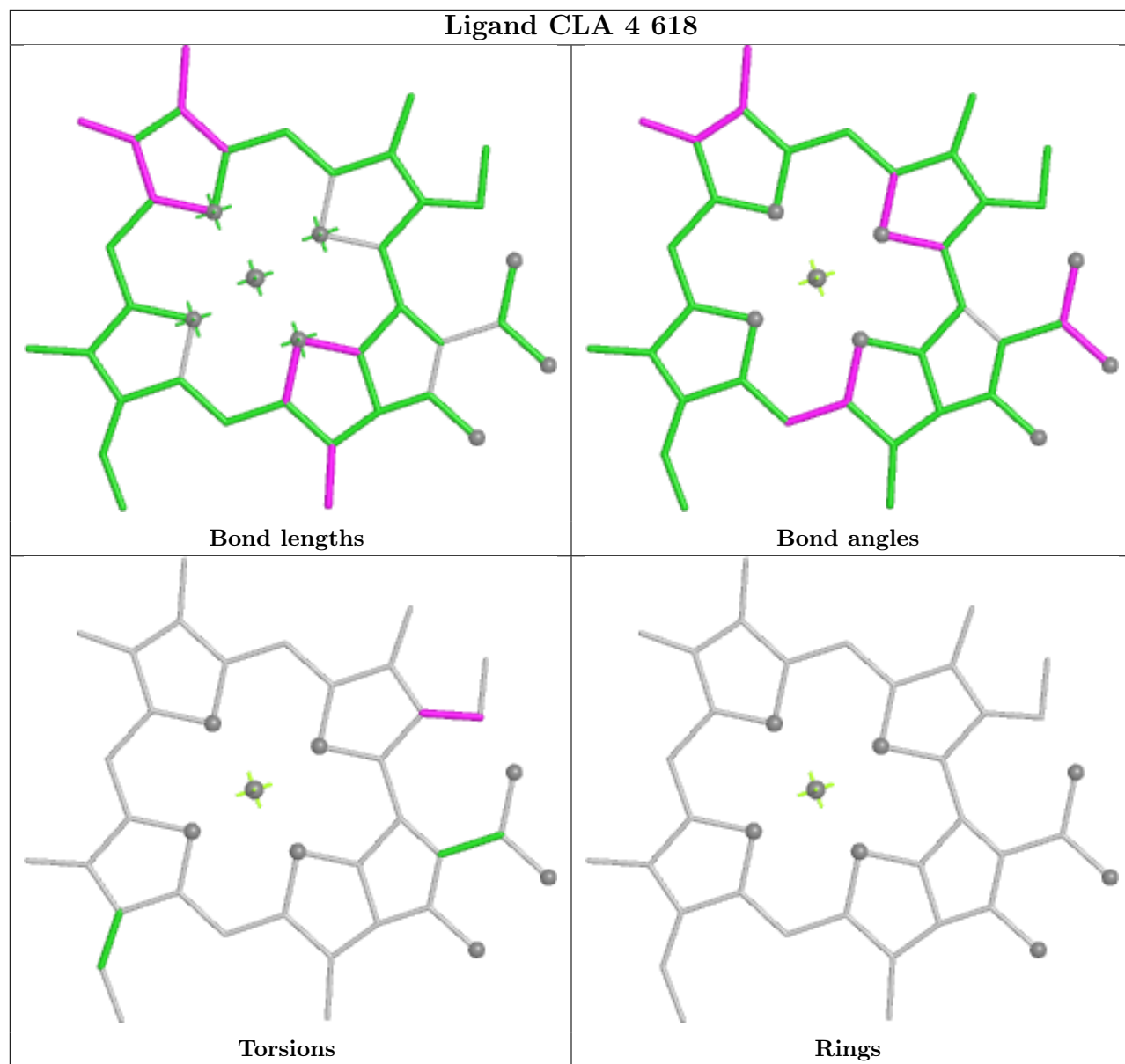
Torsions



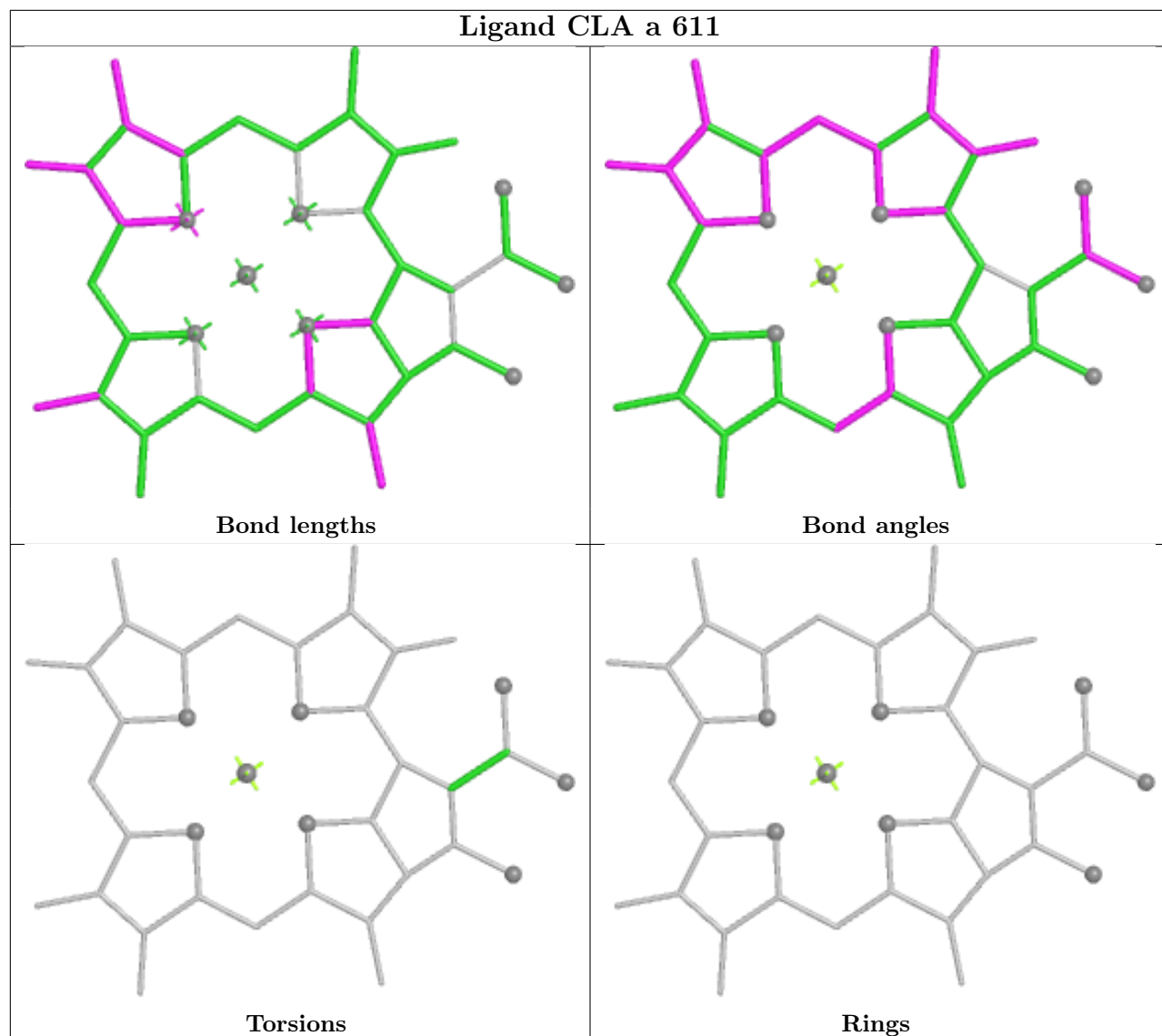
Rings

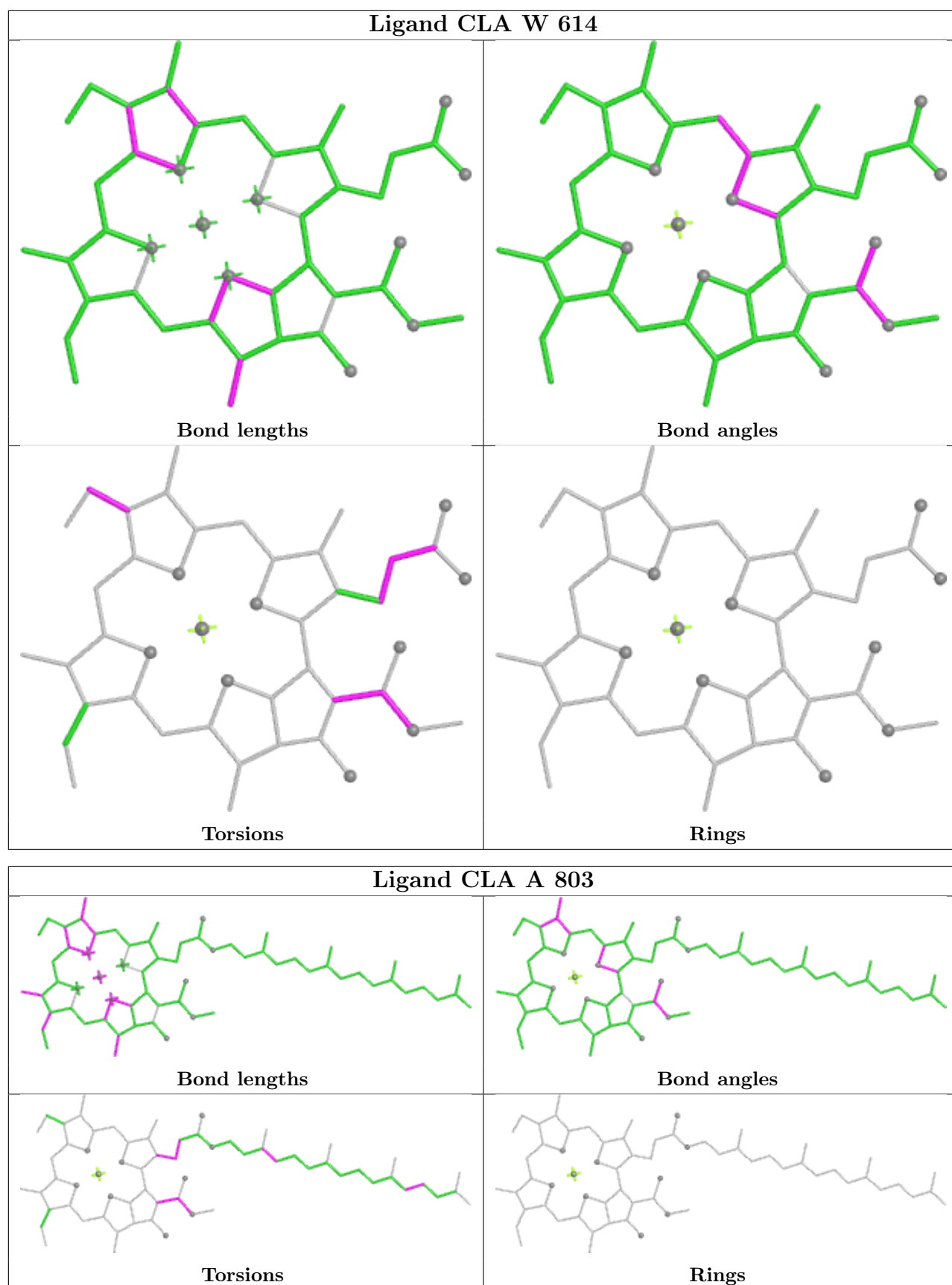
**Ligand XAT 6 621****Ligand CLA H 202**

## Ligand CLA 4 618

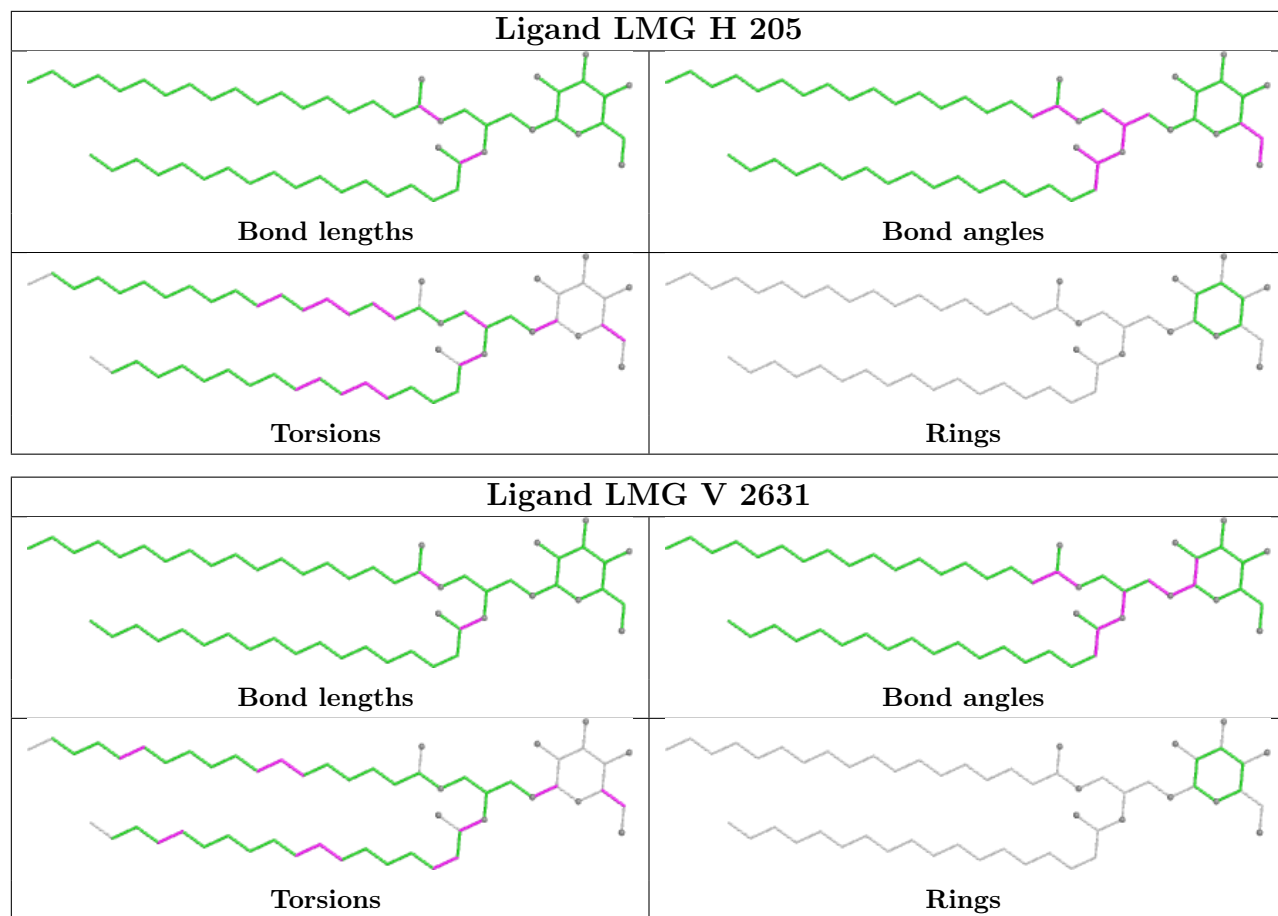


## Ligand CLA a 611

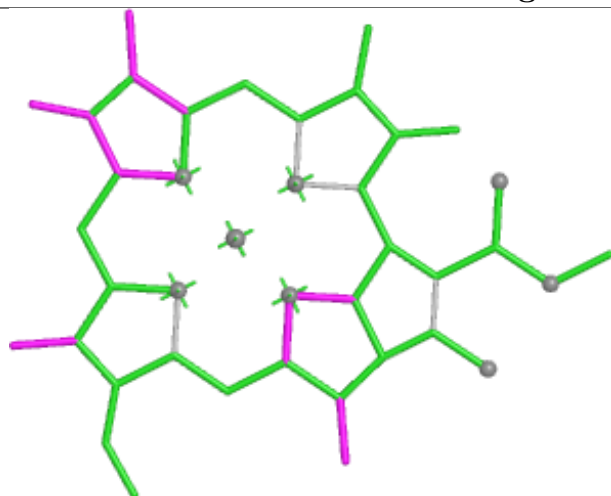








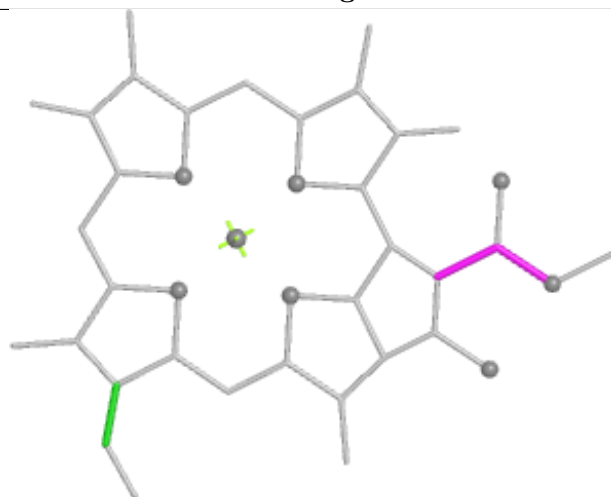
## Ligand CLA 1 609



Bond lengths



Bond angles

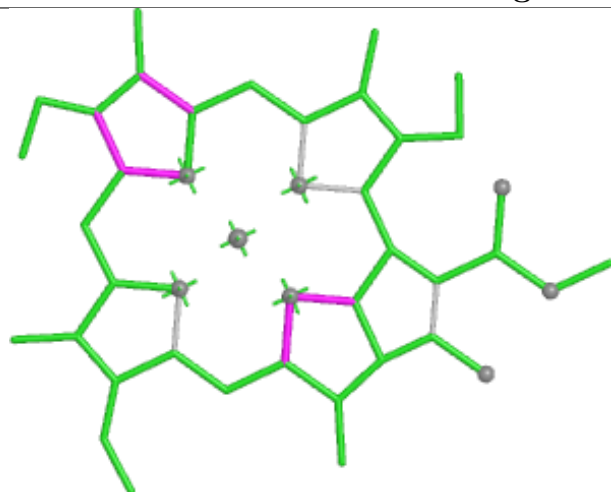


Torsions

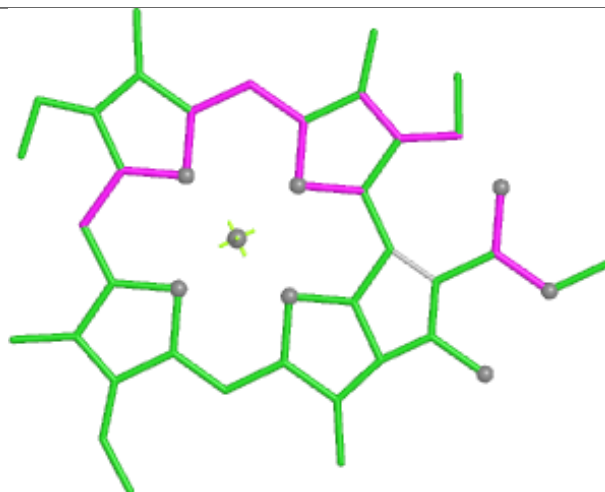


Rings

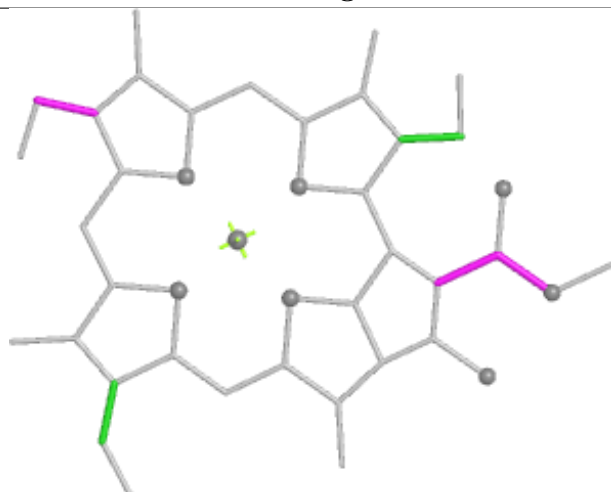
## Ligand CLA U 612



Bond lengths



Bond angles

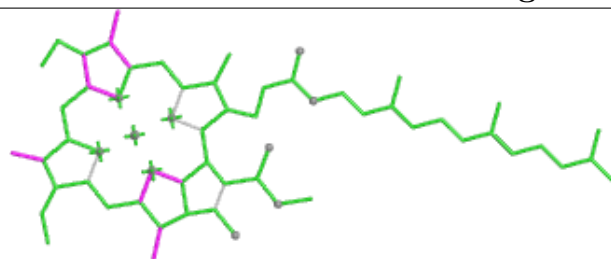


Torsions

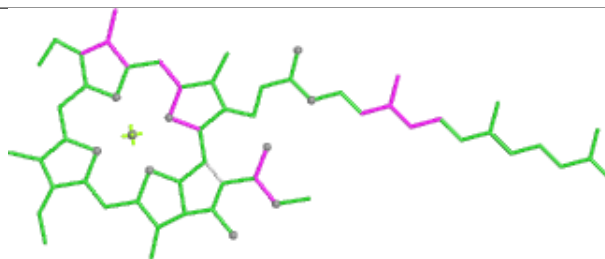


Rings

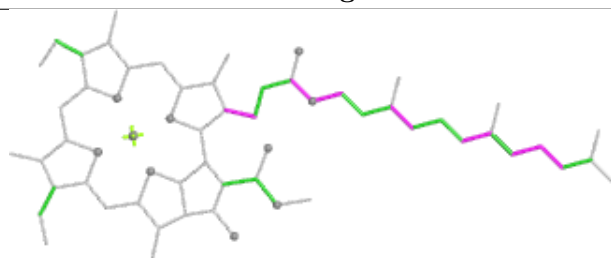
## Ligand CLA 8 610



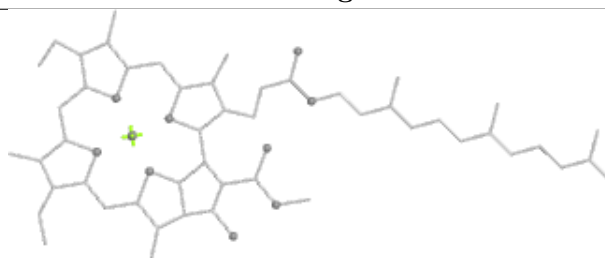
Bond lengths



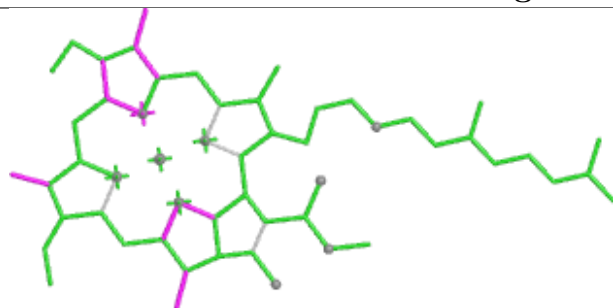
Bond angles



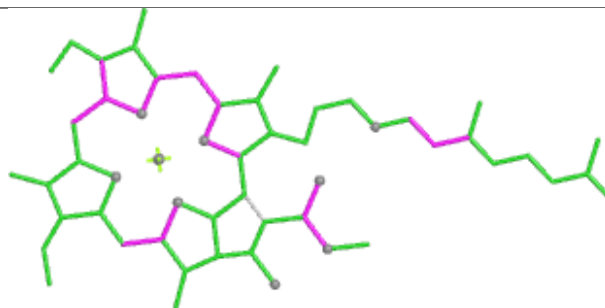
Torsions



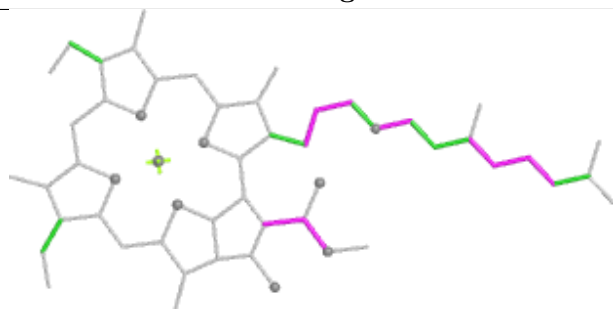
Rings

**Ligand CLA B 816**

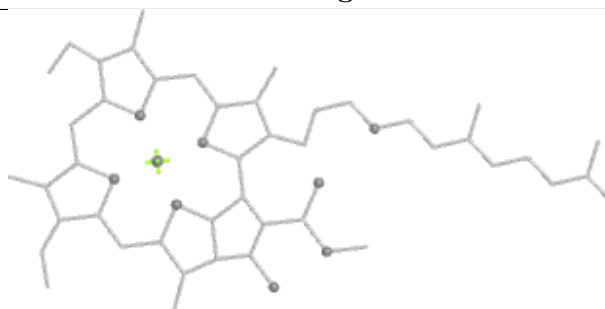
Bond lengths



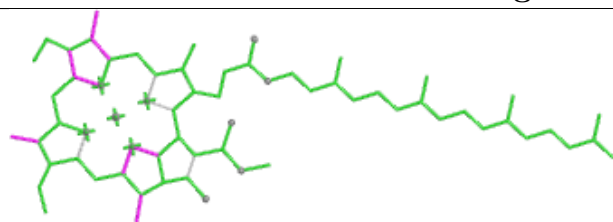
Bond angles



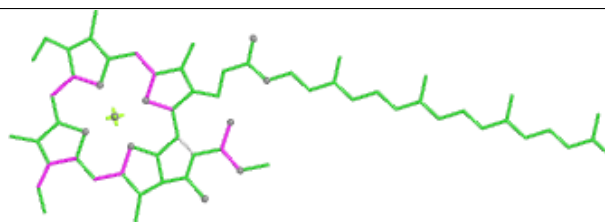
Torsions



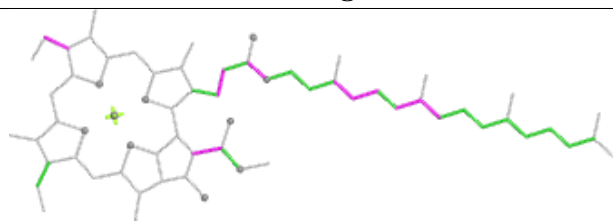
Rings

**Ligand CLA X 613**

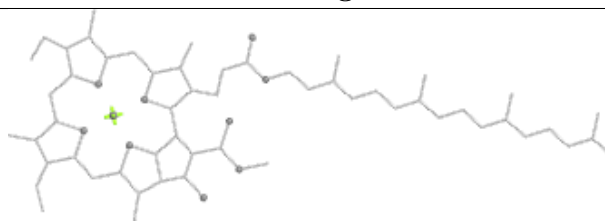
Bond lengths



Bond angles

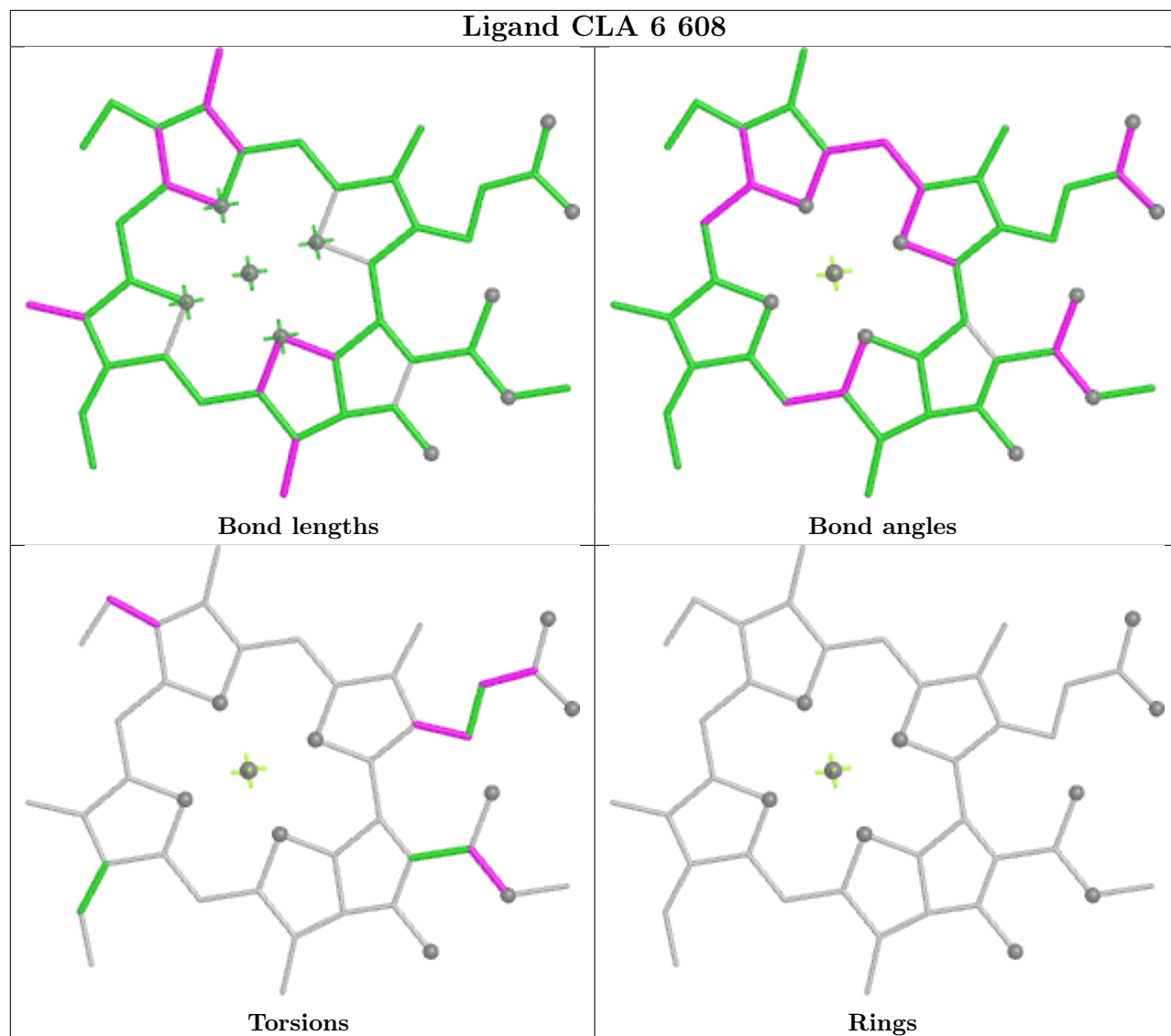


Torsions

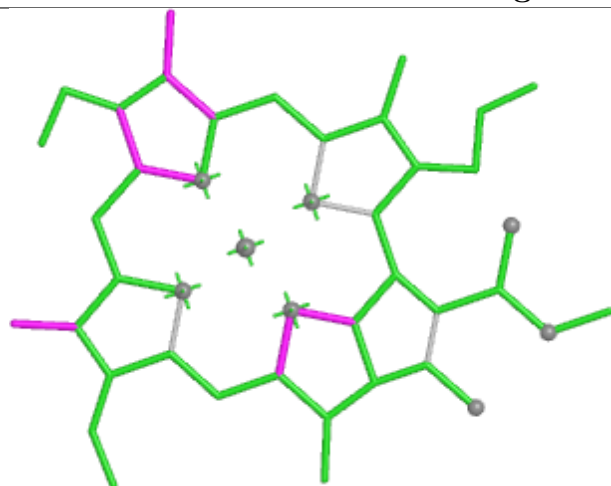


Rings

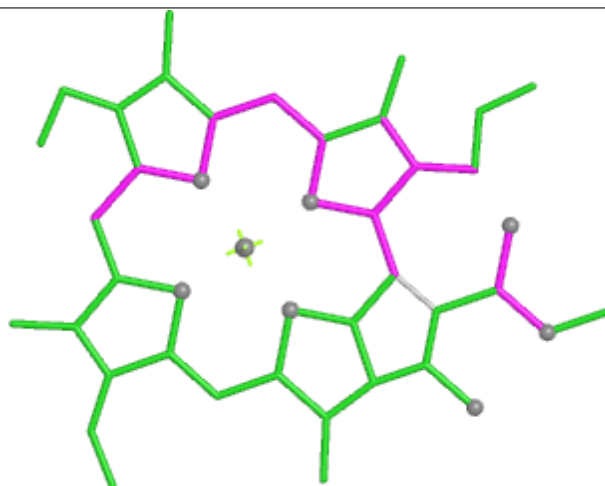
## Ligand CLA 6 608



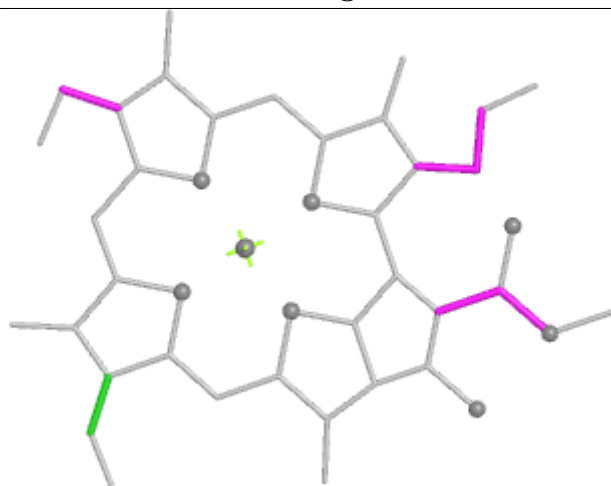
## Ligand CLA X 612



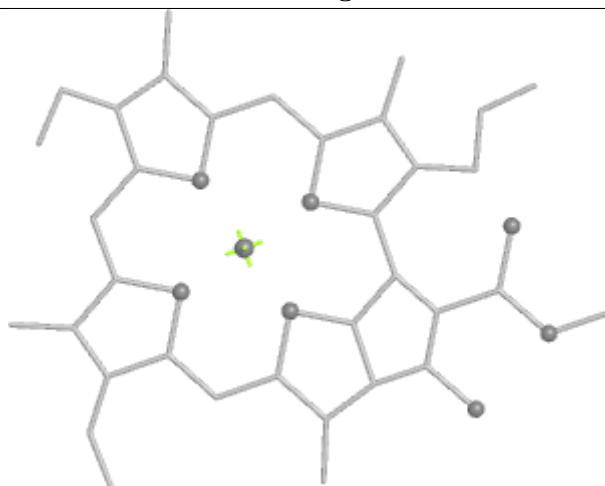
Bond lengths



Bond angles

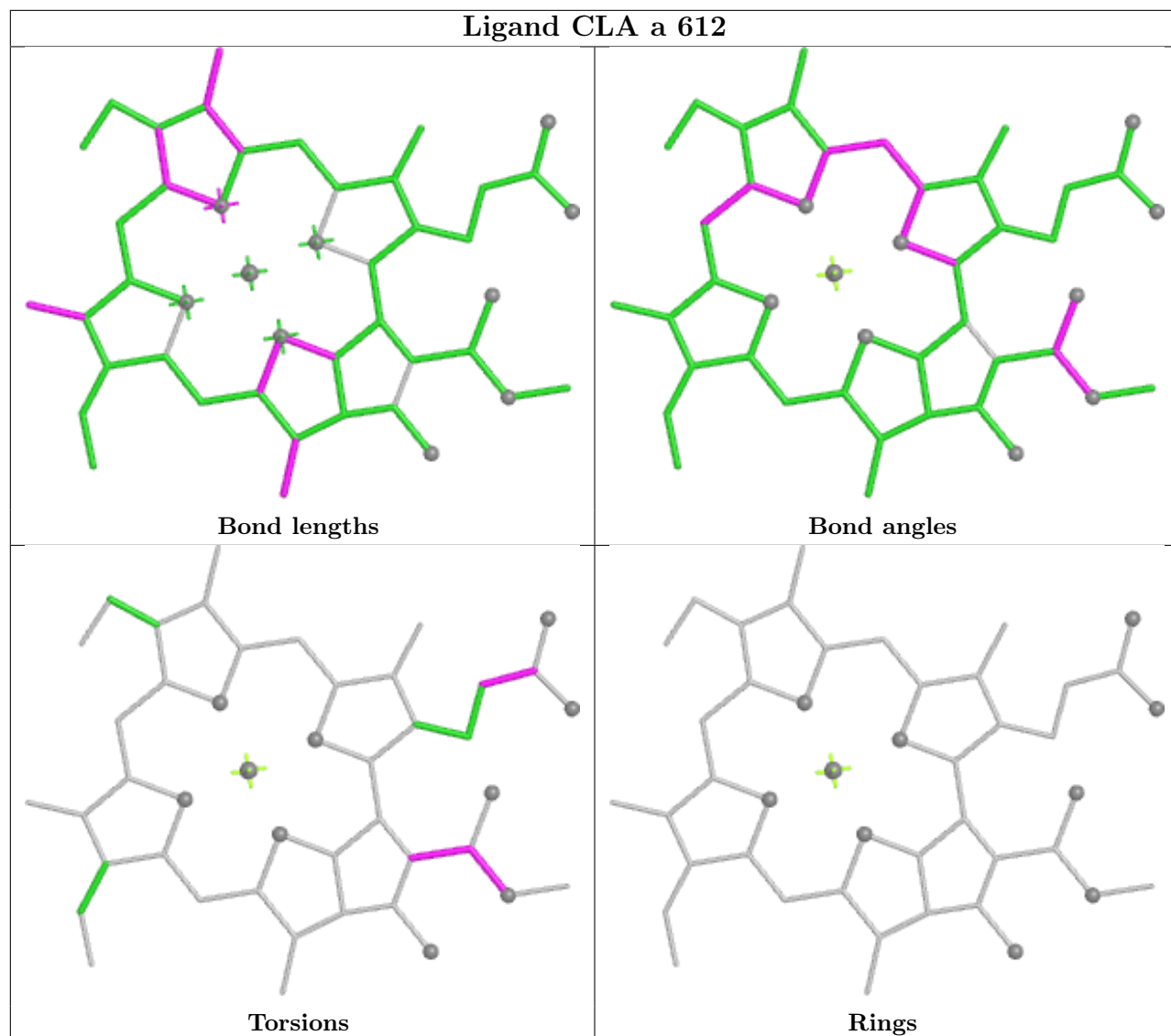


Torsions

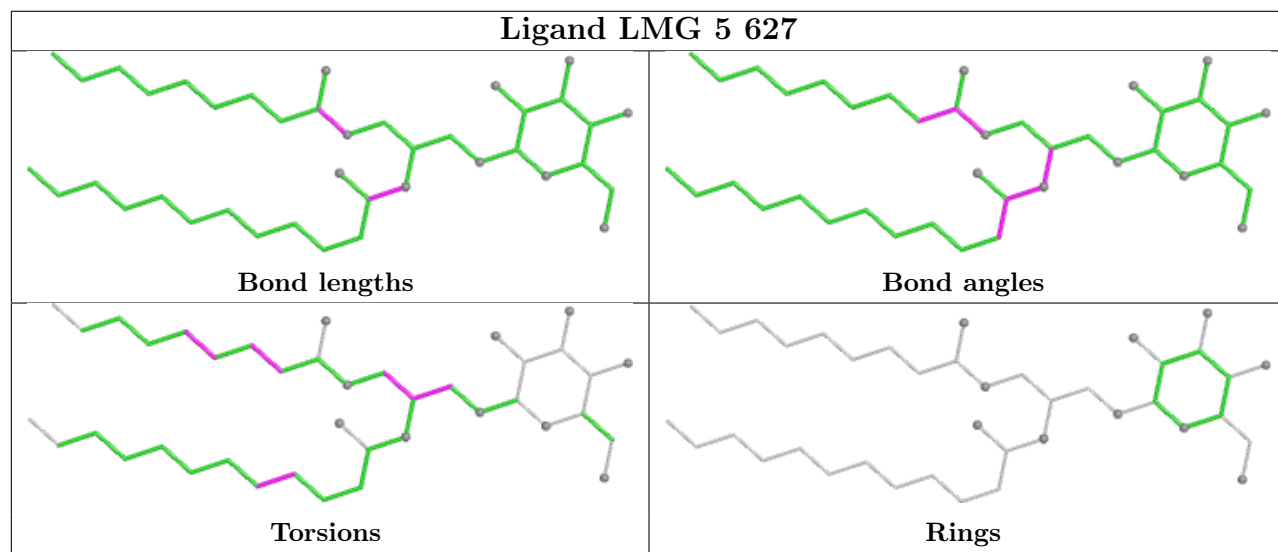


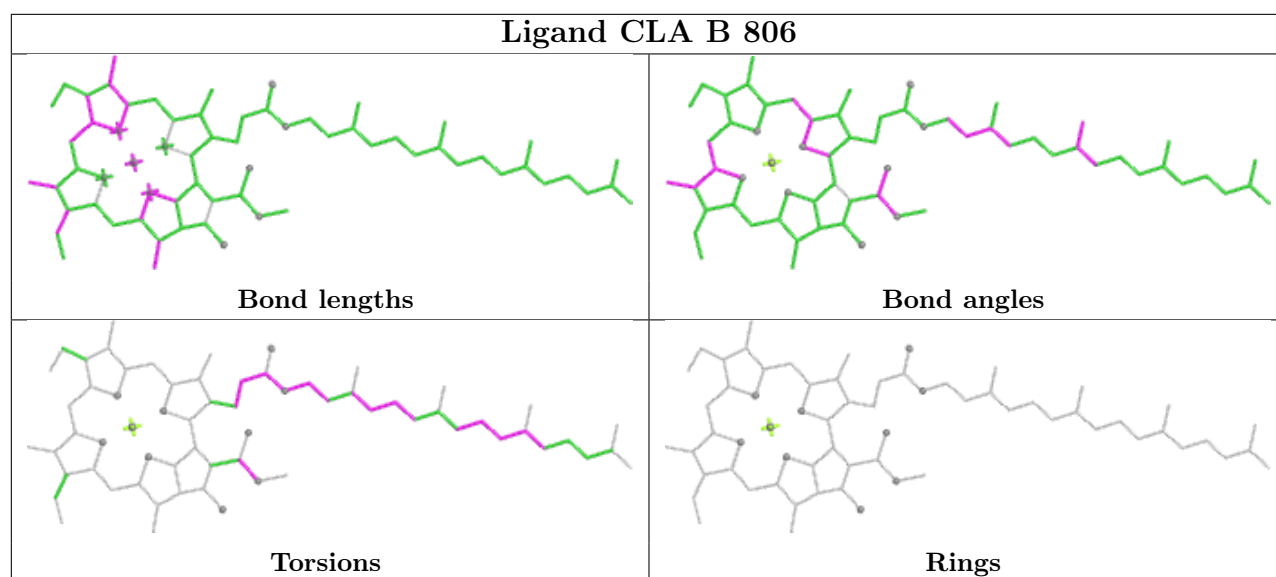
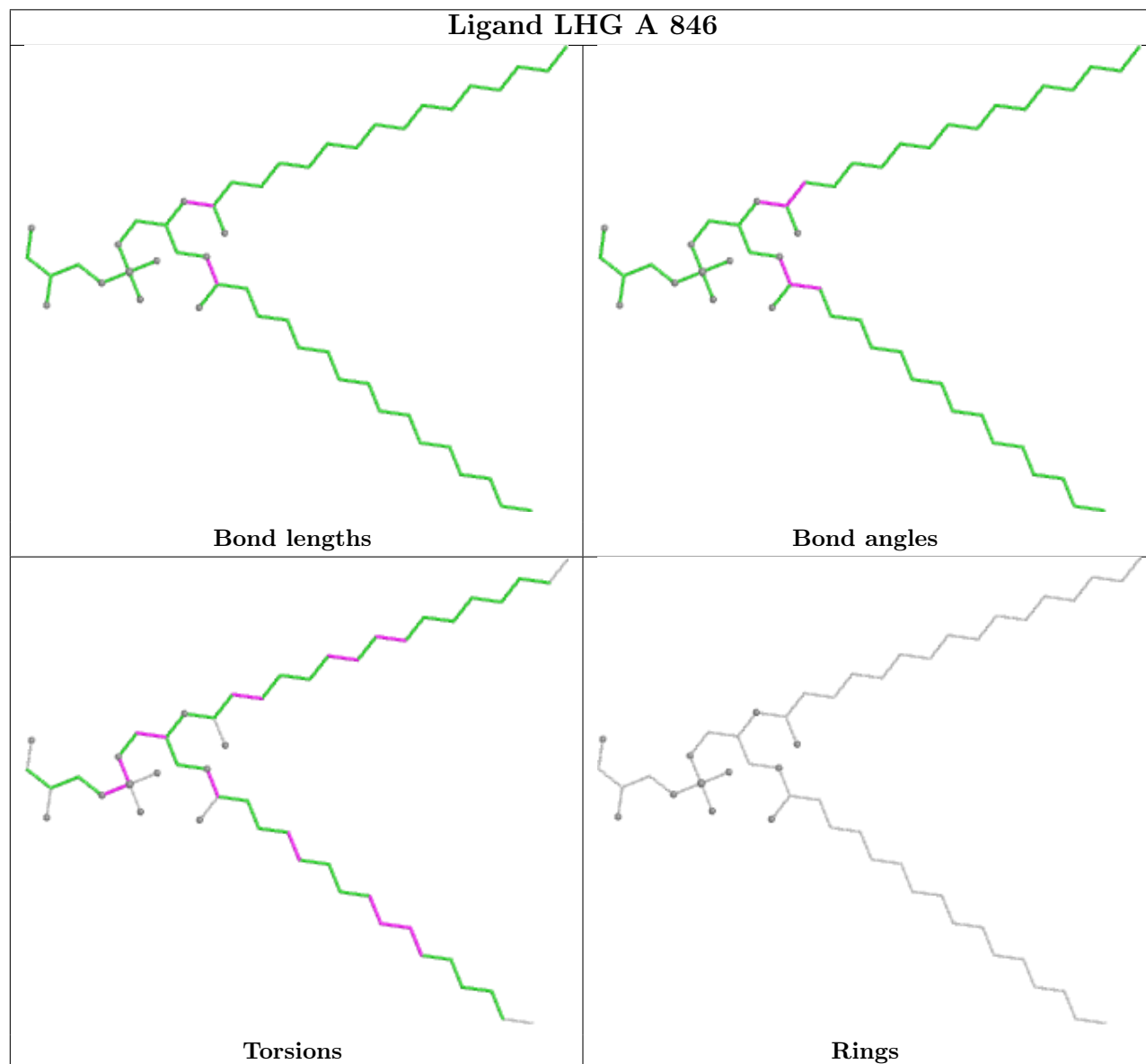
Rings

## Ligand CLA a 612

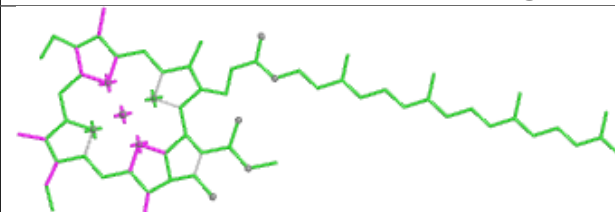
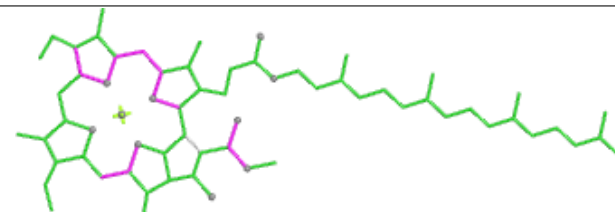
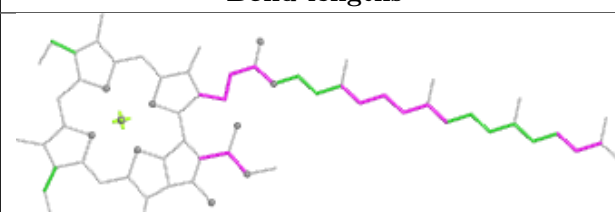
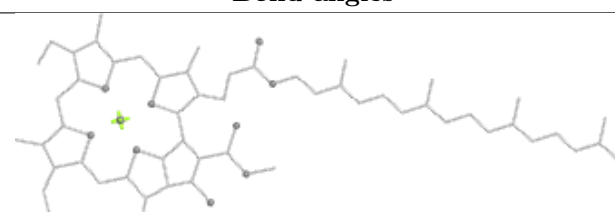
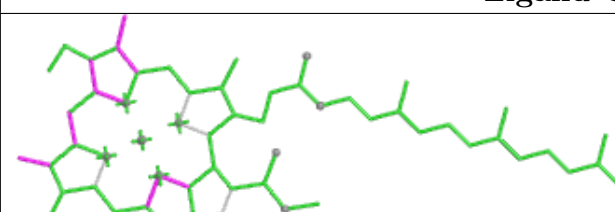
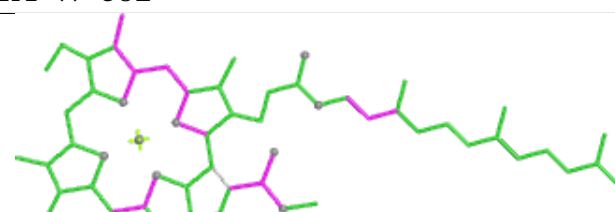
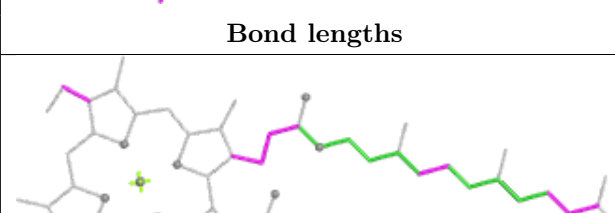
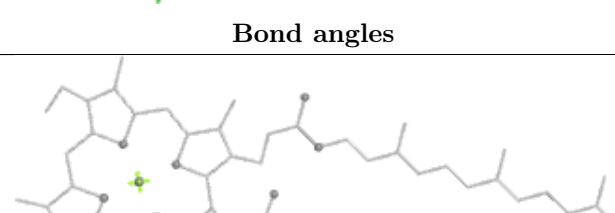
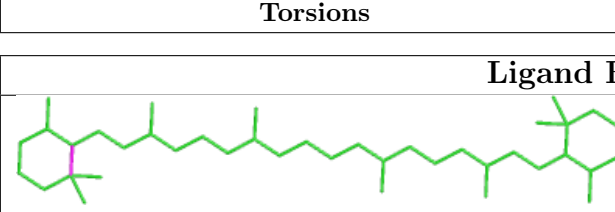
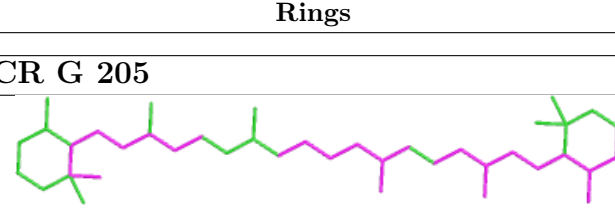


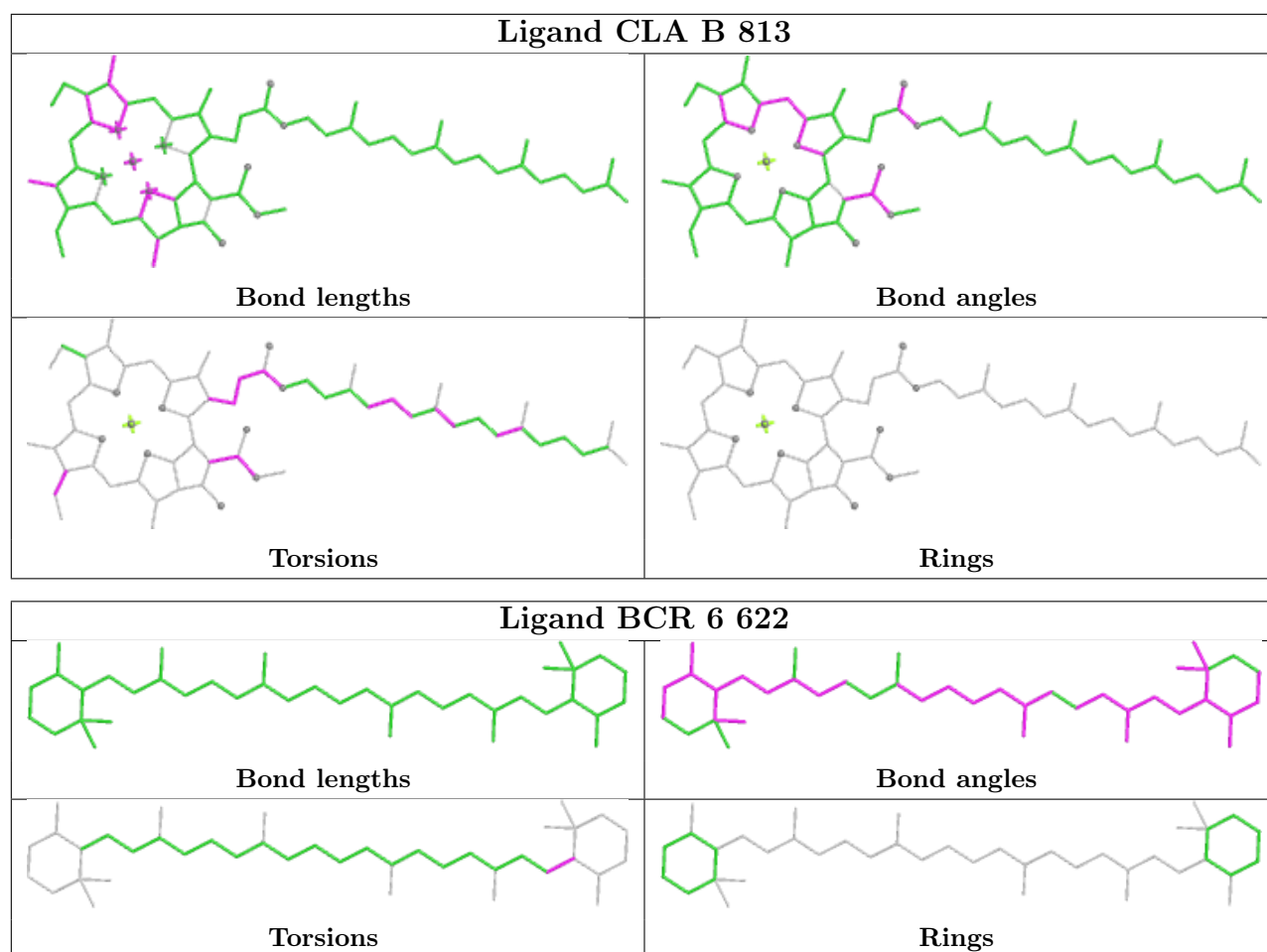
## Ligand LMG 5 627



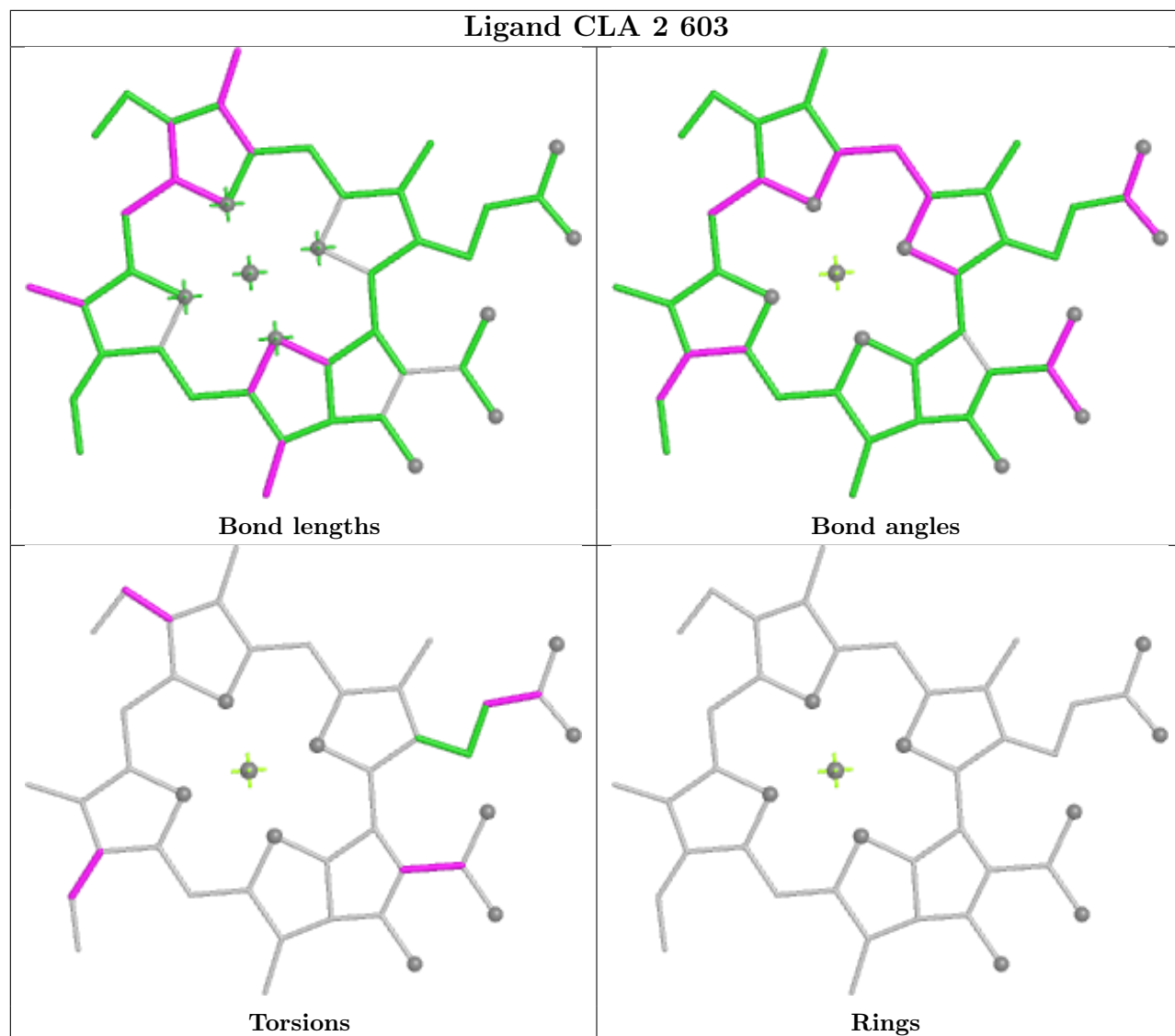




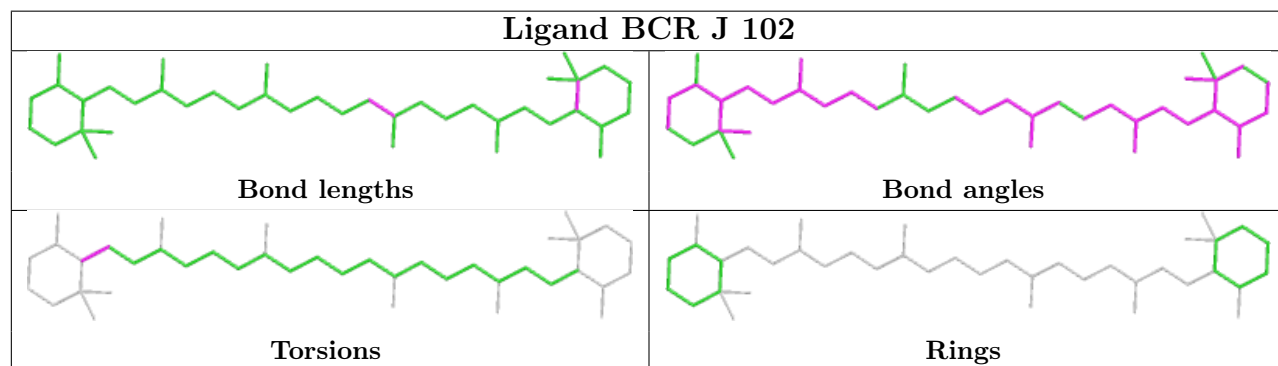
| Ligand CLA A 807                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|    |    |
| Torsions                                                                            | Rings                                                                                |
| Ligand CLA W 602                                                                    |                                                                                      |
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |
| Ligand BCR G 205                                                                    |                                                                                      |
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

