



## wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 07:53 AM JST

PDB ID : 6LY5 / pdb\_00006ly5  
EMDB ID : EMD-30012  
Title : Organization and energy transfer in a huge diatom PSI-FCPI supercomplex  
Authors : Xiong, P.; Caizhe, X.  
Deposited on : 2020-02-13  
Resolution : 2.38 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:

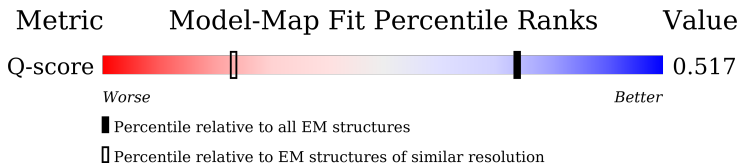
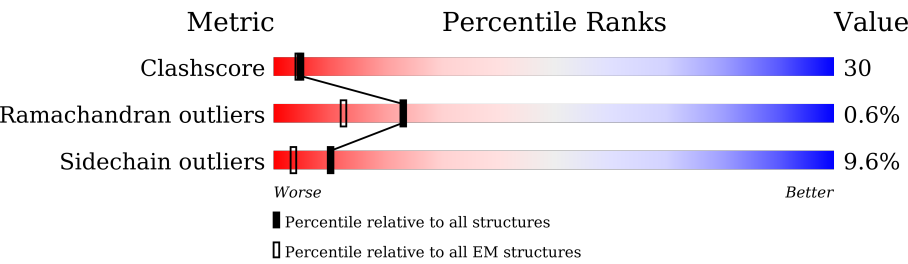
EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 i

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

The reported resolution of this entry is 2.38 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.



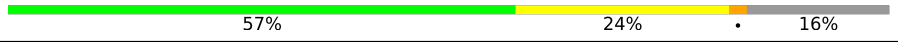
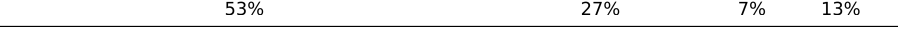
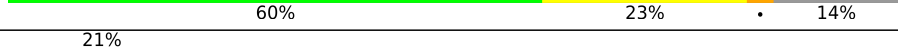
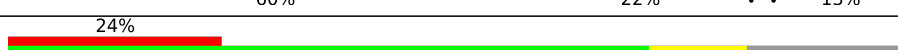
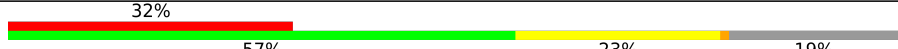
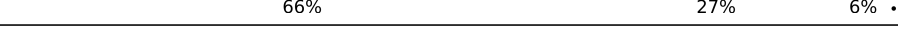
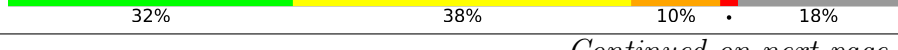
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 4811 ( 1.88 - 2.88 )                                     |

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     | 168    | <div><div>65%31%.</div></div>     |
| 2   | B     | 223    | <div><div>38%17%.41%</div></div>  |
| 3   | C     | 198    | <div><div>58%20%5%18%</div></div> |
| 4   | D     | 207    | <div><div>56%20%7%17%</div></div> |

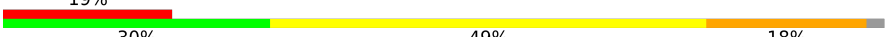
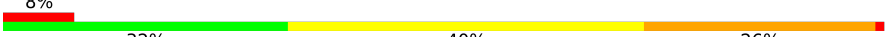
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 5   | E     | 222    |    |
| 6   | F     | 215    |    |
| 7   | G     | 245    |    |
| 8   | H     | 203    |    |
| 9   | I     | 195    |    |
| 10  | J     | 200    |    |
| 11  | K     | 207    |    |
| 12  | L     | 229    |    |
| 13  | M     | 306    |    |
| 14  | N     | 219    |   |
| 15  | O     | 205    |  |
| 15  | P     | 205    |  |
| 15  | Q     | 205    |  |
| 16  | R     | 246    |  |
| 17  | S     | 254    |  |
| 18  | T     | 207    |  |
| 19  | W     | 198    |  |
| 19  | X     | 198    |  |
| 20  | a     | 743    |  |
| 21  | b     | 733    |  |
| 22  | c     | 80     |  |
| 23  | d     | 132    |  |
| 24  | e     | 63     |  |
| 25  | f     | 162    |  |
| 26  | i     | 40     |  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 27  | j     | 42     |  |
| 28  | l     | 172    |  |
| 29  | m     | 29     |  |
| 30  | g     | 134    |  |
| 31  | h     | 139    |  |
| 32  | U     | 160    |  |
| 33  | V     | 179    |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 34  | DD6  | L     | 305 | -         | -        | X       | -                |
| 34  | DD6  | W     | 204 | -         | -        | X       | -                |
| 34  | DD6  | W     | 205 | -         | -        | X       | -                |
| 35  | A86  | Q     | 316 | -         | -        | X       | -                |
| 35  | A86  | S     | 304 | -         | -        | X       | -                |
| 35  | A86  | V     | 301 | -         | -        | X       | -                |
| 35  | A86  | X     | 314 | -         | -        | X       | -                |
| 36  | CLA  | A     | 306 | X         | -        | -       | -                |
| 36  | CLA  | C     | 207 | X         | -        | -       | -                |
| 36  | CLA  | D     | 309 | X         | -        | -       | -                |
| 36  | CLA  | E     | 313 | X         | -        | -       | -                |
| 36  | CLA  | E     | 315 | X         | -        | X       | -                |
| 36  | CLA  | F     | 317 | X         | -        | X       | -                |
| 36  | CLA  | G     | 315 | X         | -        | X       | -                |
| 36  | CLA  | I     | 305 | X         | -        | -       | -                |
| 36  | CLA  | I     | 306 | X         | -        | -       | -                |
| 36  | CLA  | I     | 308 | X         | -        | X       | -                |
| 36  | CLA  | K     | 307 | X         | -        | -       | -                |
| 36  | CLA  | K     | 310 | X         | -        | X       | -                |
| 36  | CLA  | L     | 308 | X         | -        | X       | -                |
| 36  | CLA  | O     | 316 | X         | -        | X       | -                |
| 36  | CLA  | Q     | 314 | -         | -        | X       | -                |
| 36  | CLA  | U     | 306 | X         | -        | X       | -                |
| 36  | CLA  | V     | 305 | -         | -        | X       | -                |
| 36  | CLA  | V     | 306 | -         | -        | X       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 36  | CLA  | V     | 314 | X         | -        | X       | -                |
| 36  | CLA  | W     | 212 | -         | -        | X       | -                |
| 36  | CLA  | X     | 315 | -         | -        | X       | -                |
| 36  | CLA  | a     | 802 | X         | -        | -       | -                |
| 36  | CLA  | a     | 806 | X         | -        | -       | -                |
| 36  | CLA  | a     | 816 | X         | -        | X       | -                |
| 36  | CLA  | a     | 823 | X         | -        | -       | -                |
| 36  | CLA  | a     | 825 | X         | -        | -       | -                |
| 36  | CLA  | a     | 848 | X         | -        | -       | -                |
| 36  | CLA  | b     | 816 | X         | -        | -       | -                |
| 36  | CLA  | b     | 817 | X         | -        | -       | -                |
| 36  | CLA  | b     | 836 | X         | -        | -       | -                |
| 36  | CLA  | f     | 803 | X         | -        | -       | -                |
| 36  | CLA  | f     | 804 | X         | -        | -       | -                |
| 36  | CLA  | j     | 102 | X         | -        | -       | -                |
| 36  | CLA  | l     | 205 | X         | -        | -       | -                |
| 39  | LMT  | F     | 321 | -         | -        | X       | -                |
| 39  | LMT  | h     | 205 | -         | -        | X       | -                |
| 41  | LHG  | E     | 322 | -         | -        | X       | -                |
| 41  | LHG  | f     | 808 | -         | -        | X       | -                |
| 41  | LHG  | i     | 104 | -         | -        | X       | -                |
| 42  | LMG  | J     | 318 | -         | -        | X       | -                |
| 42  | LMG  | V     | 316 | -         | -        | X       | -                |
| 42  | LMG  | j     | 105 | -         | -        | X       | -                |

## 2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 81344 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 FCPI-7.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 1   | A     | 168      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1287  | 825 | 213 | 237 | 12 |         |       |

- Molecule 2 is a protein called FCPI-1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | B     | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1013  | 662 | 166 | 176 | 9 |         |       |

- Molecule 3 is a protein called FCPI-11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | C     | 163      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1247  | 796 | 210 | 232 | 9 |         |       |

- Molecule 4 is a protein called FCPI-6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 172      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1337  | 870 | 214 | 245 | 8 |         |       |

- Molecule 5 is a protein called FCPI-5.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 5   | E     | 188      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1411  | 891 | 240 | 265 | 15 |         |       |

- Molecule 6 is a protein called FCPI-8.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 6   | F     | 180      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1375  | 880 | 230 | 253 | 12 |         |       |

- Molecule 7 is a protein called FCPI-4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | G     | 214      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1668  | 1079 | 276 | 305 | 8 |         |       |

- Molecule 8 is a protein called FCPI-10.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 8   | H     | 170      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1291  | 832 | 213 | 236 | 10 |         |       |

- Molecule 9 is a protein called FCPI-3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | I     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1250  | 807 | 208 | 228 | 7 |         |       |

- Molecule 10 is a protein called FCPI-9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | J     | 167      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1301  | 843 | 217 | 236 | 5 |         |       |

- Molecule 11 is a protein called FCPI-13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | K     | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1304  | 850 | 214 | 232 | 8 |         |       |

- Molecule 12 is a protein called FCPI-14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | L     | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1523  | 989 | 250 | 276 | 8 |         |       |

- Molecule 13 is a protein called FCPI-16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | M     | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1423  | 914 | 248 | 255 | 6 |         |       |

- Molecule 14 is a protein called FCPI-21.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | N     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1716  | 1119 | 282 | 309 | 6 |         |       |

- Molecule 15 is a protein called FCPI.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | O     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1302  | 837 | 216 | 241 | 8 |         |       |
| 15  | P     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1296  | 834 | 213 | 241 | 8 |         |       |
| 15  | Q     | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1302  | 837 | 216 | 241 | 8 |         |       |

- Molecule 16 is a protein called FCPI-24.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | R     | 211      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1628  | 1061 | 266 | 294 | 7 |         |       |

- Molecule 17 is a protein called FCPI-23.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | S     | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1722  | 1122 | 283 | 311 | 6 |         |       |

- Molecule 18 is a protein called FCPI-12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | T     | 172      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1326  | 848 | 226 | 247 | 5 |         |       |

- Molecule 19 is a protein called FCPI-17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | W     | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1239  | 799 | 203 | 233 | 4 |         |       |
| 19  | X     | 161      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1253  | 808 | 207 | 234 | 4 |         |       |

- Molecule 20 is a protein called PsaA.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 20  | a     | 742      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5858  | 3826 | 991 | 1013 | 28 |         |       |

- Molecule 21 is a protein called PsaB.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 21  | b     | 732      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 5820  | 3828 | 980 | 994 | 18 |         |       |

- Molecule 22 is a protein called PsaC.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 22  | c     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 597   | 368 | 104 | 114 | 11 |         |       |

- Molecule 23 is a protein called PsaD.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | d     | 132      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1056  | 681 | 186 | 186 | 3 |         |       |

- Molecule 24 is a protein called PsaE.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 24  | e     | 63       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 507   | 321 | 90 | 96 |         |       |

- Molecule 25 is a protein called PsaF.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | f     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1223  | 789 | 211 | 220 | 3 |         |       |

- Molecule 26 is a protein called PsaI.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26  | i     | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 256   | 176 | 40 | 38 | 2 |         |       |

- Molecule 27 is a protein called PsaJ.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 27  | j     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 324   | 219 | 50 | 54 | 1 |         |       |

- Molecule 28 is a protein called PsaL.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | l     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1094  | 726 | 178 | 187 | 3 |         |       |

- Molecule 29 is a protein called PsaM.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 29  | m     | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 198   | 130 | 32 | 34 | 2 |         |       |

- Molecule 30 is a protein called PsaS.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | g     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 402 | 134 | 134 |   |         |       |

- Molecule 31 is a protein called PsaR.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | h     | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 676   | 440 | 110 | 120 | 6 |         |       |

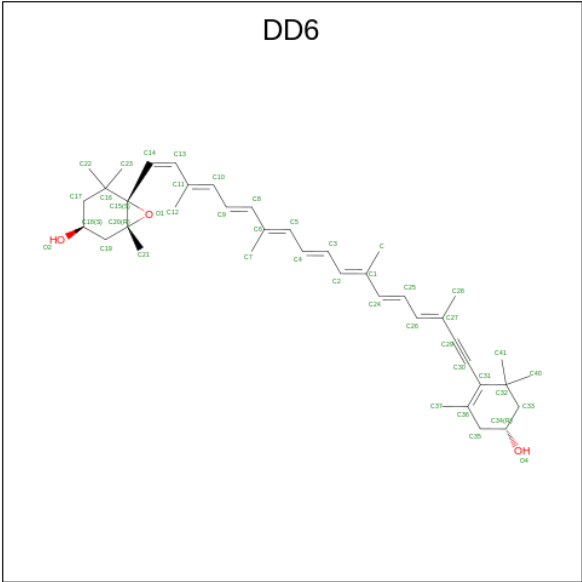
- Molecule 32 is a protein called FCPI-2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | U     | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1194  | 766 | 199 | 221 | 8 |         |       |

- Molecule 33 is a protein called FCPI-19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | V     | 179      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1361  | 871 | 234 | 252 | 4 |         |       |

- Molecule 34 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (CCD ID: DD6) (formula: C<sub>40</sub>H<sub>54</sub>O<sub>3</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 34  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 34  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 34  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 34  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 34  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 34  | C     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 34  | D     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 34  | D     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 34  | D     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 34  | D     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 34  | E     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 34  | E     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 34  | E     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |
| 34  | E     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |

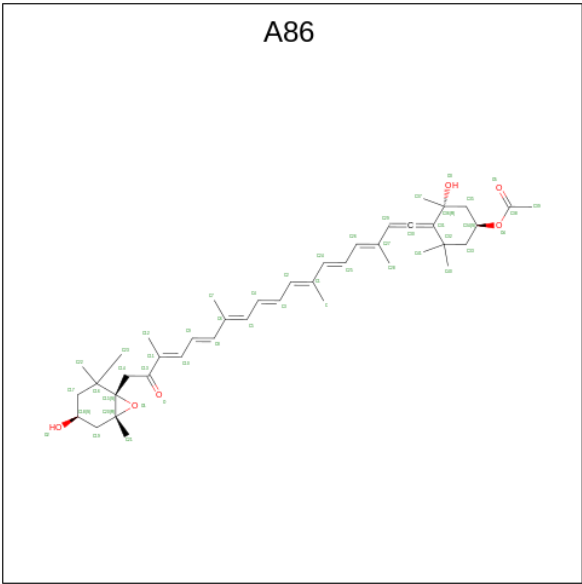
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| Mol | Chain | Residues | Atoms       |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|
| 34  | F     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | G     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | H     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | H     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | I     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | J     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | K     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | K     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | L     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | M     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | O     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | P     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | Q     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | R     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | R     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | S     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | S     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | W     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | W     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | a     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |
| 34  | j     | 1        | Total<br>43 | C<br>40 | O<br>3 | 0       |



- Molecule 35 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C<sub>42</sub>H<sub>58</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 35  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | C     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | C     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | C     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | D     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | E     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | E     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | E     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | F     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 35  | F     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | F     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | F     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | F     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | F     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | G     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | G     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | G     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | G     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | H     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | H     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | I     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | I     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | I     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | J     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | J     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | J     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | J     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | J     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | K     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | K     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 35  | K     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | K     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | M     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | M     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | M     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | M     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | O     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | O     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | O     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 35  | O     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | O     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | P     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | P     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | P     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | P     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | Q     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | Q     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | Q     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | Q     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | R     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | R     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | R     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | R     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | R     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | R     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | R     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | S     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | S     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | S     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | S     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |

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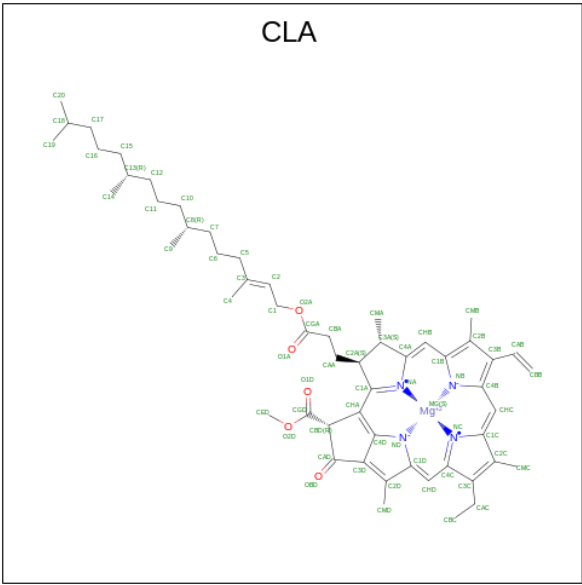
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 35  | S     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | S     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | T     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | T     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | T     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | T     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | T     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | T     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | W     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | W     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | X     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | X     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | X     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | X     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | X     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | X     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | h     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | h     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | U     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | U     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 35  | U     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | U     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | V     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | V     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | V     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |
| 35  | V     | 1        | Total | C  | O | 0       |
|     |       |          | 48    | 42 | 6 |         |

- Molecule 36 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 36  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 36  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 36  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 36  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 36  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 36  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | A     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | B     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | B     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | B     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | C     | 1        | Total<br>43 | C<br>35 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | C     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | C     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | C     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | D     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | D     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 36  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | D     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | D     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | D     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | D     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | D     | 1        | Total<br>58 | C<br>48 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | E     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | E     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | E     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | E     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | E     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | E     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | E     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | E     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | F     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | F     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | F     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 36  | F     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | F     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | F     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | F     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | F     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | G     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | G     | 1        | Total<br>58 | C<br>48 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | G     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | G     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | G     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | H     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | H     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | H     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | H     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | H     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | H     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 36  | H     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | H     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | H     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | H     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | H     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | H     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | H     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | H     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | I     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | I     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | I     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | I     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | I     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | I     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | I     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | I     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | I     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | I     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | J     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | J     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | J     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | J     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 36  | J     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | J     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | J     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | J     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | J     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | J     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | K     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | K     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | K     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | K     | 1        | Total<br>62 | C<br>52 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | K     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | K     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | K     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | K     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | K     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | L     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | L     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | L     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | L     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 36  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | L     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | M     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | M     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | M     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | M     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | M     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | M     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | M     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | M     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | M     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | M     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | N     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | N     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | N     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | N     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | N     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | N     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | N     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | N     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 36  | N     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | N     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | N     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | N     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | O     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | O     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | O     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | O     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | O     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | O     | 1        | Total<br>58 | C<br>48 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | O     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | O     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | O     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | P     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | P     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | P     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | P     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | P     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | P     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | P     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | P     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 36  | P     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | P     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | P     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | P     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | Q     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | Q     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | Q     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | Q     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | Q     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | Q     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | Q     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | Q     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | R     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | R     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | R     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | R     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | R     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | R     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | R     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | R     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | R     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 36  | R     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | R     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | R     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | S     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | S     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | S     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | S     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | S     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | S     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | S     | 1        | Total<br>45 | C<br>37 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | S     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | S     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | S     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | S     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | S     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | T     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | T     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | T     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | T     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | T     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | T     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 36  | T     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | W     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | W     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | W     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | W     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | W     | 1        | Total<br>57 | C<br>47 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | W     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | W     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | W     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | W     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | W     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | W     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | W     | 1        | Total<br>43 | C<br>35 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | X     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | X     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | X     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | X     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | X     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | X     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | X     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | X     | 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 |
|-----|-------|----------|-------|----|----|---|---|---------|
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 62    | 52 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 36  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 36  | a     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>62 | C<br>52 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>53 | C<br>43 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>58 | C<br>48 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>58 | C<br>48 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | f     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | f     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | f     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | f     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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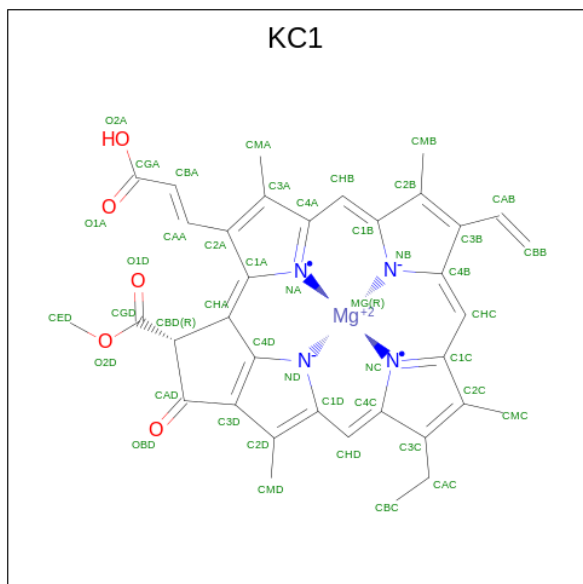
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 36  | i     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | j     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | j     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | j     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | l     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | l     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | l     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | l     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | l     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | h     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | U     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | U     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | U     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | U     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | U     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | U     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | U     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | U     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 36  | V     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | V     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 36  | V     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 36  | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 36  | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 35 | 1  | 4 | 3 |         |
| 36  | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 36  | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 36  | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 36  | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

- Molecule 37 is Chlorophyll c1 (CCD ID: KC1) (formula:  $C_{35}H_{30}MgN_4O_5$ ).



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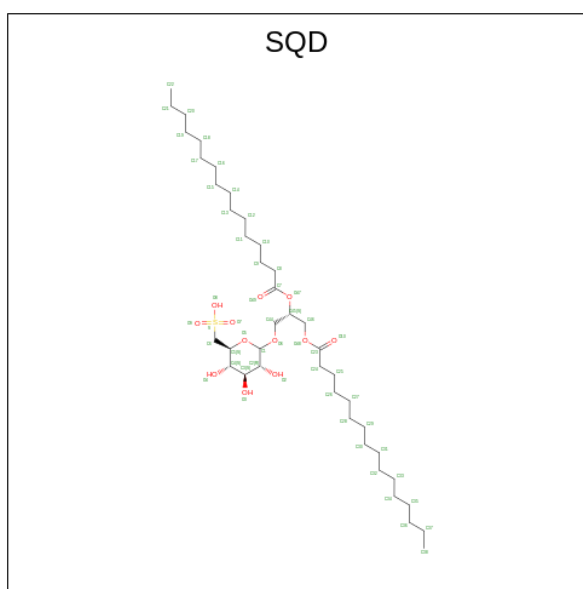
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 37  | F     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | F     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | G     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | G     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | G     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | H     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | J     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | K     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | L     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | L     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | M     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | M     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | M     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | N     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | O     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | O     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | P     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | P     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | Q     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | Q     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 37  | R     | 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 |
|-----|-------|----------|-------|----|----|---|---|---------|
| 37  | S     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 37  | T     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 37  | T     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 37  | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 37  | W     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 37  | X     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 37  | U     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 37  | V     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

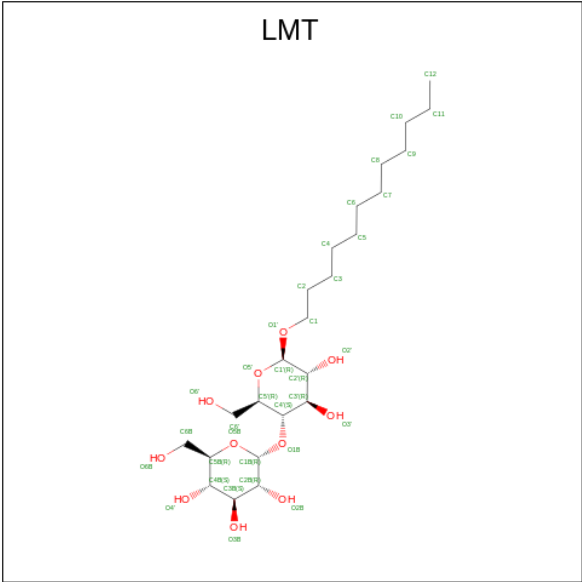
- Molecule 38 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 38  | A     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 28    | 15 | 12 | 1 |         |
| 38  | b     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 46    | 33 | 12 | 1 |         |

- Molecule 39 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).





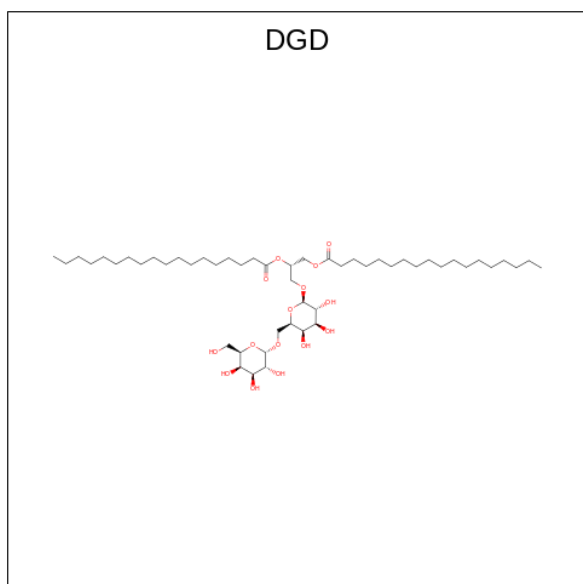
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 39  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 39  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 39  | E     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 39  | E     | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 17 | 6  |         |
| 39  | E     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 39  | F     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 39  | F     | 1        | Total | C  | O  | 0       |
|     |       |          | 33    | 22 | 11 |         |
| 39  | G     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 39  | G     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 39  | I     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 39  | I     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 39  | K     | 1        | Total | C  | O  | 0       |
|     |       |          | 31    | 20 | 11 |         |
| 39  | K     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 39  | L     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

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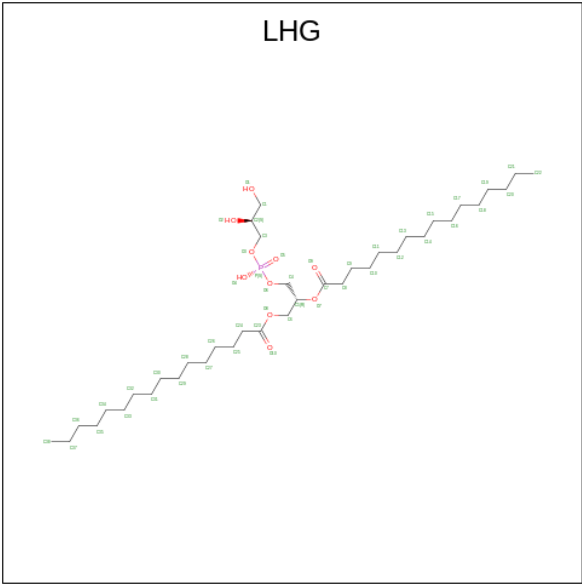
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 39  | L     | 1        | Total | C  | O  | 0       |
|     |       |          | 31    | 20 | 11 |         |
| 39  | P     | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 17 | 6  |         |
| 39  | P     | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 17 | 6  |         |
| 39  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 39  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 32    | 21 | 11 |         |
| 39  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 39  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 39  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 24    | 19 | 5  |         |
| 39  | f     | 1        | Total | C  | O  | 0       |
|     |       |          | 24    | 18 | 6  |         |
| 39  | h     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 39  | U     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 39  | U     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

- Molecule 40 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 40  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 57    | 42 | 15 |         |
| 40  | L     | 1        | Total | C  | O  | 0       |
|     |       |          | 47    | 32 | 15 |         |
| 40  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 60    | 45 | 15 |         |

- Molecule 41 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



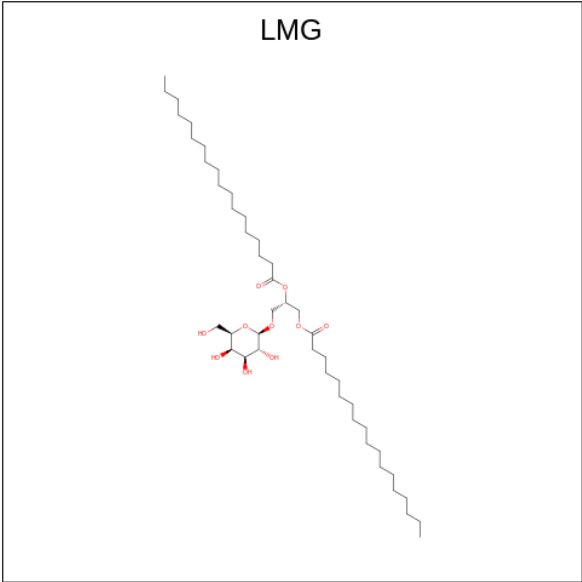
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 41  | D     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 46    | 35 | 10 | 1 |         |
| 41  | D     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 41  | E     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 41  | F     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 33    | 24 | 8  | 1 |         |
| 41  | F     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 41    | 30 | 10 | 1 |         |
| 41  | G     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 41  | G     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 40    | 29 | 10 | 1 |         |
| 41  | G     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 47    | 36 | 10 | 1 |         |

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| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 41  | I     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 41  | O     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 42    | 31 | 10 | 1 |         |
| 41  | O     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 41  | Q     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 41  | R     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 41  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 48    | 37 | 10 | 1 |         |
| 41  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 27    | 16 | 10 | 1 |         |
| 41  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 47    | 36 | 10 | 1 |         |
| 41  | b     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 41  | f     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 41  | f     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 42    | 31 | 10 | 1 |         |
| 41  | i     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 46    | 35 | 10 | 1 |         |
| 41  | j     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 41  | l     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 48    | 37 | 10 | 1 |         |

- Molecule 42 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



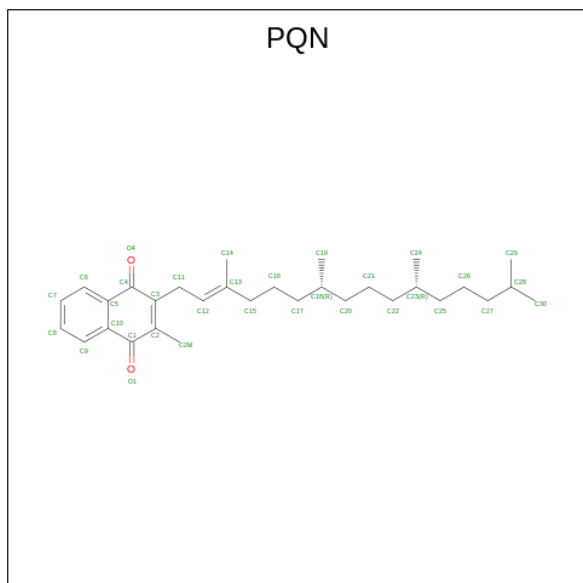
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 42  | D     | 1        | Total | C  | O  | 0       |
|     |       |          | 46    | 36 | 10 |         |
| 42  | D     | 1        | Total | C  | O  | 0       |
|     |       |          | 37    | 27 | 10 |         |
| 42  | E     | 1        | Total | C  | O  | 0       |
|     |       |          | 46    | 36 | 10 |         |
| 42  | E     | 1        | Total | C  | O  | 0       |
|     |       |          | 40    | 30 | 10 |         |
| 42  | G     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |
| 42  | G     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |
| 42  | I     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |
| 42  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |
| 42  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 44    | 34 | 10 |         |
| 42  | L     | 1        | Total | C  | O  | 0       |
|     |       |          | 33    | 23 | 10 |         |
| 42  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 54    | 44 | 10 |         |
| 42  | j     | 1        | Total | C  | O  | 0       |
|     |       |          | 52    | 42 | 10 |         |
| 42  | m     | 1        | Total | C  | O  | 0       |
|     |       |          | 37    | 27 | 10 |         |
| 42  | h     | 1        | Total | C  | O  | 0       |
|     |       |          | 45    | 35 | 10 |         |

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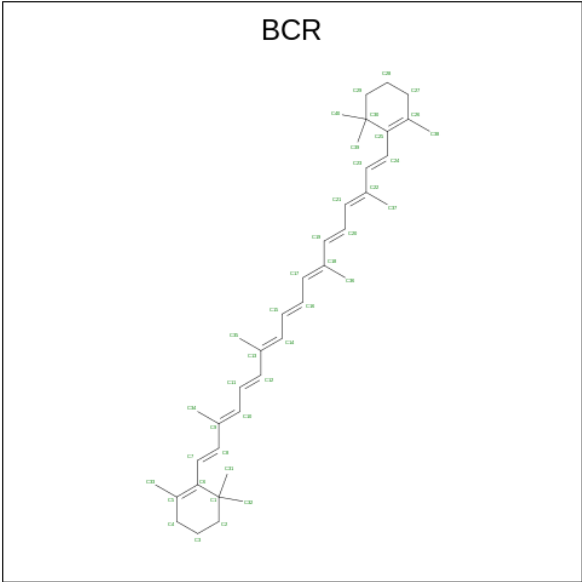
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 42  | V     | 1        | Total | C  | O  | 0       |
|     |       |          | 46    | 36 | 10 |         |
| 42  | V     | 1        | Total | C  | O  | 0       |
|     |       |          | 46    | 36 | 10 |         |

- Molecule 43 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 43  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 43  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |

- Molecule 44 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



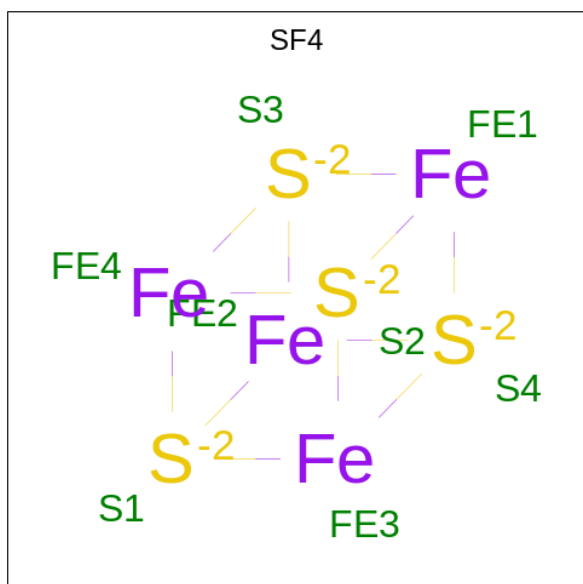
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 44  | a     | 1        | Total C<br>40 40 | 0       |
| 44  | a     | 1        | Total C<br>40 40 | 0       |
| 44  | a     | 1        | Total C<br>40 40 | 0       |
| 44  | a     | 1        | Total C<br>40 40 | 0       |
| 44  | b     | 1        | Total C<br>40 40 | 0       |
| 44  | b     | 1        | Total C<br>40 40 | 0       |
| 44  | b     | 1        | Total C<br>40 40 | 0       |
| 44  | b     | 1        | Total C<br>40 40 | 0       |
| 44  | b     | 1        | Total C<br>40 40 | 0       |
| 44  | f     | 1        | Total C<br>40 40 | 0       |
| 44  | f     | 1        | Total C<br>40 40 | 0       |
| 44  | i     | 1        | Total C<br>40 40 | 0       |
| 44  | i     | 1        | Total C<br>40 40 | 0       |
| 44  | j     | 1        | Total C<br>40 40 | 0       |

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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 44  | l     | 1        | Total C<br>40 40 | 0       |
| 44  | l     | 1        | Total C<br>40 40 | 0       |
| 44  | m     | 1        | Total C<br>40 40 | 0       |
| 44  | h     | 1        | Total C<br>40 40 | 0       |

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms               | AltConf |
|-----|-------|----------|---------------------|---------|
| 45  | b     | 1        | Total Fe S<br>8 4 4 | 0       |
| 45  | c     | 1        | Total Fe S<br>8 4 4 | 0       |
| 45  | c     | 1        | Total Fe S<br>8 4 4 | 0       |

- Molecule 46 is water.

| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 46  | a     | 64       | Total O<br>64 64 | 0       |
| 46  | b     | 72       | Total O<br>72 72 | 0       |

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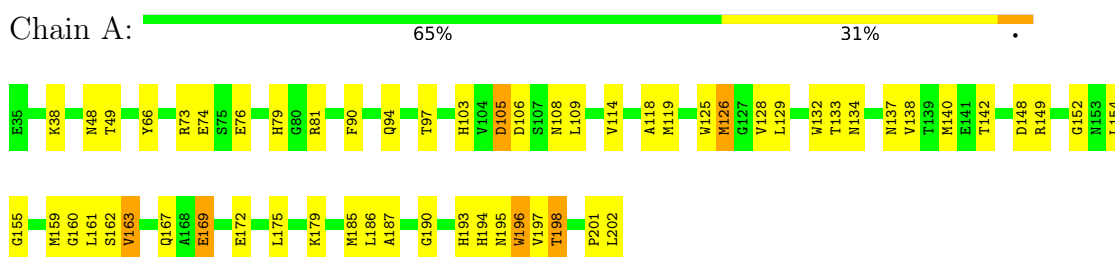
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| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 46  | c     | 7        | Total<br>7 | O<br>7 | 0       |
| 46  | d     | 4        | Total<br>4 | O<br>4 | 0       |
| 46  | f     | 2        | Total<br>2 | O<br>2 | 0       |
| 46  | j     | 1        | Total<br>1 | O<br>1 | 0       |
| 46  | l     | 3        | Total<br>3 | O<br>3 | 0       |

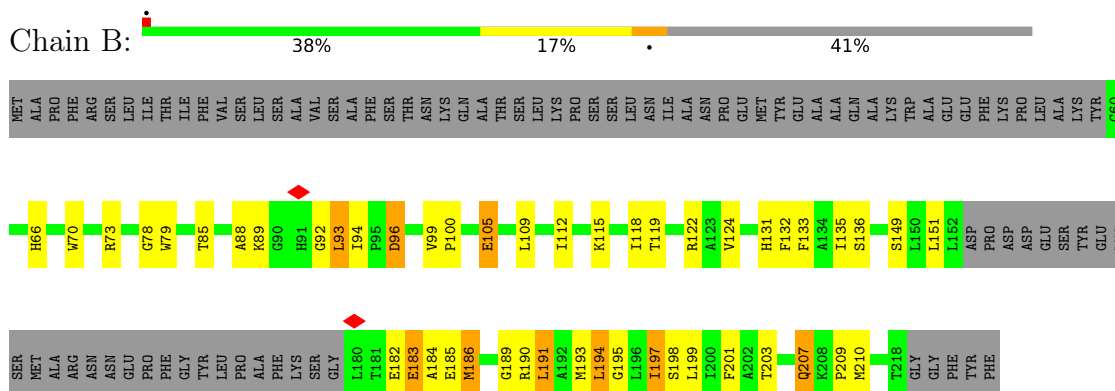
### 3 Residue-property plots

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.

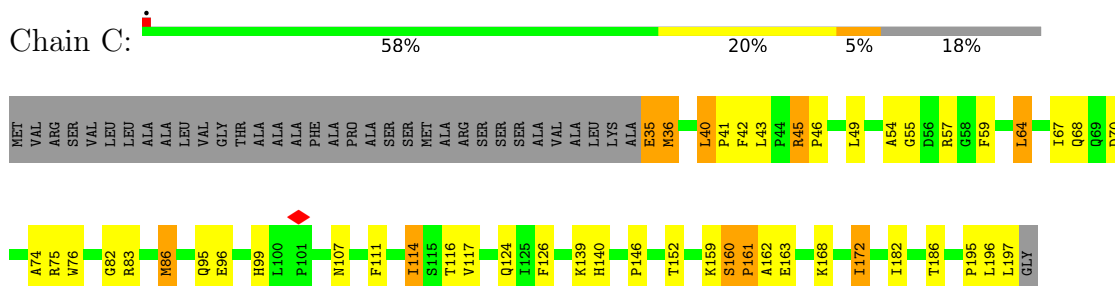
#### • Molecule 1: FCPI-7



#### • Molecule 2: FCPI-1

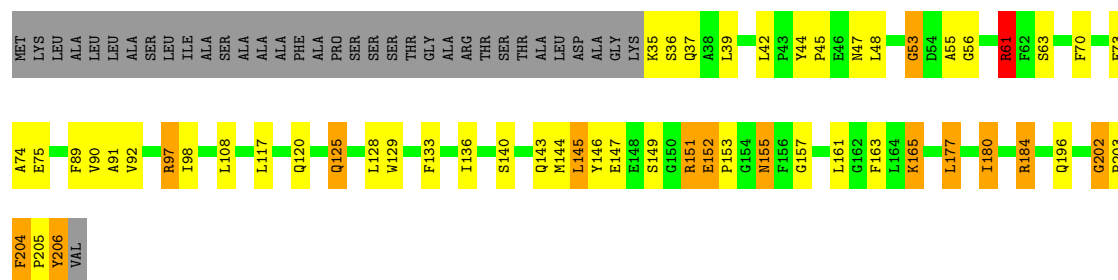


#### • Molecule 3: FCPI-11



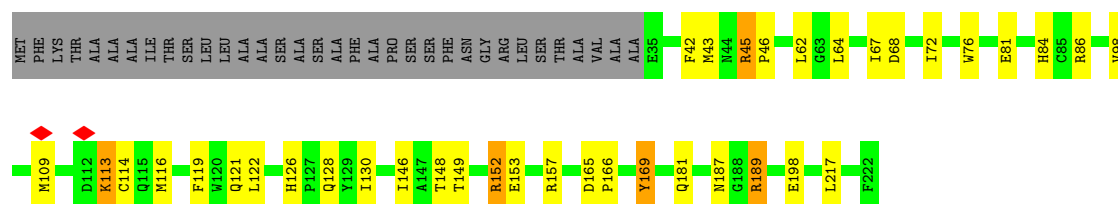
#### • Molecule 4: FCPI-6





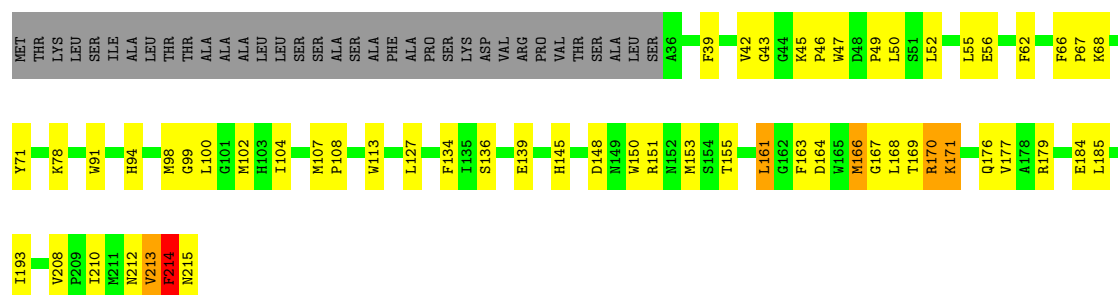
- Molecule 5: FCPI-5

Chain E: 68% 15% 15%



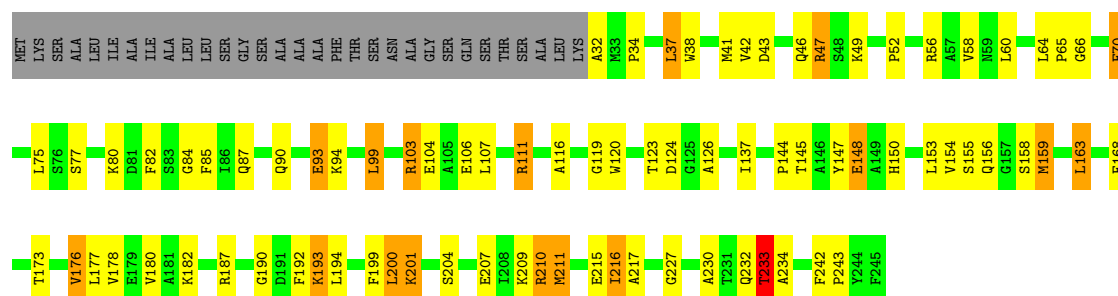
- Molecule 6: FCPI-8

Chain F: 57% 24% 16%



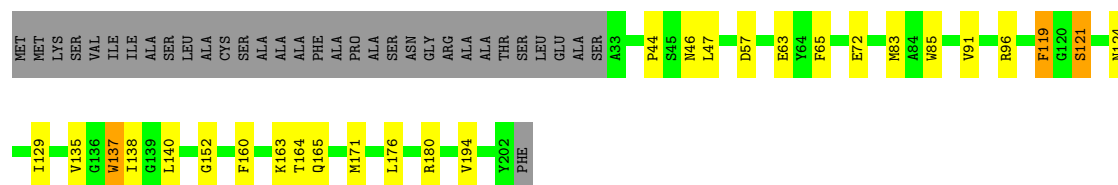
- Molecule 7: FCPI-4

Chain G: 53% 27% 7% 13%

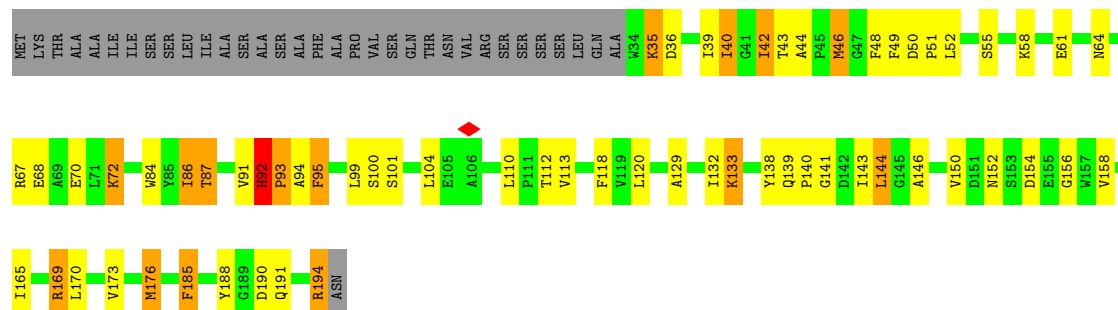


- Molecule 8: FCPI-10

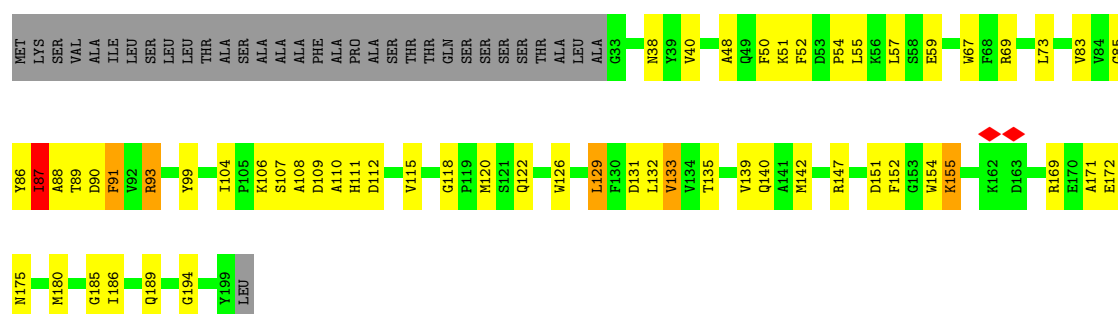
Chain H: 70% 12% 16%



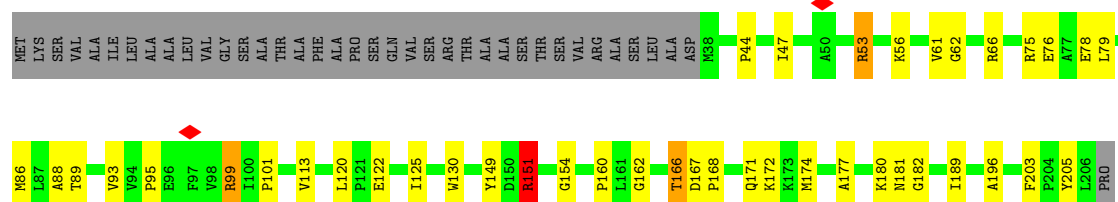
- Molecule 9: FCPI-3



- Molecule 10: FCPI-9

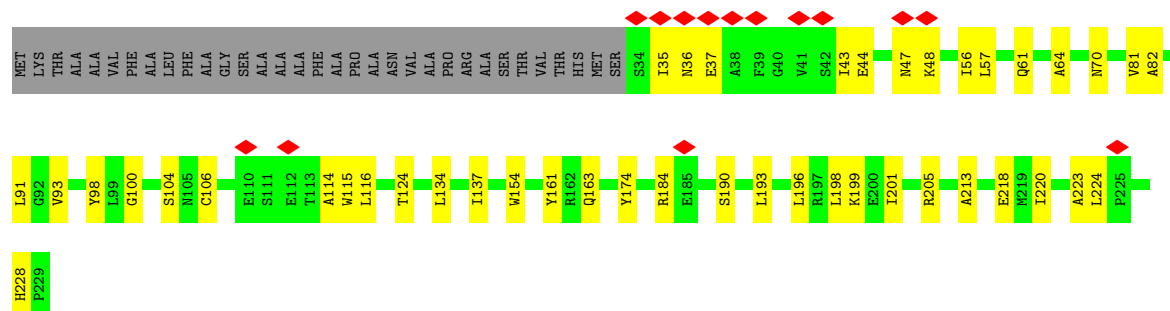


- Molecule 11: FCPI-13



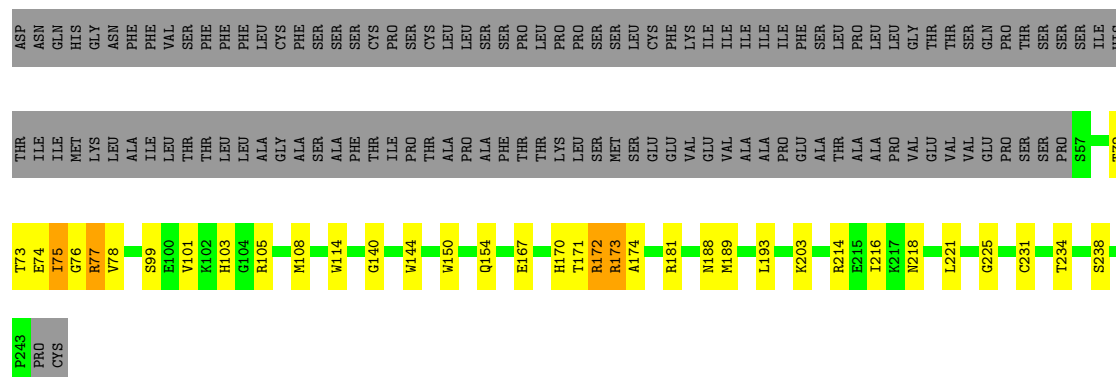
- Molecule 12: FCPI-14





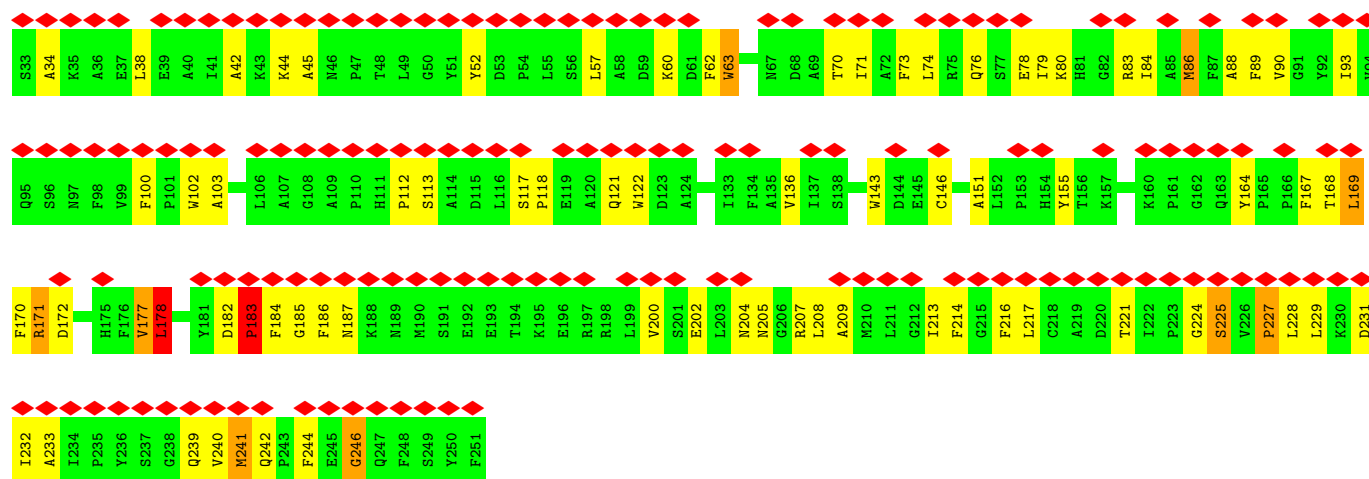
• Molecule 13: FCPI-16

Chain M: 49% 10% 39%



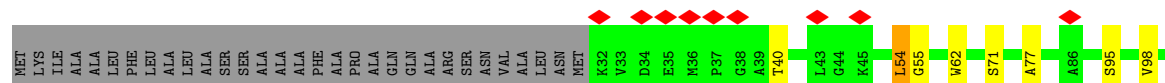
• Molecule 14: FCPI-21

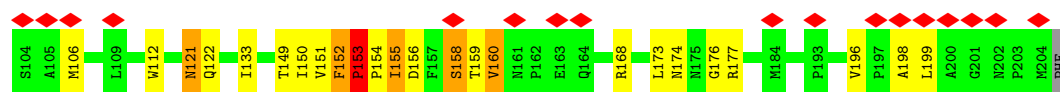
Chain N: 71% 63% 32%



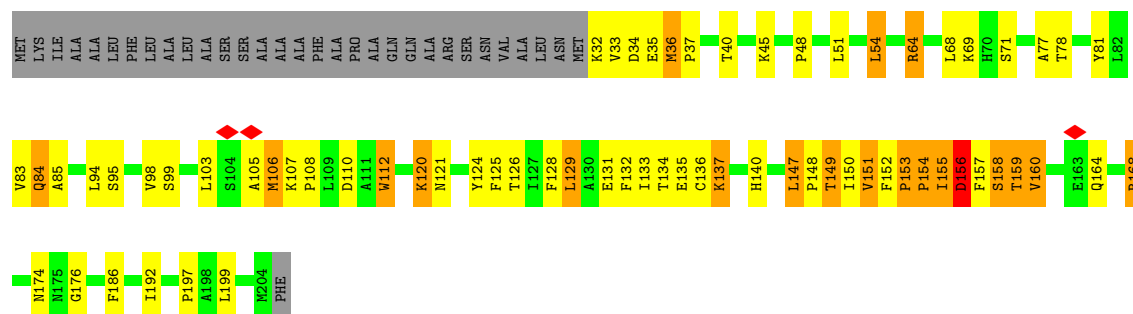
• Molecule 15: FCPI

Chain O: 13% 69% 12% 16%

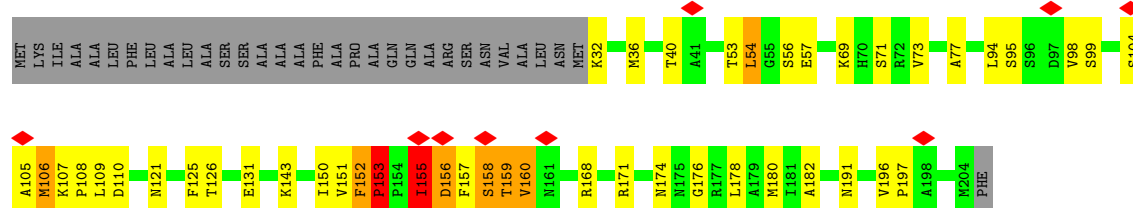




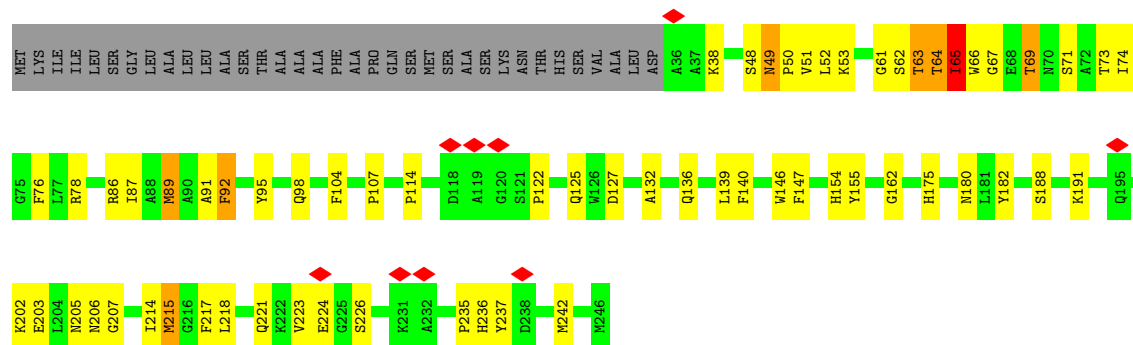
• Molecule 15: FCPI



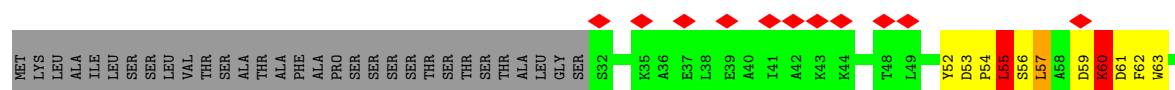
• Molecule 15: FCPI

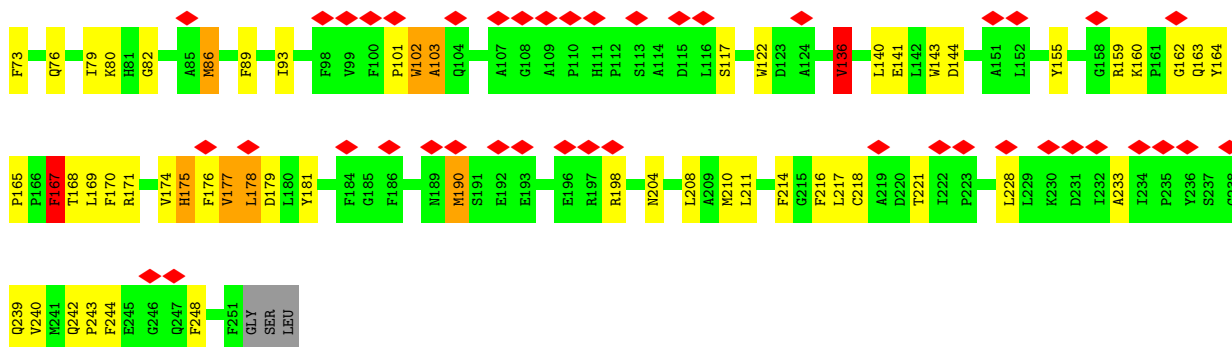


• Molecule 16: FCPI-24

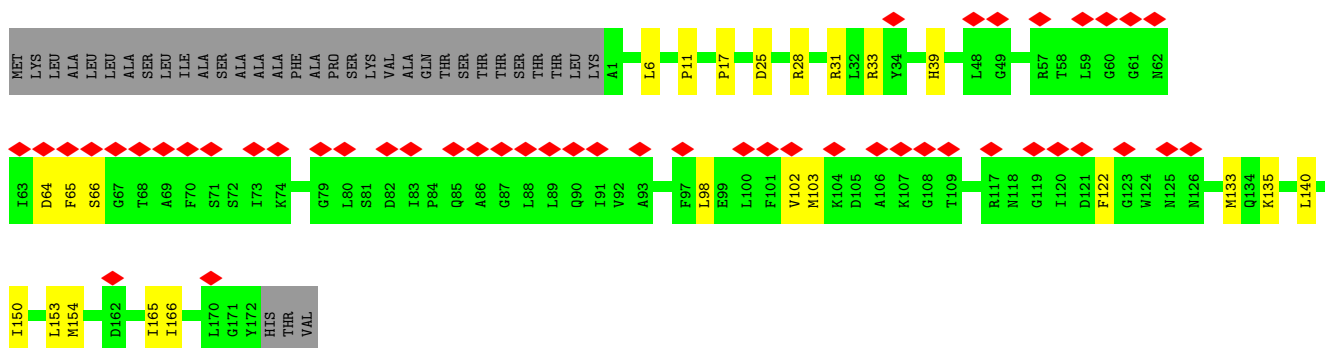


• Molecule 17: FCPI-23

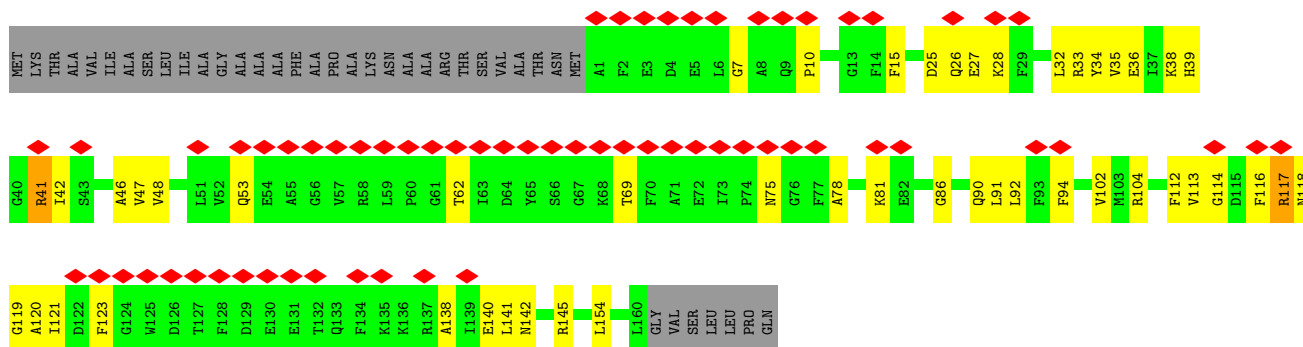




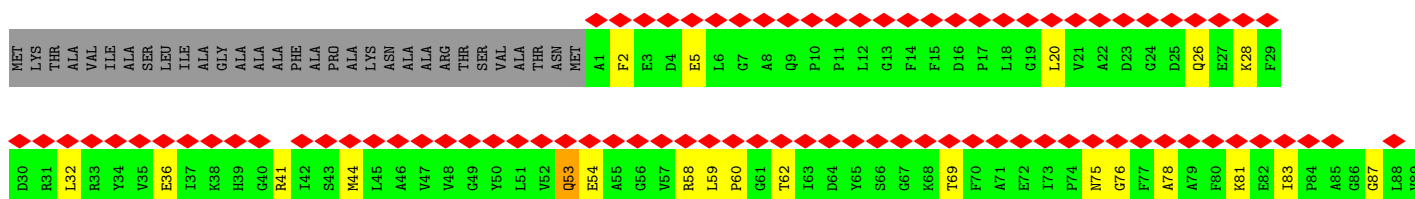
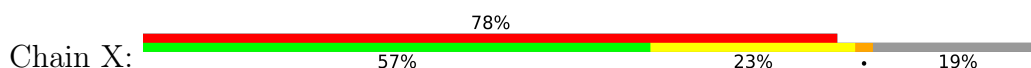
• Molecule 18: FCPI-12

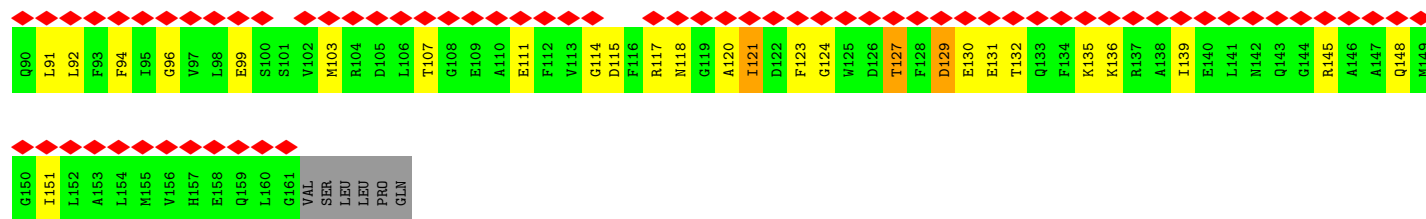


• Molecule 19: FCPI-17



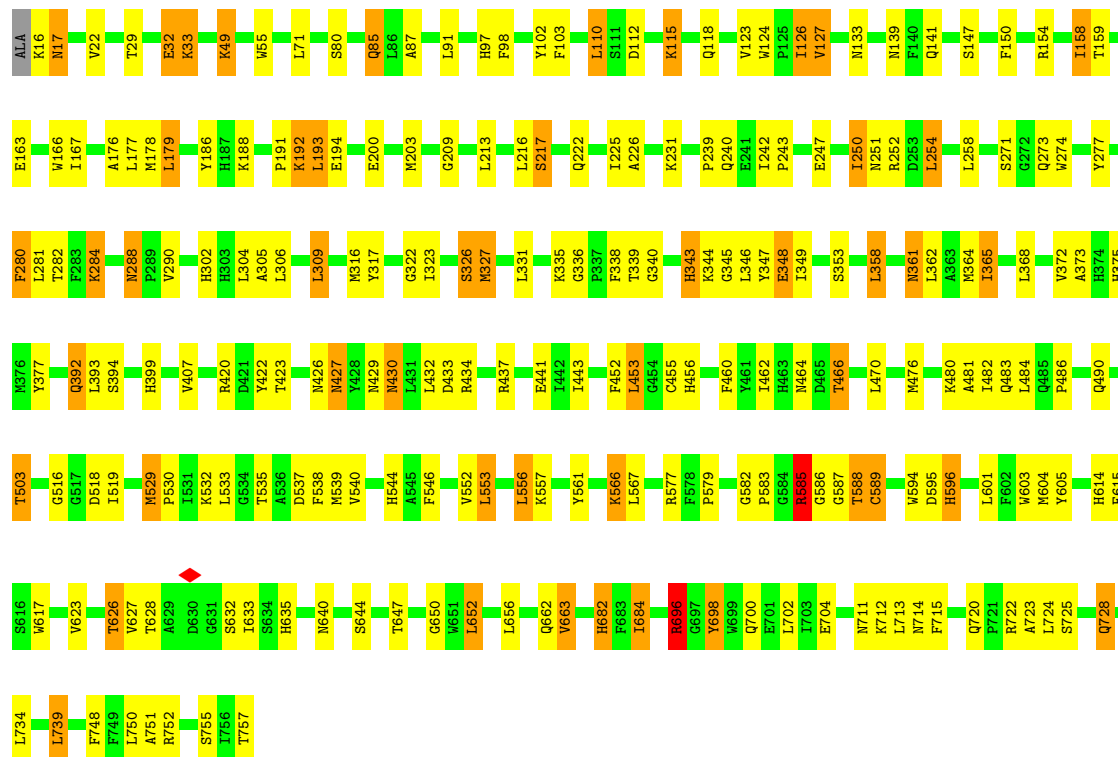
• Molecule 19: FCPI-17





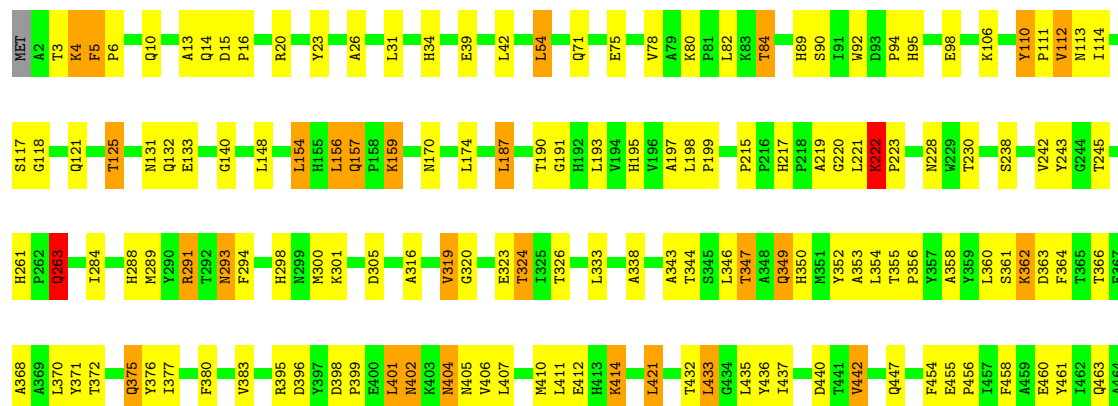
• Molecule 20: PsaA

Chain a: 69% 24% 6%

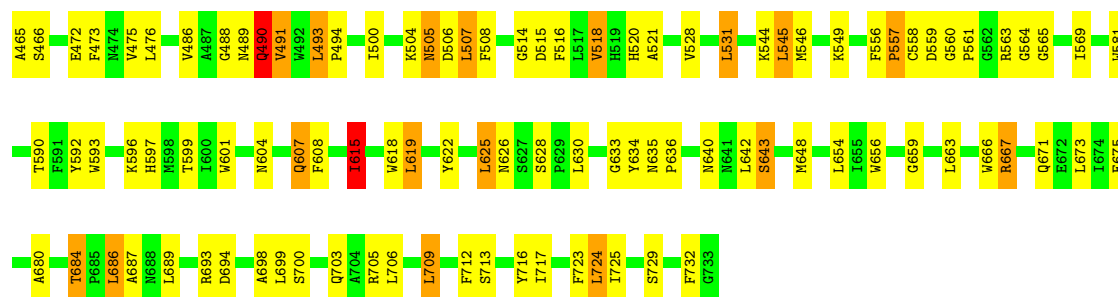


• Molecule 21: PsaB

Chain b: 66% 27% 6%



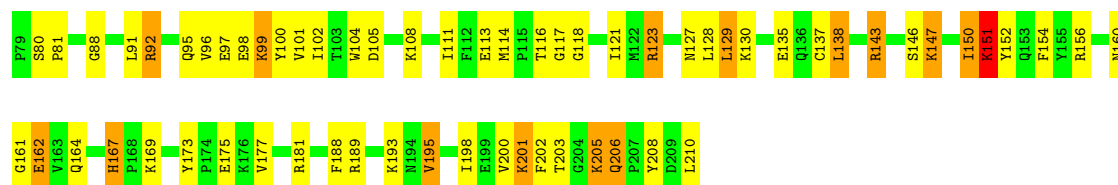




• Molecule 22: PsaC



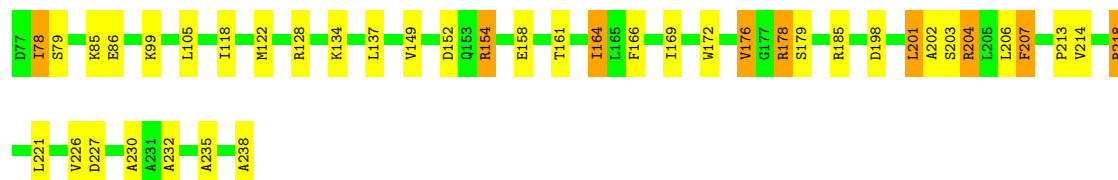
• Molecule 23: PsaD



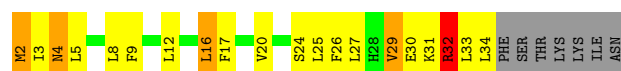
• Molecule 24: PsaE



• Molecule 25: PsaF



• Molecule 26: PsaI



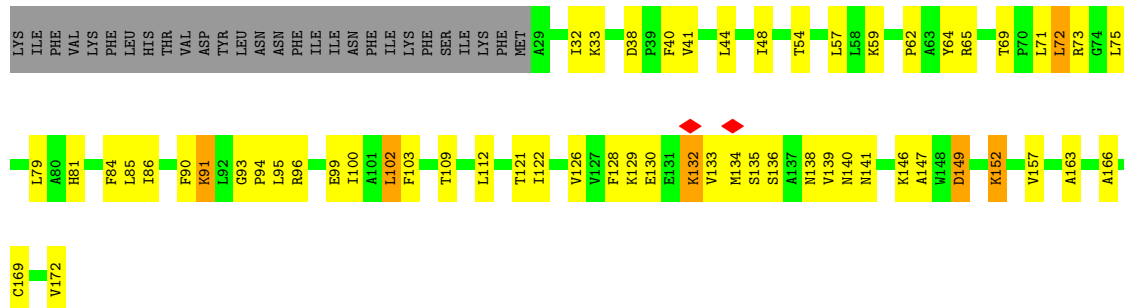
- Molecule 27: PsaJ

Chain j:  43% 38% 17% .



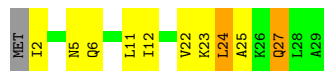
- Molecule 28: PsaL

Chain l:  49% 31% . 16%



- Molecule 29: PsaM

Chain m:  62% 28% 7% .

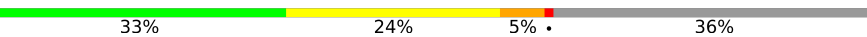


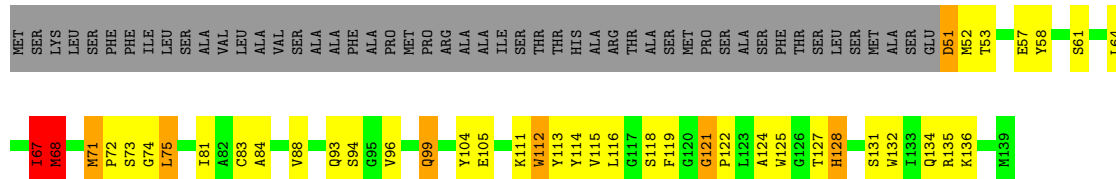
- Molecule 30: PsaS

Chain g:  90% 10%



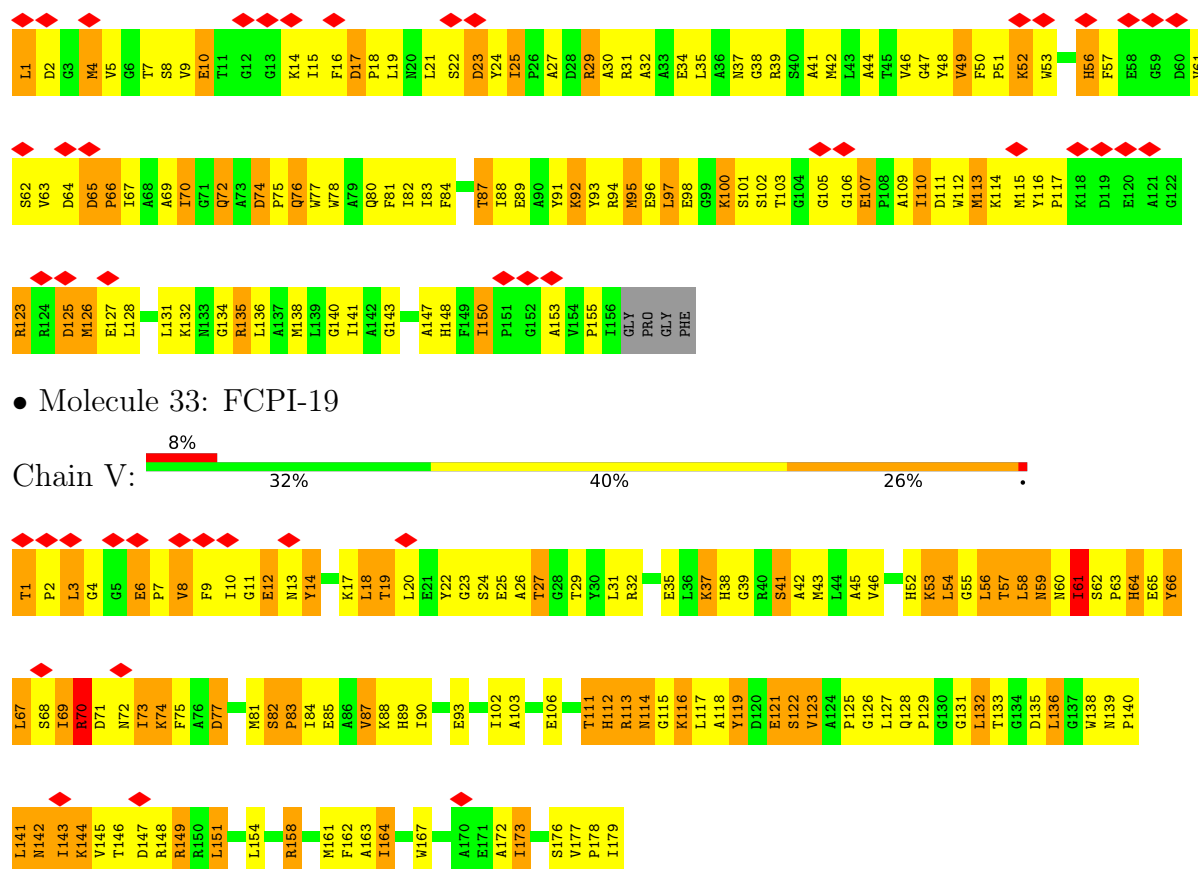
- Molecule 31: PsaR

Chain h:  33% 24% 5% . 36%



- Molecule 32: FCPI-2

Chain U:  19% 30% 49% 18% .



• Molecule 33: FCPI-19



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 164480                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | 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                    | 0.163                                   | Depositor |
| Minimum map value                    | -0.055                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.004                                   | Depositor |
| Recommended contour level            | 0.016                                   | Depositor |
| Map size (Å)                         | 567.32, 567.32, 567.32                  | wwPDB     |
| Map dimensions                       | 520, 520, 520                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.091, 1.091, 1.091                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: KC1, BCR, CLA, LMG, LMT, DGD, LHG, PQN, SQD, SF4, DD6, A86

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     | 0.50         | 0/1319        | 0.80        | 0/1786         |
| 2   | B     | 0.87         | 2/1039 (0.2%) | 1.16        | 11/1412 (0.8%) |
| 3   | C     | 0.41         | 0/1275        | 0.77        | 3/1726 (0.2%)  |
| 4   | D     | 0.49         | 0/1373        | 0.84        | 5/1860 (0.3%)  |
| 5   | E     | 0.48         | 0/1439        | 0.70        | 1/1944 (0.1%)  |
| 6   | F     | 0.43         | 0/1411        | 0.84        | 5/1908 (0.3%)  |
| 7   | G     | 0.45         | 0/1714        | 0.79        | 2/2321 (0.1%)  |
| 8   | H     | 0.48         | 0/1326        | 0.80        | 1/1798 (0.1%)  |
| 9   | I     | 0.44         | 0/1285        | 1.00        | 6/1746 (0.3%)  |
| 10  | J     | 0.50         | 1/1339 (0.1%) | 0.94        | 4/1811 (0.2%)  |
| 11  | K     | 0.49         | 0/1346        | 0.84        | 4/1826 (0.2%)  |
| 12  | L     | 0.45         | 0/1571        | 0.71        | 0/2141         |
| 13  | M     | 0.40         | 0/1464        | 0.74        | 3/1982 (0.2%)  |
| 14  | N     | 0.48         | 0/1770        | 1.01        | 7/2405 (0.3%)  |
| 15  | O     | 0.47         | 0/1335        | 0.92        | 7/1817 (0.4%)  |
| 15  | P     | 0.47         | 1/1329 (0.1%) | 1.31        | 11/1810 (0.6%) |
| 15  | Q     | 0.48         | 0/1335        | 0.92        | 8/1817 (0.4%)  |
| 16  | R     | 0.35         | 0/1680        | 0.72        | 1/2282 (0.0%)  |
| 17  | S     | 0.40         | 0/1776        | 0.89        | 3/2413 (0.1%)  |
| 18  | T     | 0.34         | 0/1353        | 0.62        | 0/1823         |
| 19  | W     | 0.48         | 1/1265 (0.1%) | 0.85        | 3/1707 (0.2%)  |
| 19  | X     | 0.50         | 2/1282 (0.2%) | 0.93        | 7/1729 (0.4%)  |
| 20  | a     | 0.47         | 0/6053        | 0.80        | 19/8238 (0.2%) |
| 21  | b     | 0.48         | 2/6031 (0.0%) | 0.85        | 20/8231 (0.2%) |
| 22  | c     | 0.45         | 0/607         | 0.82        | 2/822 (0.2%)   |
| 23  | d     | 4.08         | 2/1086 (0.2%) | 1.45        | 9/1461 (0.6%)  |
| 24  | e     | 0.40         | 0/517         | 0.58        | 0/701          |
| 25  | f     | 0.47         | 0/1248        | 0.75        | 2/1687 (0.1%)  |
| 26  | i     | 0.60         | 0/262         | 1.24        | 2/356 (0.6%)   |
| 27  | j     | 0.57         | 0/333         | 0.82        | 1/455 (0.2%)   |
| 28  | l     | 0.48         | 0/1121        | 0.83        | 2/1520 (0.1%)  |
| 29  | m     | 0.57         | 0/198         | 0.82        | 0/269          |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 31  | h     | 0.49         | 0/698           | 1.08        | 10/951 (1.1%)    |
| 32  | U     | 0.59         | 0/1225          | 2.00        | 10/1657 (0.6%)   |
| 33  | V     | 0.38         | 0/1393          | 0.88        | 5/1894 (0.3%)    |
| All | All   | 0.76         | 11/51798 (0.0%) | 0.92        | 174/70306 (0.2%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 10  | J     | 0                   | 1                   |
| 12  | L     | 0                   | 2                   |
| 14  | N     | 0                   | 7                   |
| 15  | O     | 0                   | 1                   |
| 15  | P     | 0                   | 1                   |
| 15  | Q     | 0                   | 1                   |
| 17  | S     | 0                   | 2                   |
| 19  | W     | 0                   | 3                   |
| 23  | d     | 0                   | 5                   |
| 30  | g     | 0                   | 1                   |
| 33  | V     | 0                   | 1                   |
| All | All   | 0                   | 25                  |

The worst 5 of 11 bond length outliers are listed below:

| Mol | Chain | Res    | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|-------|-------|-------------|----------|
| 23  | d     | 151[A] | LYS  | CA-C  | 94.74 | 2.66        | 1.52     |
| 23  | d     | 151[B] | LYS  | CA-C  | 94.74 | 2.66        | 1.52     |
| 2   | B     | 186    | MET  | C-N   | 22.66 | 1.54        | 1.33     |
| 15  | P     | 156    | ASP  | C-N   | 9.60  | 1.48        | 1.33     |
| 2   | B     | 183    | GLU  | C-N   | -8.62 | 1.21        | 1.33     |

The worst 5 of 174 bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|--------|------|---------|--------|-------------|----------|
| 32  | U     | 65     | ASP  | CA-C-N  | 48.07  | 179.93      | 119.84   |
| 32  | U     | 65     | ASP  | C-N-CA  | 48.07  | 179.93      | 119.84   |
| 23  | d     | 151[A] | LYS  | CB-CA-C | -26.47 | 64.81       | 109.80   |
| 23  | d     | 151[B] | LYS  | CB-CA-C | -26.47 | 64.81       | 109.80   |
| 15  | P     | 156    | ASP  | O-C-N   | -23.88 | 90.36       | 123.07   |

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 10  | J     | 91  | PHE  | Mainchain |
| 12  | L     | 228 | HIS  | Peptide   |
| 12  | L     | 47  | ASN  | Peptide   |
| 14  | N     | 112 | PRO  | Peptide   |
| 14  | N     | 172 | ASP  | Peptide   |

## 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     | 1287  | 0        | 1265     | 83      | 0            |
| 2   | B     | 1013  | 0        | 1016     | 100     | 0            |
| 3   | C     | 1247  | 0        | 1240     | 72      | 0            |
| 4   | D     | 1337  | 0        | 1310     | 69      | 0            |
| 5   | E     | 1411  | 0        | 1376     | 46      | 0            |
| 6   | F     | 1375  | 0        | 1345     | 82      | 0            |
| 7   | G     | 1668  | 0        | 1631     | 110     | 0            |
| 8   | H     | 1291  | 0        | 1258     | 47      | 0            |
| 9   | I     | 1250  | 0        | 1196     | 79      | 0            |
| 10  | J     | 1301  | 0        | 1256     | 66      | 0            |
| 11  | K     | 1304  | 0        | 1281     | 48      | 0            |
| 12  | L     | 1523  | 0        | 1488     | 71      | 0            |
| 13  | M     | 1423  | 0        | 1397     | 37      | 0            |
| 14  | N     | 1716  | 0        | 1658     | 139     | 0            |
| 15  | O     | 1302  | 0        | 1296     | 64      | 0            |
| 15  | P     | 1296  | 0        | 1291     | 125     | 0            |
| 15  | Q     | 1302  | 0        | 1300     | 115     | 0            |
| 16  | R     | 1628  | 0        | 1588     | 115     | 0            |
| 17  | S     | 1722  | 0        | 1670     | 149     | 0            |
| 18  | T     | 1326  | 0        | 1304     | 18      | 0            |
| 19  | W     | 1239  | 0        | 1208     | 55      | 0            |
| 19  | X     | 1253  | 0        | 1232     | 91      | 0            |
| 20  | a     | 5858  | 0        | 5689     | 242     | 0            |
| 21  | b     | 5820  | 0        | 5647     | 269     | 0            |
| 22  | c     | 597   | 0        | 583      | 29      | 0            |
| 23  | d     | 1056  | 0        | 1074     | 108     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24  | e     | 507   | 0        | 504      | 23      | 0            |
| 25  | f     | 1223  | 0        | 1238     | 79      | 0            |
| 26  | i     | 256   | 0        | 284      | 29      | 0            |
| 27  | j     | 324   | 0        | 338      | 48      | 0            |
| 28  | l     | 1094  | 0        | 1129     | 55      | 0            |
| 29  | m     | 198   | 0        | 213      | 27      | 0            |
| 30  | g     | 670   | 0        | 143      | 23      | 0            |
| 31  | h     | 676   | 0        | 662      | 75      | 0            |
| 32  | U     | 1194  | 0        | 1160     | 221     | 0            |
| 33  | V     | 1361  | 0        | 1354     | 361     | 0            |
| 34  | A     | 129   | 0        | 0        | 14      | 0            |
| 34  | B     | 86    | 0        | 0        | 15      | 0            |
| 34  | C     | 43    | 0        | 0        | 4       | 0            |
| 34  | D     | 172   | 0        | 0        | 19      | 0            |
| 34  | E     | 172   | 0        | 0        | 12      | 0            |
| 34  | F     | 43    | 0        | 0        | 3       | 0            |
| 34  | G     | 43    | 0        | 0        | 2       | 0            |
| 34  | H     | 86    | 0        | 0        | 6       | 0            |
| 34  | I     | 43    | 0        | 0        | 6       | 0            |
| 34  | J     | 43    | 0        | 0        | 4       | 0            |
| 34  | K     | 86    | 0        | 0        | 8       | 0            |
| 34  | L     | 43    | 0        | 0        | 25      | 0            |
| 34  | M     | 43    | 0        | 0        | 18      | 0            |
| 34  | O     | 43    | 0        | 0        | 6       | 0            |
| 34  | P     | 43    | 0        | 0        | 6       | 0            |
| 34  | Q     | 43    | 0        | 0        | 19      | 0            |
| 34  | R     | 86    | 0        | 0        | 16      | 0            |
| 34  | S     | 86    | 0        | 0        | 3       | 0            |
| 34  | W     | 86    | 0        | 0        | 45      | 0            |
| 34  | a     | 43    | 0        | 0        | 1       | 0            |
| 34  | j     | 43    | 0        | 0        | 4       | 0            |
| 35  | A     | 96    | 0        | 0        | 3       | 0            |
| 35  | B     | 96    | 0        | 0        | 19      | 0            |
| 35  | C     | 144   | 0        | 0        | 16      | 0            |
| 35  | D     | 48    | 0        | 0        | 6       | 0            |
| 35  | E     | 144   | 0        | 0        | 18      | 0            |
| 35  | F     | 288   | 0        | 0        | 12      | 0            |
| 35  | G     | 192   | 0        | 0        | 9       | 0            |
| 35  | H     | 96    | 0        | 0        | 7       | 0            |
| 35  | I     | 144   | 0        | 0        | 21      | 0            |
| 35  | J     | 240   | 0        | 0        | 29      | 0            |
| 35  | K     | 192   | 0        | 0        | 6       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 35  | L     | 240   | 0        | 0        | 14      | 0            |
| 35  | M     | 192   | 0        | 0        | 12      | 0            |
| 35  | N     | 336   | 0        | 0        | 55      | 0            |
| 35  | O     | 240   | 0        | 0        | 27      | 0            |
| 35  | P     | 192   | 0        | 0        | 6       | 0            |
| 35  | Q     | 192   | 0        | 0        | 42      | 0            |
| 35  | R     | 336   | 0        | 0        | 10      | 0            |
| 35  | S     | 288   | 0        | 0        | 27      | 0            |
| 35  | T     | 336   | 0        | 0        | 9       | 0            |
| 35  | U     | 192   | 0        | 0        | 35      | 0            |
| 35  | V     | 192   | 0        | 0        | 46      | 0            |
| 35  | W     | 96    | 0        | 0        | 1       | 0            |
| 35  | X     | 288   | 0        | 0        | 27      | 0            |
| 35  | h     | 96    | 0        | 0        | 9       | 0            |
| 36  | A     | 517   | 0        | 509      | 59      | 0            |
| 36  | B     | 329   | 0        | 299      | 34      | 0            |
| 36  | C     | 516   | 0        | 513      | 41      | 0            |
| 36  | D     | 618   | 0        | 591      | 45      | 0            |
| 36  | E     | 550   | 0        | 576      | 54      | 0            |
| 36  | F     | 452   | 0        | 431      | 57      | 0            |
| 36  | G     | 556   | 0        | 526      | 75      | 0            |
| 36  | H     | 760   | 0        | 747      | 60      | 0            |
| 36  | I     | 555   | 0        | 520      | 91      | 0            |
| 36  | J     | 562   | 0        | 540      | 30      | 0            |
| 36  | K     | 529   | 0        | 532      | 61      | 0            |
| 36  | L     | 527   | 0        | 523      | 54      | 0            |
| 36  | M     | 525   | 0        | 462      | 38      | 0            |
| 36  | N     | 601   | 0        | 503      | 65      | 0            |
| 36  | O     | 506   | 0        | 492      | 34      | 0            |
| 36  | P     | 686   | 0        | 666      | 50      | 0            |
| 36  | Q     | 458   | 0        | 441      | 78      | 0            |
| 36  | R     | 661   | 0        | 616      | 25      | 0            |
| 36  | S     | 658   | 0        | 611      | 46      | 0            |
| 36  | T     | 408   | 0        | 409      | 27      | 0            |
| 36  | U     | 449   | 0        | 427      | 96      | 0            |
| 36  | V     | 545   | 0        | 565      | 145     | 0            |
| 36  | W     | 629   | 0        | 552      | 49      | 0            |
| 36  | X     | 368   | 0        | 273      | 36      | 0            |
| 36  | a     | 2437  | 0        | 2463     | 146     | 0            |
| 36  | b     | 2337  | 0        | 2371     | 117     | 0            |
| 36  | f     | 247   | 0        | 259      | 39      | 0            |
| 36  | h     | 65    | 0        | 72       | 11      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 36  | i     | 65    | 0        | 71       | 3       | 0            |
| 36  | j     | 172   | 0        | 172      | 31      | 0            |
| 36  | l     | 294   | 0        | 291      | 24      | 0            |
| 37  | A     | 45    | 0        | 0        | 4       | 0            |
| 37  | B     | 45    | 0        | 0        | 2       | 0            |
| 37  | C     | 45    | 0        | 0        | 1       | 0            |
| 37  | D     | 45    | 0        | 0        | 0       | 0            |
| 37  | E     | 45    | 0        | 0        | 2       | 0            |
| 37  | F     | 90    | 0        | 0        | 20      | 0            |
| 37  | G     | 135   | 0        | 0        | 8       | 0            |
| 37  | H     | 45    | 0        | 0        | 0       | 0            |
| 37  | J     | 45    | 0        | 0        | 0       | 0            |
| 37  | K     | 45    | 0        | 0        | 9       | 0            |
| 37  | L     | 90    | 0        | 0        | 11      | 0            |
| 37  | M     | 135   | 0        | 0        | 7       | 0            |
| 37  | N     | 45    | 0        | 0        | 0       | 0            |
| 37  | O     | 90    | 0        | 0        | 13      | 0            |
| 37  | P     | 90    | 0        | 0        | 2       | 0            |
| 37  | Q     | 90    | 0        | 0        | 16      | 0            |
| 37  | R     | 45    | 0        | 0        | 0       | 0            |
| 37  | S     | 45    | 0        | 0        | 4       | 0            |
| 37  | T     | 90    | 0        | 0        | 18      | 0            |
| 37  | U     | 45    | 0        | 0        | 0       | 0            |
| 37  | V     | 45    | 0        | 0        | 1       | 0            |
| 37  | W     | 90    | 0        | 0        | 14      | 0            |
| 37  | X     | 45    | 0        | 0        | 0       | 0            |
| 38  | A     | 28    | 0        | 19       | 7       | 0            |
| 38  | b     | 46    | 0        | 56       | 10      | 0            |
| 39  | B     | 70    | 0        | 92       | 20      | 0            |
| 39  | E     | 93    | 0        | 118      | 25      | 0            |
| 39  | F     | 68    | 0        | 85       | 35      | 0            |
| 39  | G     | 70    | 0        | 90       | 14      | 0            |
| 39  | I     | 70    | 0        | 92       | 22      | 0            |
| 39  | K     | 66    | 0        | 81       | 14      | 0            |
| 39  | L     | 66    | 0        | 77       | 10      | 0            |
| 39  | P     | 46    | 0        | 60       | 8       | 0            |
| 39  | U     | 70    | 0        | 92       | 27      | 0            |
| 39  | a     | 102   | 0        | 129      | 25      | 0            |
| 39  | b     | 59    | 0        | 78       | 25      | 0            |
| 39  | f     | 24    | 0        | 35       | 2       | 0            |
| 39  | h     | 35    | 0        | 43       | 21      | 0            |
| 40  | C     | 57    | 0        | 75       | 19      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 40  | L     | 47    | 0        | 52       | 20      | 0            |
| 40  | b     | 60    | 0        | 81       | 4       | 0            |
| 41  | D     | 95    | 0        | 137      | 28      | 0            |
| 41  | E     | 49    | 0        | 74       | 24      | 0            |
| 41  | F     | 74    | 0        | 97       | 5       | 0            |
| 41  | G     | 136   | 0        | 194      | 27      | 0            |
| 41  | I     | 49    | 0        | 74       | 10      | 0            |
| 41  | O     | 91    | 0        | 129      | 14      | 0            |
| 41  | Q     | 49    | 0        | 72       | 19      | 0            |
| 41  | R     | 49    | 0        | 74       | 14      | 0            |
| 41  | a     | 122   | 0        | 160      | 20      | 0            |
| 41  | b     | 49    | 0        | 74       | 18      | 0            |
| 41  | f     | 91    | 0        | 129      | 41      | 0            |
| 41  | i     | 46    | 0        | 65       | 28      | 0            |
| 41  | j     | 49    | 0        | 74       | 14      | 0            |
| 41  | l     | 48    | 0        | 69       | 17      | 0            |
| 42  | D     | 83    | 0        | 109      | 17      | 0            |
| 42  | E     | 86    | 0        | 112      | 25      | 0            |
| 42  | G     | 110   | 0        | 172      | 22      | 0            |
| 42  | I     | 55    | 0        | 86       | 14      | 0            |
| 42  | J     | 99    | 0        | 147      | 36      | 0            |
| 42  | L     | 33    | 0        | 36       | 10      | 0            |
| 42  | V     | 92    | 0        | 130      | 41      | 0            |
| 42  | a     | 54    | 0        | 81       | 20      | 0            |
| 42  | h     | 45    | 0        | 63       | 7       | 0            |
| 42  | j     | 52    | 0        | 77       | 26      | 0            |
| 42  | m     | 37    | 0        | 43       | 9       | 0            |
| 43  | a     | 33    | 0        | 46       | 3       | 0            |
| 43  | b     | 33    | 0        | 46       | 3       | 0            |
| 44  | a     | 160   | 0        | 224      | 13      | 0            |
| 44  | b     | 200   | 0        | 280      | 14      | 0            |
| 44  | f     | 80    | 0        | 112      | 3       | 0            |
| 44  | h     | 40    | 0        | 56       | 4       | 0            |
| 44  | i     | 80    | 0        | 112      | 9       | 0            |
| 44  | j     | 40    | 0        | 56       | 1       | 0            |
| 44  | l     | 80    | 0        | 112      | 5       | 0            |
| 44  | m     | 40    | 0        | 56       | 11      | 0            |
| 45  | b     | 8     | 0        | 0        | 1       | 0            |
| 45  | c     | 16    | 0        | 0        | 0       | 0            |
| 46  | a     | 64    | 0        | 0        | 7       | 0            |
| 46  | b     | 72    | 0        | 0        | 13      | 0            |
| 46  | c     | 7     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 46  | d     | 4     | 0        | 0        | 0       | 0            |
| 46  | f     | 2     | 0        | 0        | 0       | 0            |
| 46  | j     | 1     | 0        | 0        | 0       | 0            |
| 46  | l     | 3     | 0        | 0        | 3       | 0            |
| All | All   | 81344 | 0        | 72580    | 4619    | 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 30.

The worst 5 of 4619 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) |
|-------------------|------------------|--------------------------|-------------------|
| 33:V:140:PRO:CB   | 35:V:303:A86:C39 | 1.75                     | 1.63              |
| 32:U:42:MET:HB3   | 35:U:304:A86:C   | 1.26                     | 1.62              |
| 36:Q:314:CLA:HED3 | 36:Q:314:CLA:C1A | 1.29                     | 1.59              |
| 33:V:69:ILE:CG2   | 36:V:309:CLA:CGA | 1.75                     | 1.59              |
| 5:E:128:GLN:HG3   | 34:E:301:DD6:C23 | 1.32                     | 1.56              |

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     | 166/168 (99%) | 150 (90%) | 14 (8%) | 2 (1%)   | 10          | 14  |
| 2   | B     | 128/223 (57%) | 121 (94%) | 7 (6%)  | 0        | 100         | 100 |
| 3   | C     | 161/198 (81%) | 150 (93%) | 9 (6%)  | 2 (1%)   | 10          | 14  |
| 4   | D     | 170/207 (82%) | 160 (94%) | 9 (5%)  | 1 (1%)   | 21          | 30  |
| 5   | E     | 186/222 (84%) | 178 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 6   | F     | 178/215 (83%) | 165 (93%) | 13 (7%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 7   | G     | 212/245 (86%)   | 197 (93%)  | 14 (7%)  | 1 (0%)   | 24          | 34  |
| 8   | H     | 168/203 (83%)   | 151 (90%)  | 17 (10%) | 0        | 100         | 100 |
| 9   | I     | 159/195 (82%)   | 146 (92%)  | 13 (8%)  | 0        | 100         | 100 |
| 10  | J     | 165/200 (82%)   | 145 (88%)  | 17 (10%) | 3 (2%)   | 6           | 8   |
| 11  | K     | 167/207 (81%)   | 152 (91%)  | 15 (9%)  | 0        | 100         | 100 |
| 12  | L     | 194/229 (85%)   | 176 (91%)  | 18 (9%)  | 0        | 100         | 100 |
| 13  | M     | 185/306 (60%)   | 169 (91%)  | 15 (8%)  | 1 (0%)   | 24          | 34  |
| 14  | N     | 217/219 (99%)   | 174 (80%)  | 40 (18%) | 3 (1%)   | 9           | 11  |
| 15  | O     | 171/205 (83%)   | 147 (86%)  | 21 (12%) | 3 (2%)   | 6           | 8   |
| 15  | P     | 171/205 (83%)   | 153 (90%)  | 16 (9%)  | 2 (1%)   | 10          | 14  |
| 15  | Q     | 171/205 (83%)   | 150 (88%)  | 19 (11%) | 2 (1%)   | 10          | 14  |
| 16  | R     | 209/246 (85%)   | 182 (87%)  | 25 (12%) | 2 (1%)   | 12          | 17  |
| 17  | S     | 218/254 (86%)   | 184 (84%)  | 29 (13%) | 5 (2%)   | 5           | 5   |
| 18  | T     | 170/207 (82%)   | 164 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 19  | W     | 158/198 (80%)   | 133 (84%)  | 25 (16%) | 0        | 100         | 100 |
| 19  | X     | 160/198 (81%)   | 146 (91%)  | 13 (8%)  | 1 (1%)   | 21          | 30  |
| 20  | a     | 740/743 (100%)  | 713 (96%)  | 26 (4%)  | 1 (0%)   | 48          | 62  |
| 21  | b     | 731/733 (100%)  | 699 (96%)  | 31 (4%)  | 1 (0%)   | 48          | 62  |
| 22  | c     | 78/80 (98%)     | 74 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 23  | d     | 131/132 (99%)   | 125 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 24  | e     | 61/63 (97%)     | 60 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 25  | f     | 160/162 (99%)   | 152 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 26  | i     | 31/40 (78%)     | 31 (100%)  | 0        | 0        | 100         | 100 |
| 27  | j     | 39/42 (93%)     | 37 (95%)   | 1 (3%)   | 1 (3%)   | 4           | 4   |
| 28  | l     | 142/172 (83%)   | 131 (92%)  | 11 (8%)  | 0        | 100         | 100 |
| 29  | m     | 26/29 (90%)     | 26 (100%)  | 0        | 0        | 100         | 100 |
| 31  | h     | 87/139 (63%)    | 87 (100%)  | 0        | 0        | 100         | 100 |
| 32  | U     | 154/160 (96%)   | 123 (80%)  | 26 (17%) | 5 (3%)   | 3           | 2   |
| 33  | V     | 177/179 (99%)   | 152 (86%)  | 20 (11%) | 5 (3%)   | 4           | 3   |
| All | All   | 6441/7429 (87%) | 5903 (92%) | 497 (8%) | 41 (1%)  | 23          | 30  |

5 of 41 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | J     | 87  | ILE  |
| 15  | O     | 153 | PRO  |
| 15  | O     | 155 | ILE  |
| 15  | Q     | 153 | PRO  |
| 17  | S     | 103 | ALA  |

### 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     | 137/137 (100%) | 128 (93%)  | 9 (7%)   | 15          | 24  |
| 2   | B     | 105/180 (58%)  | 98 (93%)   | 7 (7%)   | 15          | 23  |
| 3   | C     | 131/153 (86%)  | 122 (93%)  | 9 (7%)   | 14          | 22  |
| 4   | D     | 140/163 (86%)  | 125 (89%)  | 15 (11%) | 6           | 8   |
| 5   | E     | 142/164 (87%)  | 136 (96%)  | 6 (4%)   | 26          | 42  |
| 6   | F     | 142/169 (84%)  | 135 (95%)  | 7 (5%)   | 22          | 36  |
| 7   | G     | 172/193 (89%)  | 146 (85%)  | 26 (15%) | 3           | 3   |
| 8   | H     | 131/154 (85%)  | 129 (98%)  | 2 (2%)   | 57          | 75  |
| 9   | I     | 124/152 (82%)  | 101 (82%)  | 23 (18%) | 1           | 2   |
| 10  | J     | 130/154 (84%)  | 122 (94%)  | 8 (6%)   | 16          | 26  |
| 11  | K     | 133/160 (83%)  | 130 (98%)  | 3 (2%)   | 44          | 64  |
| 12  | L     | 159/180 (88%)  | 159 (100%) | 0        | 100         | 100 |
| 13  | M     | 142/247 (58%)  | 135 (95%)  | 7 (5%)   | 22          | 36  |
| 14  | N     | 176/176 (100%) | 170 (97%)  | 6 (3%)   | 32          | 51  |
| 15  | O     | 138/159 (87%)  | 134 (97%)  | 4 (3%)   | 37          | 57  |
| 15  | P     | 137/159 (86%)  | 120 (88%)  | 17 (12%) | 4           | 6   |
| 15  | Q     | 138/159 (87%)  | 133 (96%)  | 5 (4%)   | 31          | 49  |
| 16  | R     | 167/193 (86%)  | 160 (96%)  | 7 (4%)   | 26          | 42  |
| 17  | S     | 177/204 (87%)  | 169 (96%)  | 8 (4%)   | 24          | 39  |
| 18  | T     | 136/163 (83%)  | 135 (99%)  | 1 (1%)   | 76          | 87  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |     |
|-----|-------|-----------------|------------|-----------|-------------|-----|
| 19  | W     | 125/151 (83%)   | 125 (100%) | 0         | 100         | 100 |
| 19  | X     | 127/151 (84%)   | 125 (98%)  | 2 (2%)    | 55          | 74  |
| 20  | a     | 606/606 (100%)  | 543 (90%)  | 63 (10%)  | 7           | 9   |
| 21  | b     | 593/593 (100%)  | 517 (87%)  | 76 (13%)  | 4           | 5   |
| 22  | c     | 67/69 (97%)     | 59 (88%)   | 8 (12%)   | 5           | 6   |
| 23  | d     | 111/111 (100%)  | 88 (79%)   | 23 (21%)  | 1           | 1   |
| 24  | e     | 55/55 (100%)    | 51 (93%)   | 4 (7%)    | 13          | 20  |
| 25  | f     | 119/125 (95%)   | 105 (88%)  | 14 (12%)  | 5           | 6   |
| 26  | i     | 29/36 (81%)     | 20 (69%)   | 9 (31%)   | 0           | 0   |
| 27  | j     | 34/35 (97%)     | 29 (85%)   | 5 (15%)   | 3           | 3   |
| 28  | l     | 114/143 (80%)   | 98 (86%)   | 16 (14%)  | 3           | 4   |
| 29  | m     | 20/23 (87%)     | 17 (85%)   | 3 (15%)   | 3           | 3   |
| 31  | h     | 70/109 (64%)    | 54 (77%)   | 16 (23%)  | 1           | 1   |
| 32  | U     | 119/121 (98%)   | 82 (69%)   | 37 (31%)  | 0           | 0   |
| 33  | V     | 137/137 (100%)  | 83 (61%)   | 54 (39%)  | 0           | 0   |
| All | All   | 5183/5884 (88%) | 4683 (90%) | 500 (10%) | 10          | 11  |

5 of 500 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | a     | 728 | GLN  |
| 32  | U     | 127 | GLU  |
| 21  | b     | 491 | VAL  |
| 32  | U     | 114 | LYS  |
| 33  | V     | 74  | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | b     | 404 | ASN  |
| 33  | V     | 89  | HIS  |
| 21  | b     | 520 | HIS  |
| 25  | f     | 155 | HIS  |
| 15  | O     | 84  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

589 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 | $\# Z  > 2$ |
| 37  | KC1  | M     | 317 | -     | 49,53,53     | 2.75 | 20 (40%)    | 63,89,89    | 4.78 | 38 (60%)    |
| 36  | CLA  | a     | 819 | -     | 49,53,73     | 1.50 | 12 (24%)    | 59,89,113   | 2.16 | 8 (13%)     |
| 36  | CLA  | H     | 307 | 8     | 64,68,73     | 1.37 | 9 (14%)     | 77,107,113  | 1.87 | 20 (25%)    |
| 36  | CLA  | a     | 828 | -     | 69,73,73     | 1.21 | 9 (13%)     | 83,113,113  | 1.42 | 8 (9%)      |
| 36  | CLA  | b     | 835 | -     | 49,53,73     | 1.45 | 10 (20%)    | 59,89,113   | 1.64 | 9 (15%)     |
| 36  | CLA  | b     | 838 | 21    | 51,55,73     | 1.37 | 10 (19%)    | 61,91,113   | 1.44 | 7 (11%)     |
| 36  | CLA  | M     | 314 | -     | 45,49,73     | 1.51 | 9 (20%)     | 54,84,113   | 1.56 | 6 (11%)     |
| 36  | CLA  | U     | 313 | -     | 45,49,73     | 1.51 | 7 (15%)     | 54,84,113   | 1.70 | 9 (16%)     |
| 36  | CLA  | M     | 309 | -     | 69,73,73     | 1.24 | 10 (14%)    | 83,113,113  | 1.30 | 6 (7%)      |
| 44  | BCR  | j     | 107 | -     | 41,41,41     | 1.11 | 2 (4%)      | 56,56,56    | 1.22 | 7 (12%)     |
| 36  | CLA  | R     | 311 | 16    | 69,73,73     | 1.23 | 9 (13%)     | 83,113,113  | 1.36 | 8 (9%)      |
| 36  | CLA  | X     | 309 | 19    | 48,53,73     | 1.52 | 8 (16%)     | 57,89,113   | 1.66 | 10 (17%)    |
| 36  | CLA  | X     | 307 | 19,35 | 54,58,73     | 1.49 | 9 (16%)     | 65,95,113   | 1.76 | 12 (18%)    |
| 35  | A86  | R     | 304 | 16,36 | 44,50,50     | 1.30 | 3 (6%)      | 51,76,76    | 2.95 | 17 (33%)    |



| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 35  | A86  | V     | 302 | -     | 44,50,50     | 1.32 | 4 (9%)   | 51,76,76    | 2.92 | 21 (41%) |
| 36  | CLA  | b     | 840 | 21    | 69,73,73     | 1.23 | 11 (15%) | 83,113,113  | 1.48 | 12 (14%) |
| 36  | CLA  | T     | 313 | 18    | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.28 | 7 (8%)   |
| 35  | A86  | X     | 305 | -     | 44,50,50     | 1.29 | 4 (9%)   | 51,76,76    | 3.04 | 18 (35%) |
| 36  | CLA  | W     | 211 | 19    | 69,73,73     | 1.24 | 8 (11%)  | 83,113,113  | 1.50 | 9 (10%)  |
| 36  | CLA  | a     | 827 | 20    | 66,70,73     | 1.28 | 10 (15%) | 79,109,113  | 1.51 | 10 (12%) |
| 42  | LMG  | V     | 315 | -     | 46,46,55     | 0.98 | 2 (4%)   | 54,54,63    | 4.29 | 4 (7%)   |
| 35  | A86  | Q     | 301 | -     | 44,50,50     | 1.33 | 5 (11%)  | 51,76,76    | 2.73 | 17 (33%) |
| 36  | CLA  | P     | 312 | 15    | 50,54,73     | 1.45 | 9 (18%)  | 60,90,113   | 1.58 | 8 (13%)  |
| 35  | A86  | N     | 306 | -     | 44,50,50     | 1.22 | 3 (6%)   | 51,76,76    | 2.83 | 16 (31%) |
| 39  | LMT  | b     | 848 | -     | 36,36,36     | 0.38 | 0        | 47,47,47    | 0.67 | 1 (2%)   |
| 36  | CLA  | F     | 314 | 6,35  | 69,73,73     | 1.23 | 11 (15%) | 83,113,113  | 1.45 | 8 (9%)   |
| 42  | LMG  | J     | 318 | -     | 55,55,55     | 0.89 | 2 (3%)   | 63,63,63    | 1.02 | 3 (4%)   |
| 35  | A86  | O     | 303 | -     | 44,50,50     | 1.34 | 5 (11%)  | 51,76,76    | 2.73 | 17 (33%) |
| 36  | CLA  | W     | 212 | 19    | 69,73,73     | 1.29 | 9 (13%)  | 83,113,113  | 1.64 | 11 (13%) |
| 35  | A86  | V     | 303 | 35    | 44,50,50     | 1.28 | 4 (9%)   | 51,76,76    | 3.25 | 22 (43%) |
| 36  | CLA  | C     | 211 | -     | 69,73,73     | 1.24 | 11 (15%) | 83,113,113  | 1.36 | 7 (8%)   |
| 36  | CLA  | b     | 820 | 21    | 64,68,73     | 1.30 | 11 (17%) | 77,107,113  | 1.34 | 7 (9%)   |
| 36  | CLA  | B     | 306 | -     | 50,54,73     | 1.42 | 8 (16%)  | 60,90,113   | 1.61 | 6 (10%)  |
| 36  | CLA  | T     | 311 | 18    | 69,73,73     | 1.28 | 10 (14%) | 83,113,113  | 1.93 | 14 (16%) |
| 36  | CLA  | M     | 308 | -     | 56,60,73     | 1.39 | 11 (19%) | 67,97,113   | 1.60 | 8 (11%)  |
| 36  | CLA  | a     | 816 | 20    | 69,73,73     | 1.56 | 9 (13%)  | 83,113,113  | 2.07 | 18 (21%) |
| 37  | KC1  | P     | 315 | 35    | 49,53,53     | 2.88 | 20 (40%) | 63,89,89    | 6.04 | 39 (61%) |
| 36  | CLA  | X     | 313 | 19    | 46,50,73     | 2.14 | 12 (26%) | 55,85,113   | 4.04 | 20 (36%) |
| 35  | A86  | T     | 306 | -     | 44,50,50     | 1.23 | 4 (9%)   | 51,76,76    | 2.88 | 18 (35%) |
| 35  | A86  | L     | 319 | -     | 44,50,50     | 1.43 | 6 (13%)  | 51,76,76    | 3.47 | 24 (47%) |
| 36  | CLA  | N     | 315 | -     | 45,49,73     | 1.54 | 7 (15%)  | 54,84,113   | 1.73 | 12 (22%) |
| 36  | CLA  | b     | 826 | 21,46 | 68,72,73     | 1.33 | 12 (17%) | 81,111,113  | 2.00 | 17 (20%) |
| 36  | CLA  | W     | 207 | 34    | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.42 | 8 (9%)   |
| 35  | A86  | G     | 302 | -     | 44,50,50     | 1.18 | 3 (6%)   | 51,76,76    | 1.92 | 13 (25%) |
| 36  | CLA  | P     | 308 | -     | 65,69,73     | 1.28 | 9 (13%)  | 78,108,113  | 1.38 | 5 (6%)   |
| 36  | CLA  | Q     | 309 | 15    | 50,54,73     | 1.46 | 9 (18%)  | 60,90,113   | 1.60 | 8 (13%)  |
| 35  | A86  | O     | 305 | -     | 44,50,50     | 1.42 | 4 (9%)   | 51,76,76    | 1.95 | 16 (31%) |
| 36  | CLA  | N     | 319 | 14    | 46,50,73     | 3.35 | 13 (28%) | 55,85,113   | 5.74 | 32 (58%) |
| 36  | CLA  | M     | 312 | 13,36 | 51,55,73     | 1.46 | 9 (17%)  | 61,91,113   | 1.58 | 8 (13%)  |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 39  | LMT  | a     | 854 | -     | 36,36,36     | 0.40 | 0        | 47,47,47    | 0.75 | 0        |
| 42  | LMG  | V     | 316 | -     | 46,46,55     | 0.98 | 2 (4%)   | 54,54,63    | 1.04 | 3 (5%)   |
| 39  | LMT  | b     | 851 | -     | 24,24,36     | 0.42 | 0        | 29,29,47    | 0.81 | 0        |
| 35  | A86  | W     | 203 | 36    | 44,50,50     | 1.37 | 4 (9%)   | 51,76,76    | 2.83 | 20 (39%) |
| 36  | CLA  | P     | 309 | 41    | 69,73,73     | 1.24 | 11 (15%) | 83,113,113  | 1.37 | 7 (8%)   |
| 36  | CLA  | b     | 831 | 21    | 54,58,73     | 1.42 | 11 (20%) | 65,95,113   | 1.55 | 8 (12%)  |
| 36  | CLA  | V     | 308 | -     | 69,73,73     | 1.23 | 10 (14%) | 83,113,113  | 1.37 | 10 (12%) |
| 35  | A86  | L     | 306 | 37    | 44,50,50     | 1.24 | 3 (6%)   | 51,76,76    | 2.98 | 19 (37%) |
| 34  | DD6  | R     | 308 | -     | 39,45,45     | 2.02 | 3 (7%)   | 52,67,67    | 2.12 | 13 (25%) |
| 35  | A86  | Q     | 304 | -     | 44,50,50     | 1.39 | 6 (13%)  | 51,76,76    | 3.30 | 24 (47%) |
| 36  | CLA  | b     | 841 | 41    | 69,73,73     | 1.32 | 12 (17%) | 83,113,113  | 1.82 | 16 (19%) |
| 44  | BCR  | a     | 846 | -     | 41,41,41     | 1.15 | 3 (7%)   | 56,56,56    | 1.19 | 3 (5%)   |
| 36  | CLA  | I     | 312 | 9     | 56,60,73     | 1.41 | 9 (16%)  | 67,97,113   | 1.42 | 6 (8%)   |
| 35  | A86  | U     | 301 | -     | 44,50,50     | 1.37 | 3 (6%)   | 51,76,76    | 3.80 | 25 (49%) |
| 35  | A86  | I     | 302 | -     | 44,50,50     | 1.30 | 4 (9%)   | 51,76,76    | 2.66 | 17 (33%) |
| 36  | CLA  | b     | 824 | 21    | 57,61,73     | 2.02 | 17 (29%) | 68,98,113   | 2.57 | 25 (36%) |
| 36  | CLA  | a     | 802 | -     | 69,73,73     | 1.34 | 8 (11%)  | 83,113,113  | 1.83 | 14 (16%) |
| 36  | CLA  | V     | 310 | 33    | 69,73,73     | 1.23 | 9 (13%)  | 83,113,113  | 1.32 | 5 (6%)   |
| 35  | A86  | T     | 302 | 18    | 44,50,50     | 1.24 | 3 (6%)   | 51,76,76    | 2.85 | 21 (41%) |
| 36  | CLA  | N     | 316 | 14    | 69,73,73     | 1.25 | 9 (13%)  | 83,113,113  | 1.32 | 5 (6%)   |
| 35  | A86  | h     | 202 | -     | 44,50,50     | 1.24 | 4 (9%)   | 51,76,76    | 1.74 | 10 (19%) |
| 41  | LHG  | F     | 318 | -     | 32,32,48     | 0.88 | 1 (3%)   | 36,37,54    | 1.72 | 6 (16%)  |
| 36  | CLA  | P     | 310 | 15,41 | 69,73,73     | 1.25 | 9 (13%)  | 83,113,113  | 1.35 | 6 (7%)   |
| 35  | A86  | Q     | 303 | -     | 44,50,50     | 1.33 | 5 (11%)  | 51,76,76    | 2.05 | 15 (29%) |
| 36  | CLA  | a     | 820 | -     | 69,73,73     | 1.22 | 11 (15%) | 83,113,113  | 1.40 | 11 (13%) |
| 37  | KC1  | R     | 317 | -     | 49,53,53     | 2.71 | 19 (38%) | 63,89,89    | 5.25 | 38 (60%) |
| 35  | A86  | N     | 304 | -     | 44,50,50     | 2.90 | 7 (15%)  | 51,76,76    | 7.45 | 18 (35%) |
| 42  | LMG  | D     | 321 | -     | 37,37,55     | 1.08 | 2 (5%)   | 45,45,63    | 1.02 | 2 (4%)   |
| 36  | CLA  | f     | 804 | 46    | 69,73,73     | 1.99 | 19 (27%) | 83,113,113  | 3.08 | 32 (38%) |
| 39  | LMT  | U     | 315 | -     | 36,36,36     | 0.40 | 0        | 47,47,47    | 0.74 | 1 (2%)   |
| 36  | CLA  | J     | 312 | 10    | 69,73,73     | 1.21 | 10 (14%) | 83,113,113  | 1.41 | 8 (9%)   |
| 36  | CLA  | W     | 218 | 19    | 47,51,73     | 1.49 | 10 (21%) | 56,86,113   | 1.64 | 8 (14%)  |
| 39  | LMT  | h     | 205 | -     | 36,36,36     | 0.41 | 0        | 47,47,47    | 0.70 | 1 (2%)   |
| 36  | CLA  | K     | 315 | -     | 45,49,73     | 1.51 | 10 (22%) | 54,84,113   | 1.62 | 7 (12%)  |
| 36  | CLA  | a     | 812 | 20    | 69,73,73     | 1.23 | 10 (14%) | 83,113,113  | 1.40 | 8 (9%)   |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 43  | PQN  | b     | 842 | -     | 34,34,34     | 1.56 | 2 (5%)   | 42,45,45    | 1.19 | 4 (9%)   |
| 42  | LMG  | m     | 102 | -     | 37,37,55     | 1.08 | 2 (5%)   | 45,45,63    | 1.08 | 3 (6%)   |
| 36  | CLA  | E     | 311 | 5     | 69,73,73     | 1.23 | 10 (14%) | 83,113,113  | 1.33 | 7 (8%)   |
| 36  | CLA  | D     | 311 | 4     | 50,54,73     | 1.43 | 9 (18%)  | 60,90,113   | 1.48 | 5 (8%)   |
| 36  | CLA  | L     | 311 | -     | 69,73,73     | 1.25 | 11 (15%) | 83,113,113  | 1.34 | 10 (12%) |
| 36  | CLA  | P     | 301 | 15    | 69,73,73     | 1.23 | 11 (15%) | 83,113,113  | 1.45 | 8 (9%)   |
| 41  | LHG  | j     | 104 | -     | 48,48,48     | 0.93 | 2 (4%)   | 51,54,54    | 1.04 | 3 (5%)   |
| 34  | DD6  | H     | 303 | -     | 39,45,45     | 1.99 | 3 (7%)   | 52,67,67    | 1.97 | 12 (23%) |
| 44  | BCR  | b     | 846 | -     | 41,41,41     | 1.15 | 4 (9%)   | 56,56,56    | 1.44 | 10 (17%) |
| 36  | CLA  | V     | 306 | 33    | 69,73,73     | 1.30 | 8 (11%)  | 83,113,113  | 1.50 | 12 (14%) |
| 35  | A86  | F     | 304 | 36    | 44,50,50     | 1.25 | 4 (9%)   | 51,76,76    | 2.03 | 13 (25%) |
| 36  | CLA  | Q     | 308 | -     | 69,73,73     | 1.24 | 10 (14%) | 83,113,113  | 1.42 | 10 (12%) |
| 43  | PQN  | a     | 840 | -     | 34,34,34     | 1.58 | 2 (5%)   | 42,45,45    | 1.15 | 4 (9%)   |
| 36  | CLA  | H     | 310 | 8     | 50,54,73     | 1.74 | 12 (24%) | 60,90,113   | 2.66 | 19 (31%) |
| 41  | LHG  | b     | 850 | 36    | 48,48,48     | 0.92 | 2 (4%)   | 51,54,54    | 1.04 | 3 (5%)   |
| 36  | CLA  | b     | 815 | 21    | 69,73,73     | 1.27 | 11 (15%) | 83,113,113  | 1.36 | 7 (8%)   |
| 36  | CLA  | T     | 312 | 18    | 50,54,73     | 1.46 | 8 (16%)  | 60,90,113   | 1.64 | 10 (16%) |
| 44  | BCR  | a     | 847 | -     | 41,41,41     | 1.23 | 4 (9%)   | 56,56,56    | 1.25 | 5 (8%)   |
| 36  | CLA  | G     | 314 | 7     | 45,49,73     | 1.48 | 9 (20%)  | 54,84,113   | 1.70 | 8 (14%)  |
| 36  | CLA  | P     | 302 | -     | 46,50,73     | 1.47 | 9 (19%)  | 55,85,113   | 1.68 | 8 (14%)  |
| 35  | A86  | X     | 304 | 19    | 44,50,50     | 1.34 | 4 (9%)   | 51,76,76    | 3.26 | 20 (39%) |
| 34  | DD6  | D     | 304 | -     | 39,45,45     | 1.97 | 3 (7%)   | 52,67,67    | 1.91 | 12 (23%) |
| 34  | DD6  | E     | 303 | -     | 39,45,45     | 2.00 | 3 (7%)   | 52,67,67    | 2.00 | 10 (19%) |
| 35  | A86  | P     | 306 | -     | 44,50,50     | 1.22 | 3 (6%)   | 51,76,76    | 1.89 | 13 (25%) |
| 36  | CLA  | J     | 311 | -     | 50,54,73     | 1.47 | 10 (20%) | 60,90,113   | 1.48 | 7 (11%)  |
| 42  | LMG  | h     | 206 | -     | 45,45,55     | 0.99 | 2 (4%)   | 53,53,63    | 1.03 | 3 (5%)   |
| 35  | A86  | M     | 305 | -     | 44,50,50     | 1.34 | 4 (9%)   | 51,76,76    | 2.88 | 15 (29%) |
| 41  | LHG  | O     | 317 | -     | 41,41,48     | 1.00 | 2 (4%)   | 44,47,54    | 1.08 | 3 (6%)   |
| 36  | CLA  | I     | 306 | 9     | 69,73,73     | 1.67 | 15 (21%) | 83,113,113  | 2.48 | 24 (28%) |
| 36  | CLA  | E     | 315 | -     | 69,73,73     | 1.96 | 20 (28%) | 83,113,113  | 2.88 | 28 (33%) |
| 37  | KC1  | F     | 315 | -     | 49,53,53     | 2.67 | 17 (34%) | 63,89,89    | 5.79 | 37 (58%) |
| 36  | CLA  | W     | 210 | -     | 50,54,73     | 1.46 | 8 (16%)  | 60,90,113   | 1.87 | 15 (25%) |
| 44  | BCR  | h     | 201 | -     | 41,41,41     | 1.26 | 5 (12%)  | 56,56,56    | 1.42 | 10 (17%) |
| 35  | A86  | U     | 304 | 37,32 | 44,50,50     | 1.21 | 3 (6%)   | 51,76,76    | 2.34 | 19 (37%) |
| 36  | CLA  | K     | 316 | -     | 69,73,73     | 1.24 | 9 (13%)  | 83,113,113  | 1.29 | 5 (6%)   |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 36  | CLA  | W     | 214 | 19    | 45,49,73     | 1.66 | 8 (17%)  | 54,84,113   | 1.82 | 13 (24%) |
| 37  | KC1  | N     | 314 | 14    | 49,53,53     | 2.87 | 22 (44%) | 63,89,89    | 4.43 | 37 (58%) |
| 41  | LHG  | f     | 808 | 25    | 48,48,48     | 0.95 | 2 (4%)   | 51,54,54    | 1.02 | 3 (5%)   |
| 36  | CLA  | E     | 308 | 5     | 53,57,73     | 1.39 | 11 (20%) | 62,93,113   | 1.52 | 8 (12%)  |
| 36  | CLA  | b     | 816 | 21    | 64,68,73     | 1.99 | 17 (26%) | 77,107,113  | 1.92 | 18 (23%) |
| 45  | SF4  | b     | 803 | 21,20 | 0,12,12      | -    | -        | -           |      |          |
| 35  | A86  | J     | 305 | -     | 44,50,50     | 1.24 | 3 (6%)   | 51,76,76    | 2.08 | 15 (29%) |
| 36  | CLA  | T     | 316 | -     | 45,49,73     | 1.52 | 9 (20%)  | 54,84,113   | 1.55 | 7 (12%)  |
| 36  | CLA  | b     | 839 | -     | 69,73,73     | 1.21 | 10 (14%) | 83,113,113  | 1.43 | 8 (9%)   |
| 39  | LMT  | E     | 321 | -     | 23,23,36     | 0.45 | 0        | 28,28,47    | 0.59 | 0        |
| 36  | CLA  | E     | 312 | -     | 69,73,73     | 1.24 | 11 (15%) | 83,113,113  | 1.44 | 10 (12%) |
| 35  | A86  | E     | 302 | -     | 44,50,50     | 1.23 | 4 (9%)   | 51,76,76    | 2.19 | 13 (25%) |
| 37  | KC1  | Q     | 311 | 15    | 49,53,53     | 2.88 | 19 (38%) | 63,89,89    | 6.04 | 39 (61%) |
| 34  | DD6  | L     | 305 | -     | 39,45,45     | 2.04 | 3 (7%)   | 52,67,67    | 2.00 | 15 (28%) |
| 36  | CLA  | b     | 830 | 21    | 69,73,73     | 1.29 | 10 (14%) | 83,113,113  | 1.66 | 13 (15%) |
| 44  | BCR  | l     | 207 | -     | 41,41,41     | 1.08 | 2 (4%)   | 56,56,56    | 1.35 | 8 (14%)  |
| 35  | A86  | C     | 203 | -     | 44,50,50     | 1.24 | 4 (9%)   | 51,76,76    | 2.07 | 16 (31%) |
| 35  | A86  | S     | 308 | 37    | 44,50,50     | 1.23 | 4 (9%)   | 51,76,76    | 2.12 | 16 (31%) |
| 36  | CLA  | a     | 815 | 46    | 49,53,73     | 1.46 | 9 (18%)  | 59,89,113   | 1.53 | 5 (8%)   |
| 36  | CLA  | X     | 308 | 19    | 51,55,73     | 2.57 | 11 (21%) | 61,91,113   | 2.62 | 20 (32%) |
| 36  | CLA  | M     | 315 | 13    | 51,55,73     | 1.44 | 10 (19%) | 61,91,113   | 1.58 | 6 (9%)   |
| 36  | CLA  | J     | 308 | -     | 65,69,73     | 1.27 | 9 (13%)  | 78,108,113  | 1.63 | 10 (12%) |
| 34  | DD6  | Q     | 302 | -     | 39,45,45     | 2.04 | 3 (7%)   | 52,67,67    | 2.04 | 16 (30%) |
| 36  | CLA  | R     | 315 | -     | 69,73,73     | 1.23 | 9 (13%)  | 83,113,113  | 1.35 | 5 (6%)   |
| 37  | KC1  | L     | 317 | -     | 49,53,53     | 2.75 | 19 (38%) | 63,89,89    | 4.79 | 38 (60%) |
| 36  | CLA  | O     | 309 | -     | 69,73,73     | 1.25 | 11 (15%) | 83,113,113  | 1.42 | 11 (13%) |
| 36  | CLA  | i     | 102 | 26    | 69,73,73     | 1.24 | 10 (14%) | 83,113,113  | 1.44 | 8 (9%)   |
| 36  | CLA  | G     | 307 | -     | 45,50,73     | 2.21 | 14 (31%) | 53,85,113   | 3.15 | 17 (32%) |
| 36  | CLA  | b     | 833 | 21    | 62,66,73     | 1.31 | 10 (16%) | 74,104,113  | 1.57 | 11 (14%) |
| 36  | CLA  | P     | 318 | -     | 55,59,73     | 1.41 | 9 (16%)  | 66,96,113   | 1.45 | 6 (9%)   |
| 36  | CLA  | G     | 309 | 7     | 69,73,73     | 1.21 | 12 (17%) | 83,113,113  | 1.80 | 14 (16%) |
| 36  | CLA  | B     | 311 | 2     | 59,63,73     | 1.35 | 7 (11%)  | 71,101,113  | 1.68 | 12 (16%) |
| 37  | KC1  | E     | 309 | -     | 49,53,53     | 2.70 | 19 (38%) | 63,89,89    | 4.86 | 41 (65%) |
| 42  | LMG  | G     | 325 | -     | 55,55,55     | 0.89 | 2 (3%)   | 63,63,63    | 1.01 | 3 (4%)   |
| 36  | CLA  | U     | 305 | -     | 65,69,73     | 1.29 | 8 (12%)  | 78,108,113  | 1.34 | 5 (6%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 36  | CLA  | L     | 313 | -    | 69,73,73     | 1.20 | 8 (11%)  | 83,113,113  | 1.43 | 8 (9%)   |
| 36  | CLA  | b     | 825 | -    | 69,73,73     | 1.24 | 11 (15%) | 83,113,113  | 1.43 | 9 (10%)  |
| 35  | A86  | X     | 301 | -    | 44,50,50     | 1.55 | 5 (11%)  | 51,76,76    | 3.61 | 28 (54%) |
| 36  | CLA  | a     | 826 | 20   | 69,73,73     | 1.23 | 10 (14%) | 83,113,113  | 1.51 | 9 (10%)  |
| 36  | CLA  | N     | 317 | 14   | 58,62,73     | 1.39 | 9 (15%)  | 69,99,113   | 1.51 | 10 (14%) |
| 34  | DD6  | E     | 306 | -    | 39,45,45     | 2.03 | 3 (7%)   | 52,67,67    | 2.04 | 10 (19%) |
| 36  | CLA  | a     | 835 | 20   | 55,59,73     | 1.41 | 11 (20%) | 66,96,113   | 1.43 | 8 (12%)  |
| 35  | A86  | V     | 301 | 35   | 44,50,50     | 1.23 | 4 (9%)   | 51,76,76    | 2.22 | 16 (31%) |
| 36  | CLA  | S     | 321 | -    | 56,60,73     | 1.38 | 9 (16%)  | 67,97,113   | 1.64 | 8 (11%)  |
| 36  | CLA  | I     | 310 | 35   | 69,73,73     | 1.22 | 10 (14%) | 83,113,113  | 1.38 | 8 (9%)   |
| 37  | KC1  | H     | 313 | -    | 49,53,53     | 2.65 | 21 (42%) | 63,89,89    | 4.55 | 36 (57%) |
| 41  | LHG  | E     | 322 | -    | 48,48,48     | 0.93 | 2 (4%)   | 51,54,54    | 0.99 | 2 (3%)   |
| 36  | CLA  | O     | 310 | 15   | 50,54,73     | 1.45 | 9 (18%)  | 60,90,113   | 1.59 | 8 (13%)  |
| 36  | CLA  | X     | 306 | -    | 65,69,73     | 1.31 | 7 (10%)  | 78,108,113  | 1.37 | 6 (7%)   |
| 36  | CLA  | a     | 848 | 36   | 69,73,73     | 1.55 | 14 (20%) | 83,113,113  | 1.90 | 18 (21%) |
| 36  | CLA  | G     | 310 | 7    | 69,73,73     | 1.23 | 12 (17%) | 83,113,113  | 1.26 | 8 (9%)   |
| 36  | CLA  | G     | 319 | 7    | 54,58,73     | 2.01 | 18 (33%) | 65,95,113   | 4.02 | 30 (46%) |
| 35  | A86  | I     | 301 | -    | 44,50,50     | 1.23 | 3 (6%)   | 51,76,76    | 2.39 | 18 (35%) |
| 35  | A86  | U     | 302 | -    | 44,50,50     | 1.33 | 4 (9%)   | 51,76,76    | 3.12 | 22 (43%) |
| 35  | A86  | X     | 314 | 19   | 44,50,50     | 1.26 | 4 (9%)   | 51,76,76    | 2.07 | 13 (25%) |
| 36  | CLA  | K     | 310 | -    | 66,70,73     | 1.97 | 19 (28%) | 79,109,113  | 2.81 | 29 (36%) |
| 35  | A86  | N     | 320 | -    | 44,50,50     | 1.38 | 6 (13%)  | 51,76,76    | 3.30 | 24 (47%) |
| 36  | CLA  | M     | 316 | 36   | 46,50,73     | 1.47 | 9 (19%)  | 55,85,113   | 1.47 | 4 (7%)   |
| 42  | LMG  | a     | 852 | -    | 54,54,55     | 0.90 | 2 (3%)   | 62,62,63    | 1.03 | 3 (4%)   |
| 36  | CLA  | V     | 313 | 33   | 69,73,73     | 1.27 | 10 (14%) | 83,113,113  | 1.26 | 7 (8%)   |
| 34  | DD6  | W     | 205 | -    | 39,45,45     | 1.99 | 3 (7%)   | 52,67,67    | 2.03 | 15 (28%) |
| 34  | DD6  | K     | 305 | -    | 39,45,45     | 2.00 | 3 (7%)   | 52,67,67    | 2.00 | 14 (26%) |
| 36  | CLA  | H     | 317 | 8    | 69,73,73     | 1.25 | 10 (14%) | 83,113,113  | 1.30 | 6 (7%)   |
| 37  | KC1  | M     | 318 | -    | 49,53,53     | 4.98 | 26 (53%) | 63,89,89    | 7.21 | 36 (57%) |
| 36  | CLA  | F     | 317 | 6    | 60,64,73     | 1.97 | 16 (26%) | 72,102,113  | 2.65 | 24 (33%) |
| 35  | A86  | M     | 304 | -    | 44,50,50     | 1.23 | 3 (6%)   | 51,76,76    | 2.06 | 14 (27%) |
| 42  | LMG  | D     | 320 | 41   | 46,46,55     | 0.98 | 2 (4%)   | 54,54,63    | 1.03 | 3 (5%)   |
| 36  | CLA  | R     | 322 | 16   | 56,60,73     | 1.42 | 10 (17%) | 67,97,113   | 1.66 | 10 (14%) |
| 36  | CLA  | S     | 314 | 17   | 69,73,73     | 1.32 | 11 (15%) | 83,113,113  | 1.46 | 11 (13%) |
| 44  | BCR  | l     | 203 | -    | 41,41,41     | 1.23 | 4 (9%)   | 56,56,56    | 1.21 | 5 (8%)   |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 36  | CLA  | E     | 316 | -     | 69,73,73     | 1.24 | 8 (11%)  | 83,113,113  | 1.54 | 10 (12%) |
| 36  | CLA  | P     | 316 | -     | 45,49,73     | 1.51 | 9 (20%)  | 54,84,113   | 1.73 | 8 (14%)  |
| 39  | LMT  | P     | 320 | -     | 23,23,36     | 0.43 | 0        | 28,28,47    | 0.62 | 0        |
| 36  | CLA  | H     | 311 | -     | 69,73,73     | 1.18 | 10 (14%) | 83,113,113  | 1.43 | 9 (10%)  |
| 36  | CLA  | b     | 834 | -     | 69,73,73     | 1.25 | 10 (14%) | 83,113,113  | 1.34 | 7 (8%)   |
| 34  | DD6  | D     | 303 | -     | 39,45,45     | 2.97 | 8 (20%)  | 52,67,67    | 2.65 | 18 (34%) |
| 35  | A86  | F     | 306 | -     | 44,50,50     | 1.26 | 4 (9%)   | 51,76,76    | 2.04 | 13 (25%) |
| 35  | A86  | H     | 301 | -     | 44,50,50     | 1.29 | 3 (6%)   | 51,76,76    | 4.88 | 20 (39%) |
| 35  | A86  | S     | 304 | -     | 44,50,50     | 1.24 | 4 (9%)   | 51,76,76    | 2.13 | 16 (31%) |
| 36  | CLA  | E     | 313 | -     | 69,73,73     | 1.77 | 16 (23%) | 83,113,113  | 2.40 | 24 (28%) |
| 36  | CLA  | O     | 306 | -     | 65,69,73     | 1.28 | 9 (13%)  | 78,108,113  | 1.37 | 5 (6%)   |
| 34  | DD6  | a     | 849 | -     | 39,45,45     | 2.01 | 3 (7%)   | 52,67,67    | 1.84 | 13 (25%) |
| 36  | CLA  | R     | 319 | 16    | 49,53,73     | 1.47 | 9 (18%)  | 59,89,113   | 1.83 | 12 (20%) |
| 36  | CLA  | V     | 309 | 33    | 47,51,73     | 1.45 | 8 (17%)  | 56,86,113   | 1.89 | 11 (19%) |
| 39  | LMT  | G     | 322 | -     | 36,36,36     | 0.39 | 0        | 47,47,47    | 0.69 | 0        |
| 36  | CLA  | S     | 317 | -     | 45,49,73     | 1.52 | 8 (17%)  | 54,84,113   | 1.55 | 6 (11%)  |
| 42  | LMG  | I     | 315 | -     | 55,55,55     | 0.89 | 2 (3%)   | 63,63,63    | 1.00 | 3 (4%)   |
| 37  | KC1  | D     | 314 | 4     | 49,53,53     | 2.66 | 18 (36%) | 63,89,89    | 4.84 | 39 (61%) |
| 35  | A86  | O     | 319 | 35,36 | 44,50,50     | 1.28 | 5 (11%)  | 51,76,76    | 2.93 | 18 (35%) |
| 36  | CLA  | N     | 318 | -     | 51,55,73     | 1.44 | 9 (17%)  | 61,91,113   | 1.68 | 9 (14%)  |
| 36  | CLA  | C     | 210 | 3     | 50,54,73     | 1.49 | 9 (18%)  | 60,90,113   | 1.55 | 7 (11%)  |
| 39  | LMT  | I     | 318 | -     | 36,36,36     | 0.39 | 0        | 47,47,47    | 0.75 | 1 (2%)   |
| 35  | A86  | R     | 303 | -     | 44,50,50     | 1.36 | 5 (11%)  | 51,76,76    | 3.63 | 21 (41%) |
| 35  | A86  | T     | 307 | -     | 44,50,50     | 1.24 | 3 (6%)   | 51,76,76    | 3.14 | 21 (41%) |
| 36  | CLA  | C     | 214 | -     | 45,49,73     | 1.48 | 10 (22%) | 54,84,113   | 1.60 | 8 (14%)  |
| 36  | CLA  | a     | 825 | -     | 69,73,73     | 1.38 | 11 (15%) | 83,113,113  | 1.73 | 12 (14%) |
| 36  | CLA  | a     | 839 | 46    | 69,73,73     | 1.21 | 10 (14%) | 83,113,113  | 1.37 | 8 (9%)   |
| 36  | CLA  | E     | 317 | -     | 50,54,73     | 1.47 | 8 (16%)  | 60,90,113   | 1.44 | 6 (10%)  |
| 36  | CLA  | b     | 805 | 21,36 | 69,73,73     | 1.27 | 10 (14%) | 83,113,113  | 1.30 | 13 (15%) |
| 36  | CLA  | G     | 313 | 7     | 69,73,73     | 1.36 | 9 (13%)  | 83,113,113  | 1.85 | 16 (19%) |
| 38  | SQD  | b     | 804 | -     | 45,46,54     | 1.27 | 4 (8%)   | 54,57,65    | 1.21 | 4 (7%)   |
| 36  | CLA  | I     | 309 | 9     | 50,54,73     | 1.44 | 8 (16%)  | 60,90,113   | 1.92 | 9 (15%)  |
| 34  | DD6  | E     | 304 | -     | 39,45,45     | 1.99 | 3 (7%)   | 52,67,67    | 1.78 | 10 (19%) |
| 36  | CLA  | M     | 311 | 13,35 | 69,73,73     | 1.25 | 9 (13%)  | 83,113,113  | 1.27 | 4 (4%)   |
| 36  | CLA  | V     | 314 | -     | 69,73,73     | 1.97 | 16 (23%) | 83,113,113  | 2.90 | 24 (28%) |



| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 39  | LMT  | E     | 323 | -     | 36,36,36     | 0.35 | 0        | 47,47,47    | 0.82 | 1 (2%)   |
| 36  | CLA  | a     | 834 | 20    | 49,53,73     | 1.47 | 9 (18%)  | 59,89,113   | 1.56 | 7 (11%)  |
| 36  | CLA  | X     | 315 | -     | 45,49,73     | 1.53 | 7 (15%)  | 54,84,113   | 1.58 | 9 (16%)  |
| 35  | A86  | L     | 301 | -     | 44,50,50     | 1.25 | 4 (9%)   | 51,76,76    | 2.01 | 14 (27%) |
| 36  | CLA  | K     | 307 | -     | 65,69,73     | 1.92 | 15 (23%) | 78,108,113  | 2.89 | 22 (28%) |
| 36  | CLA  | b     | 802 | 20    | 69,73,73     | 1.22 | 10 (14%) | 83,113,113  | 1.38 | 8 (9%)   |
| 36  | CLA  | L     | 320 | 12    | 69,73,73     | 1.23 | 9 (13%)  | 83,113,113  | 1.32 | 5 (6%)   |
| 36  | CLA  | J     | 310 | -     | 69,73,73     | 1.21 | 10 (14%) | 83,113,113  | 1.36 | 7 (8%)   |
| 36  | CLA  | a     | 823 | -     | 59,63,73     | 1.71 | 13 (22%) | 71,101,113  | 2.27 | 21 (29%) |
| 35  | A86  | V     | 304 | -     | 44,50,50     | 1.48 | 6 (13%)  | 51,76,76    | 3.49 | 18 (35%) |
| 36  | CLA  | H     | 309 | 8     | 69,73,73     | 1.24 | 9 (13%)  | 83,113,113  | 1.35 | 6 (7%)   |
| 36  | CLA  | H     | 312 | 8     | 69,73,73     | 1.23 | 11 (15%) | 83,113,113  | 1.48 | 11 (13%) |
| 36  | CLA  | F     | 311 | -     | 56,60,73     | 1.36 | 9 (16%)  | 67,97,113   | 1.53 | 6 (8%)   |
| 36  | CLA  | M     | 310 | 13,35 | 50,54,73     | 2.12 | 9 (18%)  | 60,90,113   | 1.96 | 13 (21%) |
| 35  | A86  | T     | 301 | 36    | 44,50,50     | 1.25 | 4 (9%)   | 51,76,76    | 2.07 | 16 (31%) |
| 36  | CLA  | a     | 805 | 20    | 69,73,73     | 1.23 | 11 (15%) | 83,113,113  | 1.35 | 9 (10%)  |
| 36  | CLA  | b     | 818 | 21    | 59,63,73     | 1.34 | 8 (13%)  | 71,101,113  | 1.65 | 13 (18%) |
| 36  | CLA  | b     | 819 | -     | 63,67,73     | 1.33 | 8 (12%)  | 75,105,113  | 1.89 | 17 (22%) |
| 36  | CLA  | a     | 824 | -     | 69,73,73     | 1.29 | 12 (17%) | 83,113,113  | 1.80 | 19 (22%) |
| 44  | BCR  | b     | 845 | -     | 41,41,41     | 1.20 | 3 (7%)   | 56,56,56    | 1.37 | 8 (14%)  |
| 35  | A86  | C     | 202 | 3,36  | 44,50,50     | 1.40 | 5 (11%)  | 51,76,76    | 3.09 | 17 (33%) |
| 36  | CLA  | Q     | 312 | -     | 45,49,73     | 1.52 | 9 (20%)  | 54,84,113   | 1.73 | 8 (14%)  |
| 36  | CLA  | b     | 811 | 21    | 69,73,73     | 1.24 | 10 (14%) | 83,113,113  | 1.52 | 8 (9%)   |
| 35  | A86  | G     | 305 | -     | 44,50,50     | 1.23 | 3 (6%)   | 51,76,76    | 2.23 | 15 (29%) |
| 35  | A86  | I     | 304 | -     | 44,50,50     | 1.47 | 4 (9%)   | 51,76,76    | 3.38 | 21 (41%) |
| 34  | DD6  | B     | 302 | -     | 39,45,45     | 2.01 | 3 (7%)   | 52,67,67    | 2.07 | 16 (30%) |
| 35  | A86  | N     | 303 | -     | 44,50,50     | 1.31 | 5 (11%)  | 51,76,76    | 3.31 | 22 (43%) |
| 35  | A86  | E     | 307 | 36    | 44,50,50     | 1.24 | 4 (9%)   | 51,76,76    | 2.07 | 12 (23%) |
| 36  | CLA  | H     | 306 | -     | 65,69,73     | 1.27 | 10 (15%) | 78,108,113  | 1.34 | 5 (6%)   |
| 36  | CLA  | b     | 808 | 21    | 69,73,73     | 1.21 | 10 (14%) | 83,113,113  | 1.40 | 8 (9%)   |
| 35  | A86  | T     | 304 | -     | 44,50,50     | 1.11 | 3 (6%)   | 51,76,76    | 1.69 | 11 (21%) |
| 36  | CLA  | S     | 310 | 17    | 69,73,73     | 1.24 | 10 (14%) | 83,113,113  | 1.60 | 13 (15%) |
| 37  | KC1  | G     | 308 | -     | 49,53,53     | 2.71 | 20 (40%) | 63,89,89    | 4.85 | 38 (60%) |
| 36  | CLA  | I     | 308 | 9     | 69,73,73     | 1.88 | 17 (24%) | 83,113,113  | 2.71 | 24 (28%) |
| 35  | A86  | P     | 303 | -     | 44,50,50     | 1.44 | 6 (13%)  | 51,76,76    | 3.47 | 23 (45%) |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 36  | CLA  | D     | 307 | 41    | 65,69,73     | 1.25 | 9 (13%)  | 78,108,113  | 1.60 | 16 (20%) |
| 36  | CLA  | l     | 204 | 28    | 53,57,73     | 2.03 | 16 (30%) | 62,93,113   | 2.45 | 20 (32%) |
| 36  | CLA  | W     | 209 | 19    | 61,65,73     | 1.35 | 10 (16%) | 73,103,113  | 1.41 | 11 (15%) |
| 36  | CLA  | I     | 311 | 9     | 69,73,73     | 1.20 | 10 (14%) | 83,113,113  | 1.49 | 10 (12%) |
| 36  | CLA  | U     | 308 | 35,32 | 60,64,73     | 1.35 | 8 (13%)  | 72,102,113  | 1.63 | 8 (11%)  |
| 35  | A86  | R     | 302 | 16    | 44,50,50     | 1.38 | 5 (11%)  | 51,76,76    | 2.80 | 15 (29%) |
| 34  | DD6  | G     | 303 | -     | 39,45,45     | 1.99 | 3 (7%)   | 52,67,67    | 1.83 | 10 (19%) |
| 36  | CLA  | D     | 312 | -     | 69,73,73     | 1.25 | 10 (14%) | 83,113,113  | 1.32 | 8 (9%)   |
| 36  | CLA  | L     | 312 | 12    | 50,54,73     | 1.46 | 9 (18%)  | 60,90,113   | 1.77 | 8 (13%)  |
| 36  | CLA  | H     | 305 | 8     | 52,56,73     | 1.44 | 8 (15%)  | 62,92,113   | 1.48 | 7 (11%)  |
| 36  | CLA  | U     | 311 | 32    | 69,73,73     | 1.27 | 11 (15%) | 83,113,113  | 1.53 | 13 (15%) |
| 35  | A86  | H     | 304 | -     | 44,50,50     | 1.24 | 4 (9%)   | 51,76,76    | 2.31 | 17 (33%) |
| 36  | CLA  | a     | 817 | 20    | 69,73,73     | 1.26 | 10 (14%) | 83,113,113  | 1.61 | 15 (18%) |
| 36  | CLA  | R     | 316 | -     | 50,54,73     | 1.49 | 11 (22%) | 60,90,113   | 1.96 | 15 (25%) |
| 36  | CLA  | J     | 315 | 10    | 45,49,73     | 1.51 | 9 (20%)  | 54,84,113   | 1.64 | 7 (12%)  |
| 44  | BCR  | i     | 101 | -     | 41,41,41     | 1.09 | 2 (4%)   | 56,56,56    | 1.25 | 7 (12%)  |
| 36  | CLA  | J     | 316 | 10    | 50,54,73     | 1.45 | 9 (18%)  | 60,90,113   | 1.73 | 10 (16%) |
| 36  | CLA  | I     | 314 | -     | 45,49,73     | 1.50 | 8 (17%)  | 54,84,113   | 1.63 | 8 (14%)  |
| 34  | DD6  | S     | 307 | -     | 39,45,45     | 2.03 | 3 (7%)   | 52,67,67    | 2.07 | 15 (28%) |
| 35  | A86  | W     | 202 | 19,36 | 44,50,50     | 1.50 | 6 (13%)  | 51,76,76    | 3.63 | 29 (56%) |
| 36  | CLA  | a     | 830 | 20    | 54,58,73     | 1.71 | 13 (24%) | 65,95,113   | 3.30 | 20 (30%) |
| 35  | A86  | D     | 302 | -     | 44,50,50     | 1.23 | 4 (9%)   | 51,76,76    | 2.08 | 11 (21%) |
| 35  | A86  | L     | 304 | -     | 44,50,50     | 1.39 | 4 (9%)   | 51,76,76    | 2.99 | 15 (29%) |
| 36  | CLA  | j     | 101 | 1,27  | 69,73,73     | 1.24 | 10 (14%) | 83,113,113  | 1.27 | 7 (8%)   |
| 41  | LHG  | a     | 843 | 36    | 26,26,48     | 1.24 | 2 (7%)   | 29,32,54    | 1.31 | 2 (6%)   |
| 41  | LHG  | a     | 842 | -     | 47,47,48     | 0.76 | 1 (2%)   | 50,53,54    | 1.27 | 4 (8%)   |
| 36  | CLA  | J     | 307 | 10    | 65,69,73     | 1.27 | 10 (15%) | 78,108,113  | 1.45 | 12 (15%) |
| 37  | KC1  | B     | 310 | 2     | 49,53,53     | 2.88 | 20 (40%) | 63,89,89    | 4.55 | 36 (57%) |
| 36  | CLA  | V     | 307 | -     | 55,59,73     | 1.42 | 9 (16%)  | 66,96,113   | 1.38 | 6 (9%)   |
| 36  | CLA  | D     | 306 | 4     | 49,53,73     | 1.53 | 11 (22%) | 59,89,113   | 1.65 | 9 (15%)  |
| 36  | CLA  | F     | 312 | -     | 69,73,73     | 1.23 | 9 (13%)  | 83,113,113  | 1.33 | 7 (8%)   |
| 36  | CLA  | B     | 305 | 2     | 69,73,73     | 1.24 | 9 (13%)  | 83,113,113  | 1.38 | 10 (12%) |
| 35  | A86  | F     | 302 | -     | 44,50,50     | 1.24 | 4 (9%)   | 51,76,76    | 1.92 | 11 (21%) |
| 35  | A86  | O     | 301 | -     | 44,50,50     | 1.25 | 4 (9%)   | 51,76,76    | 2.07 | 14 (27%) |
| 36  | CLA  | D     | 313 | -     | 69,73,73     | 1.20 | 11 (15%) | 83,113,113  | 1.51 | 12 (14%) |



| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 36  | CLA  | G     | 312 | 7     | 62,66,73     | 1.28 | 11 (17%) | 74,104,113  | 1.47 | 6 (8%)   |
| 36  | CLA  | S     | 319 | 17    | 69,73,73     | 1.28 | 10 (14%) | 83,113,113  | 1.48 | 9 (10%)  |
| 36  | CLA  | I     | 305 | -     | 65,69,73     | 1.86 | 13 (20%) | 78,108,113  | 1.63 | 11 (14%) |
| 34  | DD6  | O     | 304 | -     | 39,45,45     | 1.90 | 3 (7%)   | 52,67,67    | 2.00 | 14 (26%) |
| 34  | DD6  | W     | 204 | 36    | 39,45,45     | 2.04 | 3 (7%)   | 52,67,67    | 2.01 | 13 (25%) |
| 36  | CLA  | N     | 311 | 14    | 50,54,73     | 1.45 | 7 (14%)  | 60,90,113   | 1.72 | 8 (13%)  |
| 36  | CLA  | a     | 803 | 36,20 | 59,63,73     | 1.32 | 11 (18%) | 71,101,113  | 1.55 | 12 (16%) |
| 44  | BCR  | i     | 103 | -     | 41,41,41     | 1.19 | 3 (7%)   | 56,56,56    | 1.32 | 7 (12%)  |
| 35  | A86  | K     | 301 | -     | 44,50,50     | 1.25 | 4 (9%)   | 51,76,76    | 2.26 | 13 (25%) |
| 35  | A86  | G     | 306 | -     | 44,50,50     | 1.21 | 4 (9%)   | 51,76,76    | 2.34 | 18 (35%) |
| 42  | LMG  | j     | 105 | -     | 52,52,55     | 0.91 | 2 (3%)   | 60,60,63    | 1.00 | 3 (5%)   |
| 36  | CLA  | a     | 807 | 20    | 69,73,73     | 1.20 | 11 (15%) | 83,113,113  | 1.49 | 12 (14%) |
| 37  | KC1  | W     | 217 | -     | 49,53,53     | 2.87 | 18 (36%) | 63,89,89    | 4.42 | 37 (58%) |
| 44  | BCR  | a     | 845 | -     | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 1.19 | 5 (8%)   |
| 39  | LMT  | P     | 321 | -     | 23,23,36     | 0.43 | 0        | 28,28,47    | 0.61 | 0        |
| 36  | CLA  | a     | 811 | 20    | 58,62,73     | 1.34 | 9 (15%)  | 69,99,113   | 1.44 | 6 (8%)   |
| 36  | CLA  | N     | 310 | 14    | 45,49,73     | 1.73 | 10 (22%) | 54,84,113   | 2.52 | 18 (33%) |
| 34  | DD6  | P     | 305 | -     | 39,45,45     | 2.02 | 3 (7%)   | 52,67,67    | 2.06 | 16 (30%) |
| 36  | CLA  | H     | 318 | -     | 54,58,73     | 1.42 | 12 (22%) | 65,95,113   | 1.51 | 8 (12%)  |
| 36  | CLA  | a     | 813 | 20    | 49,53,73     | 1.50 | 11 (22%) | 59,89,113   | 1.75 | 11 (18%) |
| 36  | CLA  | D     | 309 | 4     | 59,63,73     | 2.08 | 18 (30%) | 71,101,113  | 3.19 | 29 (40%) |
| 36  | CLA  | b     | 801 | 46    | 69,73,73     | 1.29 | 12 (17%) | 83,113,113  | 1.39 | 10 (12%) |
| 37  | KC1  | U     | 312 | 35,32 | 49,53,53     | 2.95 | 21 (42%) | 63,89,89    | 4.31 | 34 (53%) |
| 36  | CLA  | j     | 106 | 27    | 46,50,73     | 1.46 | 10 (21%) | 55,85,113   | 1.59 | 7 (12%)  |
| 41  | LHG  | G     | 301 | -     | 48,48,48     | 0.77 | 2 (4%)   | 51,54,54    | 1.28 | 6 (11%)  |
| 36  | CLA  | b     | 822 | 21    | 50,54,73     | 1.43 | 10 (20%) | 60,90,113   | 1.50 | 8 (13%)  |
| 36  | CLA  | j     | 102 | -     | 69,73,73     | 1.63 | 13 (18%) | 83,113,113  | 2.19 | 18 (21%) |
| 36  | CLA  | U     | 307 | -     | 54,58,73     | 1.38 | 10 (18%) | 65,95,113   | 1.39 | 4 (6%)   |
| 41  | LHG  | a     | 850 | -     | 46,46,48     | 0.96 | 2 (4%)   | 49,52,54    | 1.04 | 3 (6%)   |
| 36  | CLA  | T     | 314 | -     | 69,73,73     | 1.22 | 8 (11%)  | 83,113,113  | 1.53 | 11 (13%) |
| 39  | LMT  | L     | 303 | -     | 36,36,36     | 1.33 | 6 (16%)  | 47,47,47    | 0.96 | 1 (2%)   |
| 36  | CLA  | G     | 311 | -     | 69,73,73     | 1.25 | 9 (13%)  | 83,113,113  | 1.32 | 8 (9%)   |
| 40  | DGD  | C     | 215 | -     | 58,58,67     | 0.90 | 2 (3%)   | 72,72,81    | 0.96 | 3 (4%)   |
| 41  | LHG  | Q     | 315 | 36    | 48,48,48     | 0.93 | 2 (4%)   | 51,54,54    | 1.04 | 3 (5%)   |
| 34  | DD6  | j     | 103 | -     | 39,45,45     | 1.99 | 3 (7%)   | 52,67,67    | 1.83 | 12 (23%) |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 36  | CLA  | R     | 318 | 35    | 45,49,73     | 1.53 | 9 (20%)  | 54,84,113   | 1.57 | 9 (16%)  |
| 36  | CLA  | b     | 812 | 21    | 69,73,73     | 1.23 | 10 (14%) | 83,113,113  | 1.48 | 14 (16%) |
| 37  | KC1  | L     | 315 | 12,35 | 49,53,53     | 2.80 | 18 (36%) | 63,89,89    | 5.32 | 39 (61%) |
| 35  | A86  | X     | 303 | 36    | 44,50,50     | 1.47 | 5 (11%)  | 51,76,76    | 3.76 | 24 (47%) |
| 36  | CLA  | Q     | 310 | 15    | 69,73,73     | 2.74 | 17 (24%) | 83,113,113  | 2.82 | 23 (27%) |
| 36  | CLA  | I     | 307 | 9     | 58,62,73     | 1.33 | 11 (18%) | 69,99,113   | 1.49 | 9 (13%)  |
| 36  | CLA  | O     | 311 | -     | 62,66,73     | 1.29 | 9 (14%)  | 74,104,113  | 1.37 | 5 (6%)   |
| 36  | CLA  | S     | 313 | -     | 50,54,73     | 1.45 | 7 (14%)  | 60,90,113   | 1.81 | 12 (20%) |
| 36  | CLA  | b     | 829 | 21    | 69,73,73     | 1.25 | 11 (15%) | 83,113,113  | 1.31 | 6 (7%)   |
| 37  | KC1  | O     | 313 | 15    | 49,53,53     | 2.88 | 20 (40%) | 63,89,89    | 6.04 | 39 (61%) |
| 39  | LMT  | a     | 853 | -     | 33,33,36     | 0.42 | 0        | 44,44,47    | 0.74 | 1 (2%)   |
| 35  | A86  | P     | 304 | -     | 44,50,50     | 1.33 | 5 (11%)  | 51,76,76    | 2.74 | 17 (33%) |
| 36  | CLA  | L     | 308 | -     | 65,69,73     | 1.92 | 14 (21%) | 78,108,113  | 2.83 | 22 (28%) |
| 36  | CLA  | b     | 823 | 21    | 59,63,73     | 1.30 | 10 (16%) | 71,101,113  | 1.45 | 7 (9%)   |
| 42  | LMG  | E     | 319 | -     | 40,40,55     | 1.04 | 2 (5%)   | 48,48,63    | 1.11 | 3 (6%)   |
| 36  | CLA  | a     | 810 | 36,20 | 66,70,73     | 1.21 | 9 (13%)  | 79,109,113  | 1.43 | 6 (7%)   |
| 34  | DD6  | D     | 305 | -     | 39,45,45     | 2.00 | 3 (7%)   | 52,67,67    | 1.63 | 9 (17%)  |
| 41  | LHG  | D     | 318 | 36    | 45,45,48     | 0.30 | 0        | 48,51,54    | 0.39 | 0        |
| 37  | KC1  | C     | 213 | 3     | 49,53,53     | 2.74 | 18 (36%) | 63,89,89    | 4.34 | 34 (53%) |
| 34  | DD6  | H     | 302 | -     | 39,45,45     | 1.98 | 3 (7%)   | 52,67,67    | 1.92 | 15 (28%) |
| 34  | DD6  | F     | 303 | -     | 39,45,45     | 2.00 | 3 (7%)   | 52,67,67    | 1.91 | 14 (26%) |
| 36  | CLA  | A     | 314 | 1     | 69,73,73     | 1.32 | 8 (11%)  | 83,113,113  | 1.81 | 9 (10%)  |
| 37  | KC1  | F     | 308 | 6     | 49,53,53     | 2.73 | 20 (40%) | 63,89,89    | 5.24 | 36 (57%) |
| 34  | DD6  | J     | 304 | -     | 39,45,45     | 2.00 | 3 (7%)   | 52,67,67    | 1.87 | 12 (23%) |
| 36  | CLA  | E     | 314 | -     | 69,73,73     | 1.21 | 11 (15%) | 83,113,113  | 1.51 | 13 (15%) |
| 36  | CLA  | b     | 817 | 21    | 63,67,73     | 1.73 | 14 (22%) | 75,105,113  | 2.17 | 18 (24%) |
| 36  | CLA  | N     | 307 | -     | 65,69,73     | 1.29 | 8 (12%)  | 78,108,113  | 1.34 | 4 (5%)   |
| 36  | CLA  | L     | 314 | 12    | 69,73,73     | 1.23 | 9 (13%)  | 83,113,113  | 1.45 | 10 (12%) |
| 36  | CLA  | a     | 809 | -     | 60,64,73     | 1.29 | 10 (16%) | 72,102,113  | 1.41 | 8 (11%)  |
| 39  | LMT  | F     | 321 | -     | 34,34,36     | 0.65 | 0        | 45,45,47    | 1.61 | 6 (13%)  |
| 39  | LMT  | U     | 314 | -     | 36,36,36     | 0.40 | 0        | 47,47,47    | 0.69 | 1 (2%)   |
| 36  | CLA  | f     | 802 | 21    | 69,73,73     | 1.28 | 10 (14%) | 83,113,113  | 1.42 | 8 (9%)   |
| 41  | LHG  | O     | 318 | 15    | 48,48,48     | 0.88 | 3 (6%)   | 51,54,54    | 1.22 | 4 (7%)   |
| 36  | CLA  | F     | 310 | 6     | 60,64,73     | 1.30 | 10 (16%) | 72,102,113  | 1.50 | 13 (18%) |
| 36  | CLA  | I     | 313 | -     | 45,49,73     | 1.49 | 10 (22%) | 54,84,113   | 1.58 | 6 (11%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 36  | CLA  | a     | 821 | 20   | 53,57,73     | 1.38 | 11 (20%) | 62,93,113   | 1.53 | 7 (11%)  |
| 39  | LMT  | E     | 320 | -    | 36,36,36     | 0.37 | 0        | 47,47,47    | 0.67 | 0        |
| 36  | CLA  | a     | 814 | 20   | 54,58,73     | 1.40 | 11 (20%) | 65,95,113   | 1.72 | 7 (10%)  |
| 36  | CLA  | L     | 316 | -    | 45,49,73     | 1.53 | 7 (15%)  | 54,84,113   | 1.58 | 6 (11%)  |
| 35  | A86  | F     | 307 | -    | 44,50,50     | 1.31 | 3 (6%)   | 51,76,76    | 3.94 | 22 (43%) |
| 36  | CLA  | b     | 832 | 21   | 53,57,73     | 1.33 | 11 (20%) | 62,93,113   | 1.55 | 8 (12%)  |
| 36  | CLA  | B     | 308 | 2    | 69,73,73     | 1.28 | 9 (13%)  | 83,113,113  | 1.47 | 12 (14%) |
| 37  | KC1  | J     | 314 | -    | 49,53,53     | 2.70 | 18 (36%) | 63,89,89    | 5.38 | 38 (60%) |
| 36  | CLA  | b     | 837 | 21   | 69,73,73     | 1.21 | 10 (14%) | 83,113,113  | 1.46 | 12 (14%) |
| 36  | CLA  | D     | 315 | -    | 45,49,73     | 1.47 | 10 (22%) | 54,84,113   | 1.80 | 9 (16%)  |
| 39  | LMT  | G     | 323 | -    | 36,36,36     | 0.39 | 0        | 47,47,47    | 0.82 | 0        |
| 36  | CLA  | K     | 309 | 11   | 63,67,73     | 1.31 | 10 (15%) | 75,105,113  | 1.34 | 7 (9%)   |
| 36  | CLA  | a     | 806 | -    | 69,73,73     | 1.46 | 10 (14%) | 83,113,113  | 1.97 | 19 (22%) |
| 37  | KC1  | T     | 315 | -    | 49,53,53     | 2.75 | 18 (36%) | 63,89,89    | 5.01 | 36 (57%) |
| 35  | A86  | T     | 305 | 18   | 44,50,50     | 1.48 | 5 (11%)  | 51,76,76    | 3.68 | 22 (43%) |
| 36  | CLA  | b     | 807 | 21   | 49,53,73     | 1.42 | 11 (22%) | 59,89,113   | 1.57 | 8 (13%)  |
| 41  | LHG  | l     | 208 | -    | 47,47,48     | 0.95 | 2 (4%)   | 50,53,54    | 1.02 | 3 (6%)   |
| 34  | DD6  | I     | 303 | -    | 39,45,45     | 2.03 | 3 (7%)   | 52,67,67    | 1.95 | 15 (28%) |
| 35  | A86  | O     | 302 | -    | 44,50,50     | 1.44 | 6 (13%)  | 51,76,76    | 3.47 | 23 (45%) |
| 36  | CLA  | a     | 837 | 20   | 69,73,73     | 1.20 | 9 (13%)  | 83,113,113  | 1.40 | 8 (9%)   |
| 36  | CLA  | C     | 208 | 3    | 69,73,73     | 1.25 | 10 (14%) | 83,113,113  | 1.36 | 8 (9%)   |
| 41  | LHG  | G     | 321 | 36   | 46,46,48     | 0.96 | 2 (4%)   | 49,52,54    | 1.06 | 2 (4%)   |
| 36  | CLA  | A     | 310 | -    | 69,73,73     | 1.23 | 11 (15%) | 83,113,113  | 1.36 | 8 (9%)   |
| 36  | CLA  | b     | 828 | 21   | 69,73,73     | 1.30 | 10 (14%) | 83,113,113  | 1.43 | 13 (15%) |
| 45  | SF4  | c     | 101 | 22   | 0,12,12      | -    | -        | -           | -    | -        |
| 42  | LMG  | L     | 321 | 40   | 33,33,55     | 1.13 | 2 (6%)   | 41,41,63    | 1.15 | 3 (7%)   |
| 36  | CLA  | l     | 201 | -    | 69,73,73     | 1.23 | 10 (14%) | 83,113,113  | 1.44 | 12 (14%) |
| 35  | A86  | h     | 204 | -    | 44,50,50     | 1.23 | 4 (9%)   | 51,76,76    | 2.14 | 11 (21%) |
| 36  | CLA  | a     | 829 | 20   | 69,73,73     | 1.27 | 9 (13%)  | 83,113,113  | 1.62 | 14 (16%) |
| 36  | CLA  | h     | 203 | 31   | 69,73,73     | 1.21 | 10 (14%) | 83,113,113  | 1.47 | 9 (10%)  |
| 36  | CLA  | O     | 308 | 15   | 69,73,73     | 1.26 | 9 (13%)  | 83,113,113  | 1.43 | 7 (8%)   |
| 36  | CLA  | a     | 808 | 20   | 69,73,73     | 1.23 | 11 (15%) | 83,113,113  | 1.41 | 9 (10%)  |
| 41  | LHG  | I     | 316 | -    | 48,48,48     | 0.95 | 2 (4%)   | 51,54,54    | 1.00 | 2 (3%)   |
| 36  | CLA  | W     | 208 | -    | 49,53,73     | 1.48 | 10 (20%) | 59,89,113   | 1.48 | 4 (6%)   |
| 36  | CLA  | S     | 309 | -    | 65,69,73     | 1.30 | 11 (16%) | 78,108,113  | 1.30 | 8 (10%)  |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 44  | BCR  | a     | 844 | -     | 41,41,41     | 1.07 | 2 (4%)   | 56,56,56    | 1.29 | 5 (8%)   |
| 36  | CLA  | S     | 312 | 17    | 69,73,73     | 1.27 | 9 (13%)  | 83,113,113  | 1.37 | 10 (12%) |
| 39  | LMT  | K     | 318 | -     | 36,36,36     | 0.41 | 0        | 47,47,47    | 0.72 | 1 (2%)   |
| 36  | CLA  | Q     | 305 | -     | 65,69,73     | 1.28 | 9 (13%)  | 78,108,113  | 1.37 | 5 (6%)   |
| 35  | A86  | S     | 301 | -     | 44,50,50     | 1.46 | 4 (9%)   | 51,76,76    | 3.73 | 26 (50%) |
| 36  | CLA  | a     | 801 | 20    | 69,73,73     | 1.30 | 9 (13%)  | 83,113,113  | 1.53 | 13 (15%) |
| 35  | A86  | N     | 305 | -     | 44,50,50     | 1.65 | 8 (18%)  | 51,76,76    | 2.29 | 17 (33%) |
| 36  | CLA  | f     | 803 | -     | 69,73,73     | 1.81 | 17 (24%) | 83,113,113  | 2.56 | 27 (32%) |
| 36  | CLA  | K     | 311 | 11    | 50,54,73     | 1.46 | 9 (18%)  | 60,90,113   | 1.51 | 8 (13%)  |
| 36  | CLA  | a     | 804 | 20    | 69,73,73     | 1.25 | 10 (14%) | 83,113,113  | 1.42 | 12 (14%) |
| 37  | KC1  | M     | 313 | 13,36 | 49,53,53     | 2.71 | 19 (38%) | 63,89,89    | 5.30 | 40 (63%) |
| 36  | CLA  | L     | 309 | 12    | 69,73,73     | 1.23 | 10 (14%) | 83,113,113  | 1.34 | 9 (10%)  |
| 36  | CLA  | O     | 307 | -     | 69,73,73     | 1.24 | 11 (15%) | 83,113,113  | 1.36 | 7 (8%)   |
| 35  | A86  | S     | 302 | -     | 44,50,50     | 1.20 | 3 (6%)   | 51,76,76    | 2.68 | 15 (29%) |
| 35  | A86  | E     | 305 | 5     | 44,50,50     | 1.23 | 4 (9%)   | 51,76,76    | 2.04 | 14 (27%) |
| 36  | CLA  | A     | 306 | -     | 65,69,73     | 1.94 | 18 (27%) | 78,108,113  | 2.78 | 29 (37%) |
| 35  | A86  | K     | 302 | -     | 44,50,50     | 1.38 | 4 (9%)   | 51,76,76    | 3.29 | 20 (39%) |
| 36  | CLA  | O     | 312 | -     | 43,48,73     | 1.79 | 12 (27%) | 52,82,113   | 1.53 | 10 (19%) |
| 37  | KC1  | P     | 317 | 15    | 49,53,53     | 2.60 | 19 (38%) | 63,89,89    | 5.00 | 37 (58%) |
| 35  | A86  | C     | 204 | -     | 44,50,50     | 1.84 | 14 (31%) | 51,76,76    | 2.68 | 16 (31%) |
| 36  | CLA  | b     | 810 | 21    | 69,73,73     | 1.18 | 9 (13%)  | 83,113,113  | 1.32 | 6 (7%)   |
| 36  | CLA  | K     | 312 | -     | 69,73,73     | 1.21 | 10 (14%) | 83,113,113  | 1.33 | 6 (7%)   |
| 36  | CLA  | J     | 309 | 10    | 69,73,73     | 1.25 | 10 (14%) | 83,113,113  | 1.26 | 8 (9%)   |
| 37  | KC1  | T     | 310 | 18    | 49,53,53     | 4.55 | 27 (55%) | 63,89,89    | 6.90 | 40 (63%) |
| 36  | CLA  | S     | 311 | 35    | 50,54,73     | 1.50 | 10 (20%) | 60,90,113   | 1.55 | 9 (15%)  |
| 35  | A86  | J     | 301 | -     | 44,50,50     | 1.26 | 4 (9%)   | 51,76,76    | 2.23 | 18 (35%) |
| 36  | CLA  | N     | 313 | 14    | 45,49,73     | 1.58 | 8 (17%)  | 54,84,113   | 1.78 | 15 (27%) |
| 44  | BCR  | b     | 843 | -     | 41,41,41     | 1.18 | 3 (7%)   | 56,56,56    | 1.18 | 5 (8%)   |
| 36  | CLA  | H     | 315 | 8     | 69,73,73     | 1.26 | 10 (14%) | 83,113,113  | 1.53 | 13 (15%) |
| 35  | A86  | S     | 303 | 17    | 44,50,50     | 1.32 | 5 (11%)  | 51,76,76    | 3.30 | 22 (43%) |
| 44  | BCR  | m     | 101 | -     | 41,41,41     | 1.15 | 4 (9%)   | 56,56,56    | 1.34 | 7 (12%)  |
| 36  | CLA  | R     | 314 | 16    | 50,54,73     | 1.48 | 9 (18%)  | 60,90,113   | 1.75 | 9 (15%)  |
| 36  | CLA  | D     | 317 | -     | 62,66,73     | 1.30 | 10 (16%) | 74,104,113  | 1.40 | 6 (8%)   |
| 36  | CLA  | T     | 308 | 18    | 65,69,73     | 1.28 | 7 (10%)  | 78,108,113  | 1.43 | 7 (8%)   |
| 36  | CLA  | H     | 316 | -     | 69,73,73     | 1.23 | 10 (14%) | 83,113,113  | 1.38 | 5 (6%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 35  | A86  | L     | 307 | -    | 44,50,50     | 1.24 | 4 (9%)   | 51,76,76    | 1.93 | 11 (21%) |
| 36  | CLA  | b     | 813 | 21   | 58,62,73     | 1.40 | 13 (22%) | 73,100,113  | 1.40 | 10 (13%) |
| 41  | LHG  | f     | 809 | -    | 41,41,48     | 1.01 | 2 (4%)   | 44,47,54    | 1.09 | 3 (6%)   |
| 39  | LMT  | F     | 320 | -    | 36,36,36     | 0.38 | 0        | 47,47,47    | 0.67 | 1 (2%)   |
| 37  | KC1  | G     | 317 | -    | 49,53,53     | 2.71 | 20 (40%) | 63,89,89    | 4.44 | 38 (60%) |
| 39  | LMT  | B     | 312 | -    | 36,36,36     | 0.42 | 0        | 47,47,47    | 0.66 | 1 (2%)   |
| 36  | CLA  | B     | 307 | -    | 50,54,73     | 1.45 | 8 (16%)  | 60,90,113   | 1.52 | 7 (11%)  |
| 35  | A86  | R     | 309 | -    | 44,50,50     | 1.23 | 4 (9%)   | 51,76,76    | 2.84 | 16 (31%) |
| 37  | KC1  | K     | 314 | 11   | 49,53,53     | 2.65 | 18 (36%) | 63,89,89    | 5.06 | 38 (60%) |
| 36  | CLA  | H     | 308 | 8    | 67,72,73     | 1.27 | 12 (17%) | 80,112,113  | 1.33 | 11 (13%) |
| 37  | KC1  | X     | 311 | -    | 49,53,53     | 2.86 | 19 (38%) | 63,89,89    | 4.42 | 36 (57%) |
| 41  | LHG  | i     | 104 | -    | 45,45,48     | 0.98 | 2 (4%)   | 48,51,54    | 1.03 | 2 (4%)   |
| 35  | A86  | R     | 301 | -    | 44,50,50     | 1.47 | 4 (9%)   | 51,76,76    | 3.48 | 24 (47%) |
| 36  | CLA  | J     | 317 | 10   | 51,55,73     | 1.42 | 10 (19%) | 61,91,113   | 1.42 | 5 (8%)   |
| 36  | CLA  | l     | 206 | 46   | 54,58,73     | 1.36 | 10 (18%) | 65,95,113   | 1.48 | 7 (10%)  |
| 36  | CLA  | W     | 206 | 19   | 65,69,73     | 1.26 | 6 (9%)   | 78,108,113  | 1.47 | 6 (7%)   |
| 42  | LMG  | G     | 324 | -    | 55,55,55     | 0.90 | 2 (3%)   | 63,63,63    | 1.00 | 3 (4%)   |
| 36  | CLA  | a     | 836 | -    | 69,73,73     | 1.17 | 10 (14%) | 83,113,113  | 1.56 | 10 (12%) |
| 36  | CLA  | V     | 311 | 33   | 69,73,73     | 1.24 | 10 (14%) | 83,113,113  | 1.62 | 15 (18%) |
| 36  | CLA  | P     | 313 | -    | 69,73,73     | 1.23 | 9 (13%)  | 83,113,113  | 1.32 | 4 (4%)   |
| 36  | CLA  | a     | 831 | -    | 69,73,73     | 1.25 | 10 (14%) | 83,113,113  | 1.27 | 10 (12%) |
| 36  | CLA  | D     | 308 | -    | 69,73,73     | 1.27 | 11 (15%) | 83,113,113  | 1.54 | 13 (15%) |
| 36  | CLA  | a     | 833 | 20   | 54,58,73     | 1.37 | 10 (18%) | 65,95,113   | 1.64 | 8 (12%)  |
| 38  | SQD  | A     | 315 | -    | 27,28,54     | 1.50 | 4 (14%)  | 36,39,65    | 1.29 | 5 (13%)  |
| 36  | CLA  | W     | 215 | -    | 52,56,73     | 1.63 | 10 (19%) | 62,92,113   | 1.42 | 8 (12%)  |
| 44  | BCR  | b     | 844 | -    | 41,41,41     | 1.11 | 3 (7%)   | 56,56,56    | 1.31 | 5 (8%)   |
| 36  | CLA  | U     | 306 | 32   | 69,73,73     | 1.92 | 17 (24%) | 83,113,113  | 2.65 | 25 (30%) |
| 36  | CLA  | M     | 307 | -    | 69,73,73     | 1.25 | 12 (17%) | 83,113,113  | 1.46 | 9 (10%)  |
| 34  | DD6  | A     | 301 | -    | 39,45,45     | 2.04 | 3 (7%)   | 52,67,67    | 2.08 | 15 (28%) |
| 40  | DGD  | b     | 849 | -    | 61,61,67     | 1.05 | 7 (11%)  | 75,75,81    | 1.49 | 11 (14%) |
| 36  | CLA  | R     | 321 | 16   | 69,73,73     | 1.27 | 9 (13%)  | 83,113,113  | 1.44 | 10 (12%) |
| 35  | A86  | J     | 302 | -    | 44,50,50     | 1.26 | 4 (9%)   | 51,76,76    | 2.08 | 12 (23%) |
| 36  | CLA  | P     | 314 | -    | 64,68,73     | 1.43 | 11 (17%) | 77,107,113  | 1.67 | 16 (20%) |
| 35  | A86  | M     | 302 | -    | 44,50,50     | 1.29 | 4 (9%)   | 51,76,76    | 2.78 | 16 (31%) |
| 36  | CLA  | G     | 315 | 7    | 60,64,73     | 1.92 | 15 (25%) | 72,102,113  | 2.85 | 23 (31%) |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 36  | CLA  | K     | 313 | -     | 69,73,73     | 1.30 | 13 (18%) | 83,113,113  | 1.48 | 11 (13%) |
| 36  | CLA  | P     | 311 | -     | 69,73,73     | 1.24 | 10 (14%) | 83,113,113  | 1.42 | 10 (12%) |
| 36  | CLA  | M     | 306 | 37,13 | 59,63,73     | 1.33 | 9 (15%)  | 71,101,113  | 1.58 | 10 (14%) |
| 36  | CLA  | b     | 821 | 46    | 69,73,73     | 1.22 | 10 (14%) | 83,113,113  | 1.42 | 8 (9%)   |
| 37  | KC1  | Q     | 313 | -     | 49,53,53     | 2.89 | 19 (38%) | 63,89,89    | 6.04 | 39 (61%) |
| 36  | CLA  | V     | 305 | 35    | 65,69,73     | 1.38 | 7 (10%)  | 78,108,113  | 1.45 | 9 (11%)  |
| 36  | CLA  | U     | 309 | 32    | 50,54,73     | 1.52 | 7 (14%)  | 60,90,113   | 1.71 | 10 (16%) |
| 36  | CLA  | D     | 316 | -     | 56,60,73     | 1.37 | 9 (16%)  | 67,97,113   | 1.69 | 12 (17%) |
| 34  | DD6  | B     | 304 | -     | 39,45,45     | 2.01 | 3 (7%)   | 52,67,67    | 2.14 | 16 (30%) |
| 35  | A86  | U     | 303 | 36    | 44,50,50     | 1.23 | 4 (9%)   | 51,76,76    | 2.00 | 14 (27%) |
| 36  | CLA  | N     | 309 | 14    | 55,59,73     | 1.41 | 8 (14%)  | 66,96,113   | 1.74 | 8 (12%)  |
| 35  | A86  | A     | 316 | -     | 44,50,50     | 1.23 | 4 (9%)   | 51,76,76    | 2.16 | 16 (31%) |
| 36  | CLA  | Q     | 314 | -     | 69,73,73     | 1.27 | 8 (11%)  | 83,113,113  | 3.97 | 14 (16%) |
| 42  | LMG  | J     | 319 | -     | 44,44,55     | 0.99 | 2 (4%)   | 52,52,63    | 1.11 | 3 (5%)   |
| 35  | A86  | J     | 303 | -     | 44,50,50     | 1.41 | 4 (9%)   | 51,76,76    | 2.80 | 20 (39%) |
| 35  | A86  | N     | 301 | -     | 44,50,50     | 1.46 | 4 (9%)   | 51,76,76    | 3.73 | 26 (50%) |
| 36  | CLA  | a     | 818 | 20    | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.54 | 11 (13%) |
| 37  | KC1  | V     | 312 | 33    | 49,53,53     | 2.86 | 20 (40%) | 63,89,89    | 4.75 | 36 (57%) |
| 36  | CLA  | S     | 320 | -     | 69,73,73     | 1.26 | 9 (13%)  | 83,113,113  | 1.30 | 7 (8%)   |
| 34  | DD6  | A     | 304 | -     | 39,45,45     | 2.00 | 3 (7%)   | 52,67,67    | 1.90 | 12 (23%) |
| 36  | CLA  | T     | 309 | 18    | 69,73,73     | 1.23 | 9 (13%)  | 83,113,113  | 1.41 | 8 (9%)   |
| 41  | LHG  | F     | 319 | -     | 40,40,48     | 1.03 | 2 (5%)   | 43,46,54    | 1.10 | 3 (6%)   |
| 36  | CLA  | b     | 836 | 21    | 62,66,73     | 2.02 | 15 (24%) | 74,104,113  | 3.01 | 24 (32%) |
| 36  | CLA  | X     | 312 | -     | 45,49,73     | 1.52 | 9 (20%)  | 54,84,113   | 1.71 | 8 (14%)  |
| 34  | DD6  | K     | 304 | -     | 39,45,45     | 2.02 | 3 (7%)   | 52,67,67    | 1.87 | 13 (25%) |
| 34  | DD6  | A     | 303 | -     | 39,45,45     | 2.00 | 3 (7%)   | 52,67,67    | 1.86 | 9 (17%)  |
| 45  | SF4  | c     | 102 | -     | 0,12,12      | -    | -        | -           | -    | -        |
| 34  | DD6  | S     | 306 | -     | 39,45,45     | 1.96 | 3 (7%)   | 52,67,67    | 2.00 | 13 (25%) |
| 34  | DD6  | R     | 307 | -     | 39,45,45     | 2.00 | 2 (5%)   | 52,67,67    | 2.11 | 15 (28%) |
| 36  | CLA  | A     | 313 | -     | 45,49,73     | 1.51 | 9 (20%)  | 54,84,113   | 1.71 | 7 (12%)  |
| 44  | BCR  | f     | 801 | -     | 41,41,41     | 1.12 | 2 (4%)   | 56,56,56    | 1.19 | 5 (8%)   |
| 35  | A86  | K     | 306 | 11    | 44,50,50     | 1.22 | 3 (6%)   | 51,76,76    | 3.50 | 21 (41%) |
| 42  | LMG  | E     | 318 | -     | 46,46,55     | 0.98 | 2 (4%)   | 54,54,63    | 1.06 | 2 (3%)   |
| 36  | CLA  | C     | 212 | 35    | 69,73,73     | 1.22 | 11 (15%) | 83,113,113  | 1.54 | 13 (15%) |
| 36  | CLA  | R     | 310 | -     | 65,69,73     | 1.28 | 10 (15%) | 78,108,113  | 1.39 | 7 (8%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 37  | KC1  | G     | 318 | -    | 49,53,53     | 2.74 | 20 (40%) | 63,89,89    | 4.46 | 41 (65%) |
| 39  | LMT  | f     | 807 | -    | 24,24,36     | 0.43 | 0        | 29,29,47    | 0.58 | 0        |
| 35  | A86  | F     | 301 | -    | 44,50,50     | 1.24 | 4 (9%)   | 51,76,76    | 2.32 | 16 (31%) |
| 44  | BCR  | b     | 847 | -    | 41,41,41     | 1.18 | 3 (7%)   | 56,56,56    | 1.26 | 7 (12%)  |
| 36  | CLA  | F     | 316 | 6    | 45,49,73     | 1.48 | 10 (22%) | 54,84,113   | 1.50 | 7 (12%)  |
| 37  | KC1  | A     | 312 | 1    | 49,53,53     | 2.73 | 18 (36%) | 63,89,89    | 6.28 | 44 (69%) |
| 36  | CLA  | N     | 308 | 14   | 69,73,73     | 1.40 | 8 (11%)  | 83,113,113  | 1.80 | 20 (24%) |
| 34  | DD6  | C     | 201 | -    | 39,45,45     | 2.03 | 3 (7%)   | 52,67,67    | 1.92 | 13 (25%) |
| 35  | A86  | X     | 302 | 35   | 44,50,50     | 1.22 | 4 (9%)   | 51,76,76    | 2.97 | 18 (35%) |
| 36  | CLA  | G     | 316 | -    | 53,57,73     | 1.40 | 10 (18%) | 62,93,113   | 1.49 | 5 (8%)   |
| 35  | A86  | P     | 307 | -    | 44,50,50     | 1.22 | 3 (6%)   | 51,76,76    | 2.05 | 13 (25%) |
| 44  | BCR  | f     | 806 | -    | 41,41,41     | 1.18 | 3 (7%)   | 56,56,56    | 1.23 | 7 (12%)  |
| 35  | A86  | G     | 304 | -    | 44,50,50     | 1.43 | 5 (11%)  | 51,76,76    | 3.69 | 25 (49%) |
| 41  | LHG  | D     | 319 | 42   | 48,48,48     | 0.93 | 2 (4%)   | 51,54,54    | 1.06 | 3 (5%)   |
| 36  | CLA  | a     | 838 | 20   | 69,73,73     | 1.21 | 10 (14%) | 83,113,113  | 1.36 | 8 (9%)   |
| 36  | CLA  | C     | 209 | -    | 69,73,73     | 1.26 | 10 (14%) | 83,113,113  | 1.40 | 9 (10%)  |
| 41  | LHG  | G     | 320 | -    | 39,39,48     | 1.04 | 2 (5%)   | 42,45,54    | 1.11 | 3 (7%)   |
| 37  | KC1  | S     | 316 | -    | 49,53,53     | 2.83 | 20 (40%) | 63,89,89    | 5.25 | 40 (63%) |
| 35  | A86  | B     | 301 | -    | 44,50,50     | 1.23 | 4 (9%)   | 51,76,76    | 1.98 | 13 (25%) |
| 39  | LMT  | L     | 318 | -    | 32,32,36     | 0.45 | 0        | 43,43,47    | 0.79 | 1 (2%)   |
| 36  | CLA  | a     | 841 | 41   | 56,60,73     | 1.41 | 10 (17%) | 67,97,113   | 1.55 | 9 (13%)  |
| 35  | A86  | N     | 302 | -    | 44,50,50     | 1.19 | 3 (6%)   | 51,76,76    | 2.68 | 15 (29%) |
| 36  | CLA  | F     | 313 | -    | 56,60,73     | 1.34 | 9 (16%)  | 67,97,113   | 1.46 | 8 (11%)  |
| 36  | CLA  | F     | 309 | -    | 69,73,73     | 1.25 | 10 (14%) | 83,113,113  | 1.43 | 12 (14%) |
| 36  | CLA  | C     | 206 | -    | 65,69,73     | 1.27 | 8 (12%)  | 78,108,113  | 1.38 | 5 (6%)   |
| 36  | CLA  | E     | 310 | -    | 69,73,73     | 1.29 | 8 (11%)  | 83,113,113  | 1.43 | 10 (12%) |
| 36  | CLA  | D     | 310 | -    | 69,73,73     | 1.18 | 8 (11%)  | 83,113,113  | 1.45 | 9 (10%)  |
| 36  | CLA  | P     | 319 | -    | 64,68,73     | 1.97 | 13 (20%) | 77,107,113  | 2.21 | 16 (20%) |
| 36  | CLA  | R     | 313 | -    | 69,73,73     | 1.23 | 11 (15%) | 83,113,113  | 1.25 | 8 (9%)   |
| 36  | CLA  | b     | 809 | 21   | 69,73,73     | 1.22 | 11 (15%) | 83,113,113  | 1.30 | 6 (7%)   |
| 36  | CLA  | b     | 827 | -    | 69,73,73     | 1.33 | 10 (14%) | 83,113,113  | 1.40 | 9 (10%)  |
| 36  | CLA  | O     | 316 | -    | 69,73,73     | 1.84 | 15 (21%) | 83,113,113  | 2.88 | 27 (32%) |
| 35  | A86  | F     | 305 | -    | 44,50,50     | 1.35 | 6 (13%)  | 51,76,76    | 2.84 | 20 (39%) |
| 36  | CLA  | J     | 313 | -    | 69,73,73     | 1.24 | 10 (14%) | 83,113,113  | 1.37 | 7 (8%)   |
| 35  | A86  | M     | 301 | -    | 44,50,50     | 1.36 | 4 (9%)   | 51,76,76    | 3.39 | 22 (43%) |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 35  | A86  | K     | 303 | -     | 44,50,50     | 1.31 | 4 (9%)   | 51,76,76    | 2.80 | 17 (33%) |
| 36  | CLA  | C     | 205 | -     | 47,51,73     | 1.45 | 9 (19%)  | 56,86,113   | 1.56 | 9 (16%)  |
| 36  | CLA  | b     | 814 | 21    | 59,63,73     | 1.32 | 10 (16%) | 71,101,113  | 1.38 | 6 (8%)   |
| 36  | CLA  | L     | 310 | -     | 58,62,73     | 1.38 | 9 (15%)  | 69,99,113   | 1.31 | 5 (7%)   |
| 36  | CLA  | A     | 309 | 1     | 50,54,73     | 1.45 | 9 (18%)  | 60,90,113   | 1.48 | 5 (8%)   |
| 36  | CLA  | A     | 311 | -     | 69,73,73     | 1.23 | 10 (14%) | 83,113,113  | 1.36 | 6 (7%)   |
| 41  | LHG  | R     | 323 | -     | 48,48,48     | 0.94 | 2 (4%)   | 51,54,54    | 1.04 | 3 (5%)   |
| 35  | A86  | Q     | 316 | 15,36 | 44,50,50     | 1.65 | 8 (18%)  | 51,76,76    | 2.29 | 17 (33%) |
| 36  | CLA  | N     | 312 | -     | 51,55,73     | 1.37 | 8 (15%)  | 61,91,113   | 1.49 | 4 (6%)   |
| 36  | CLA  | S     | 318 | -     | 46,50,73     | 1.48 | 6 (13%)  | 55,85,113   | 1.60 | 6 (10%)  |
| 35  | A86  | R     | 305 | -     | 44,50,50     | 1.22 | 4 (9%)   | 51,76,76    | 1.81 | 11 (21%) |
| 36  | CLA  | Q     | 306 | -     | 69,73,73     | 1.23 | 11 (15%) | 83,113,113  | 1.37 | 7 (8%)   |
| 36  | CLA  | R     | 320 | 16    | 49,53,73     | 1.51 | 11 (22%) | 59,89,113   | 1.71 | 13 (22%) |
| 36  | CLA  | a     | 822 | -     | 55,59,73     | 1.60 | 11 (20%) | 66,96,113   | 2.18 | 18 (27%) |
| 35  | A86  | T     | 303 | -     | 44,50,50     | 1.22 | 4 (9%)   | 51,76,76    | 3.14 | 21 (41%) |
| 36  | CLA  | B     | 309 | 2     | 56,60,73     | 1.78 | 11 (19%) | 67,97,113   | 2.23 | 20 (29%) |
| 35  | A86  | S     | 305 | -     | 44,50,50     | 1.27 | 3 (6%)   | 51,76,76    | 2.95 | 20 (39%) |
| 36  | CLA  | H     | 314 | -     | 45,49,73     | 1.49 | 11 (24%) | 54,84,113   | 1.72 | 8 (14%)  |
| 39  | LMT  | a     | 851 | -     | 36,36,36     | 0.43 | 0        | 47,47,47    | 0.74 | 1 (2%)   |
| 36  | CLA  | l     | 202 | 21,28 | 69,73,73     | 1.26 | 11 (15%) | 83,113,113  | 1.33 | 9 (10%)  |
| 39  | LMT  | K     | 317 | -     | 32,32,36     | 0.43 | 0        | 43,43,47    | 0.70 | 0        |
| 39  | LMT  | I     | 317 | -     | 36,36,36     | 0.41 | 0        | 47,47,47    | 0.75 | 1 (2%)   |
| 36  | CLA  | S     | 315 | 17    | 47,51,73     | 1.51 | 8 (17%)  | 56,86,113   | 1.97 | 10 (17%) |
| 36  | CLA  | X     | 310 | 19    | 45,49,73     | 1.55 | 8 (17%)  | 54,84,113   | 2.03 | 9 (16%)  |
| 37  | KC1  | O     | 315 | 15    | 49,53,53     | 2.88 | 19 (38%) | 63,89,89    | 6.04 | 39 (61%) |
| 36  | CLA  | a     | 832 | -     | 69,73,73     | 1.22 | 9 (13%)  | 83,113,113  | 1.52 | 12 (14%) |
| 35  | A86  | B     | 303 | -     | 44,50,50     | 1.30 | 3 (6%)   | 51,76,76    | 4.01 | 27 (52%) |
| 35  | A86  | J     | 306 | -     | 44,50,50     | 1.25 | 3 (6%)   | 51,76,76    | 1.96 | 11 (21%) |
| 36  | CLA  | Q     | 307 | 15    | 54,58,73     | 1.40 | 10 (18%) | 63,94,113   | 1.46 | 5 (7%)   |
| 36  | CLA  | O     | 314 | -     | 45,49,73     | 1.51 | 9 (20%)  | 54,84,113   | 1.72 | 8 (14%)  |
| 39  | LMT  | B     | 313 | -     | 36,36,36     | 0.43 | 0        | 47,47,47    | 0.73 | 1 (2%)   |
| 36  | CLA  | C     | 207 | -     | 69,73,73     | 1.98 | 17 (24%) | 83,113,113  | 2.97 | 26 (31%) |
| 37  | KC1  | W     | 213 | -     | 49,53,53     | 2.86 | 20 (40%) | 63,89,89    | 4.90 | 35 (55%) |
| 36  | CLA  | A     | 305 | 1     | 53,57,73     | 1.41 | 9 (16%)  | 62,93,113   | 1.42 | 6 (9%)   |
| 34  | DD6  | D     | 301 | -     | 39,45,45     | 2.01 | 3 (7%)   | 52,67,67    | 1.99 | 13 (25%) |



| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 36  | CLA  | U     | 310 | -     | 69,73,73     | 1.25 | 8 (11%)  | 83,113,113  | 1.53 | 12 (14%) |
| 36  | CLA  | A     | 307 | -     | 64,68,73     | 1.27 | 10 (15%) | 77,107,113  | 1.38 | 9 (11%)  |
| 36  | CLA  | l     | 205 | -     | 69,73,73     | 1.54 | 14 (20%) | 83,113,113  | 2.13 | 17 (20%) |
| 36  | CLA  | K     | 308 | -     | 69,73,73     | 1.24 | 9 (13%)  | 83,113,113  | 1.38 | 9 (10%)  |
| 40  | DGD  | L     | 302 | 42    | 48,48,67     | 0.98 | 2 (4%)   | 62,62,81    | 1.05 | 4 (6%)   |
| 36  | CLA  | W     | 201 | 19    | 52,56,73     | 1.43 | 8 (15%)  | 62,92,113   | 1.43 | 5 (8%)   |
| 34  | DD6  | E     | 301 | -     | 39,45,45     | 1.98 | 3 (7%)   | 52,67,67    | 1.93 | 10 (19%) |
| 36  | CLA  | A     | 308 | -     | 69,73,73     | 1.22 | 9 (13%)  | 83,113,113  | 1.44 | 10 (12%) |
| 36  | CLA  | R     | 312 | 16    | 69,73,73     | 1.25 | 9 (13%)  | 83,113,113  | 1.51 | 10 (12%) |
| 36  | CLA  | f     | 805 | 25    | 56,60,73     | 1.34 | 10 (17%) | 67,97,113   | 1.52 | 8 (11%)  |
| 34  | DD6  | M     | 303 | -     | 39,45,45     | 2.03 | 3 (7%)   | 52,67,67    | 1.96 | 11 (21%) |
| 36  | CLA  | b     | 806 | -     | 69,73,73     | 1.28 | 9 (13%)  | 83,113,113  | 1.60 | 13 (15%) |
| 35  | A86  | A     | 302 | -     | 44,50,50     | 1.61 | 6 (13%)  | 51,76,76    | 4.76 | 25 (49%) |
| 36  | CLA  | W     | 216 | 19,35 | 49,53,73     | 1.95 | 10 (20%) | 59,89,113   | 3.01 | 15 (25%) |
| 35  | A86  | R     | 306 | -     | 44,50,50     | 1.34 | 4 (9%)   | 51,76,76    | 2.91 | 16 (31%) |

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   |
|-----|------|-------|-----|-------|---------|---------------|---------|
| 37  | KC1  | M     | 317 | -     | -       | 3/15/71/71    | -       |
| 36  | CLA  | a     | 819 | -     | -       | 5/15/91/115   | -       |
| 36  | CLA  | H     | 307 | 8     | -       | 5/33/109/115  | -       |
| 36  | CLA  | a     | 828 | -     | -       | 20/39/115/115 | -       |
| 36  | CLA  | b     | 835 | -     | -       | 5/15/91/115   | -       |
| 36  | CLA  | b     | 838 | 21    | -       | 3/18/94/115   | -       |
| 36  | CLA  | M     | 314 | -     | -       | 4/10/86/115   | -       |
| 36  | CLA  | U     | 313 | -     | -       | 4/10/86/115   | -       |
| 36  | CLA  | M     | 309 | -     | -       | 15/39/115/115 | -       |
| 44  | BCR  | j     | 107 | -     | -       | 5/29/63/63    | 0/2/2/2 |
| 36  | CLA  | R     | 311 | 16    | -       | 13/39/115/115 | -       |
| 36  | CLA  | X     | 309 | 19    | -       | 8/15/91/115   | -       |
| 36  | CLA  | X     | 307 | 19,35 | -       | 6/21/97/115   | -       |
| 35  | A86  | R     | 304 | 16,36 | -       | 8/34/90/90    | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 35  | A86  | V     | 302 | -     | -         | 5/34/90/90    | 0/3/3/3 |
| 36  | CLA  | b     | 840 | 21    | -         | 12/39/115/115 | -       |
| 36  | CLA  | T     | 313 | 18    | -         | 8/39/115/115  | -       |
| 35  | A86  | X     | 305 | -     | -         | 8/34/90/90    | 0/3/3/3 |
| 36  | CLA  | W     | 211 | 19    | -         | 10/39/115/115 | -       |
| 36  | CLA  | a     | 827 | 20    | -         | 14/36/112/115 | -       |
| 42  | LMG  | V     | 315 | -     | -         | 24/41/61/70   | 0/1/1/1 |
| 35  | A86  | Q     | 301 | -     | -         | 6/34/90/90    | 0/3/3/3 |
| 36  | CLA  | P     | 312 | 15    | -         | 9/17/93/115   | -       |
| 35  | A86  | N     | 306 | -     | -         | 8/34/90/90    | 0/3/3/3 |
| 39  | LMT  | b     | 848 | -     | -         | 12/21/61/61   | 0/2/2/2 |
| 36  | CLA  | F     | 314 | 6,35  | -         | 16/39/115/115 | -       |
| 42  | LMG  | J     | 318 | -     | -         | 28/50/70/70   | 0/1/1/1 |
| 35  | A86  | O     | 303 | -     | -         | 6/34/90/90    | 0/3/3/3 |
| 36  | CLA  | W     | 212 | 19    | -         | 15/39/115/115 | -       |
| 35  | A86  | V     | 303 | 35    | -         | 8/34/90/90    | 0/3/3/3 |
| 36  | CLA  | C     | 211 | -     | -         | 13/39/115/115 | -       |
| 36  | CLA  | b     | 820 | 21    | -         | 17/33/109/115 | -       |
| 36  | CLA  | B     | 306 | -     | -         | 6/17/93/115   | -       |
| 36  | CLA  | T     | 311 | 18    | -         | 13/39/115/115 | -       |
| 36  | CLA  | M     | 308 | -     | -         | 7/24/100/115  | -       |
| 36  | CLA  | a     | 816 | 20    | 1/1/15/20 | 21/39/115/115 | -       |
| 37  | KC1  | P     | 315 | 35    | -         | 2/15/71/71    | -       |
| 36  | CLA  | X     | 313 | 19    | -         | 6/12/88/115   | -       |
| 35  | A86  | T     | 306 | -     | -         | 6/34/90/90    | 0/3/3/3 |
| 35  | A86  | L     | 319 | -     | -         | 9/34/90/90    | 0/3/3/3 |
| 36  | CLA  | N     | 315 | -     | -         | 0/10/86/115   | -       |
| 36  | CLA  | b     | 826 | 21,46 | -         | 11/38/114/115 | -       |
| 36  | CLA  | W     | 207 | 34    | -         | 17/39/115/115 | -       |
| 35  | A86  | G     | 302 | -     | -         | 7/34/90/90    | 0/3/3/3 |
| 36  | CLA  | P     | 308 | -     | -         | 11/35/111/115 | -       |
| 36  | CLA  | Q     | 309 | 15    | -         | 9/17/93/115   | -       |
| 35  | A86  | O     | 305 | -     | -         | 14/34/90/90   | 0/3/3/3 |
| 36  | CLA  | N     | 319 | 14    | -         | 5/12/88/115   | -       |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 36  | CLA  | M     | 312 | 13,36 | -         | 12/18/94/115  | -       |
| 39  | LMT  | a     | 854 | -     | -         | 16/21/61/61   | 0/2/2/2 |
| 42  | LMG  | V     | 316 | -     | -         | 24/41/61/70   | 0/1/1/1 |
| 39  | LMT  | b     | 851 | -     | -         | 7/15/35/61    | 0/1/1/2 |
| 35  | A86  | W     | 203 | 36    | -         | 6/34/90/90    | 0/3/3/3 |
| 36  | CLA  | P     | 309 | 41    | -         | 14/39/115/115 | -       |
| 36  | CLA  | b     | 831 | 21    | -         | 9/21/97/115   | -       |
| 36  | CLA  | V     | 308 | -     | -         | 18/39/115/115 | -       |
| 35  | A86  | L     | 306 | 37    | -         | 10/34/90/90   | 0/3/3/3 |
| 34  | DD6  | R     | 308 | -     | -         | 10/26/80/80   | 0/3/3/3 |
| 35  | A86  | Q     | 304 | -     | -         | 10/34/90/90   | 0/3/3/3 |
| 36  | CLA  | b     | 841 | 41    | -         | 9/39/115/115  | -       |
| 44  | BCR  | a     | 846 | -     | -         | 7/29/63/63    | 0/2/2/2 |
| 36  | CLA  | I     | 312 | 9     | -         | 4/24/100/115  | -       |
| 35  | A86  | U     | 301 | -     | -         | 8/34/90/90    | 0/3/3/3 |
| 35  | A86  | I     | 302 | -     | -         | 7/34/90/90    | 0/3/3/3 |
| 36  | CLA  | b     | 824 | 21    | -         | 14/25/101/115 | -       |
| 36  | CLA  | a     | 802 | -     | 1/1/15/20 | 11/39/115/115 | -       |
| 36  | CLA  | V     | 310 | 33    | -         | 8/39/115/115  | -       |
| 35  | A86  | T     | 302 | 18    | -         | 7/34/90/90    | 0/3/3/3 |
| 36  | CLA  | N     | 316 | 14    | -         | 13/39/115/115 | -       |
| 35  | A86  | h     | 202 | -     | -         | 3/34/90/90    | 1/3/3/3 |
| 41  | LHG  | F     | 318 | -     | -         | 15/34/34/53   | -       |
| 36  | CLA  | P     | 310 | 15,41 | -         | 13/39/115/115 | -       |
| 35  | A86  | Q     | 303 | -     | -         | 8/34/90/90    | 0/3/3/3 |
| 36  | CLA  | a     | 820 | -     | -         | 11/39/115/115 | -       |
| 37  | KC1  | R     | 317 | -     | -         | 3/15/71/71    | -       |
| 35  | A86  | N     | 304 | -     | -         | 8/34/90/90    | 0/3/3/3 |
| 42  | LMG  | D     | 321 | -     | -         | 21/32/52/70   | 0/1/1/1 |
| 36  | CLA  | f     | 804 | 46    | 1/1/15/20 | 10/39/115/115 | -       |
| 39  | LMT  | U     | 315 | -     | -         | 17/21/61/61   | 0/2/2/2 |
| 36  | CLA  | J     | 312 | 10    | -         | 10/39/115/115 | -       |
| 36  | CLA  | W     | 218 | 19    | -         | 9/13/89/115   | -       |
| 39  | LMT  | h     | 205 | -     | -         | 10/21/61/61   | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 36  | CLA  | K     | 315 | -    | -         | 3/10/86/115   | -       |
| 36  | CLA  | a     | 812 | 20   | -         | 14/39/115/115 | -       |
| 43  | PQN  | b     | 842 | -    | -         | 11/23/43/43   | 0/2/2/2 |
| 42  | LMG  | m     | 102 | -    | -         | 14/32/52/70   | 0/1/1/1 |
| 36  | CLA  | E     | 311 | 5    | -         | 16/39/115/115 | -       |
| 36  | CLA  | D     | 311 | 4    | -         | 7/17/93/115   | -       |
| 36  | CLA  | L     | 311 | -    | -         | 14/39/115/115 | -       |
| 36  | CLA  | P     | 301 | 15   | -         | 18/39/115/115 | -       |
| 41  | LHG  | j     | 104 | -    | -         | 32/53/53/53   | -       |
| 34  | DD6  | H     | 303 | -    | -         | 6/26/80/80    | 0/3/3/3 |
| 44  | BCR  | b     | 846 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 36  | CLA  | V     | 306 | 33   | -         | 19/39/115/115 | -       |
| 35  | A86  | F     | 304 | 36   | -         | 4/34/90/90    | 0/3/3/3 |
| 36  | CLA  | Q     | 308 | -    | -         | 20/39/115/115 | -       |
| 43  | PQN  | a     | 840 | -    | -         | 7/23/43/43    | 0/2/2/2 |
| 36  | CLA  | H     | 310 | 8    | -         | 7/17/93/115   | -       |
| 41  | LHG  | b     | 850 | 36   | -         | 27/53/53/53   | -       |
| 36  | CLA  | b     | 815 | 21   | -         | 19/39/115/115 | -       |
| 36  | CLA  | T     | 312 | 18   | -         | 7/17/93/115   | -       |
| 44  | BCR  | a     | 847 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 36  | CLA  | G     | 314 | 7    | -         | 4/10/86/115   | -       |
| 36  | CLA  | P     | 302 | -    | -         | 5/12/88/115   | -       |
| 35  | A86  | X     | 304 | 19   | -         | 7/34/90/90    | 0/3/3/3 |
| 34  | DD6  | D     | 304 | -    | -         | 8/26/80/80    | 0/3/3/3 |
| 34  | DD6  | E     | 303 | -    | -         | 7/26/80/80    | 0/3/3/3 |
| 35  | A86  | P     | 306 | -    | -         | 3/34/90/90    | 0/3/3/3 |
| 36  | CLA  | J     | 311 | -    | -         | 5/17/93/115   | -       |
| 42  | LMG  | h     | 206 | -    | -         | 24/40/60/70   | 0/1/1/1 |
| 35  | A86  | M     | 305 | -    | -         | 8/34/90/90    | 0/3/3/3 |
| 41  | LHG  | O     | 317 | -    | -         | 33/46/46/53   | -       |
| 36  | CLA  | I     | 306 | 9    | 1/1/15/20 | 15/39/115/115 | -       |
| 36  | CLA  | E     | 315 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 37  | KC1  | F     | 315 | -    | -         | 3/15/71/71    | -       |
| 36  | CLA  | W     | 210 | -    | -         | 9/17/93/115   | -       |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 44  | BCR  | h     | 201 | -     | -         | 9/29/63/63    | 0/2/2/2 |
| 35  | A86  | U     | 304 | 37,32 | -         | 11/34/90/90   | 0/3/3/3 |
| 36  | CLA  | K     | 316 | -     | -         | 12/39/115/115 | -       |
| 36  | CLA  | W     | 214 | 19    | -         | 5/10/86/115   | -       |
| 37  | KC1  | N     | 314 | 14    | -         | 7/15/71/71    | -       |
| 41  | LHG  | f     | 808 | 25    | -         | 29/53/53/53   | -       |
| 36  | CLA  | E     | 308 | 5     | -         | 10/20/96/115  | -       |
| 36  | CLA  | b     | 816 | 21    | 1/1/14/20 | 17/33/109/115 | -       |
| 45  | SF4  | b     | 803 | 21,20 | -         | -             | 0/6/5/5 |
| 35  | A86  | J     | 305 | -     | -         | 6/34/90/90    | 0/3/3/3 |
| 36  | CLA  | T     | 316 | -     | -         | 2/10/86/115   | -       |
| 36  | CLA  | b     | 839 | -     | -         | 6/39/115/115  | -       |
| 39  | LMT  | E     | 321 | -     | -         | 9/15/35/61    | 0/1/1/2 |
| 36  | CLA  | E     | 312 | -     | -         | 15/39/115/115 | -       |
| 35  | A86  | E     | 302 | -     | -         | 4/34/90/90    | 0/3/3/3 |
| 37  | KC1  | Q     | 311 | 15    | -         | 2/15/71/71    | -       |
| 34  | DD6  | L     | 305 | -     | -         | 7/26/80/80    | 0/3/3/3 |
| 36  | CLA  | b     | 830 | 21    | -         | 5/39/115/115  | -       |
| 44  | BCR  | l     | 207 | -     | -         | 7/29/63/63    | 0/2/2/2 |
| 35  | A86  | C     | 203 | -     | -         | 8/34/90/90    | 1/3/3/3 |
| 35  | A86  | S     | 308 | 37    | -         | 12/34/90/90   | 0/3/3/3 |
| 36  | CLA  | a     | 815 | 46    | -         | 5/15/91/115   | -       |
| 36  | CLA  | X     | 308 | 19    | -         | 12/18/94/115  | -       |
| 36  | CLA  | M     | 315 | 13    | -         | 8/18/94/115   | -       |
| 36  | CLA  | J     | 308 | -     | -         | 14/35/111/115 | -       |
| 34  | DD6  | Q     | 302 | -     | -         | 8/26/80/80    | 0/3/3/3 |
| 36  | CLA  | R     | 315 | -     | -         | 13/39/115/115 | -       |
| 37  | KC1  | L     | 317 | -     | -         | 3/15/71/71    | -       |
| 36  | CLA  | O     | 309 | -     | -         | 19/39/115/115 | -       |
| 36  | CLA  | i     | 102 | 26    | -         | 20/39/115/115 | -       |
| 36  | CLA  | G     | 307 | -     | -         | 2/11/87/115   | -       |
| 36  | CLA  | b     | 833 | 21    | -         | 11/31/107/115 | -       |
| 36  | CLA  | P     | 318 | -     | -         | 8/23/99/115   | -       |
| 36  | CLA  | G     | 309 | 7     | -         | 13/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 36  | CLA  | B     | 311 | 2    | -         | 13/27/103/115 | -       |
| 37  | KC1  | E     | 309 | -    | -         | 5/15/71/71    | -       |
| 42  | LMG  | G     | 325 | -    | -         | 27/50/70/70   | 0/1/1/1 |
| 36  | CLA  | U     | 305 | -    | -         | 13/35/111/115 | -       |
| 36  | CLA  | L     | 313 | -    | -         | 8/39/115/115  | -       |
| 36  | CLA  | b     | 825 | -    | -         | 13/39/115/115 | -       |
| 35  | A86  | X     | 301 | -    | -         | 8/34/90/90    | 0/3/3/3 |
| 36  | CLA  | a     | 826 | 20   | -         | 12/39/115/115 | -       |
| 36  | CLA  | N     | 317 | 14   | -         | 10/26/102/115 | -       |
| 34  | DD6  | E     | 306 | -    | -         | 4/26/80/80    | 0/3/3/3 |
| 36  | CLA  | a     | 835 | 20   | -         | 2/23/99/115   | -       |
| 35  | A86  | V     | 301 | 35   | -         | 10/34/90/90   | 1/3/3/3 |
| 36  | CLA  | S     | 321 | -    | -         | 12/24/100/115 | -       |
| 36  | CLA  | I     | 310 | 35   | -         | 11/39/115/115 | -       |
| 37  | KC1  | H     | 313 | -    | -         | 6/15/71/71    | -       |
| 41  | LHG  | E     | 322 | -    | -         | 28/53/53/53   | -       |
| 36  | CLA  | O     | 310 | 15   | -         | 9/17/93/115   | -       |
| 36  | CLA  | a     | 848 | 36   | 1/1/15/20 | 13/39/115/115 | -       |
| 36  | CLA  | X     | 306 | -    | -         | 11/35/111/115 | -       |
| 36  | CLA  | G     | 310 | 7    | -         | 5/39/115/115  | -       |
| 36  | CLA  | G     | 319 | 7    | -         | 8/21/97/115   | -       |
| 35  | A86  | I     | 301 | -    | -         | 10/34/90/90   | 0/3/3/3 |
| 35  | A86  | U     | 302 | -    | -         | 9/34/90/90    | 0/3/3/3 |
| 36  | CLA  | K     | 310 | -    | 1/1/14/20 | 16/36/112/115 | -       |
| 35  | A86  | X     | 314 | 19   | -         | 3/34/90/90    | 1/3/3/3 |
| 35  | A86  | N     | 320 | -    | -         | 10/34/90/90   | 0/3/3/3 |
| 36  | CLA  | M     | 316 | 36   | -         | 6/12/88/115   | -       |
| 42  | LMG  | a     | 852 | -    | -         | 26/49/69/70   | 0/1/1/1 |
| 36  | CLA  | V     | 313 | 33   | -         | 15/39/115/115 | -       |
| 34  | DD6  | W     | 205 | -    | -         | 8/26/80/80    | 0/3/3/3 |
| 34  | DD6  | K     | 305 | -    | -         | 0/26/80/80    | 0/3/3/3 |
| 36  | CLA  | H     | 317 | 8    | -         | 10/39/115/115 | -       |
| 37  | KC1  | M     | 318 | -    | -         | 10/15/71/71   | -       |
| 36  | CLA  | F     | 317 | 6    | 1/1/13/20 | 10/29/105/115 | -       |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 35  | A86  | M     | 304 | -     | -         | 14/34/90/90   | 0/3/3/3 |
| 42  | LMG  | D     | 320 | 41    | -         | 24/41/61/70   | 0/1/1/1 |
| 36  | CLA  | R     | 322 | 16    | -         | 13/24/100/115 | -       |
| 36  | CLA  | S     | 314 | 17    | -         | 11/39/115/115 | -       |
| 44  | BCR  | I     | 203 | -     | -         | 10/29/63/63   | 0/2/2/2 |
| 36  | CLA  | E     | 316 | -     | -         | 19/39/115/115 | -       |
| 36  | CLA  | P     | 316 | -     | -         | 5/10/86/115   | -       |
| 39  | LMT  | P     | 320 | -     | -         | 8/14/34/61    | 0/1/1/2 |
| 36  | CLA  | H     | 311 | -     | -         | 9/39/115/115  | -       |
| 36  | CLA  | b     | 834 | -     | -         | 10/39/115/115 | -       |
| 34  | DD6  | D     | 303 | -     | -         | 9/26/80/80    | 0/3/3/3 |
| 35  | A86  | F     | 306 | -     | -         | 0/34/90/90    | 1/3/3/3 |
| 36  | CLA  | E     | 313 | -     | 1/1/15/20 | 10/39/115/115 | -       |
| 35  | A86  | H     | 301 | -     | -         | 5/34/90/90    | 0/3/3/3 |
| 35  | A86  | S     | 304 | -     | -         | 9/34/90/90    | 0/3/3/3 |
| 36  | CLA  | O     | 306 | -     | -         | 11/35/111/115 | -       |
| 34  | DD6  | a     | 849 | -     | -         | 6/26/80/80    | 0/3/3/3 |
| 36  | CLA  | R     | 319 | 16    | -         | 7/15/91/115   | -       |
| 36  | CLA  | V     | 309 | 33    | -         | 4/13/89/115   | -       |
| 39  | LMT  | G     | 322 | -     | -         | 17/21/61/61   | 0/2/2/2 |
| 36  | CLA  | S     | 317 | -     | -         | 5/10/86/115   | -       |
| 42  | LMG  | I     | 315 | -     | -         | 32/50/70/70   | 0/1/1/1 |
| 37  | KC1  | D     | 314 | 4     | -         | 5/15/71/71    | -       |
| 35  | A86  | O     | 319 | 35,36 | -         | 8/34/90/90    | 0/3/3/3 |
| 36  | CLA  | N     | 318 | -     | -         | 7/18/94/115   | -       |
| 36  | CLA  | C     | 210 | 3     | -         | 6/17/93/115   | -       |
| 39  | LMT  | I     | 318 | -     | -         | 17/21/61/61   | 0/2/2/2 |
| 35  | A86  | R     | 303 | -     | -         | 7/34/90/90    | 0/3/3/3 |
| 35  | A86  | T     | 307 | -     | -         | 9/34/90/90    | 0/3/3/3 |
| 36  | CLA  | C     | 214 | -     | -         | 4/10/86/115   | -       |
| 36  | CLA  | a     | 825 | -     | 1/1/15/20 | 15/39/115/115 | -       |
| 36  | CLA  | a     | 839 | 46    | -         | 15/39/115/115 | -       |
| 36  | CLA  | E     | 317 | -     | -         | 7/17/93/115   | -       |
| 36  | CLA  | b     | 805 | 21,36 | -         | 18/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 36  | CLA  | G     | 313 | 7     | -         | 18/39/115/115 | -       |
| 38  | SQD  | b     | 804 | -     | -         | 23/41/61/69   | 0/1/1/1 |
| 36  | CLA  | I     | 309 | 9     | -         | 8/17/93/115   | -       |
| 36  | CLA  | V     | 314 | -     | 1/1/15/20 | 17/39/115/115 | -       |
| 34  | DD6  | E     | 304 | -     | -         | 4/26/80/80    | 0/3/3/3 |
| 36  | CLA  | M     | 311 | 13,35 | -         | 10/39/115/115 | -       |
| 39  | LMT  | E     | 323 | -     | -         | 11/21/61/61   | 0/2/2/2 |
| 36  | CLA  | a     | 834 | 20    | -         | 7/15/91/115   | -       |
| 36  | CLA  | X     | 315 | -     | -         | 3/10/86/115   | -       |
| 35  | A86  | L     | 301 | -     | -         | 5/34/90/90    | 1/3/3/3 |
| 36  | CLA  | K     | 307 | -     | 1/1/14/20 | 21/35/111/115 | -       |
| 36  | CLA  | b     | 802 | 20    | -         | 11/39/115/115 | -       |
| 36  | CLA  | L     | 320 | 12    | -         | 11/39/115/115 | -       |
| 36  | CLA  | a     | 823 | -     | 1/1/13/20 | 12/27/103/115 | -       |
| 36  | CLA  | J     | 310 | -     | -         | 11/39/115/115 | -       |
| 35  | A86  | V     | 304 | -     | -         | 9/34/90/90    | 0/3/3/3 |
| 36  | CLA  | H     | 309 | 8     | -         | 17/39/115/115 | -       |
| 36  | CLA  | H     | 312 | 8     | -         | 17/39/115/115 | -       |
| 36  | CLA  | F     | 311 | -     | -         | 10/24/100/115 | -       |
| 36  | CLA  | M     | 310 | 13,35 | -         | 7/17/93/115   | -       |
| 35  | A86  | T     | 301 | 36    | -         | 4/34/90/90    | 1/3/3/3 |
| 36  | CLA  | a     | 805 | 20    | -         | 18/39/115/115 | -       |
| 36  | CLA  | b     | 818 | 21    | -         | 4/27/103/115  | -       |
| 36  | CLA  | b     | 819 | -     | -         | 7/32/108/115  | -       |
| 36  | CLA  | a     | 824 | -     | -         | 11/39/115/115 | -       |
| 44  | BCR  | b     | 845 | -     | -         | 7/29/63/63    | 0/2/2/2 |
| 35  | A86  | C     | 202 | 3,36  | -         | 8/34/90/90    | 0/3/3/3 |
| 36  | CLA  | Q     | 312 | -     | -         | 5/10/86/115   | -       |
| 36  | CLA  | b     | 811 | 21    | -         | 12/39/115/115 | -       |
| 35  | A86  | G     | 305 | -     | -         | 4/34/90/90    | 0/3/3/3 |
| 35  | A86  | I     | 304 | -     | -         | 9/34/90/90    | 0/3/3/3 |
| 34  | DD6  | B     | 302 | -     | -         | 4/26/80/80    | 0/3/3/3 |
| 35  | A86  | N     | 303 | -     | -         | 4/34/90/90    | 0/3/3/3 |
| 35  | A86  | E     | 307 | 36    | -         | 3/34/90/90    | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 36  | CLA  | H     | 306 | -     | -         | 8/35/111/115  | -       |
| 36  | CLA  | b     | 808 | 21    | -         | 14/39/115/115 | -       |
| 35  | A86  | T     | 304 | -     | -         | 0/34/90/90    | 0/3/3/3 |
| 36  | CLA  | S     | 310 | 17    | -         | 16/39/115/115 | -       |
| 37  | KC1  | G     | 308 | -     | -         | 5/15/71/71    | -       |
| 36  | CLA  | I     | 308 | 9     | 1/1/15/20 | 19/39/115/115 | -       |
| 35  | A86  | P     | 303 | -     | -         | 9/34/90/90    | 0/3/3/3 |
| 36  | CLA  | D     | 307 | 41    | -         | 19/35/111/115 | -       |
| 36  | CLA  | l     | 204 | 28    | -         | 8/20/96/115   | -       |
| 36  | CLA  | W     | 209 | 19    | -         | 15/30/106/115 | -       |
| 36  | CLA  | I     | 311 | 9     | -         | 17/39/115/115 | -       |
| 36  | CLA  | U     | 308 | 35,32 | -         | 12/29/105/115 | -       |
| 35  | A86  | R     | 302 | 16    | -         | 6/34/90/90    | 0/3/3/3 |
| 34  | DD6  | G     | 303 | -     | -         | 4/26/80/80    | 0/3/3/3 |
| 36  | CLA  | D     | 312 | -     | -         | 13/39/115/115 | -       |
| 36  | CLA  | L     | 312 | 12    | -         | 8/17/93/115   | -       |
| 36  | CLA  | H     | 305 | 8     | -         | 8/19/95/115   | -       |
| 36  | CLA  | U     | 311 | 32    | -         | 21/39/115/115 | -       |
| 35  | A86  | H     | 304 | -     | -         | 8/34/90/90    | 0/3/3/3 |
| 36  | CLA  | a     | 817 | 20    | -         | 17/39/115/115 | -       |
| 36  | CLA  | R     | 316 | -     | -         | 8/17/93/115   | -       |
| 36  | CLA  | J     | 315 | 10    | -         | 2/10/86/115   | -       |
| 44  | BCR  | i     | 101 | -     | -         | 2/29/63/63    | 0/2/2/2 |
| 36  | CLA  | J     | 316 | 10    | -         | 8/17/93/115   | -       |
| 36  | CLA  | I     | 314 | -     | -         | 2/10/86/115   | -       |
| 34  | DD6  | S     | 307 | -     | -         | 6/26/80/80    | 0/3/3/3 |
| 35  | A86  | W     | 202 | 19,36 | -         | 8/34/90/90    | 0/3/3/3 |
| 36  | CLA  | a     | 830 | 20    | -         | 12/21/97/115  | -       |
| 35  | A86  | D     | 302 | -     | -         | 7/34/90/90    | 0/3/3/3 |
| 35  | A86  | L     | 304 | -     | -         | 6/34/90/90    | 0/3/3/3 |
| 36  | CLA  | j     | 101 | 1,27  | -         | 19/39/115/115 | -       |
| 41  | LHG  | a     | 843 | 36    | -         | 10/31/31/53   | -       |
| 41  | LHG  | a     | 842 | -     | -         | 24/52/52/53   | -       |
| 36  | CLA  | J     | 307 | 10    | -         | 11/35/111/115 | -       |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 37  | KC1  | B     | 310 | 2     | -         | 3/15/71/71    | -       |
| 36  | CLA  | V     | 307 | -     | -         | 7/23/99/115   | -       |
| 36  | CLA  | D     | 306 | 4     | -         | 6/15/91/115   | -       |
| 36  | CLA  | F     | 312 | -     | -         | 22/39/115/115 | -       |
| 36  | CLA  | B     | 305 | 2     | -         | 24/39/115/115 | -       |
| 35  | A86  | F     | 302 | -     | -         | 8/34/90/90    | 0/3/3/3 |
| 35  | A86  | O     | 301 | -     | -         | 4/34/90/90    | 0/3/3/3 |
| 36  | CLA  | D     | 313 | -     | -         | 8/39/115/115  | -       |
| 36  | CLA  | G     | 312 | 7     | -         | 6/31/107/115  | -       |
| 36  | CLA  | S     | 319 | 17    | -         | 8/39/115/115  | -       |
| 36  | CLA  | I     | 305 | -     | 1/1/14/20 | 10/35/111/115 | -       |
| 34  | DD6  | O     | 304 | -     | -         | 5/26/80/80    | 0/3/3/3 |
| 34  | DD6  | W     | 204 | 36    | -         | 7/26/80/80    | 0/3/3/3 |
| 36  | CLA  | N     | 311 | 14    | -         | 6/17/93/115   | -       |
| 36  | CLA  | a     | 803 | 36,20 | -         | 5/27/103/115  | -       |
| 44  | BCR  | i     | 103 | -     | -         | 11/29/63/63   | 0/2/2/2 |
| 35  | A86  | K     | 301 | -     | -         | 6/34/90/90    | 1/3/3/3 |
| 35  | A86  | G     | 306 | -     | -         | 6/34/90/90    | 1/3/3/3 |
| 42  | LMG  | j     | 105 | -     | -         | 31/47/67/70   | 0/1/1/1 |
| 36  | CLA  | a     | 807 | 20    | -         | 13/39/115/115 | -       |
| 37  | KC1  | W     | 217 | -     | -         | 4/15/71/71    | -       |
| 44  | BCR  | a     | 845 | -     | -         | 9/29/63/63    | 0/2/2/2 |
| 39  | LMT  | P     | 321 | -     | -         | 10/14/34/61   | 0/1/1/2 |
| 36  | CLA  | a     | 811 | 20    | -         | 6/26/102/115  | -       |
| 36  | CLA  | N     | 310 | 14    | -         | 1/10/86/115   | -       |
| 34  | DD6  | P     | 305 | -     | -         | 2/26/80/80    | 0/3/3/3 |
| 36  | CLA  | H     | 318 | -     | -         | 10/21/97/115  | -       |
| 36  | CLA  | a     | 813 | 20    | -         | 2/15/91/115   | -       |
| 36  | CLA  | D     | 309 | 4     | 1/1/13/20 | 8/27/103/115  | -       |
| 36  | CLA  | b     | 801 | 46    | -         | 8/39/115/115  | -       |
| 37  | KC1  | U     | 312 | 35,32 | -         | 4/15/71/71    | -       |
| 36  | CLA  | j     | 106 | 27    | -         | 8/12/88/115   | -       |
| 41  | LHG  | G     | 301 | -     | -         | 24/53/53/53   | -       |
| 36  | CLA  | j     | 102 | -     | 1/1/15/20 | 13/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 36  | CLA  | b     | 822 | 21    | -         | 7/17/93/115   | -       |
| 36  | CLA  | U     | 307 | -     | -         | 3/21/97/115   | -       |
| 41  | LHG  | a     | 850 | -     | -         | 36/51/51/53   | -       |
| 36  | CLA  | T     | 314 | -     | -         | 15/39/115/115 | -       |
| 39  | LMT  | L     | 303 | -     | -         | 10/21/61/61   | 0/2/2/2 |
| 36  | CLA  | G     | 311 | -     | -         | 17/39/115/115 | -       |
| 40  | DGD  | C     | 215 | -     | -         | 31/46/86/95   | 0/2/2/2 |
| 41  | LHG  | Q     | 315 | 36    | -         | 33/53/53/53   | -       |
| 34  | DD6  | j     | 103 | -     | -         | 9/26/80/80    | 0/3/3/3 |
| 36  | CLA  | R     | 318 | 35    | -         | 4/10/86/115   | -       |
| 36  | CLA  | b     | 812 | 21    | -         | 6/39/115/115  | -       |
| 37  | KC1  | L     | 315 | 12,35 | -         | 6/15/71/71    | -       |
| 35  | A86  | X     | 303 | 36    | -         | 9/34/90/90    | 0/3/3/3 |
| 36  | CLA  | Q     | 310 | 15    | -         | 22/39/115/115 | -       |
| 36  | CLA  | I     | 307 | 9     | -         | 4/26/102/115  | -       |
| 36  | CLA  | O     | 311 | -     | -         | 9/31/107/115  | -       |
| 36  | CLA  | S     | 313 | -     | -         | 8/17/93/115   | -       |
| 36  | CLA  | b     | 829 | 21    | -         | 11/39/115/115 | -       |
| 37  | KC1  | O     | 313 | 15    | -         | 2/15/71/71    | -       |
| 39  | LMT  | a     | 853 | -     | -         | 10/18/58/61   | 0/2/2/2 |
| 35  | A86  | P     | 304 | -     | -         | 6/34/90/90    | 0/3/3/3 |
| 36  | CLA  | L     | 308 | -     | 1/1/14/20 | 22/35/111/115 | -       |
| 36  | CLA  | b     | 823 | 21    | -         | 4/27/103/115  | -       |
| 42  | LMG  | E     | 319 | -     | -         | 23/35/55/70   | 0/1/1/1 |
| 36  | CLA  | a     | 810 | 36,20 | -         | 17/36/112/115 | -       |
| 34  | DD6  | D     | 305 | -     | -         | 3/26/80/80    | 0/3/3/3 |
| 41  | LHG  | D     | 318 | 36    | -         | 30/50/50/53   | -       |
| 37  | KC1  | C     | 213 | 3     | -         | 6/15/71/71    | -       |
| 34  | DD6  | H     | 302 | -     | -         | 2/26/80/80    | 0/3/3/3 |
| 34  | DD6  | F     | 303 | -     | -         | 8/26/80/80    | 0/3/3/3 |
| 36  | CLA  | A     | 314 | 1     | -         | 22/39/115/115 | -       |
| 37  | KC1  | F     | 308 | 6     | -         | 7/15/71/71    | -       |
| 34  | DD6  | J     | 304 | -     | -         | 5/26/80/80    | 0/3/3/3 |
| 36  | CLA  | b     | 817 | 21    | 1/1/13/20 | 9/32/108/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 36  | CLA  | E     | 314 | -    | -         | 8/39/115/115  | -       |
| 36  | CLA  | N     | 307 | -    | -         | 9/35/111/115  | -       |
| 36  | CLA  | L     | 314 | 12   | -         | 19/39/115/115 | -       |
| 36  | CLA  | a     | 809 | -    | -         | 11/29/105/115 | -       |
| 39  | LMT  | F     | 321 | -    | -         | 11/19/59/61   | 0/2/2/2 |
| 39  | LMT  | U     | 314 | -    | -         | 14/21/61/61   | 0/2/2/2 |
| 36  | CLA  | f     | 802 | 21   | -         | 16/39/115/115 | -       |
| 41  | LHG  | O     | 318 | 15   | -         | 30/53/53/53   | -       |
| 36  | CLA  | F     | 310 | 6    | -         | 10/29/105/115 | -       |
| 36  | CLA  | I     | 313 | -    | -         | 5/10/86/115   | -       |
| 36  | CLA  | a     | 821 | 20   | -         | 4/20/96/115   | -       |
| 39  | LMT  | E     | 320 | -    | -         | 13/21/61/61   | 0/2/2/2 |
| 36  | CLA  | a     | 814 | 20   | -         | 4/21/97/115   | -       |
| 36  | CLA  | L     | 316 | -    | -         | 3/10/86/115   | -       |
| 35  | A86  | F     | 307 | -    | -         | 6/34/90/90    | 0/3/3/3 |
| 36  | CLA  | b     | 832 | 21   | -         | 4/20/96/115   | -       |
| 36  | CLA  | B     | 308 | 2    | -         | 14/39/115/115 | -       |
| 37  | KC1  | J     | 314 | -    | -         | 4/15/71/71    | -       |
| 36  | CLA  | b     | 837 | 21   | -         | 8/39/115/115  | -       |
| 36  | CLA  | D     | 315 | -    | -         | 2/10/86/115   | -       |
| 39  | LMT  | G     | 323 | -    | -         | 16/21/61/61   | 0/2/2/2 |
| 36  | CLA  | K     | 309 | 11   | -         | 14/32/108/115 | -       |
| 36  | CLA  | a     | 806 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 37  | KC1  | T     | 315 | -    | -         | 7/15/71/71    | -       |
| 35  | A86  | T     | 305 | 18   | -         | 7/34/90/90    | 0/3/3/3 |
| 36  | CLA  | b     | 807 | 21   | -         | 3/15/91/115   | -       |
| 41  | LHG  | l     | 208 | -    | -         | 34/52/52/53   | -       |
| 34  | DD6  | I     | 303 | -    | -         | 4/26/80/80    | 0/3/3/3 |
| 35  | A86  | O     | 302 | -    | -         | 9/34/90/90    | 0/3/3/3 |
| 36  | CLA  | a     | 837 | 20   | -         | 10/39/115/115 | -       |
| 36  | CLA  | C     | 208 | 3    | -         | 19/39/115/115 | -       |
| 41  | LHG  | G     | 321 | 36   | -         | 27/51/51/53   | -       |
| 36  | CLA  | A     | 310 | -    | -         | 11/39/115/115 | -       |
| 36  | CLA  | b     | 828 | 21   | -         | 14/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 45  | SF4  | c     | 101 | 22    | -         | -             | 0/6/5/5 |
| 42  | LMG  | L     | 321 | 40    | -         | 15/28/48/70   | 0/1/1/1 |
| 36  | CLA  | l     | 201 | -     | -         | 16/39/115/115 | -       |
| 35  | A86  | h     | 204 | -     | -         | 1/34/90/90    | 0/3/3/3 |
| 36  | CLA  | a     | 829 | 20    | -         | 13/39/115/115 | -       |
| 36  | CLA  | h     | 203 | 31    | -         | 20/39/115/115 | -       |
| 36  | CLA  | O     | 308 | 15    | -         | 15/39/115/115 | -       |
| 36  | CLA  | a     | 808 | 20    | -         | 11/39/115/115 | -       |
| 41  | LHG  | I     | 316 | -     | -         | 30/53/53/53   | -       |
| 36  | CLA  | W     | 208 | -     | -         | 7/15/91/115   | -       |
| 36  | CLA  | S     | 309 | -     | -         | 10/35/111/115 | -       |
| 44  | BCR  | a     | 844 | -     | -         | 6/29/63/63    | 0/2/2/2 |
| 36  | CLA  | S     | 312 | 17    | -         | 17/39/115/115 | -       |
| 39  | LMT  | K     | 318 | -     | -         | 12/21/61/61   | 0/2/2/2 |
| 36  | CLA  | Q     | 305 | -     | -         | 11/35/111/115 | -       |
| 35  | A86  | S     | 301 | -     | -         | 8/34/90/90    | 0/3/3/3 |
| 36  | CLA  | a     | 801 | 20    | -         | 12/39/115/115 | -       |
| 35  | A86  | N     | 305 | -     | -         | 2/34/90/90    | 0/3/3/3 |
| 36  | CLA  | f     | 803 | -     | 1/1/15/20 | 13/39/115/115 | -       |
| 36  | CLA  | K     | 311 | 11    | -         | 8/17/93/115   | -       |
| 36  | CLA  | a     | 804 | 20    | -         | 18/39/115/115 | -       |
| 37  | KC1  | M     | 313 | 13,36 | -         | 5/15/71/71    | -       |
| 36  | CLA  | L     | 309 | 12    | -         | 12/39/115/115 | -       |
| 36  | CLA  | O     | 307 | -     | -         | 14/39/115/115 | -       |
| 35  | A86  | S     | 302 | -     | -         | 6/34/90/90    | 0/3/3/3 |
| 35  | A86  | E     | 305 | 5     | -         | 5/34/90/90    | 0/3/3/3 |
| 36  | CLA  | A     | 306 | -     | 1/1/14/20 | 19/35/111/115 | -       |
| 35  | A86  | K     | 302 | -     | -         | 8/34/90/90    | 0/3/3/3 |
| 36  | CLA  | O     | 312 | -     | -         | 6/10/82/115   | -       |
| 37  | KC1  | P     | 317 | 15    | -         | 4/15/71/71    | -       |
| 35  | A86  | C     | 204 | -     | -         | 12/34/90/90   | 0/3/3/3 |
| 36  | CLA  | b     | 810 | 21    | -         | 10/39/115/115 | -       |
| 36  | CLA  | K     | 312 | -     | -         | 7/39/115/115  | -       |
| 36  | CLA  | J     | 309 | 10    | -         | 10/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 37  | KC1  | T     | 310 | 18   | -       | 11/15/71/71   | -       |
| 36  | CLA  | S     | 311 | 35   | -       | 4/17/93/115   | -       |
| 35  | A86  | J     | 301 | -    | -       | 11/34/90/90   | 0/3/3/3 |
| 36  | CLA  | N     | 313 | 14   | -       | 2/10/86/115   | -       |
| 44  | BCR  | b     | 843 | -    | -       | 9/29/63/63    | 0/2/2/2 |
| 36  | CLA  | H     | 315 | 8    | -       | 15/39/115/115 | -       |
| 35  | A86  | S     | 303 | 17   | -       | 4/34/90/90    | 0/3/3/3 |
| 44  | BCR  | m     | 101 | -    | -       | 9/29/63/63    | 0/2/2/2 |
| 36  | CLA  | R     | 314 | 16   | -       | 11/17/93/115  | -       |
| 36  | CLA  | D     | 317 | -    | -       | 12/31/107/115 | -       |
| 36  | CLA  | T     | 308 | 18   | -       | 10/35/111/115 | -       |
| 36  | CLA  | H     | 316 | -    | -       | 18/39/115/115 | -       |
| 35  | A86  | L     | 307 | -    | -       | 8/34/90/90    | 1/3/3/3 |
| 36  | CLA  | b     | 813 | 21   | -       | 3/25/101/115  | -       |
| 41  | LHG  | f     | 809 | -    | -       | 28/46/46/53   | -       |
| 39  | LMT  | F     | 320 | -    | -       | 12/21/61/61   | 0/2/2/2 |
| 37  | KC1  | G     | 317 | -    | -       | 6/15/71/71    | -       |
| 39  | LMT  | B     | 312 | -    | -       | 14/21/61/61   | 0/2/2/2 |
| 36  | CLA  | B     | 307 | -    | -       | 7/17/93/115   | -       |
| 35  | A86  | R     | 309 | -    | -       | 8/34/90/90    | 0/3/3/3 |
| 37  | KC1  | K     | 314 | 11   | -       | 5/15/71/71    | -       |
| 36  | CLA  | H     | 308 | 8    | -       | 15/37/113/115 | -       |
| 37  | KC1  | X     | 311 | -    | -       | 3/15/71/71    | -       |
| 41  | LHG  | i     | 104 | -    | -       | 29/50/50/53   | -       |
| 35  | A86  | R     | 301 | -    | -       | 9/34/90/90    | 0/3/3/3 |
| 36  | CLA  | J     | 317 | 10   | -       | 5/18/94/115   | -       |
| 36  | CLA  | l     | 206 | 46   | -       | 6/21/97/115   | -       |
| 36  | CLA  | W     | 206 | 19   | -       | 10/35/111/115 | -       |
| 42  | LMG  | G     | 324 | -    | -       | 31/50/70/70   | 0/1/1/1 |
| 36  | CLA  | a     | 836 | -    | -       | 11/39/115/115 | -       |
| 36  | CLA  | V     | 311 | 33   | -       | 13/39/115/115 | -       |
| 36  | CLA  | P     | 313 | -    | -       | 12/39/115/115 | -       |
| 36  | CLA  | a     | 831 | -    | -       | 16/39/115/115 | -       |
| 36  | CLA  | D     | 308 | -    | -       | 16/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 36  | CLA  | a     | 833 | 20    | -         | 4/21/97/115   | -       |
| 38  | SQD  | A     | 315 | -     | -         | 11/22/42/69   | 0/1/1/1 |
| 36  | CLA  | W     | 215 | -     | -         | 6/19/95/115   | -       |
| 44  | BCR  | b     | 844 | -     | -         | 6/29/63/63    | 0/2/2/2 |
| 36  | CLA  | U     | 306 | 32    | 1/1/15/20 | 20/39/115/115 | -       |
| 36  | CLA  | M     | 307 | -     | -         | 12/39/115/115 | -       |
| 34  | DD6  | A     | 301 | -     | -         | 7/26/80/80    | 0/3/3/3 |
| 40  | DGD  | b     | 849 | -     | -         | 21/49/89/95   | 0/2/2/2 |
| 36  | CLA  | R     | 321 | 16    | -         | 9/39/115/115  | -       |
| 35  | A86  | J     | 302 | -     | -         | 5/34/90/90    | 1/3/3/3 |
| 36  | CLA  | P     | 314 | -     | -         | 23/33/109/115 | -       |
| 35  | A86  | M     | 302 | -     | -         | 7/34/90/90    | 0/3/3/3 |
| 36  | CLA  | G     | 315 | 7     | 1/1/13/20 | 11/29/105/115 | -       |
| 36  | CLA  | K     | 313 | -     | -         | 13/39/115/115 | -       |
| 36  | CLA  | P     | 311 | -     | -         | 19/39/115/115 | -       |
| 36  | CLA  | M     | 306 | 37,13 | -         | 10/27/103/115 | -       |
| 36  | CLA  | b     | 821 | 46    | -         | 13/39/115/115 | -       |
| 37  | KC1  | Q     | 313 | -     | -         | 2/15/71/71    | -       |
| 36  | CLA  | V     | 305 | 35    | -         | 13/35/111/115 | -       |
| 36  | CLA  | U     | 309 | 32    | -         | 6/17/93/115   | -       |
| 36  | CLA  | D     | 316 | -     | -         | 11/24/100/115 | -       |
| 34  | DD6  | B     | 304 | -     | -         | 2/26/80/80    | 0/3/3/3 |
| 35  | A86  | U     | 303 | 36    | -         | 17/34/90/90   | 0/3/3/3 |
| 36  | CLA  | N     | 309 | 14    | -         | 8/23/99/115   | -       |
| 35  | A86  | A     | 316 | -     | -         | 9/34/90/90    | 0/3/3/3 |
| 36  | CLA  | Q     | 314 | -     | -         | 22/39/115/115 | -       |
| 42  | LMG  | J     | 319 | -     | -         | 23/39/59/70   | 0/1/1/1 |
| 35  | A86  | J     | 303 | -     | -         | 7/34/90/90    | 0/3/3/3 |
| 35  | A86  | N     | 301 | -     | -         | 8/34/90/90    | 0/3/3/3 |
| 36  | CLA  | a     | 818 | 20    | -         | 14/39/115/115 | -       |
| 37  | KC1  | V     | 312 | 33    | -         | 7/15/71/71    | -       |
| 36  | CLA  | S     | 320 | -     | -         | 18/39/115/115 | -       |
| 34  | DD6  | A     | 304 | -     | -         | 4/26/80/80    | 0/3/3/3 |
| 36  | CLA  | T     | 309 | 18    | -         | 20/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 41  | LHG  | F     | 319 | -    | -         | 33/45/45/53   | -       |
| 36  | CLA  | b     | 836 | 21   | 1/1/13/20 | 9/31/107/115  | -       |
| 36  | CLA  | X     | 312 | -    | -         | 3/10/86/115   | -       |
| 34  | DD6  | K     | 304 | -    | -         | 2/26/80/80    | 0/3/3/3 |
| 34  | DD6  | A     | 303 | -    | -         | 5/26/80/80    | 0/3/3/3 |
| 45  | SF4  | c     | 102 | -    | -         | -             | 0/6/5/5 |
| 34  | DD6  | S     | 306 | -    | -         | 5/26/80/80    | 0/3/3/3 |
| 34  | DD6  | R     | 307 | -    | -         | 11/26/80/80   | 0/3/3/3 |
| 36  | CLA  | A     | 313 | -    | -         | 4/10/86/115   | -       |
| 44  | BCR  | f     | 801 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 35  | A86  | K     | 306 | 11   | -         | 8/34/90/90    | 0/3/3/3 |
| 42  | LMG  | E     | 318 | -    | -         | 24/41/61/70   | 0/1/1/1 |
| 36  | CLA  | C     | 212 | 35   | -         | 25/39/115/115 | -       |
| 36  | CLA  | R     | 310 | -    | -         | 18/35/111/115 | -       |
| 37  | KC1  | G     | 318 | -    | -         | 5/15/71/71    | -       |
| 39  | LMT  | f     | 807 | -    | -         | 7/15/35/61    | 0/1/1/2 |
| 35  | A86  | F     | 301 | -    | -         | 4/34/90/90    | 0/3/3/3 |
| 44  | BCR  | b     | 847 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 36  | CLA  | F     | 316 | 6    | -         | 3/10/86/115   | -       |
| 37  | KC1  | A     | 312 | 1    | -         | 2/15/71/71    | -       |
| 36  | CLA  | N     | 308 | 14   | -         | 17/39/115/115 | -       |
| 34  | DD6  | C     | 201 | -    | -         | 7/26/80/80    | 0/3/3/3 |
| 35  | A86  | X     | 302 | 35   | -         | 6/34/90/90    | 0/3/3/3 |
| 36  | CLA  | G     | 316 | -    | -         | 10/20/96/115  | -       |
| 35  | A86  | P     | 307 | -    | -         | 2/34/90/90    | 0/3/3/3 |
| 44  | BCR  | f     | 806 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 35  | A86  | G     | 304 | -    | -         | 8/34/90/90    | 0/3/3/3 |
| 41  | LHG  | D     | 319 | 42   | -         | 30/53/53/53   | -       |
| 36  | CLA  | a     | 838 | 20   | -         | 8/39/115/115  | -       |
| 36  | CLA  | C     | 209 | -    | -         | 12/39/115/115 | -       |
| 41  | LHG  | G     | 320 | -    | -         | 18/44/44/53   | -       |
| 37  | KC1  | S     | 316 | -    | -         | 6/15/71/71    | -       |
| 35  | A86  | B     | 301 | -    | -         | 10/34/90/90   | 0/3/3/3 |
| 39  | LMT  | L     | 318 | -    | -         | 13/17/57/61   | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 36  | CLA  | a     | 841 | 41    | -         | 7/24/100/115  | -       |
| 35  | A86  | N     | 302 | -     | -         | 6/34/90/90    | 0/3/3/3 |
| 36  | CLA  | F     | 313 | -     | -         | 8/24/100/115  | -       |
| 36  | CLA  | F     | 309 | -     | -         | 13/39/115/115 | -       |
| 36  | CLA  | C     | 206 | -     | -         | 17/35/111/115 | -       |
| 36  | CLA  | E     | 310 | -     | -         | 7/39/115/115  | -       |
| 36  | CLA  | D     | 310 | -     | -         | 9/39/115/115  | -       |
| 36  | CLA  | P     | 319 | -     | -         | 16/33/109/115 | -       |
| 36  | CLA  | R     | 313 | -     | -         | 15/39/115/115 | -       |
| 36  | CLA  | b     | 809 | 21    | -         | 18/39/115/115 | -       |
| 36  | CLA  | b     | 827 | -     | -         | 10/39/115/115 | -       |
| 36  | CLA  | O     | 316 | -     | 1/1/15/20 | 28/39/115/115 | -       |
| 35  | A86  | F     | 305 | -     | -         | 8/34/90/90    | 0/3/3/3 |
| 36  | CLA  | J     | 313 | -     | -         | 15/39/115/115 | -       |
| 35  | A86  | M     | 301 | -     | -         | 8/34/90/90    | 0/3/3/3 |
| 35  | A86  | K     | 303 | -     | -         | 5/34/90/90    | 0/3/3/3 |
| 36  | CLA  | C     | 205 | -     | -         | 4/13/89/115   | -       |
| 36  | CLA  | b     | 814 | 21    | -         | 5/27/103/115  | -       |
| 36  | CLA  | L     | 310 | -     | -         | 4/26/102/115  | -       |
| 36  | CLA  | A     | 309 | 1     | -         | 9/17/93/115   | -       |
| 36  | CLA  | A     | 311 | -     | -         | 20/39/115/115 | -       |
| 41  | LHG  | R     | 323 | -     | -         | 29/53/53/53   | -       |
| 35  | A86  | Q     | 316 | 15,36 | -         | 2/34/90/90    | 0/3/3/3 |
| 36  | CLA  | N     | 312 | -     | -         | 9/18/94/115   | -       |
| 36  | CLA  | S     | 318 | -     | -         | 9/12/88/115   | -       |
| 35  | A86  | R     | 305 | -     | -         | 5/34/90/90    | 0/3/3/3 |
| 36  | CLA  | Q     | 306 | -     | -         | 14/39/115/115 | -       |
| 36  | CLA  | R     | 320 | 16    | -         | 5/15/91/115   | -       |
| 36  | CLA  | a     | 822 | -     | -         | 4/23/99/115   | -       |
| 35  | A86  | T     | 303 | -     | -         | 6/34/90/90    | 0/3/3/3 |
| 36  | CLA  | B     | 309 | 2     | -         | 6/24/100/115  | -       |
| 35  | A86  | S     | 305 | -     | -         | 9/34/90/90    | 0/3/3/3 |
| 36  | CLA  | H     | 314 | -     | -         | 3/10/86/115   | -       |
| 39  | LMT  | a     | 851 | -     | -         | 15/21/61/61   | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 36  | CLA  | I     | 202 | 21,28 | -         | 13/39/115/115 | -       |
| 39  | LMT  | K     | 317 | -     | -         | 14/17/57/61   | 0/2/2/2 |
| 39  | LMT  | I     | 317 | -     | -         | 13/21/61/61   | 0/2/2/2 |
| 36  | CLA  | S     | 315 | 17    | -         | 5/13/89/115   | -       |
| 36  | CLA  | X     | 310 | 19    | -         | 4/10/86/115   | -       |
| 37  | KC1  | O     | 315 | 15    | -         | 2/15/71/71    | -       |
| 36  | CLA  | a     | 832 | -     | -         | 16/39/115/115 | -       |
| 35  | A86  | B     | 303 | -     | -         | 13/34/90/90   | 0/3/3/3 |
| 35  | A86  | J     | 306 | -     | -         | 10/34/90/90   | 0/3/3/3 |
| 36  | CLA  | Q     | 307 | 15    | -         | 6/21/97/115   | -       |
| 36  | CLA  | O     | 314 | -     | -         | 5/10/86/115   | -       |
| 39  | LMT  | B     | 313 | -     | -         | 16/21/61/61   | 0/2/2/2 |
| 36  | CLA  | C     | 207 | -     | 1/1/15/20 | 16/39/115/115 | -       |
| 37  | KC1  | W     | 213 | -     | -         | 5/15/71/71    | -       |
| 36  | CLA  | A     | 305 | 1     | -         | 6/20/96/115   | -       |
| 34  | DD6  | D     | 301 | -     | -         | 11/26/80/80   | 0/3/3/3 |
| 36  | CLA  | U     | 310 | -     | -         | 19/39/115/115 | -       |
| 36  | CLA  | I     | 205 | -     | 1/1/15/20 | 14/39/115/115 | -       |
| 36  | CLA  | A     | 307 | -     | -         | 10/33/109/115 | -       |
| 36  | CLA  | K     | 308 | -     | -         | 11/39/115/115 | -       |
| 40  | DGD  | L     | 302 | 42    | -         | 21/36/76/95   | 0/2/2/2 |
| 36  | CLA  | W     | 201 | 19    | -         | 4/19/95/115   | -       |
| 34  | DD6  | E     | 301 | -     | -         | 4/26/80/80    | 0/3/3/3 |
| 36  | CLA  | A     | 308 | -     | -         | 13/39/115/115 | -       |
| 36  | CLA  | R     | 312 | 16    | -         | 14/39/115/115 | -       |
| 36  | CLA  | f     | 805 | 25    | -         | 9/24/100/115  | -       |
| 34  | DD6  | M     | 303 | -     | -         | 3/26/80/80    | 0/3/3/3 |
| 36  | CLA  | b     | 806 | -     | -         | 14/39/115/115 | -       |
| 35  | A86  | A     | 302 | -     | -         | 9/34/90/90    | 0/3/3/3 |
| 36  | CLA  | W     | 216 | 19,35 | -         | 5/15/91/115   | -       |
| 35  | A86  | R     | 306 | -     | -         | 8/34/90/90    | 0/3/3/3 |

The worst 5 of 4701 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 37  | M     | 318 | KC1  | C4C-NC  | 17.10 | 1.63        | 1.37     |
| 36  | Q     | 310 | CLA  | CAA-C2A | 15.78 | 1.83        | 1.54     |
| 37  | M     | 318 | KC1  | C1A-NA  | 15.77 | 1.68        | 1.38     |
| 37  | T     | 310 | KC1  | C1A-NA  | 14.39 | 1.66        | 1.38     |
| 37  | T     | 310 | KC1  | C4C-NC  | 13.45 | 1.57        | 1.37     |

The worst 5 of 7313 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 35  | N     | 304 | A86  | O1-C20-C21  | -47.08 | 58.64       | 115.06   |
| 36  | Q     | 314 | CLA  | C4-C3-C5    | -24.40 | 74.22       | 115.27   |
| 37  | M     | 318 | KC1  | C1D-ND-C4D  | -22.78 | 90.15       | 106.33   |
| 42  | V     | 315 | LMG  | O7-C10-C11  | 22.29  | 159.53      | 111.50   |
| 35  | A     | 302 | A86  | C33-C32-C31 | -21.39 | 88.43       | 109.21   |

5 of 29 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 36  | A     | 306 | CLA  | C8   |
| 36  | C     | 207 | CLA  | C8   |
| 36  | D     | 309 | CLA  | C8   |
| 36  | E     | 313 | CLA  | C8   |
| 36  | E     | 315 | CLA  | C8   |

5 of 6194 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | A     | 301 | DD6  | C10-C11-C13-C14 |
| 34  | A     | 301 | DD6  | C12-C11-C13-C14 |
| 34  | A     | 301 | DD6  | C13-C14-C15-C20 |
| 34  | A     | 301 | DD6  | C13-C14-C15-O1  |
| 34  | A     | 303 | DD6  | C10-C11-C13-C14 |

5 of 11 ring outliers are listed below:

| Mol | Chain | Res | Type | Atoms                   |
|-----|-------|-----|------|-------------------------|
| 35  | V     | 301 | A86  | C31-C32-C33-C34-C35-C36 |
| 35  | J     | 302 | A86  | C31-C32-C33-C34-C35-C36 |
| 35  | K     | 301 | A86  | C31-C32-C33-C34-C35-C36 |
| 35  | G     | 306 | A86  | C31-C32-C33-C34-C35-C36 |
| 35  | T     | 301 | A86  | C31-C32-C33-C34-C35-C36 |

498 monomers are involved in 2732 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 36  | a     | 819 | CLA  | 10      | 0            |
| 36  | H     | 307 | CLA  | 10      | 0            |
| 36  | a     | 828 | CLA  | 1       | 0            |
| 36  | b     | 838 | CLA  | 1       | 0            |
| 36  | U     | 313 | CLA  | 1       | 0            |
| 36  | M     | 309 | CLA  | 8       | 0            |
| 44  | j     | 107 | BCR  | 1       | 0            |
| 36  | R     | 311 | CLA  | 1       | 0            |
| 36  | X     | 309 | CLA  | 2       | 0            |
| 36  | X     | 307 | CLA  | 3       | 0            |
| 35  | R     | 304 | A86  | 2       | 0            |
| 36  | b     | 840 | CLA  | 3       | 0            |
| 36  | T     | 313 | CLA  | 13      | 0            |
| 35  | X     | 305 | A86  | 2       | 0            |
| 36  | W     | 211 | CLA  | 1       | 0            |
| 36  | a     | 827 | CLA  | 2       | 0            |
| 42  | V     | 315 | LMG  | 14      | 0            |
| 35  | N     | 306 | A86  | 1       | 0            |
| 39  | b     | 848 | LMT  | 5       | 0            |
| 36  | F     | 314 | CLA  | 6       | 0            |
| 42  | J     | 318 | LMG  | 24      | 0            |
| 36  | W     | 212 | CLA  | 23      | 0            |
| 35  | V     | 303 | A86  | 13      | 0            |
| 36  | C     | 211 | CLA  | 1       | 0            |
| 36  | b     | 820 | CLA  | 6       | 0            |
| 36  | T     | 311 | CLA  | 4       | 0            |
| 36  | a     | 816 | CLA  | 30      | 0            |
| 37  | P     | 315 | KC1  | 2       | 0            |
| 35  | T     | 306 | A86  | 1       | 0            |
| 36  | N     | 315 | CLA  | 1       | 0            |
| 36  | b     | 826 | CLA  | 1       | 0            |
| 36  | W     | 207 | CLA  | 8       | 0            |
| 35  | G     | 302 | A86  | 2       | 0            |
| 36  | P     | 308 | CLA  | 1       | 0            |
| 35  | O     | 305 | A86  | 13      | 0            |
| 36  | N     | 319 | CLA  | 14      | 0            |
| 36  | M     | 312 | CLA  | 3       | 0            |
| 39  | a     | 854 | LMT  | 5       | 0            |
| 42  | V     | 316 | LMG  | 28      | 0            |
| 39  | b     | 851 | LMT  | 20      | 0            |
| 35  | W     | 203 | A86  | 1       | 0            |
| 36  | P     | 309 | CLA  | 2       | 0            |
| 36  | b     | 831 | CLA  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 36  | V     | 308 | CLA  | 12      | 0            |
| 34  | R     | 308 | DD6  | 5       | 0            |
| 35  | Q     | 304 | A86  | 1       | 0            |
| 36  | b     | 841 | CLA  | 7       | 0            |
| 44  | a     | 846 | BCR  | 2       | 0            |
| 36  | I     | 312 | CLA  | 16      | 0            |
| 35  | U     | 301 | A86  | 1       | 0            |
| 35  | I     | 302 | A86  | 17      | 0            |
| 36  | b     | 824 | CLA  | 4       | 0            |
| 36  | a     | 802 | CLA  | 4       | 0            |
| 36  | V     | 310 | CLA  | 15      | 0            |
| 36  | N     | 316 | CLA  | 6       | 0            |
| 35  | h     | 202 | A86  | 5       | 0            |
| 41  | F     | 318 | LHG  | 1       | 0            |
| 36  | P     | 310 | CLA  | 2       | 0            |
| 35  | Q     | 303 | A86  | 14      | 0            |
| 35  | N     | 304 | A86  | 14      | 0            |
| 42  | D     | 321 | LMG  | 5       | 0            |
| 36  | f     | 804 | CLA  | 12      | 0            |
| 39  | U     | 315 | LMT  | 17      | 0            |
| 36  | J     | 312 | CLA  | 5       | 0            |
| 36  | W     | 218 | CLA  | 4       | 0            |
| 39  | h     | 205 | LMT  | 21      | 0            |
| 36  | K     | 315 | CLA  | 2       | 0            |
| 36  | a     | 812 | CLA  | 1       | 0            |
| 43  | b     | 842 | PQN  | 3       | 0            |
| 42  | m     | 102 | LMG  | 9       | 0            |
| 36  | E     | 311 | CLA  | 6       | 0            |
| 36  | D     | 311 | CLA  | 5       | 0            |
| 36  | L     | 311 | CLA  | 2       | 0            |
| 36  | P     | 301 | CLA  | 9       | 0            |
| 41  | j     | 104 | LHG  | 14      | 0            |
| 34  | H     | 303 | DD6  | 5       | 0            |
| 44  | b     | 846 | BCR  | 4       | 0            |
| 36  | V     | 306 | CLA  | 22      | 0            |
| 36  | Q     | 308 | CLA  | 7       | 0            |
| 43  | a     | 840 | PQN  | 3       | 0            |
| 36  | H     | 310 | CLA  | 9       | 0            |
| 41  | b     | 850 | LHG  | 18      | 0            |
| 36  | b     | 815 | CLA  | 2       | 0            |
| 36  | T     | 312 | CLA  | 1       | 0            |
| 44  | a     | 847 | BCR  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 36  | G     | 314 | CLA  | 1       | 0            |
| 36  | P     | 302 | CLA  | 6       | 0            |
| 34  | D     | 304 | DD6  | 2       | 0            |
| 34  | E     | 303 | DD6  | 4       | 0            |
| 35  | P     | 306 | A86  | 4       | 0            |
| 36  | J     | 311 | CLA  | 3       | 0            |
| 42  | h     | 206 | LMG  | 7       | 0            |
| 41  | O     | 317 | LHG  | 8       | 0            |
| 36  | I     | 306 | CLA  | 14      | 0            |
| 36  | E     | 315 | CLA  | 29      | 0            |
| 37  | F     | 315 | KC1  | 5       | 0            |
| 44  | h     | 201 | BCR  | 4       | 0            |
| 35  | U     | 304 | A86  | 15      | 0            |
| 36  | K     | 316 | CLA  | 3       | 0            |
| 41  | f     | 808 | LHG  | 23      | 0            |
| 36  | E     | 308 | CLA  | 3       | 0            |
| 36  | b     | 816 | CLA  | 9       | 0            |
| 45  | b     | 803 | SF4  | 1       | 0            |
| 35  | J     | 305 | A86  | 6       | 0            |
| 36  | T     | 316 | CLA  | 1       | 0            |
| 36  | b     | 839 | CLA  | 1       | 0            |
| 39  | E     | 321 | LMT  | 8       | 0            |
| 36  | E     | 312 | CLA  | 1       | 0            |
| 37  | Q     | 311 | KC1  | 8       | 0            |
| 34  | L     | 305 | DD6  | 25      | 0            |
| 36  | b     | 830 | CLA  | 1       | 0            |
| 44  | l     | 207 | BCR  | 4       | 0            |
| 35  | C     | 203 | A86  | 12      | 0            |
| 35  | S     | 308 | A86  | 5       | 0            |
| 36  | a     | 815 | CLA  | 3       | 0            |
| 36  | X     | 308 | CLA  | 4       | 0            |
| 36  | M     | 315 | CLA  | 2       | 0            |
| 36  | J     | 308 | CLA  | 8       | 0            |
| 34  | Q     | 302 | DD6  | 19      | 0            |
| 37  | L     | 317 | KC1  | 2       | 0            |
| 36  | O     | 309 | CLA  | 8       | 0            |
| 36  | i     | 102 | CLA  | 3       | 0            |
| 36  | G     | 307 | CLA  | 12      | 0            |
| 36  | b     | 833 | CLA  | 8       | 0            |
| 36  | P     | 318 | CLA  | 1       | 0            |
| 36  | G     | 309 | CLA  | 4       | 0            |
| 36  | B     | 311 | CLA  | 7       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 37  | E     | 309 | KC1  | 2       | 0            |
| 42  | G     | 325 | LMG  | 14      | 0            |
| 36  | U     | 305 | CLA  | 3       | 0            |
| 36  | b     | 825 | CLA  | 3       | 0            |
| 36  | a     | 826 | CLA  | 2       | 0            |
| 36  | N     | 317 | CLA  | 3       | 0            |
| 34  | E     | 306 | DD6  | 4       | 0            |
| 36  | a     | 835 | CLA  | 1       | 0            |
| 35  | V     | 301 | A86  | 27      | 0            |
| 36  | S     | 321 | CLA  | 7       | 0            |
| 36  | I     | 310 | CLA  | 4       | 0            |
| 41  | E     | 322 | LHG  | 24      | 0            |
| 36  | a     | 848 | CLA  | 10      | 0            |
| 36  | G     | 310 | CLA  | 1       | 0            |
| 36  | G     | 319 | CLA  | 4       | 0            |
| 35  | I     | 301 | A86  | 4       | 0            |
| 35  | U     | 302 | A86  | 4       | 0            |
| 35  | X     | 314 | A86  | 24      | 0            |
| 36  | K     | 310 | CLA  | 21      | 0            |
| 36  | M     | 316 | CLA  | 3       | 0            |
| 42  | a     | 852 | LMG  | 20      | 0            |
| 36  | V     | 313 | CLA  | 12      | 0            |
| 34  | W     | 205 | DD6  | 23      | 0            |
| 34  | K     | 305 | DD6  | 4       | 0            |
| 36  | H     | 317 | CLA  | 1       | 0            |
| 37  | M     | 318 | KC1  | 6       | 0            |
| 36  | F     | 317 | CLA  | 29      | 0            |
| 35  | M     | 304 | A86  | 12      | 0            |
| 42  | D     | 320 | LMG  | 12      | 0            |
| 36  | R     | 322 | CLA  | 1       | 0            |
| 36  | S     | 314 | CLA  | 3       | 0            |
| 44  | l     | 203 | BCR  | 1       | 0            |
| 36  | E     | 316 | CLA  | 3       | 0            |
| 36  | P     | 316 | CLA  | 4       | 0            |
| 39  | P     | 320 | LMT  | 6       | 0            |
| 36  | H     | 311 | CLA  | 3       | 0            |
| 36  | b     | 834 | CLA  | 3       | 0            |
| 34  | D     | 303 | DD6  | 5       | 0            |
| 35  | S     | 304 | A86  | 21      | 0            |
| 36  | E     | 313 | CLA  | 7       | 0            |
| 36  | O     | 306 | CLA  | 1       | 0            |
| 34  | a     | 849 | DD6  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 36  | V     | 309 | CLA  | 7       | 0            |
| 39  | G     | 322 | LMT  | 10      | 0            |
| 42  | I     | 315 | LMG  | 14      | 0            |
| 35  | O     | 319 | A86  | 1       | 0            |
| 36  | N     | 318 | CLA  | 15      | 0            |
| 36  | C     | 210 | CLA  | 6       | 0            |
| 39  | I     | 318 | LMT  | 7       | 0            |
| 35  | R     | 303 | A86  | 1       | 0            |
| 36  | a     | 825 | CLA  | 2       | 0            |
| 36  | a     | 839 | CLA  | 1       | 0            |
| 36  | E     | 317 | CLA  | 1       | 0            |
| 36  | b     | 805 | CLA  | 2       | 0            |
| 36  | G     | 313 | CLA  | 18      | 0            |
| 38  | b     | 804 | SQD  | 10      | 0            |
| 36  | I     | 309 | CLA  | 17      | 0            |
| 36  | M     | 311 | CLA  | 3       | 0            |
| 36  | V     | 314 | CLA  | 31      | 0            |
| 39  | E     | 323 | LMT  | 5       | 0            |
| 36  | a     | 834 | CLA  | 2       | 0            |
| 36  | X     | 315 | CLA  | 24      | 0            |
| 35  | L     | 301 | A86  | 5       | 0            |
| 36  | K     | 307 | CLA  | 15      | 0            |
| 36  | b     | 802 | CLA  | 3       | 0            |
| 36  | L     | 320 | CLA  | 2       | 0            |
| 36  | J     | 310 | CLA  | 4       | 0            |
| 36  | a     | 823 | CLA  | 1       | 0            |
| 35  | V     | 304 | A86  | 6       | 0            |
| 36  | H     | 312 | CLA  | 2       | 0            |
| 36  | F     | 311 | CLA  | 2       | 0            |
| 36  | M     | 310 | CLA  | 1       | 0            |
| 35  | T     | 301 | A86  | 2       | 0            |
| 36  | a     | 805 | CLA  | 1       | 0            |
| 36  | b     | 818 | CLA  | 3       | 0            |
| 36  | b     | 819 | CLA  | 3       | 0            |
| 36  | a     | 824 | CLA  | 2       | 0            |
| 44  | b     | 845 | BCR  | 1       | 0            |
| 36  | b     | 811 | CLA  | 1       | 0            |
| 35  | G     | 305 | A86  | 3       | 0            |
| 34  | B     | 302 | DD6  | 5       | 0            |
| 35  | N     | 303 | A86  | 15      | 0            |
| 35  | E     | 307 | A86  | 14      | 0            |
| 36  | b     | 808 | CLA  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 35  | T     | 304 | A86  | 5       | 0            |
| 37  | G     | 308 | KC1  | 2       | 0            |
| 36  | I     | 308 | CLA  | 29      | 0            |
| 36  | D     | 307 | CLA  | 12      | 0            |
| 36  | l     | 204 | CLA  | 6       | 0            |
| 36  | W     | 209 | CLA  | 7       | 0            |
| 36  | I     | 311 | CLA  | 1       | 0            |
| 36  | U     | 308 | CLA  | 19      | 0            |
| 34  | G     | 303 | DD6  | 2       | 0            |
| 36  | D     | 312 | CLA  | 2       | 0            |
| 36  | L     | 312 | CLA  | 1       | 0            |
| 36  | H     | 305 | CLA  | 2       | 0            |
| 36  | U     | 311 | CLA  | 16      | 0            |
| 35  | H     | 304 | A86  | 7       | 0            |
| 36  | a     | 817 | CLA  | 3       | 0            |
| 36  | R     | 316 | CLA  | 1       | 0            |
| 36  | J     | 315 | CLA  | 3       | 0            |
| 44  | i     | 101 | BCR  | 4       | 0            |
| 36  | I     | 314 | CLA  | 2       | 0            |
| 34  | S     | 307 | DD6  | 1       | 0            |
| 36  | a     | 830 | CLA  | 4       | 0            |
| 35  | D     | 302 | A86  | 6       | 0            |
| 35  | L     | 304 | A86  | 1       | 0            |
| 36  | j     | 101 | CLA  | 11      | 0            |
| 41  | a     | 843 | LHG  | 5       | 0            |
| 36  | J     | 307 | CLA  | 1       | 0            |
| 37  | B     | 310 | KC1  | 2       | 0            |
| 36  | V     | 307 | CLA  | 1       | 0            |
| 36  | D     | 306 | CLA  | 5       | 0            |
| 36  | F     | 312 | CLA  | 6       | 0            |
| 36  | B     | 305 | CLA  | 3       | 0            |
| 35  | F     | 302 | A86  | 2       | 0            |
| 35  | O     | 301 | A86  | 13      | 0            |
| 36  | D     | 313 | CLA  | 3       | 0            |
| 36  | S     | 319 | CLA  | 2       | 0            |
| 36  | I     | 305 | CLA  | 5       | 0            |
| 34  | O     | 304 | DD6  | 6       | 0            |
| 34  | W     | 204 | DD6  | 22      | 0            |
| 36  | a     | 803 | CLA  | 5       | 0            |
| 44  | i     | 103 | BCR  | 5       | 0            |
| 35  | K     | 301 | A86  | 4       | 0            |
| 35  | G     | 306 | A86  | 4       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 42  | j     | 105 | LMG  | 26      | 0            |
| 36  | a     | 807 | CLA  | 1       | 0            |
| 37  | W     | 217 | KC1  | 14      | 0            |
| 44  | a     | 845 | BCR  | 3       | 0            |
| 39  | P     | 321 | LMT  | 2       | 0            |
| 36  | a     | 811 | CLA  | 3       | 0            |
| 36  | N     | 310 | CLA  | 6       | 0            |
| 34  | P     | 305 | DD6  | 6       | 0            |
| 36  | H     | 318 | CLA  | 4       | 0            |
| 36  | a     | 813 | CLA  | 12      | 0            |
| 36  | D     | 309 | CLA  | 10      | 0            |
| 36  | b     | 801 | CLA  | 1       | 0            |
| 36  | j     | 106 | CLA  | 1       | 0            |
| 41  | G     | 301 | LHG  | 3       | 0            |
| 36  | b     | 822 | CLA  | 2       | 0            |
| 36  | j     | 102 | CLA  | 19      | 0            |
| 36  | U     | 307 | CLA  | 11      | 0            |
| 41  | a     | 850 | LHG  | 15      | 0            |
| 36  | T     | 314 | CLA  | 1       | 0            |
| 39  | L     | 303 | LMT  | 1       | 0            |
| 36  | G     | 311 | CLA  | 11      | 0            |
| 40  | C     | 215 | DGD  | 19      | 0            |
| 41  | Q     | 315 | LHG  | 19      | 0            |
| 34  | j     | 103 | DD6  | 4       | 0            |
| 36  | b     | 812 | CLA  | 2       | 0            |
| 37  | L     | 315 | KC1  | 9       | 0            |
| 36  | Q     | 310 | CLA  | 9       | 0            |
| 36  | I     | 307 | CLA  | 6       | 0            |
| 36  | O     | 311 | CLA  | 3       | 0            |
| 36  | S     | 313 | CLA  | 1       | 0            |
| 36  | b     | 829 | CLA  | 3       | 0            |
| 37  | O     | 313 | KC1  | 1       | 0            |
| 39  | a     | 853 | LMT  | 12      | 0            |
| 36  | L     | 308 | CLA  | 36      | 0            |
| 36  | b     | 823 | CLA  | 11      | 0            |
| 42  | E     | 319 | LMG  | 6       | 0            |
| 36  | a     | 810 | CLA  | 4       | 0            |
| 41  | D     | 318 | LHG  | 16      | 0            |
| 37  | C     | 213 | KC1  | 1       | 0            |
| 34  | H     | 302 | DD6  | 1       | 0            |
| 34  | F     | 303 | DD6  | 3       | 0            |
| 36  | A     | 314 | CLA  | 20      | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 37  | F     | 308 | KC1  | 15      | 0            |
| 34  | J     | 304 | DD6  | 4       | 0            |
| 36  | E     | 314 | CLA  | 4       | 0            |
| 36  | b     | 817 | CLA  | 6       | 0            |
| 36  | L     | 314 | CLA  | 2       | 0            |
| 36  | a     | 809 | CLA  | 5       | 0            |
| 39  | F     | 321 | LMT  | 25      | 0            |
| 39  | U     | 314 | LMT  | 15      | 0            |
| 36  | f     | 802 | CLA  | 4       | 0            |
| 41  | O     | 318 | LHG  | 6       | 0            |
| 36  | I     | 313 | CLA  | 2       | 0            |
| 36  | a     | 821 | CLA  | 2       | 0            |
| 39  | E     | 320 | LMT  | 16      | 0            |
| 36  | B     | 308 | CLA  | 7       | 0            |
| 36  | b     | 837 | CLA  | 2       | 0            |
| 36  | D     | 315 | CLA  | 1       | 0            |
| 39  | G     | 323 | LMT  | 4       | 0            |
| 36  | K     | 309 | CLA  | 6       | 0            |
| 36  | a     | 806 | CLA  | 19      | 0            |
| 37  | T     | 315 | KC1  | 1       | 0            |
| 36  | b     | 807 | CLA  | 4       | 0            |
| 41  | l     | 208 | LHG  | 17      | 0            |
| 34  | I     | 303 | DD6  | 6       | 0            |
| 36  | C     | 208 | CLA  | 5       | 0            |
| 41  | G     | 321 | LHG  | 10      | 0            |
| 36  | A     | 310 | CLA  | 1       | 0            |
| 36  | b     | 828 | CLA  | 4       | 0            |
| 42  | L     | 321 | LMG  | 10      | 0            |
| 36  | l     | 201 | CLA  | 6       | 0            |
| 35  | h     | 204 | A86  | 4       | 0            |
| 36  | a     | 829 | CLA  | 1       | 0            |
| 36  | h     | 203 | CLA  | 11      | 0            |
| 36  | O     | 308 | CLA  | 6       | 0            |
| 36  | a     | 808 | CLA  | 7       | 0            |
| 41  | I     | 316 | LHG  | 10      | 0            |
| 36  | W     | 208 | CLA  | 1       | 0            |
| 36  | S     | 309 | CLA  | 5       | 0            |
| 44  | a     | 844 | BCR  | 7       | 0            |
| 36  | S     | 312 | CLA  | 3       | 0            |
| 39  | K     | 318 | LMT  | 8       | 0            |
| 36  | Q     | 305 | CLA  | 4       | 0            |
| 36  | a     | 801 | CLA  | 6       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 35  | N     | 305 | A86  | 20      | 0            |
| 36  | f     | 803 | CLA  | 3       | 0            |
| 36  | K     | 311 | CLA  | 5       | 0            |
| 36  | a     | 804 | CLA  | 3       | 0            |
| 37  | M     | 313 | KC1  | 1       | 0            |
| 36  | L     | 309 | CLA  | 10      | 0            |
| 35  | S     | 302 | A86  | 1       | 0            |
| 35  | E     | 305 | A86  | 4       | 0            |
| 36  | A     | 306 | CLA  | 17      | 0            |
| 36  | O     | 312 | CLA  | 2       | 0            |
| 35  | C     | 204 | A86  | 4       | 0            |
| 36  | b     | 810 | CLA  | 2       | 0            |
| 36  | K     | 312 | CLA  | 3       | 0            |
| 36  | J     | 309 | CLA  | 2       | 0            |
| 37  | T     | 310 | KC1  | 17      | 0            |
| 36  | S     | 311 | CLA  | 8       | 0            |
| 35  | J     | 301 | A86  | 14      | 0            |
| 36  | N     | 313 | CLA  | 5       | 0            |
| 44  | b     | 843 | BCR  | 6       | 0            |
| 36  | H     | 315 | CLA  | 3       | 0            |
| 44  | m     | 101 | BCR  | 11      | 0            |
| 36  | R     | 314 | CLA  | 3       | 0            |
| 36  | D     | 317 | CLA  | 1       | 0            |
| 36  | T     | 308 | CLA  | 3       | 0            |
| 36  | H     | 316 | CLA  | 2       | 0            |
| 35  | L     | 307 | A86  | 8       | 0            |
| 36  | b     | 813 | CLA  | 1       | 0            |
| 41  | f     | 809 | LHG  | 20      | 0            |
| 39  | F     | 320 | LMT  | 19      | 0            |
| 37  | G     | 317 | KC1  | 6       | 0            |
| 39  | B     | 312 | LMT  | 15      | 0            |
| 36  | B     | 307 | CLA  | 1       | 0            |
| 37  | K     | 314 | KC1  | 9       | 0            |
| 36  | H     | 308 | CLA  | 19      | 0            |
| 41  | i     | 104 | LHG  | 28      | 0            |
| 36  | J     | 317 | CLA  | 1       | 0            |
| 36  | l     | 206 | CLA  | 1       | 0            |
| 36  | W     | 206 | CLA  | 1       | 0            |
| 42  | G     | 324 | LMG  | 17      | 0            |
| 36  | a     | 836 | CLA  | 6       | 0            |
| 36  | V     | 311 | CLA  | 16      | 0            |
| 36  | P     | 313 | CLA  | 7       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 36  | a     | 831 | CLA  | 1       | 0            |
| 36  | D     | 308 | CLA  | 6       | 0            |
| 36  | a     | 833 | CLA  | 2       | 0            |
| 38  | A     | 315 | SQD  | 7       | 0            |
| 36  | W     | 215 | CLA  | 3       | 0            |
| 44  | b     | 844 | BCR  | 2       | 0            |
| 36  | U     | 306 | CLA  | 31      | 0            |
| 36  | M     | 307 | CLA  | 18      | 0            |
| 34  | A     | 301 | DD6  | 8       | 0            |
| 40  | b     | 849 | DGD  | 4       | 0            |
| 36  | R     | 321 | CLA  | 2       | 0            |
| 35  | J     | 302 | A86  | 3       | 0            |
| 36  | P     | 314 | CLA  | 5       | 0            |
| 36  | G     | 315 | CLA  | 24      | 0            |
| 36  | K     | 313 | CLA  | 6       | 0            |
| 36  | M     | 306 | CLA  | 1       | 0            |
| 36  | b     | 821 | CLA  | 1       | 0            |
| 37  | Q     | 313 | KC1  | 8       | 0            |
| 36  | V     | 305 | CLA  | 32      | 0            |
| 36  | U     | 309 | CLA  | 4       | 0            |
| 36  | D     | 316 | CLA  | 1       | 0            |
| 34  | B     | 304 | DD6  | 10      | 0            |
| 35  | U     | 303 | A86  | 15      | 0            |
| 36  | N     | 309 | CLA  | 6       | 0            |
| 35  | A     | 316 | A86  | 2       | 0            |
| 36  | Q     | 314 | CLA  | 50      | 0            |
| 42  | J     | 319 | LMG  | 12      | 0            |
| 35  | N     | 301 | A86  | 2       | 0            |
| 36  | a     | 818 | CLA  | 3       | 0            |
| 37  | V     | 312 | KC1  | 1       | 0            |
| 36  | S     | 320 | CLA  | 2       | 0            |
| 34  | A     | 304 | DD6  | 2       | 0            |
| 36  | T     | 309 | CLA  | 4       | 0            |
| 41  | F     | 319 | LHG  | 4       | 0            |
| 36  | b     | 836 | CLA  | 20      | 0            |
| 34  | K     | 304 | DD6  | 4       | 0            |
| 34  | A     | 303 | DD6  | 4       | 0            |
| 34  | S     | 306 | DD6  | 2       | 0            |
| 34  | R     | 307 | DD6  | 11      | 0            |
| 36  | A     | 313 | CLA  | 3       | 0            |
| 44  | f     | 801 | BCR  | 2       | 0            |
| 42  | E     | 318 | LMG  | 19      | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 36  | C     | 212 | CLA  | 6       | 0            |
| 36  | R     | 310 | CLA  | 9       | 0            |
| 39  | f     | 807 | LMT  | 2       | 0            |
| 35  | F     | 301 | A86  | 10      | 0            |
| 44  | b     | 847 | BCR  | 1       | 0            |
| 36  | F     | 316 | CLA  | 3       | 0            |
| 37  | A     | 312 | KC1  | 4       | 0            |
| 36  | N     | 308 | CLA  | 4       | 0            |
| 34  | C     | 201 | DD6  | 4       | 0            |
| 35  | X     | 302 | A86  | 1       | 0            |
| 36  | G     | 316 | CLA  | 3       | 0            |
| 35  | P     | 307 | A86  | 2       | 0            |
| 44  | f     | 806 | BCR  | 1       | 0            |
| 41  | D     | 319 | LHG  | 12      | 0            |
| 36  | a     | 838 | CLA  | 1       | 0            |
| 36  | C     | 209 | CLA  | 1       | 0            |
| 41  | G     | 320 | LHG  | 14      | 0            |
| 37  | S     | 316 | KC1  | 4       | 0            |
| 35  | B     | 301 | A86  | 11      | 0            |
| 39  | L     | 318 | LMT  | 9       | 0            |
| 36  | a     | 841 | CLA  | 3       | 0            |
| 35  | N     | 302 | A86  | 4       | 0            |
| 36  | F     | 313 | CLA  | 6       | 0            |
| 36  | F     | 309 | CLA  | 5       | 0            |
| 36  | C     | 206 | CLA  | 3       | 0            |
| 36  | E     | 310 | CLA  | 1       | 0            |
| 36  | D     | 310 | CLA  | 1       | 0            |
| 36  | P     | 319 | CLA  | 13      | 0            |
| 36  | R     | 313 | CLA  | 2       | 0            |
| 36  | b     | 809 | CLA  | 2       | 0            |
| 36  | O     | 316 | CLA  | 22      | 0            |
| 36  | J     | 313 | CLA  | 5       | 0            |
| 35  | K     | 303 | A86  | 2       | 0            |
| 36  | C     | 205 | CLA  | 14      | 0            |
| 36  | b     | 814 | CLA  | 2       | 0            |
| 36  | L     | 310 | CLA  | 1       | 0            |
| 36  | A     | 309 | CLA  | 6       | 0            |
| 36  | A     | 311 | CLA  | 3       | 0            |
| 41  | R     | 323 | LHG  | 14      | 0            |
| 35  | Q     | 316 | A86  | 27      | 0            |
| 36  | N     | 312 | CLA  | 6       | 0            |
| 36  | S     | 318 | CLA  | 3       | 0            |

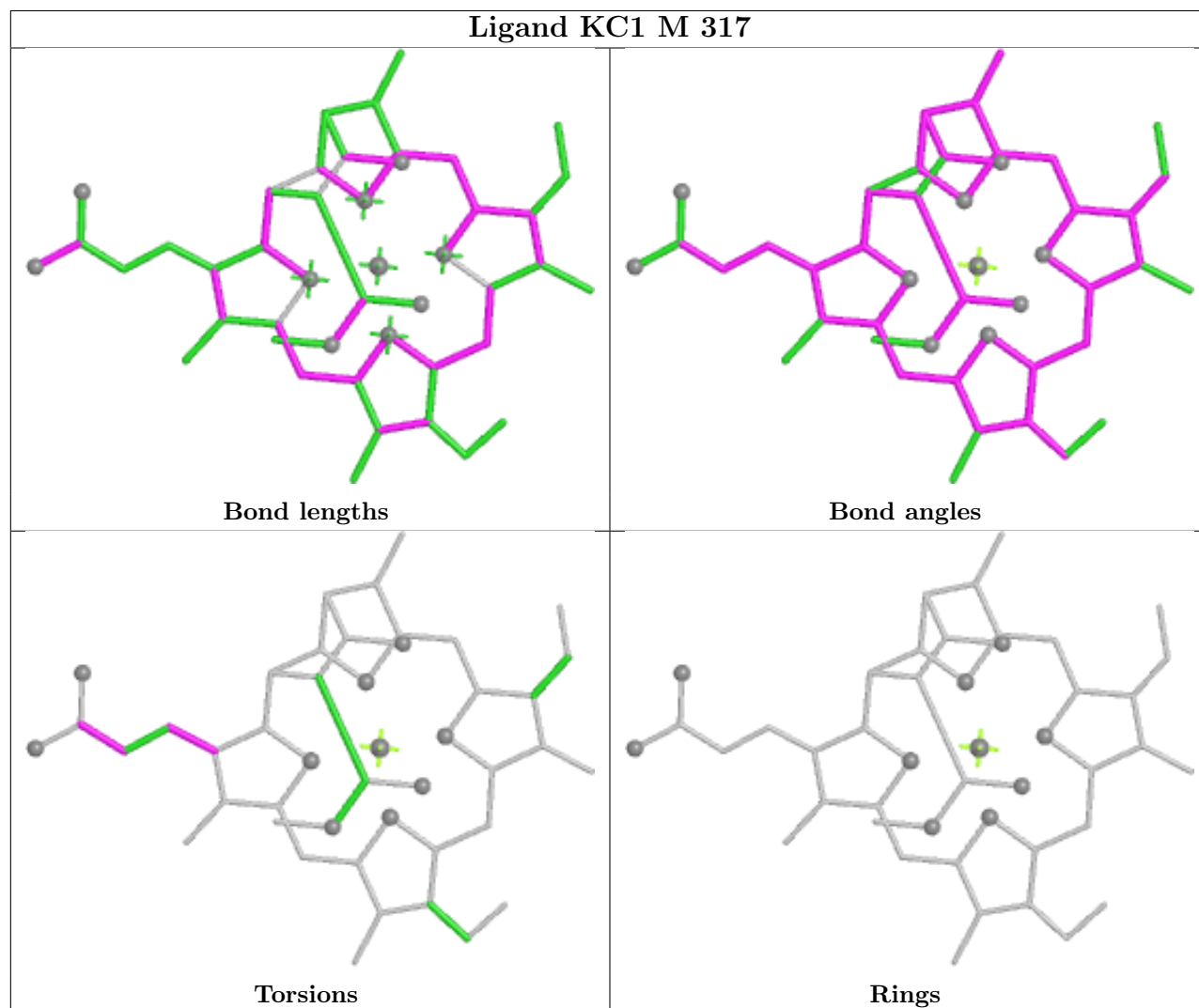
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 35  | R     | 305 | A86  | 7       | 0            |
| 36  | Q     | 306 | CLA  | 3       | 0            |
| 36  | R     | 320 | CLA  | 7       | 0            |
| 36  | a     | 822 | CLA  | 3       | 0            |
| 35  | T     | 303 | A86  | 1       | 0            |
| 36  | B     | 309 | CLA  | 16      | 0            |
| 36  | H     | 314 | CLA  | 6       | 0            |
| 39  | a     | 851 | LMT  | 8       | 0            |
| 36  | l     | 202 | CLA  | 8       | 0            |
| 39  | K     | 317 | LMT  | 6       | 0            |
| 39  | I     | 317 | LMT  | 15      | 0            |
| 36  | S     | 315 | CLA  | 15      | 0            |
| 36  | X     | 310 | CLA  | 3       | 0            |
| 37  | O     | 315 | KC1  | 12      | 0            |
| 36  | a     | 832 | CLA  | 3       | 0            |
| 35  | B     | 303 | A86  | 8       | 0            |
| 35  | J     | 306 | A86  | 6       | 0            |
| 36  | Q     | 307 | CLA  | 5       | 0            |
| 39  | B     | 313 | LMT  | 5       | 0            |
| 36  | C     | 207 | CLA  | 7       | 0            |
| 36  | A     | 305 | CLA  | 4       | 0            |
| 34  | D     | 301 | DD6  | 12      | 0            |
| 36  | U     | 310 | CLA  | 15      | 0            |
| 36  | A     | 307 | CLA  | 3       | 0            |
| 36  | l     | 205 | CLA  | 3       | 0            |
| 36  | K     | 308 | CLA  | 2       | 0            |
| 40  | L     | 302 | DGD  | 20      | 0            |
| 36  | W     | 201 | CLA  | 1       | 0            |
| 34  | E     | 301 | DD6  | 4       | 0            |
| 36  | A     | 308 | CLA  | 2       | 0            |
| 36  | f     | 805 | CLA  | 20      | 0            |
| 34  | M     | 303 | DD6  | 18      | 0            |
| 36  | b     | 806 | CLA  | 2       | 0            |
| 35  | A     | 302 | A86  | 1       | 0            |
| 36  | W     | 216 | CLA  | 1       | 0            |

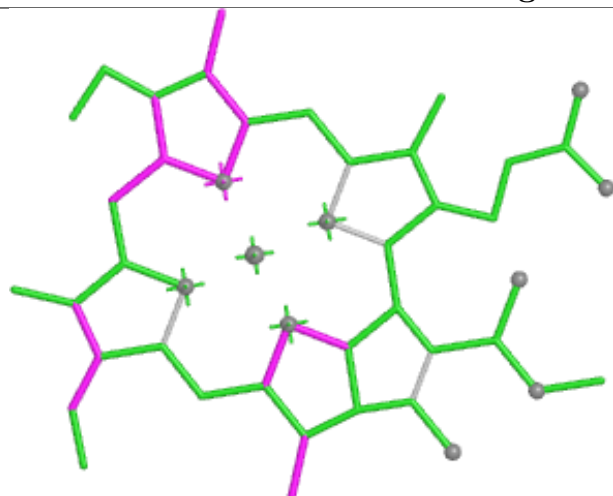
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

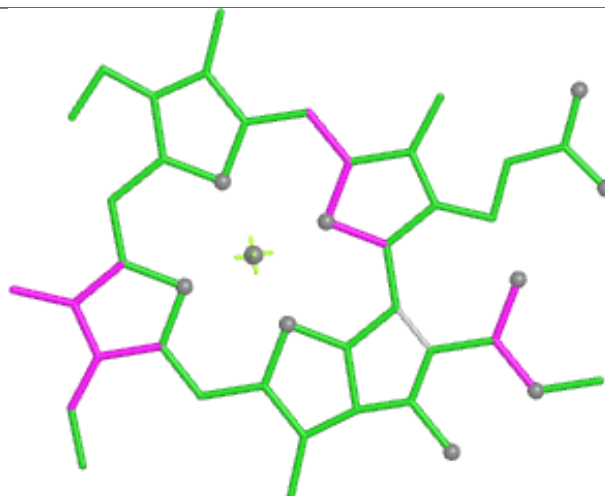




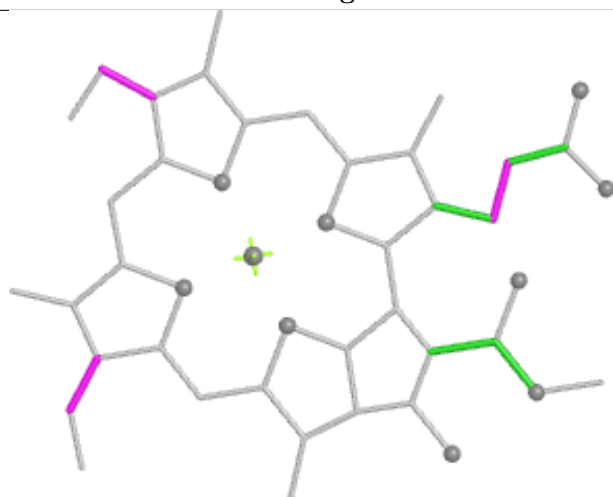
## Ligand CLA a 819



Bond lengths



Bond angles

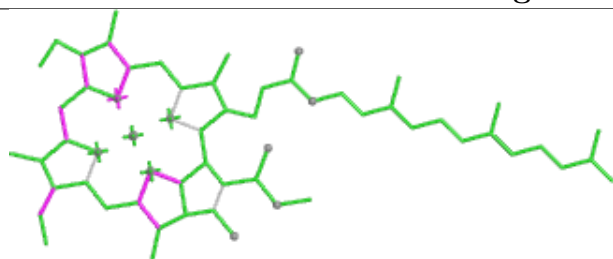


Torsions

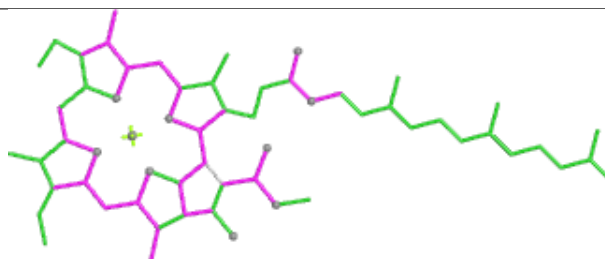


Rings

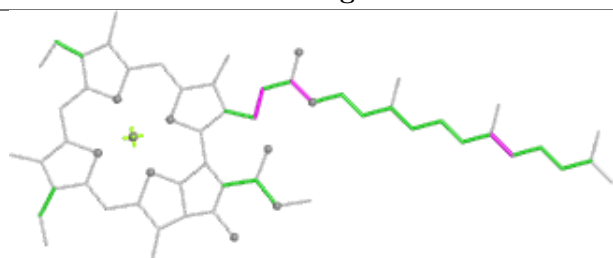
## Ligand CLA H 307



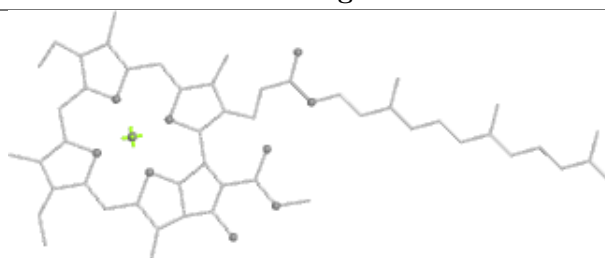
Bond lengths



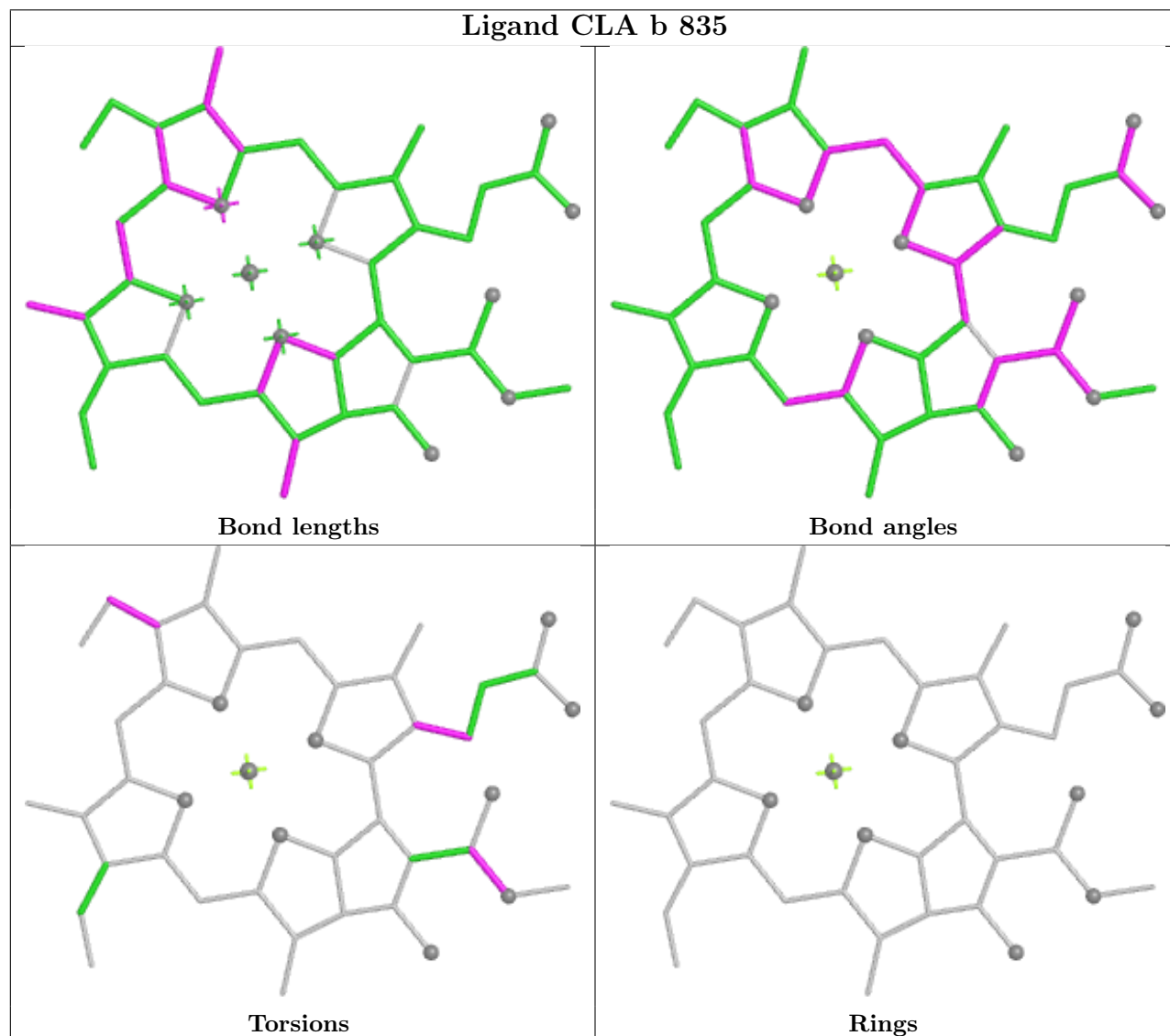
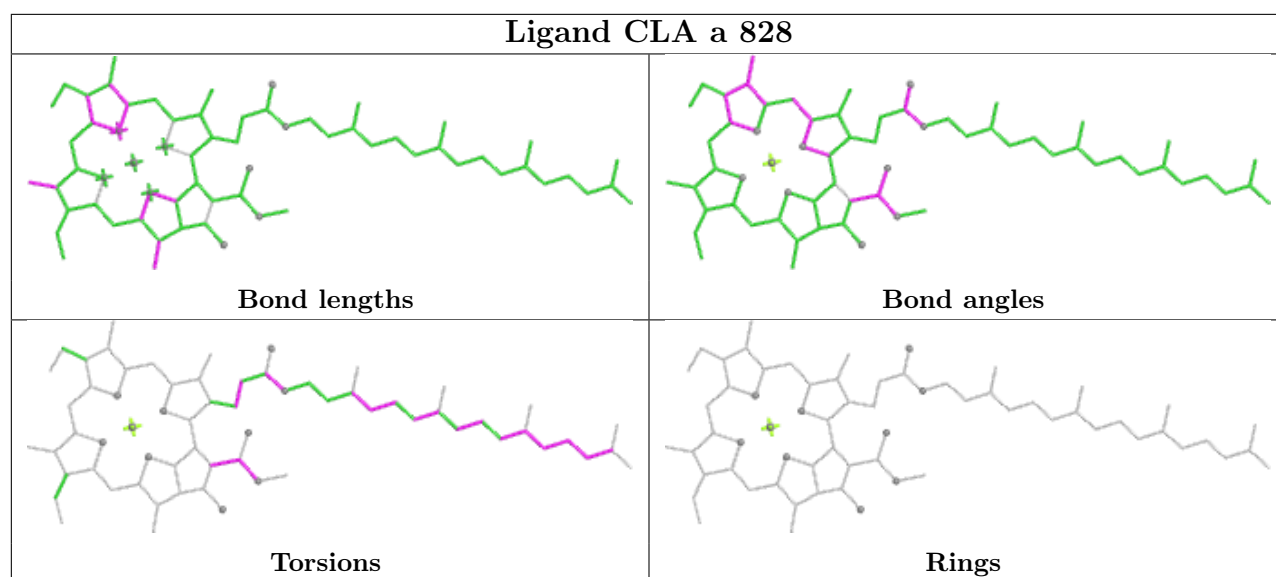
Bond angles