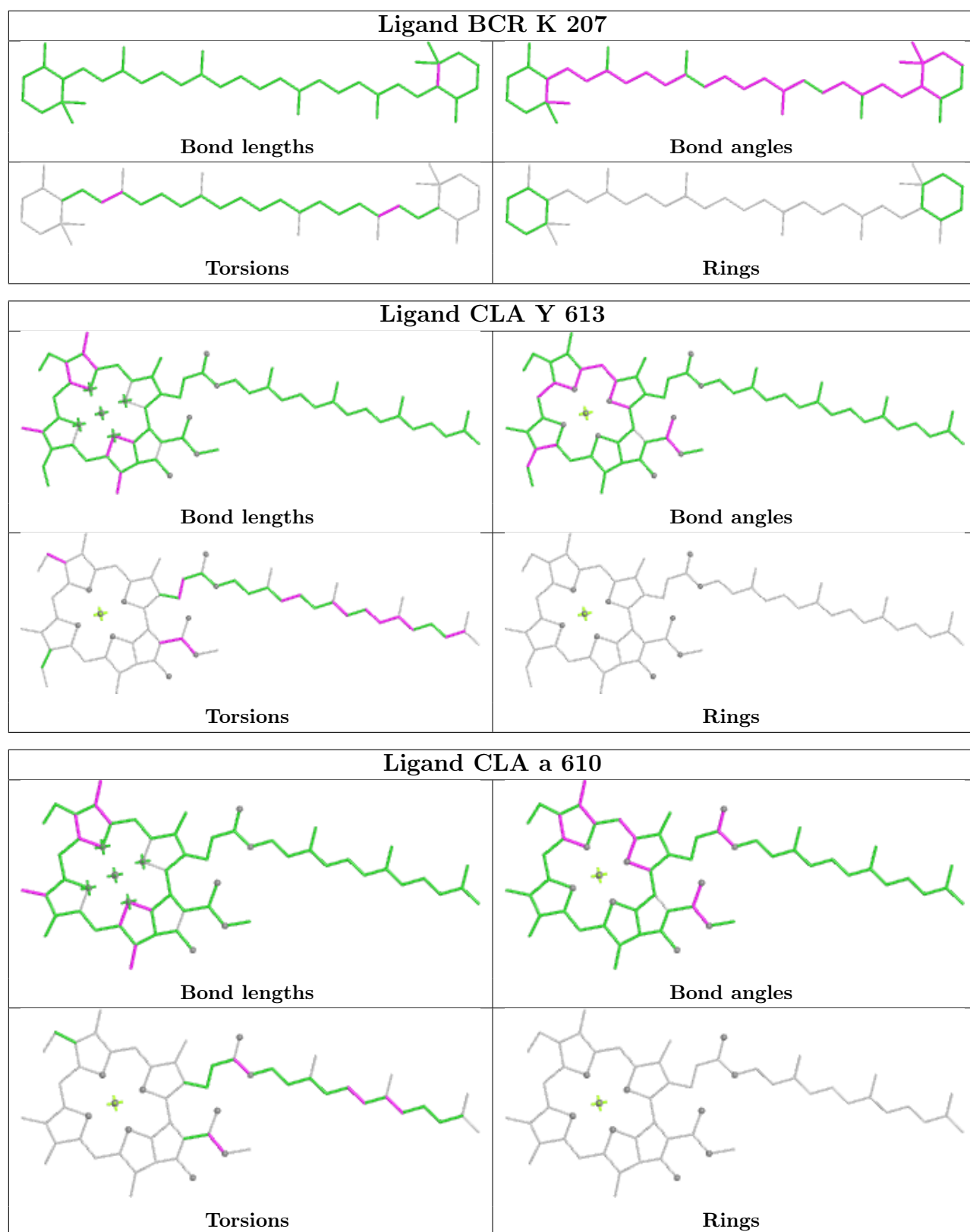


## Ligand CLA 2 603

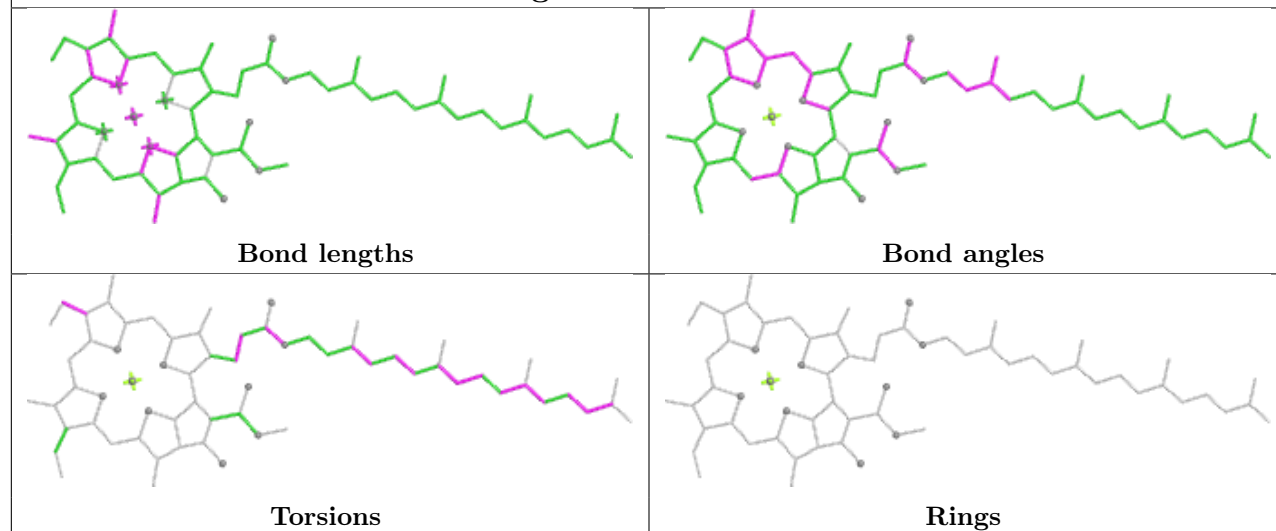


## Ligand BCR J 102

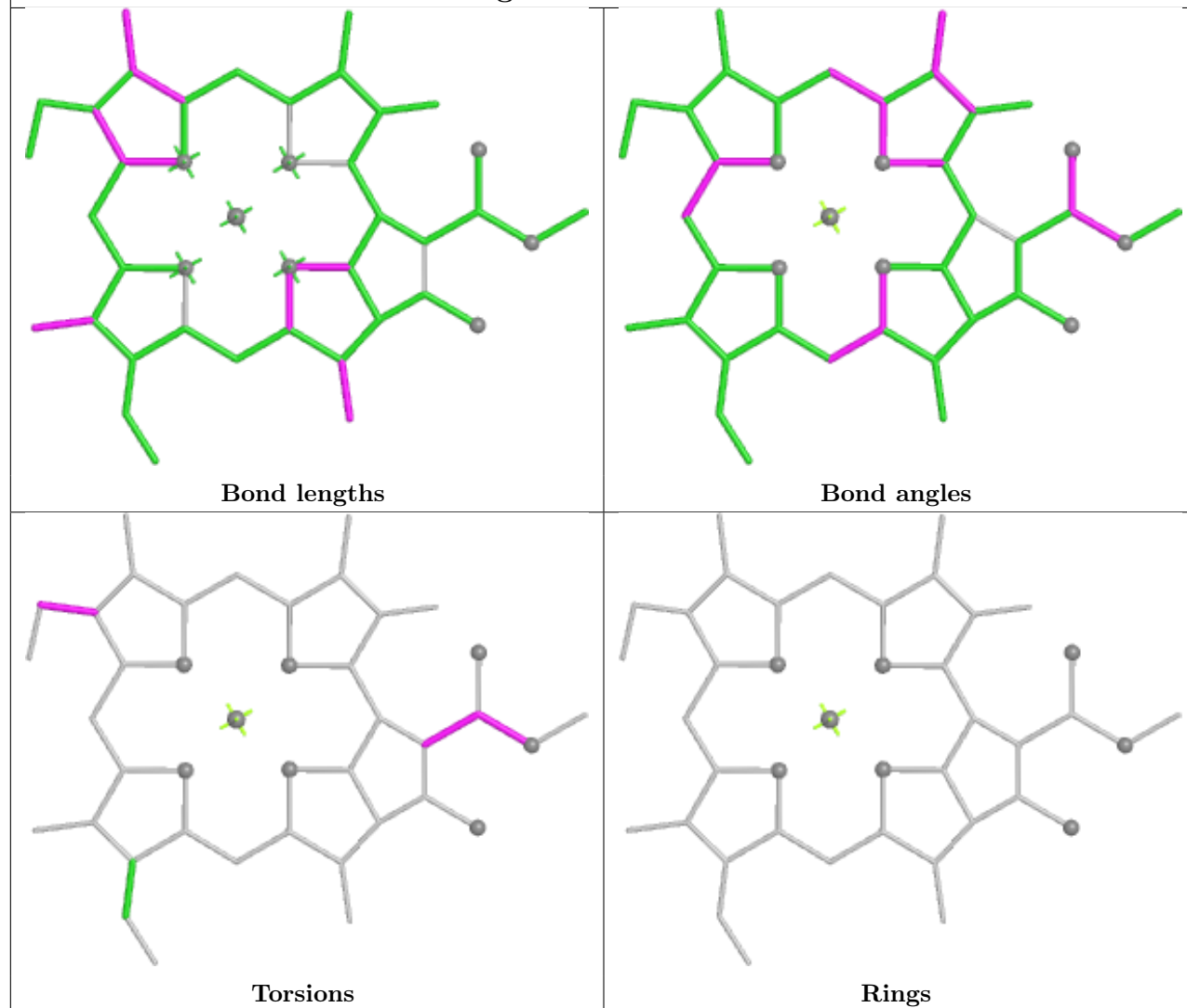




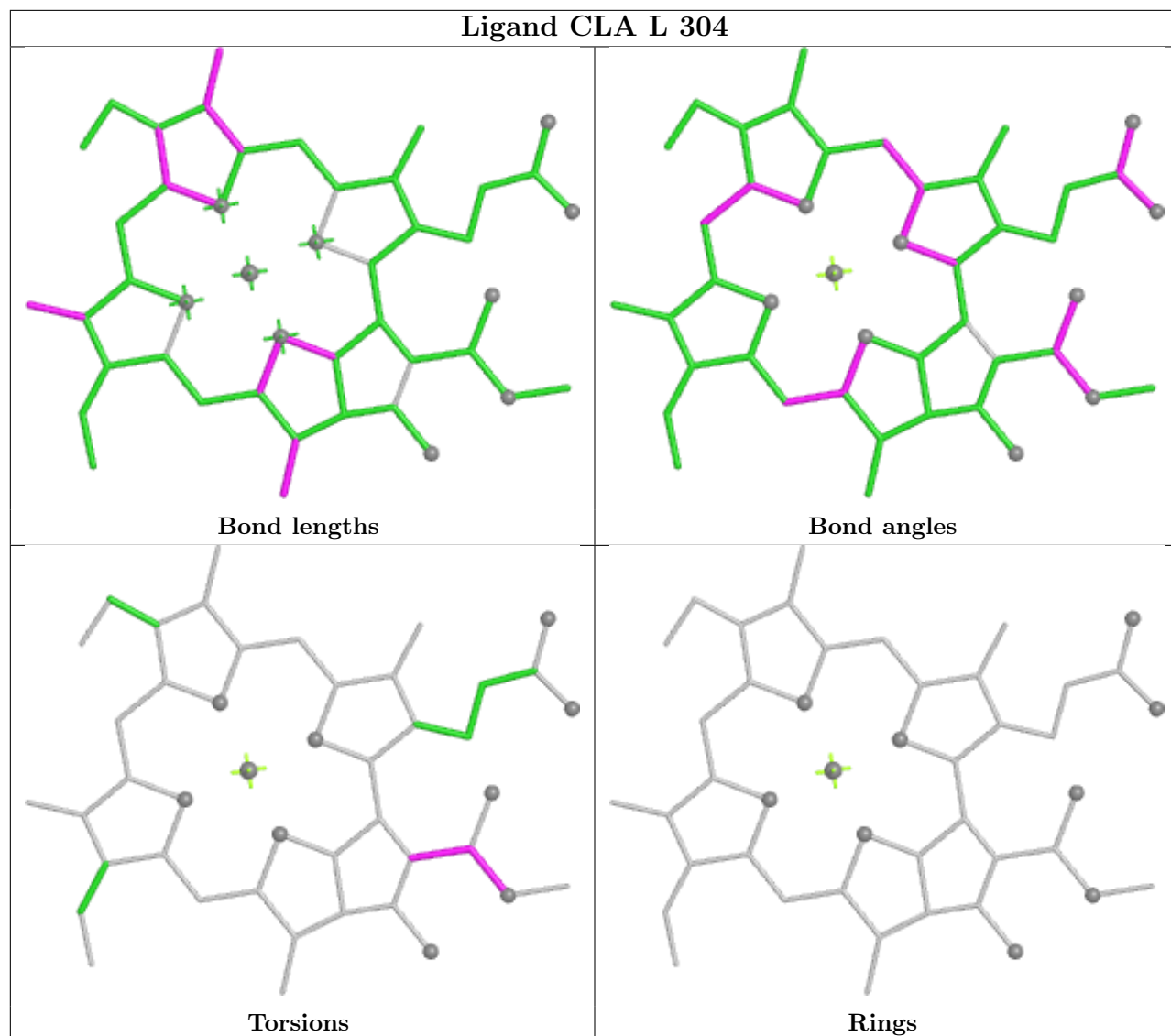
## Ligand CLA A 842



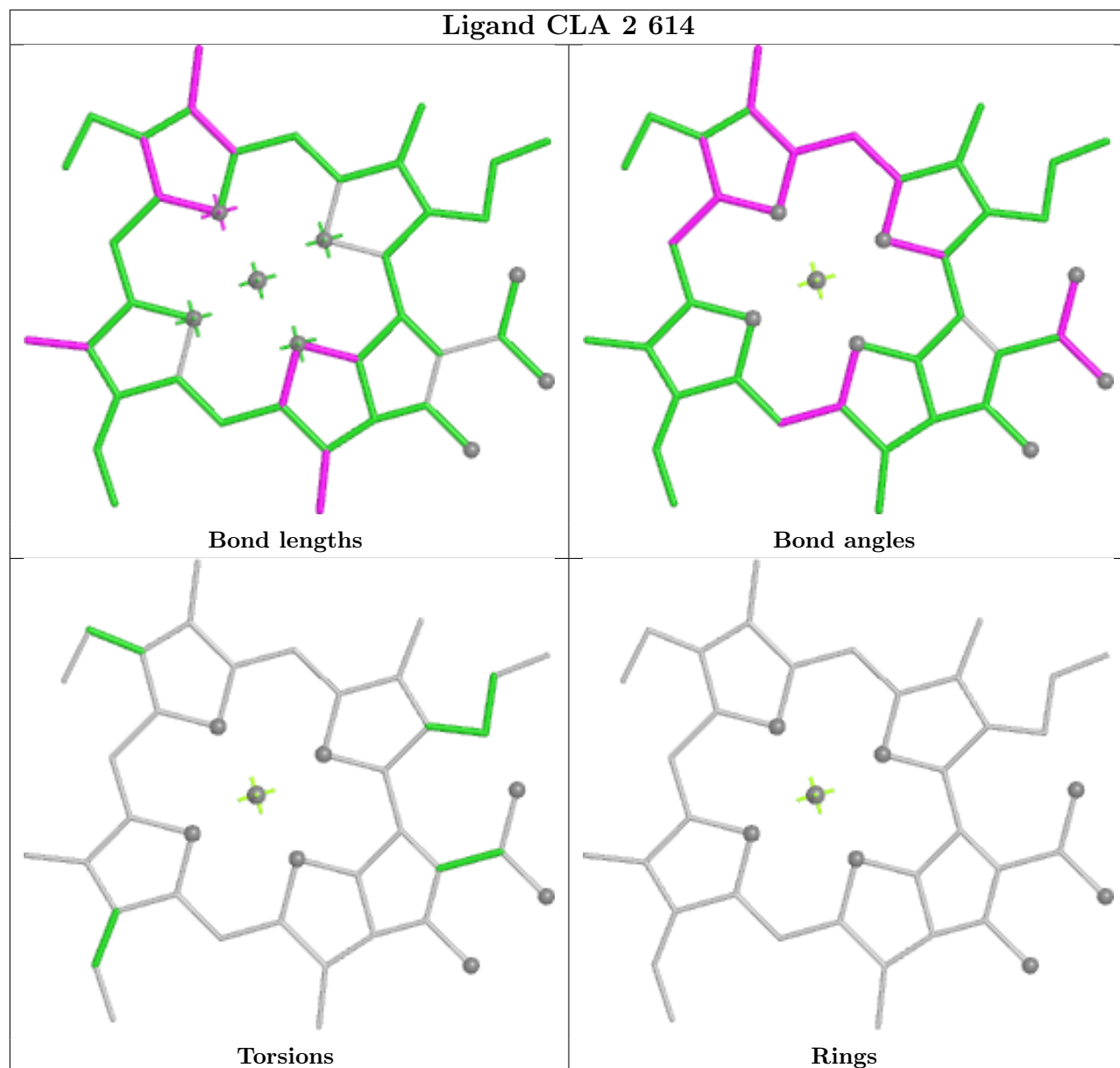
## Ligand CLA F 304



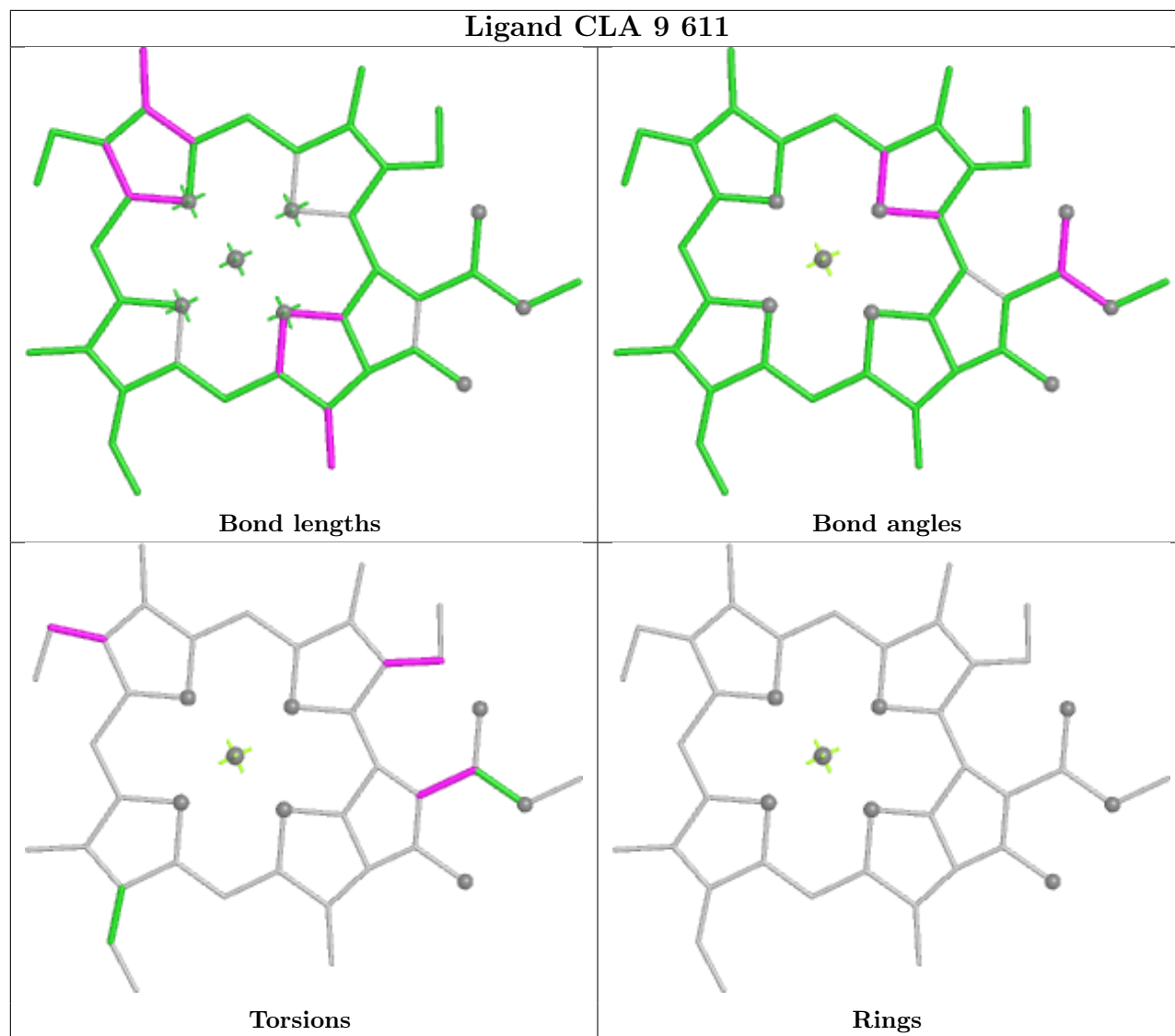
## Ligand CLA L 304



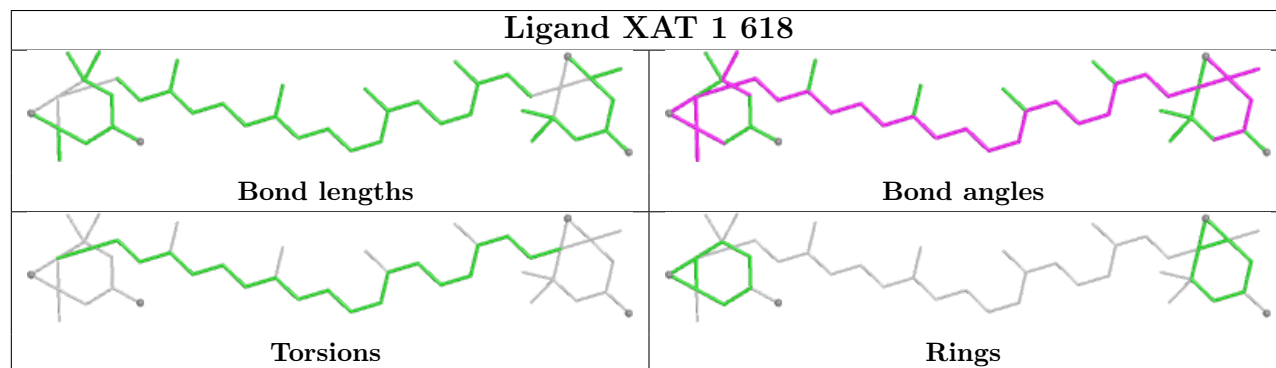
## Ligand CLA 2 614



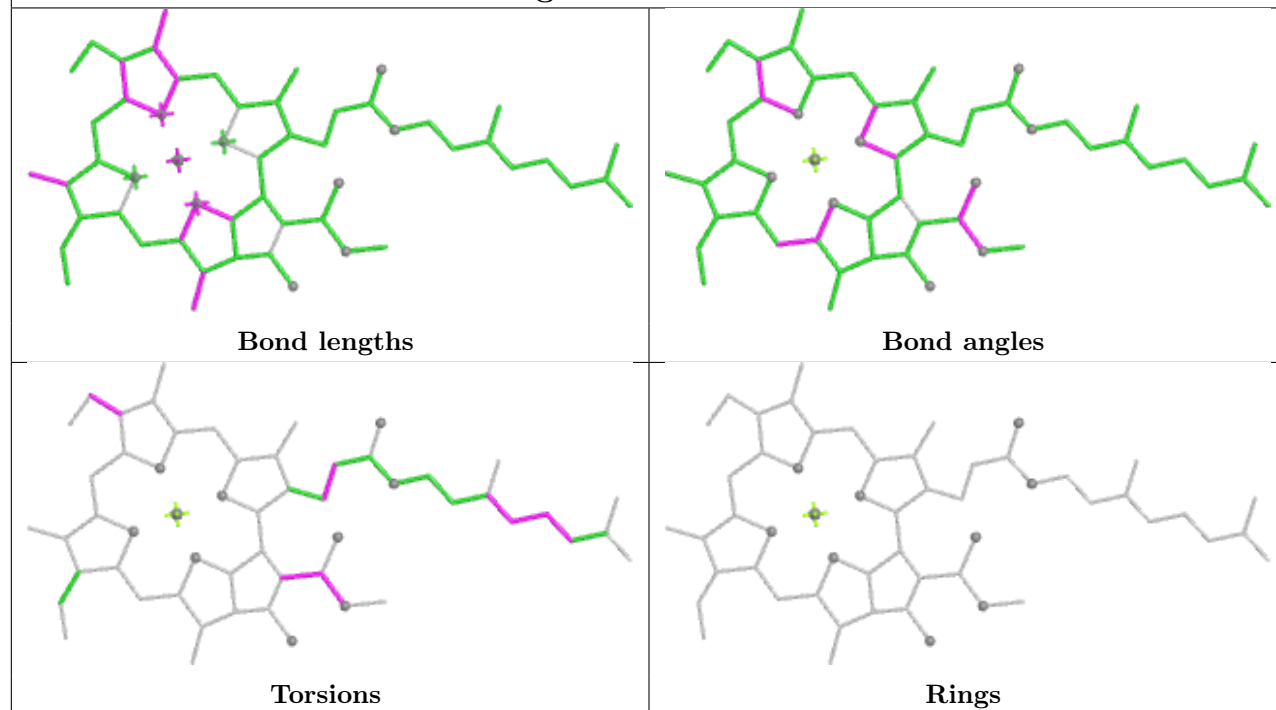
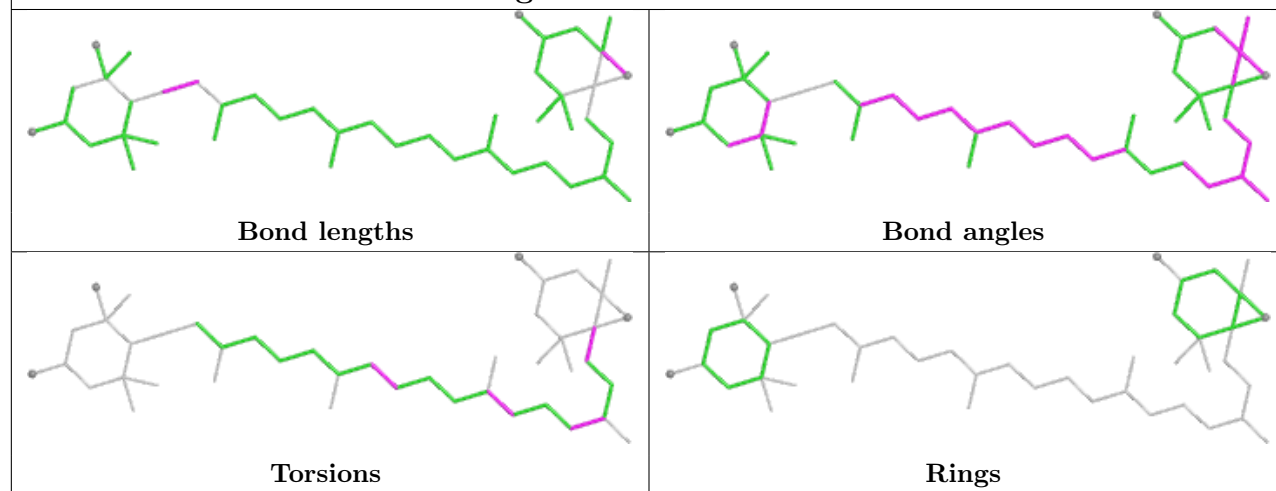
## Ligand CLA 9 611

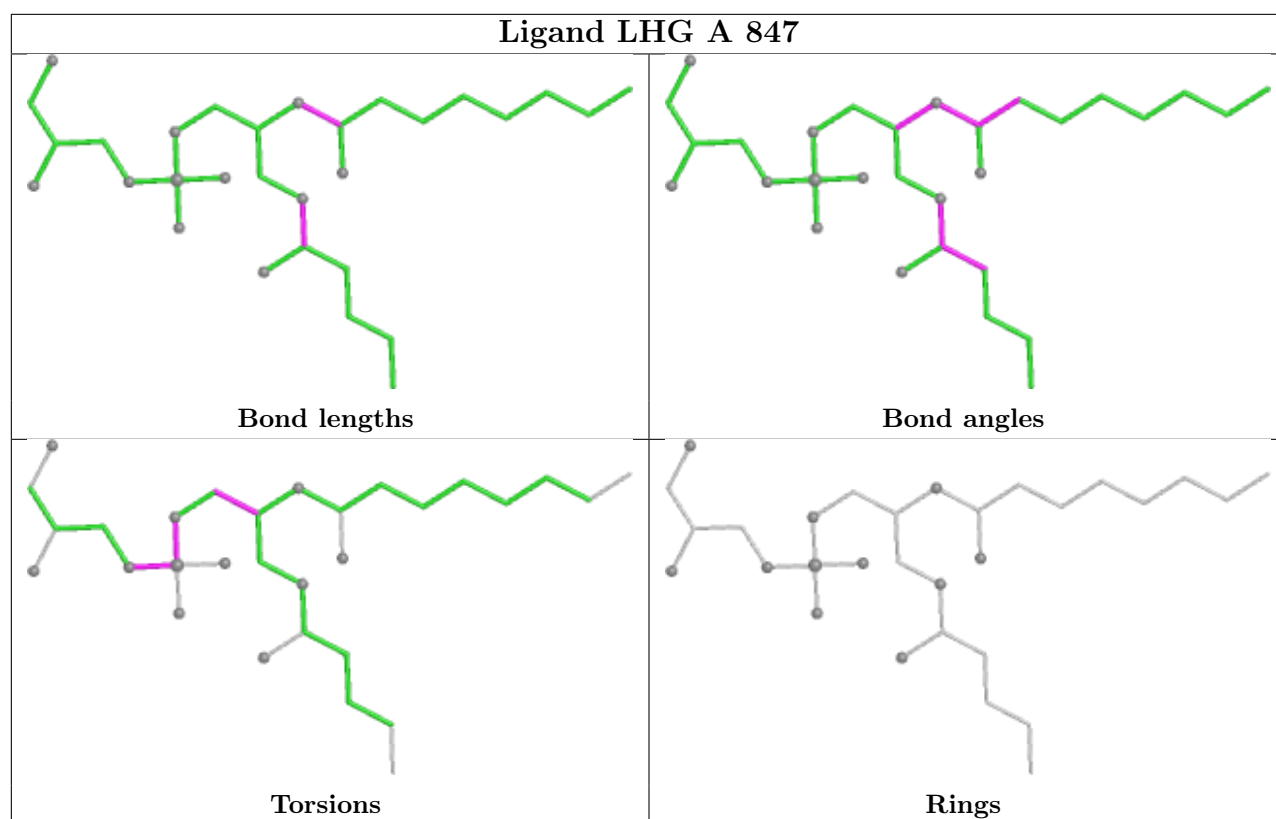
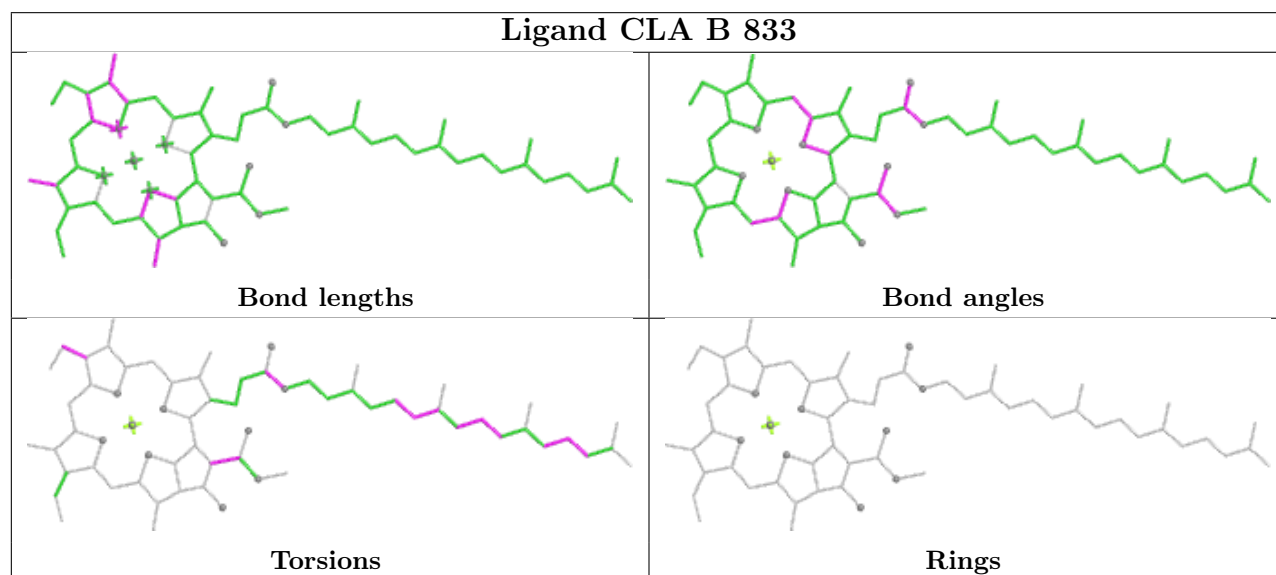
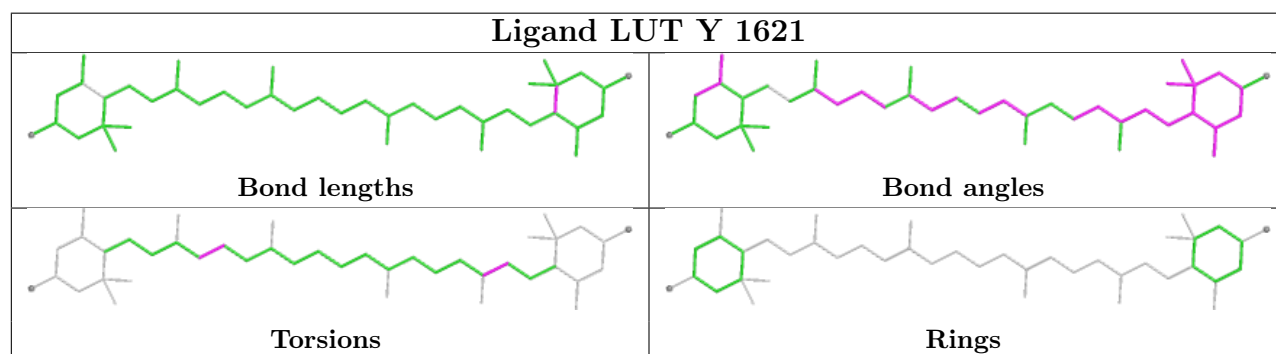


## Ligand XAT 1 618

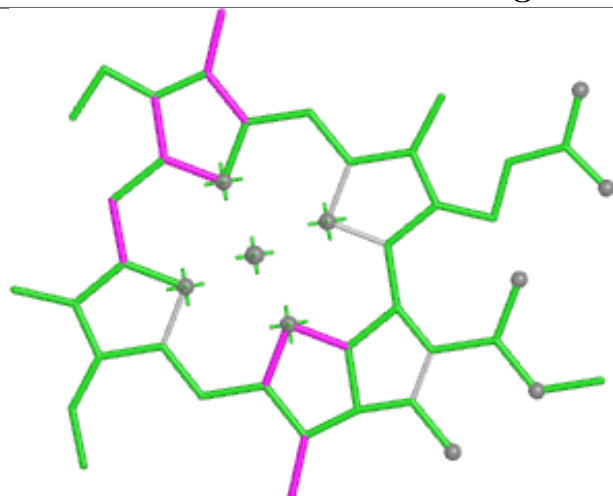




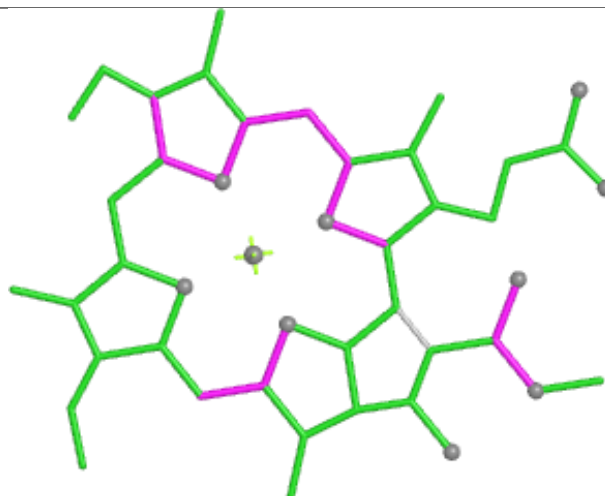
**Ligand CLA 3 608****Ligand NEX W 1623**



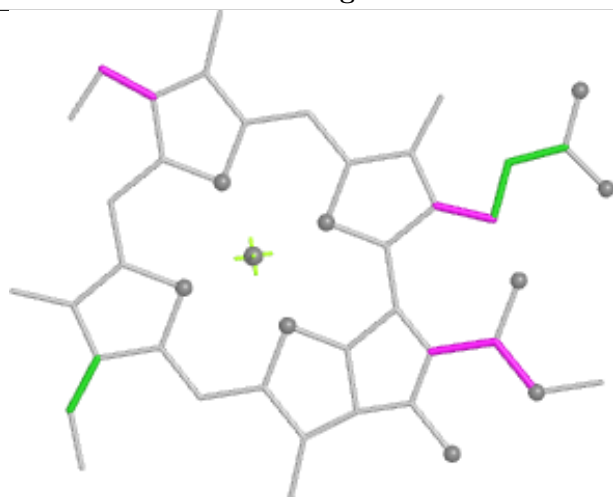
## Ligand CLA V 614



Bond lengths



Bond angles

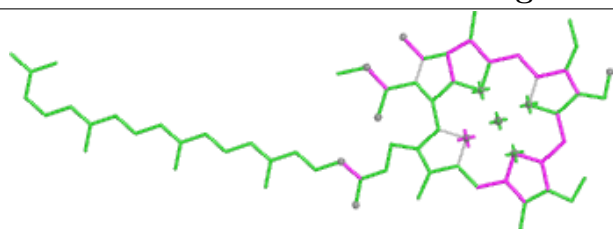


Torsions

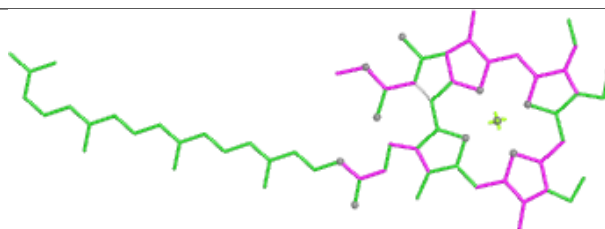


Rings

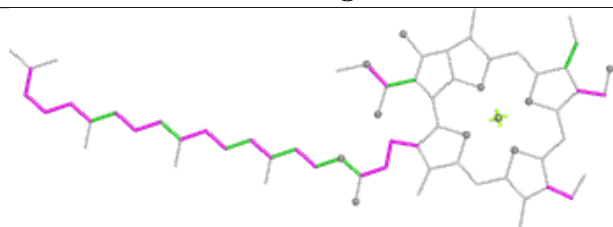
## Ligand CHL Z 607



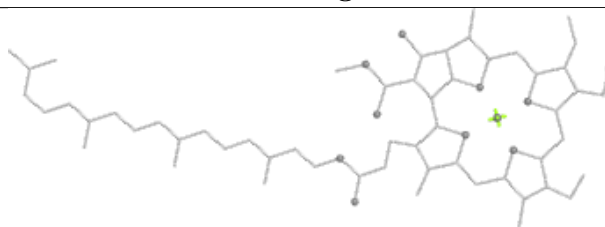
Bond lengths



Bond angles

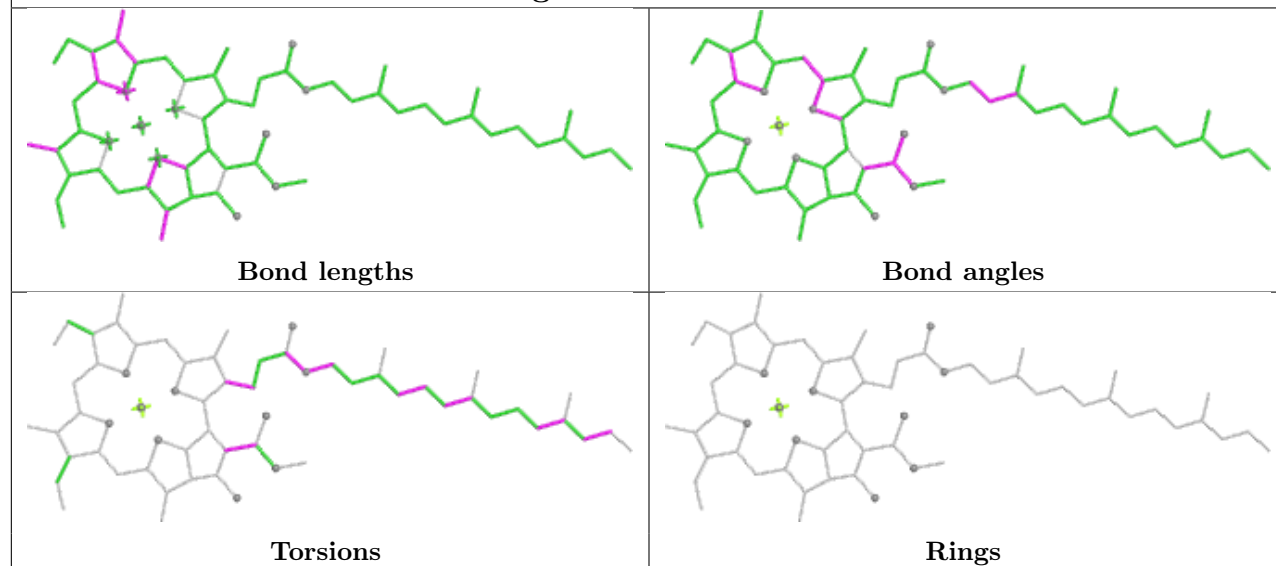


Torsions

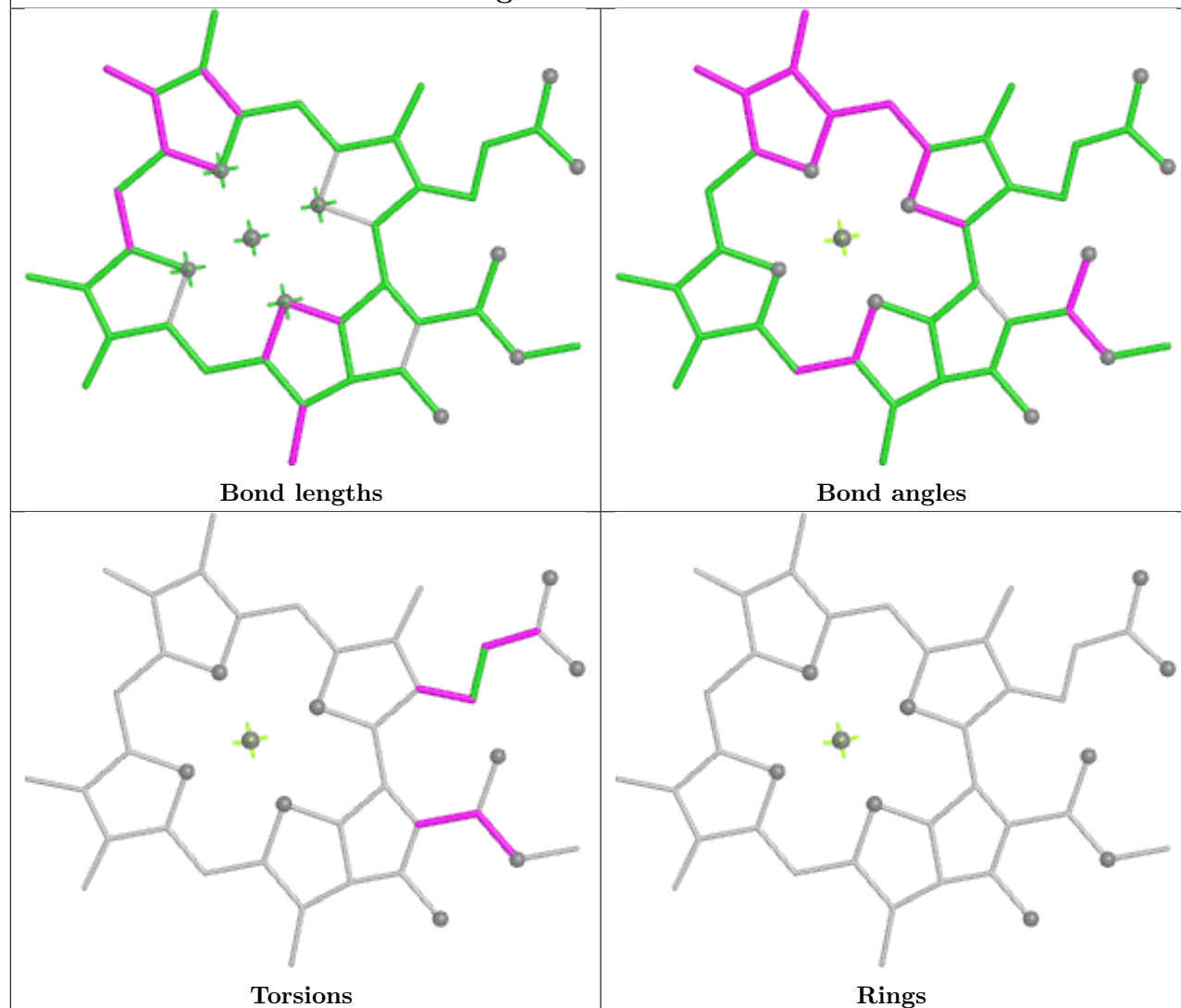


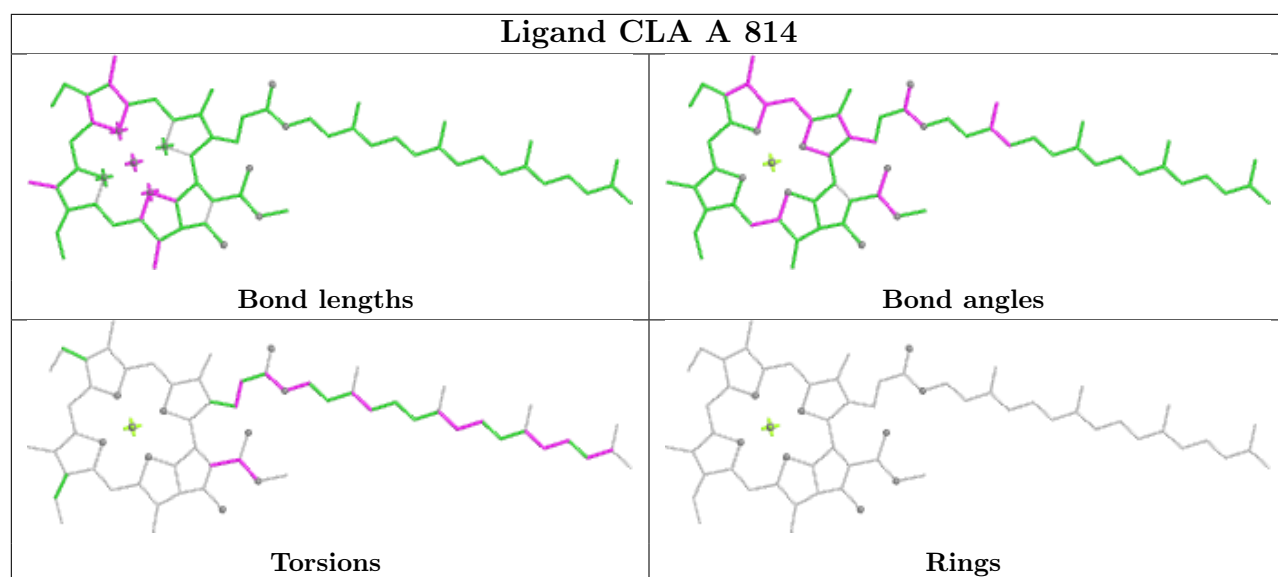
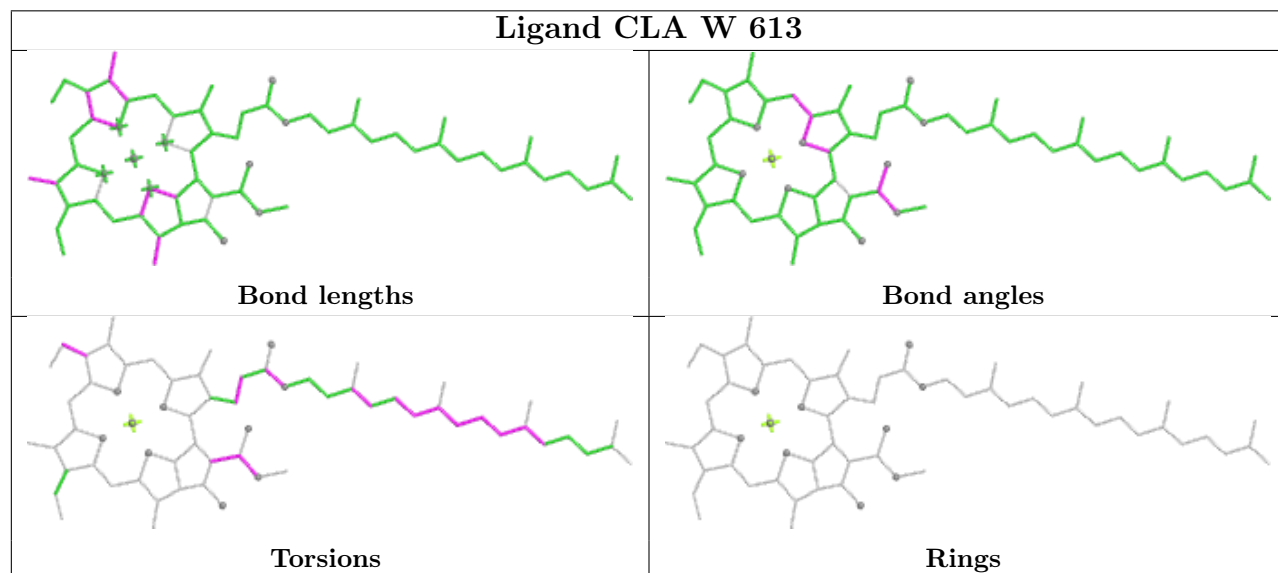
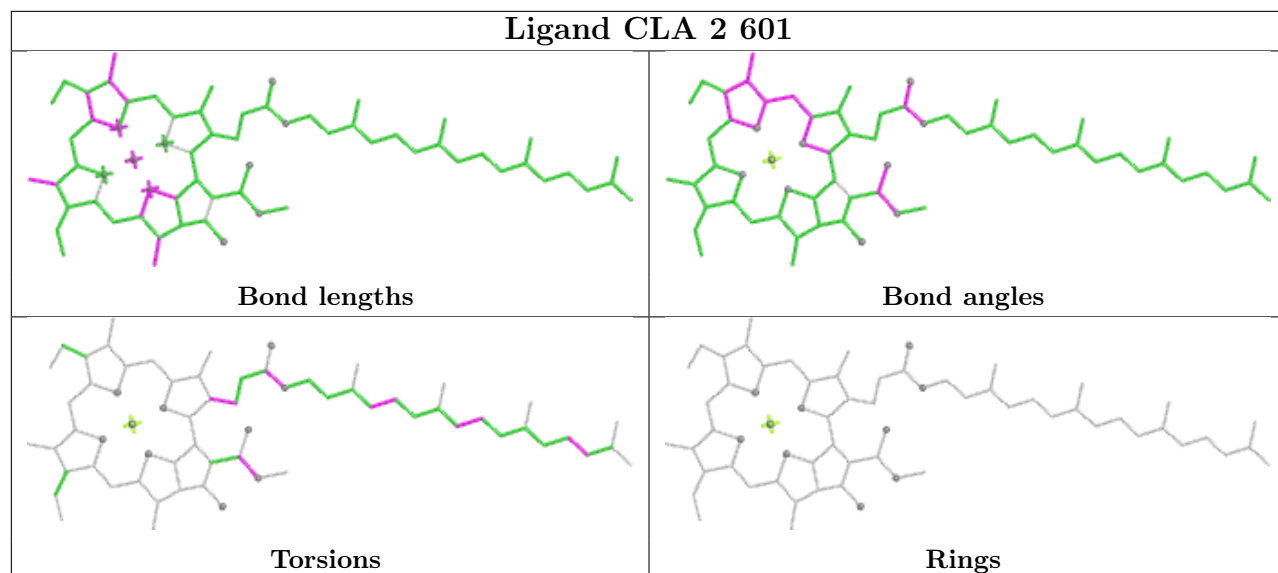
Rings

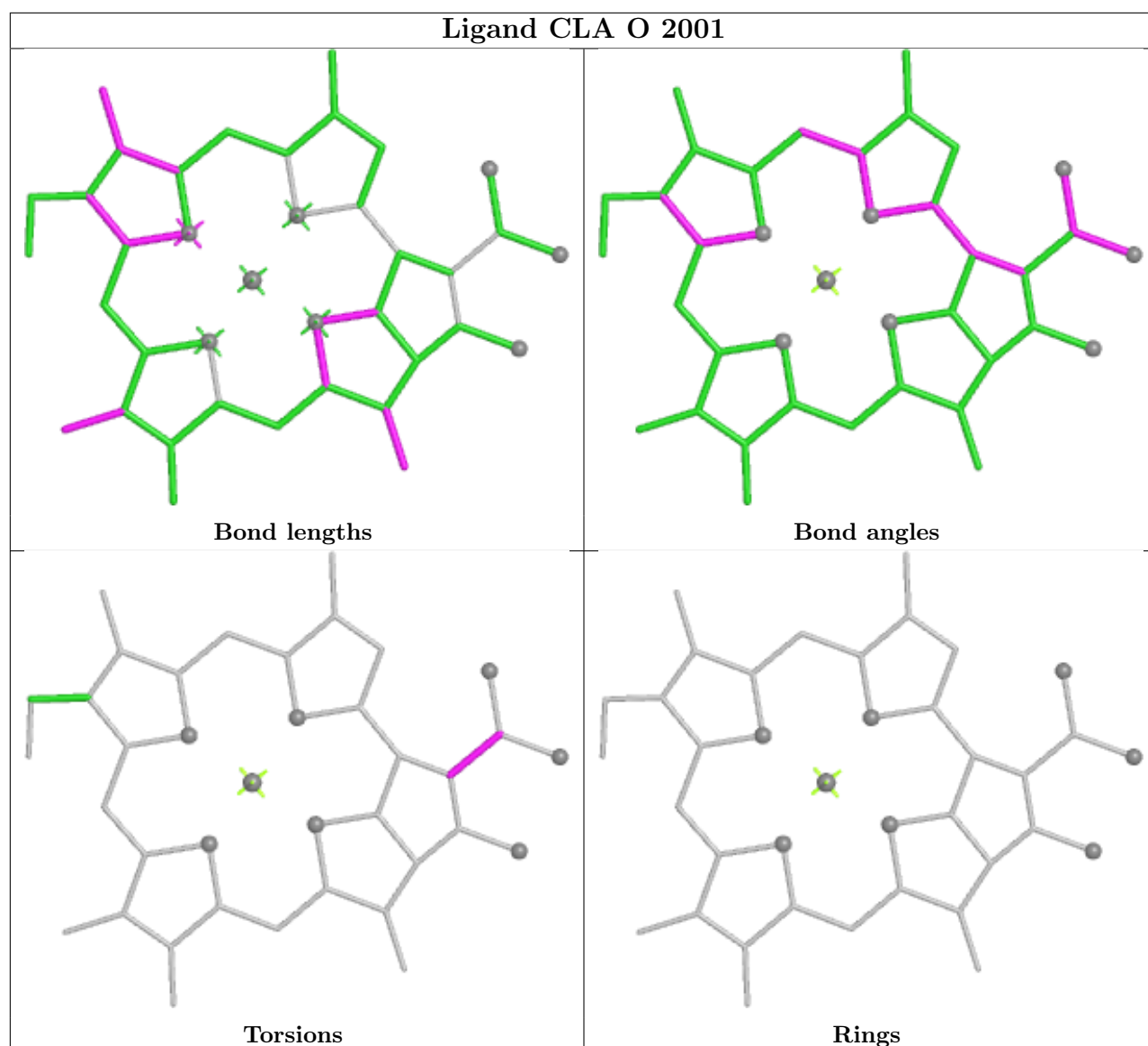
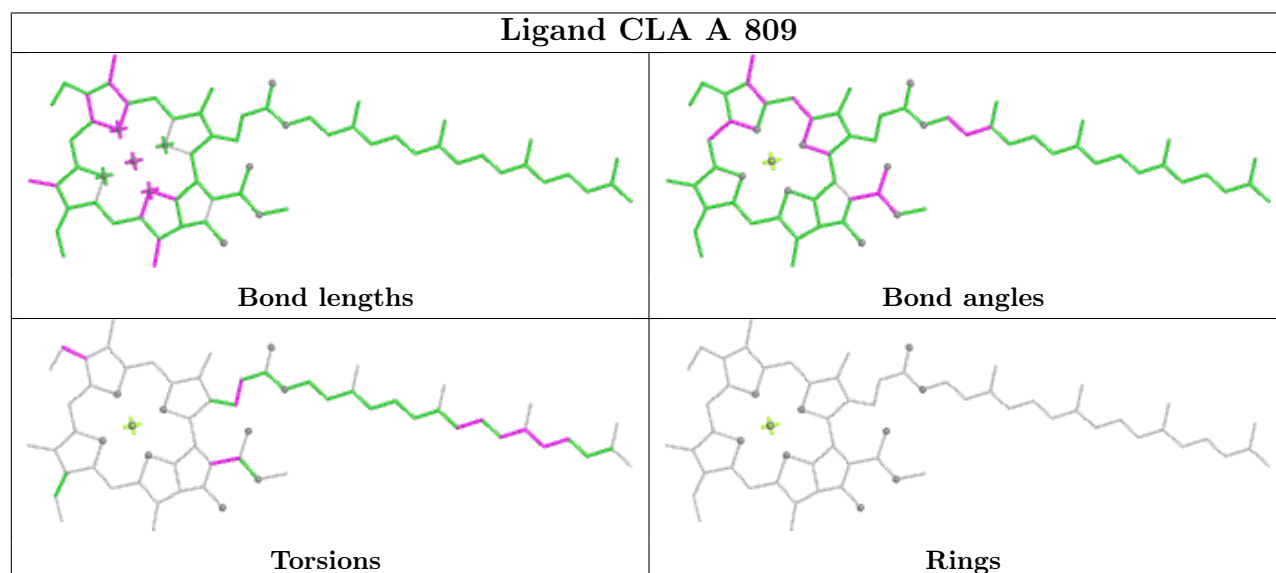
## Ligand CLA B 826