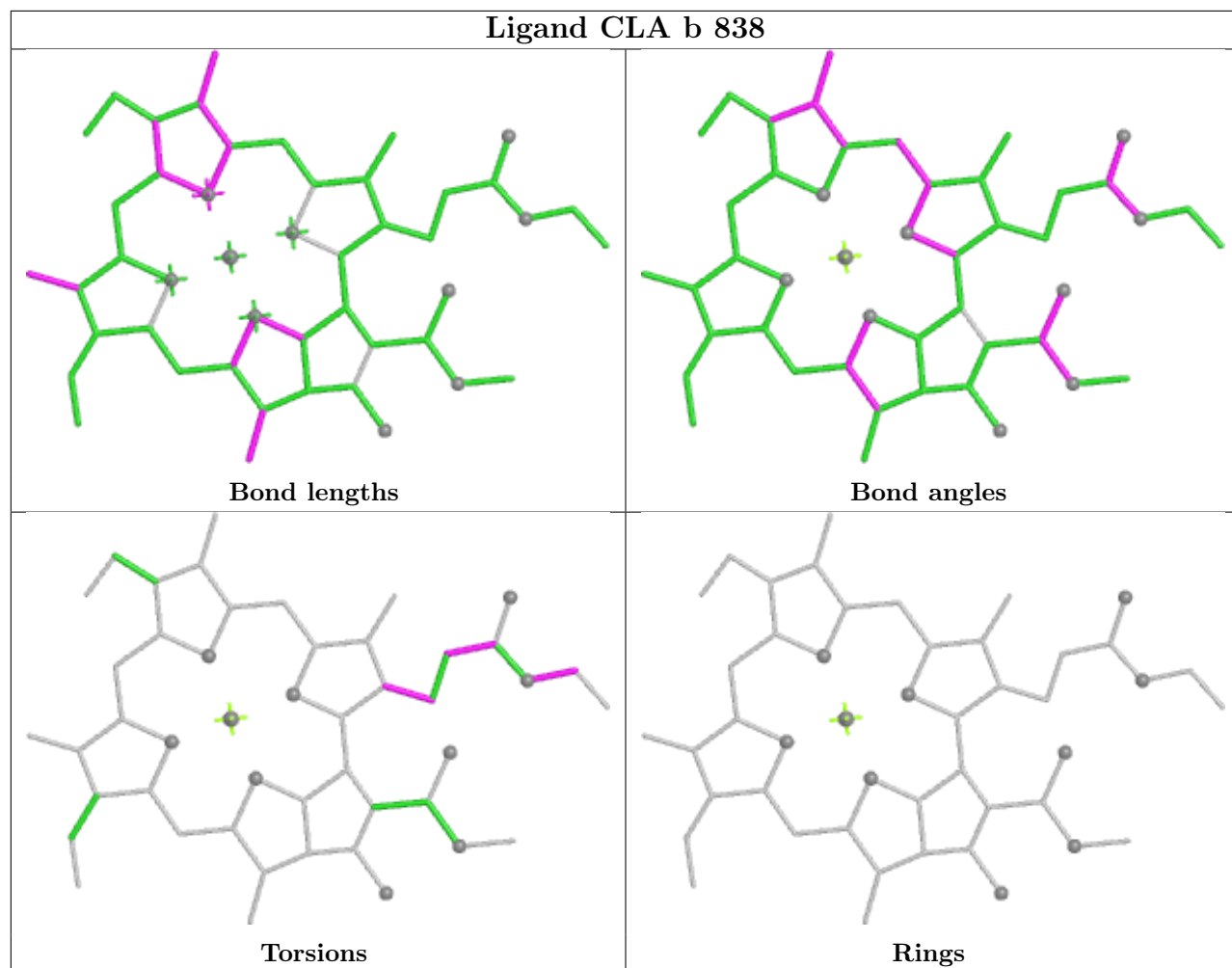
Torsions

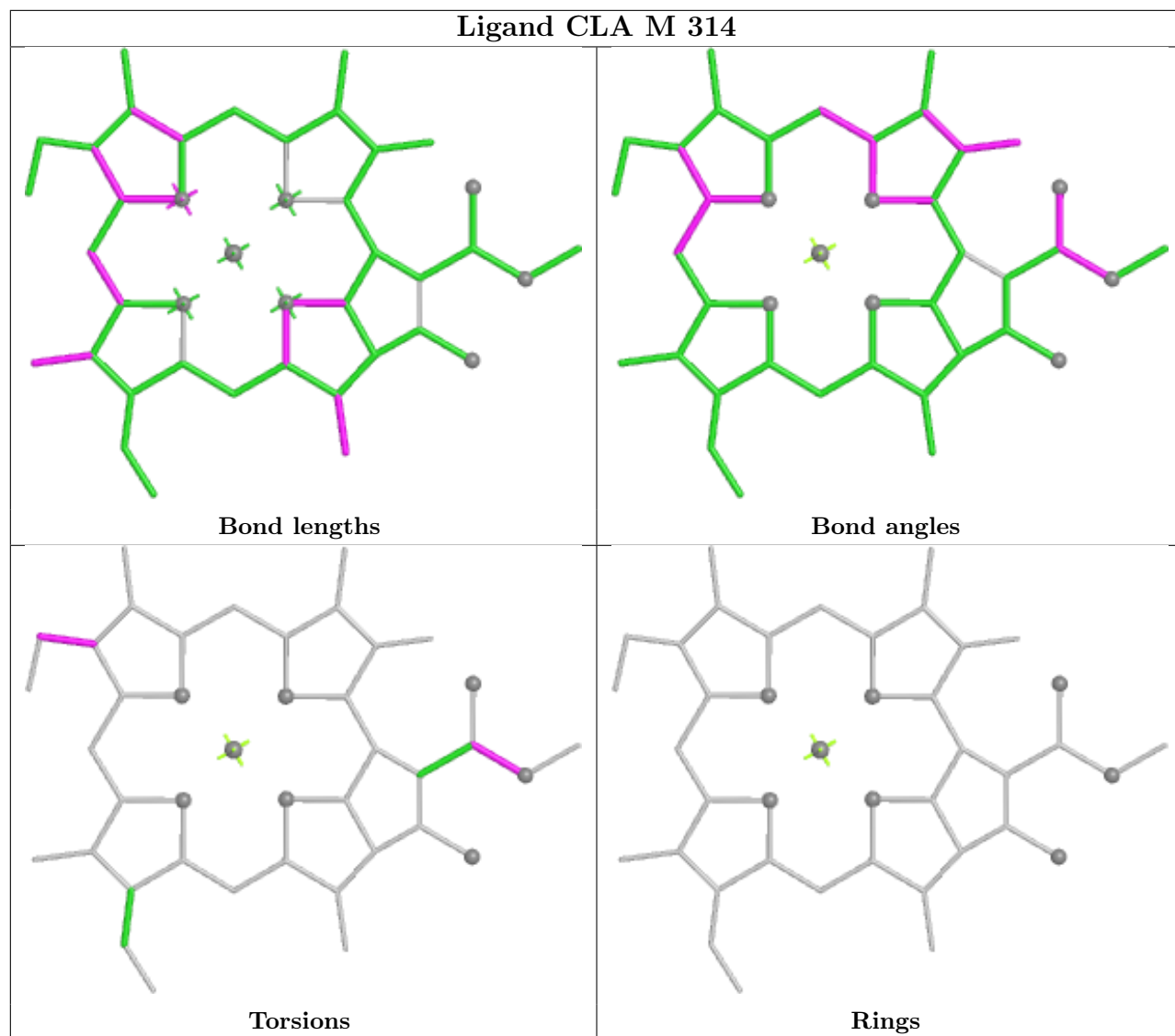


Rings

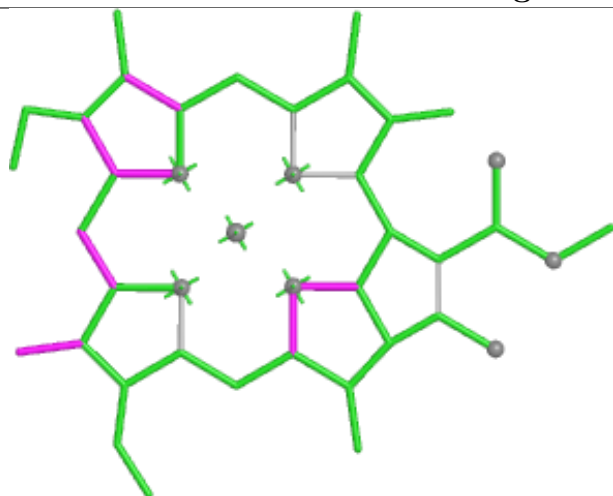


## Ligand CLA b 838

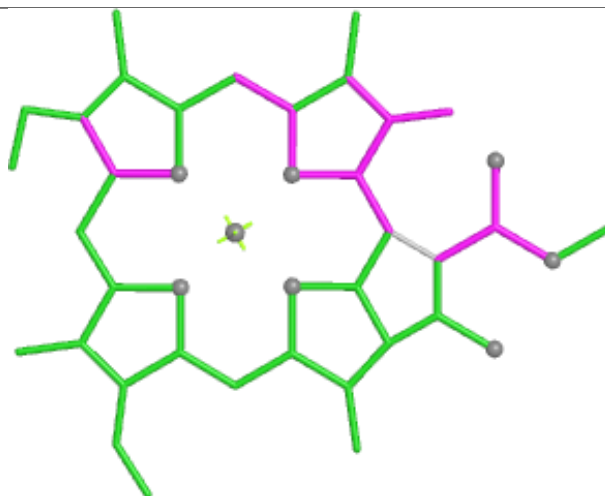




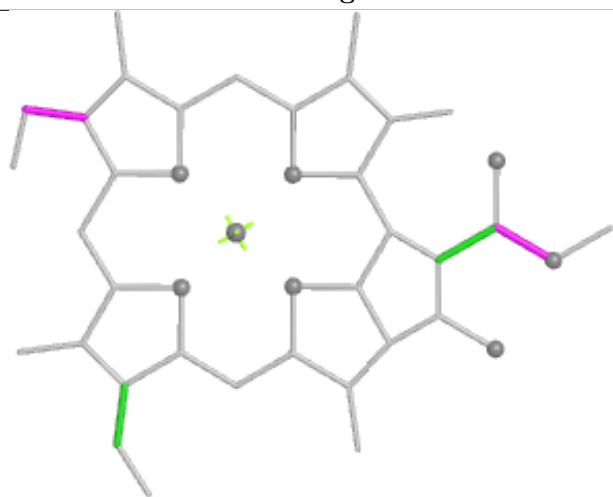
## Ligand CLA U 313



Bond lengths



Bond angles

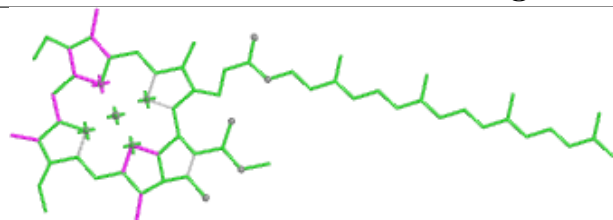


Torsions

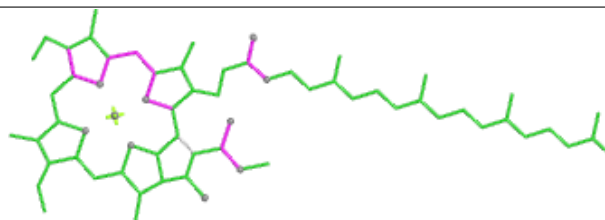


Rings

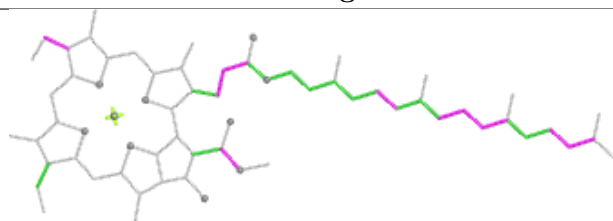
## Ligand CLA M 309



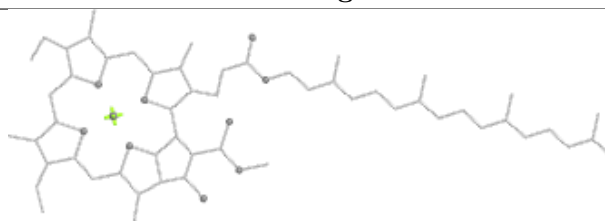
Bond lengths



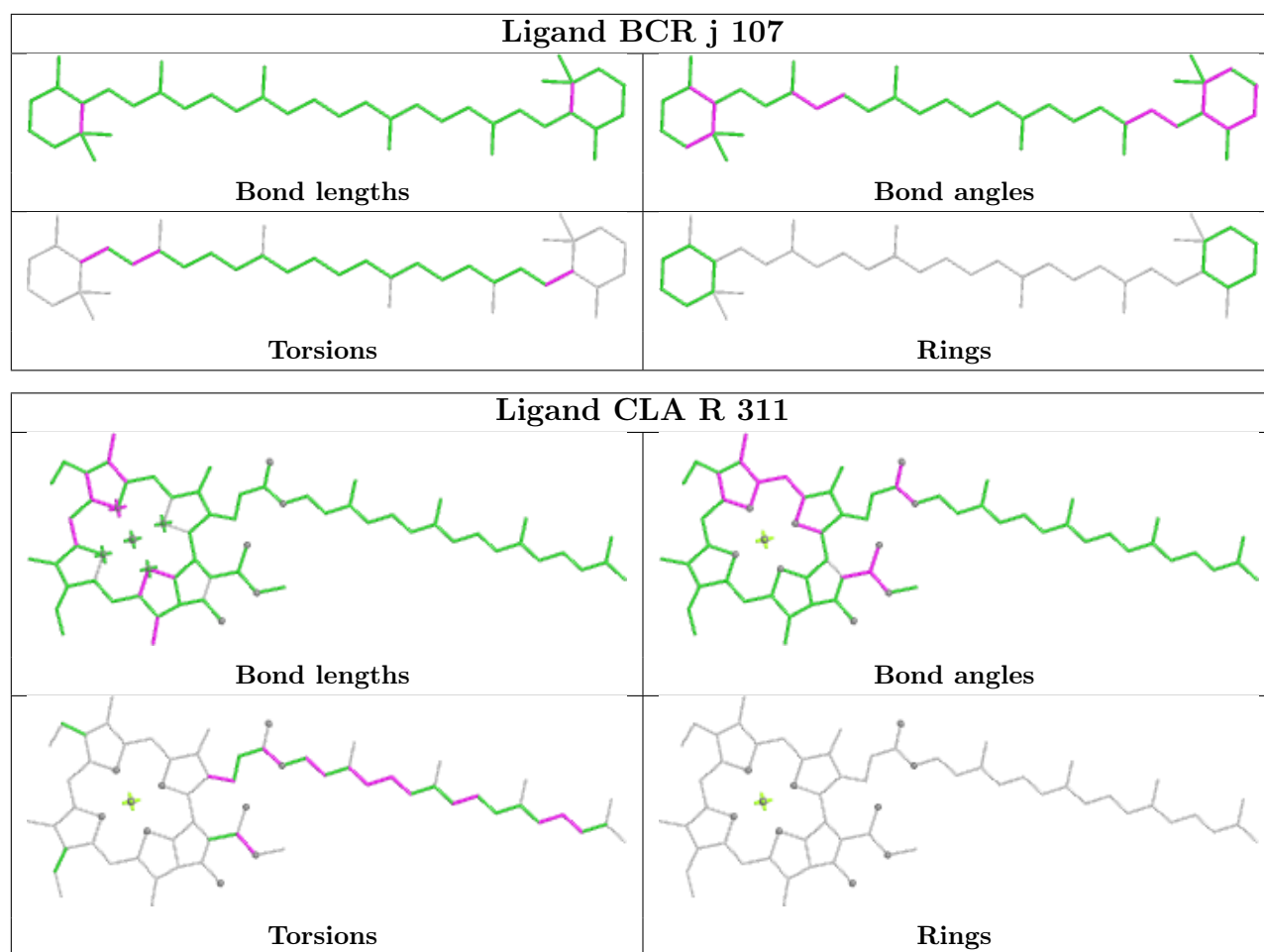
Bond angles



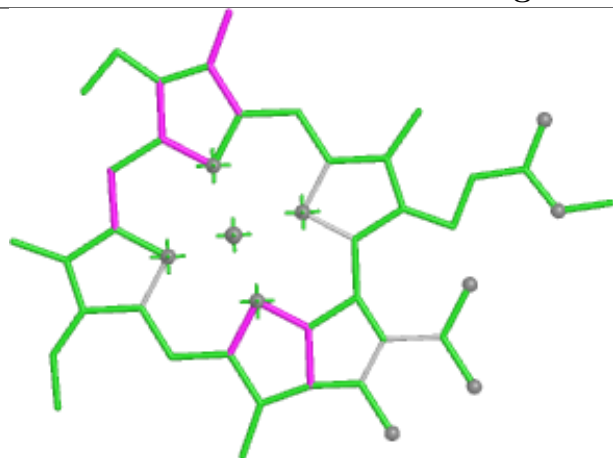
Torsions



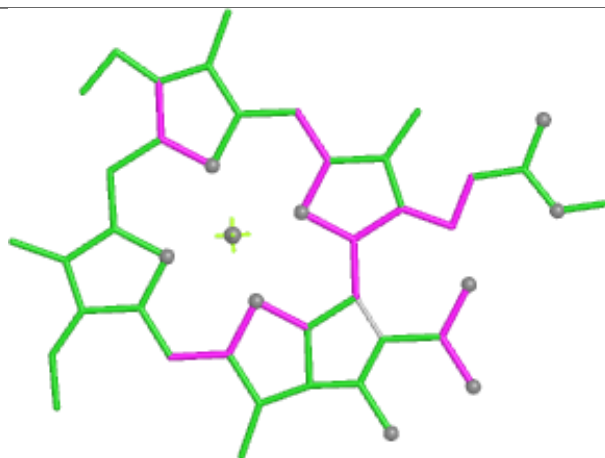
Rings



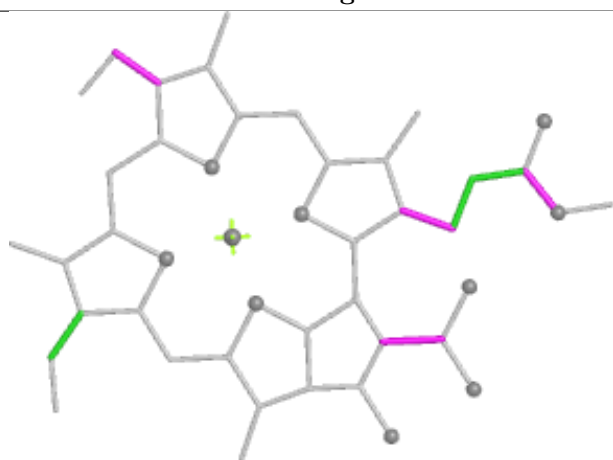
## Ligand CLA X 309



Bond lengths



Bond angles

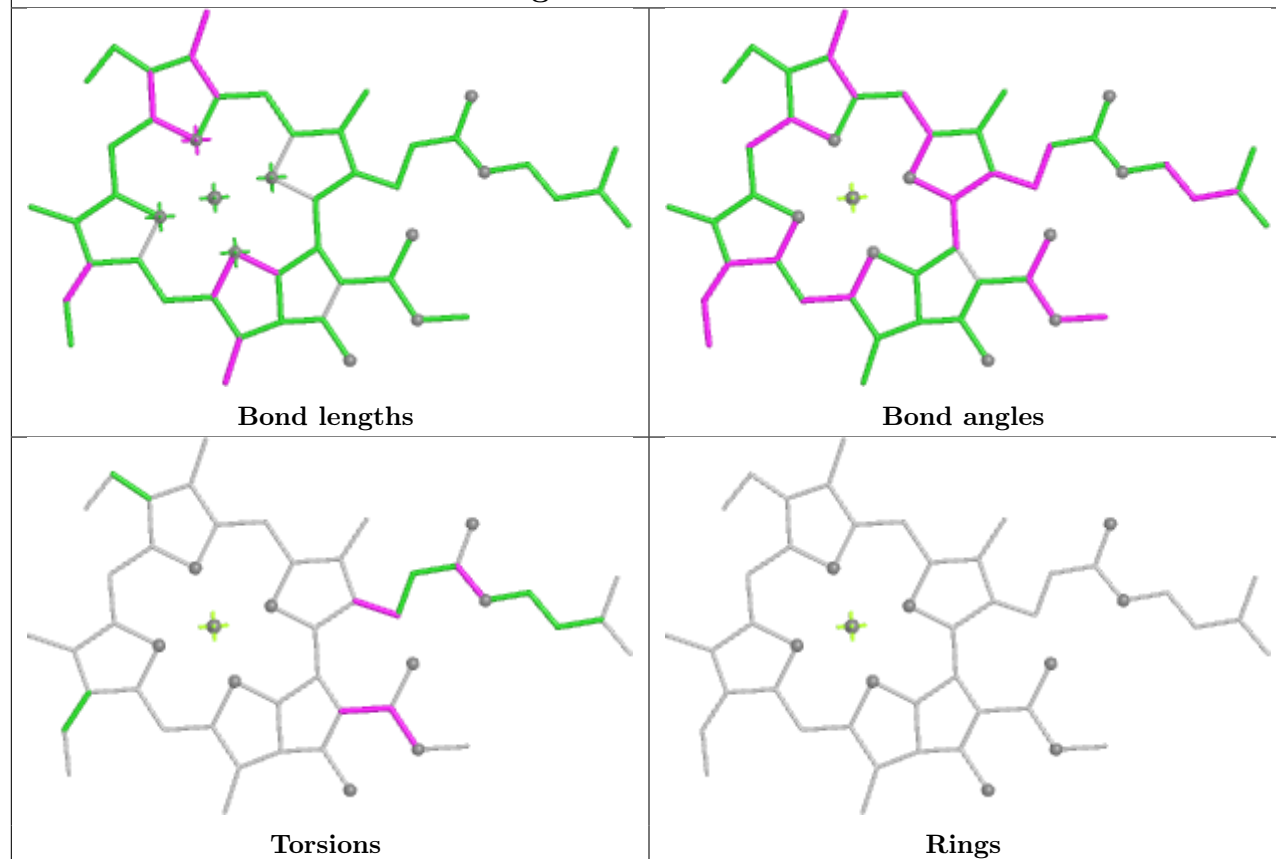


Torsions

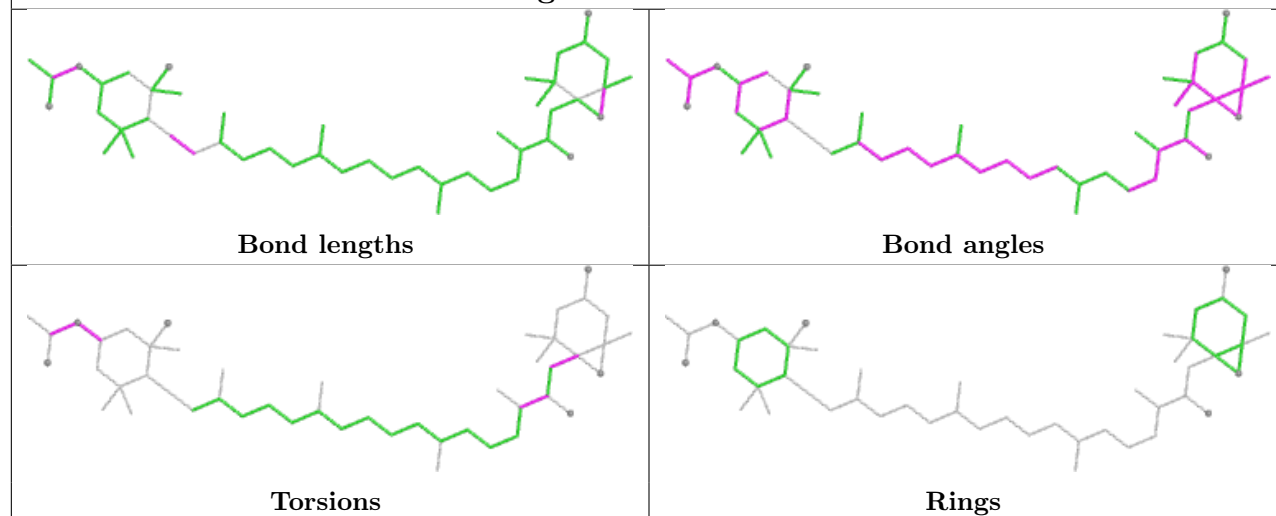


Rings

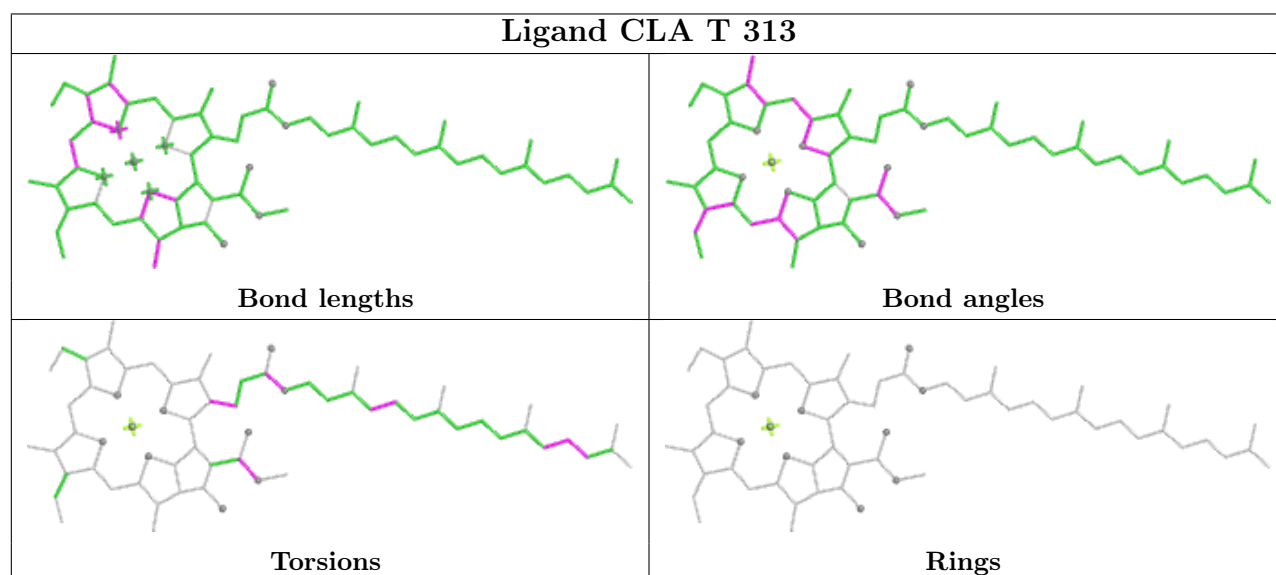
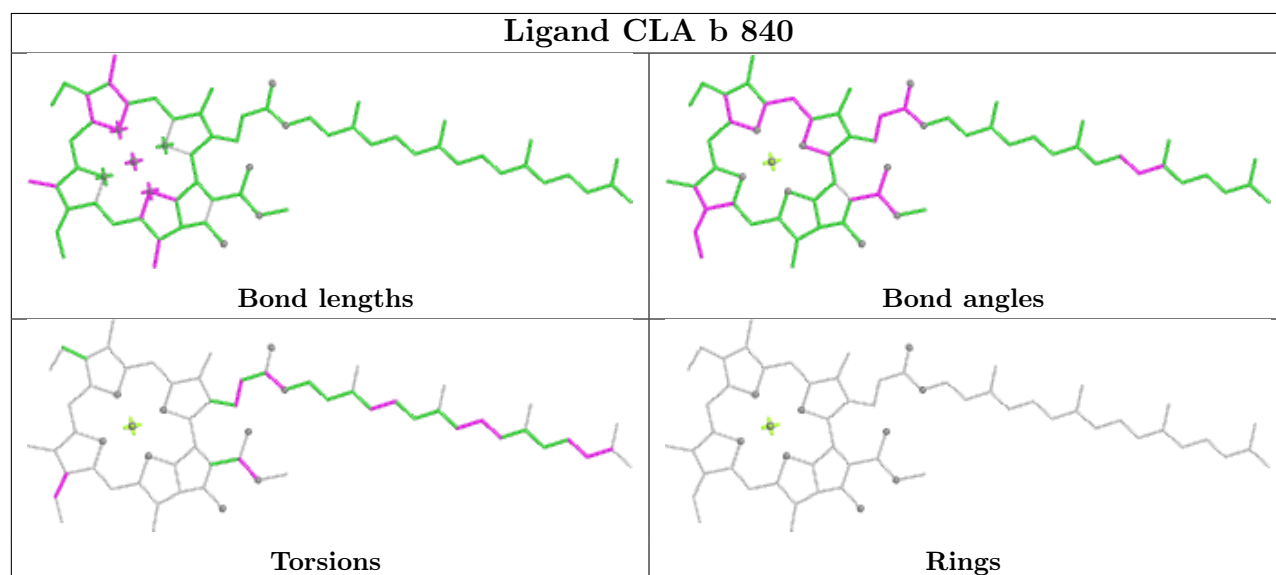
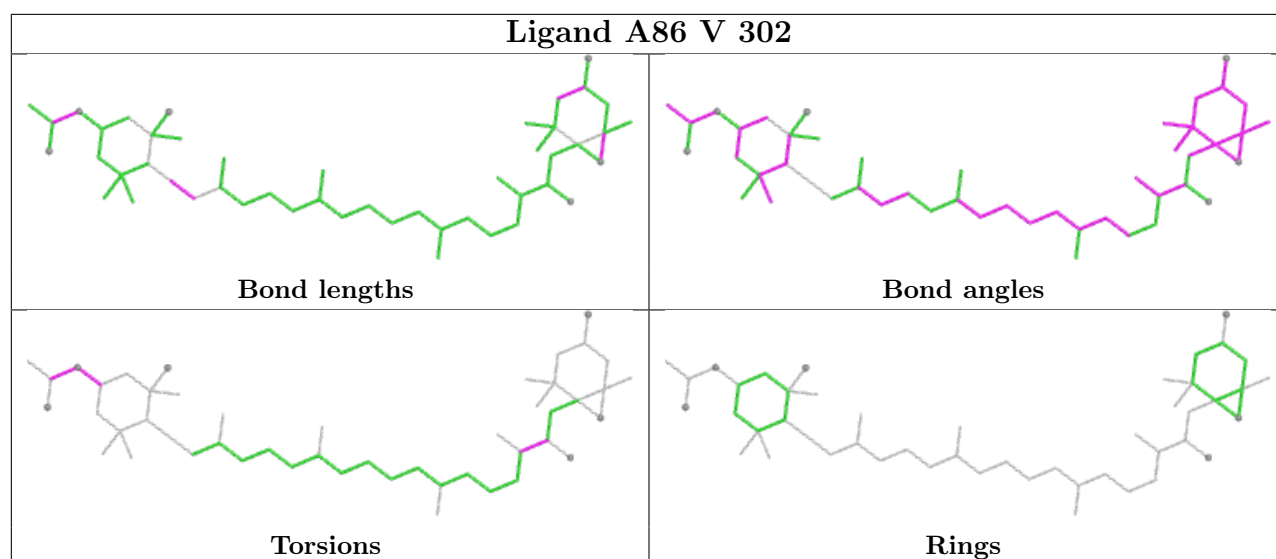
## Ligand CLA X 307

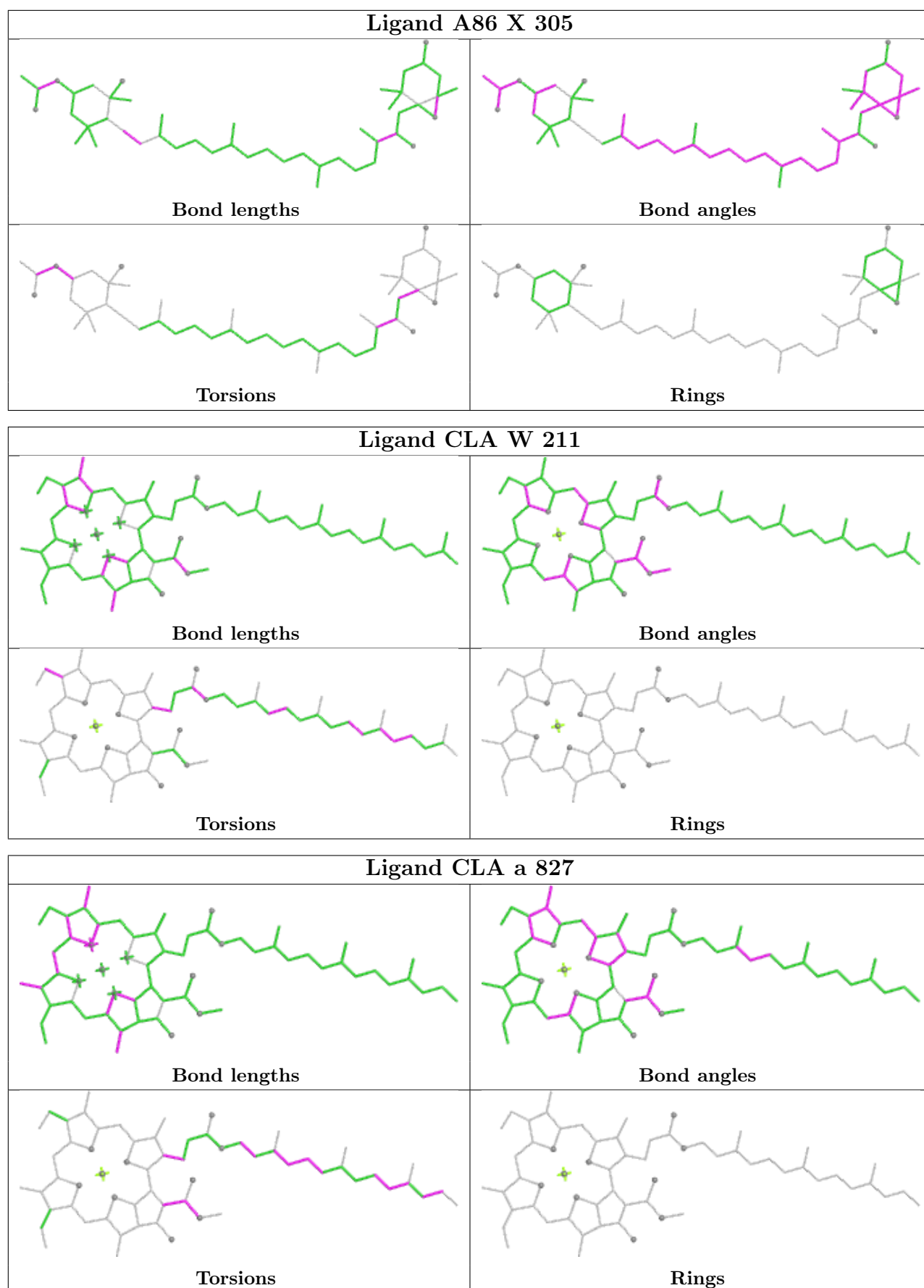


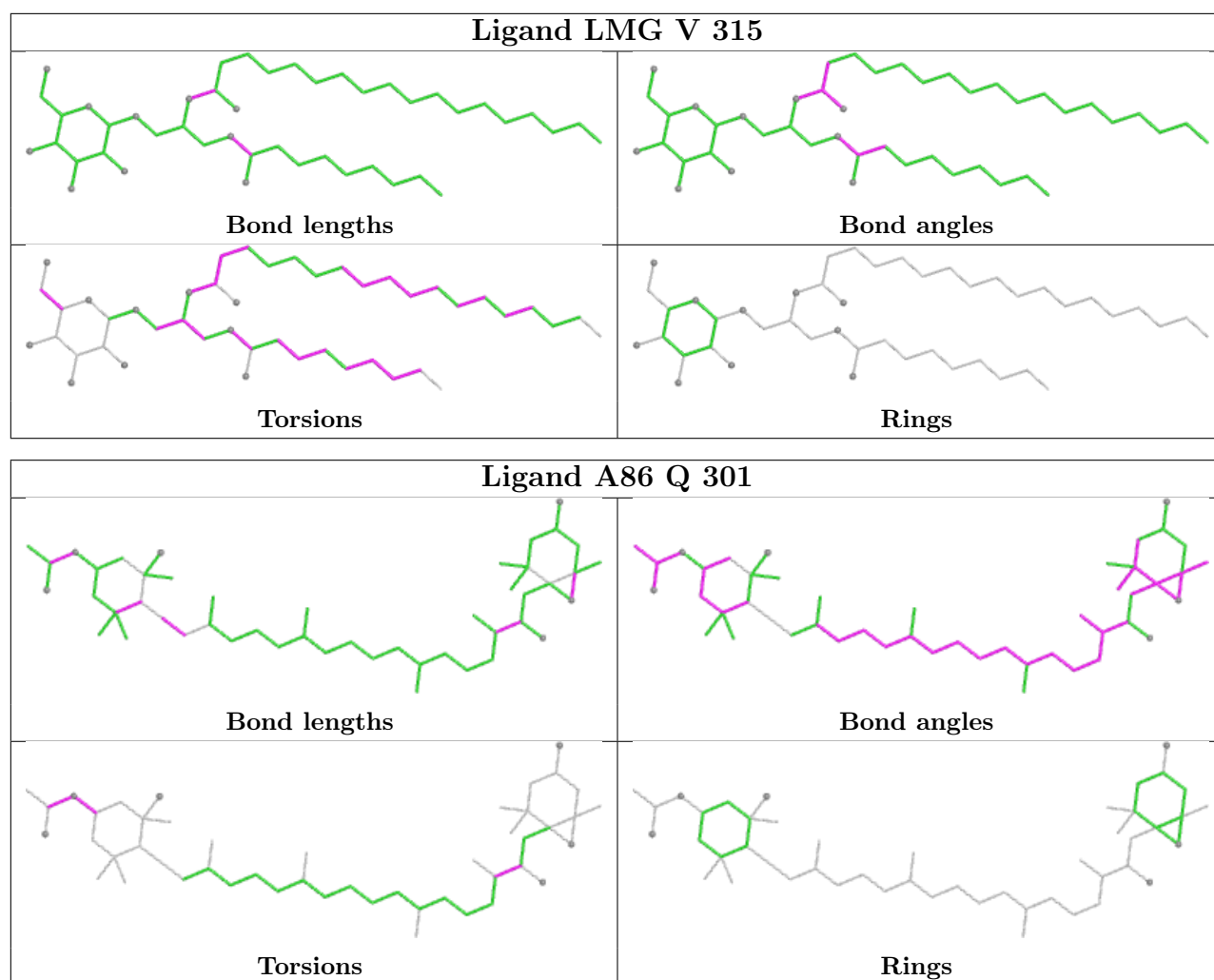
## Ligand A86 R 304



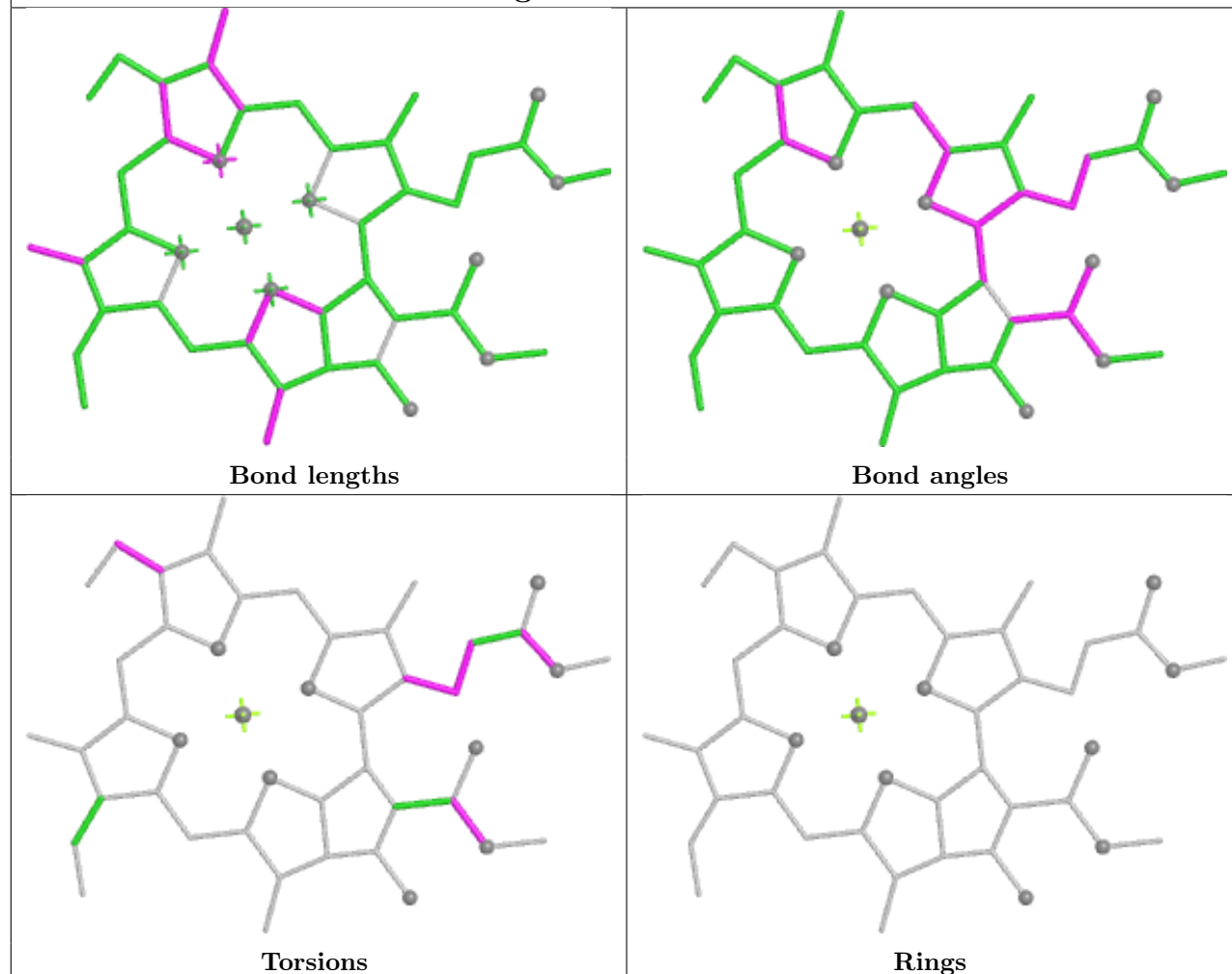




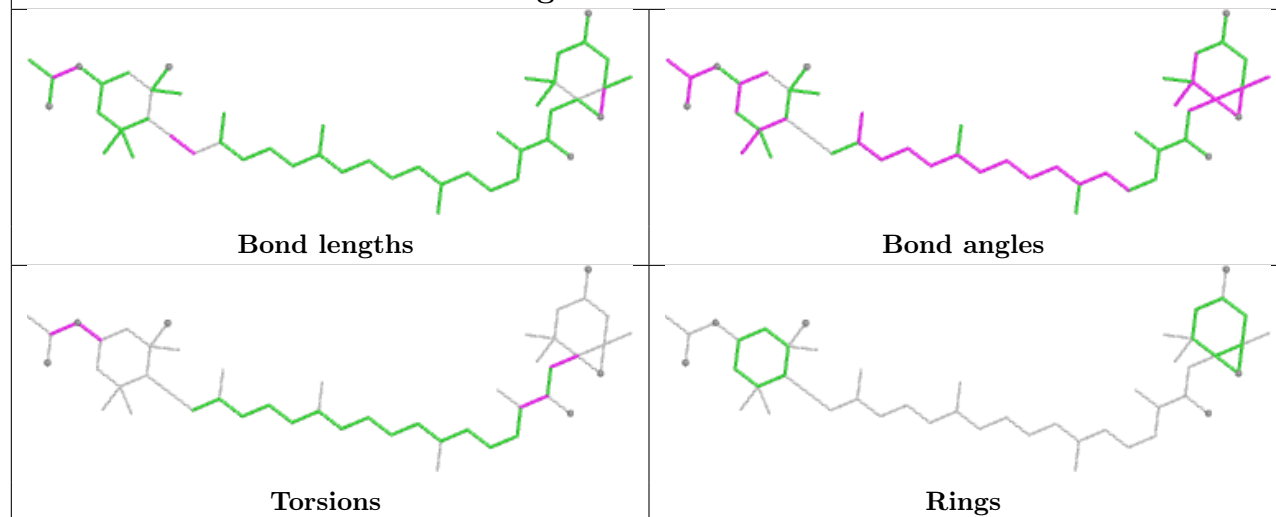


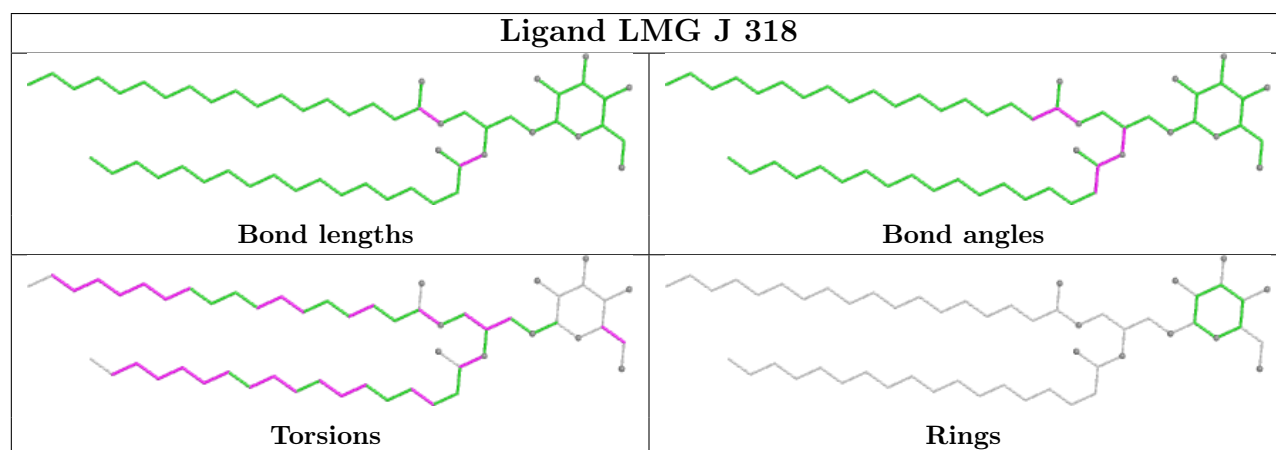
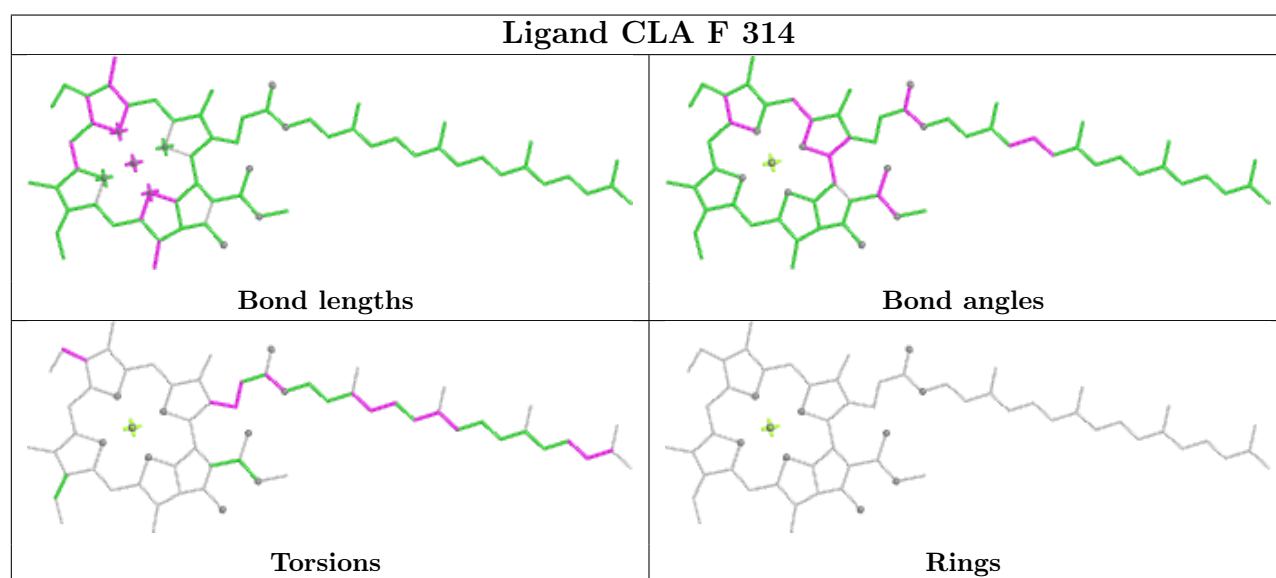
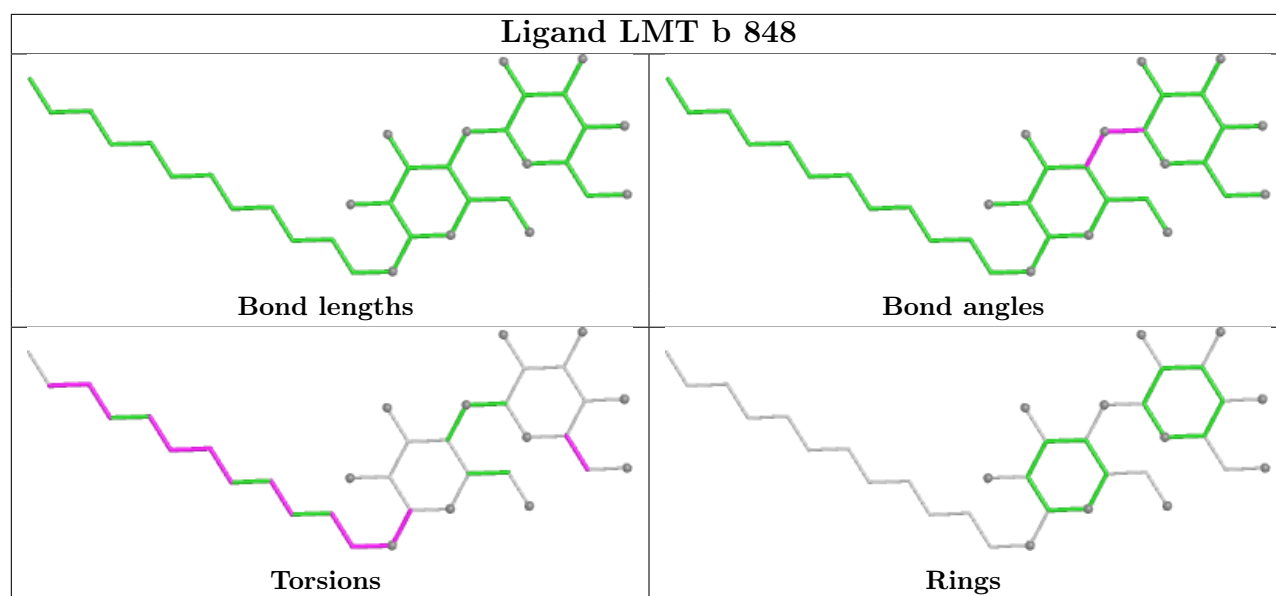


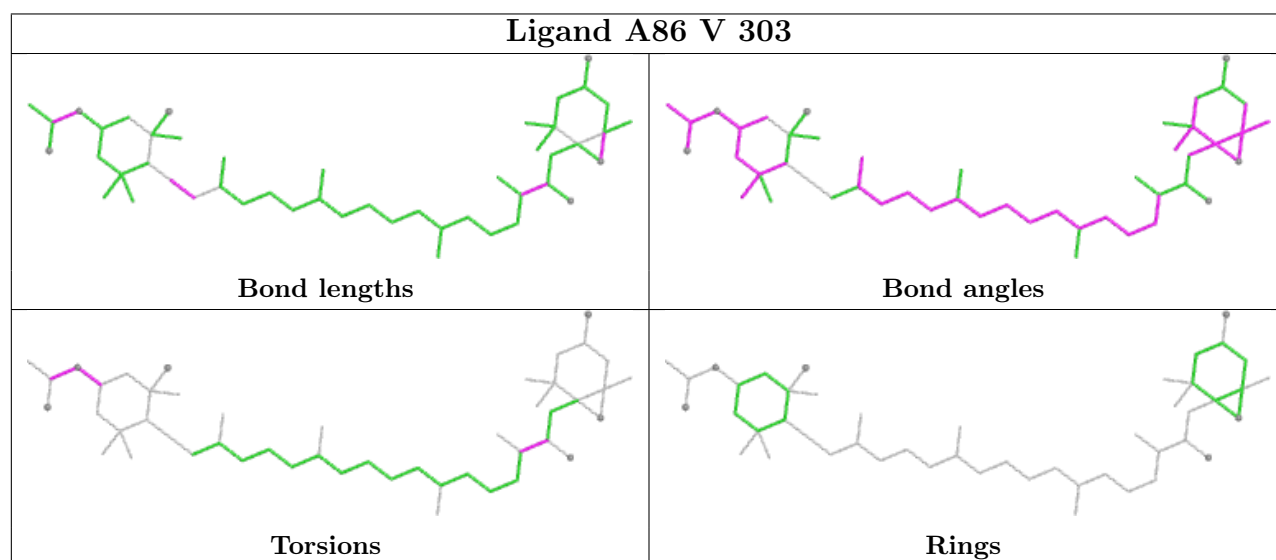
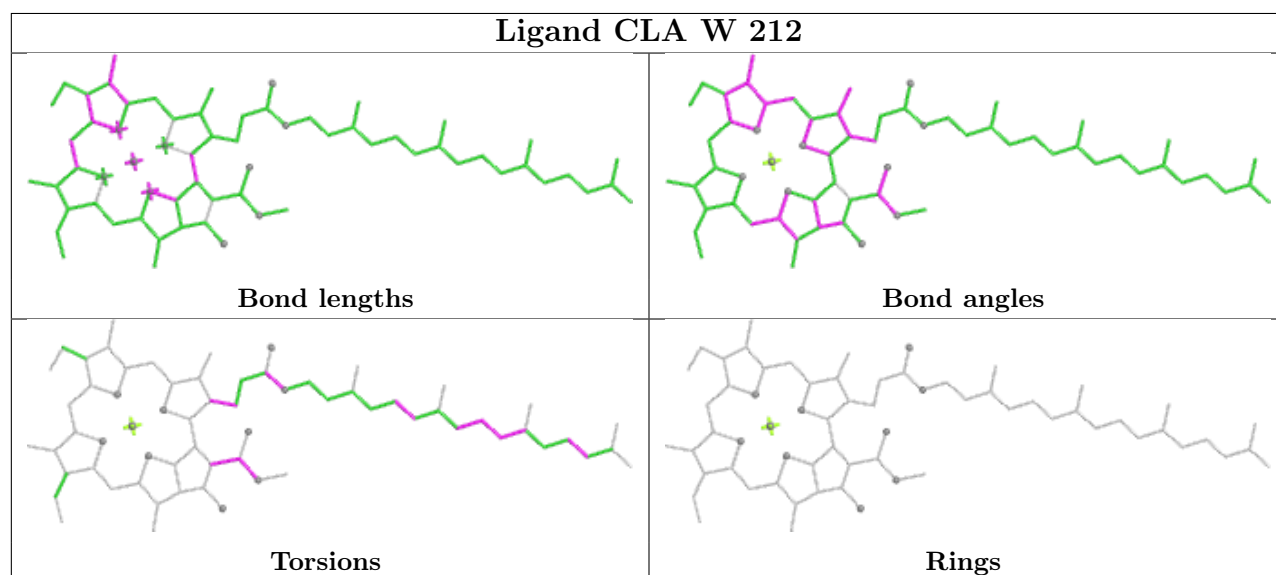
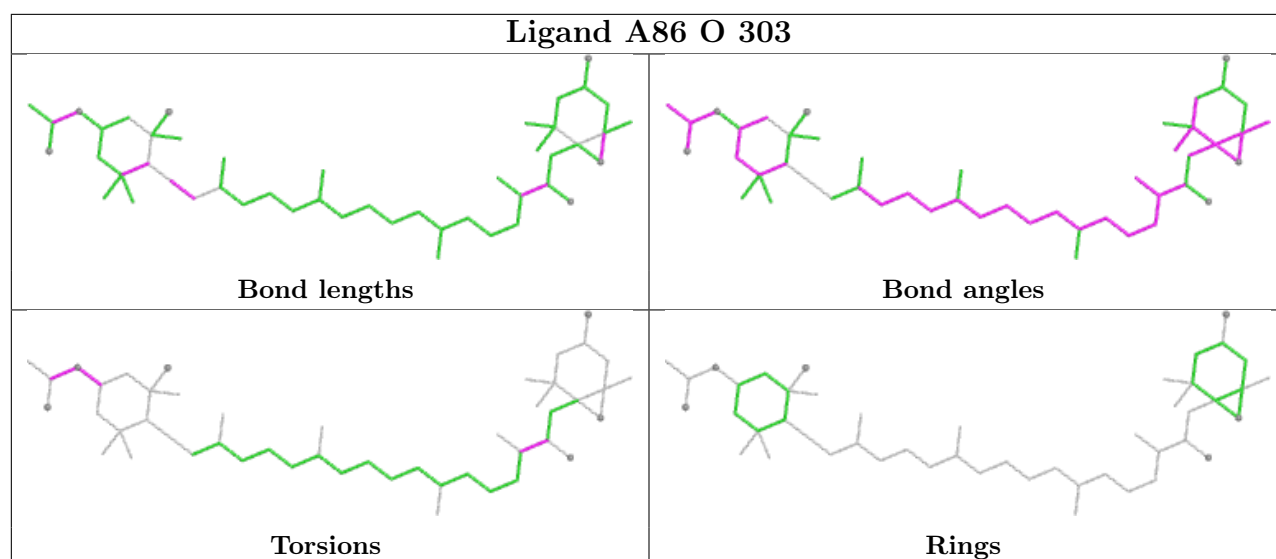
## Ligand CLA P 312

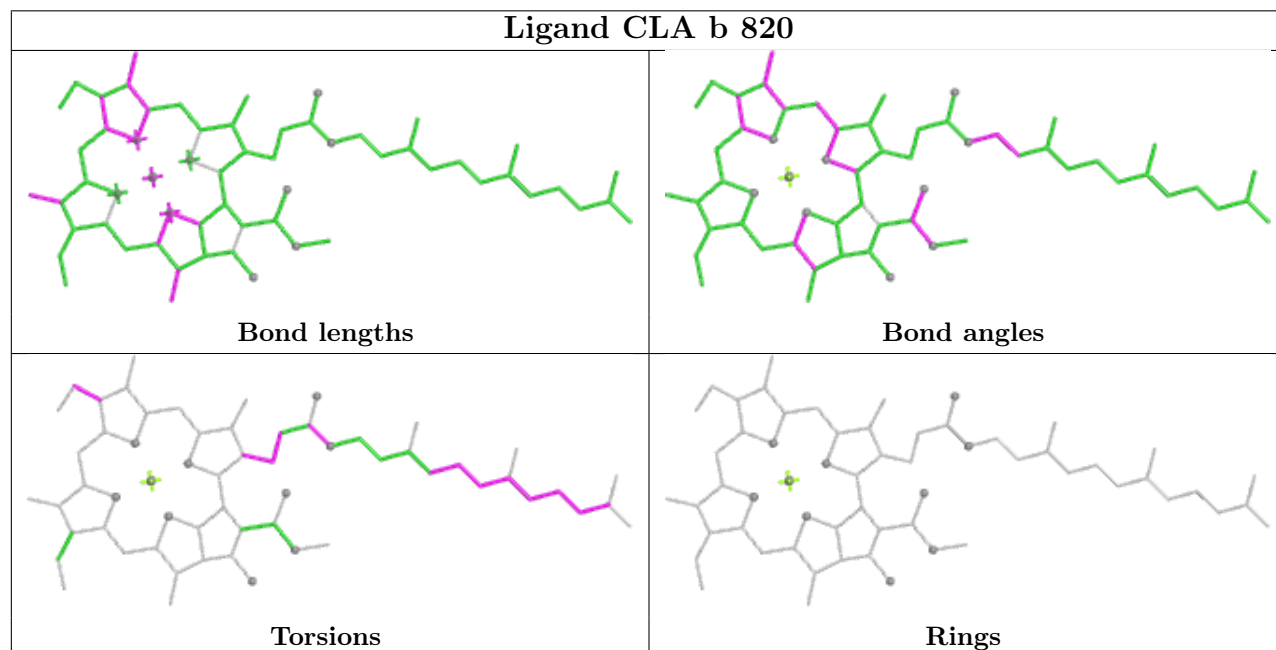
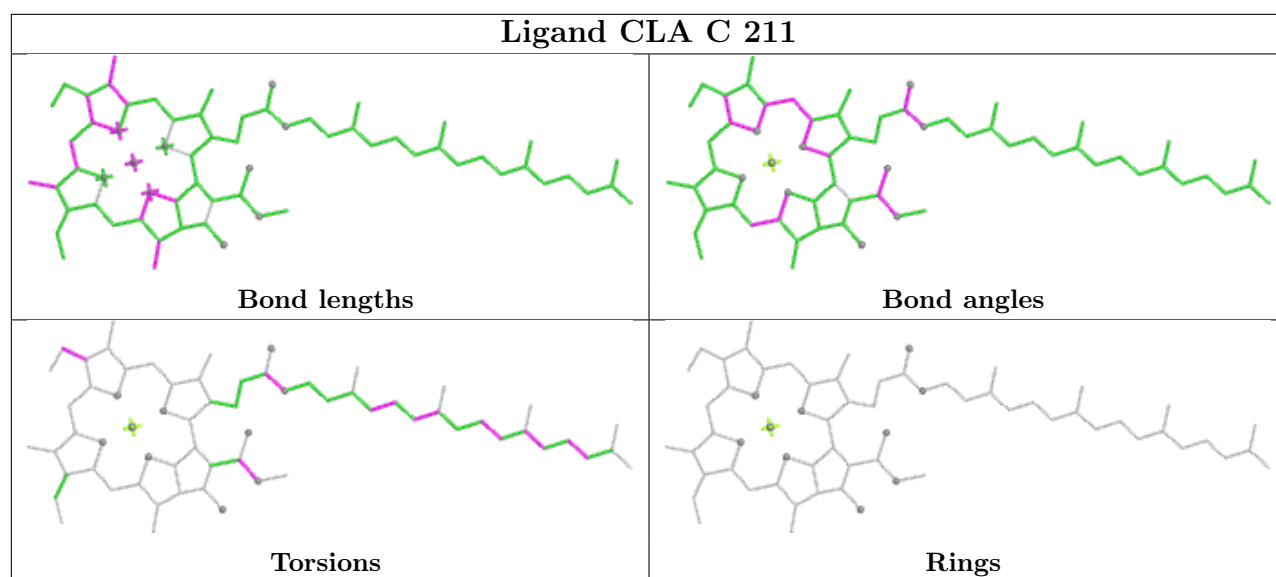


## Ligand A86 N 306

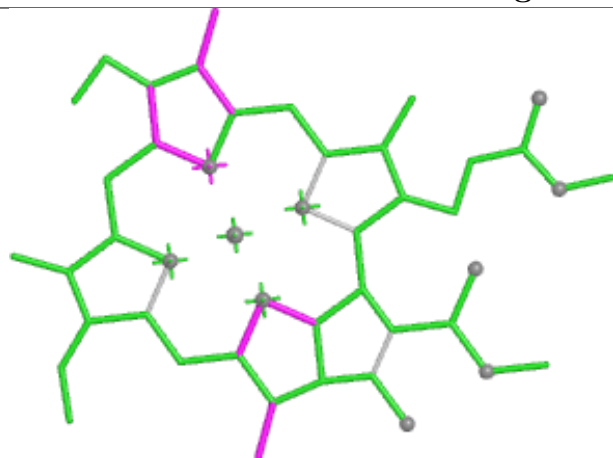




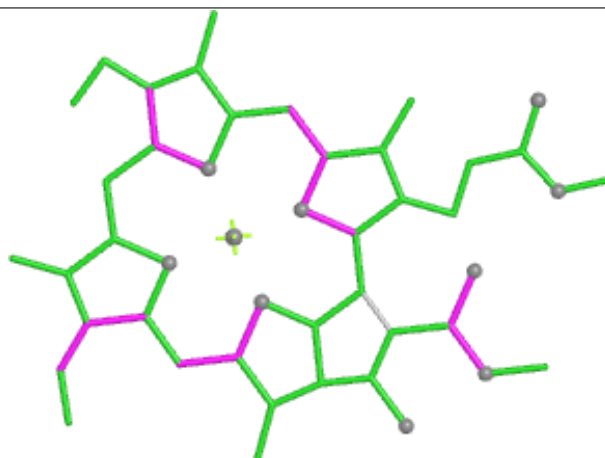




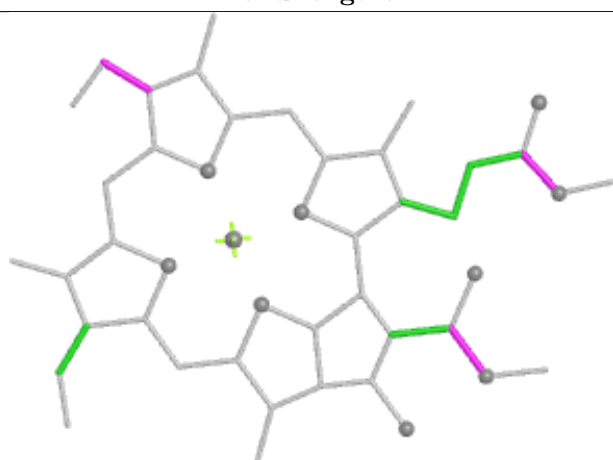
## Ligand CLA B 306



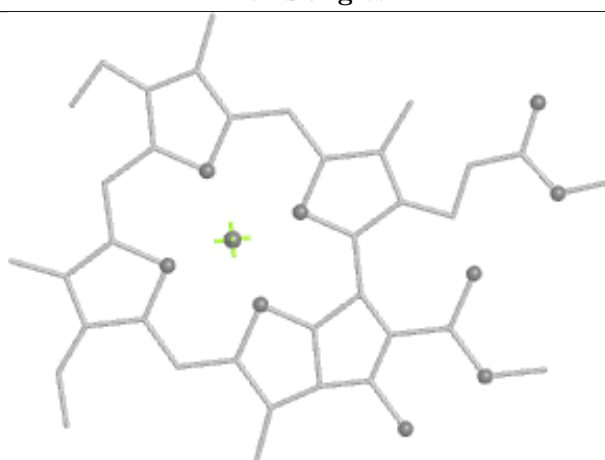
Bond lengths



Bond angles

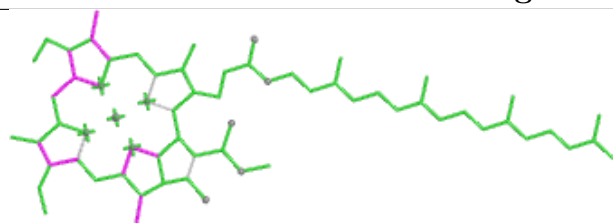


Torsions

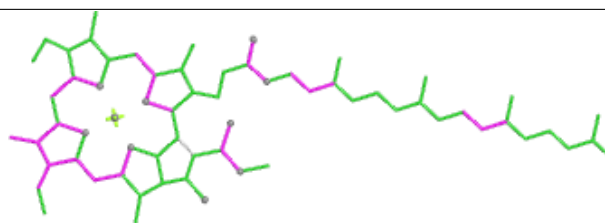


Rings

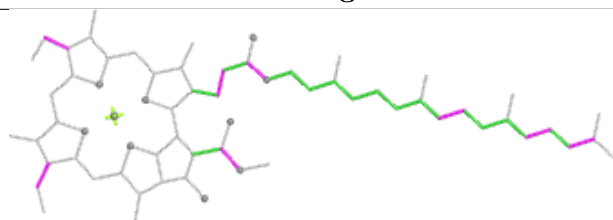
## Ligand CLA T 311



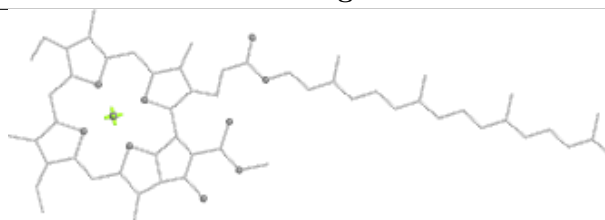
Bond lengths



Bond angles

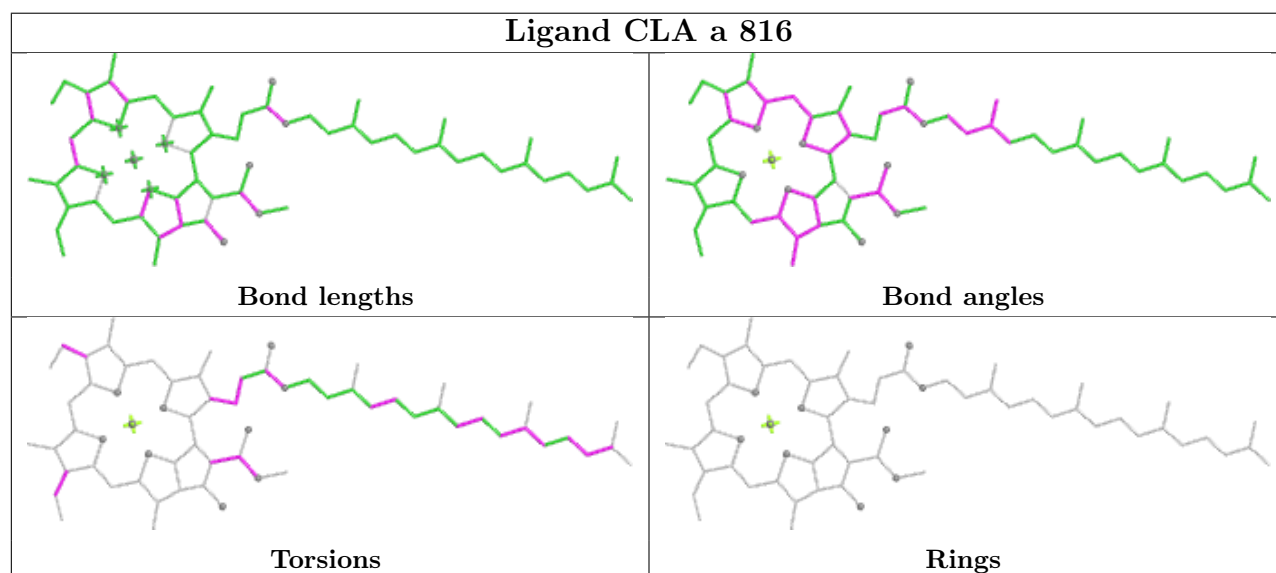
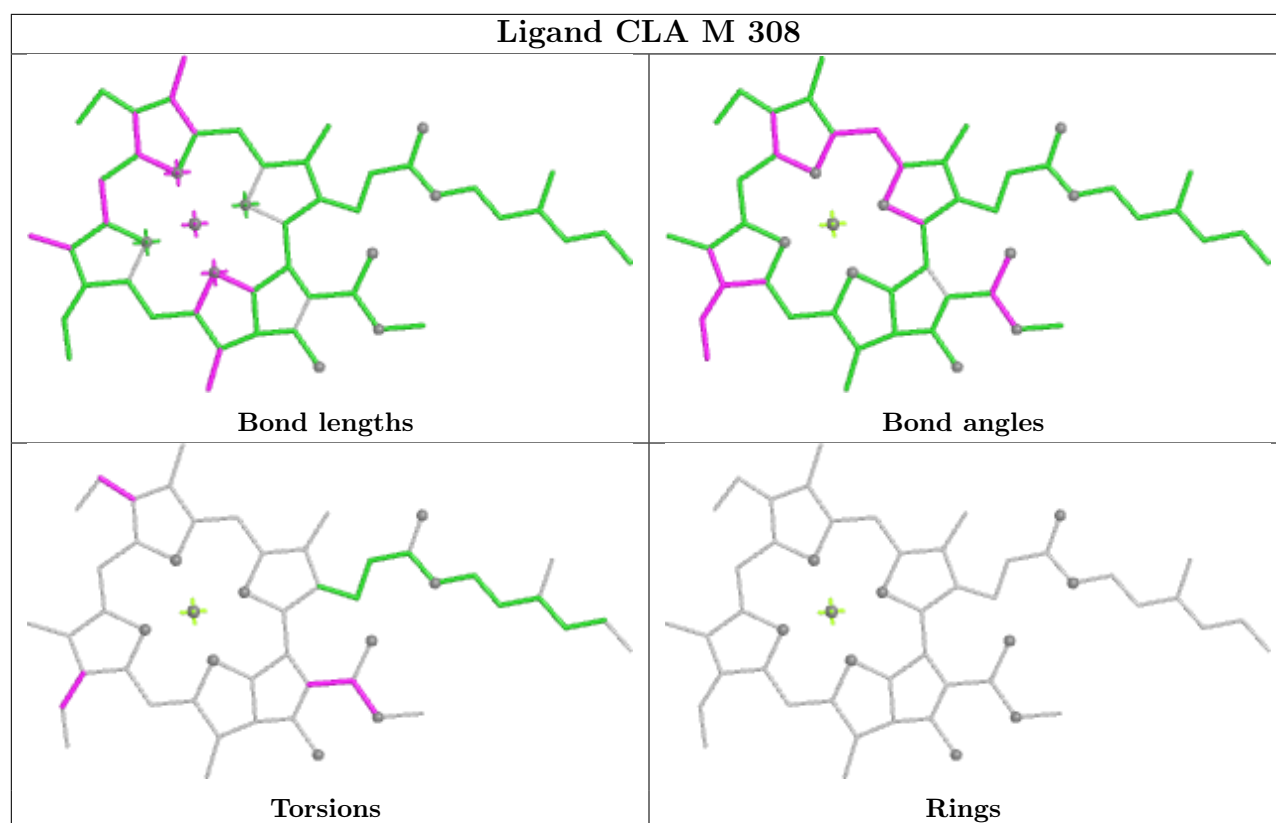


Torsions

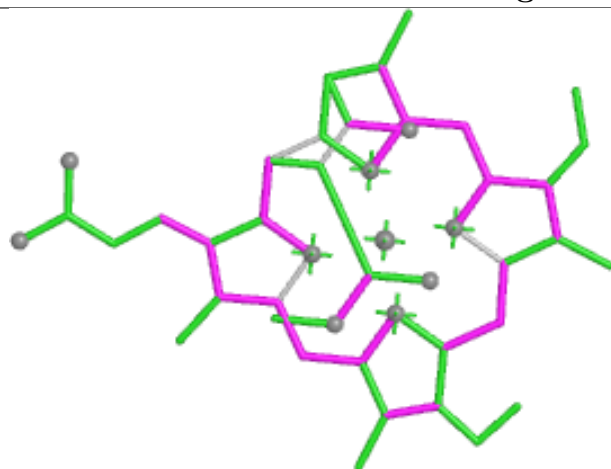


Rings

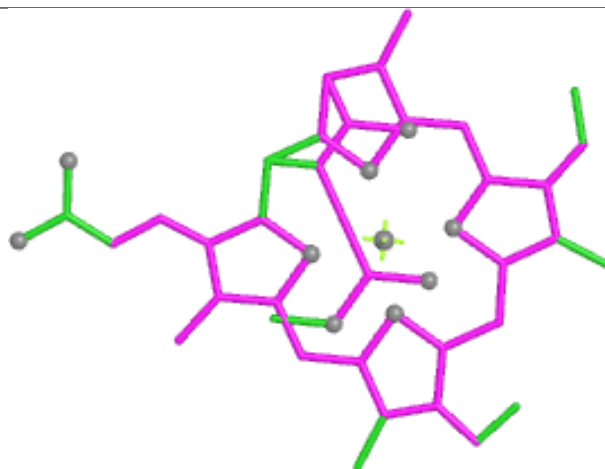




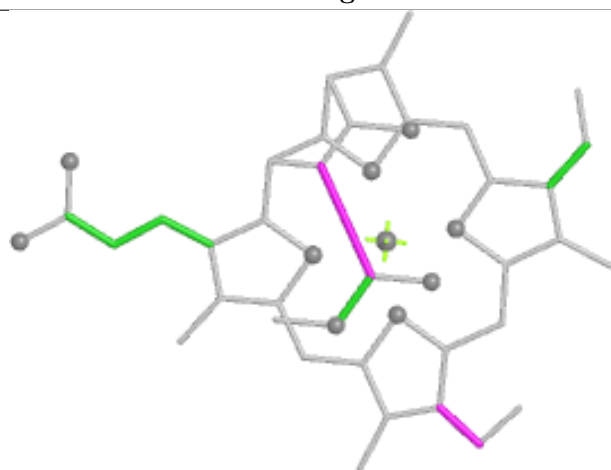
## Ligand KC1 P 315



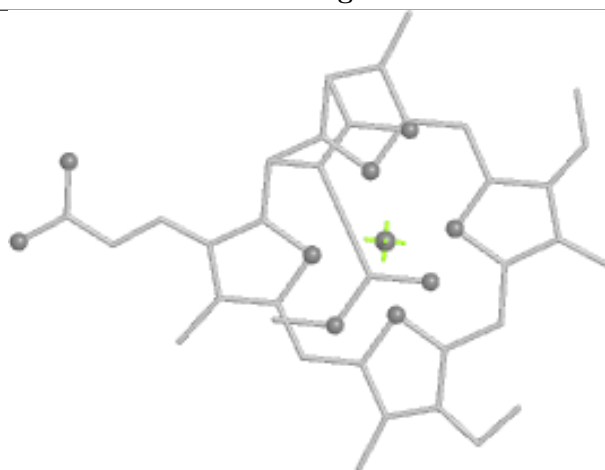
Bond lengths



Bond angles

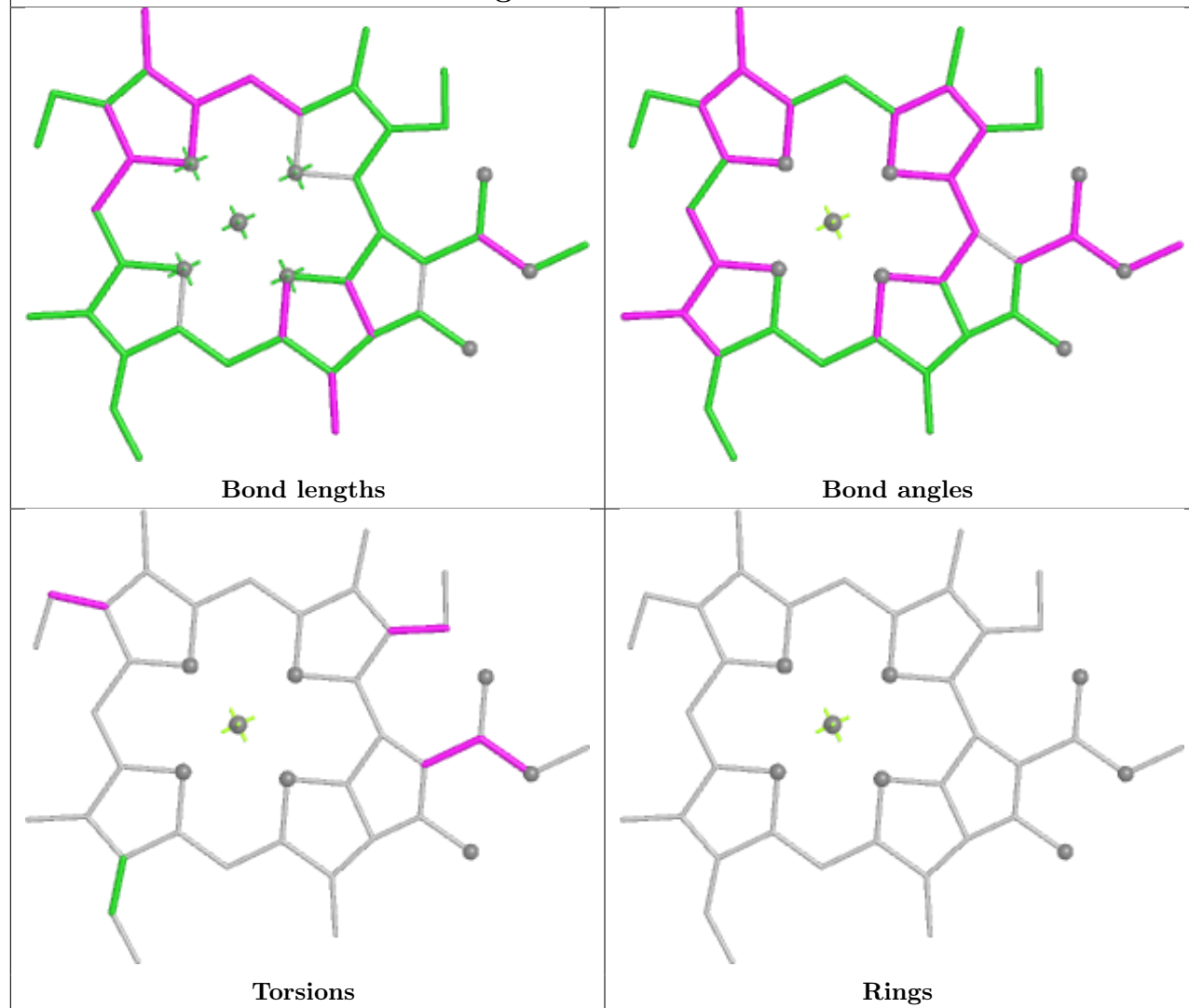


Torsions

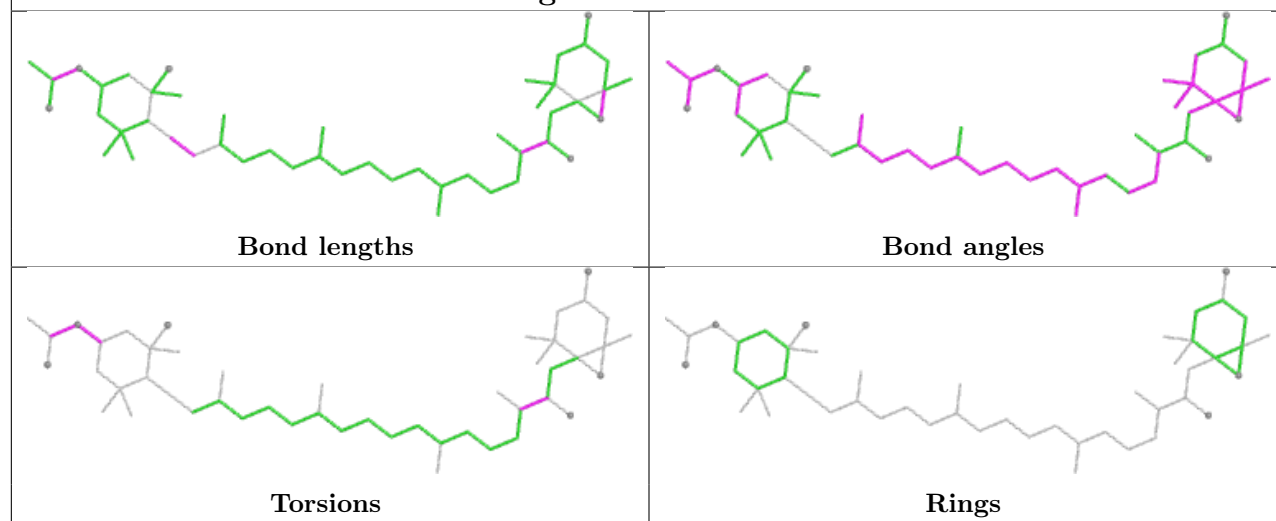


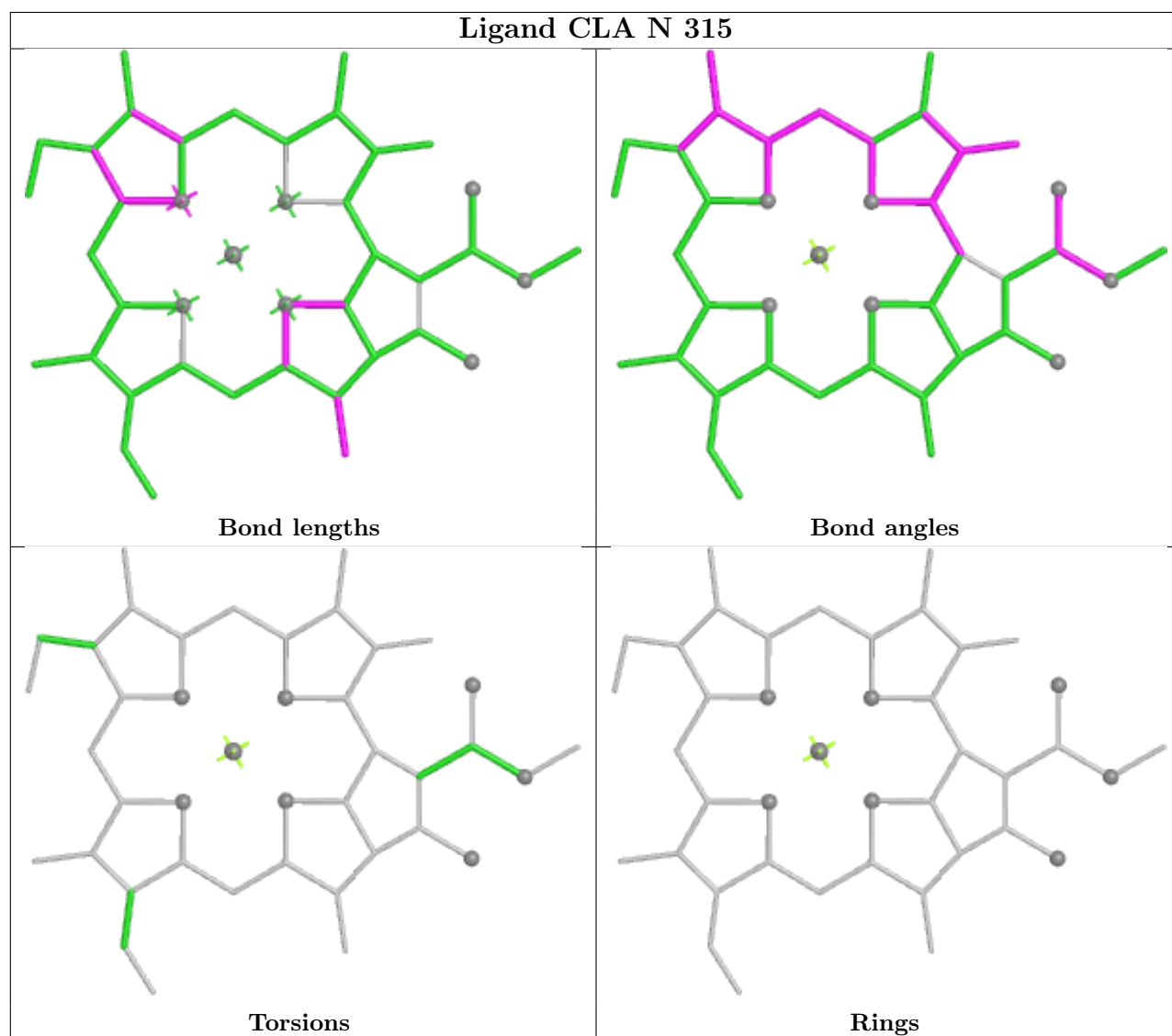
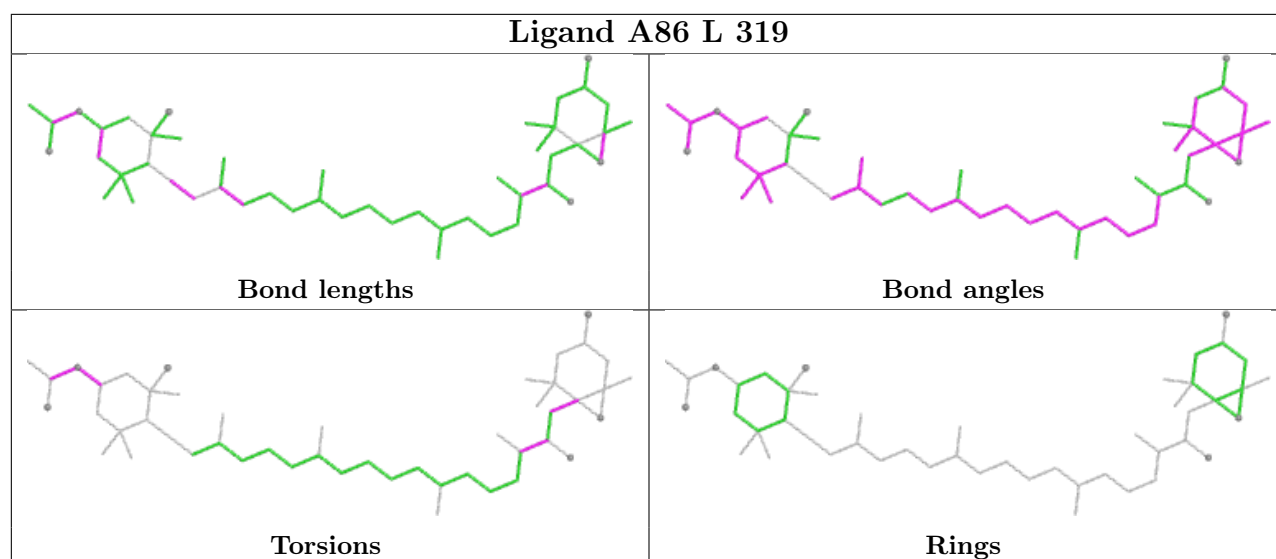
Rings

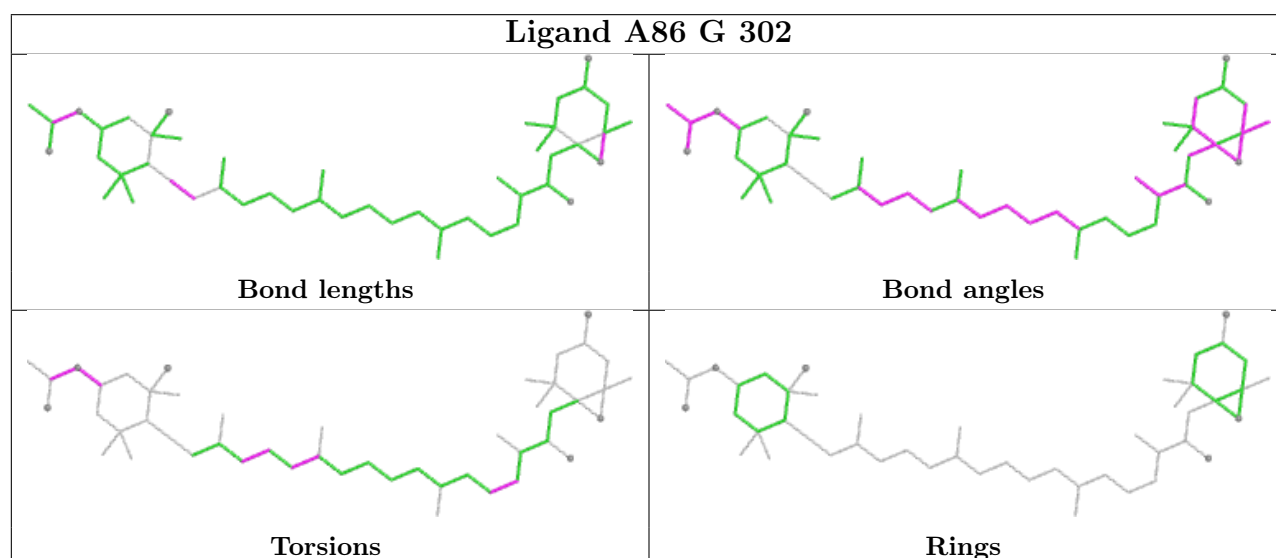
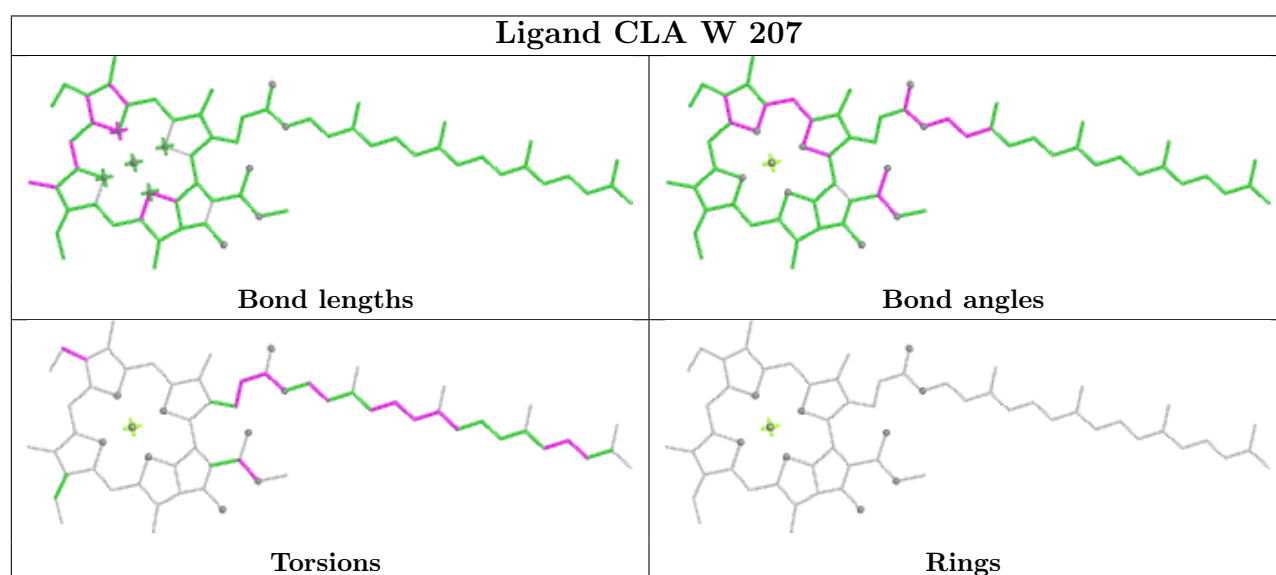
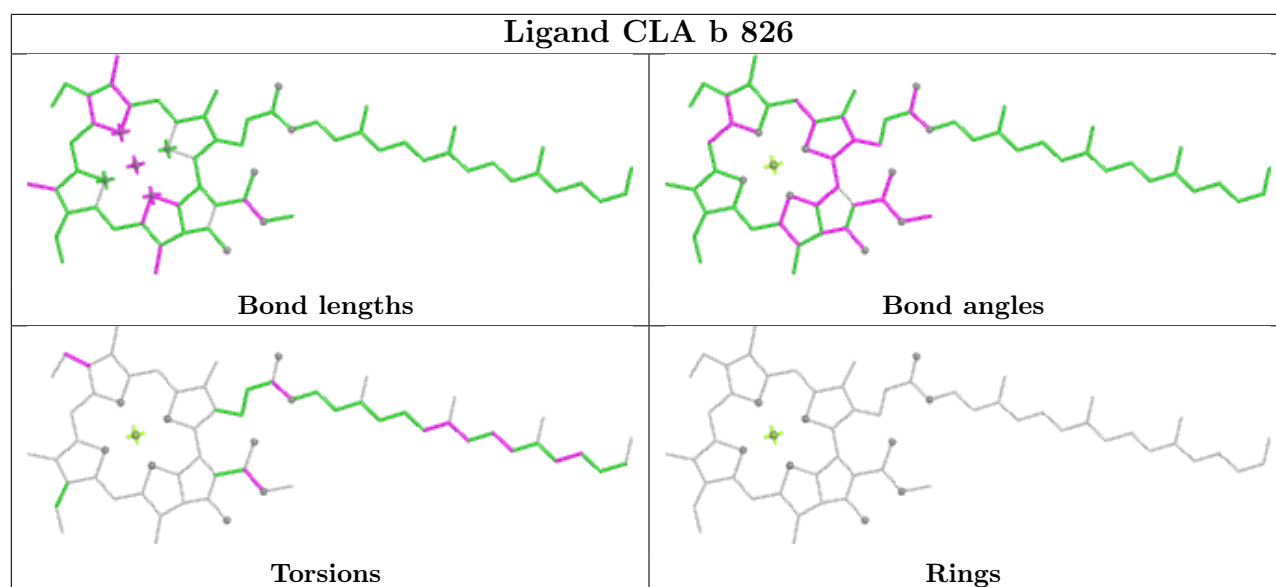
## Ligand CLA X 313



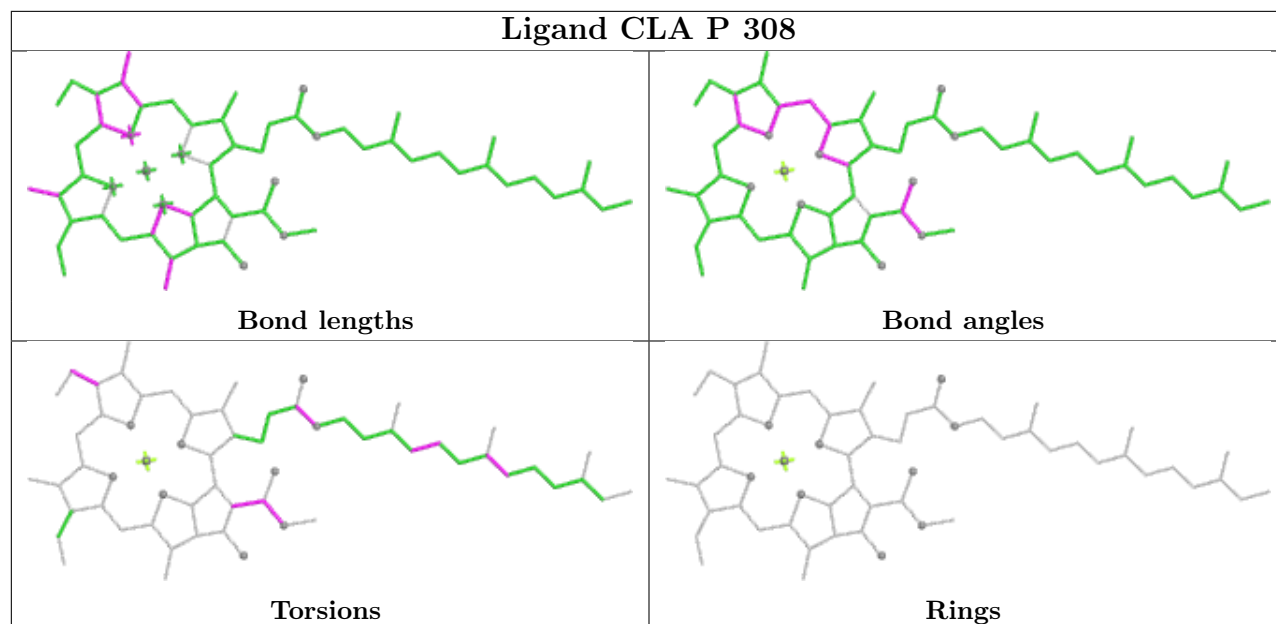
## Ligand A86 T 306



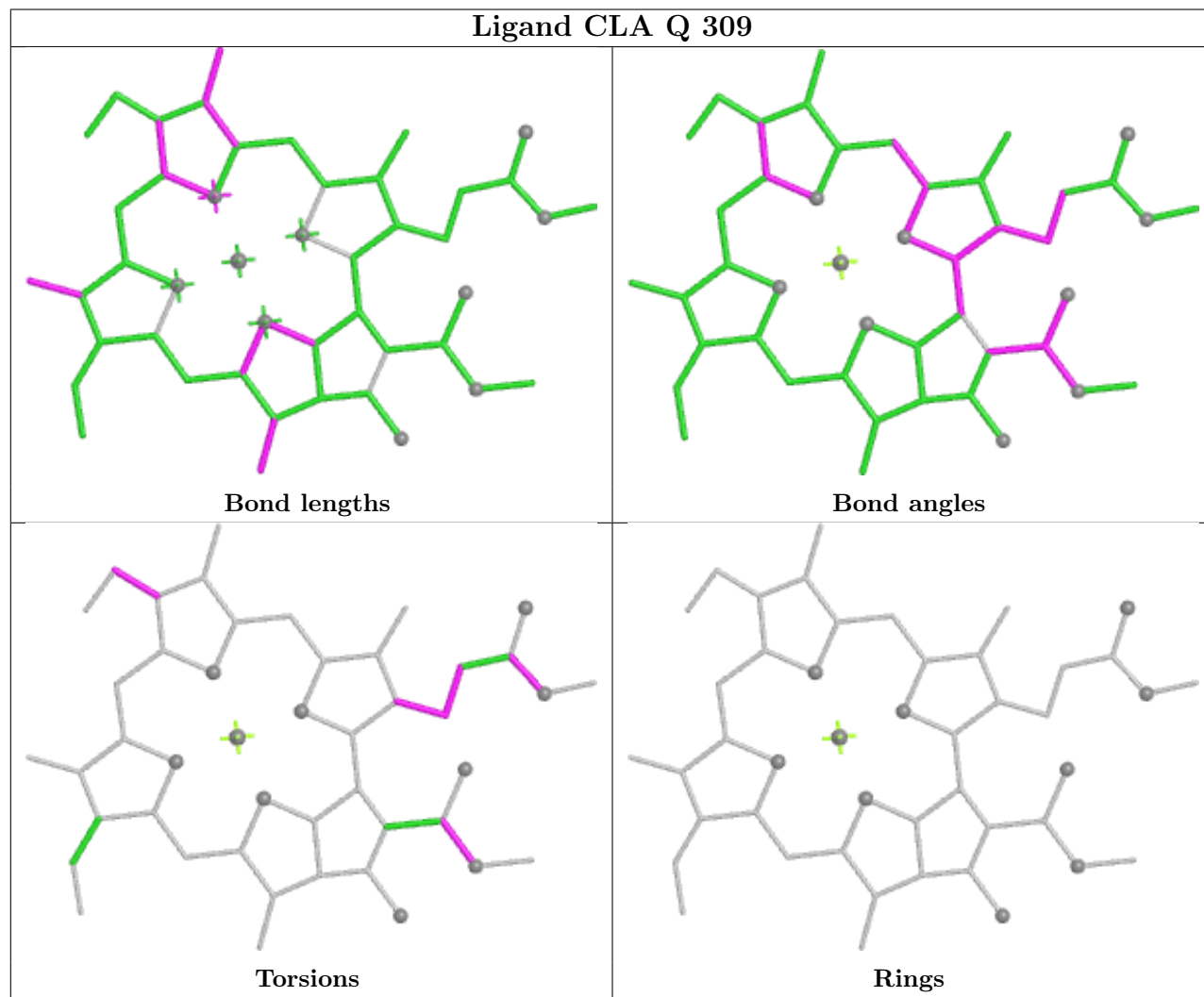


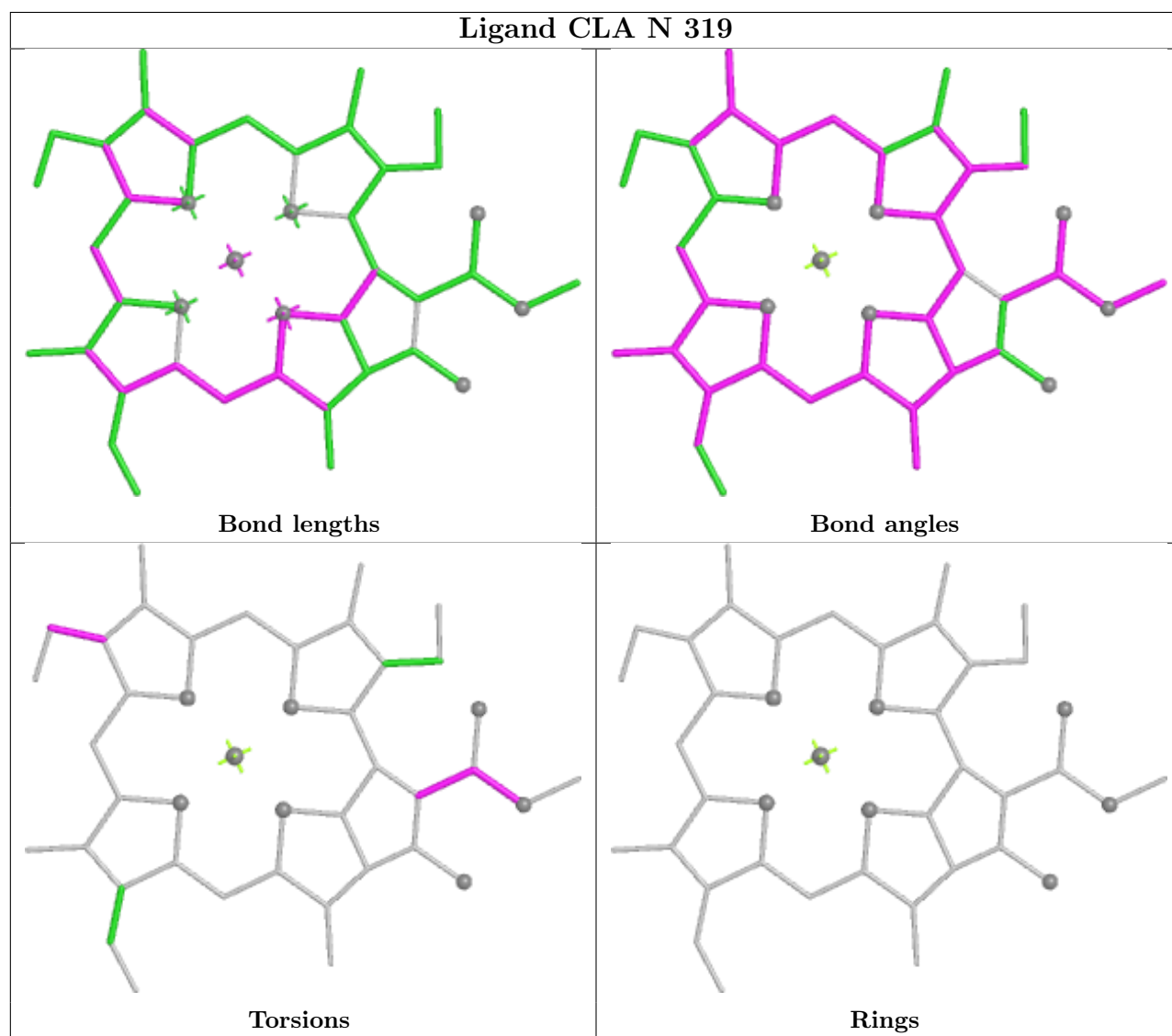
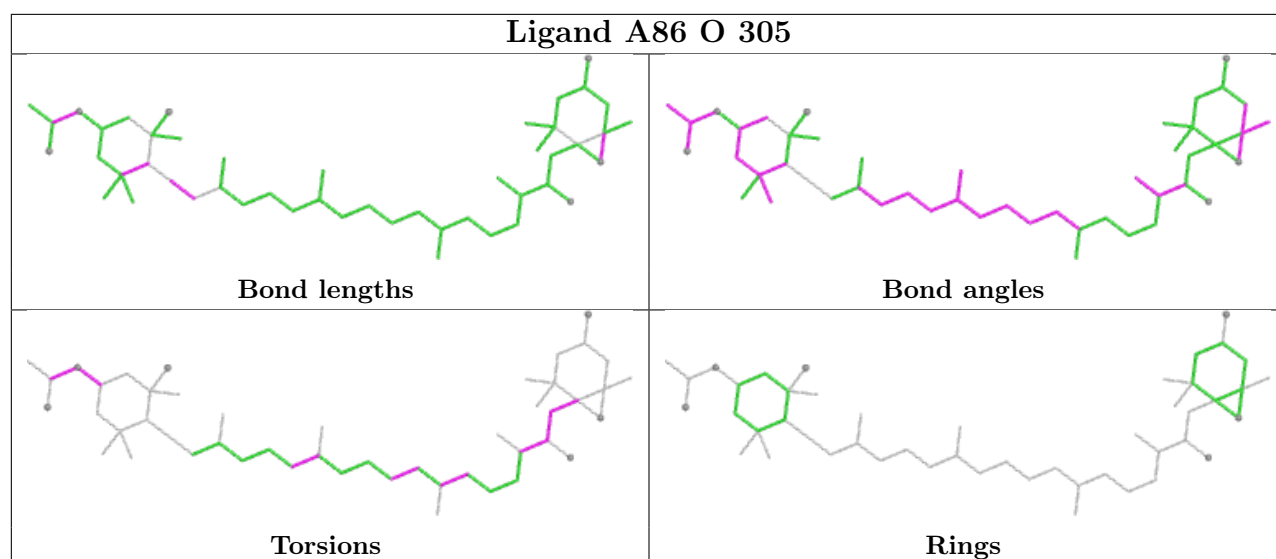


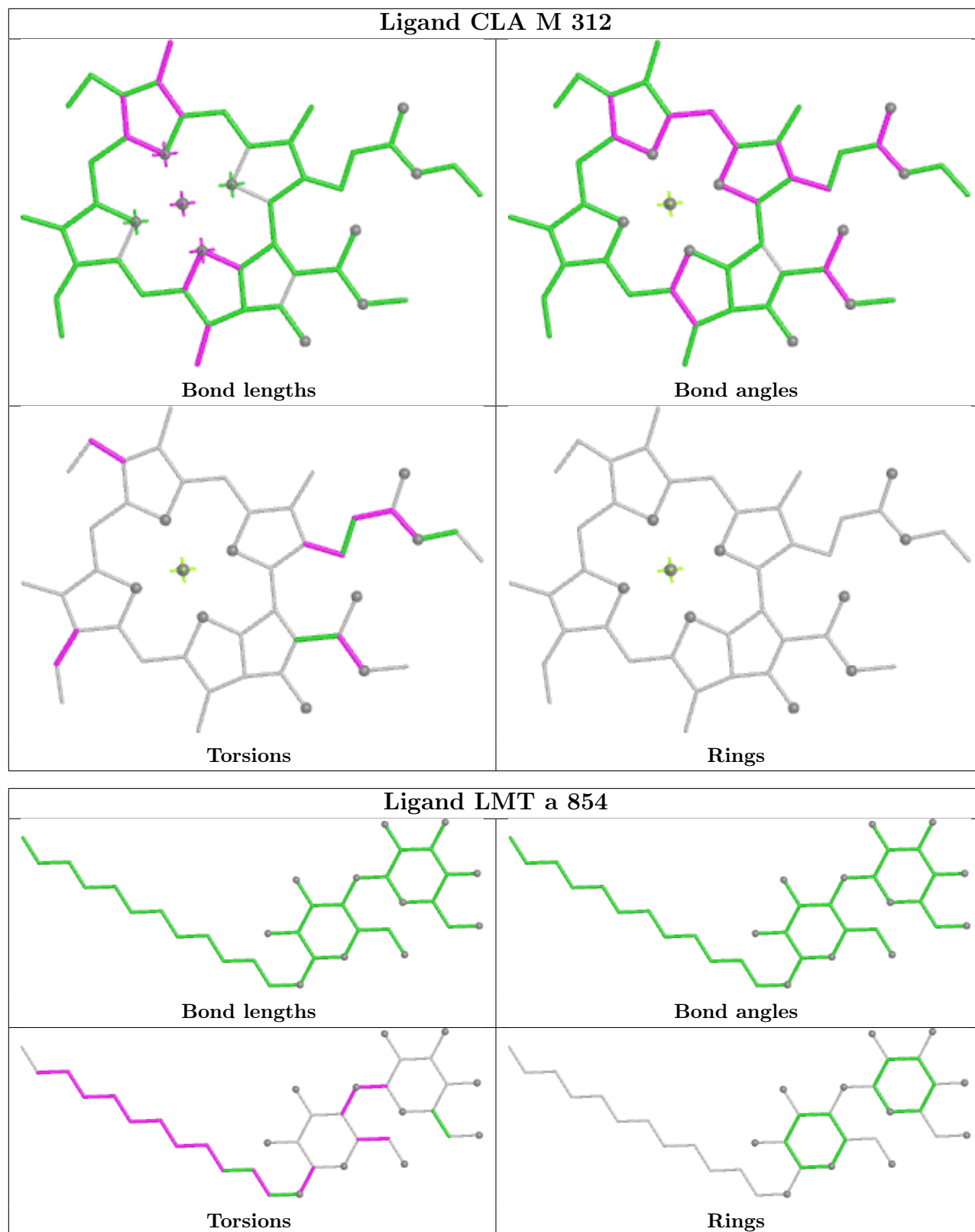
## Ligand CLA P 308



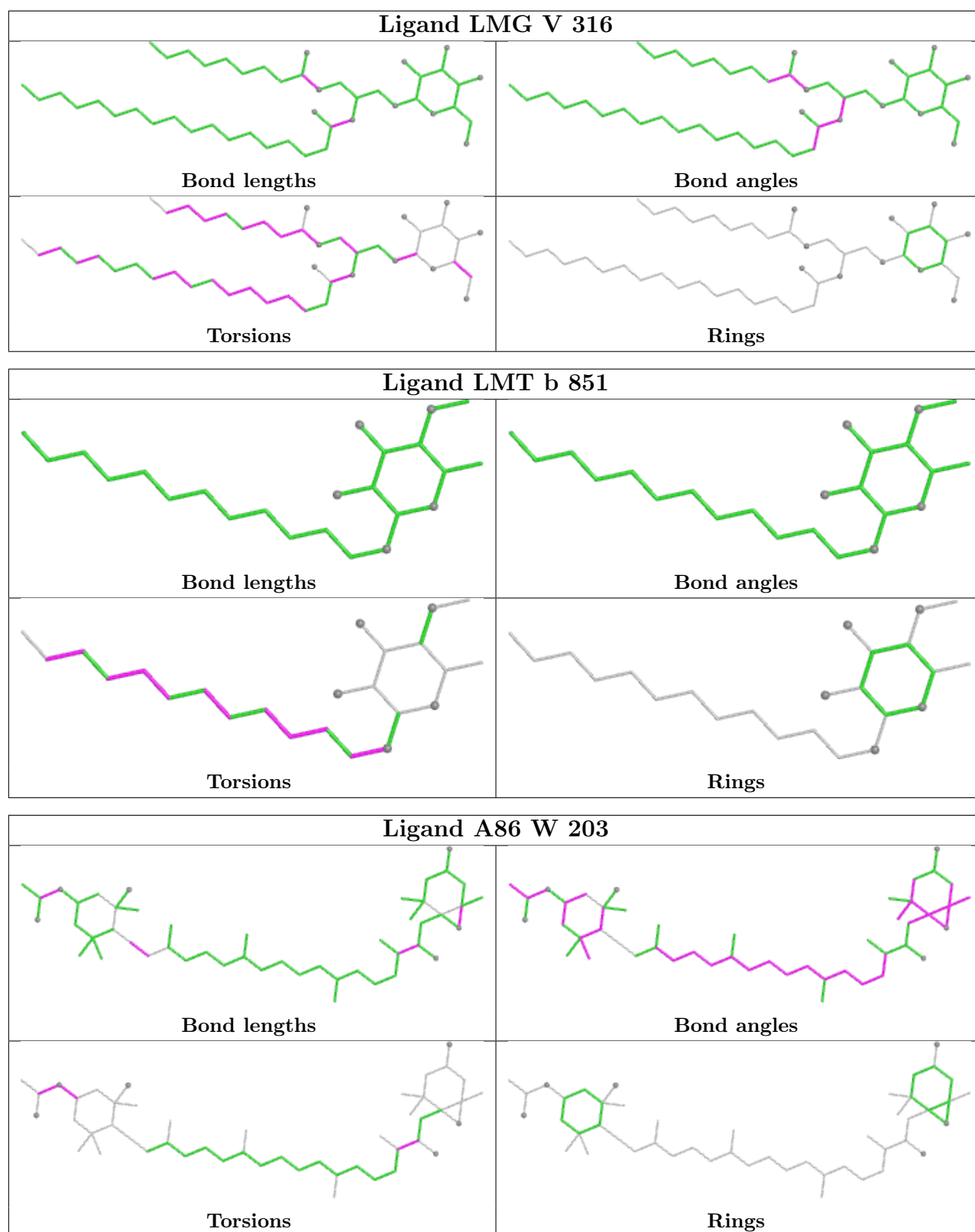
## Ligand CLA Q 309



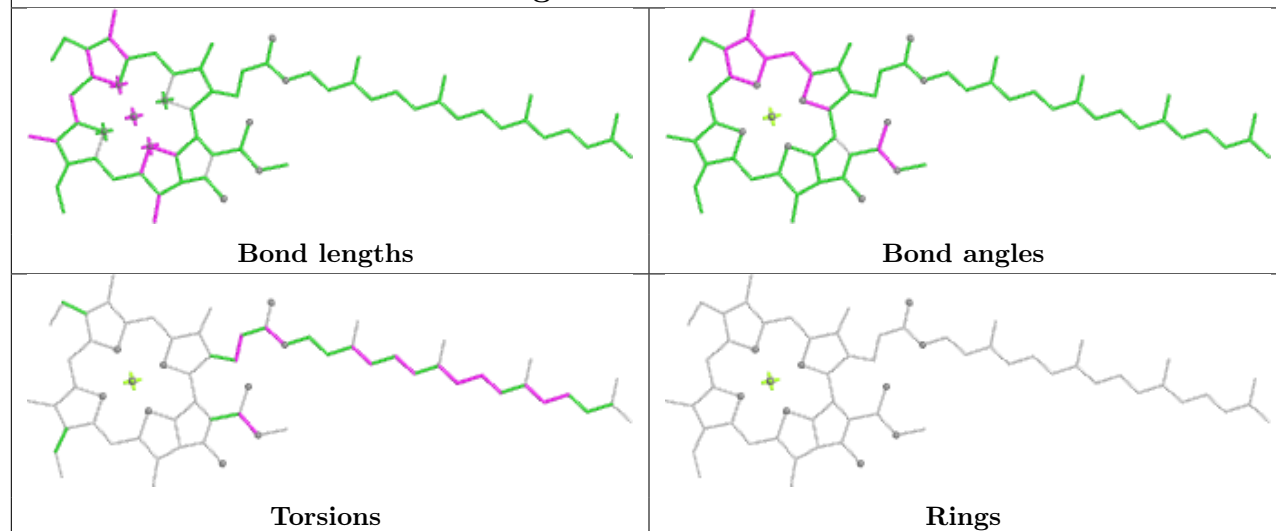




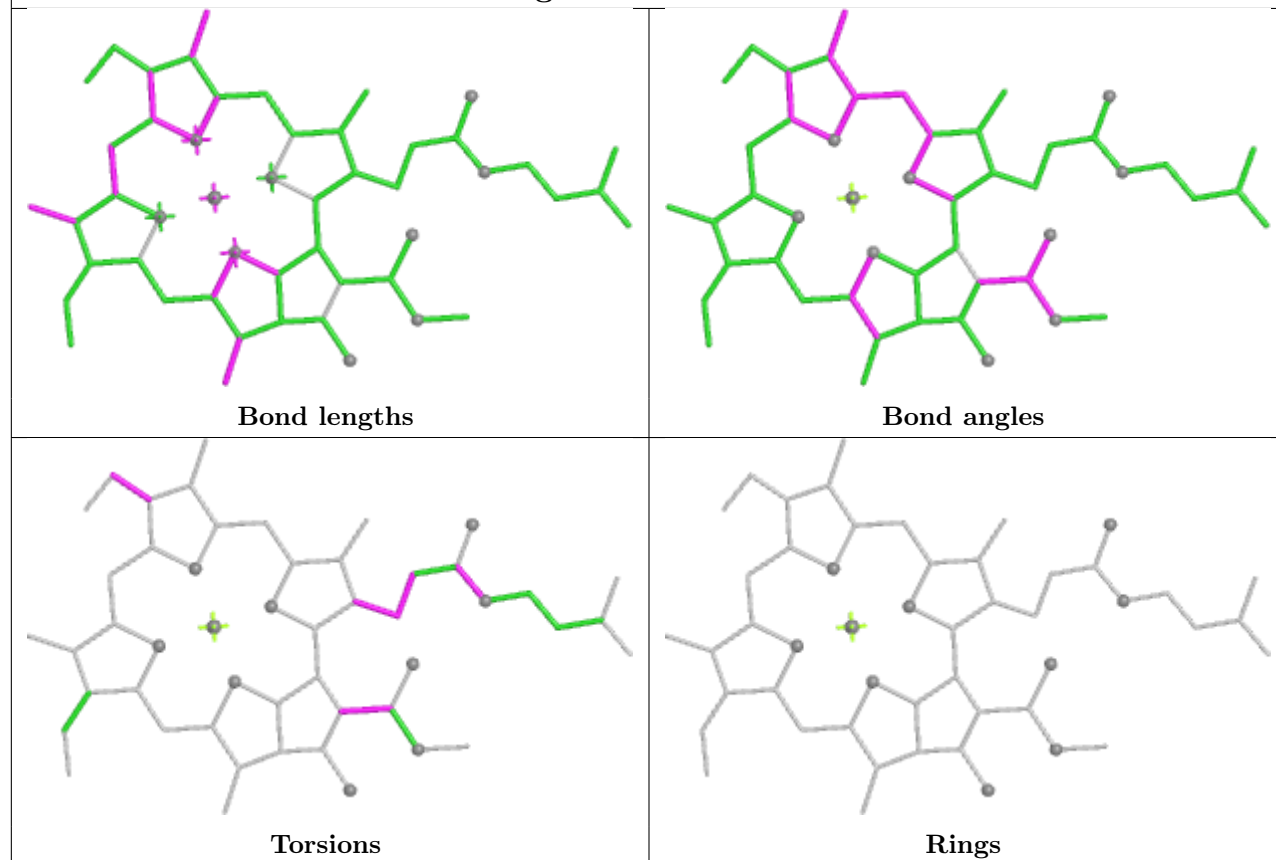


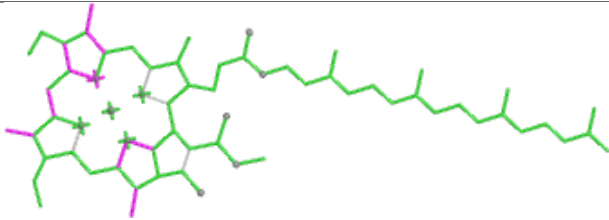
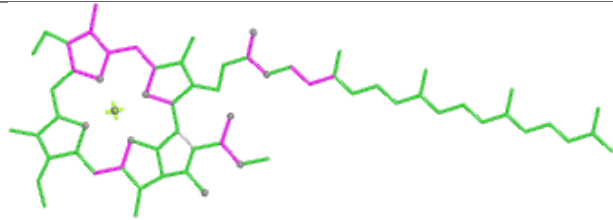
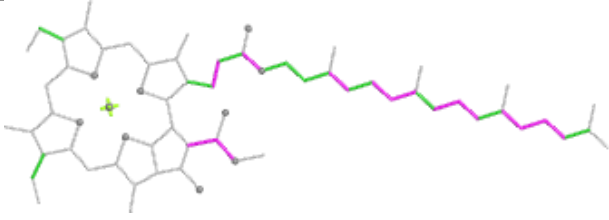
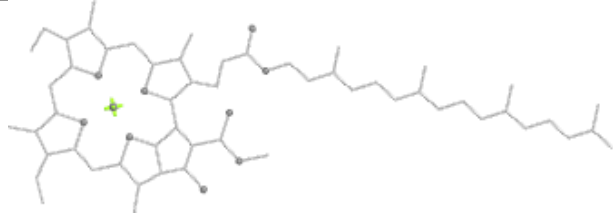


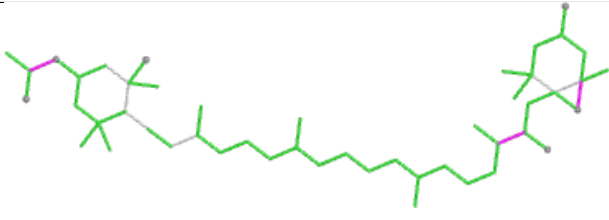
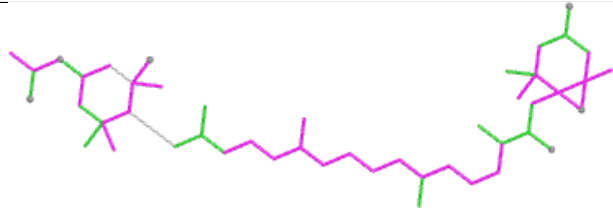
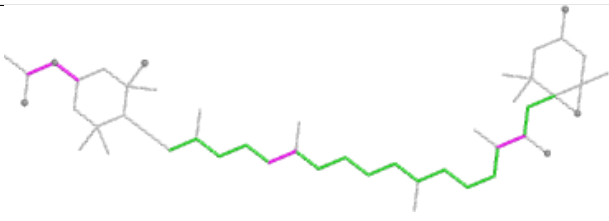
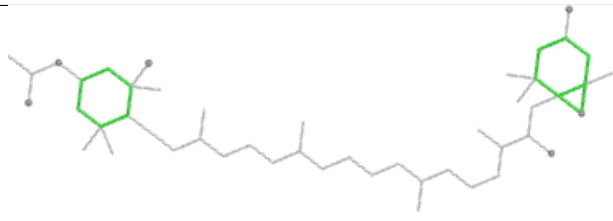
## Ligand CLA P 309

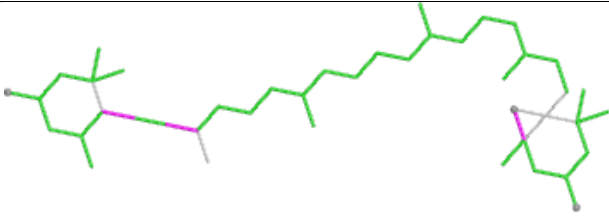
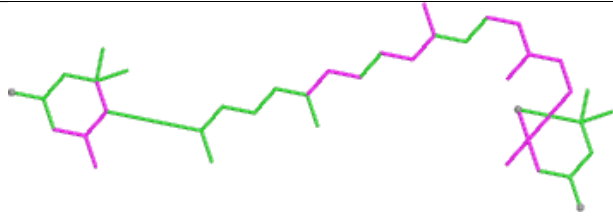
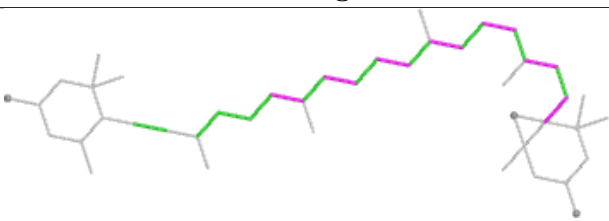
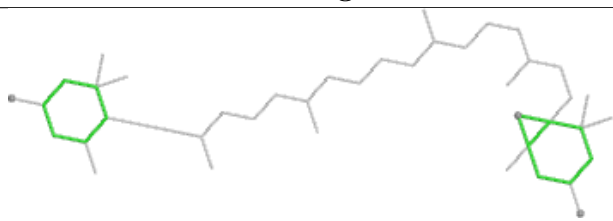


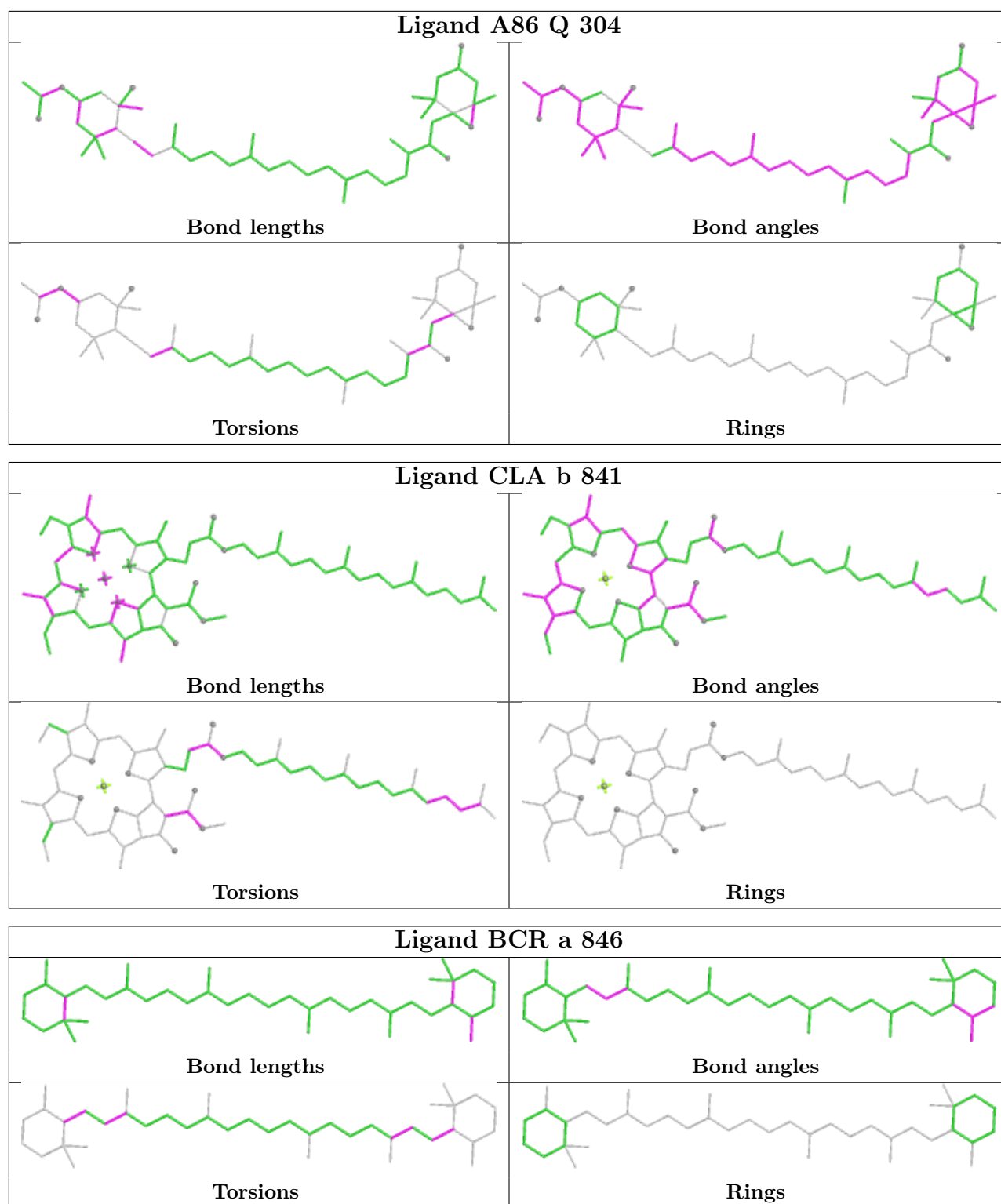
## Ligand CLA b 831

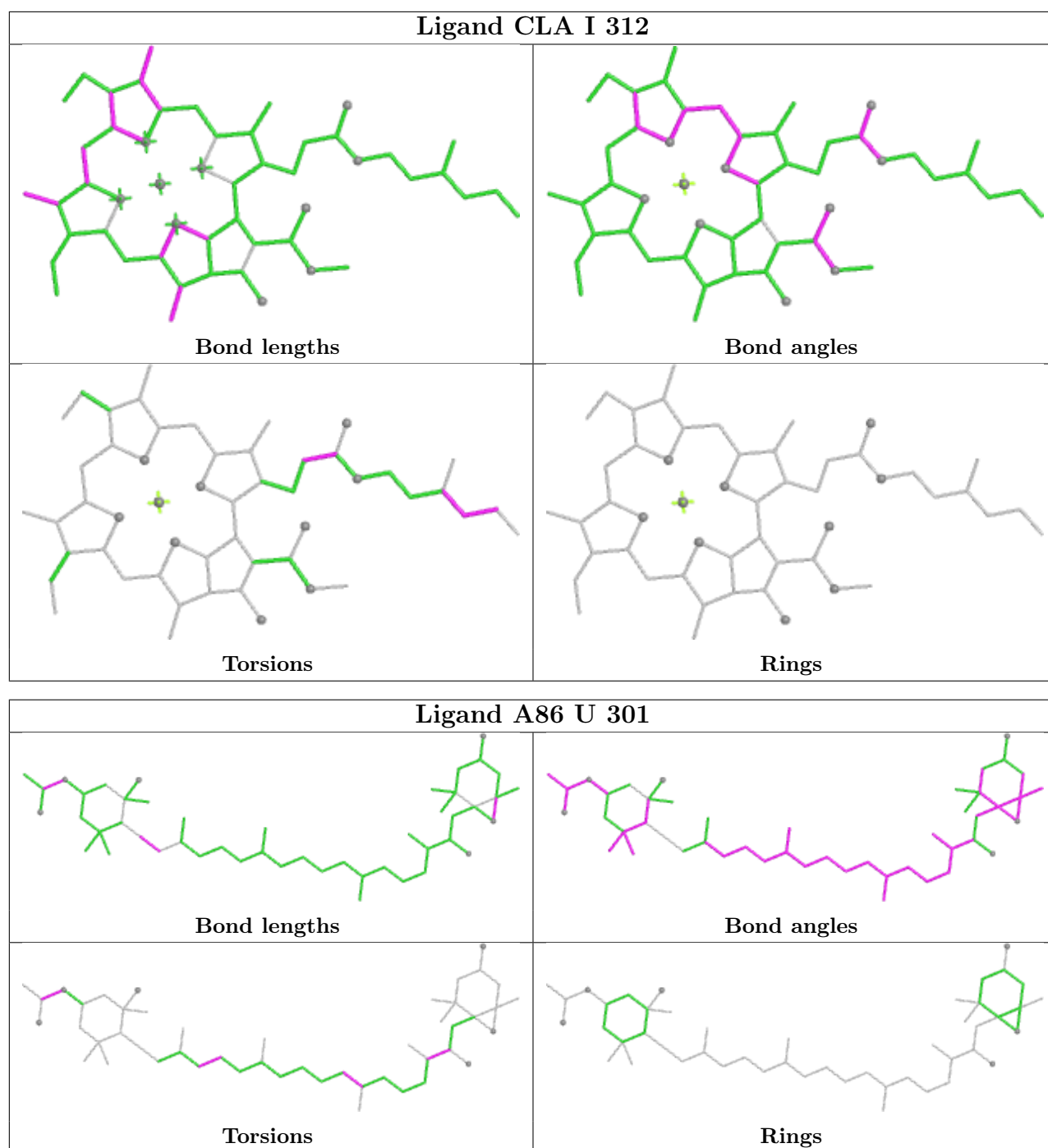


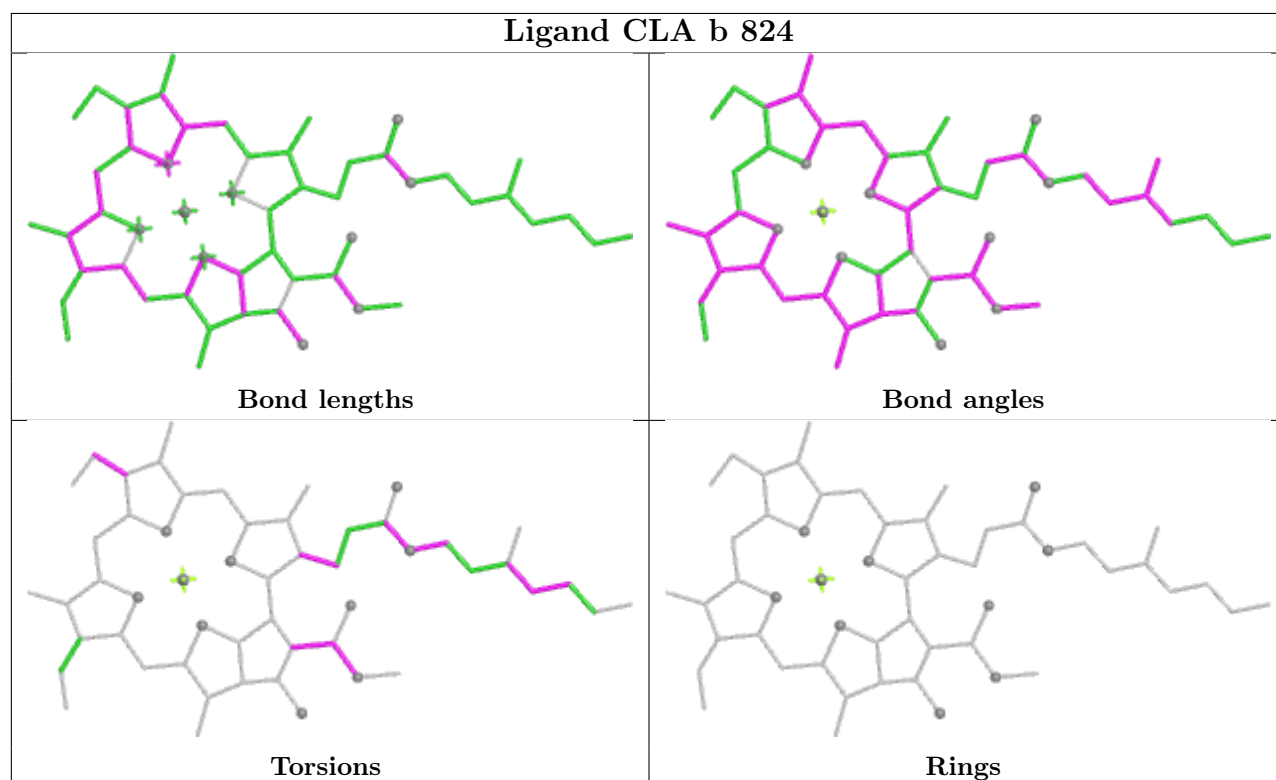
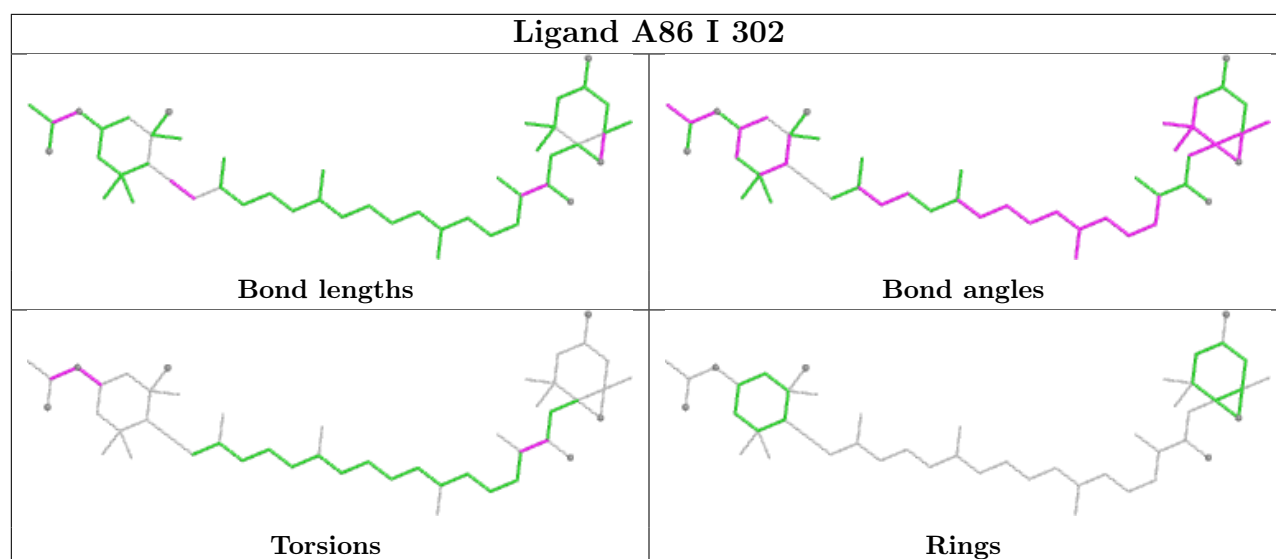
| Ligand CLA V 308                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

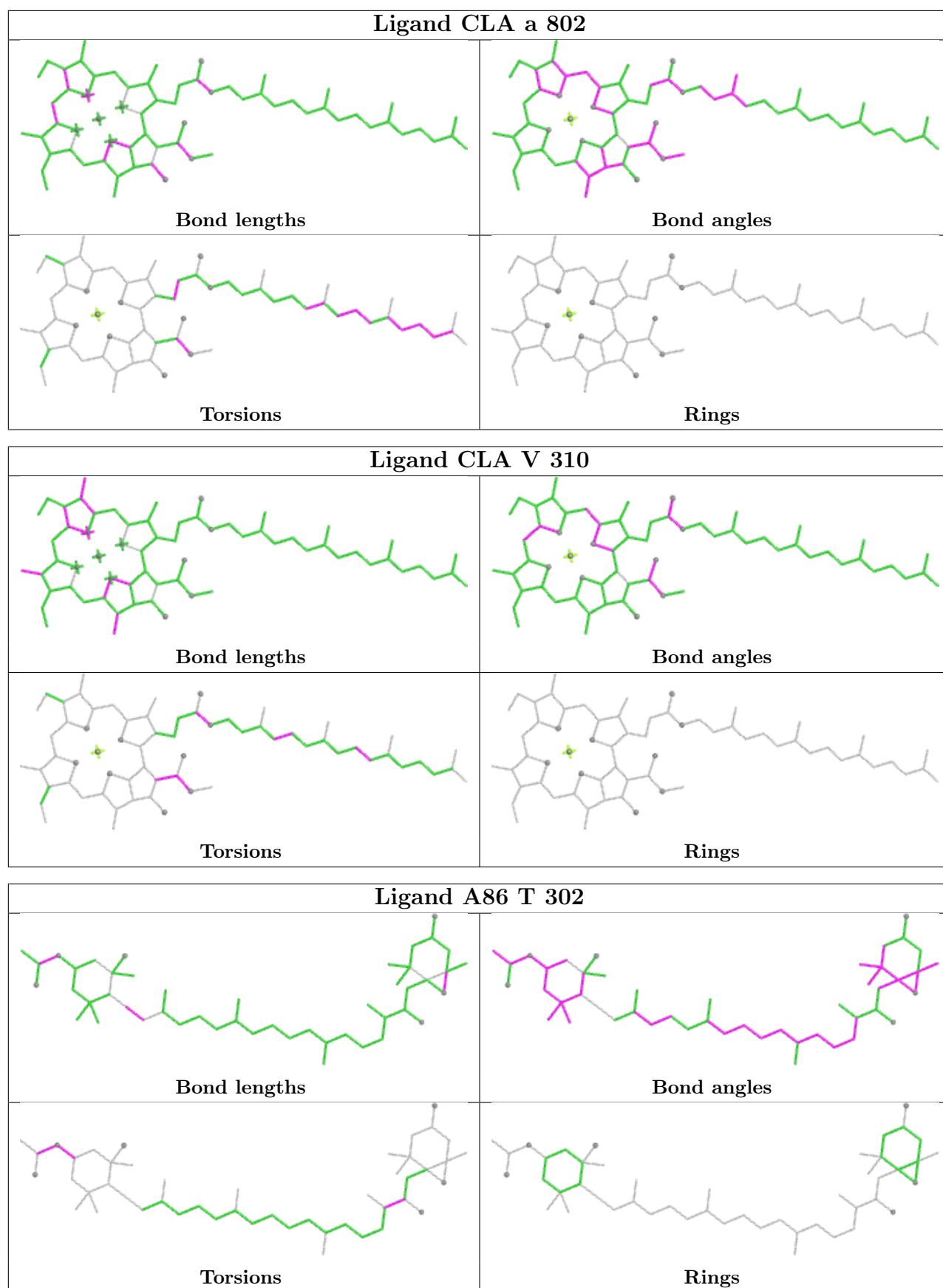
| Ligand A86 L 306                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

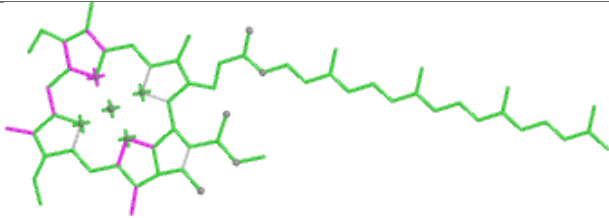
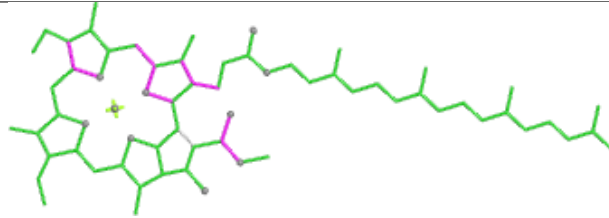
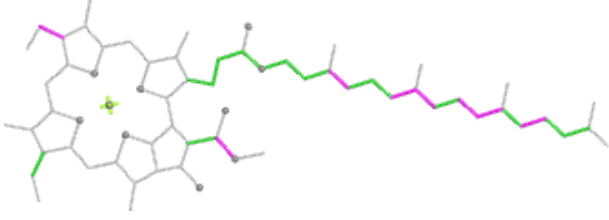
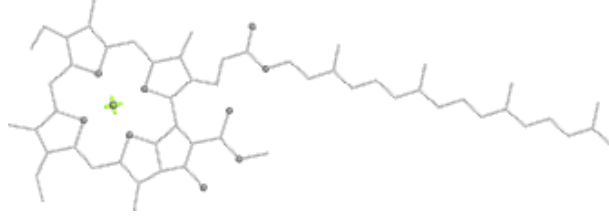
| Ligand DD6 R 308                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

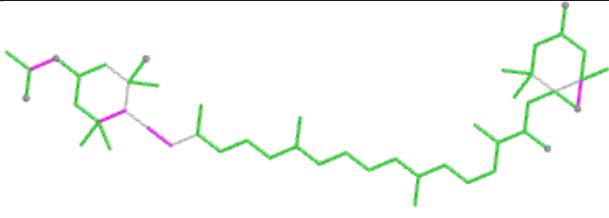
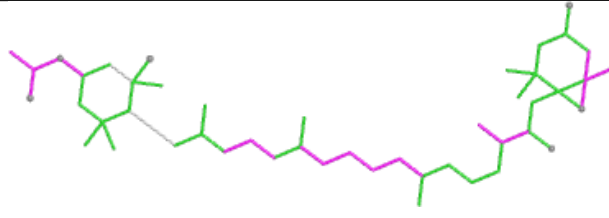
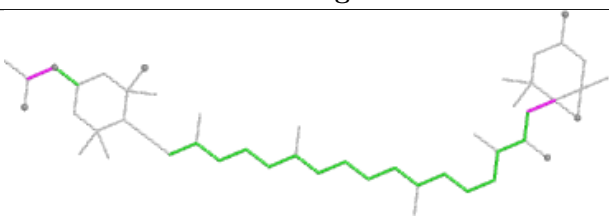
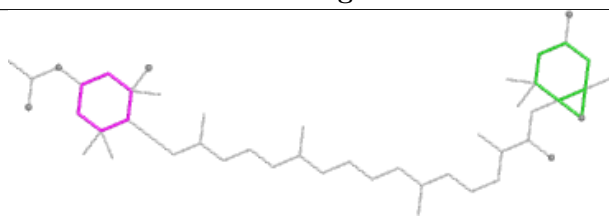


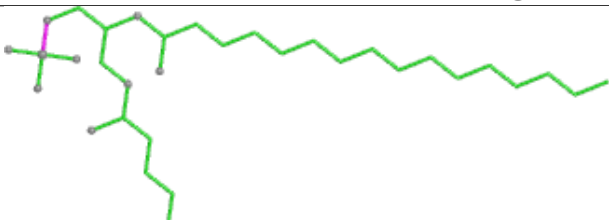
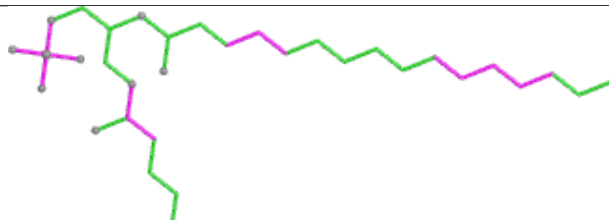
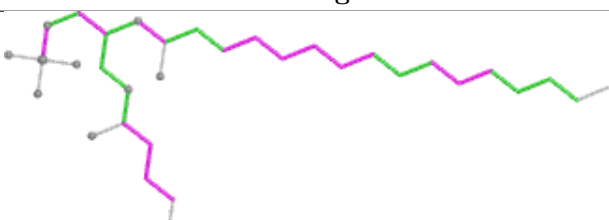
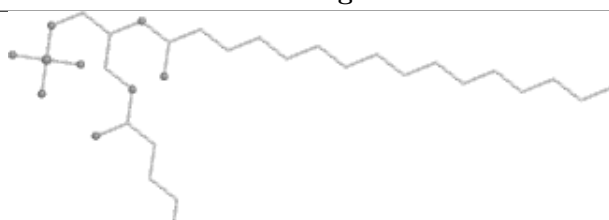






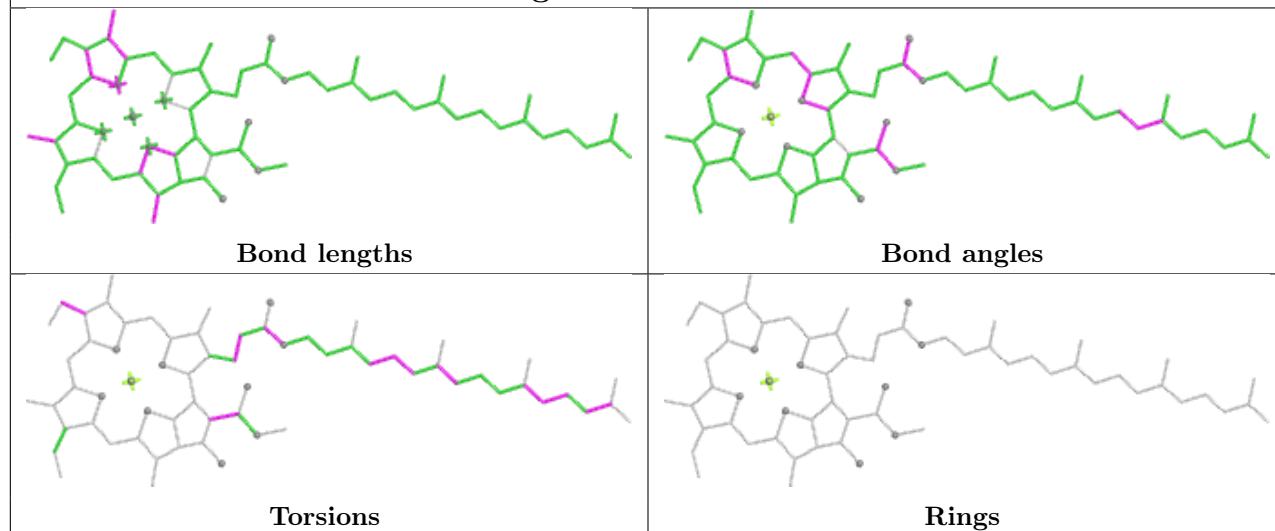
| Ligand CLA N 316                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand A86 h 202                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

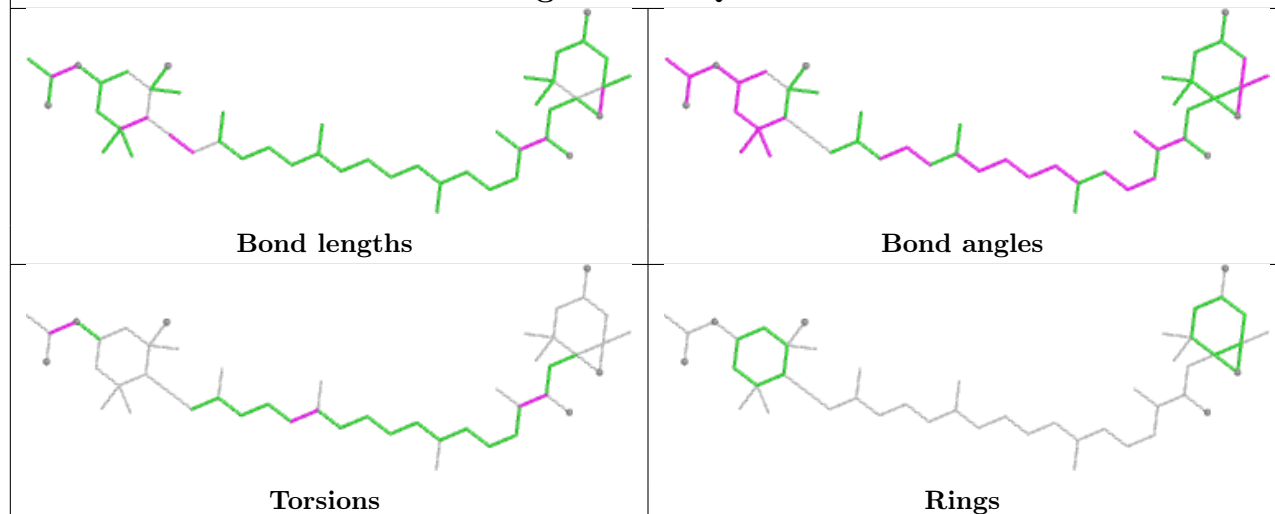
| Ligand LHG F 318                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



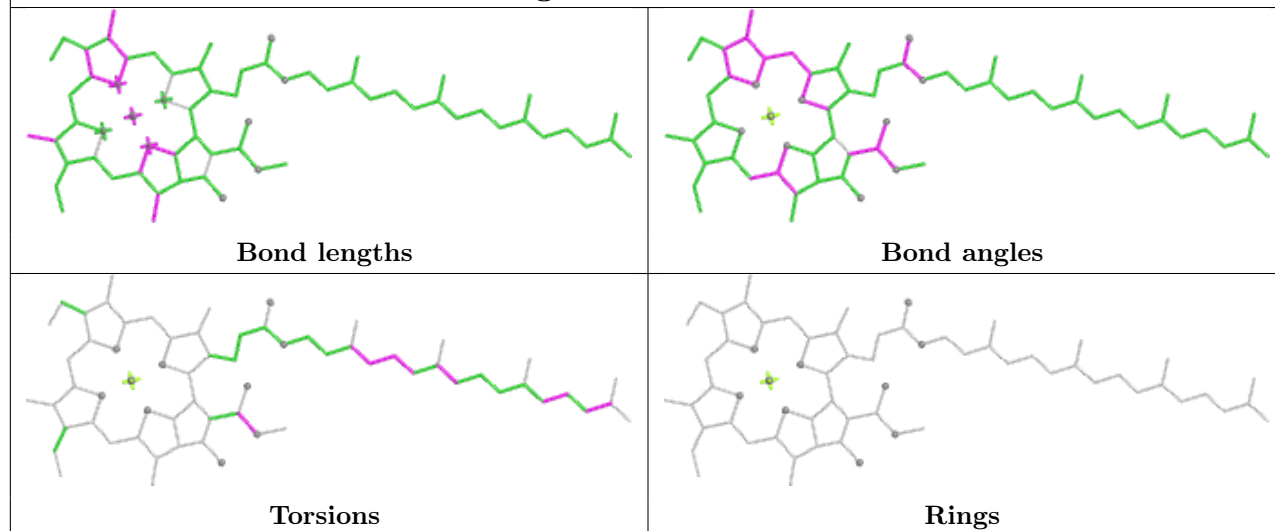
## Ligand CLA P 310



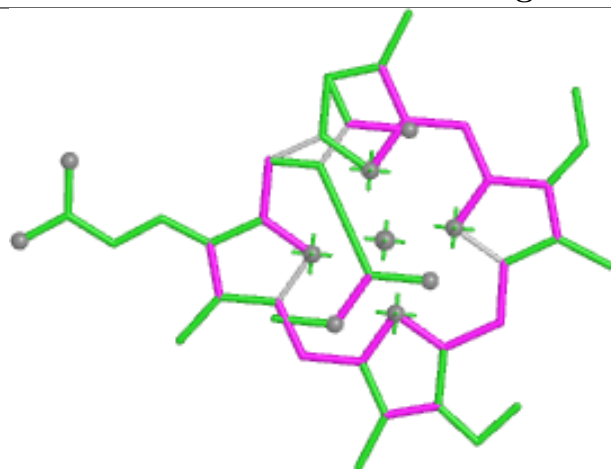
## Ligand A86 Q 303



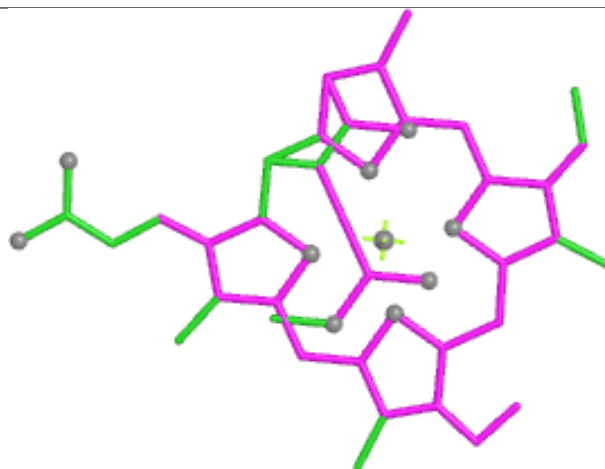
## Ligand CLA a 820



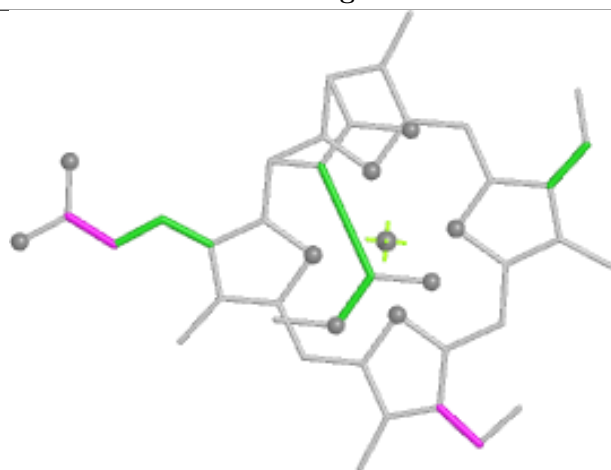
## Ligand KC1 R 317



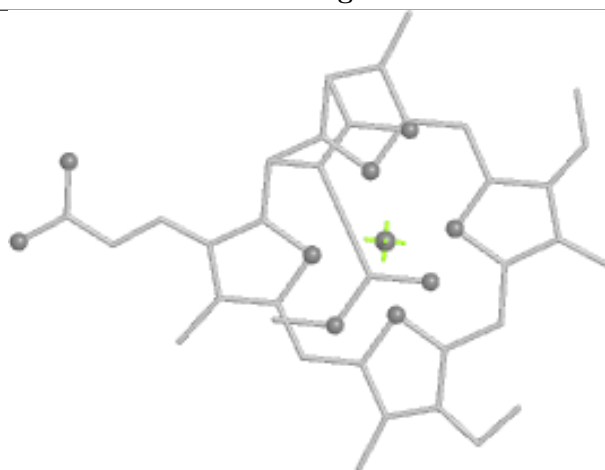
Bond lengths



Bond angles

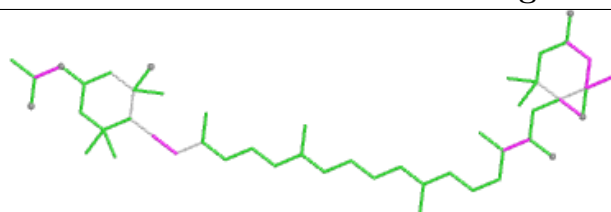


Torsions

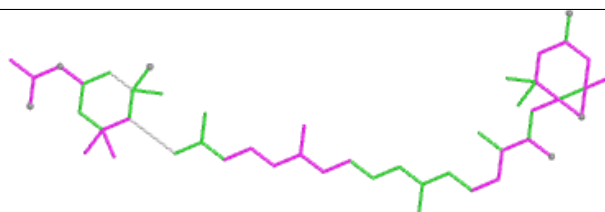


Rings

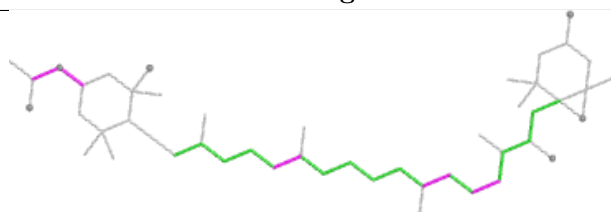
## Ligand A86 N 304



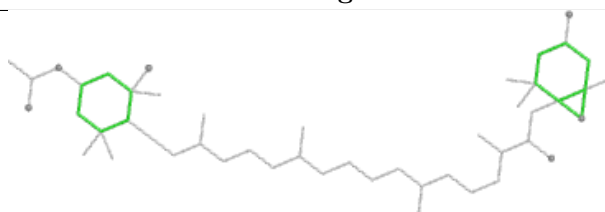
Bond lengths



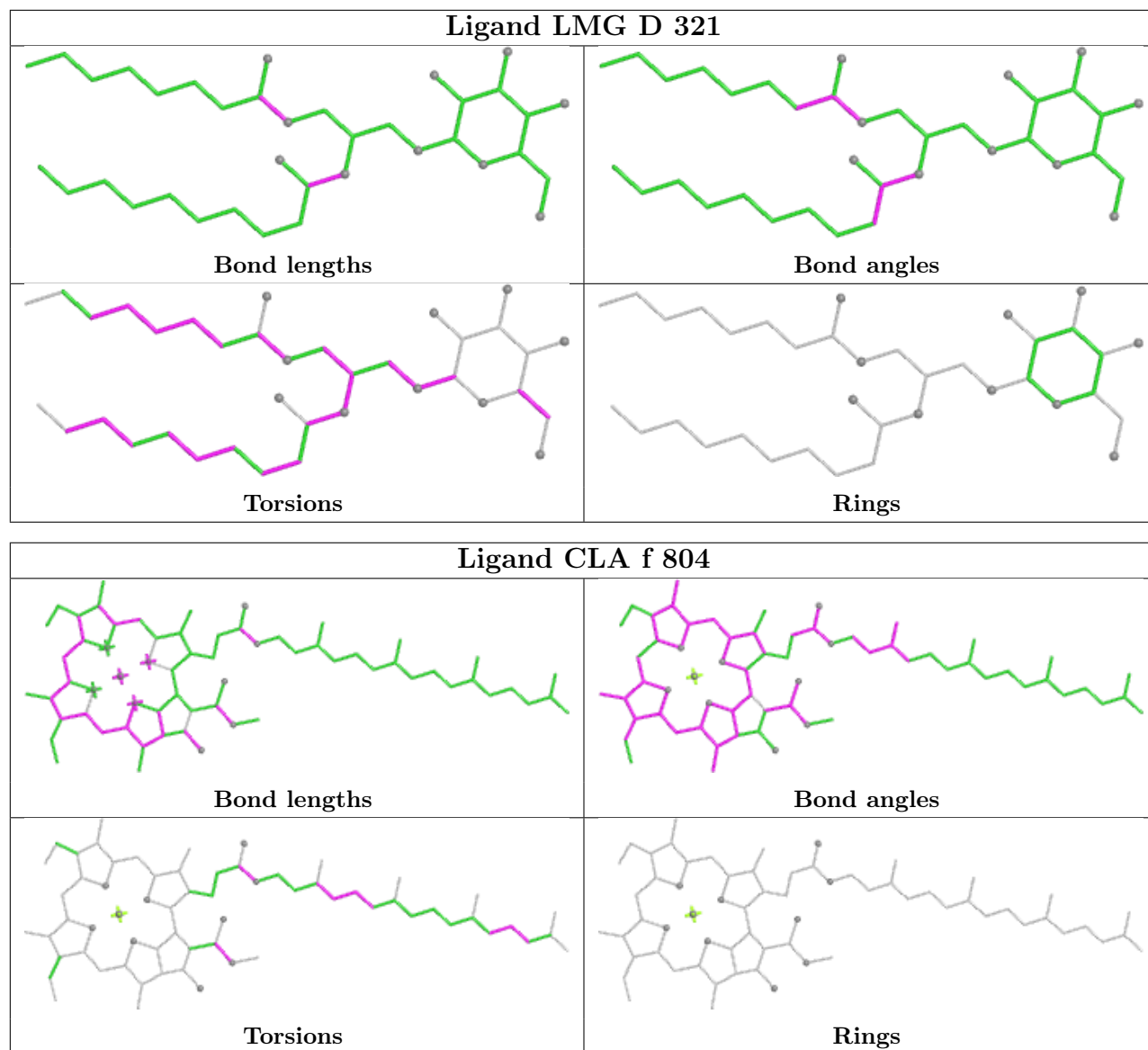
Bond angles

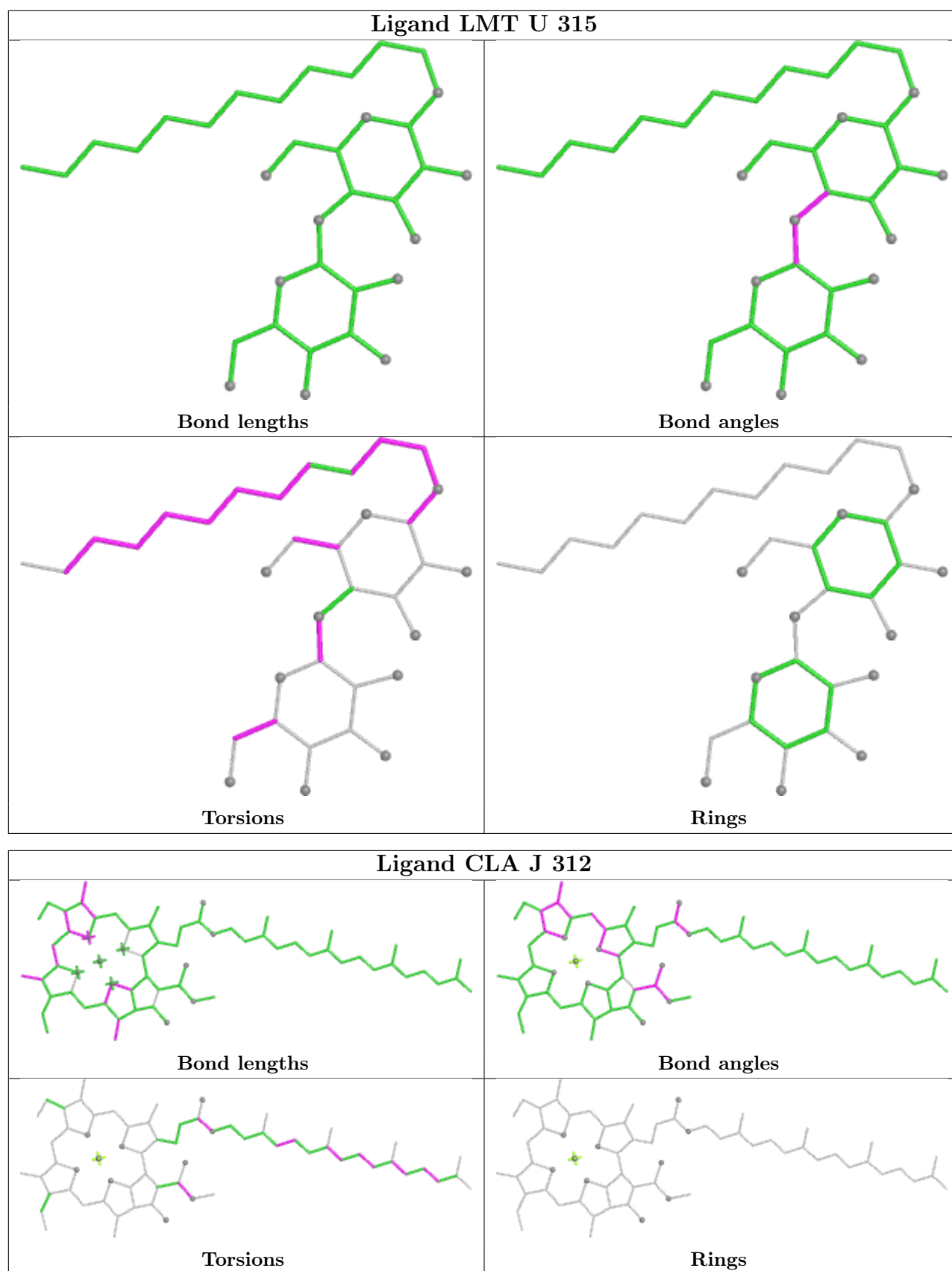


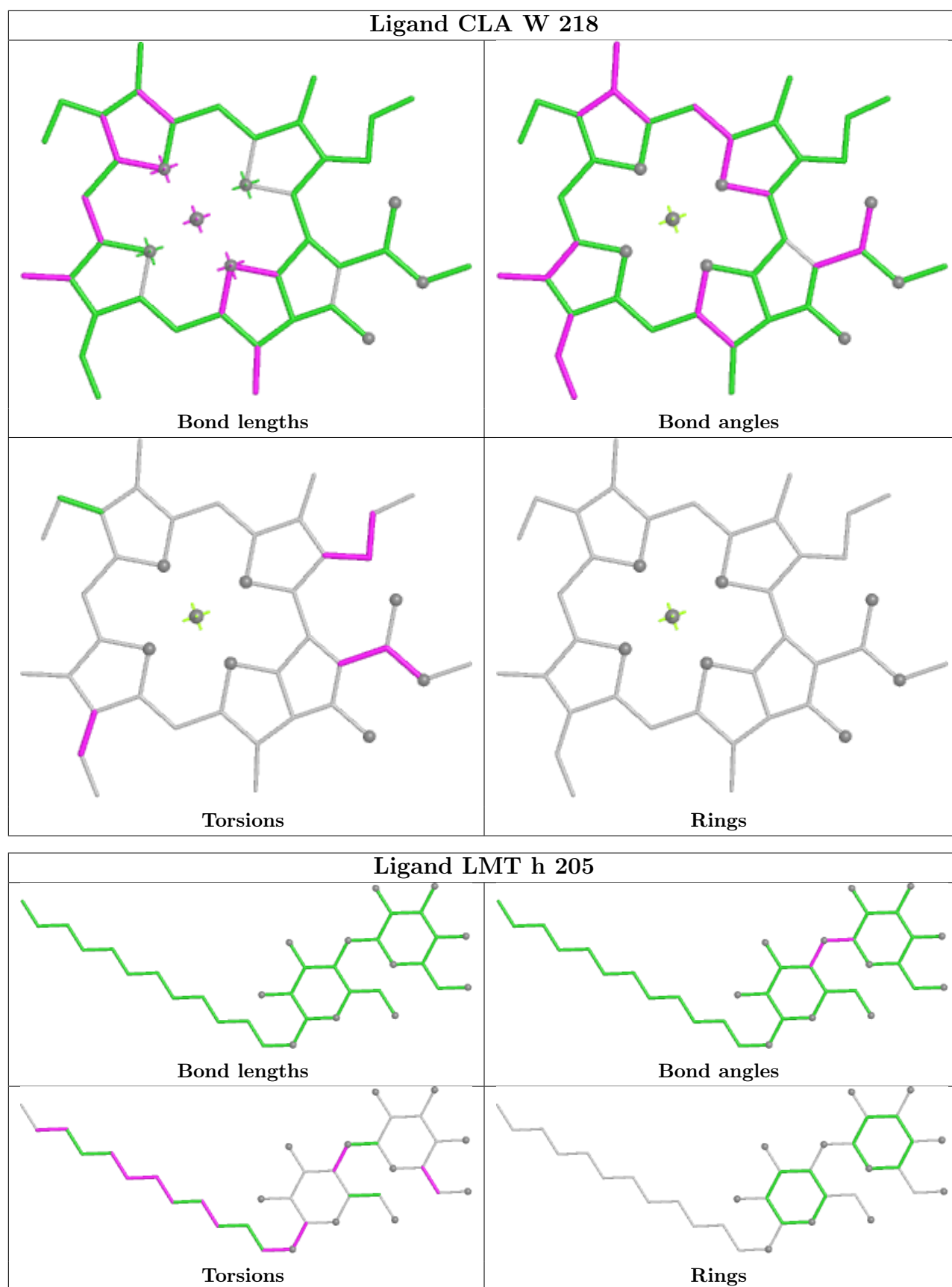
Torsions

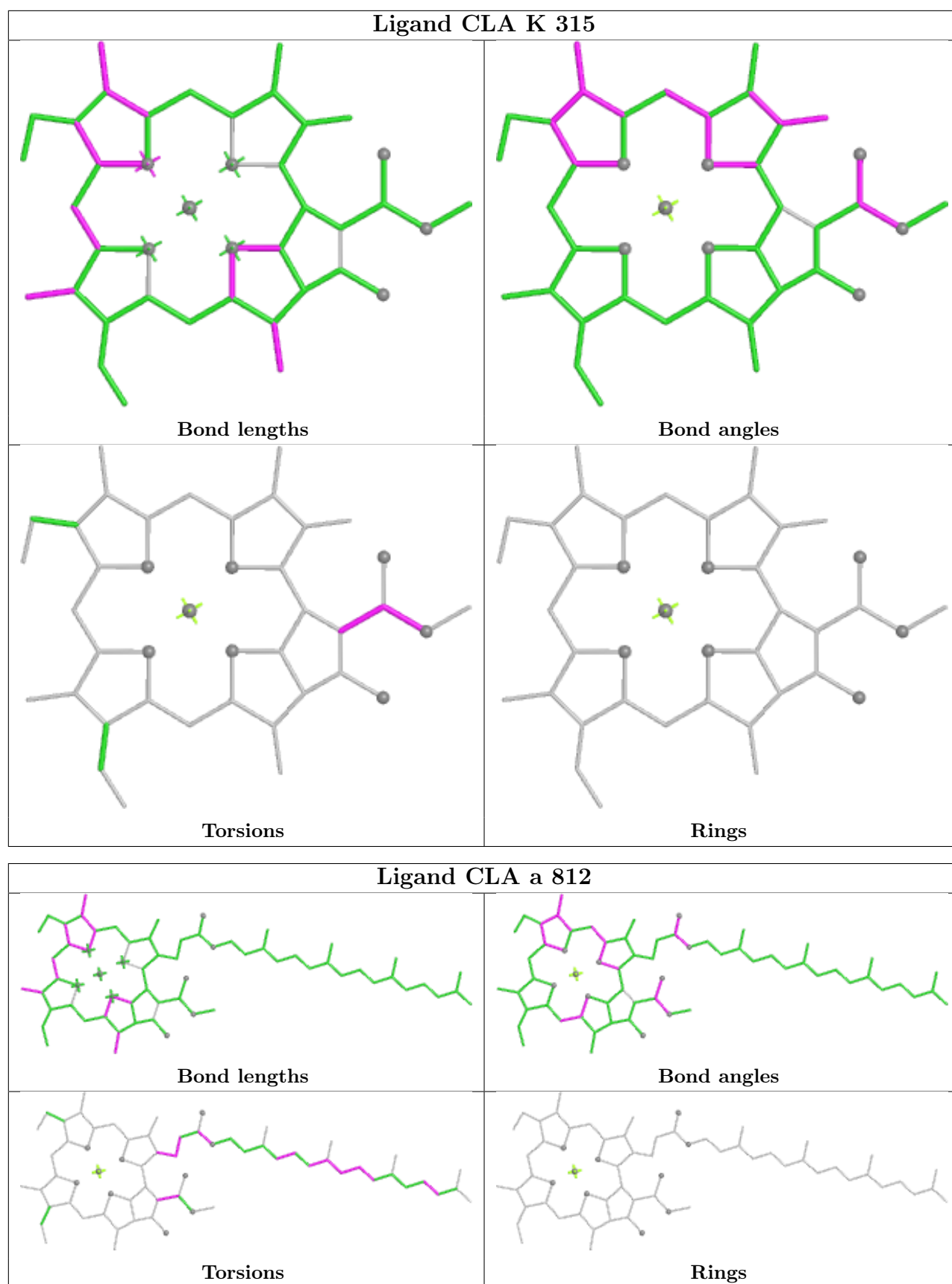


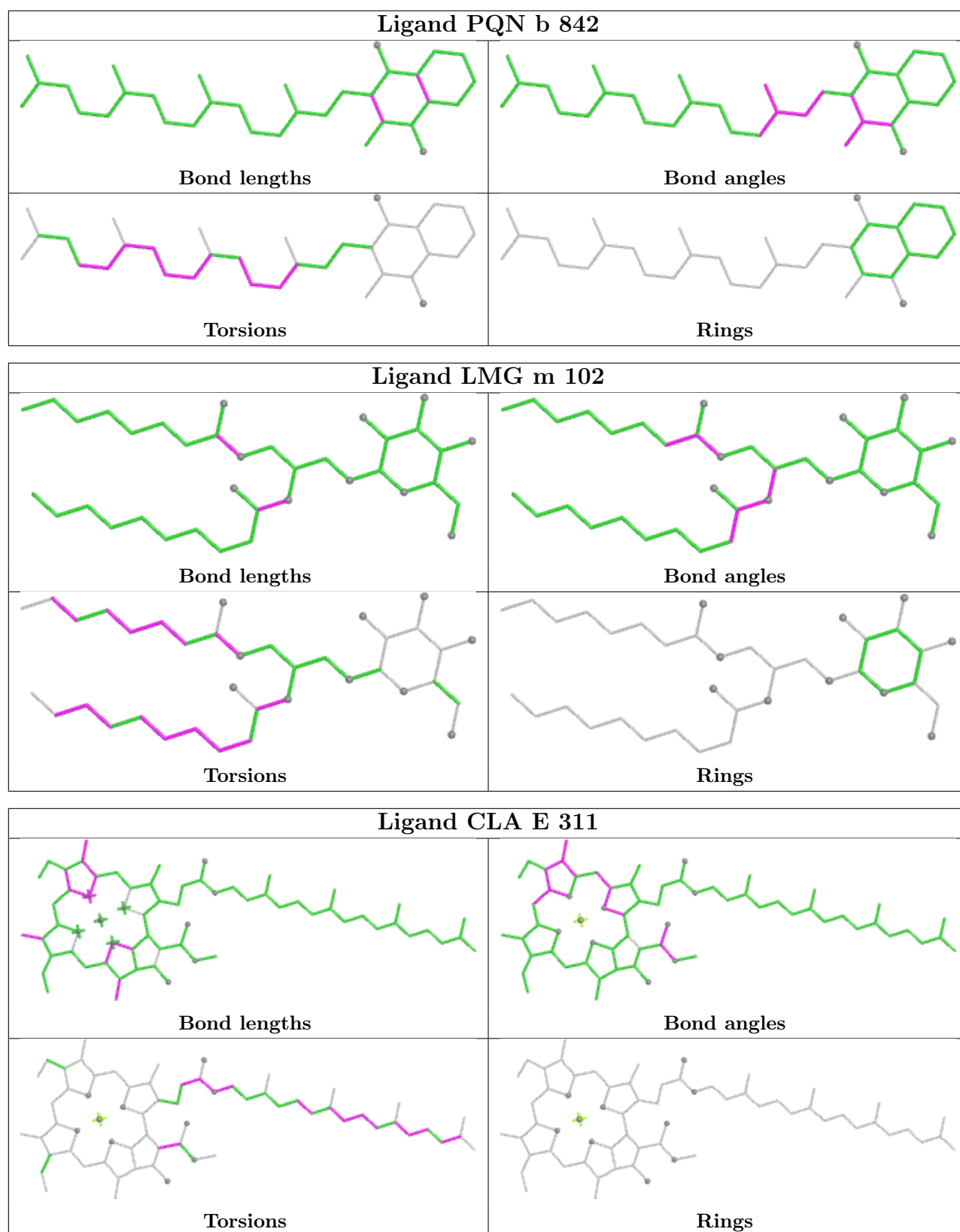
Rings



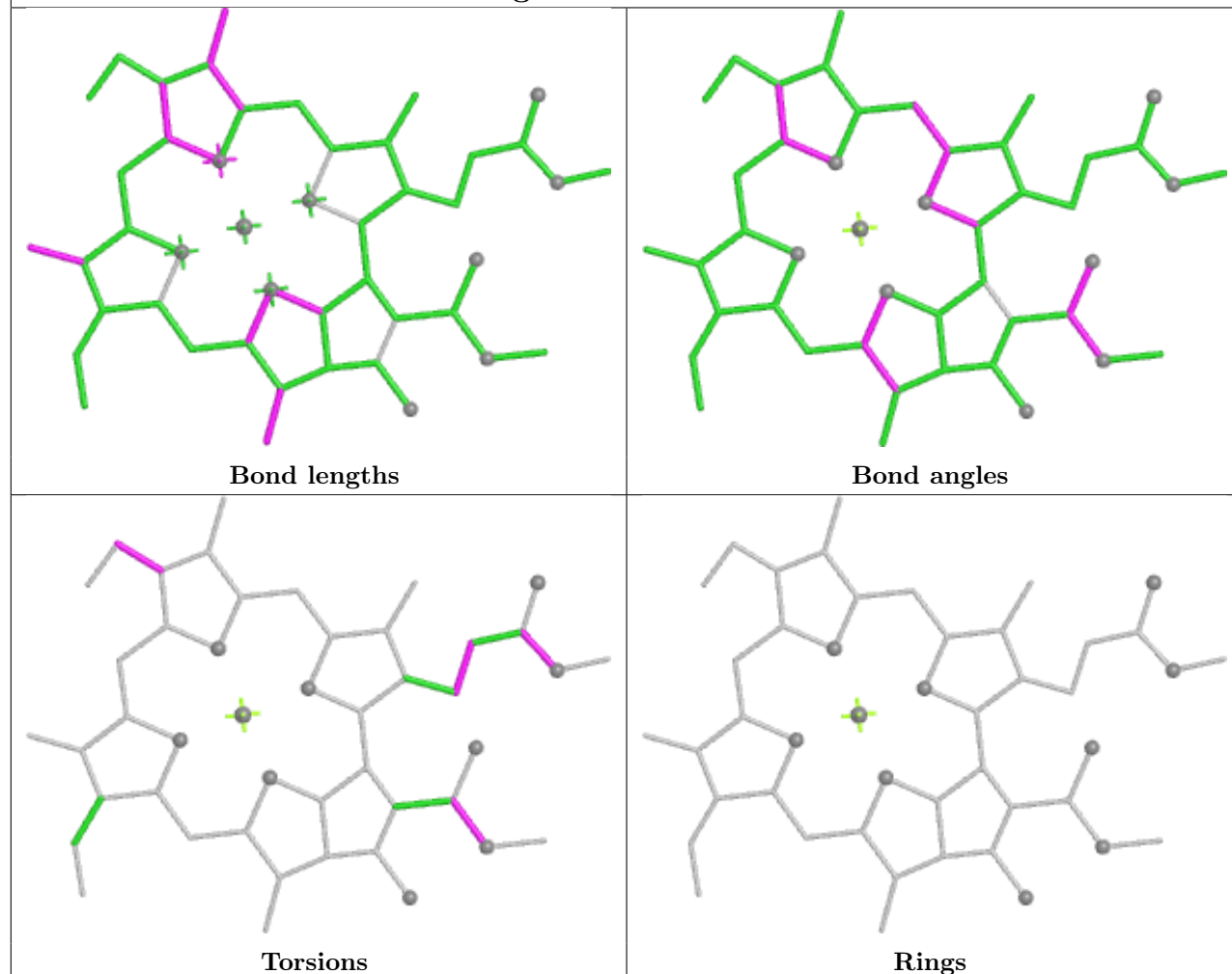




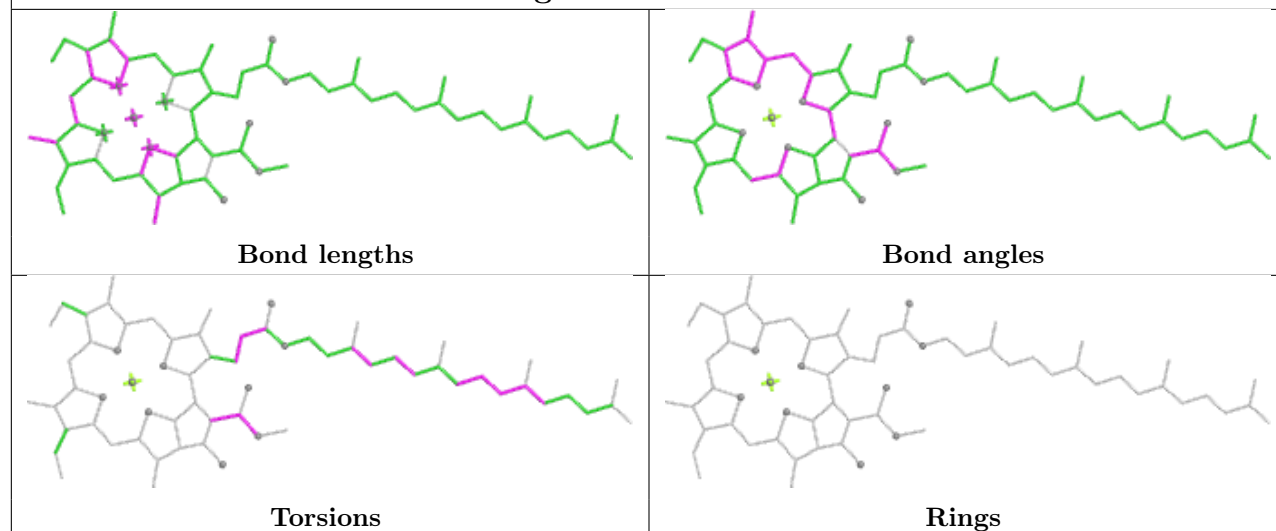




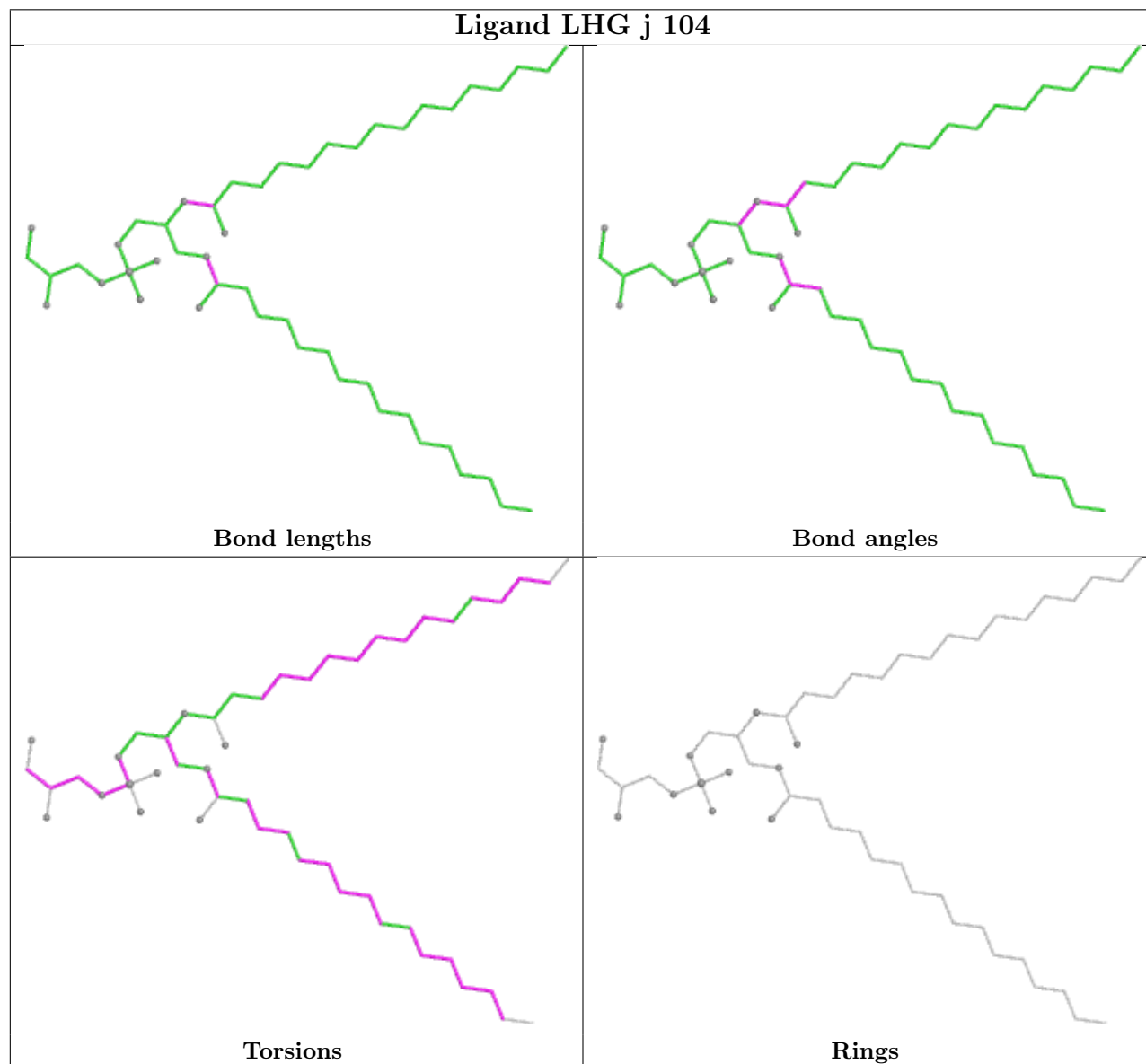
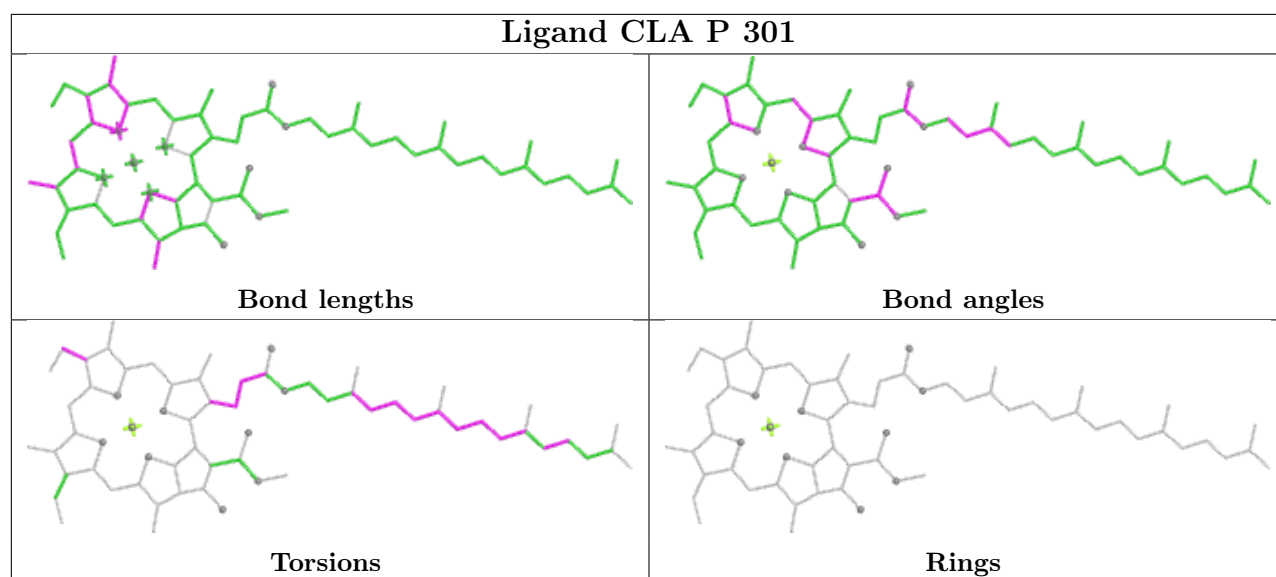
## Ligand CLA D 311

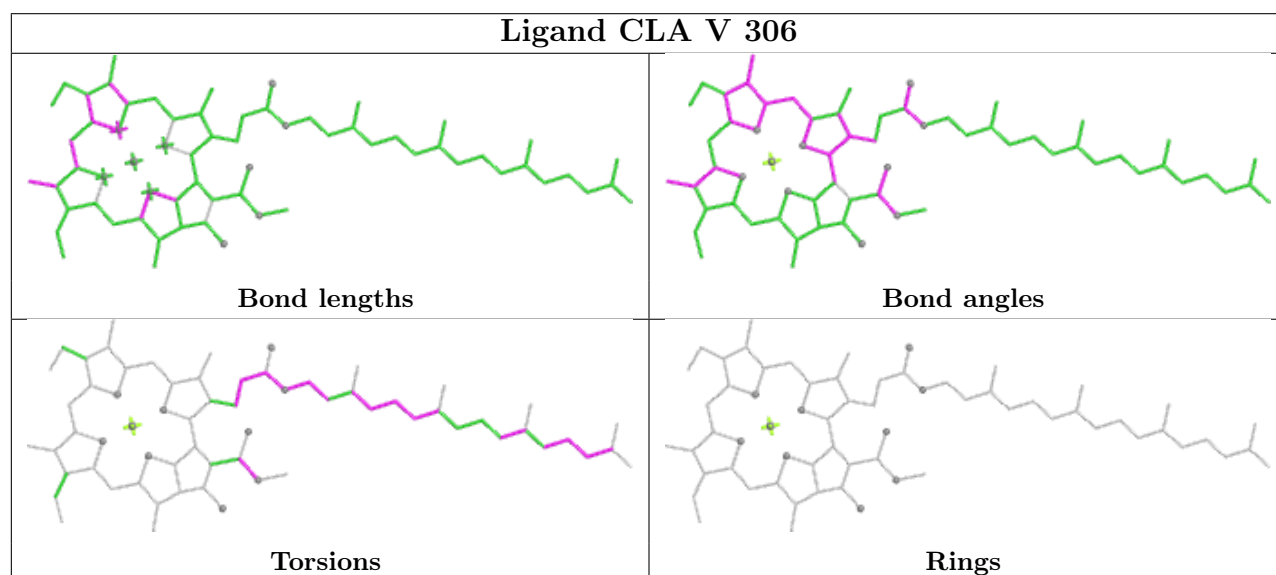
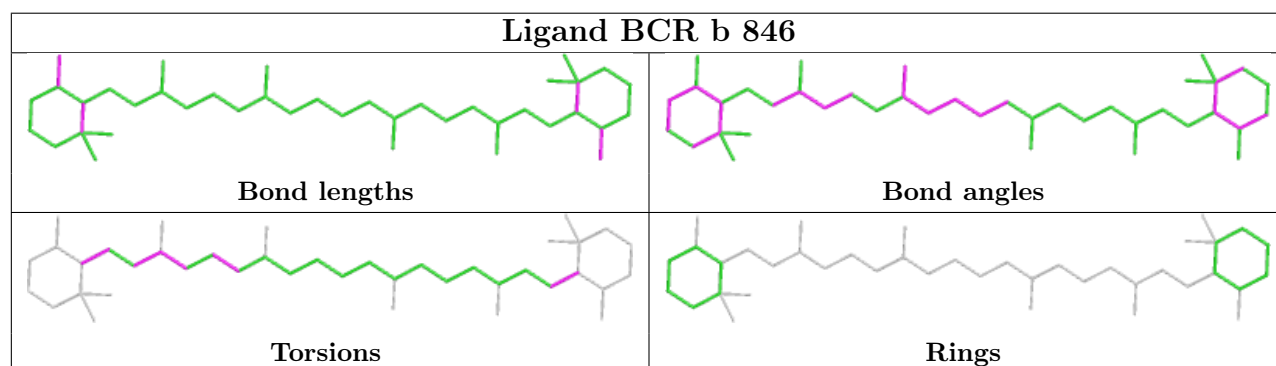
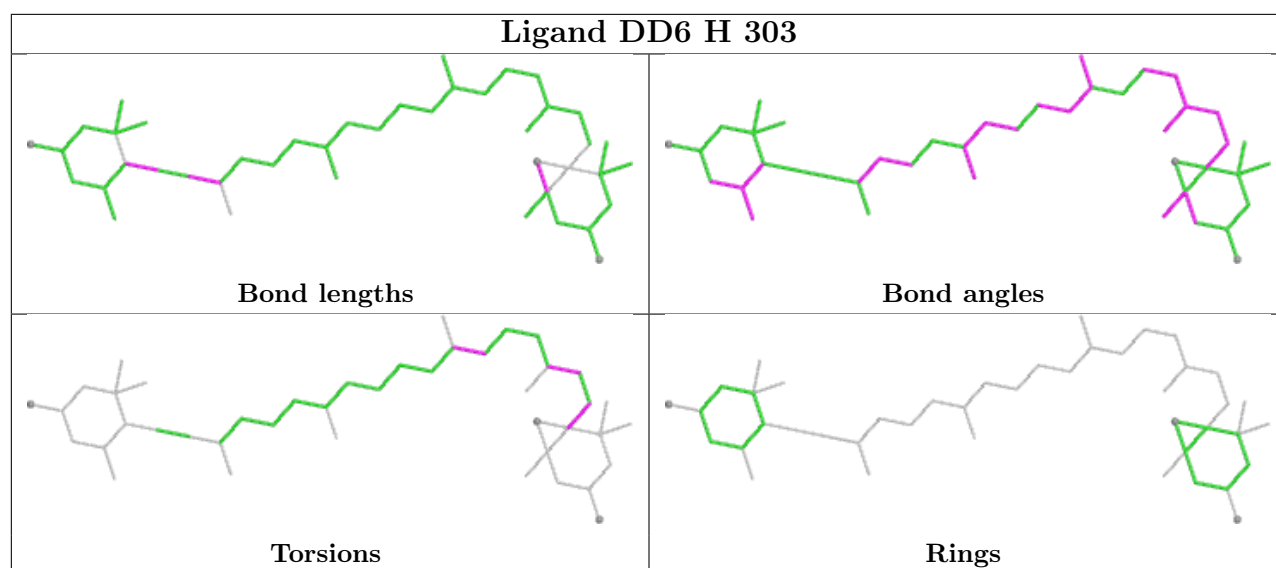


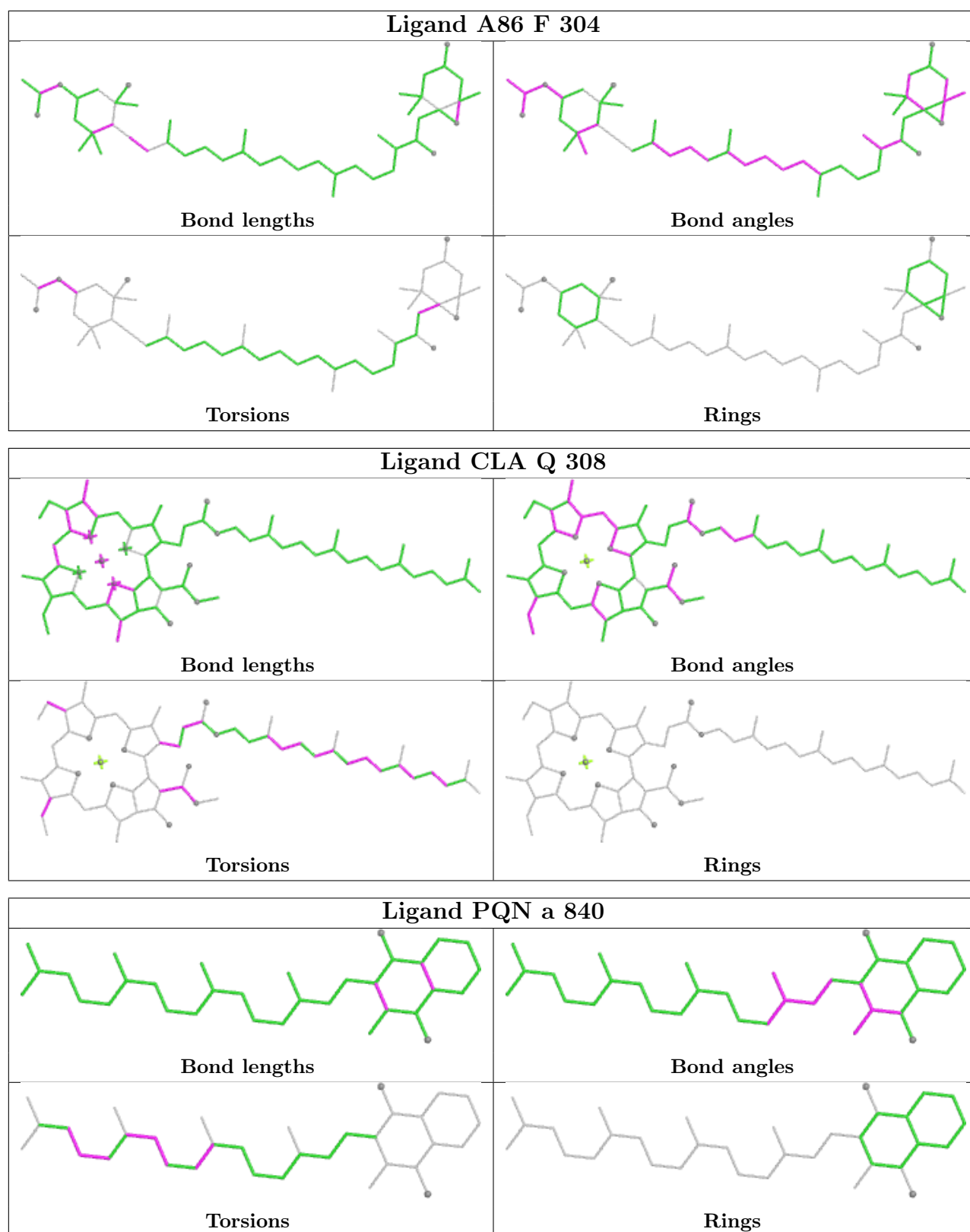
## Ligand CLA L 311



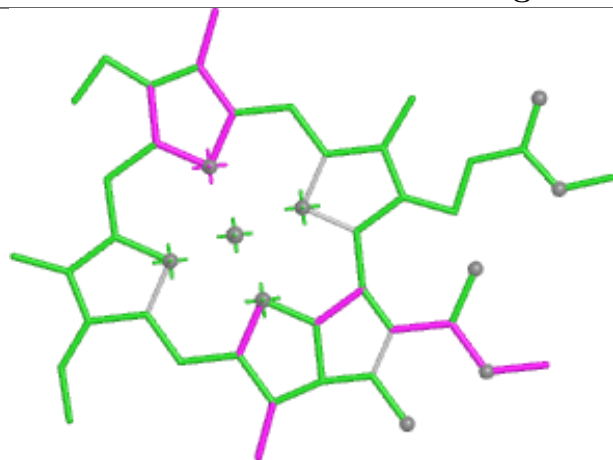




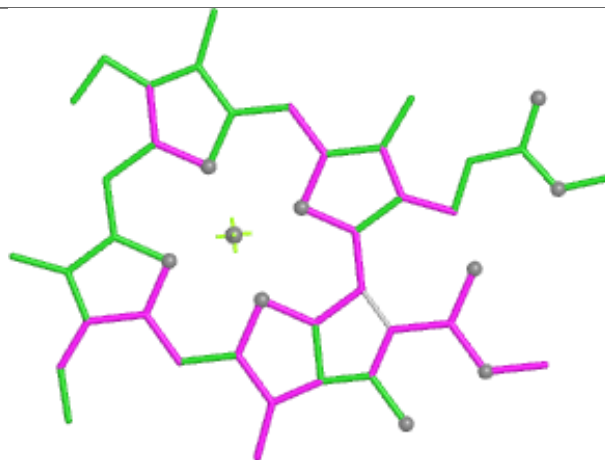




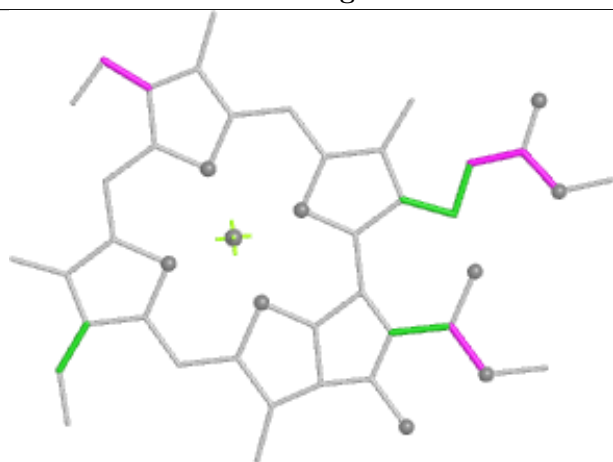
## Ligand CLA H 310



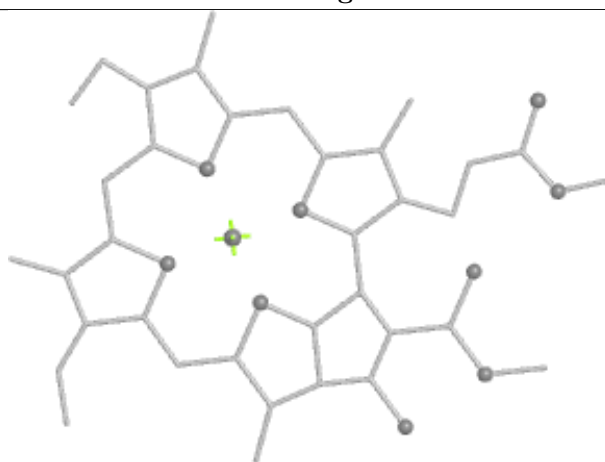
Bond lengths



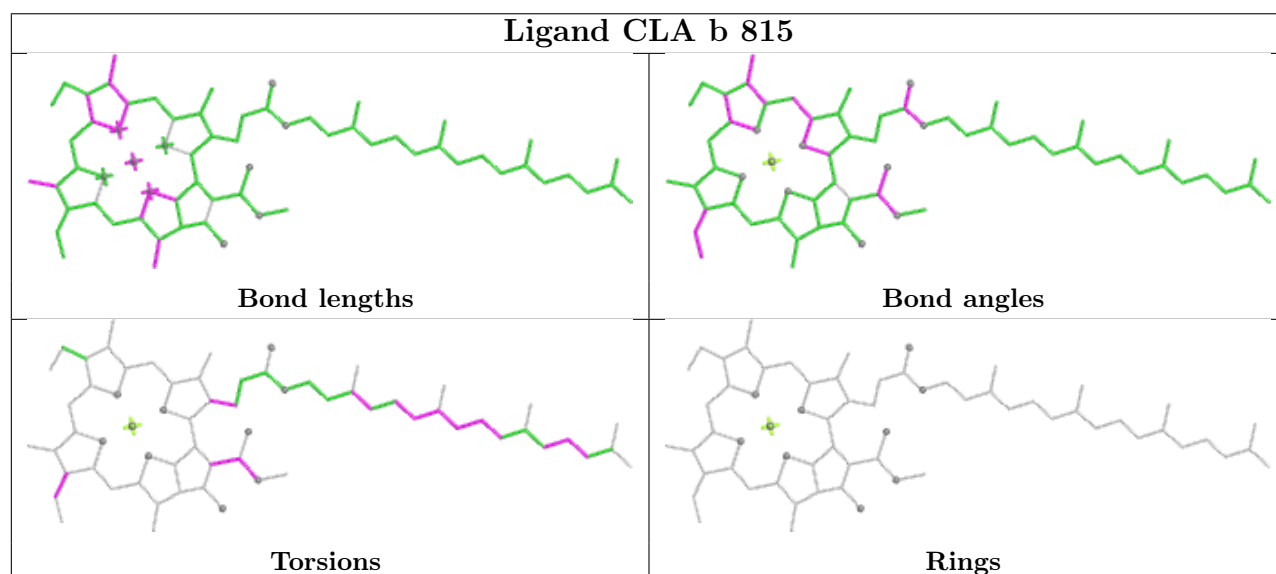
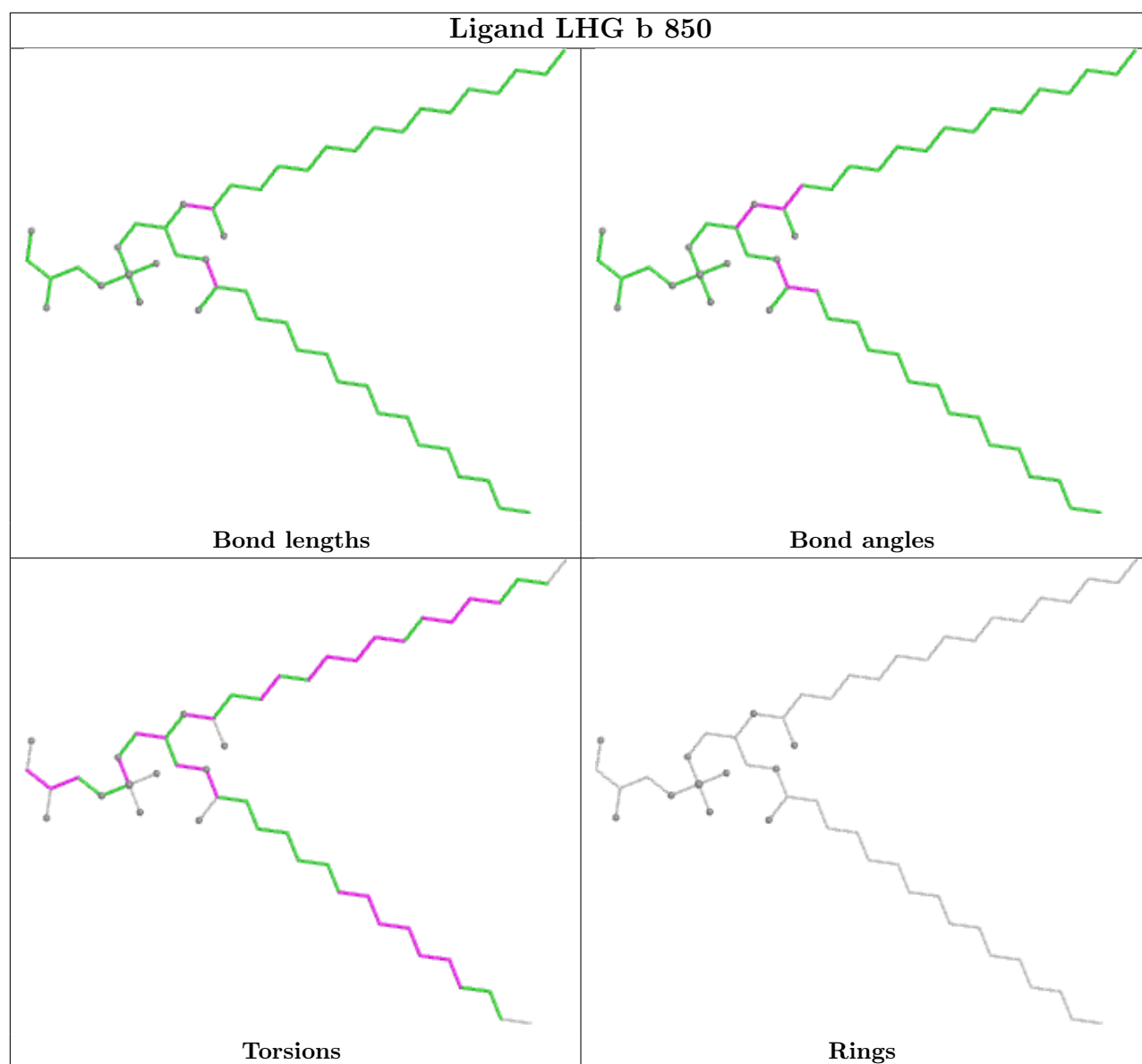
Bond angles



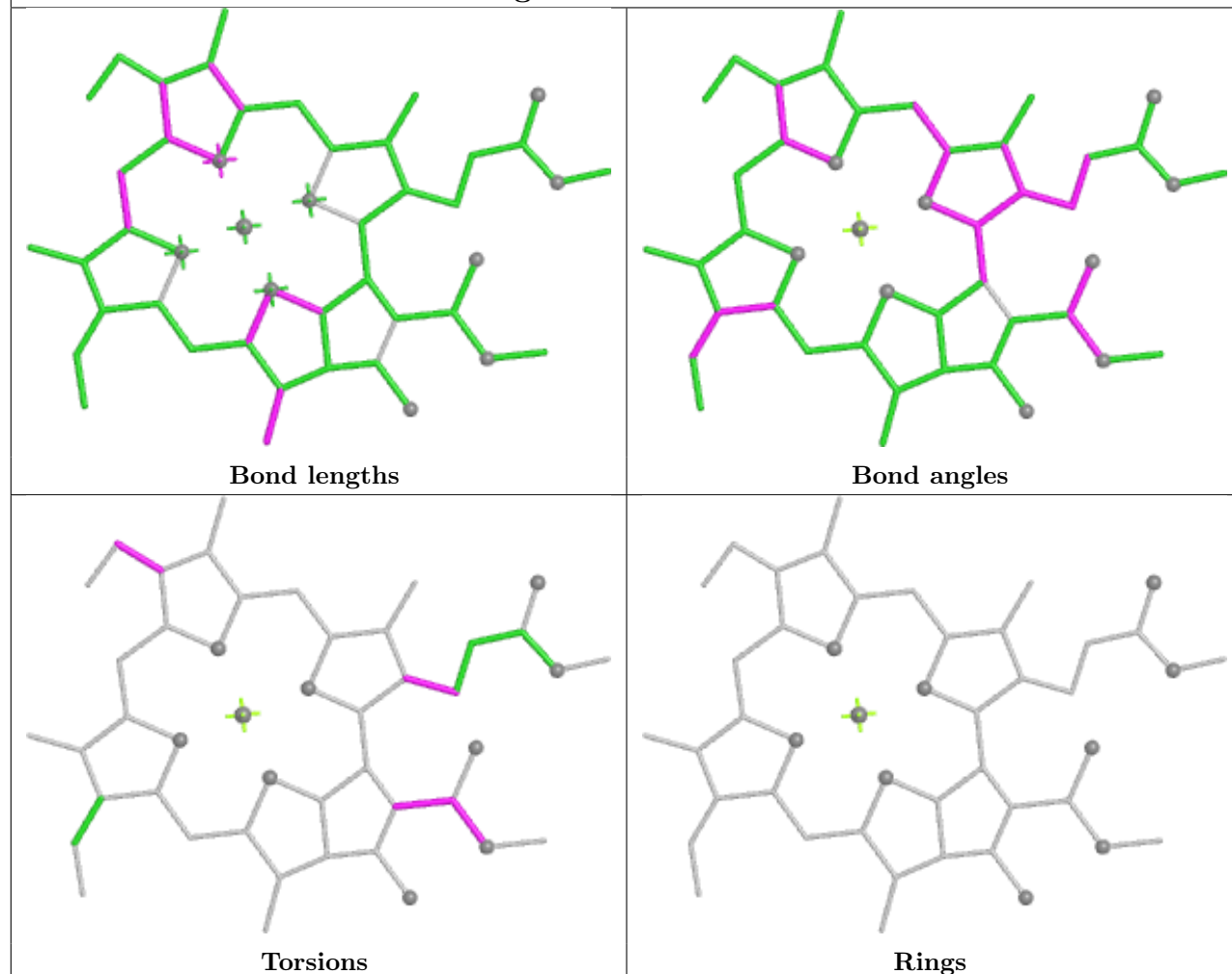
Torsions



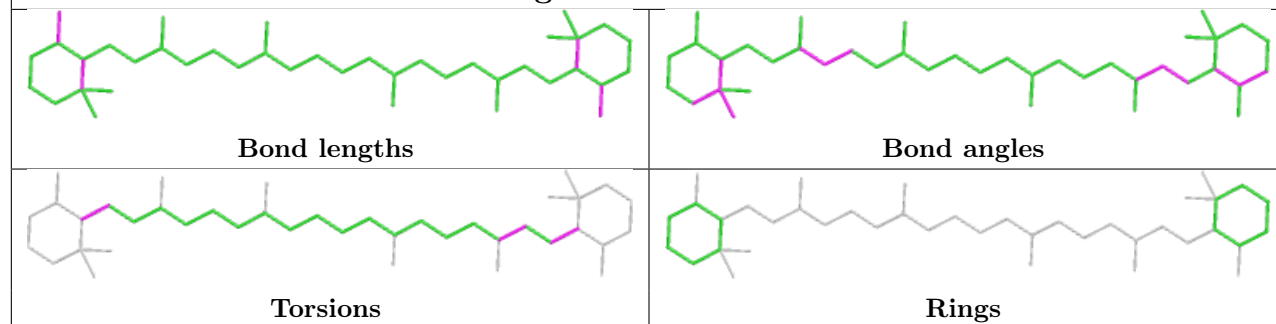
Rings

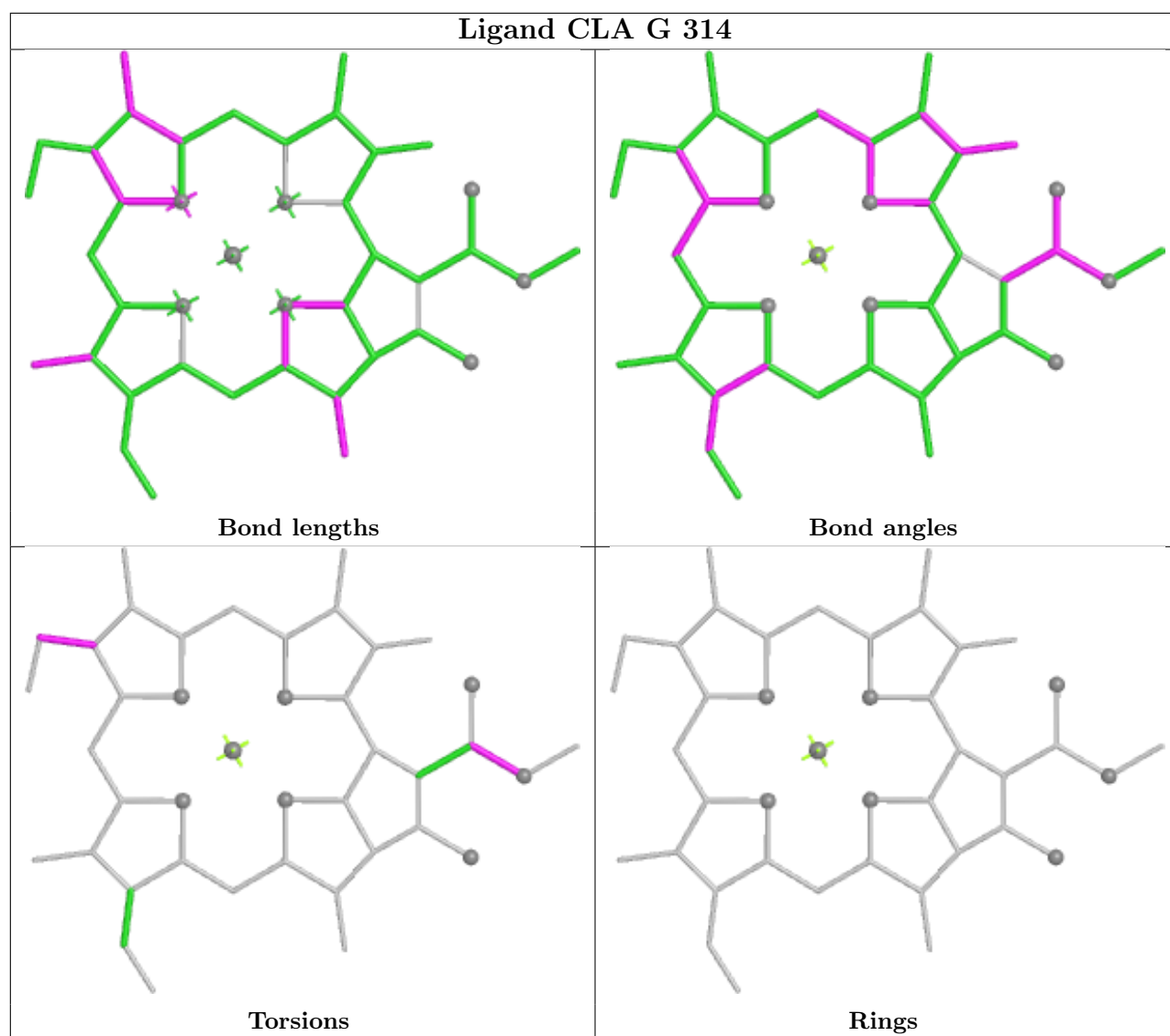


## Ligand CLA T 312

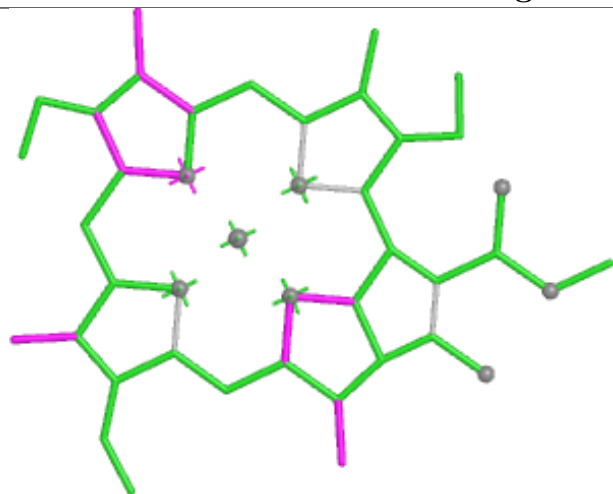


## Ligand BCR a 847

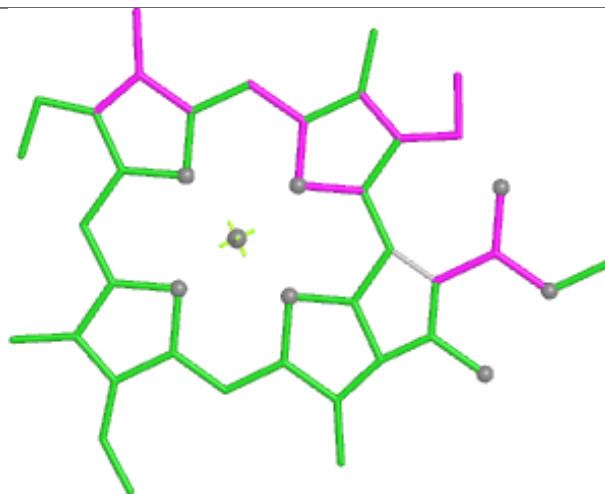




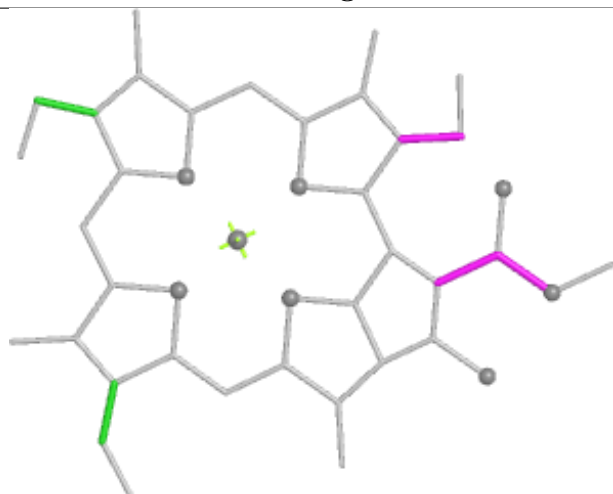
## Ligand CLA P 302



Bond lengths



Bond angles

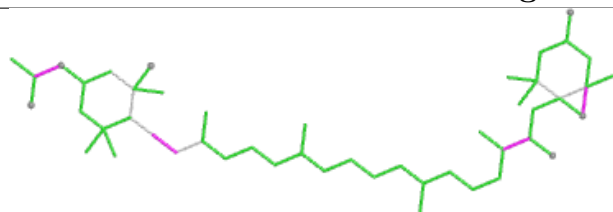


Torsions

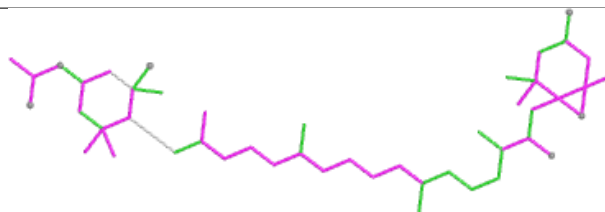


Rings

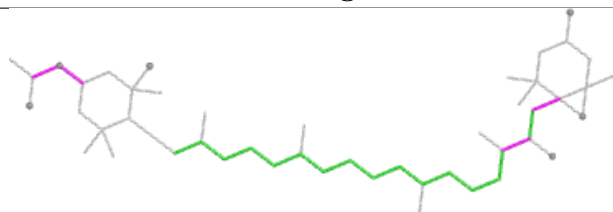
## Ligand A86 X 304



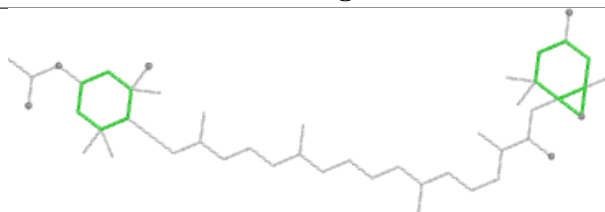
Bond lengths



Bond angles

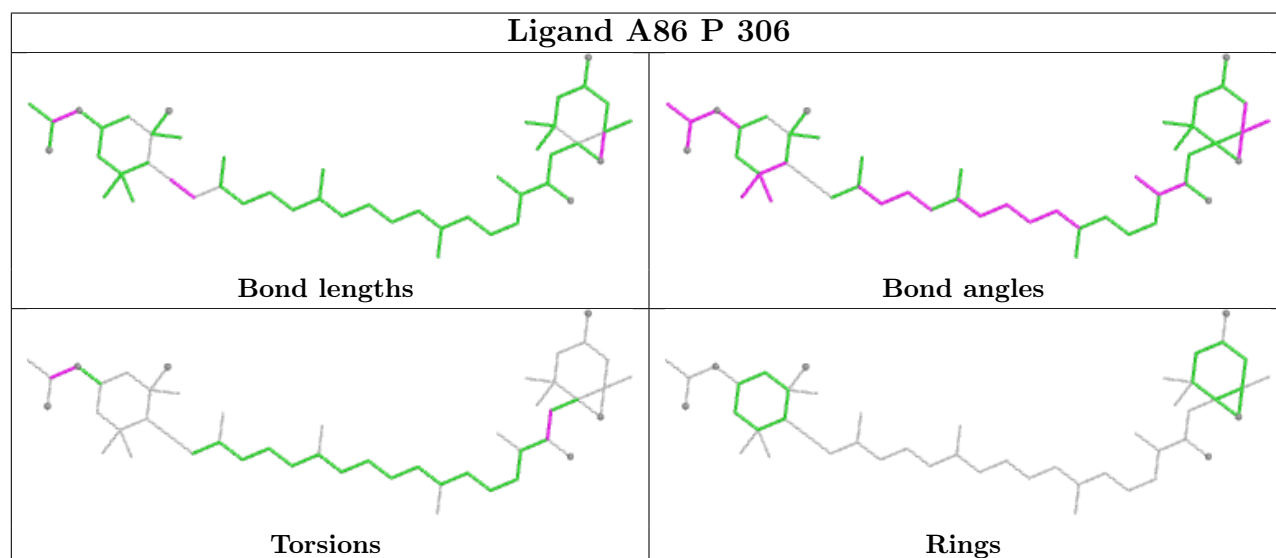
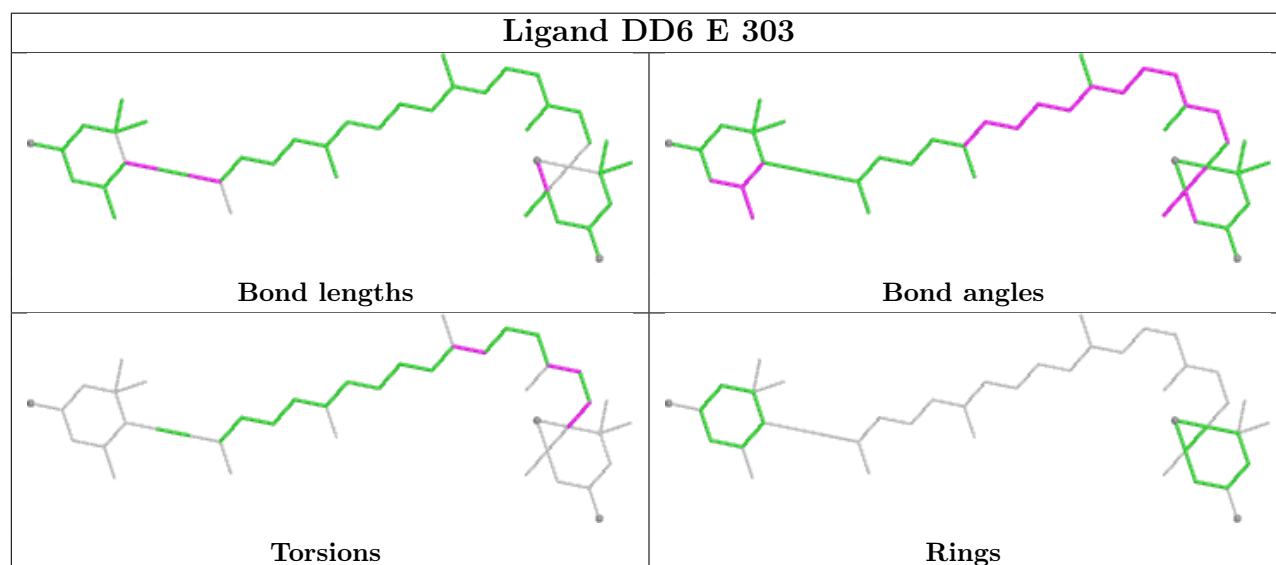
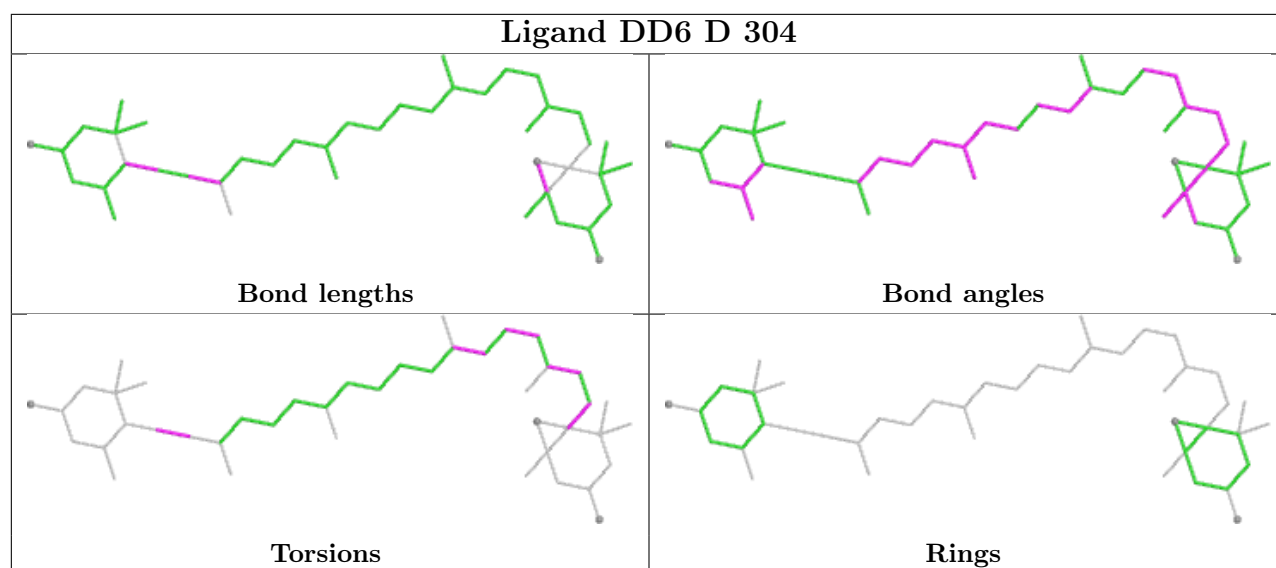


Torsions

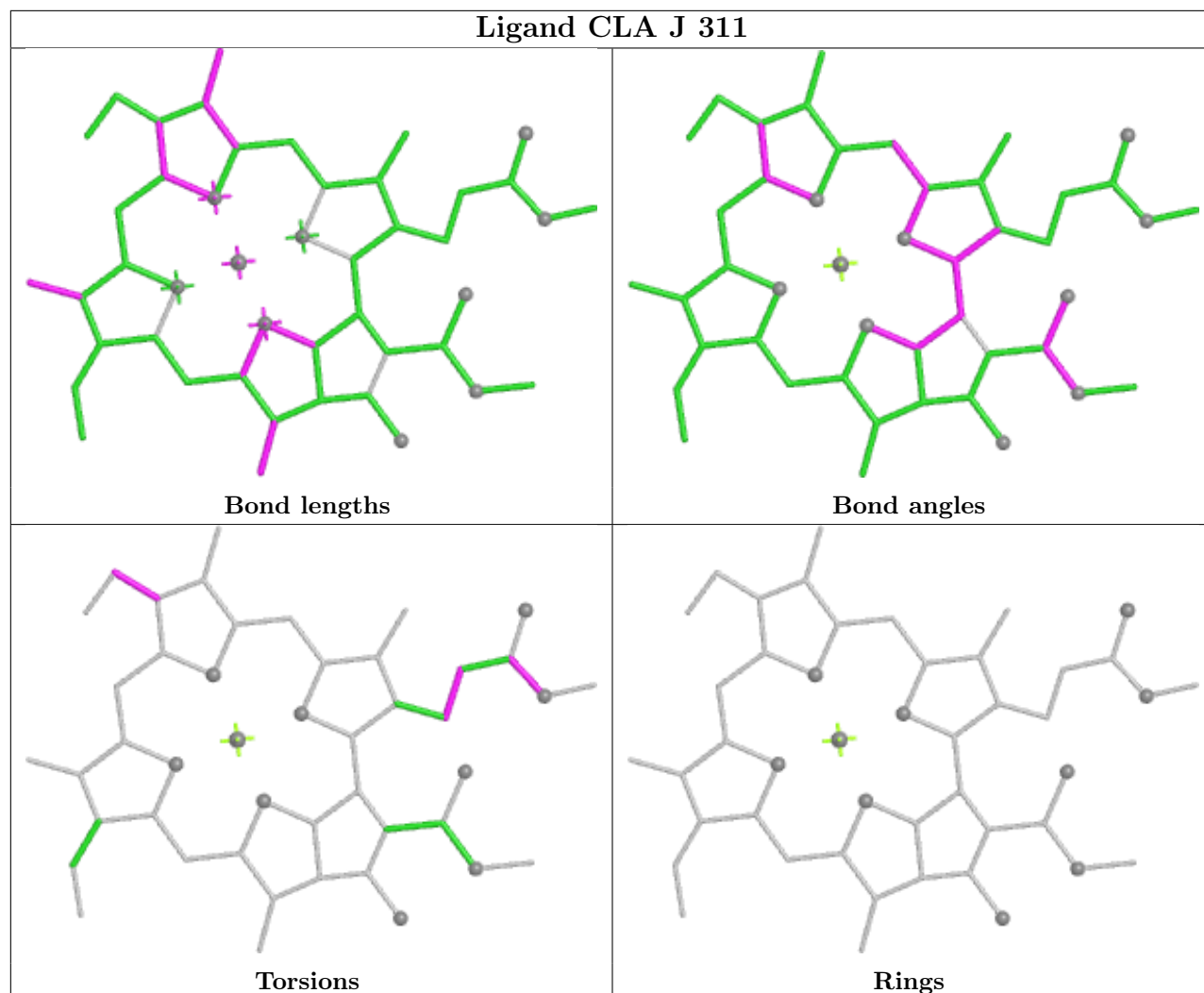


Rings

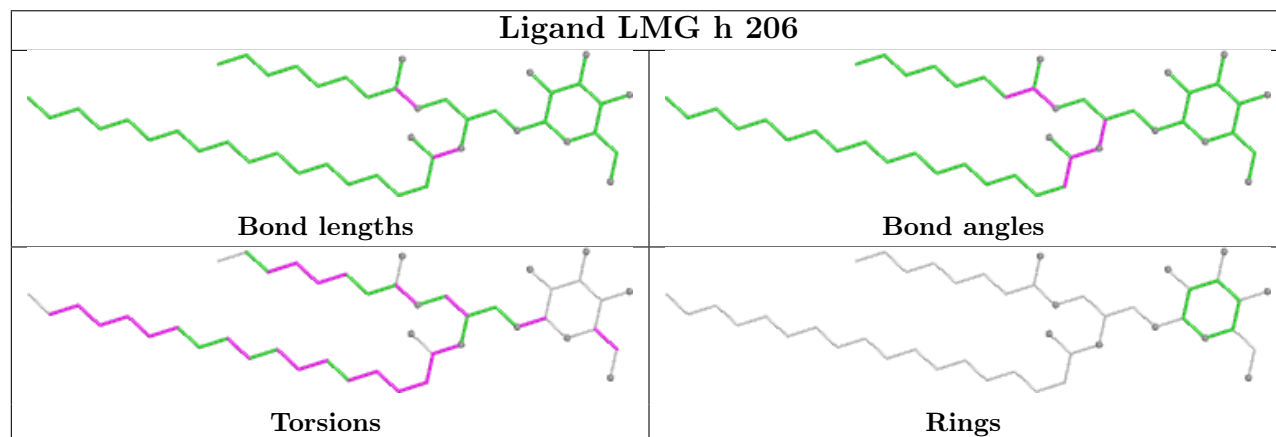


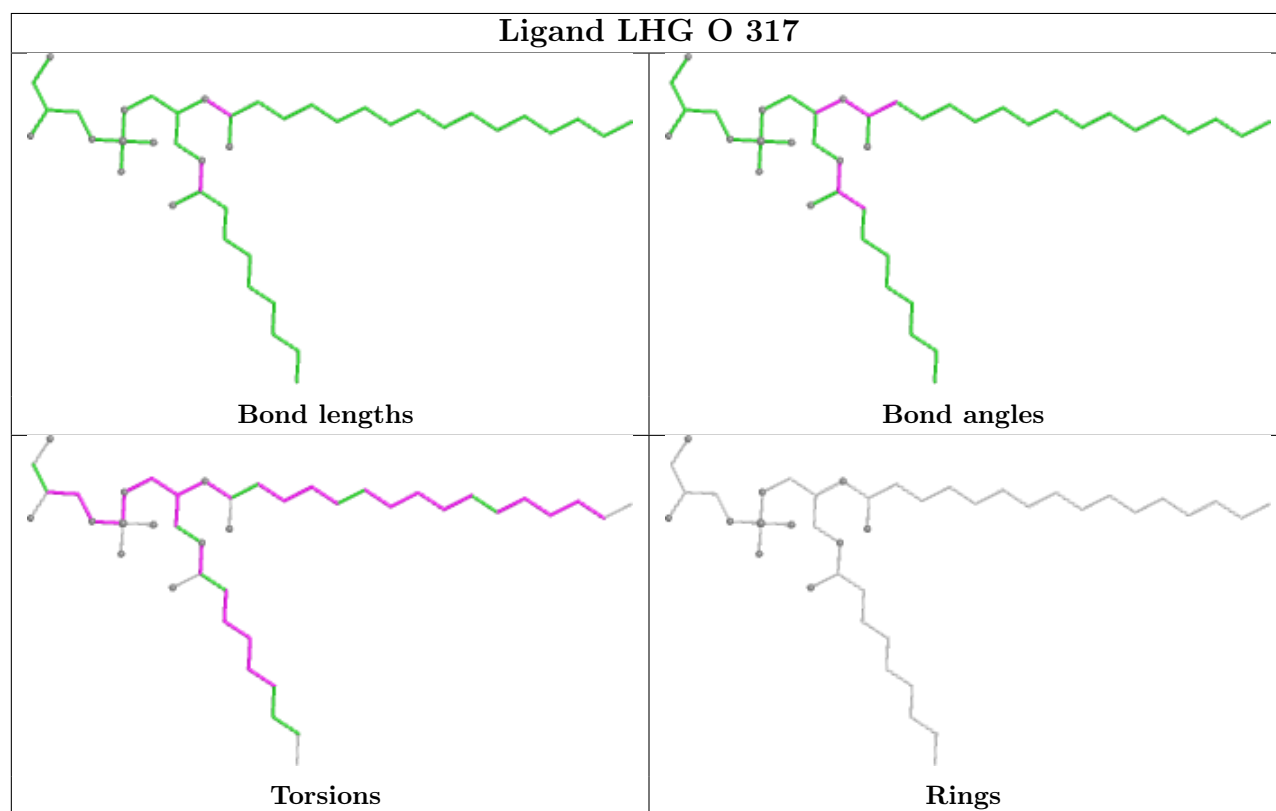
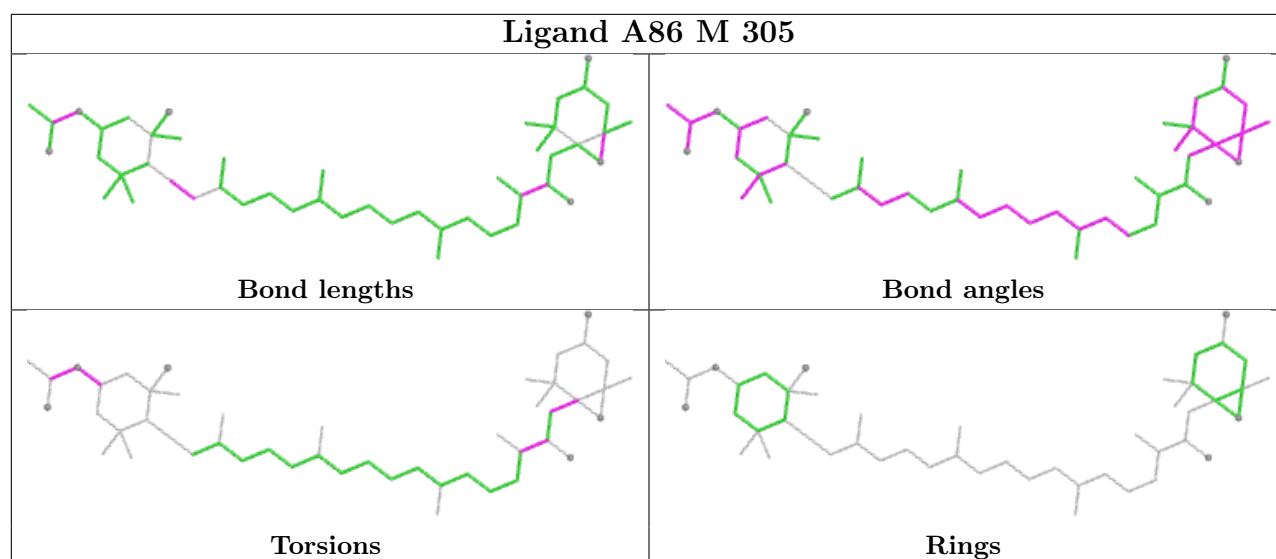


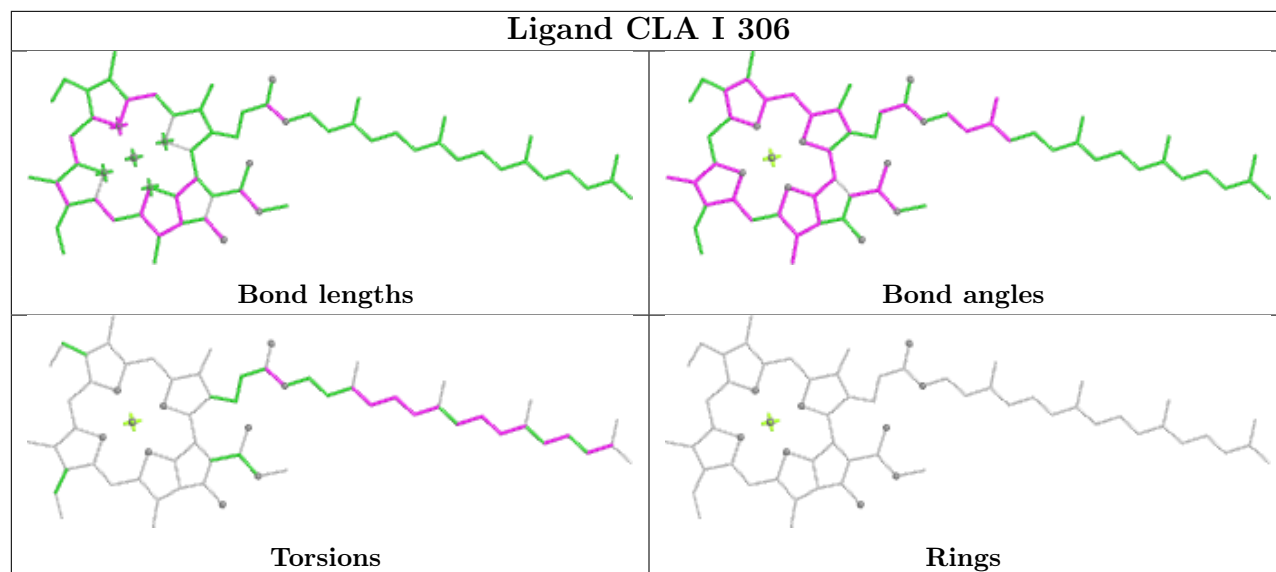
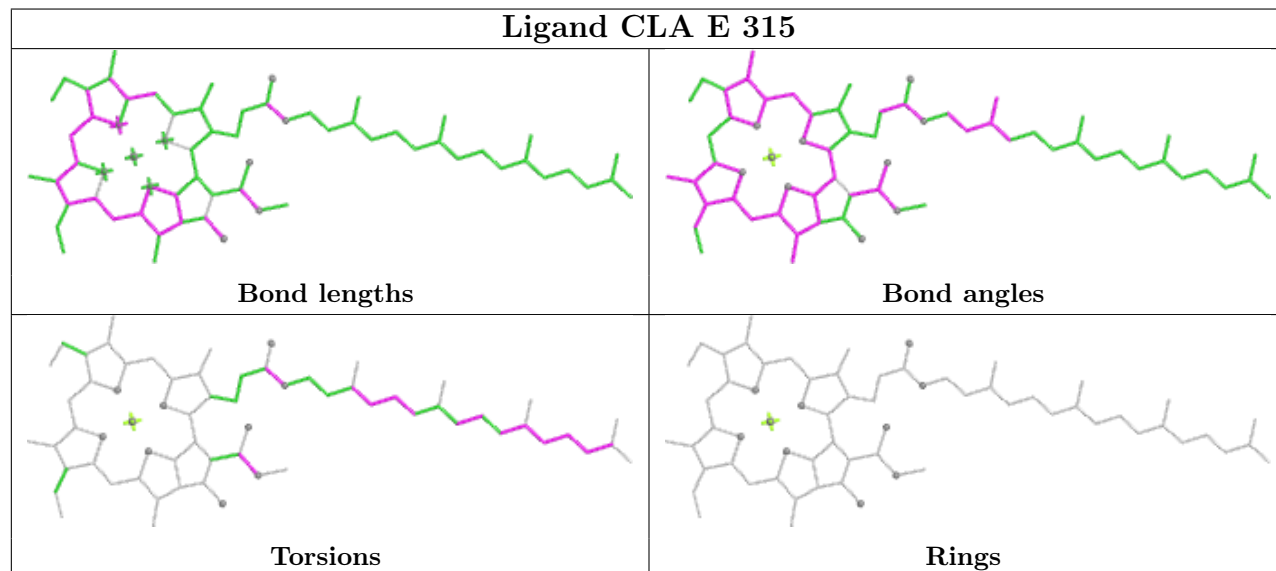
## Ligand CLA J 311



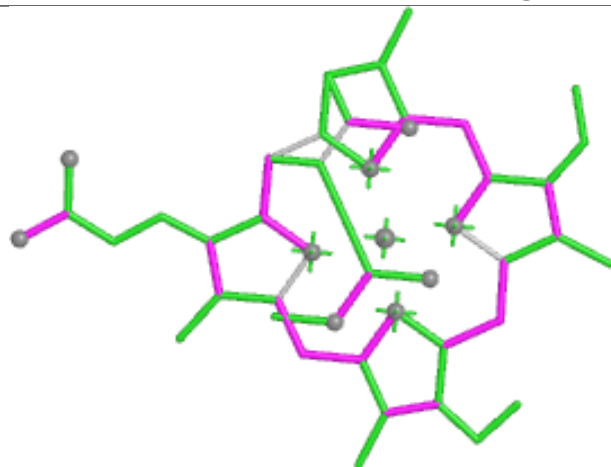
## Ligand LMG h 206





**Ligand CLA I 306****Ligand CLA E 315**

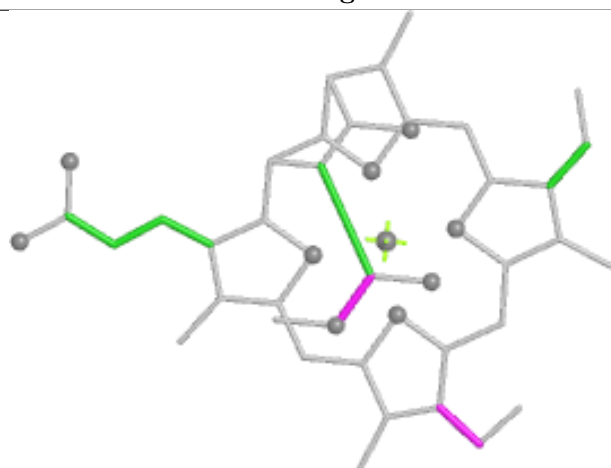
## Ligand KC1 F 315



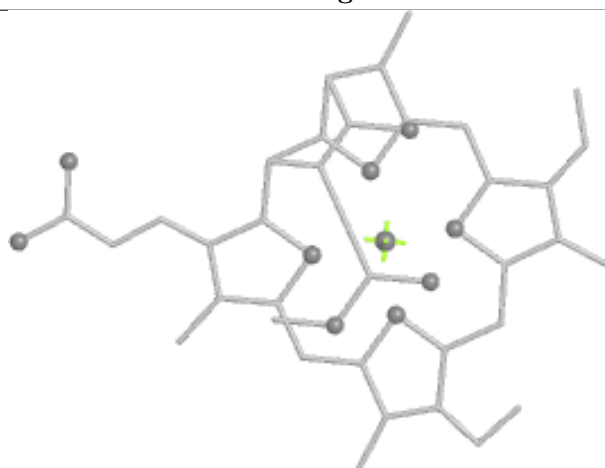
Bond lengths



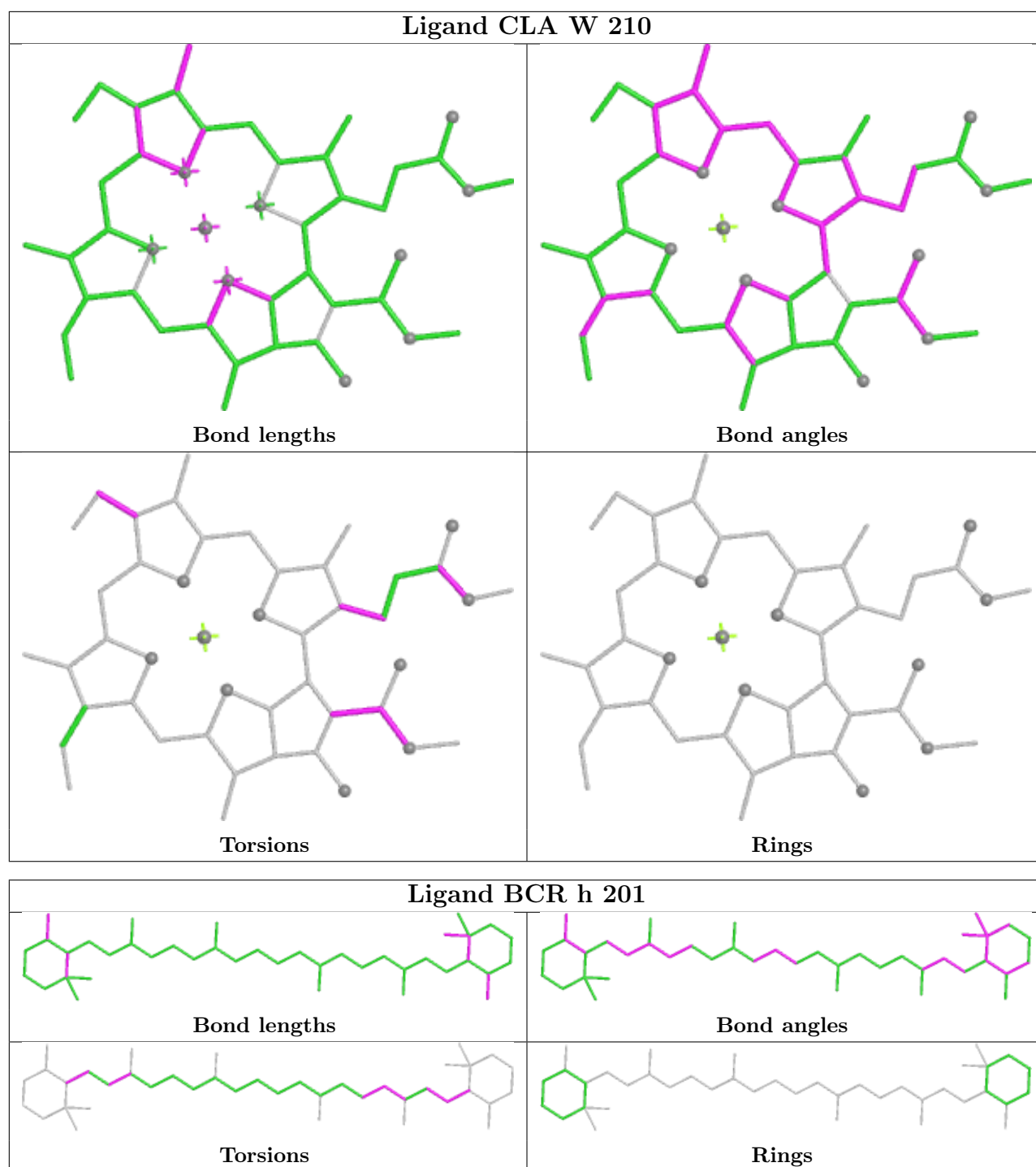
Bond angles

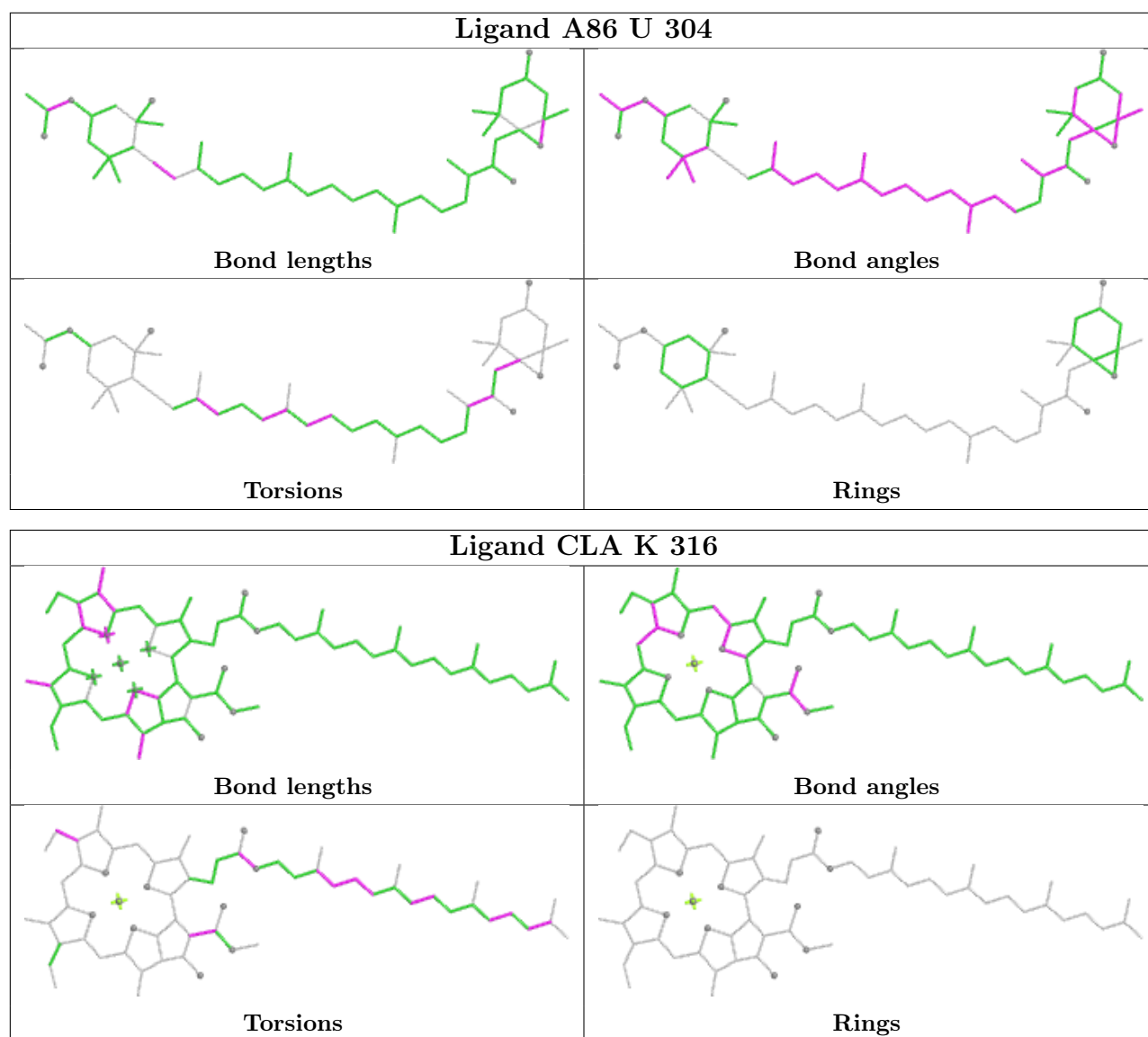


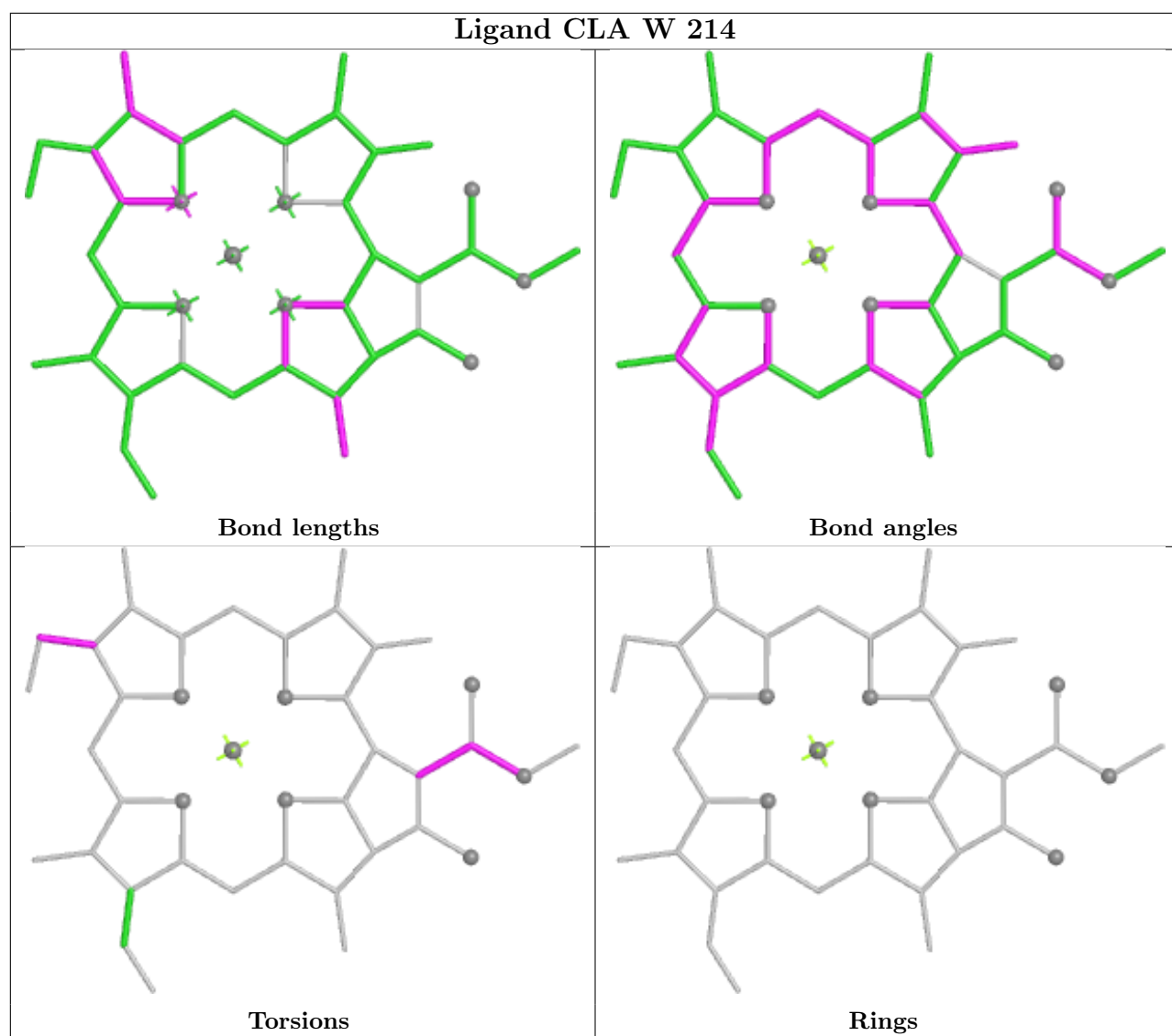
Torsions



Rings

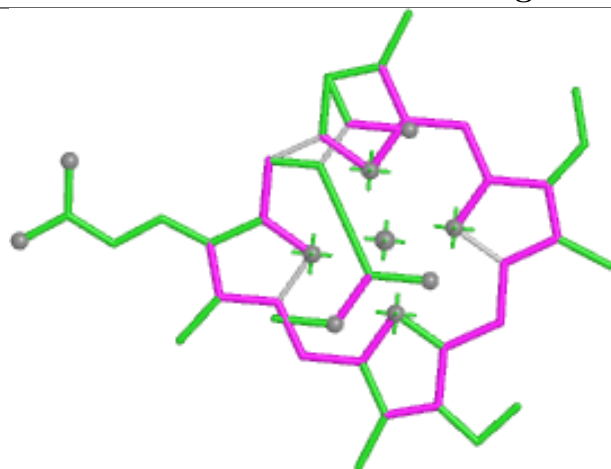




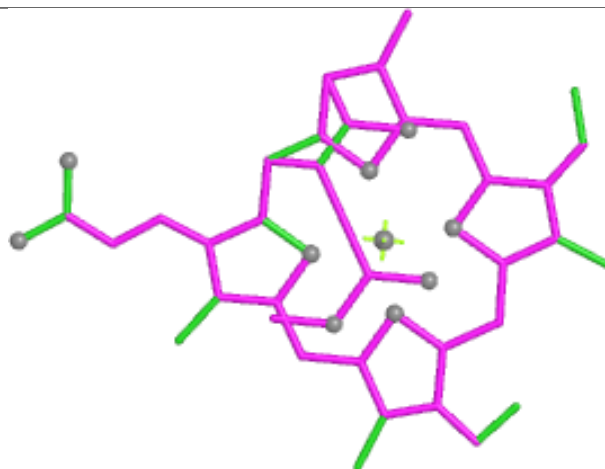




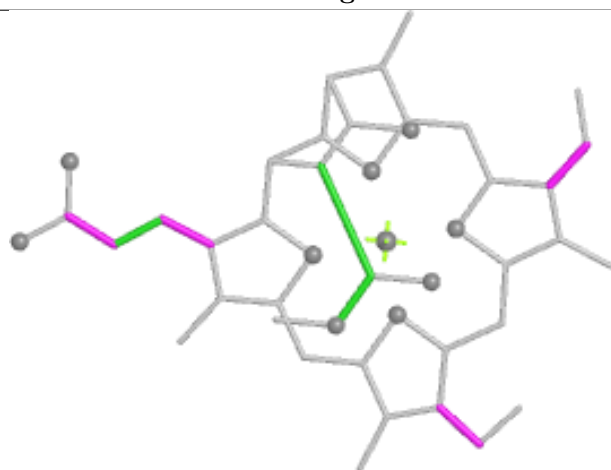
## Ligand KC1 N 314



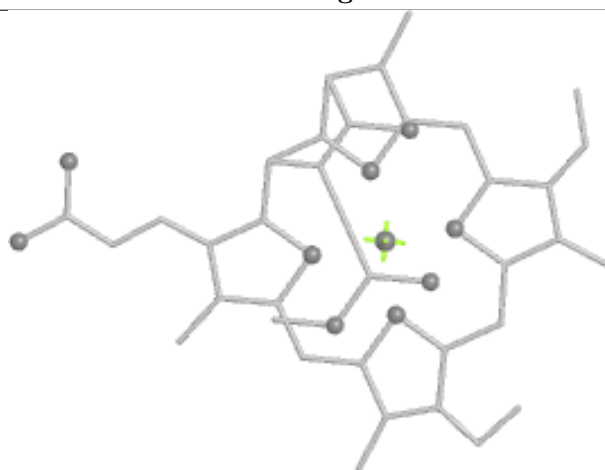
Bond lengths



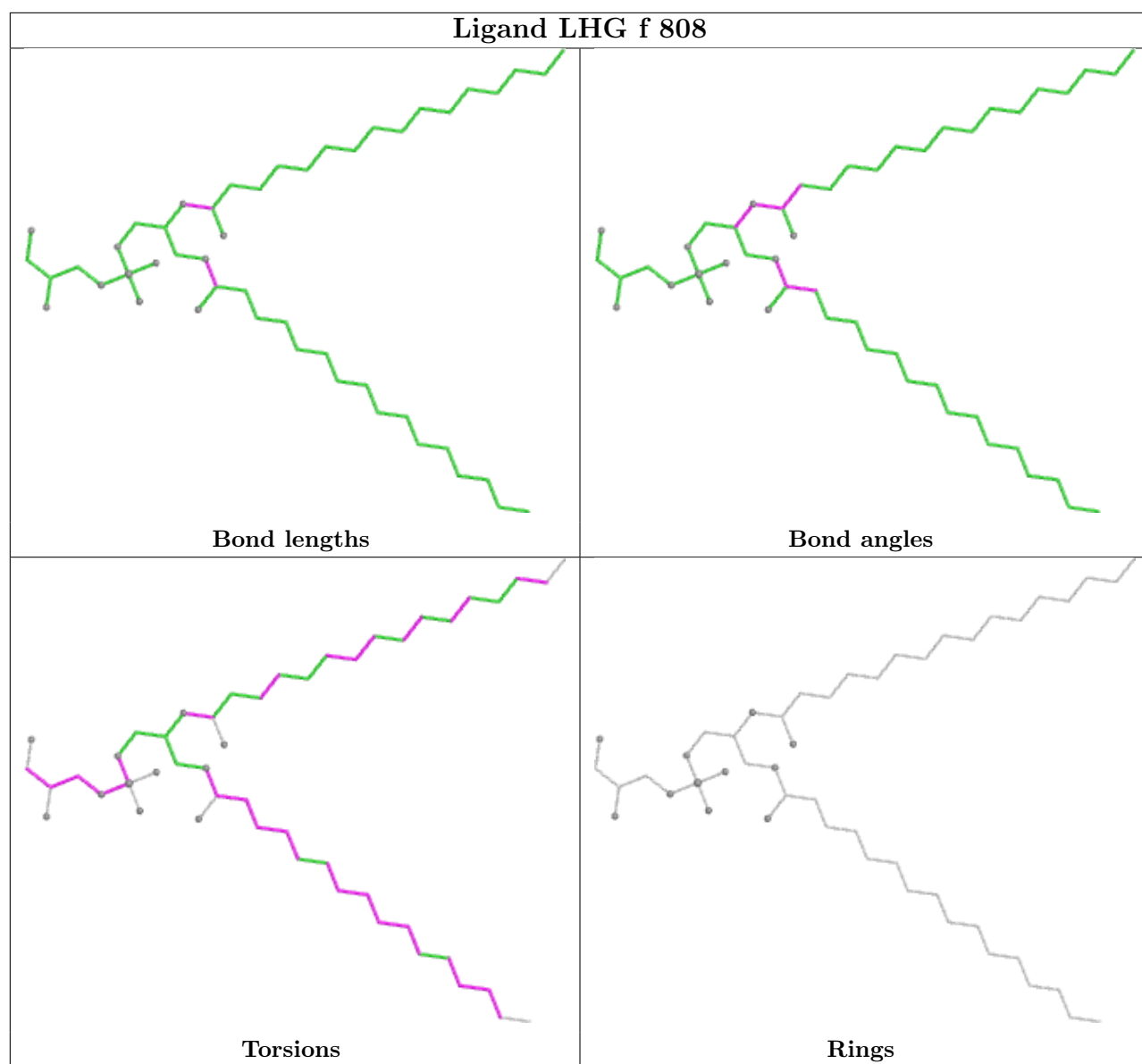
Bond angles



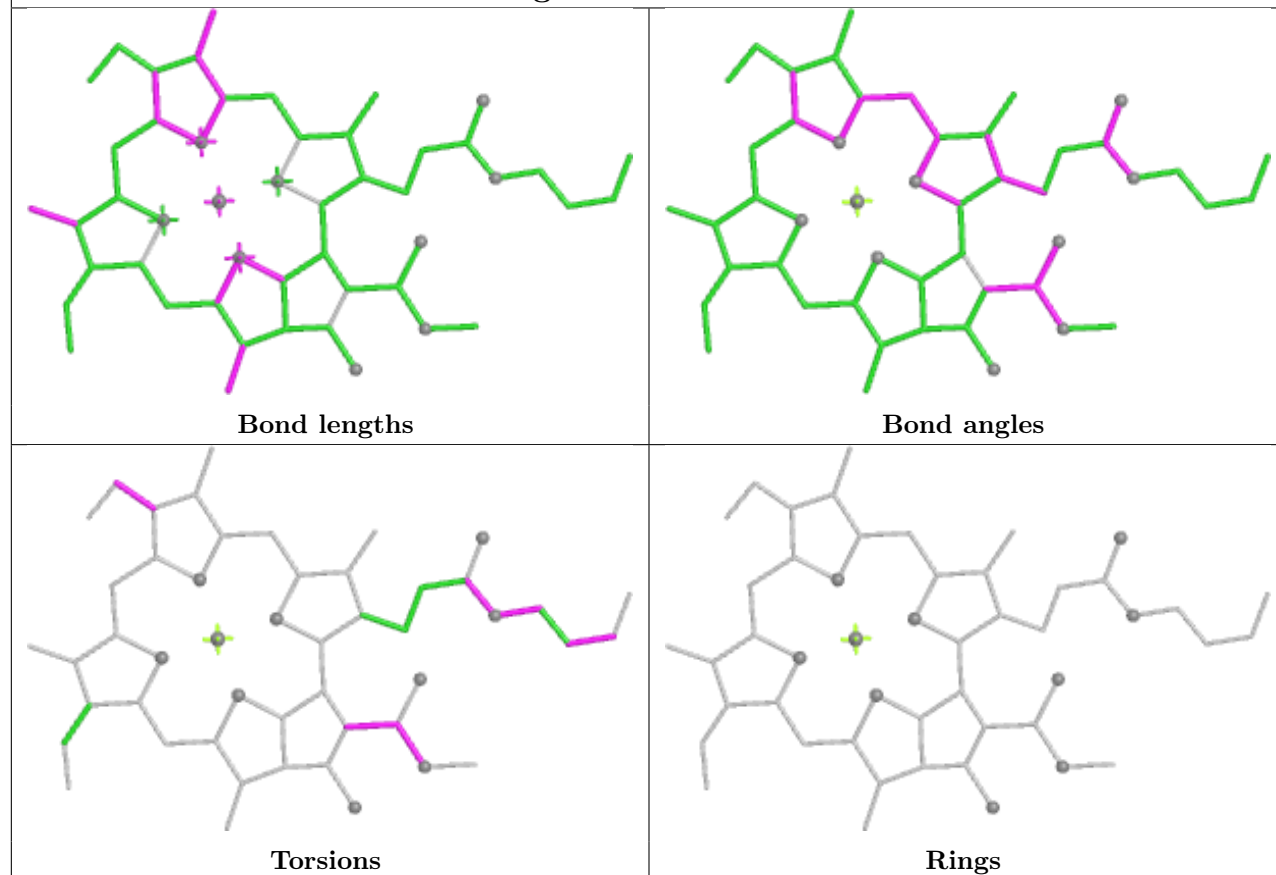
Torsions



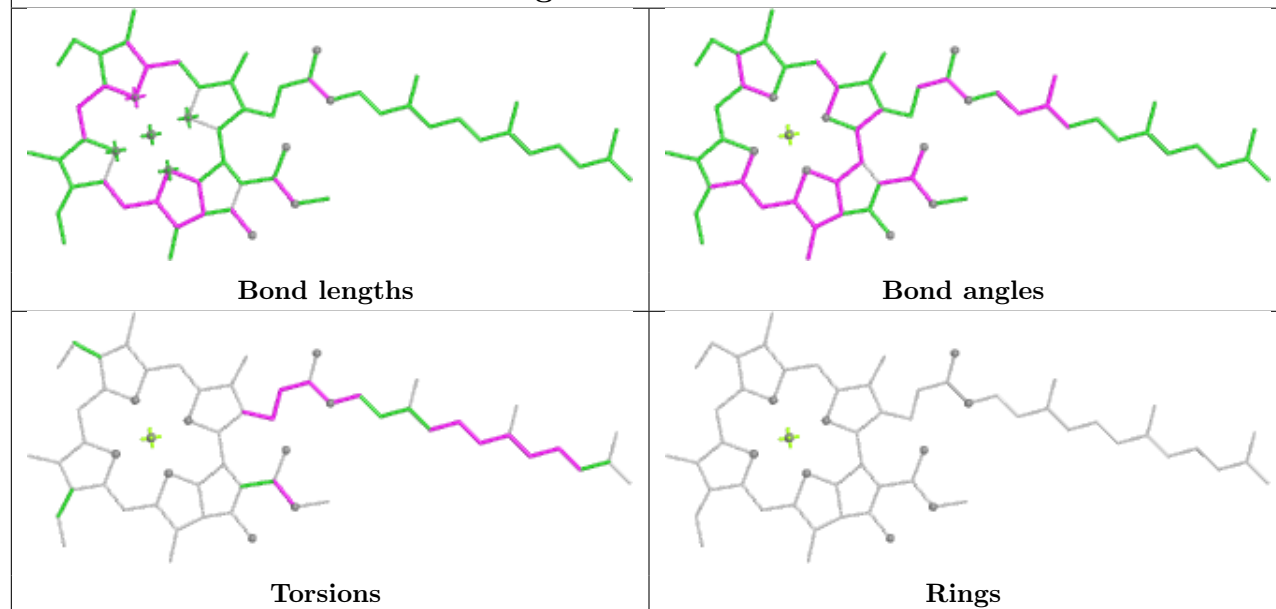
Rings

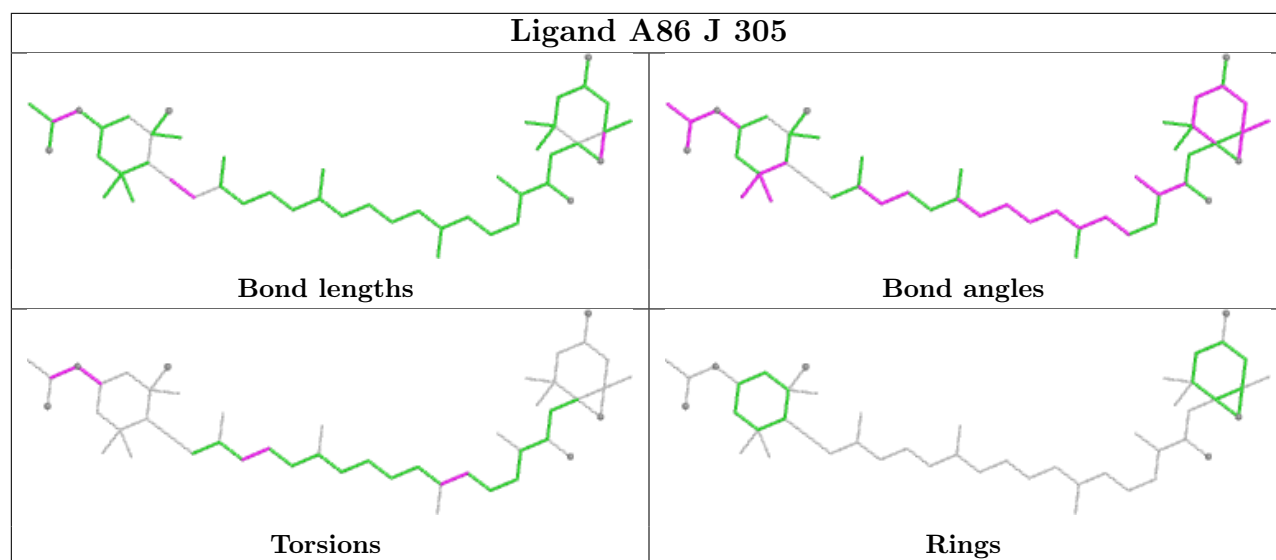
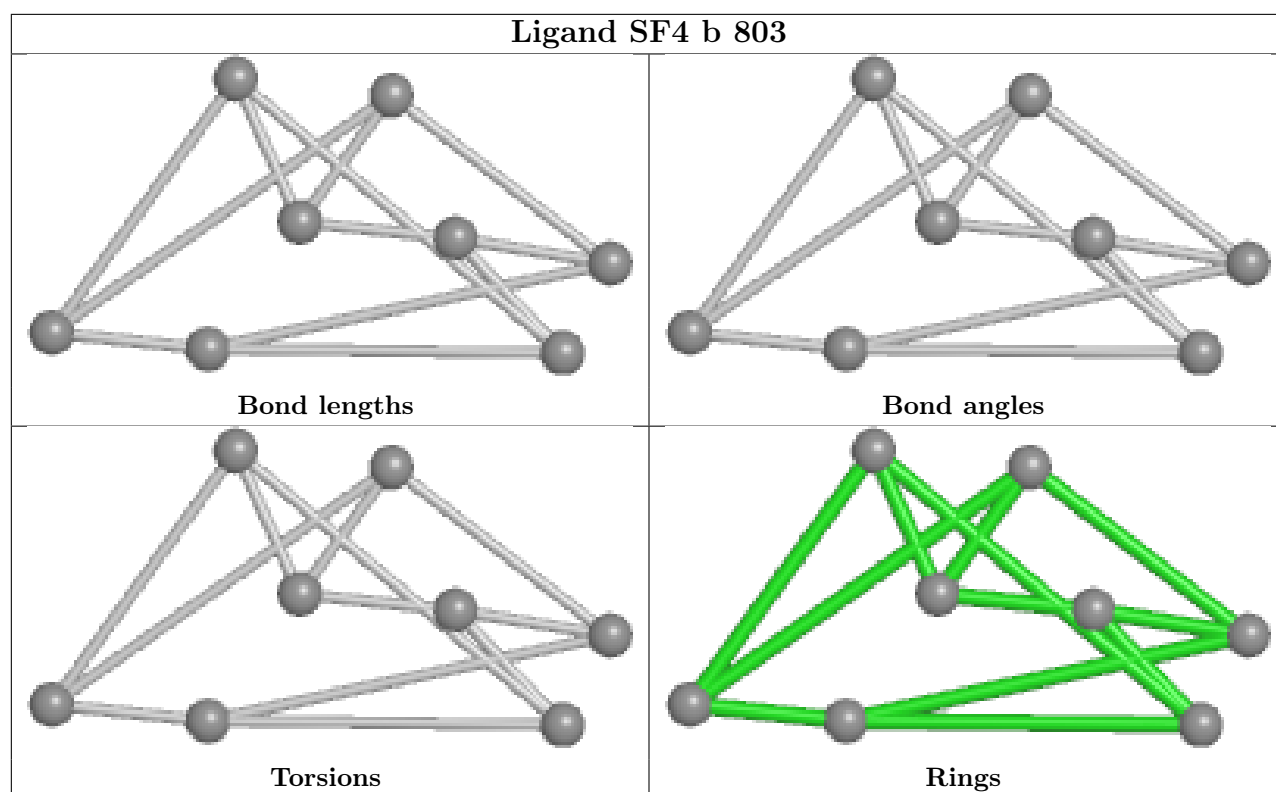


## Ligand CLA E 308

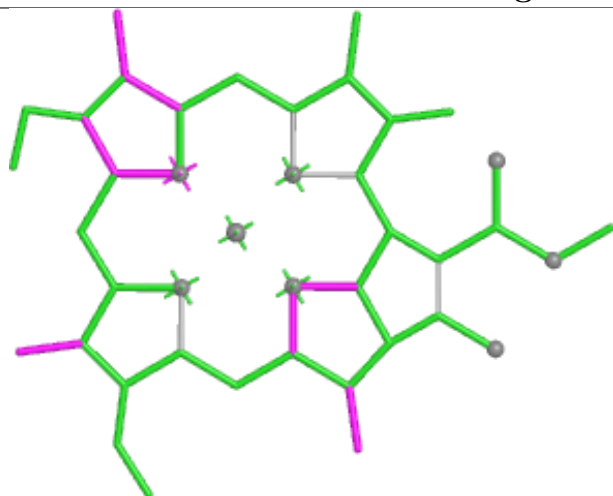


## Ligand CLA b 816

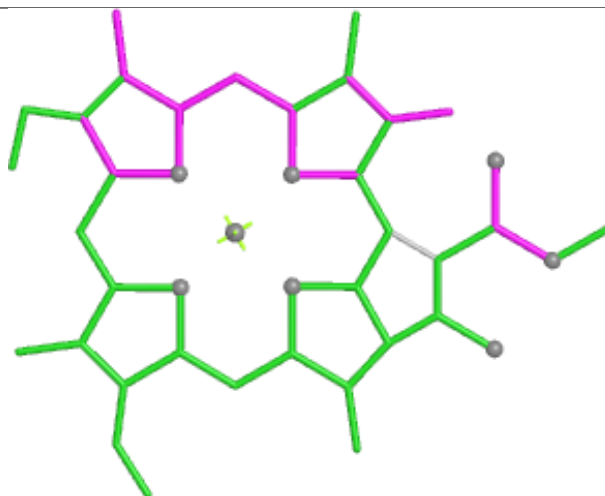




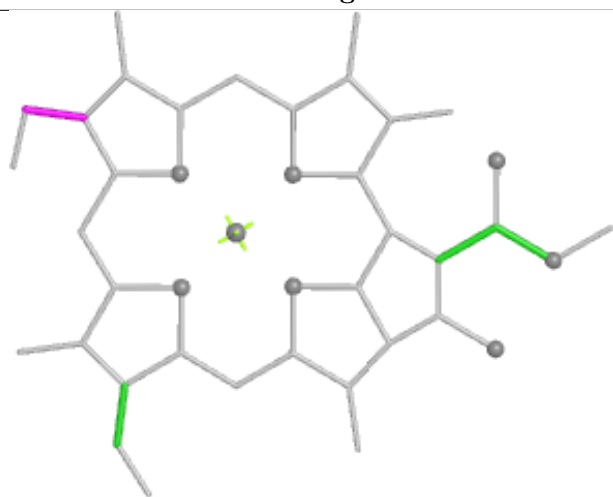
## Ligand CLA T 316



Bond lengths



Bond angles

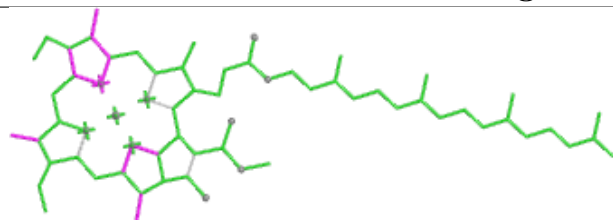


Torsions

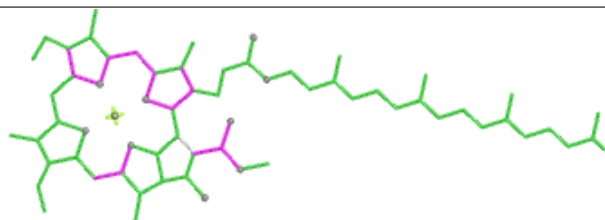


Rings

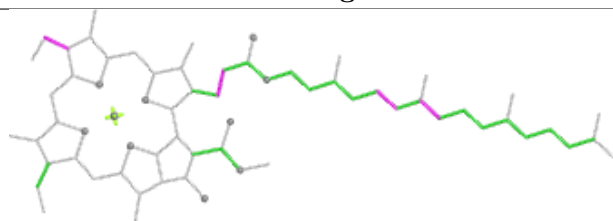
## Ligand CLA b 839



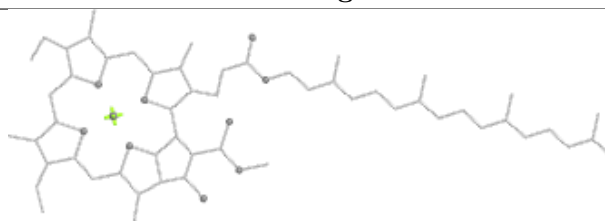
Bond lengths



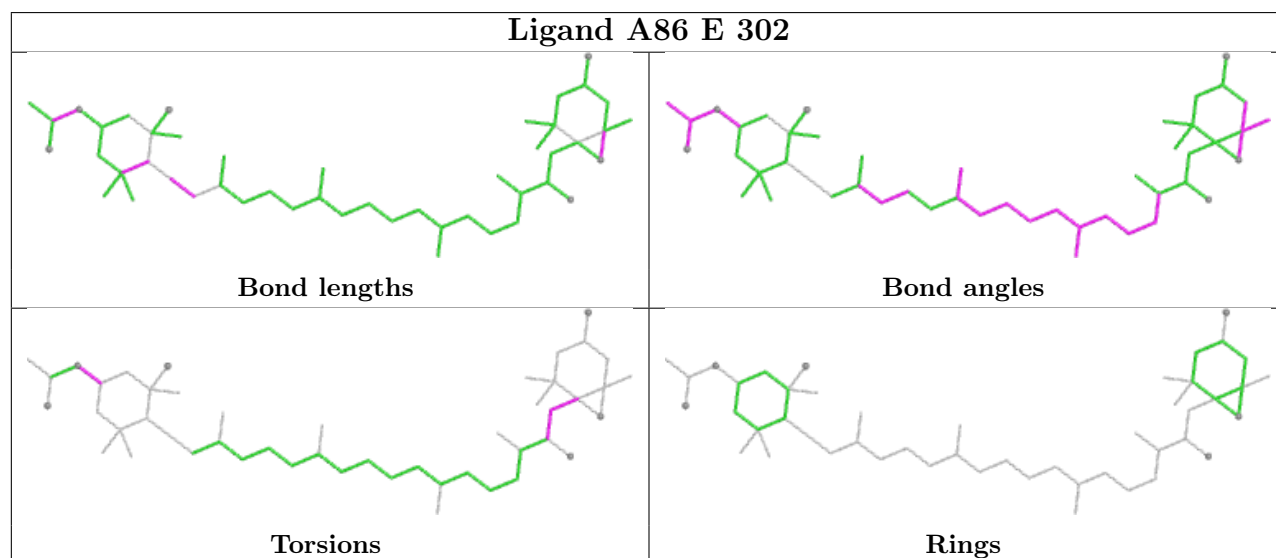
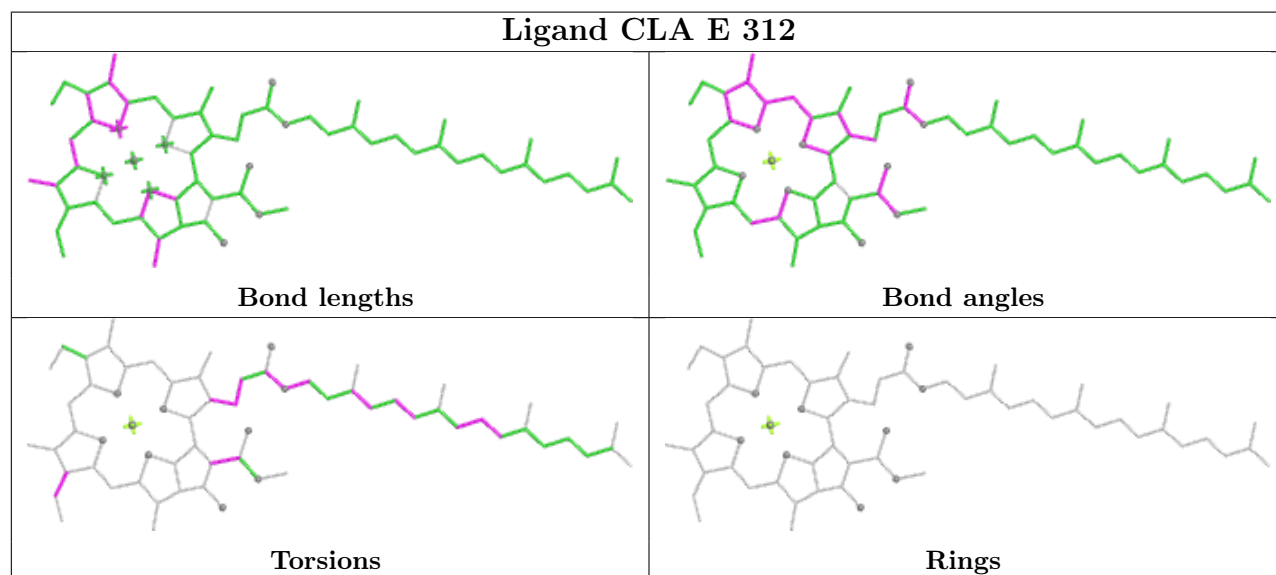
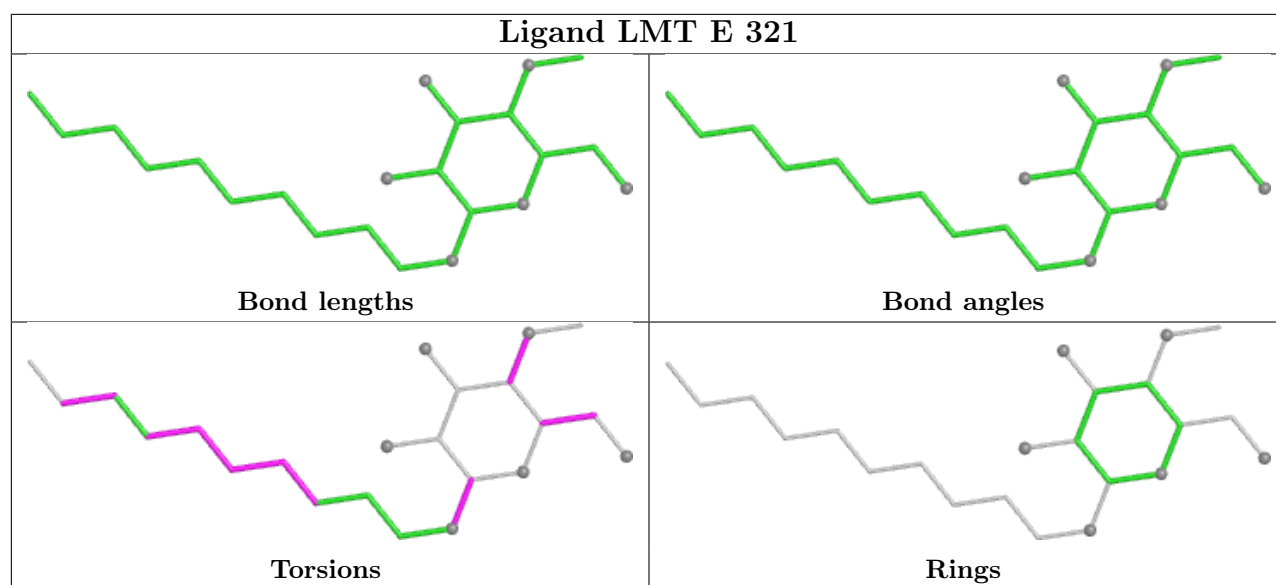
Bond angles

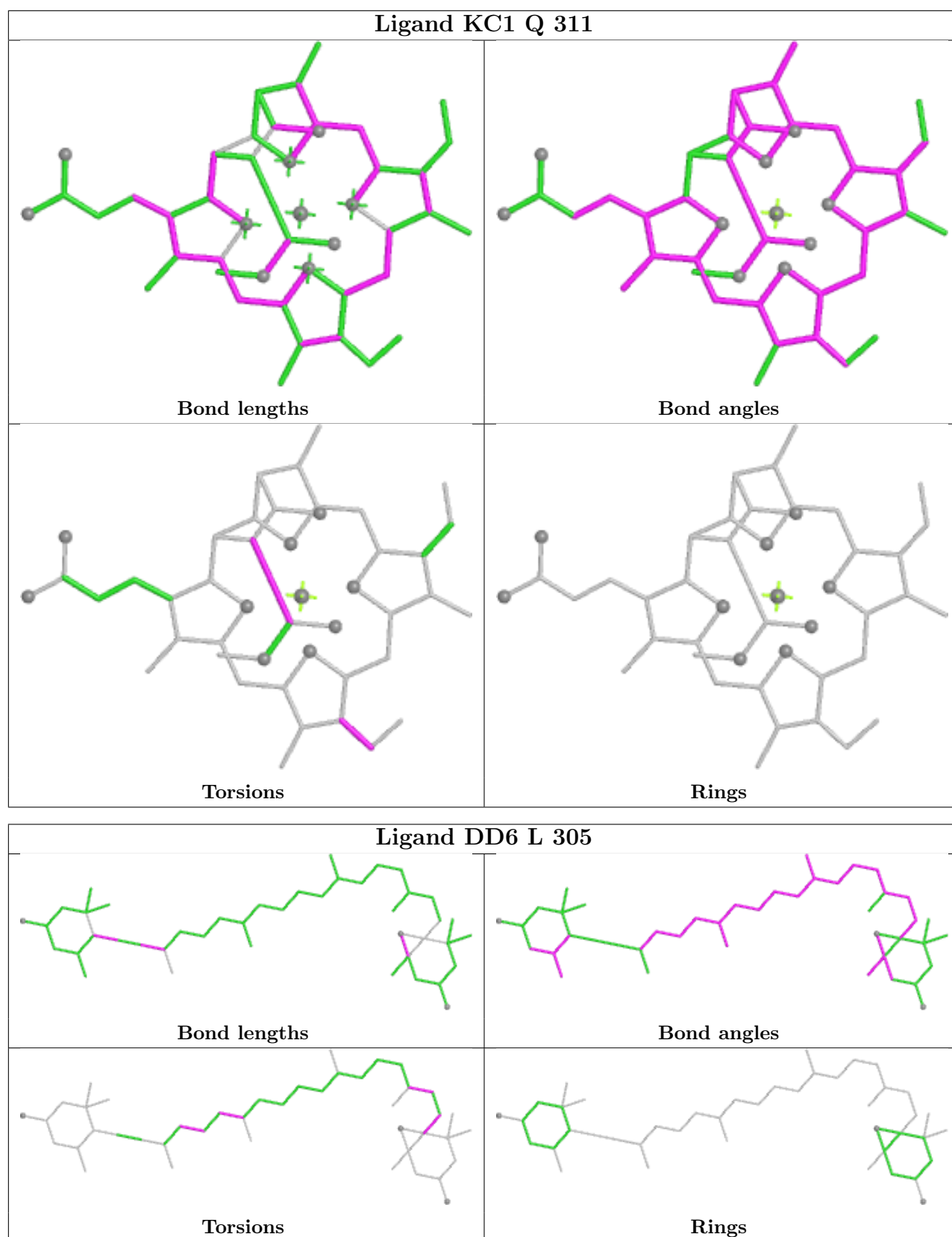


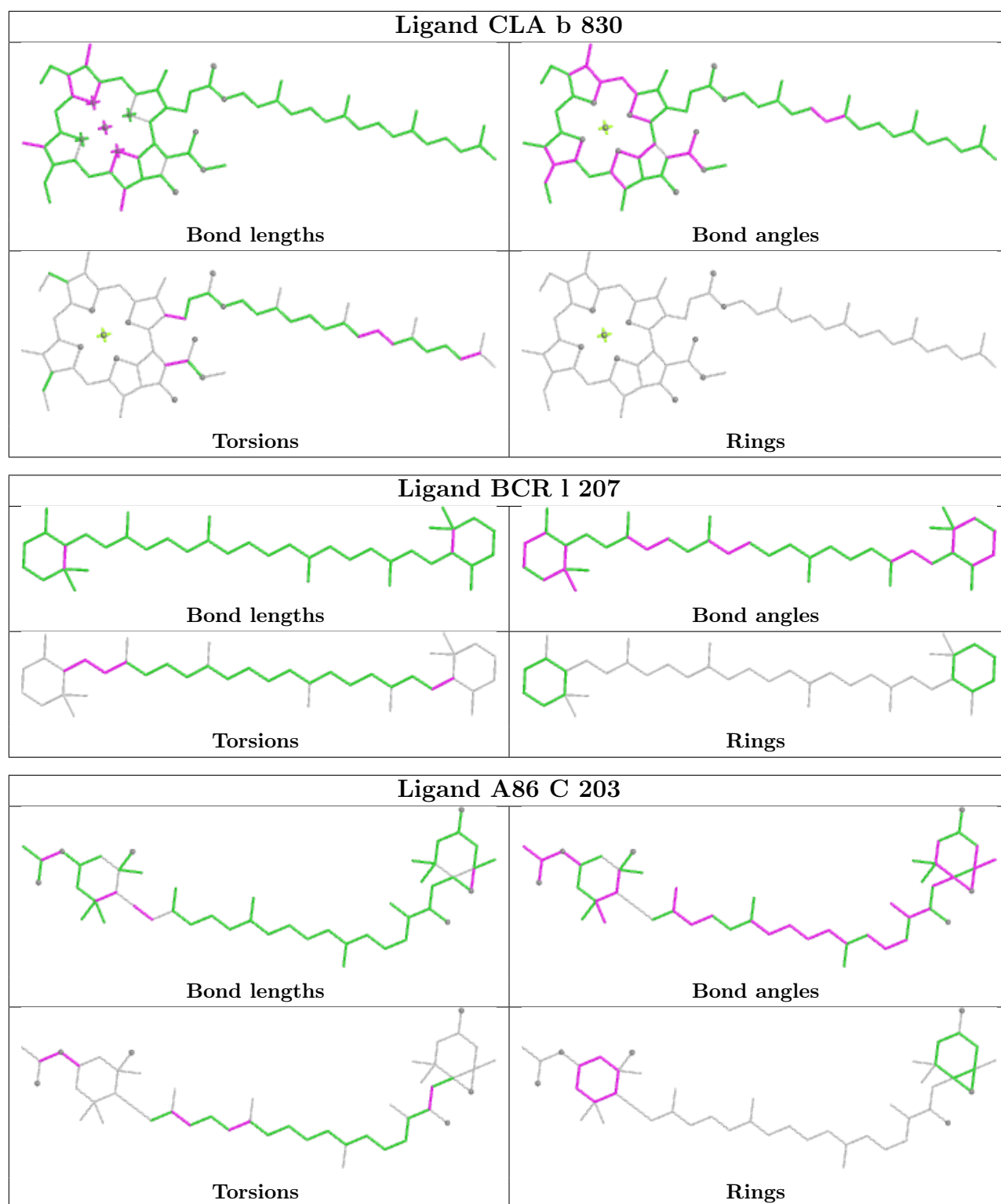
Torsions



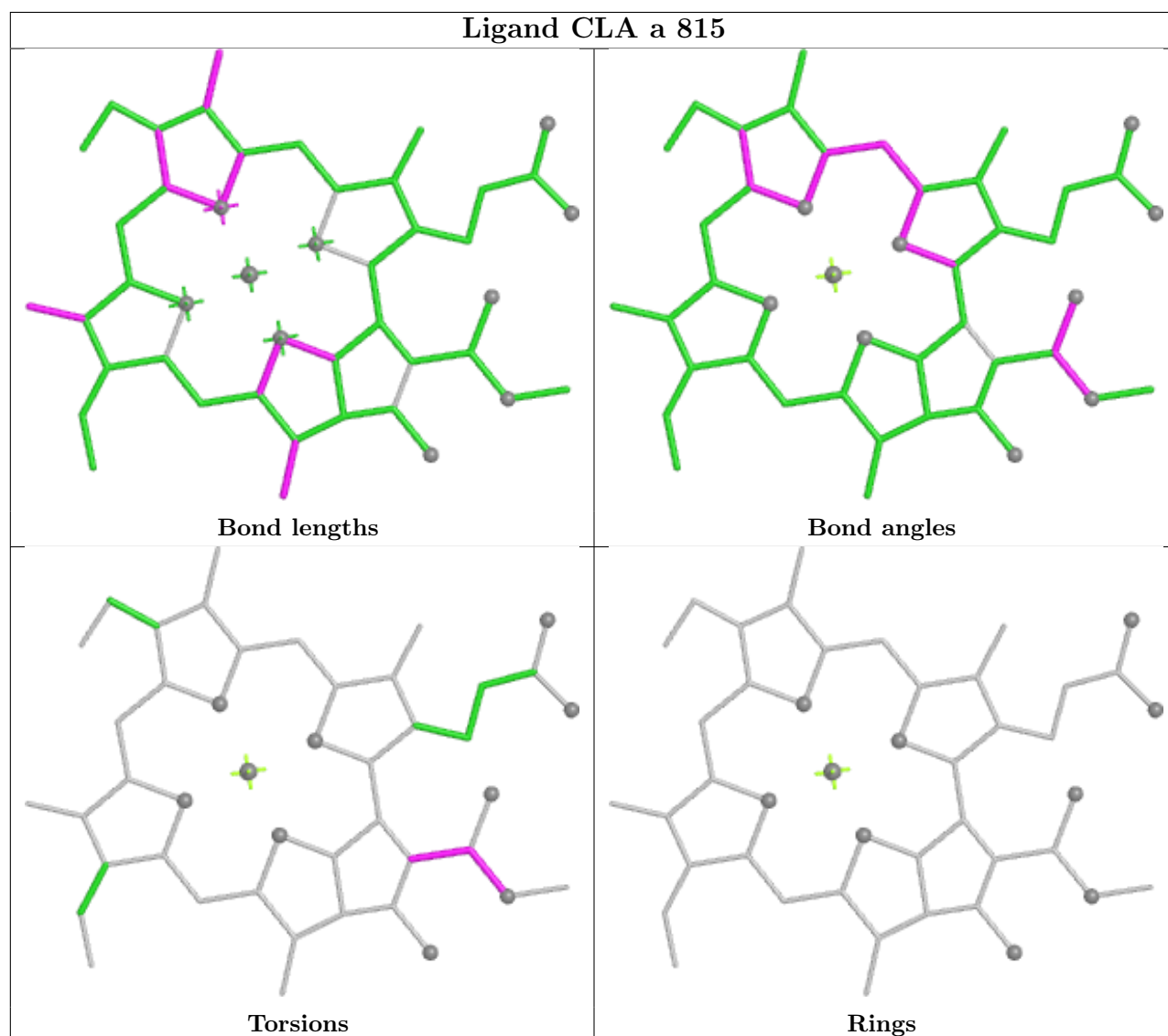
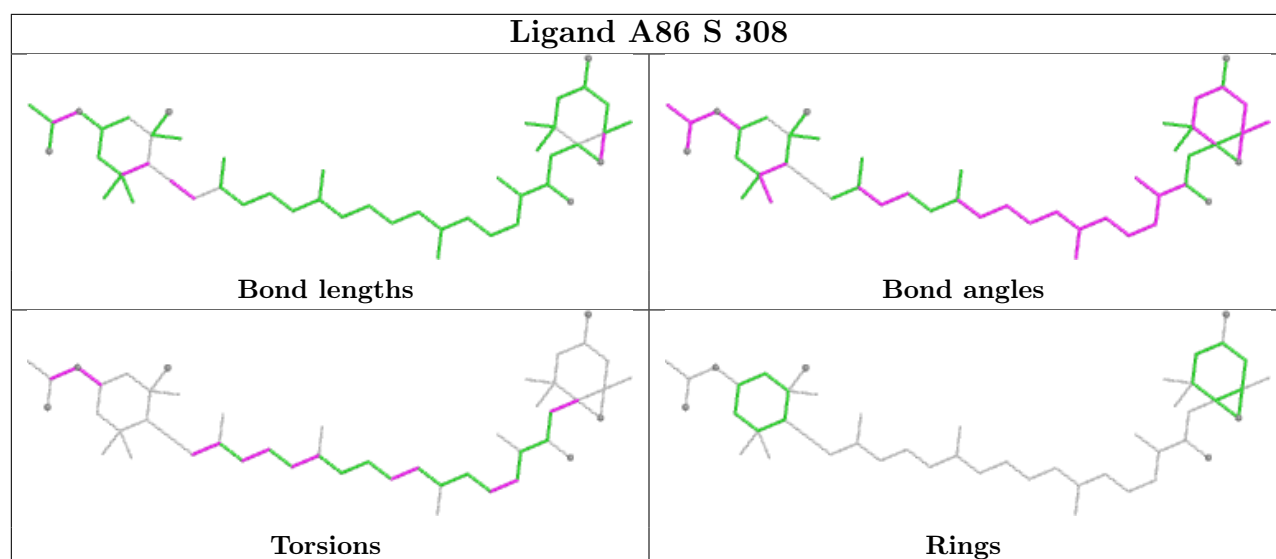
Rings