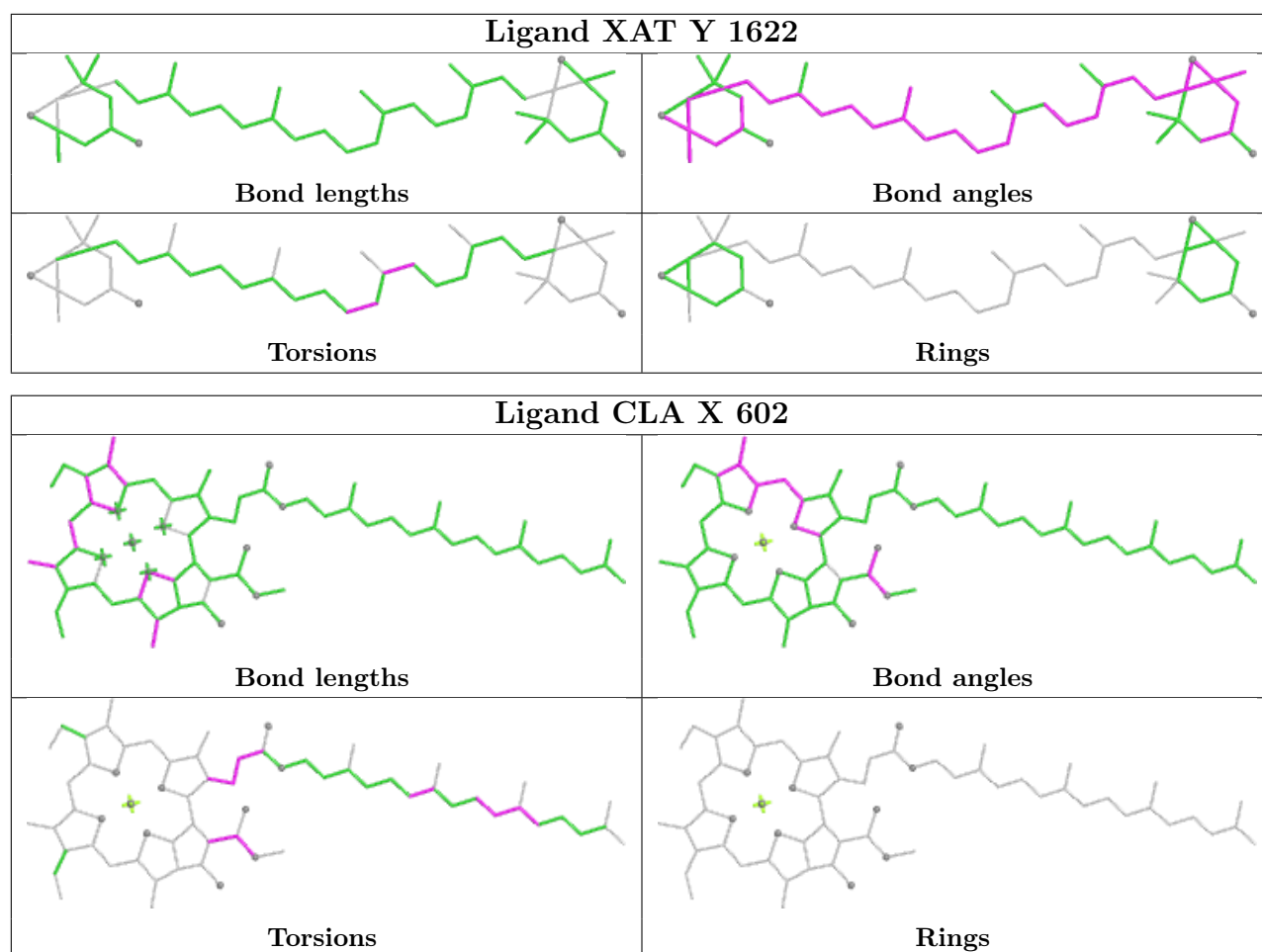


## Ligand CLA 1 616

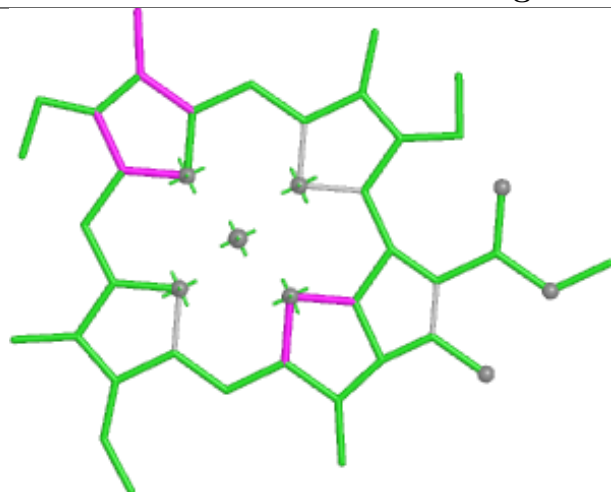




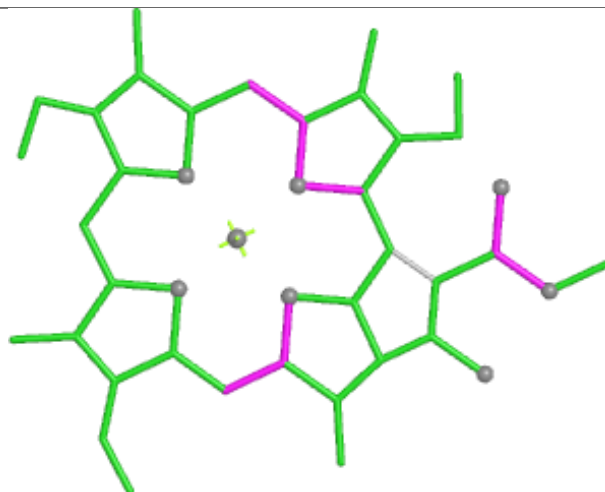




## Ligand CLA U 611



Bond lengths



Bond angles

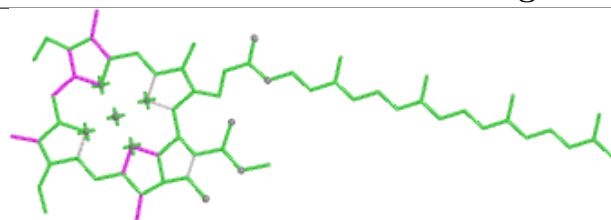


Torsions

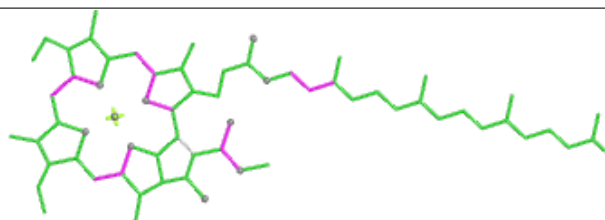


Rings

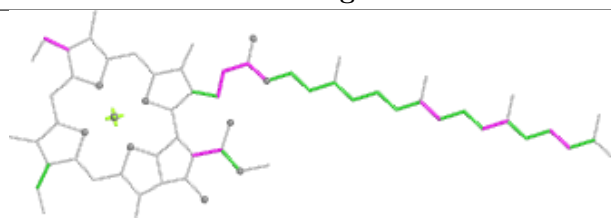
## Ligand CLA 9 613



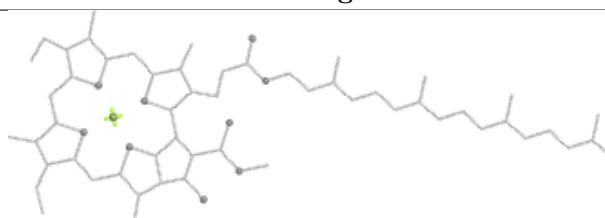
Bond lengths



Bond angles

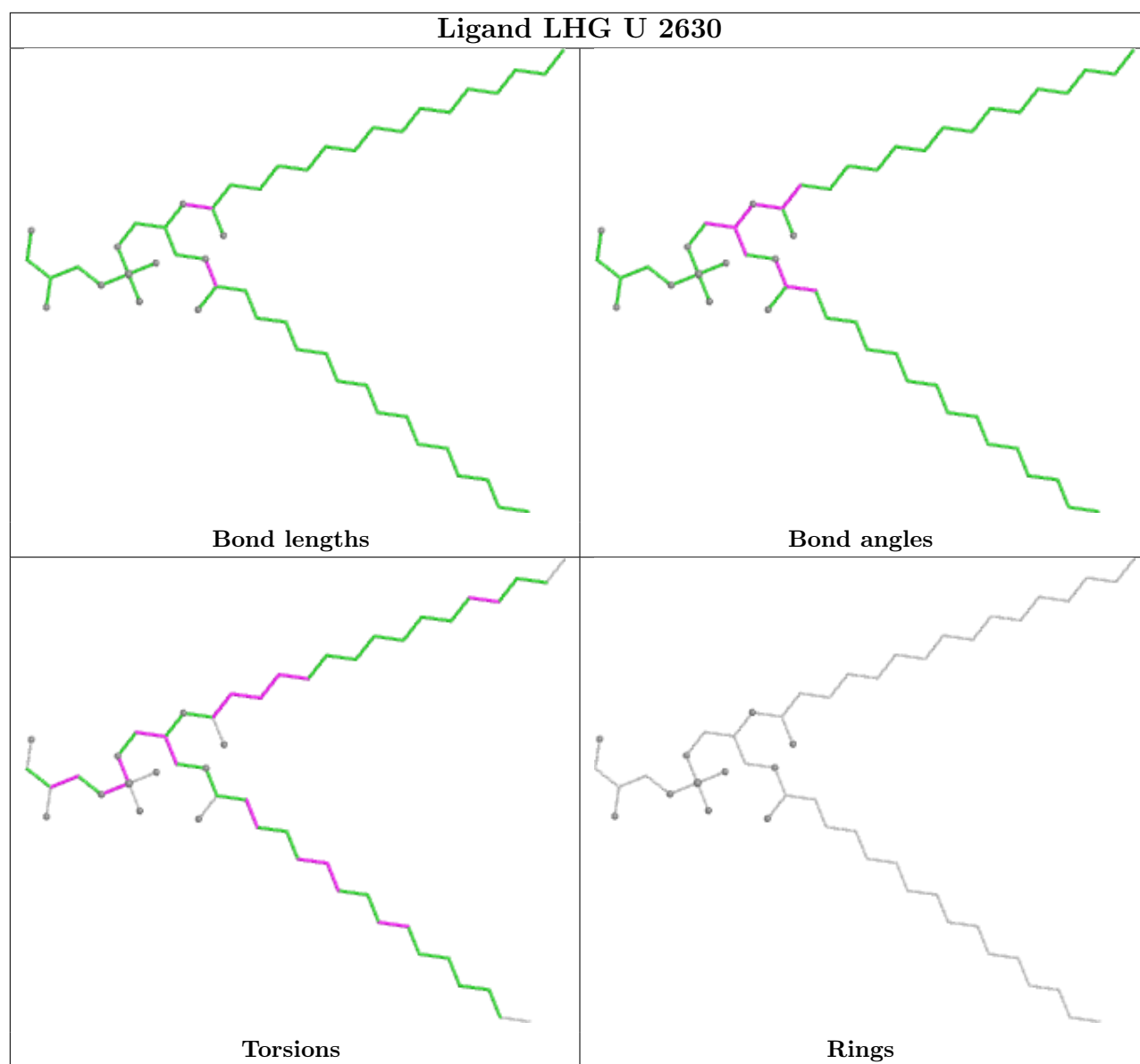
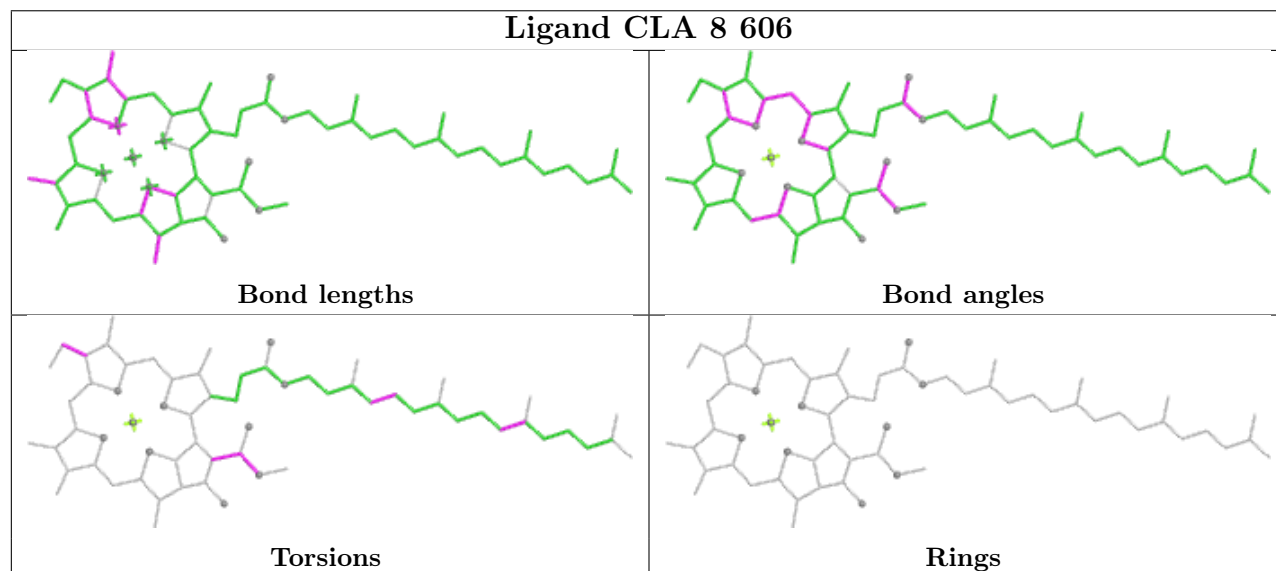


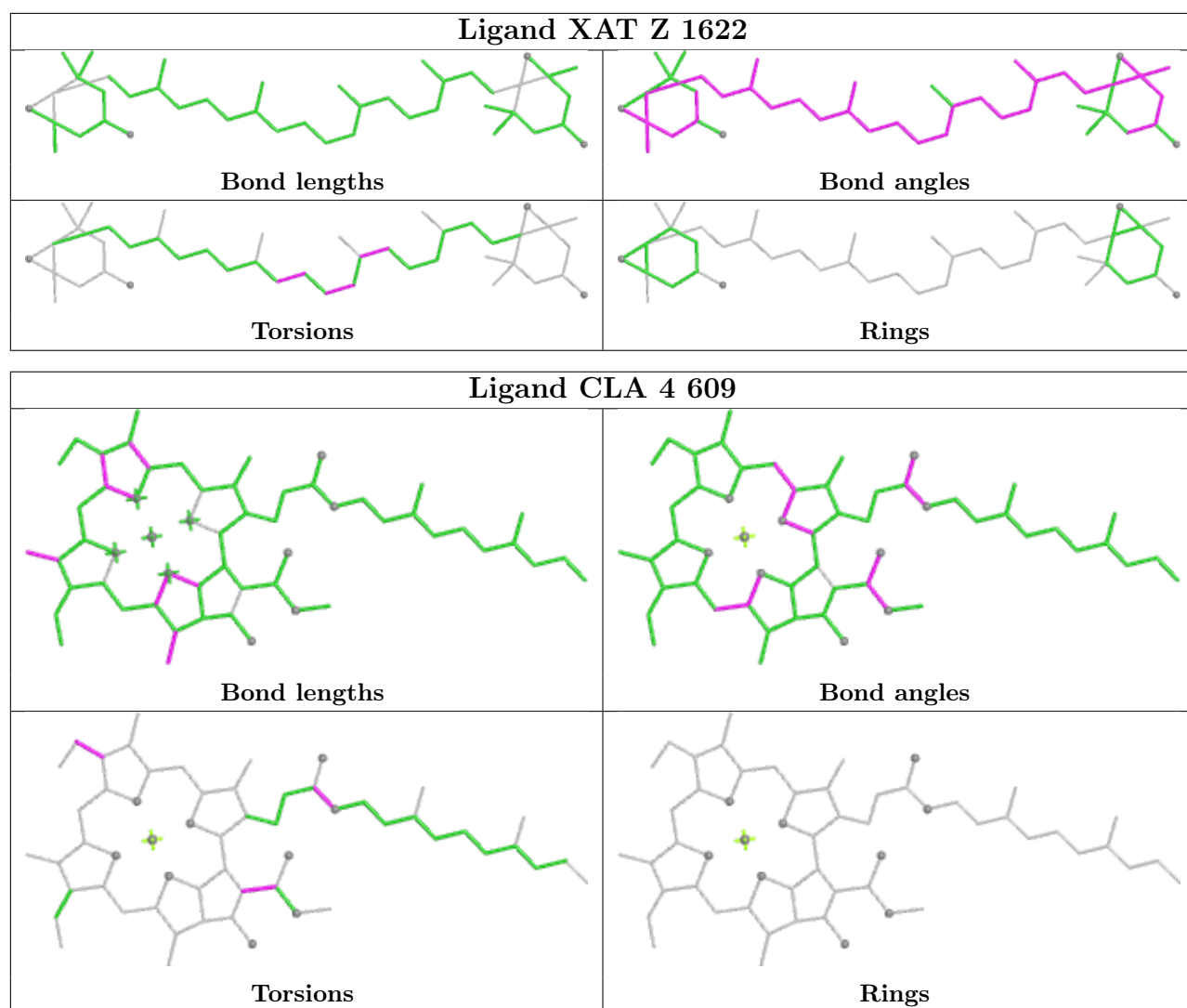
Torsions

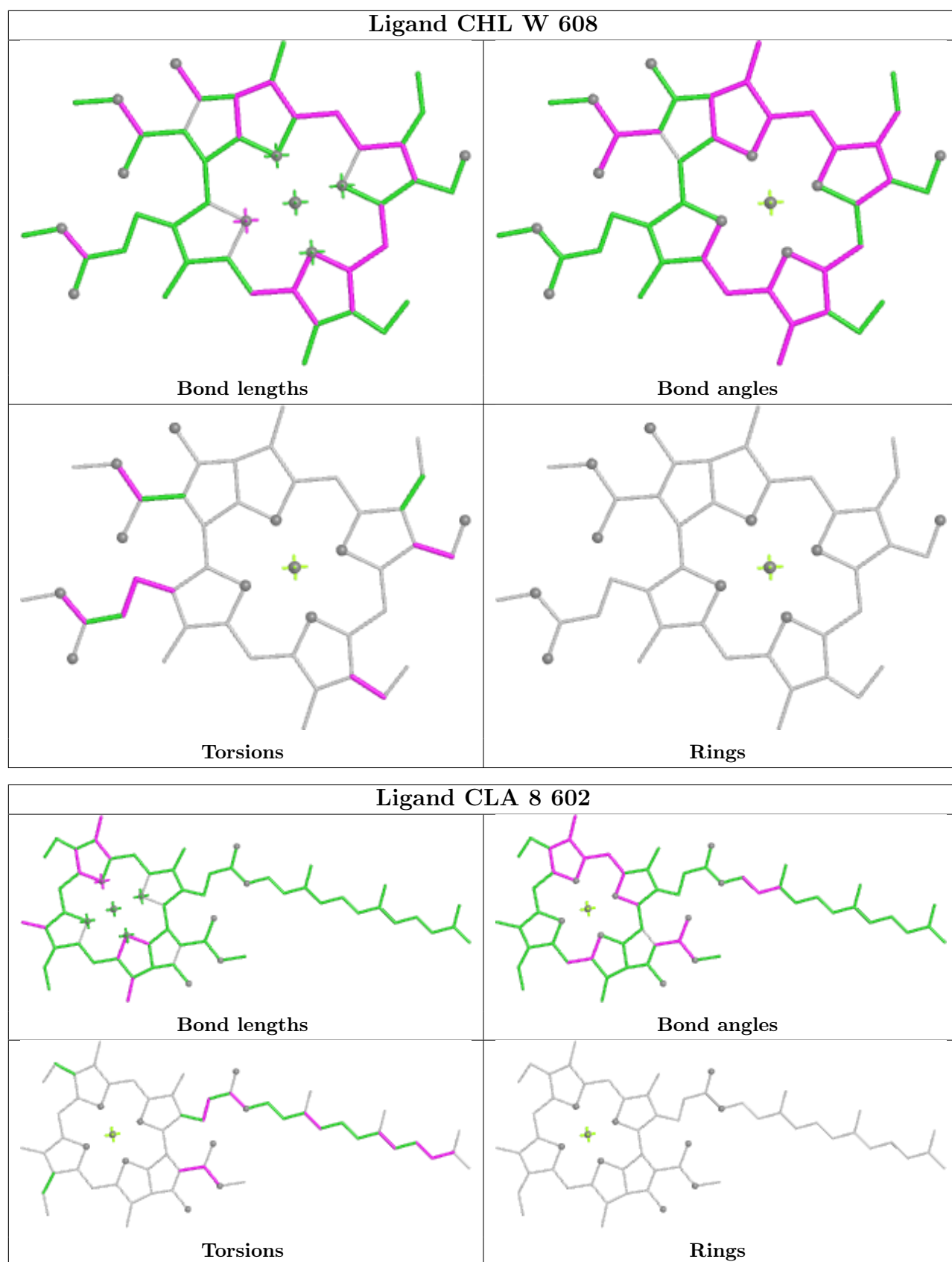


Rings

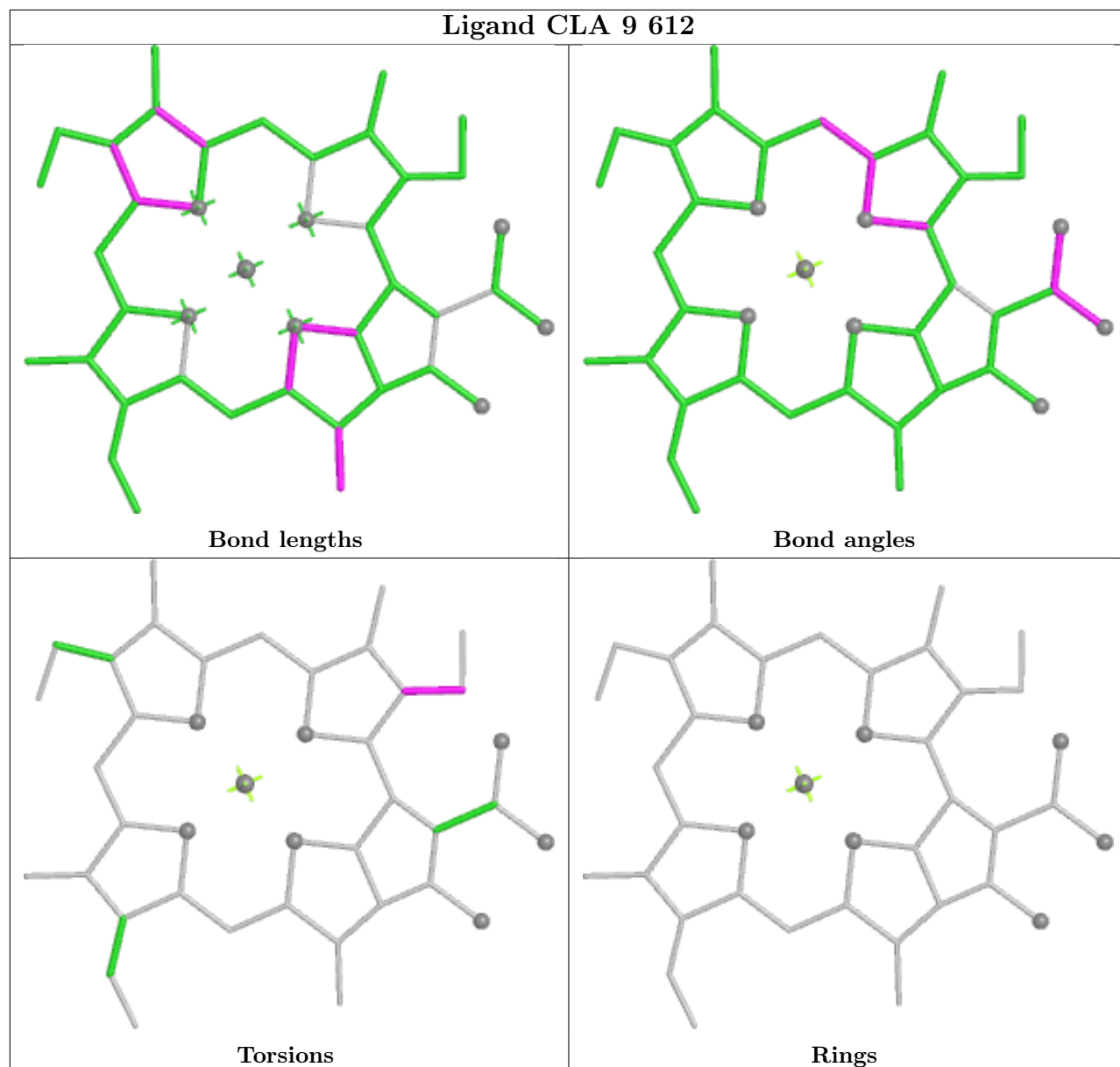


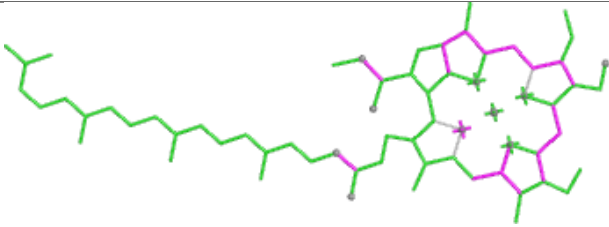
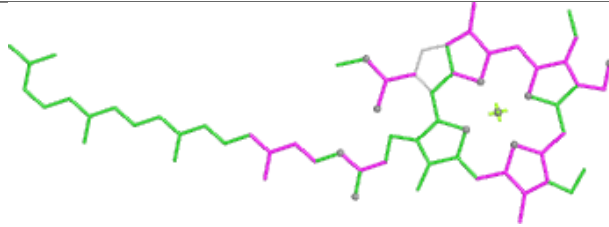
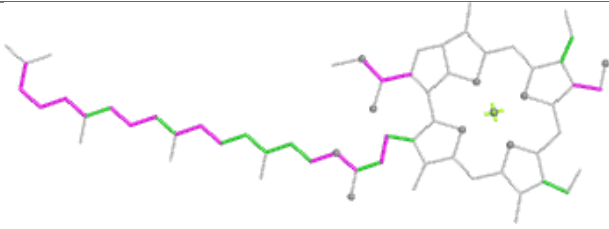
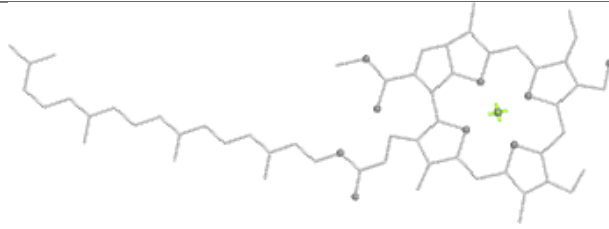
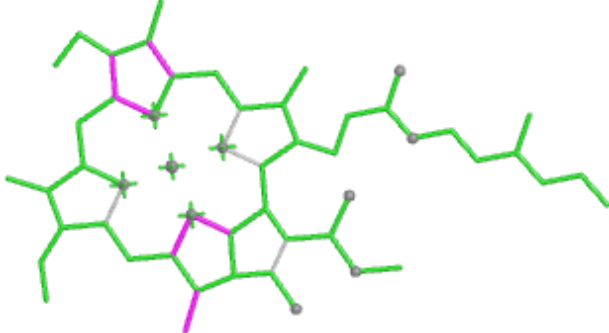
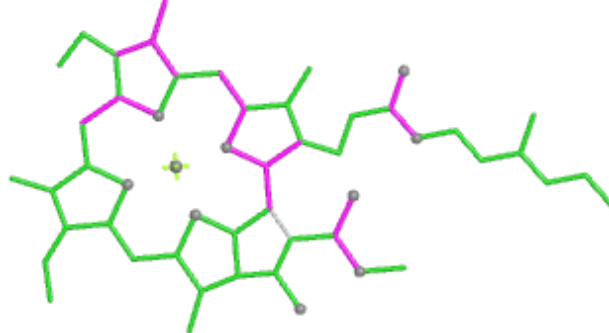
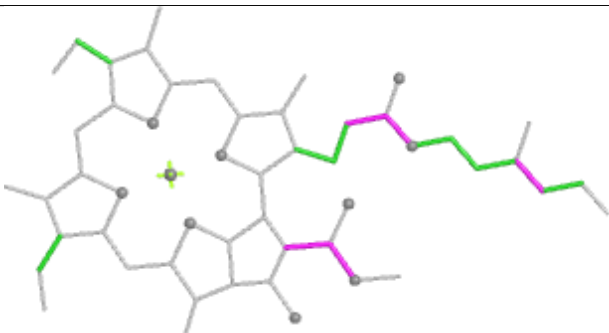
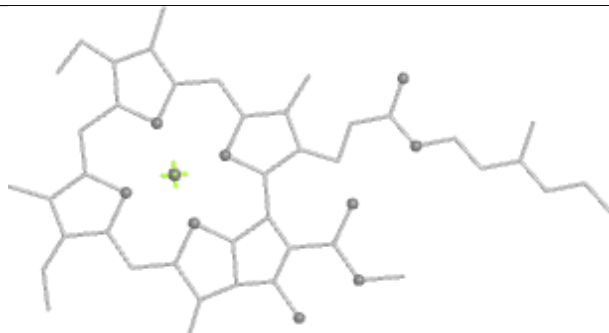
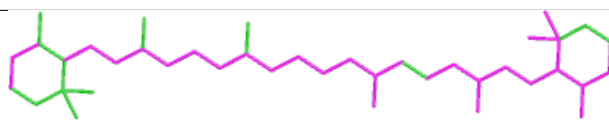
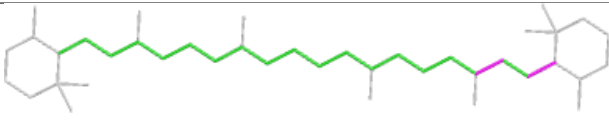
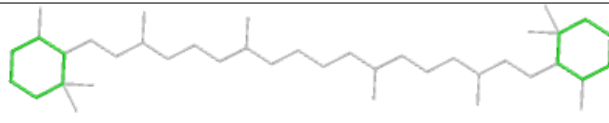


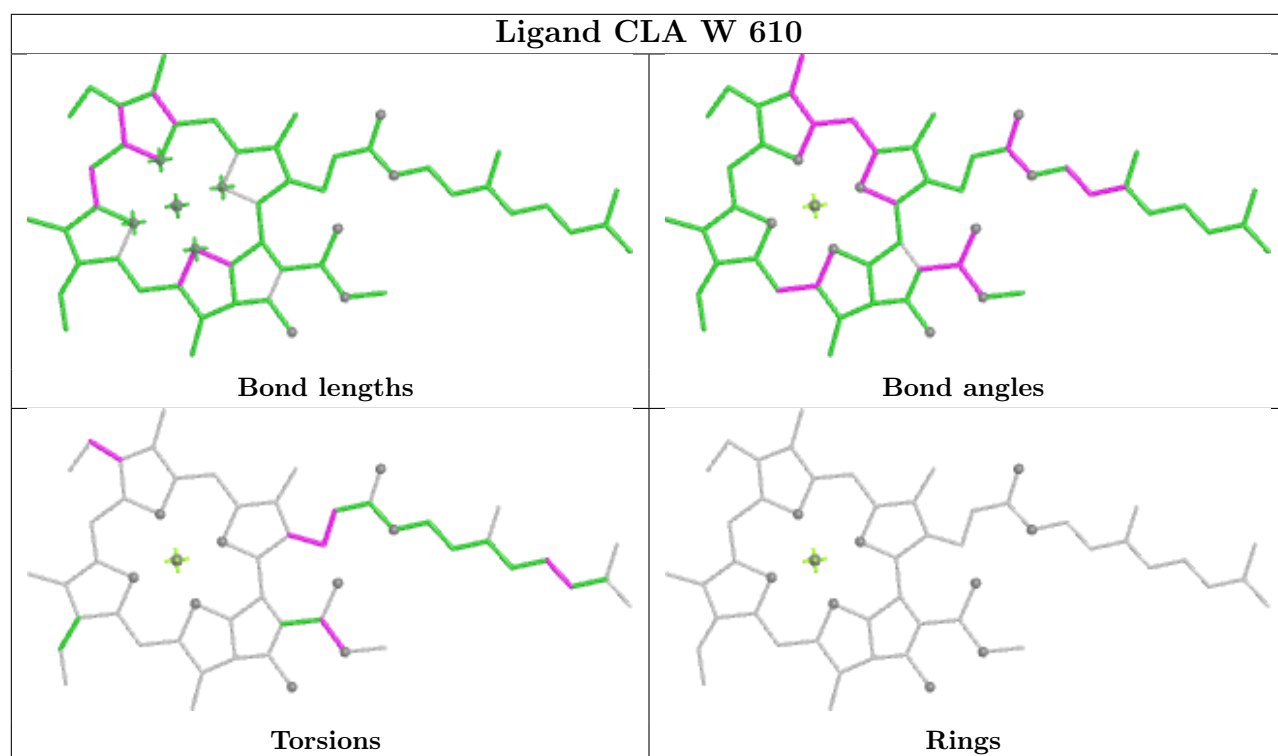




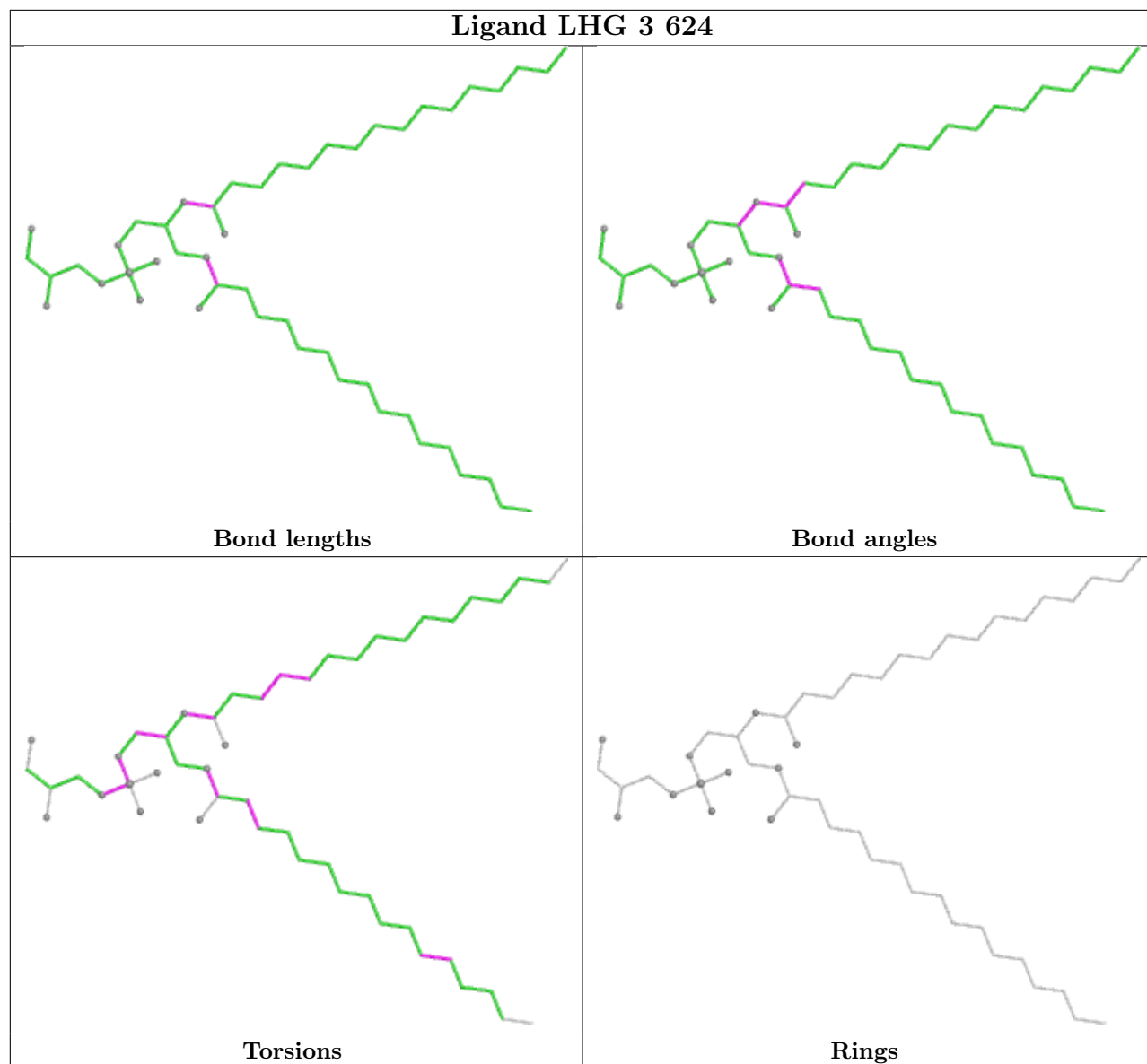
## Ligand CLA 9 612



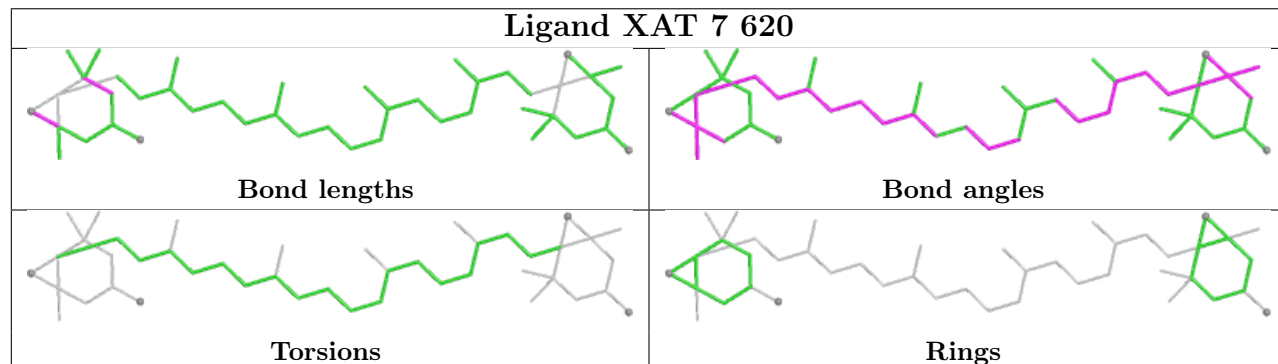
| Ligand CHL X 608                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand CLA W 603                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>  |  <p>Bond angles</p>  |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand BCR 3 620                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |



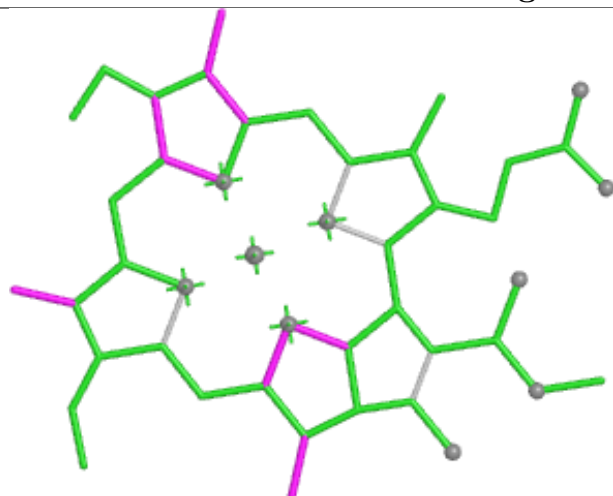
## Ligand LHG 3 624



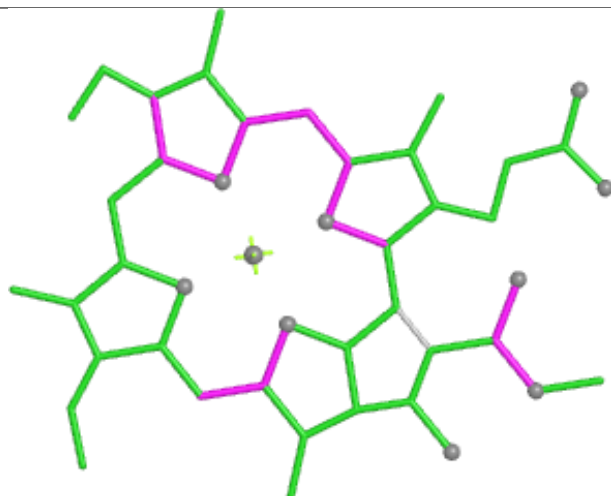
## Ligand XAT 7 620



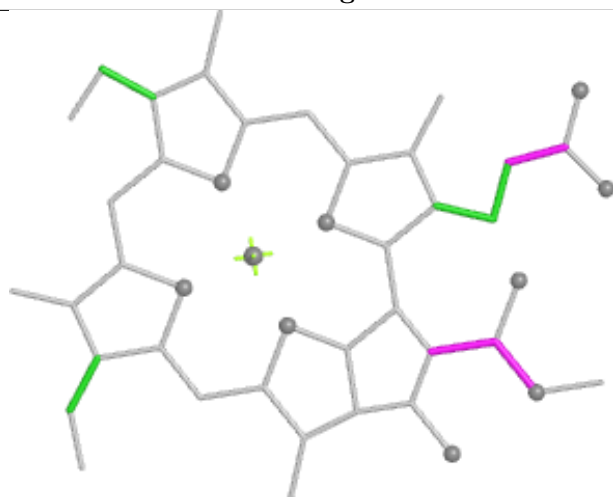
## Ligand CLA 4 607



Bond lengths



Bond angles



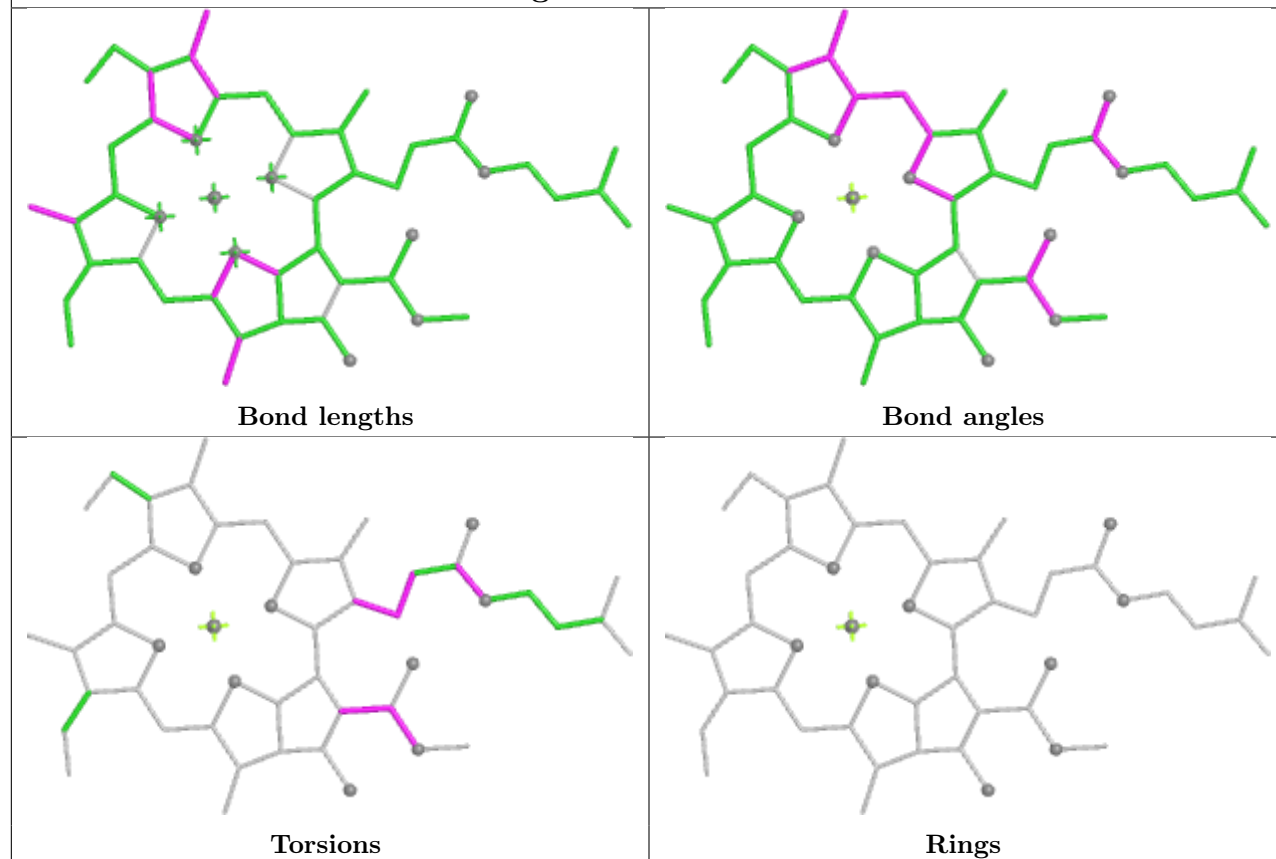
Torsions



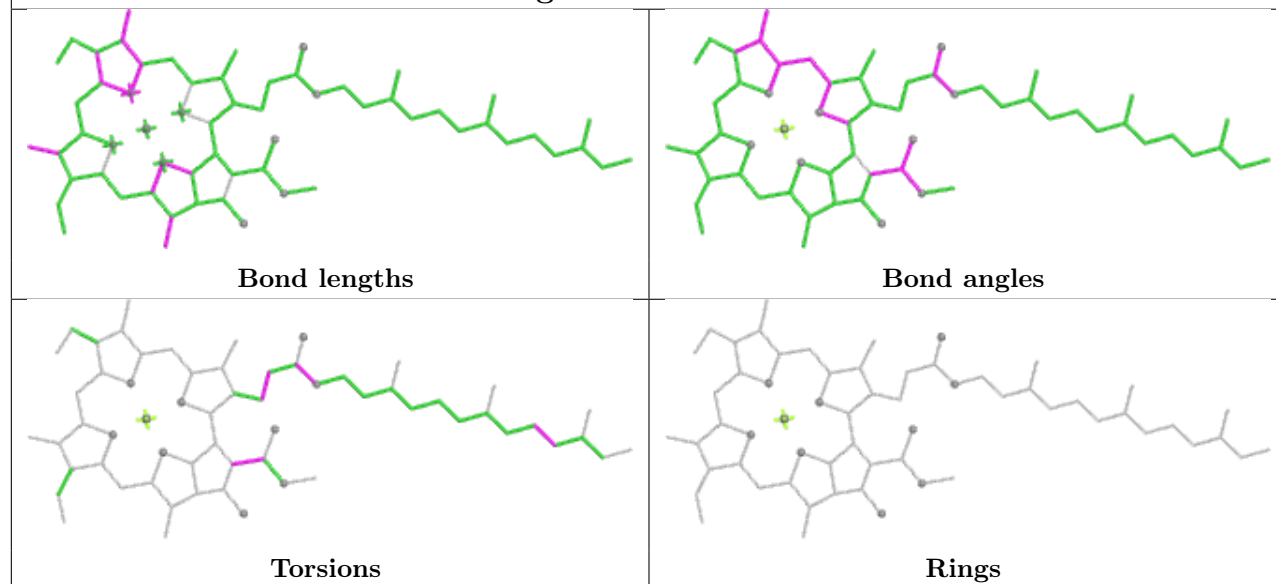
Rings



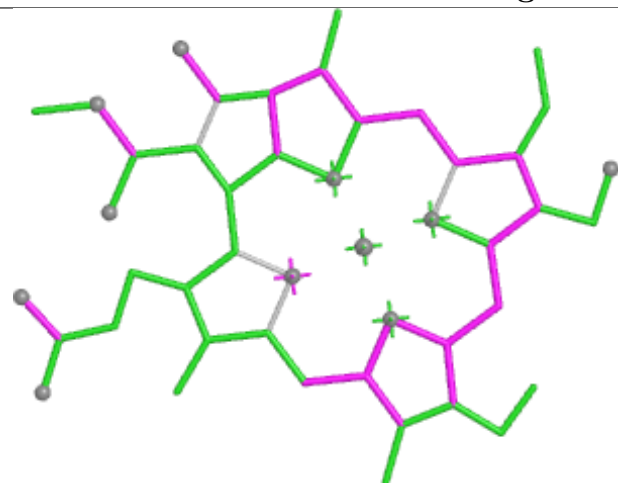
## Ligand CLA V 604



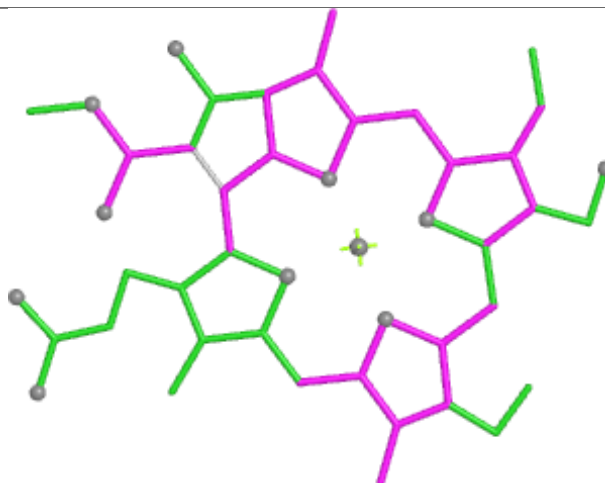
## Ligand CLA 1 602



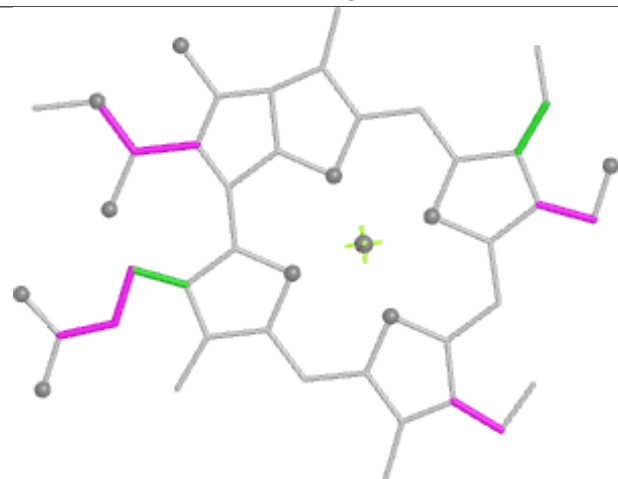
## Ligand CHL X 605



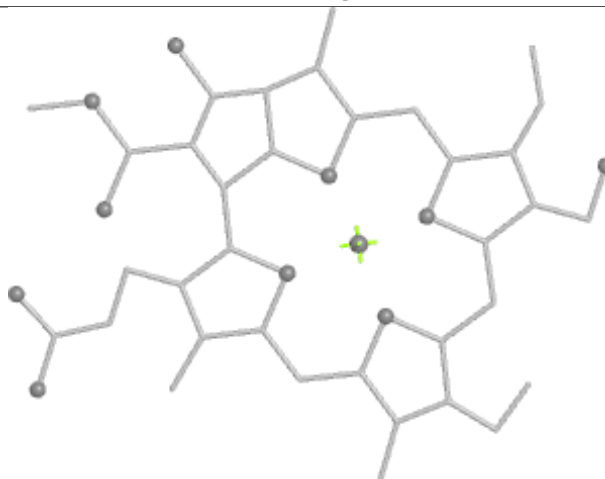
Bond lengths



Bond angles

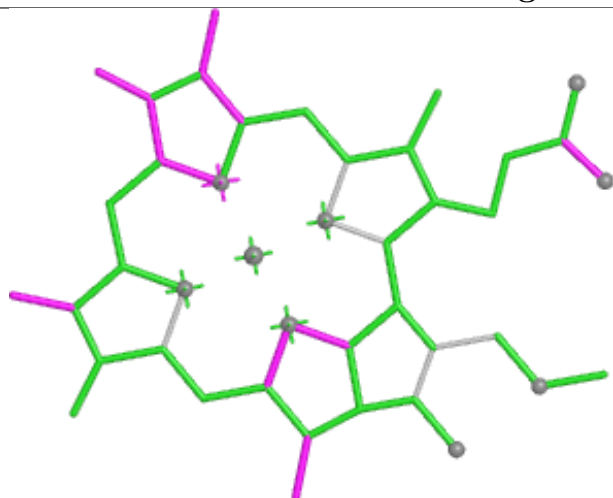


Torsions

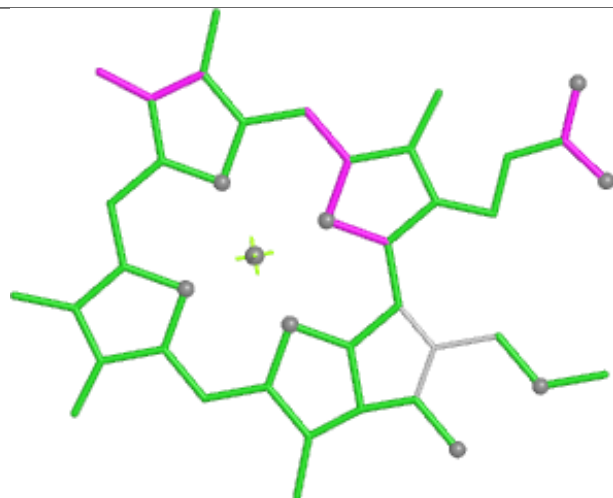


Rings

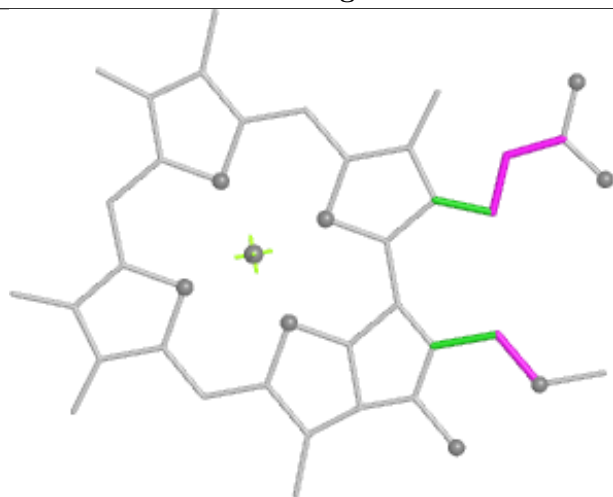
## Ligand CLA 5 616



Bond lengths



Bond angles

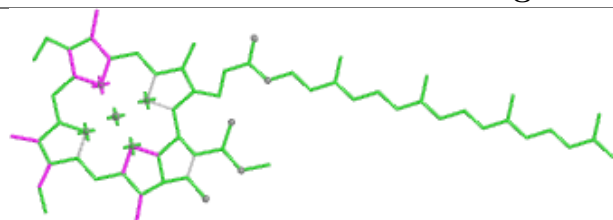


Torsions

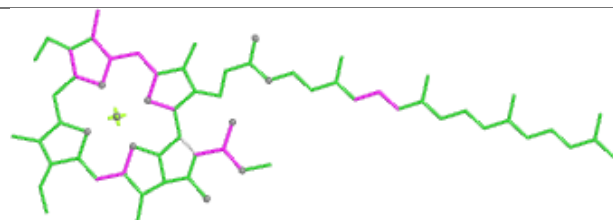


Rings

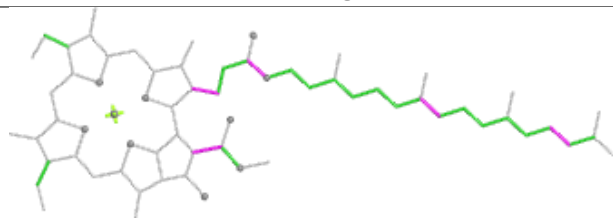
## Ligand CLA A 820



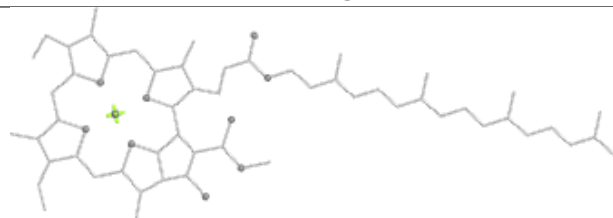
Bond lengths



Bond angles

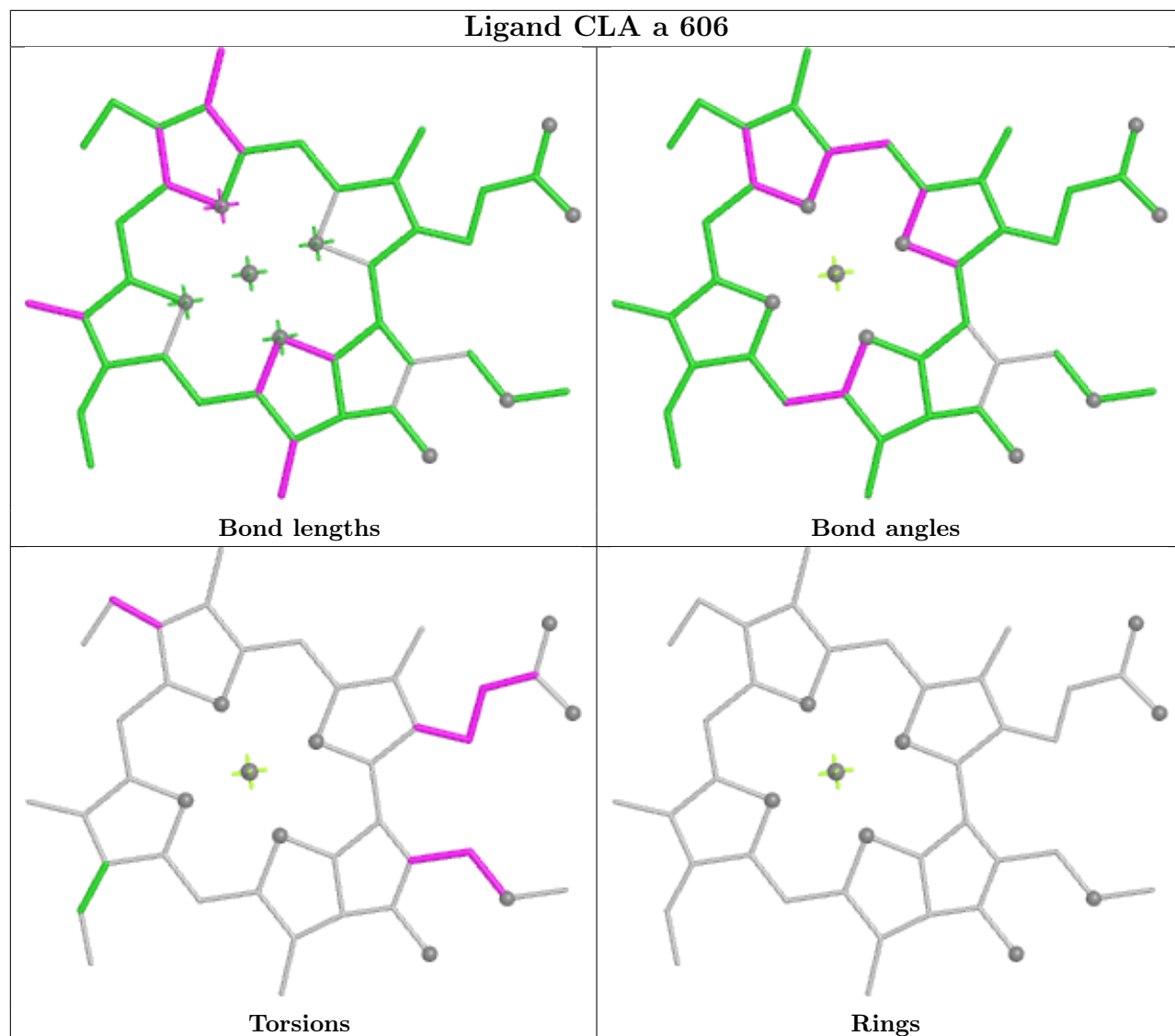


Torsions

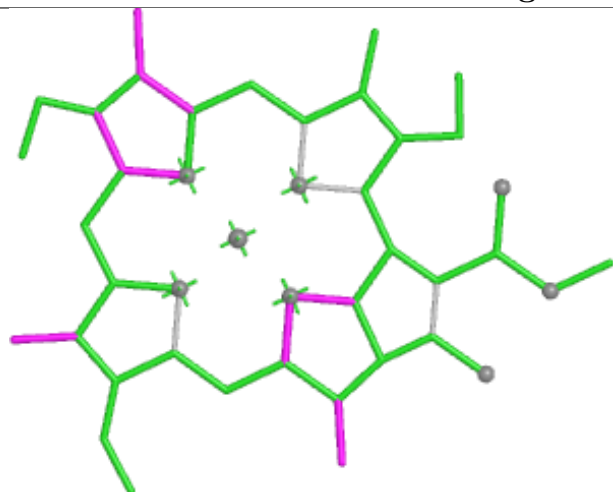


Rings

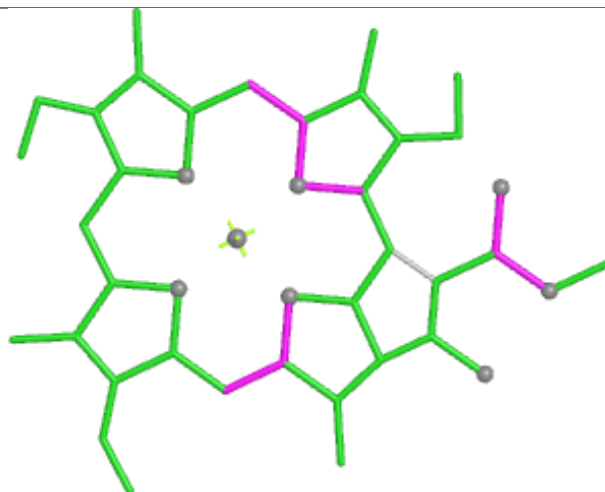
## Ligand CLA a 606



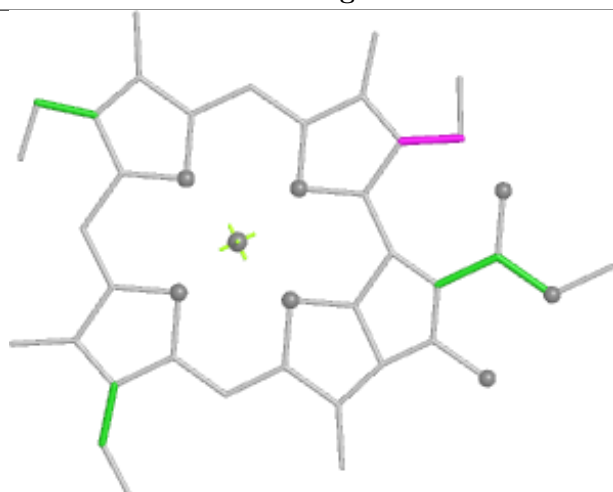
## Ligand CLA 7 607



Bond lengths



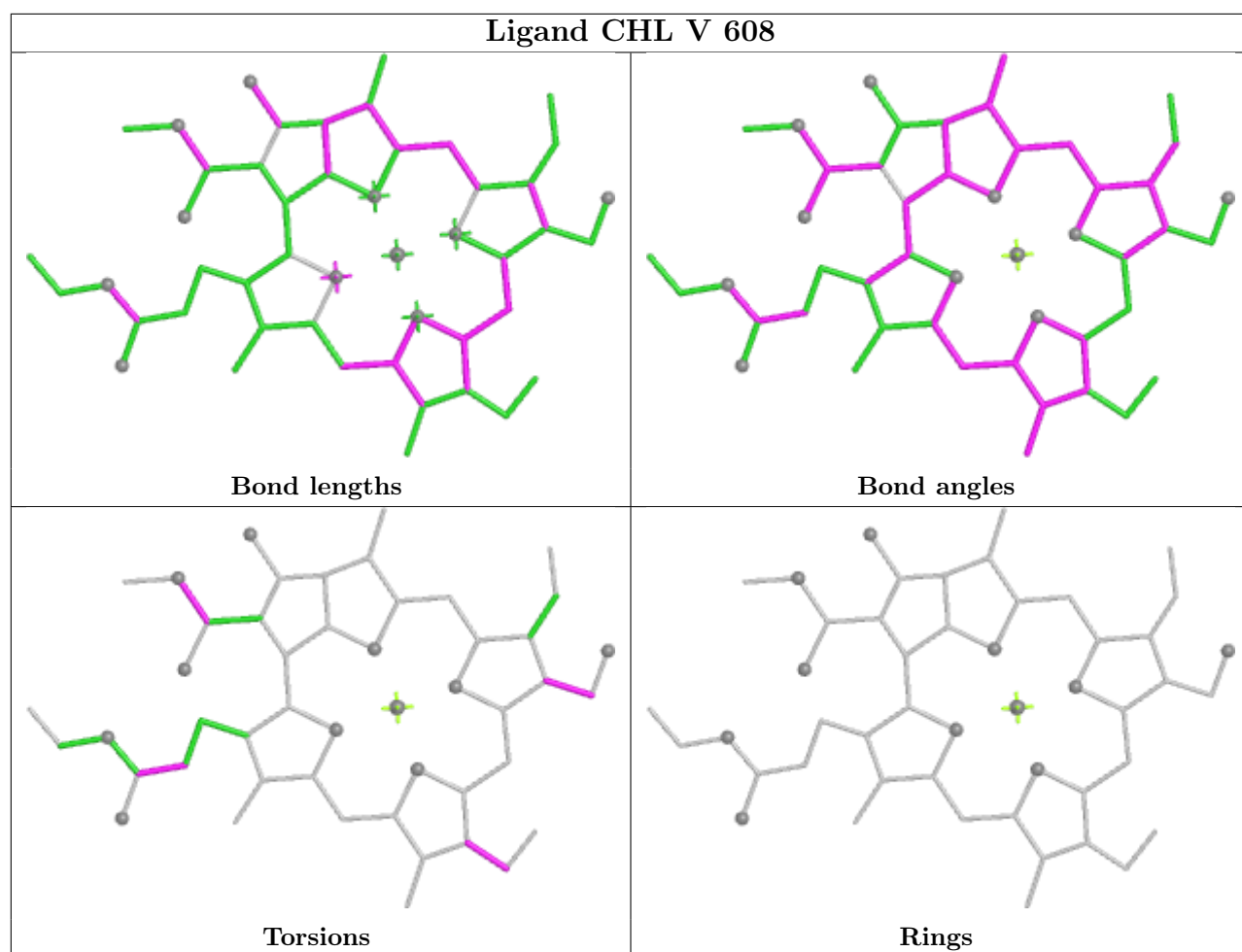
Bond angles



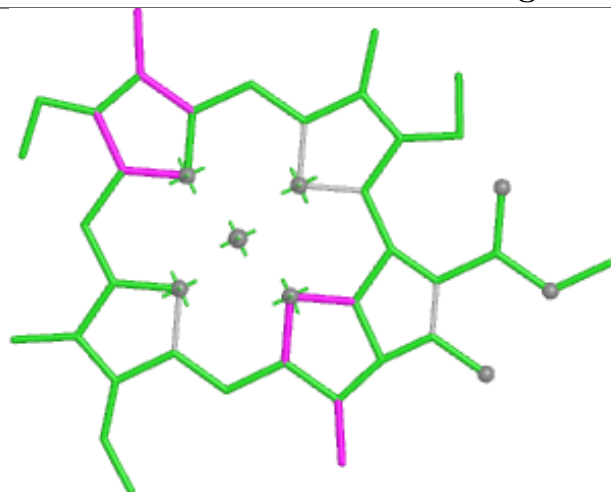
Torsions



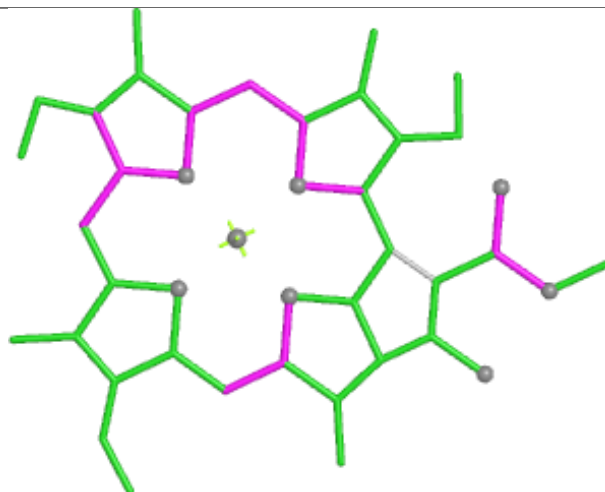
Rings



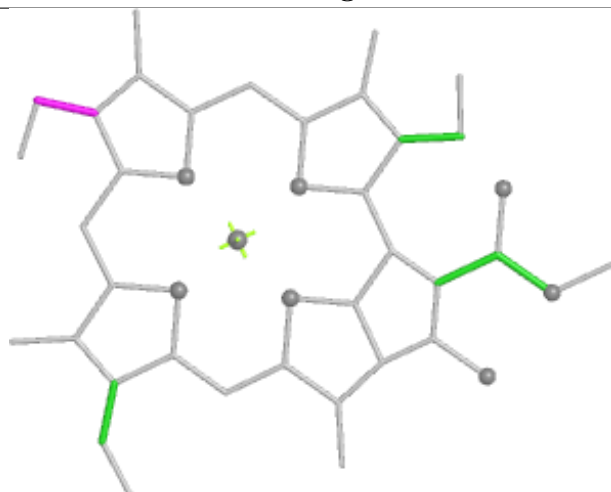
## Ligand CLA 5 611



Bond lengths



Bond angles

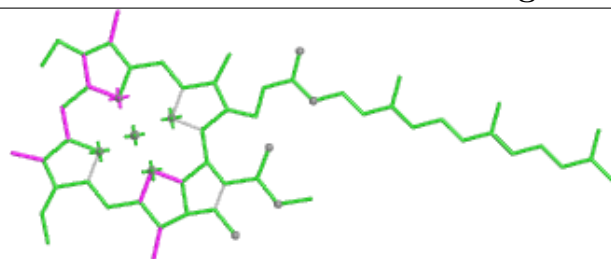


Torsions

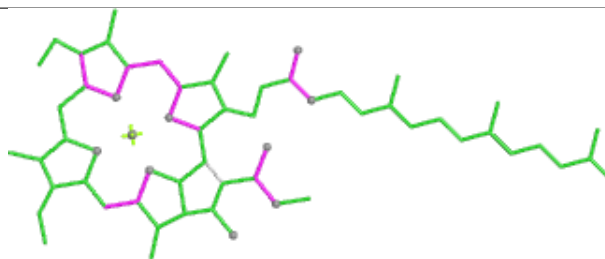


Rings

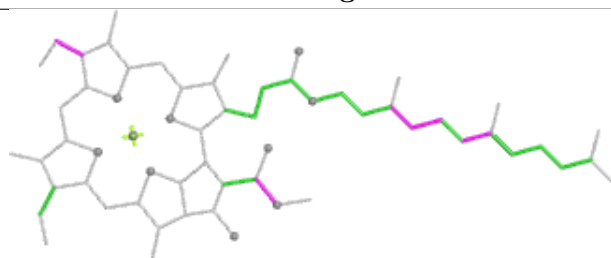
## Ligand CLA 4 602



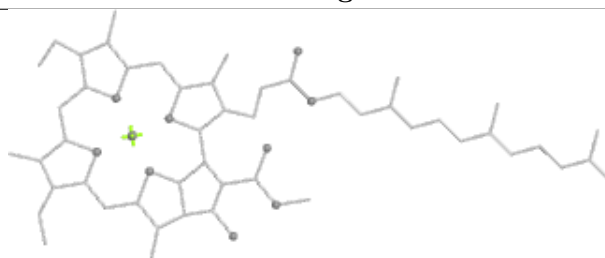
Bond lengths



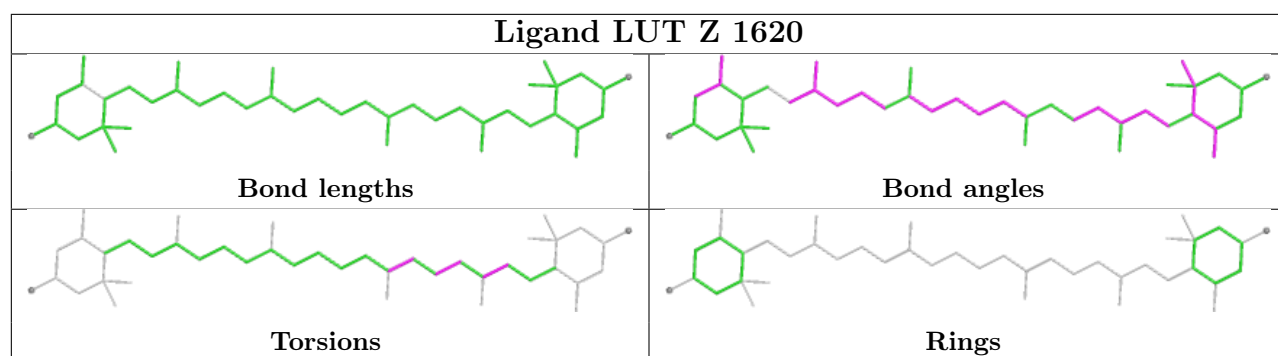
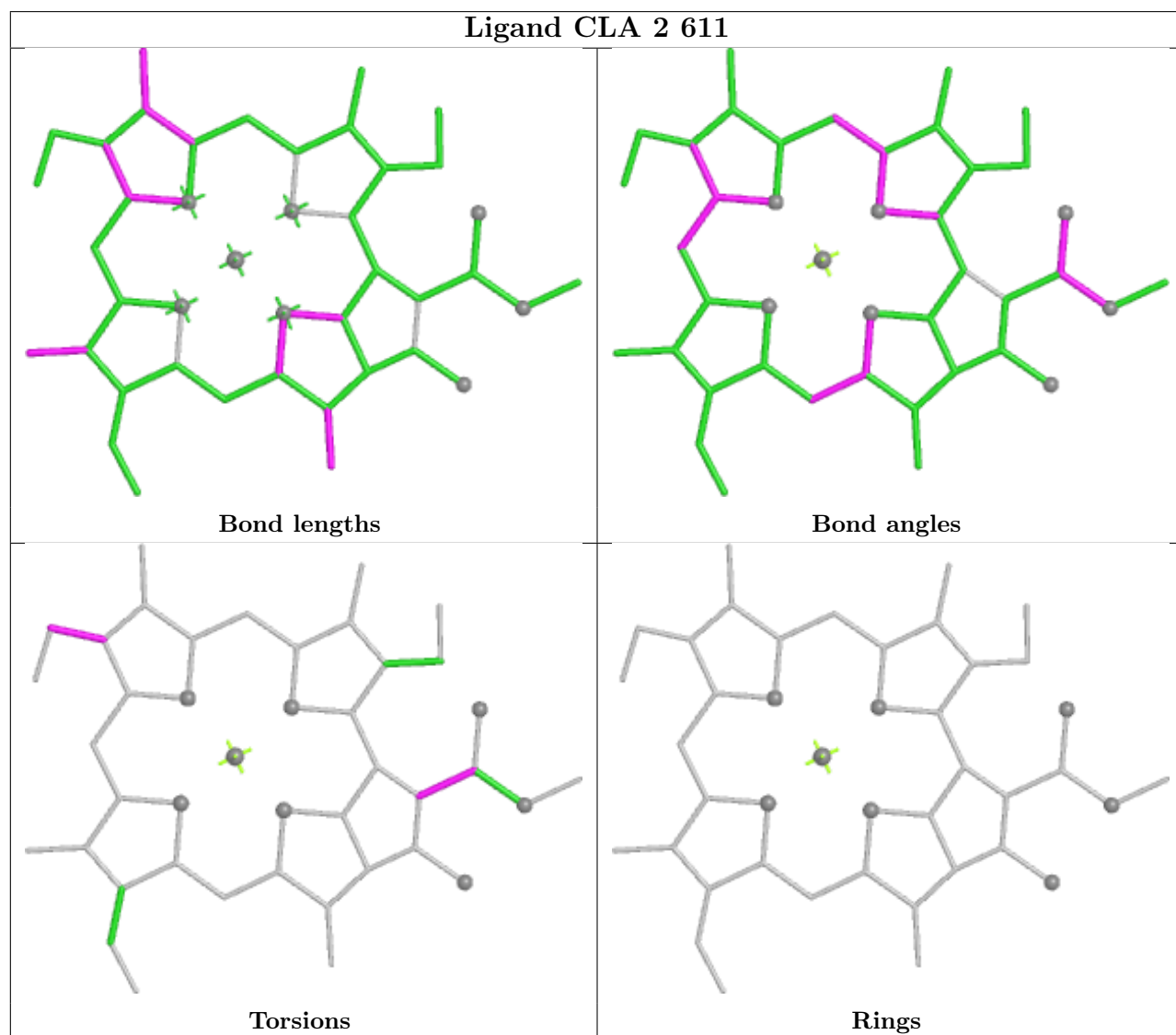
Bond angles



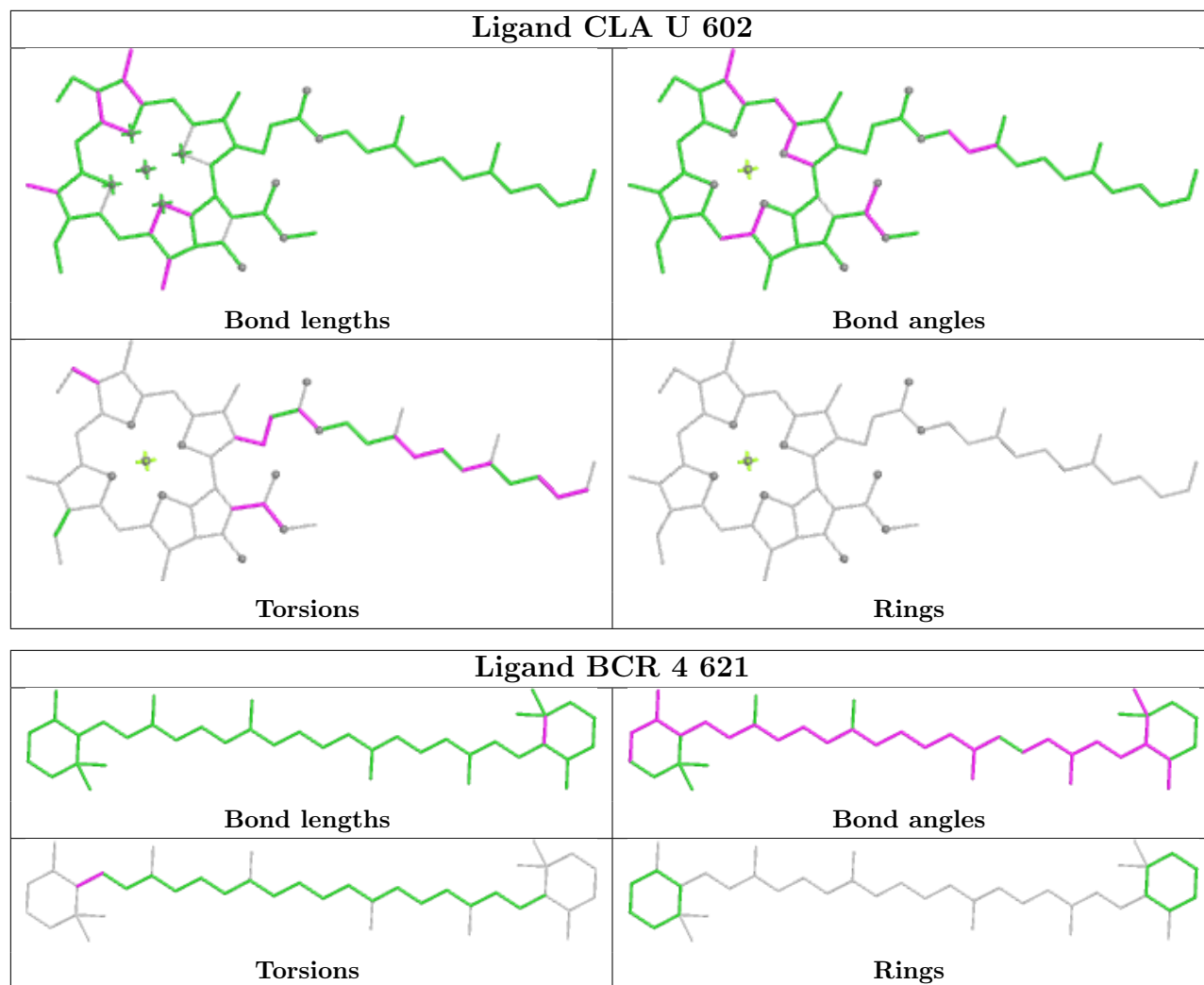
Torsions



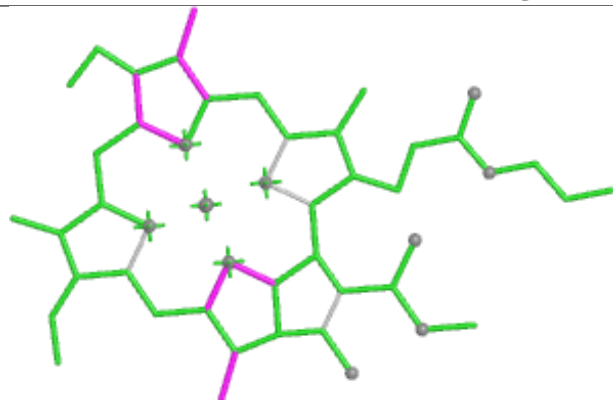
Rings



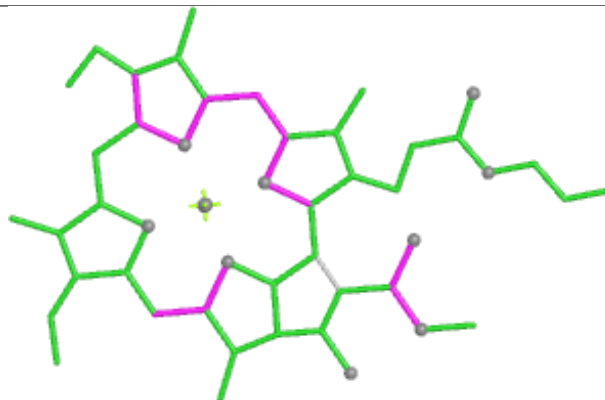




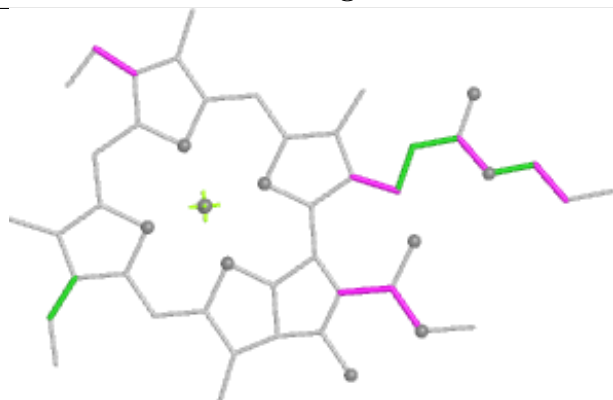
## Ligand CLA Z 614



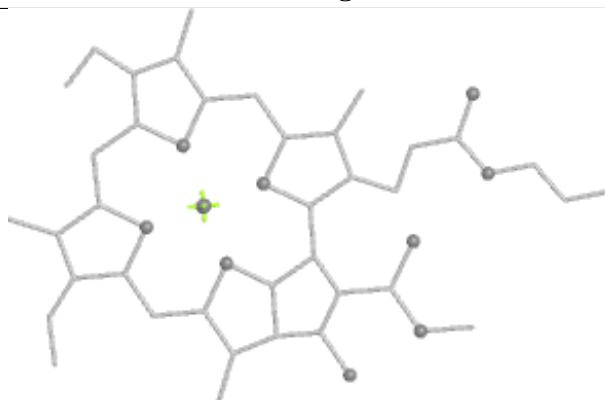
Bond lengths



Bond angles

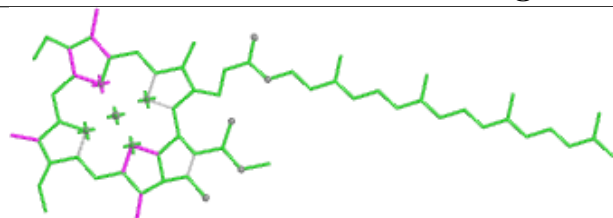


Torsions

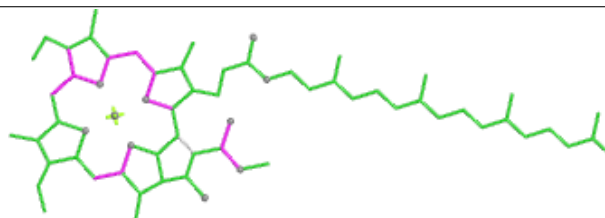


Rings

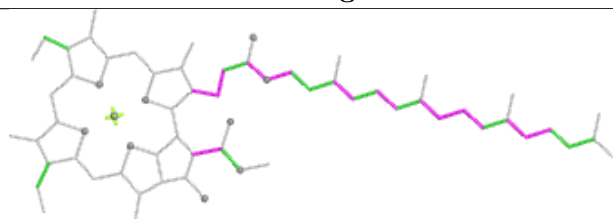
## Ligand CLA B 828



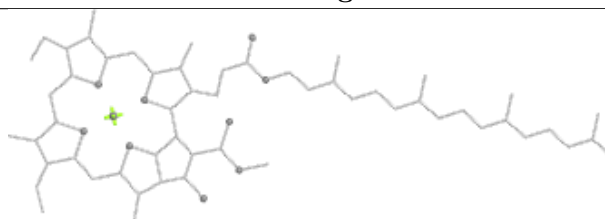
Bond lengths



Bond angles

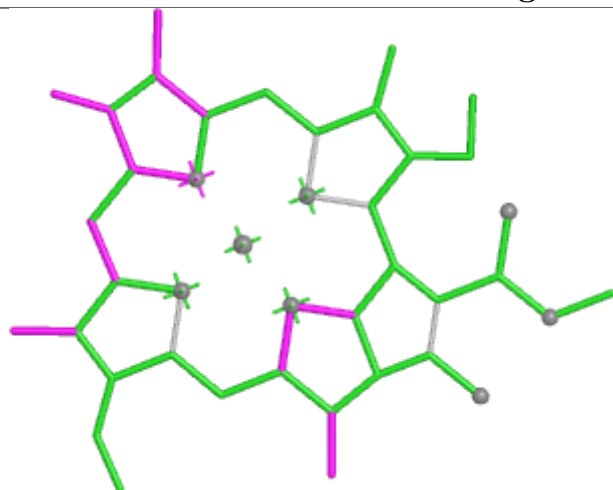


Torsions

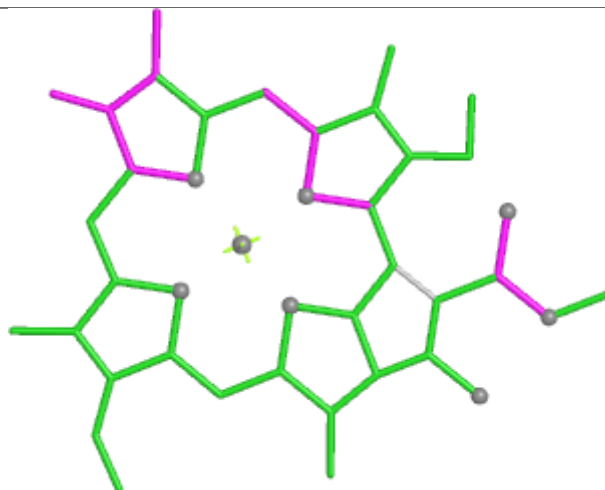


Rings

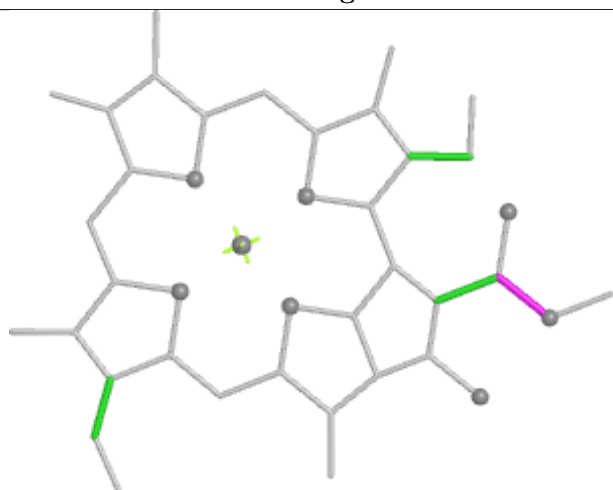
## Ligand CLA 8 607



Bond lengths



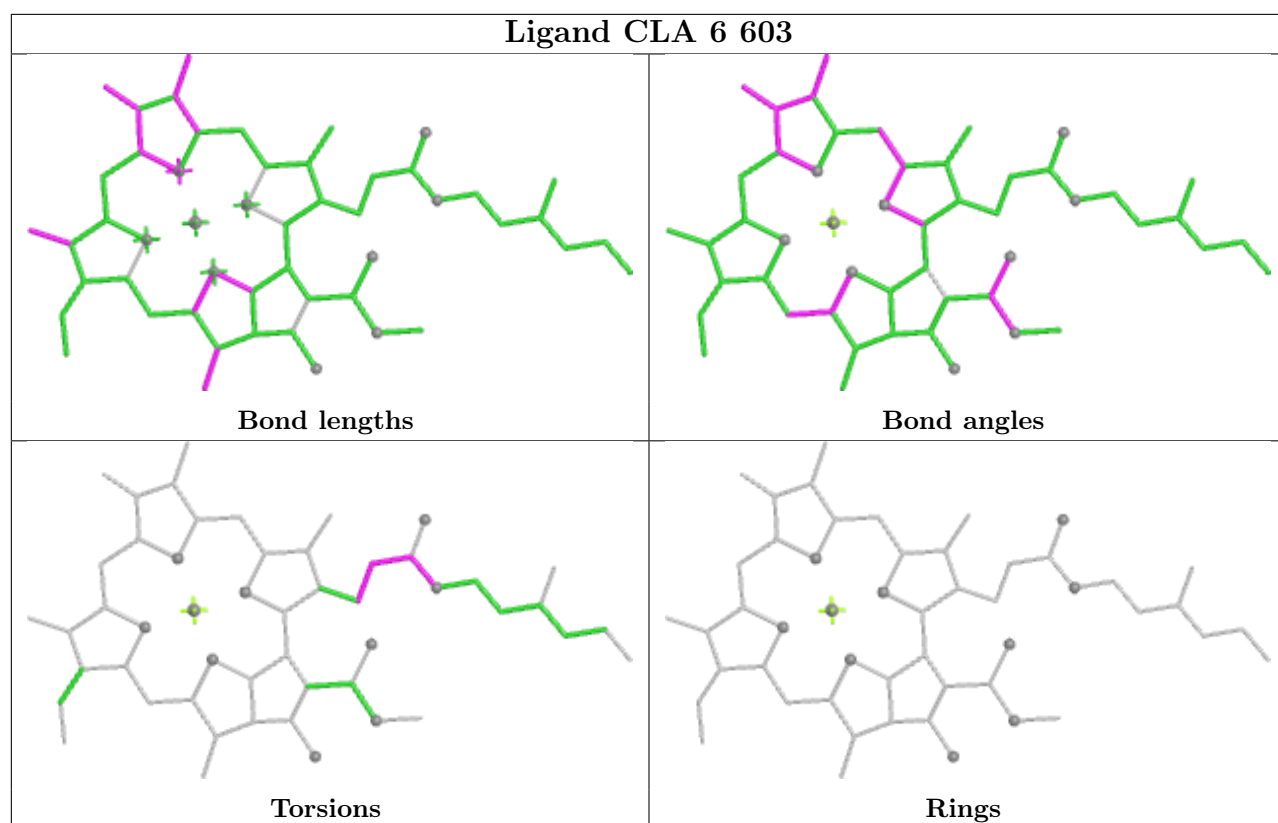
Bond angles



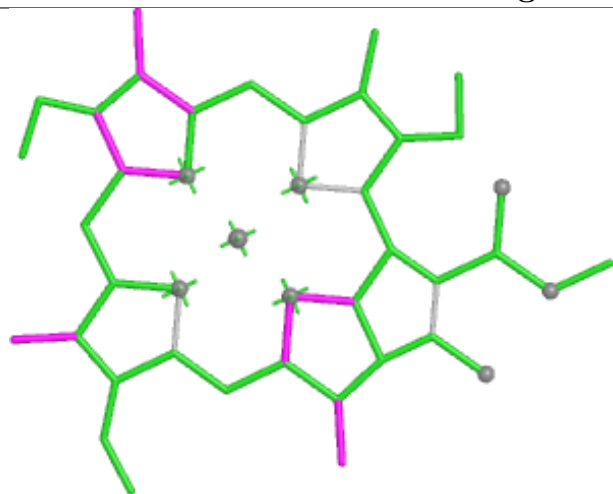
Torsions



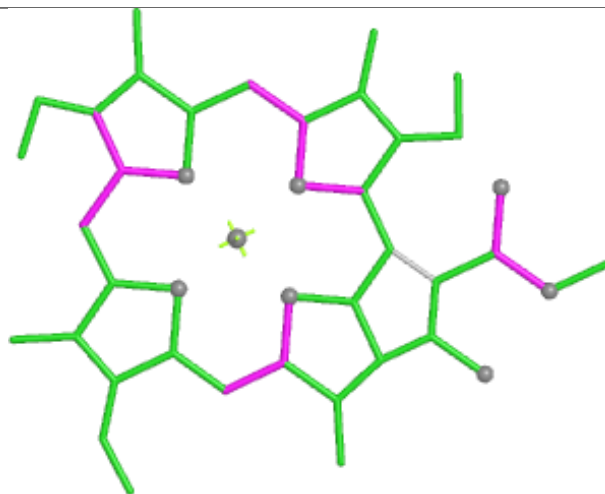
Rings



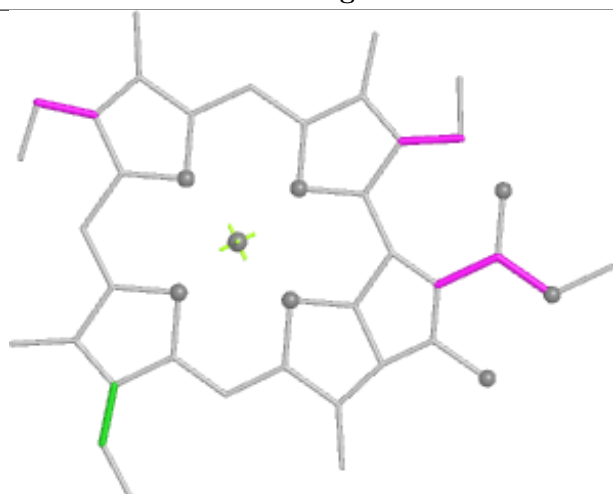
## Ligand CLA J 101



Bond lengths



Bond angles

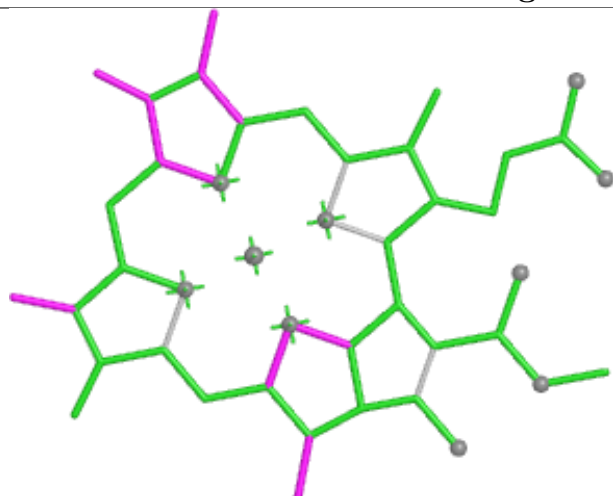


Torsions

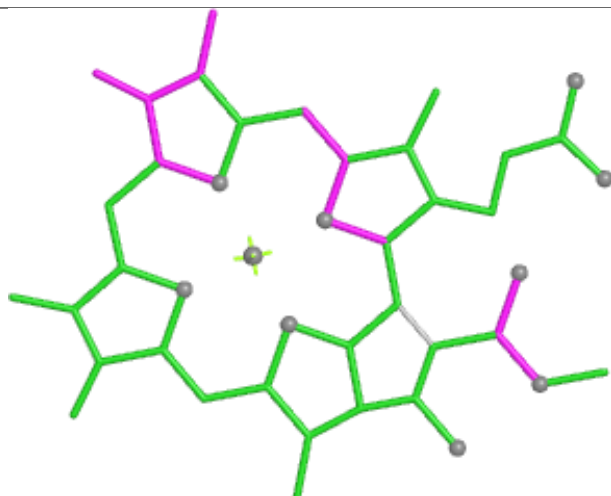


Rings

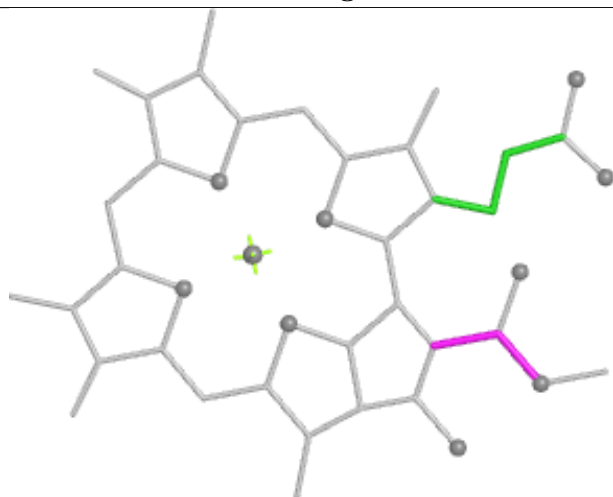
## Ligand CLA 2 616



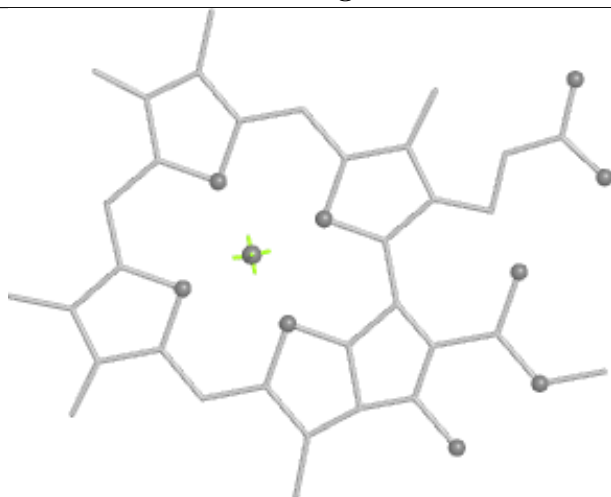
Bond lengths



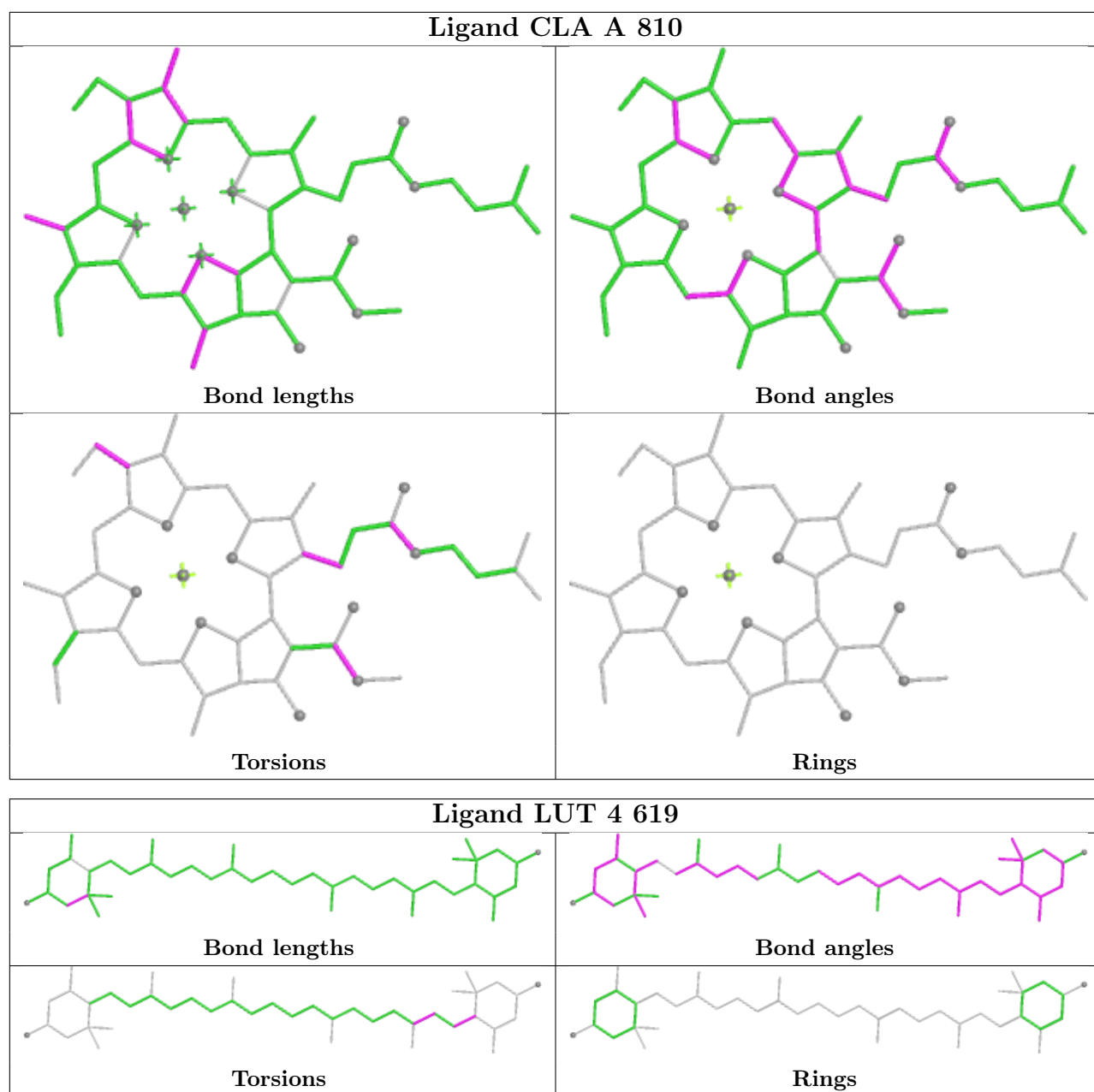
Bond angles



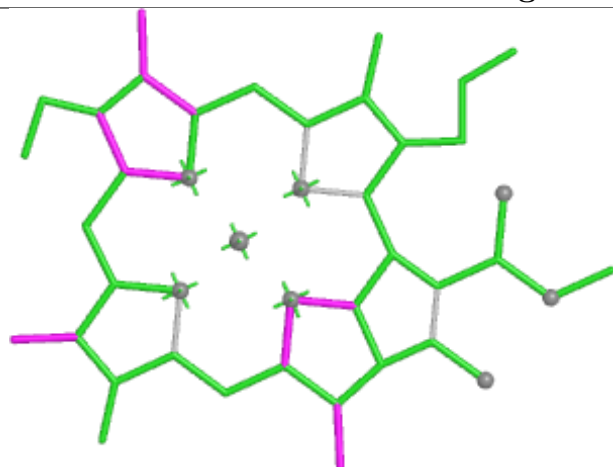
Torsions



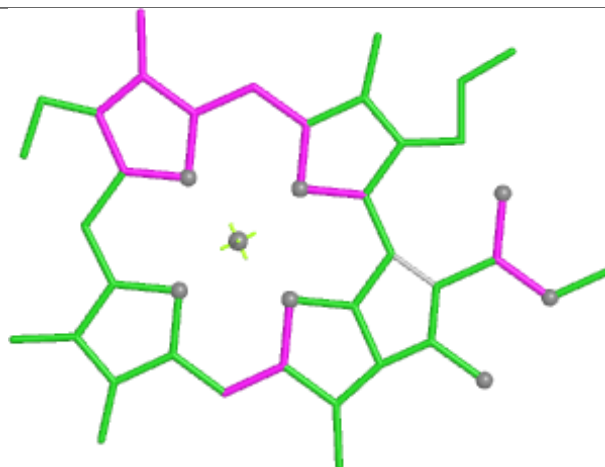
Rings



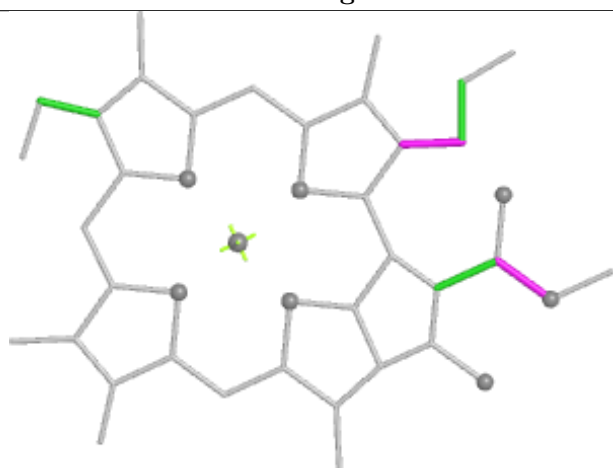
## Ligand CLA 2 604



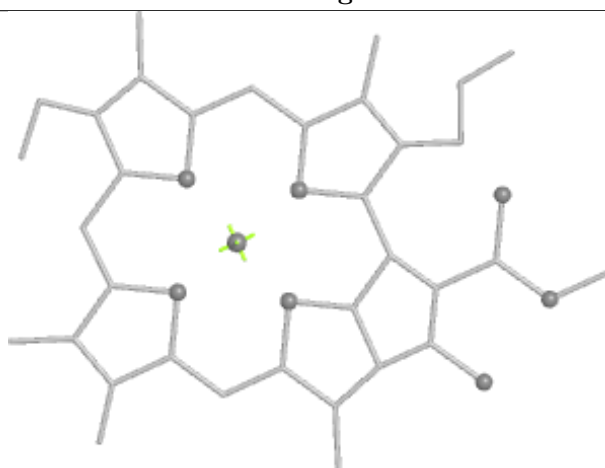
Bond lengths



Bond angles



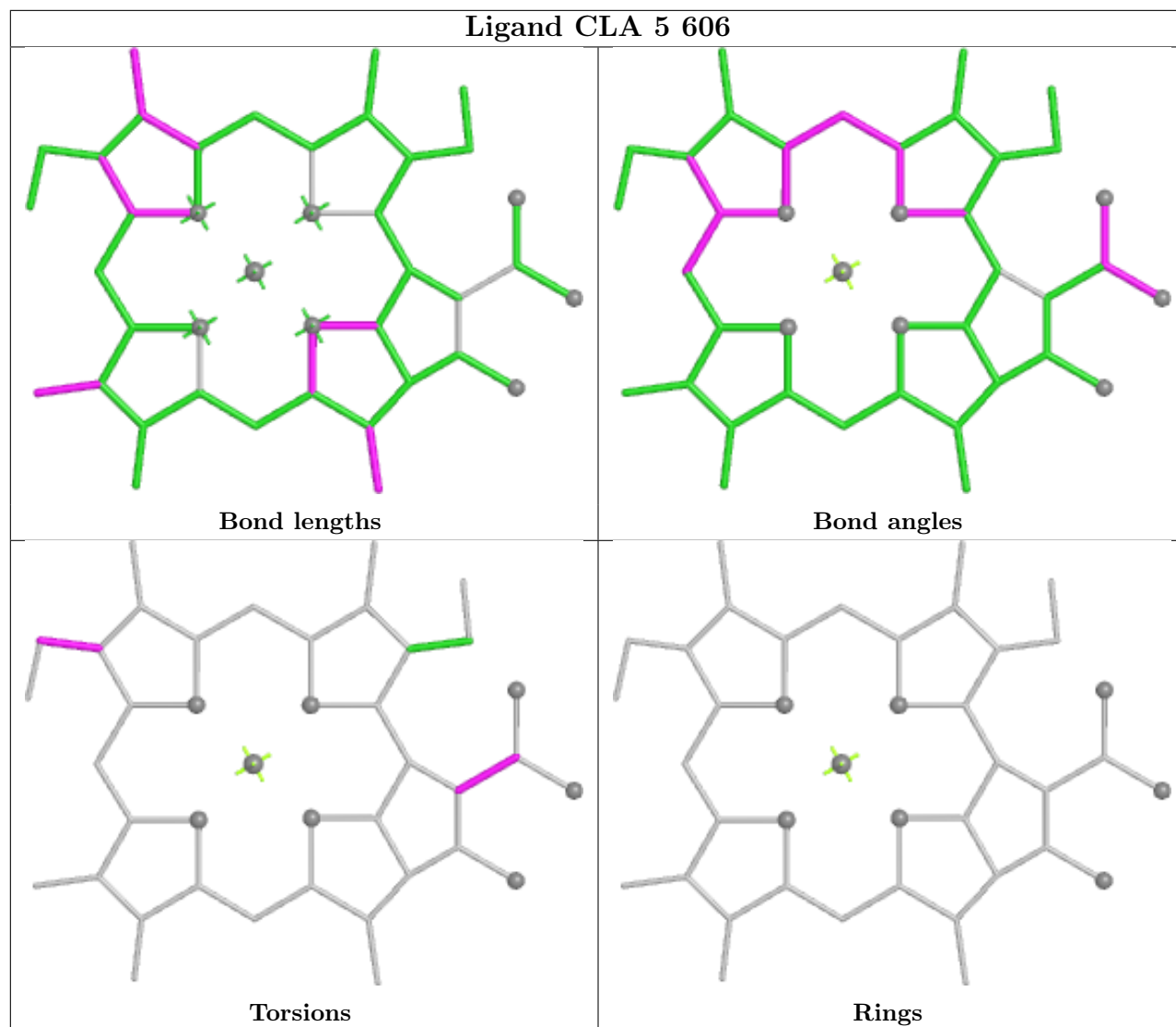
Torsions



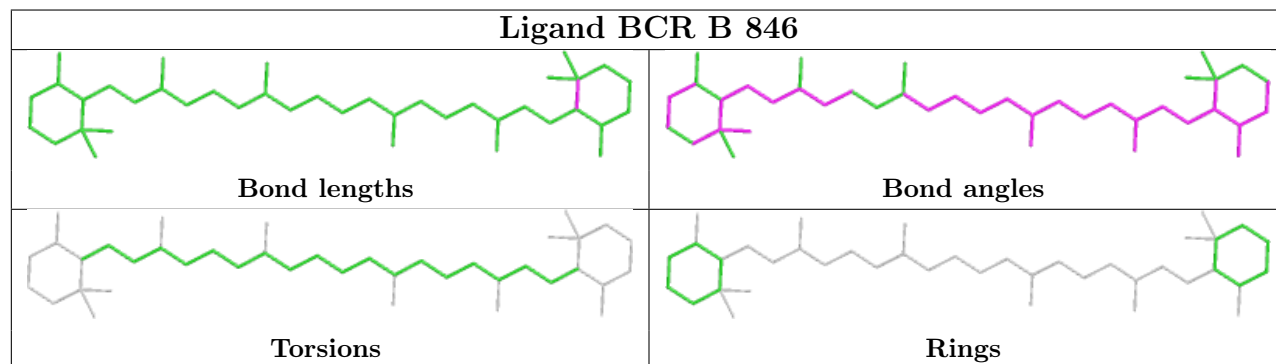
Rings

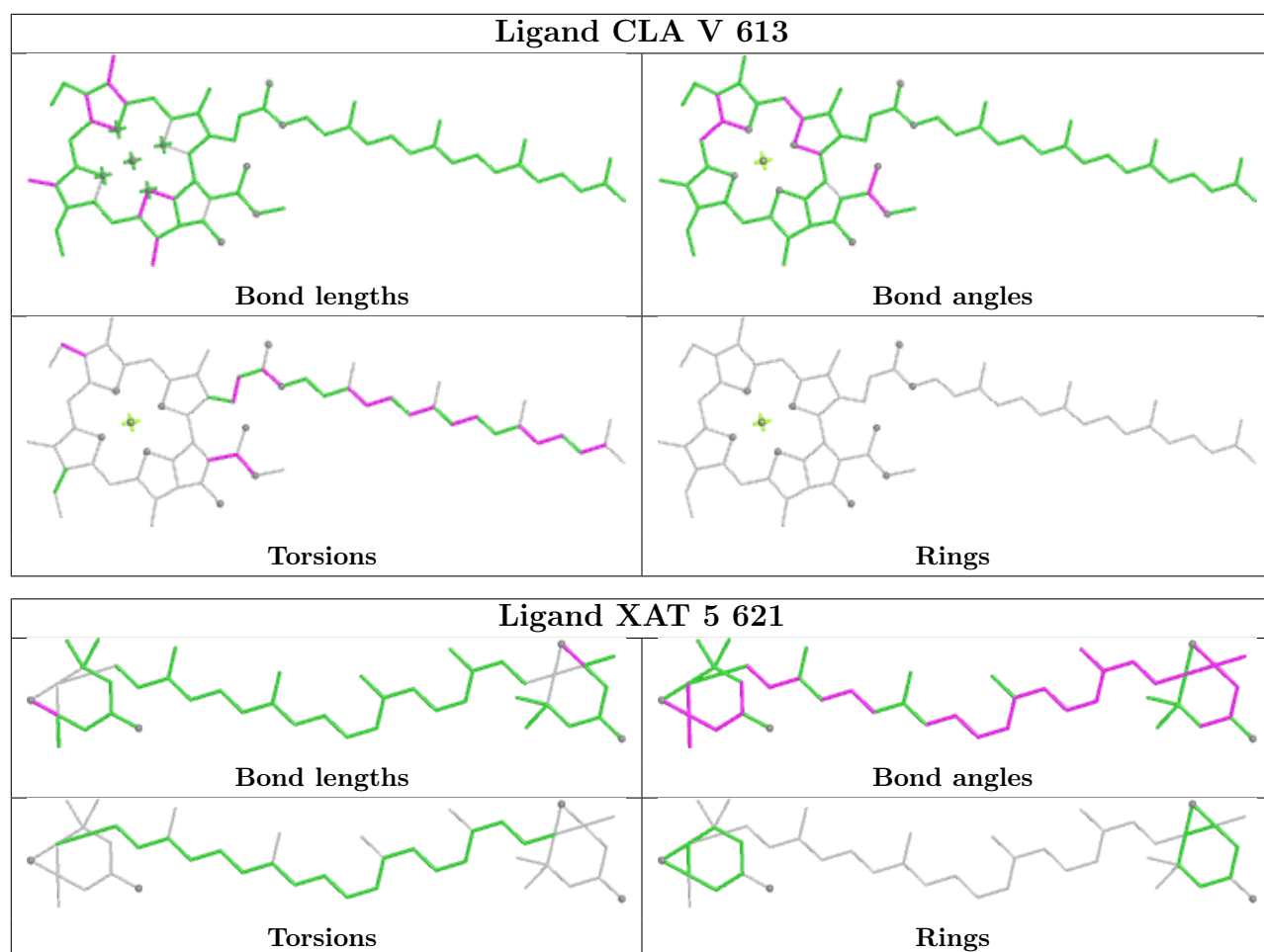


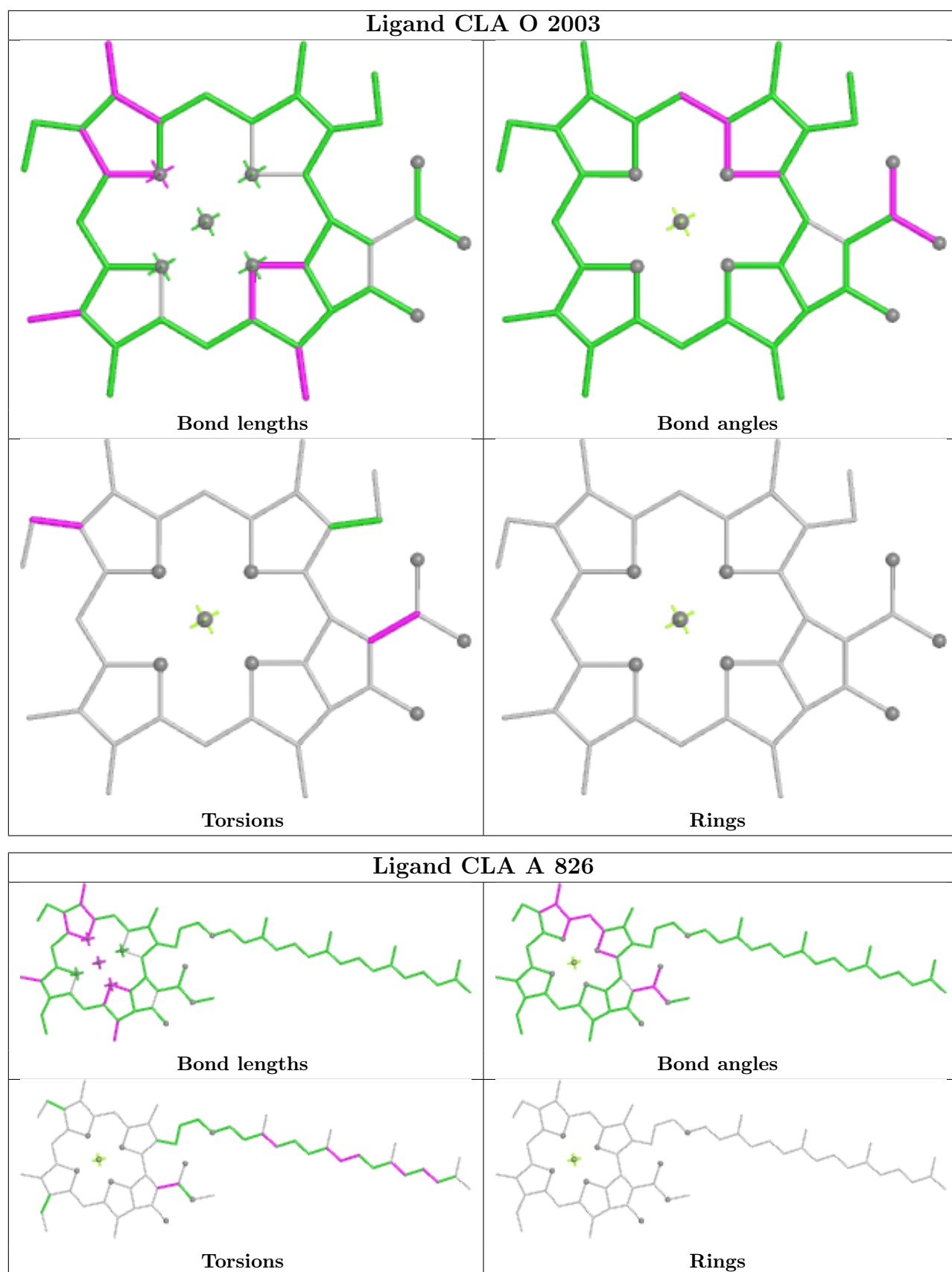
## Ligand CLA 5 606



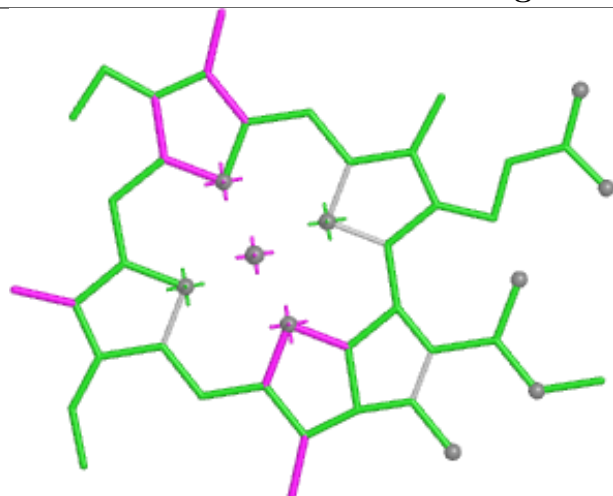
## Ligand BCR B 846



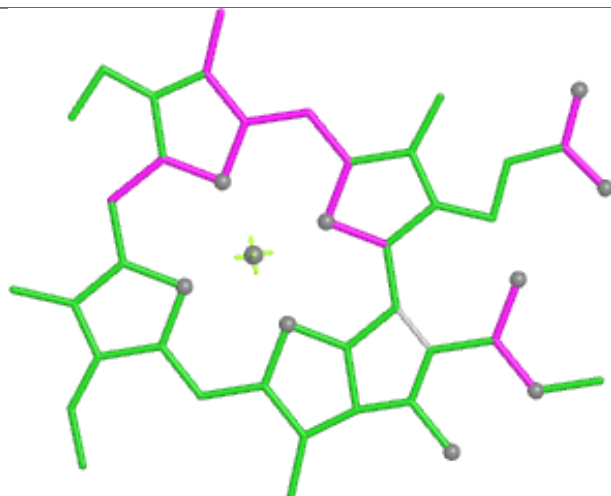




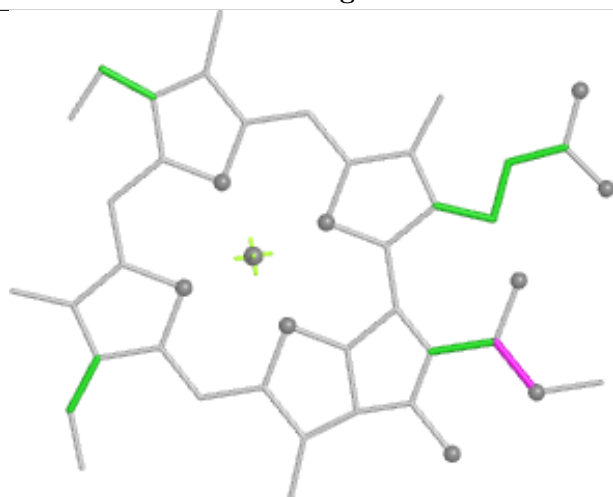
## Ligand CLA B 835



Bond lengths



Bond angles

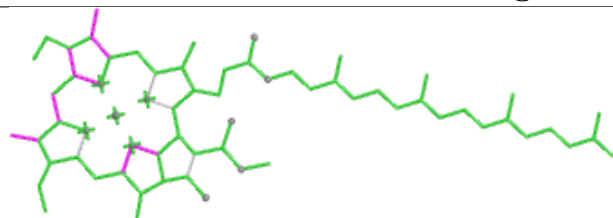


Torsions

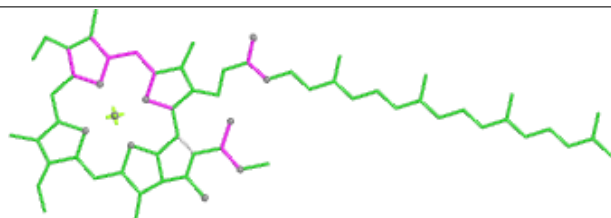


Rings

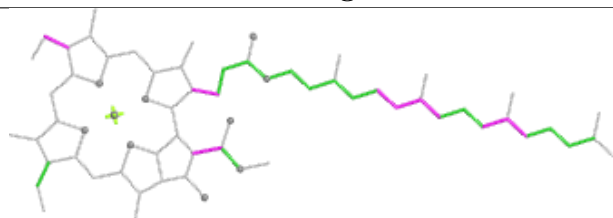
## Ligand CLA X 610



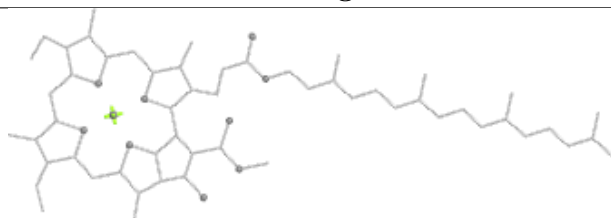
Bond lengths



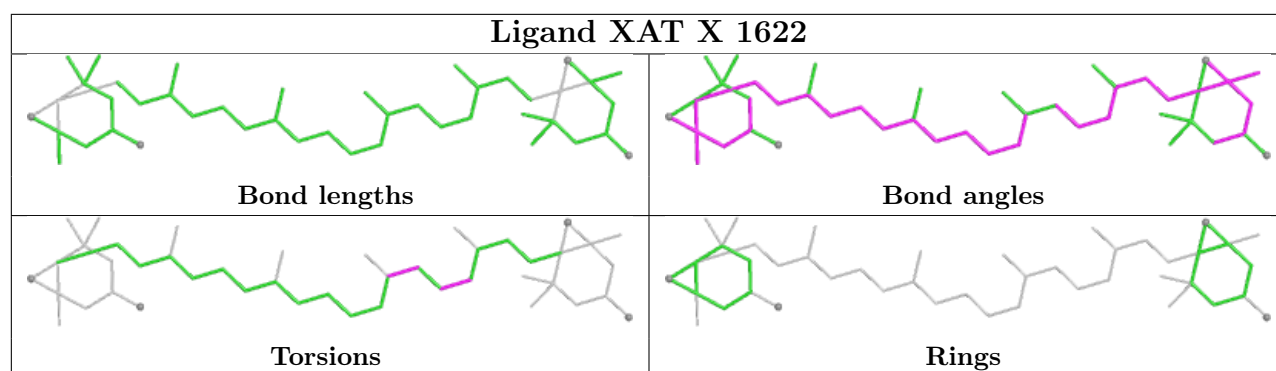
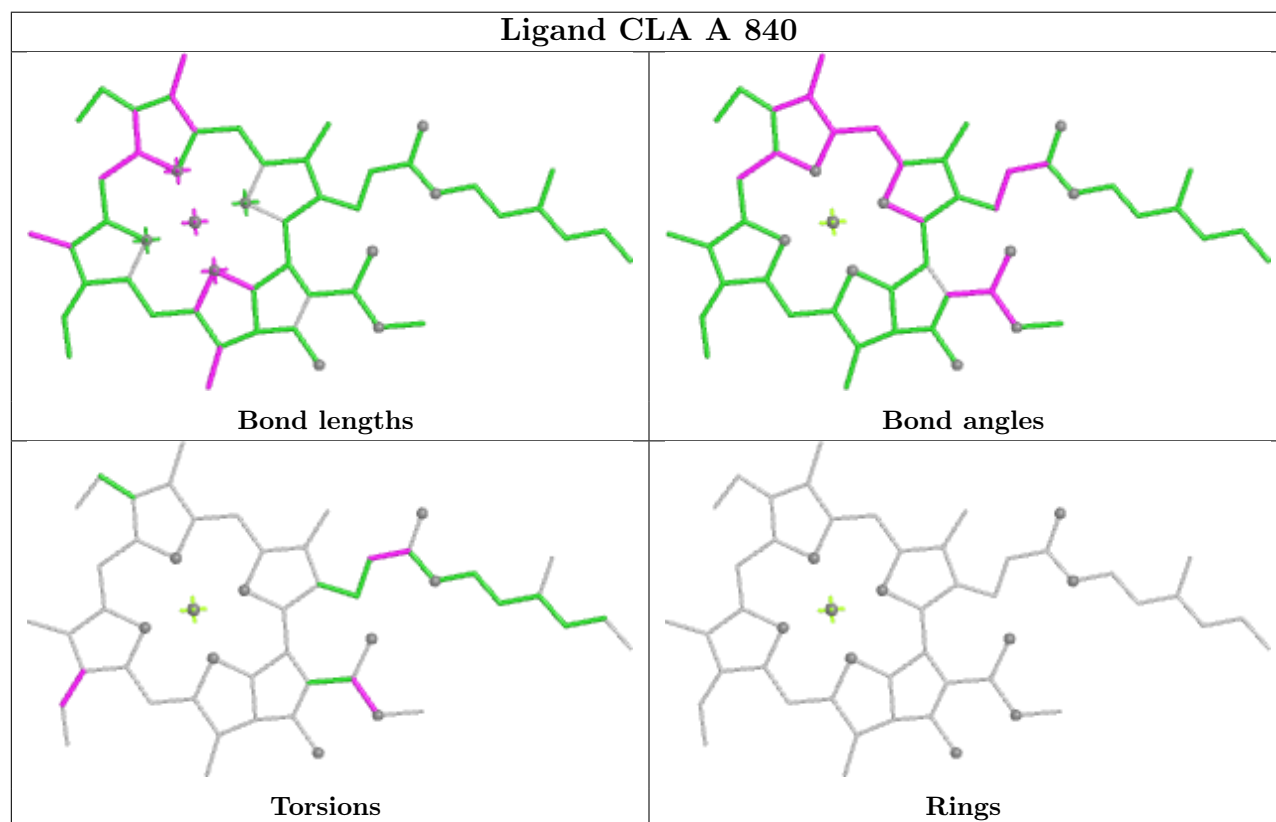
Bond angles