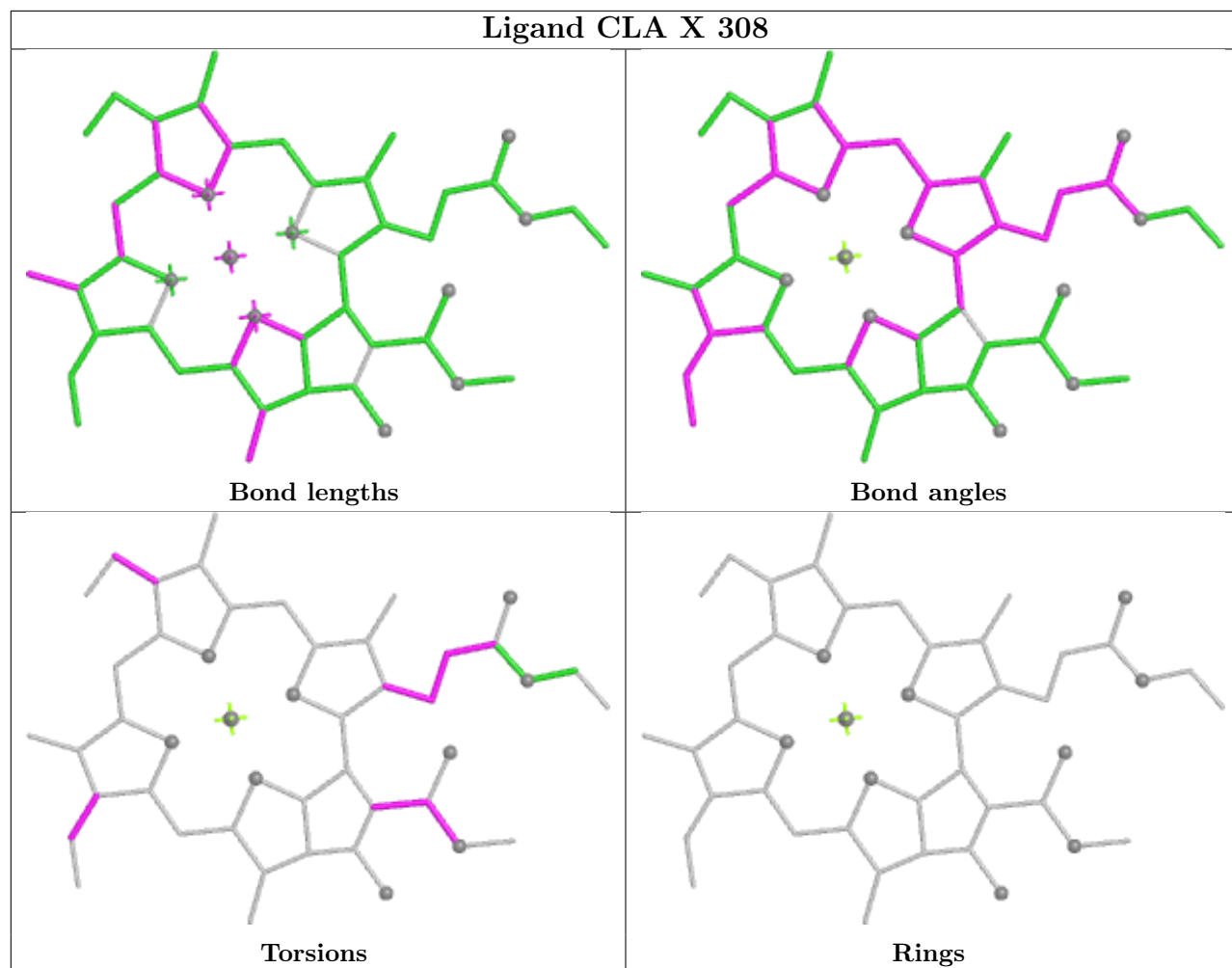


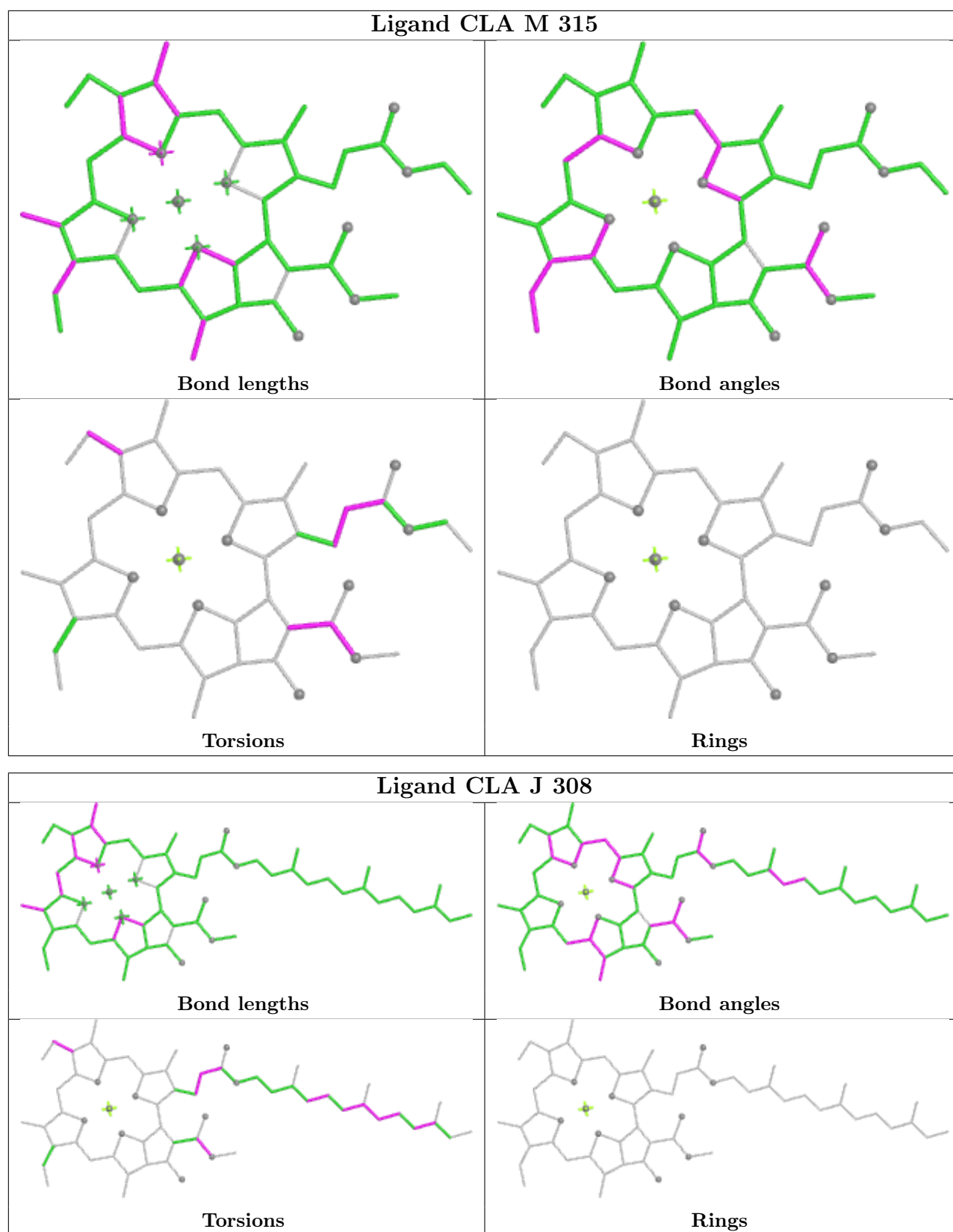


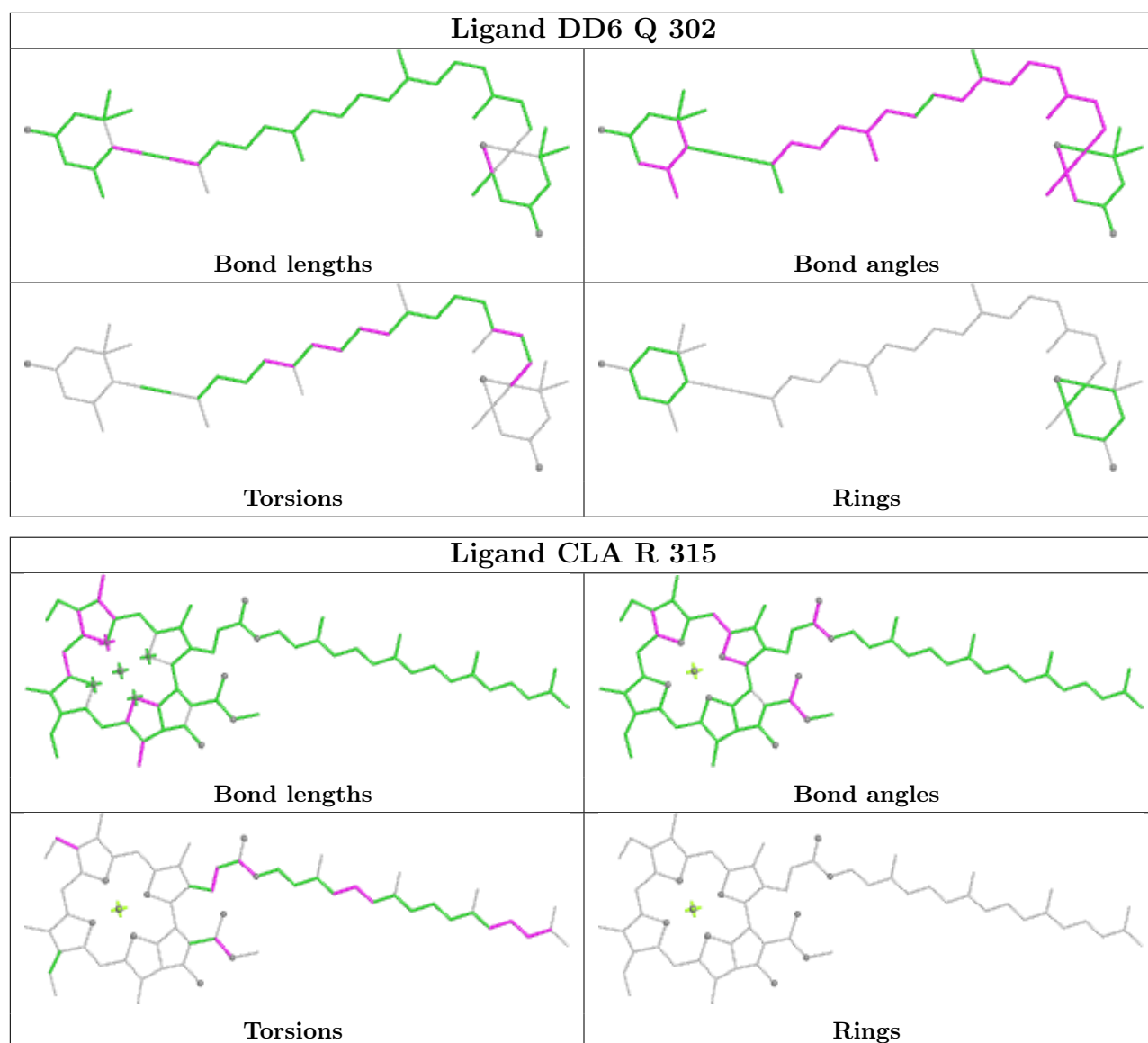




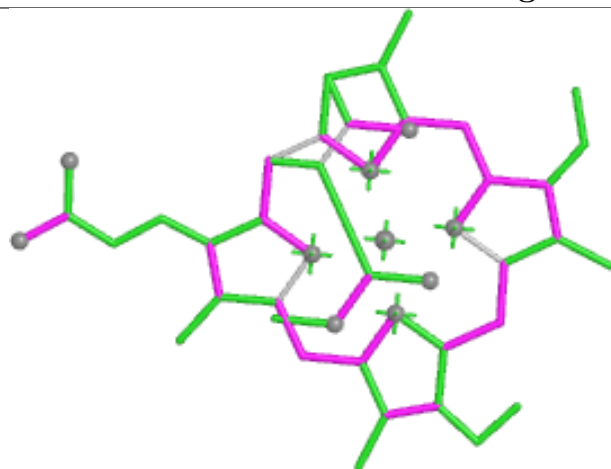
## Ligand CLA X 308



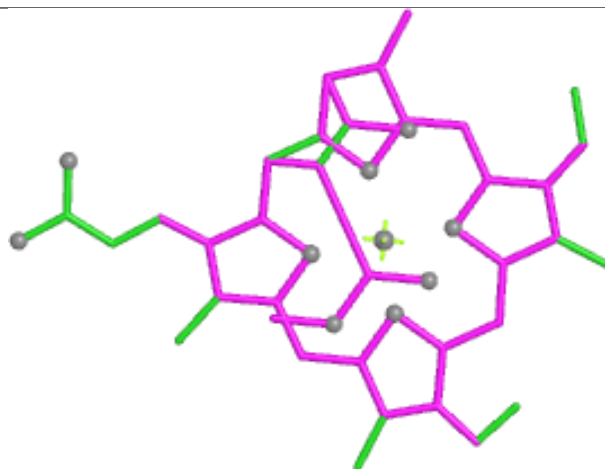




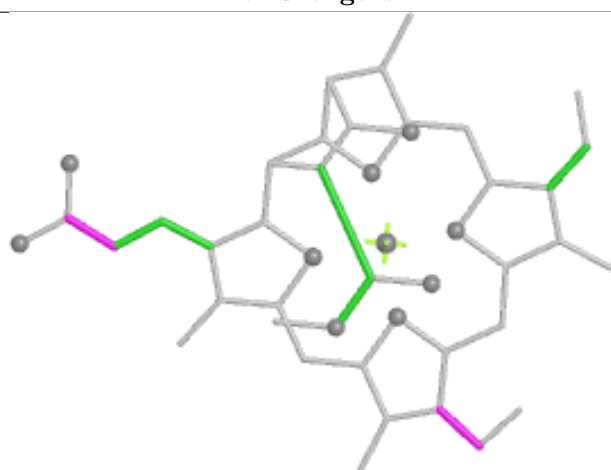
## Ligand KC1 L 317



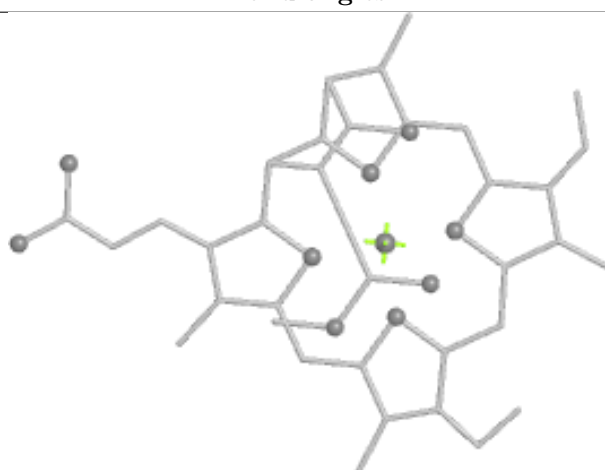
Bond lengths



Bond angles

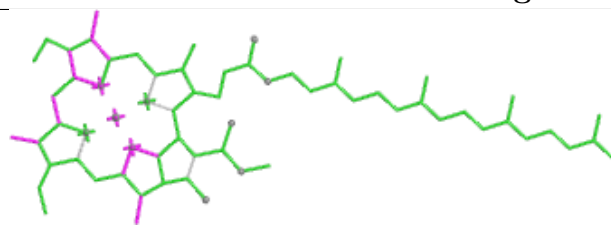


Torsions

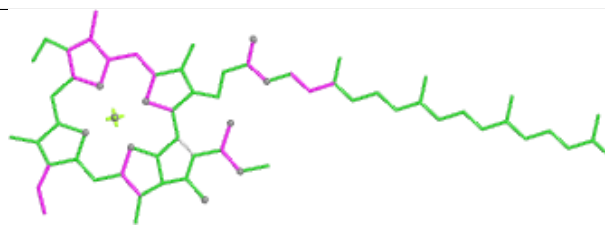


Rings

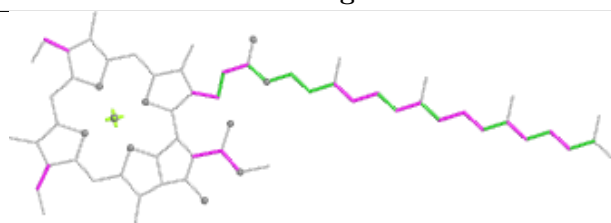
## Ligand CLA O 309



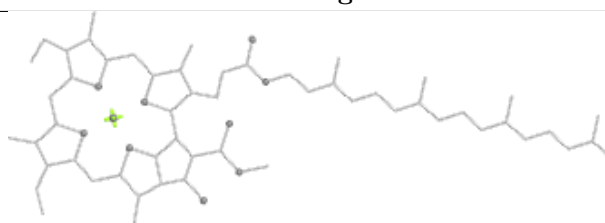
Bond lengths



Bond angles

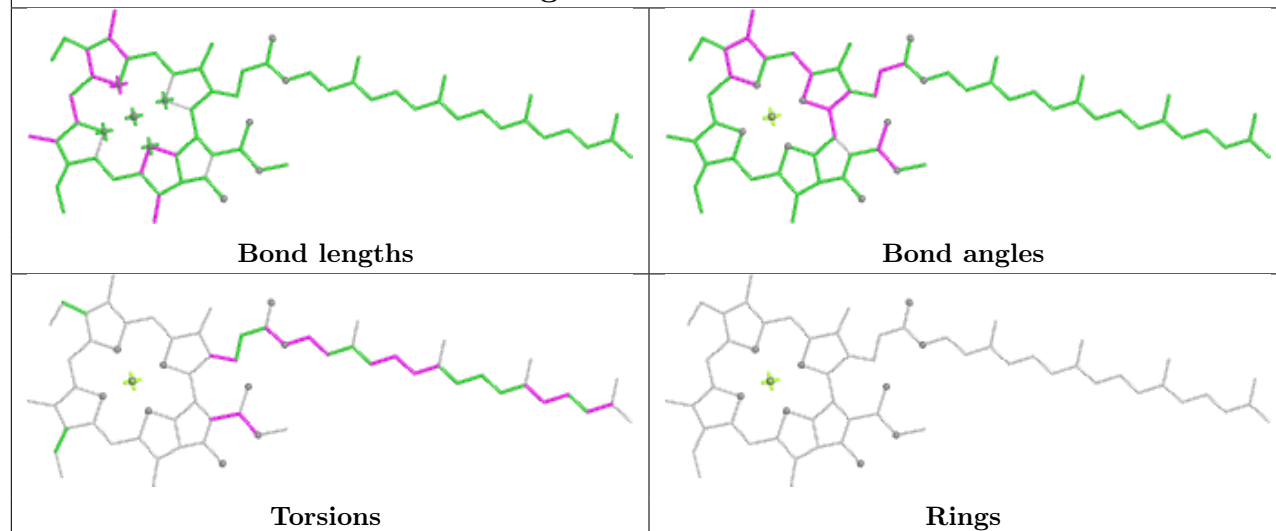


Torsions

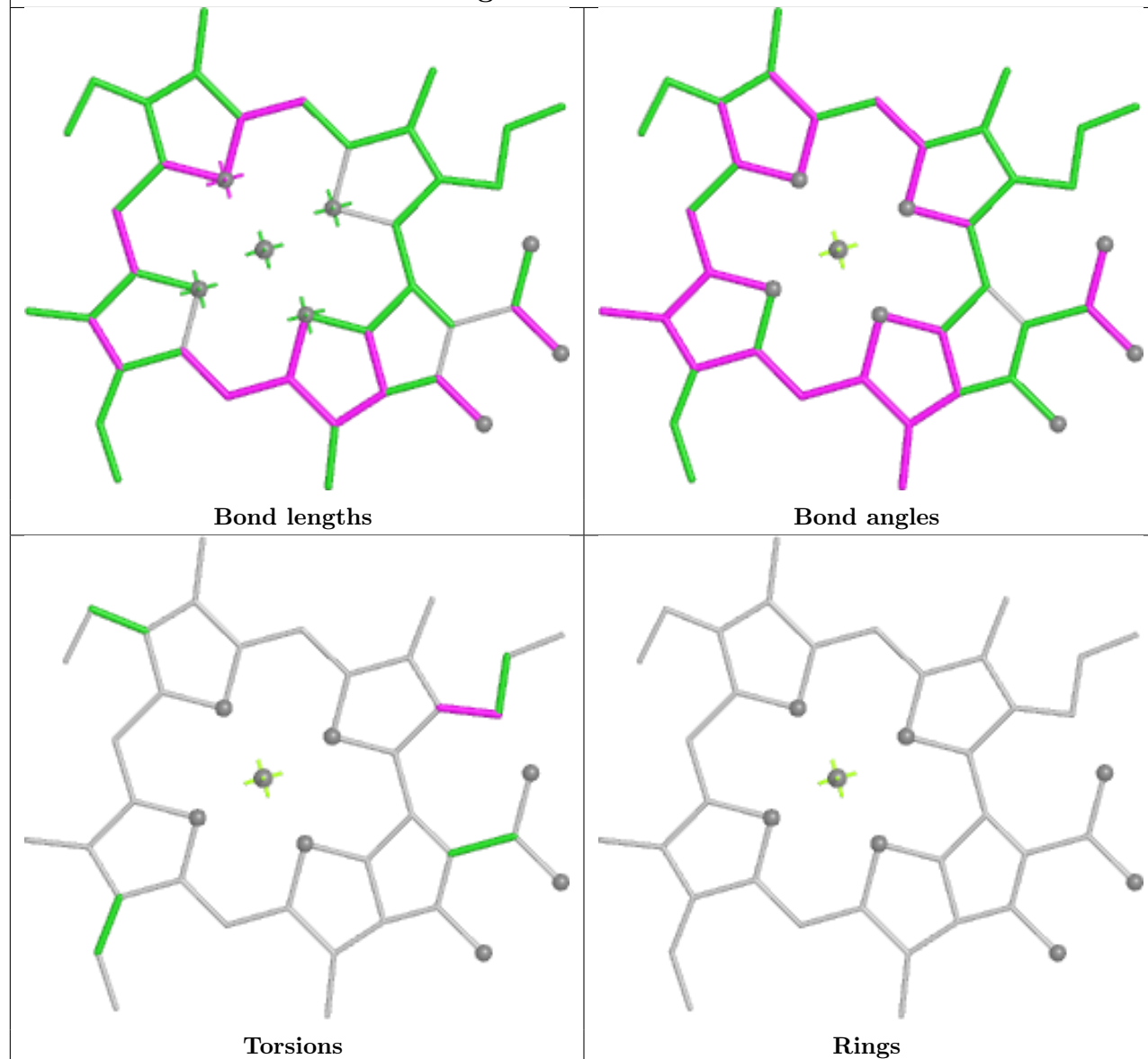


Rings

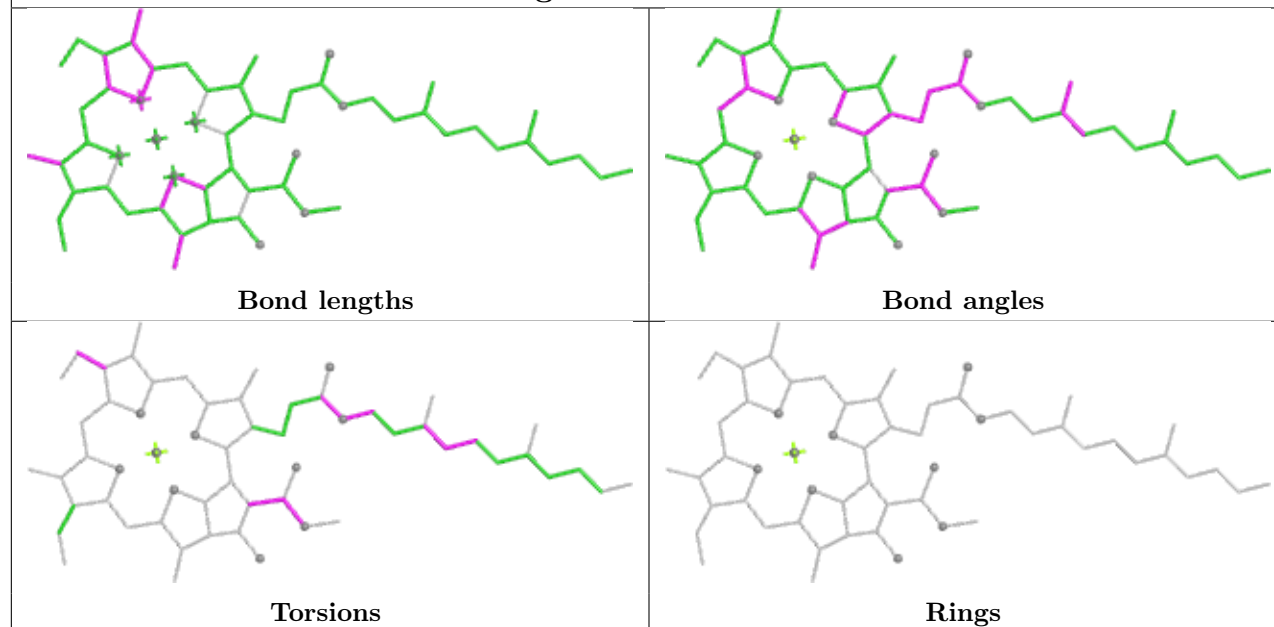
## Ligand CLA i 102



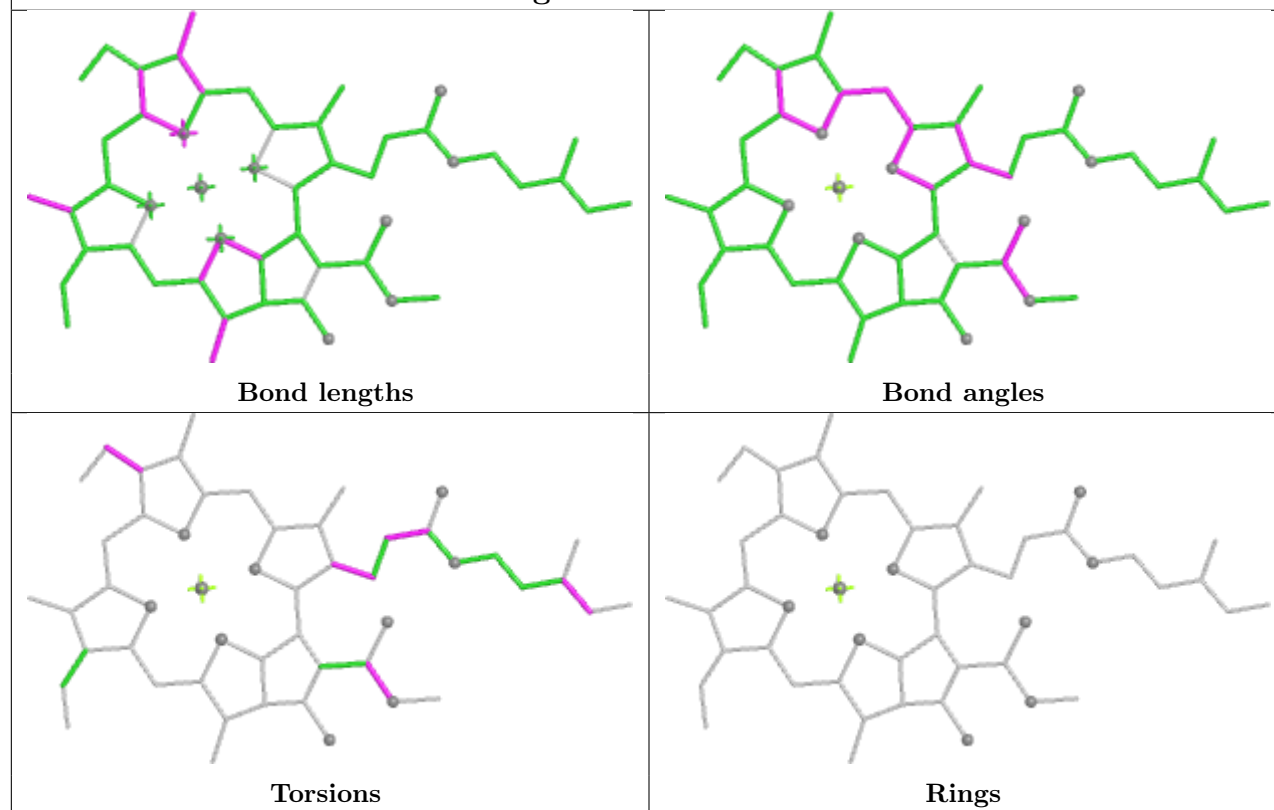
## Ligand CLA G 307

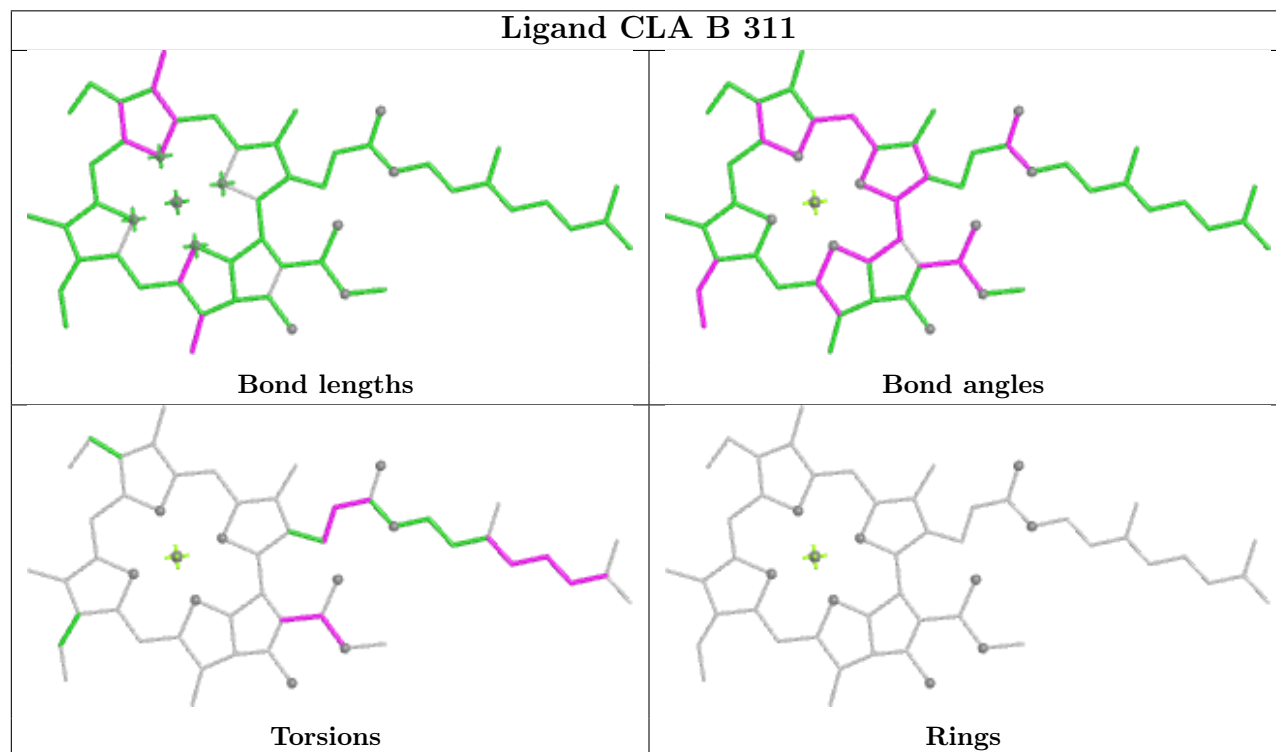
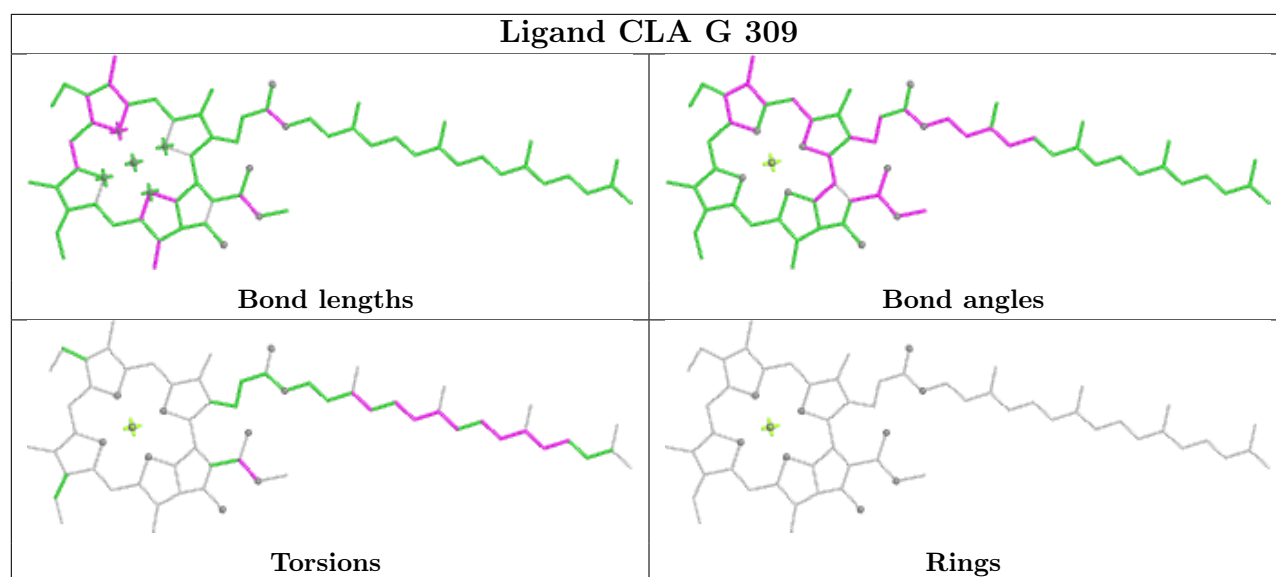


## Ligand CLA b 833



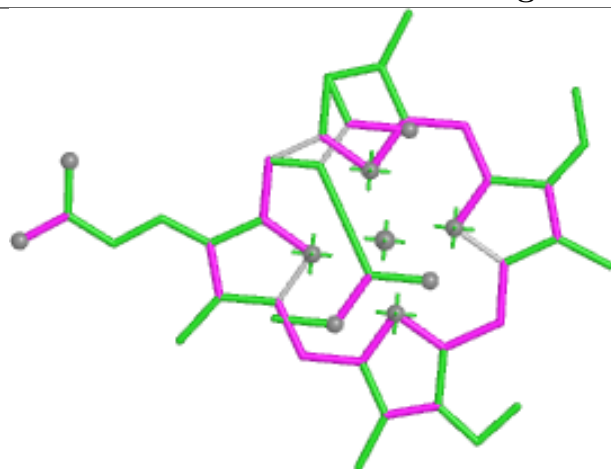
## Ligand CLA P 318



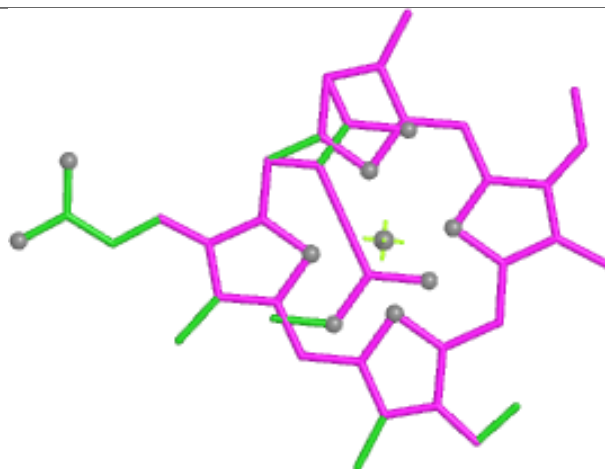




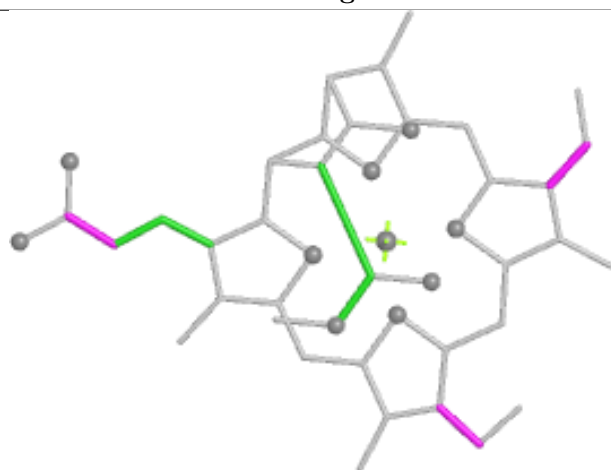
## Ligand KC1 E 309



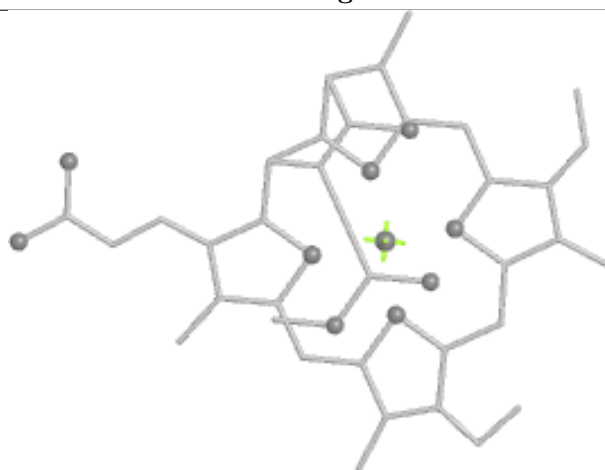
Bond lengths



Bond angles



Torsions



Rings

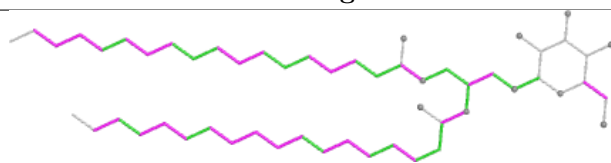
## Ligand LMG G 325



Bond lengths



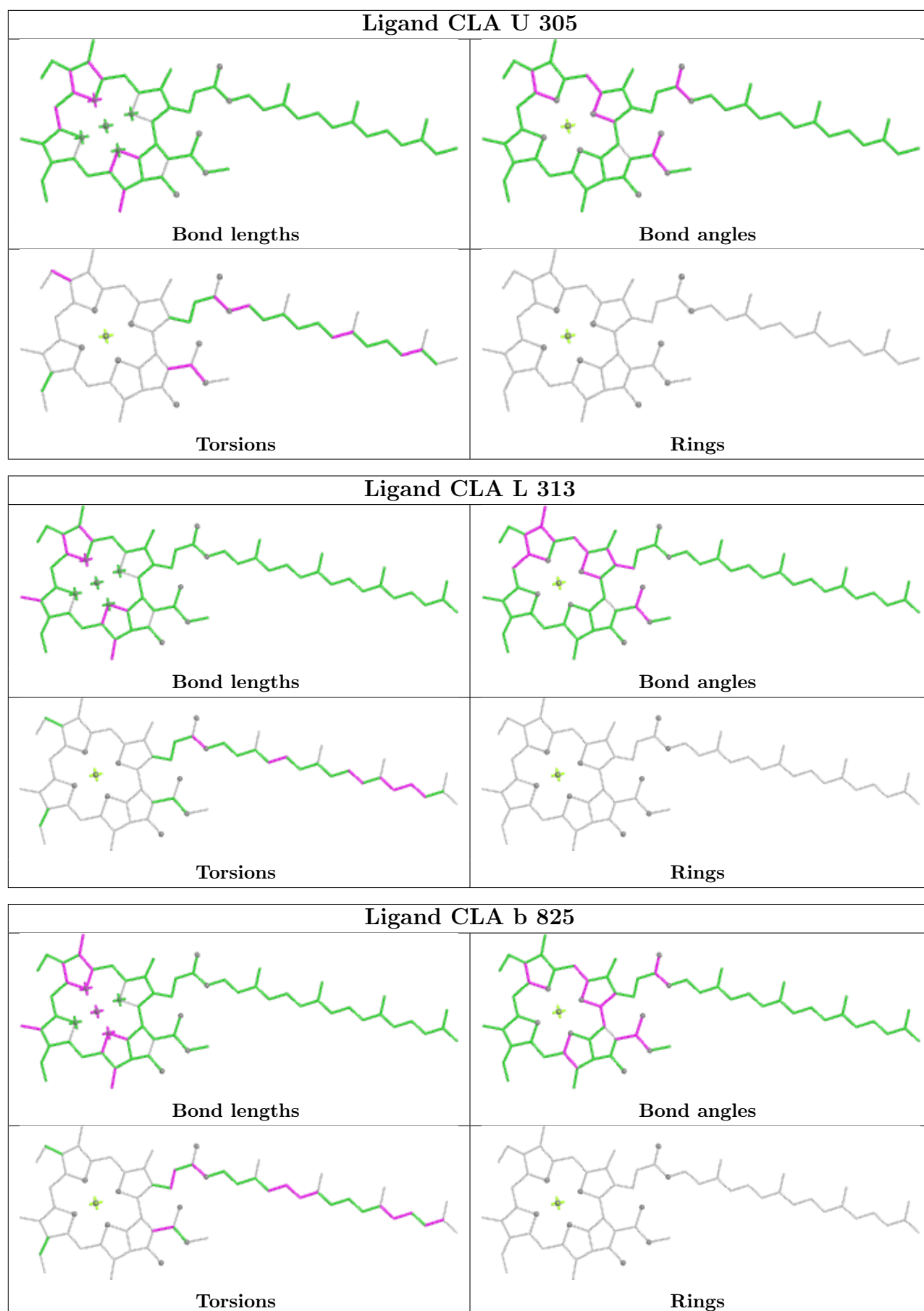
Bond angles

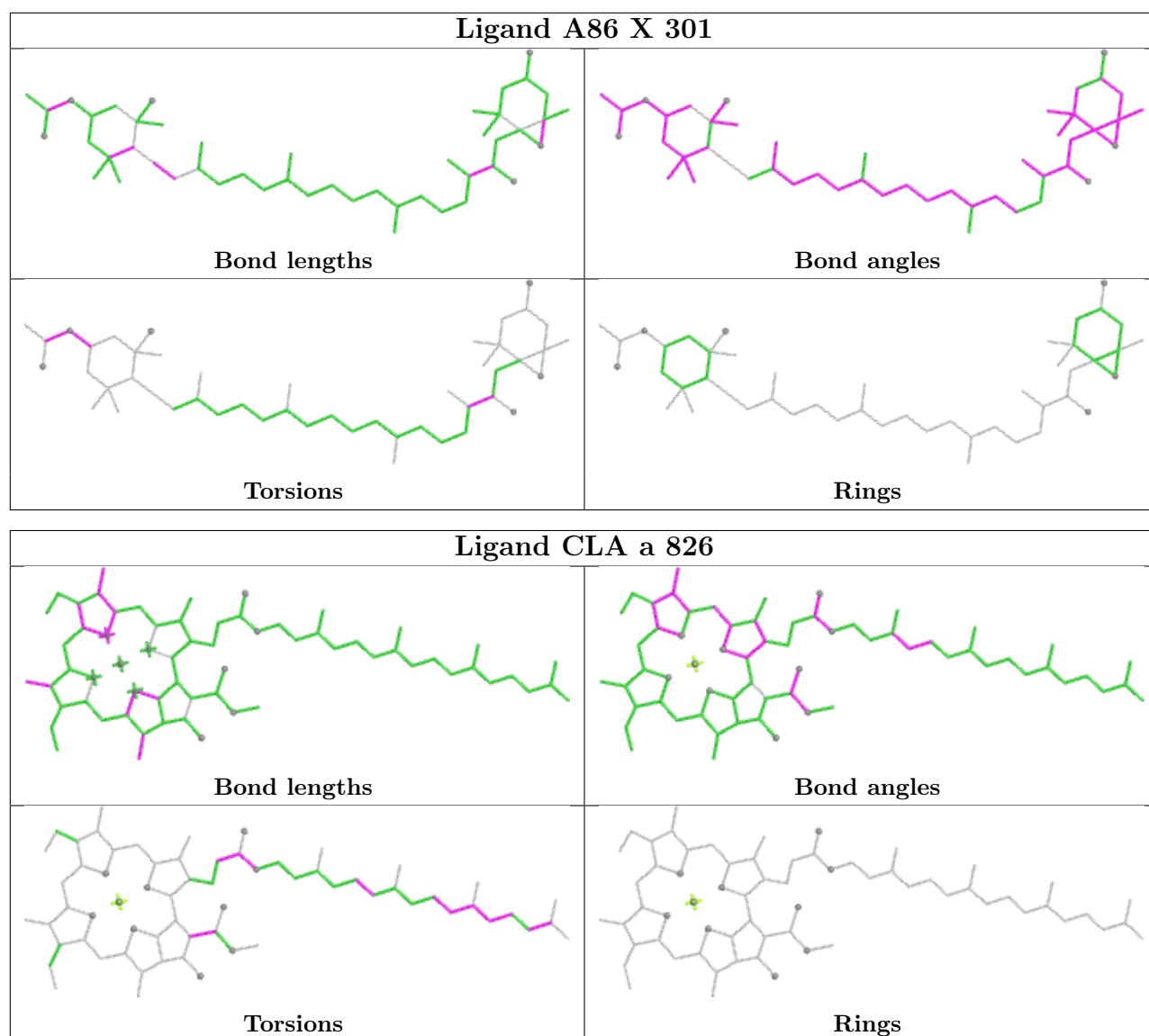


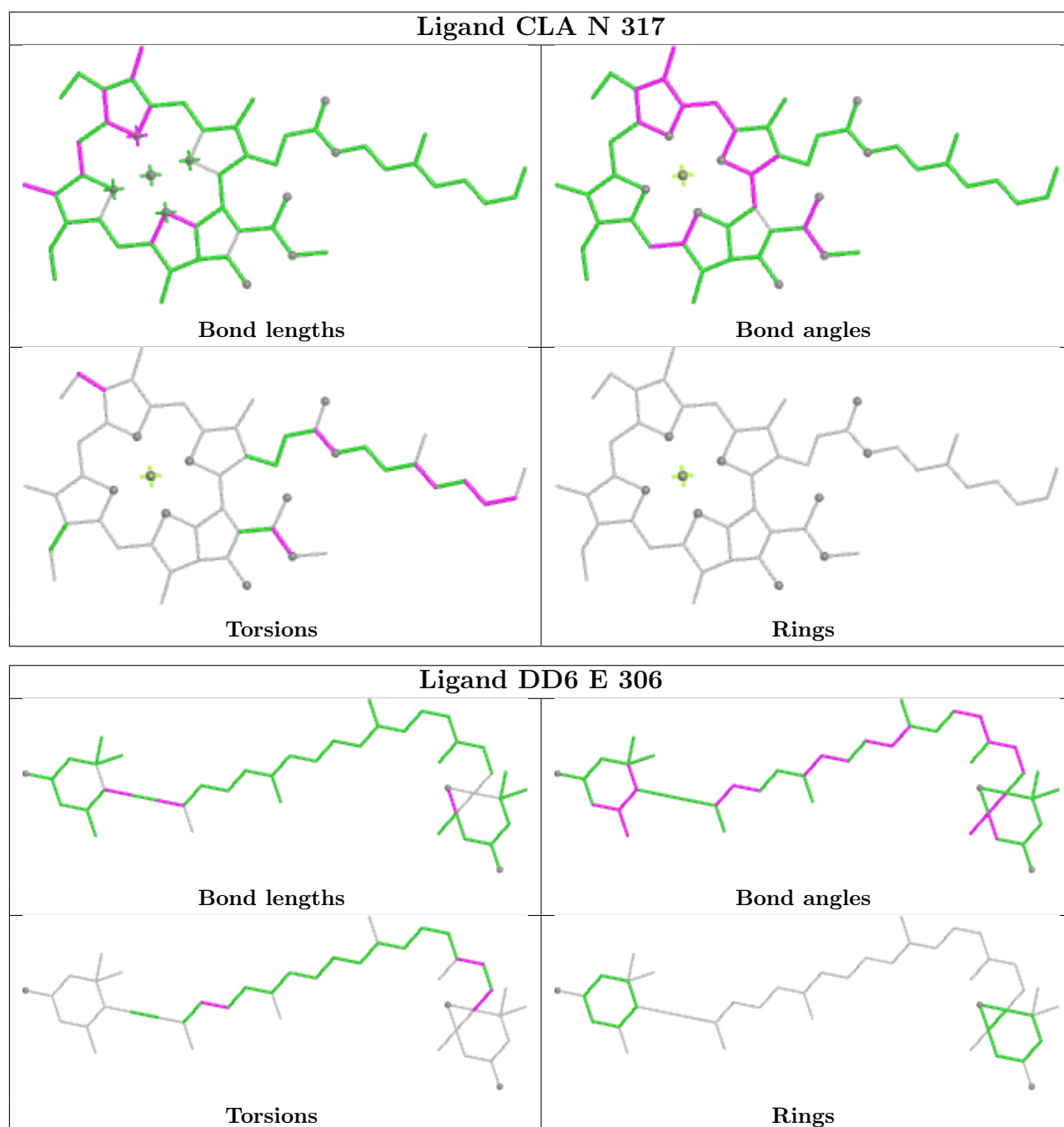
Torsions

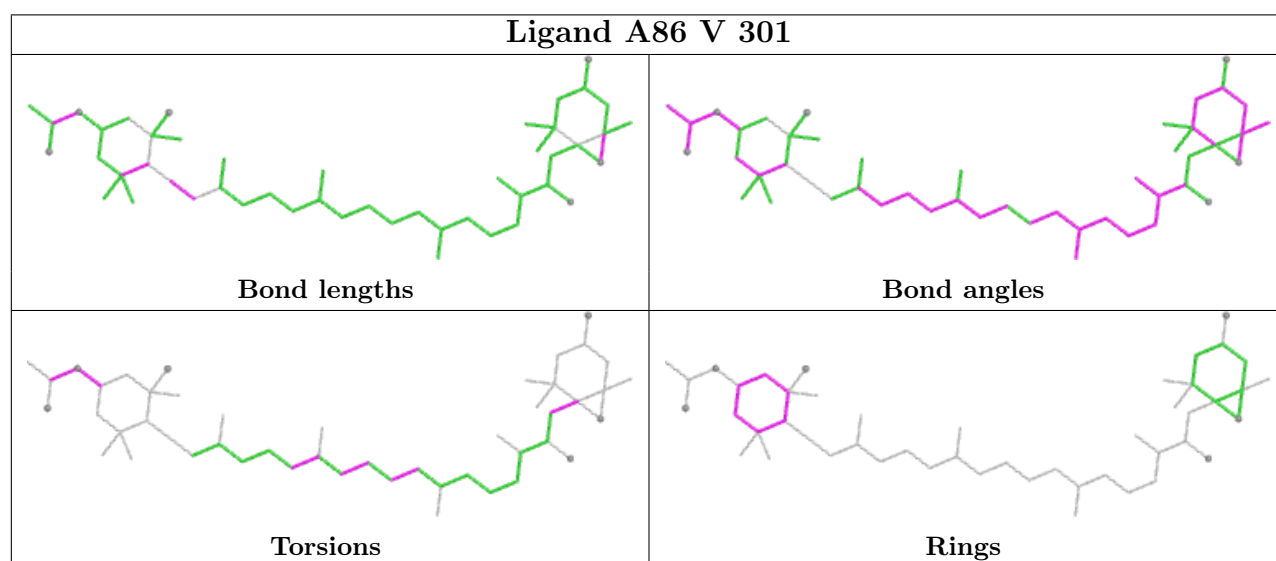
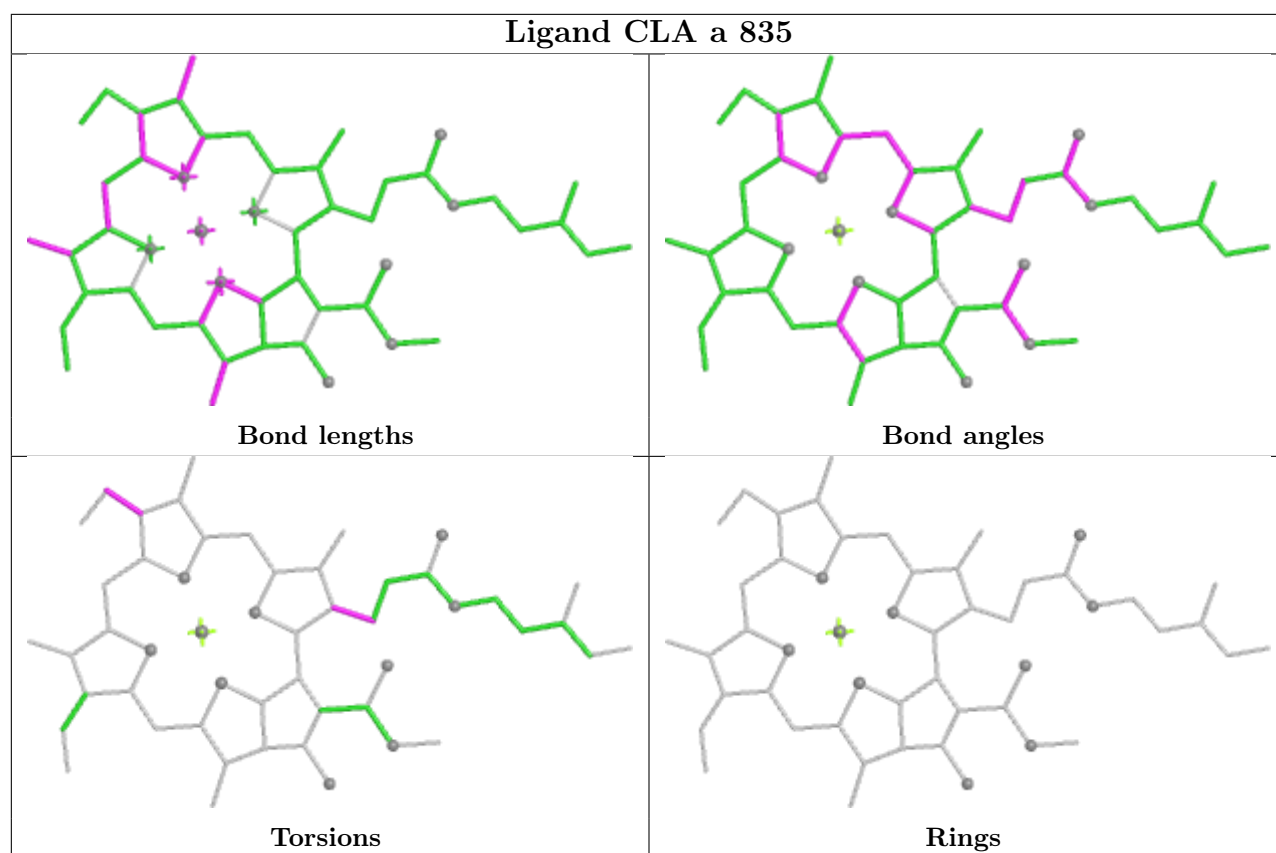


Rings

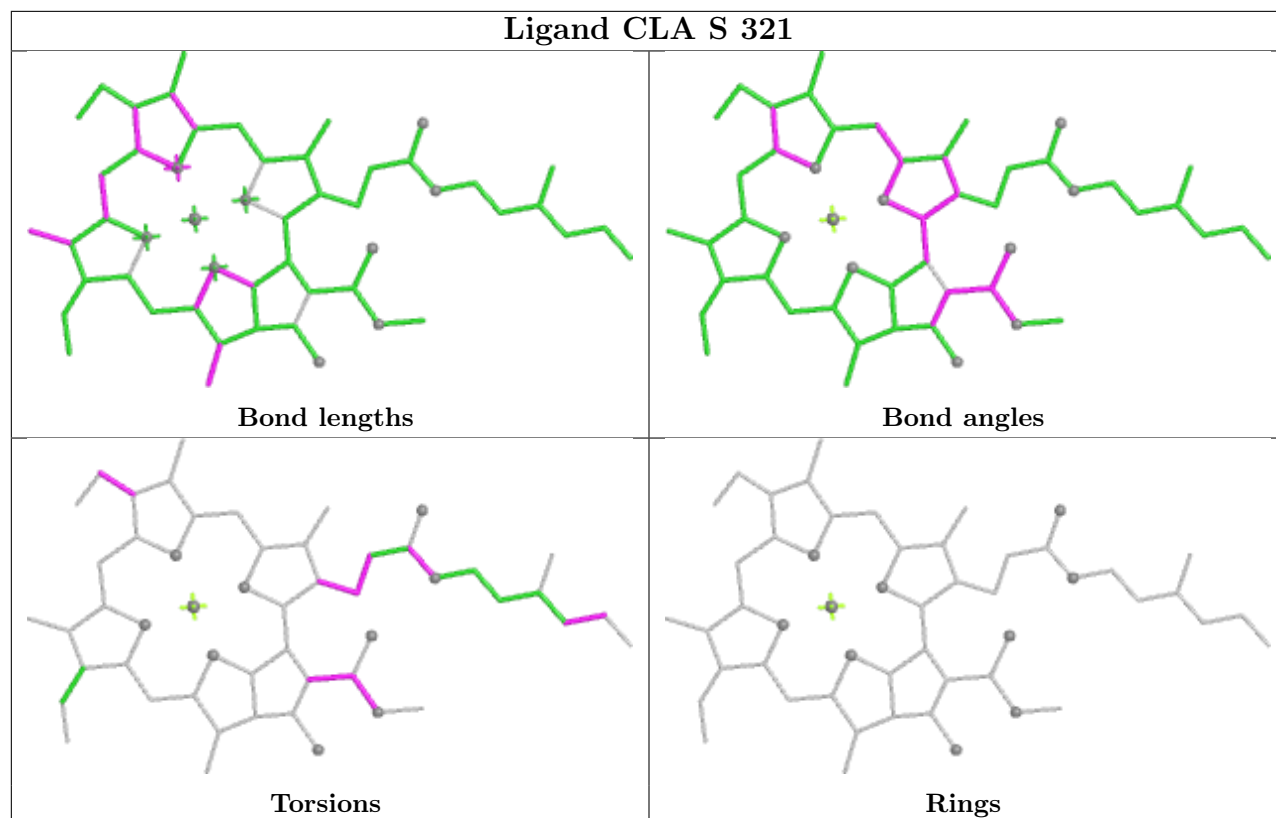




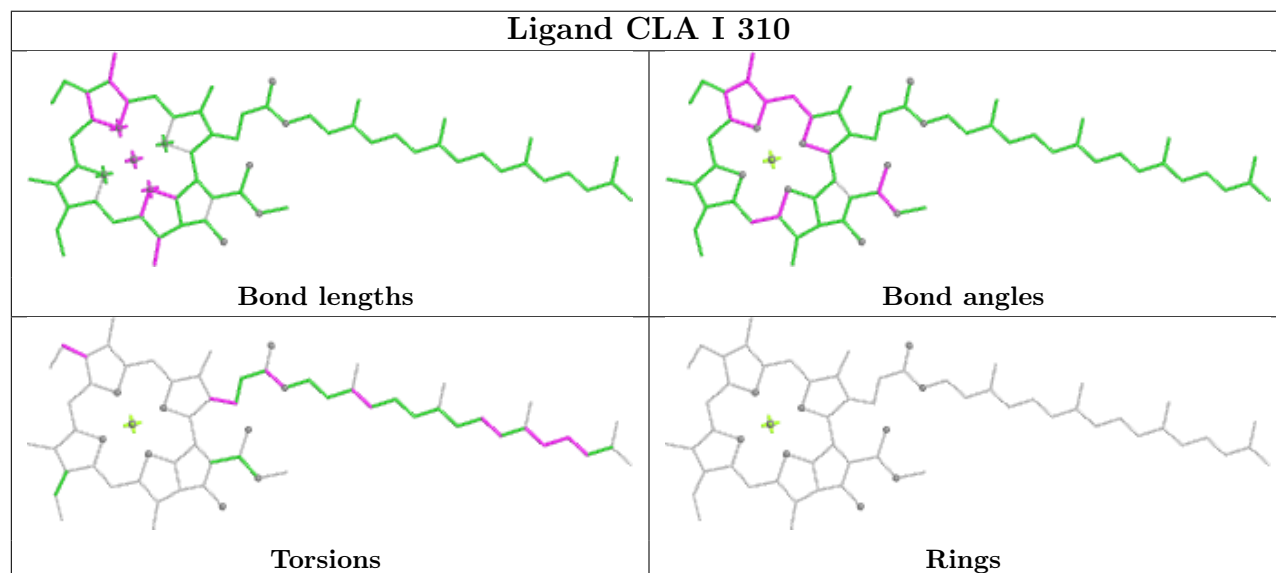




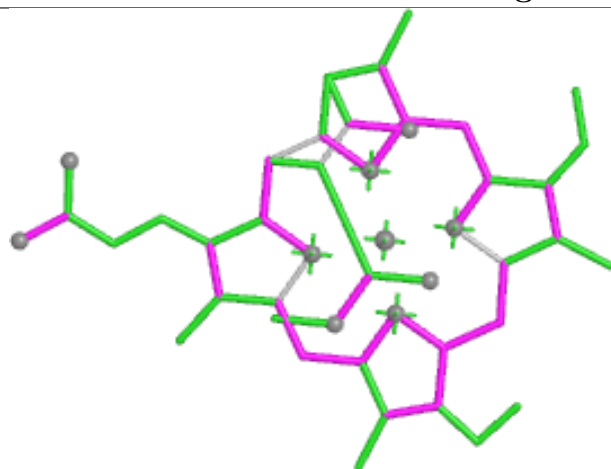
## Ligand CLA S 321



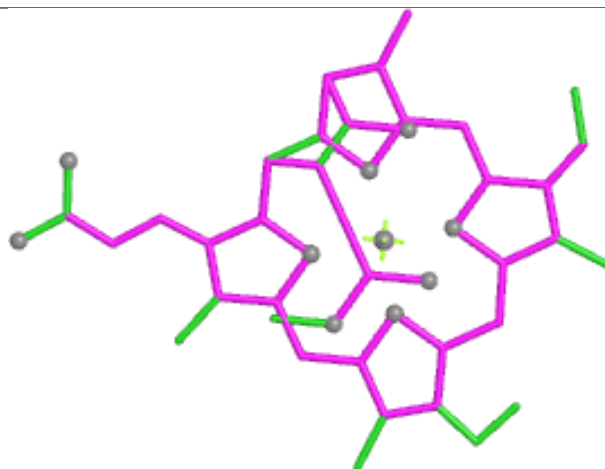
## Ligand CLA I 310



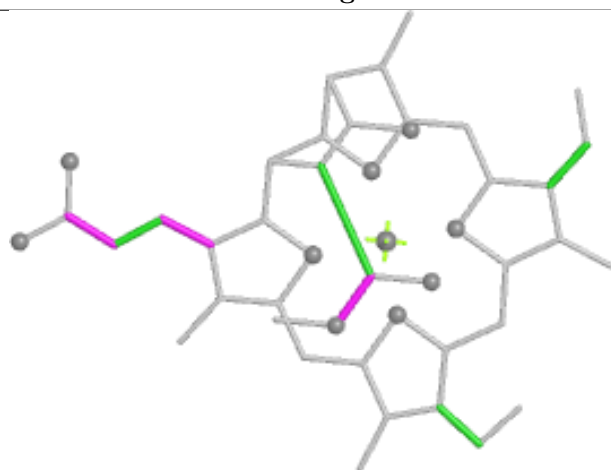
## Ligand KC1 H 313



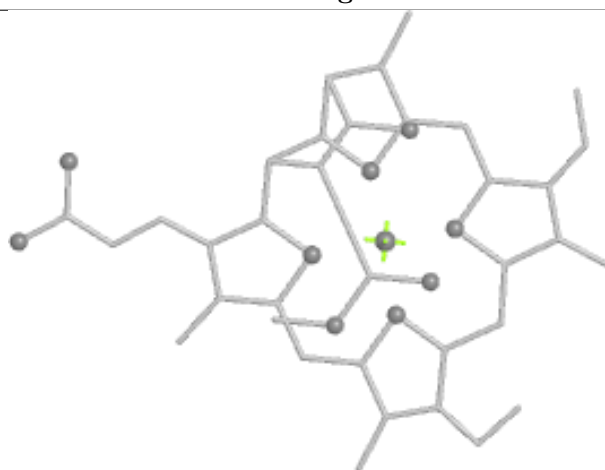
Bond lengths



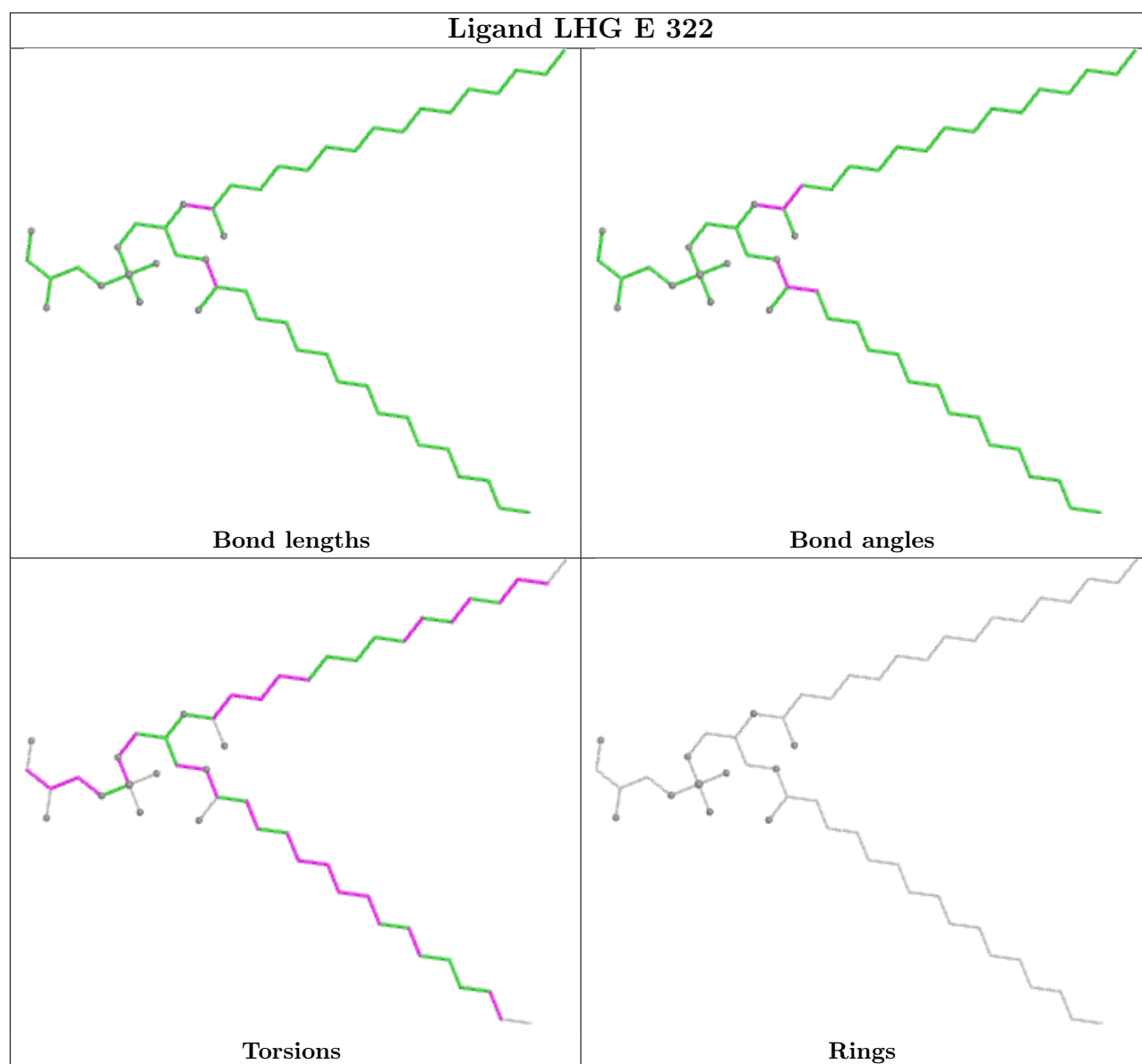
Bond angles



Torsions

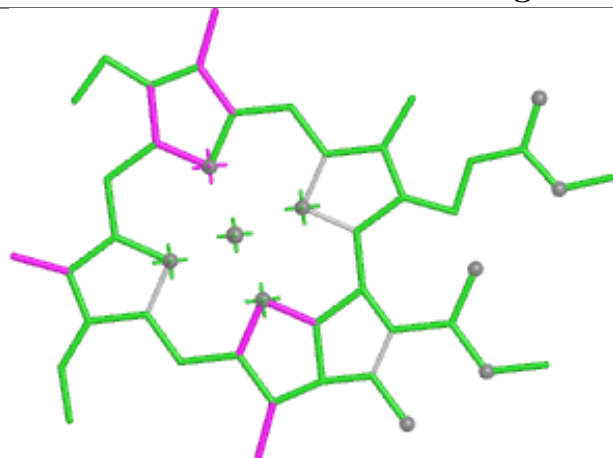


Rings

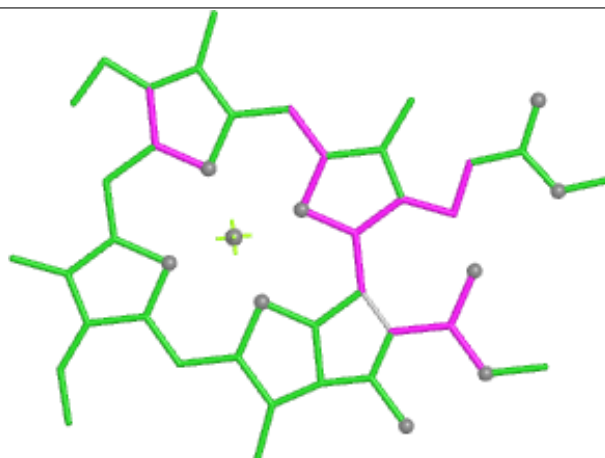




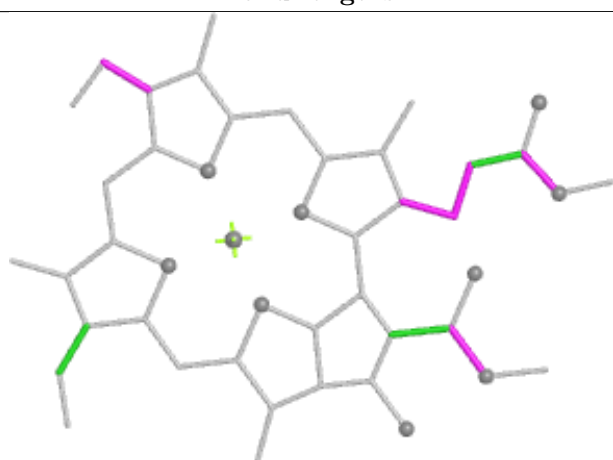
## Ligand CLA O 310



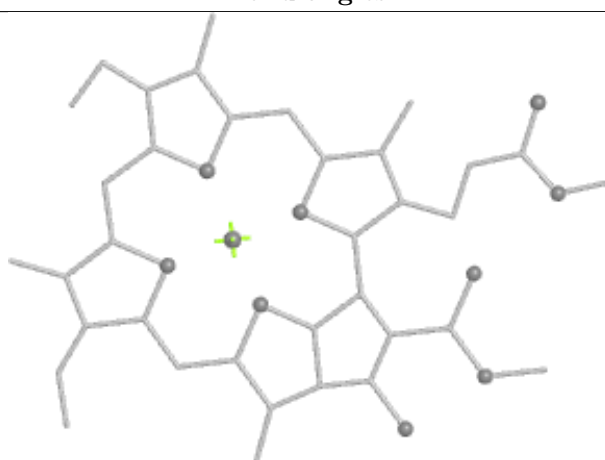
Bond lengths



Bond angles

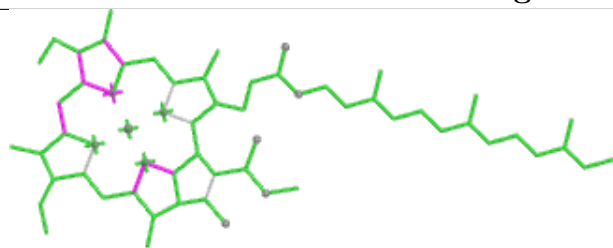


Torsions

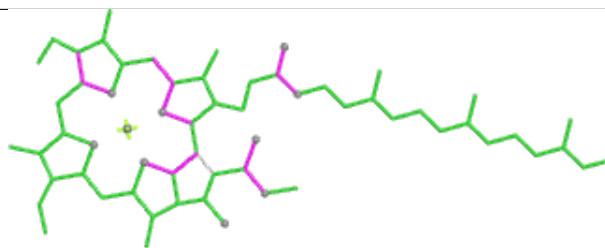


Rings

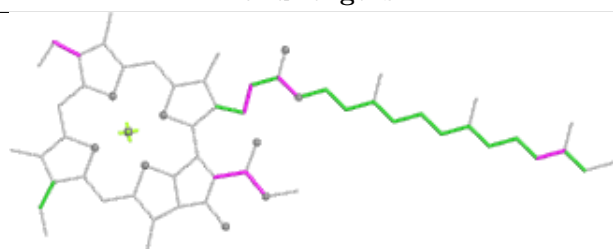
## Ligand CLA X 306



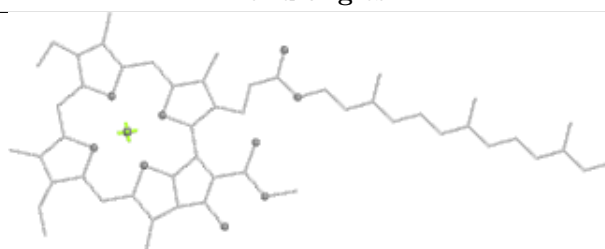
Bond lengths



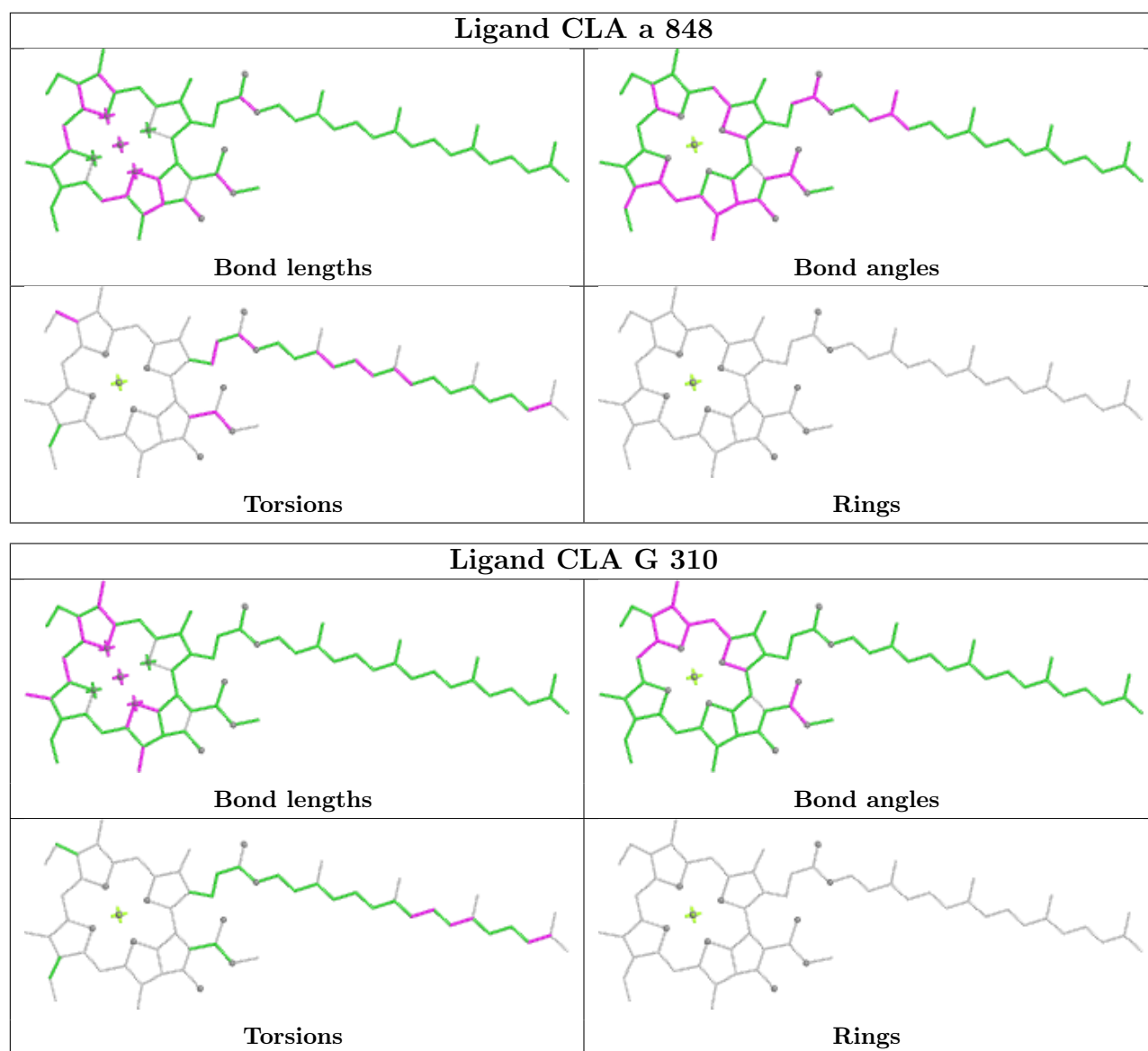
Bond angles



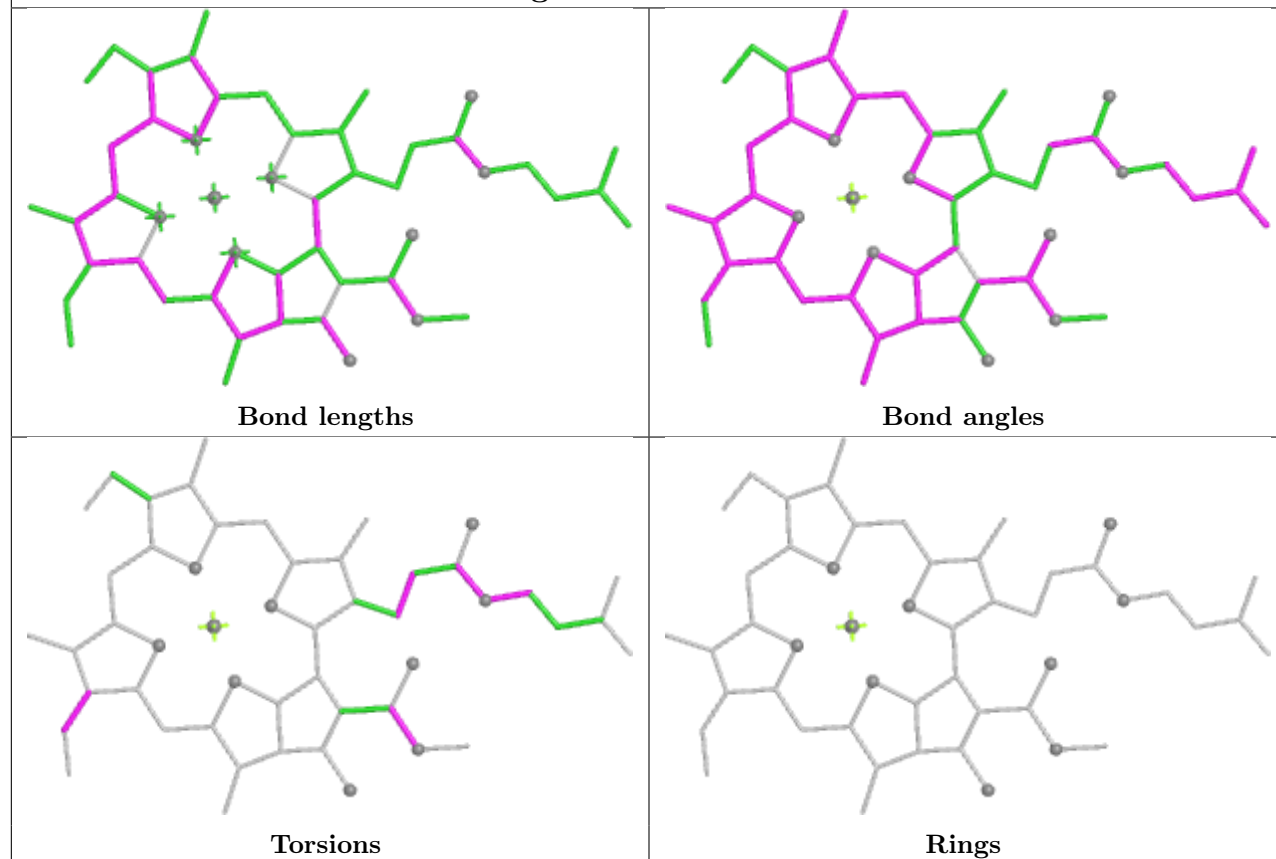
Torsions



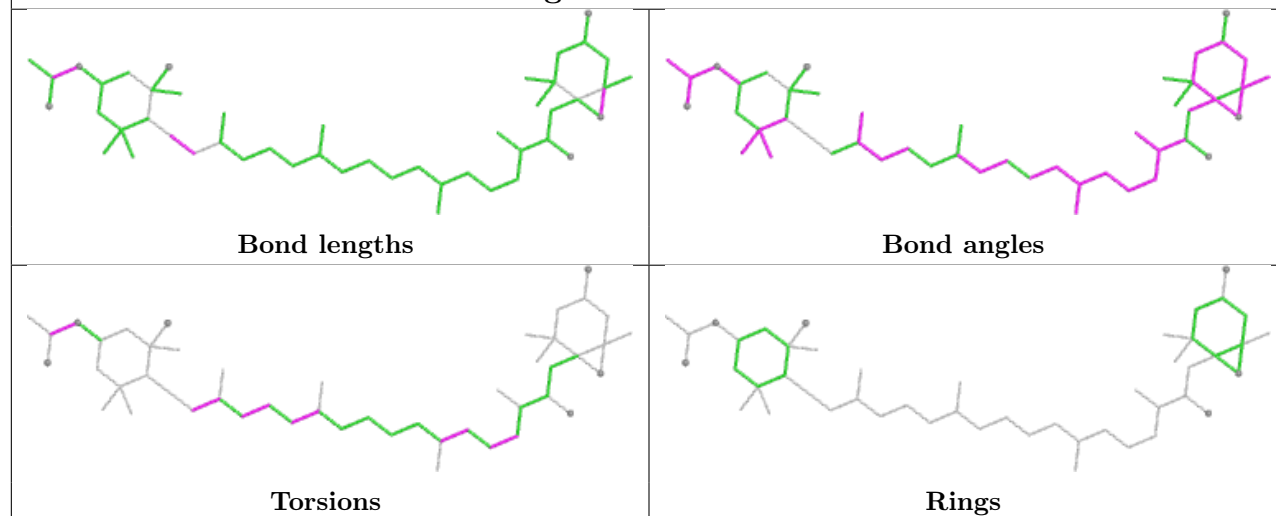
Rings

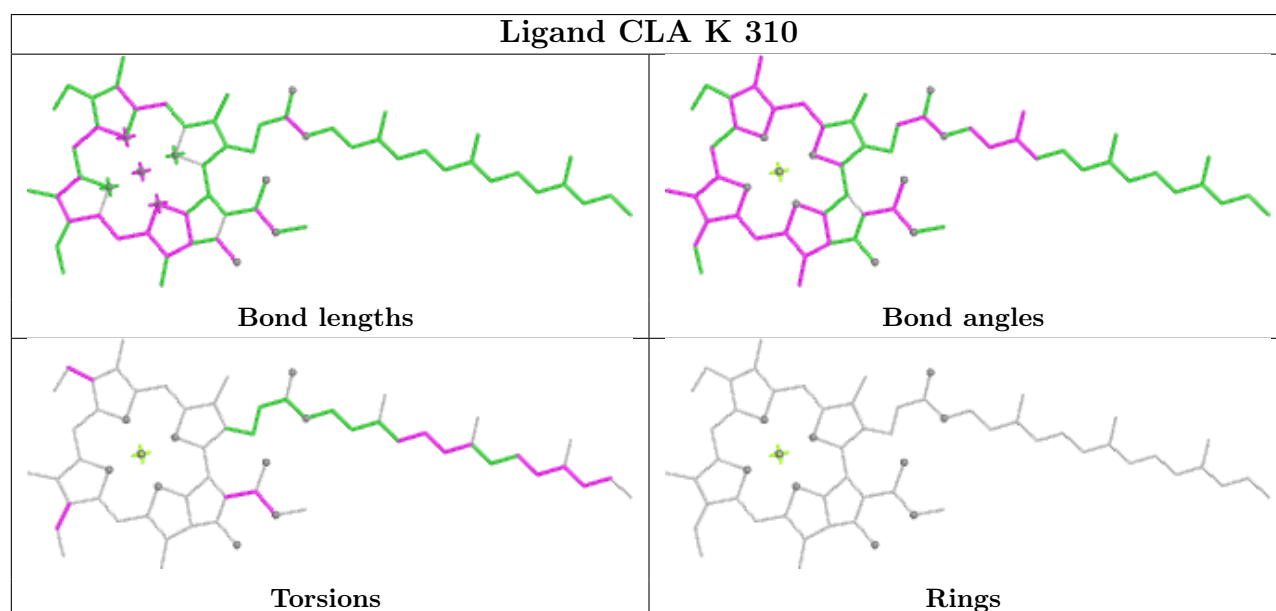
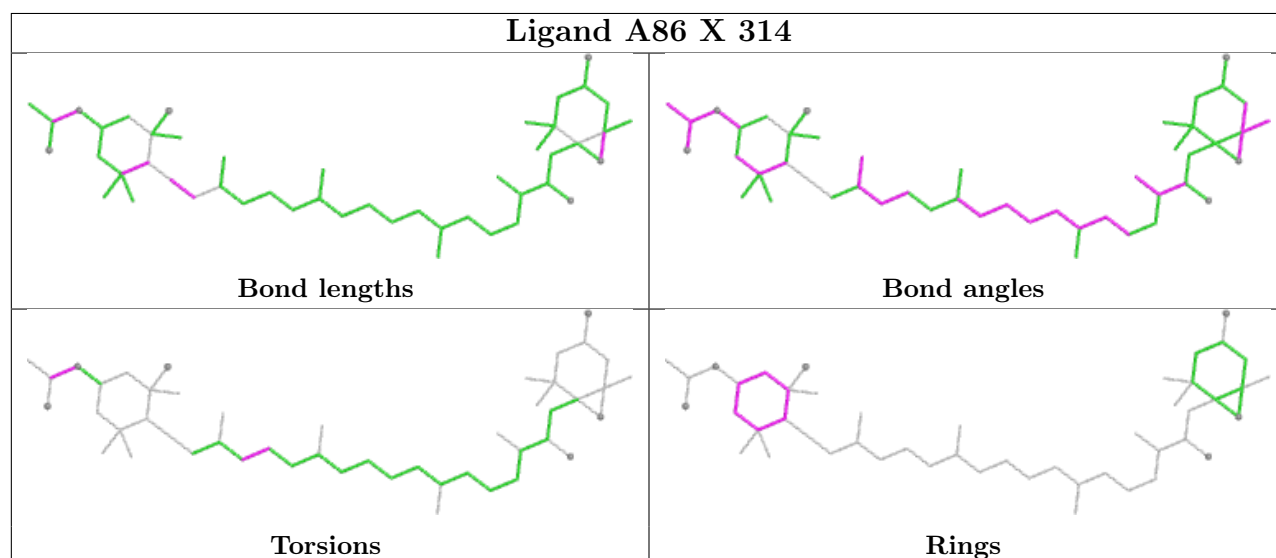
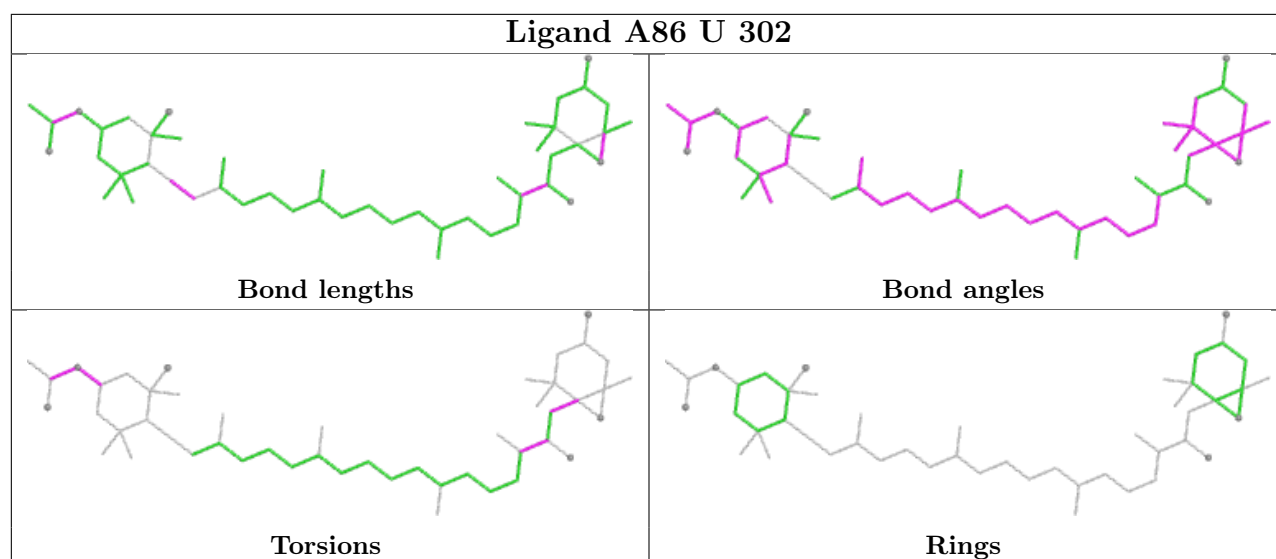


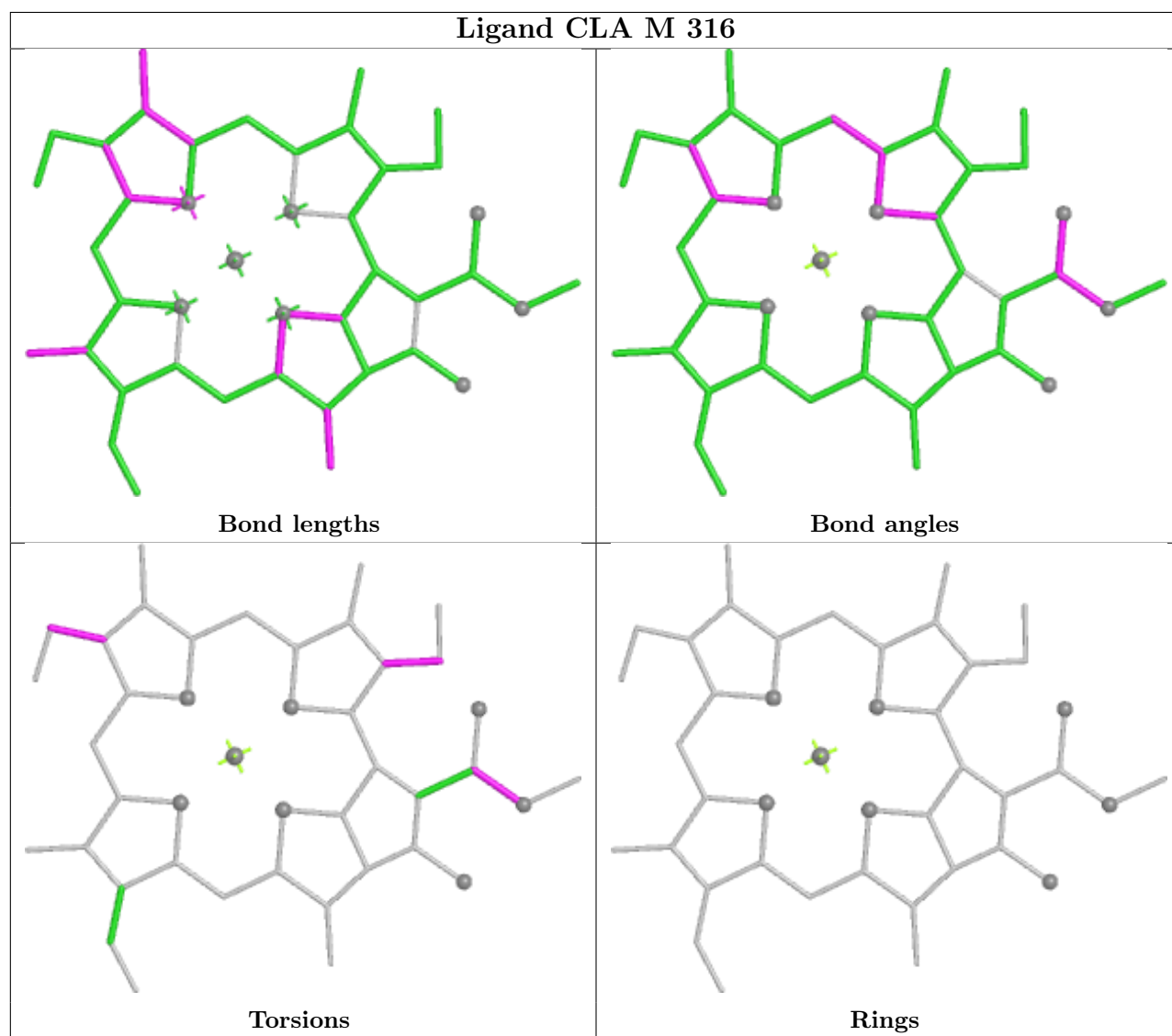
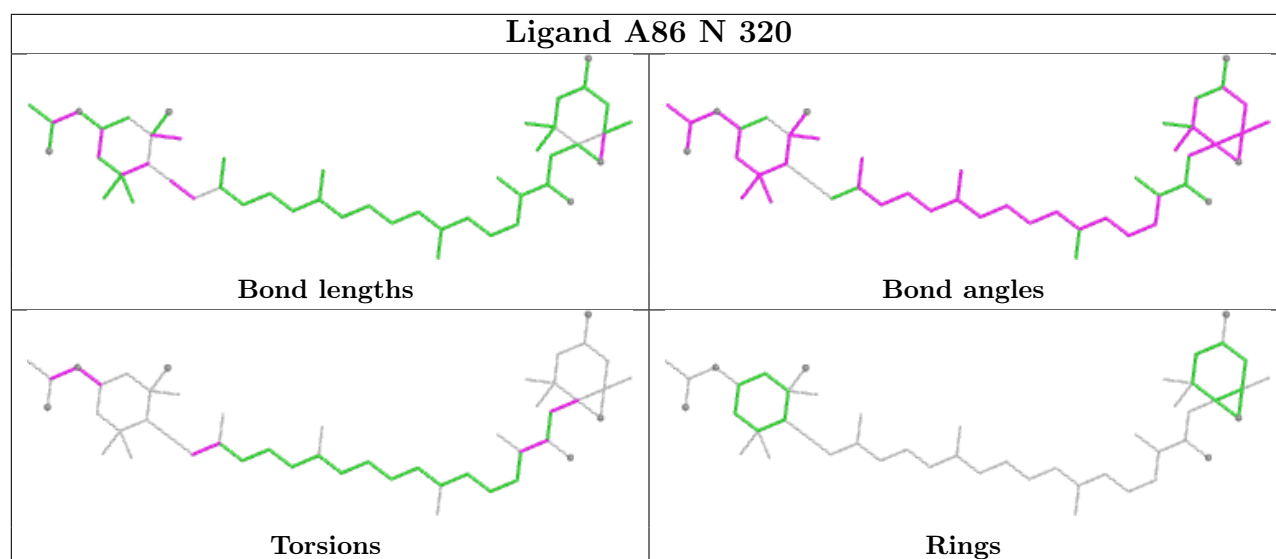
## Ligand CLA G 319

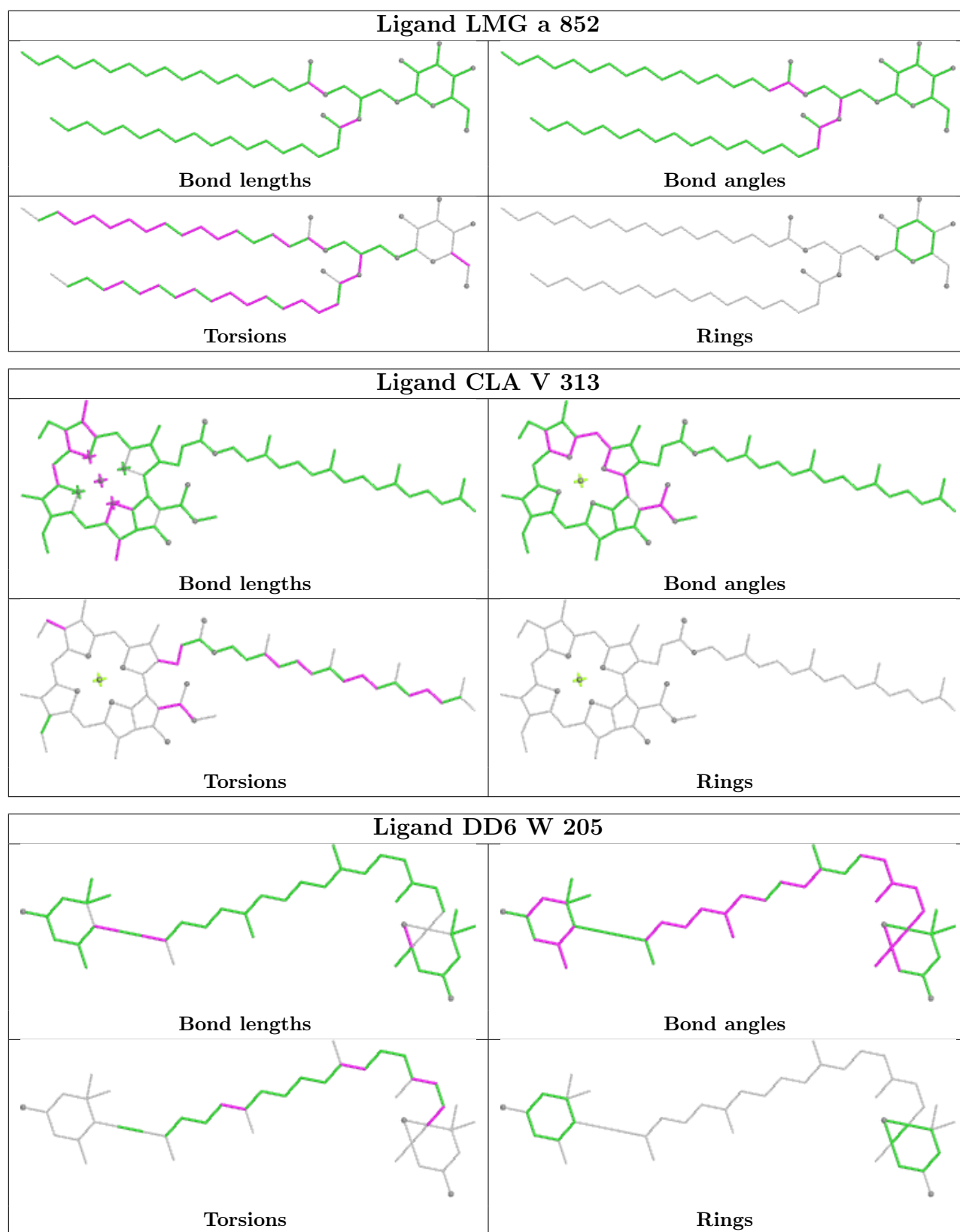


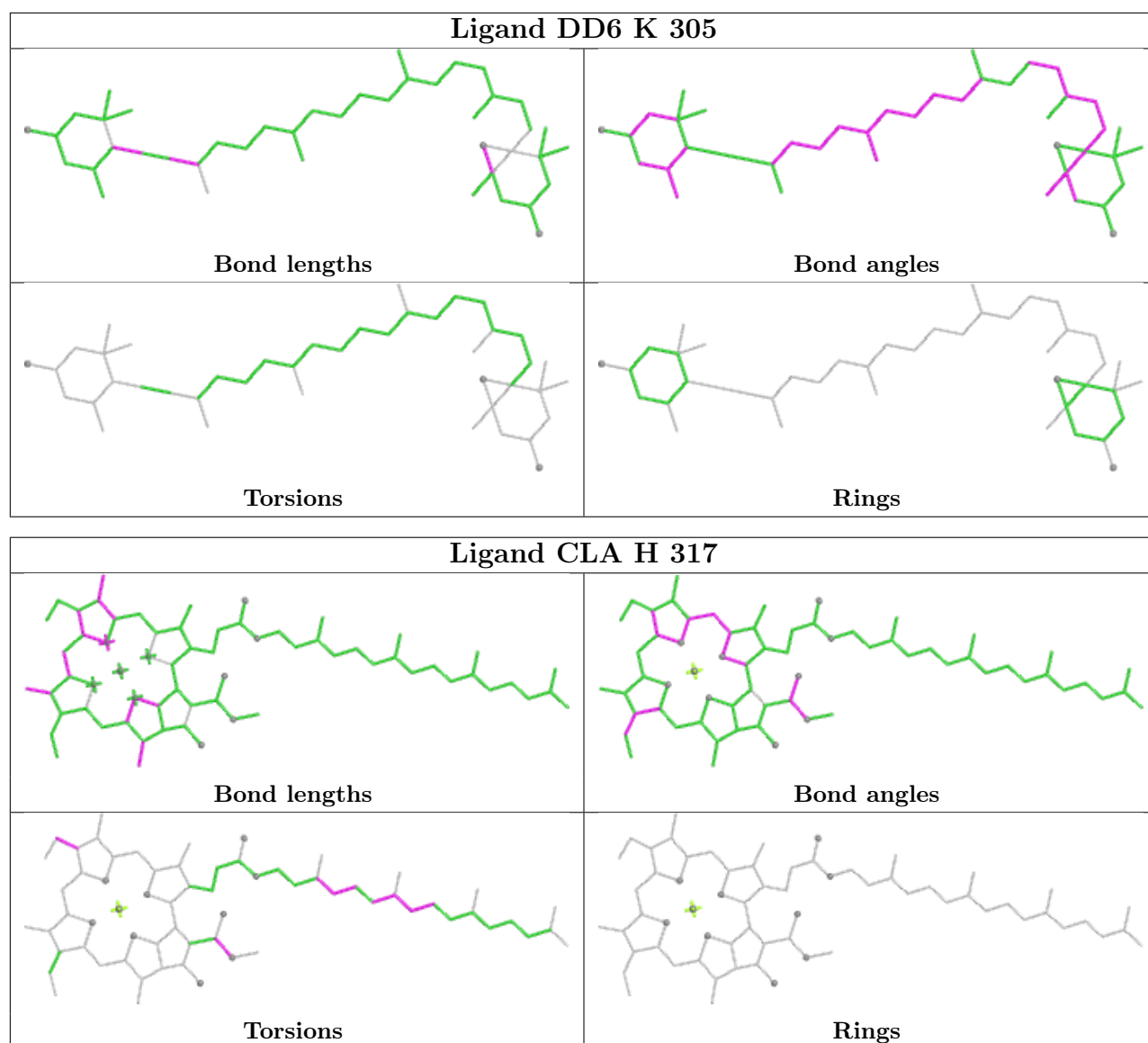
## Ligand A86 I 301



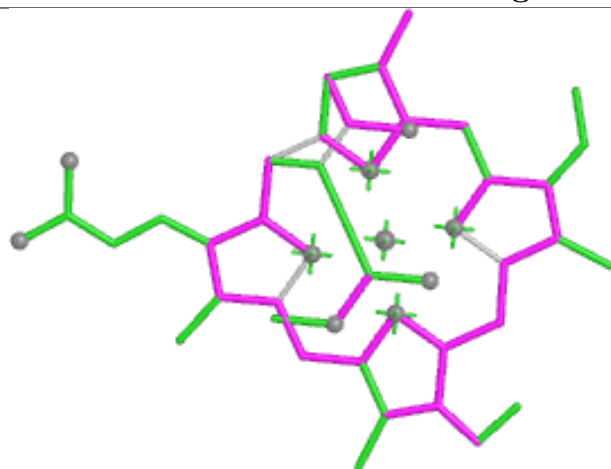




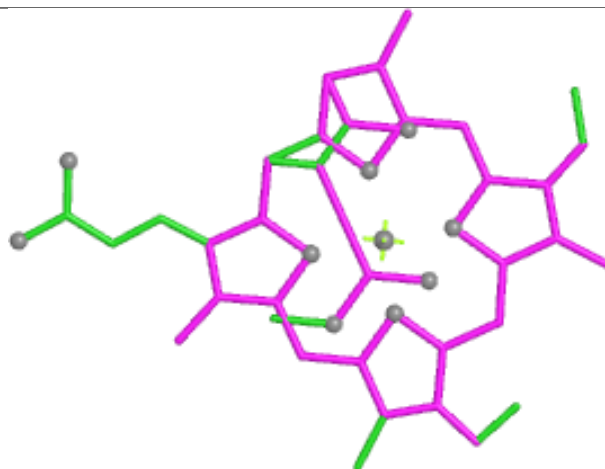




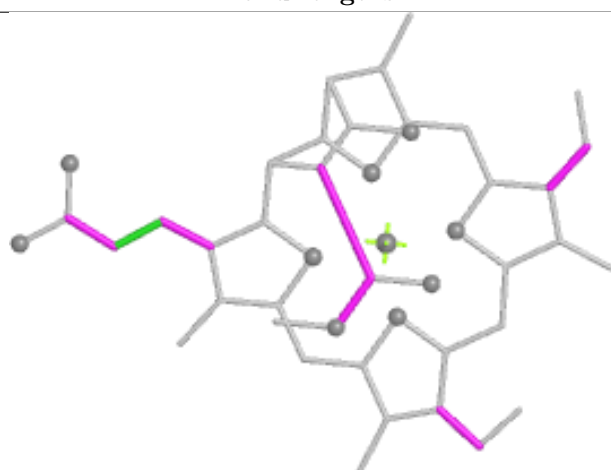
## Ligand KC1 M 318



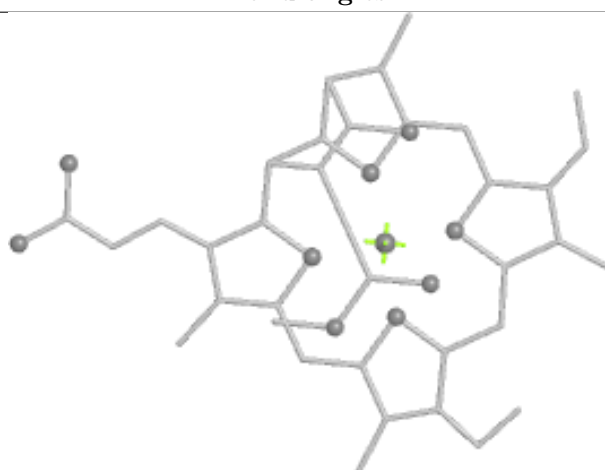
Bond lengths



Bond angles

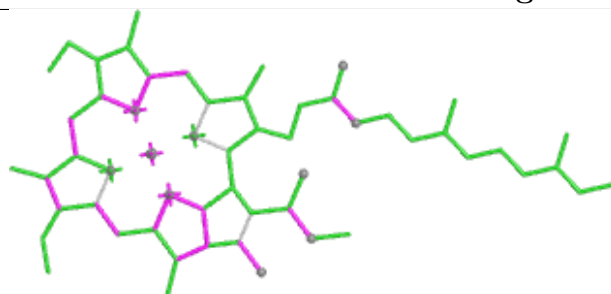


Torsions

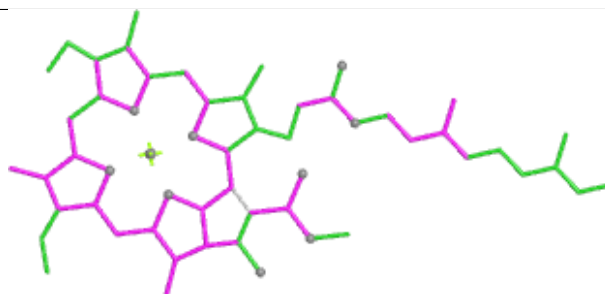


Rings

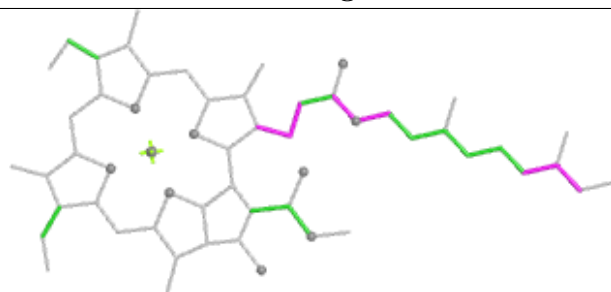
## Ligand CLA F 317



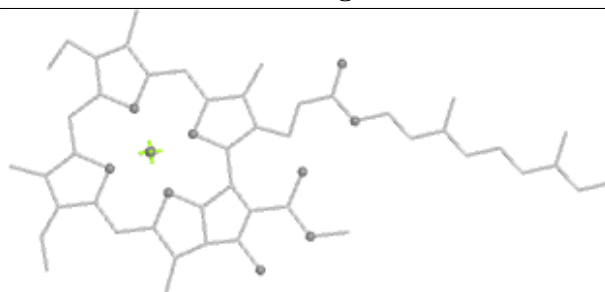
Bond lengths



Bond angles

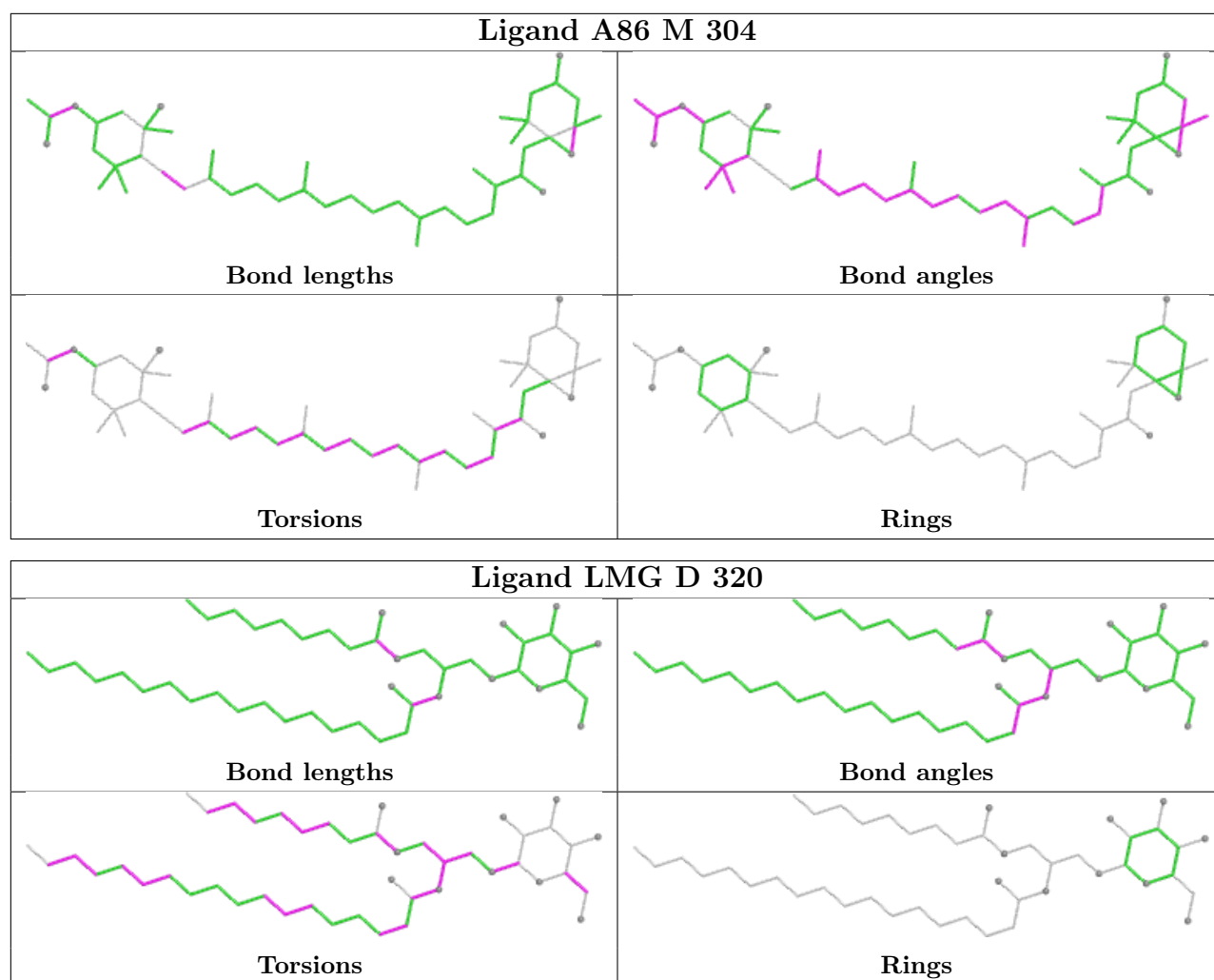


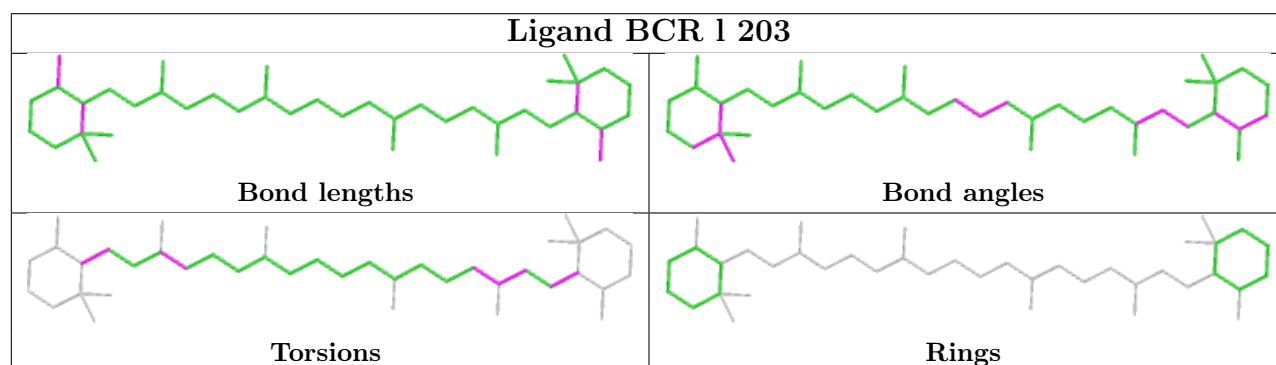
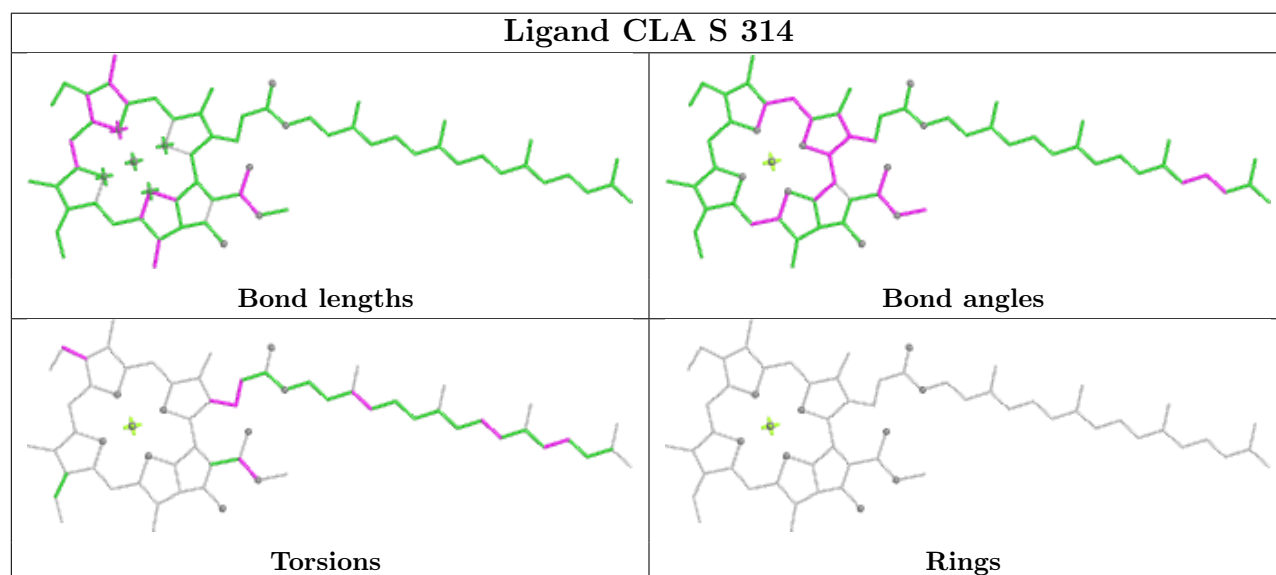
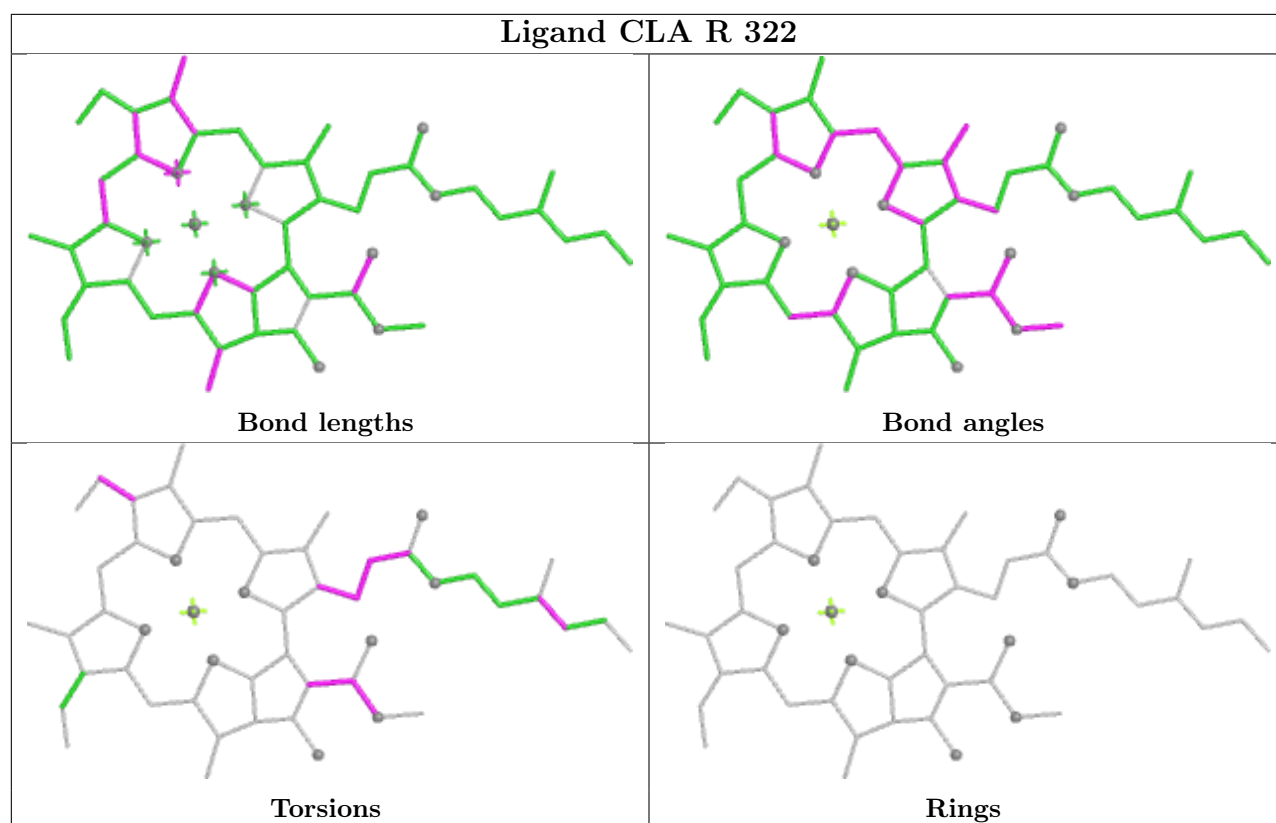
Torsions

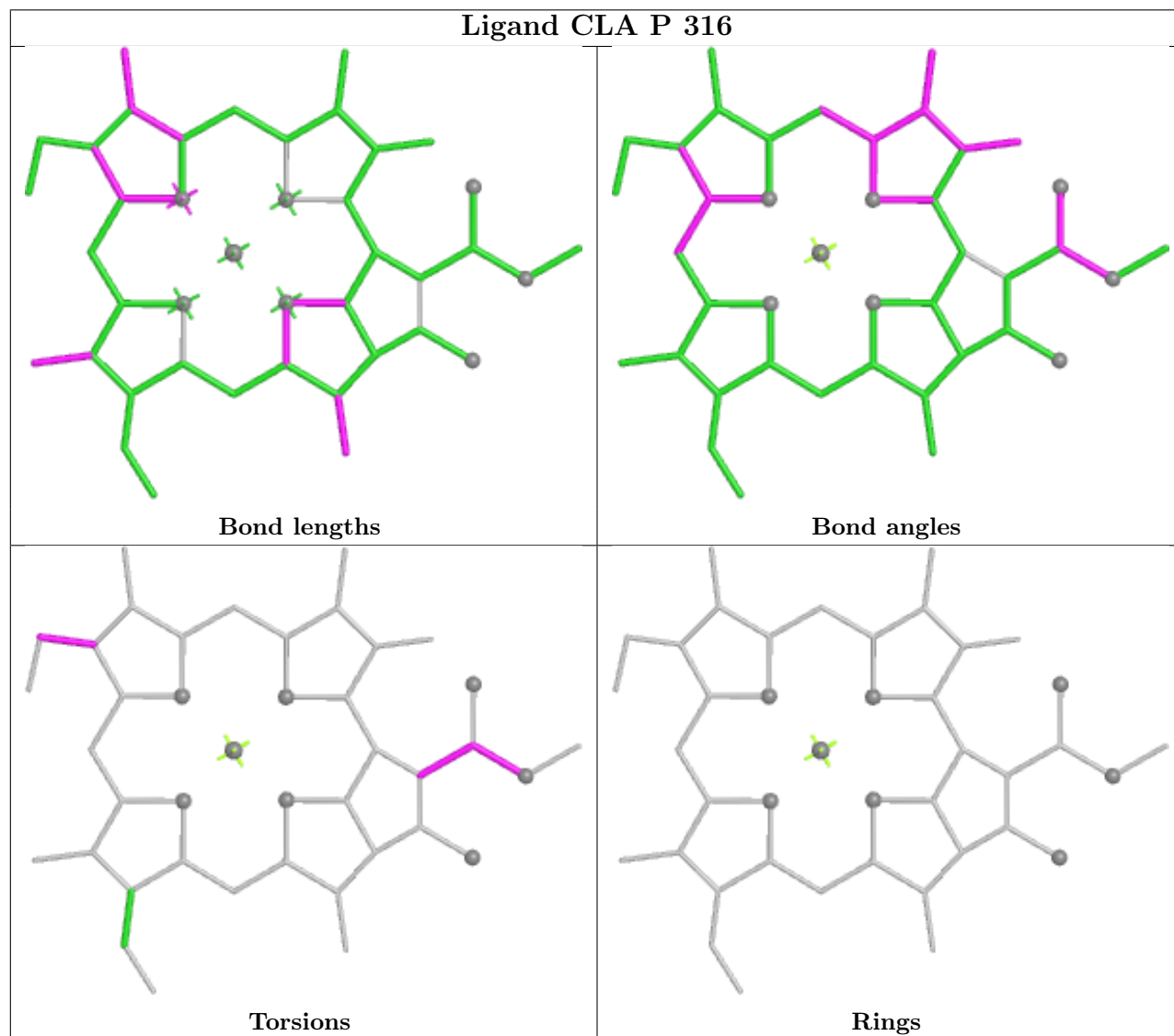
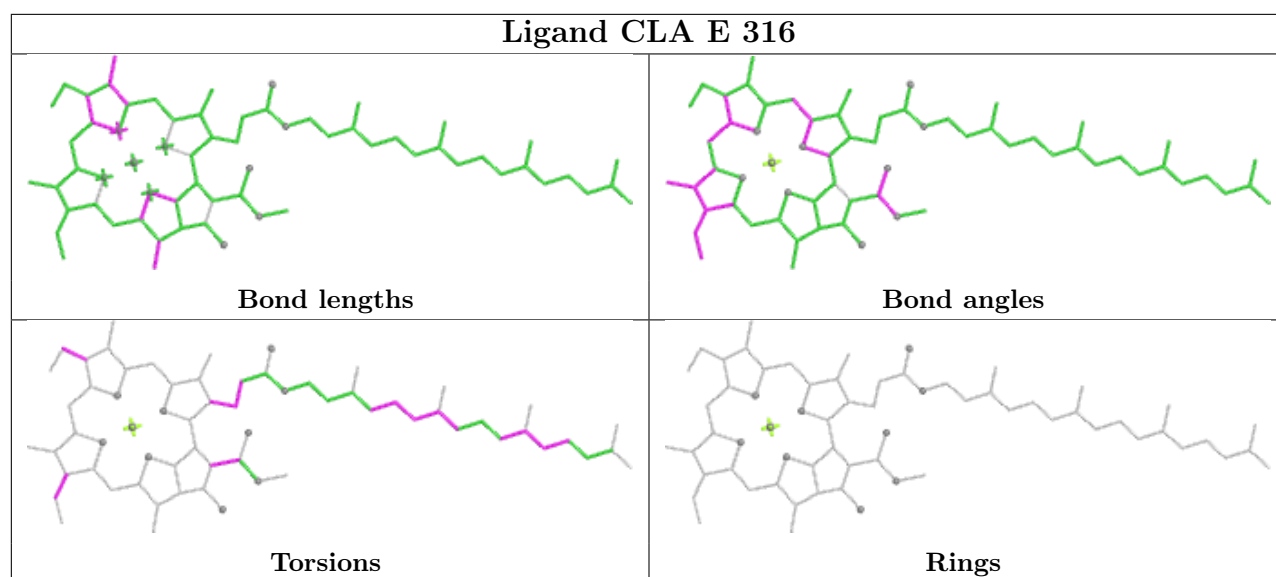


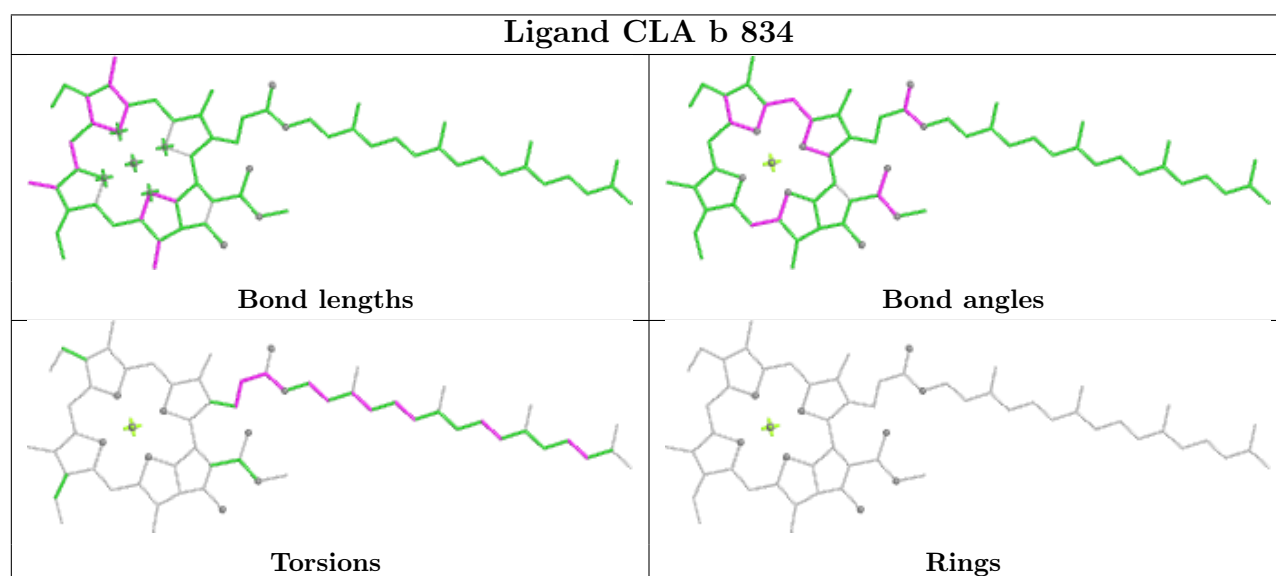
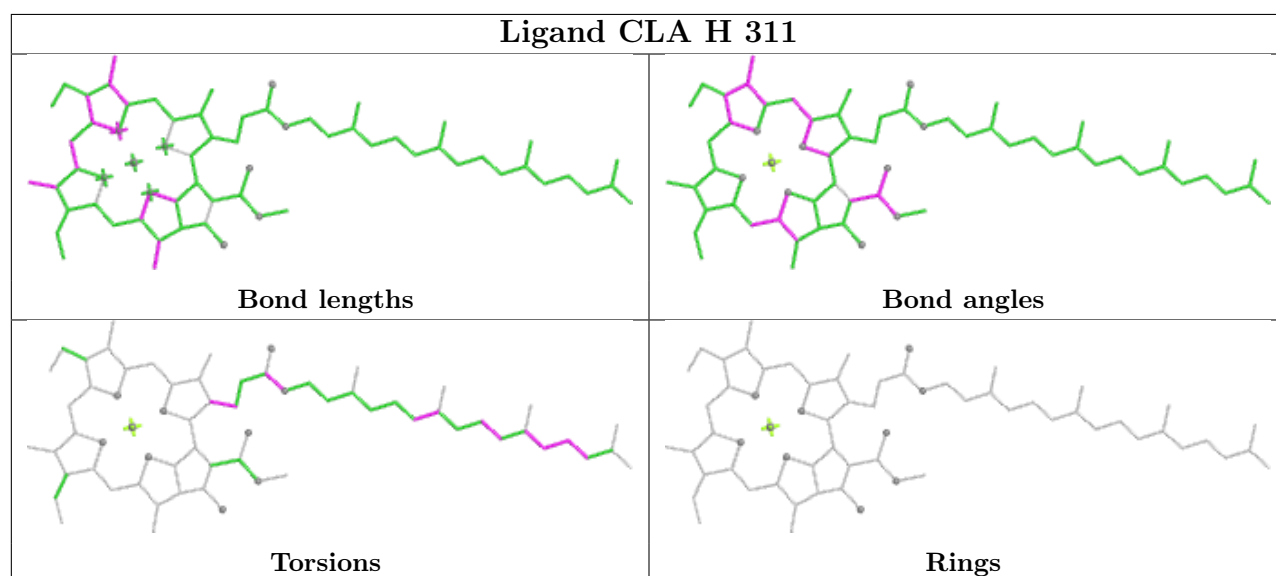
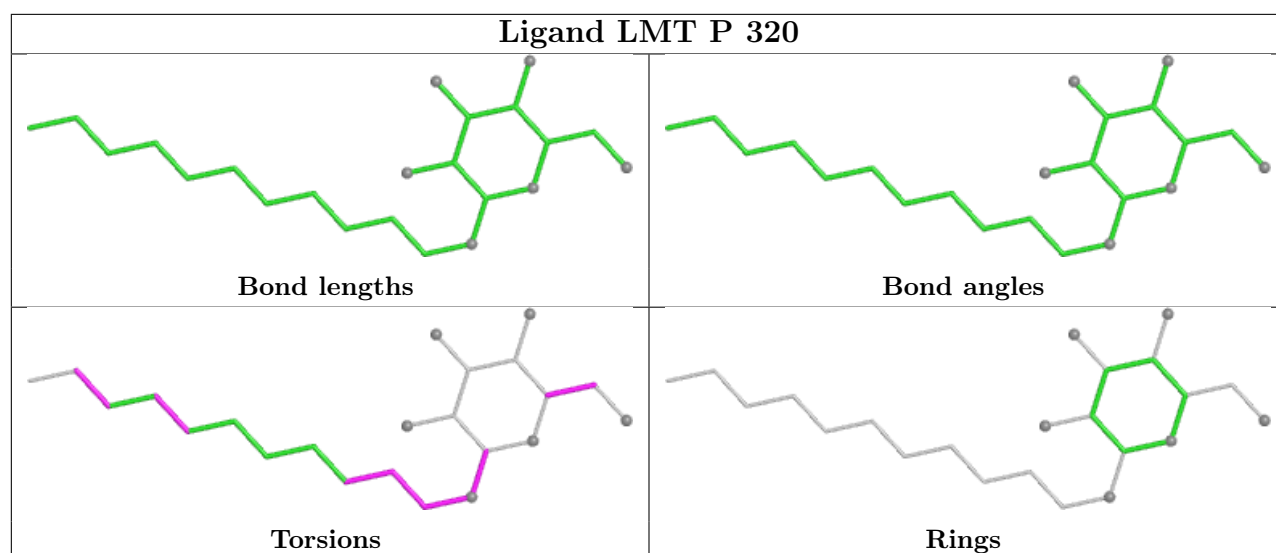
Rings

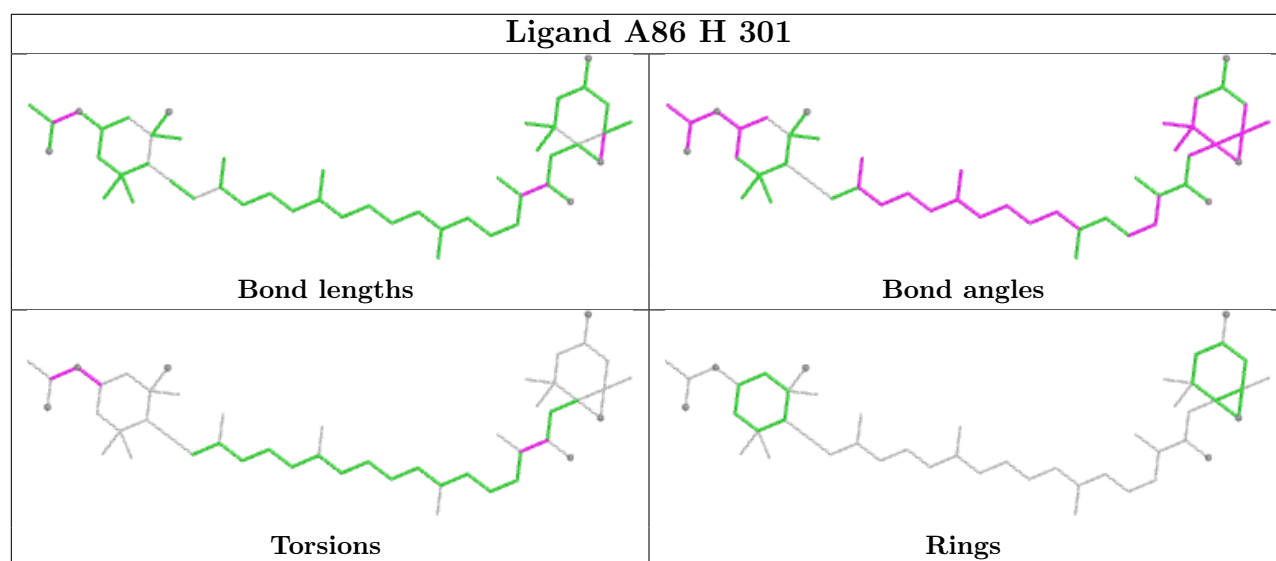
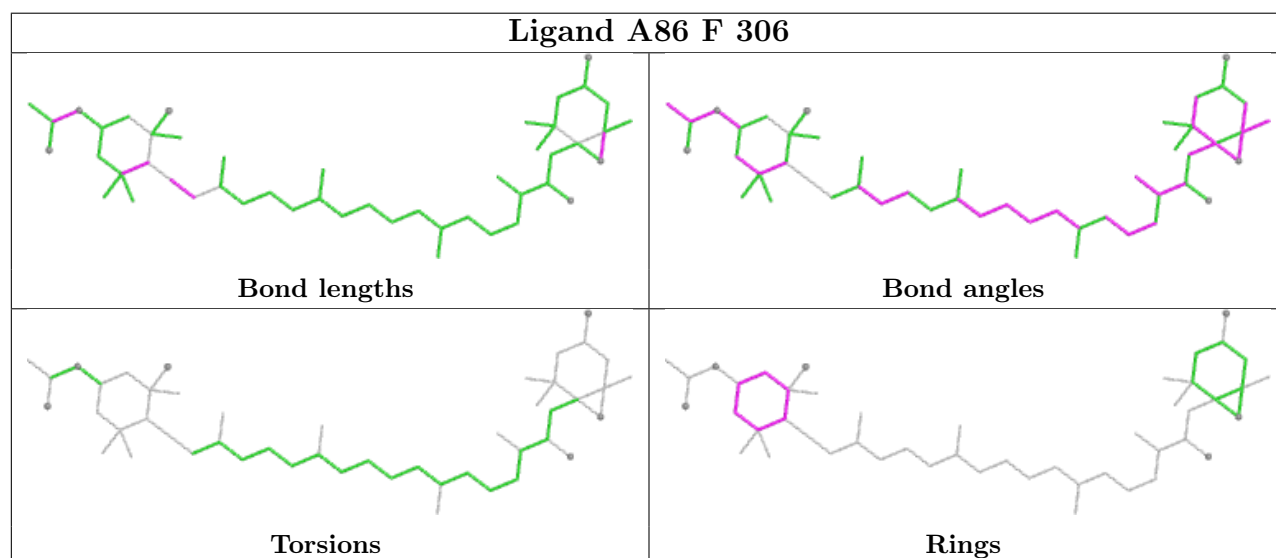
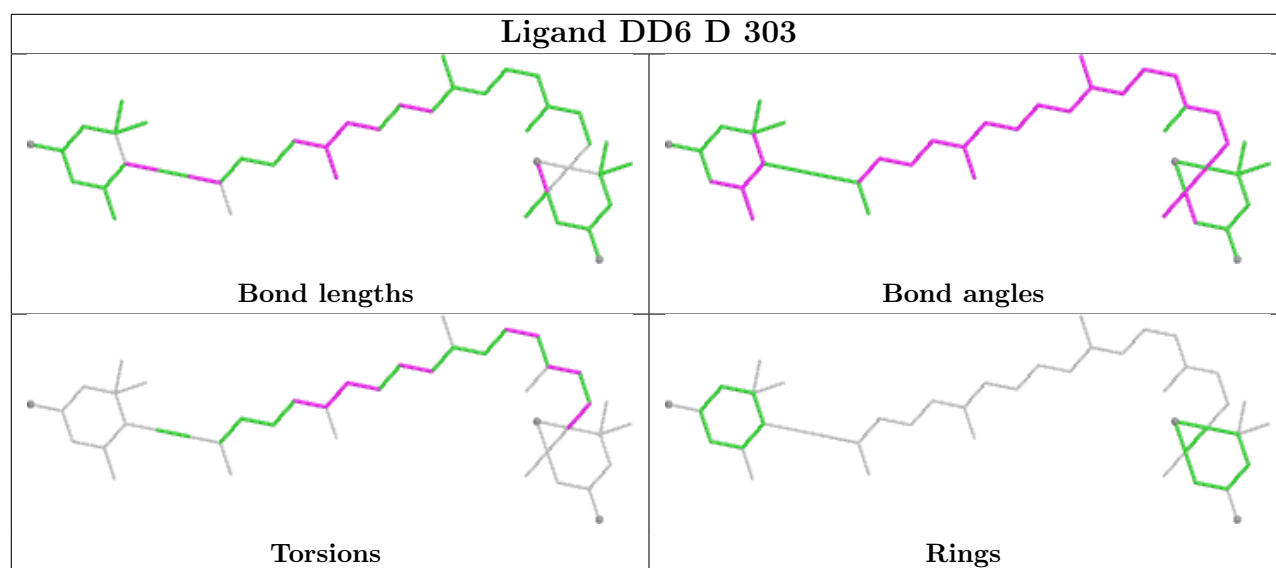


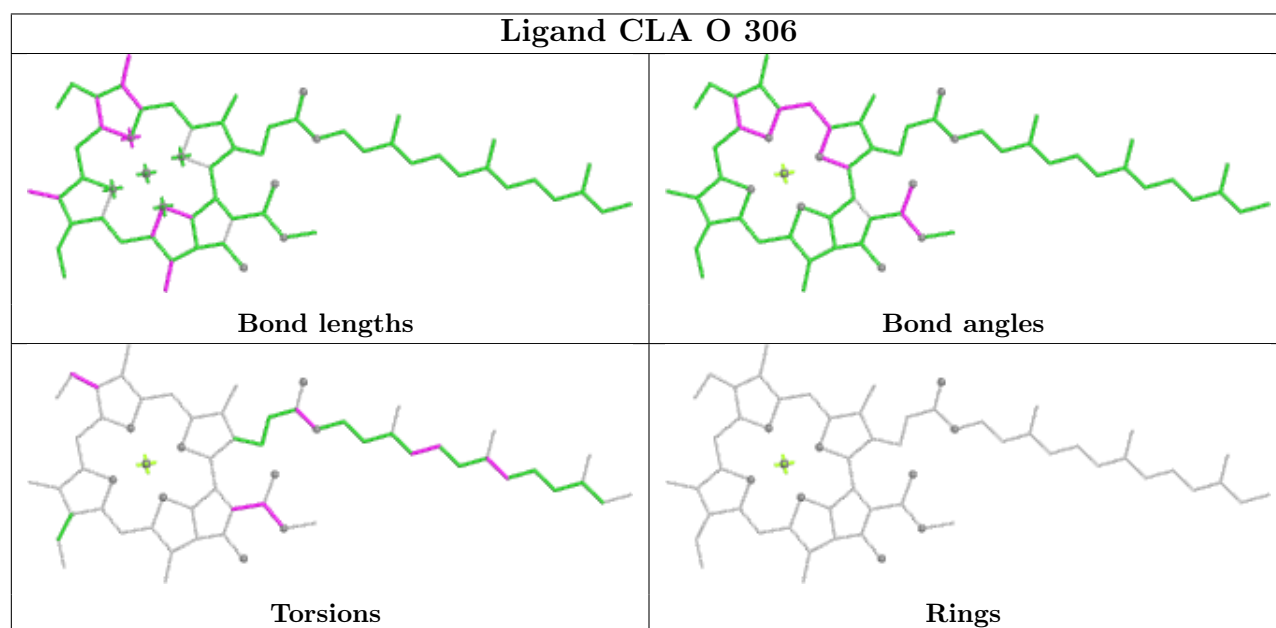
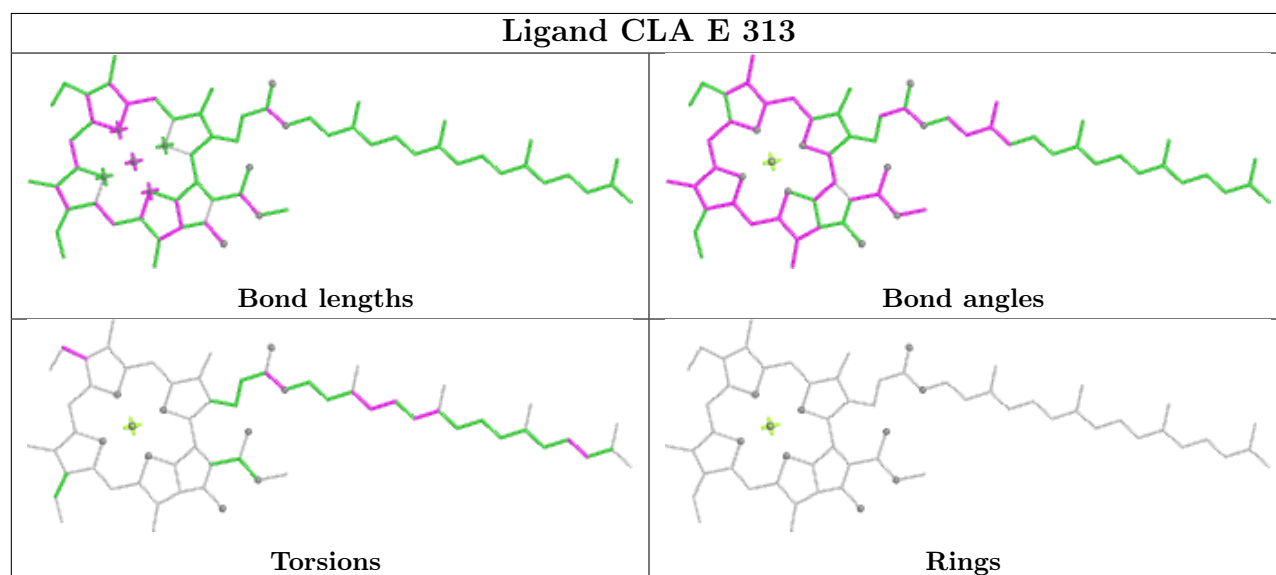
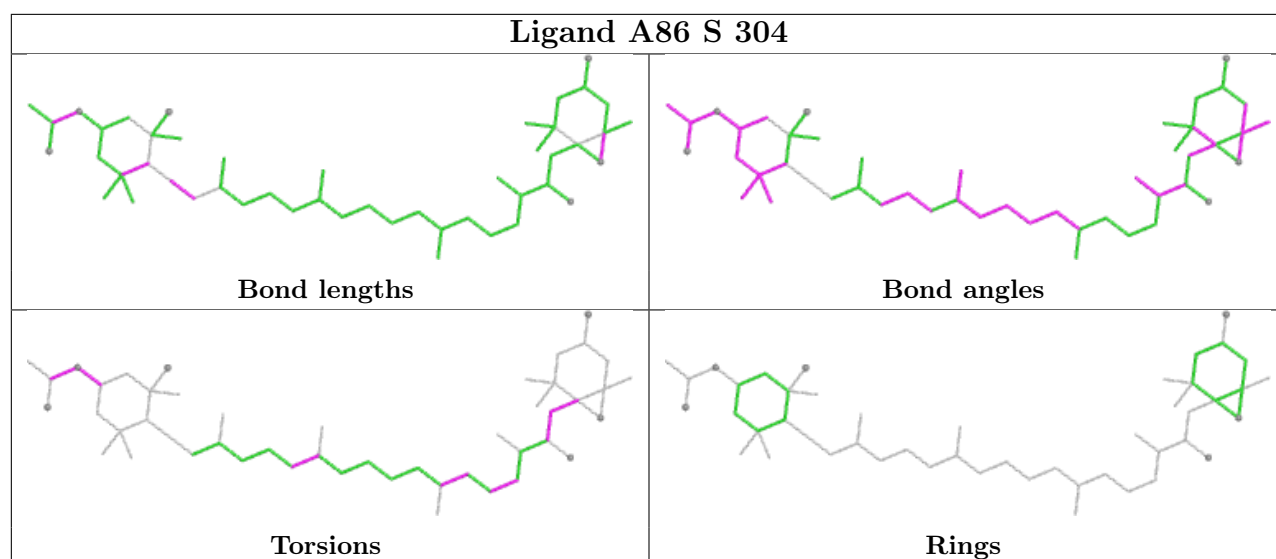


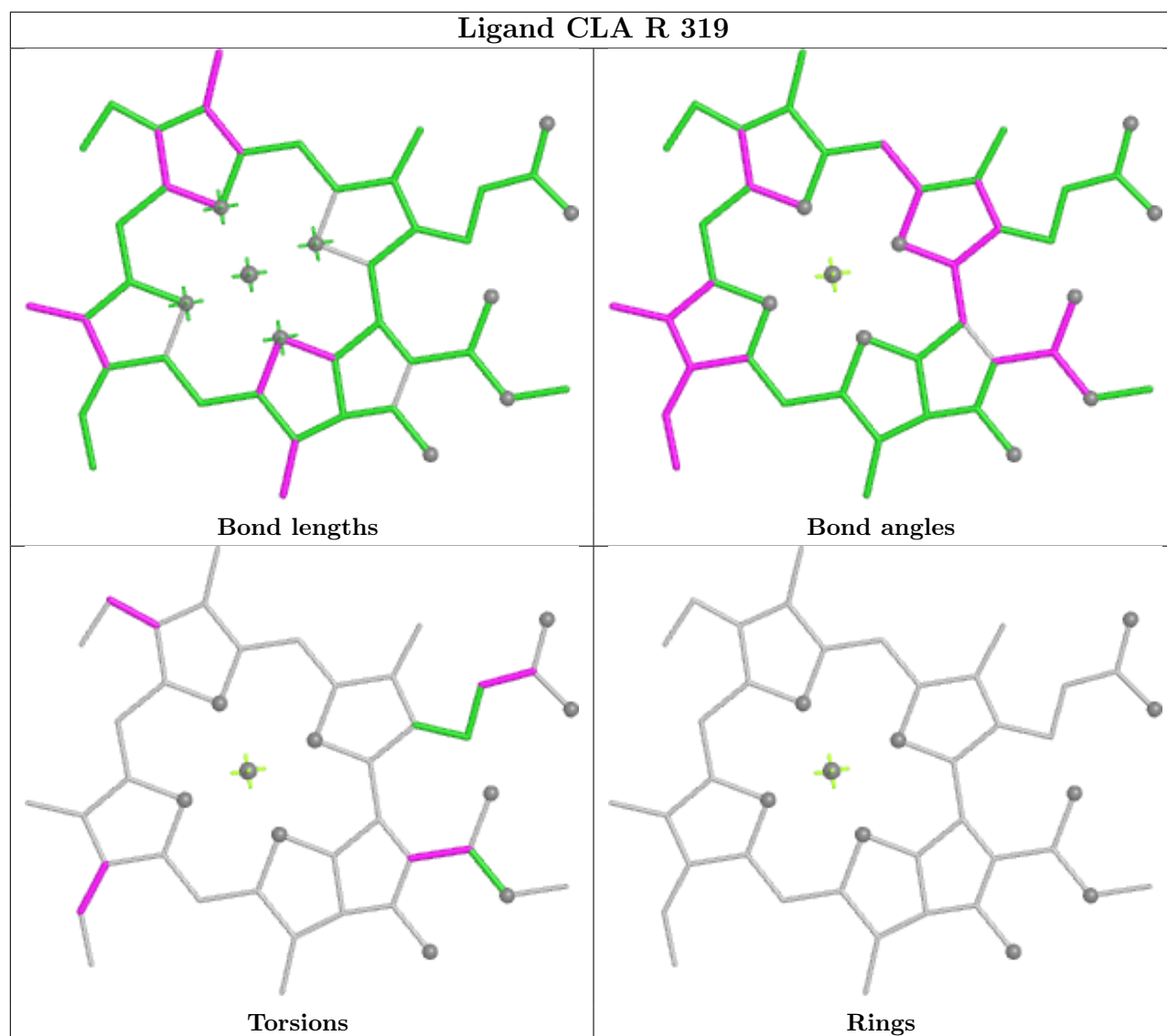
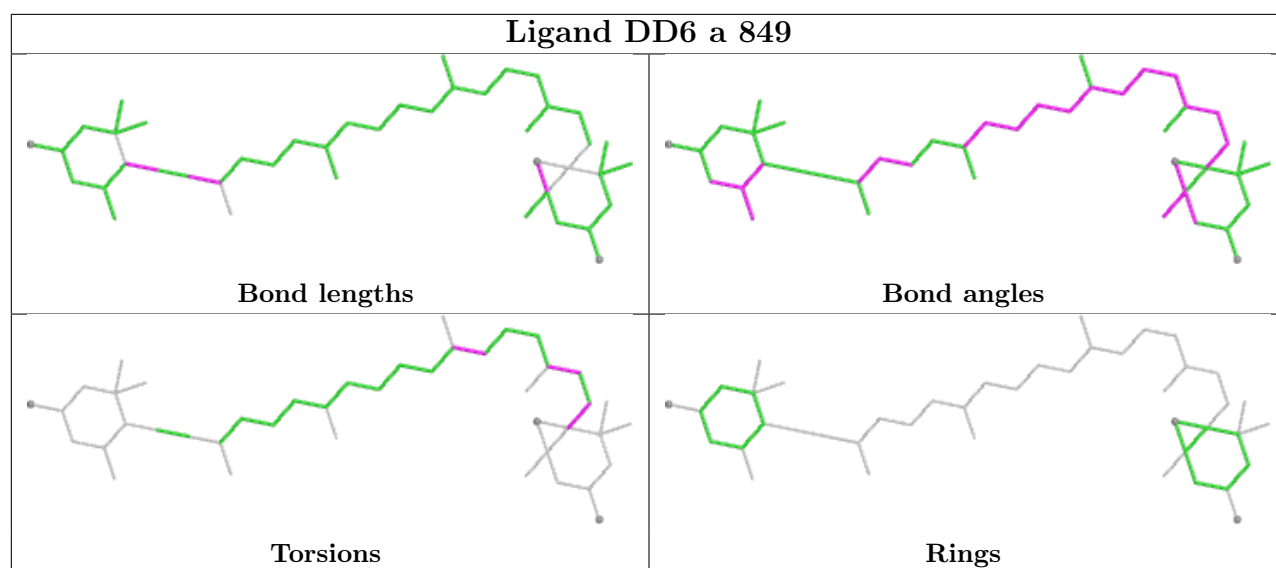


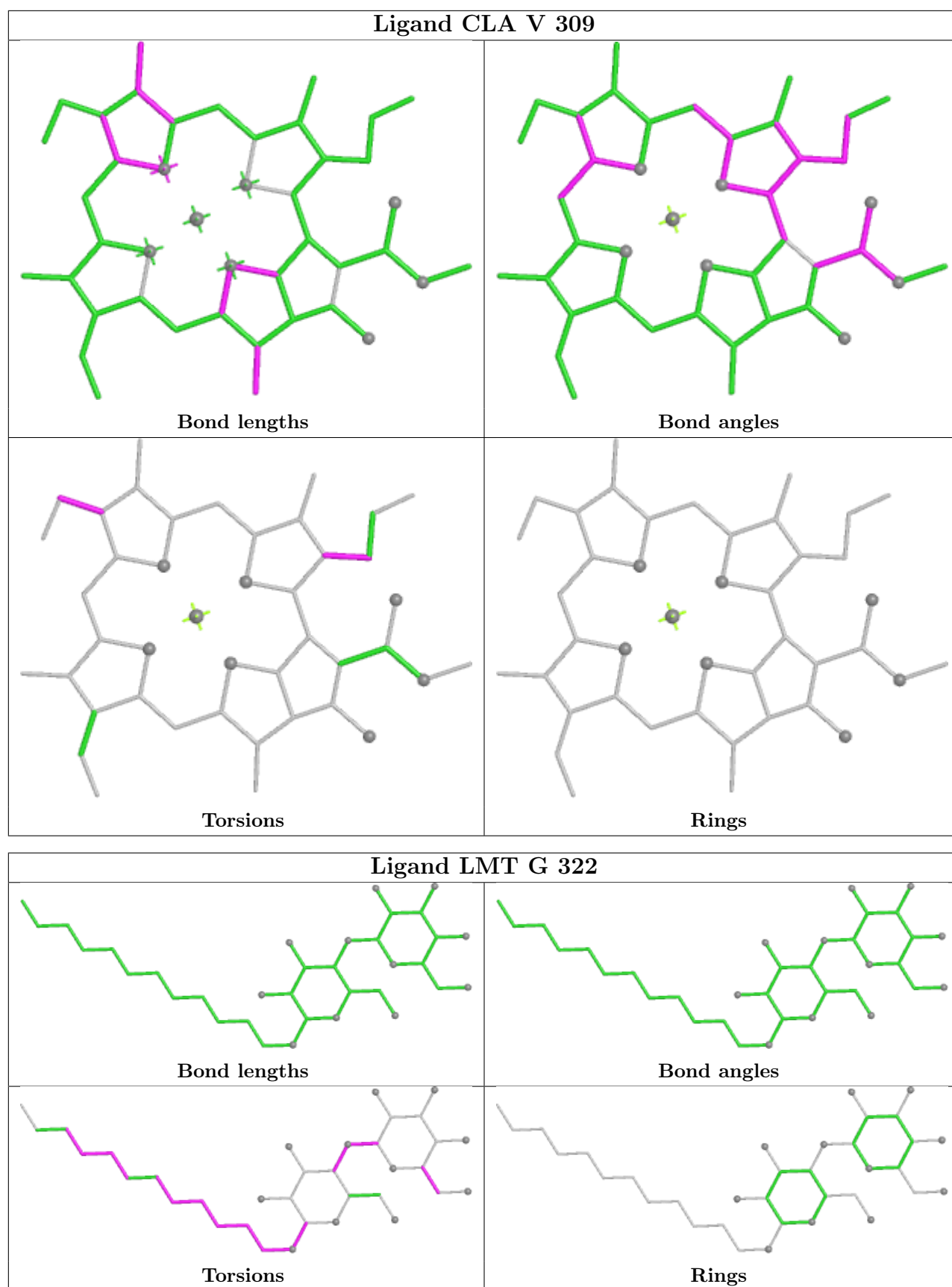






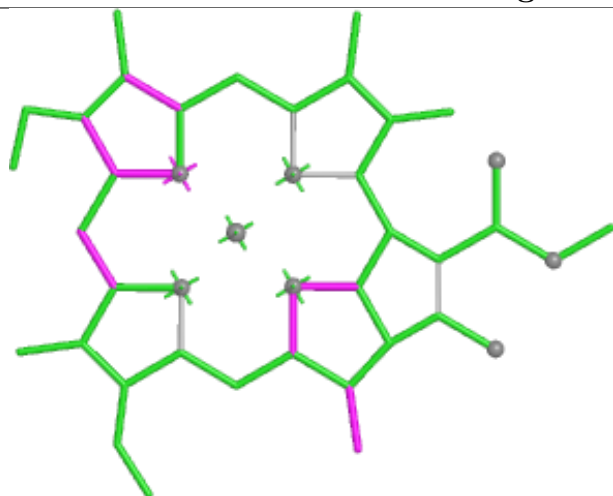








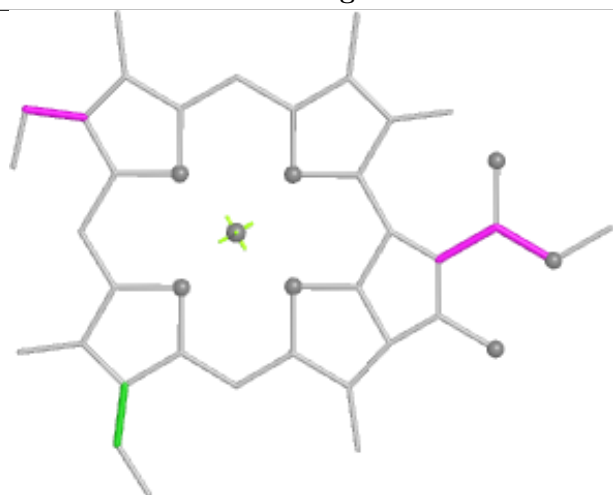
## Ligand CLA S 317



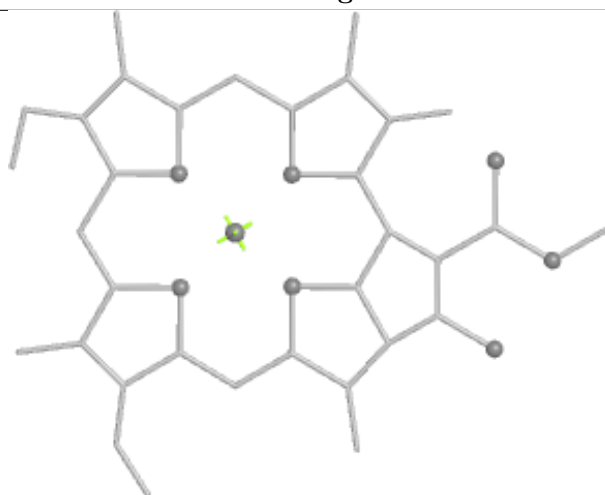
Bond lengths



Bond angles

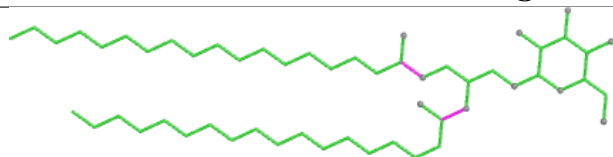


Torsions

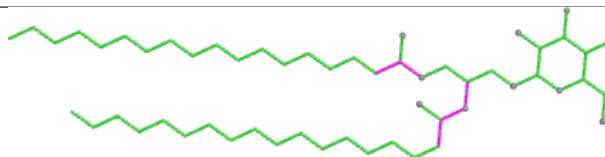


Rings

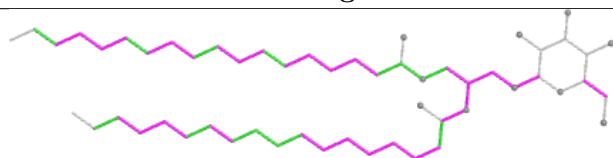
## Ligand LMG I 315



Bond lengths



Bond angles

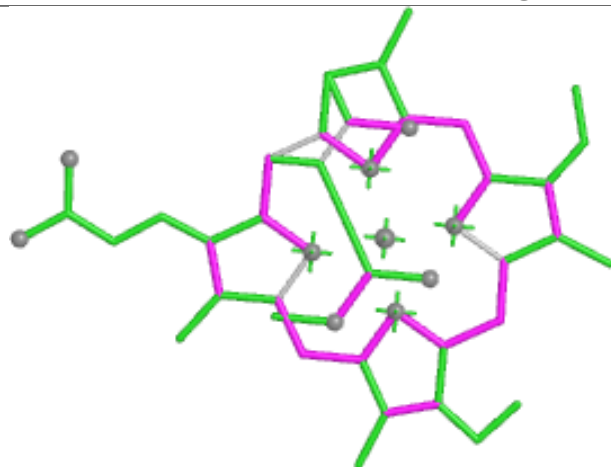


Torsions

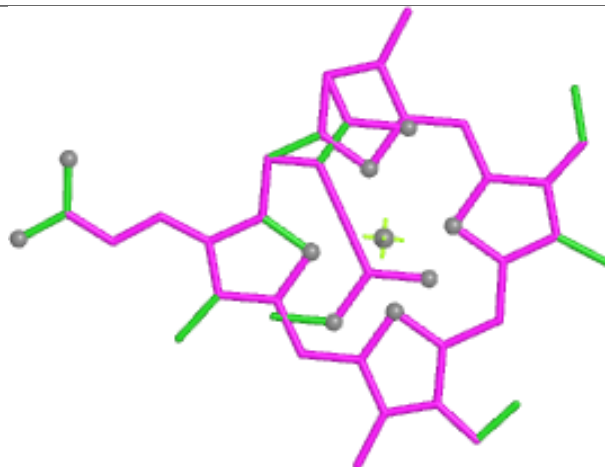


Rings

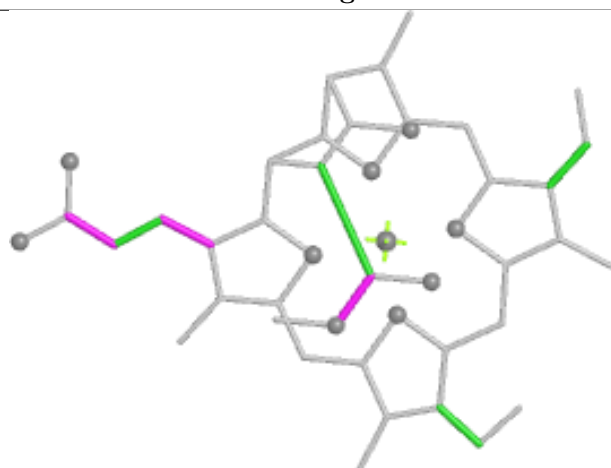
## Ligand KC1 D 314



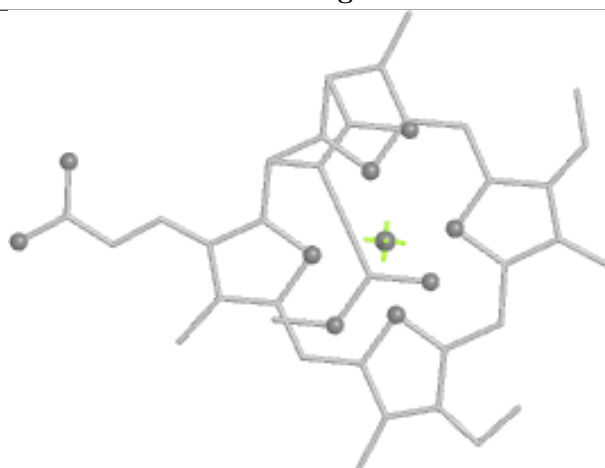
Bond lengths



Bond angles

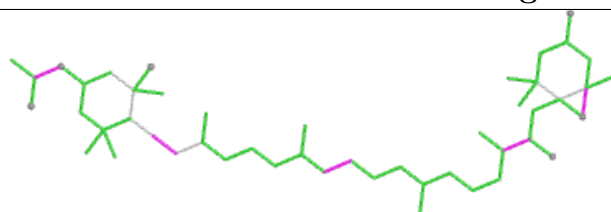


Torsions

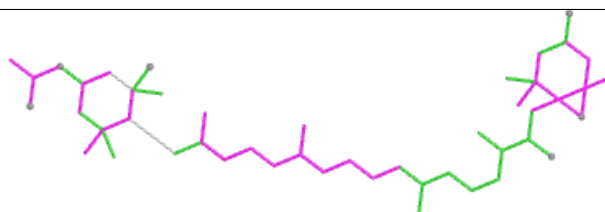


Rings

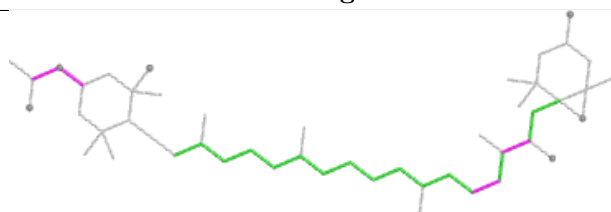
## Ligand A86 O 319



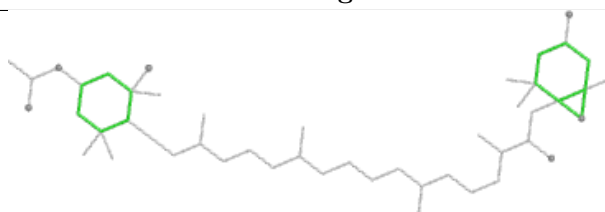
Bond lengths



Bond angles

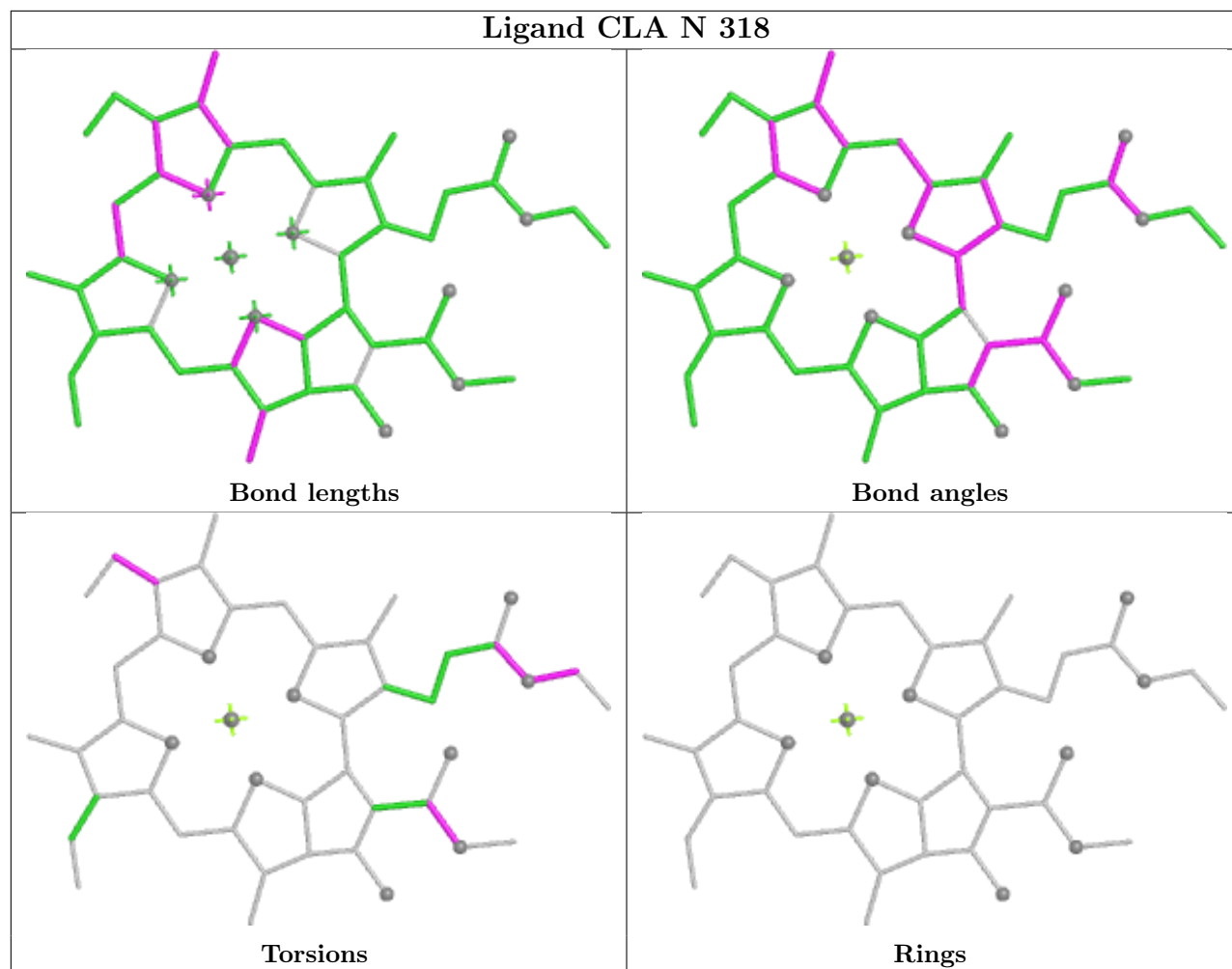


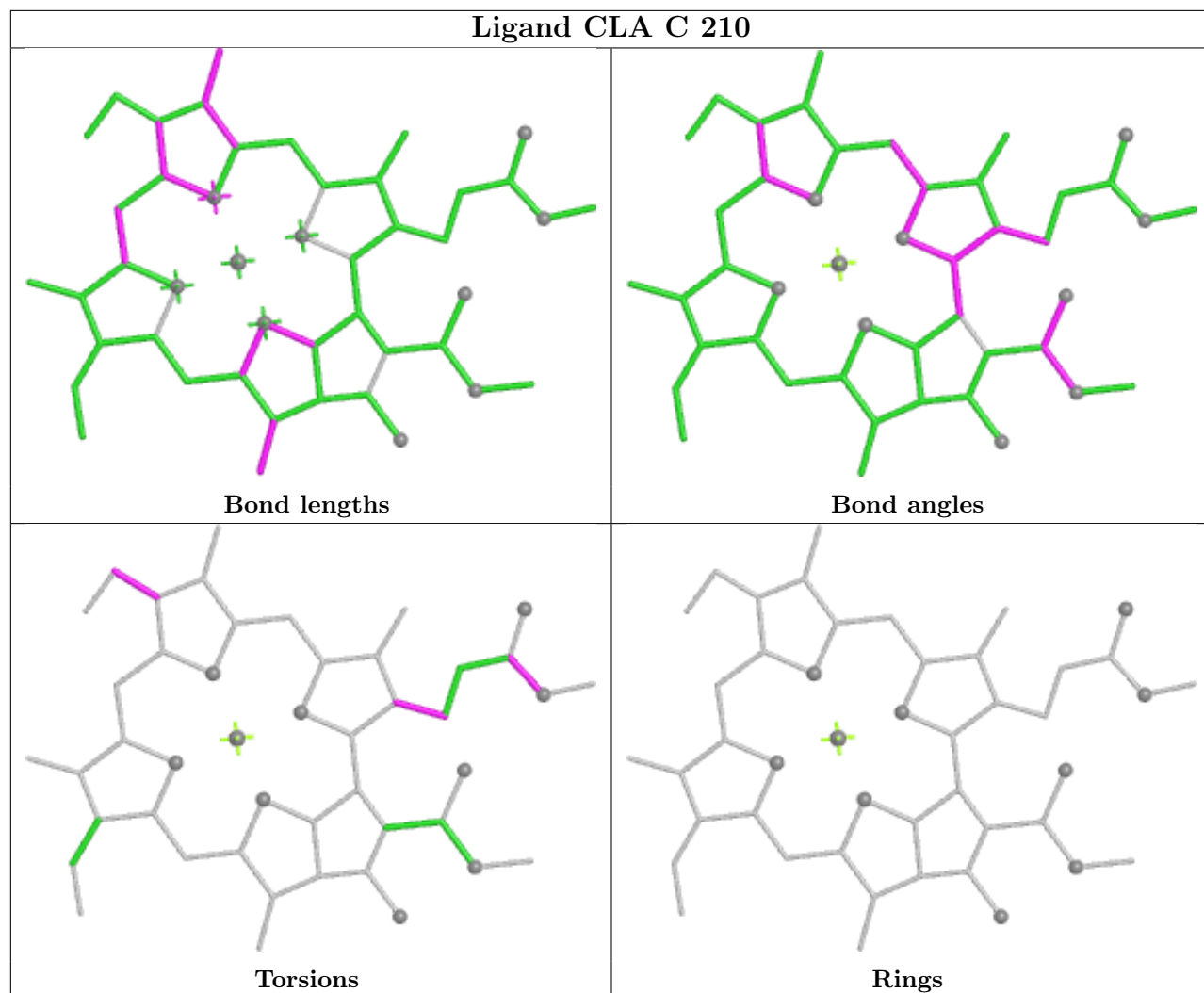
Torsions

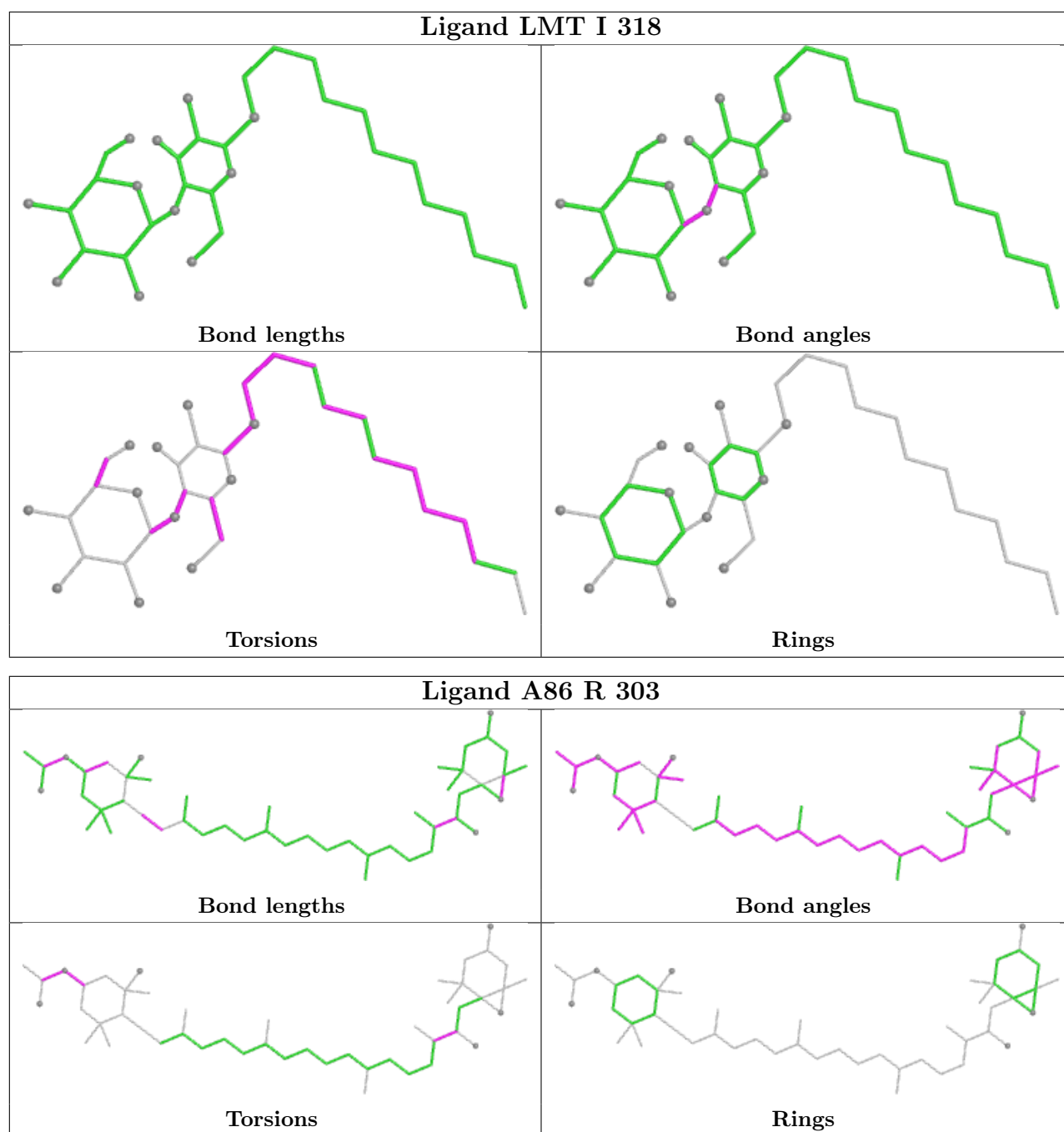


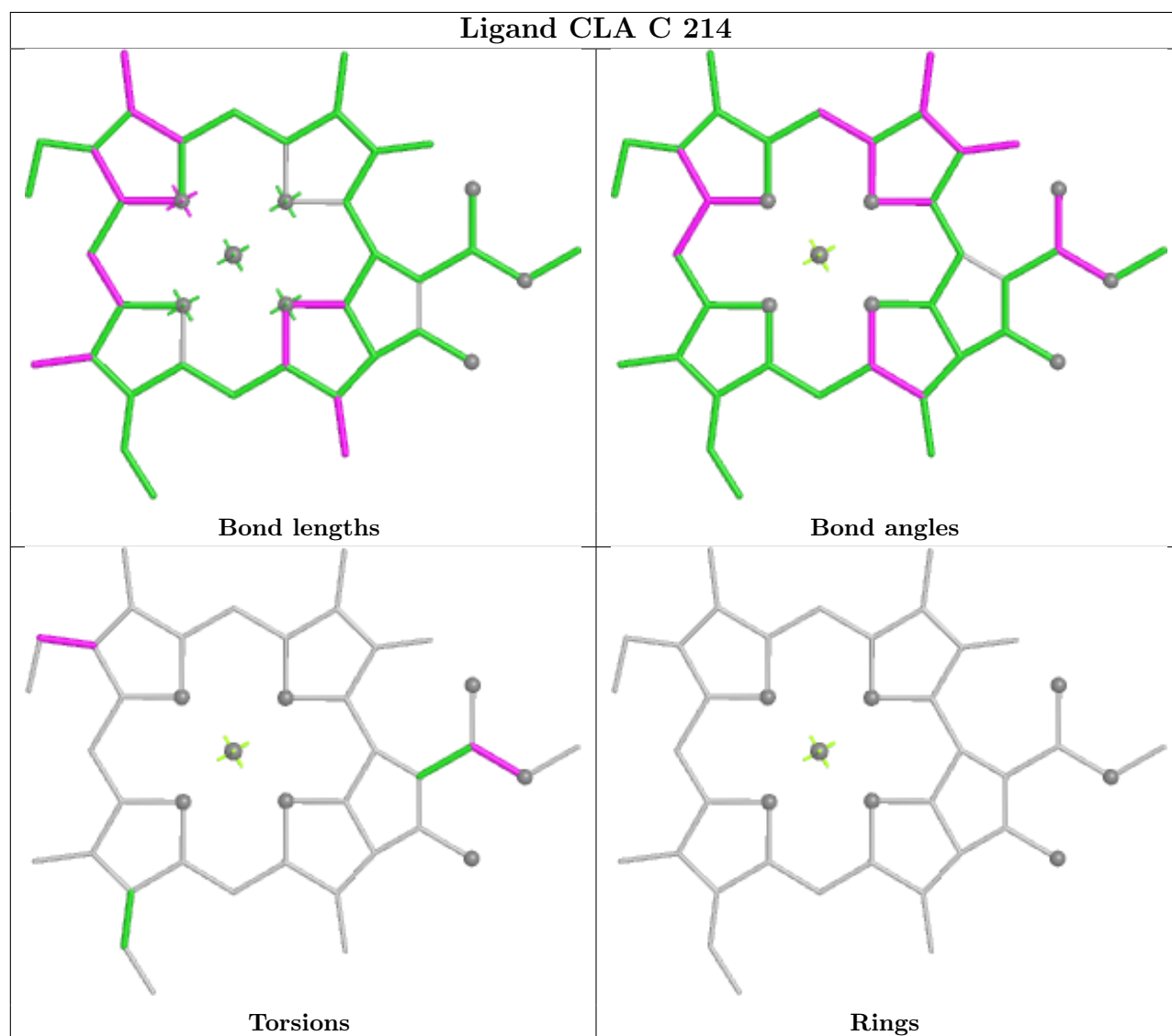
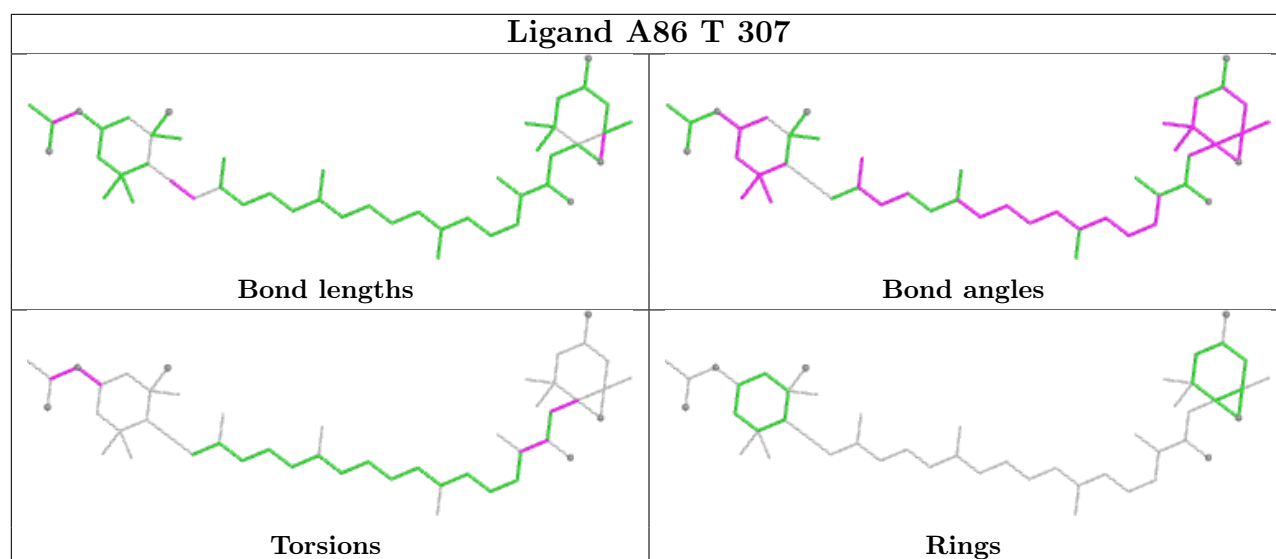
Rings

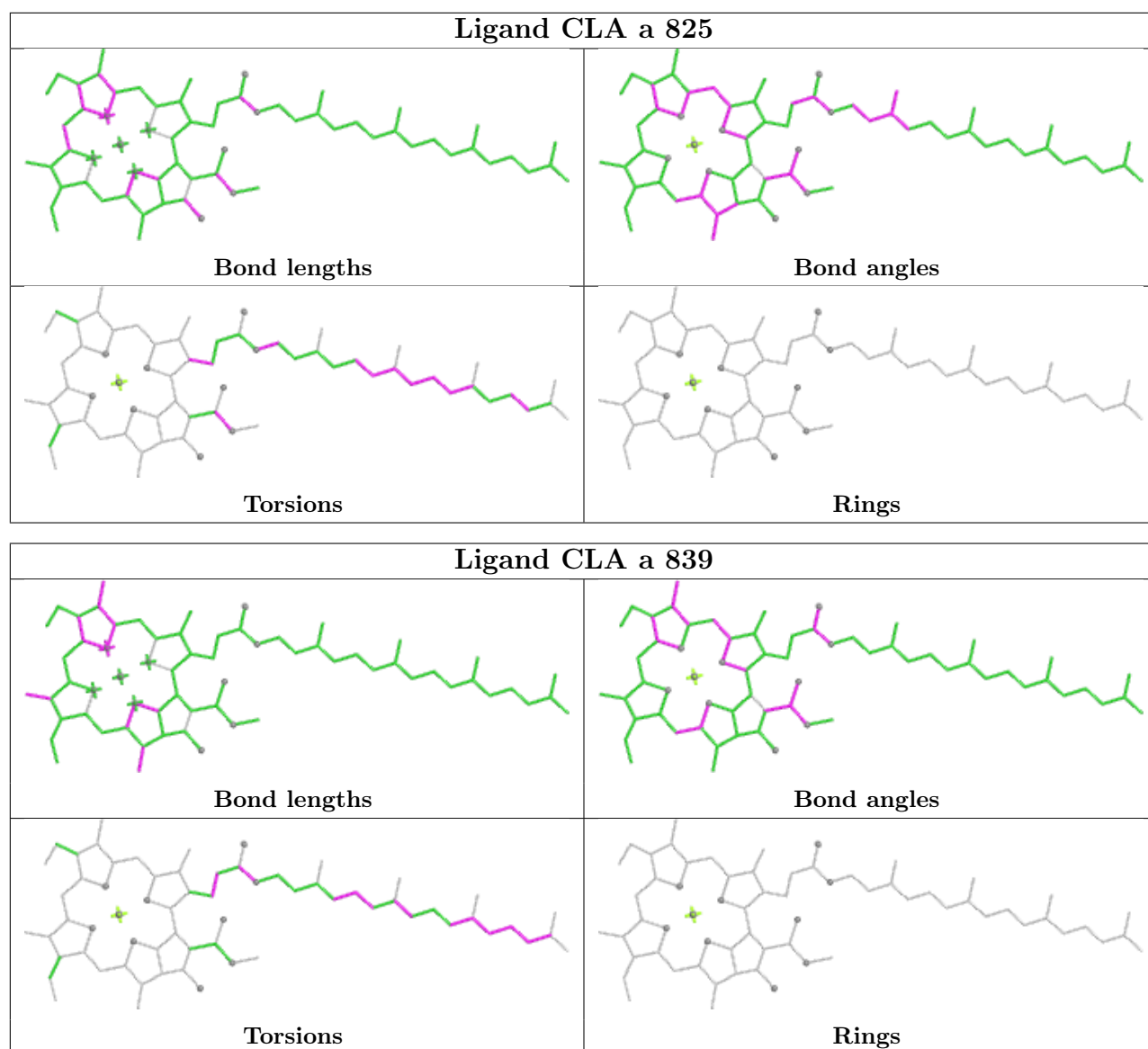
## Ligand CLA N 318



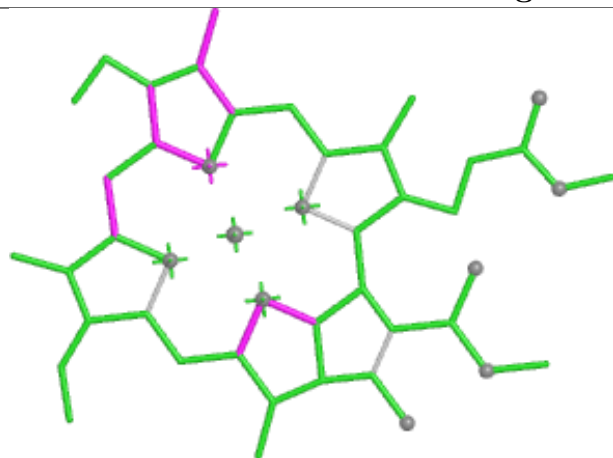




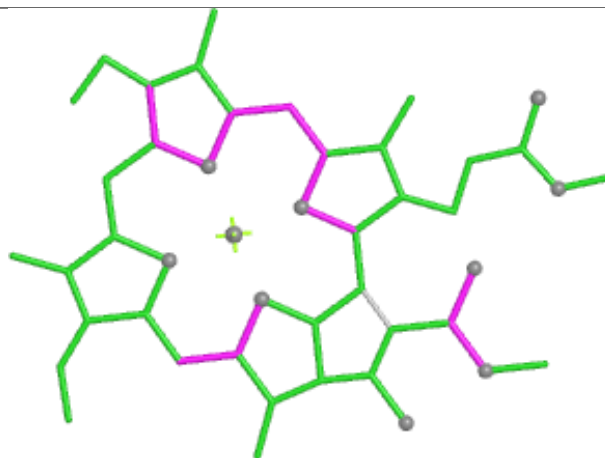




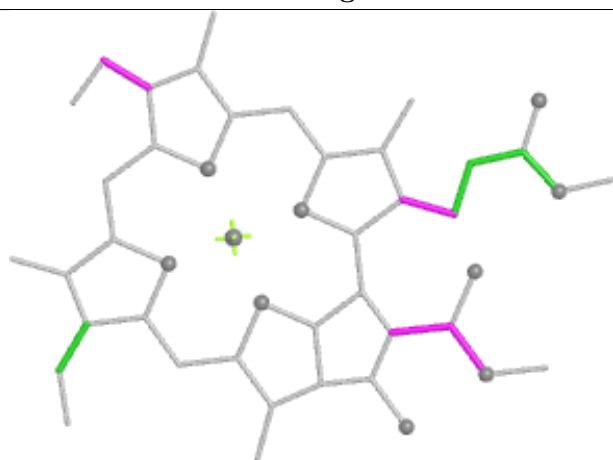
## Ligand CLA E 317



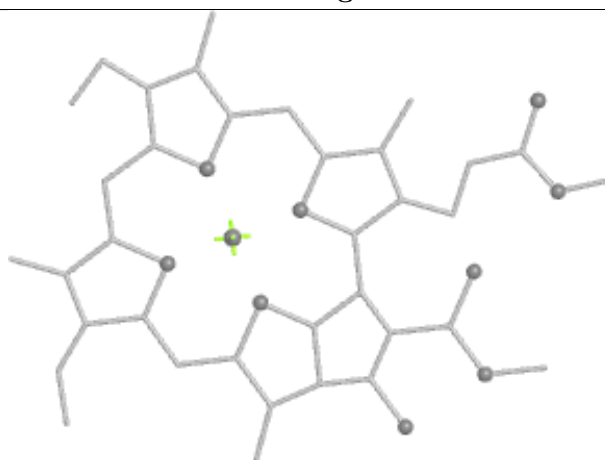
Bond lengths



Bond angles

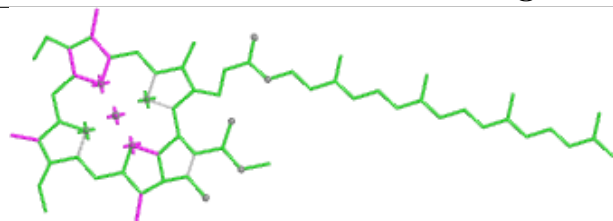


Torsions

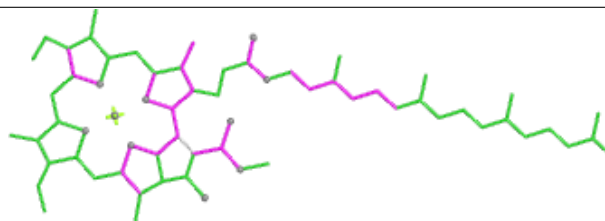


Rings

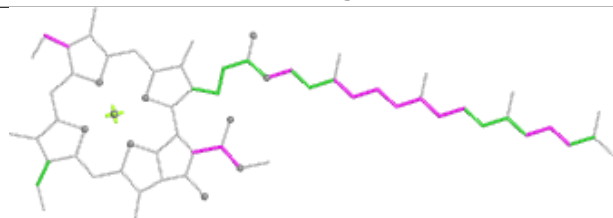
## Ligand CLA b 805



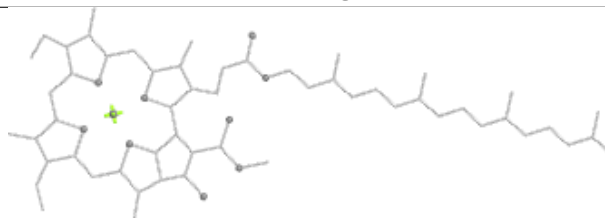
Bond lengths



Bond angles

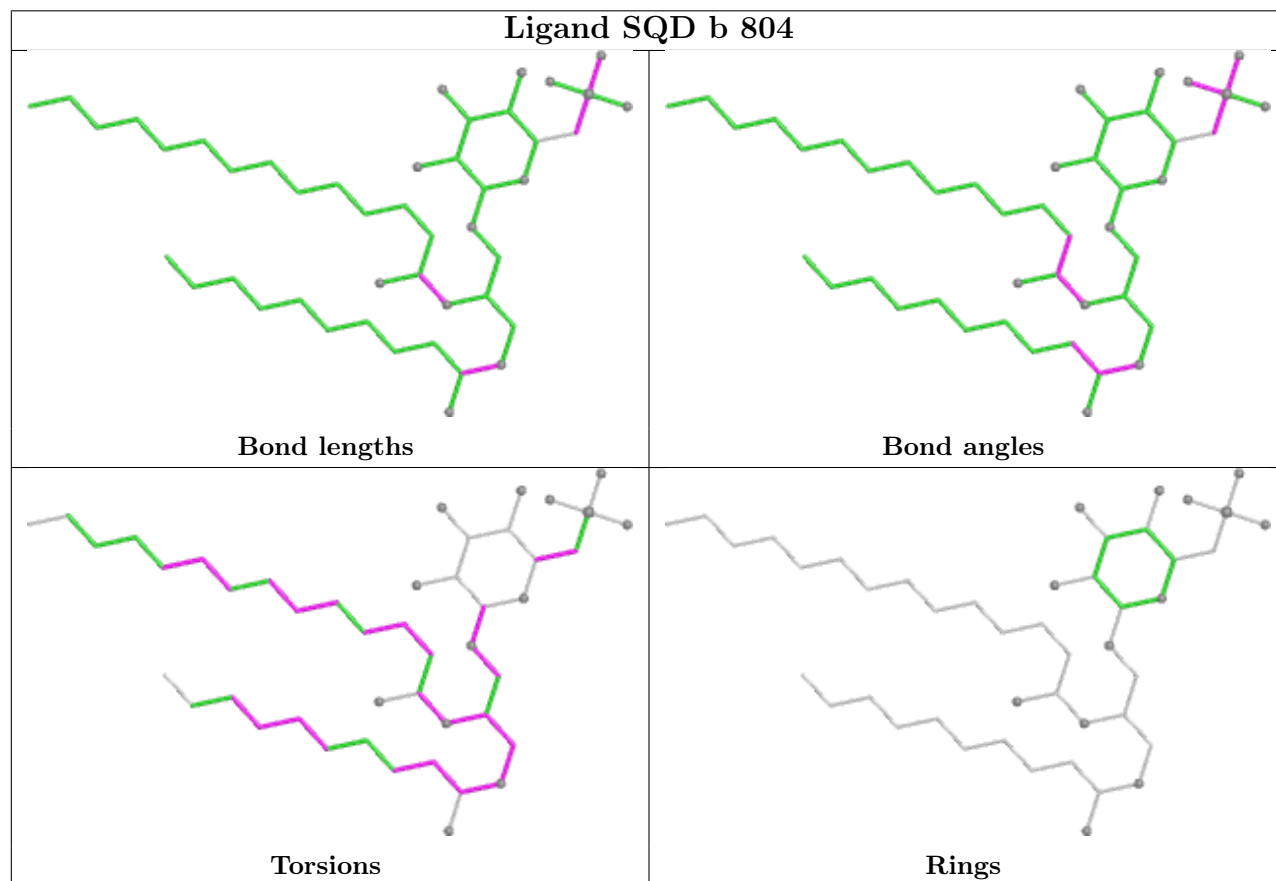
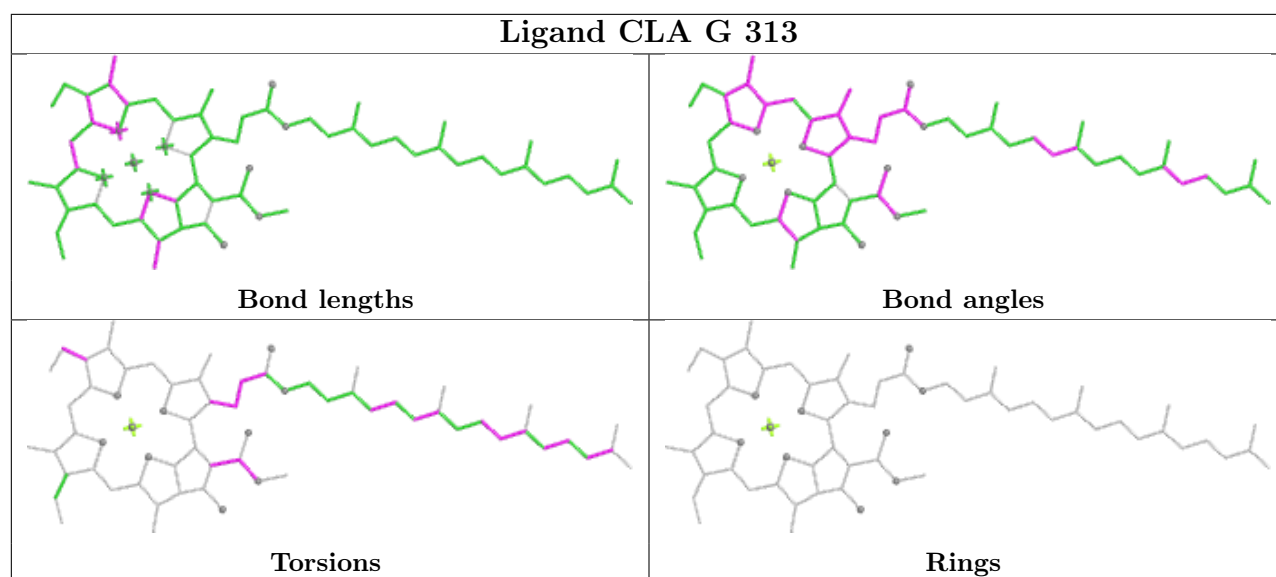


Torsions

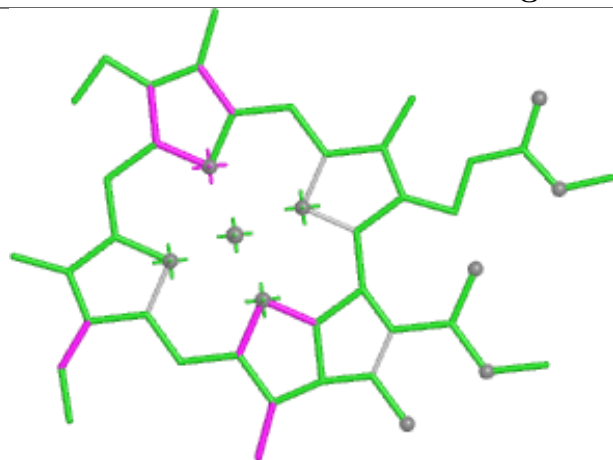


Rings

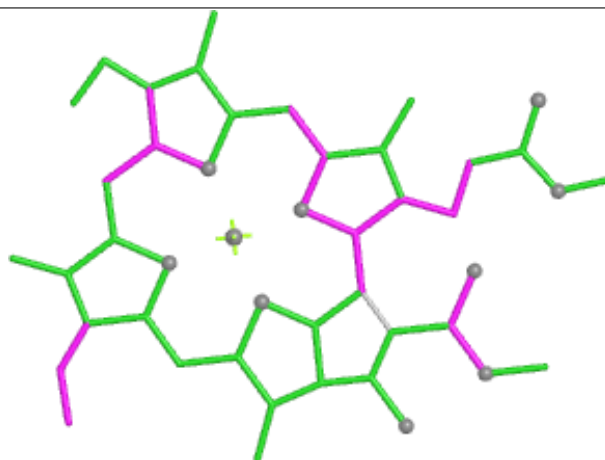




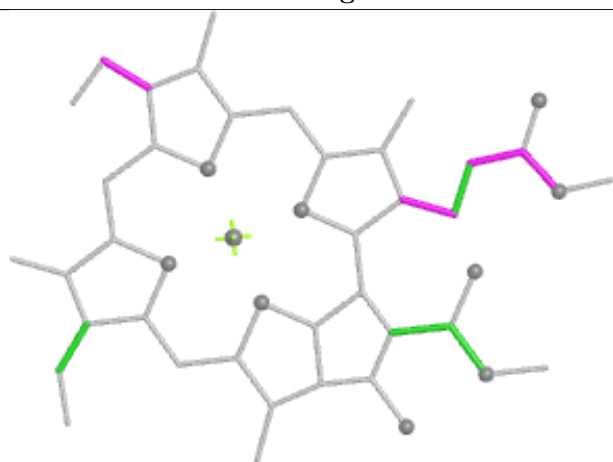
## Ligand CLA I 309



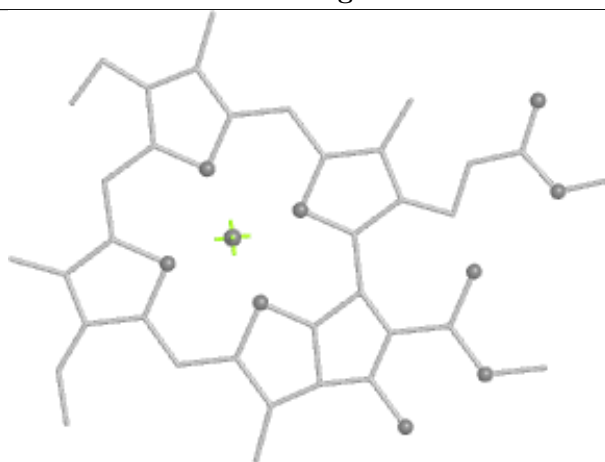
Bond lengths



Bond angles

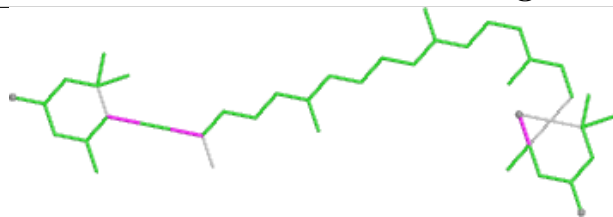


Torsions

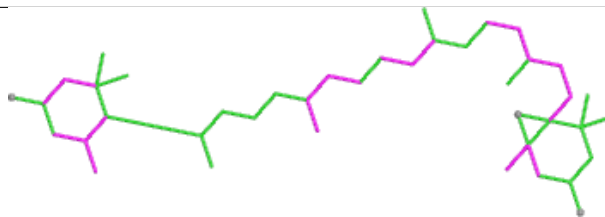


Rings

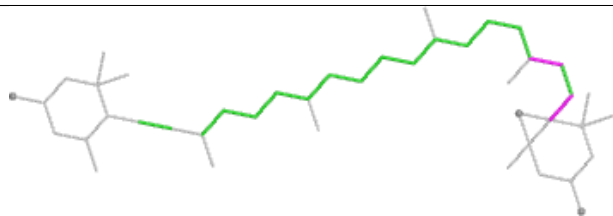
## Ligand DD6 E 304



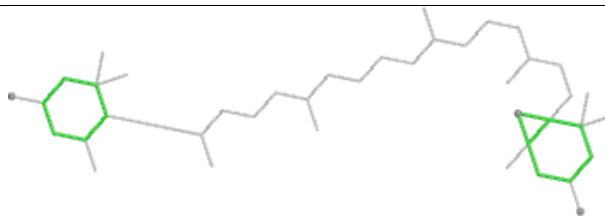
Bond lengths



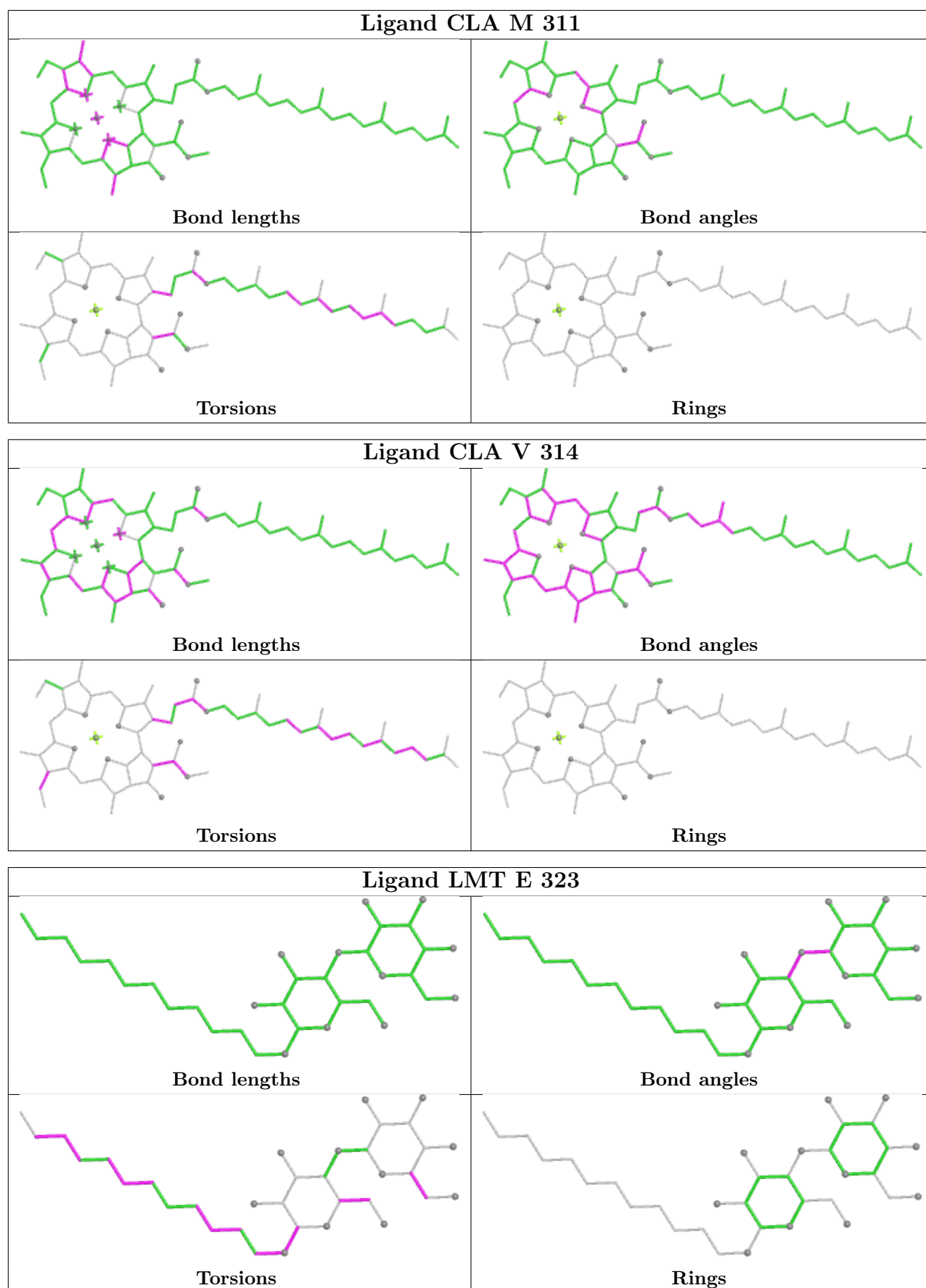
Bond angles



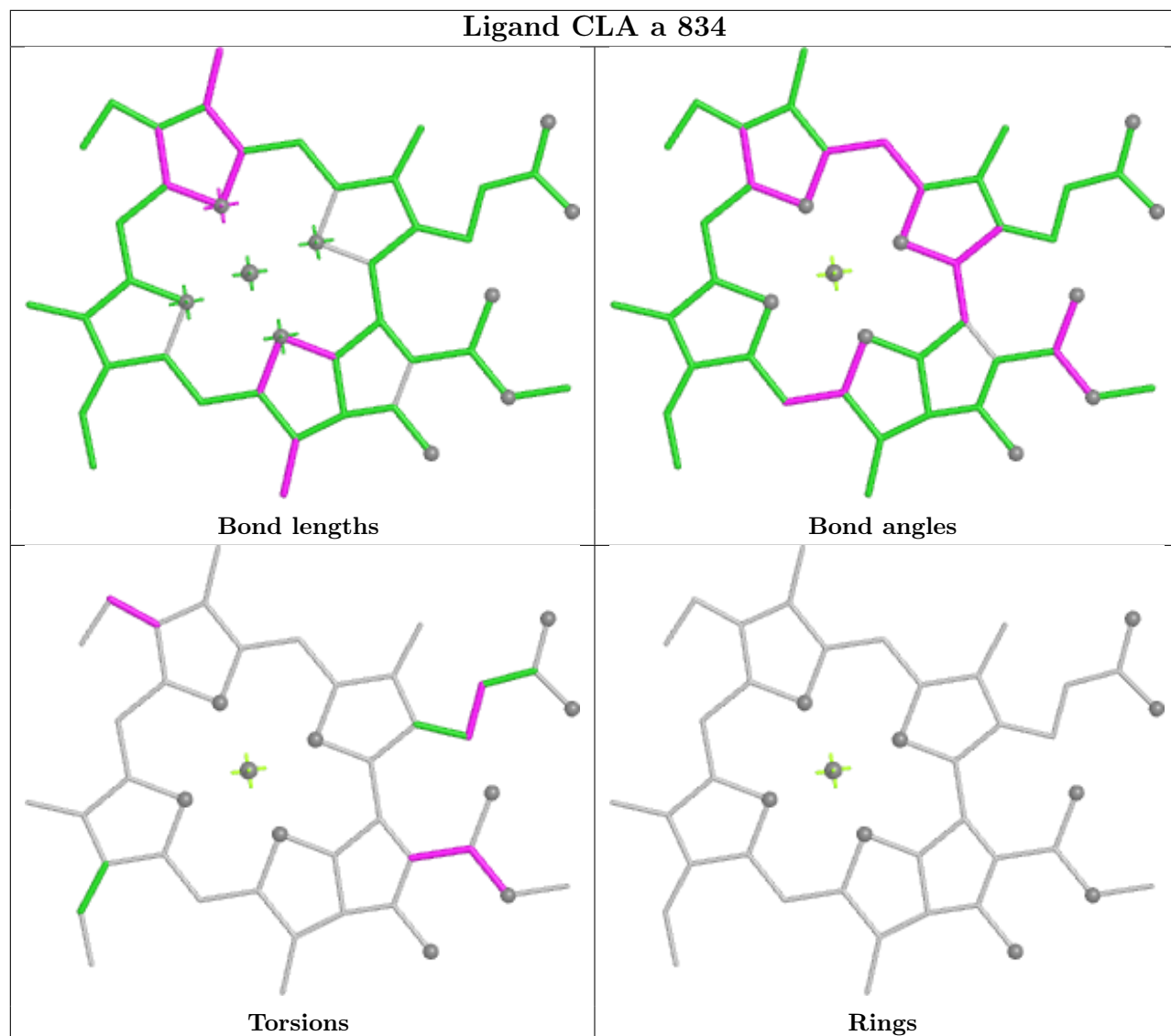
Torsions



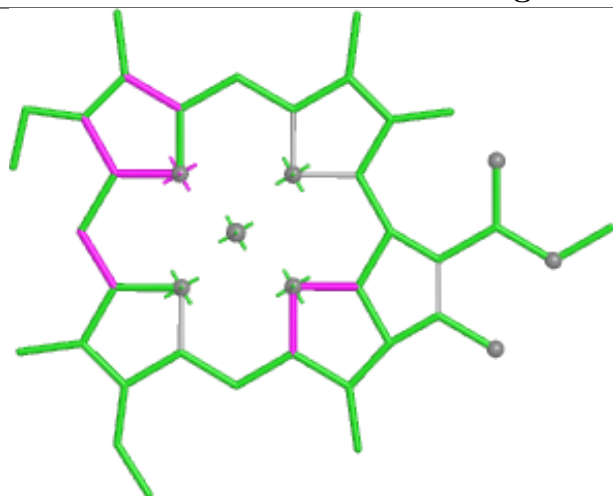
Rings



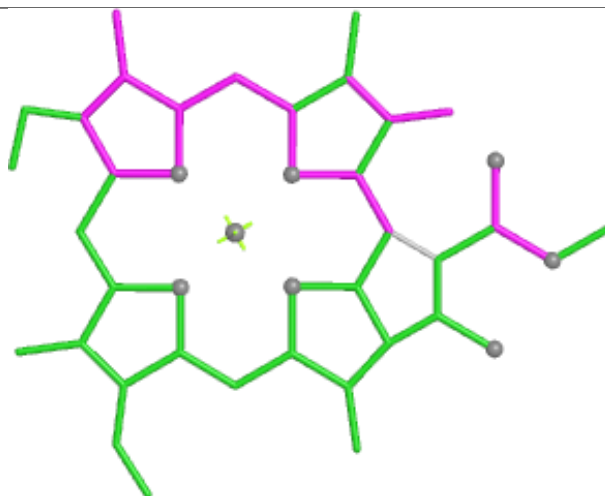
## Ligand CLA a 834



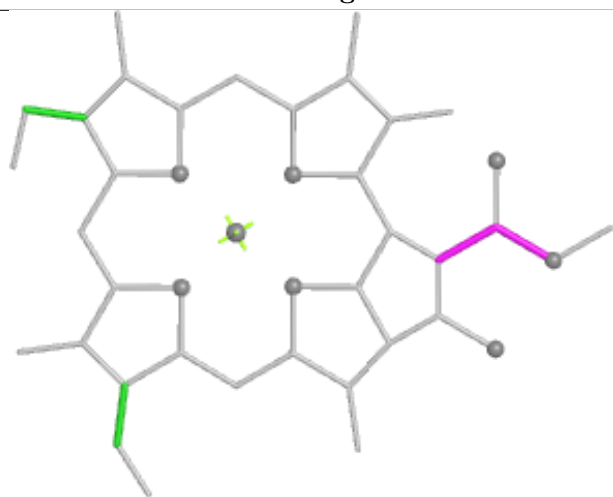
## Ligand CLA X 315



Bond lengths



Bond angles

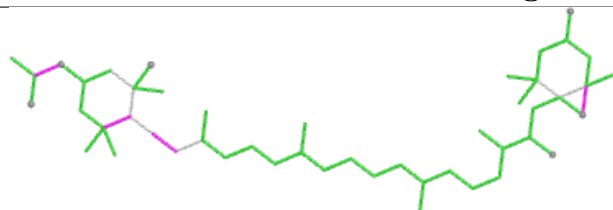


Torsions

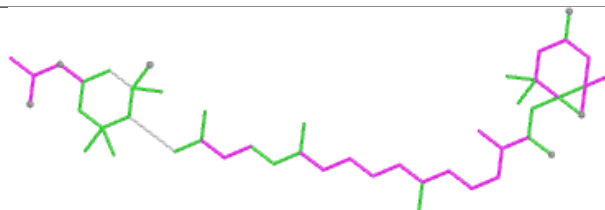


Rings

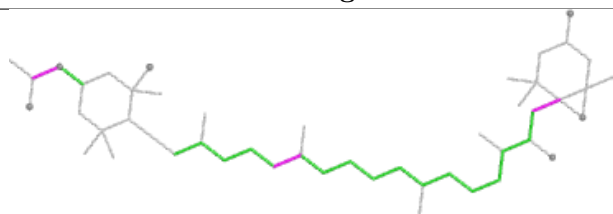
## Ligand A86 L 301



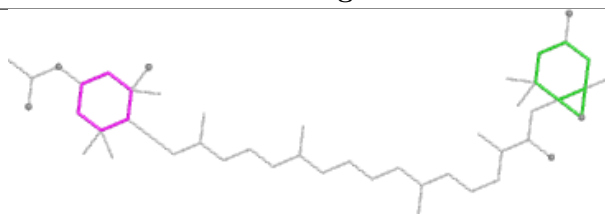
Bond lengths



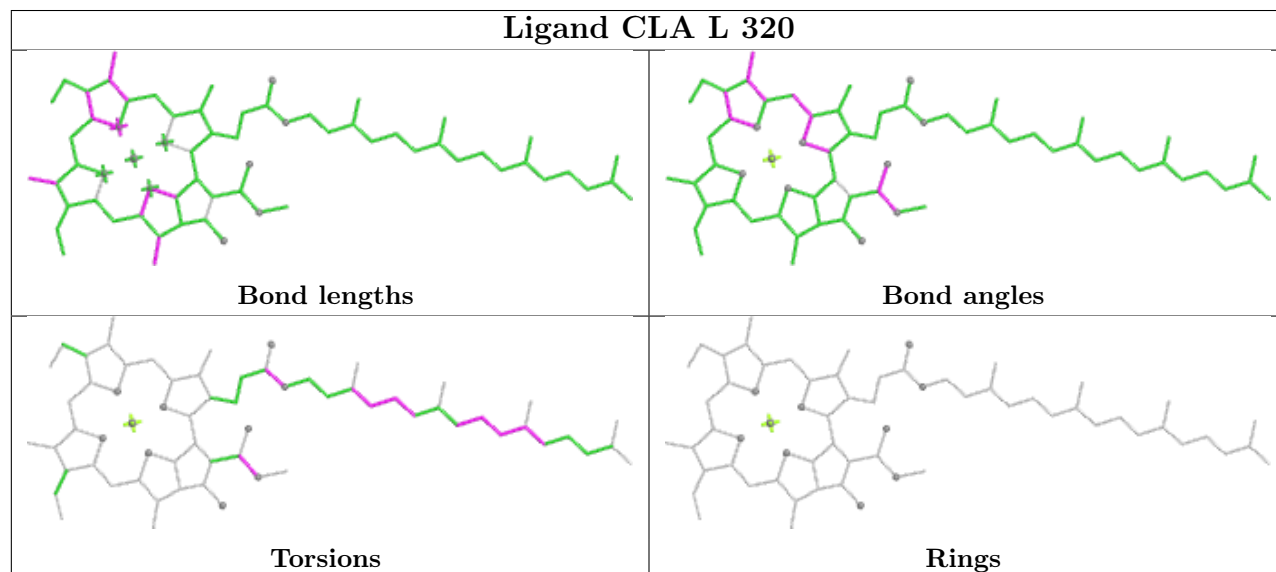
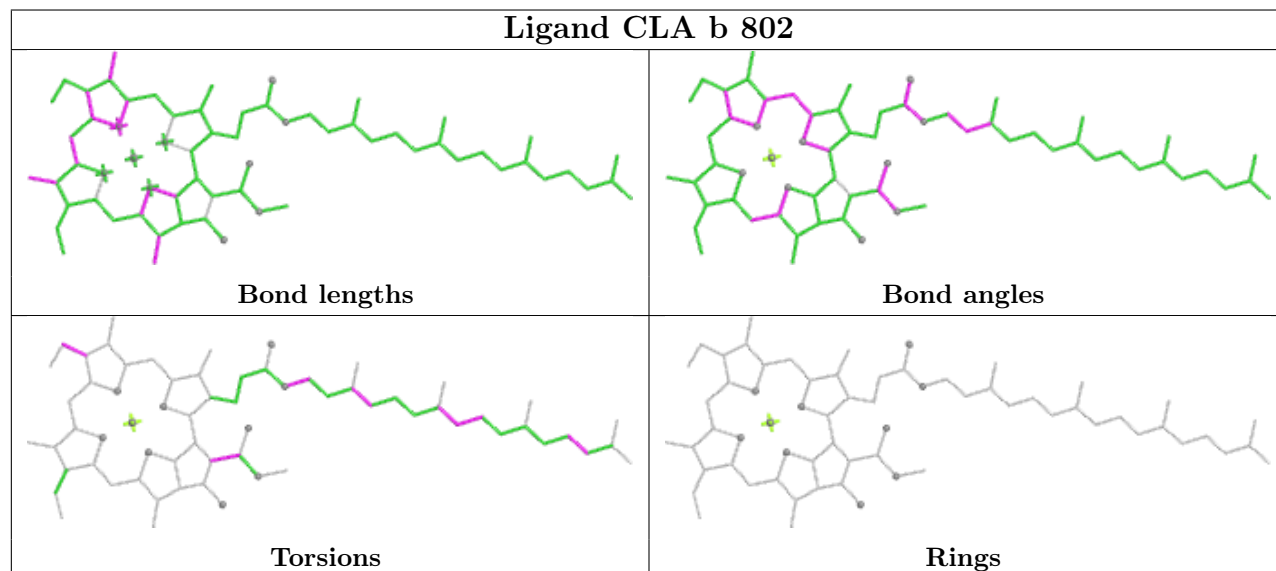
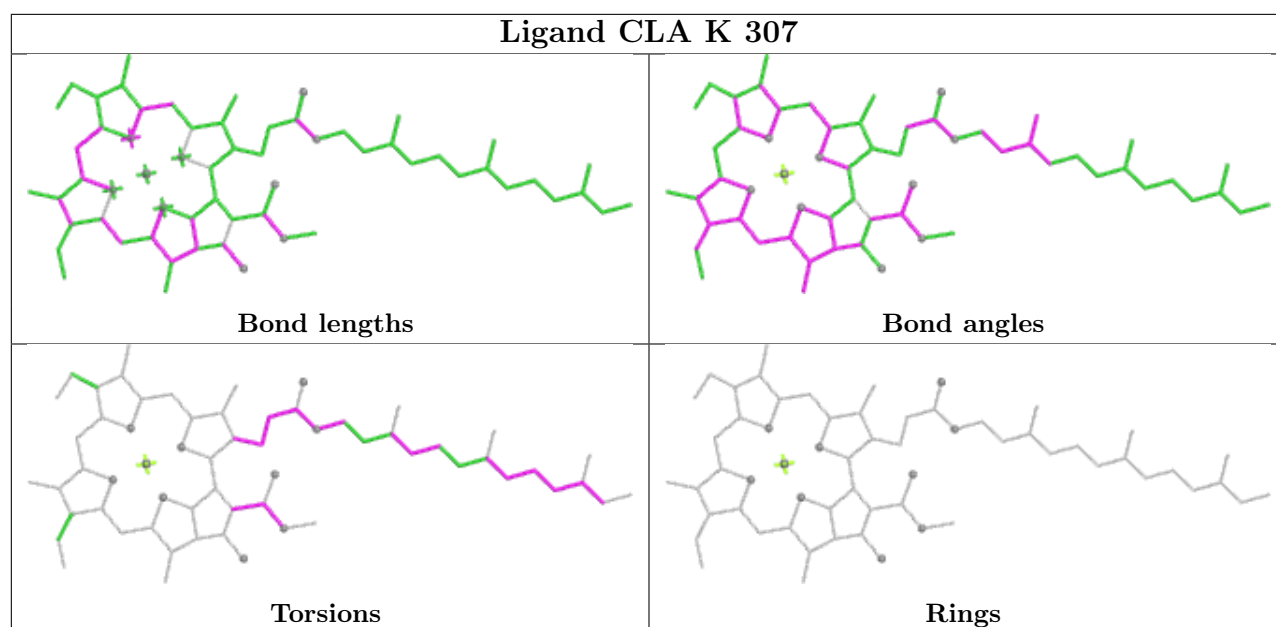
Bond angles

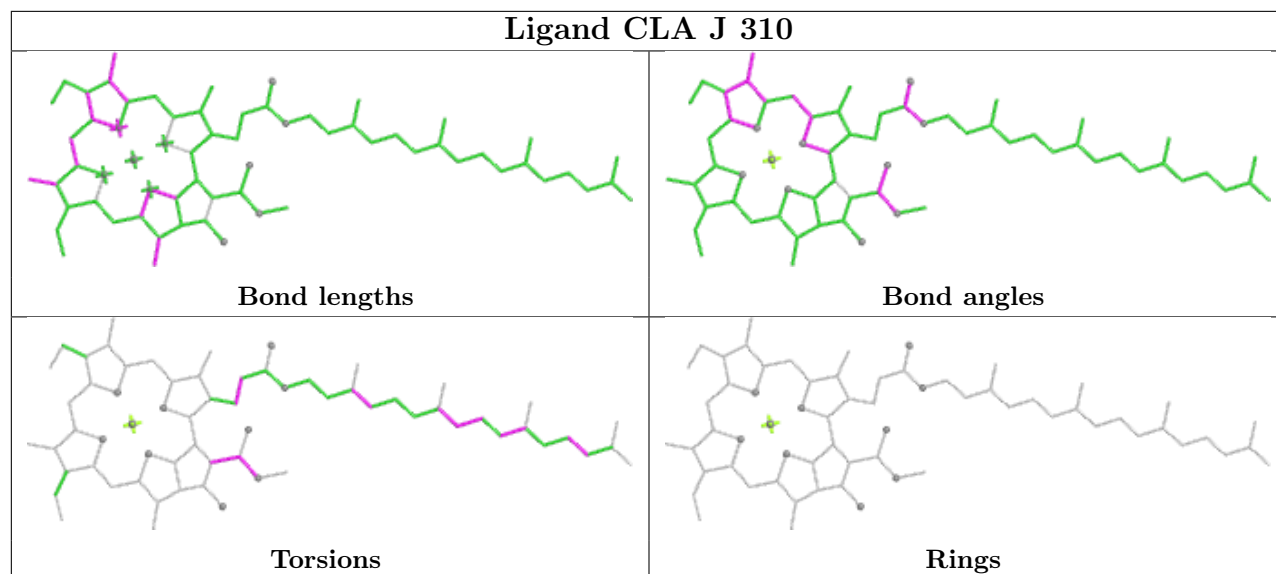
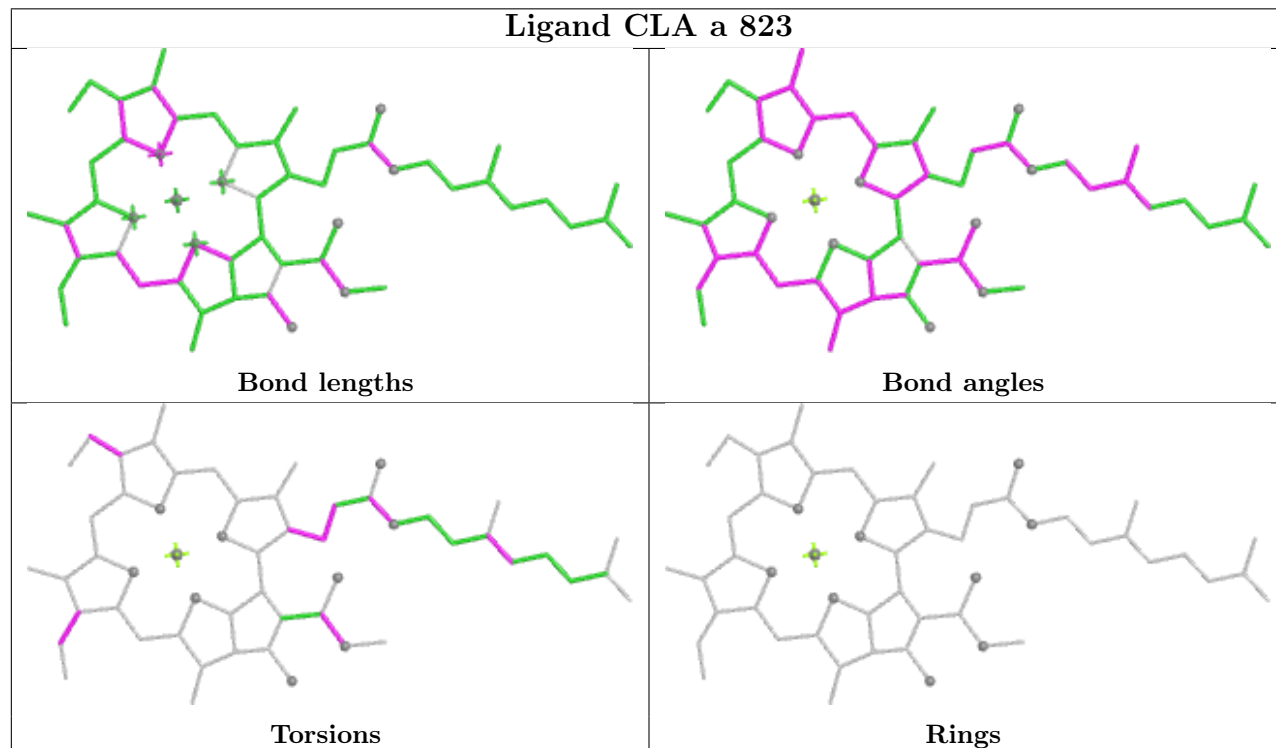


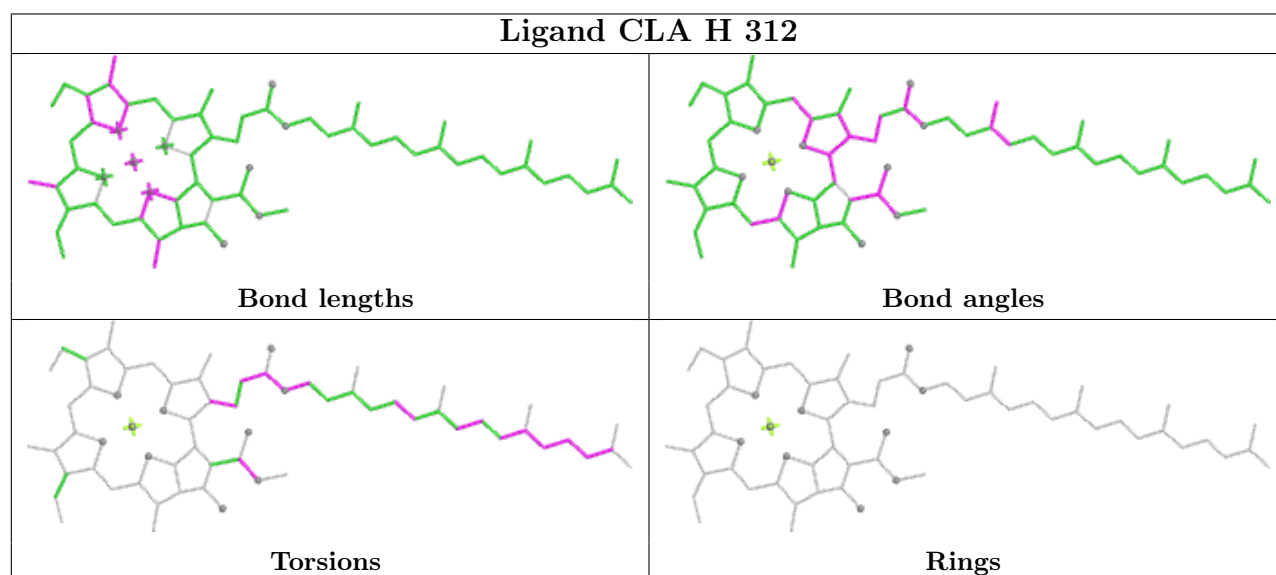
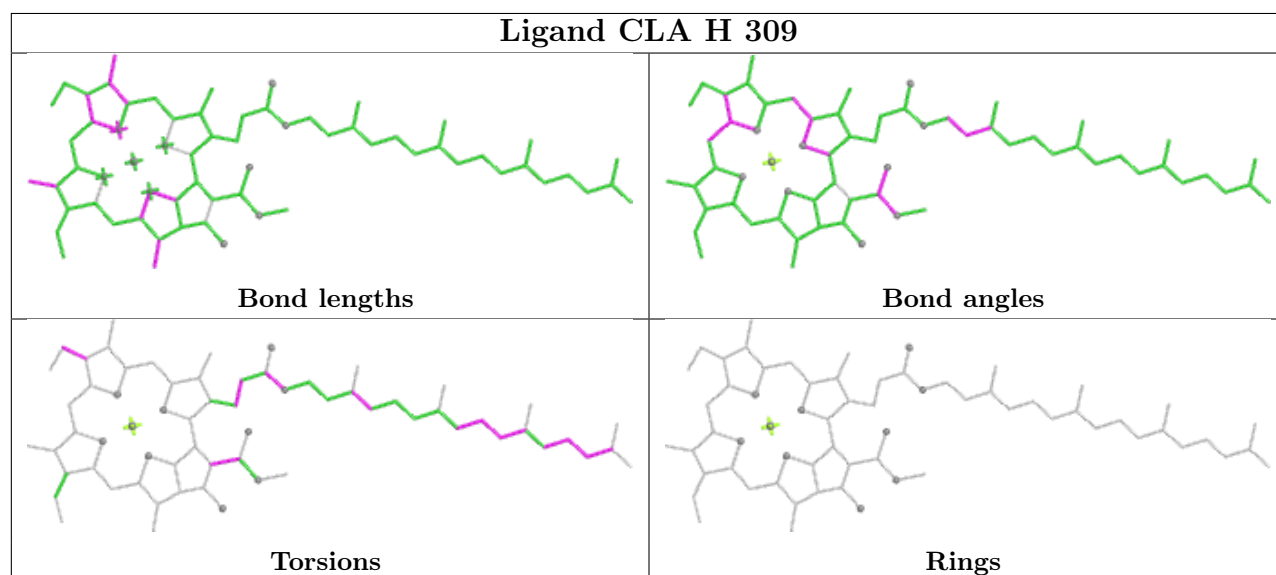
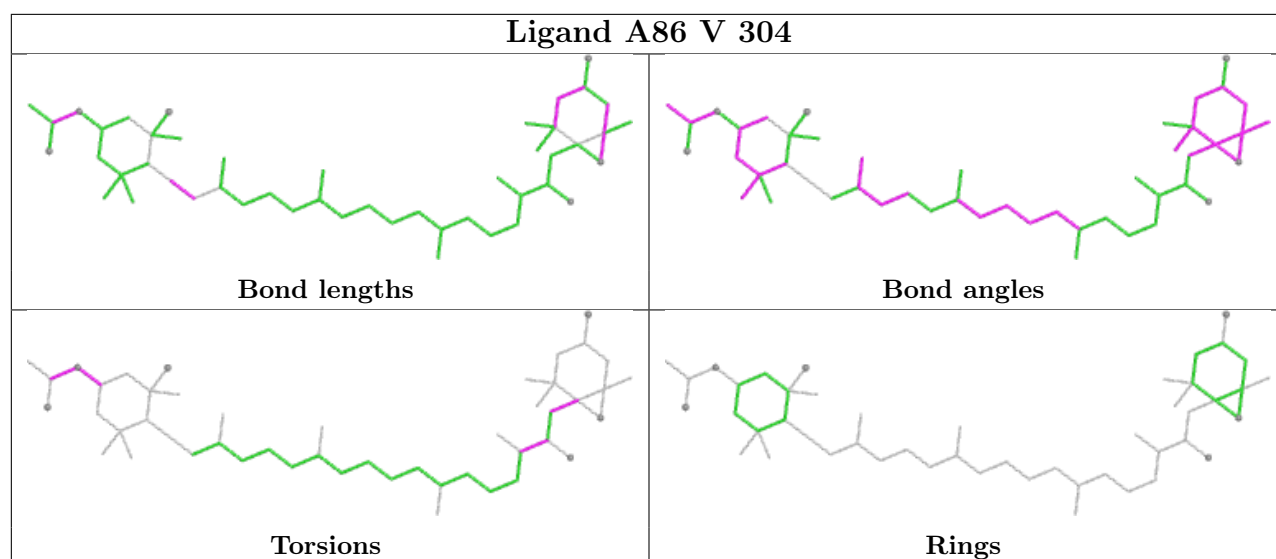
Torsions



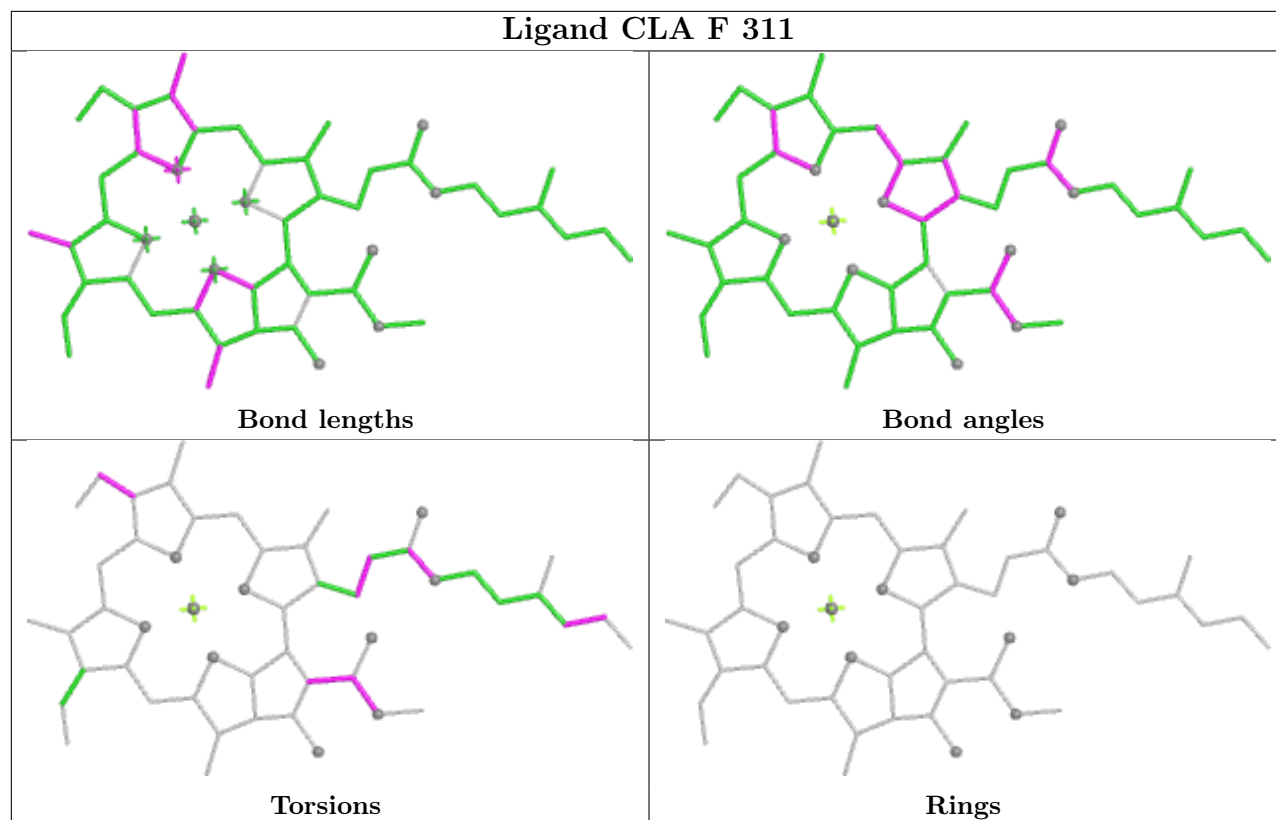
Rings

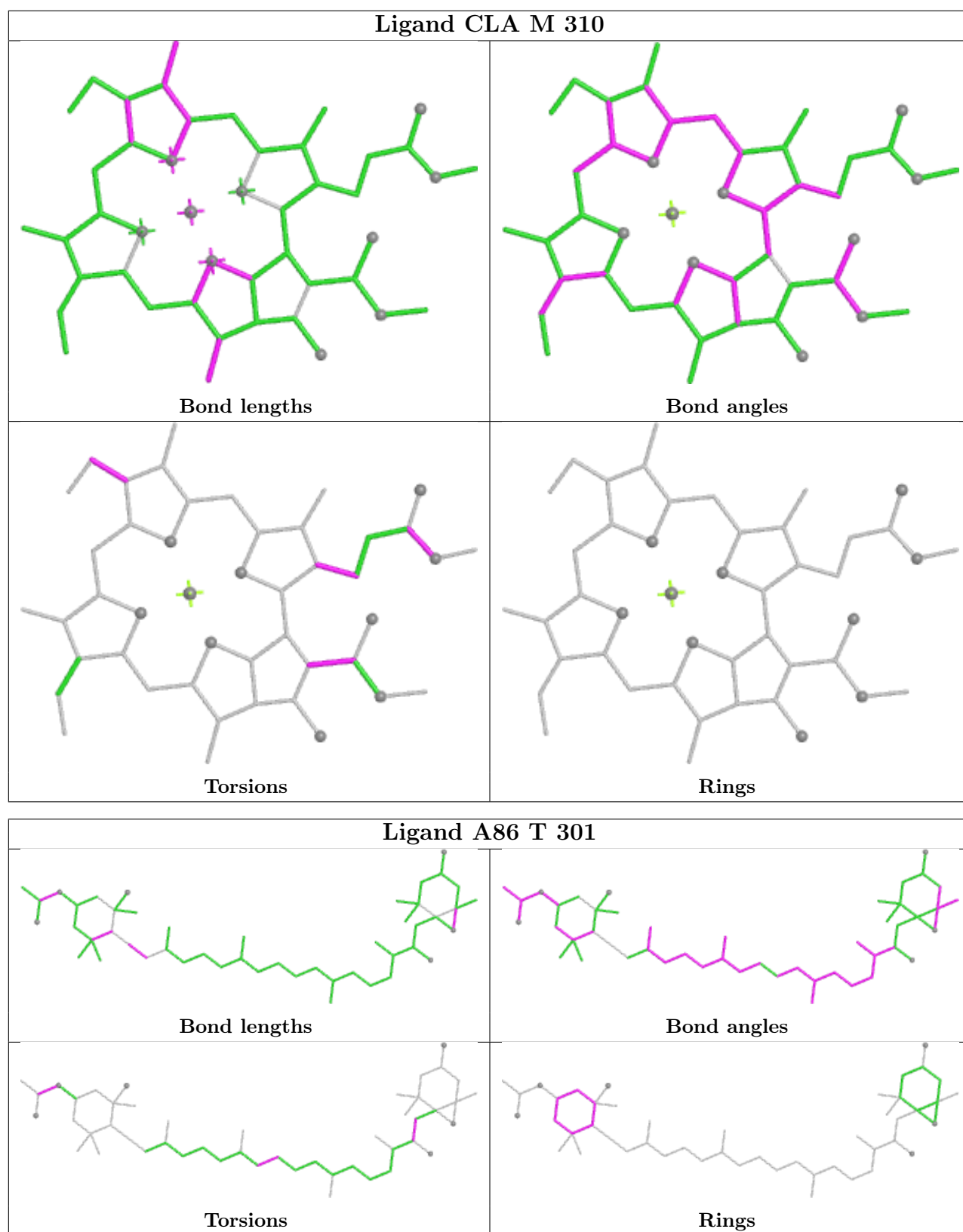


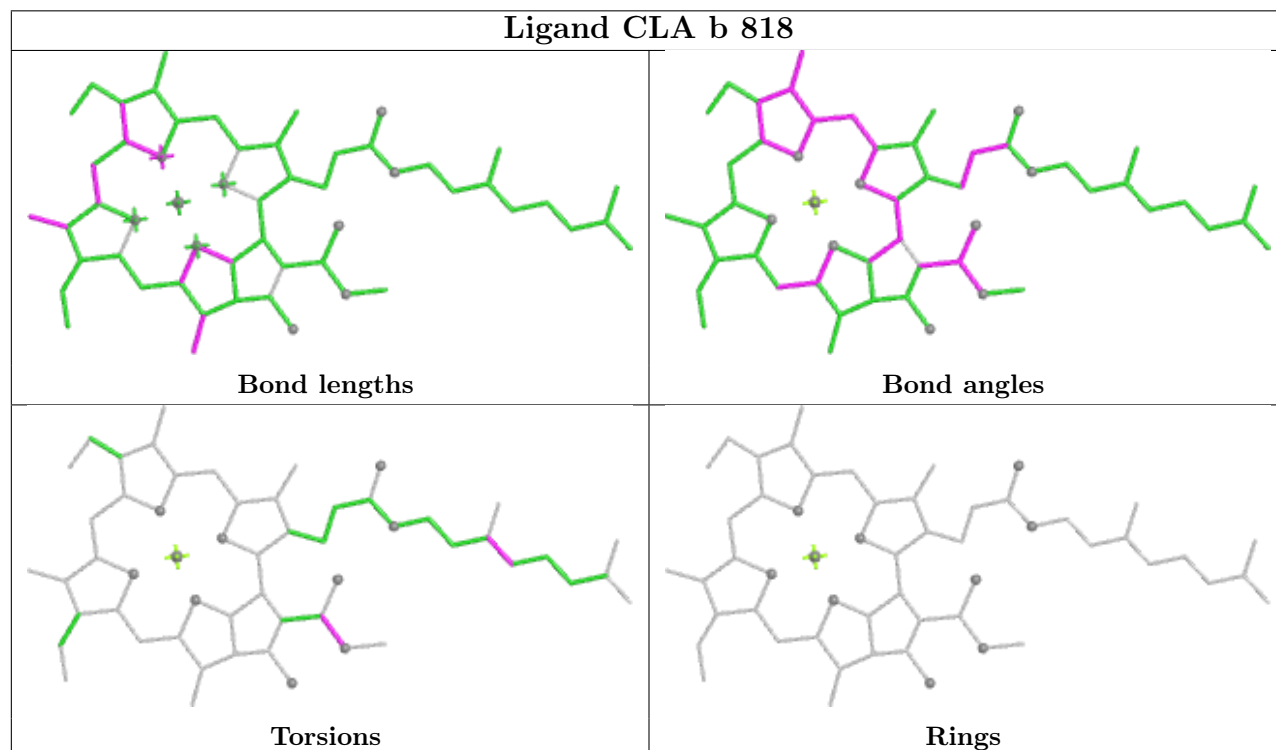
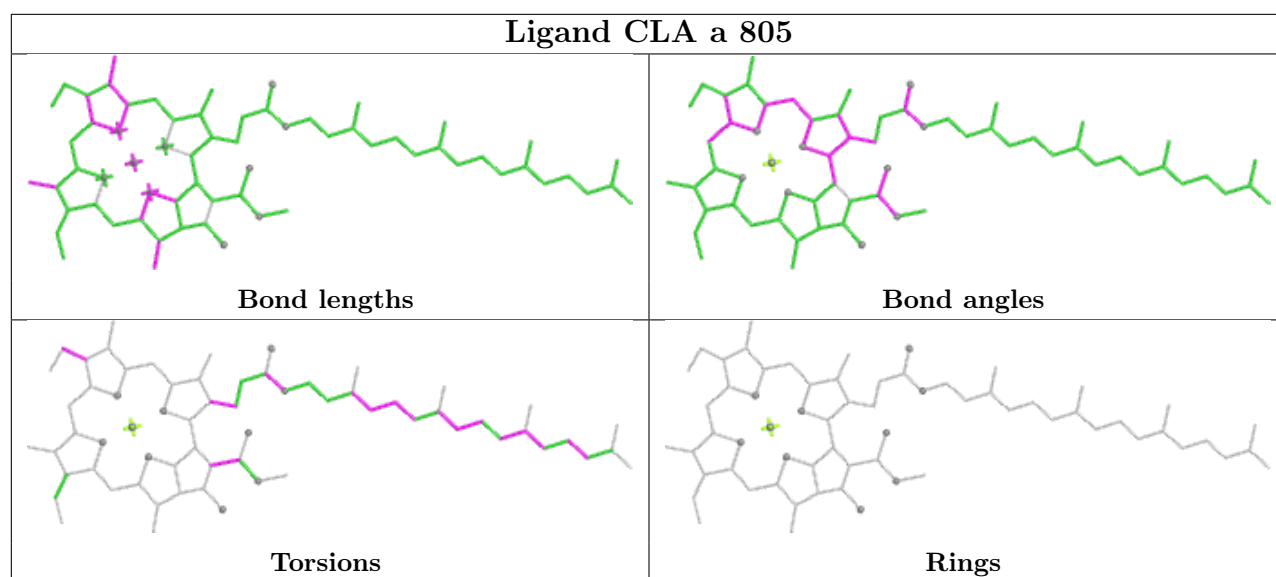
**Ligand CLA J 310****Ligand CLA a 823**



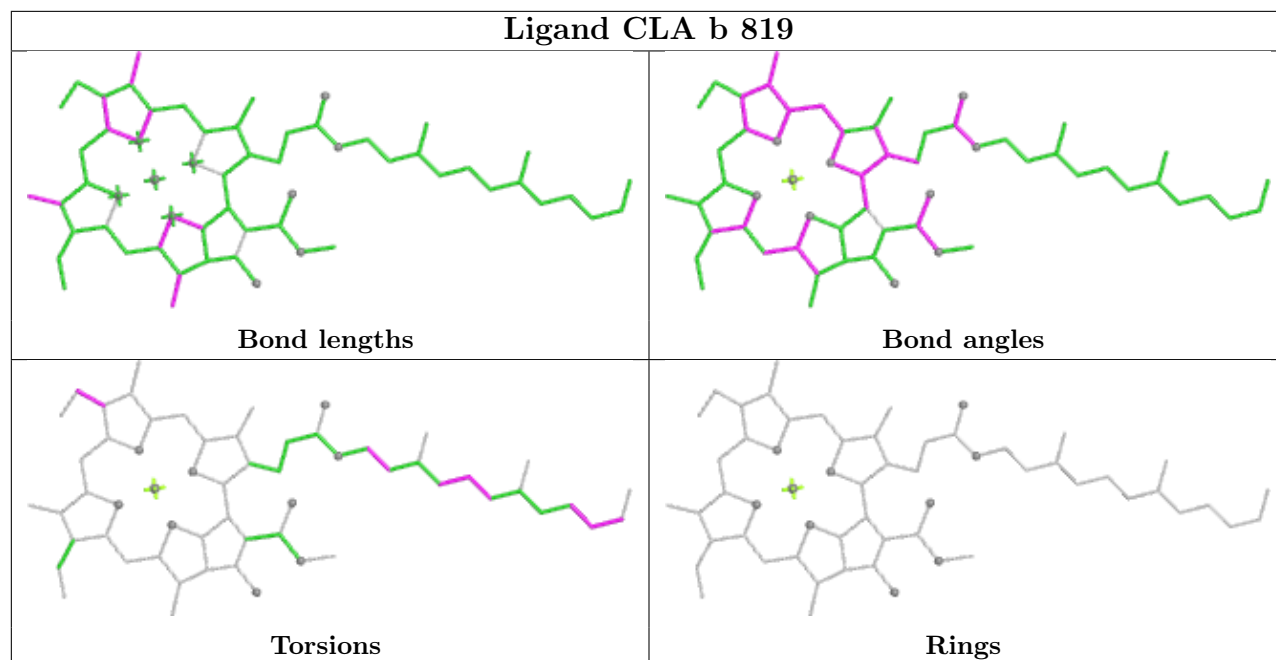




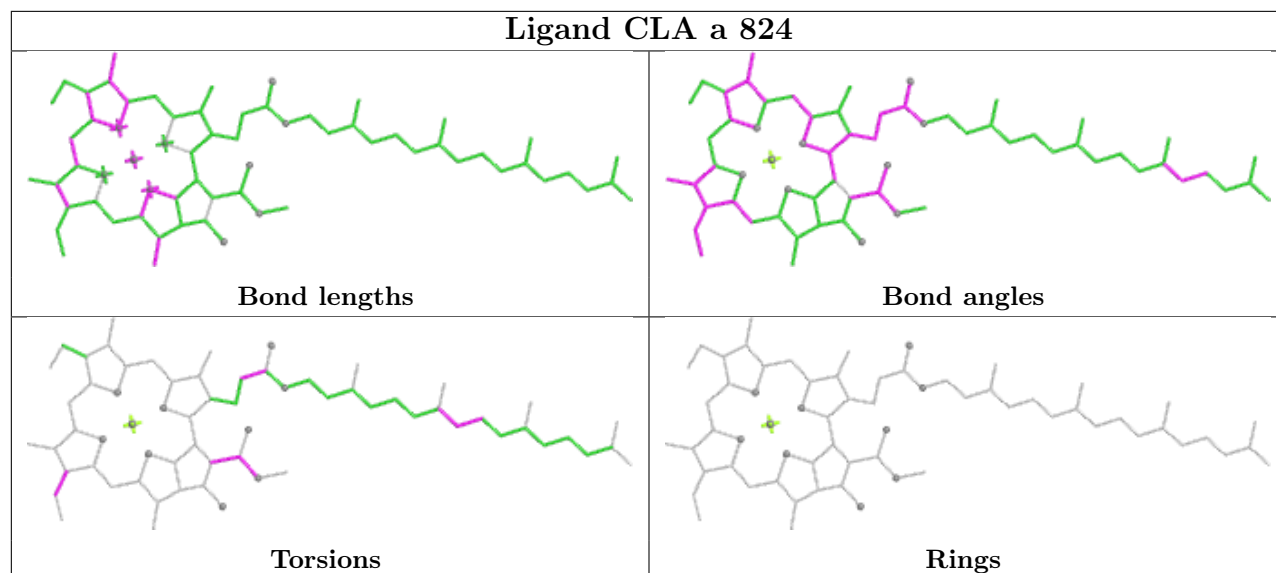




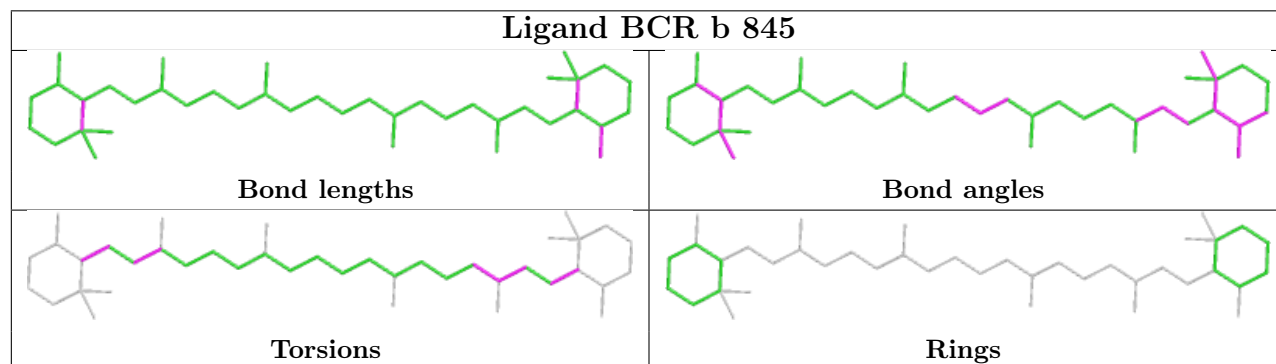
## Ligand CLA b 819

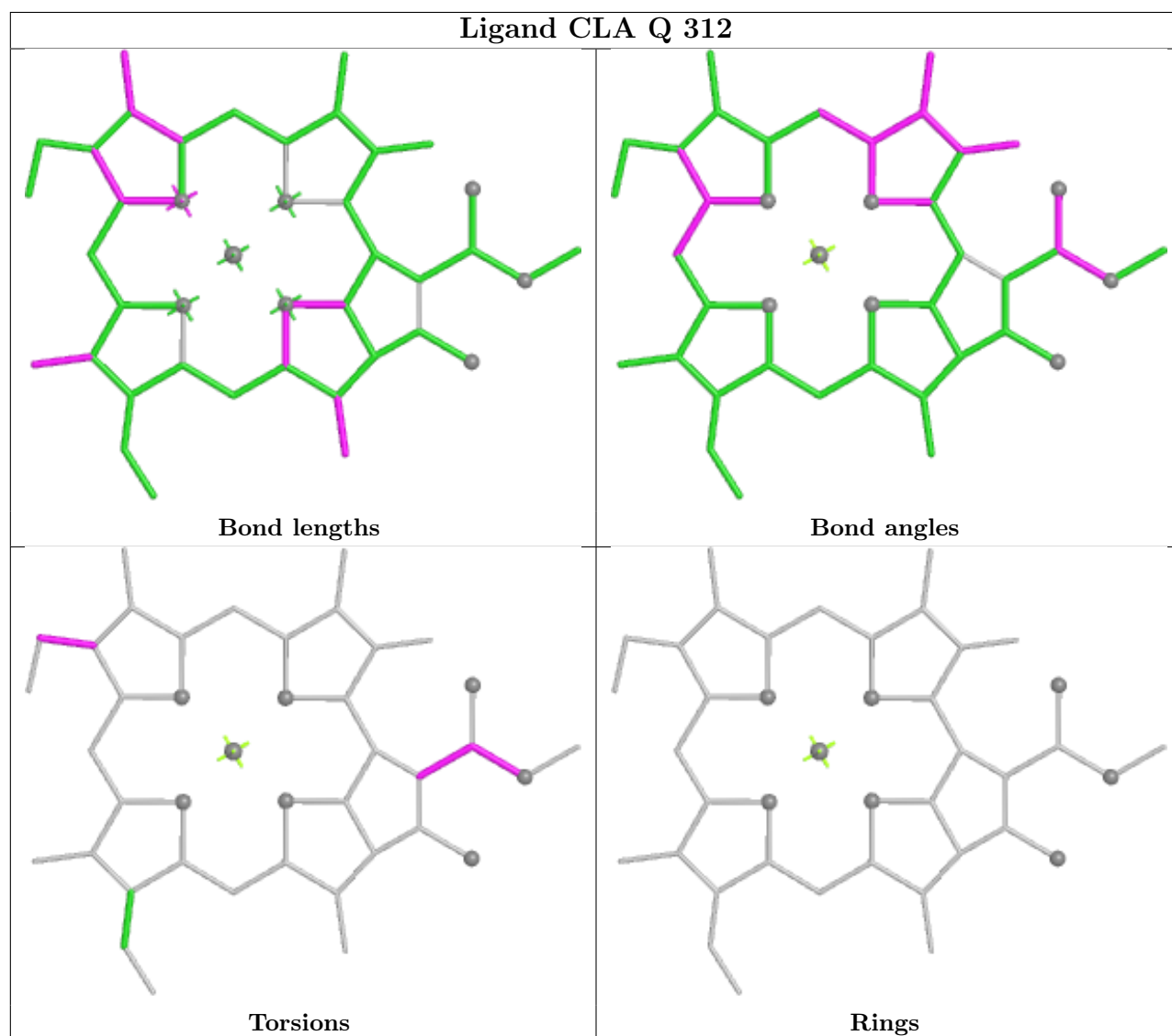
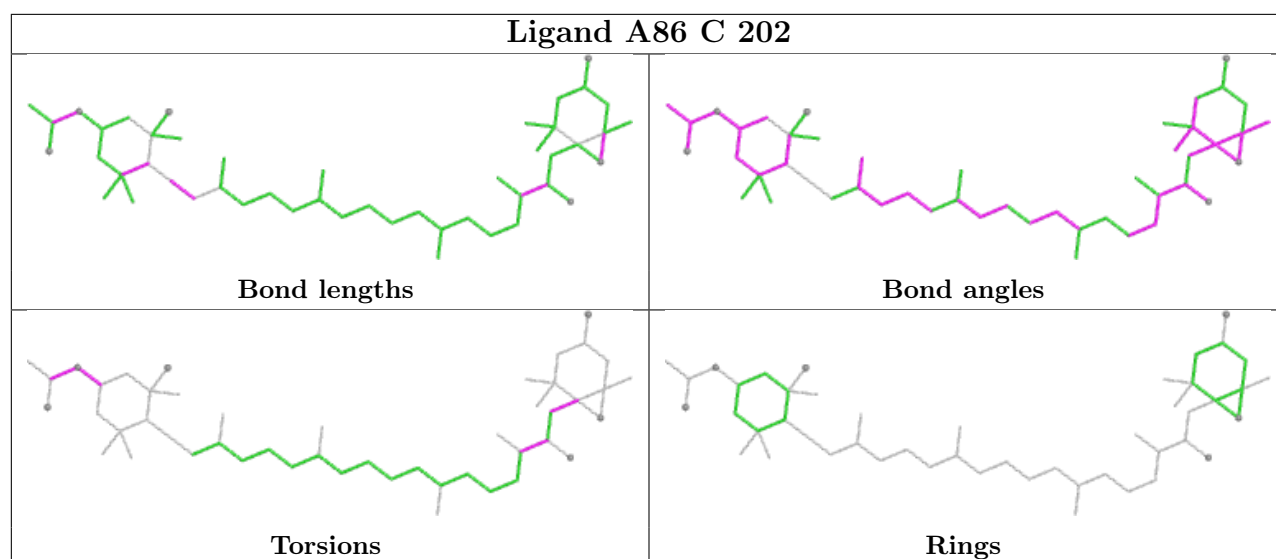


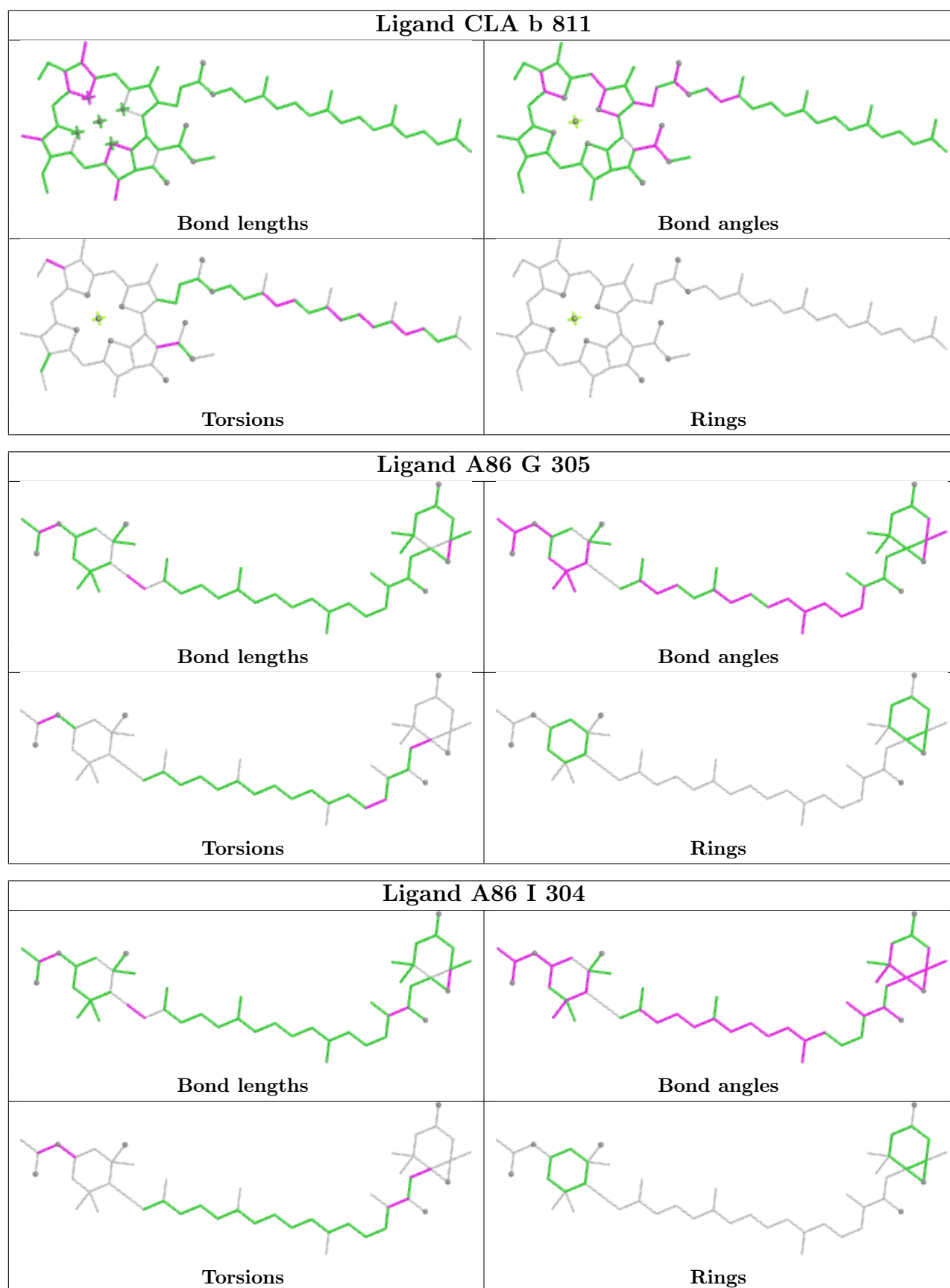
## Ligand CLA a 824

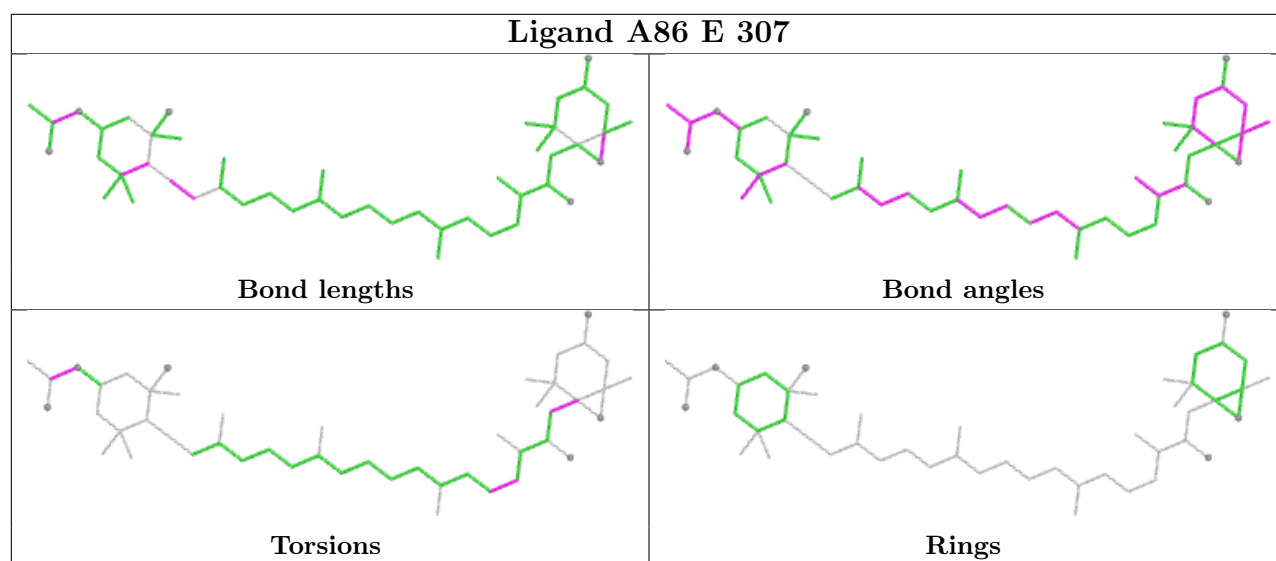
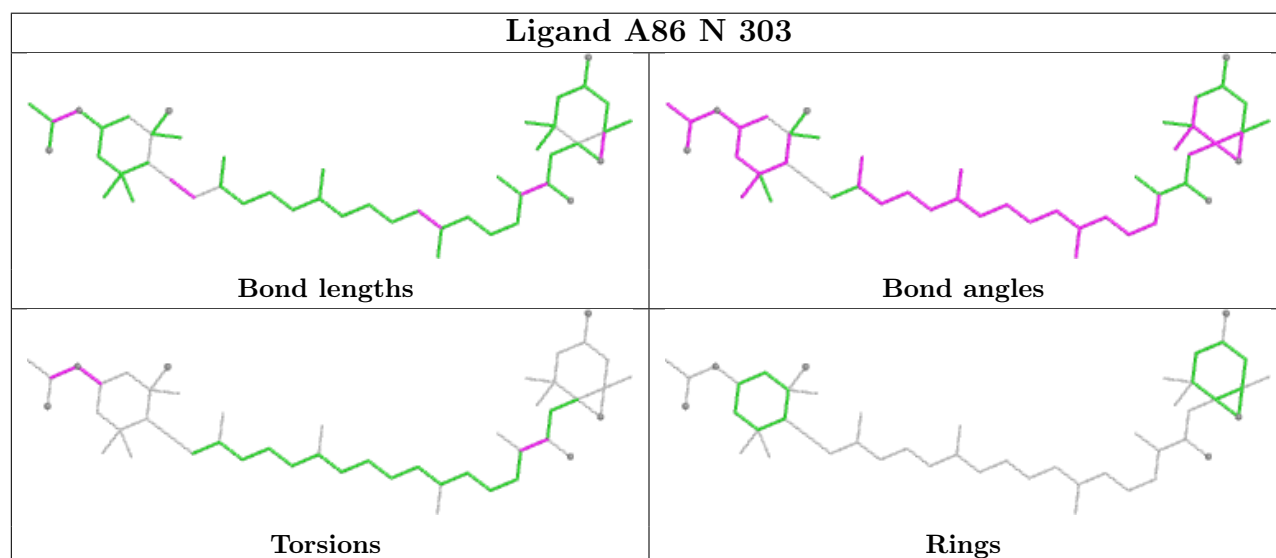
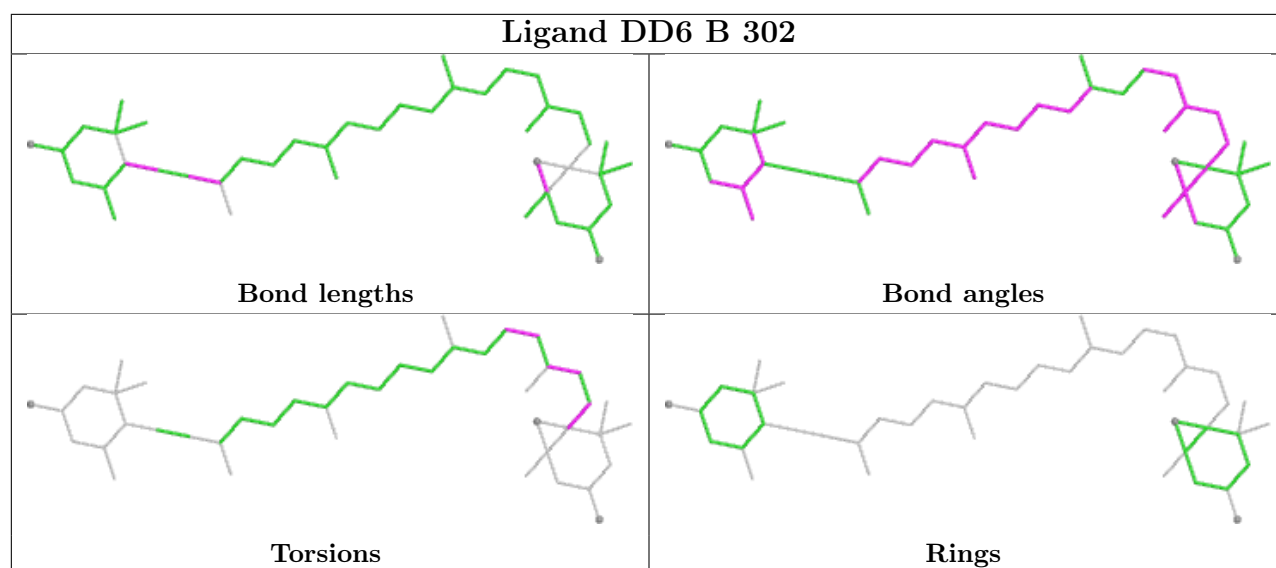


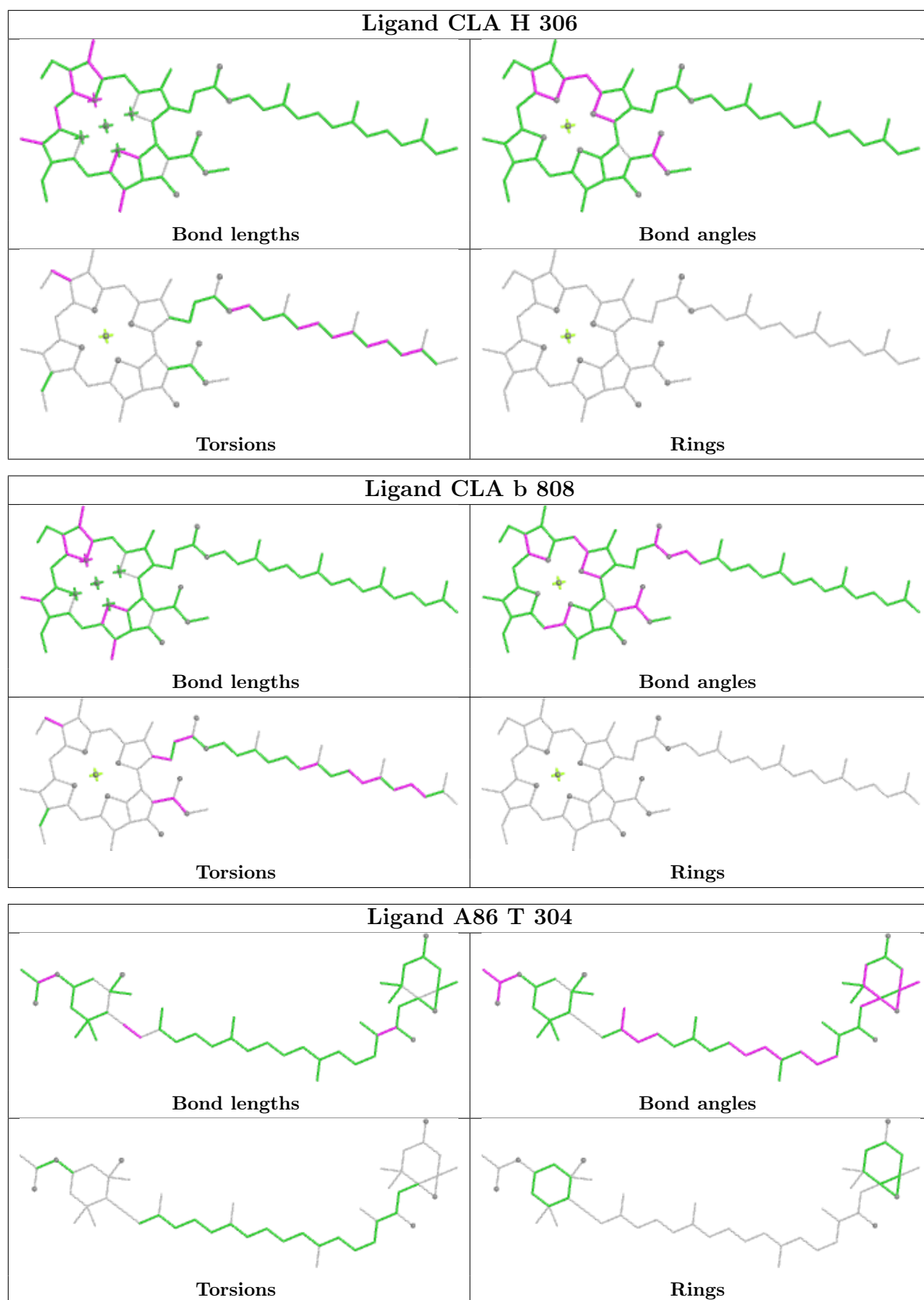
## Ligand BCR b 845





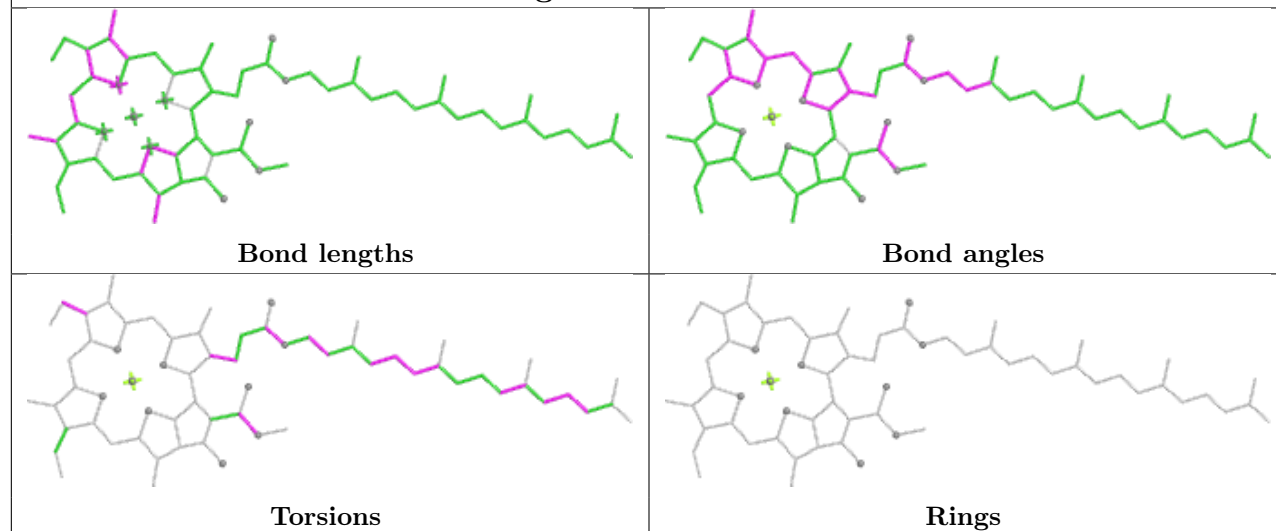




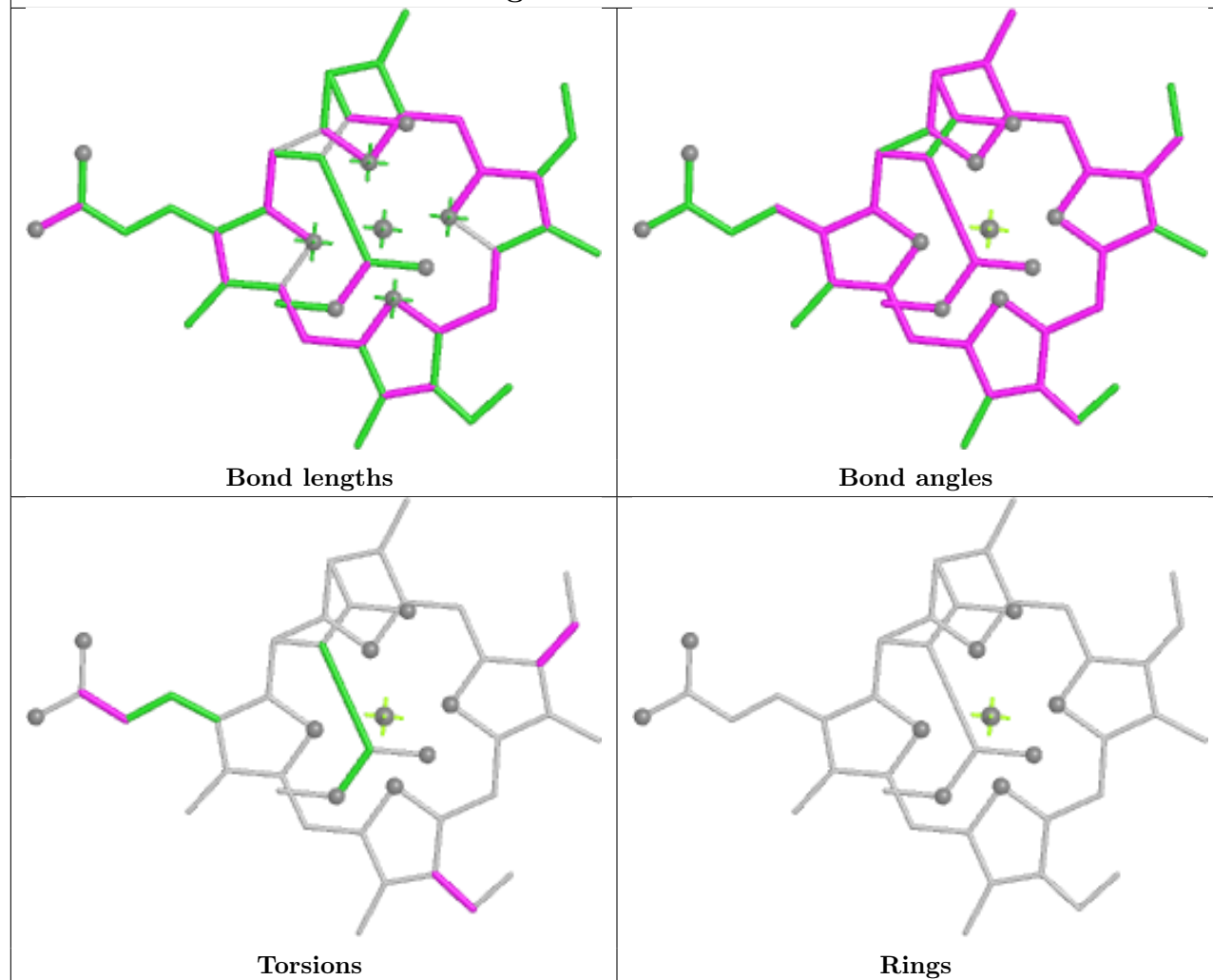


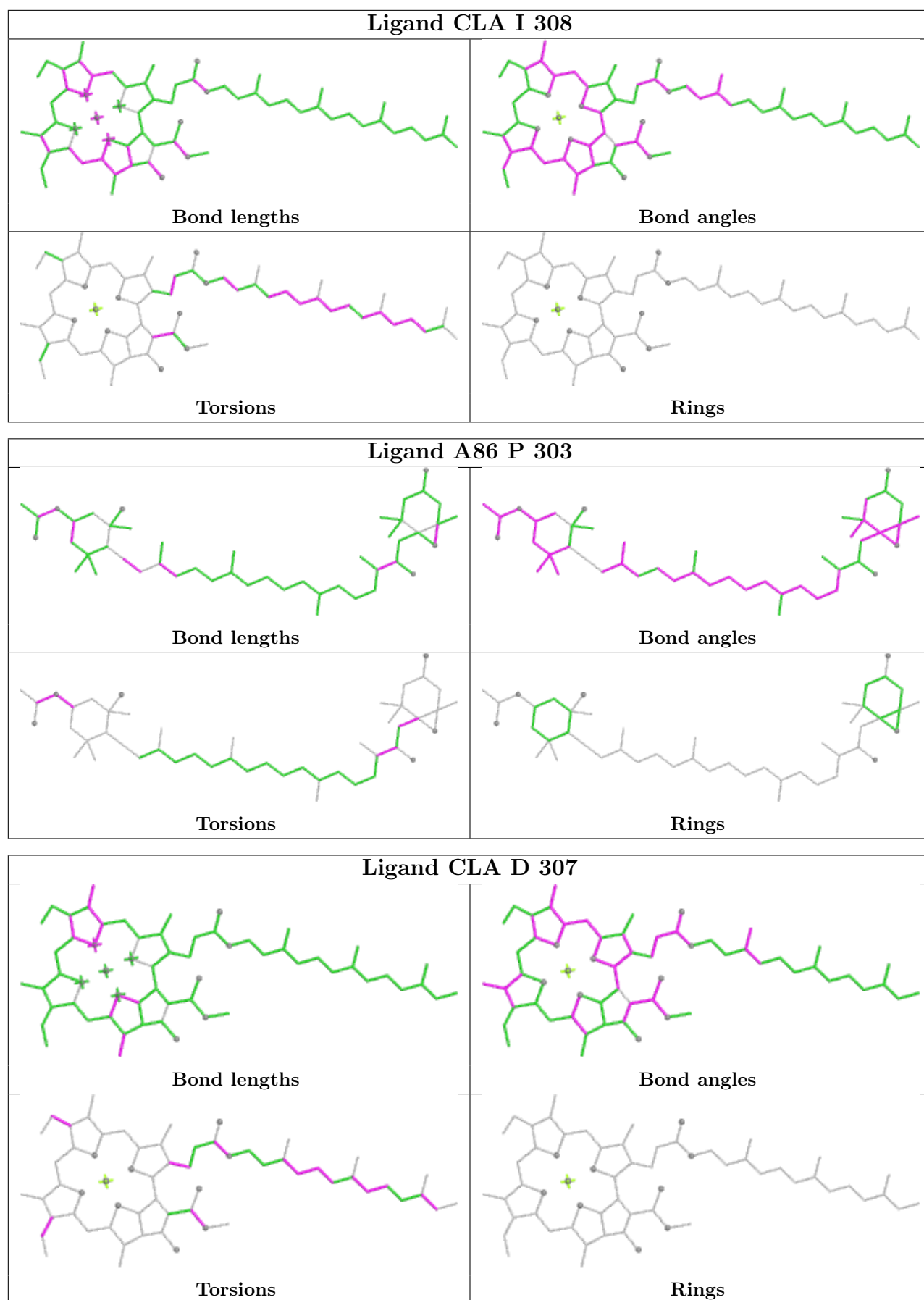


## Ligand CLA S 310

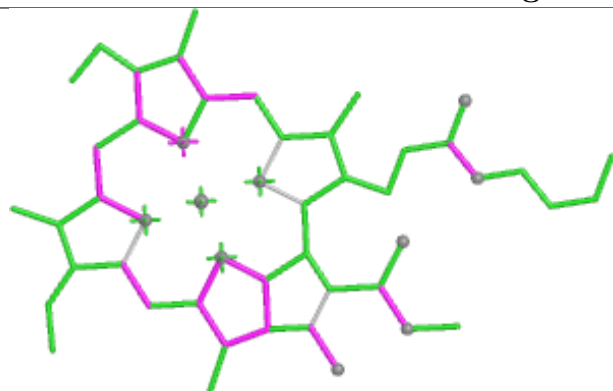


## Ligand KC1 G 308

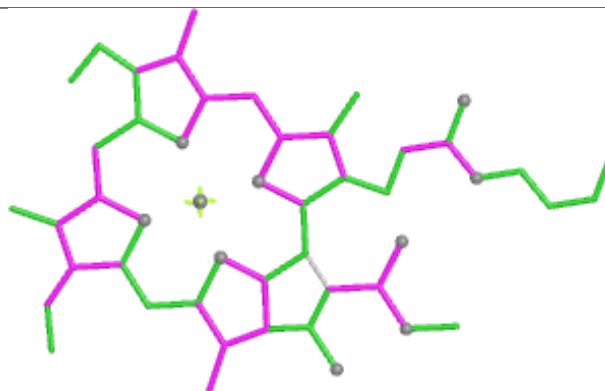




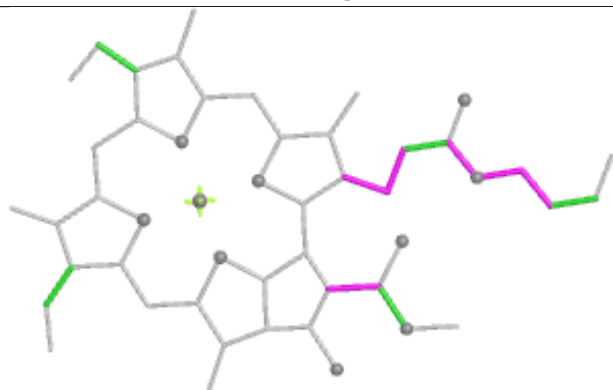
## Ligand CLA I 204



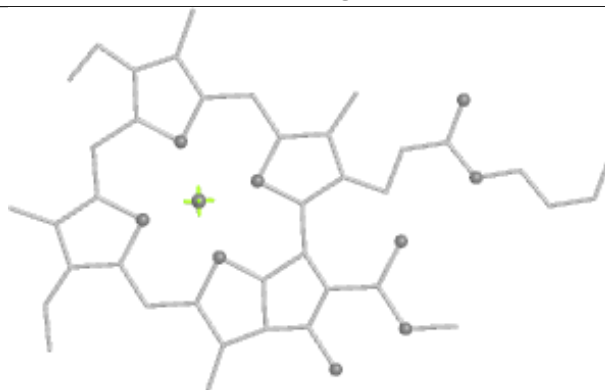
Bond lengths



Bond angles

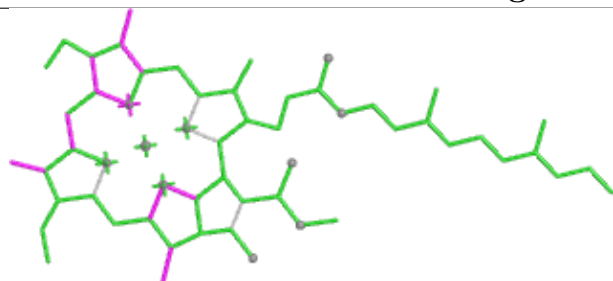


Torsions

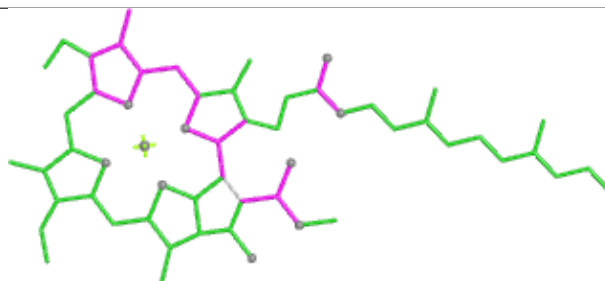


Rings

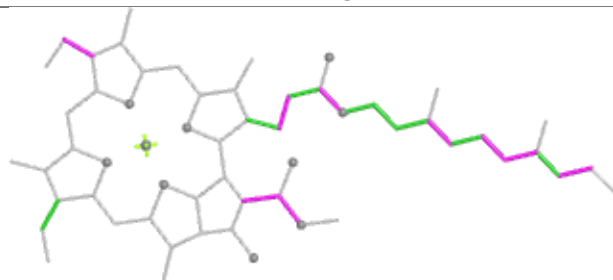
## Ligand CLA W 209



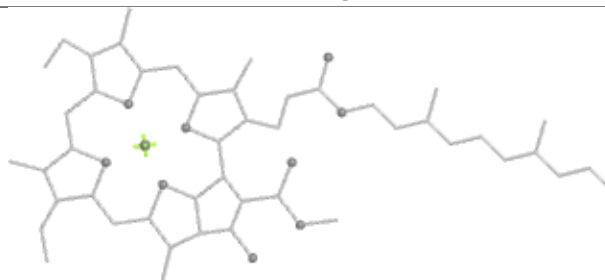
Bond lengths



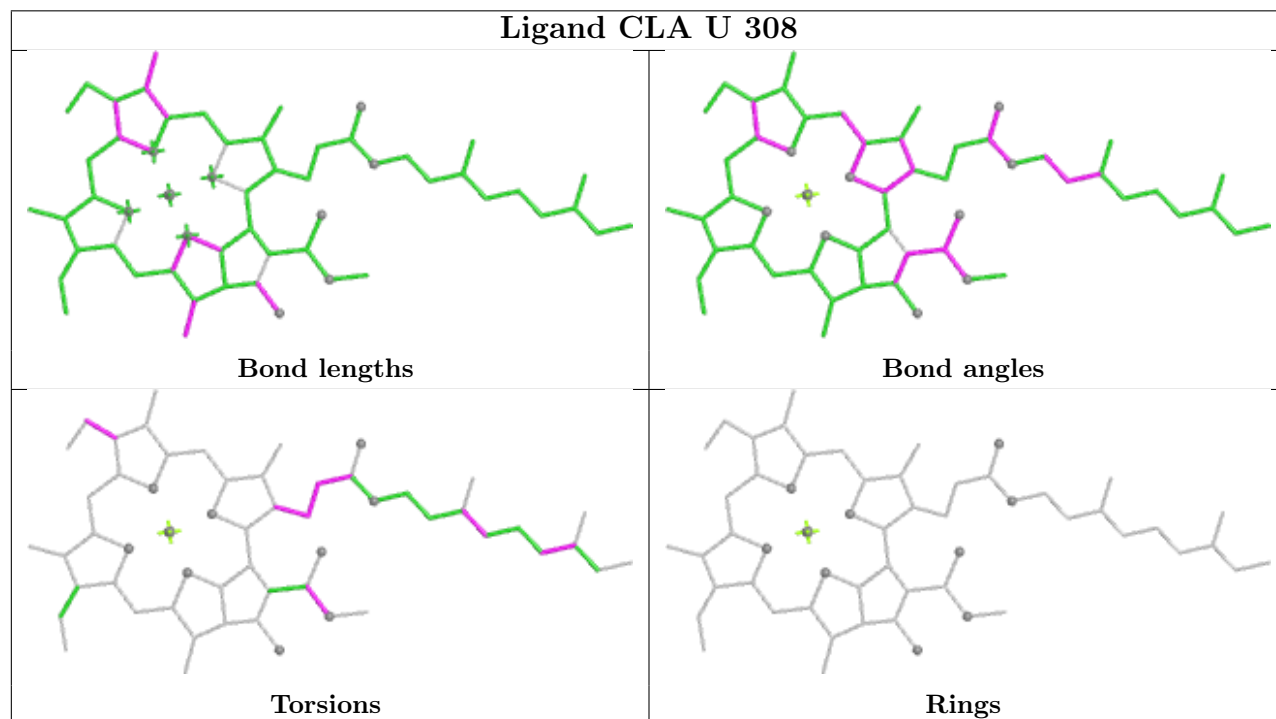
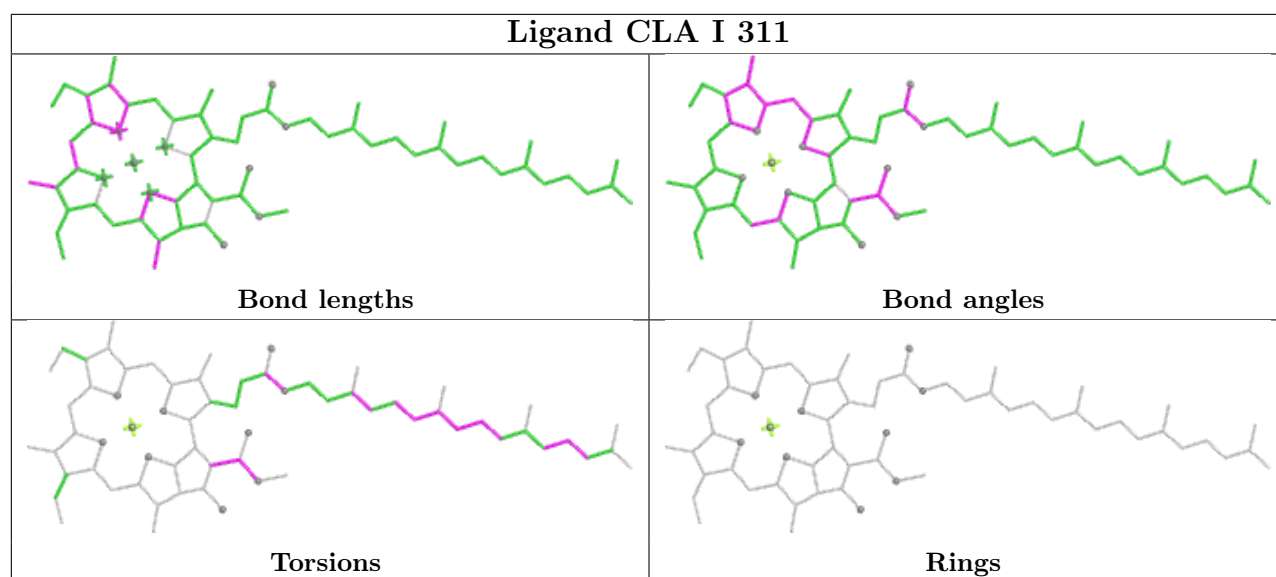
Bond angles