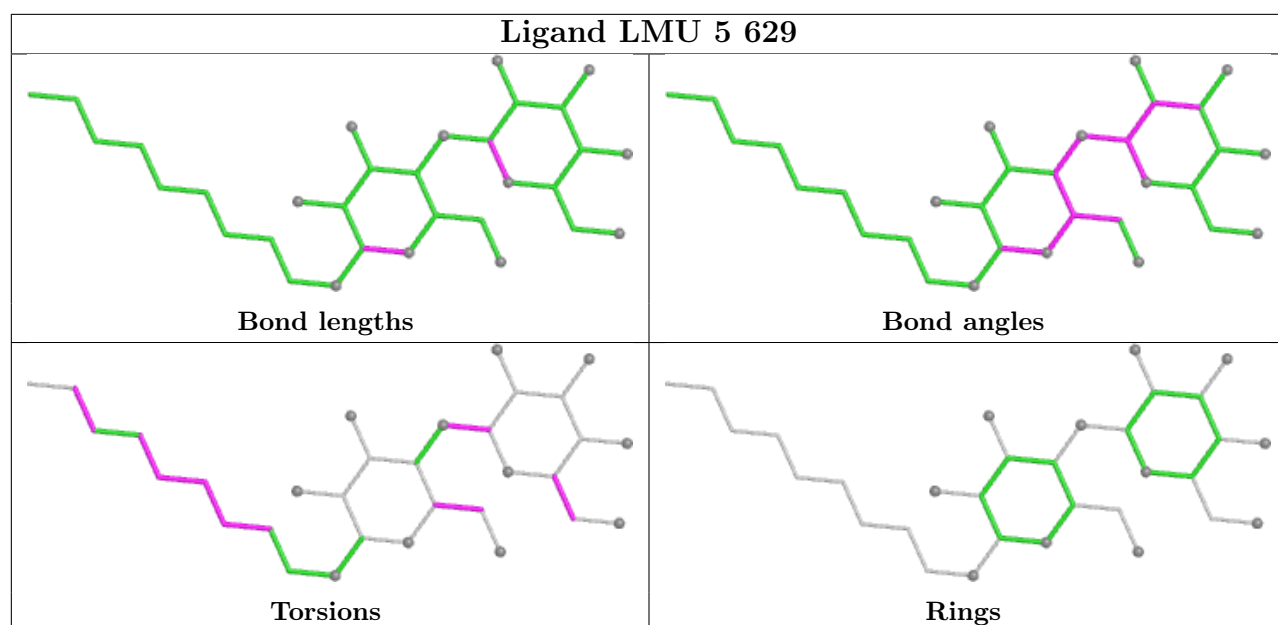
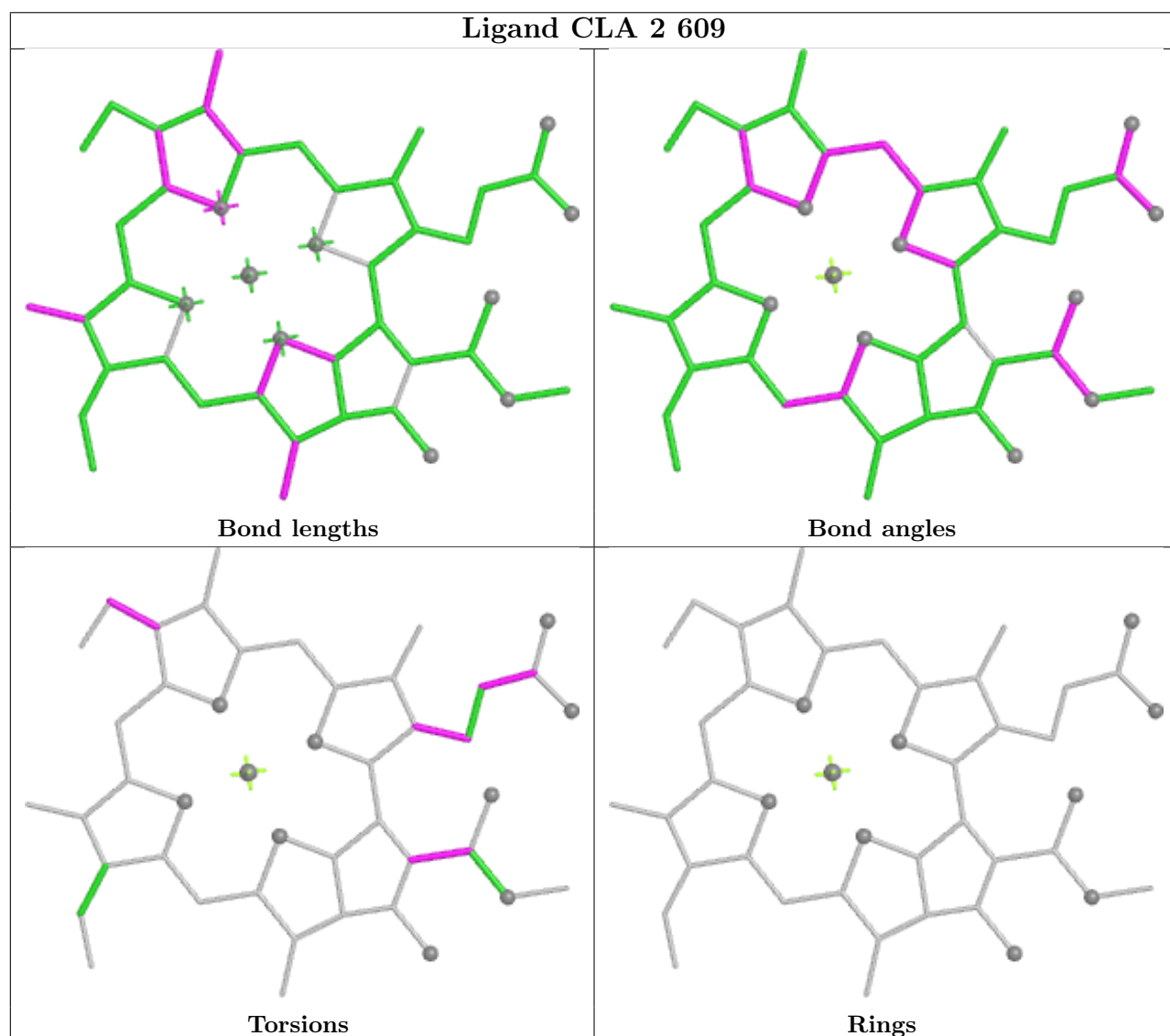


Torsions

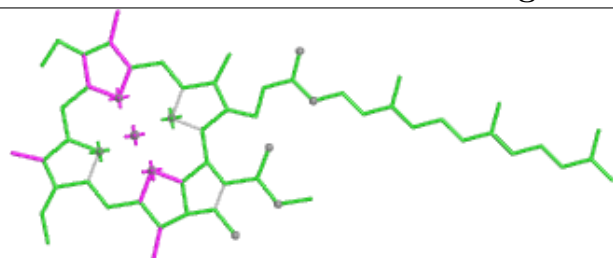


Rings

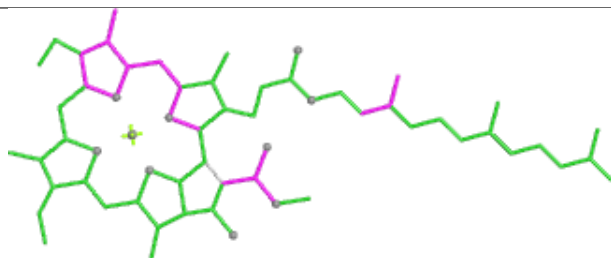




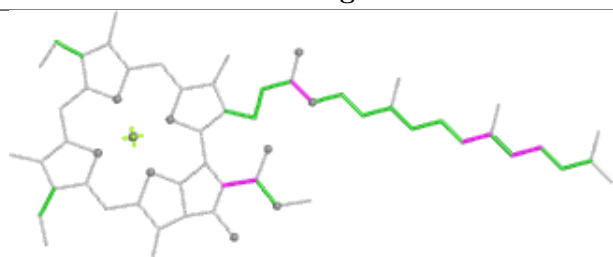
## Ligand CLA 7 601



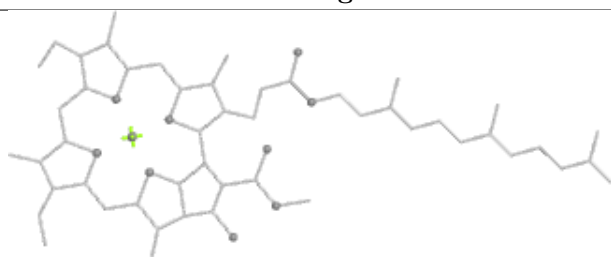
Bond lengths



Bond angles

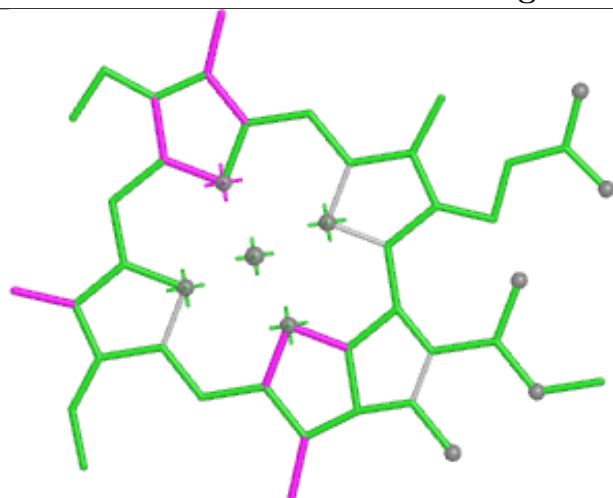


Torsions

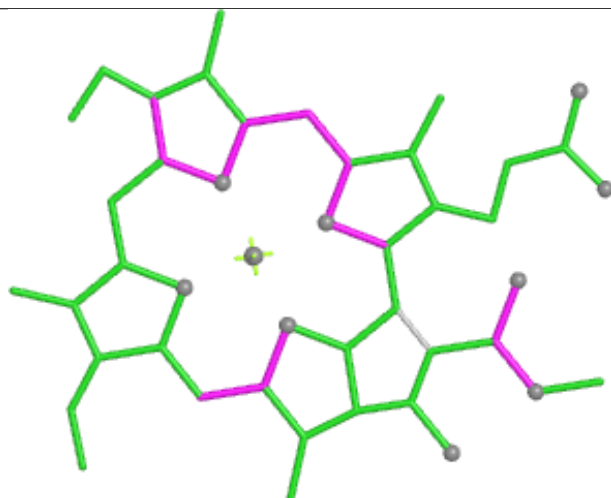


Rings

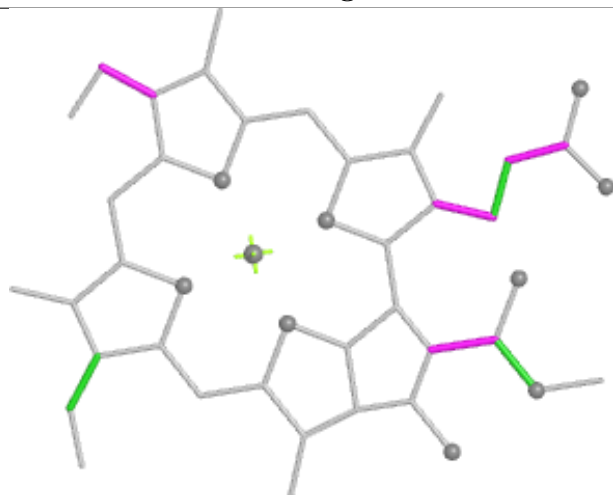
## Ligand CLA 6 609



Bond lengths



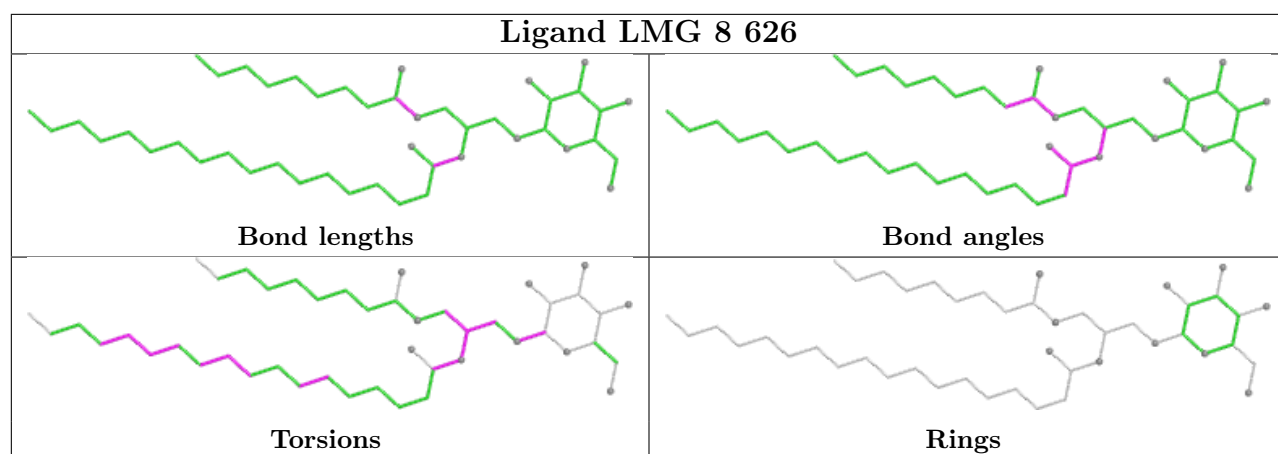
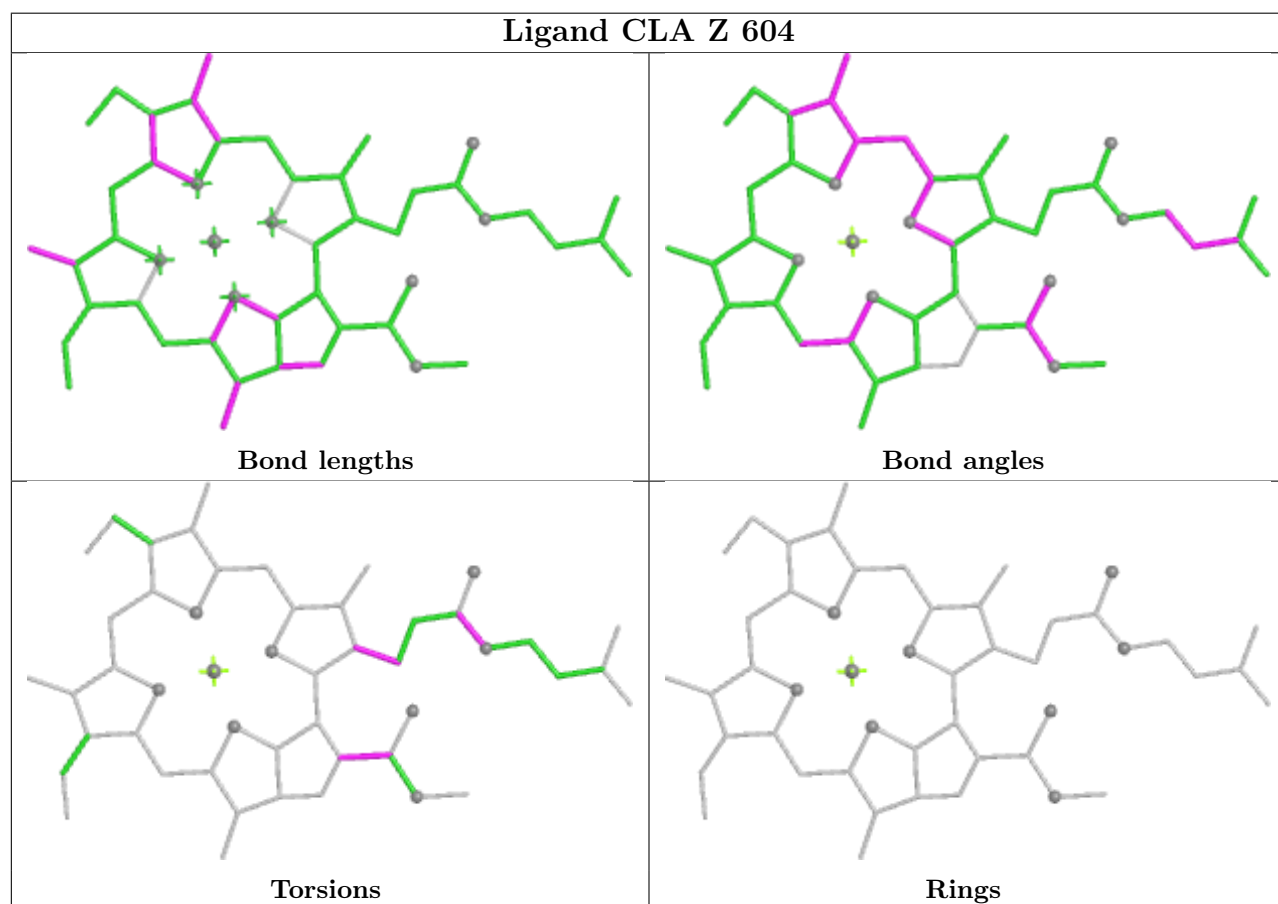
Bond angles



Torsions

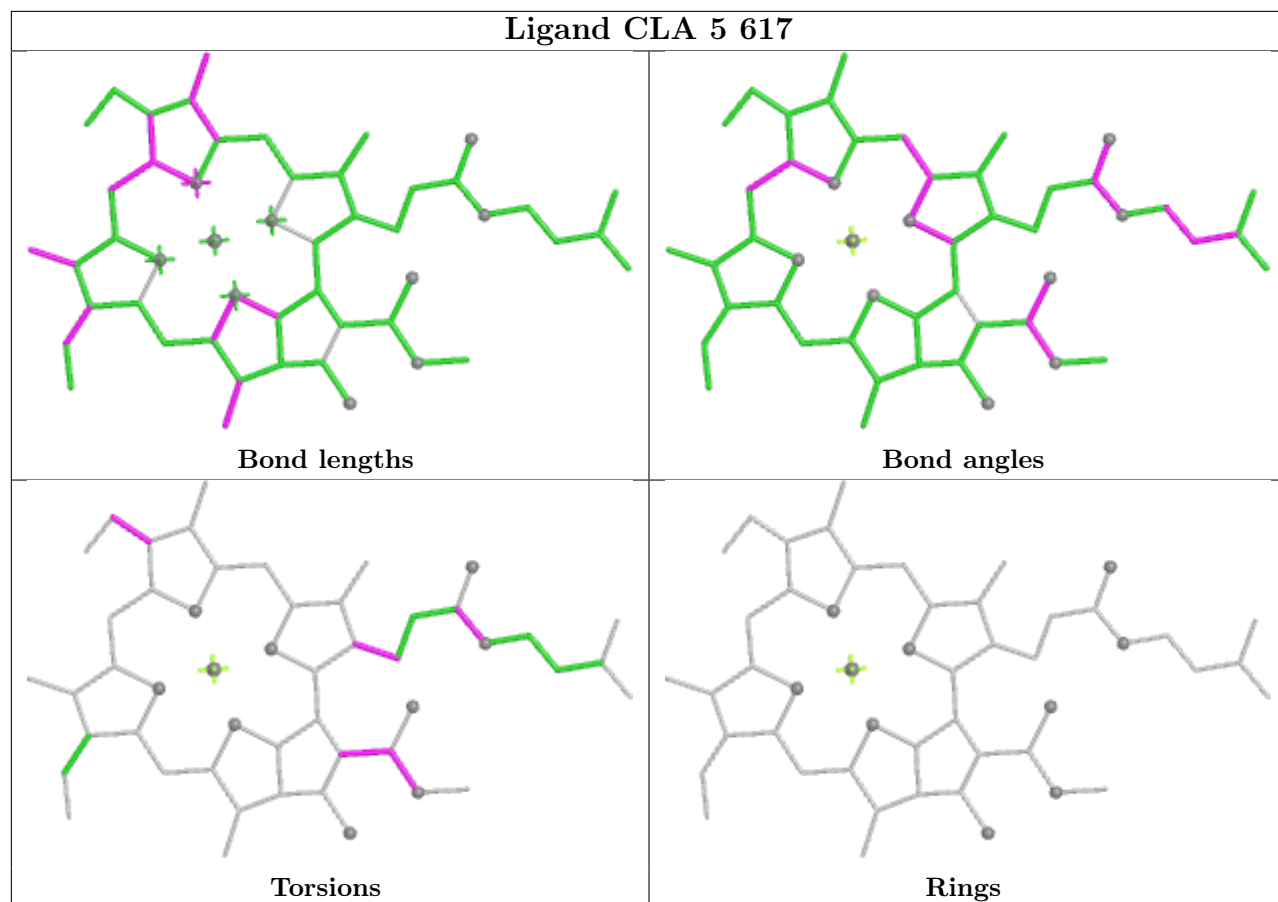


Rings

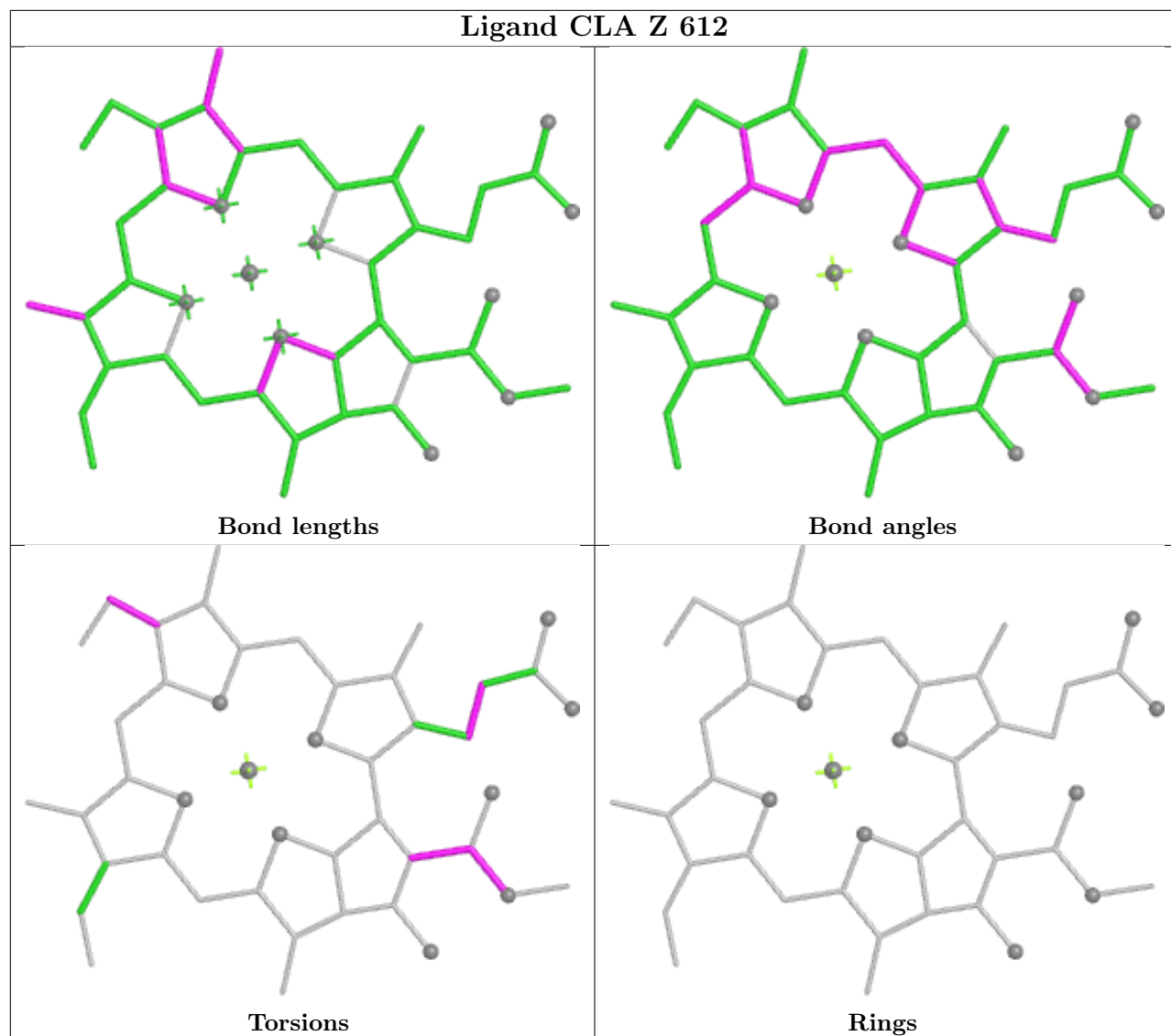




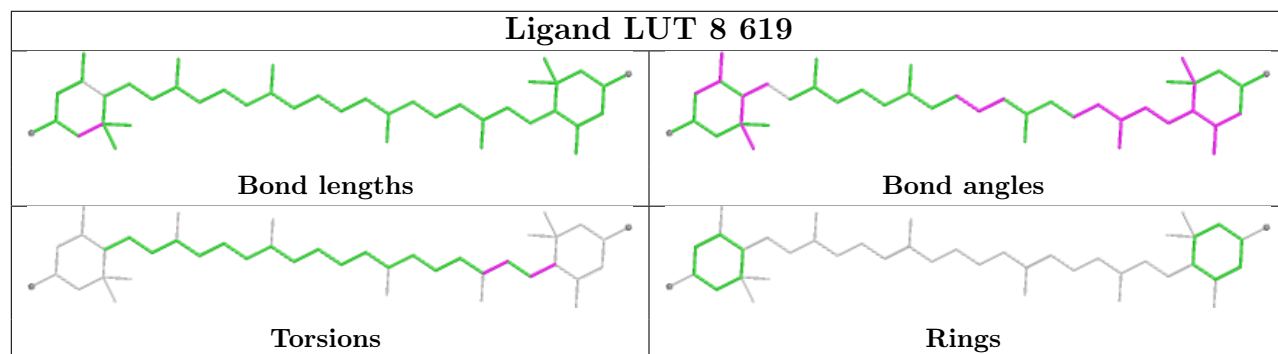
## Ligand CLA 5 617

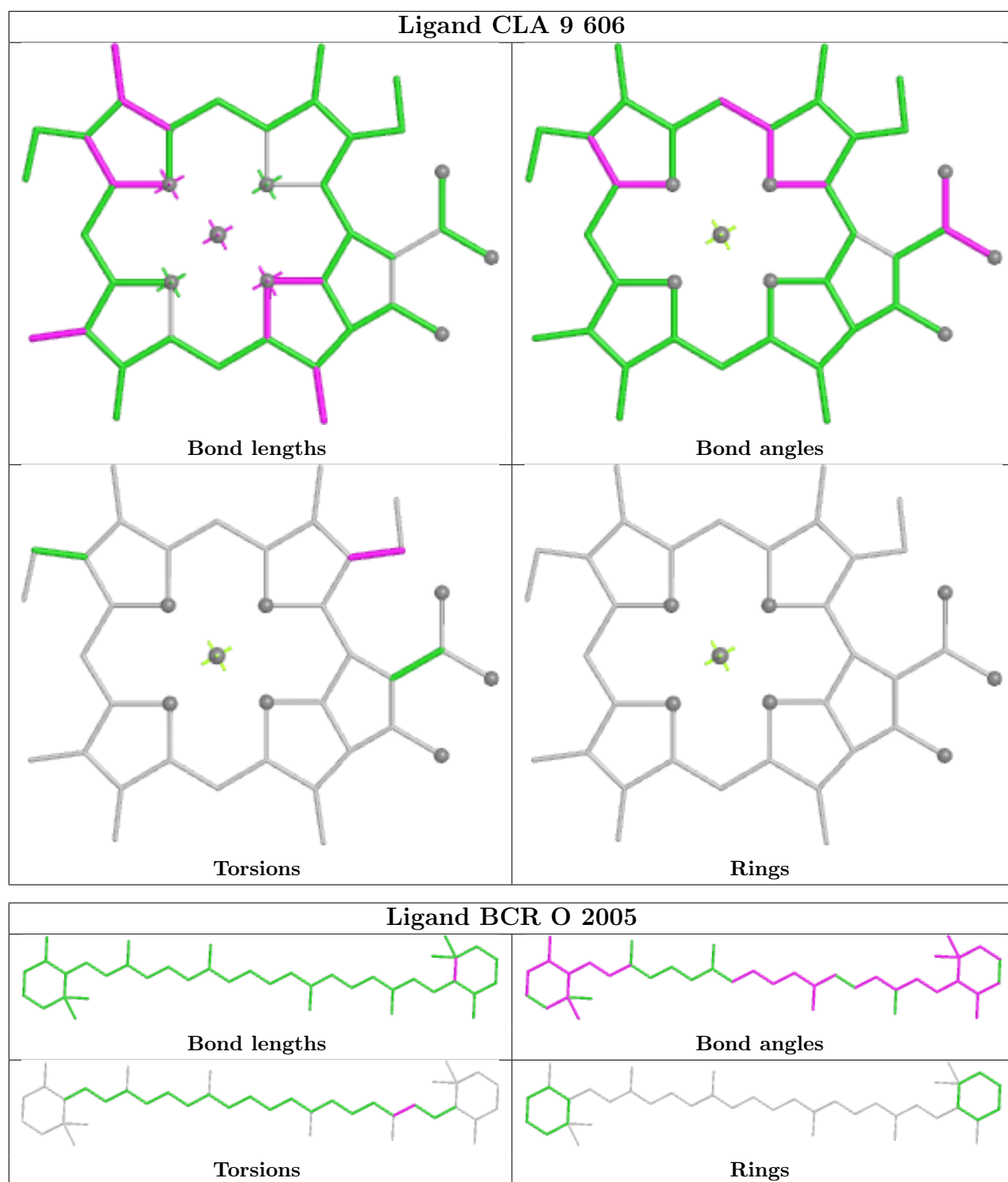


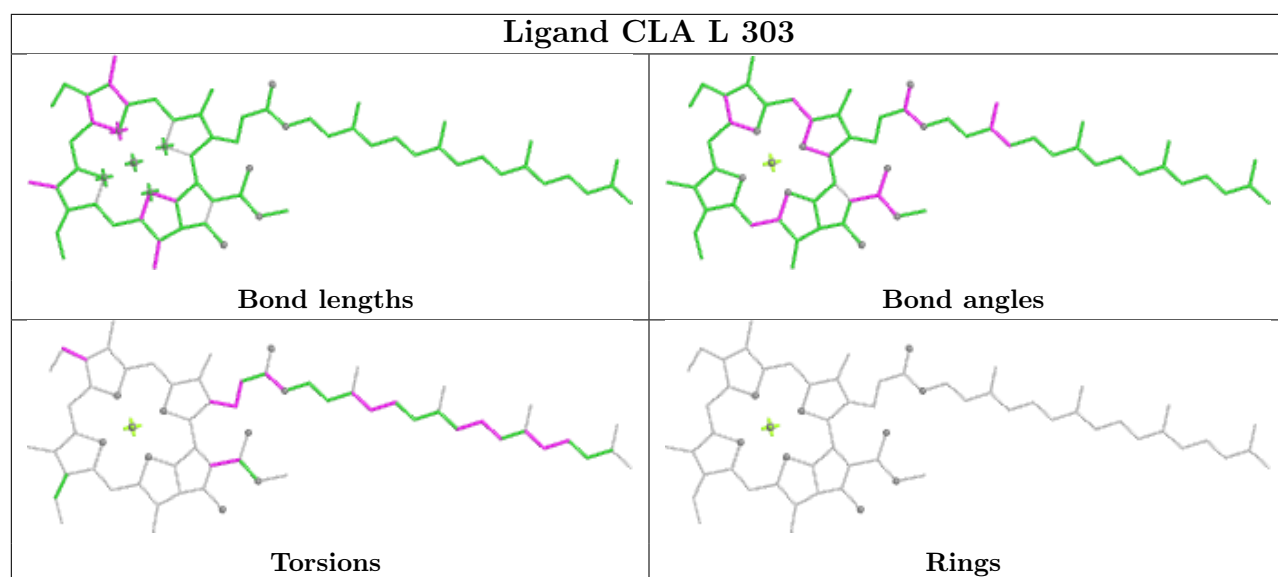
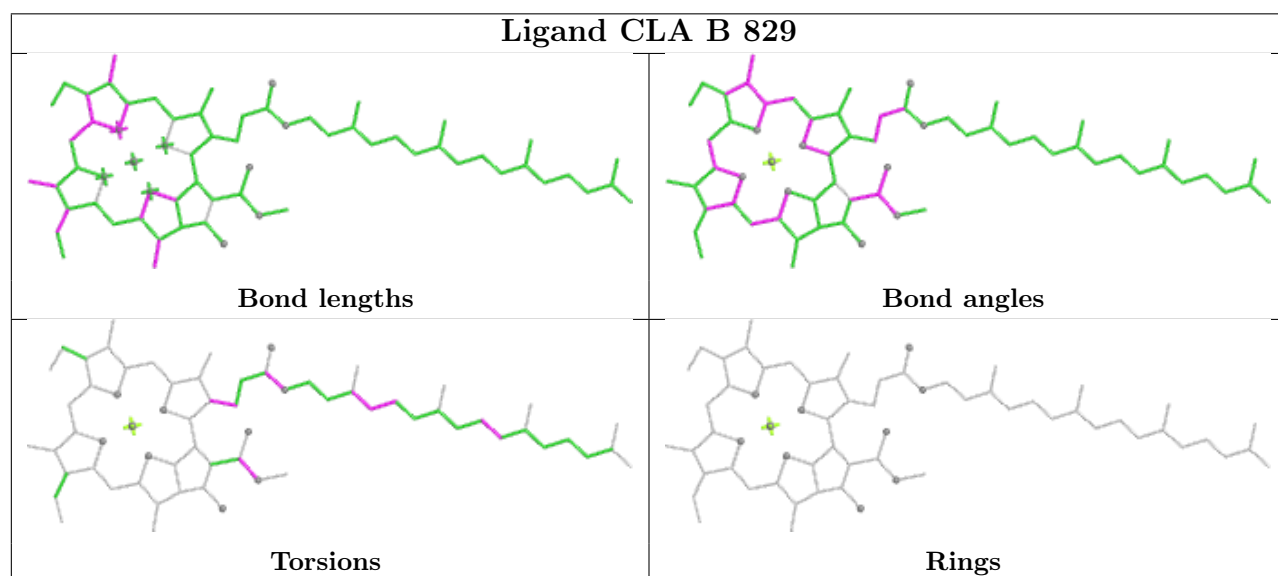
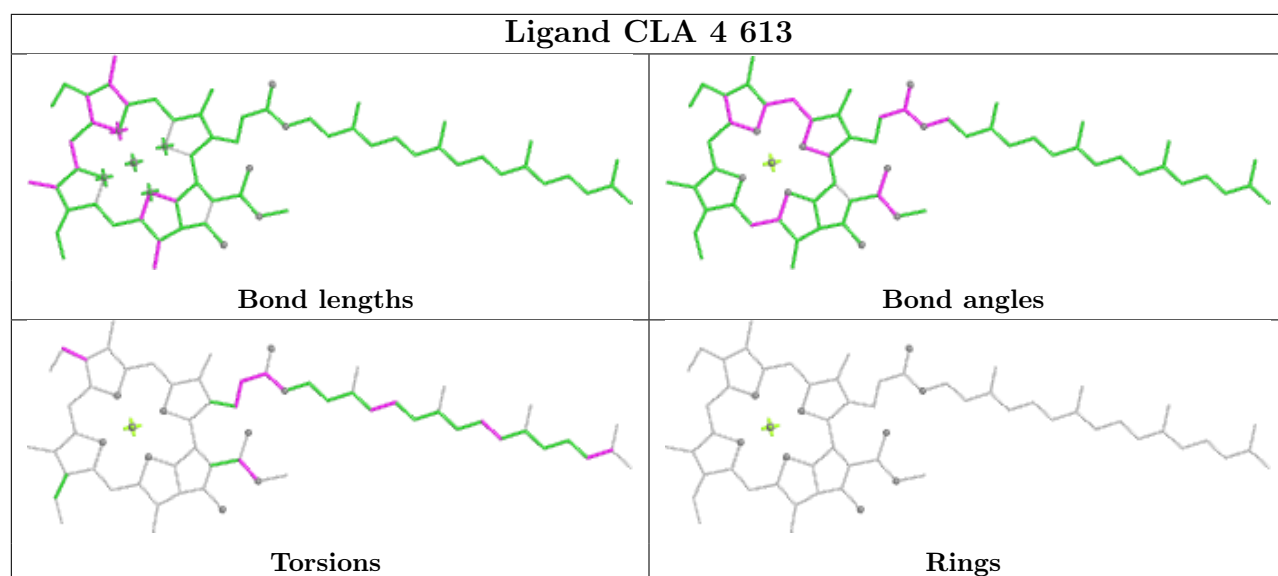
## Ligand CLA Z 612

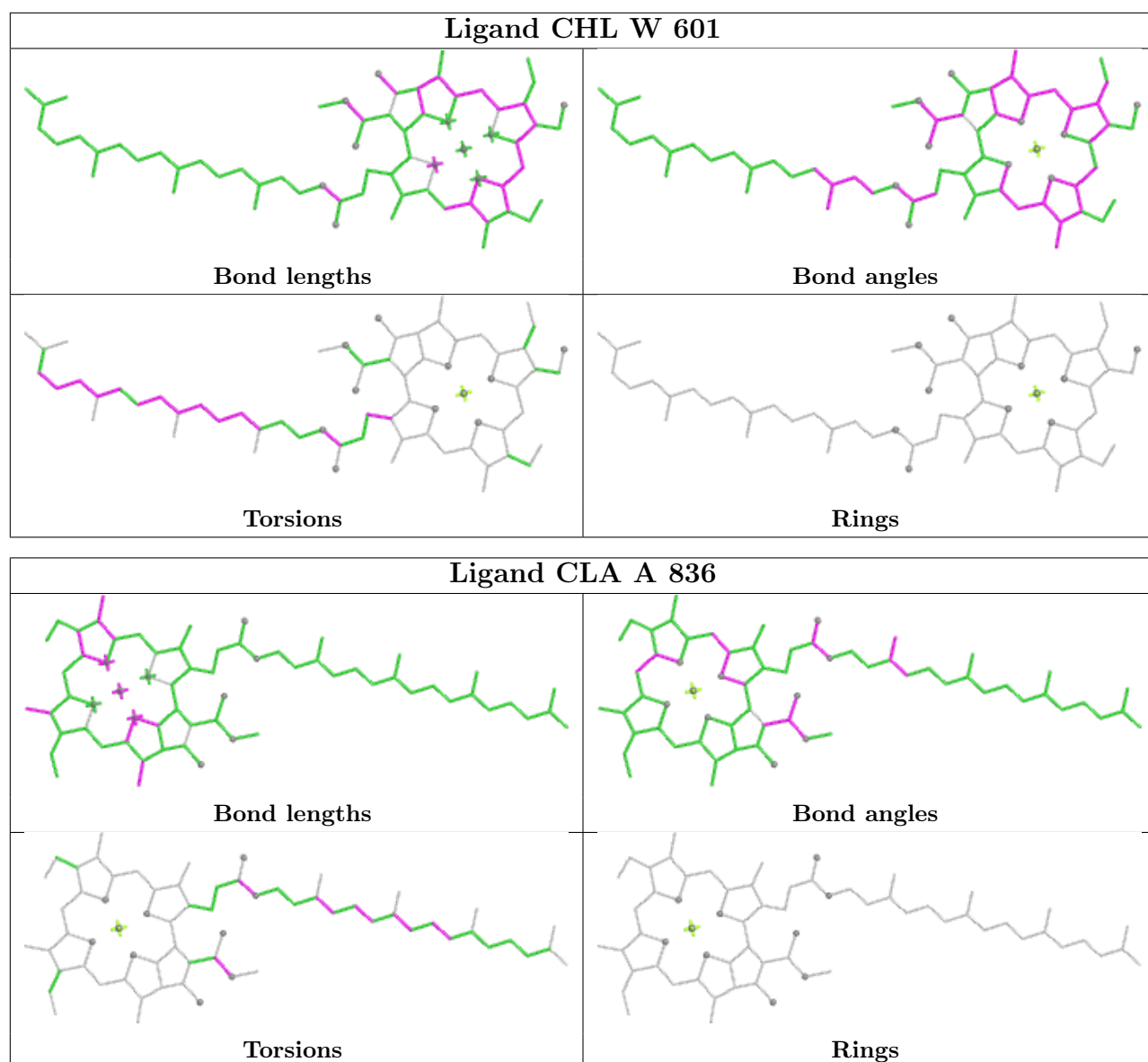


## Ligand LUT 8 619

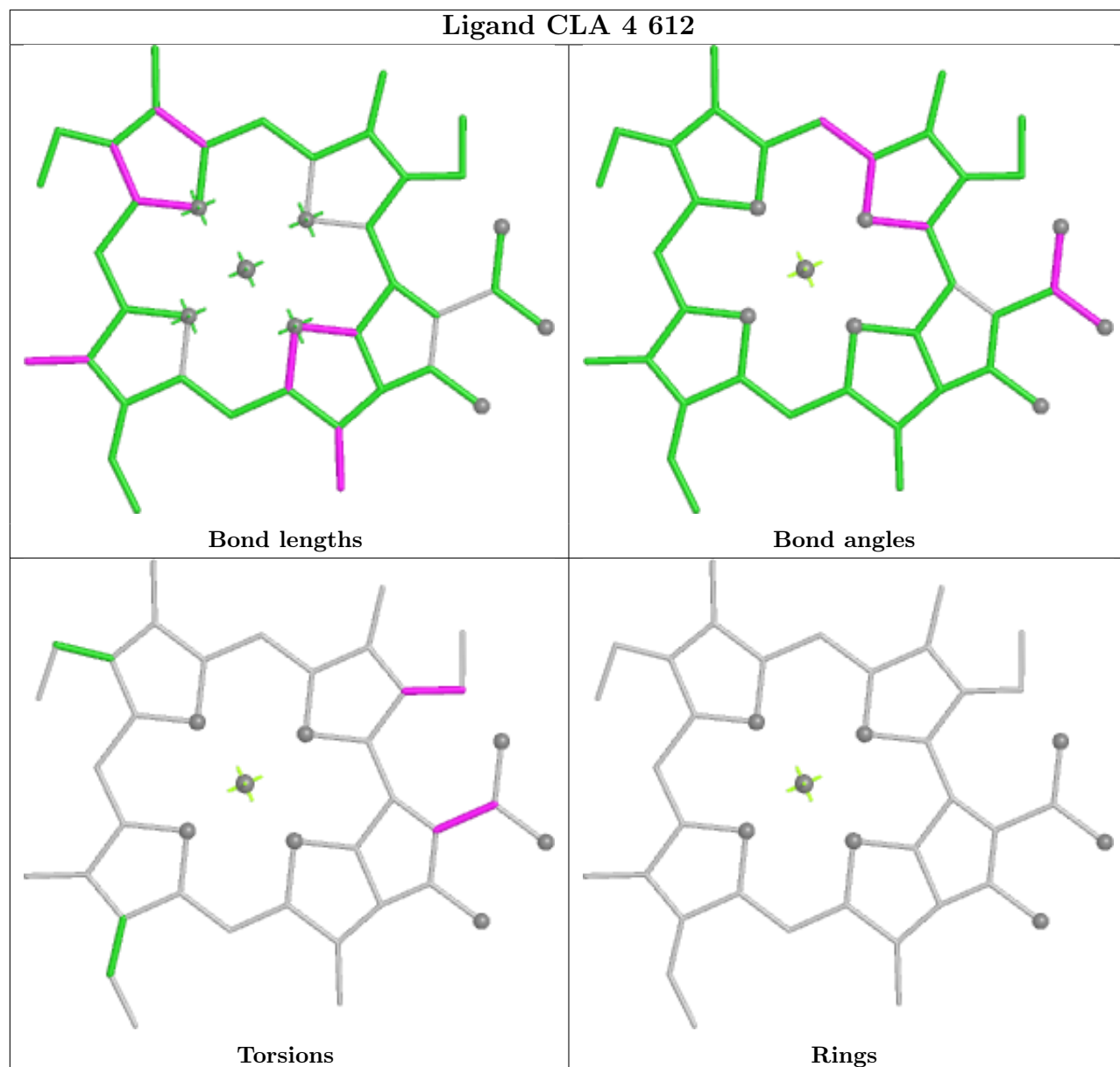




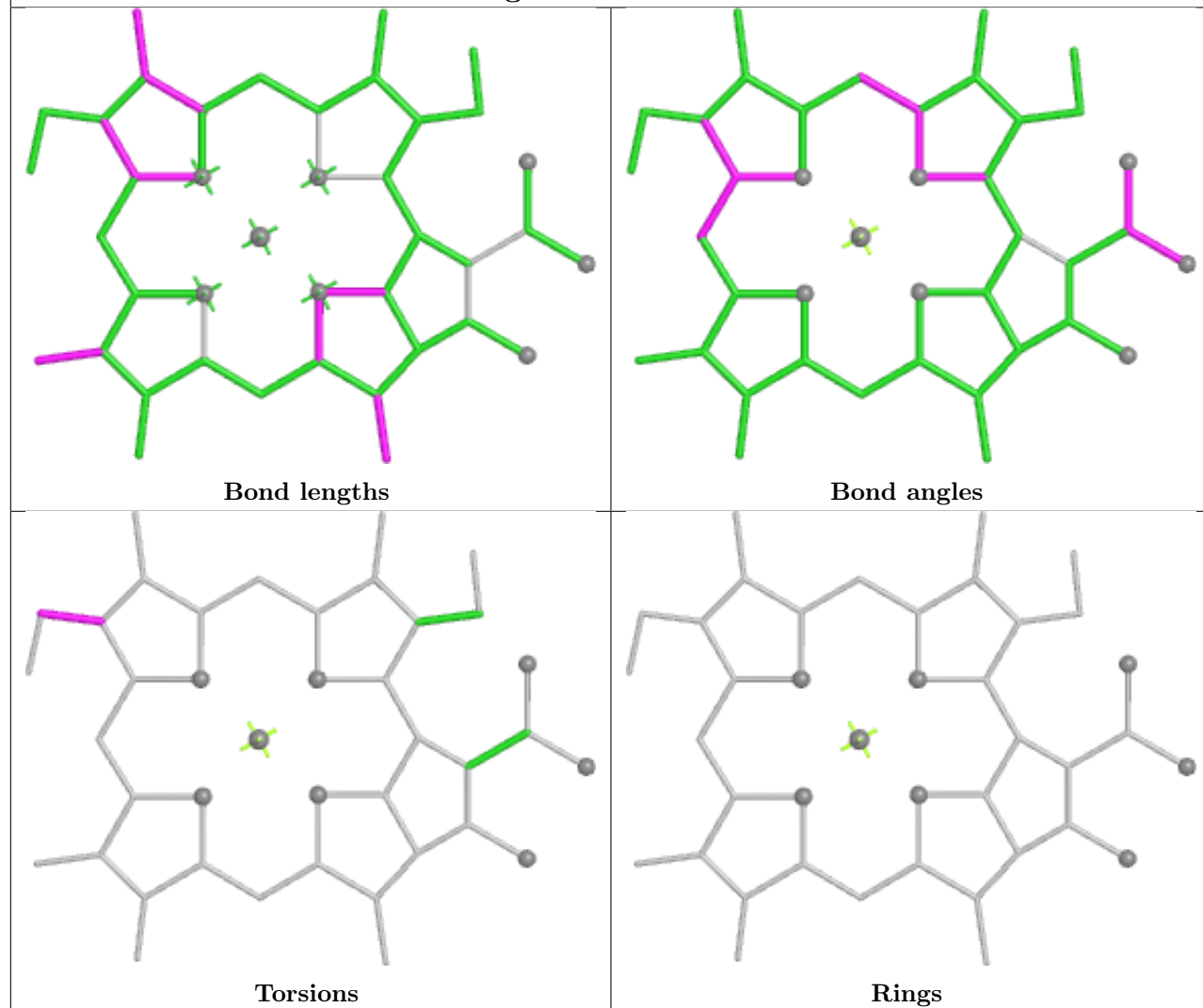




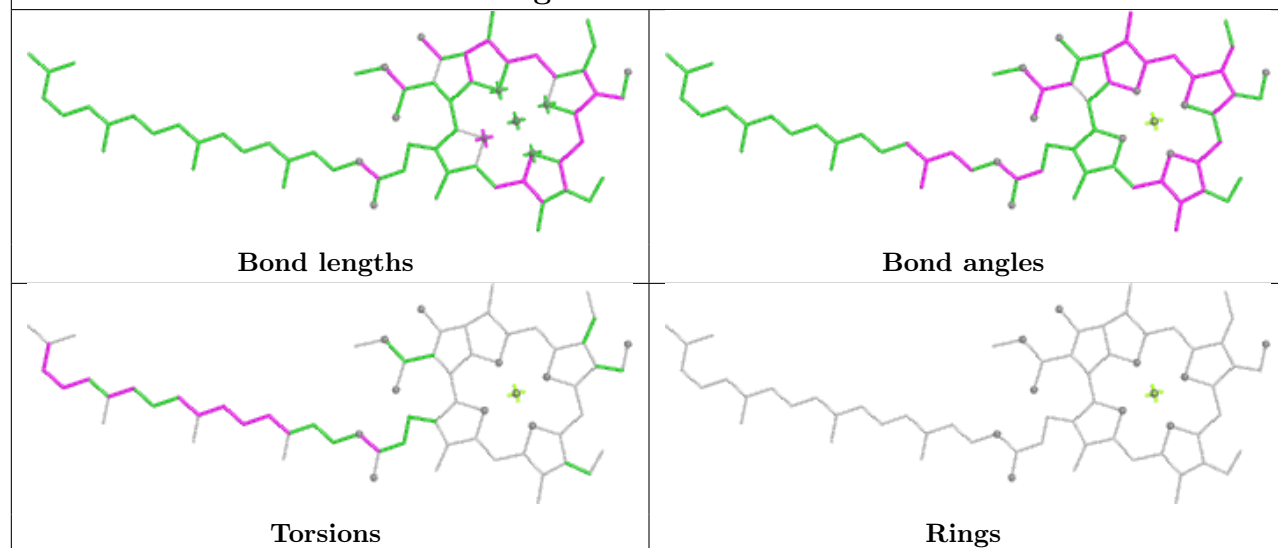
## Ligand CLA 4 612



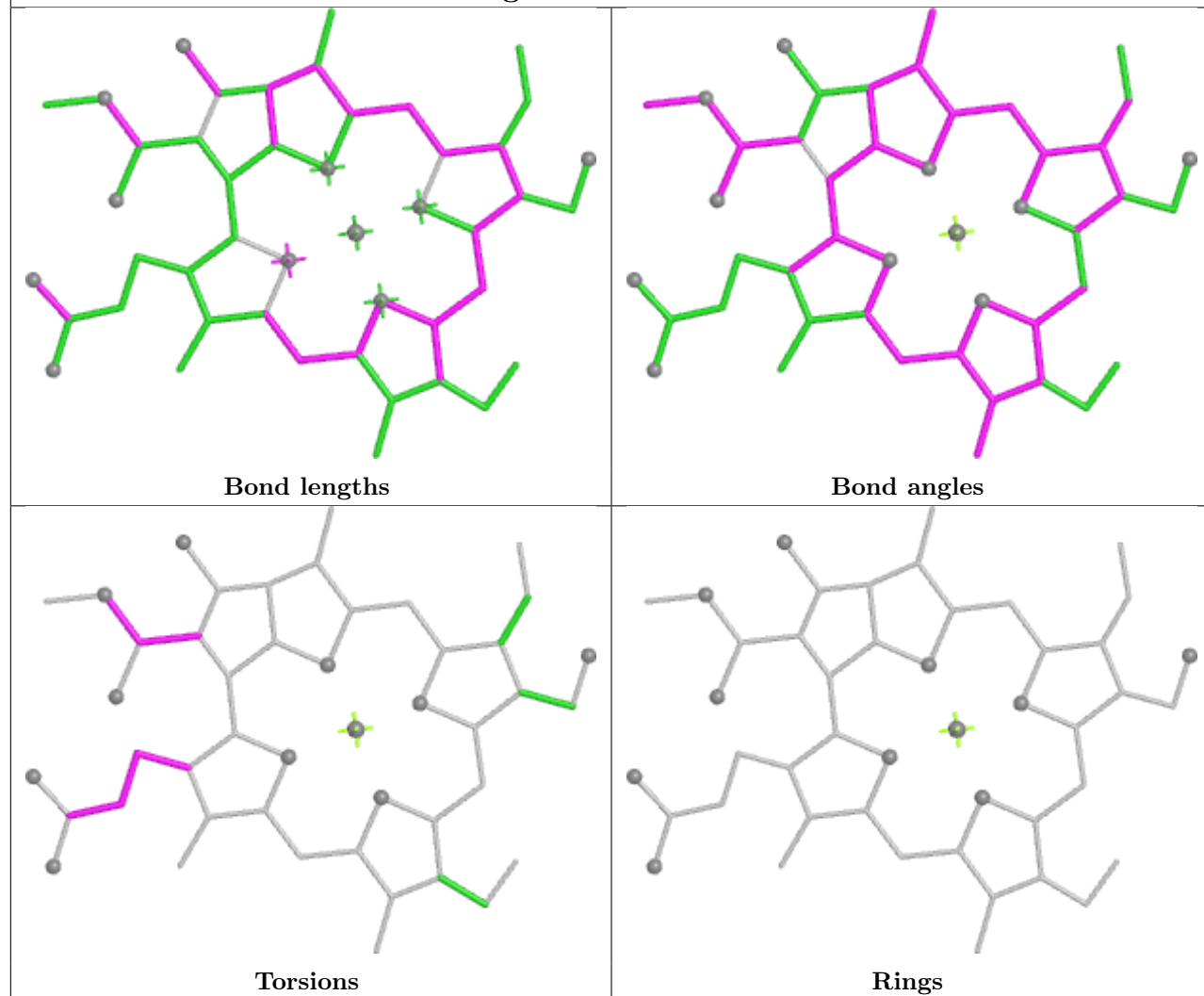
## Ligand CLA 6 606



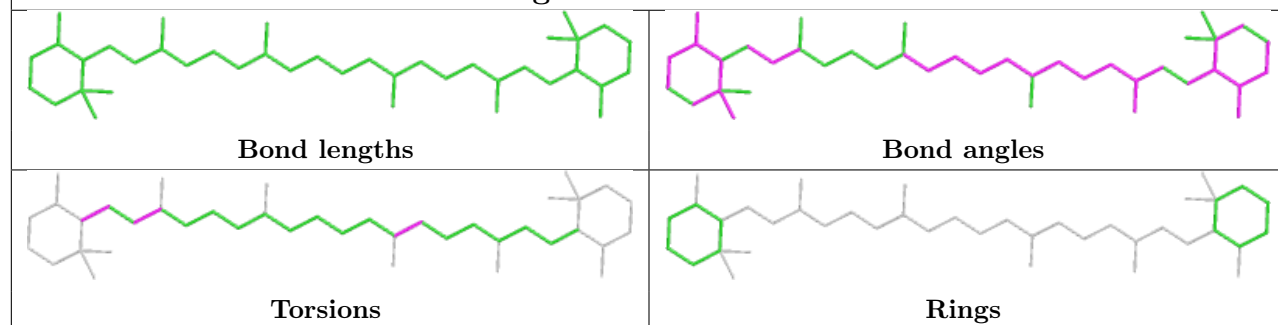
## Ligand CHL Z 601



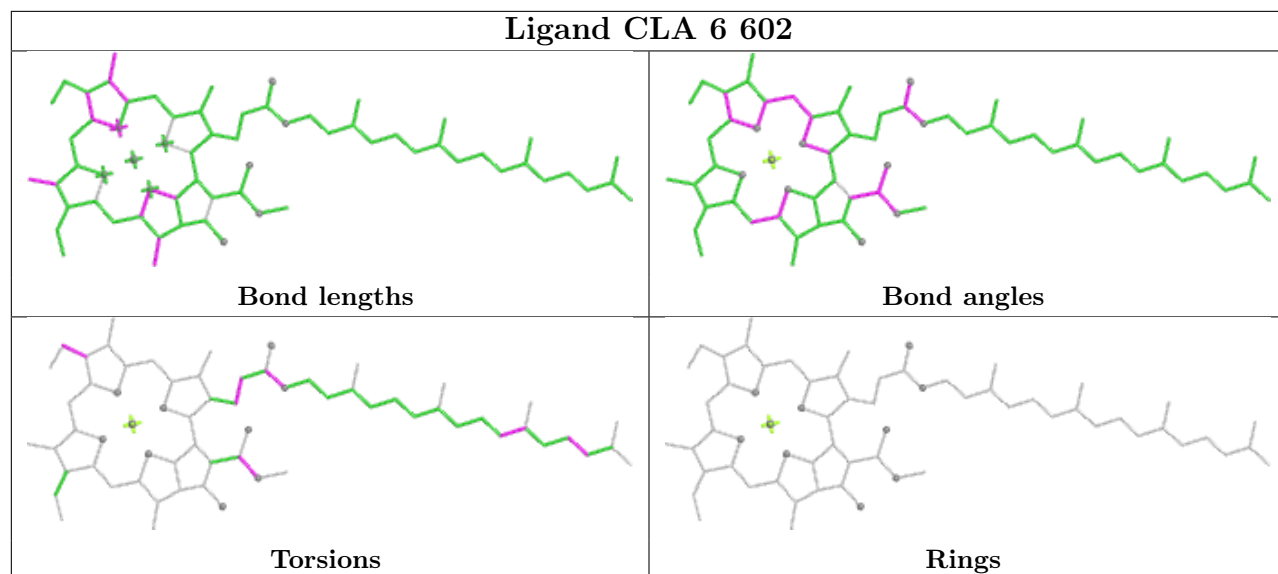
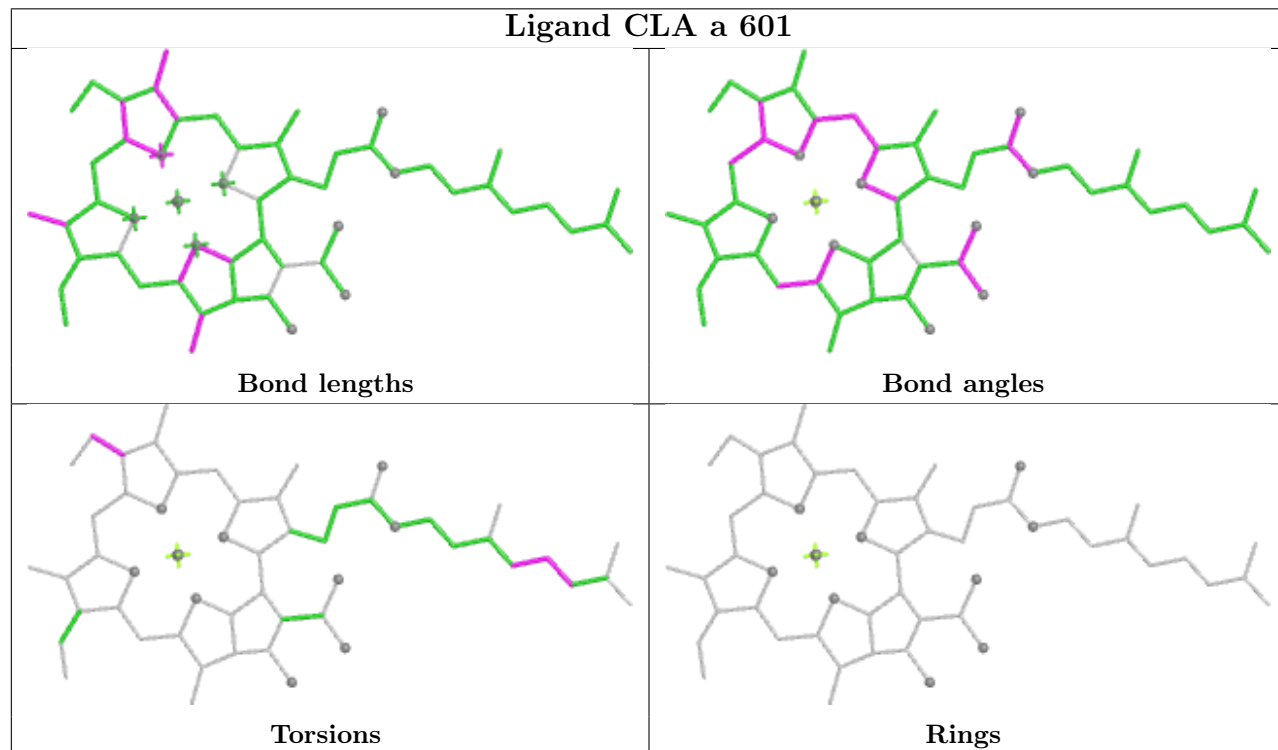
## Ligand CHL Z 606

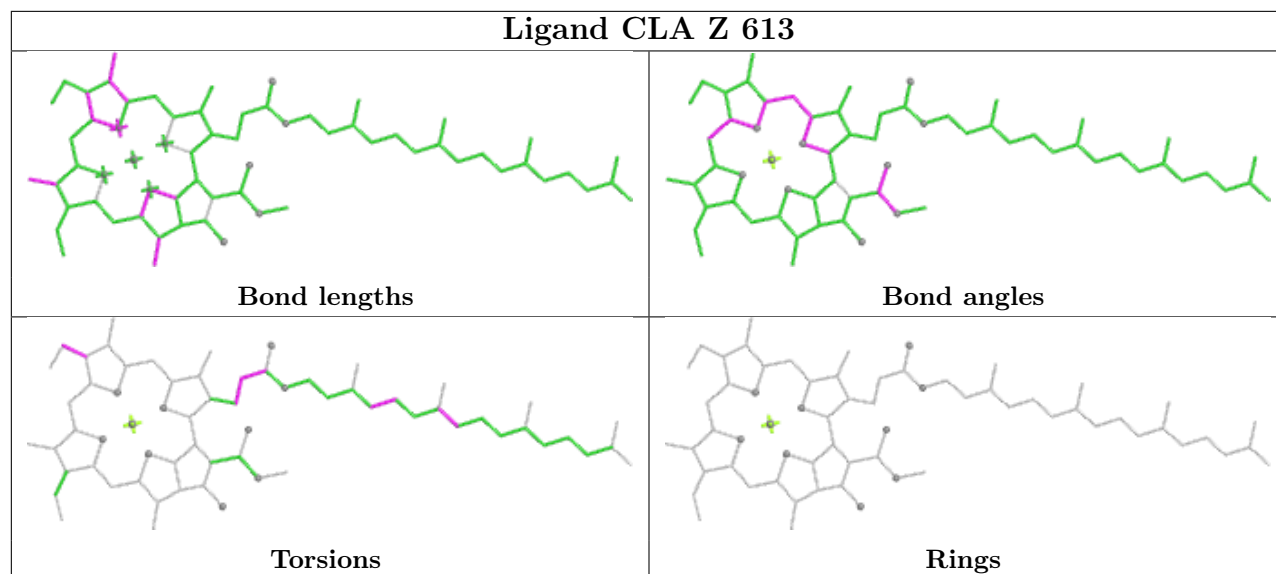
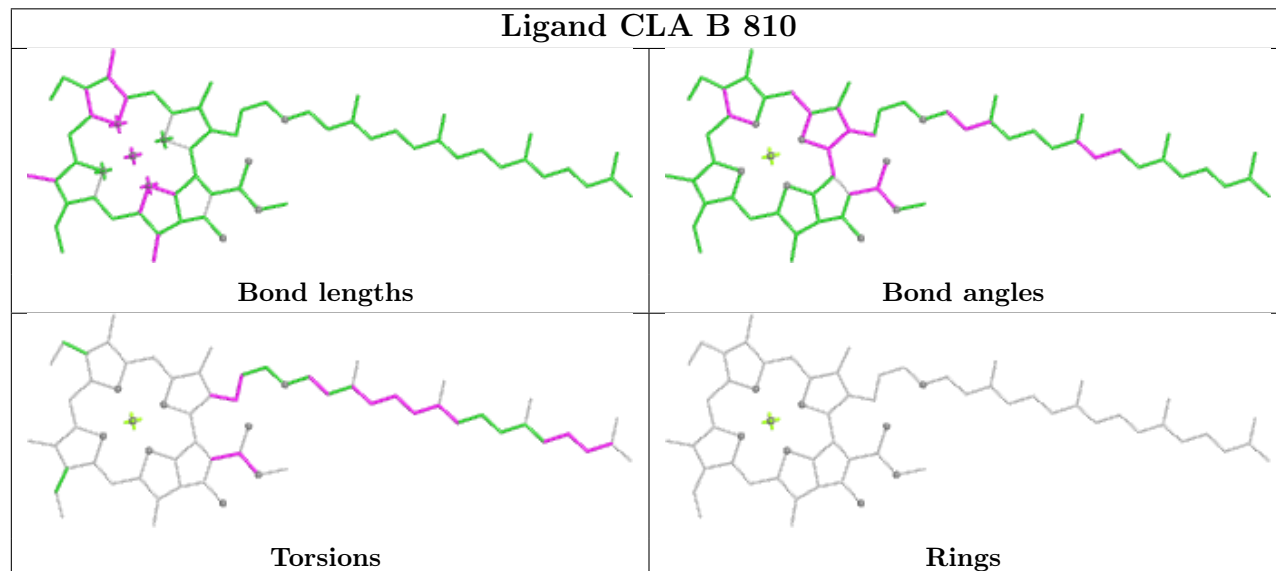


## Ligand BCR L 308

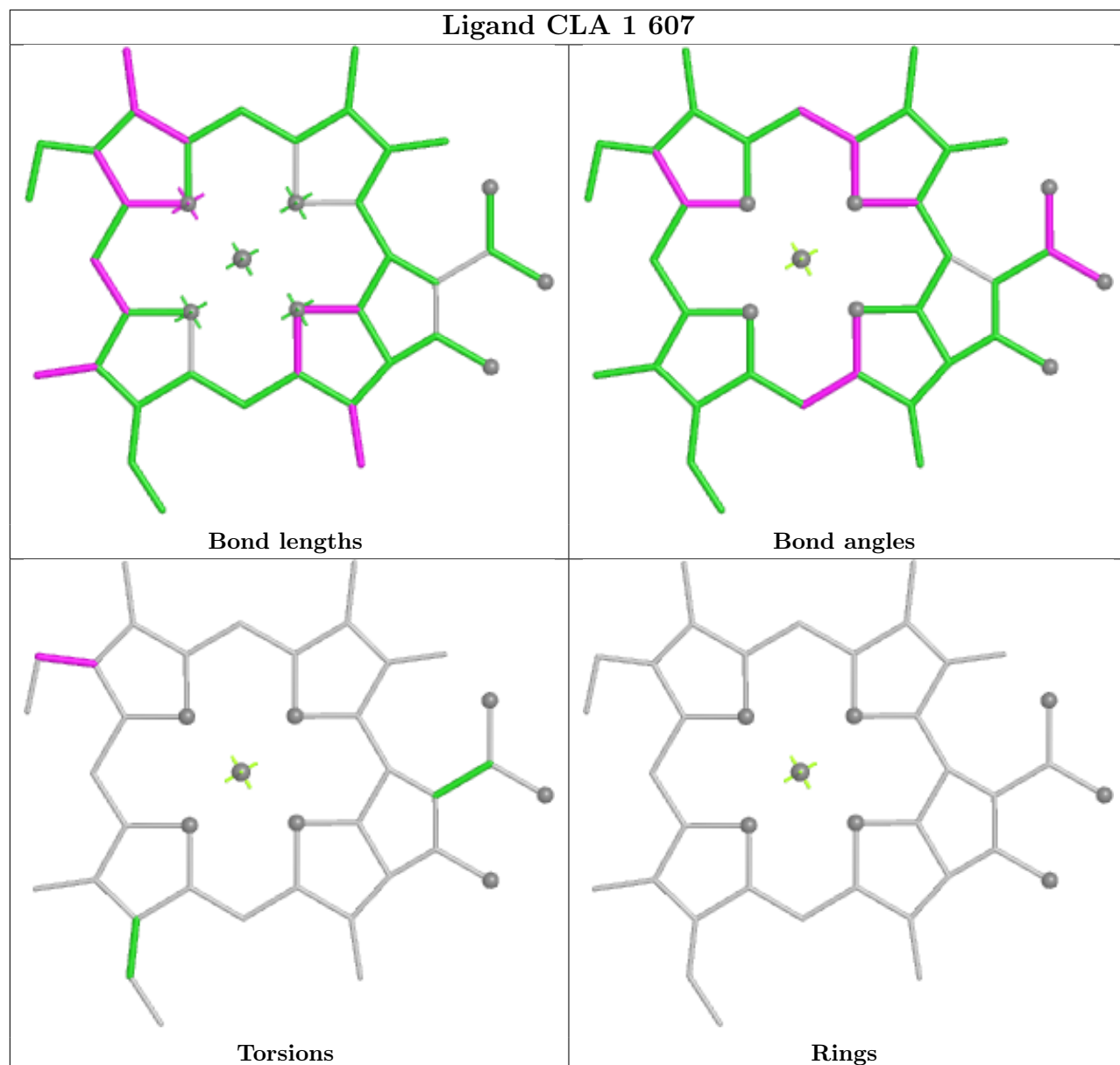




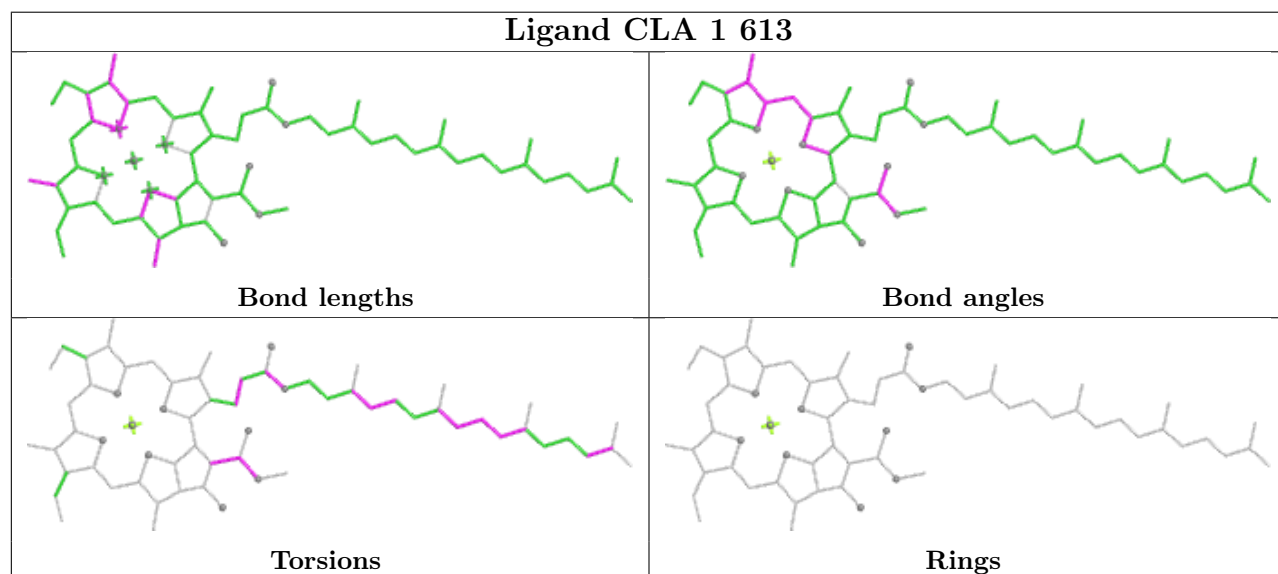
**Ligand CLA 6 602****Ligand CLA a 601**

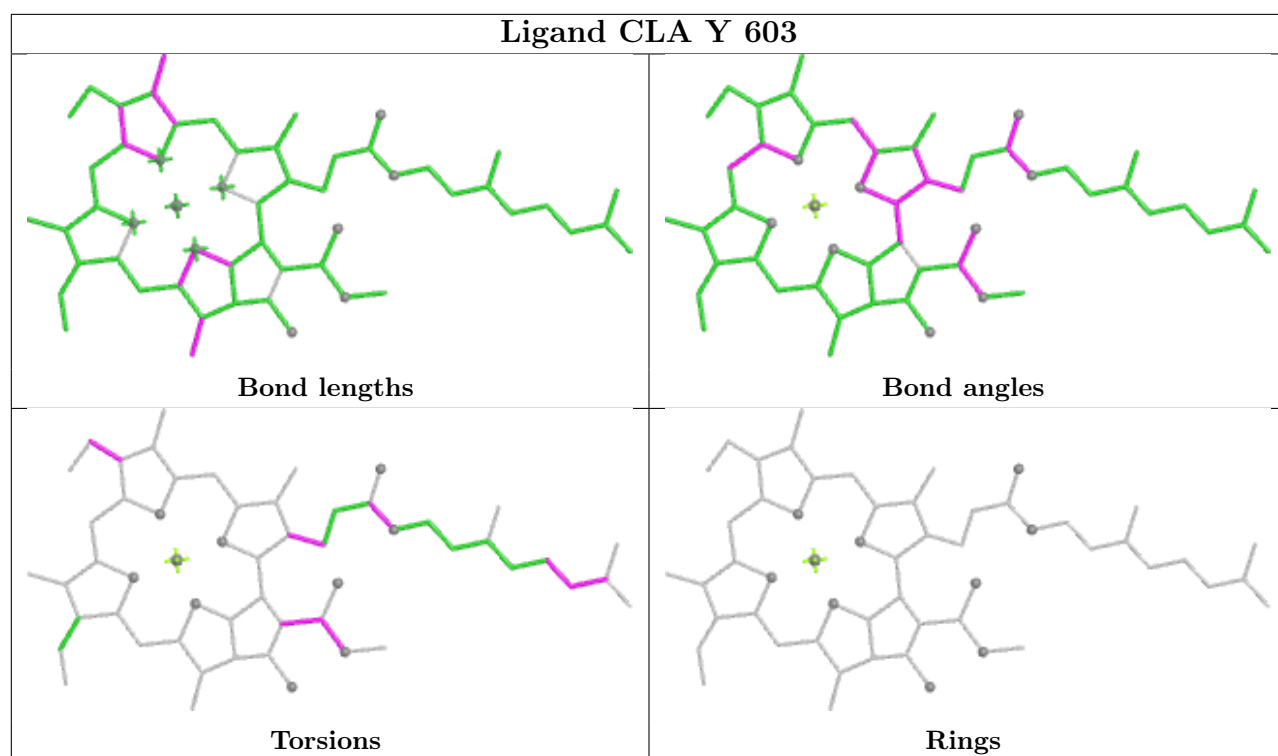
**Ligand CLA Z 613****Ligand CLA B 810**

## Ligand CLA 1 607

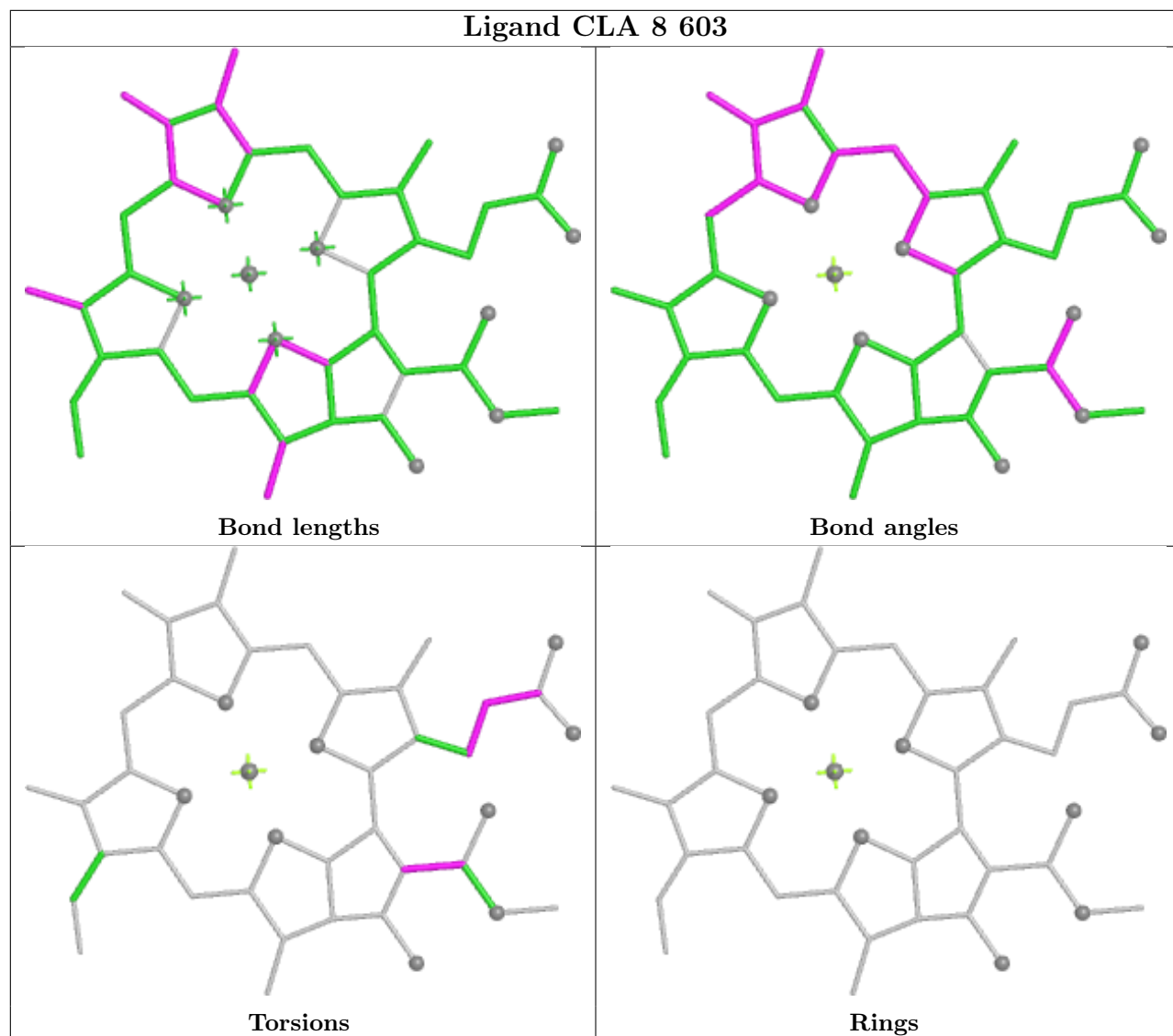


## Ligand CLA 1 613

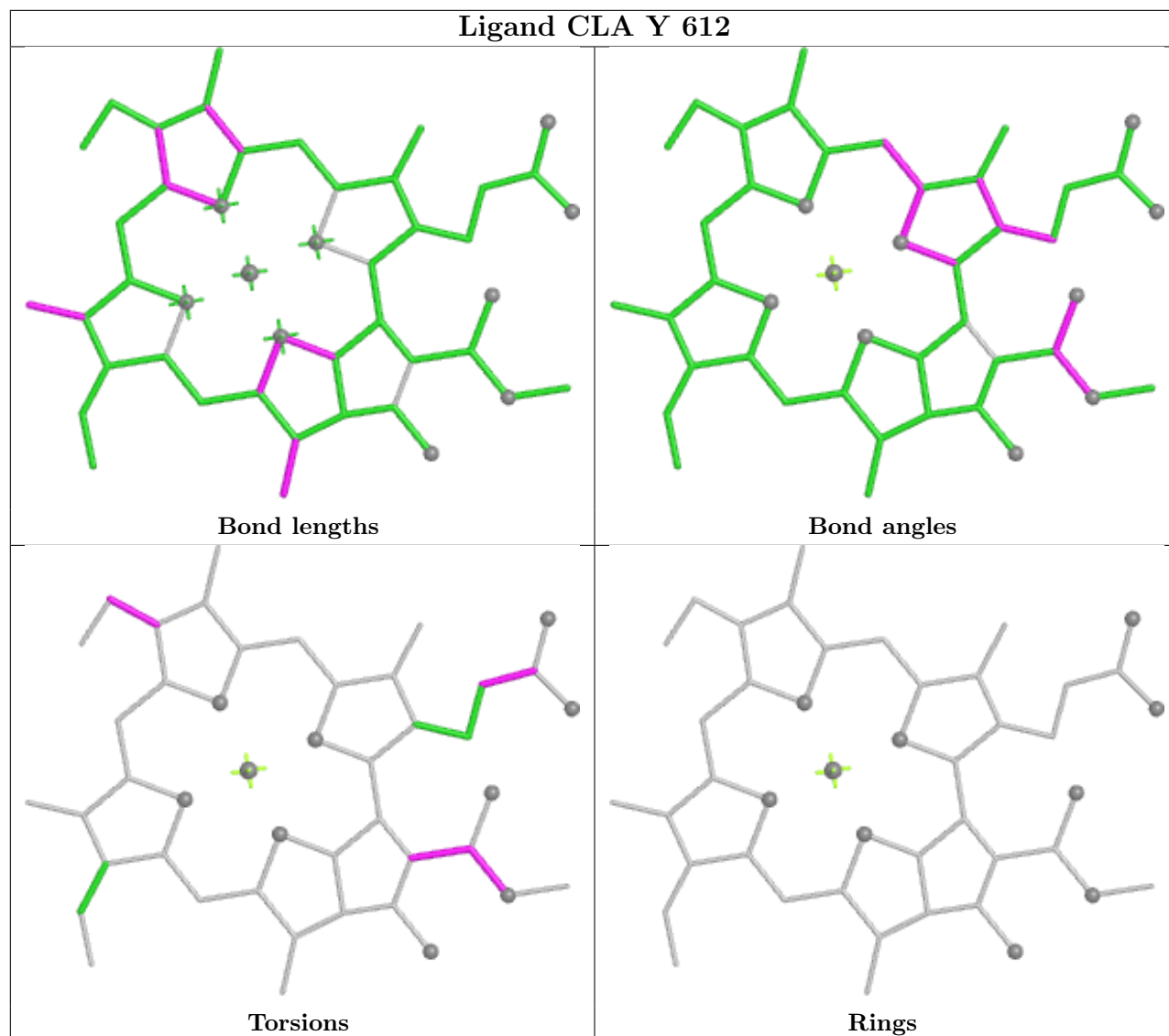




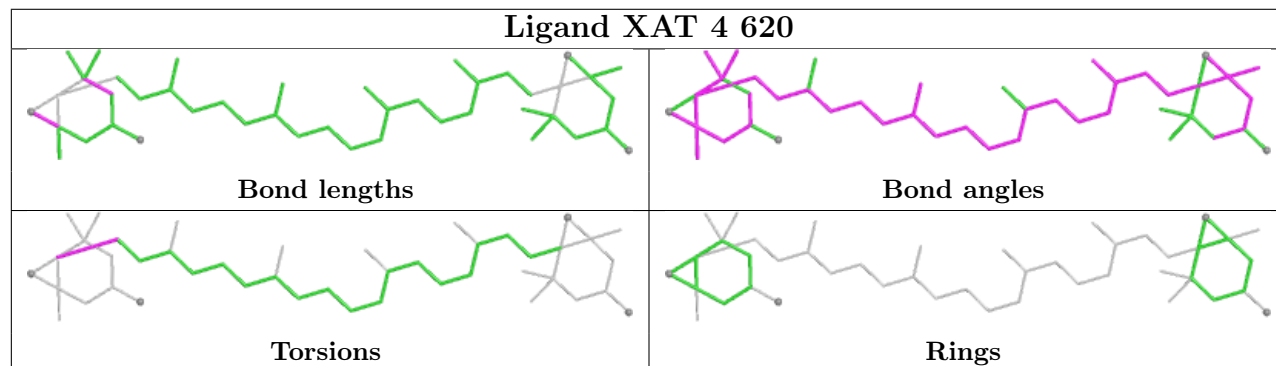
## Ligand CLA 8 603

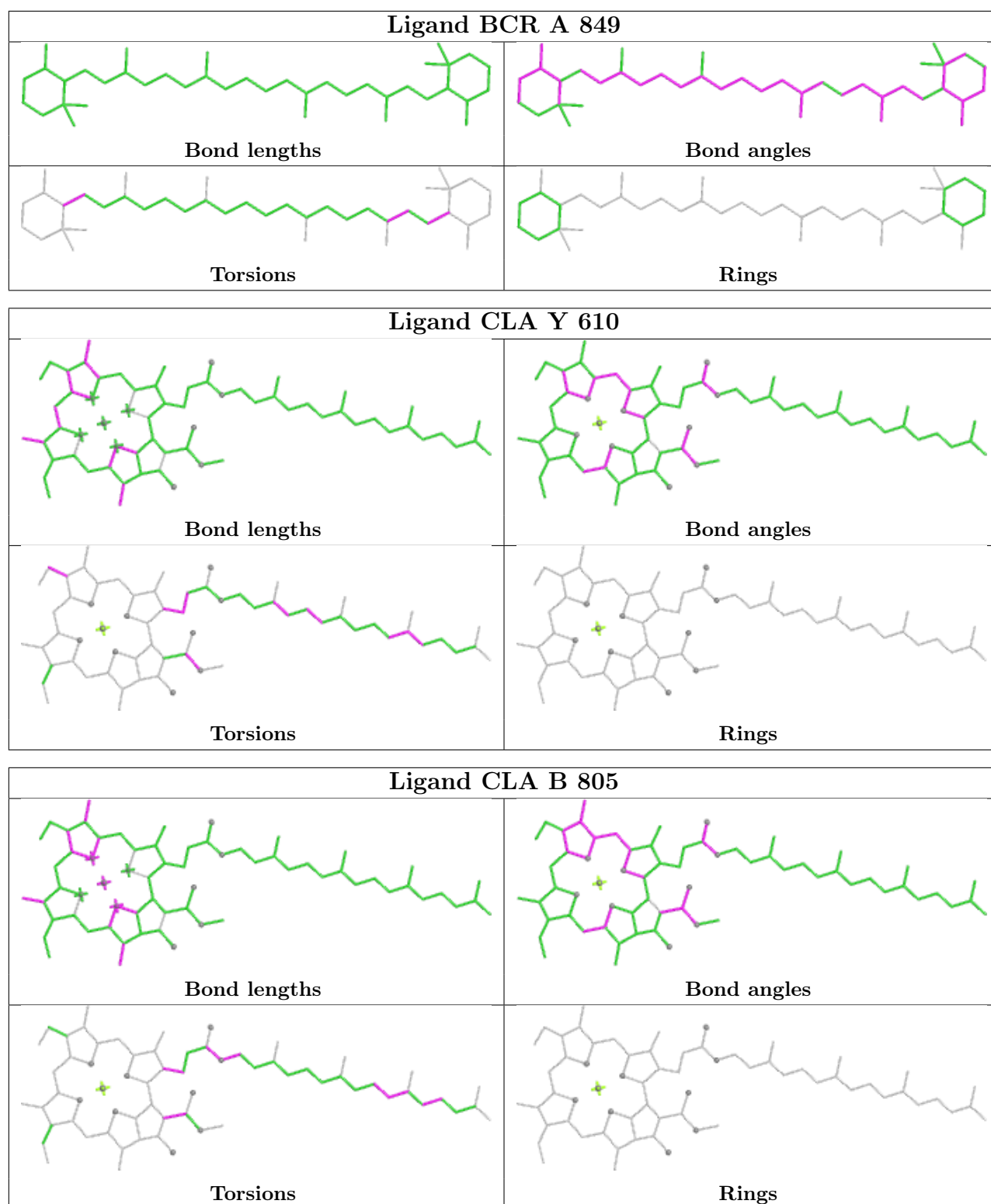


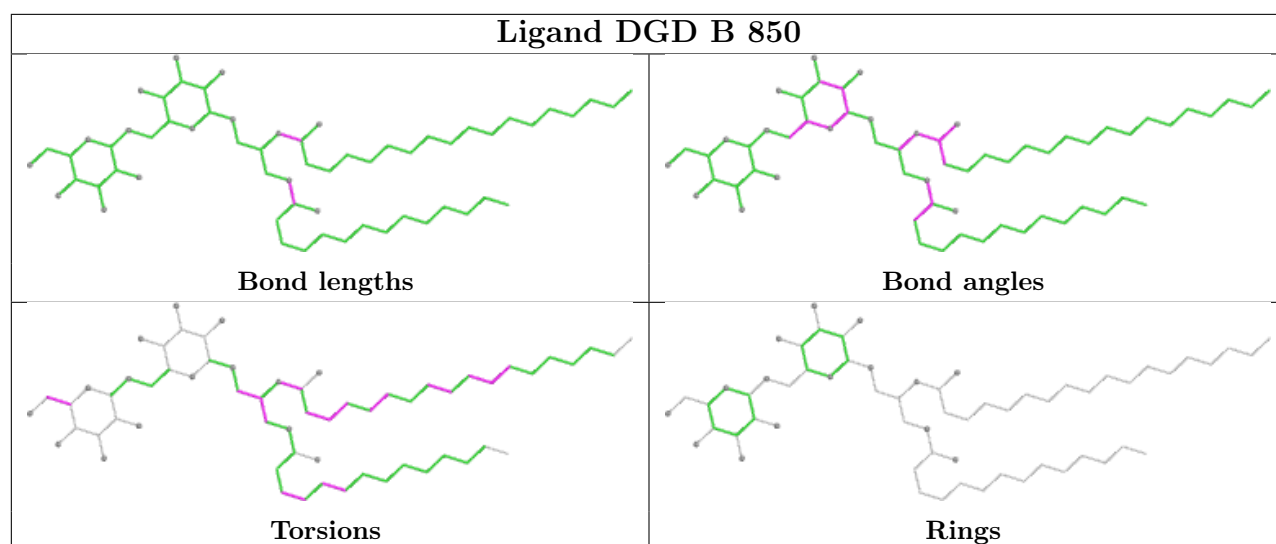
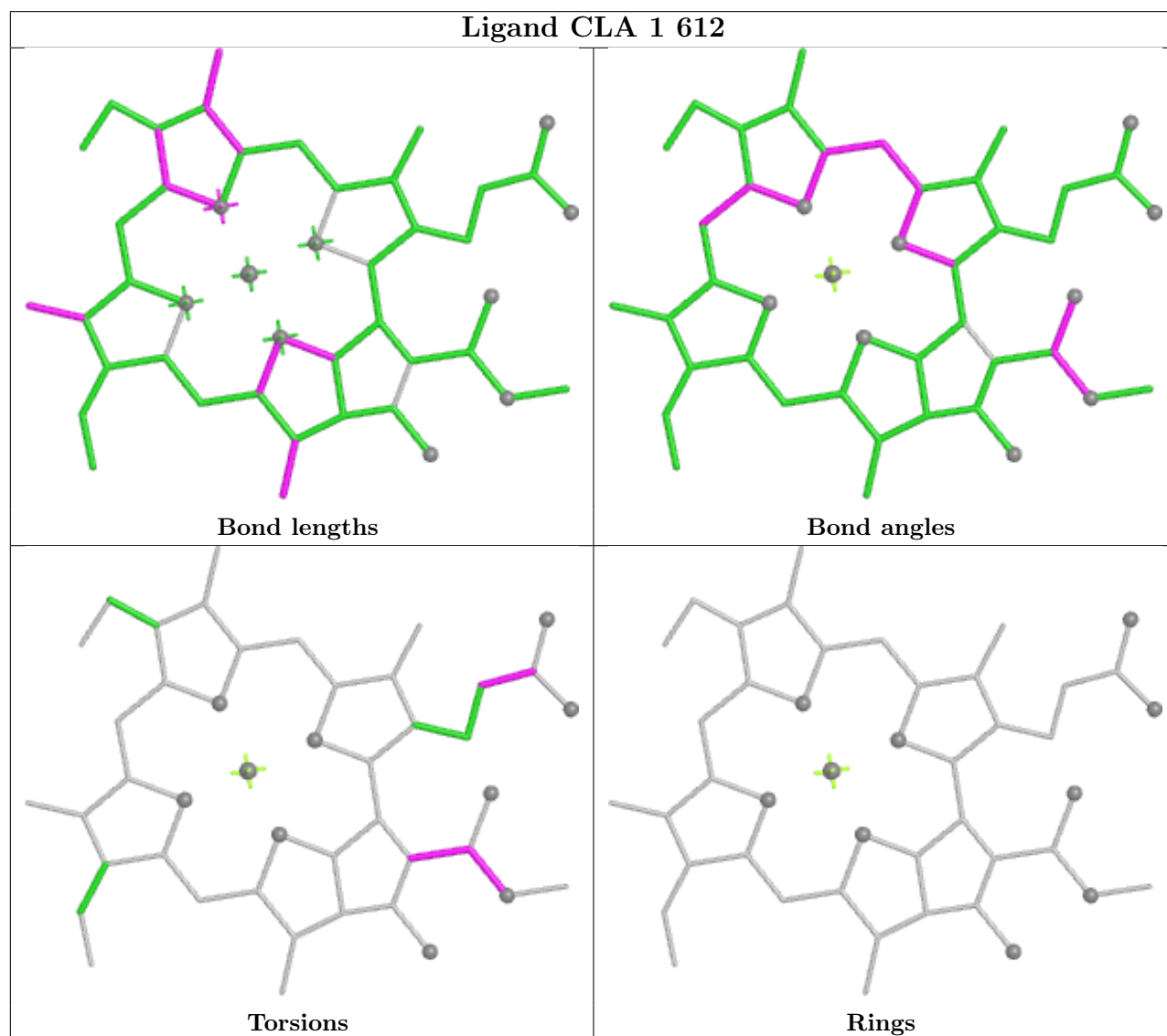
## Ligand CLA Y 612



## Ligand XAT 4 620

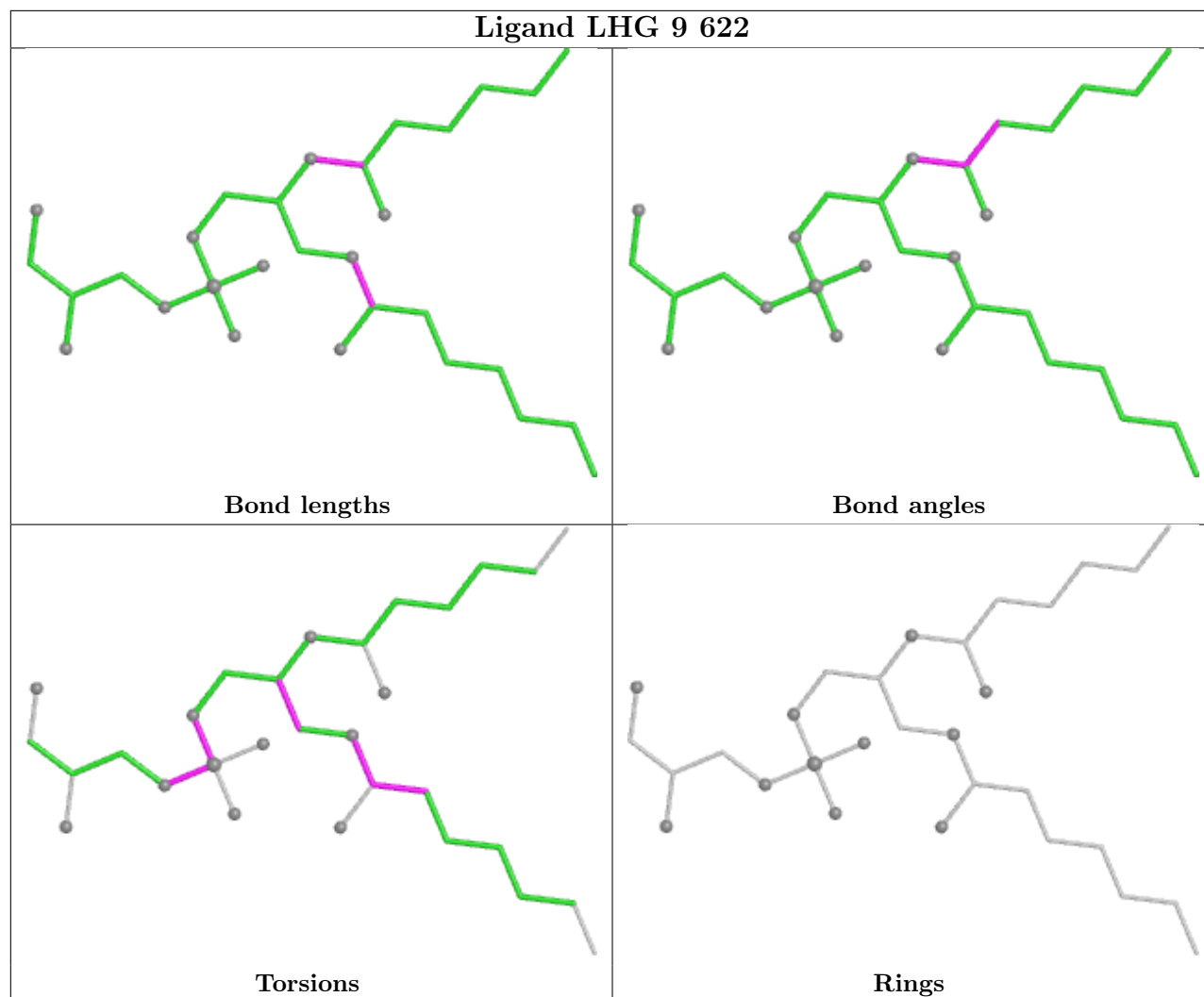




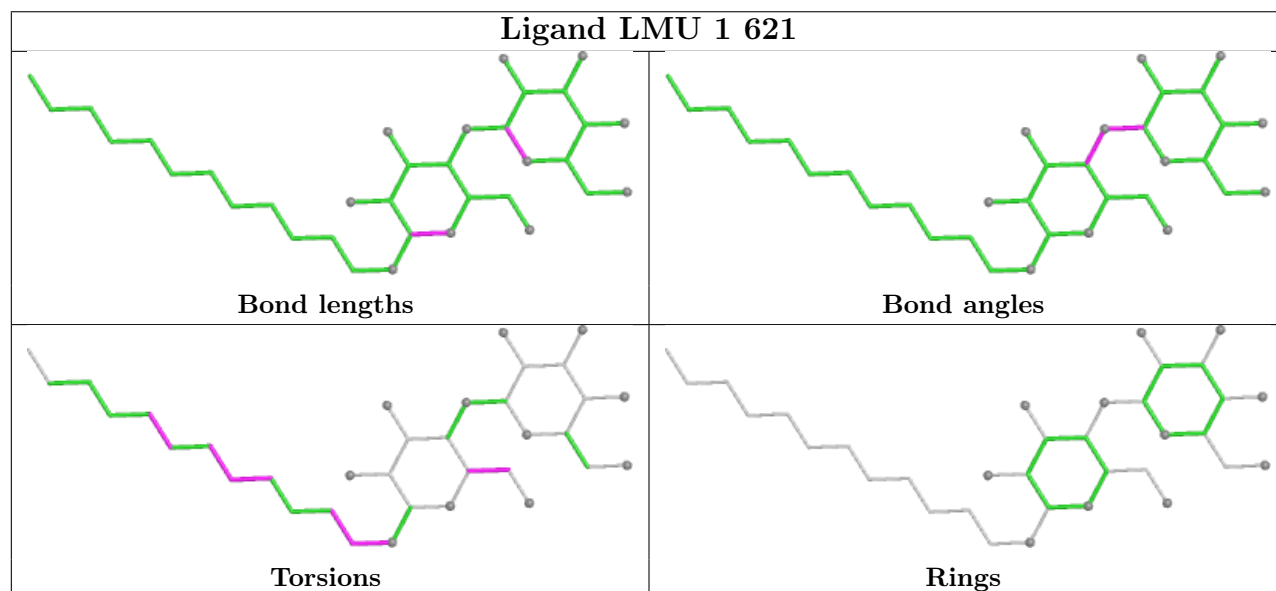




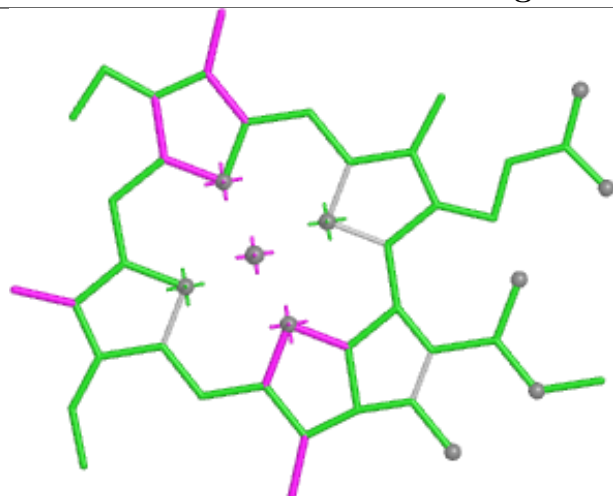
## Ligand LHG 9 622



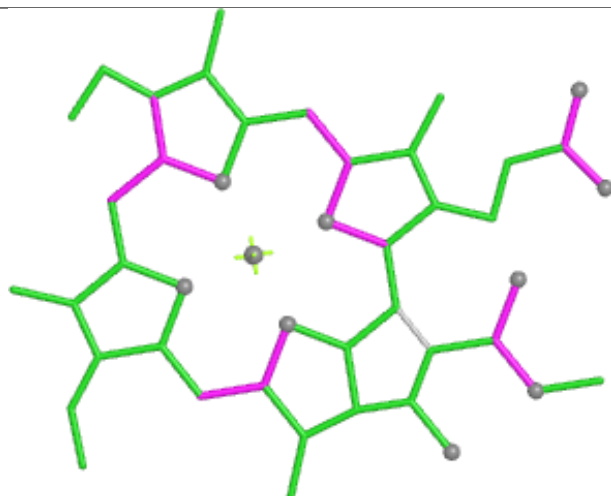
## Ligand LMU 1 621



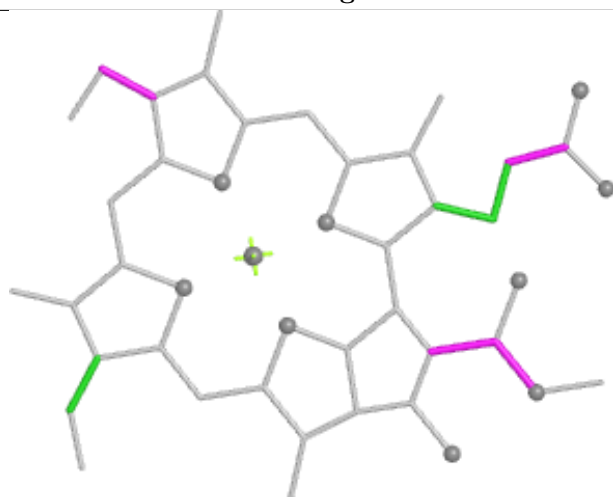
## Ligand CLA B 823



Bond lengths



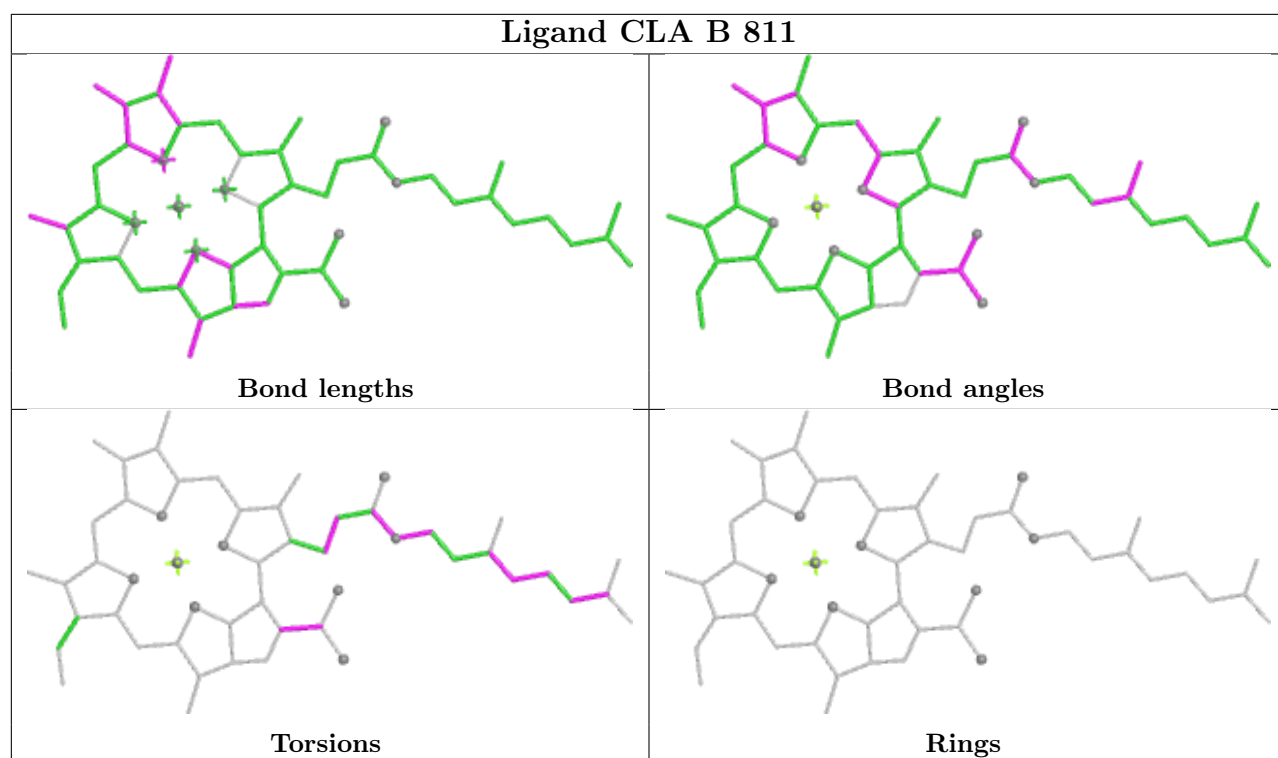
Bond angles



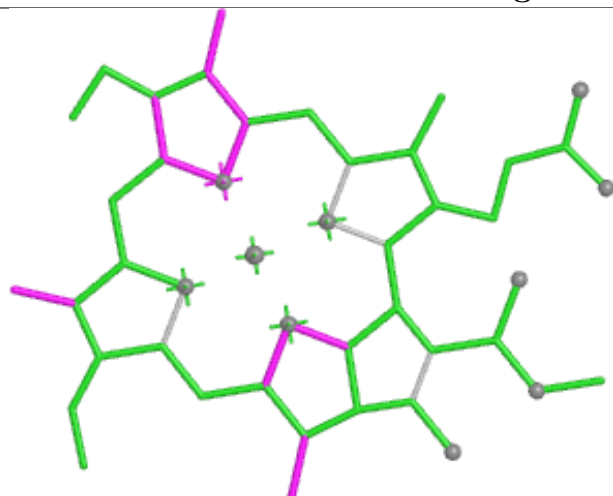
Torsions



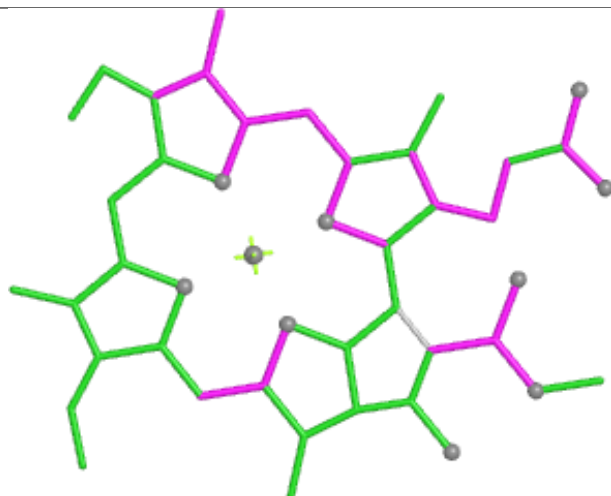
Rings



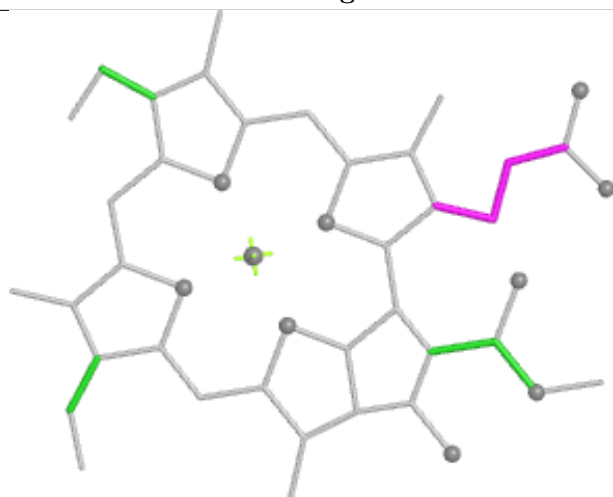
## Ligand CLA A 833



Bond lengths



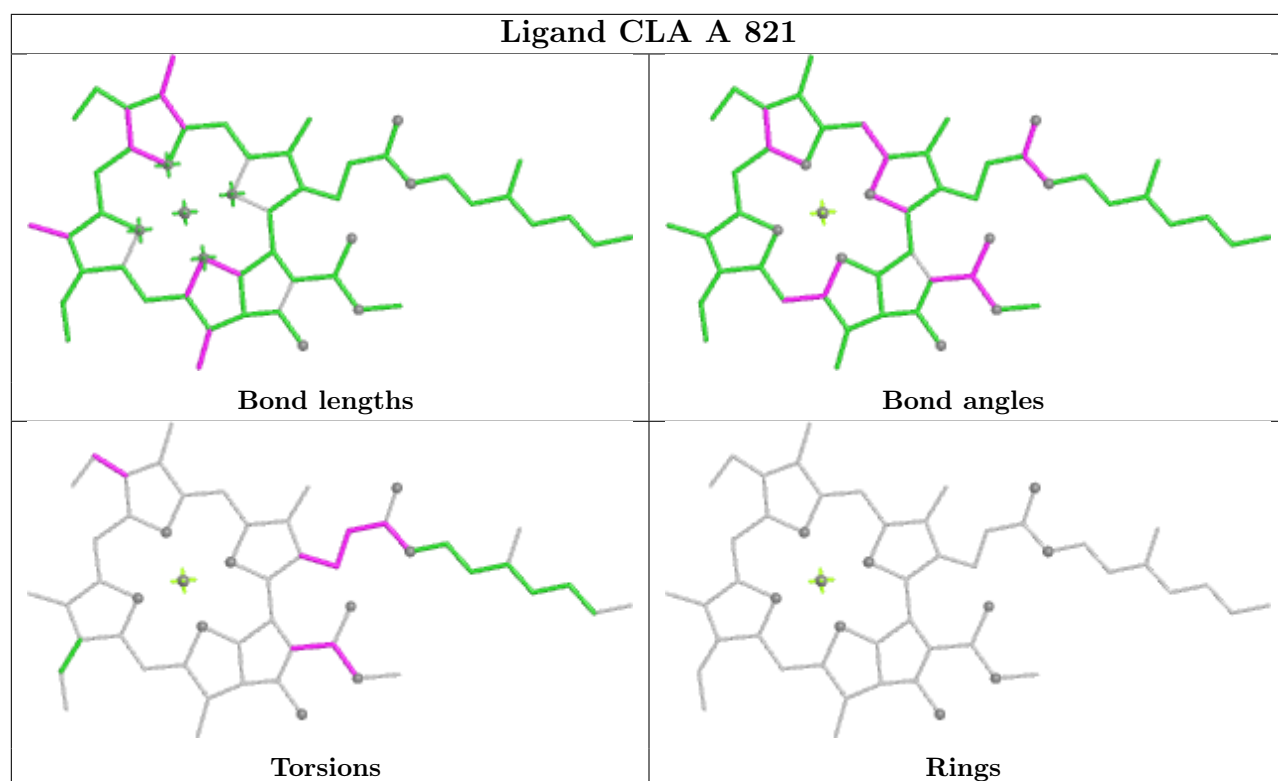
Bond angles



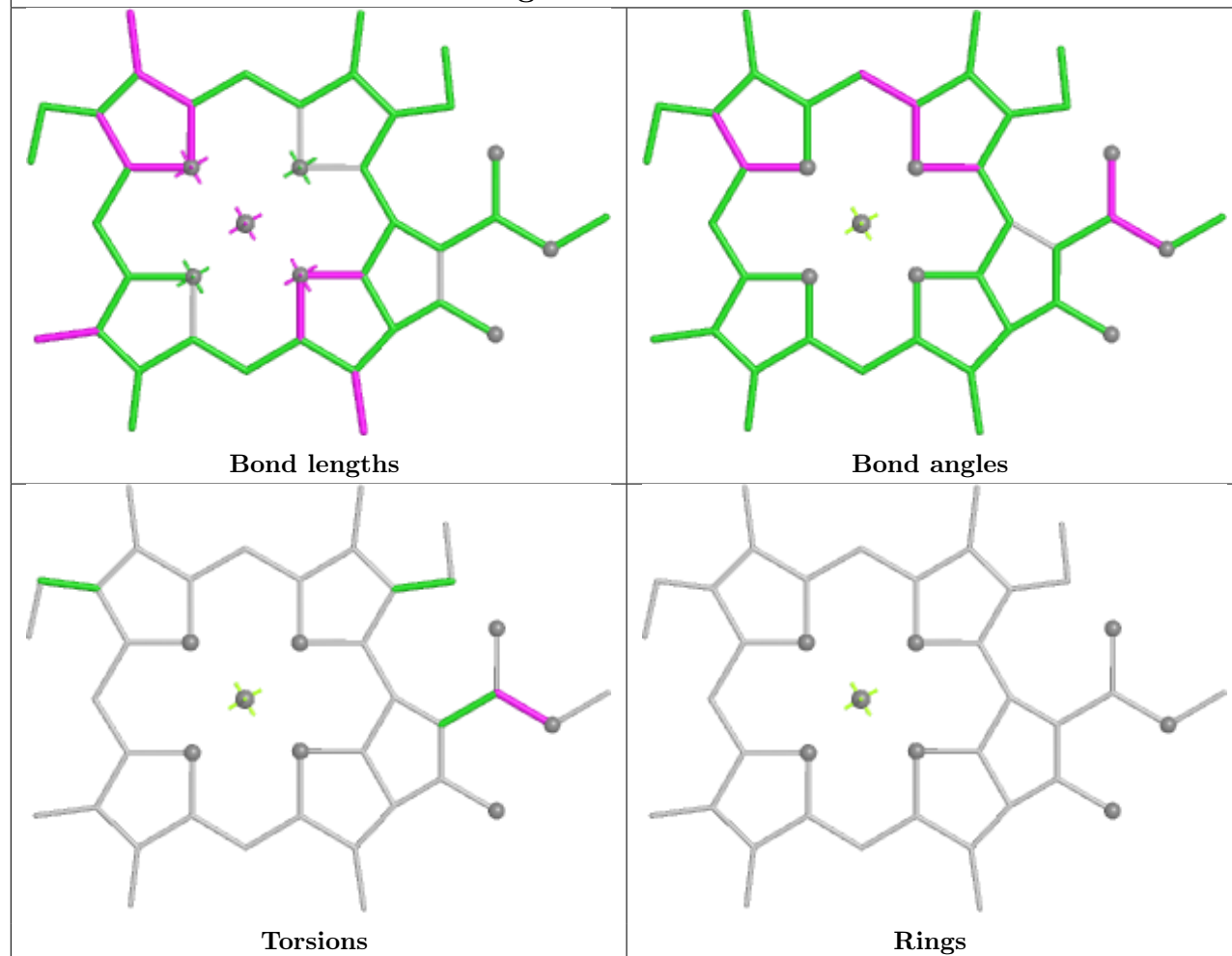
Torsions



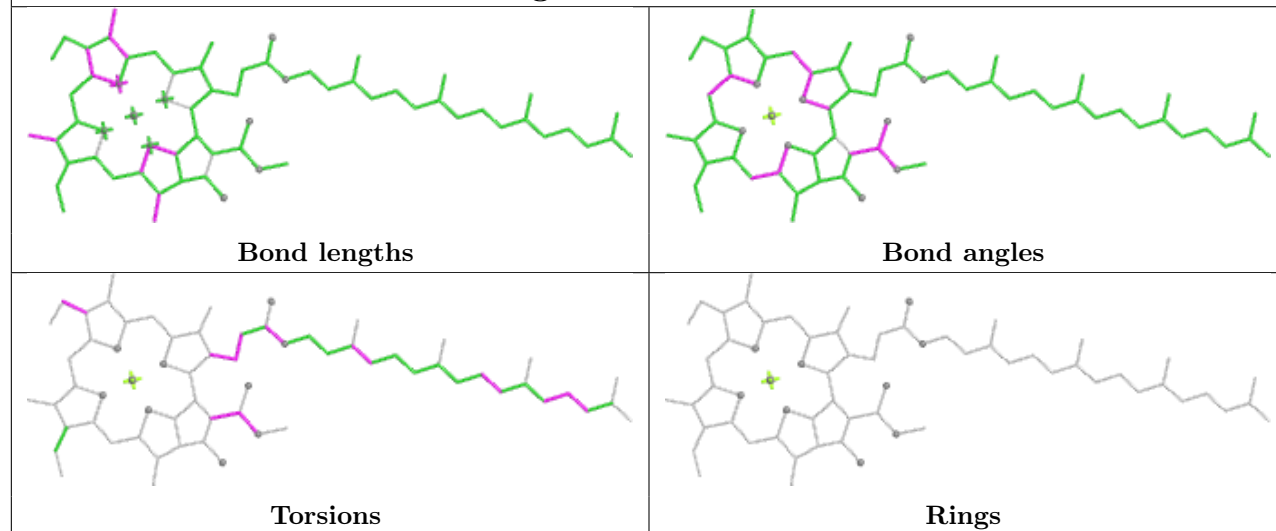
Rings

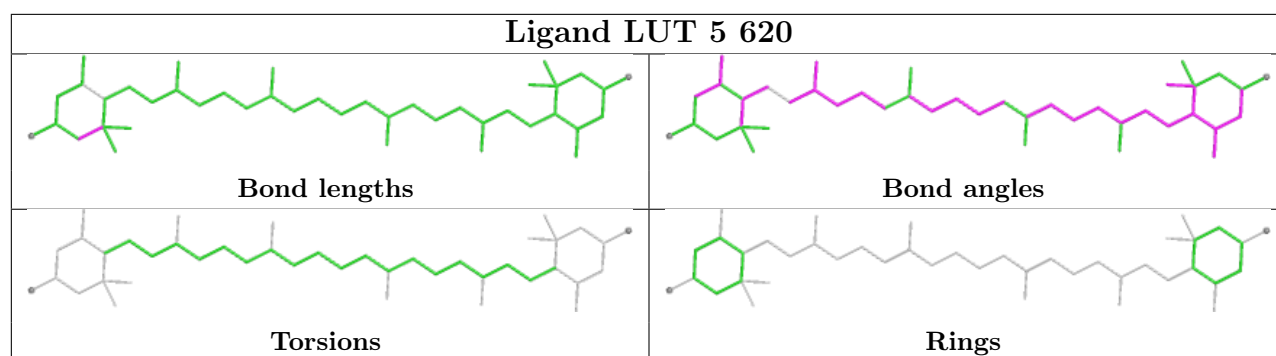
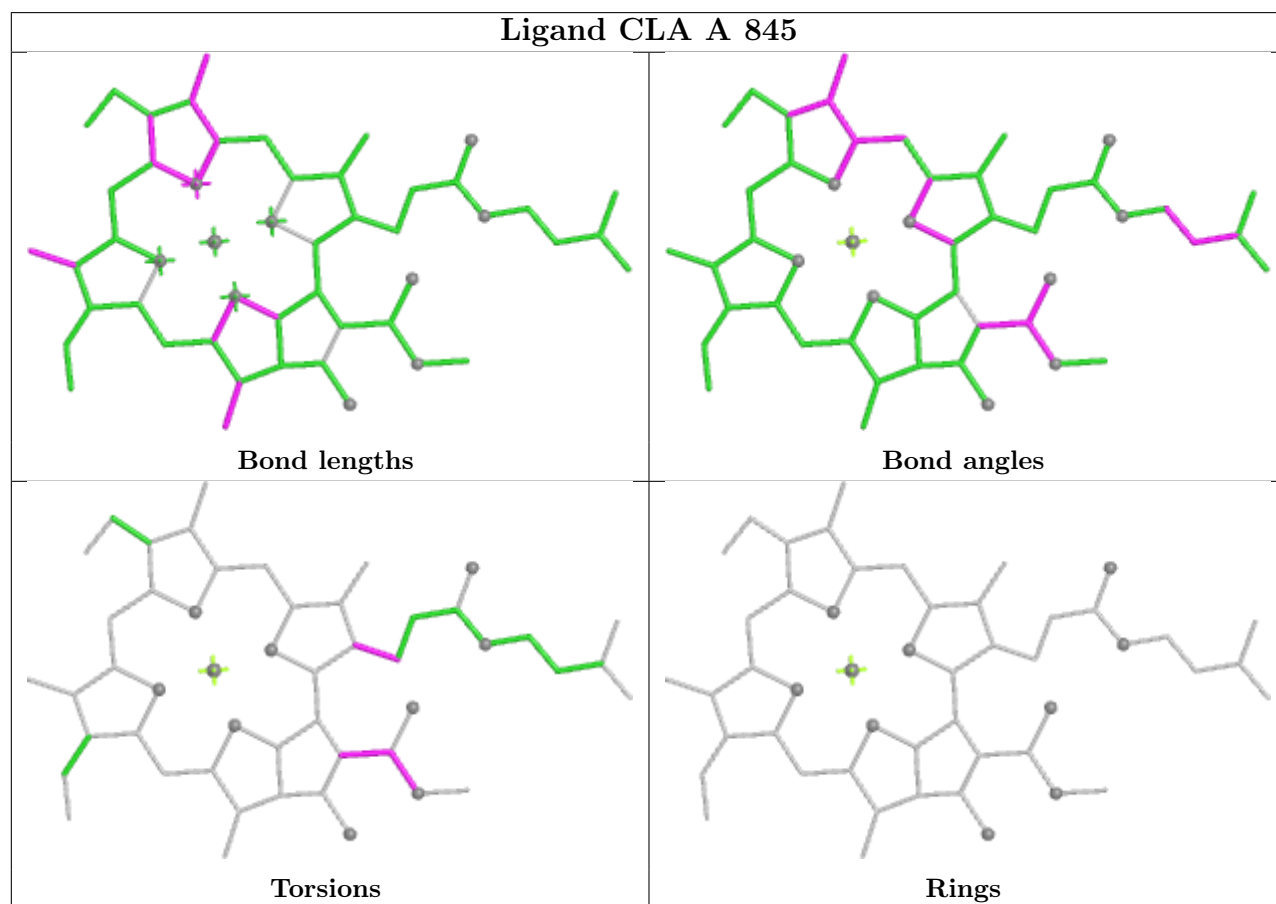
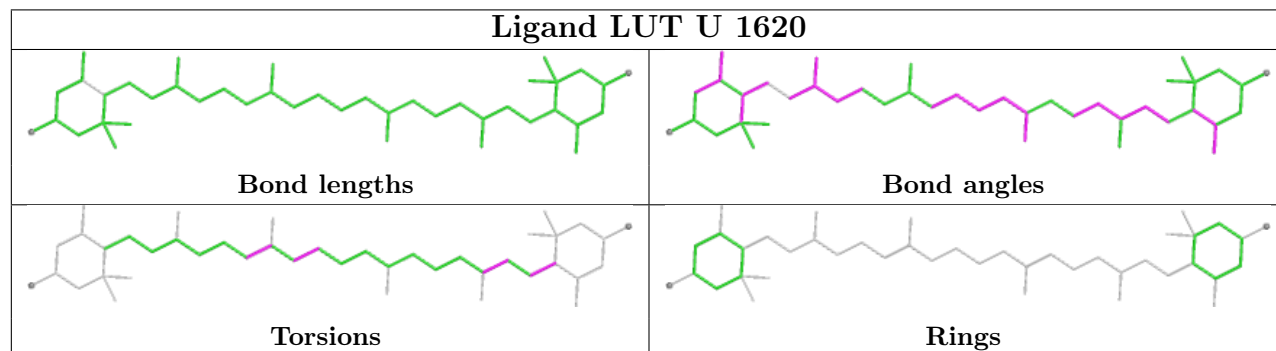