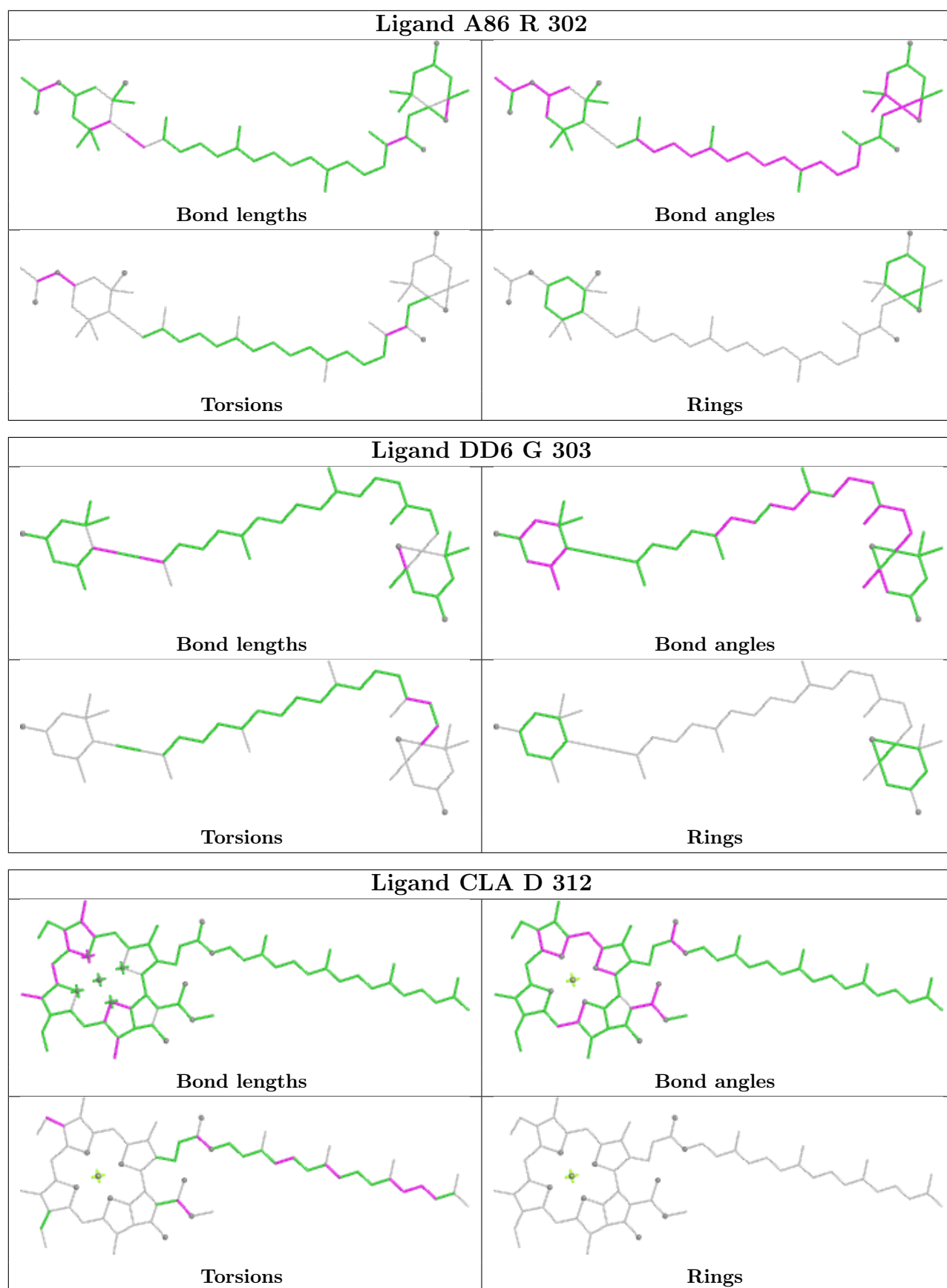


Torsions

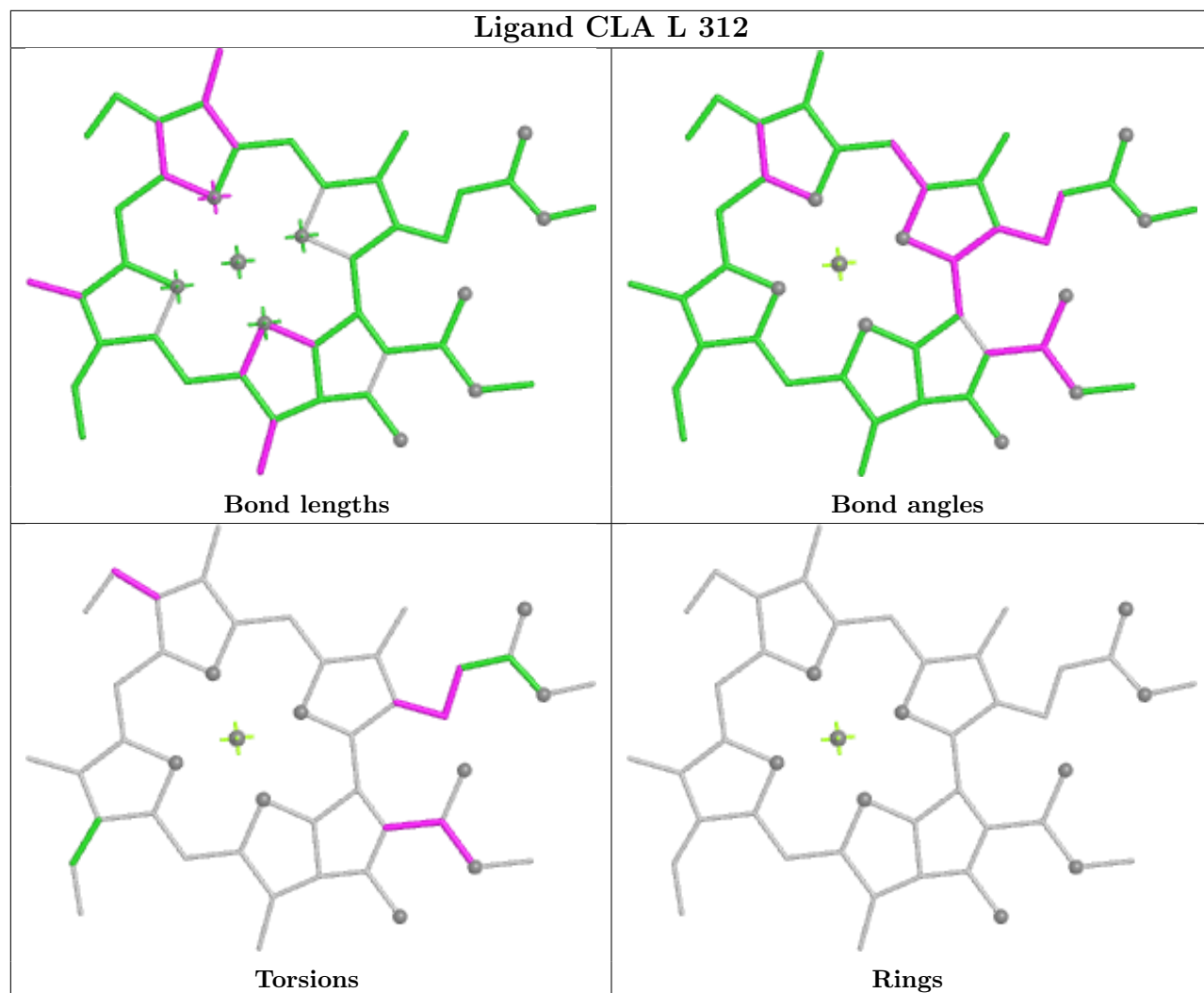


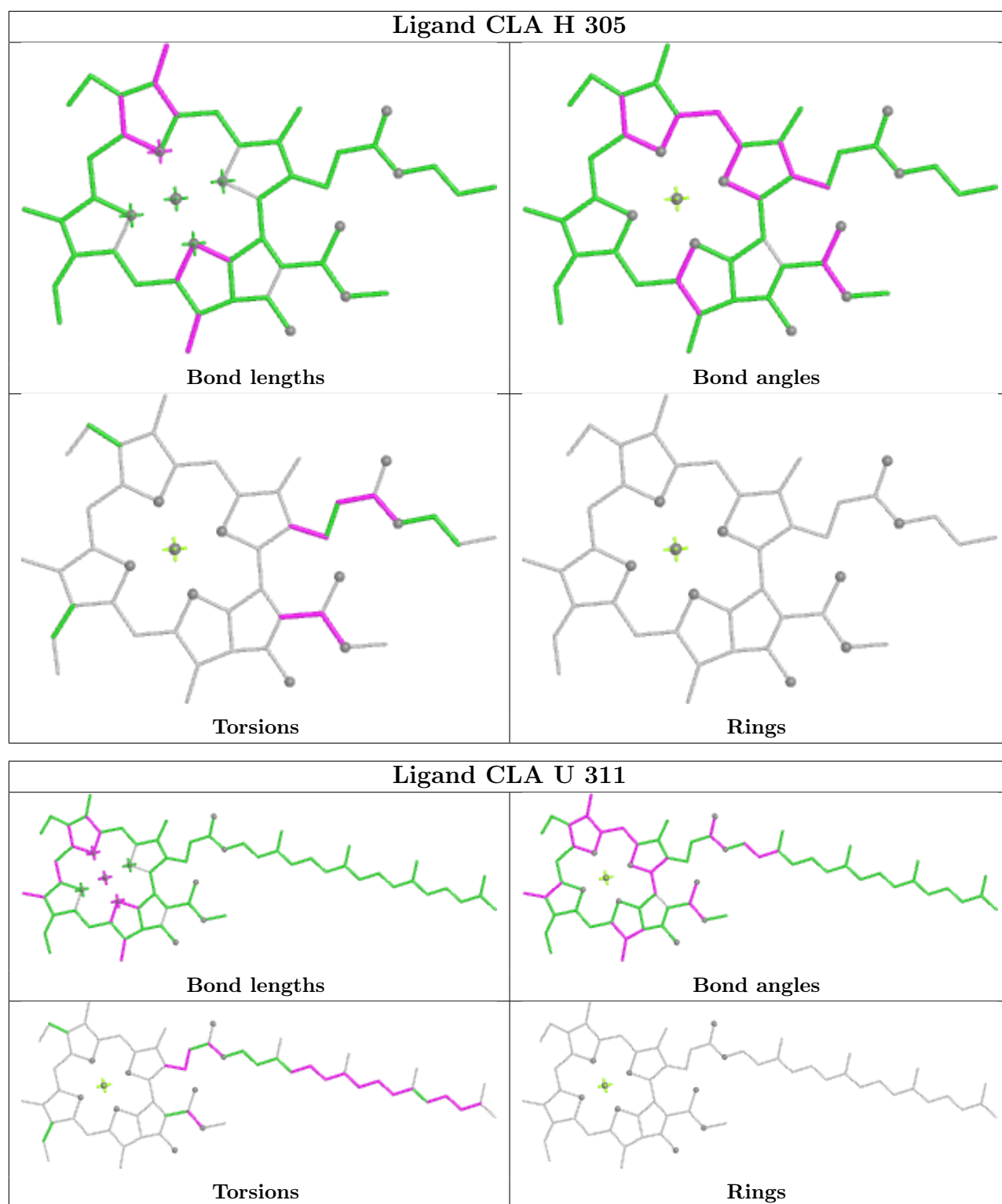
Rings

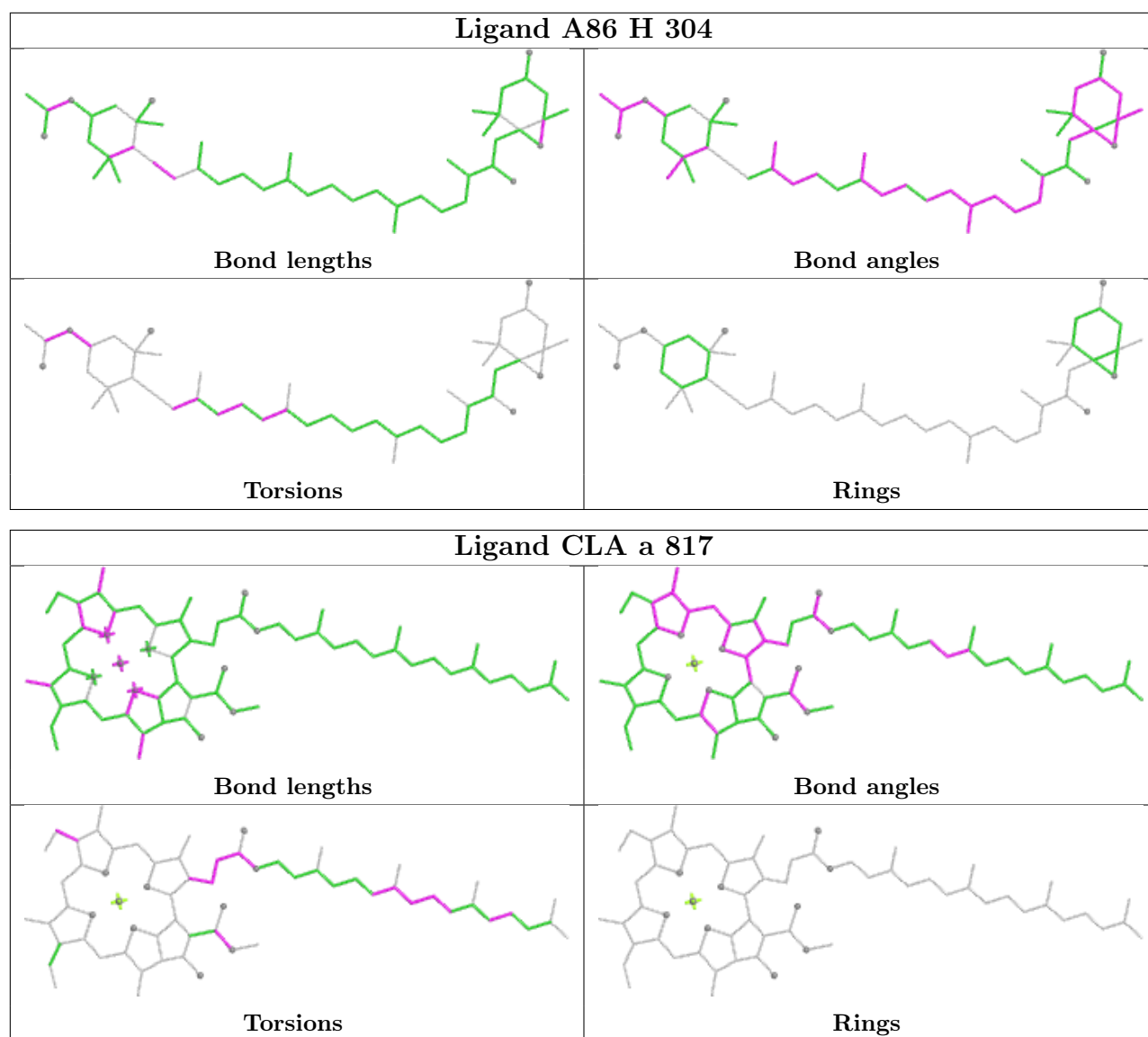




## Ligand CLA L 312

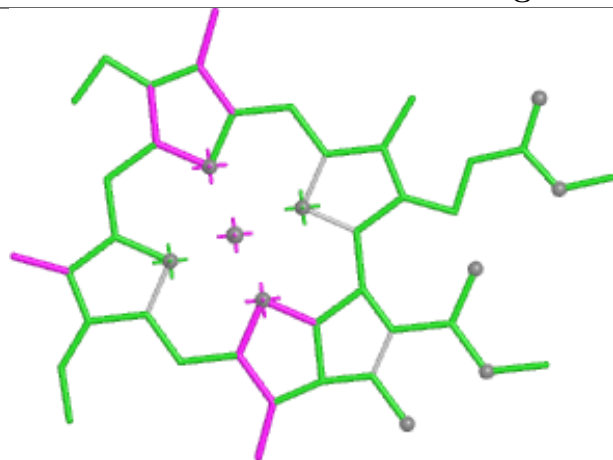




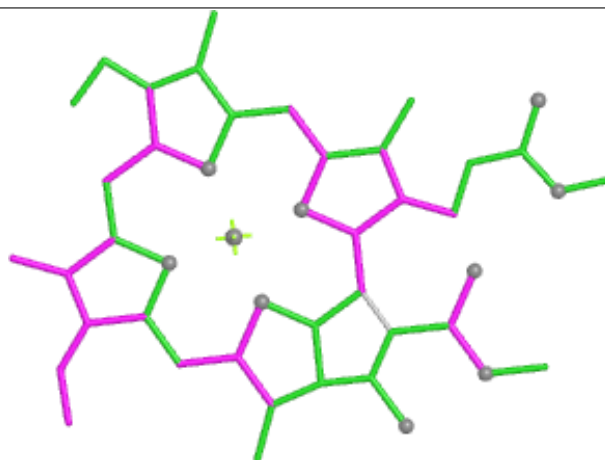




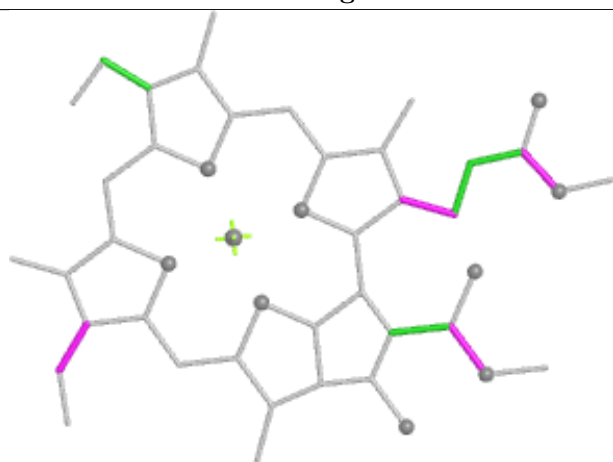
## Ligand CLA R 316



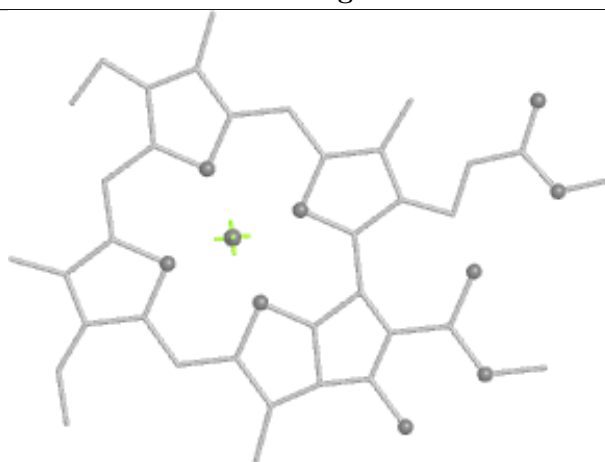
Bond lengths



Bond angles

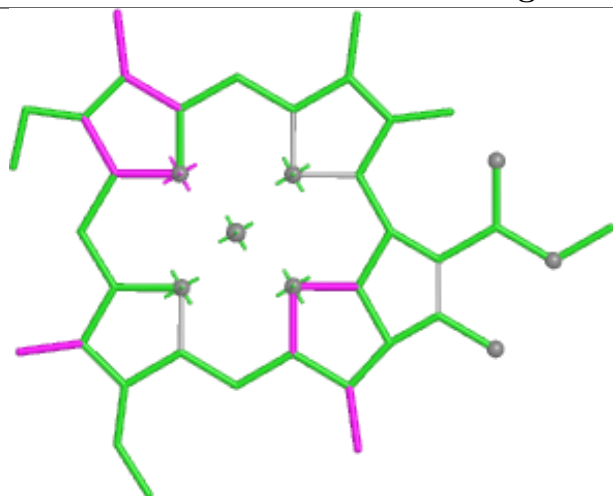


Torsions

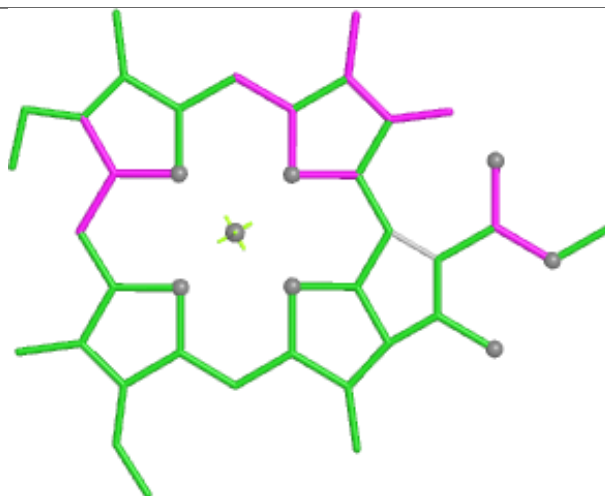


Rings

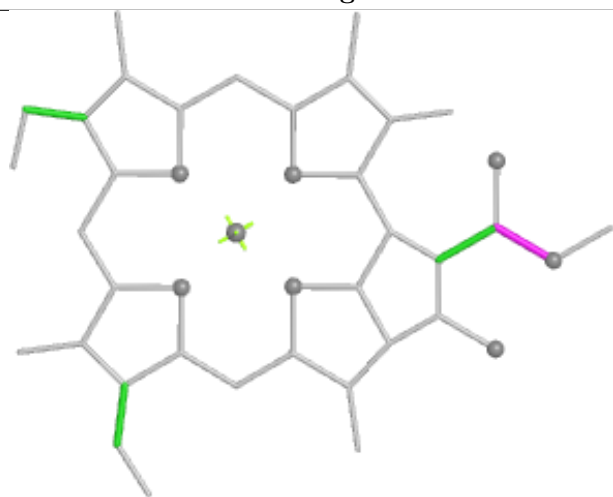
## Ligand CLA J 315



Bond lengths



Bond angles

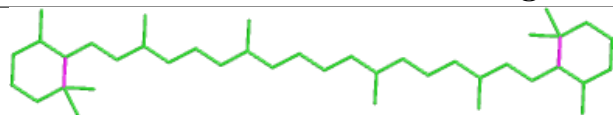


Torsions

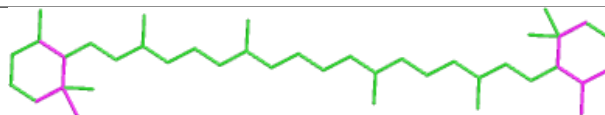


Rings

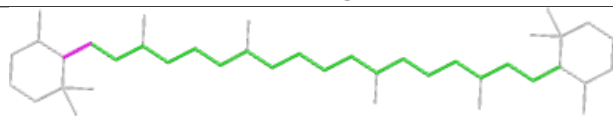
## Ligand BCR i 101



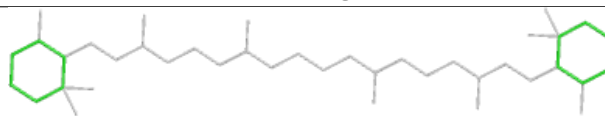
Bond lengths



Bond angles

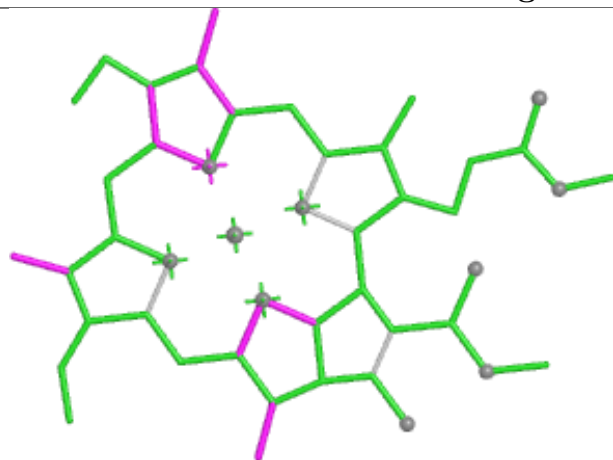


Torsions

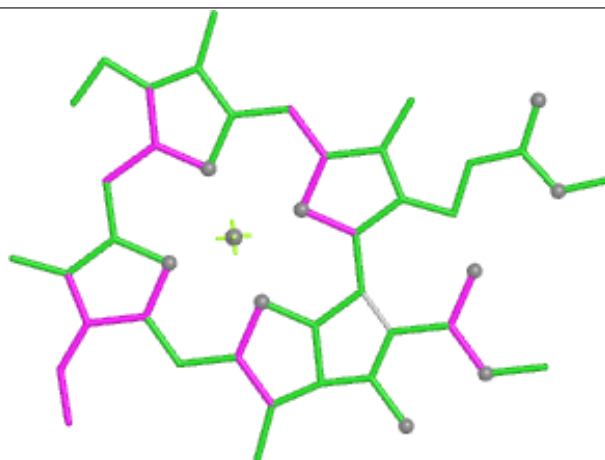


Rings

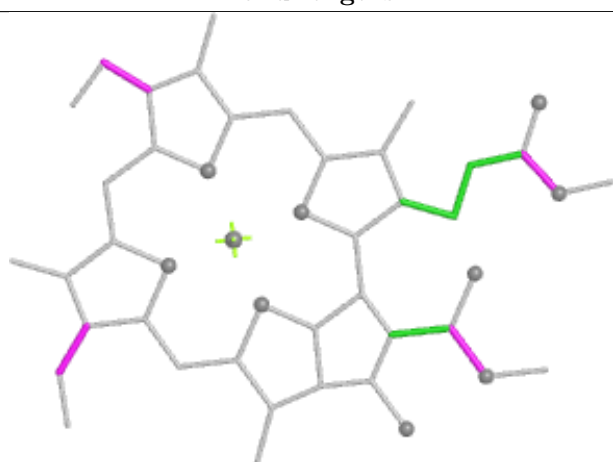
## Ligand CLA J 316



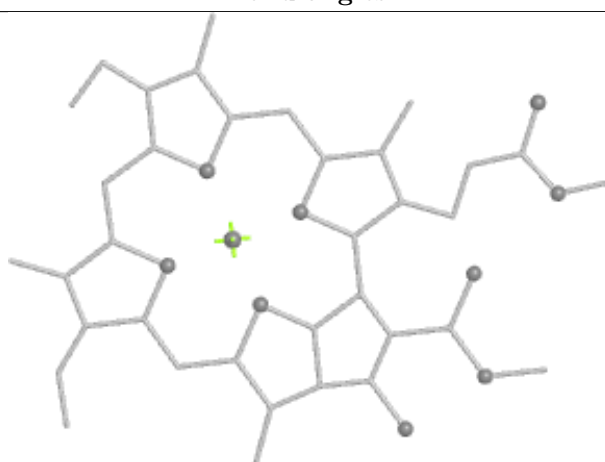
Bond lengths



Bond angles

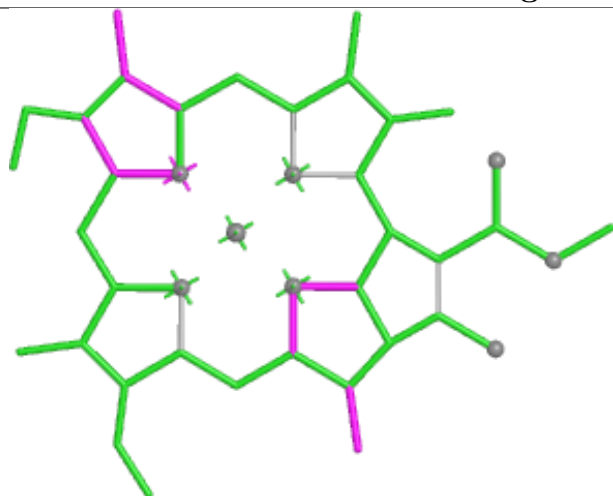


Torsions

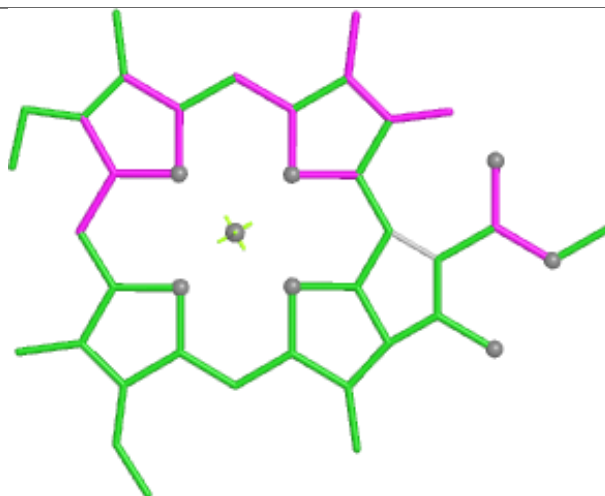


Rings

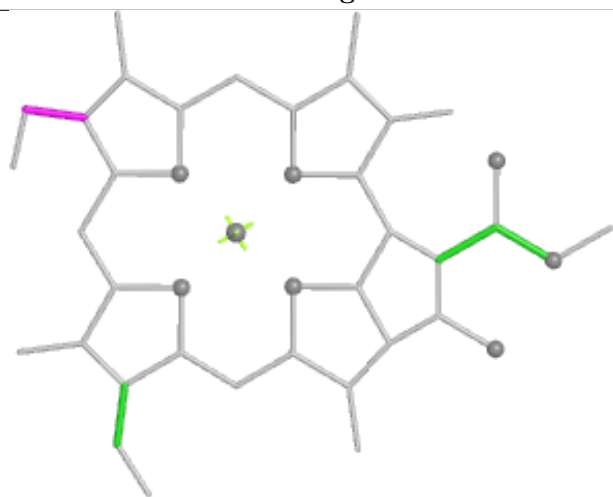
## Ligand CLA I 314



Bond lengths



Bond angles

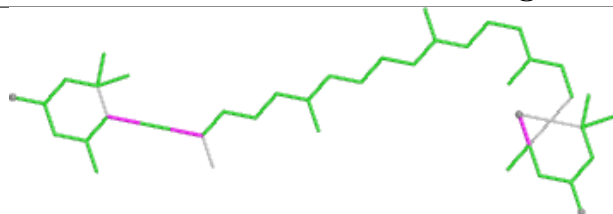


Torsions

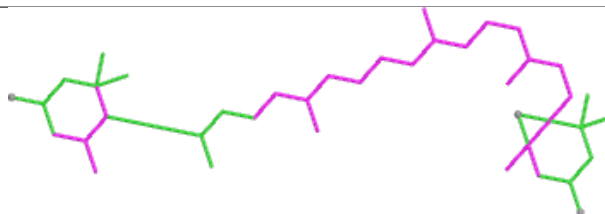


Rings

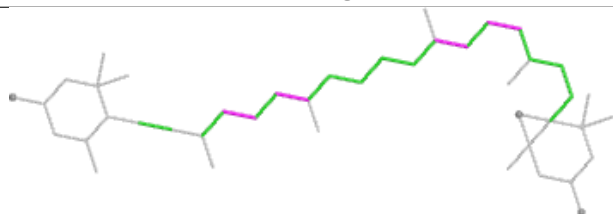
## Ligand DD6 S 307



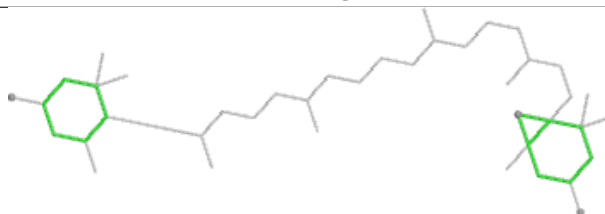
Bond lengths



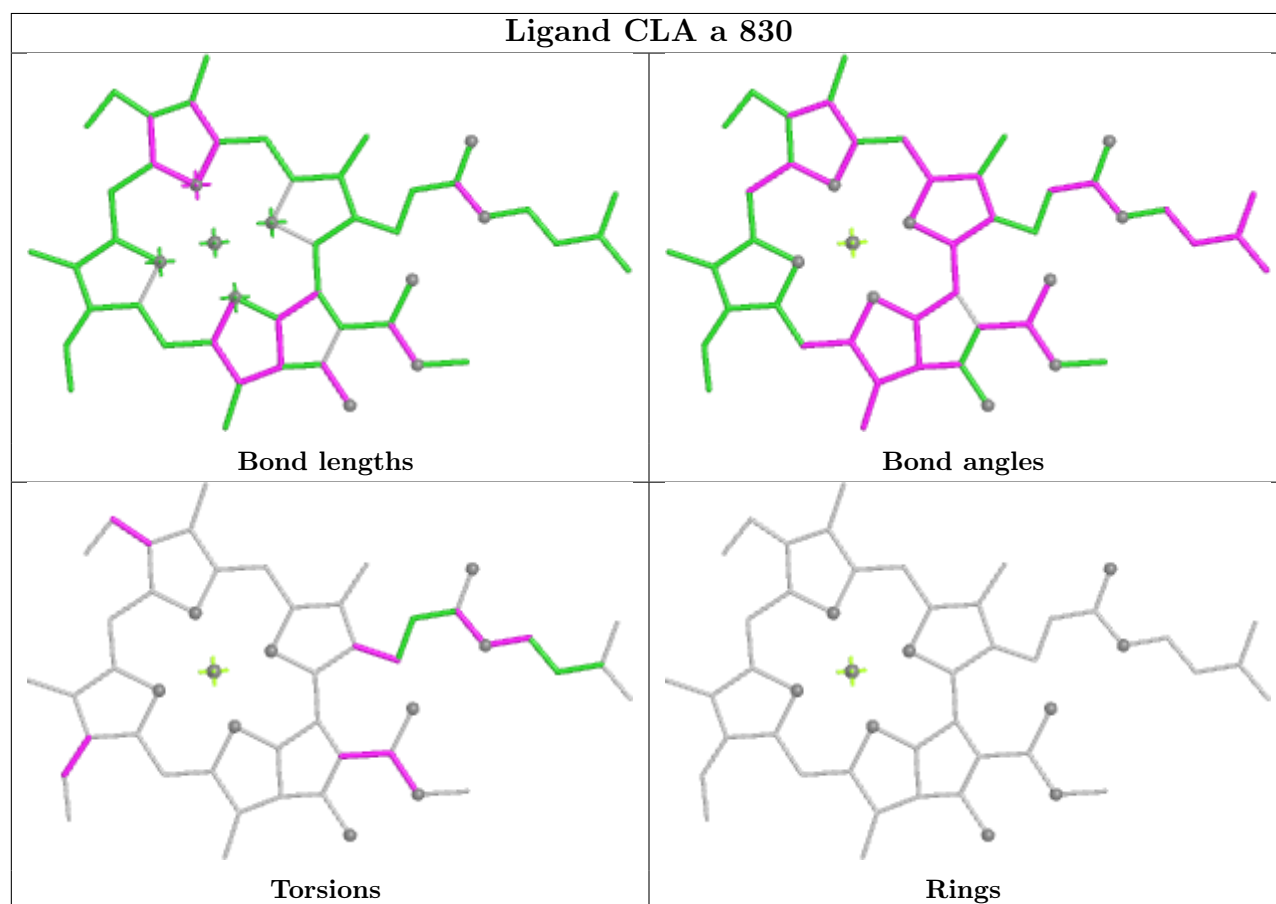
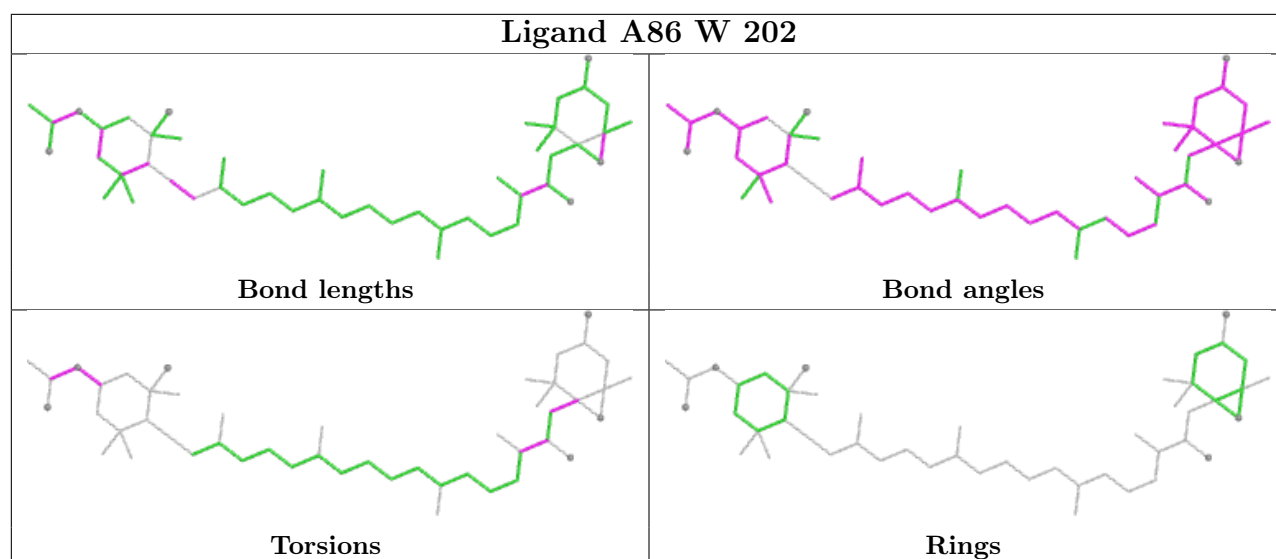
Bond angles

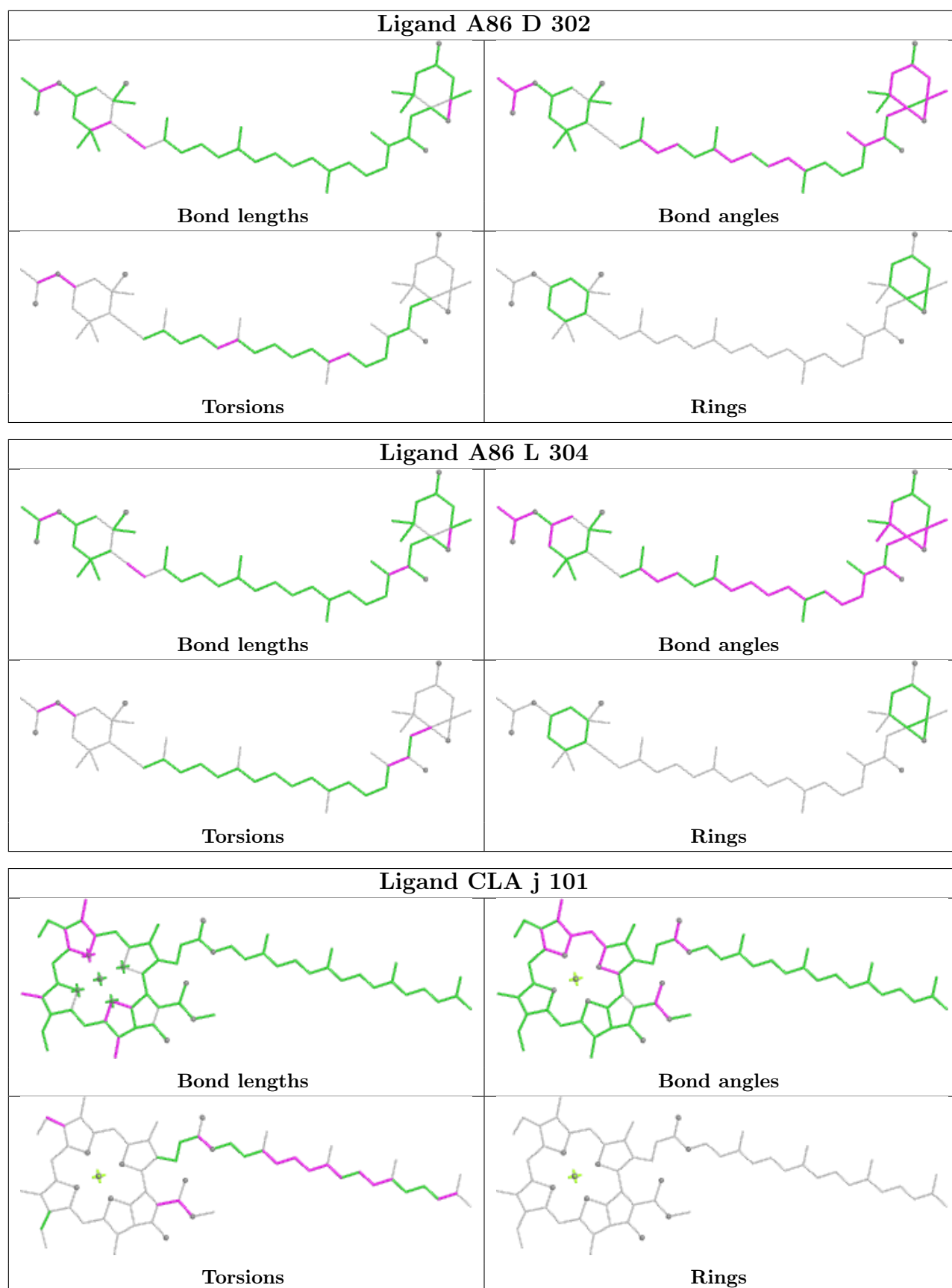


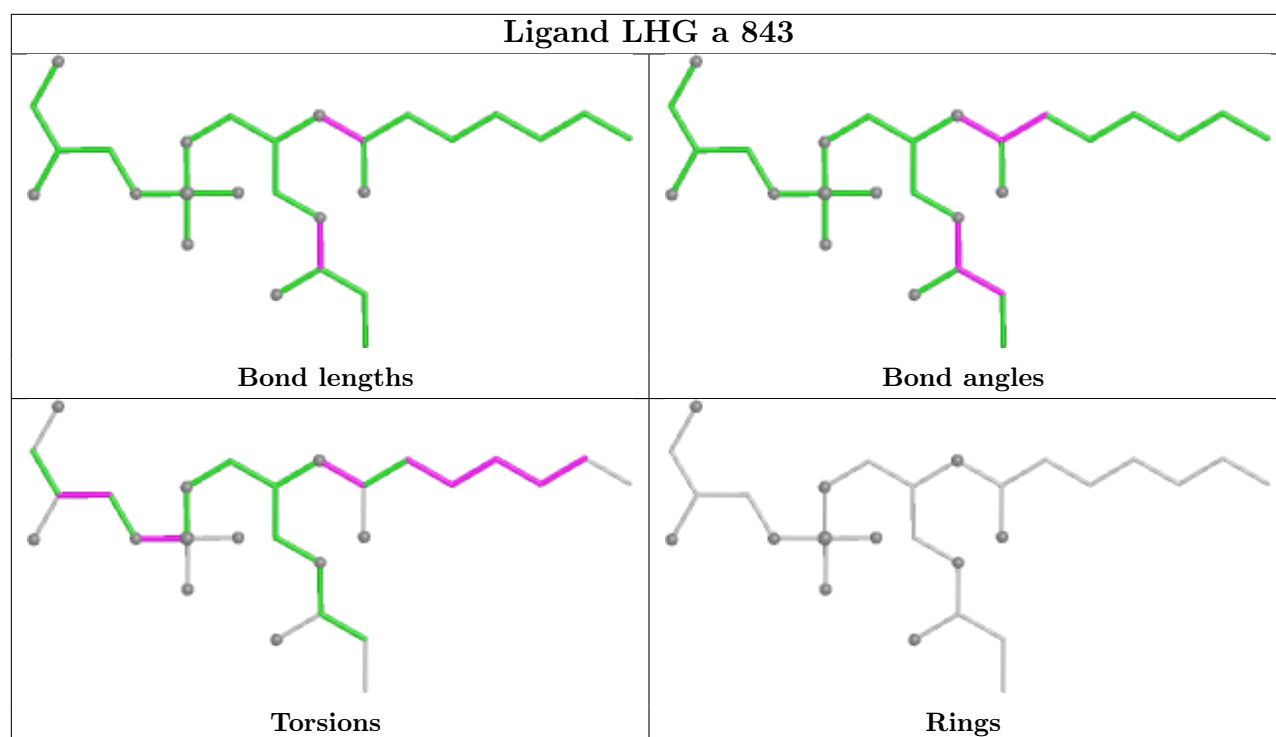
Torsions

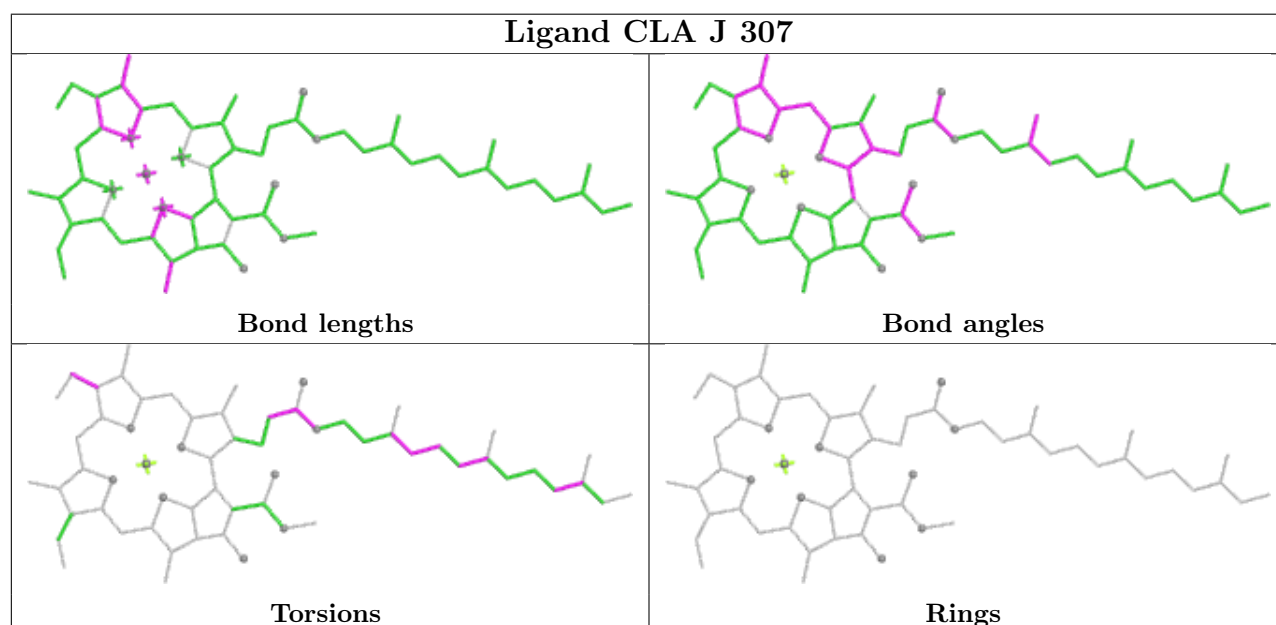
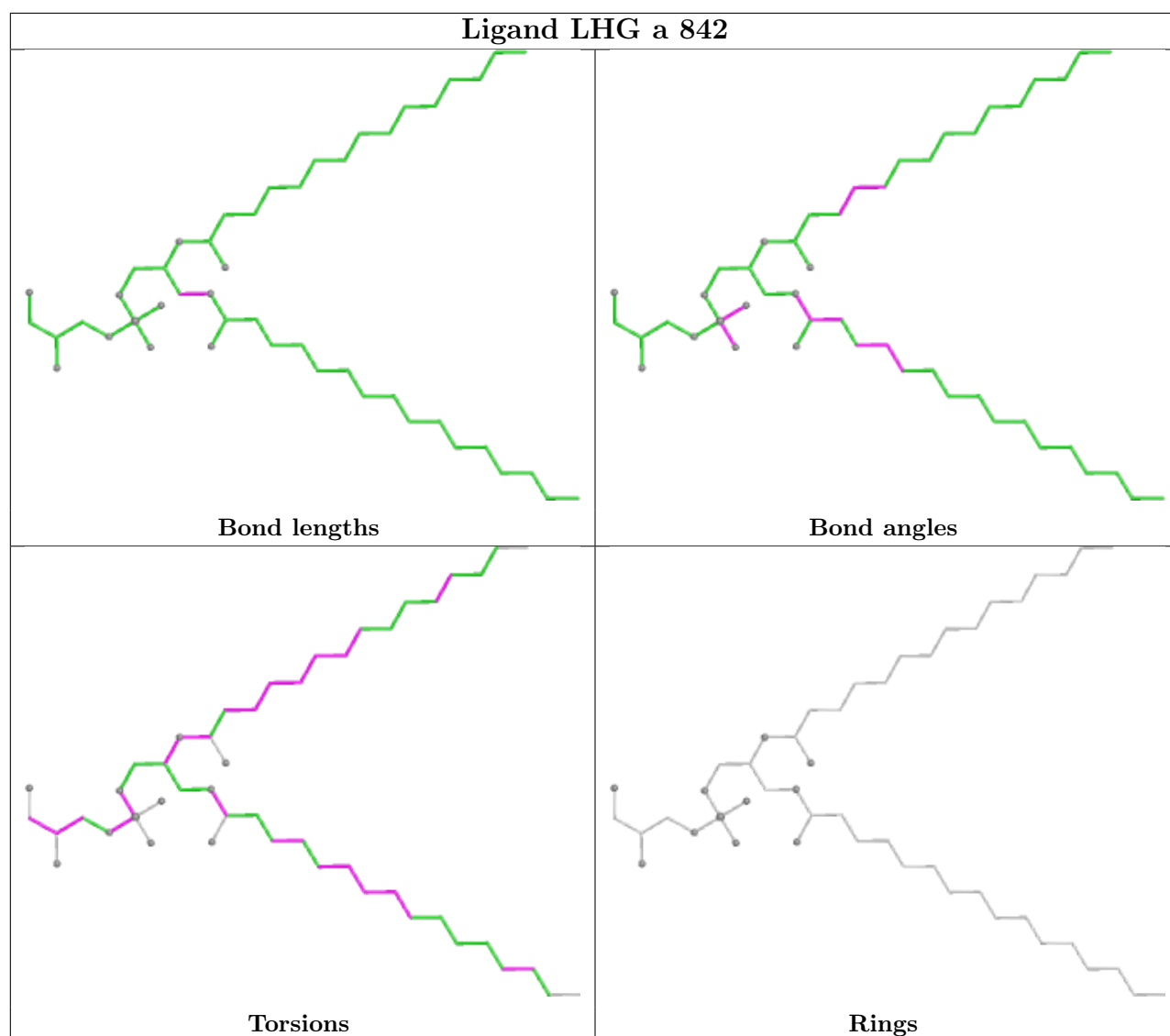


Rings



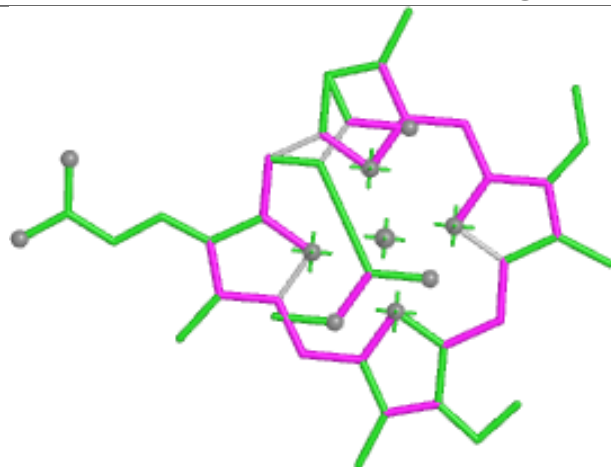




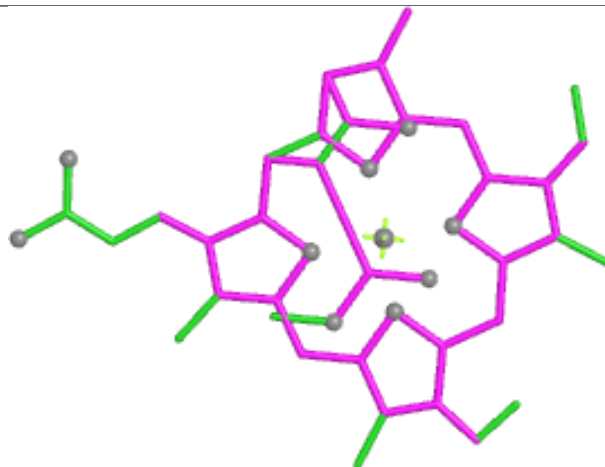




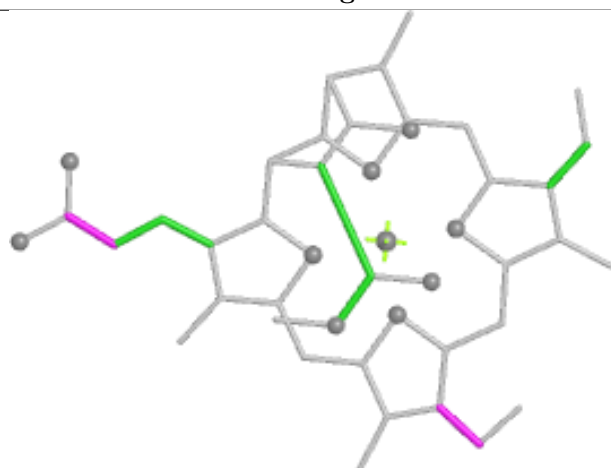
## Ligand KC1 B 310



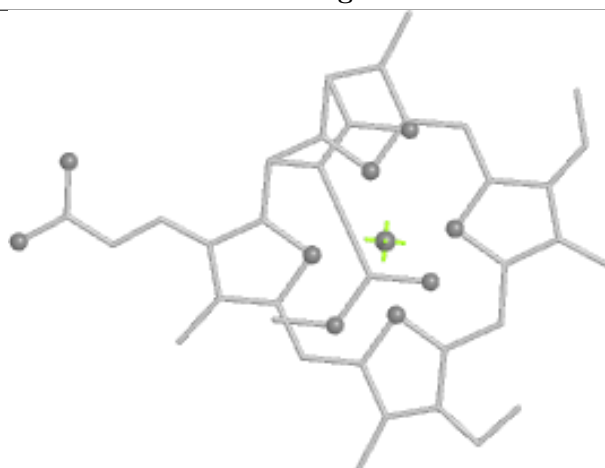
Bond lengths



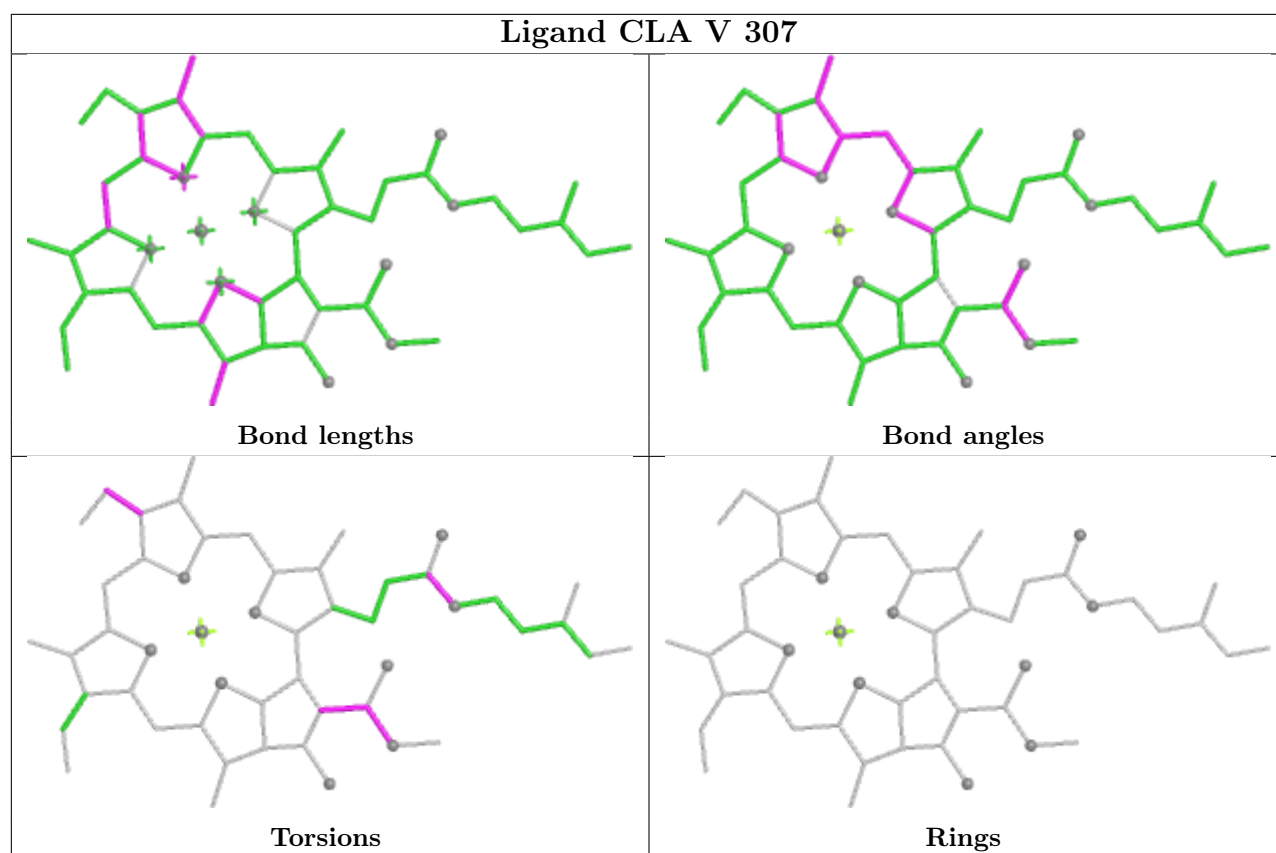
Bond angles



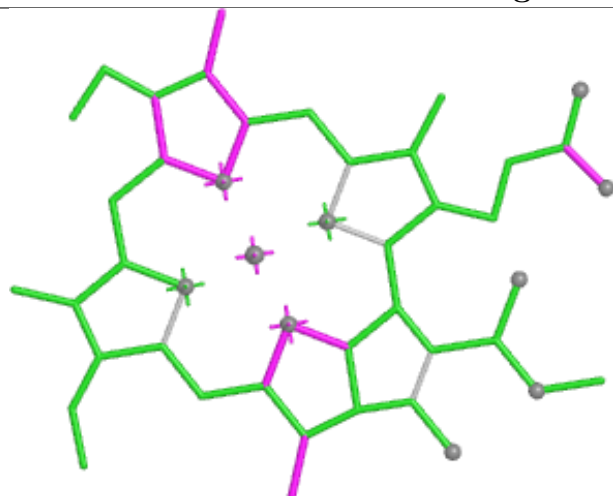
Torsions



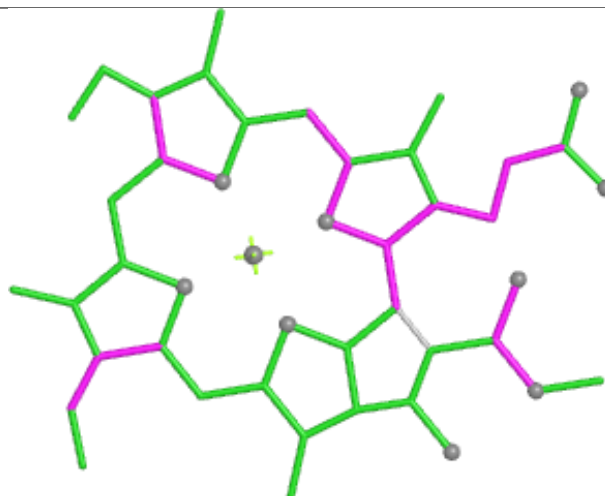
Rings



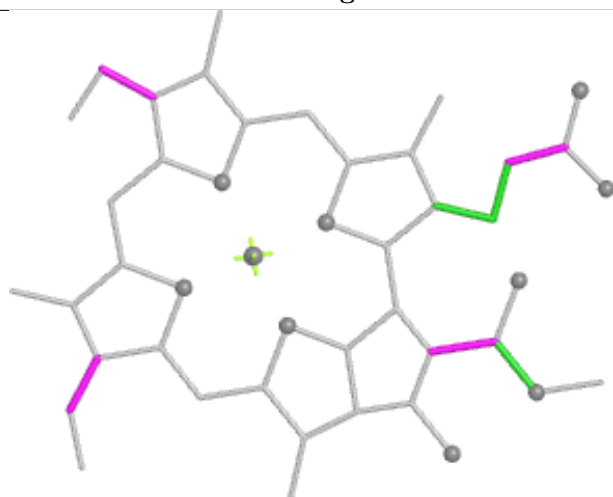
## Ligand CLA D 306



Bond lengths



Bond angles

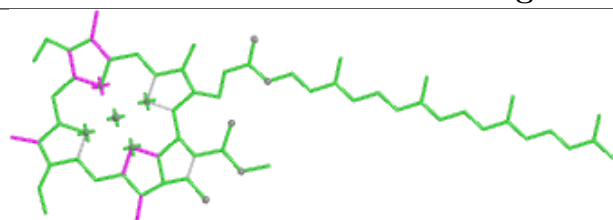


Torsions

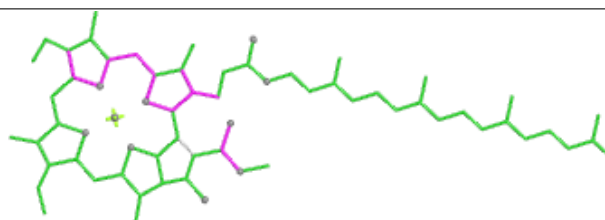


Rings

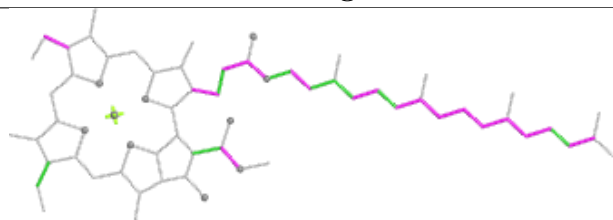
## Ligand CLA F 312



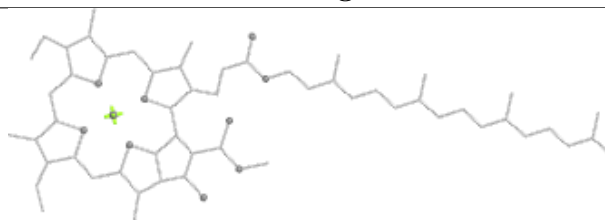
Bond lengths



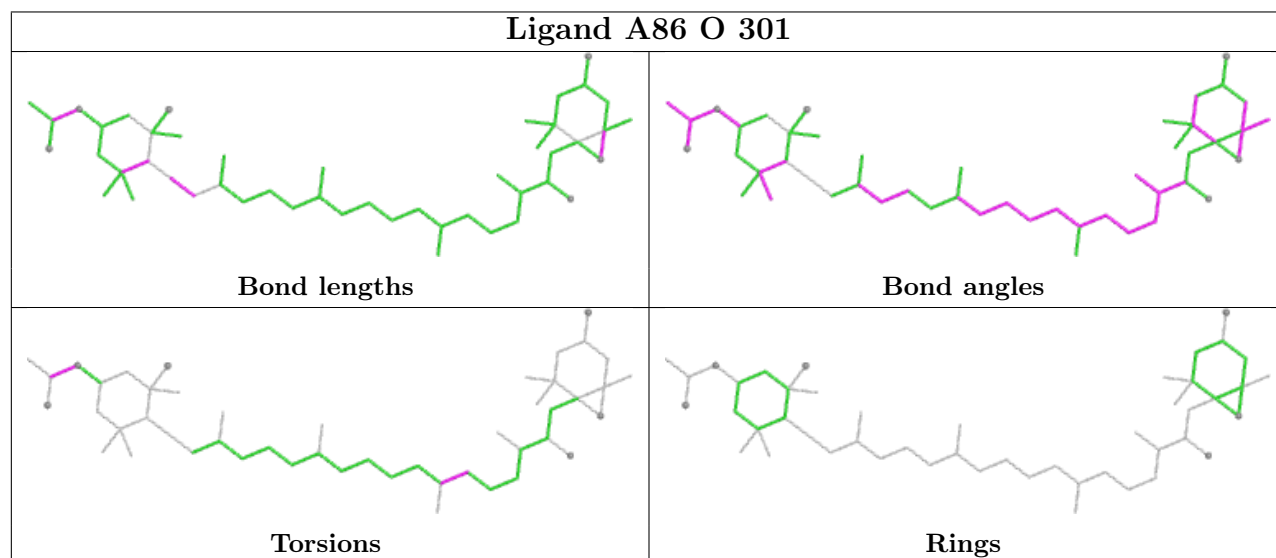
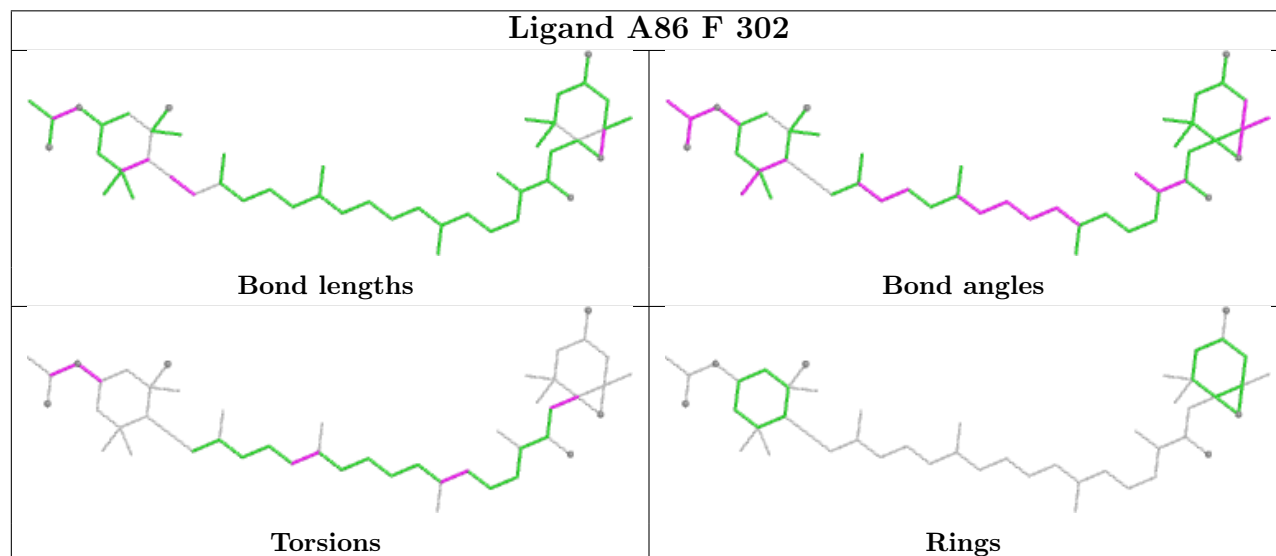
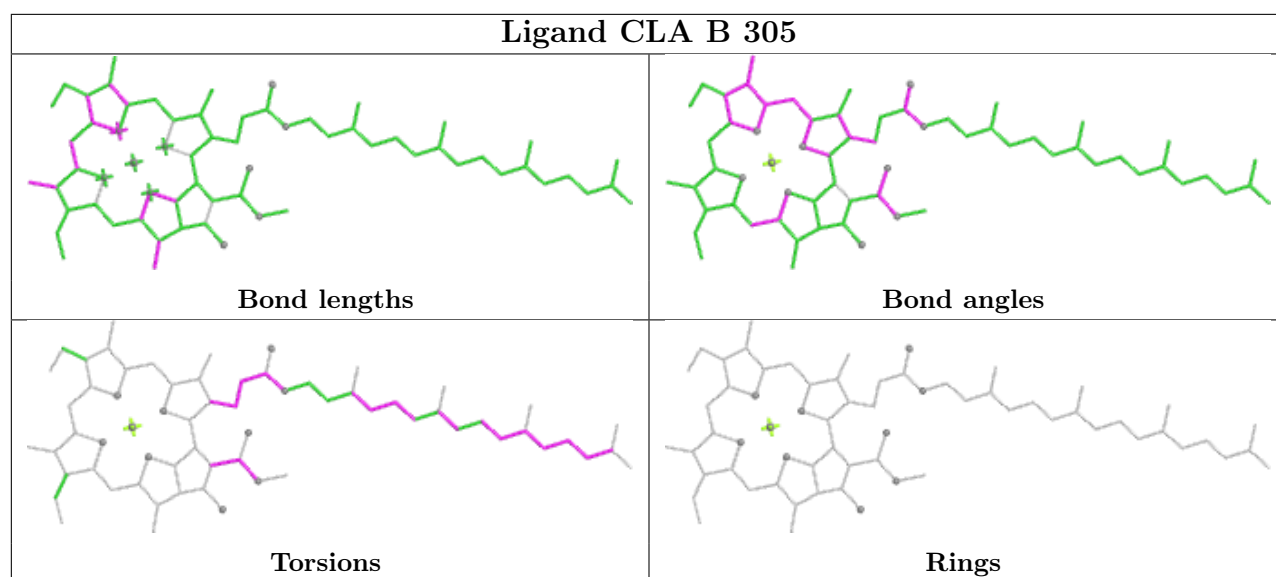
Bond angles

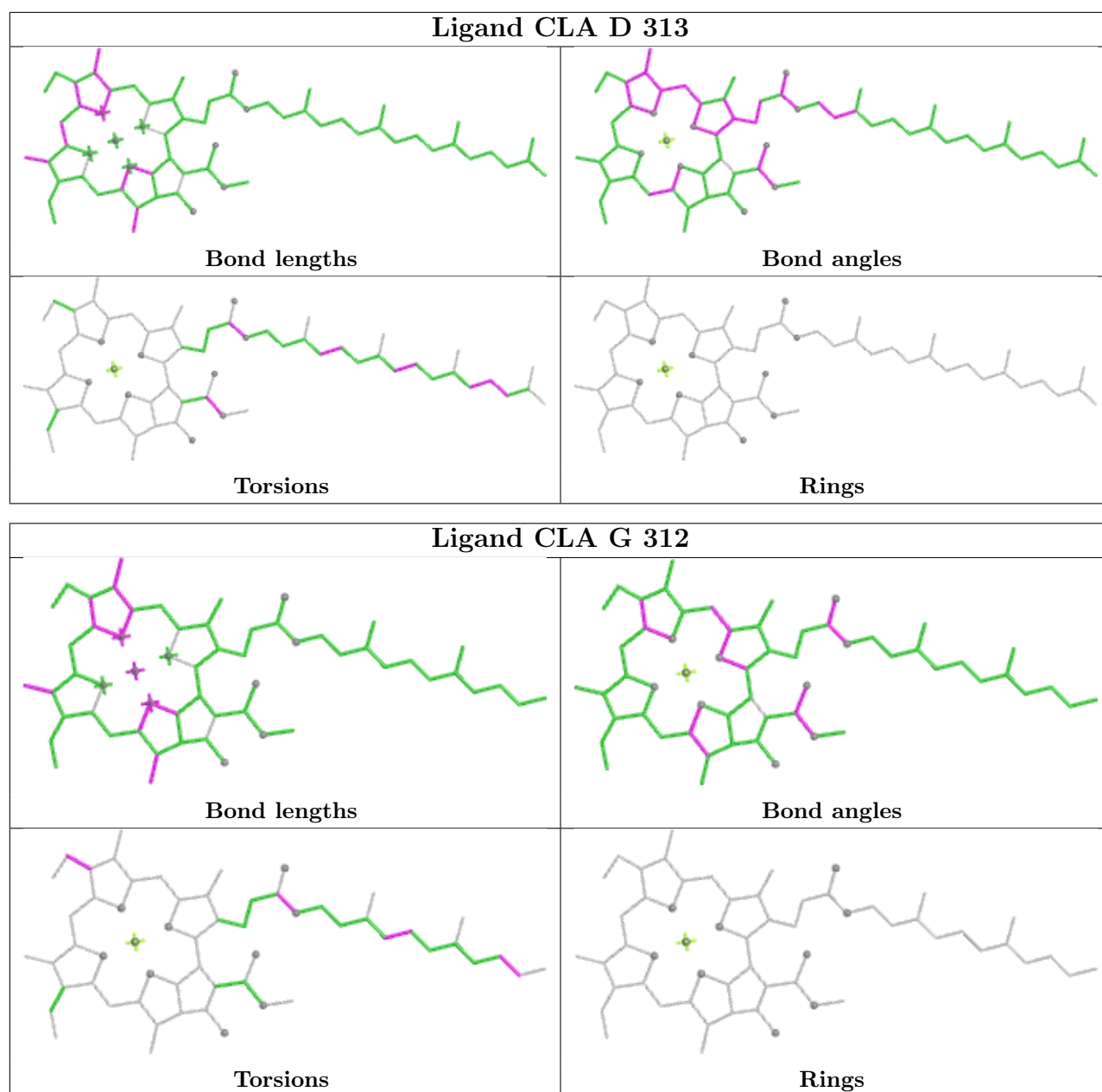


Torsions

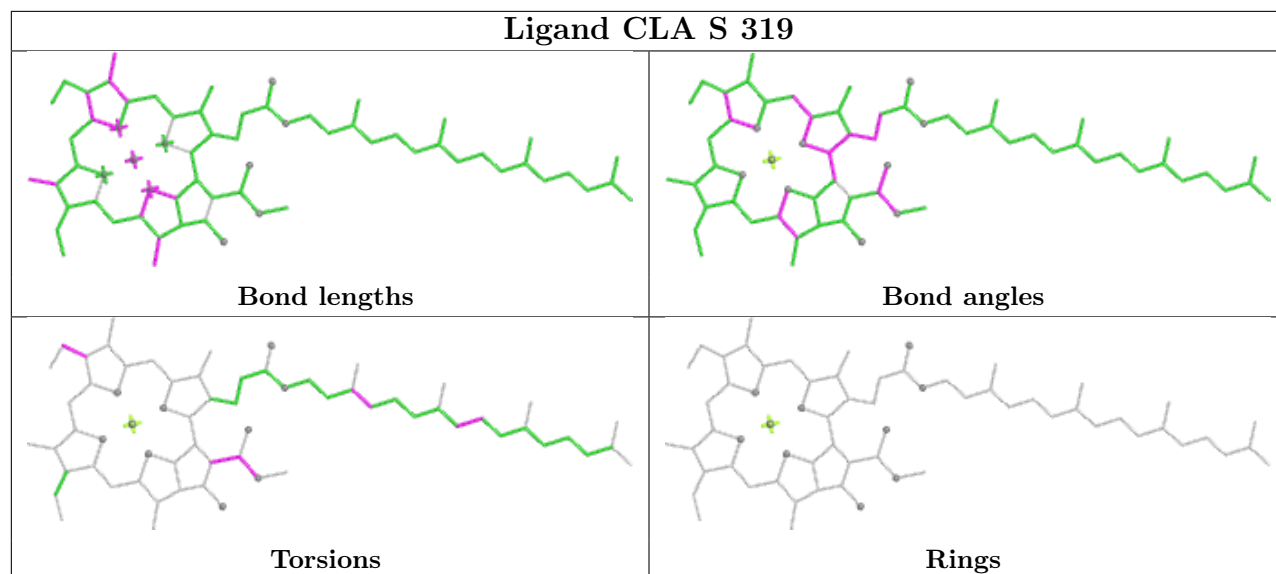


Rings

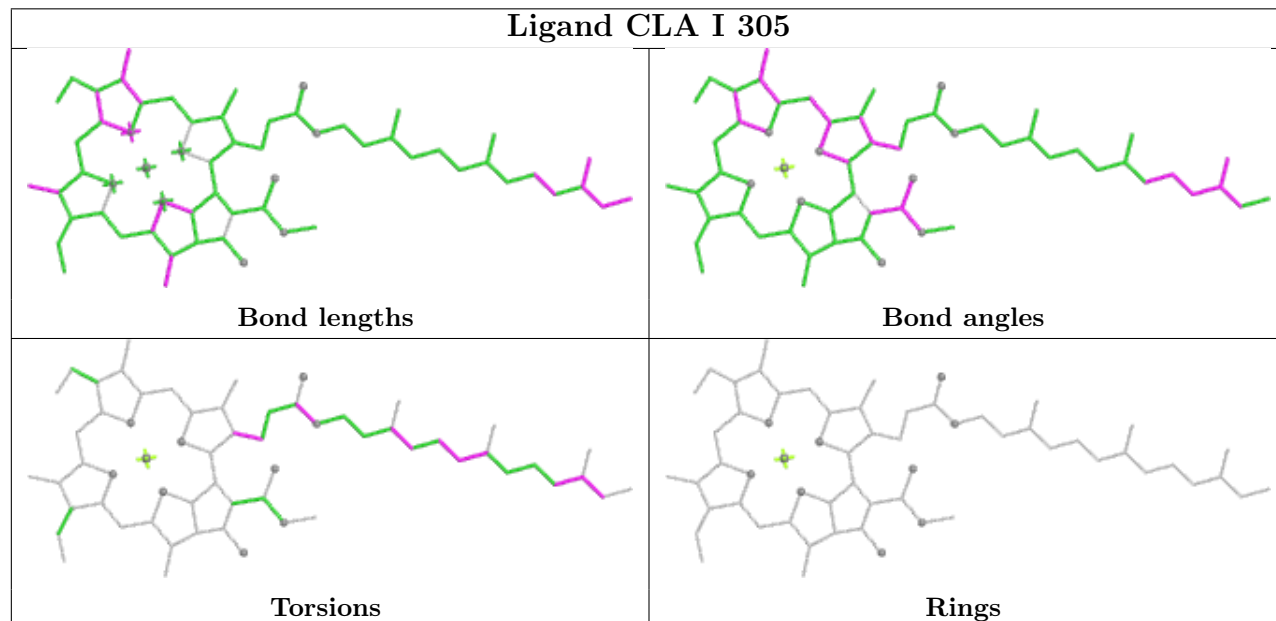




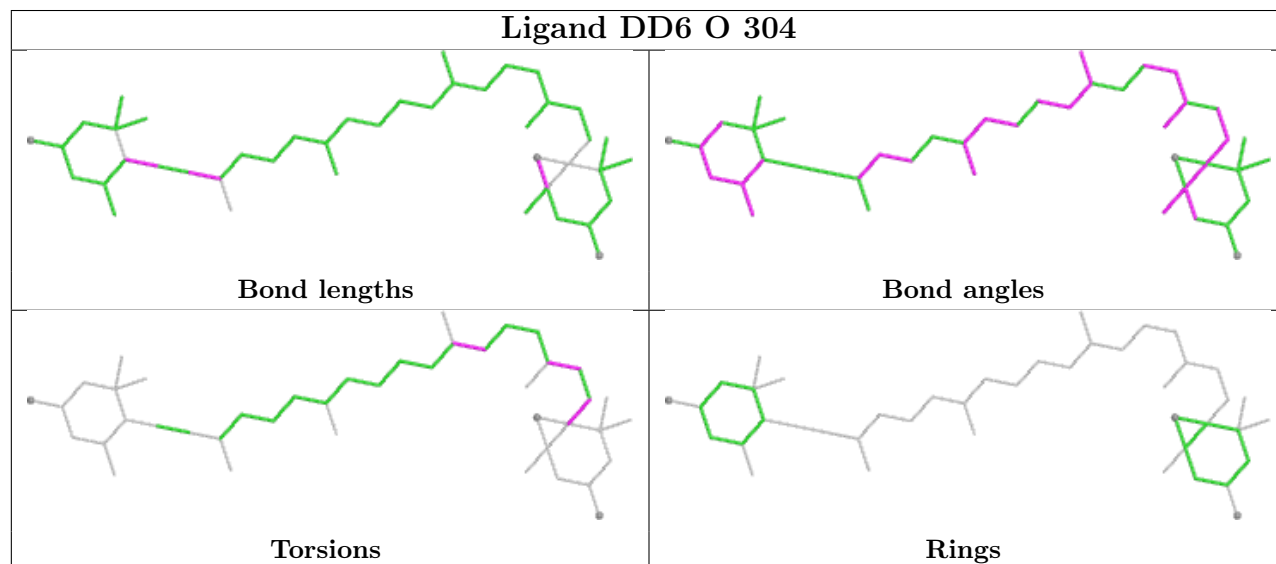
## Ligand CLA S 319

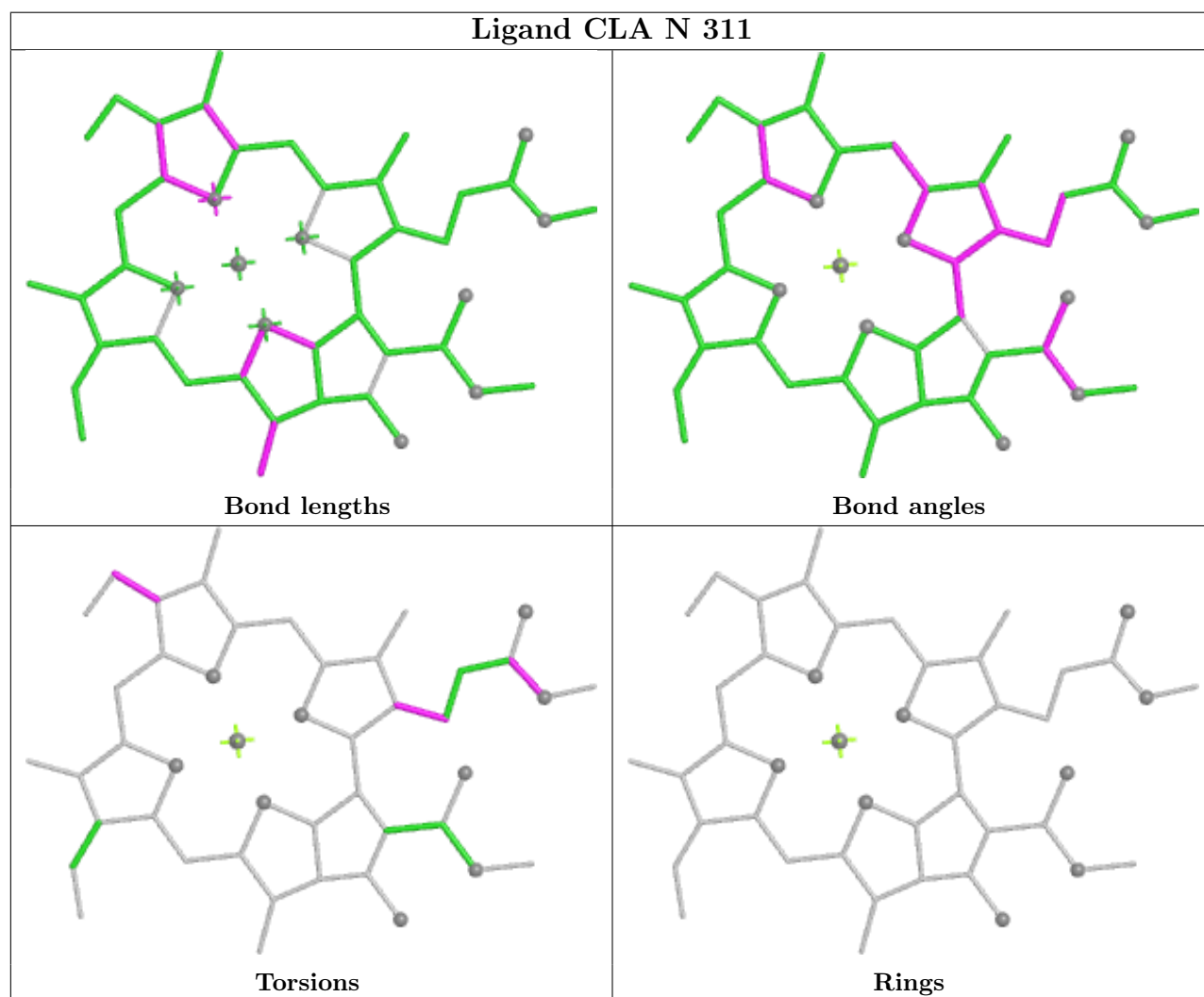
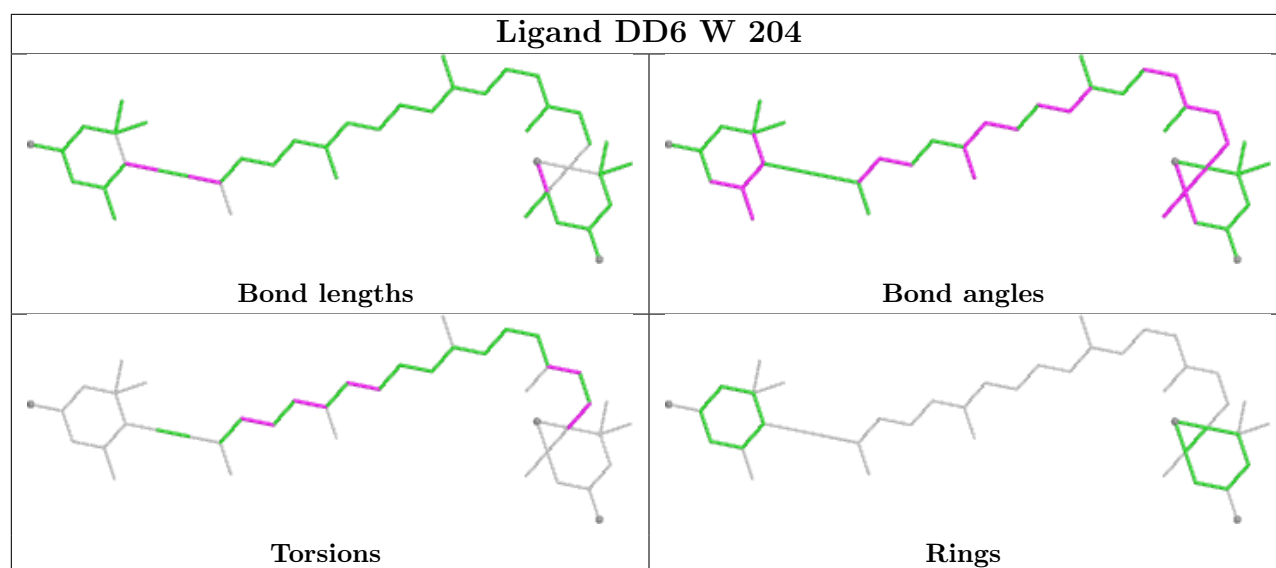


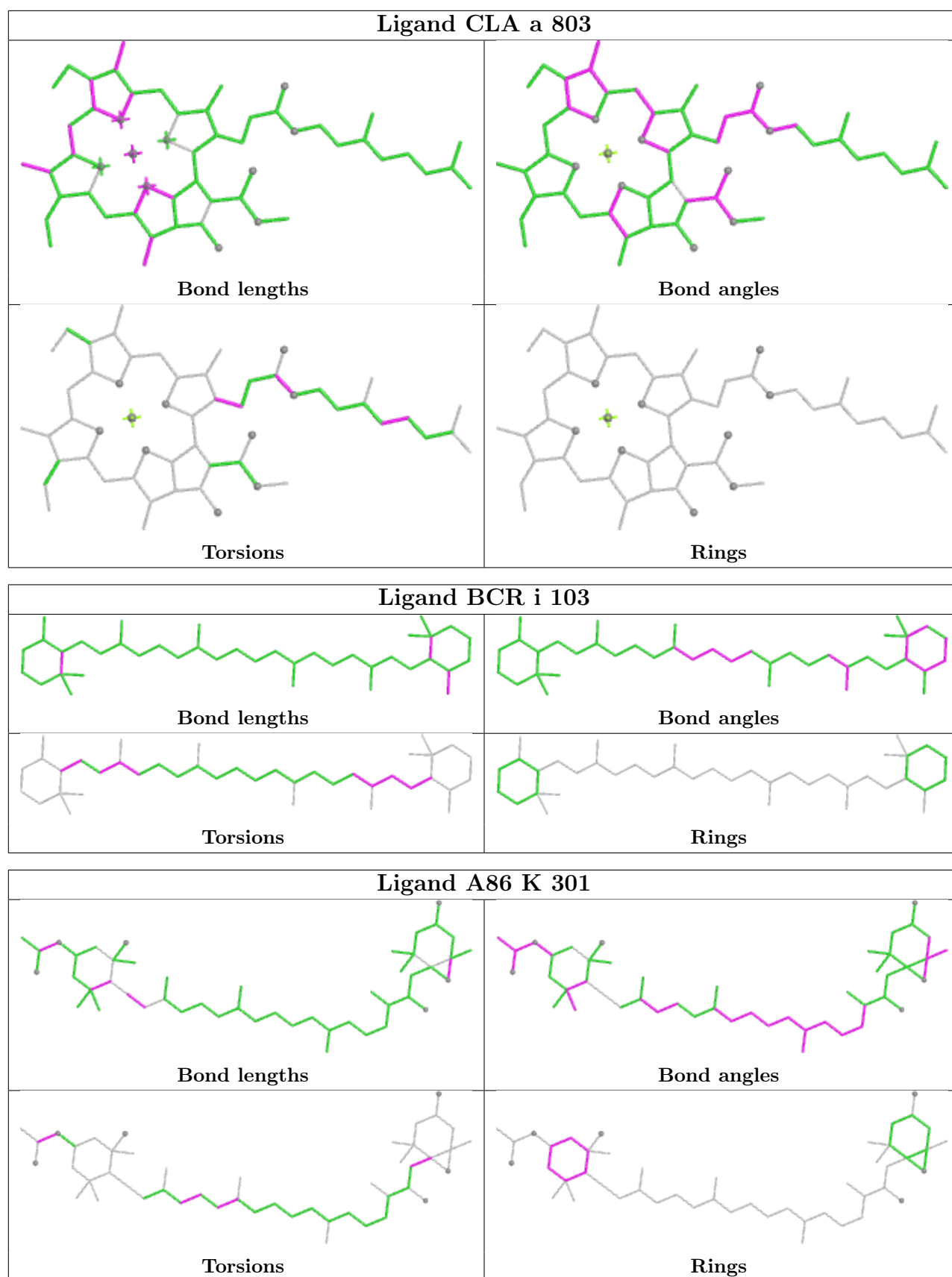
## Ligand CLA I 305



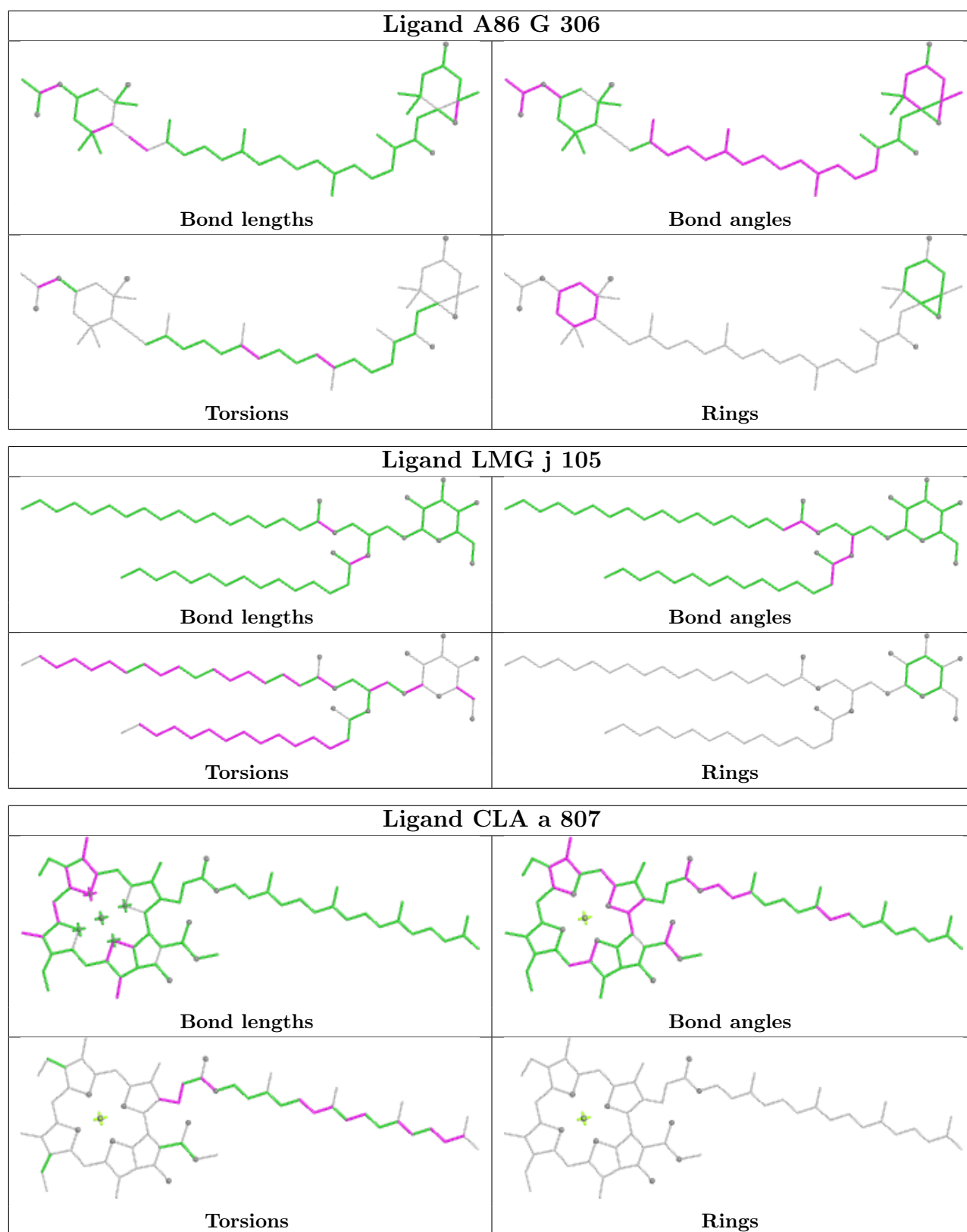
## Ligand DD6 O 304

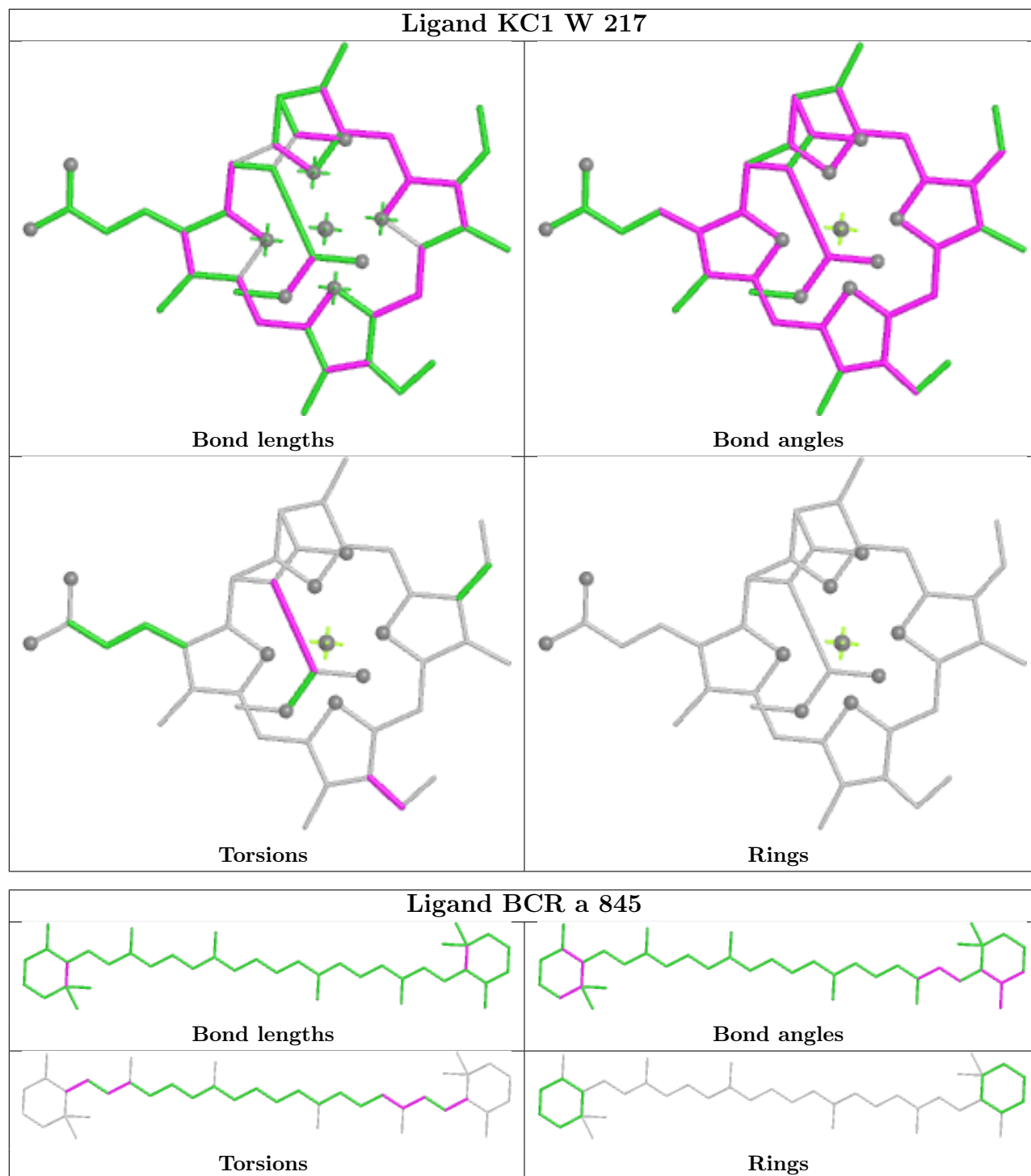


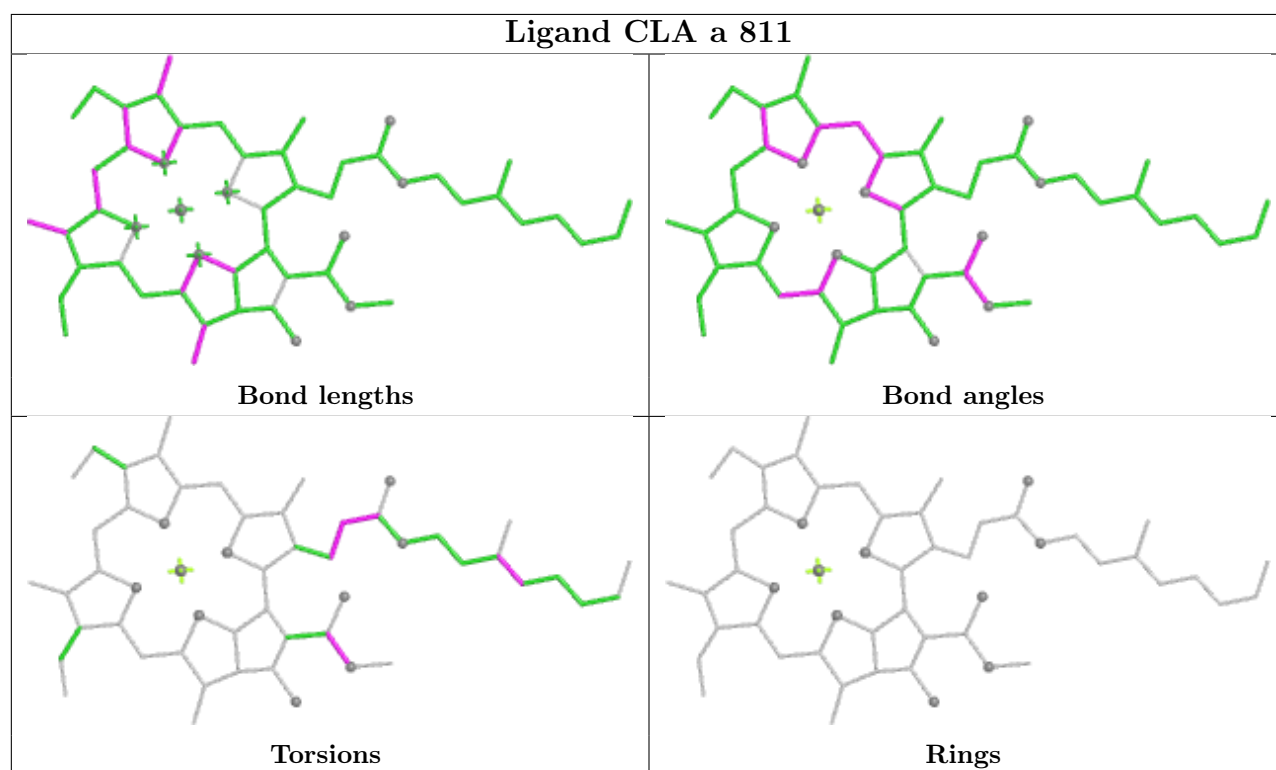
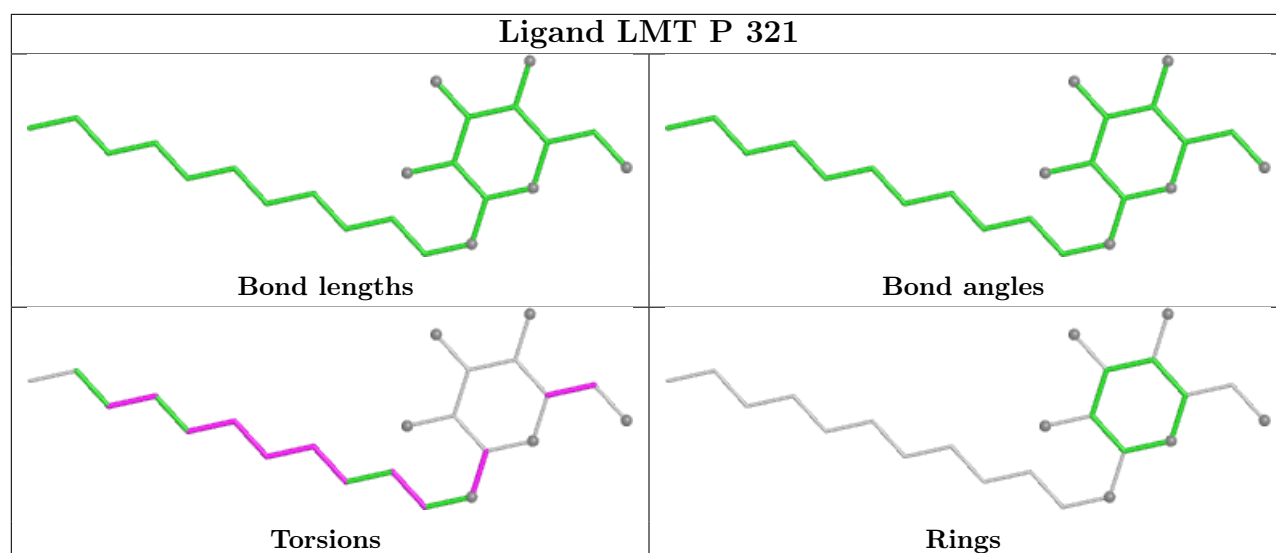




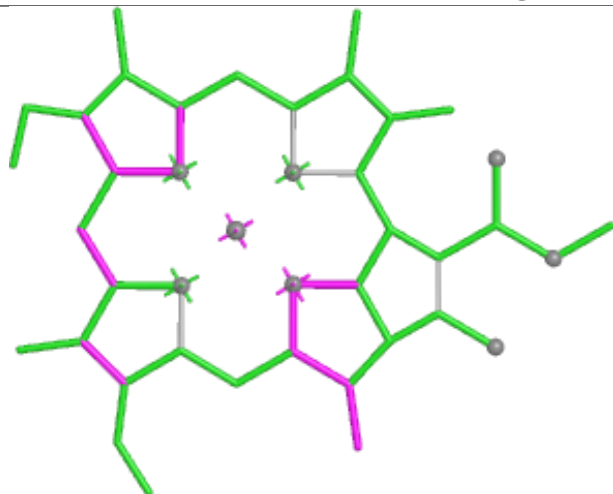








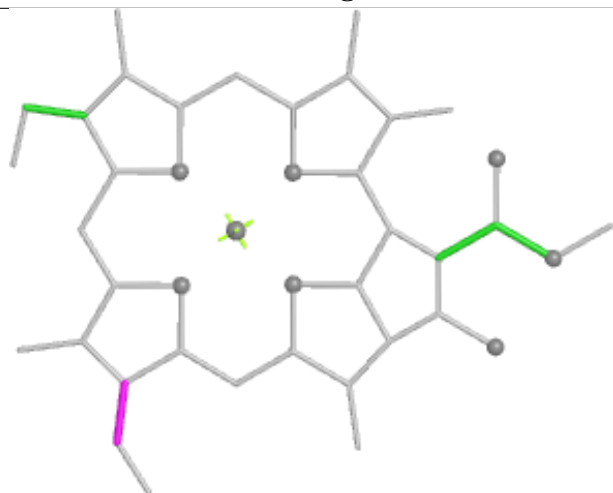
## Ligand CLA N 310



Bond lengths



Bond angles

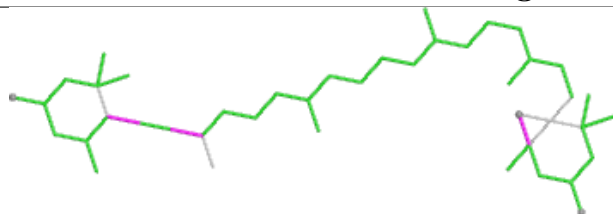


Torsions

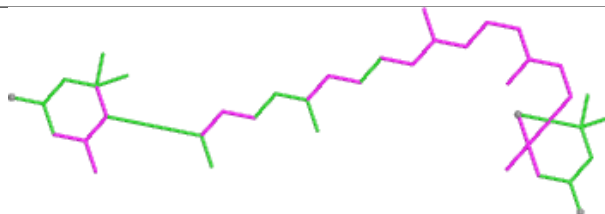


Rings

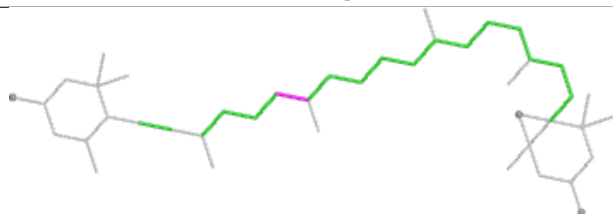
## Ligand DD6 P 305



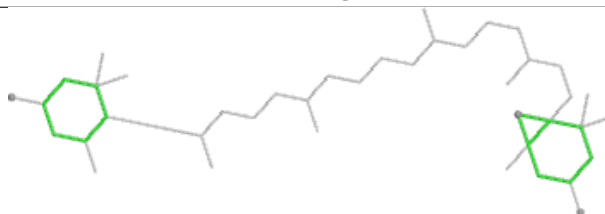
Bond lengths



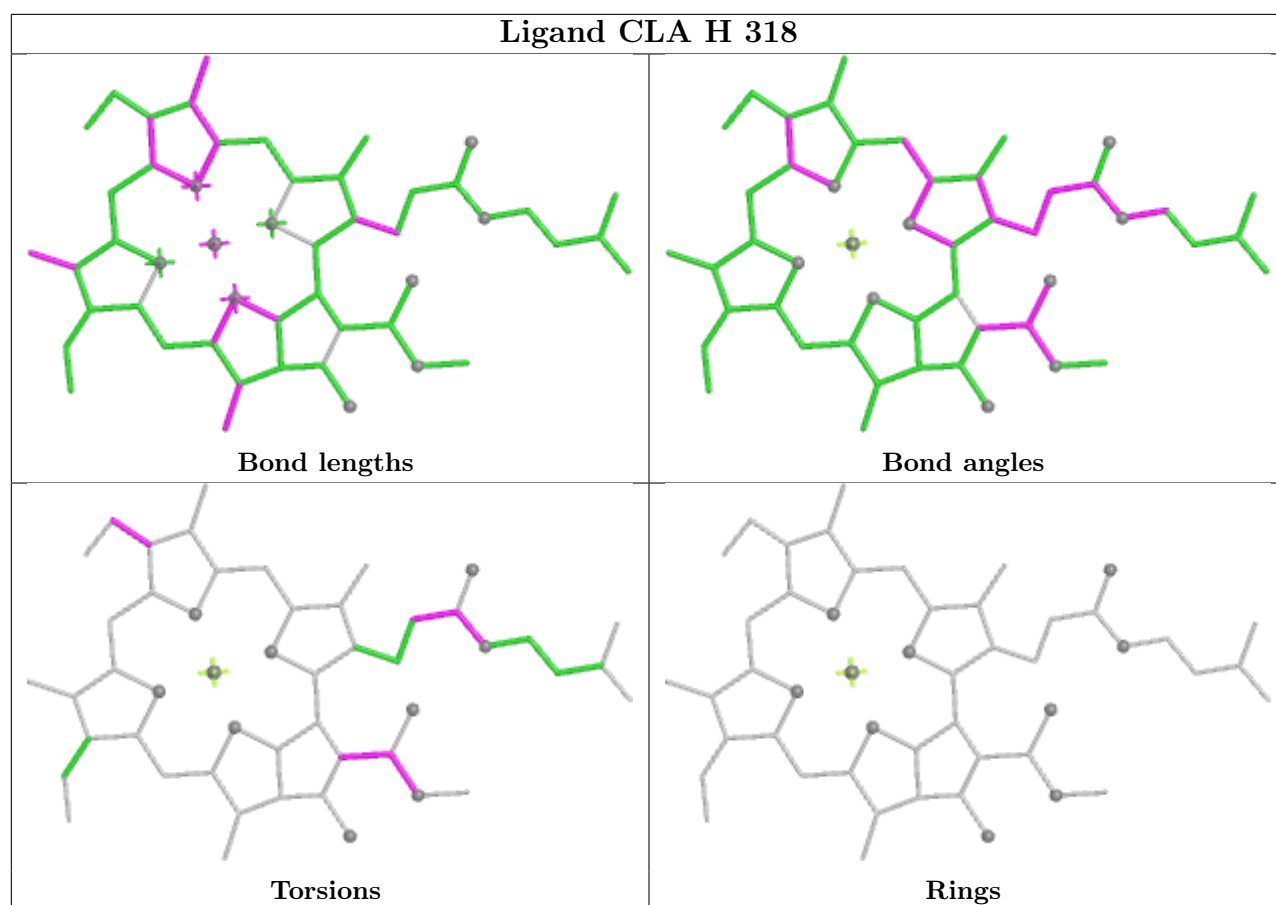
Bond angles



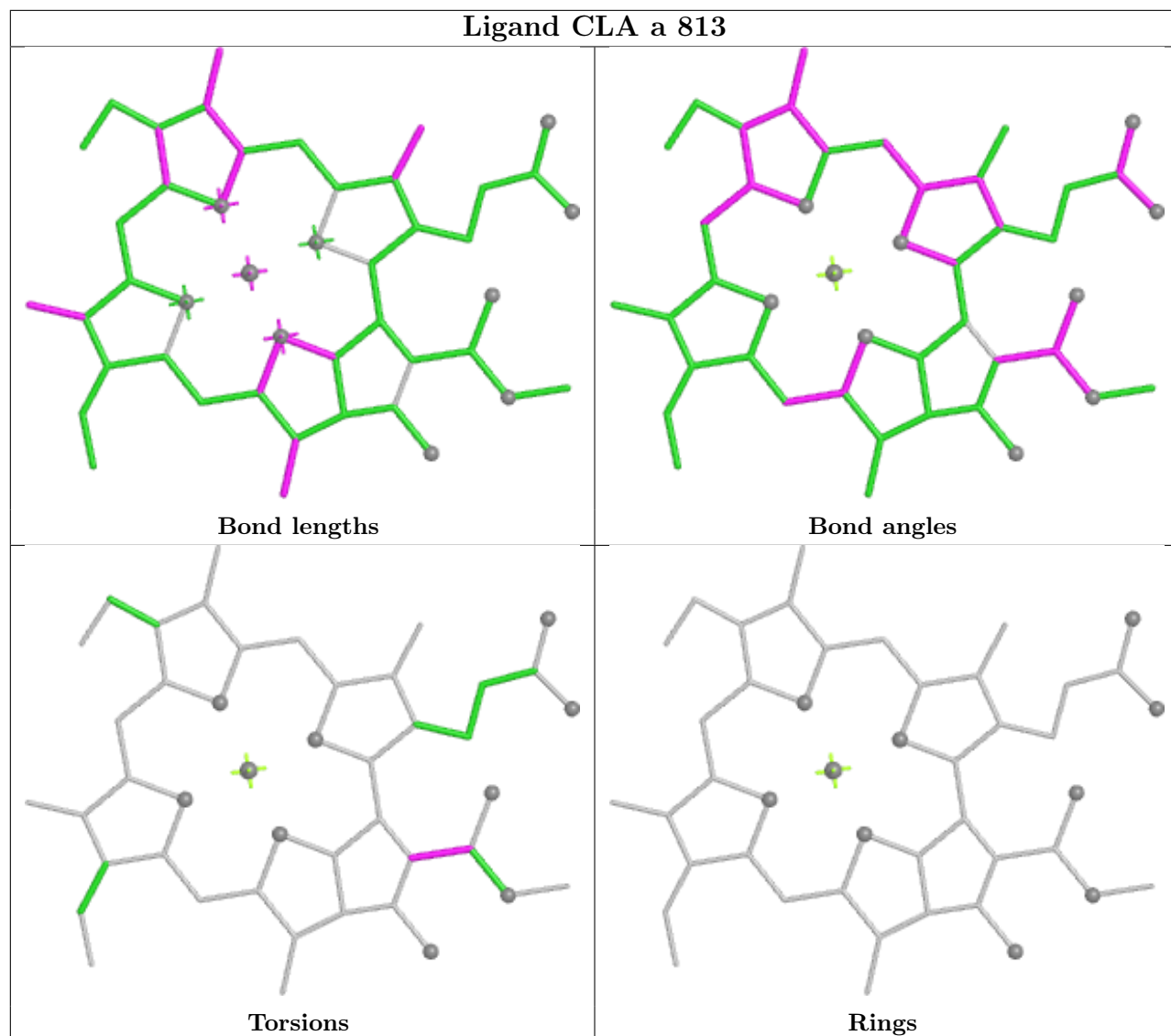
Torsions

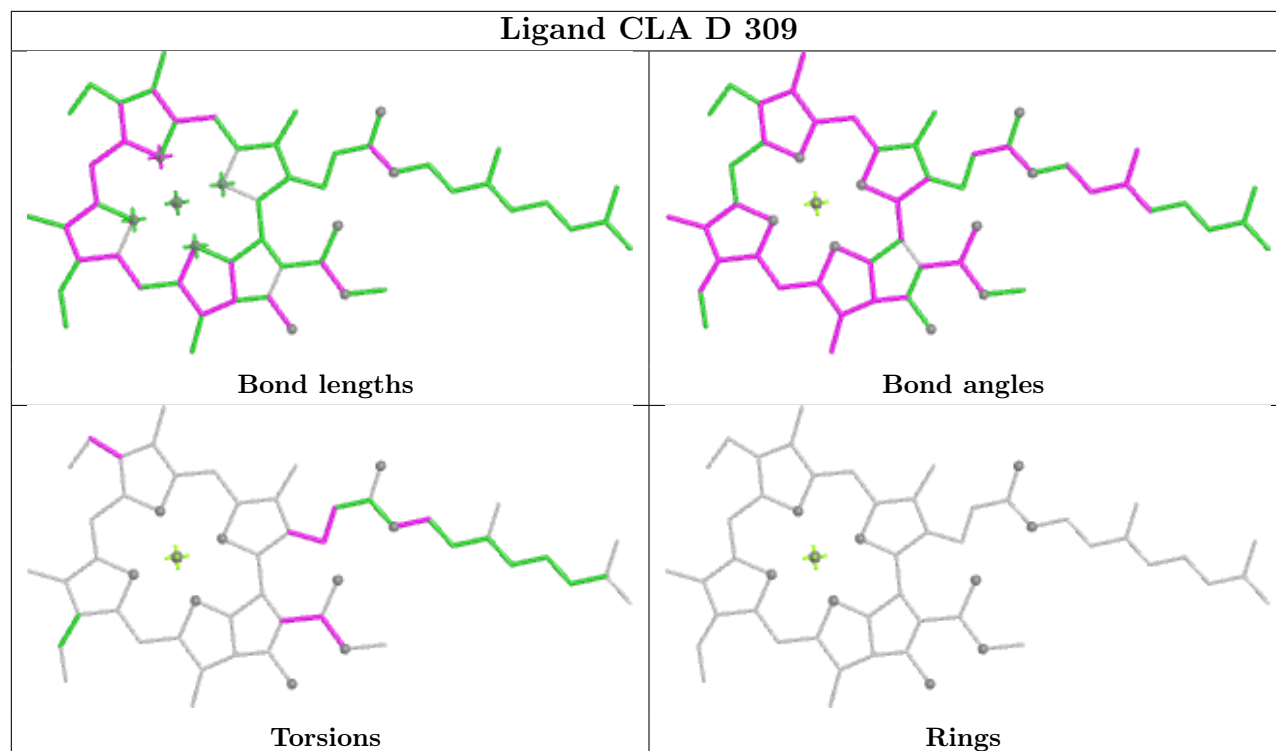
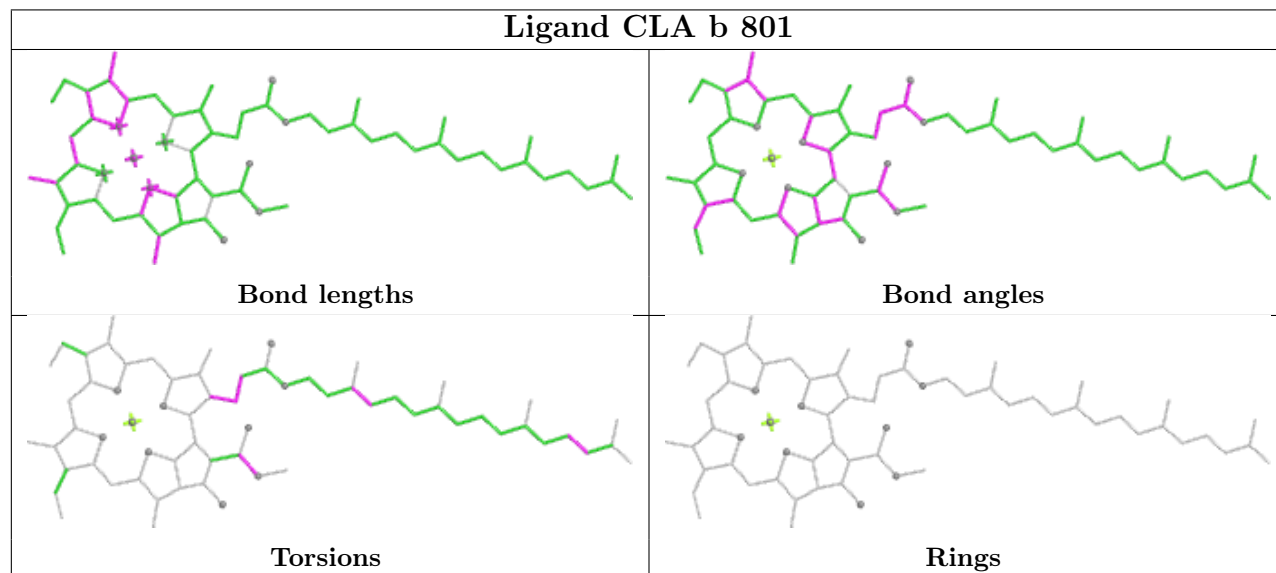


Rings

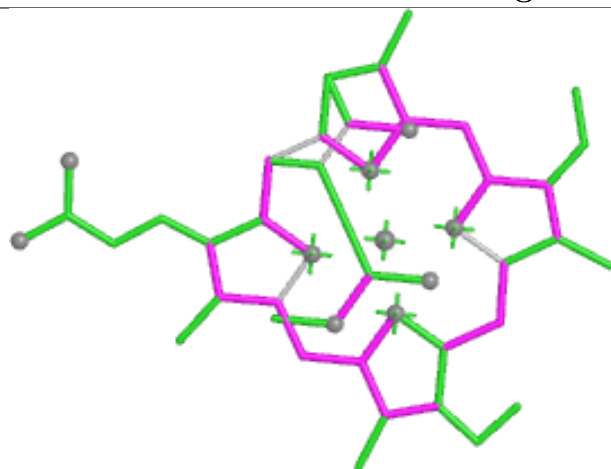


## Ligand CLA a 813

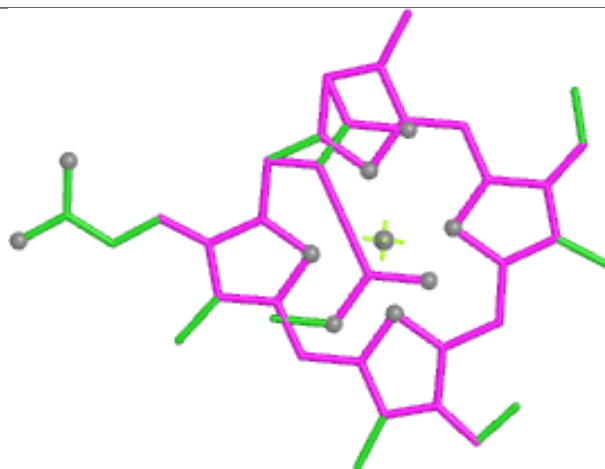


**Ligand CLA D 309****Ligand CLA b 801**

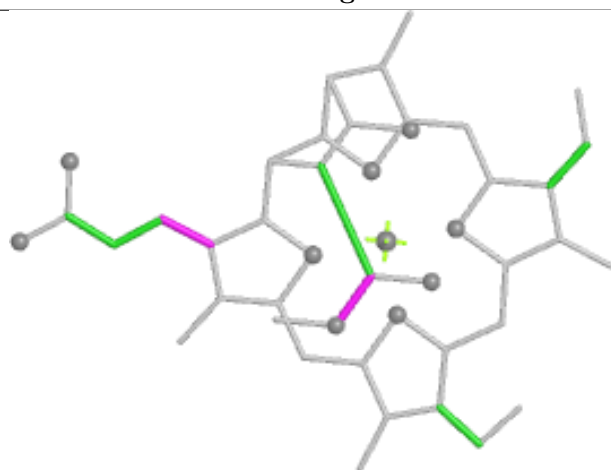
## Ligand KC1 U 312



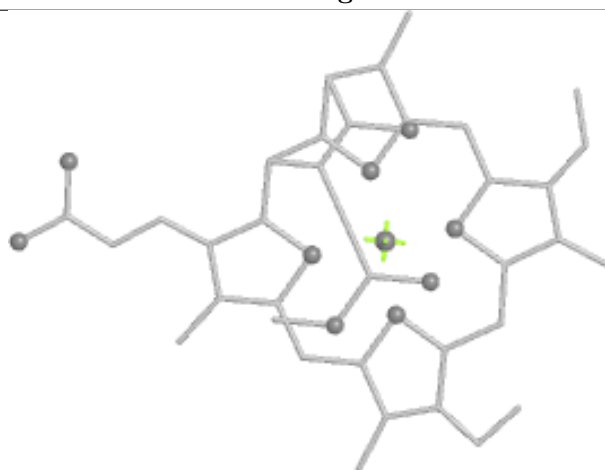
Bond lengths



Bond angles



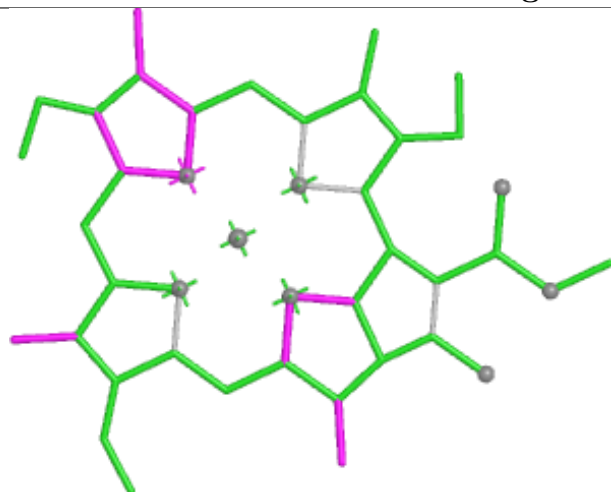
Torsions



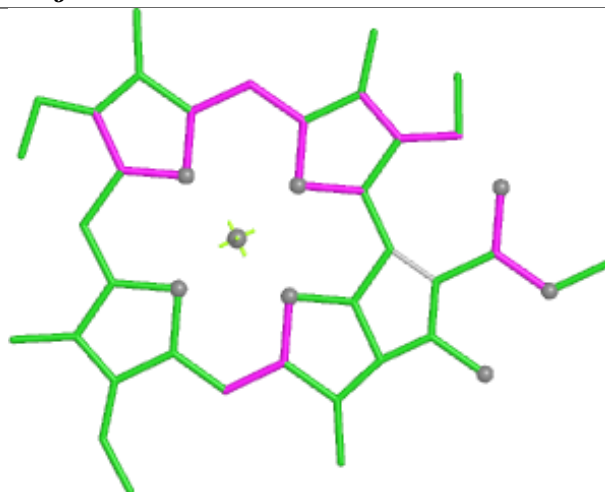
Rings



## Ligand CLA j 106



Bond lengths



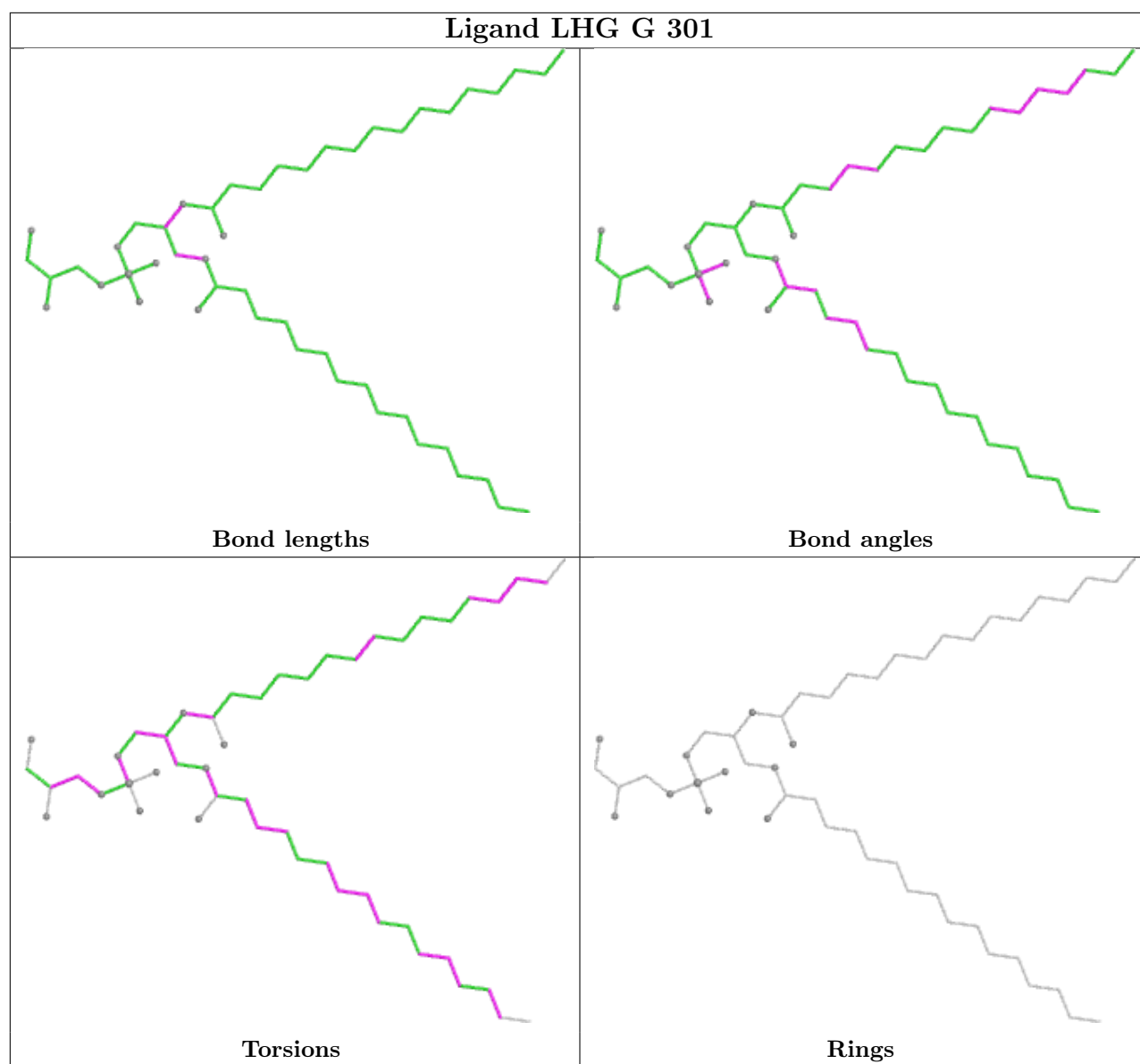
Bond angles



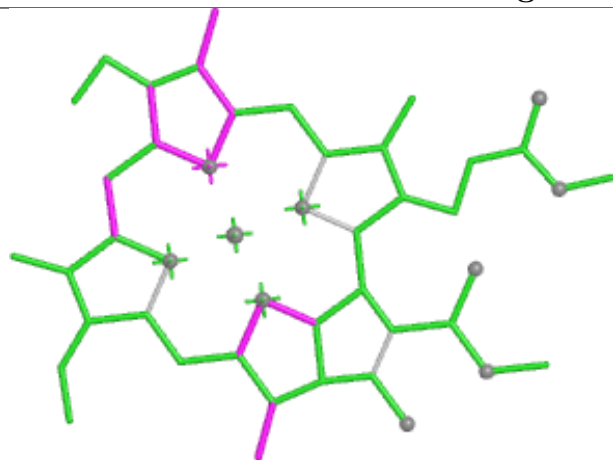
Torsions



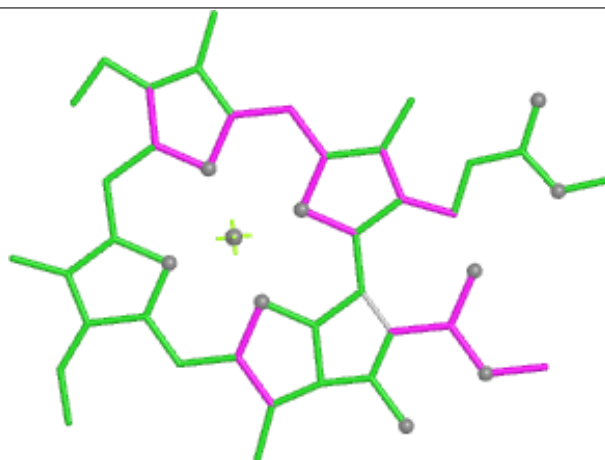
Rings



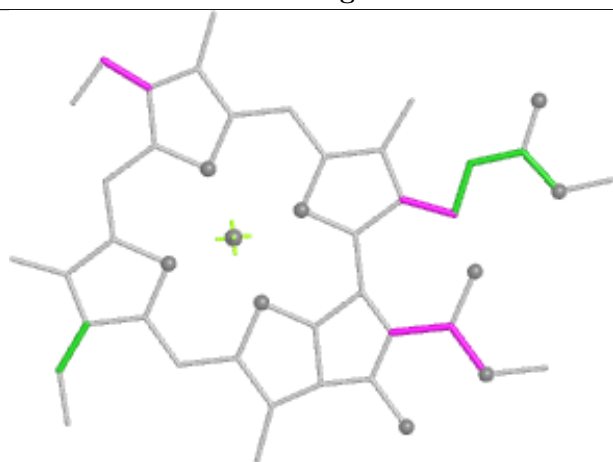
## Ligand CLA b 822



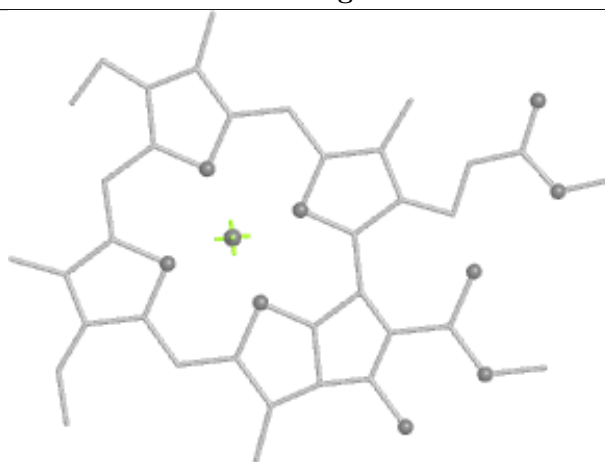
Bond lengths



Bond angles

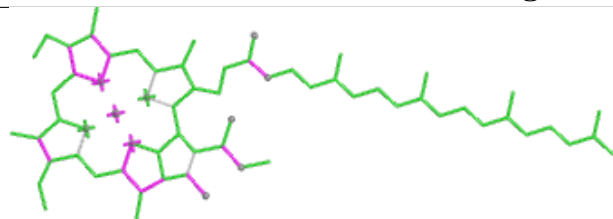


Torsions

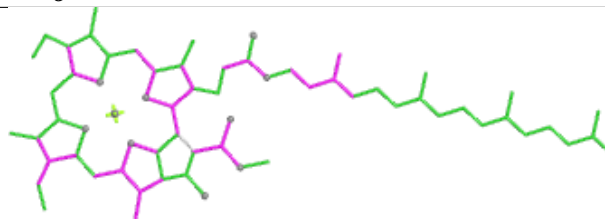


Rings

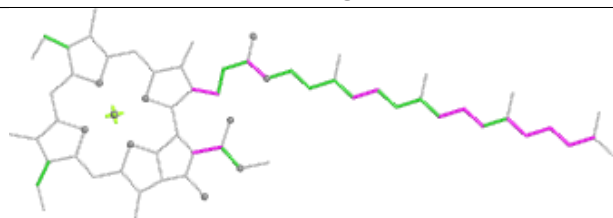
## Ligand CLA j 102



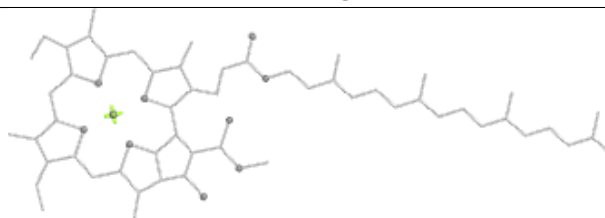
Bond lengths



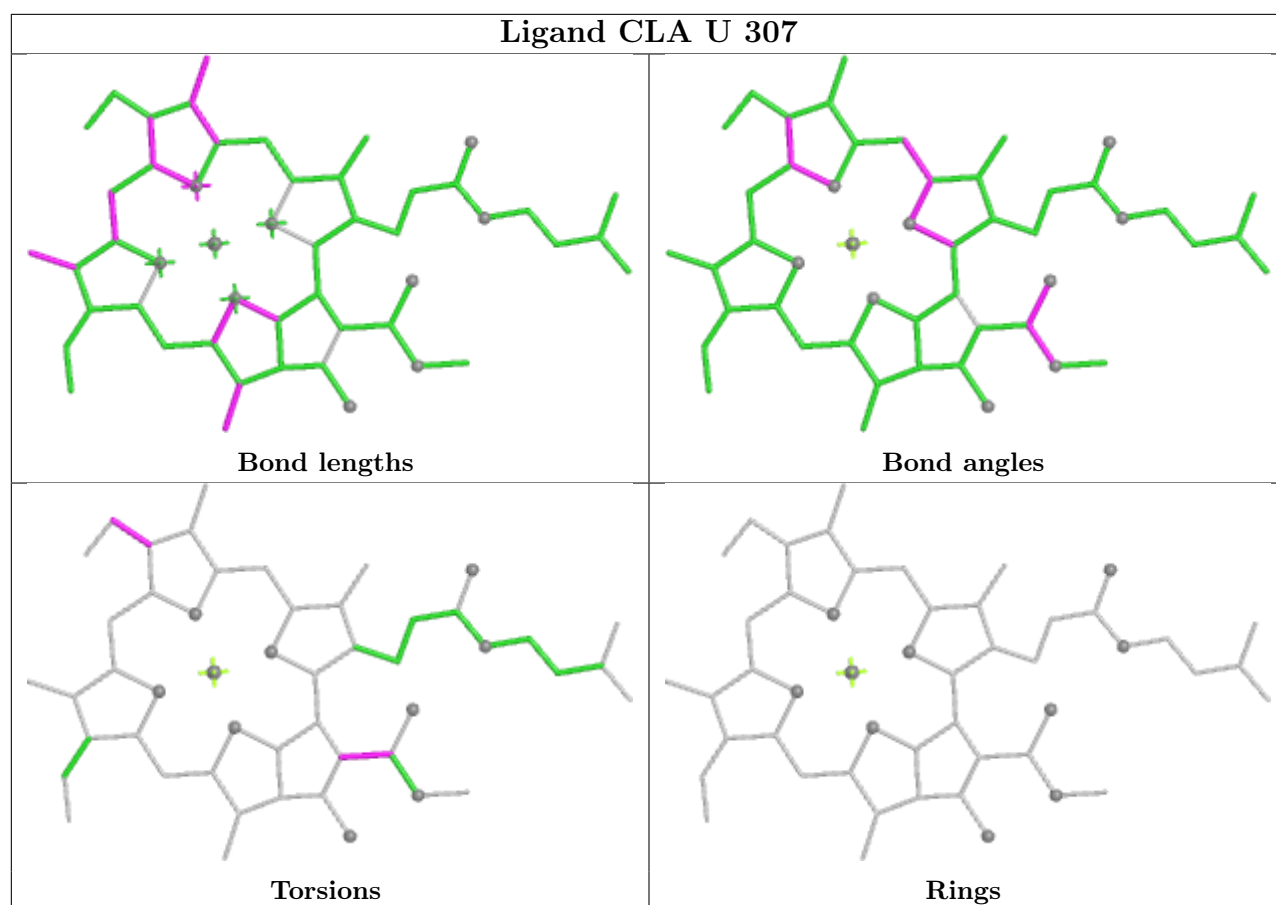
Bond angles

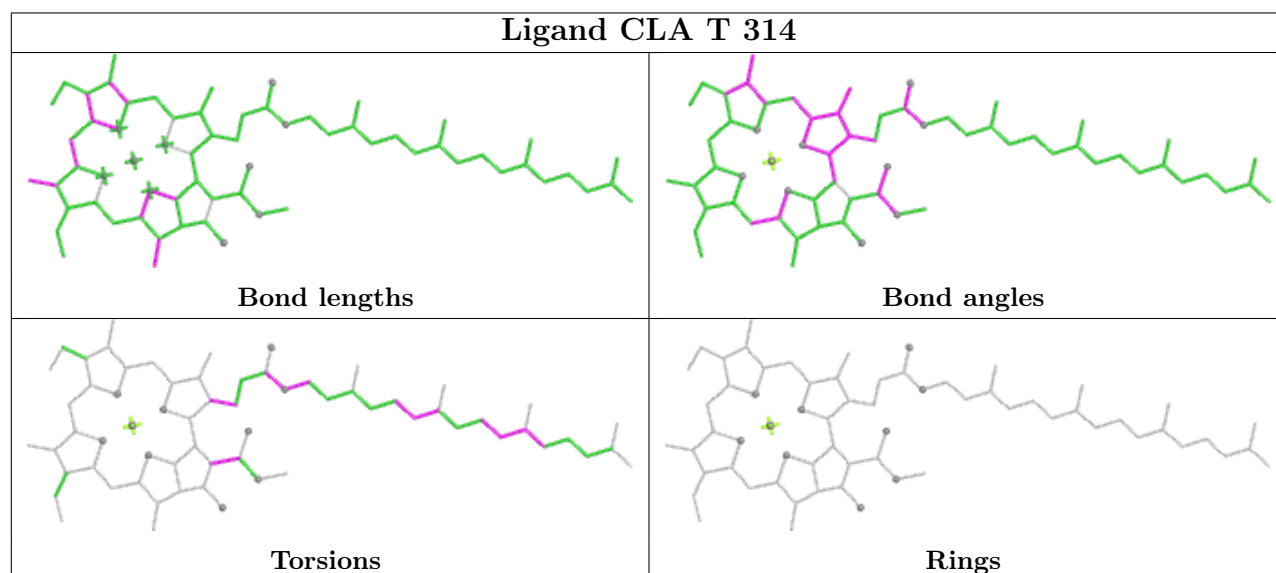
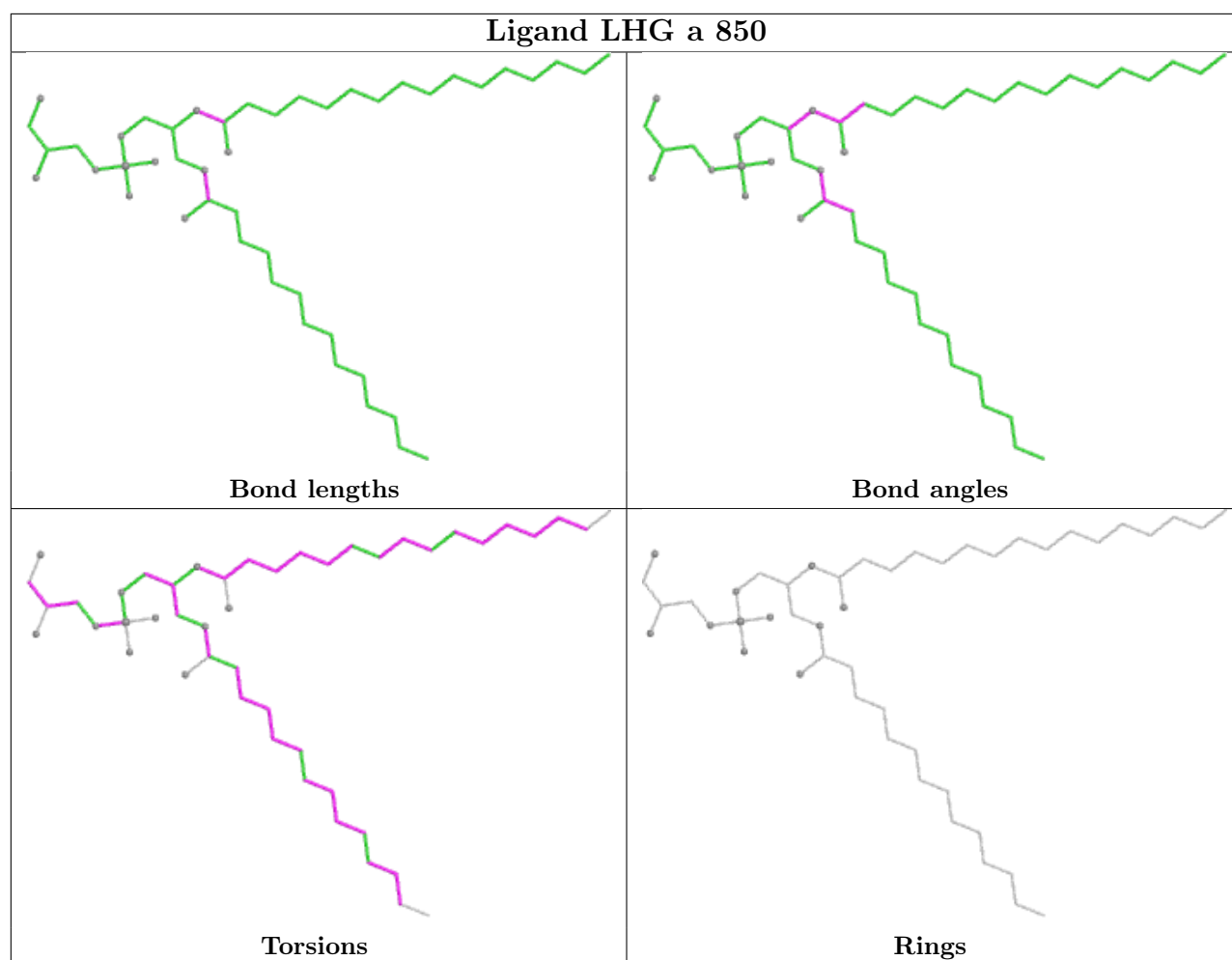


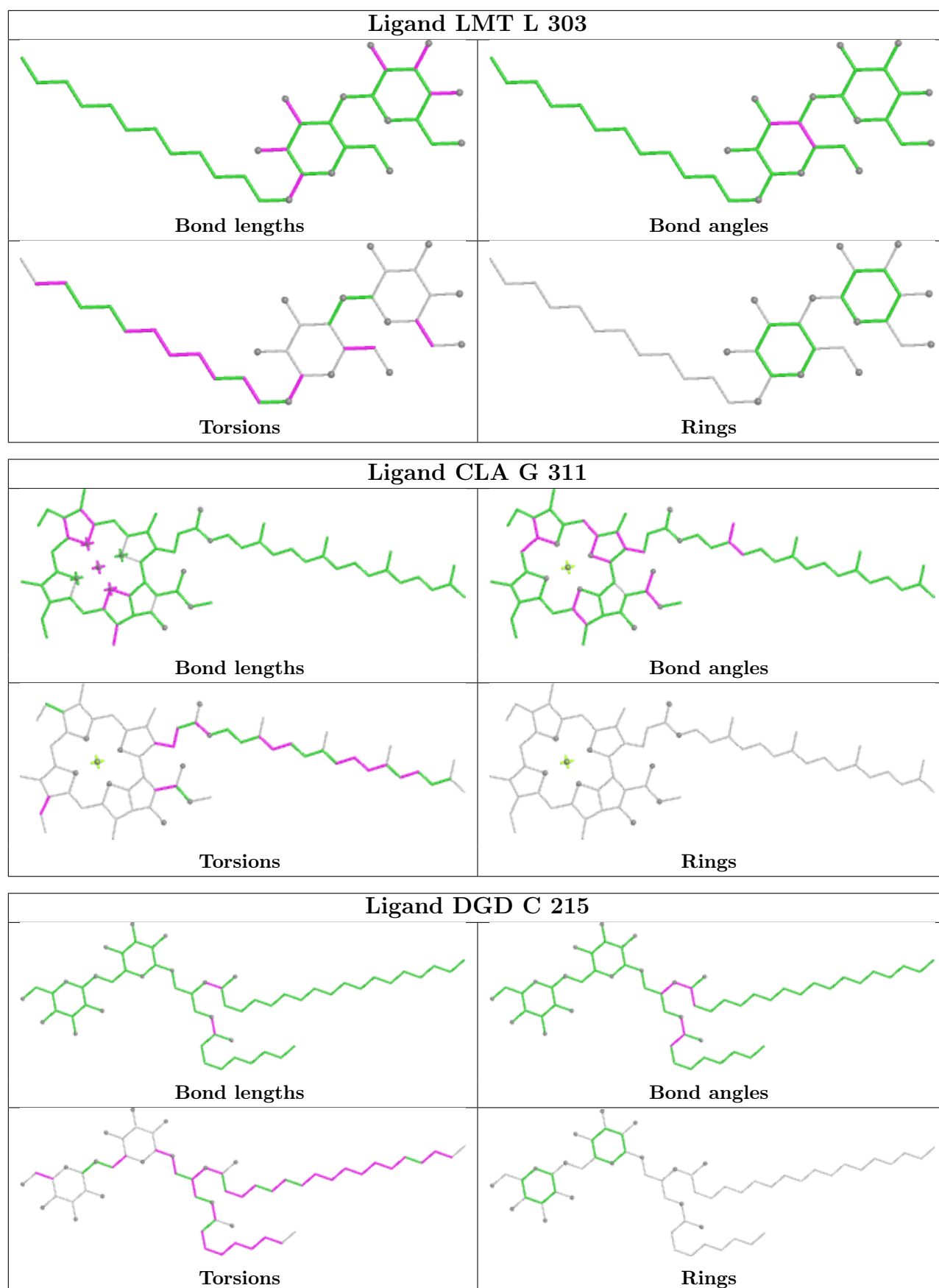
Torsions

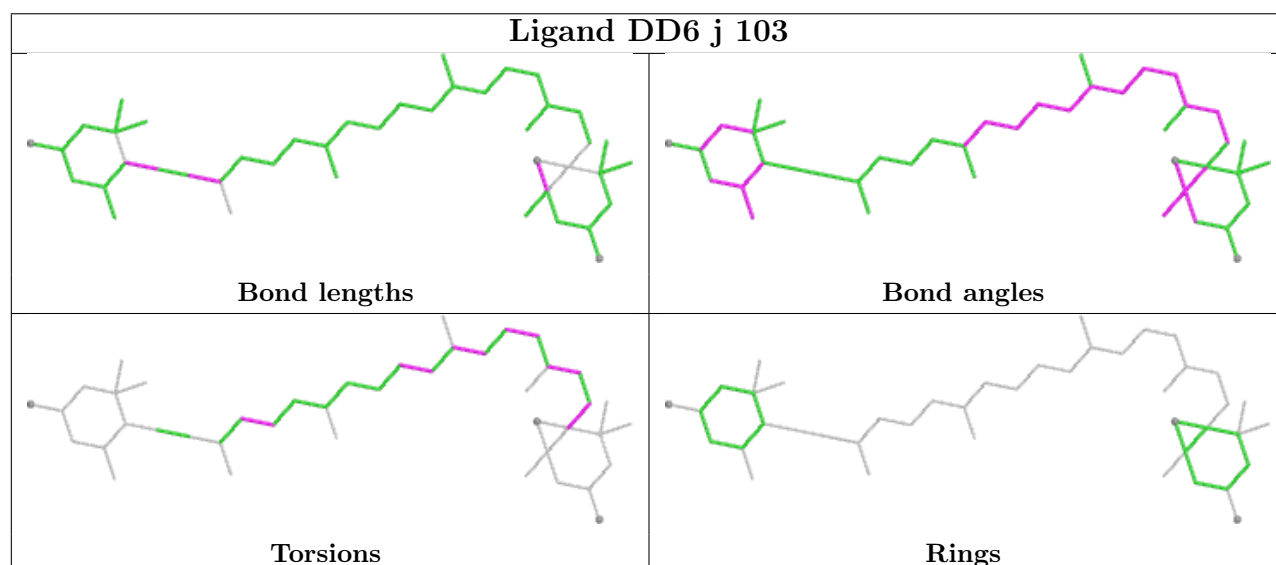
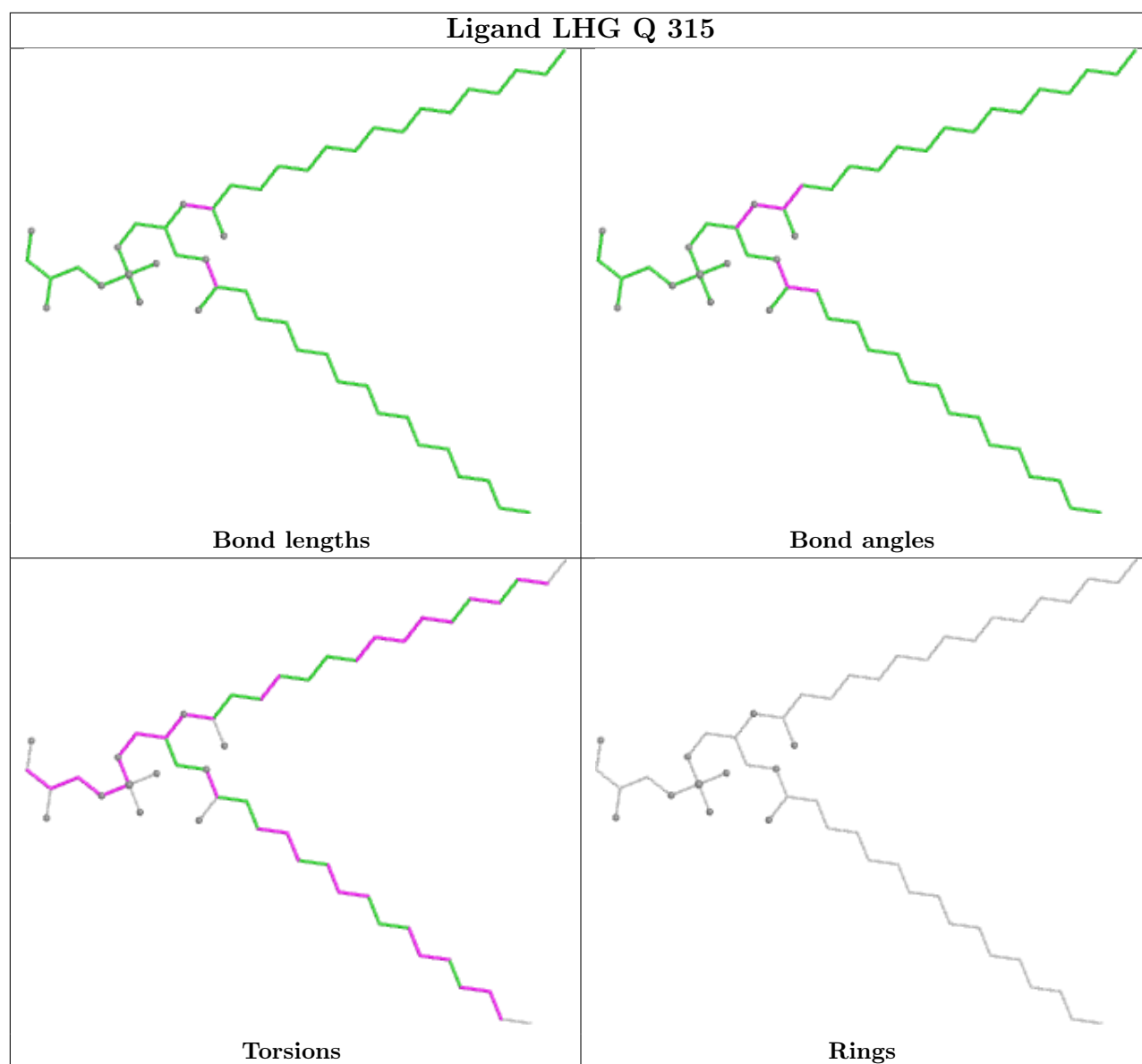


Rings

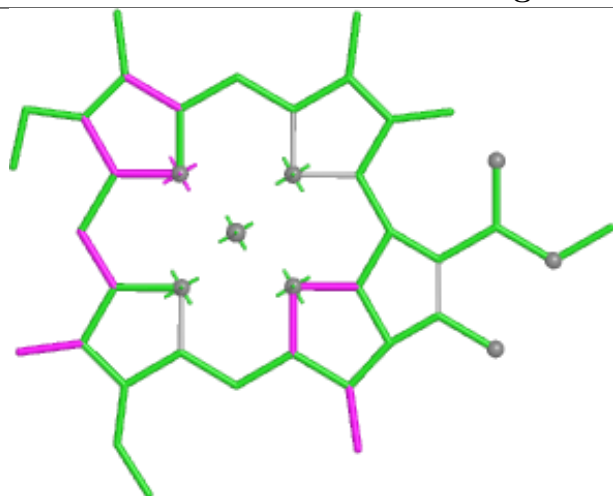




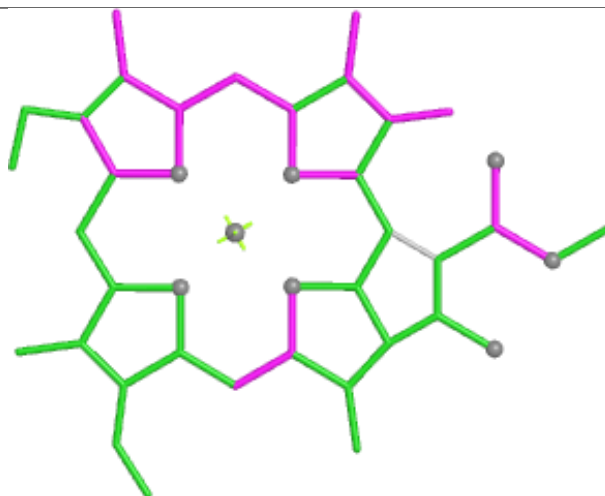




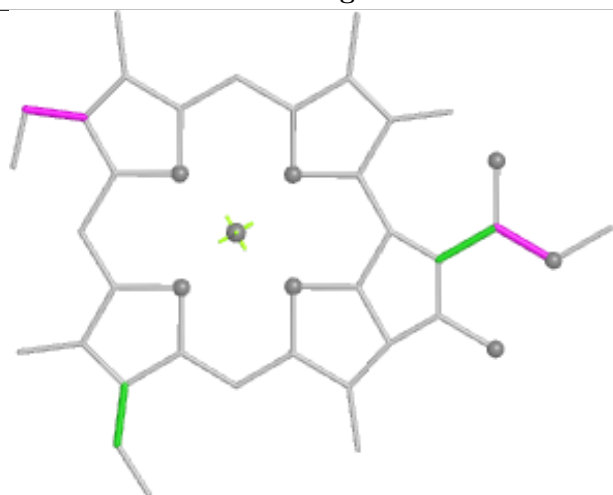
## Ligand CLA R 318



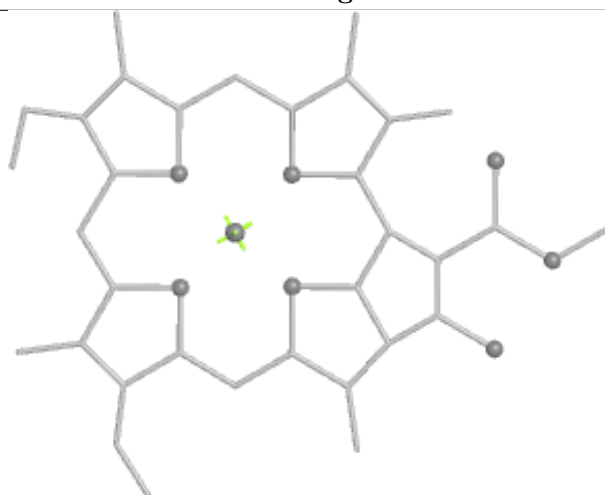
Bond lengths



Bond angles

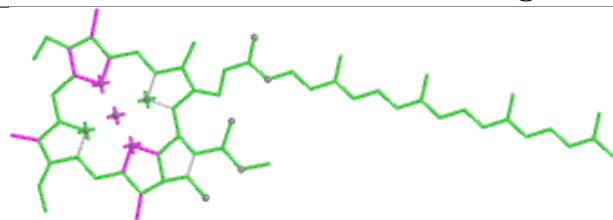


Torsions

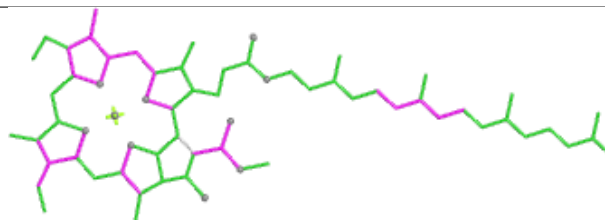


Rings

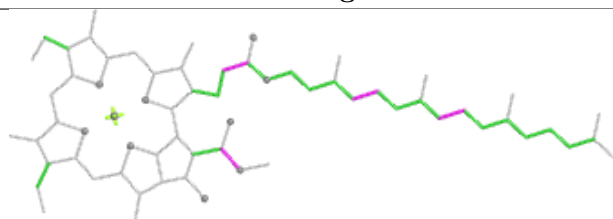
## Ligand CLA b 812



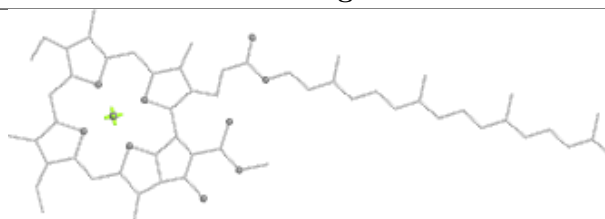
Bond lengths



Bond angles



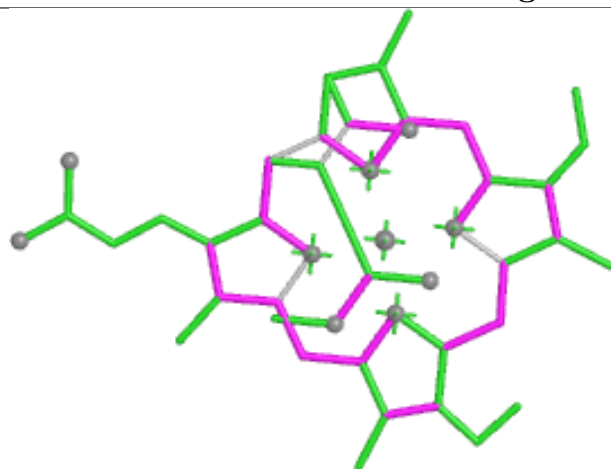
Torsions



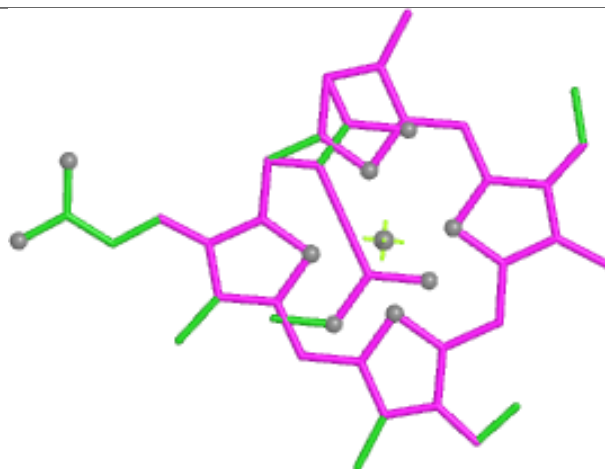
Rings



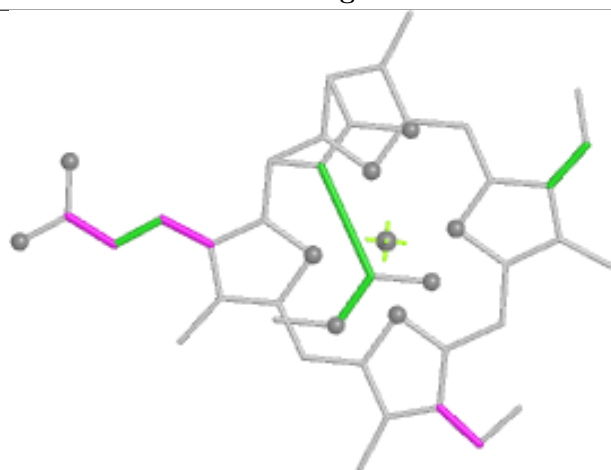
## Ligand KC1 L 315



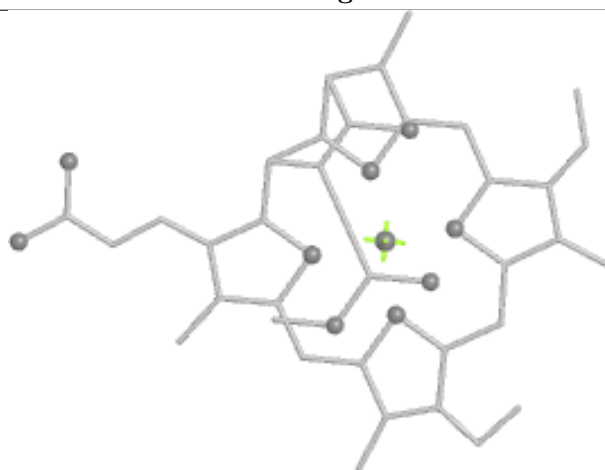
Bond lengths



Bond angles

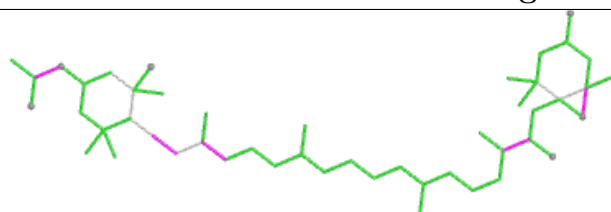


Torsions

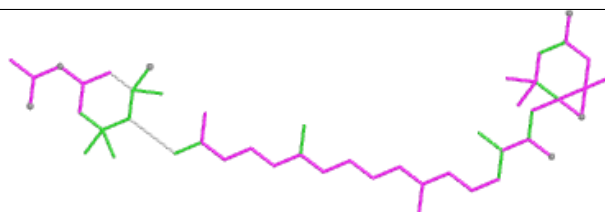


Rings

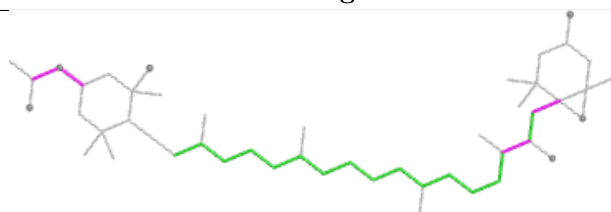
## Ligand A86 X 303



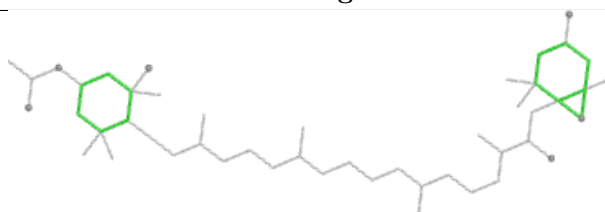
Bond lengths



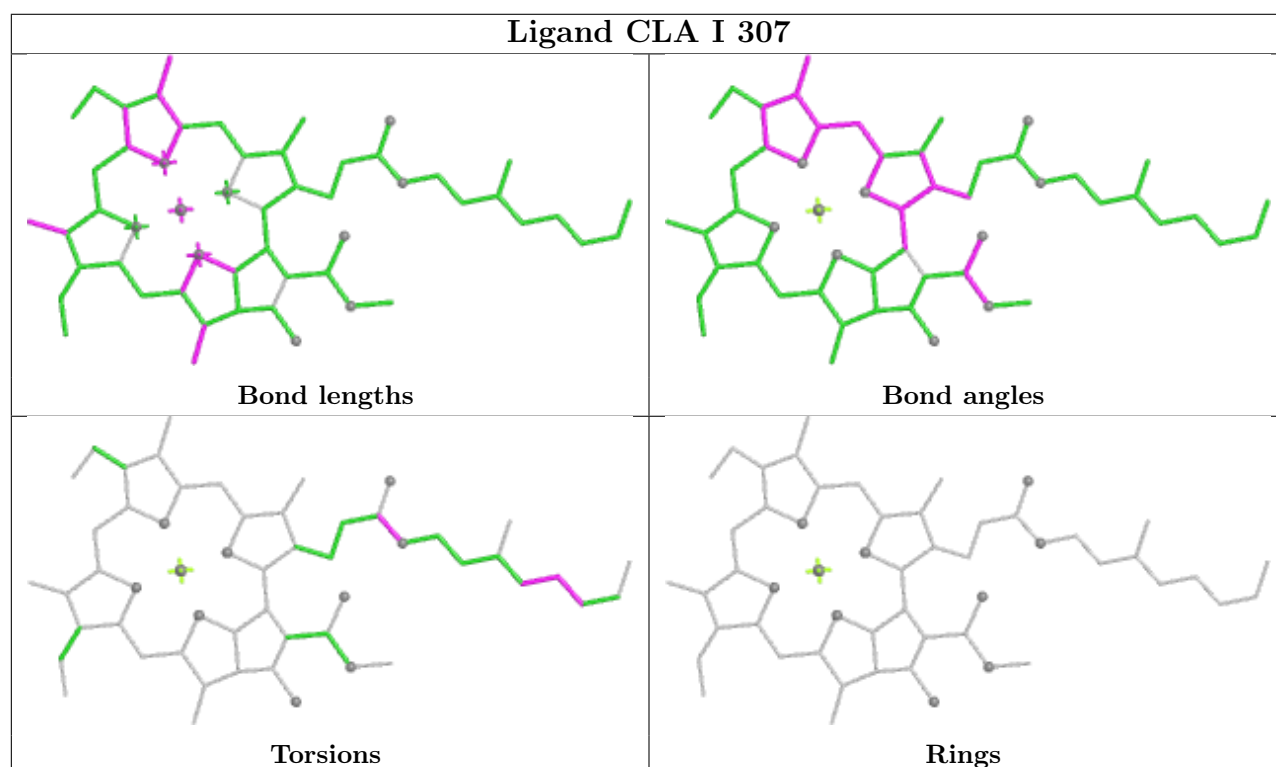
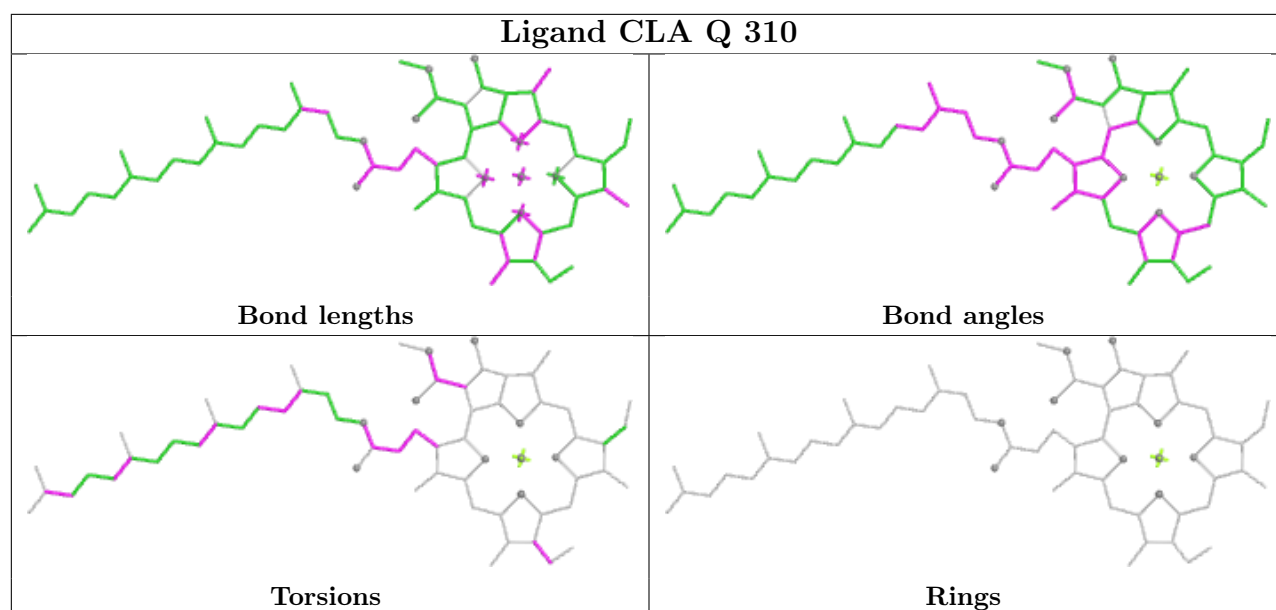
Bond angles