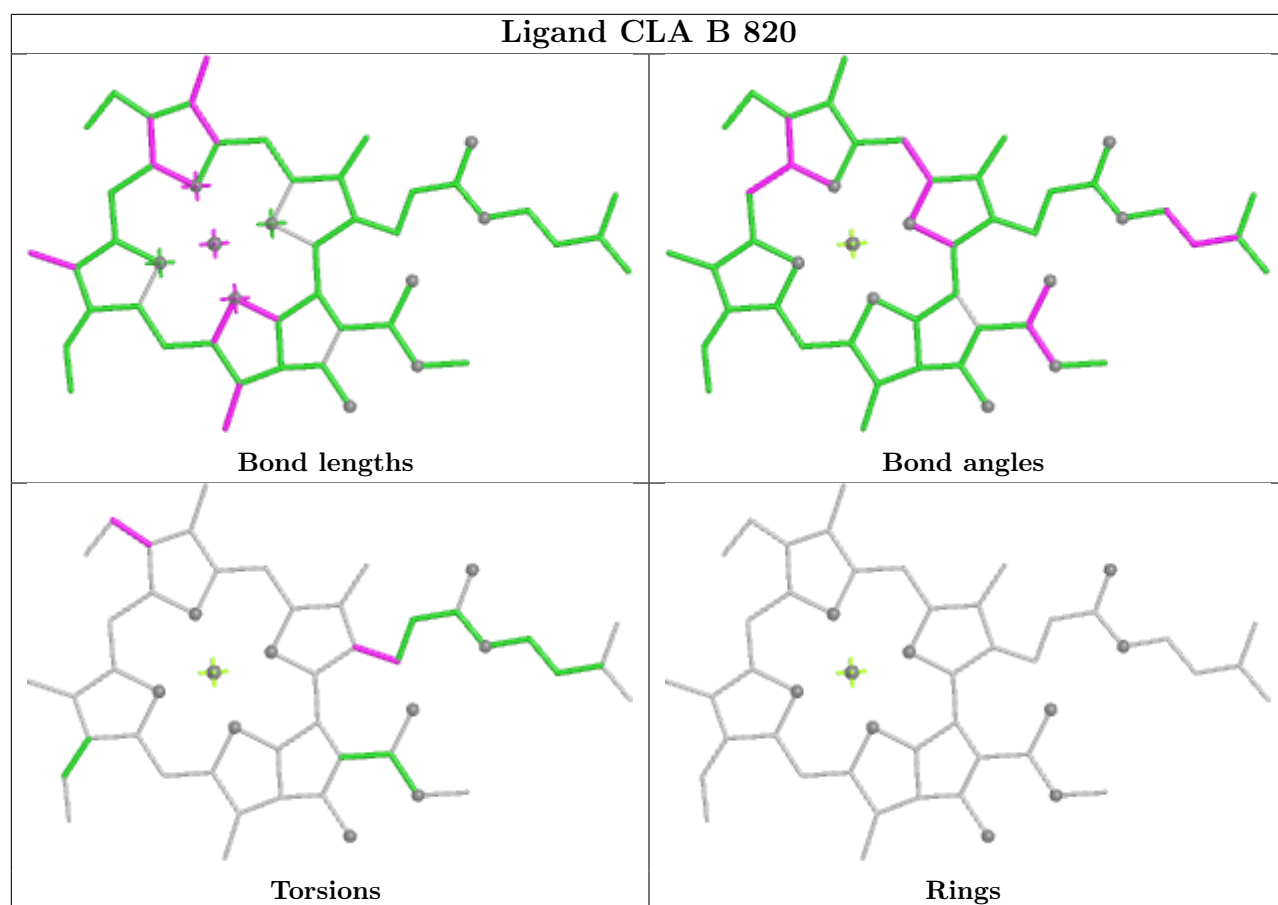
## Ligand CLA 7 606



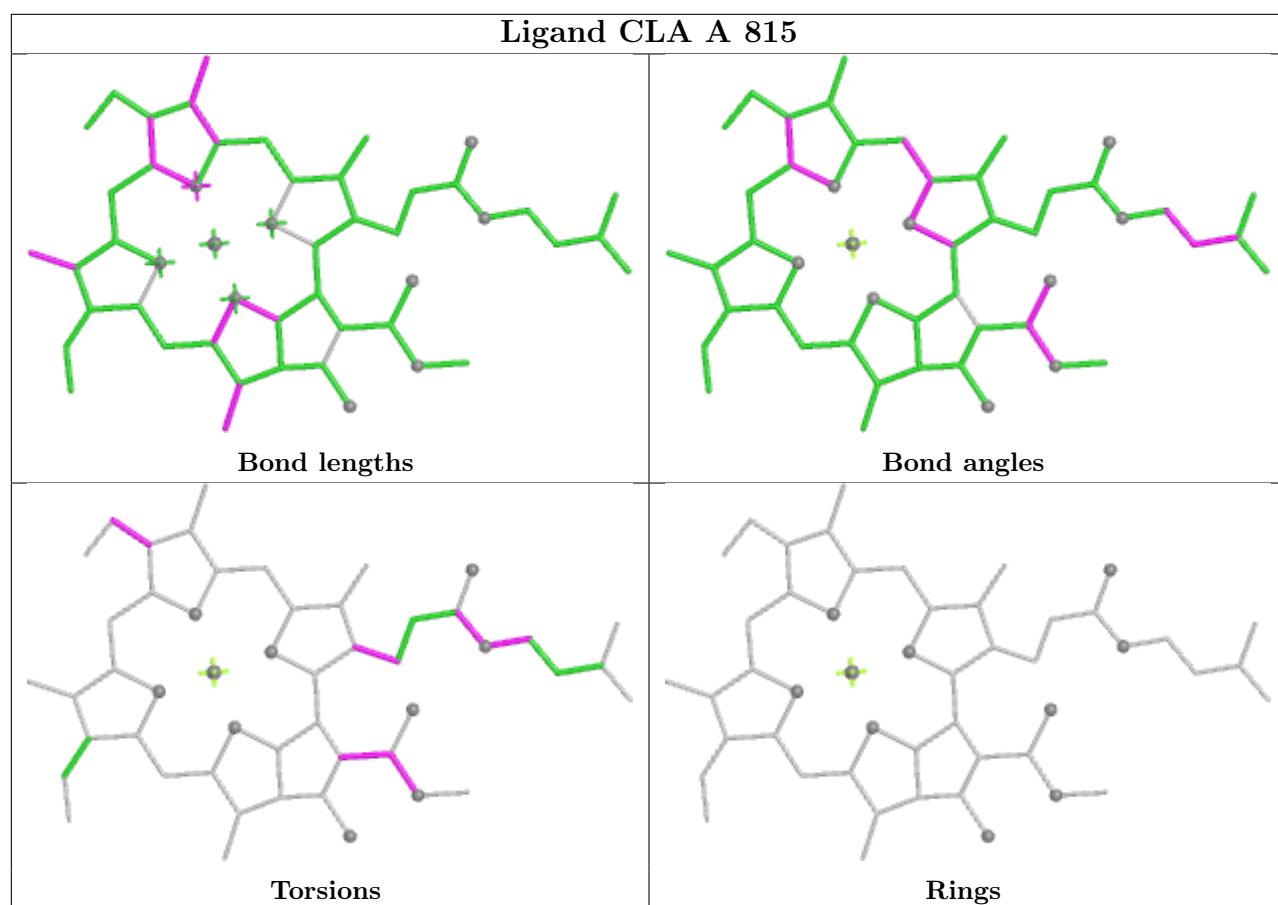
## Ligand CLA A 825



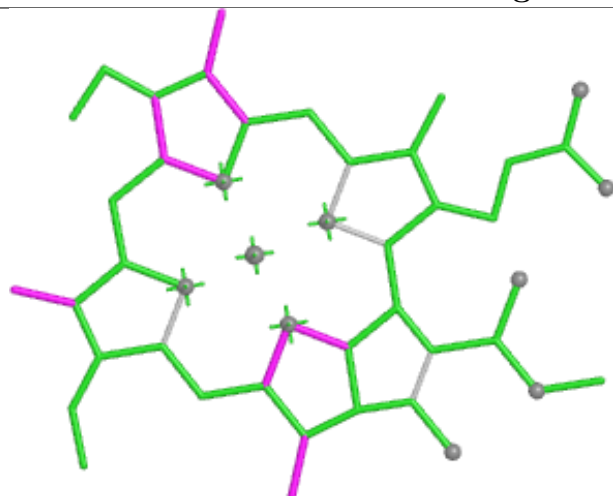




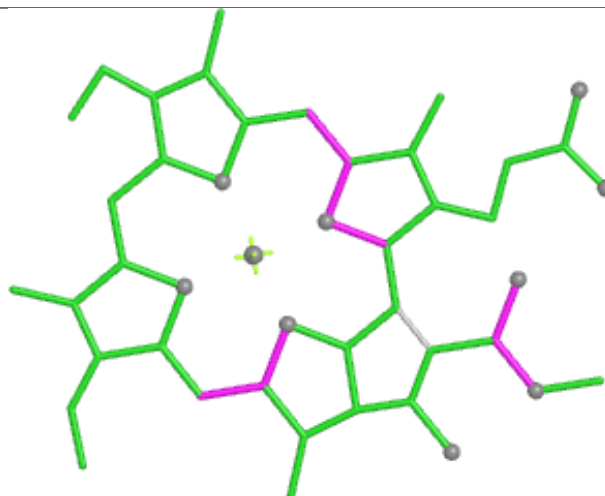




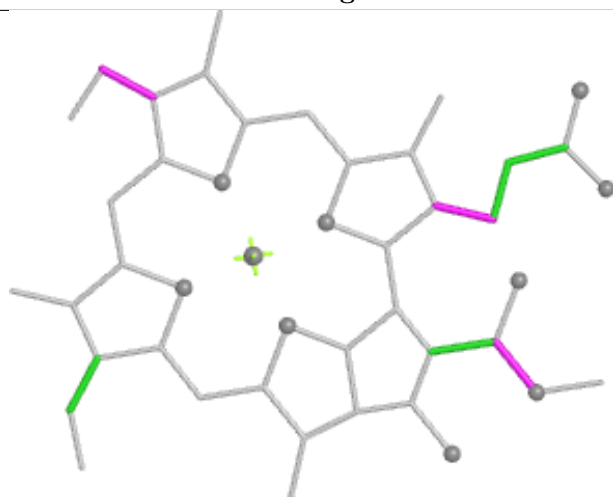
## Ligand CLA K 206



Bond lengths



Bond angles

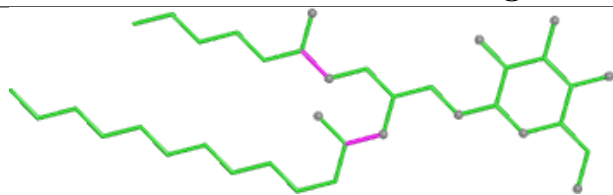


Torsions

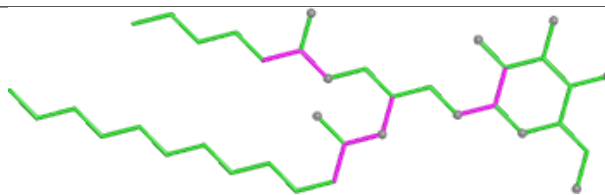


Rings

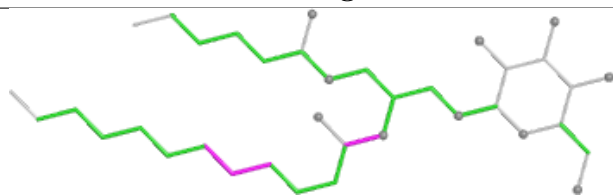
## Ligand LMG L 2631



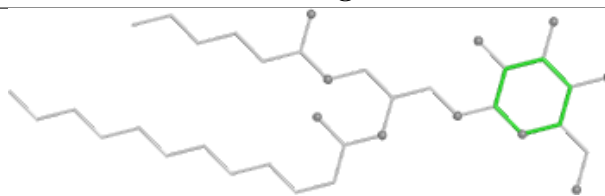
Bond lengths



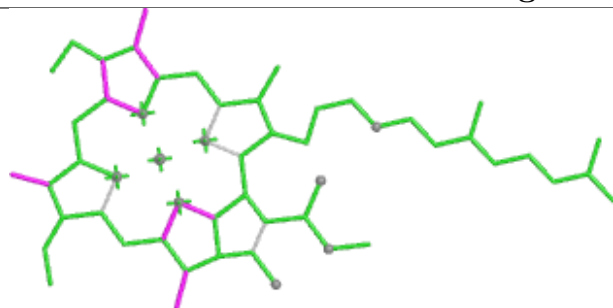
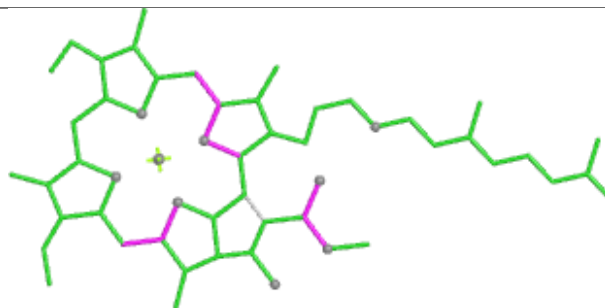
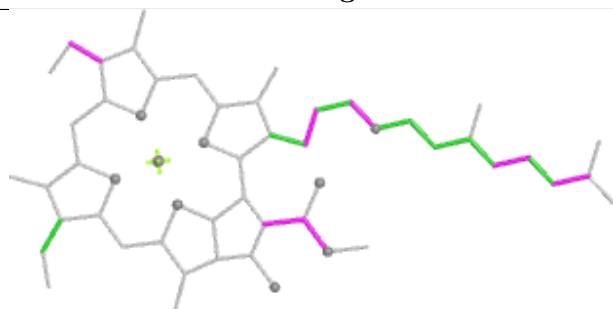
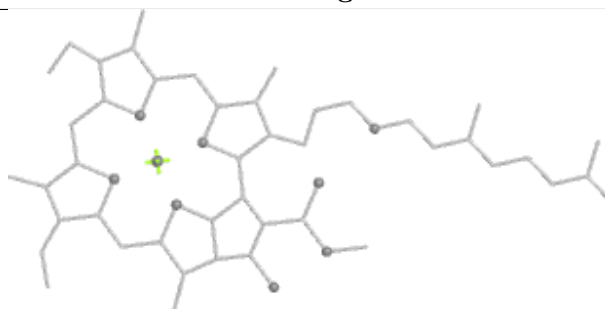
Bond angles



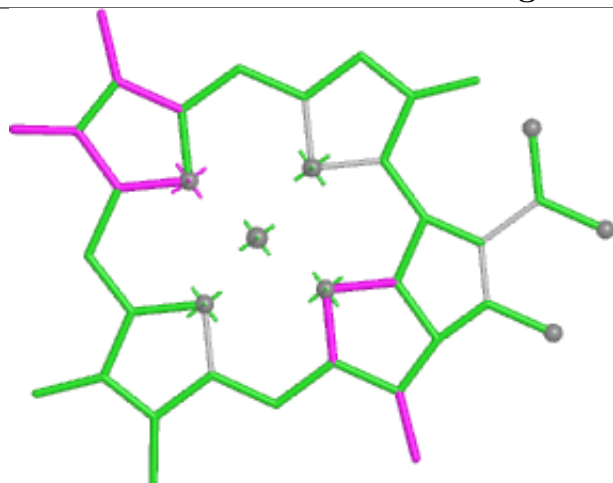
Torsions



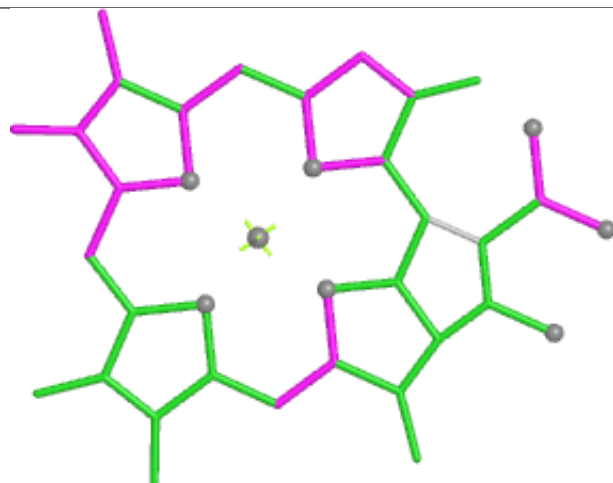
Rings

**Ligand CLA a 603****Bond lengths****Bond angles****Torsions****Rings**

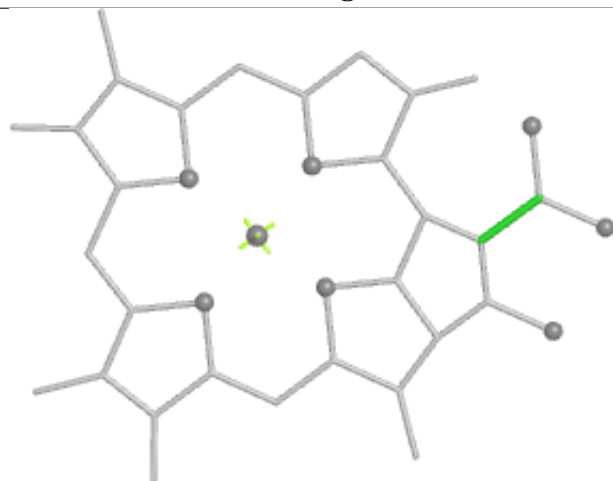
## Ligand CLA 1 614



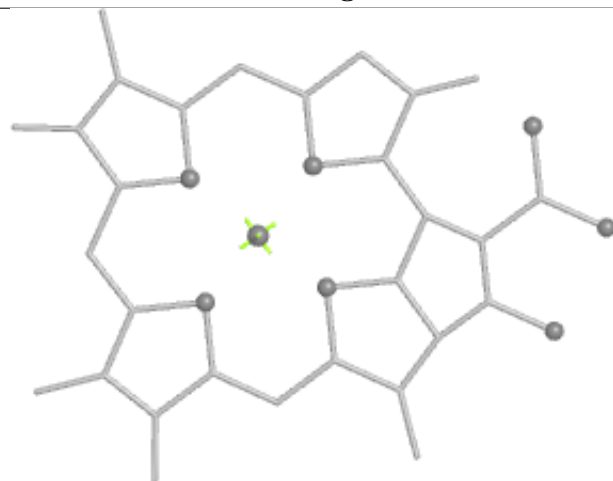
Bond lengths



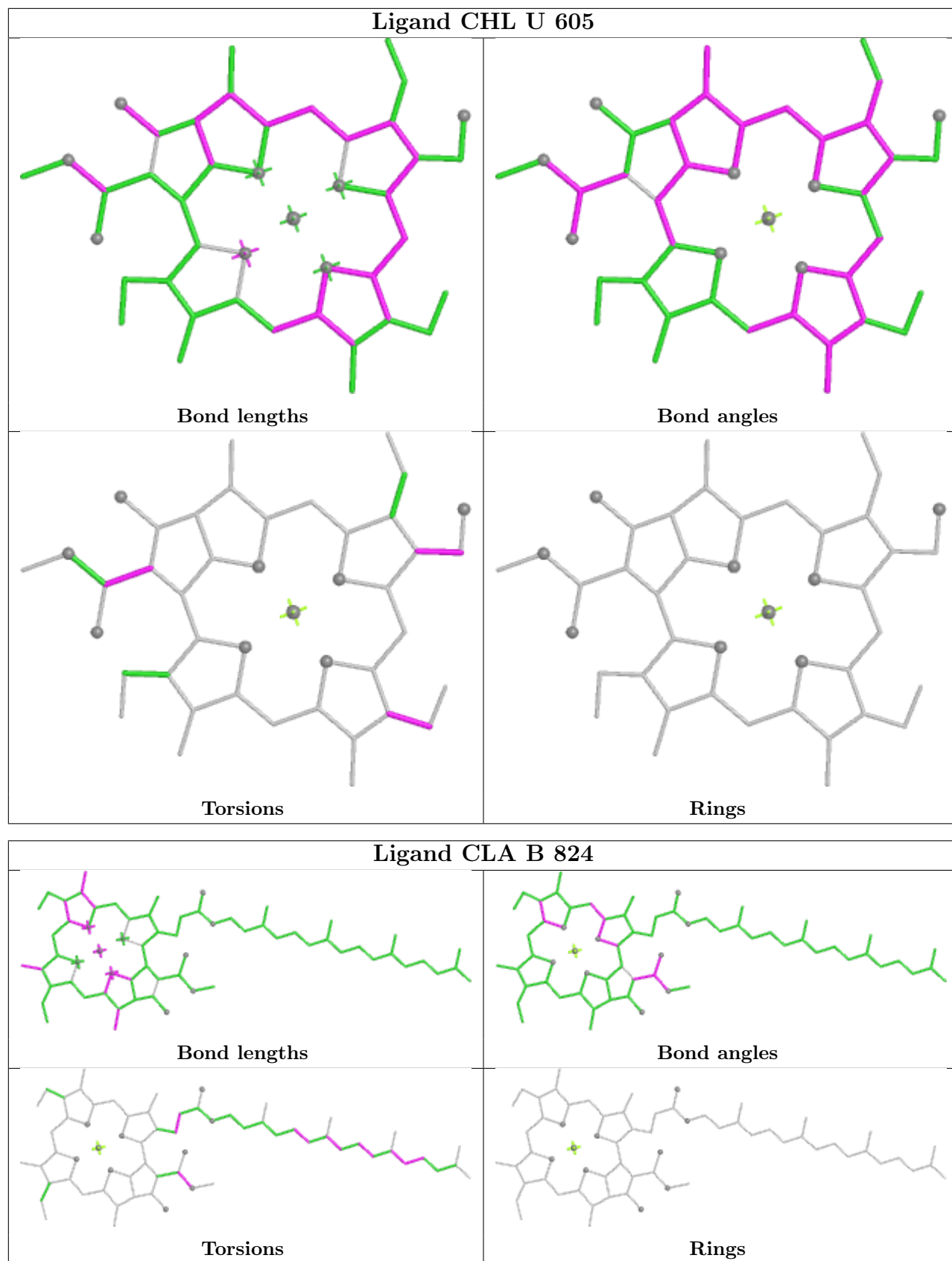
Bond angles

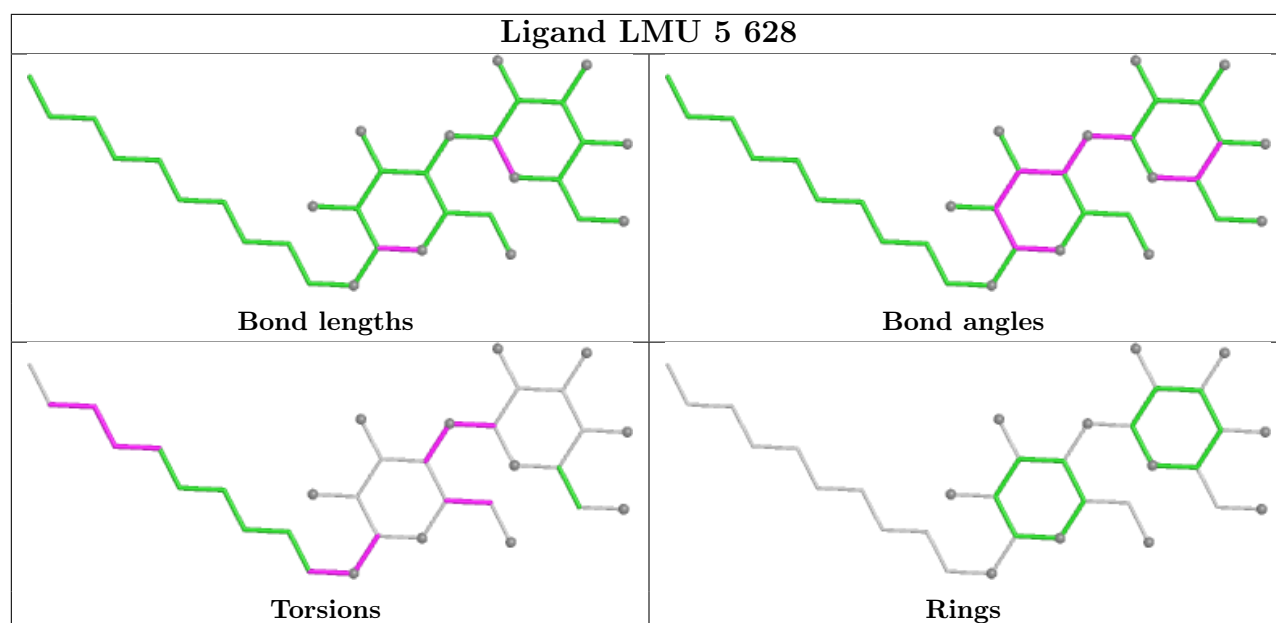
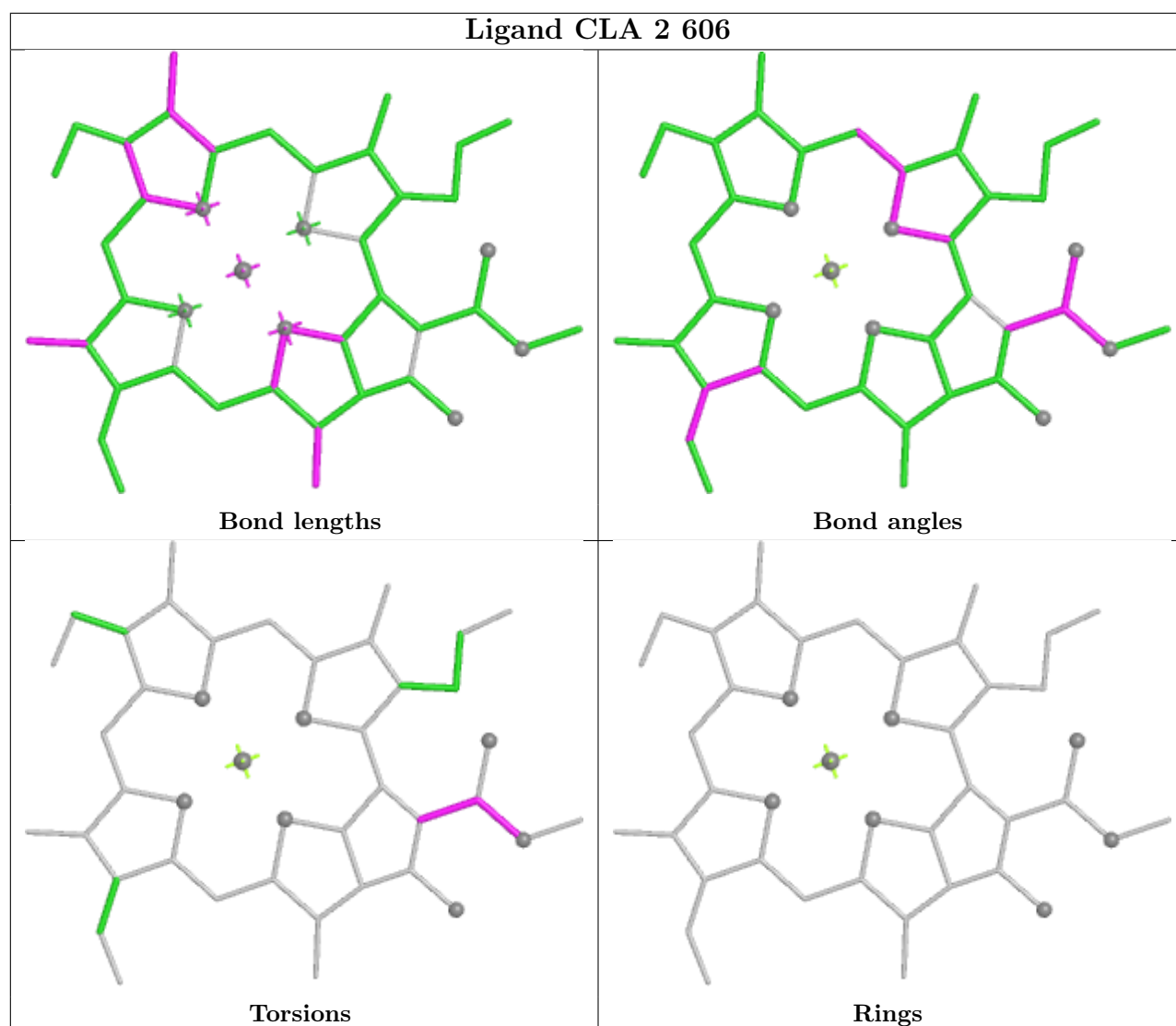


Torsions

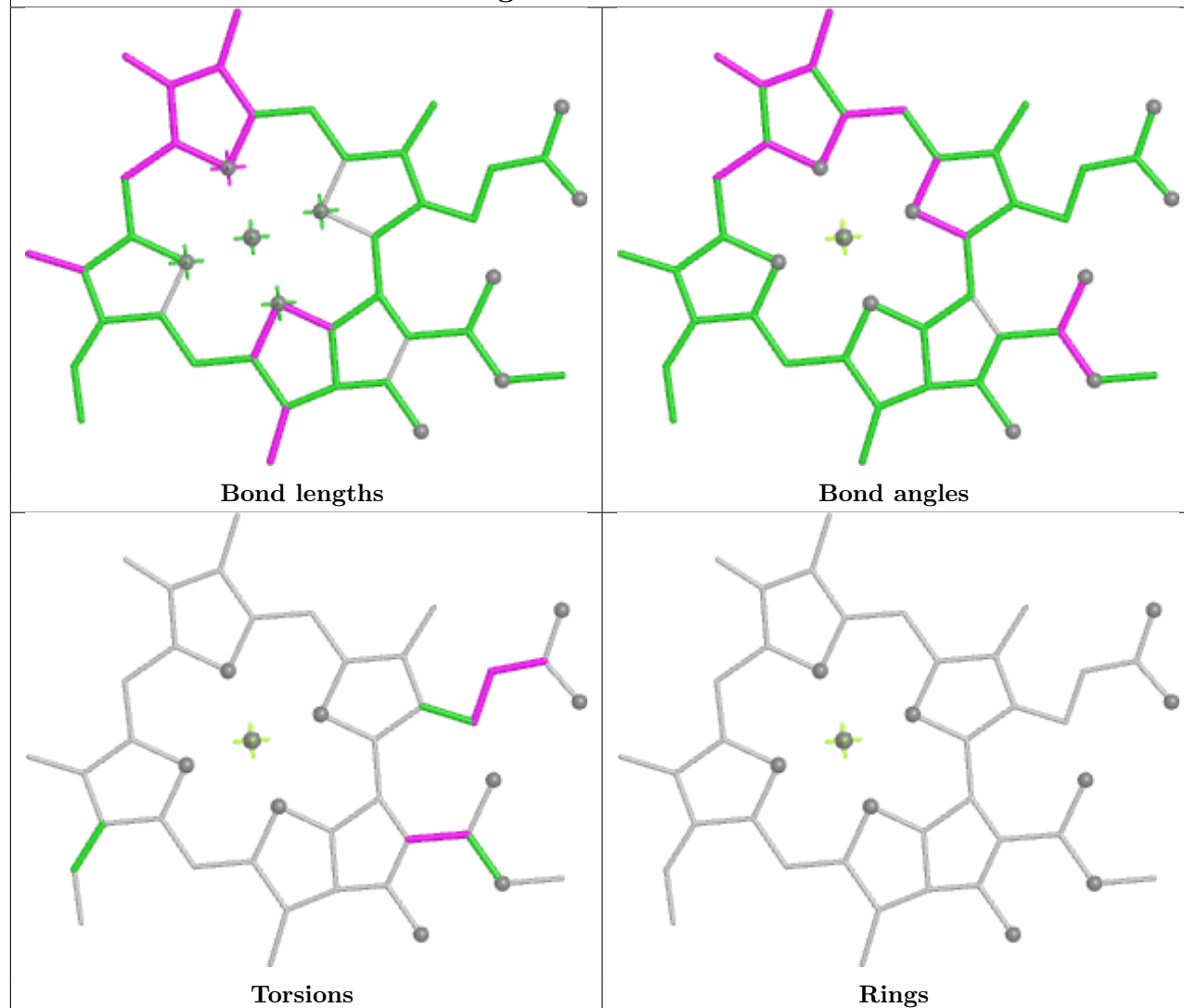


Rings

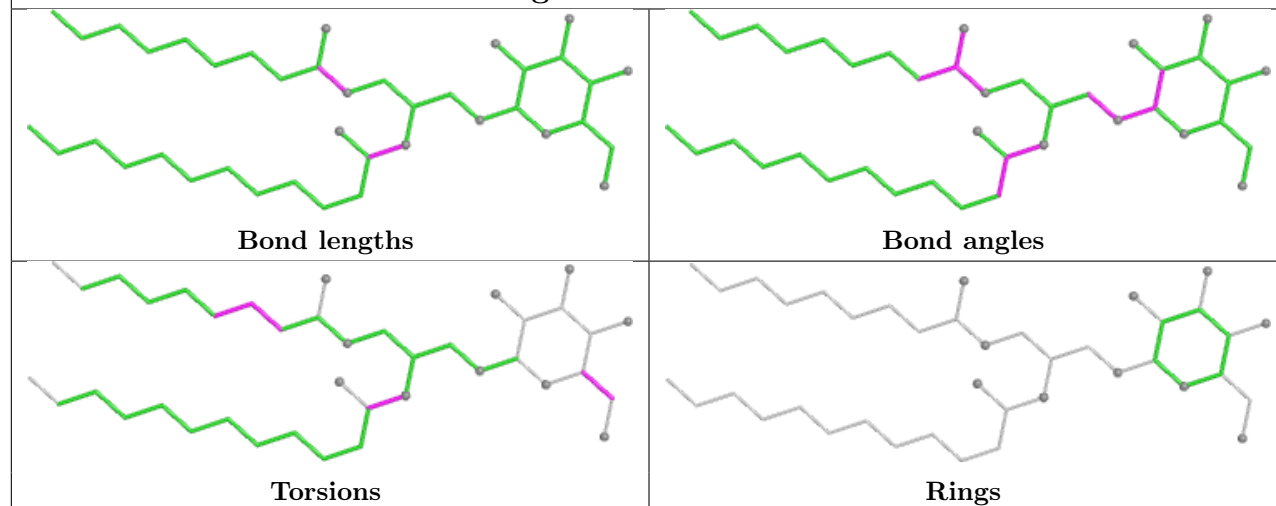


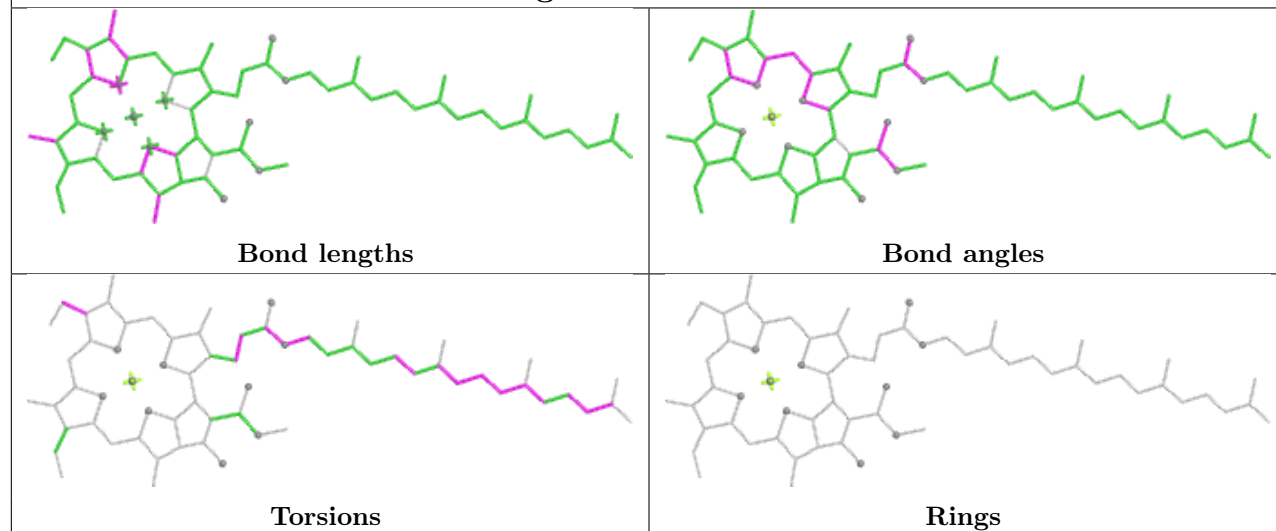
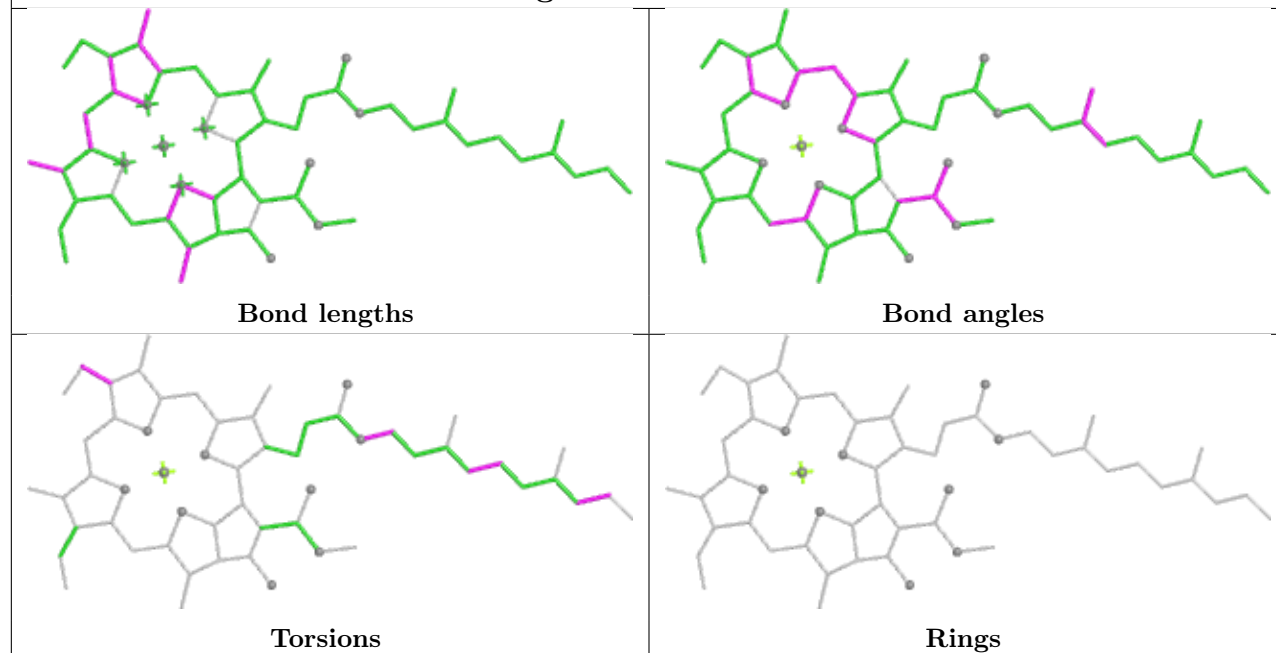
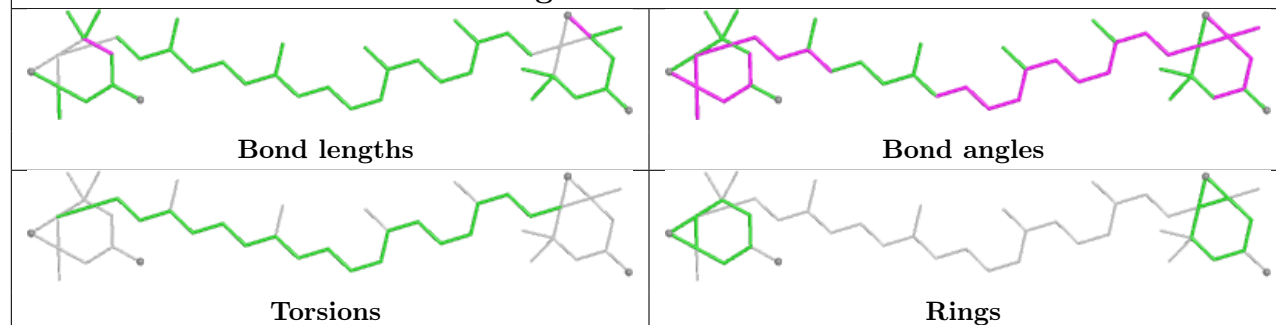


## Ligand CLA 9 603

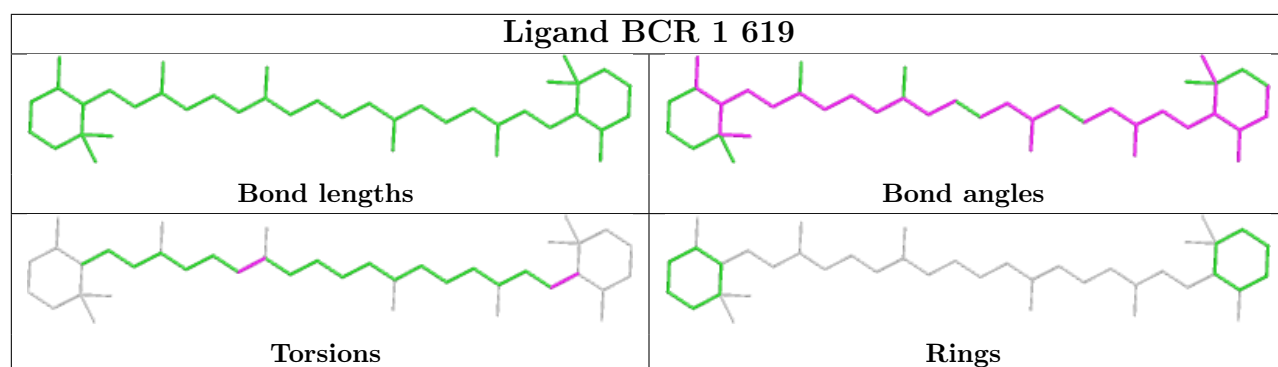
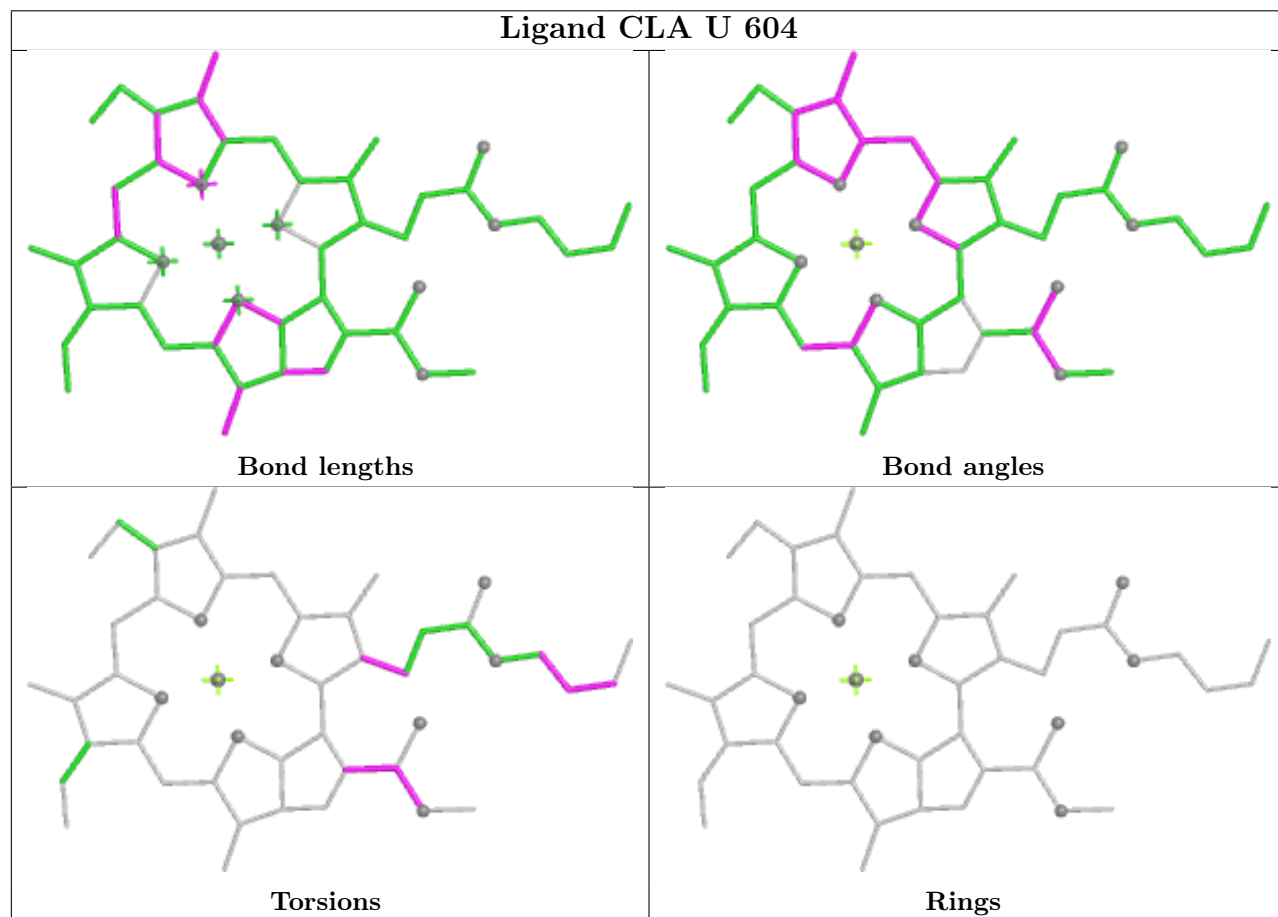


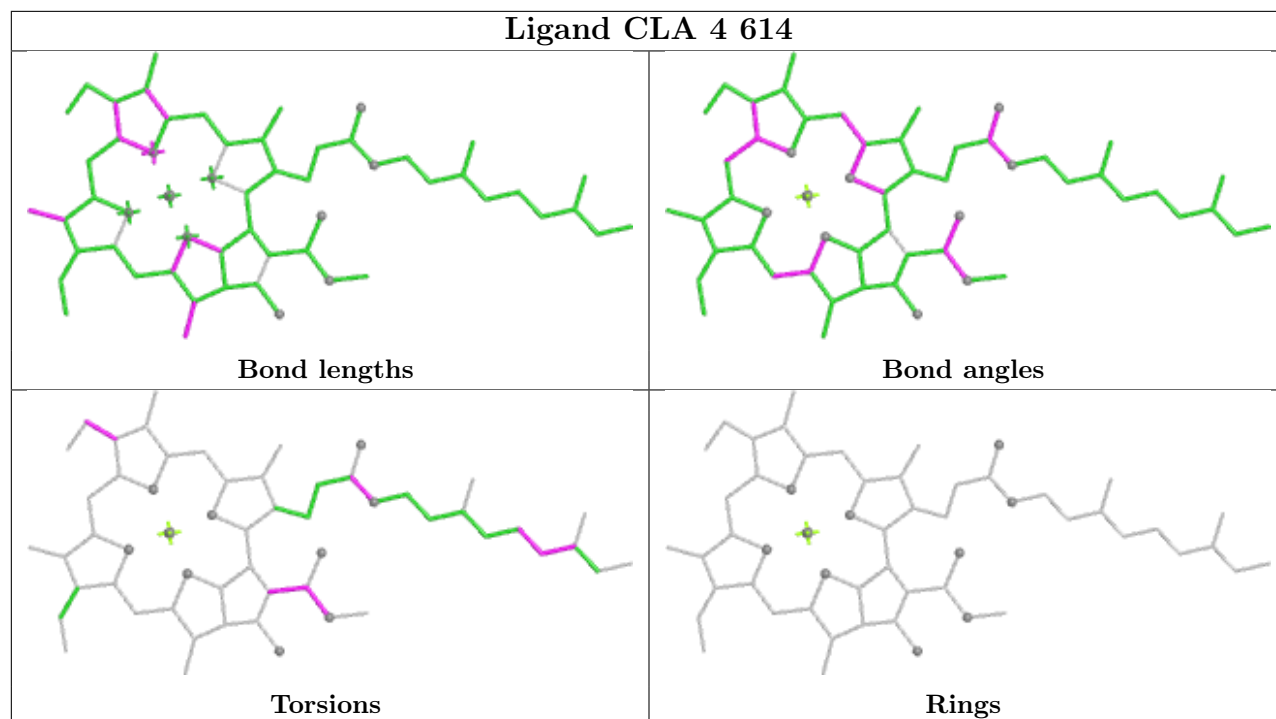
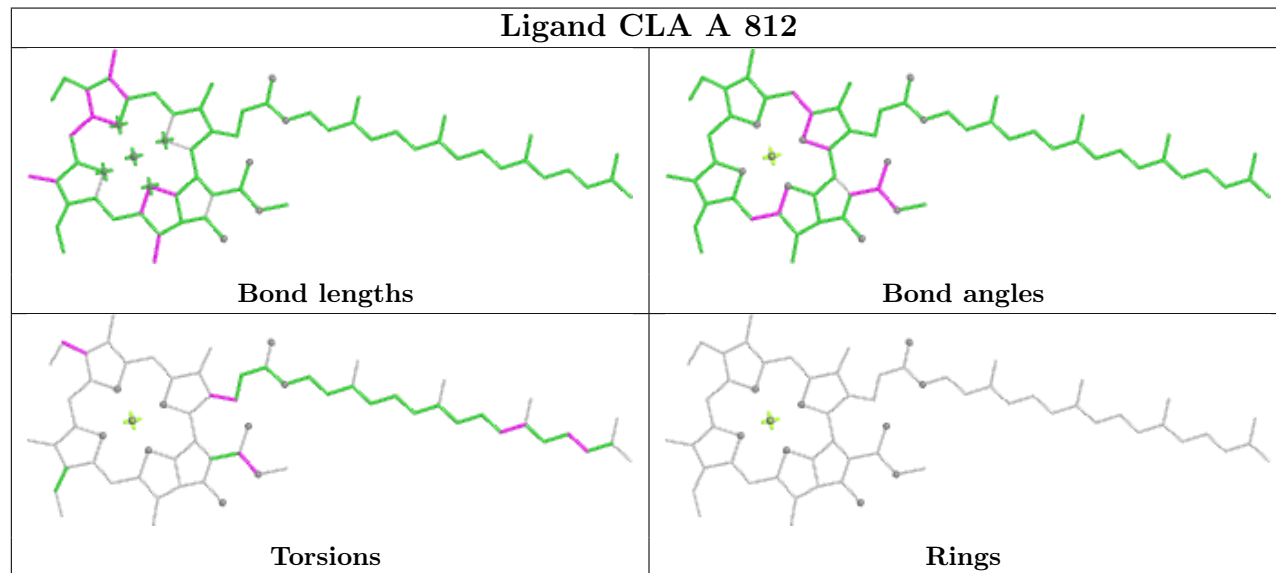
## Ligand LMG 4 624



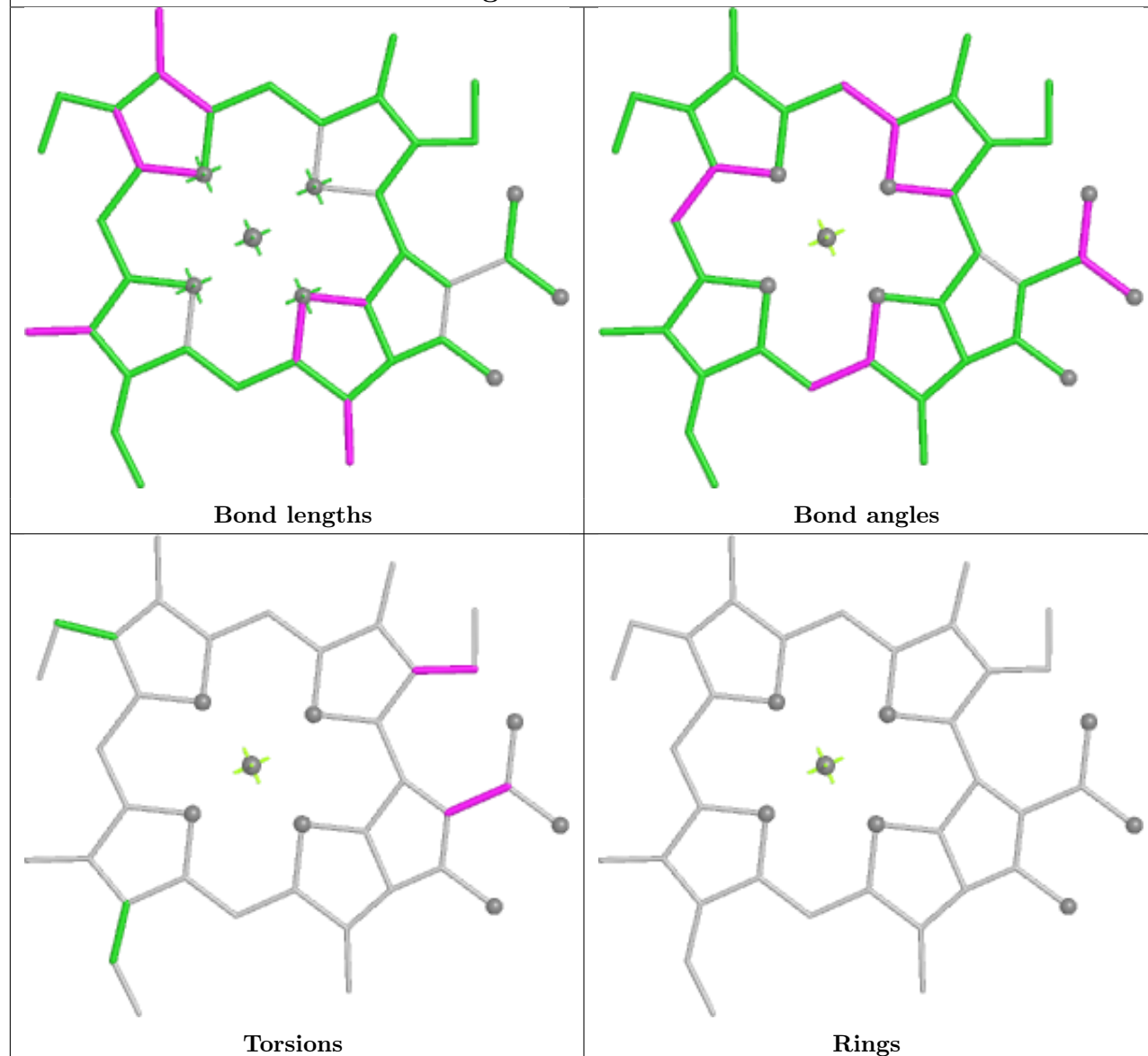
**Ligand CLA 8 613****Ligand CLA 9 610****Ligand XAT 3 619**



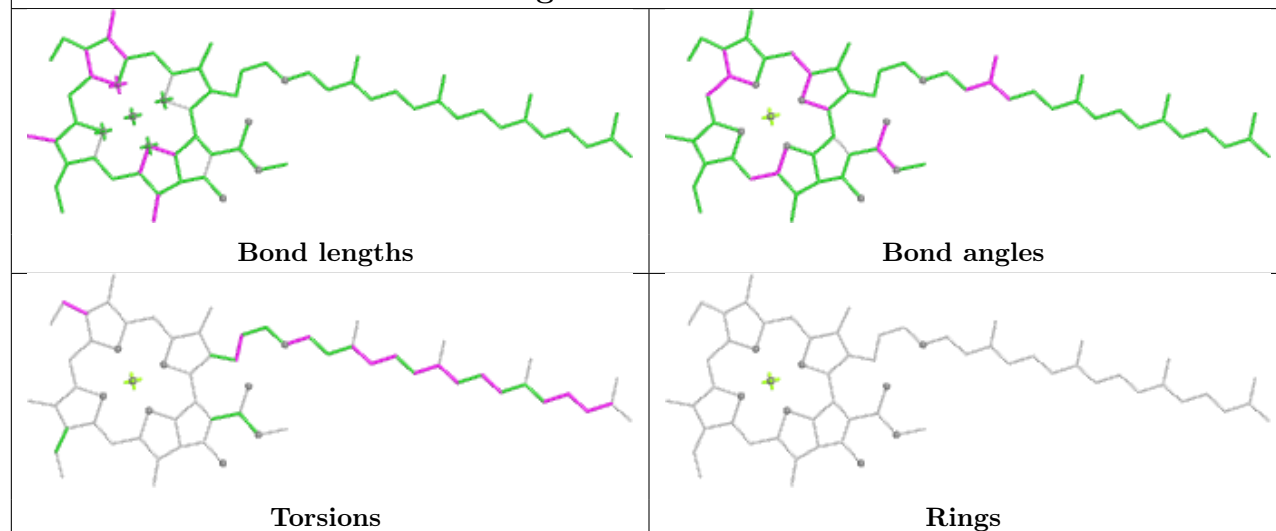


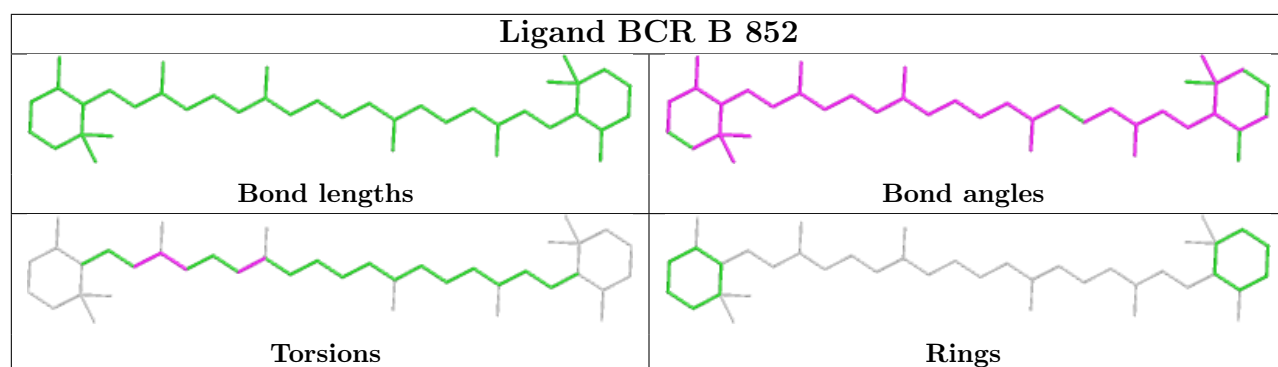
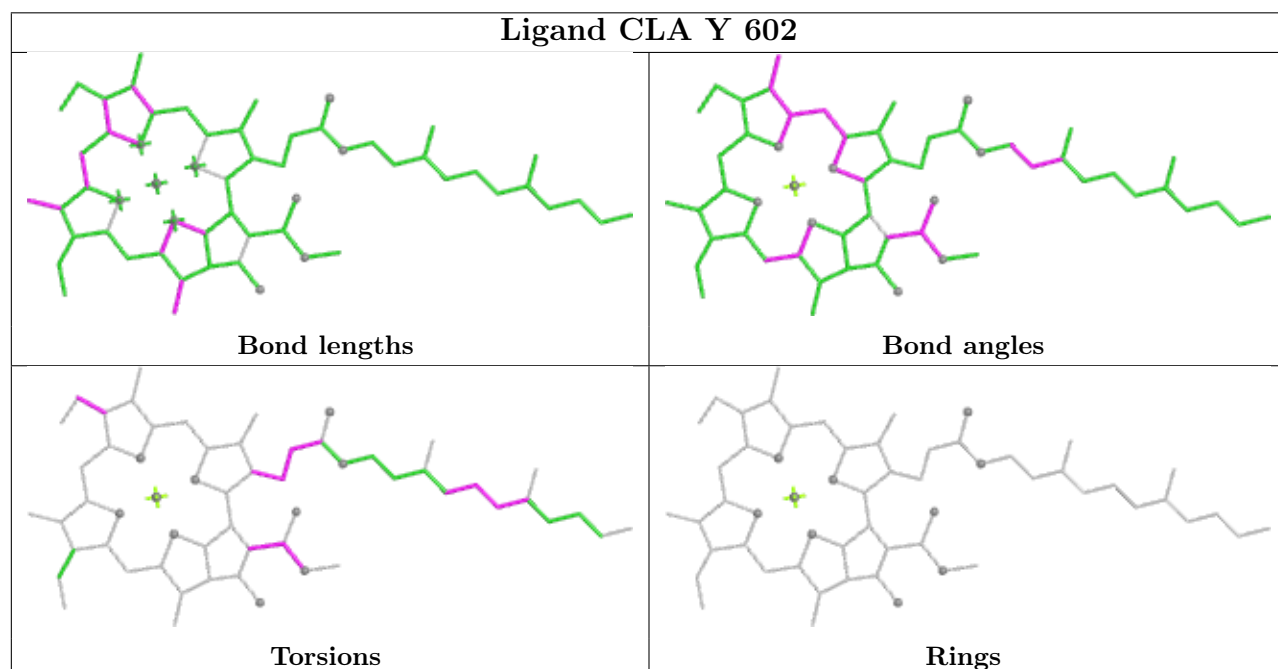
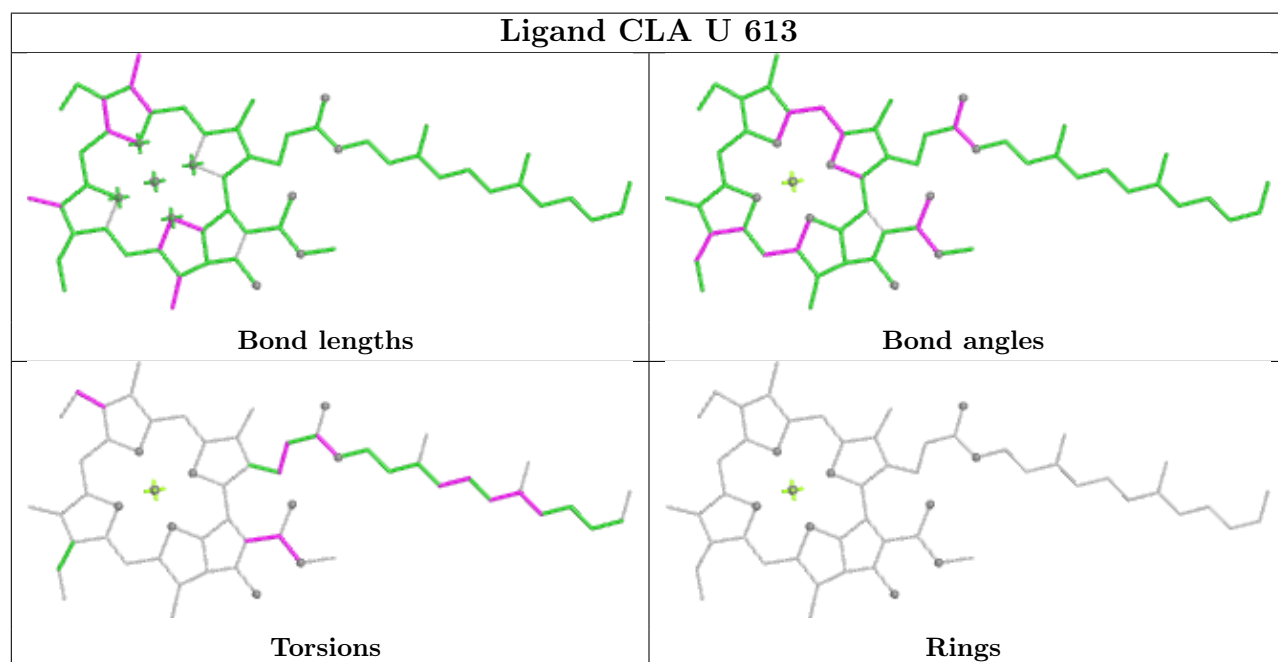
**Ligand CLA 4 614****Ligand CLA A 812**

## Ligand CLA 6 612

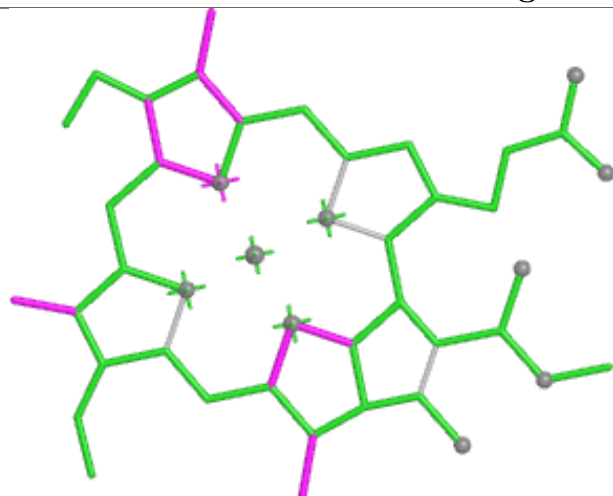


## Ligand CLA 5 613

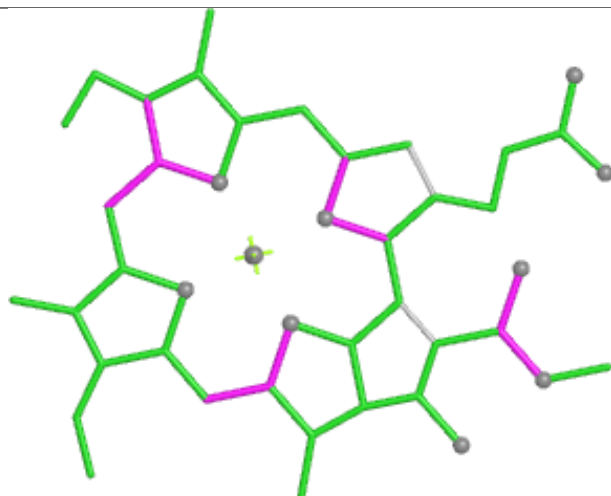




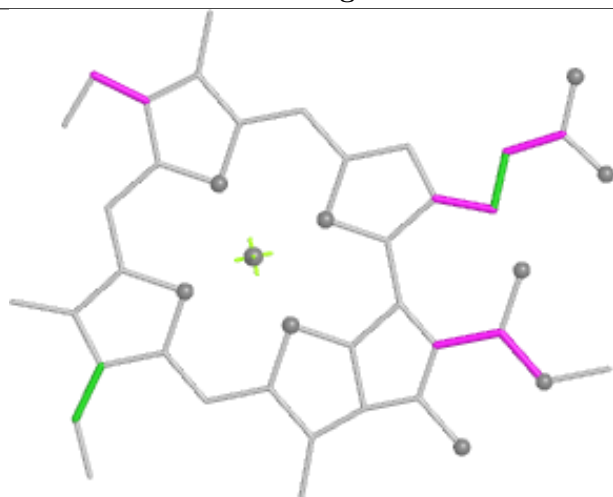
## Ligand CLA 5 614



Bond lengths



Bond angles

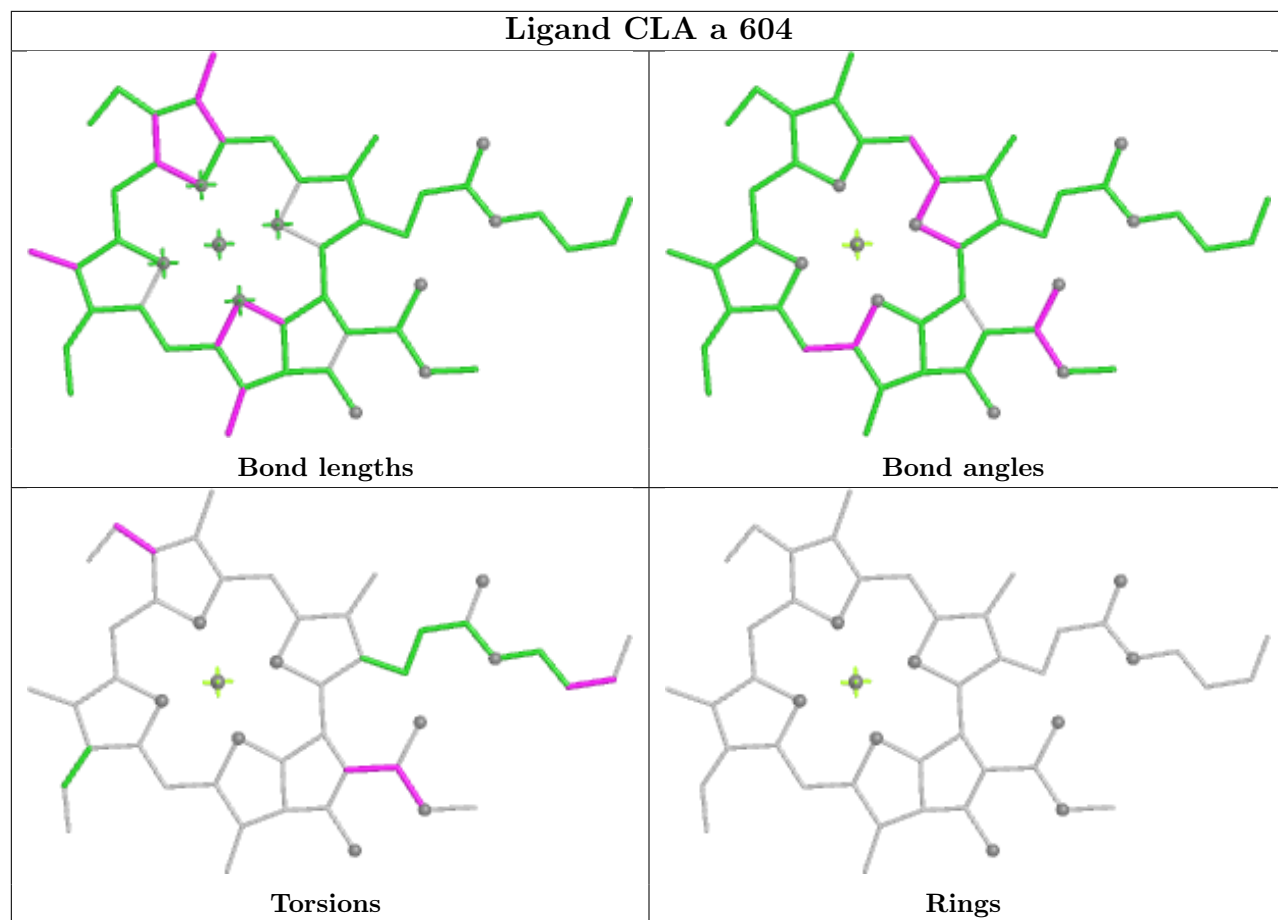


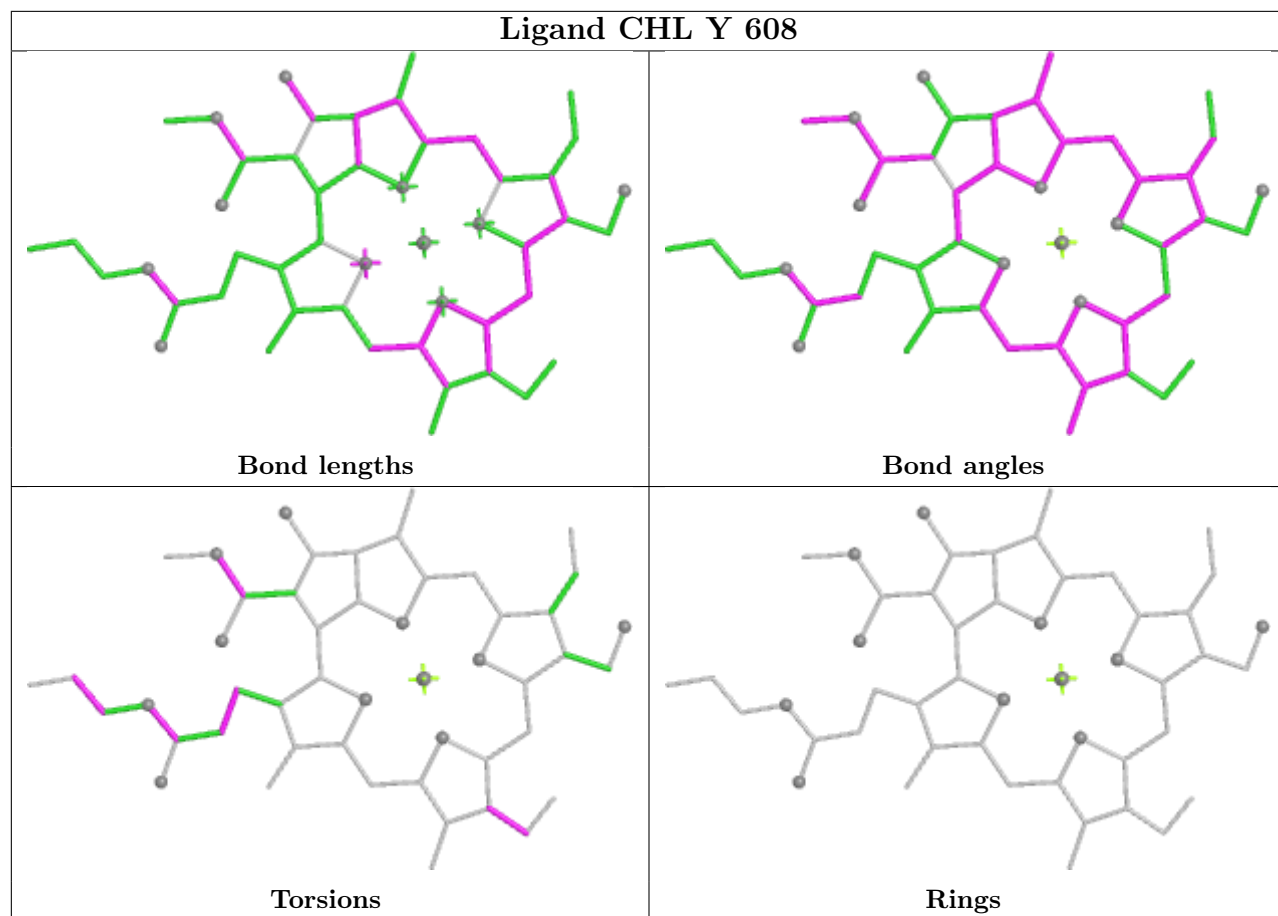
Torsions



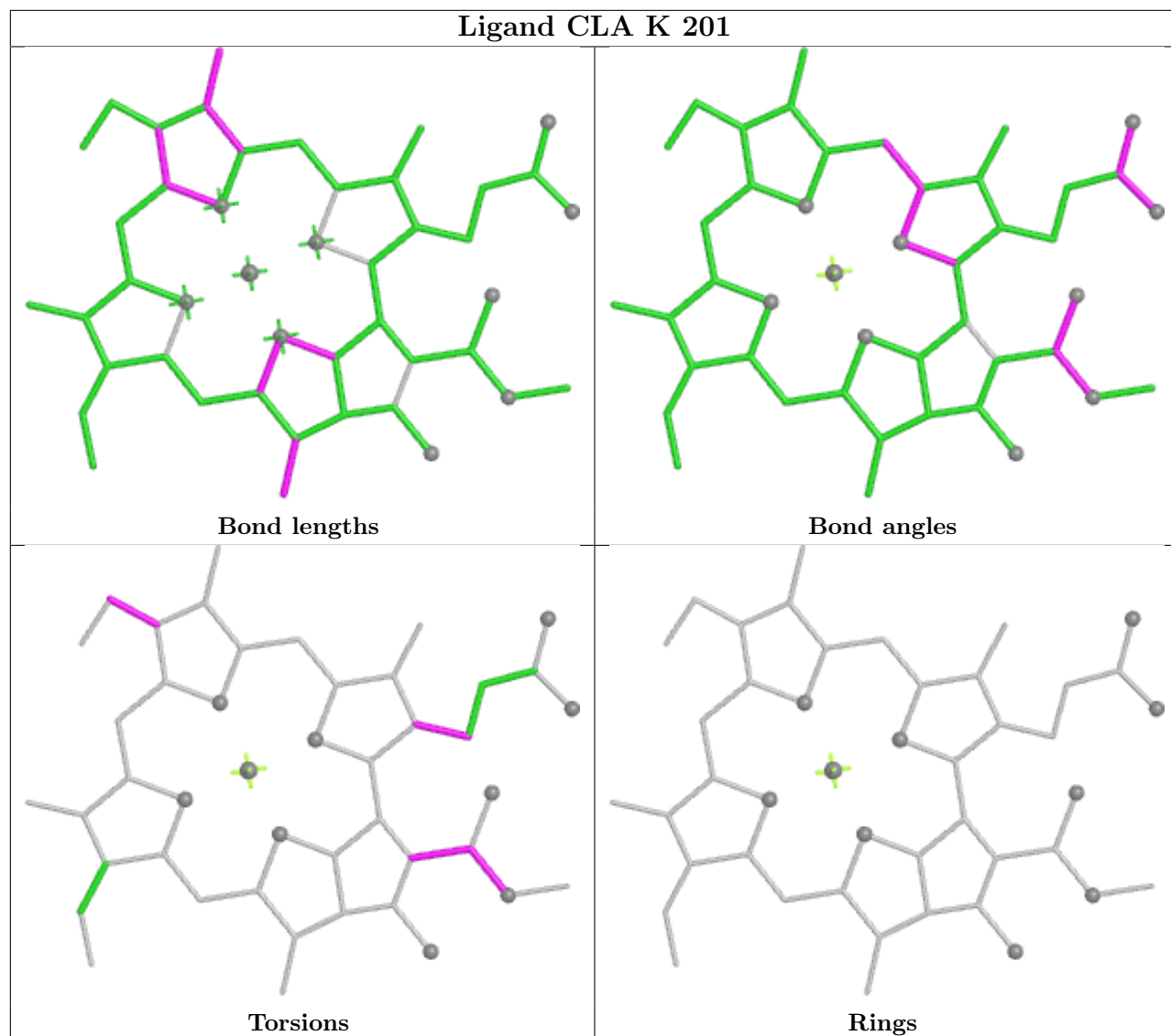
Rings

## Ligand CLA a 604

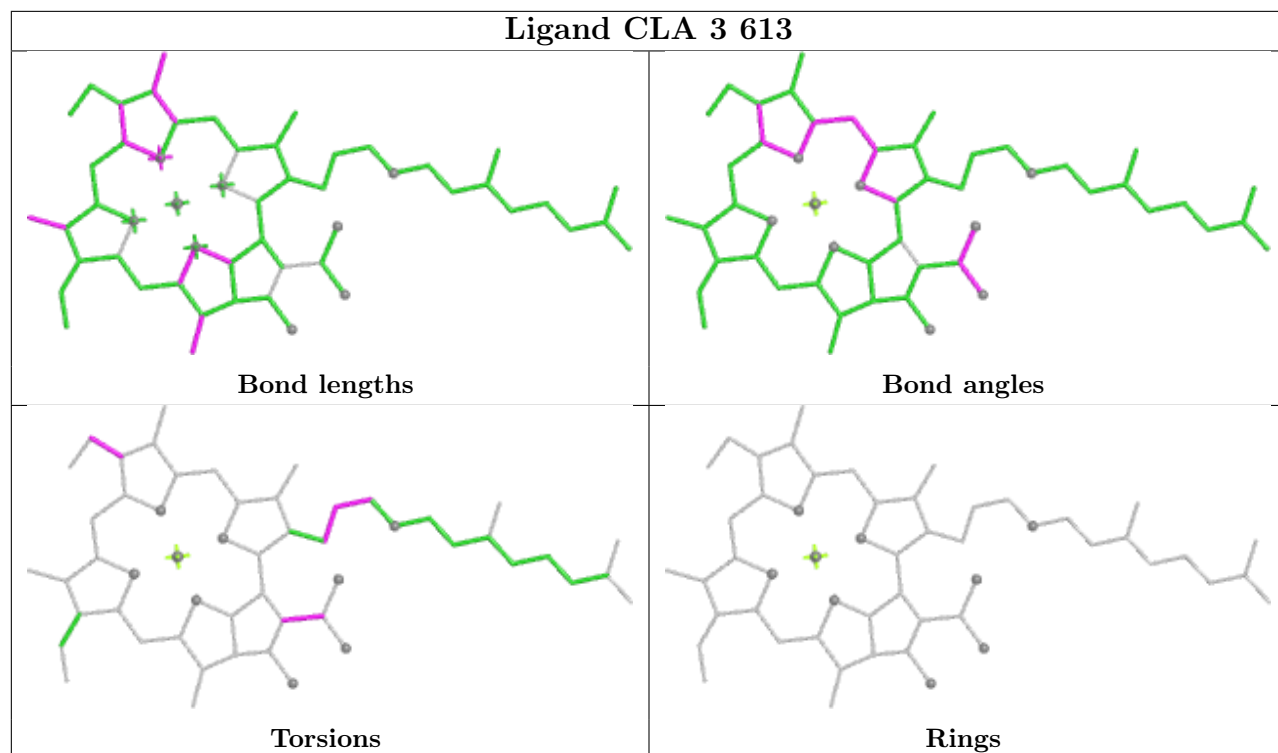
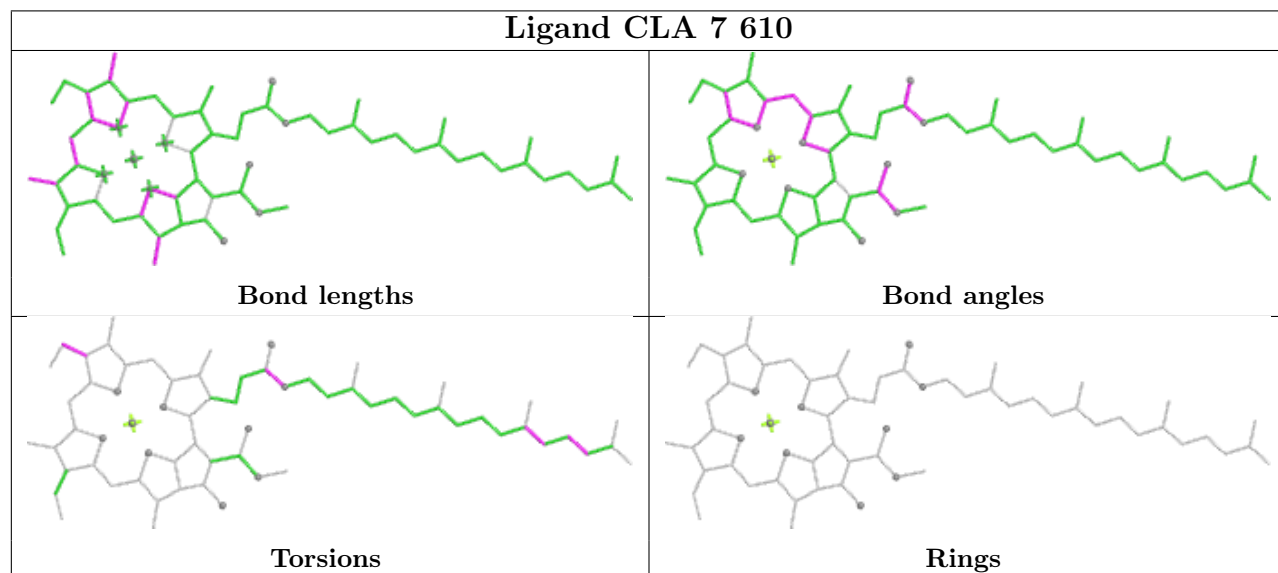




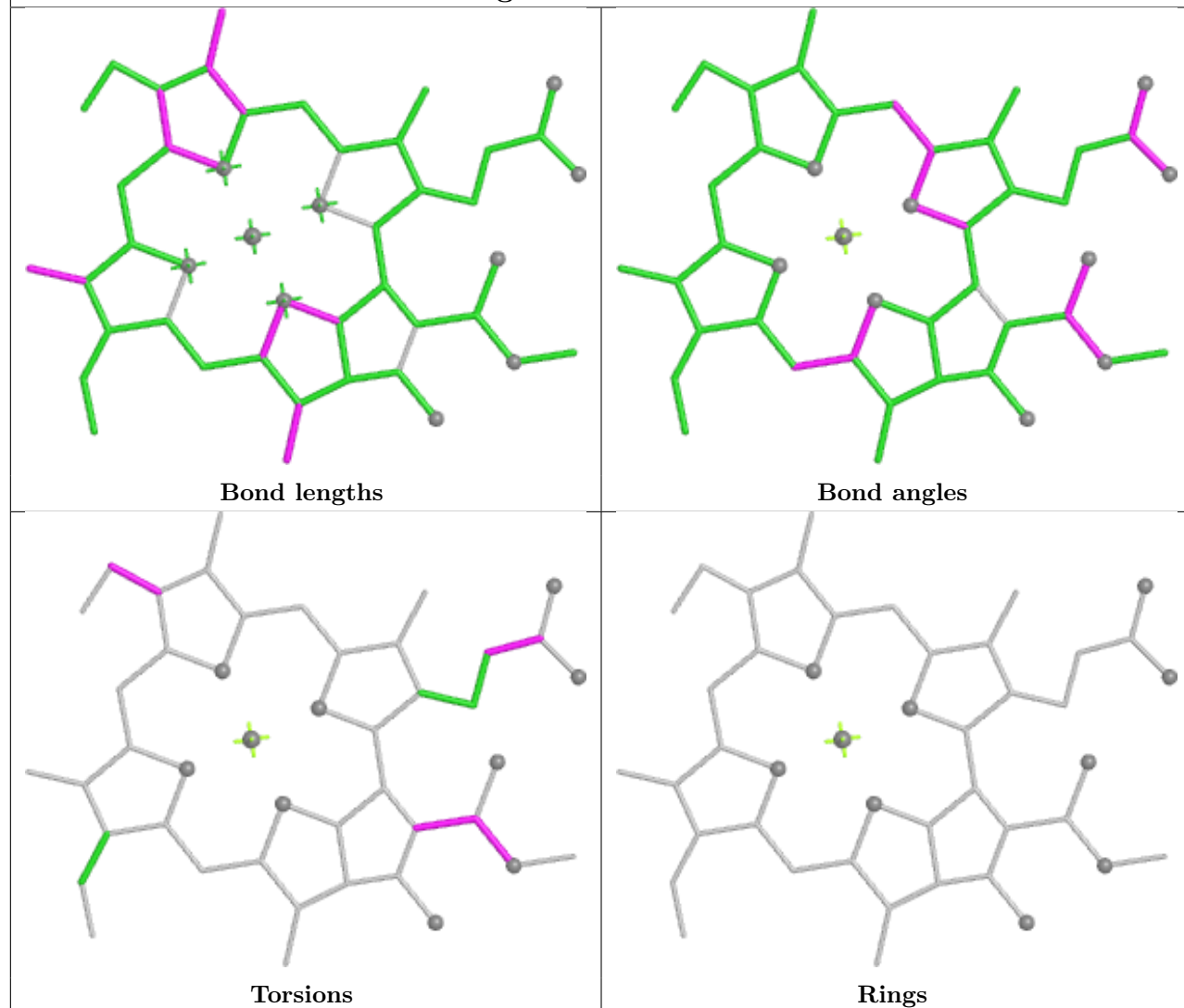
## Ligand CLA K 201



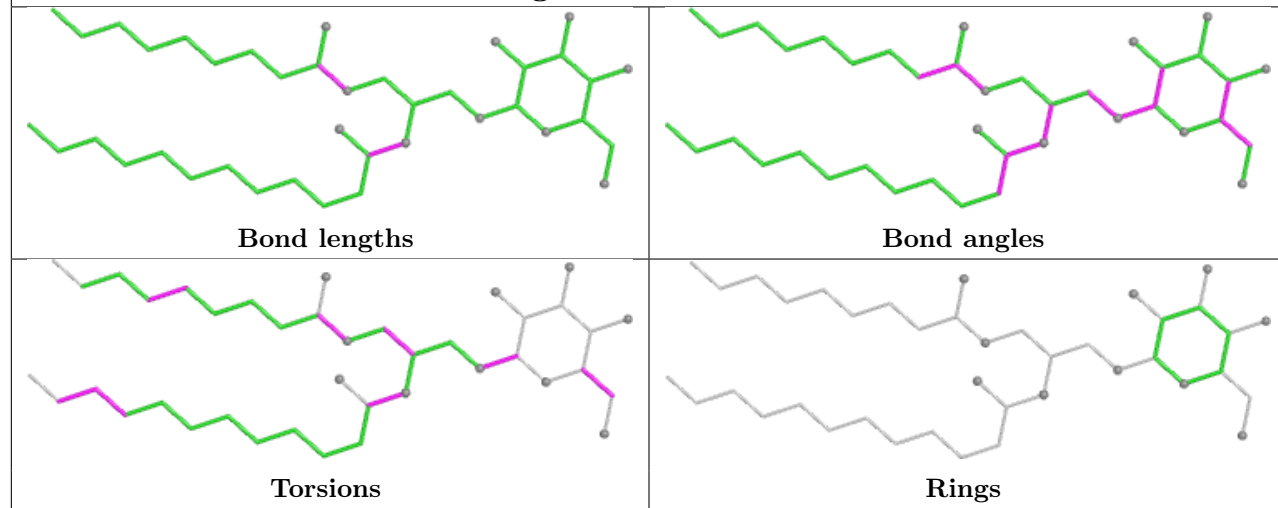


**Ligand CLA 3 613****Ligand CLA 7 610**

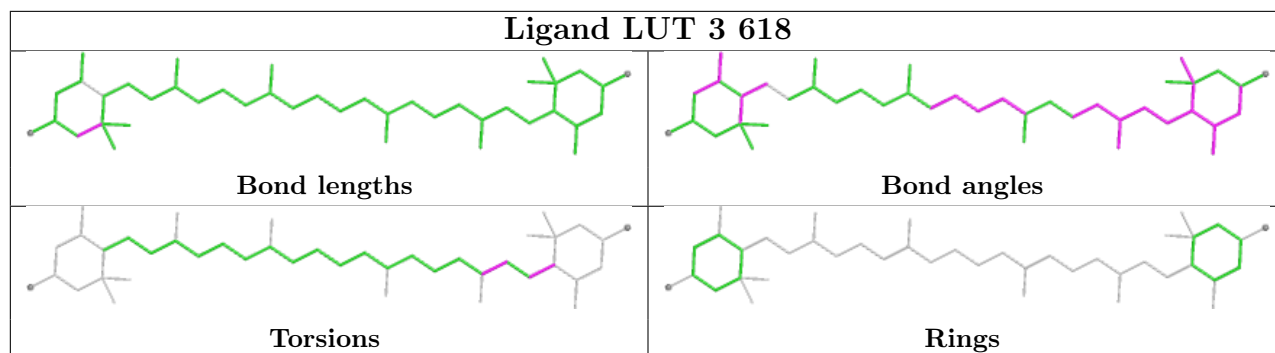
## Ligand CLA 9 601



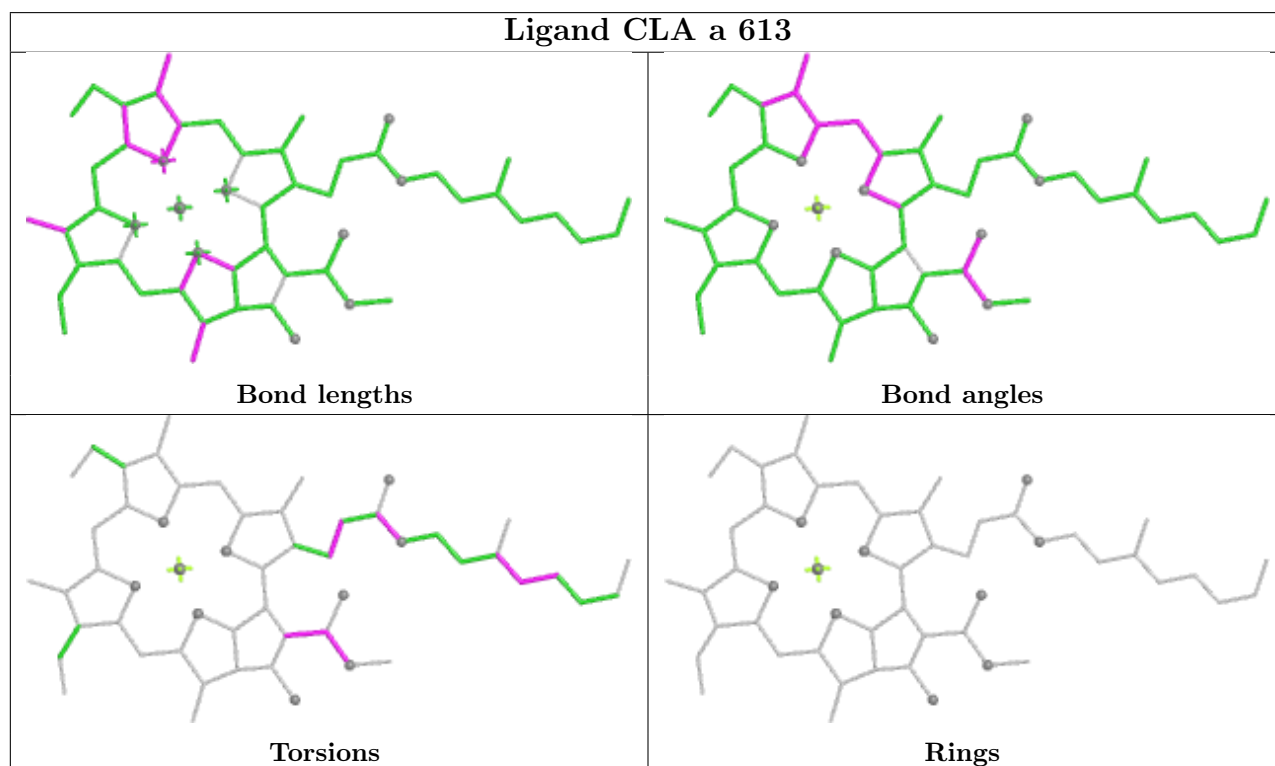
## Ligand LMG J 104



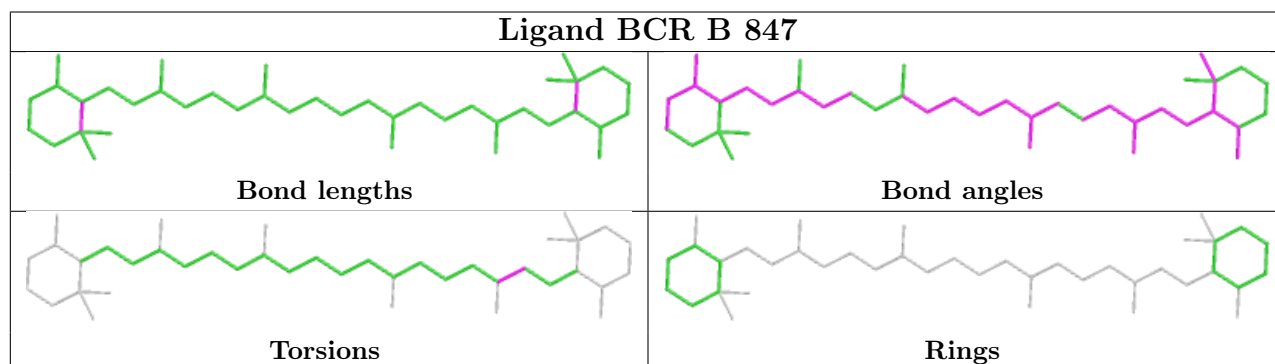
## Ligand LUT 3 618

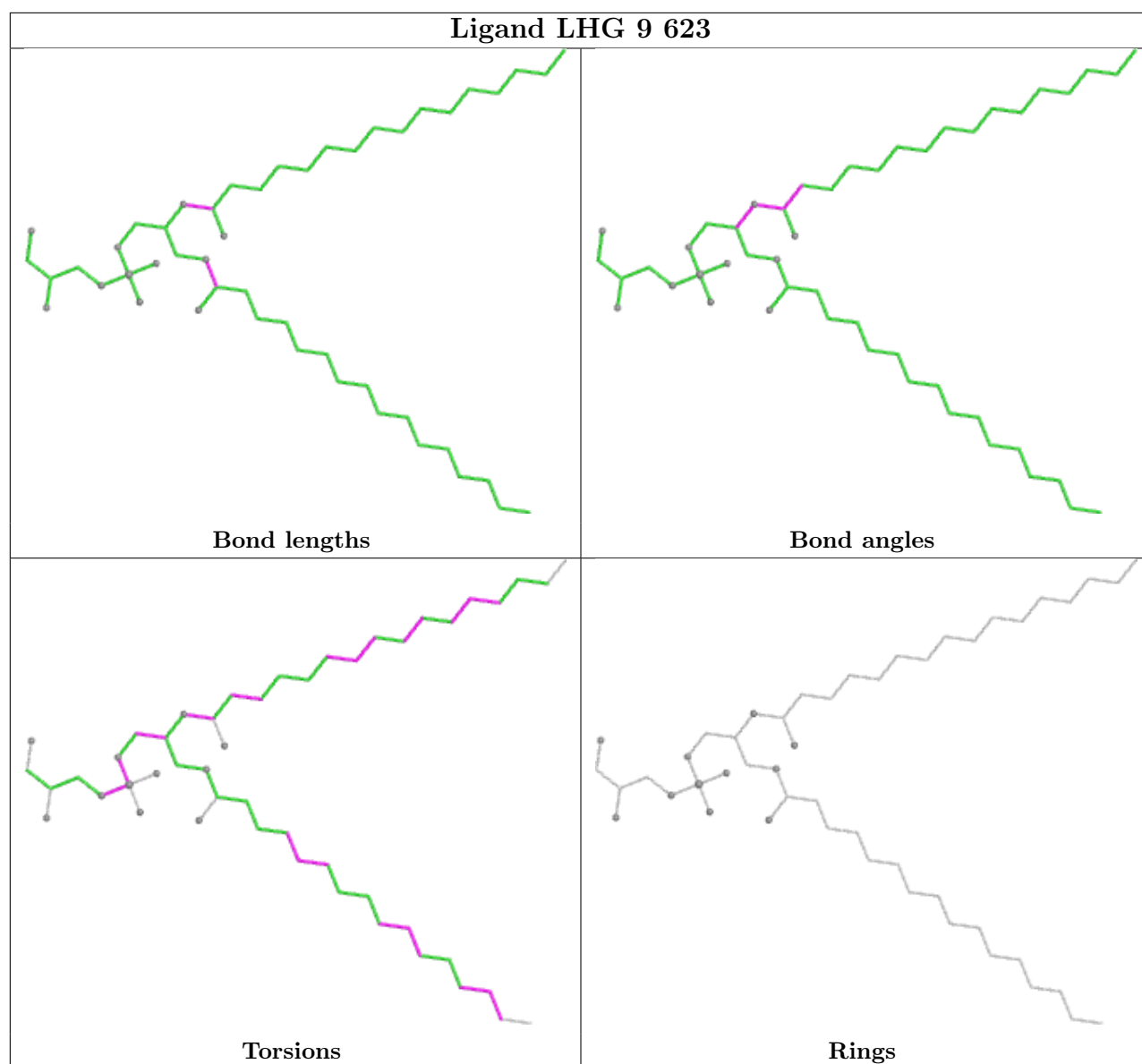


## Ligand CLA a 613



## Ligand BCR B 847





## 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.

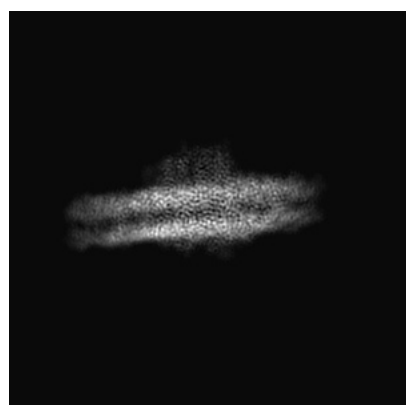
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30926. 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](#)

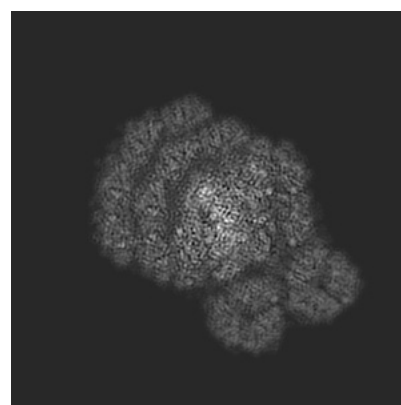
#### 6.1.1 Primary map



X



Y

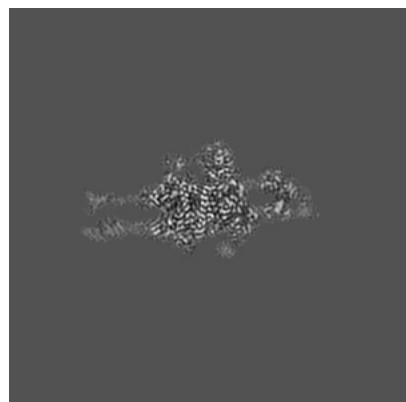


Z

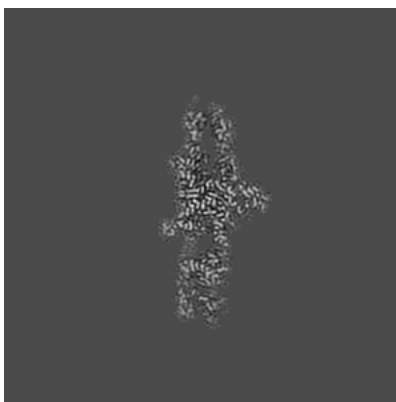
The images above show the map projected in three orthogonal directions.

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

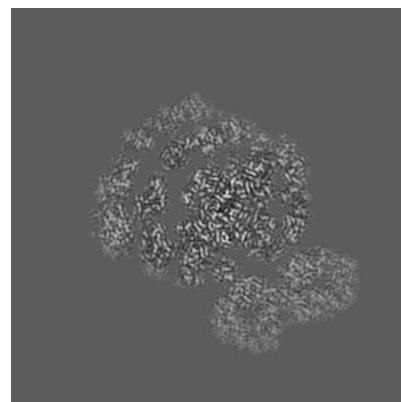
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

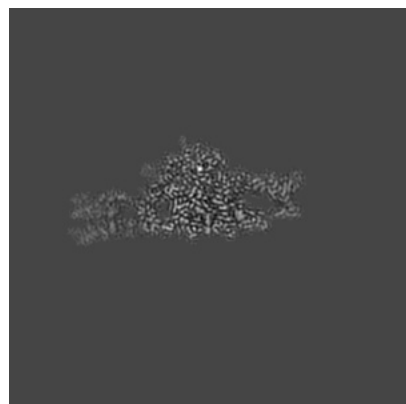


Z Index: 180

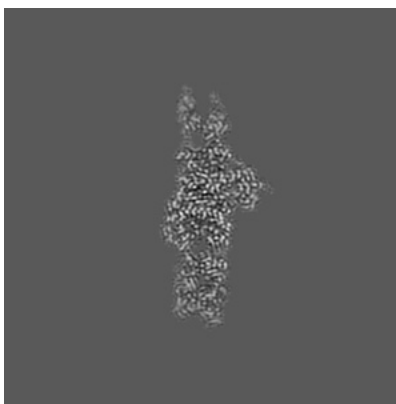
The images above show central slices of the map in three orthogonal directions.

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

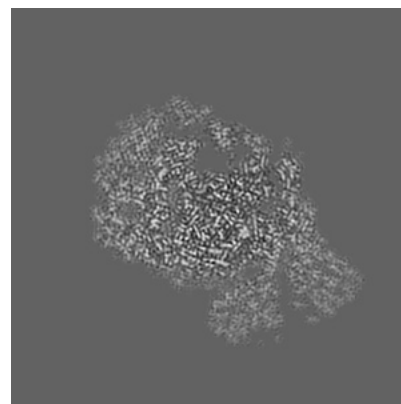
### 6.3.1 Primary map



X Index: 194



Y Index: 153

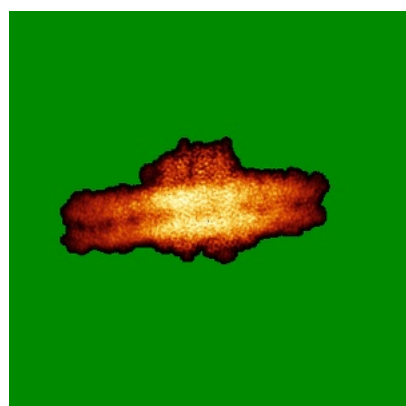


Z Index: 190

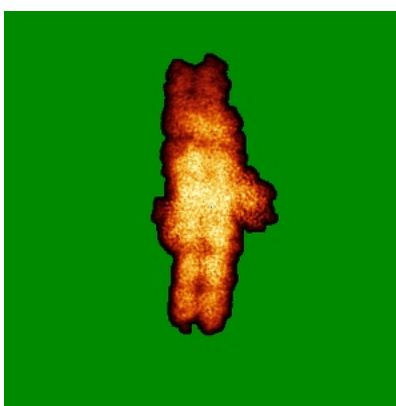
The images above show the largest variance slices of the map in three orthogonal directions.

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

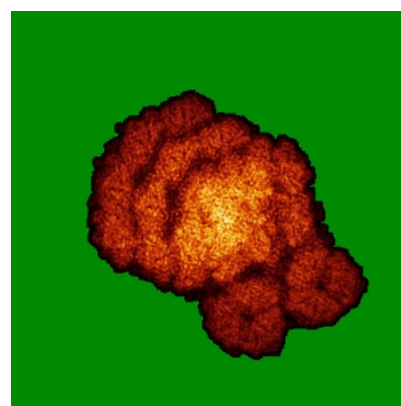
### 6.4.1 Primary map



X



Y

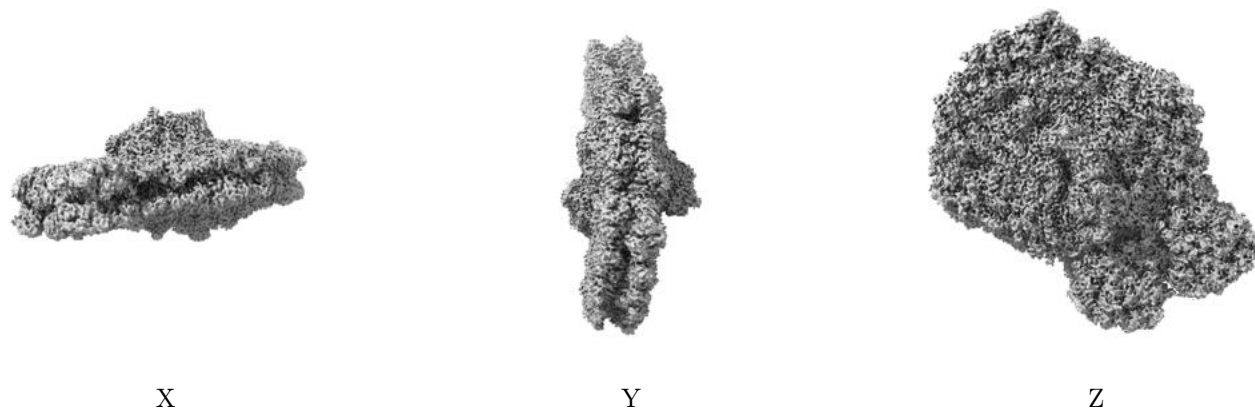


Z

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

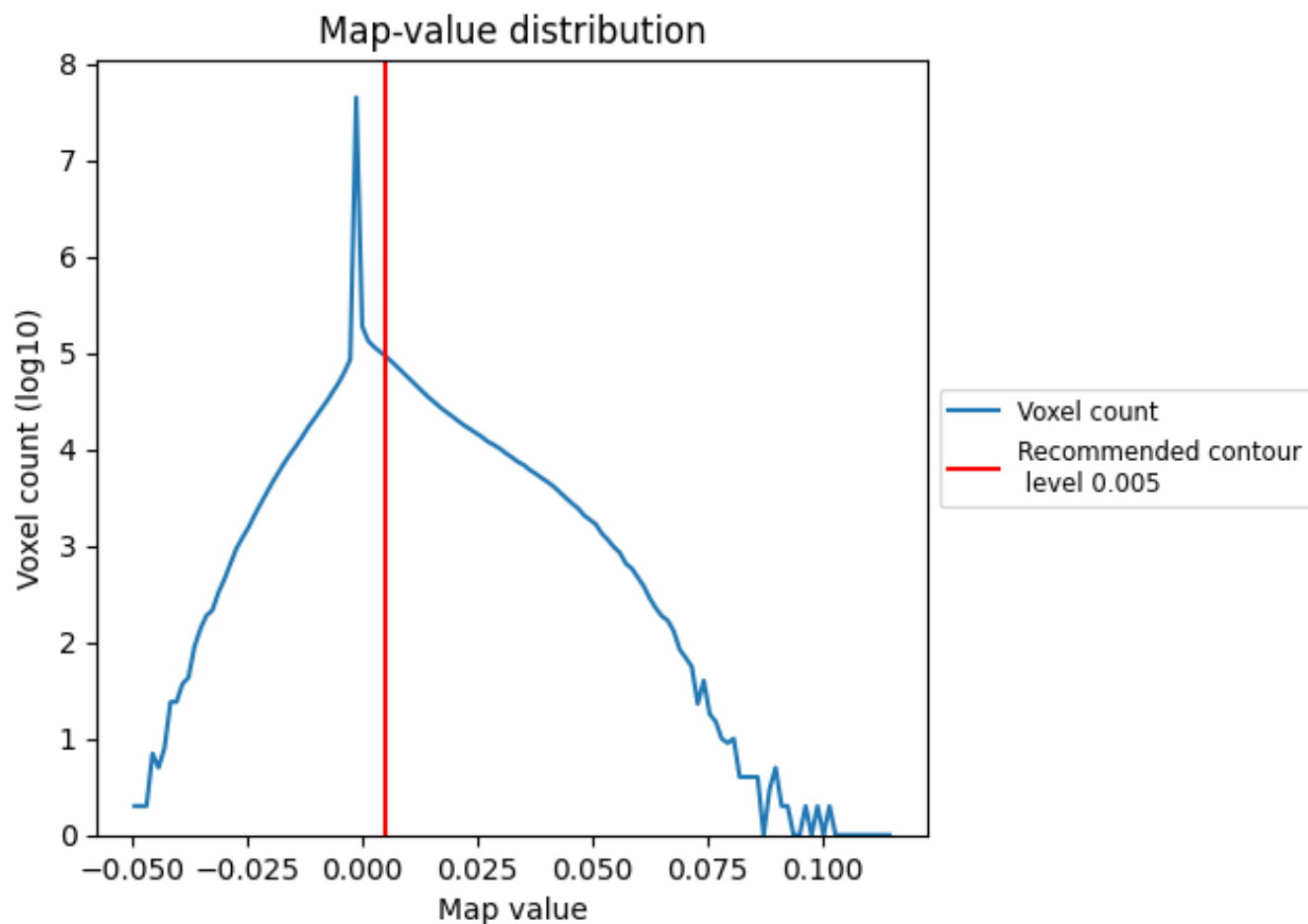
## 6.6 Mask visualisation [i](#)

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.

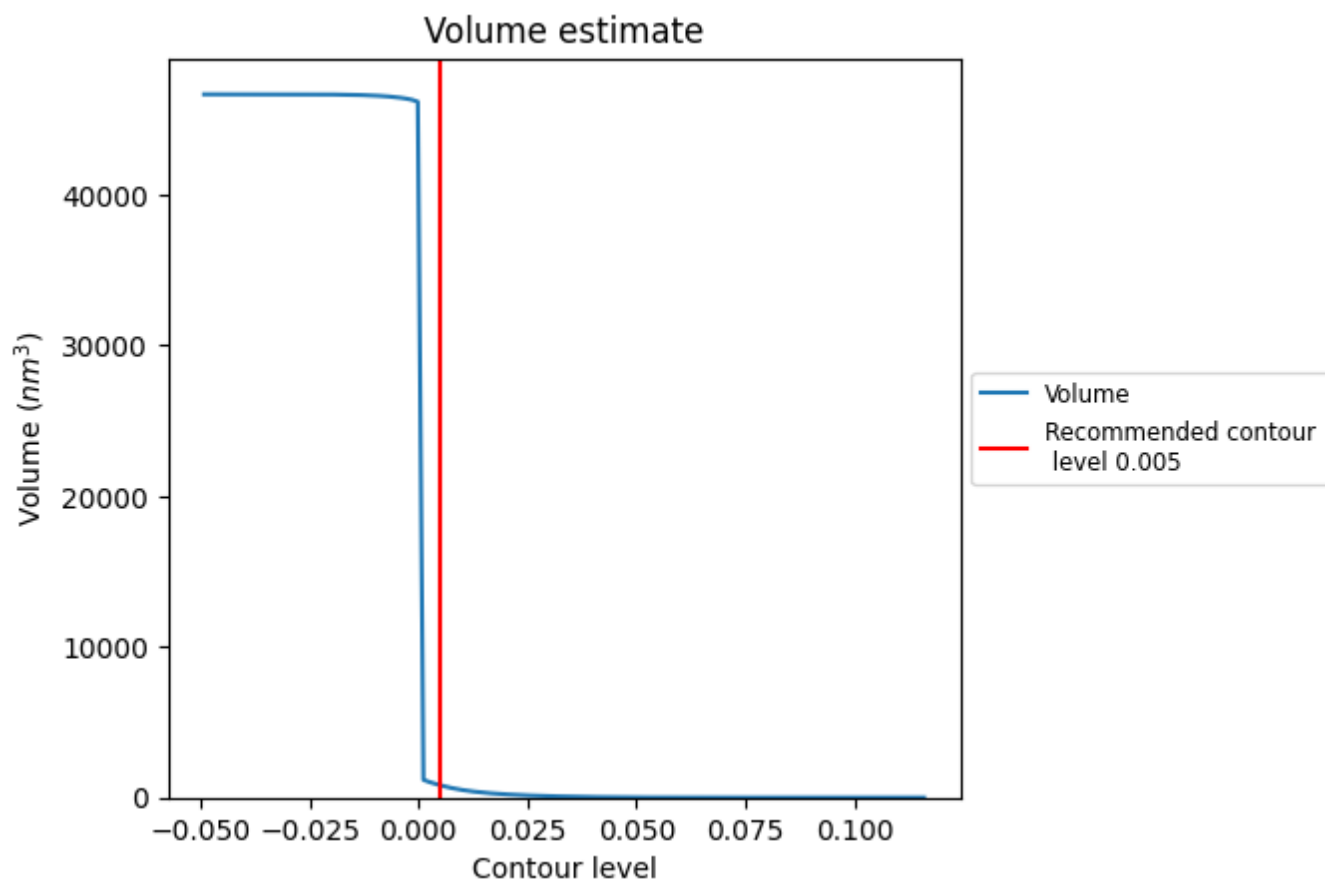
### 7.1 Map-value distribution [i](#)



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.



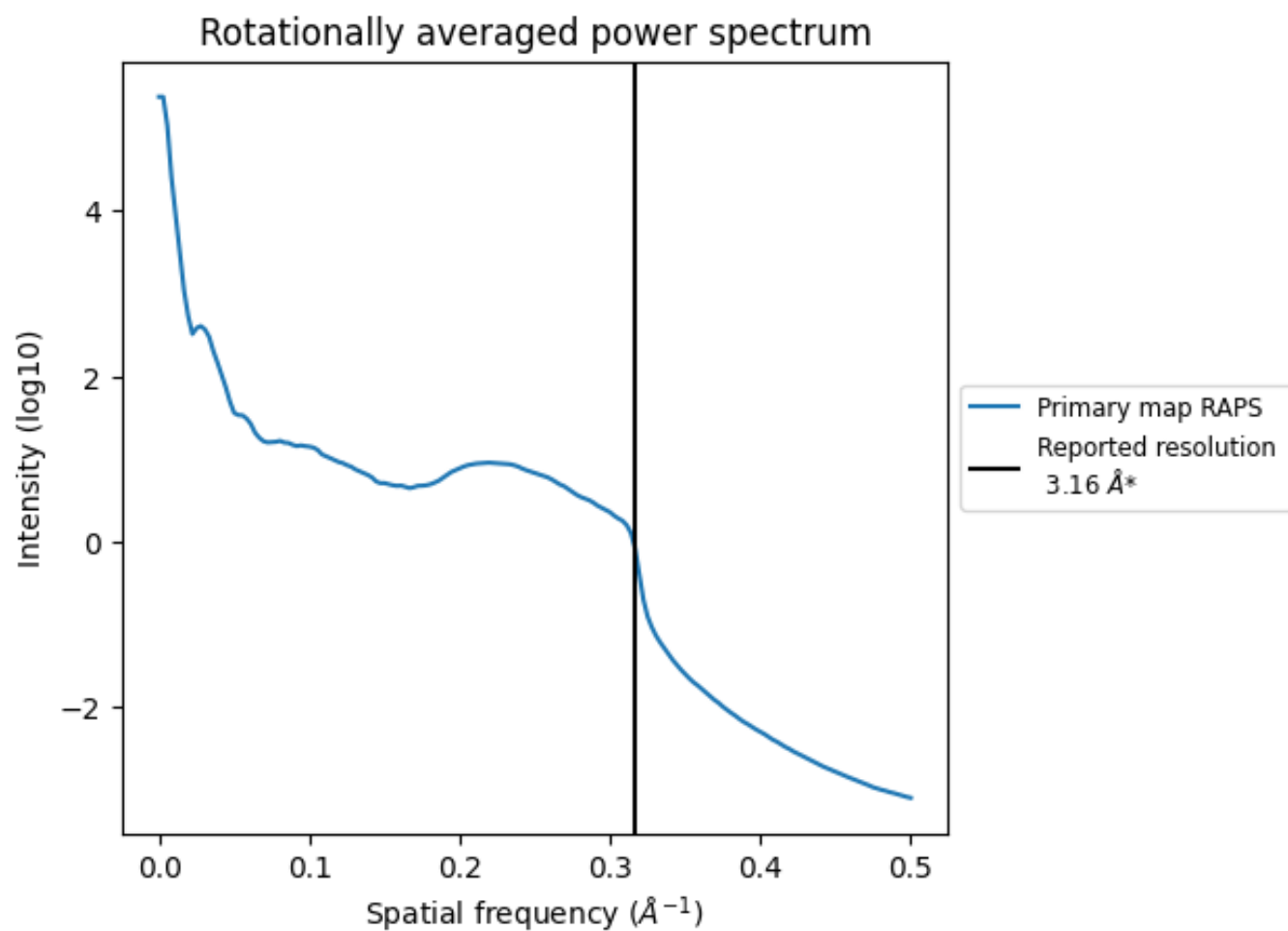
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 811  $\text{nm}^3$ ; this corresponds to an approximate mass of 733 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 0.316  $\text{\AA}^{-1}$

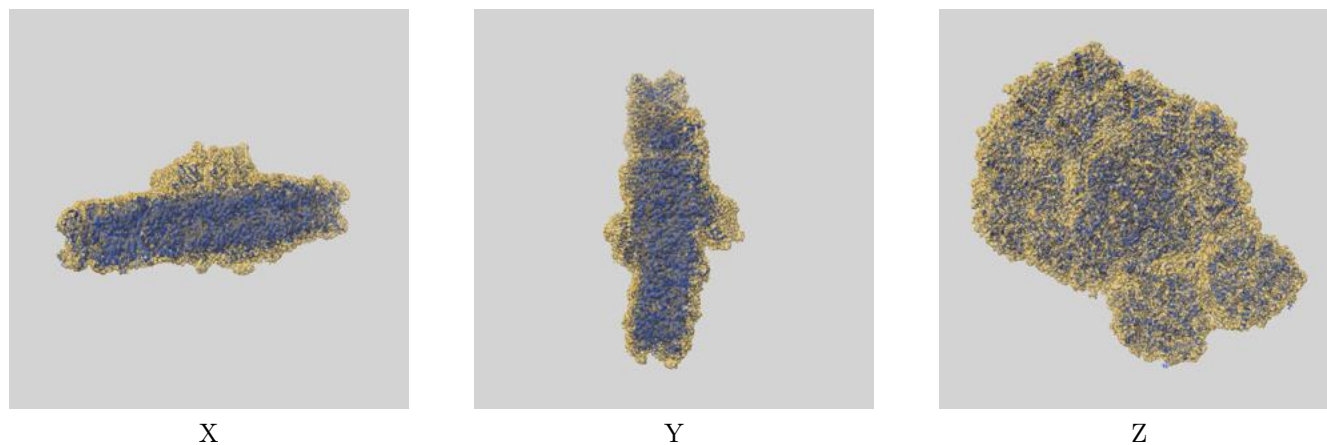
## 8 Fourier-Shell correlation

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

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

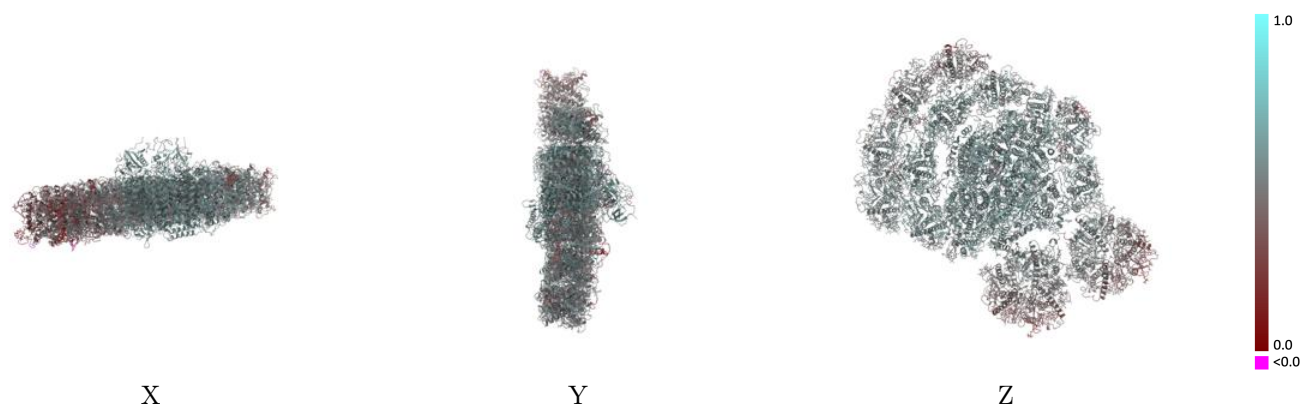
This section contains information regarding the fit between EMDB map EMD-30926 and PDB model 7DZ8. Per-residue inclusion information can be found in section [3](#) on page [37](#).

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



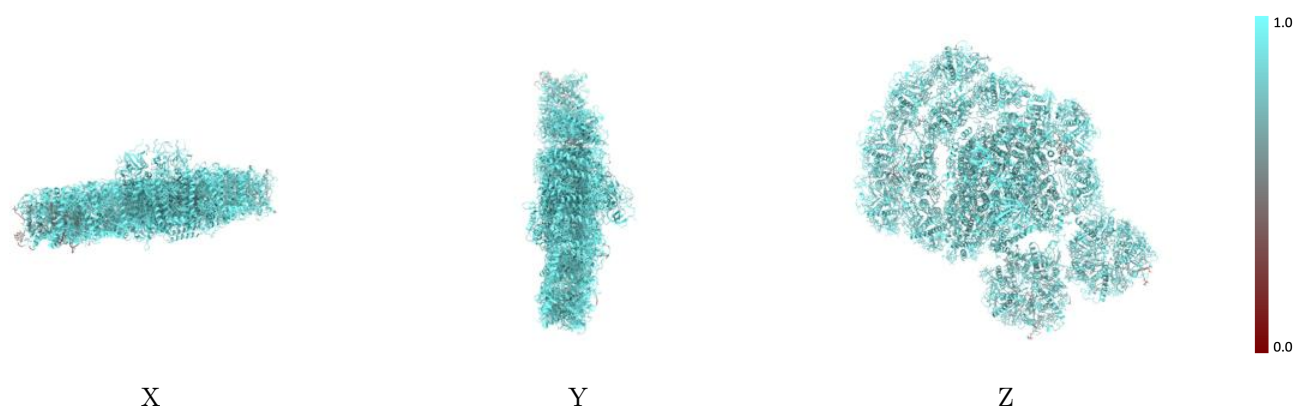
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



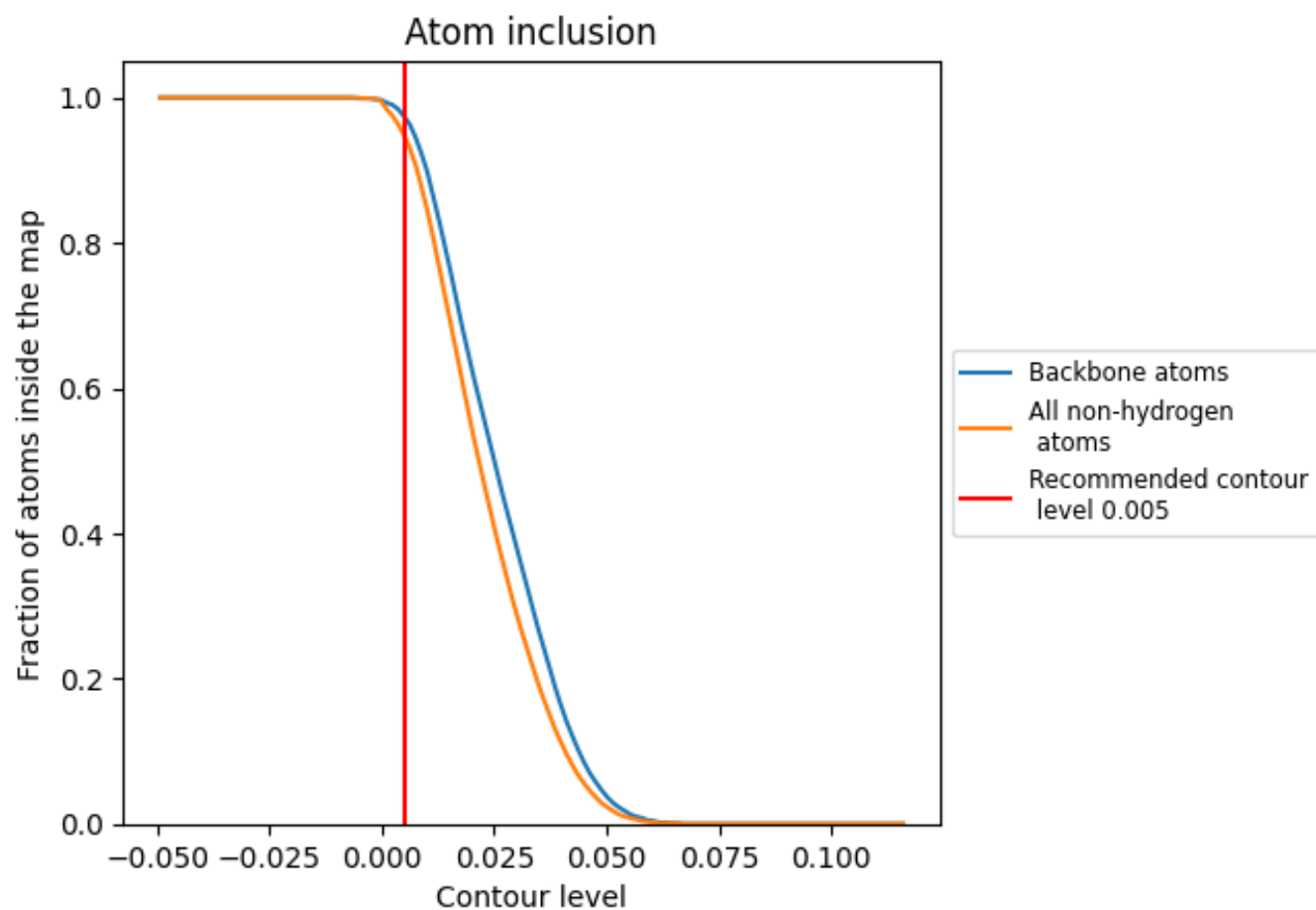
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

## 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 (0.005) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9480   |  0.5180   |
| 1     |  0.9450   |  0.5180   |
| 2     |  0.9720   |  0.5370   |
| 3     |  0.9620   |  0.5530   |
| 4     |  0.9300   |  0.4740   |
| 5     |  0.9380   |  0.5160   |
| 6     |  0.9480   |  0.5130   |
| 7     |  0.9750   |  0.5640   |
| 8     |  0.9680   |  0.5530   |
| 9     |  0.9410   |  0.5060   |
| A     |  0.9810   |  0.5850   |
| B     |  0.9750   |  0.5810   |
| C     |  0.9700   |  0.5390   |
| D     |  0.9900   |  0.5690   |
| E     |  0.9900  |  0.5660  |
| F     |  0.9890 |  0.5650 |
| G     |  0.9410 |  0.5040 |
| H     |  0.9700 |  0.5480 |
| I     |  0.9430 |  0.5380 |
| J     |  0.9610 |  0.5550 |
| K     |  0.9690 |  0.5310 |
| L     |  0.9740 |  0.5570 |
| O     |  0.9750 |  0.5400 |
| U     |  0.9200 |  0.4270 |
| V     |  0.9480 |  0.4950 |
| W     |  0.8530 |  0.3620 |
| X     |  0.8550 |  0.3700 |
| Y     |  0.8830 |  0.4070 |
| Z     |  0.9350 |  0.4990 |
| a     |  0.8970 |  0.4270 |