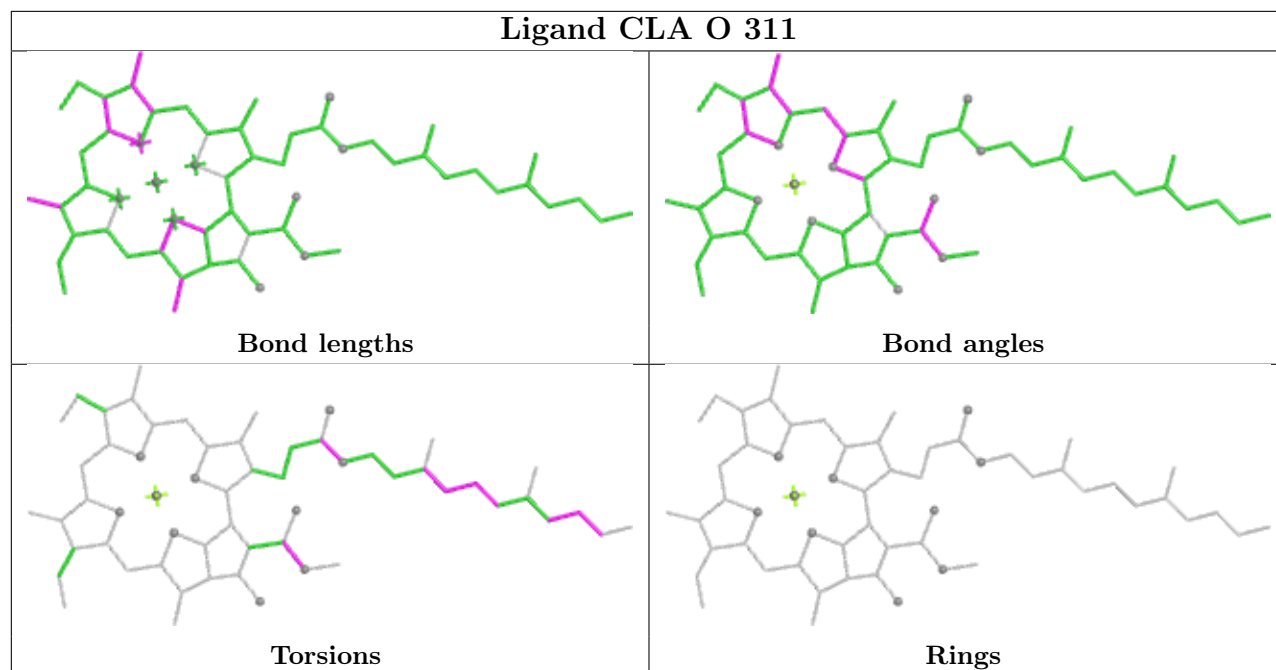
Torsions



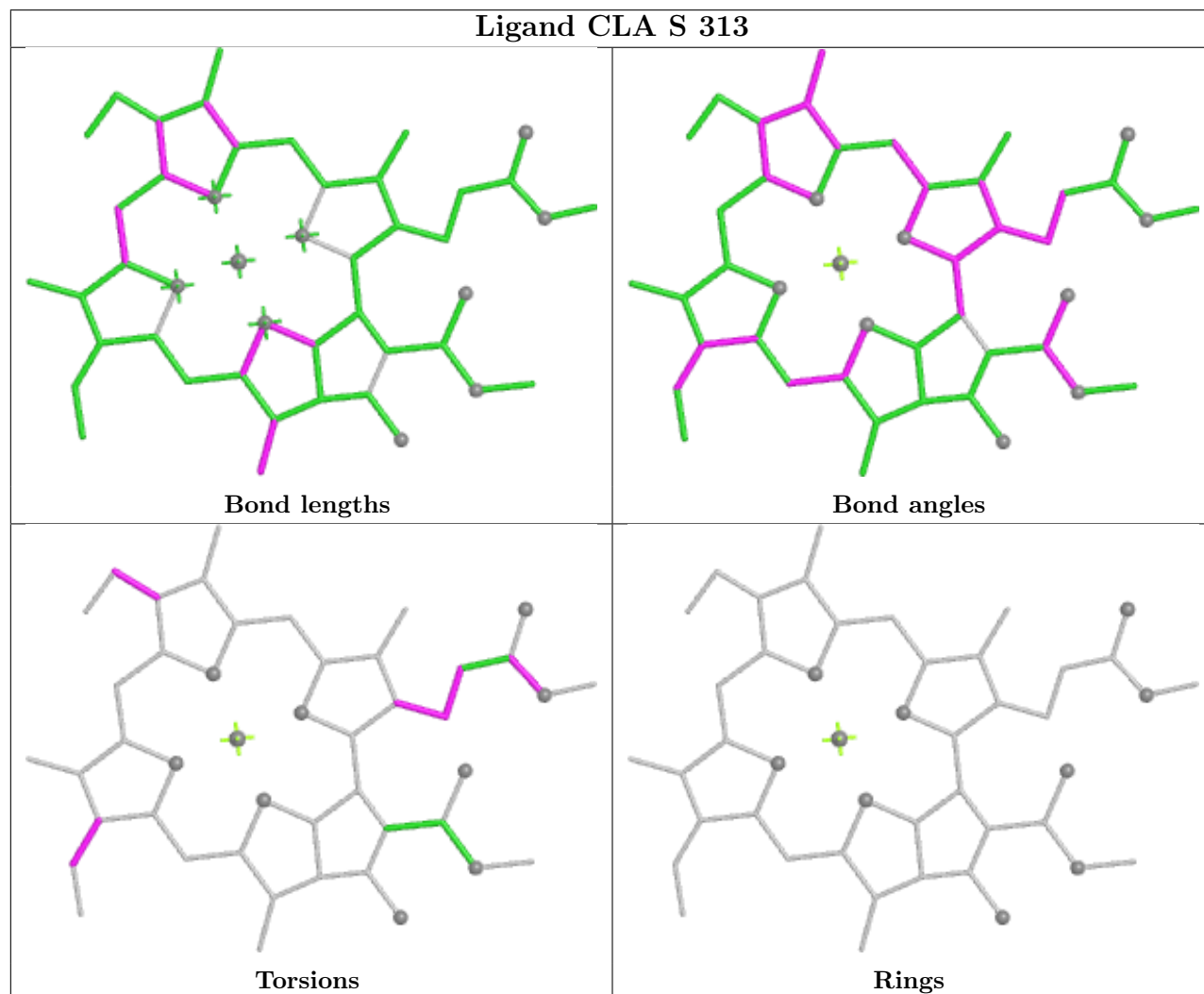
Rings



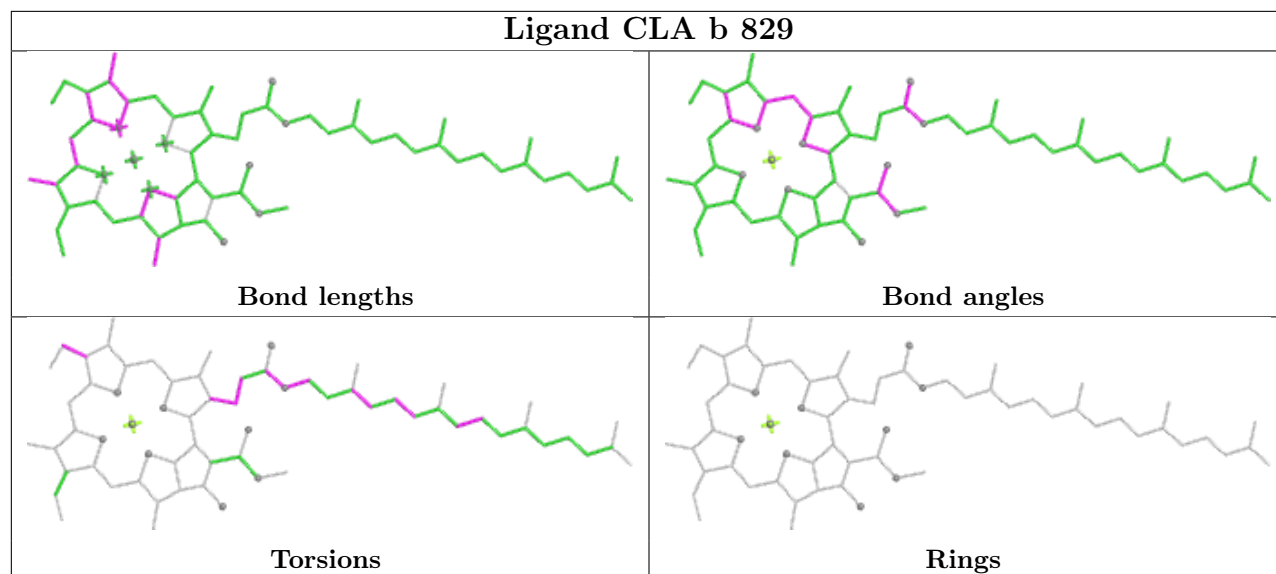
## Ligand CLA O 311



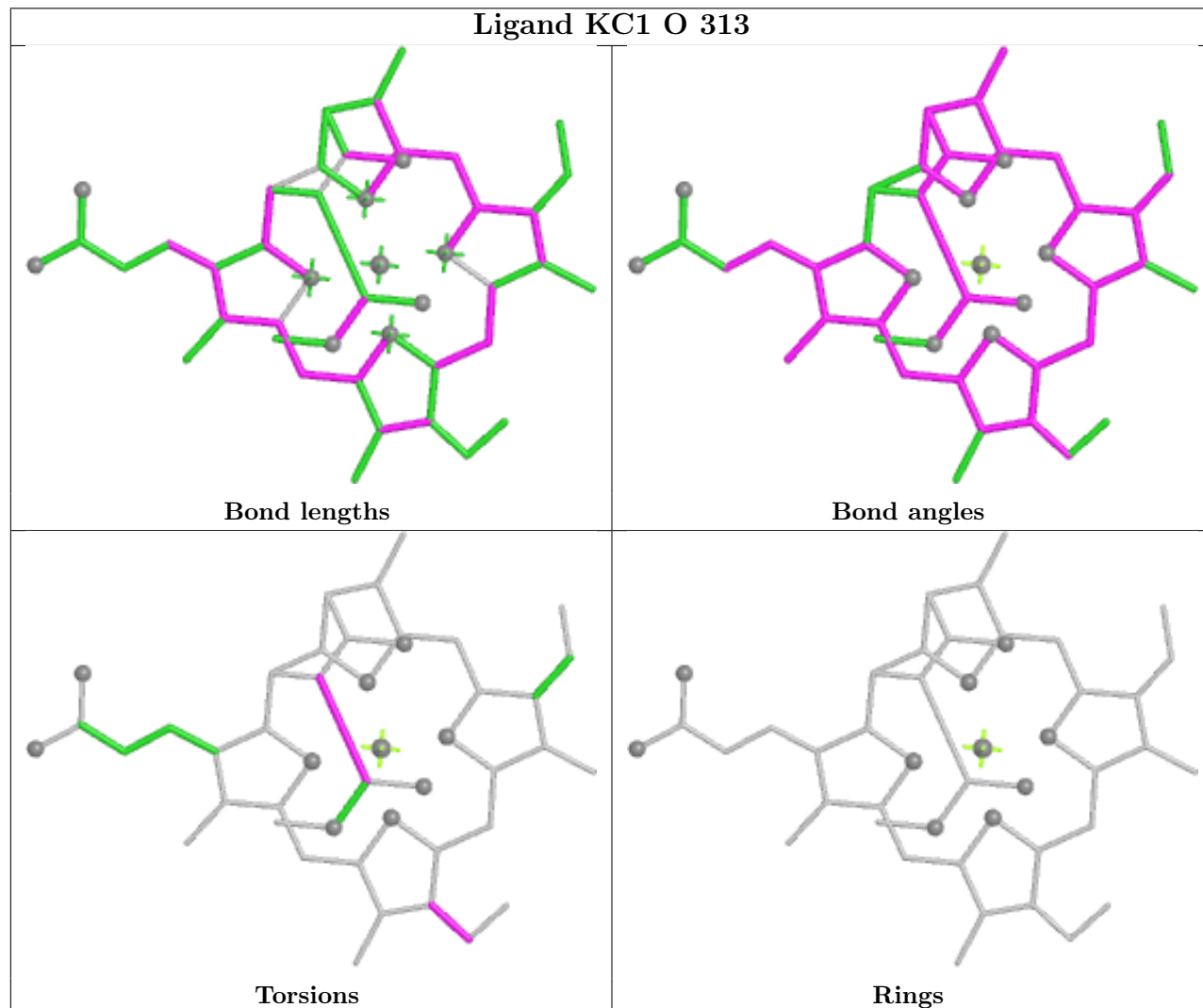
## Ligand CLA S 313

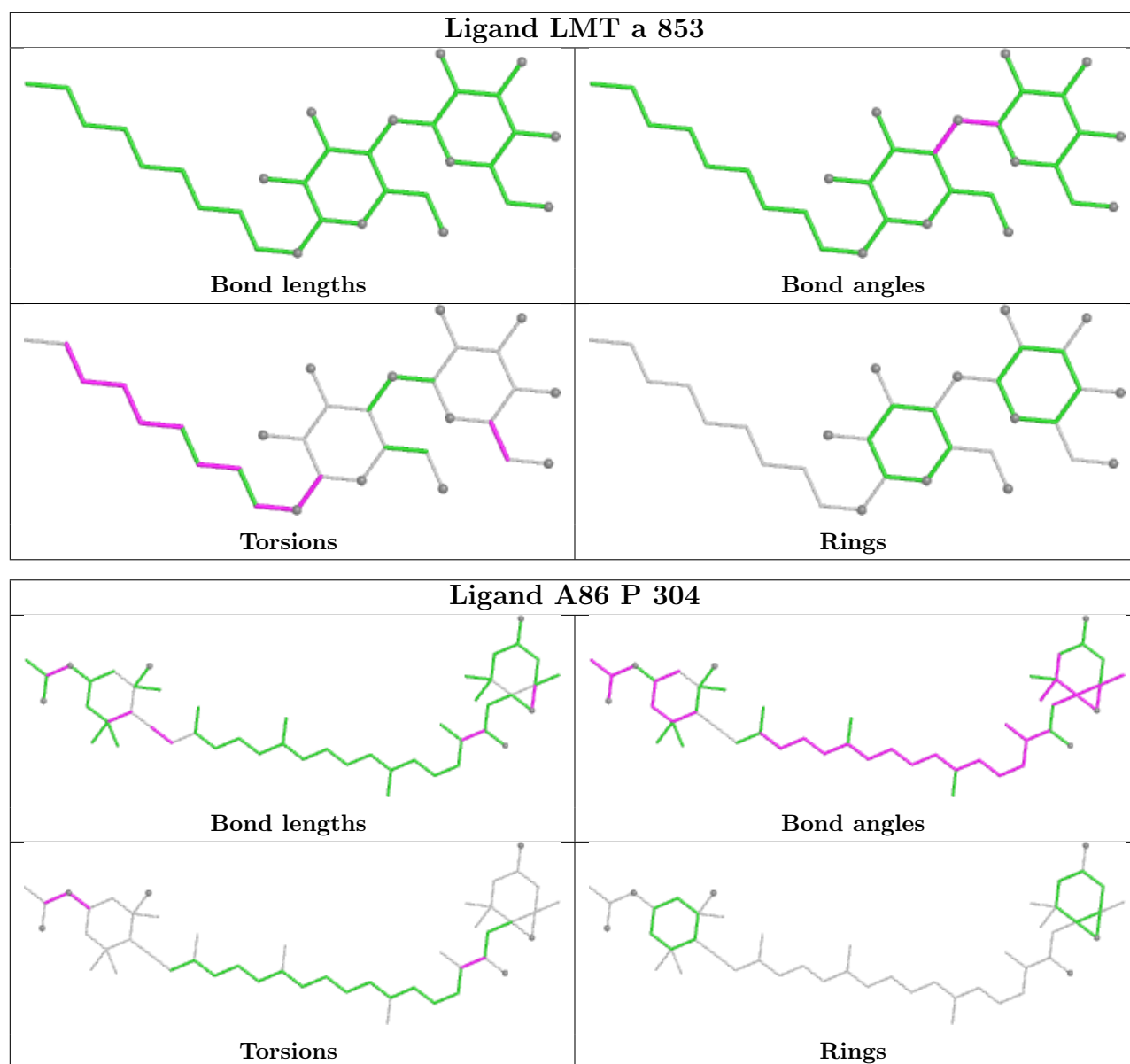


## Ligand CLA b 829

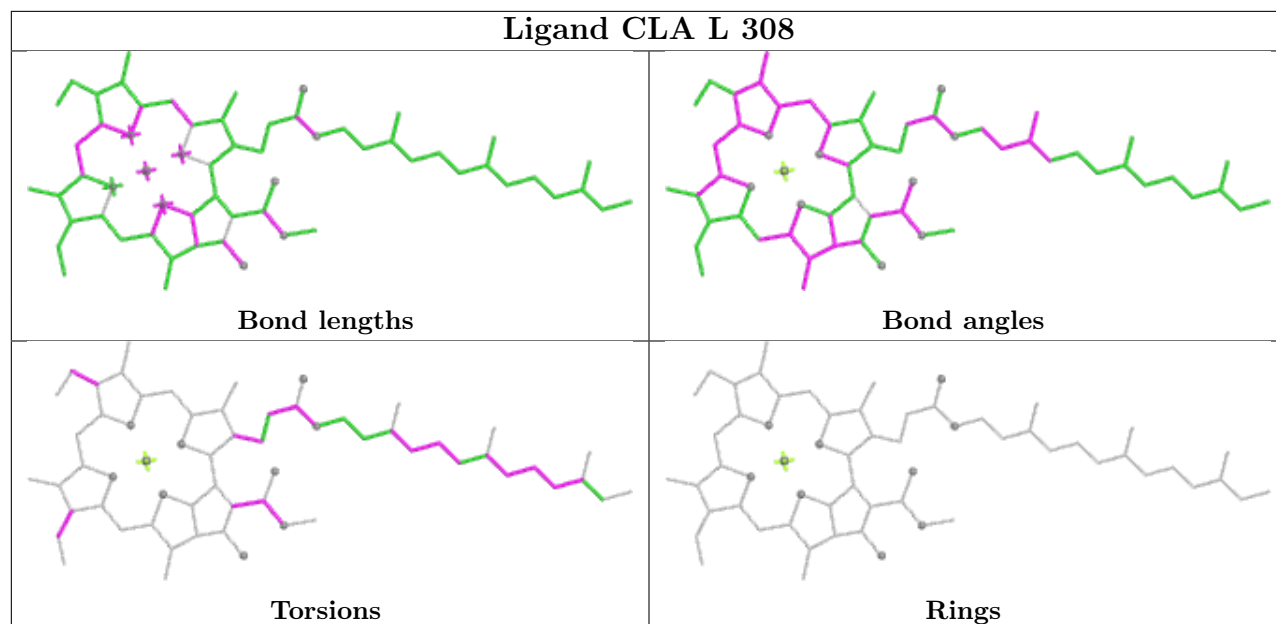


## Ligand KC1 O 313

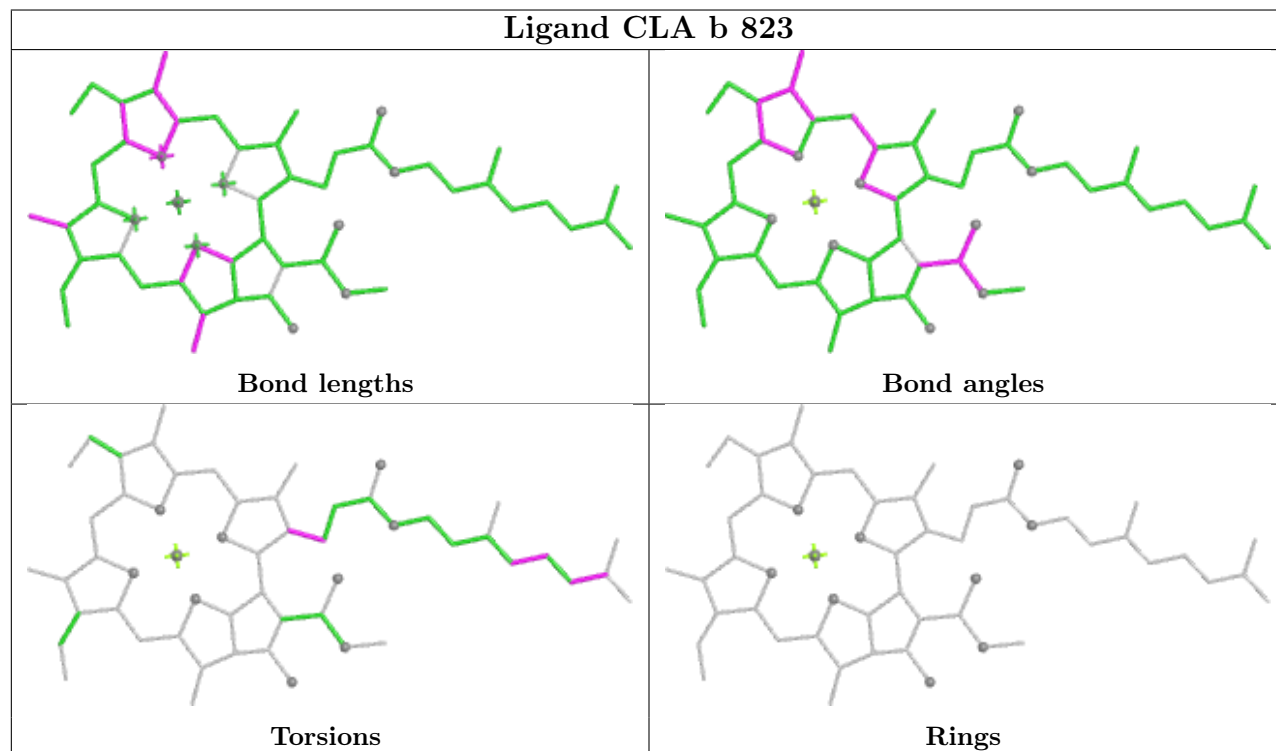


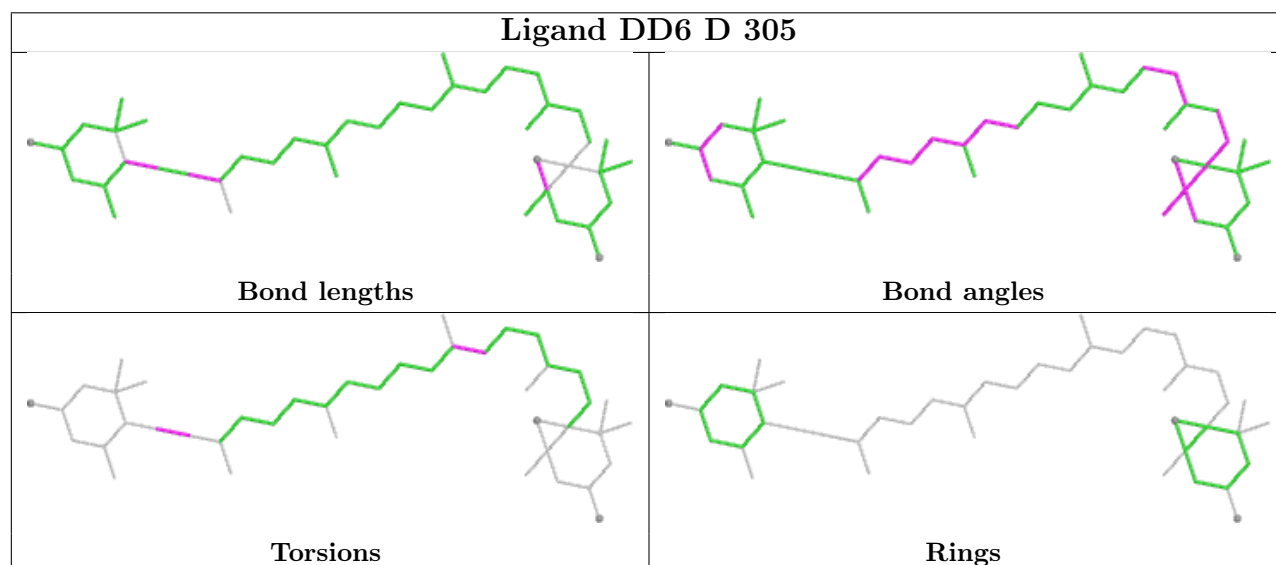
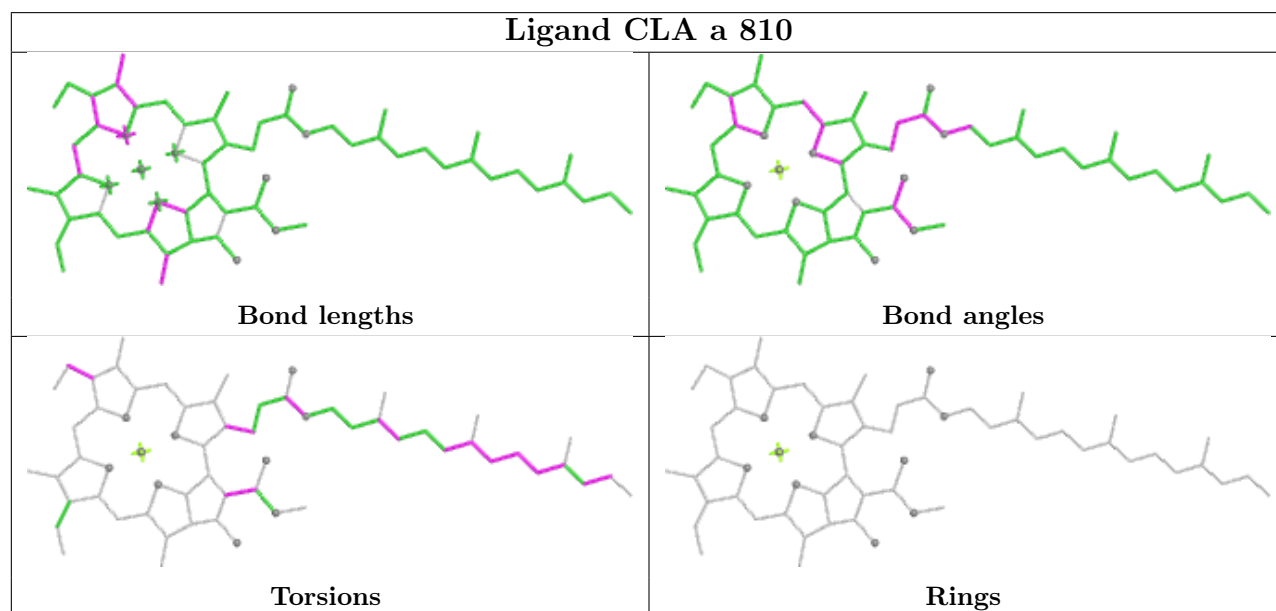
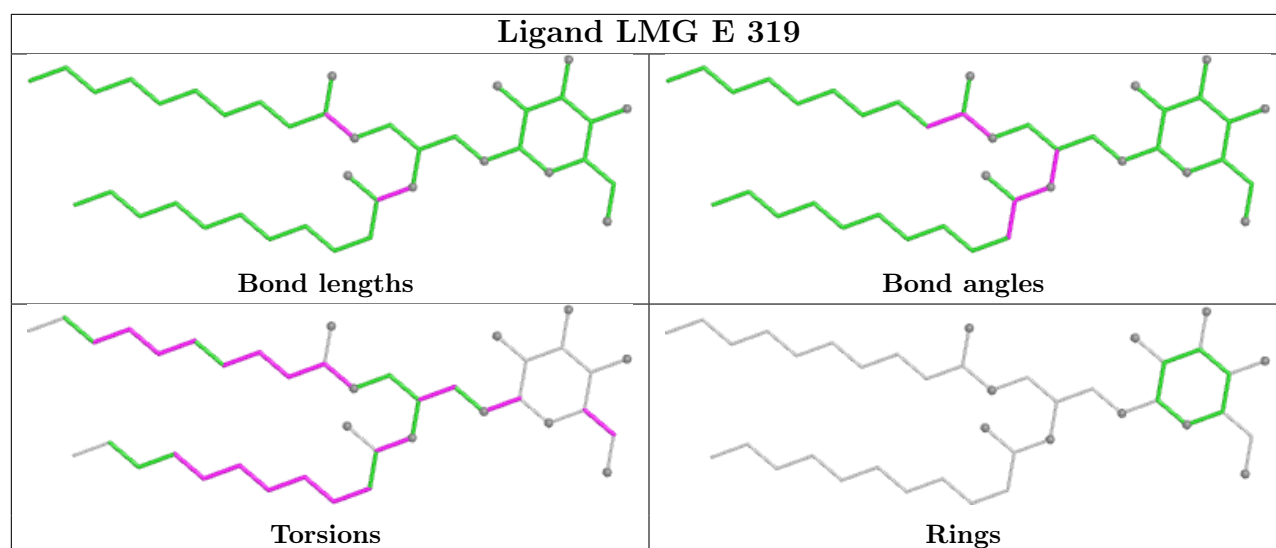


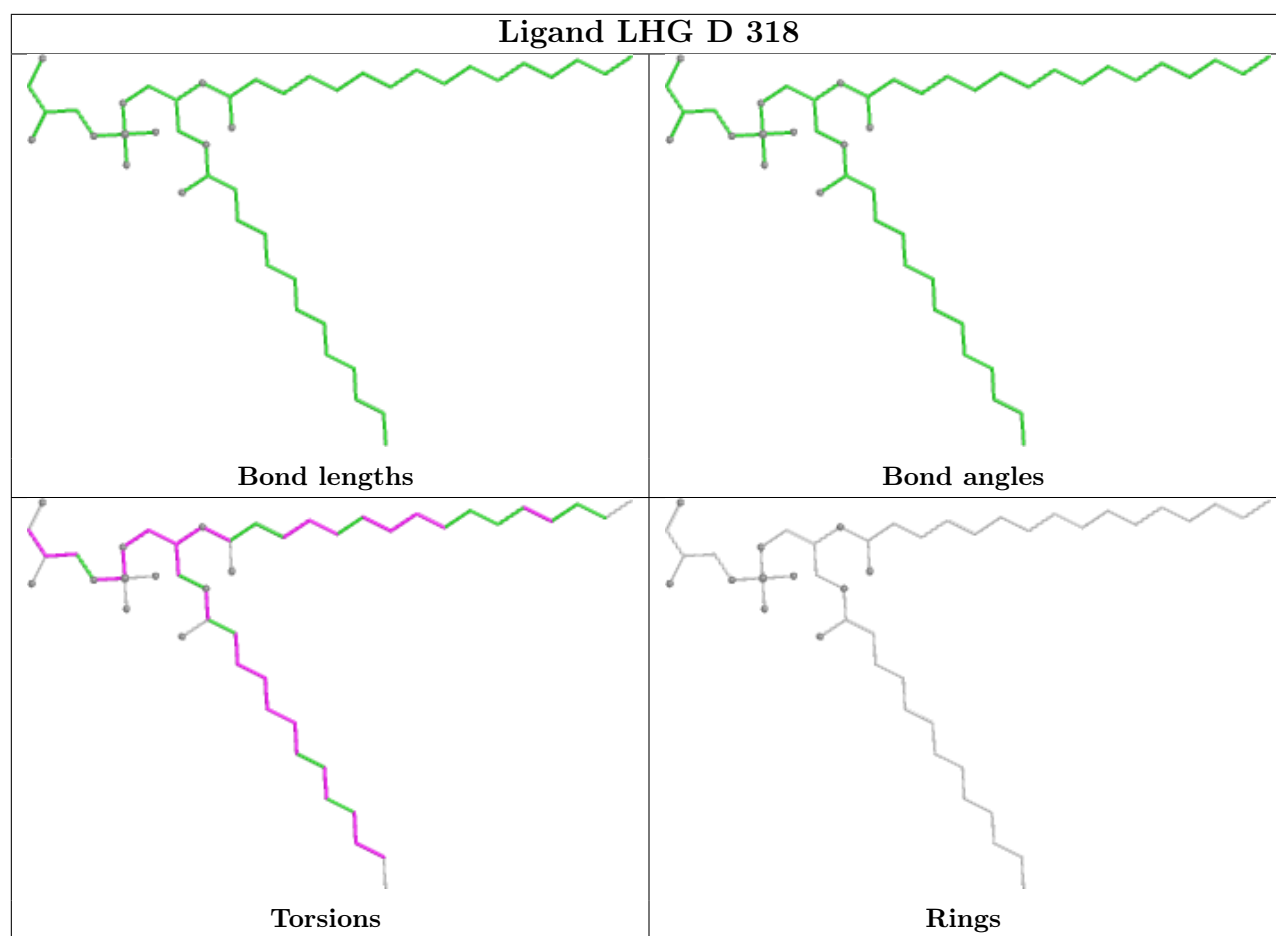
## Ligand CLA L 308



## Ligand CLA b 823

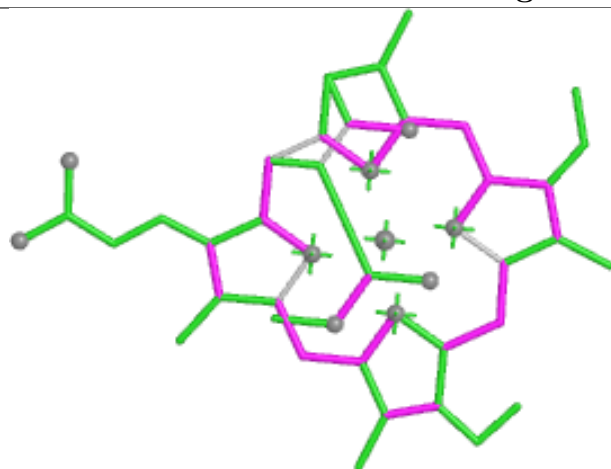




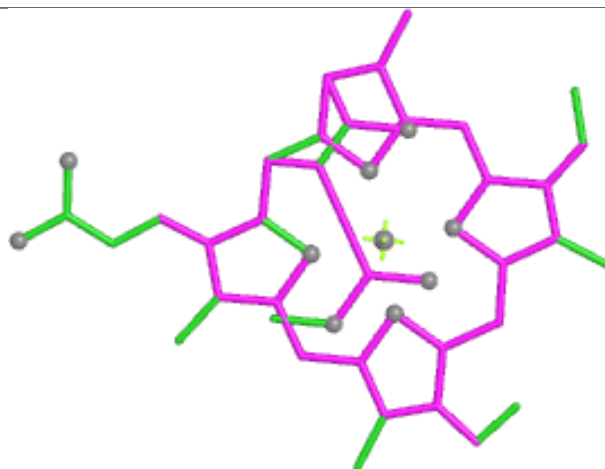




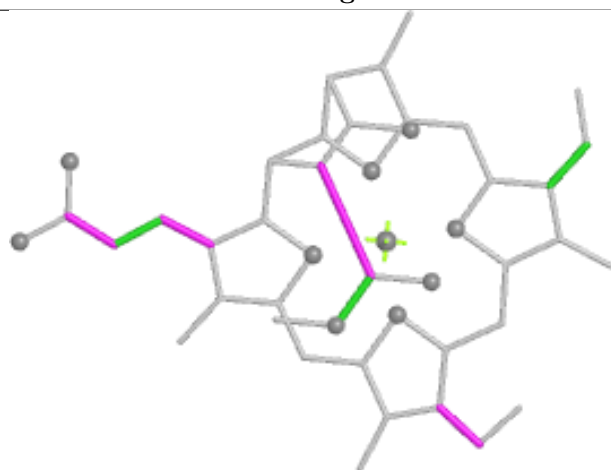
## Ligand KC1 C 213



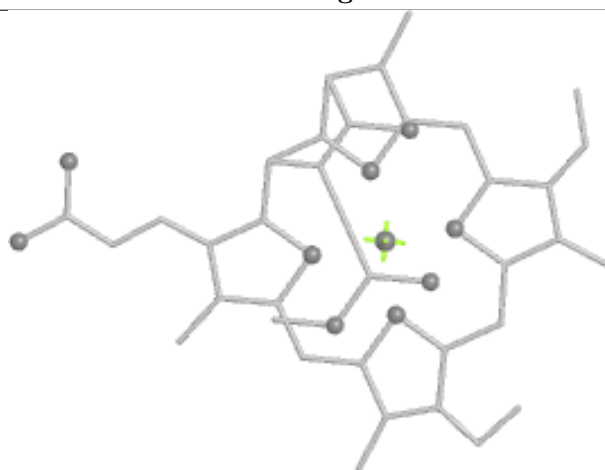
Bond lengths



Bond angles



Torsions



Rings

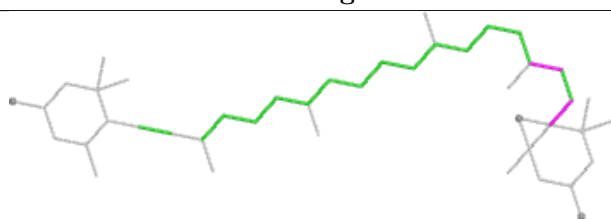
## Ligand DD6 H 302



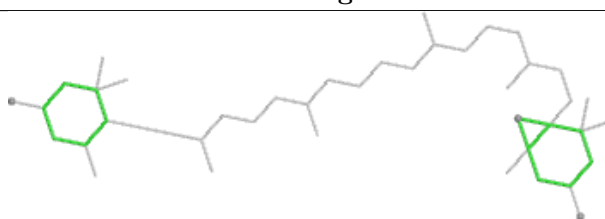
Bond lengths



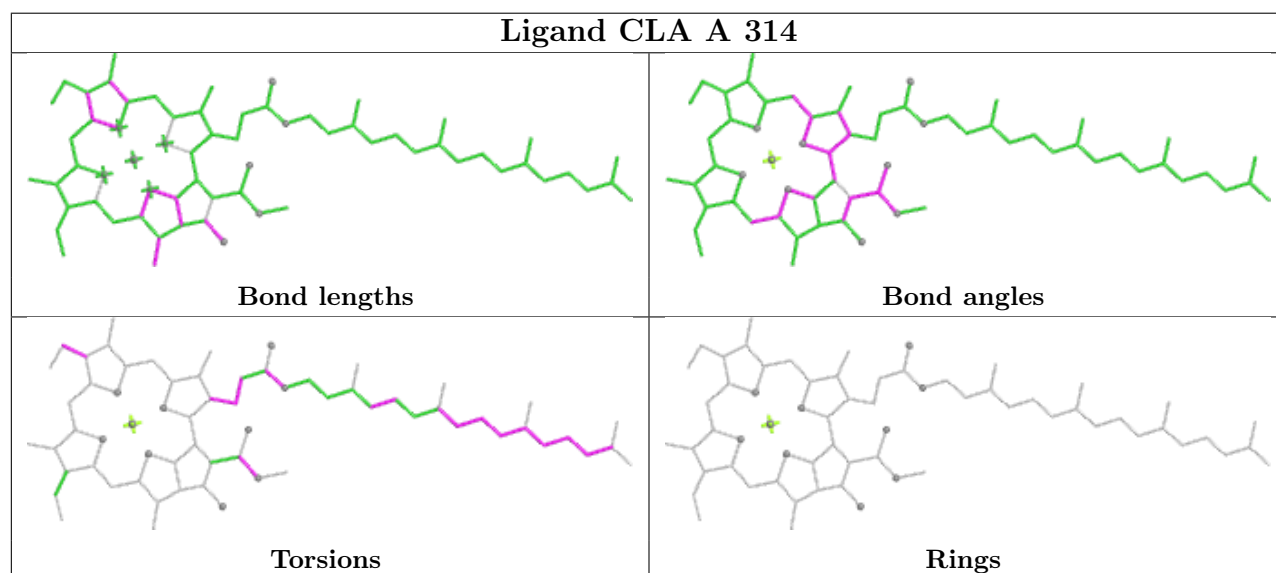
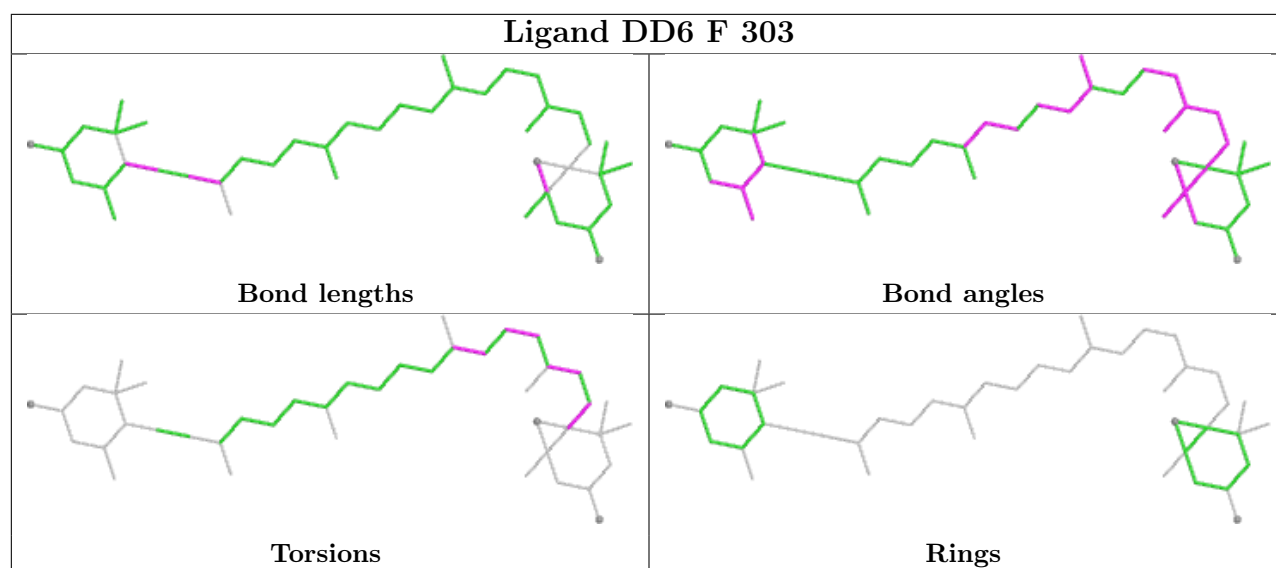
Bond angles



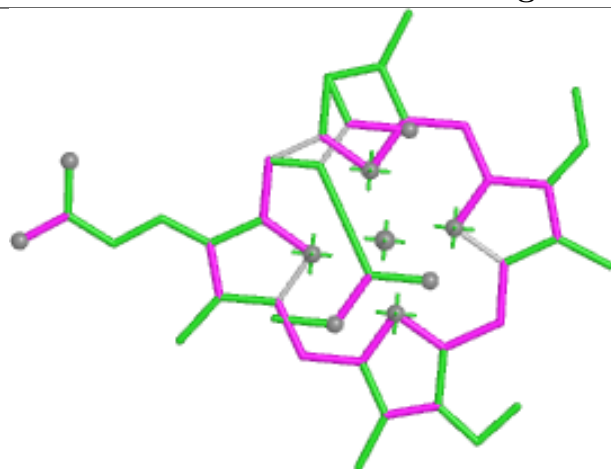
Torsions



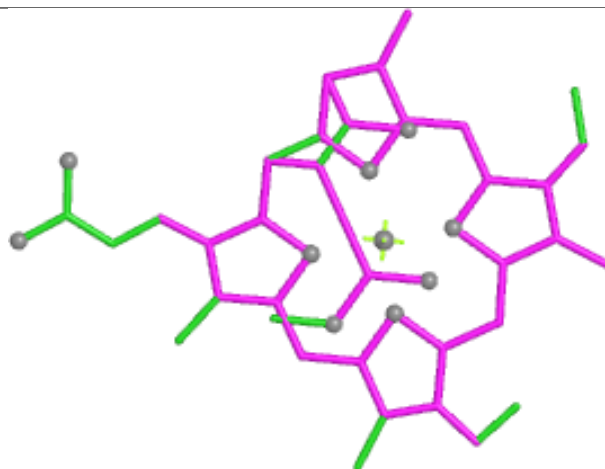
Rings



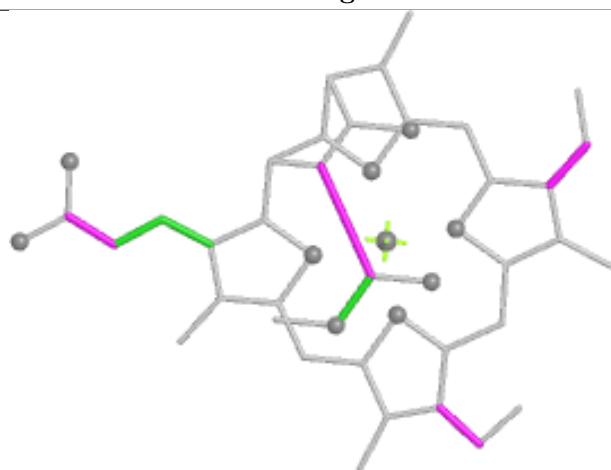
## Ligand KC1 F 308



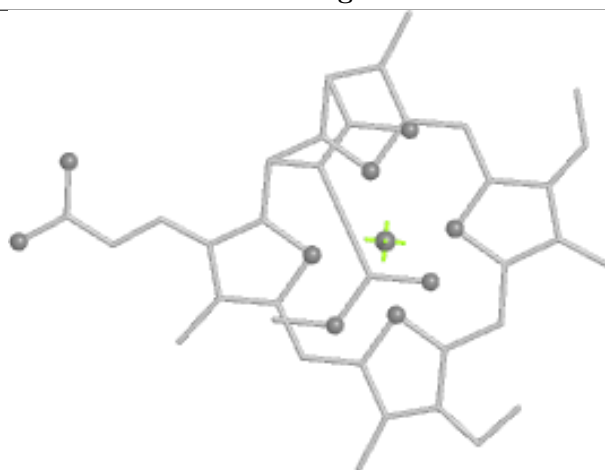
Bond lengths



Bond angles



Torsions

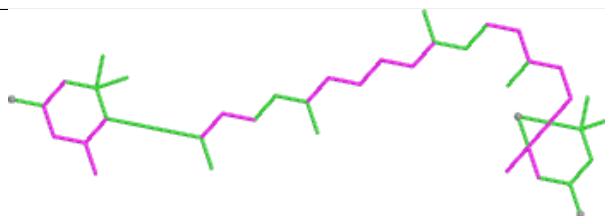


Rings

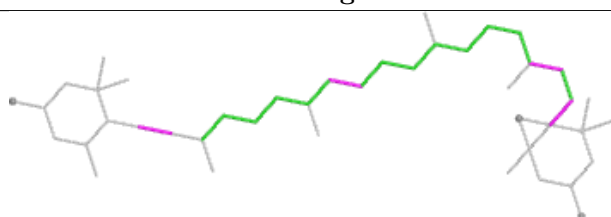
## Ligand DD6 J 304



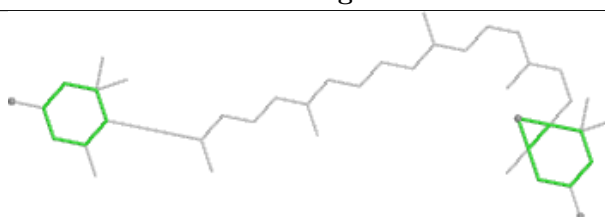
Bond lengths



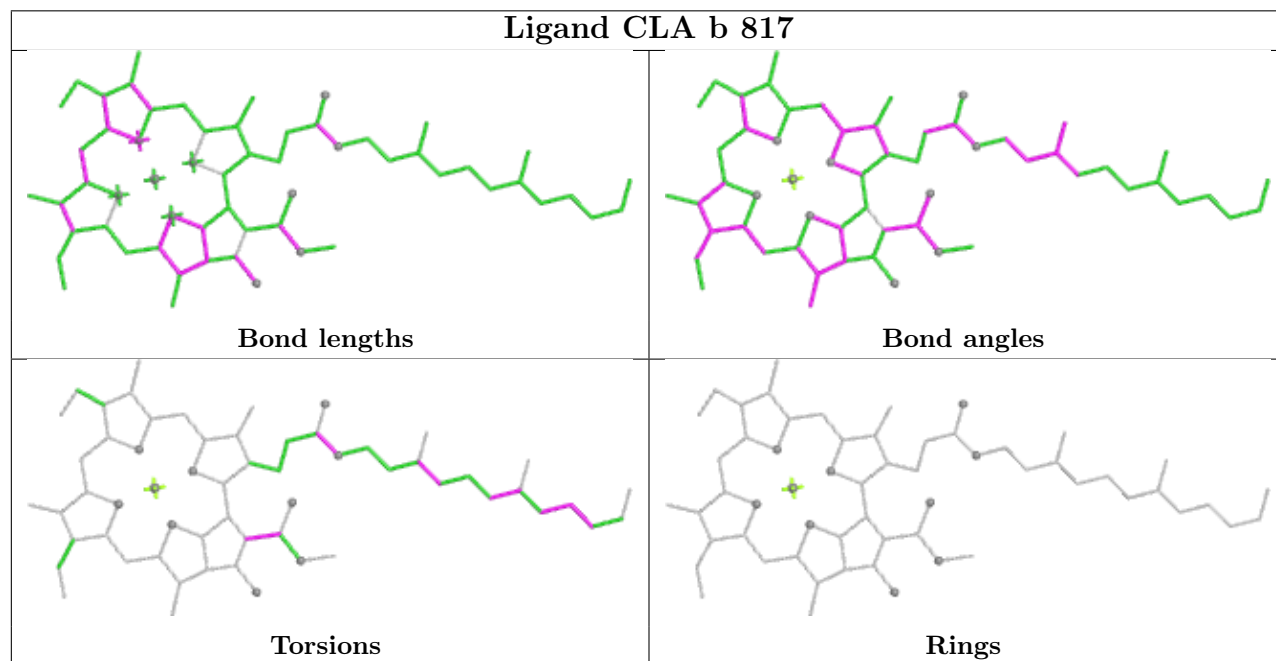
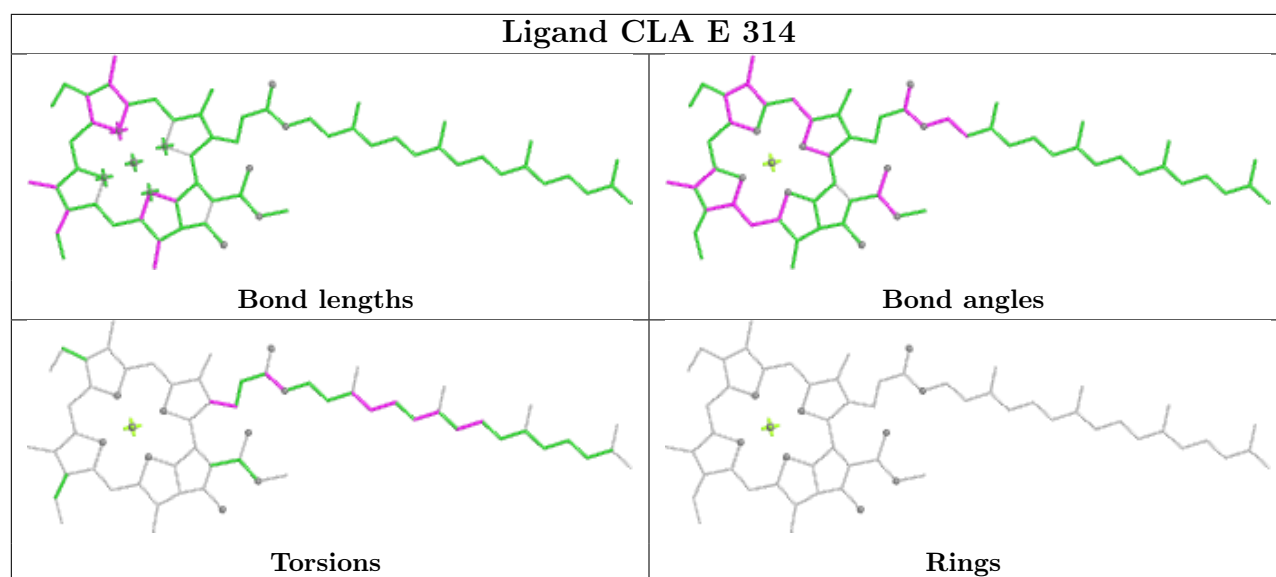
Bond angles

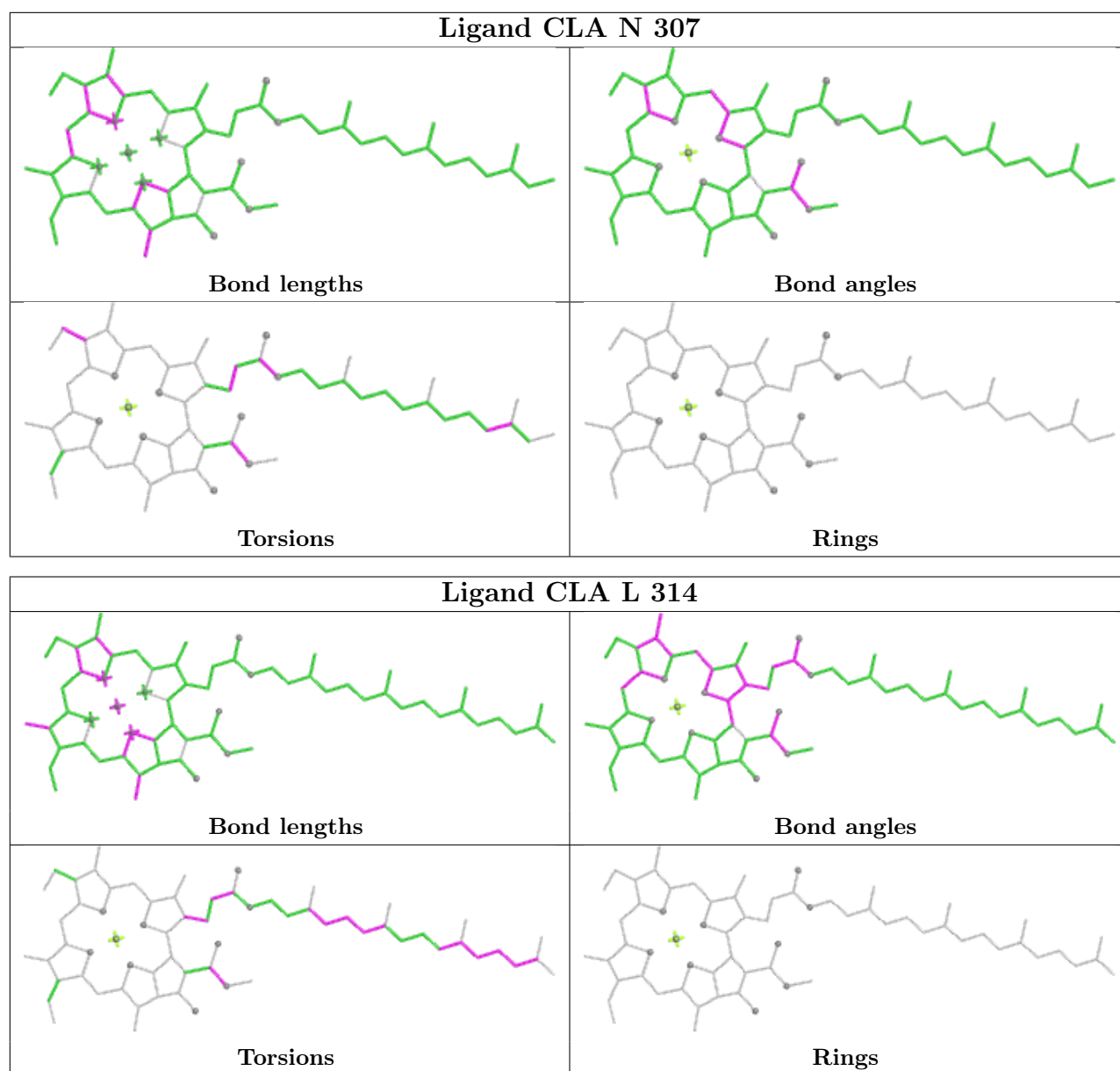


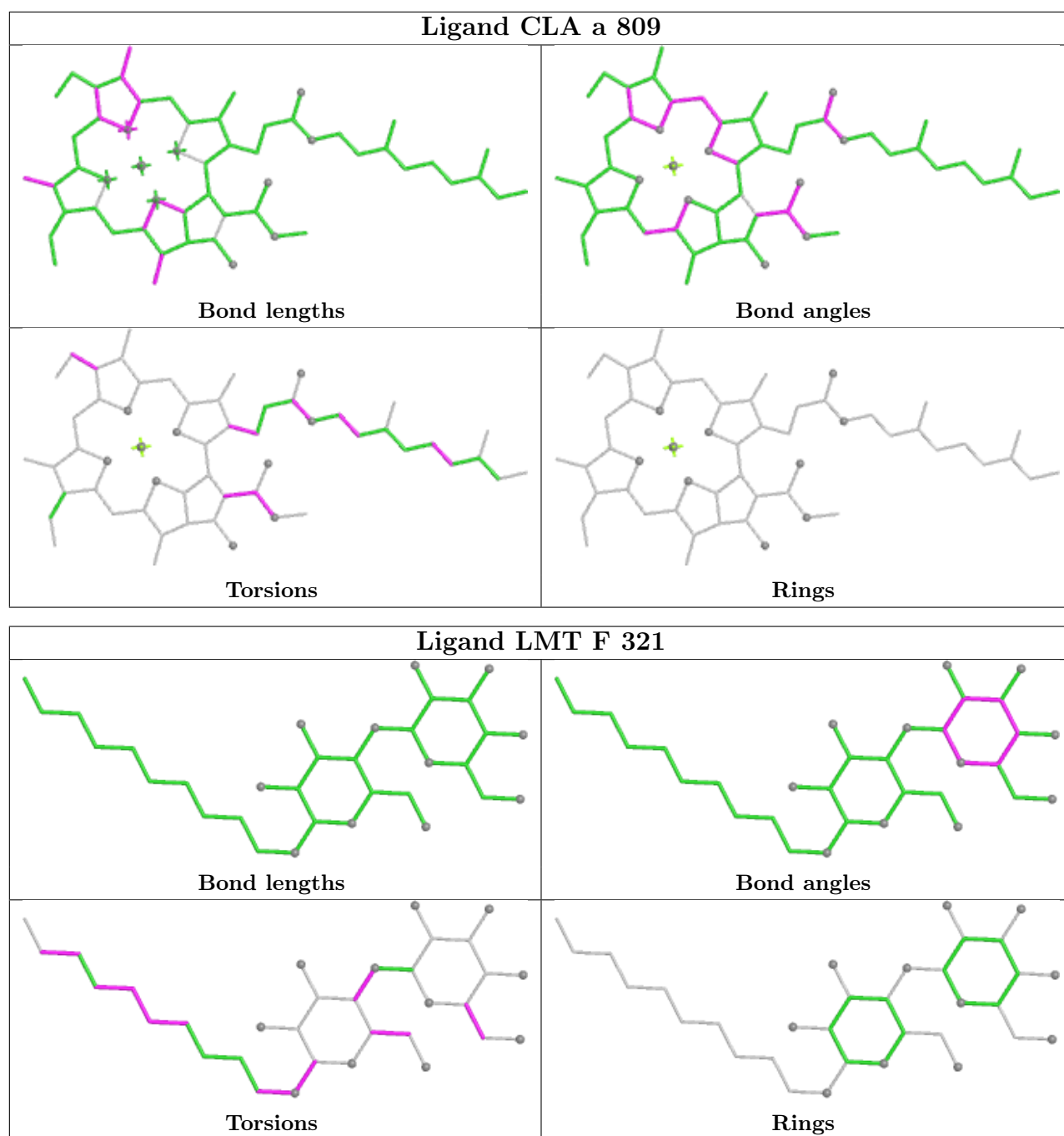
Torsions

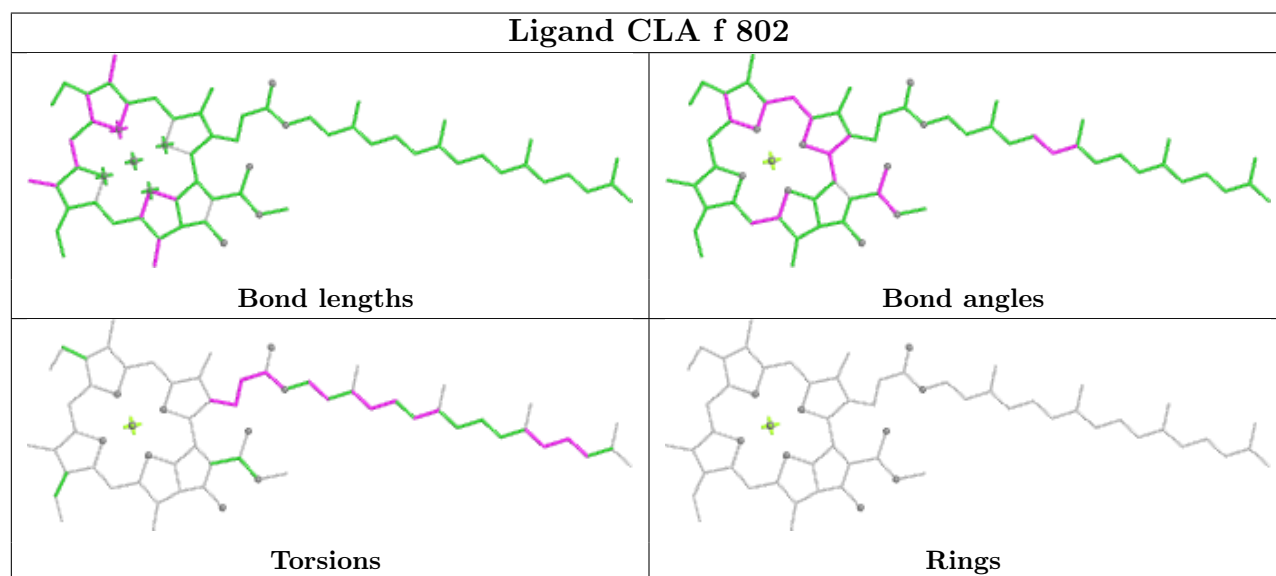
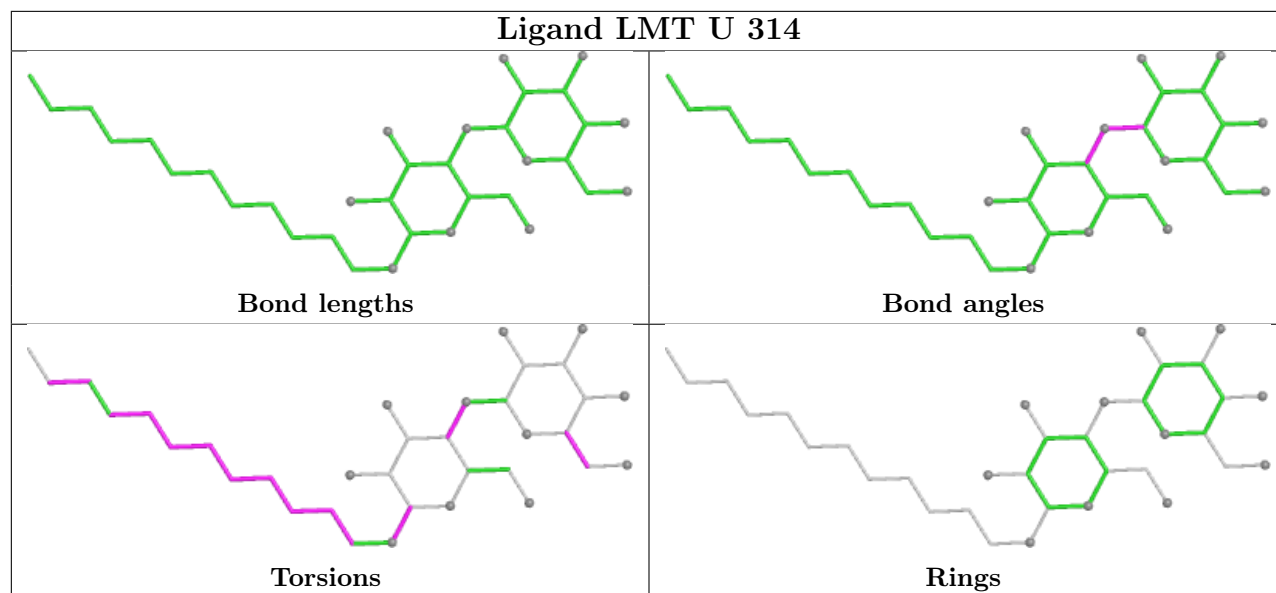


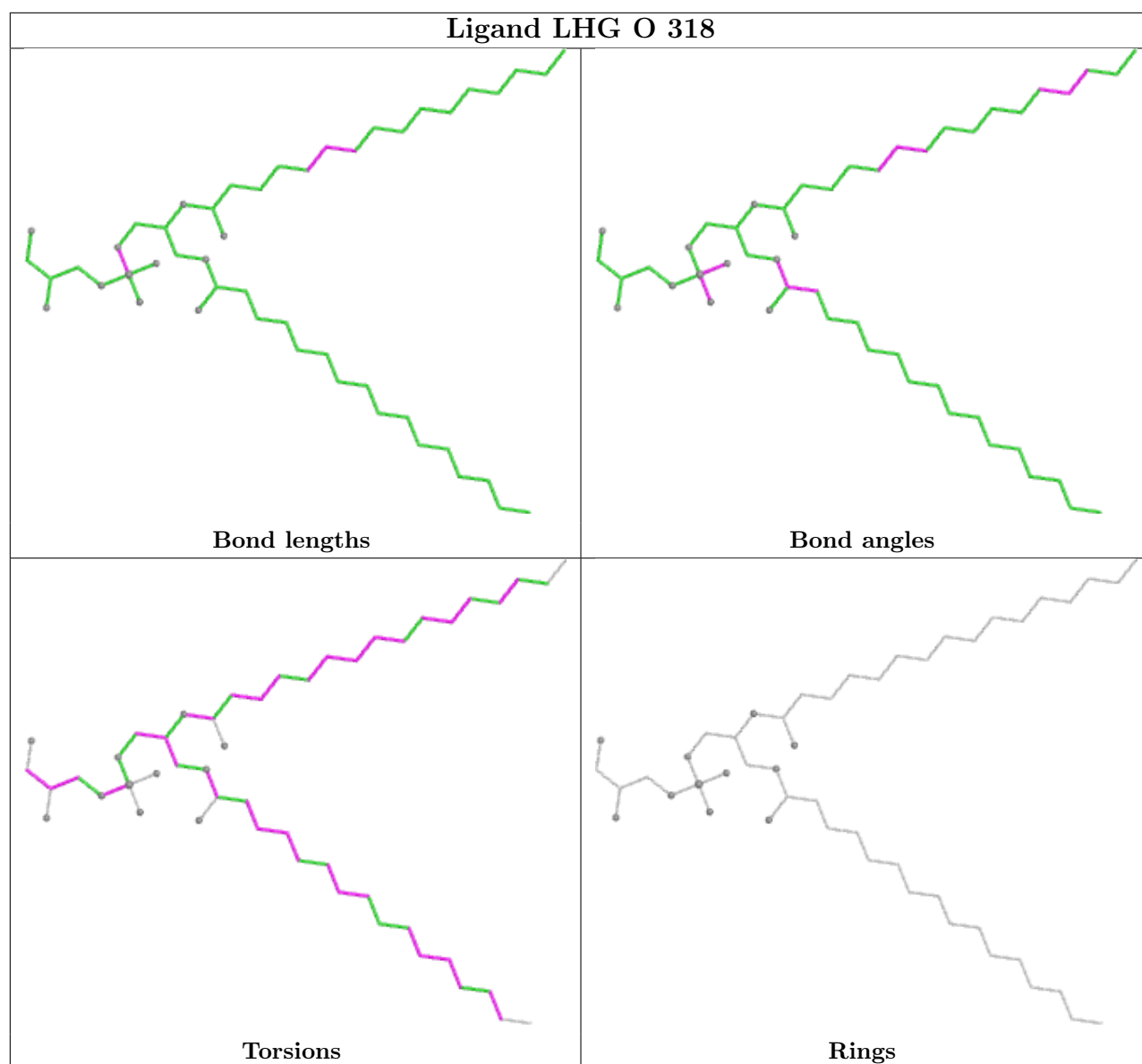
Rings



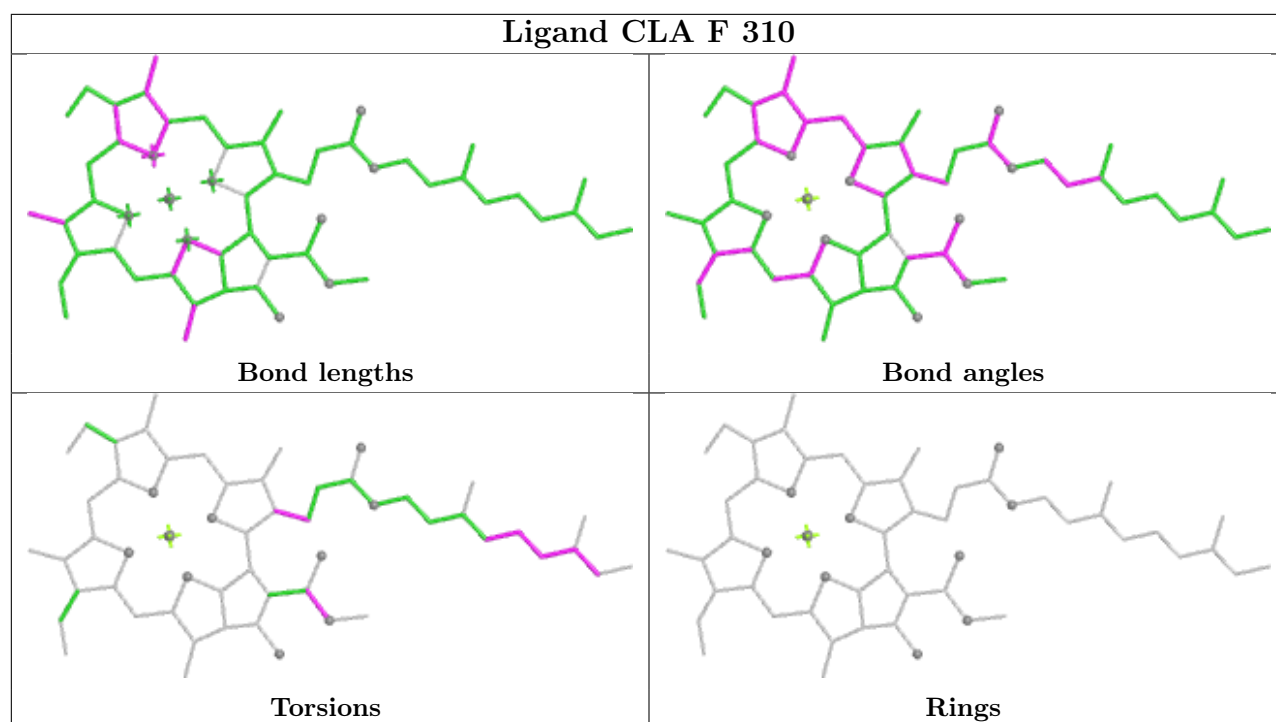




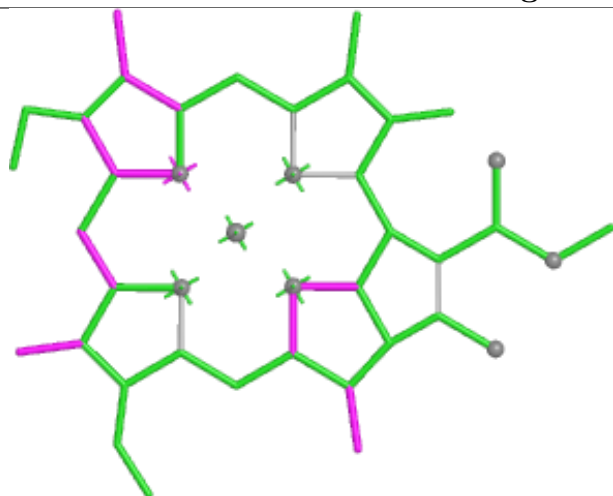




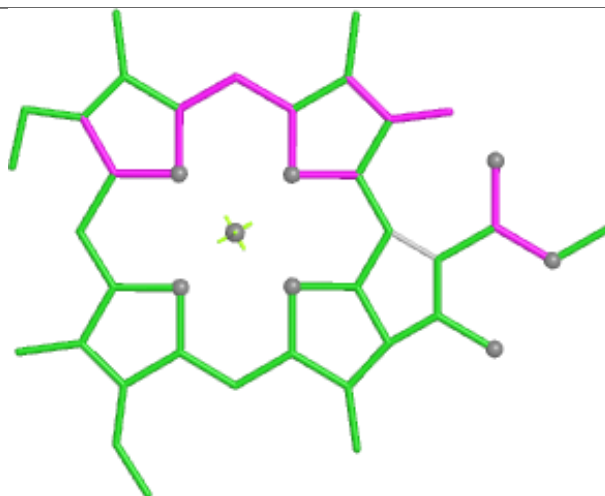




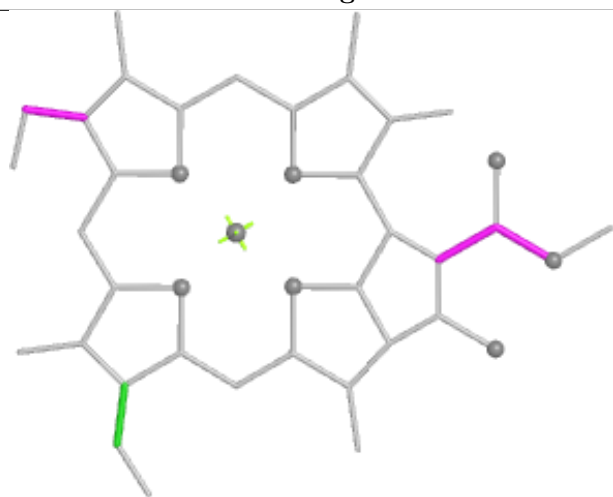
## Ligand CLA I 313



Bond lengths



Bond angles

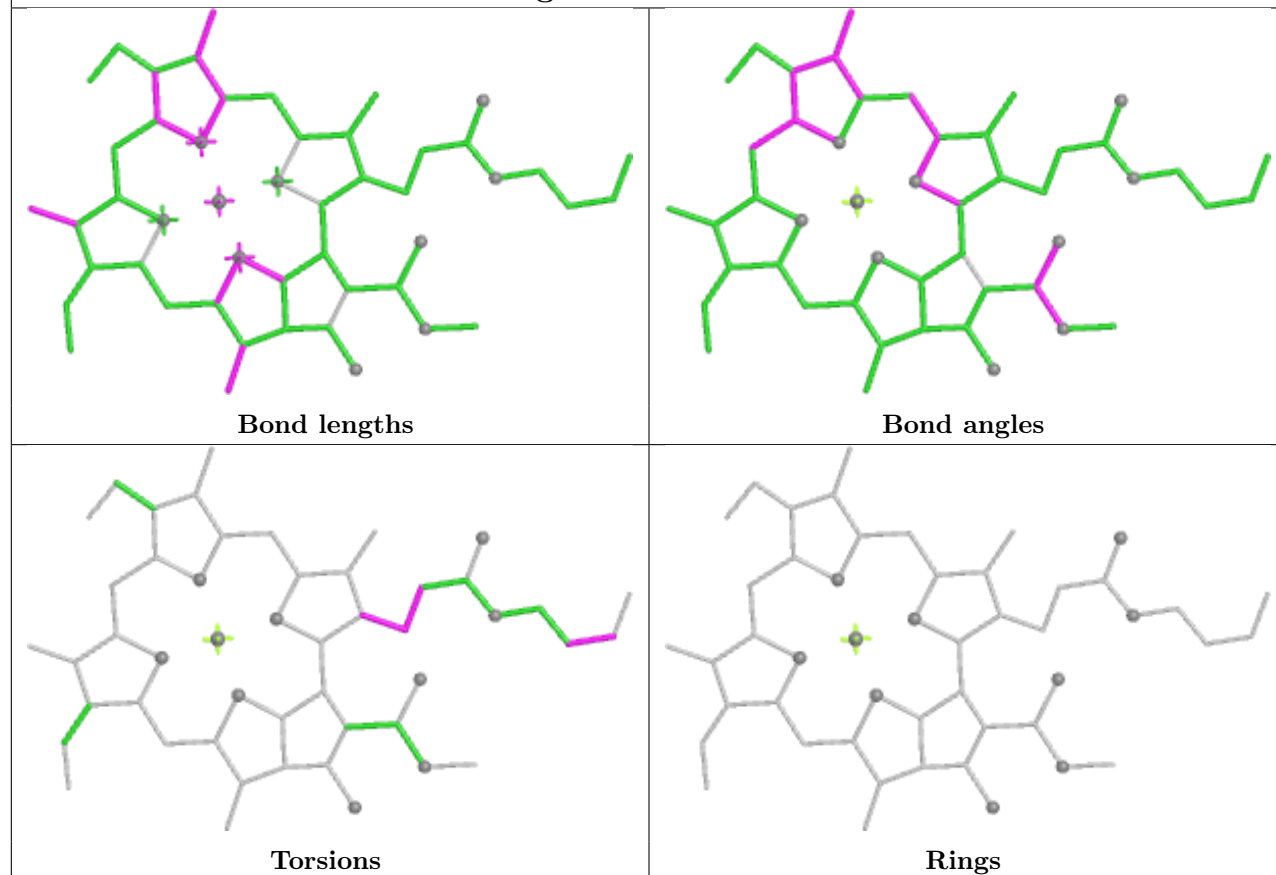


Torsions

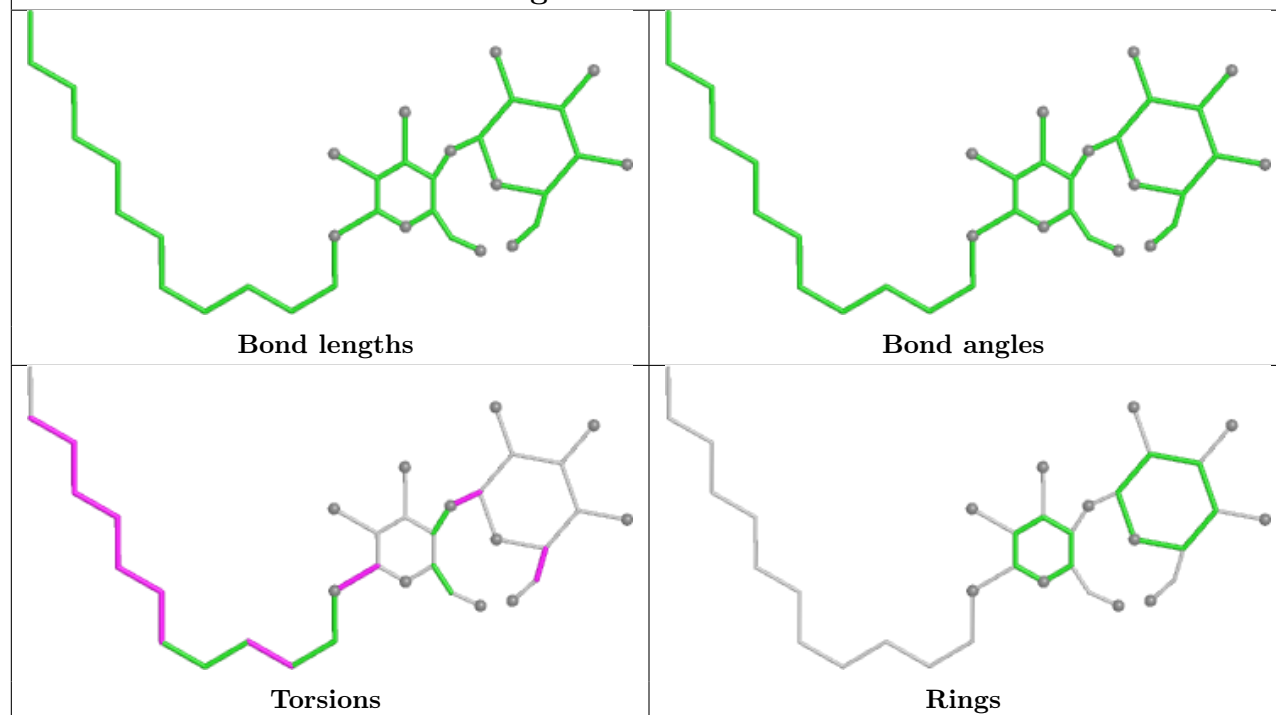


Rings

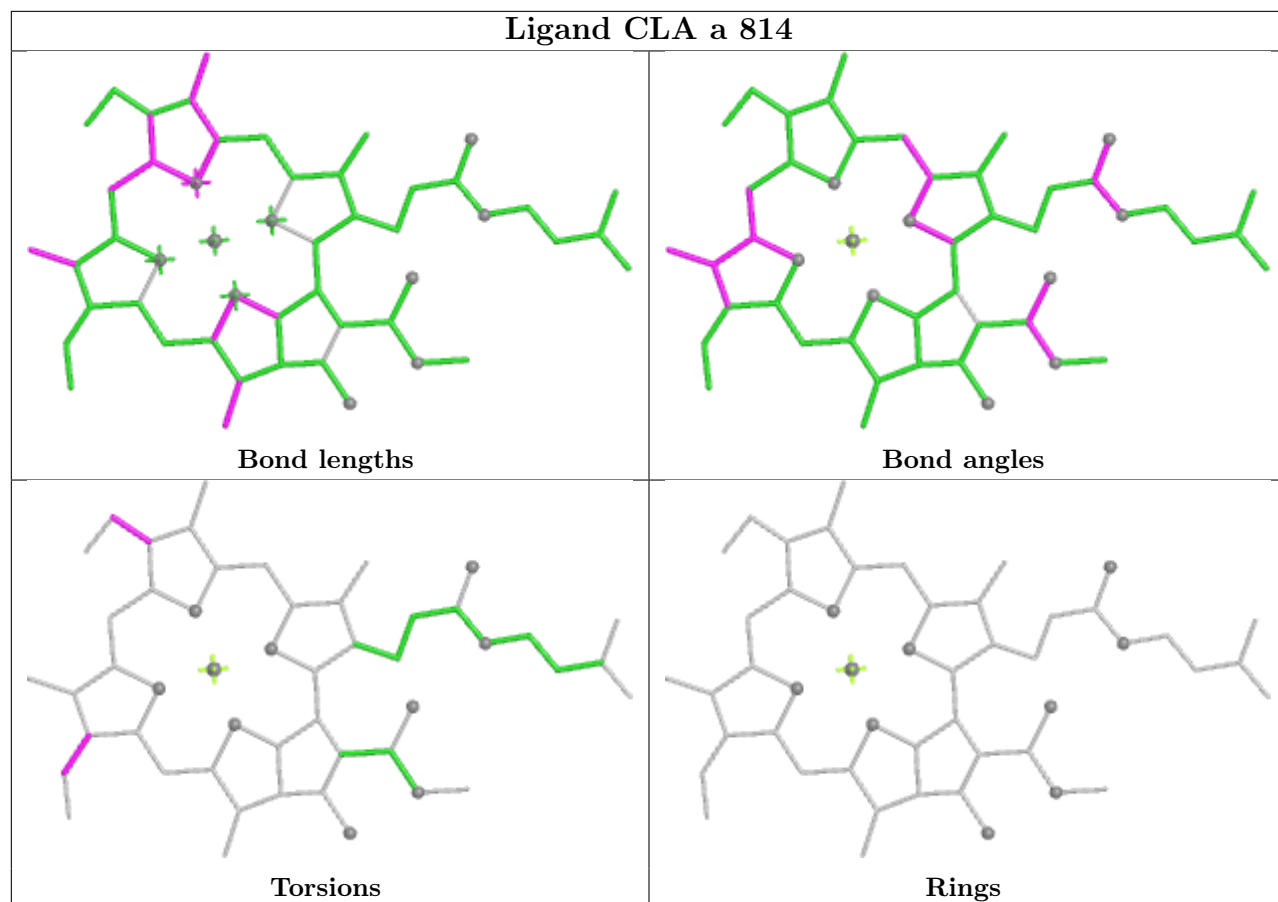
## Ligand CLA a 821



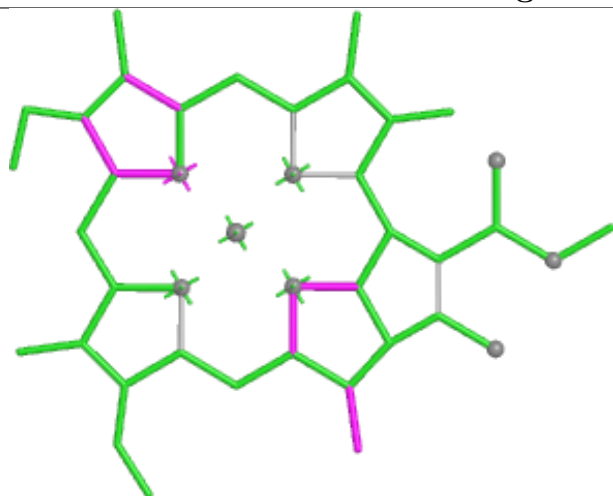
## Ligand LMT E 320



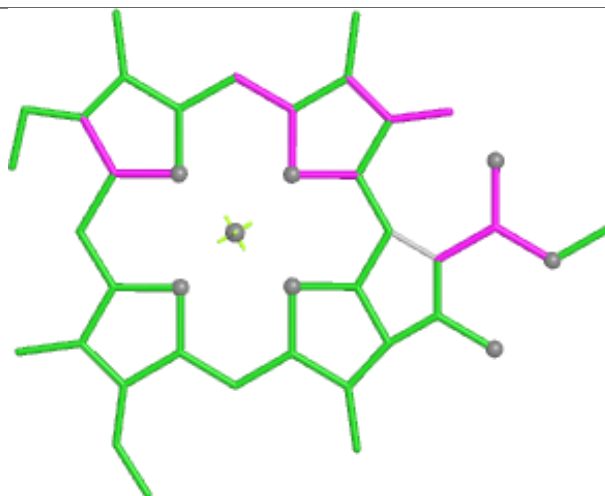
## Ligand CLA a 814



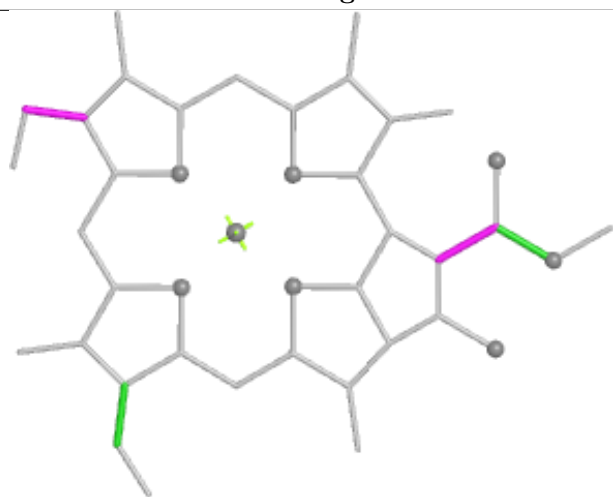
## Ligand CLA L 316



Bond lengths



Bond angles

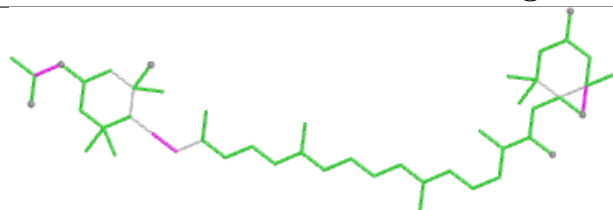


Torsions

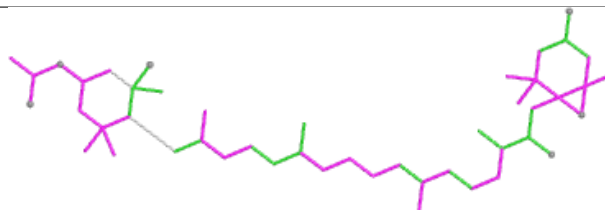


Rings

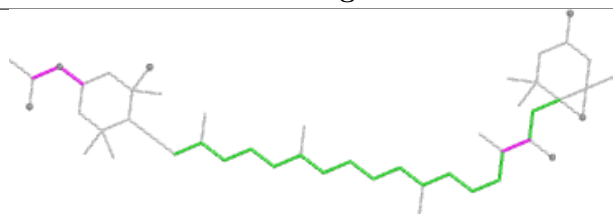
## Ligand A86 F 307



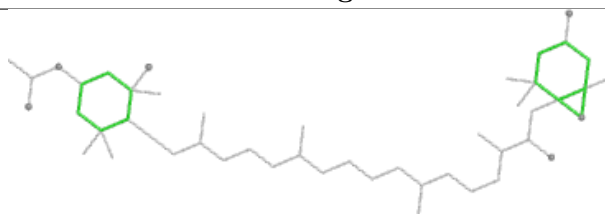
Bond lengths



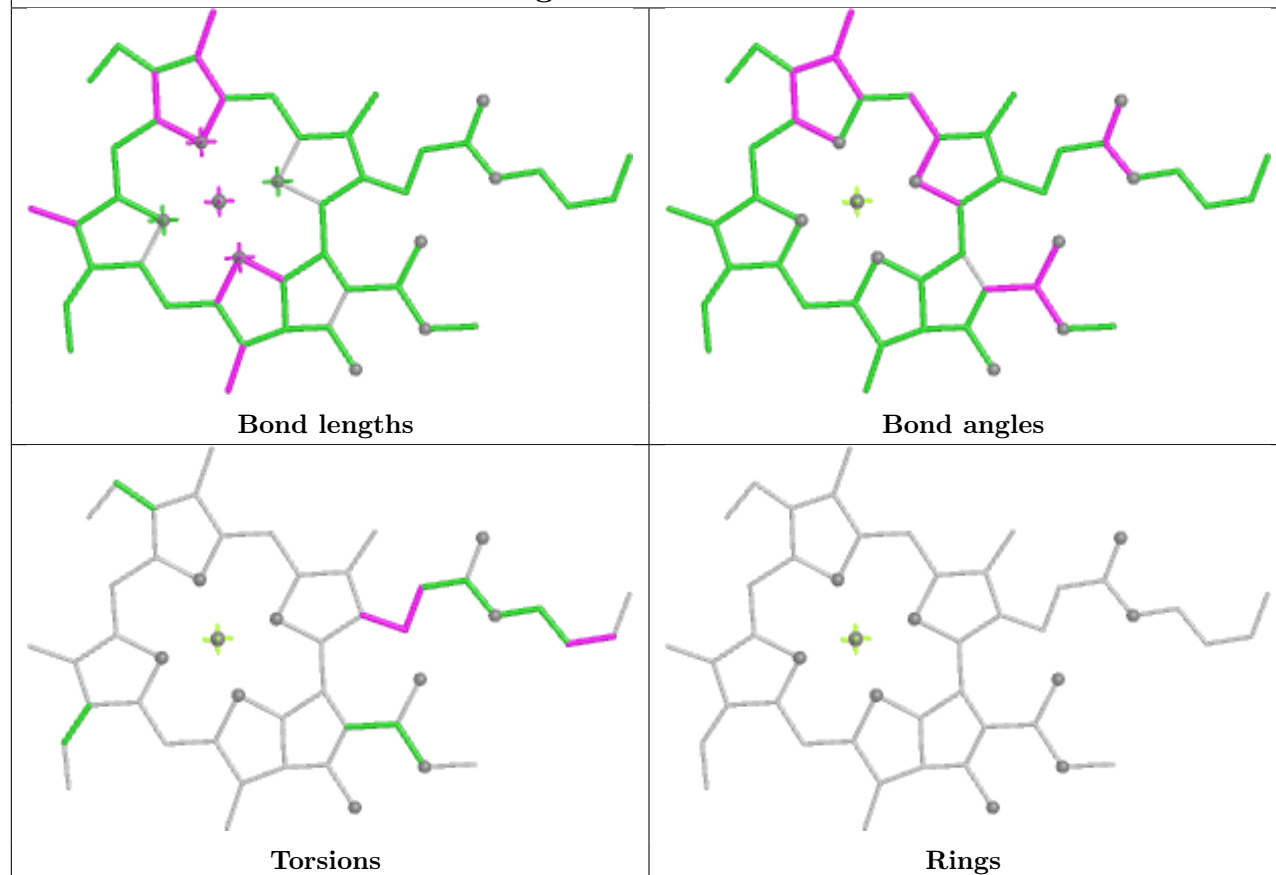
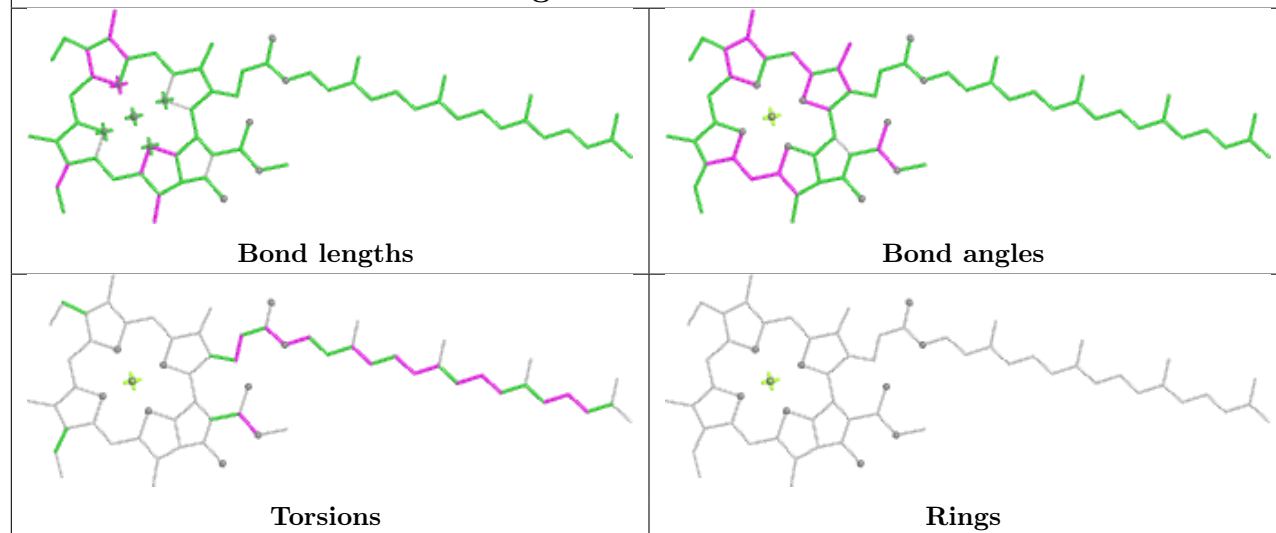
Bond angles



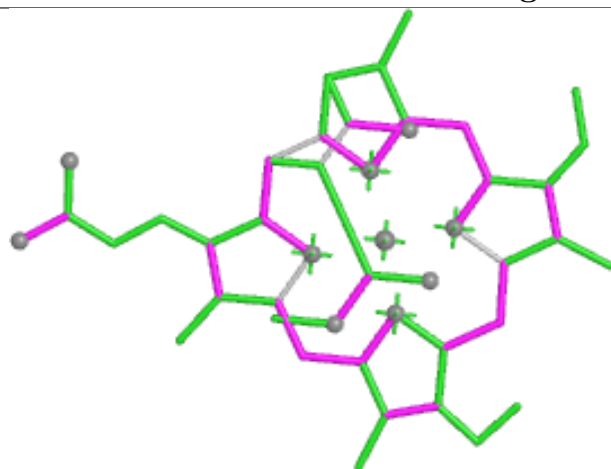
Torsions



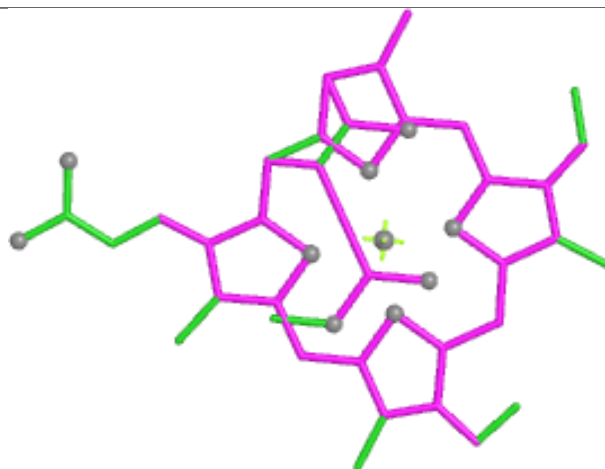
Rings

**Ligand CLA b 832****Ligand CLA B 308**

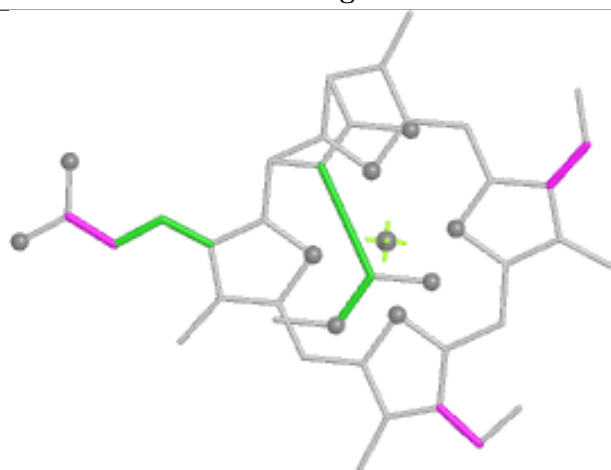
## Ligand KC1 J 314



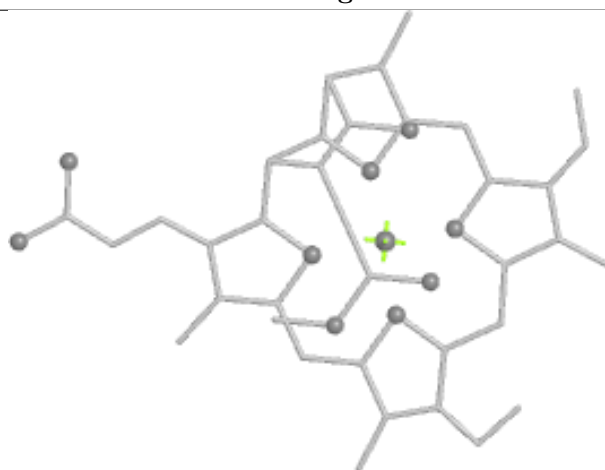
Bond lengths



Bond angles

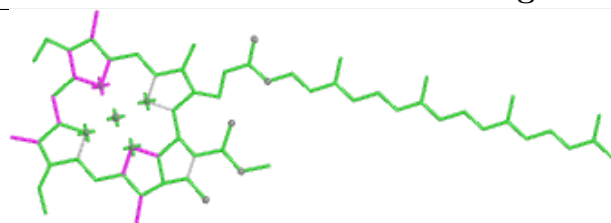


Torsions

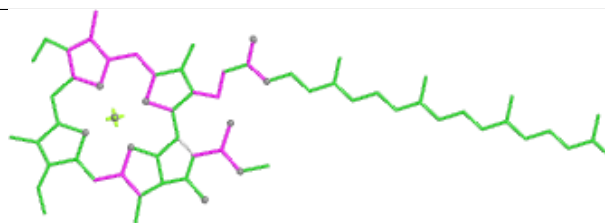


Rings

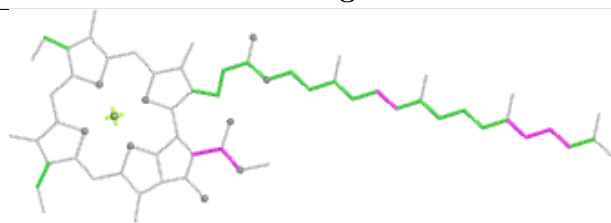
## Ligand CLA b 837



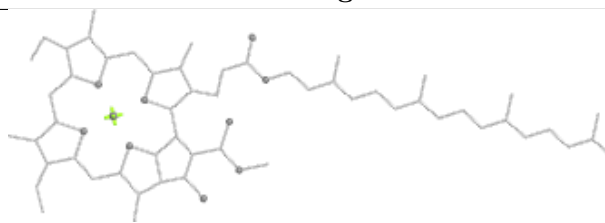
Bond lengths



Bond angles

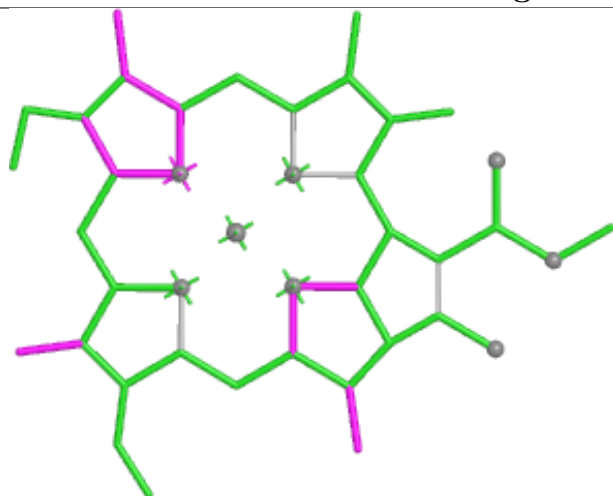


Torsions

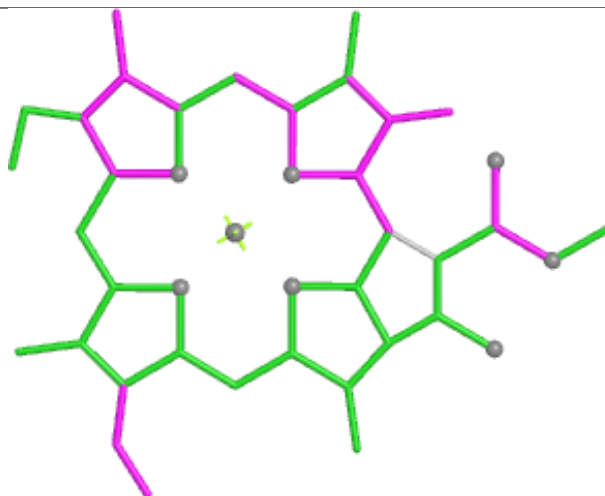


Rings

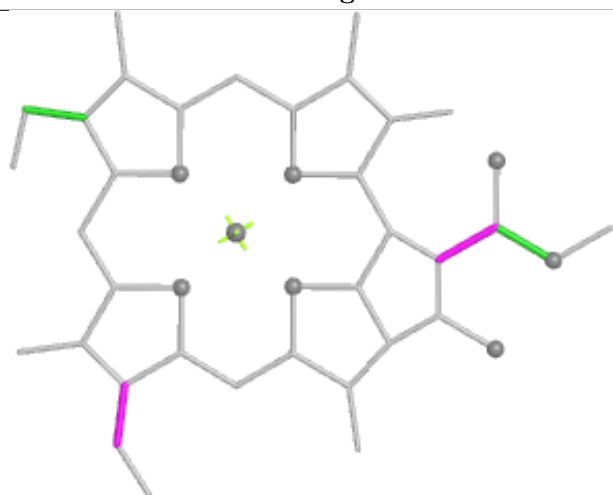
## Ligand CLA D 315



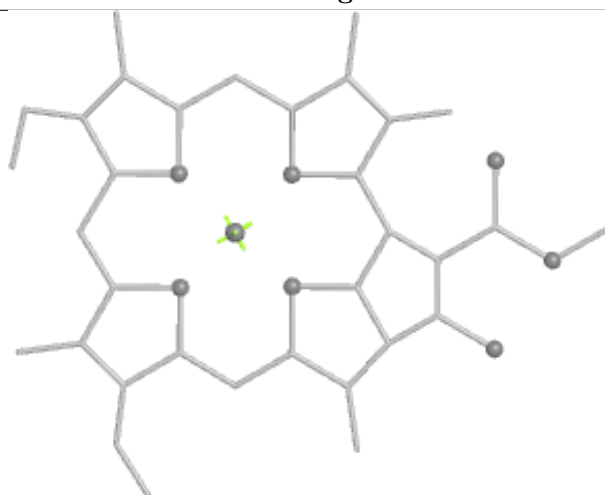
Bond lengths



Bond angles

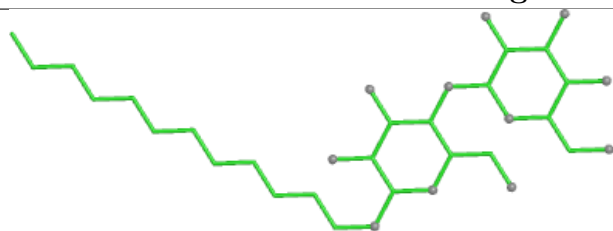


Torsions

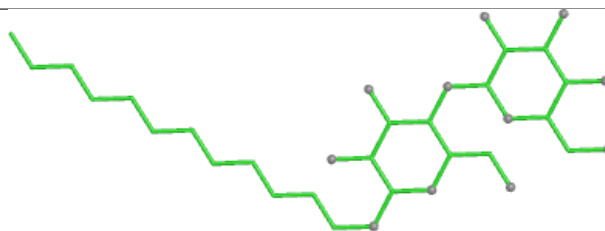


Rings

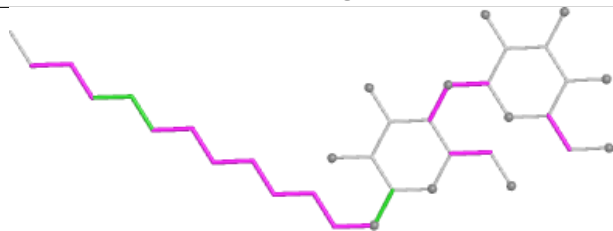
## Ligand LMT G 323



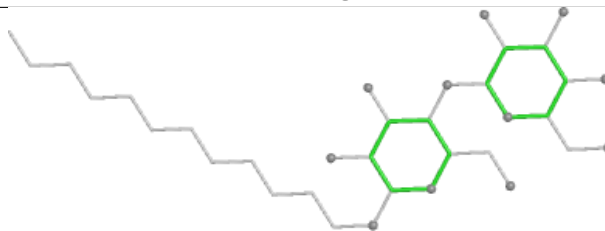
Bond lengths



Bond angles



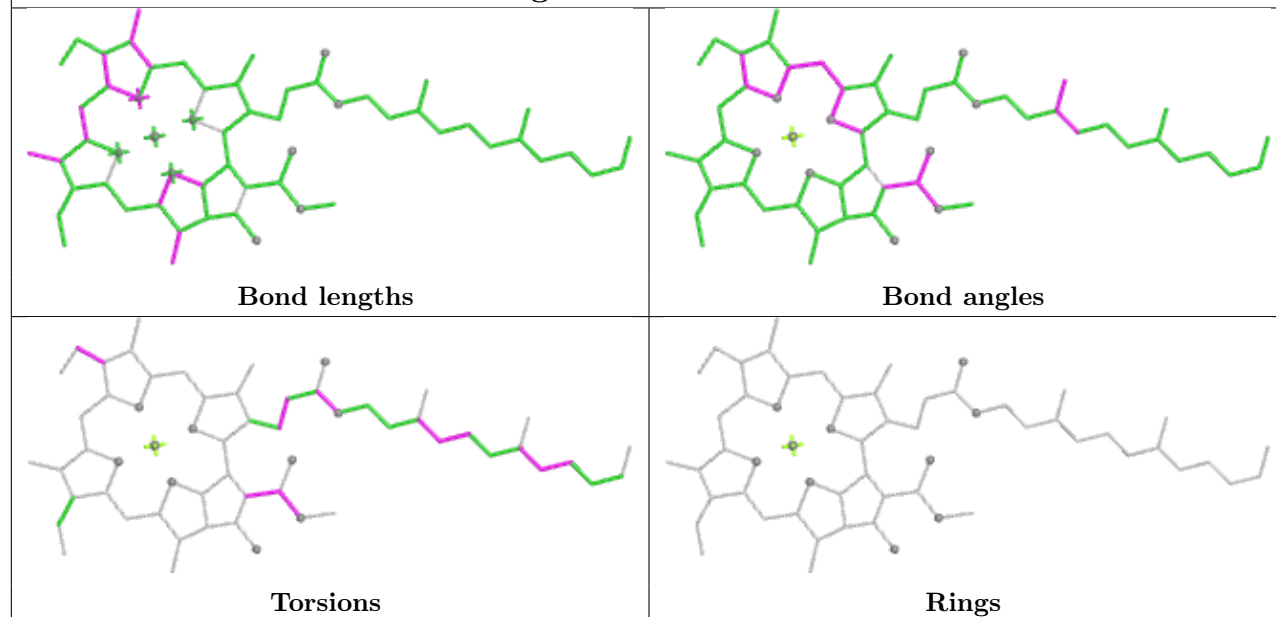
Torsions



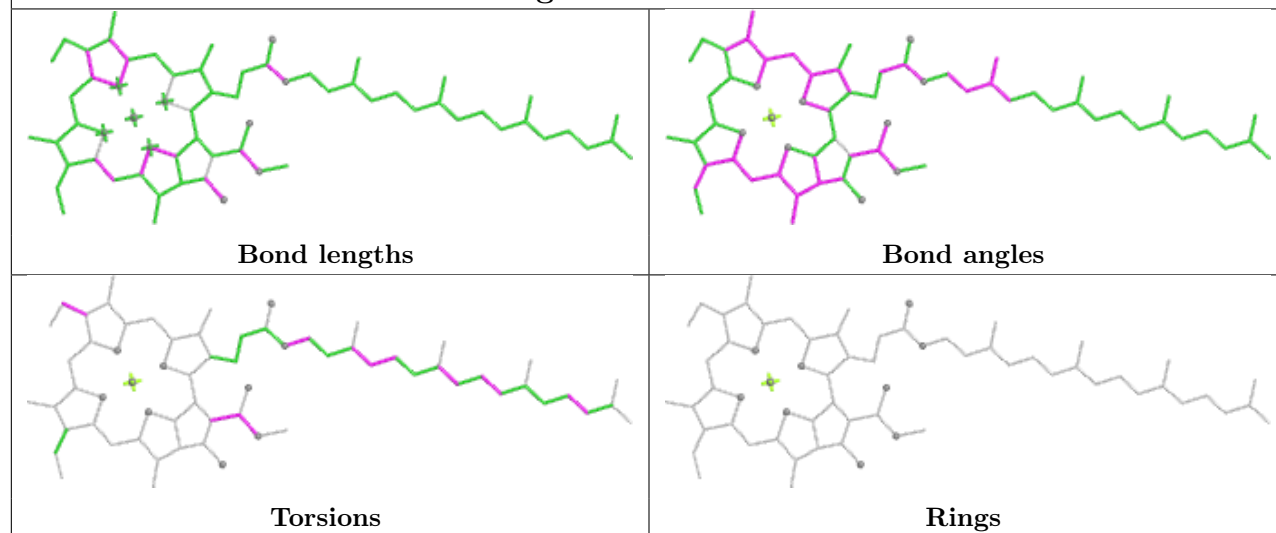
Rings



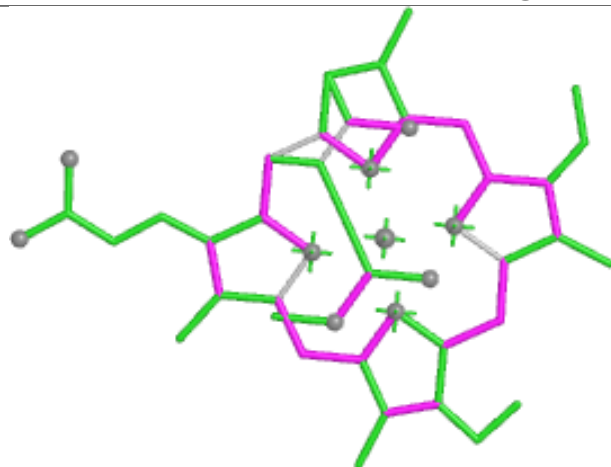
## Ligand CLA K 309



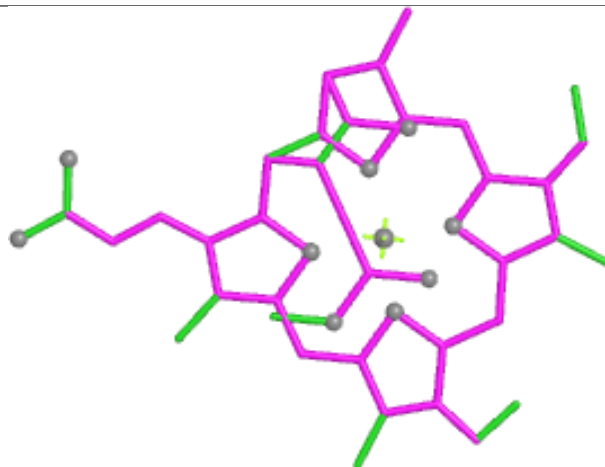
## Ligand CLA a 806



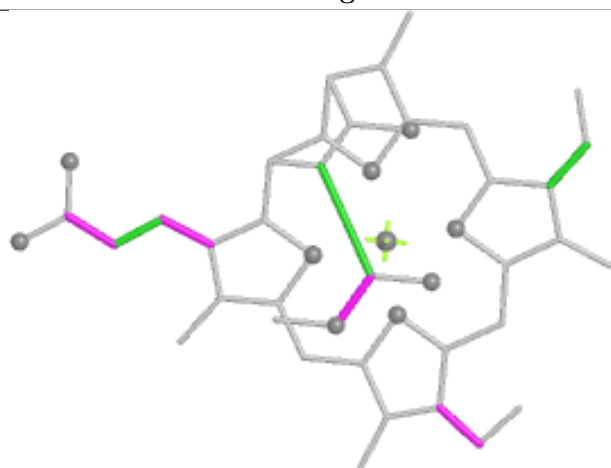
## Ligand KC1 T 315



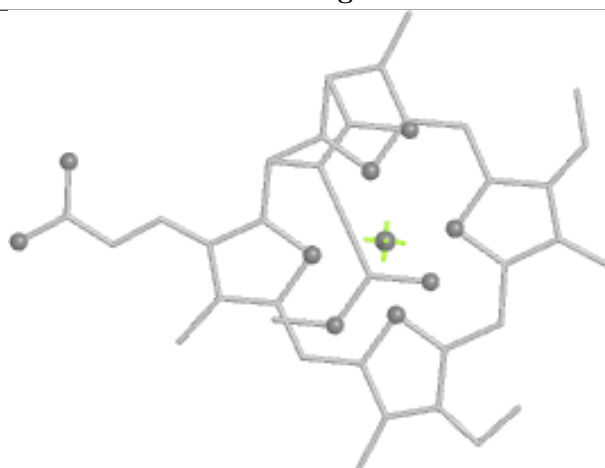
Bond lengths



Bond angles

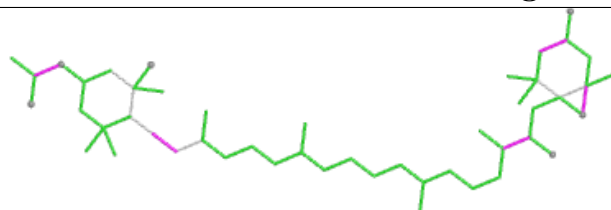


Torsions

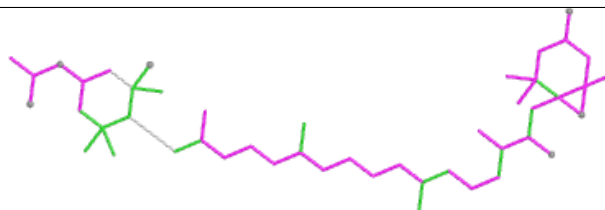


Rings

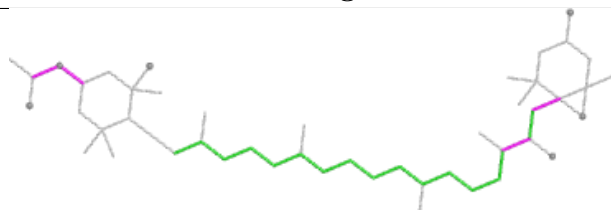
## Ligand A86 T 305



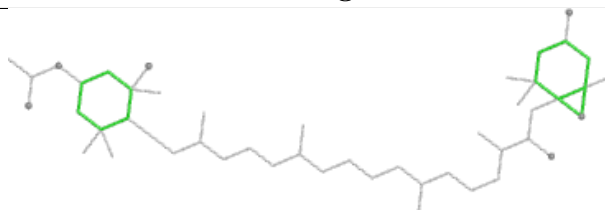
Bond lengths



Bond angles

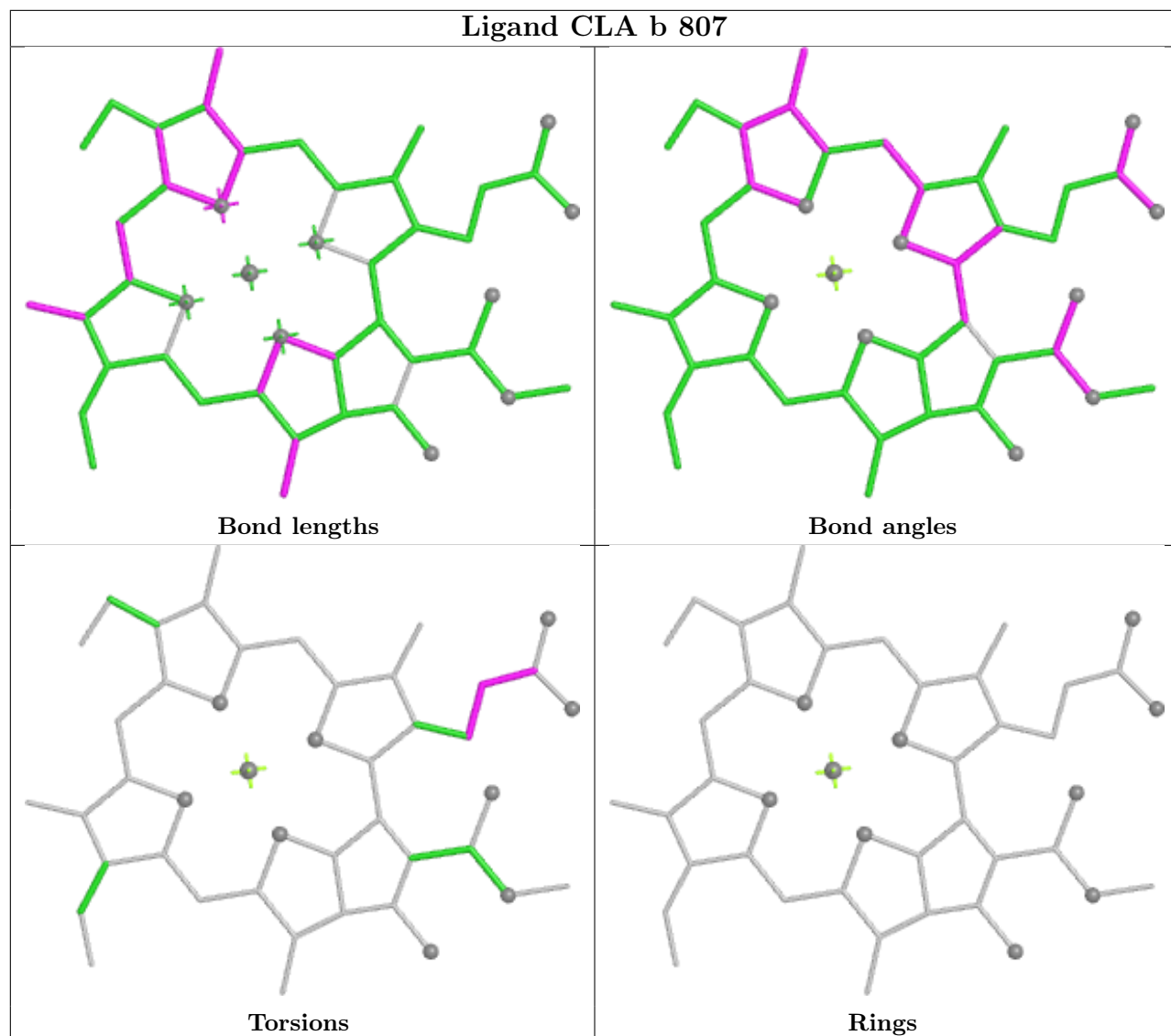


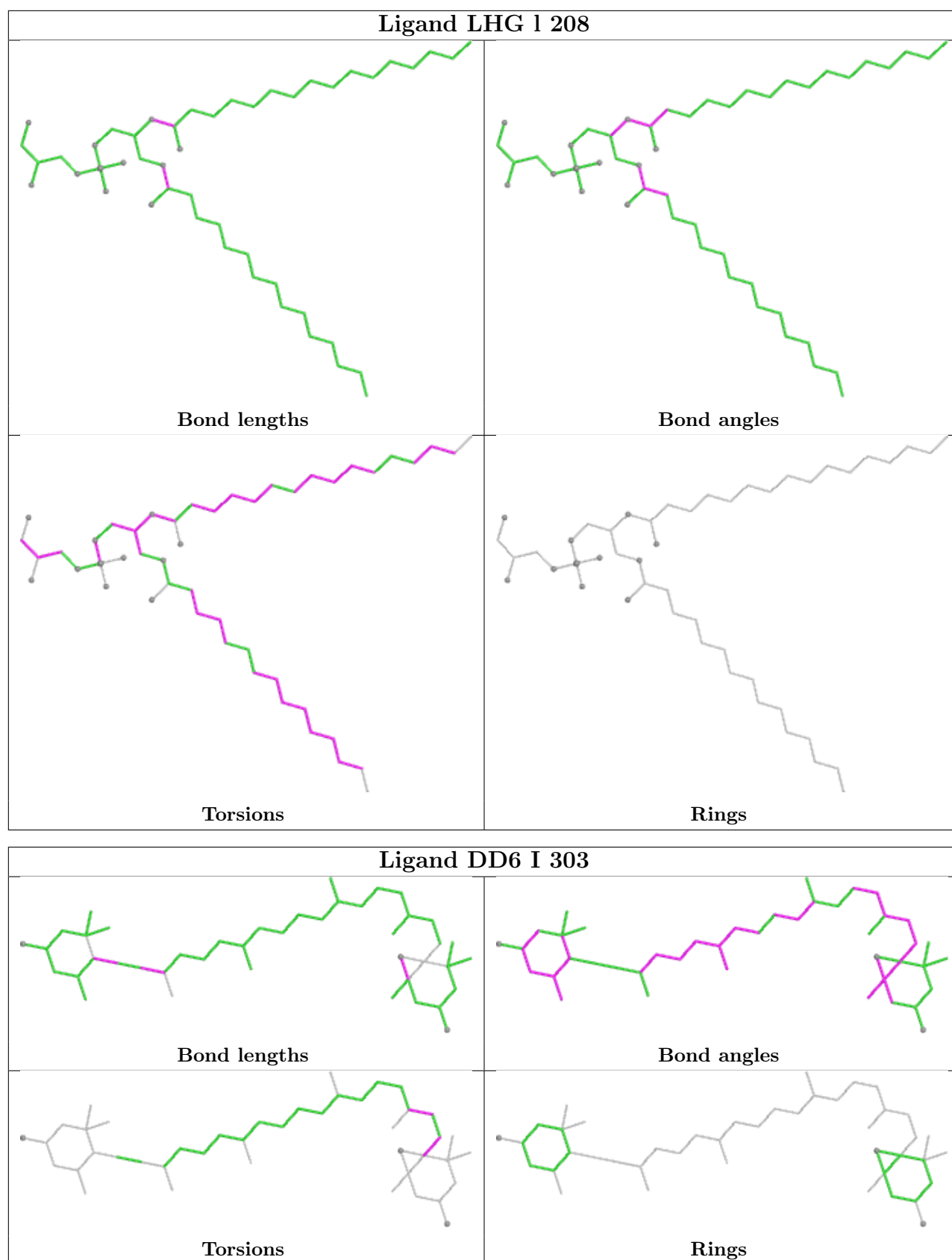
Torsions

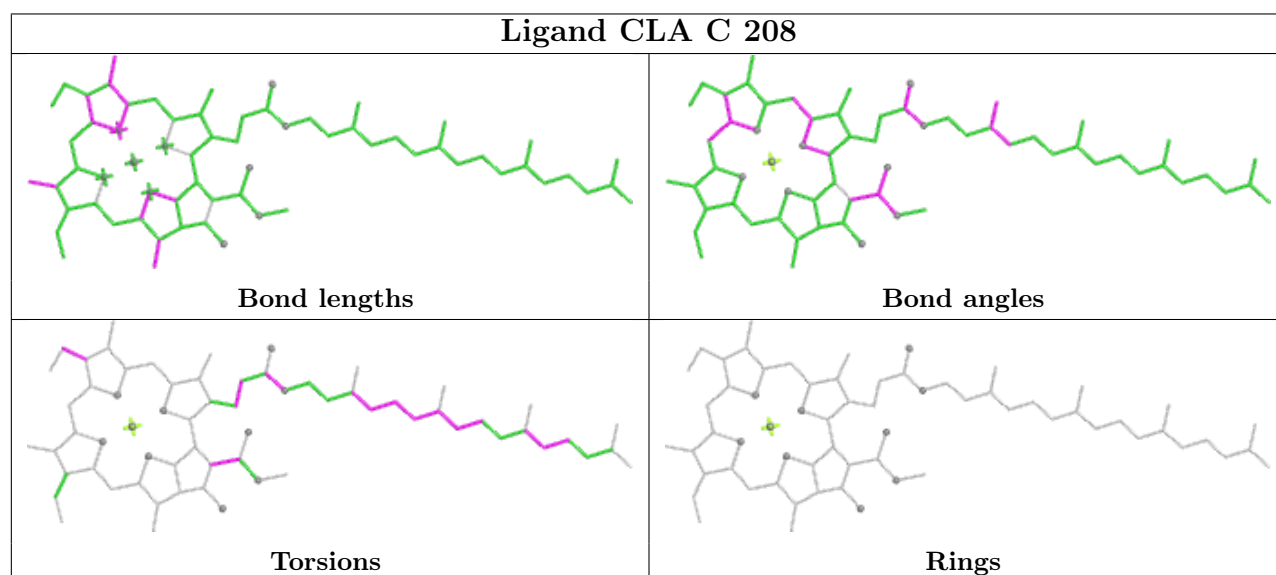
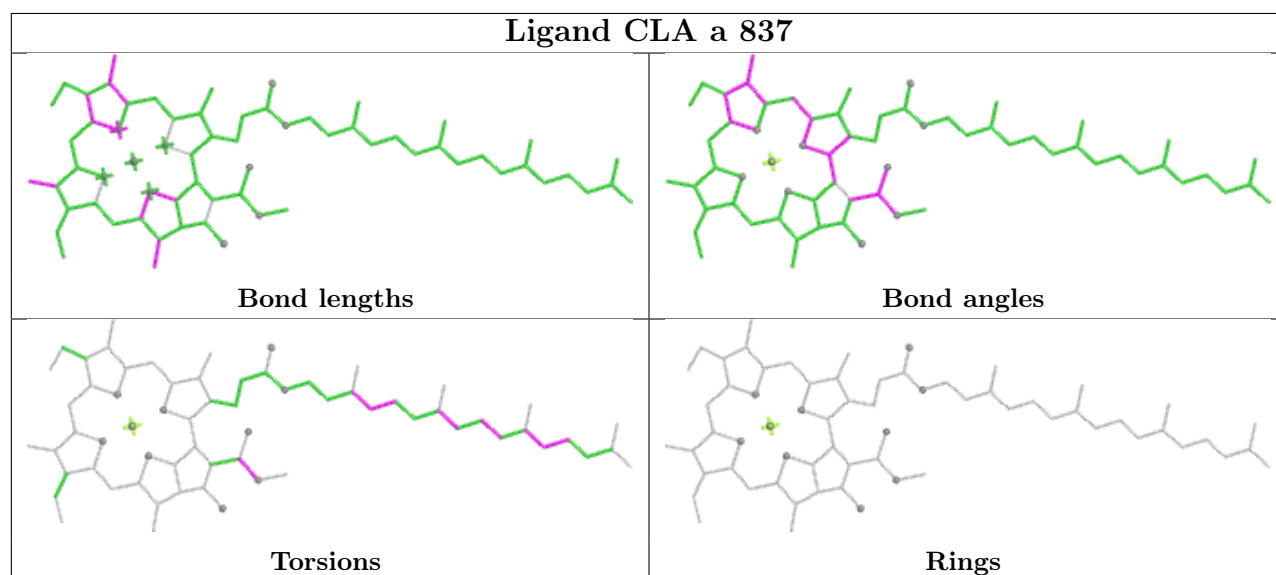
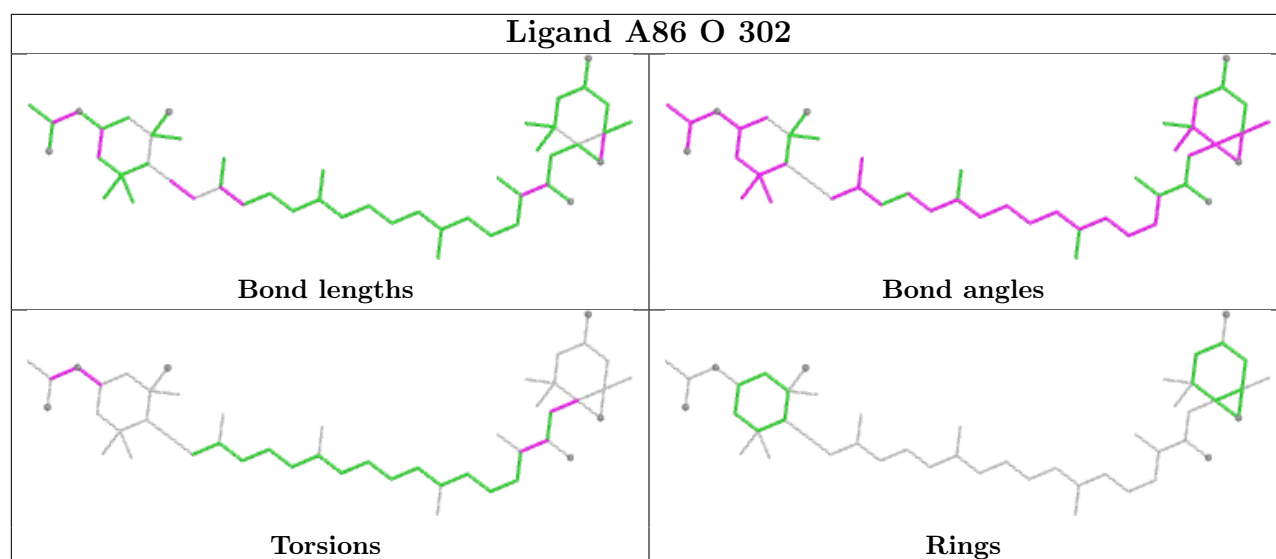


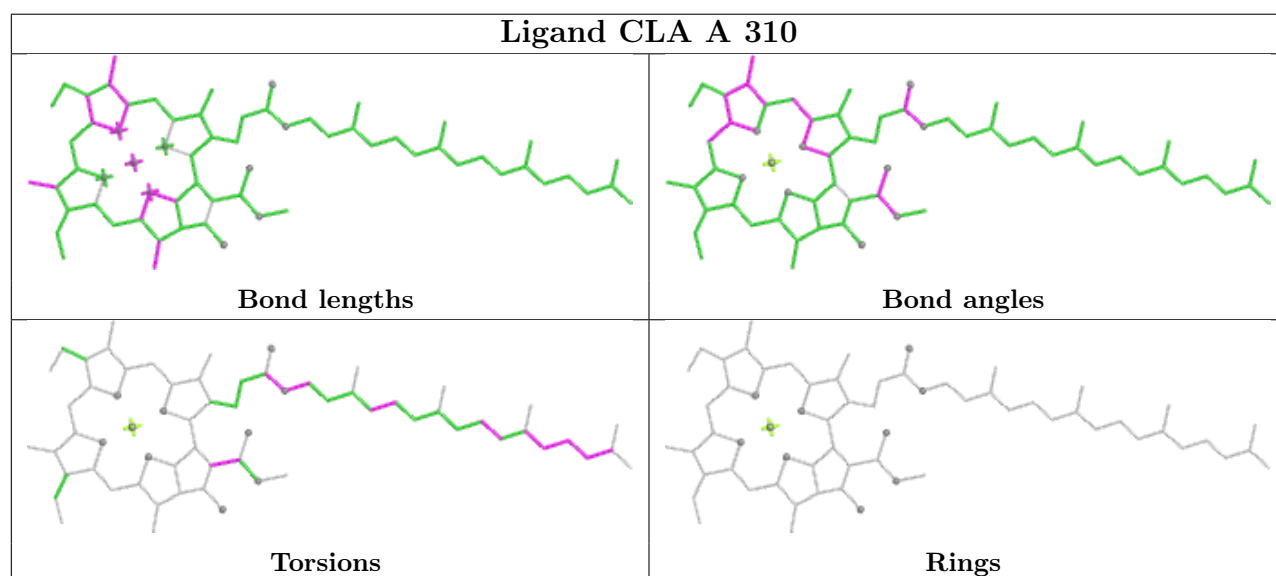
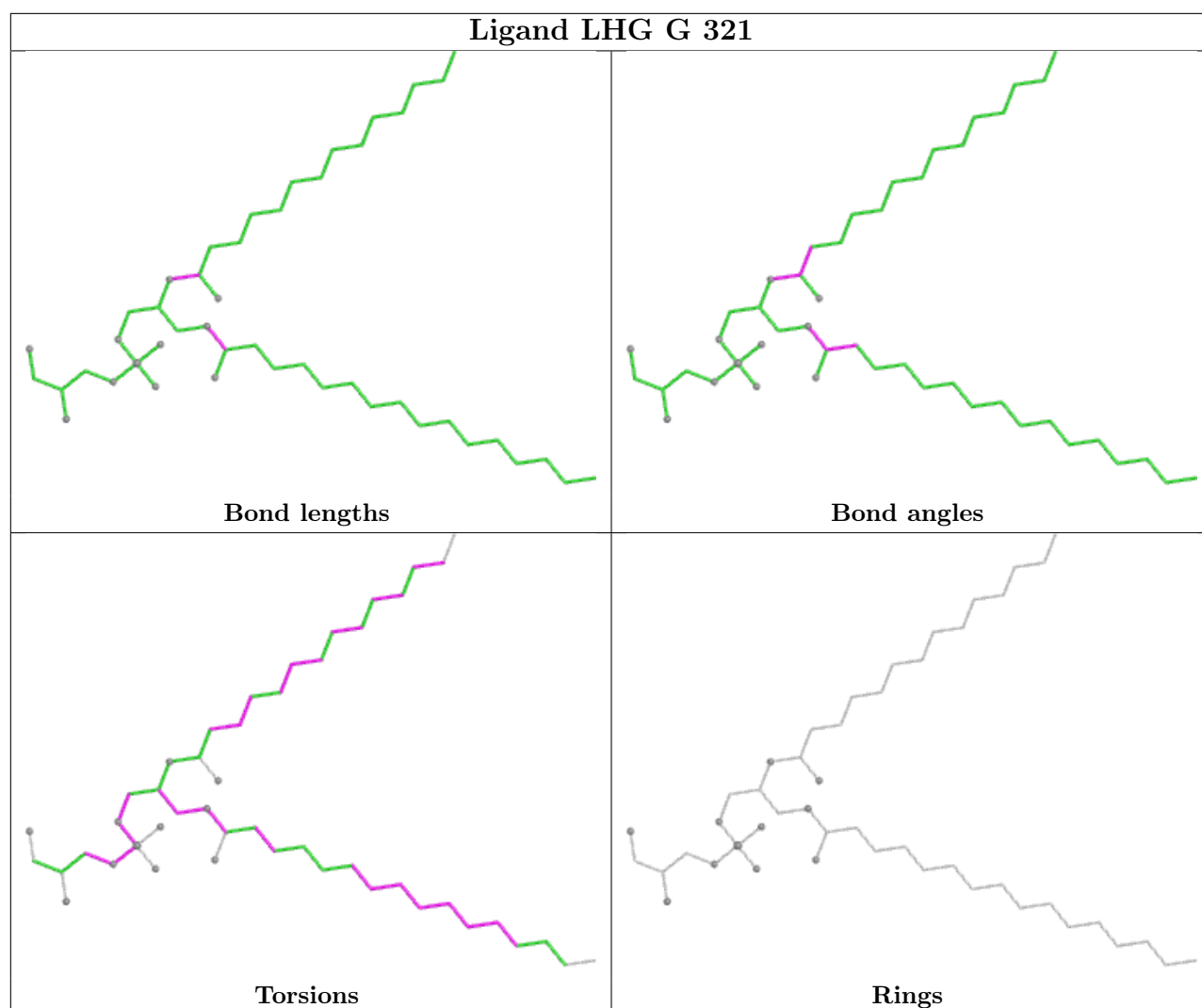
Rings

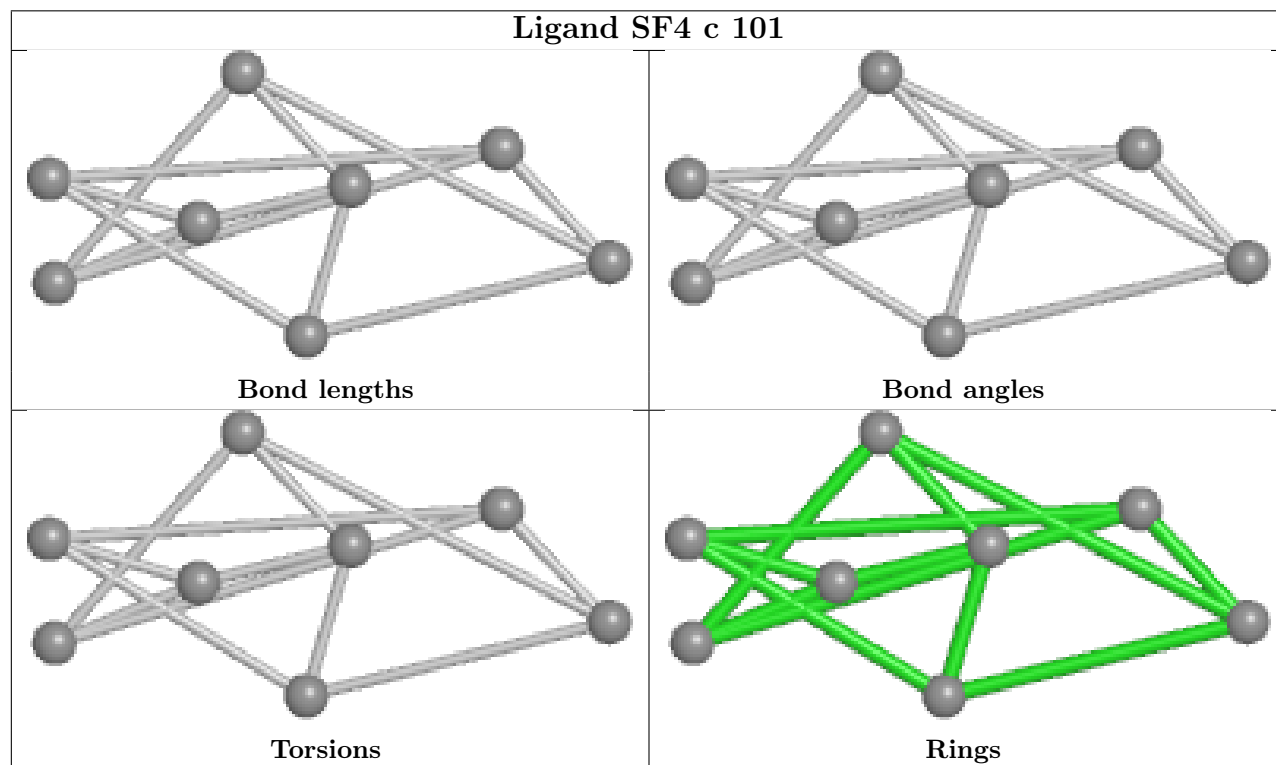
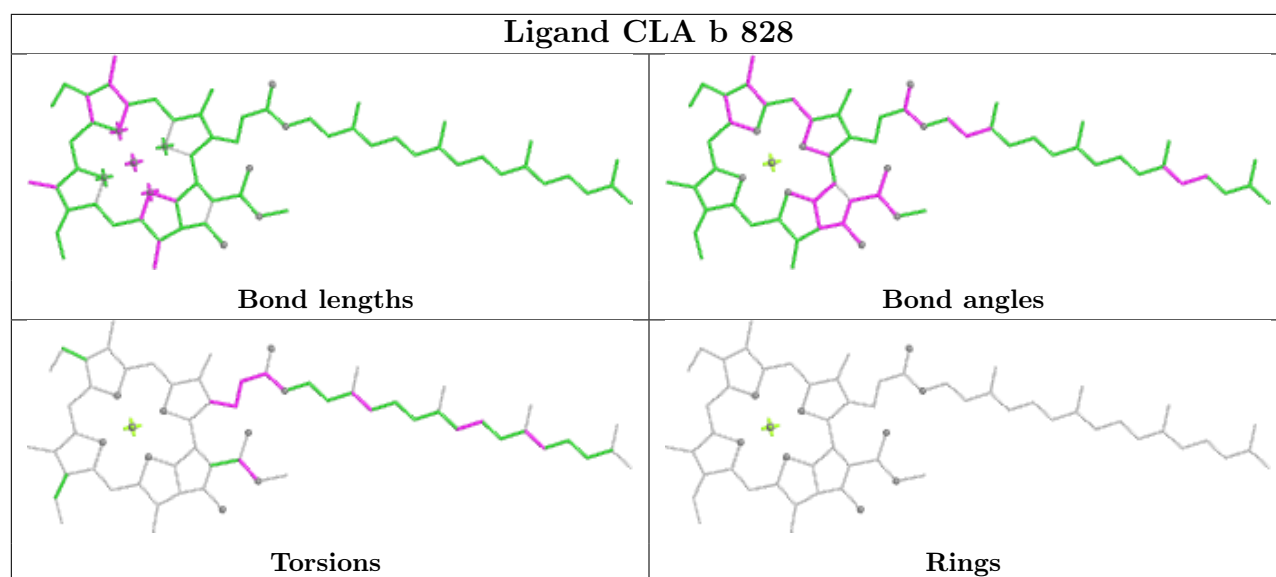
## Ligand CLA b 807

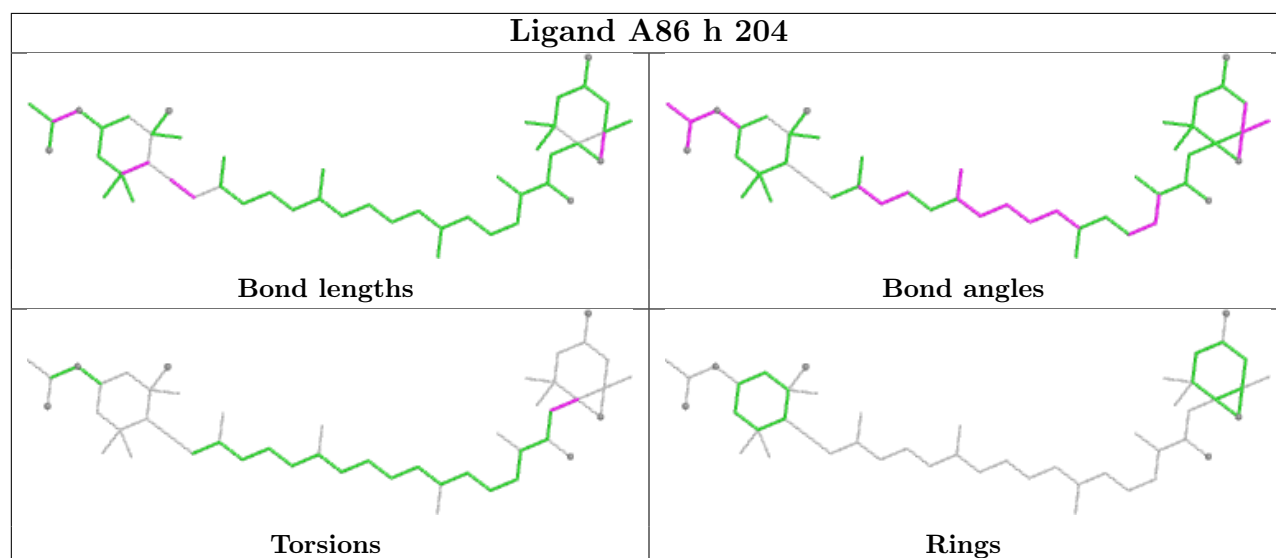
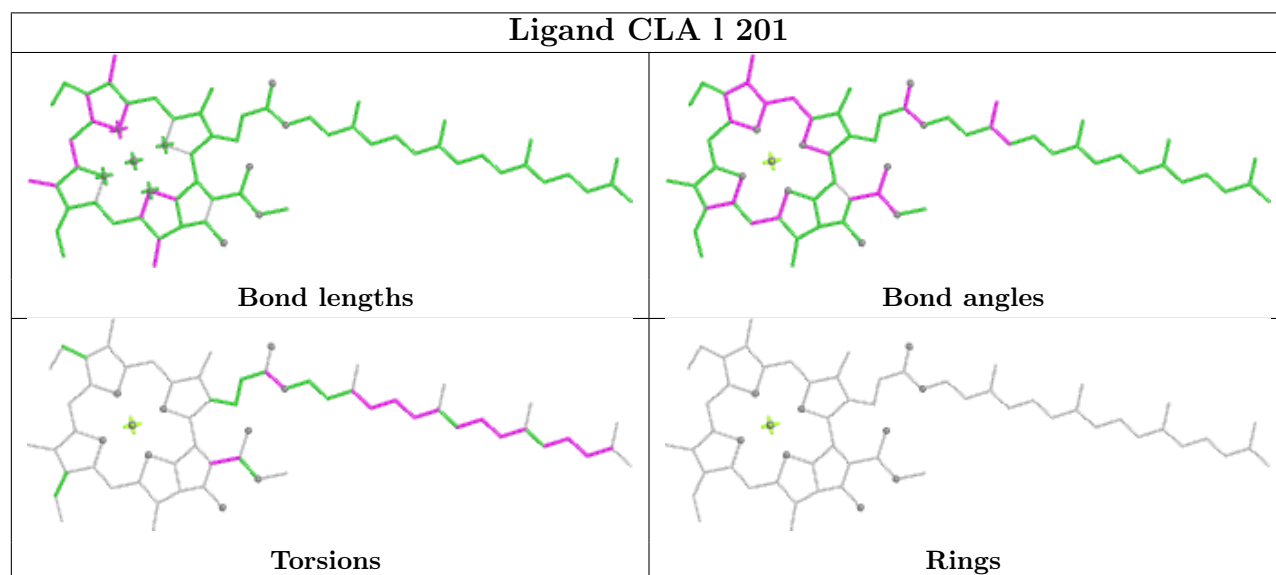
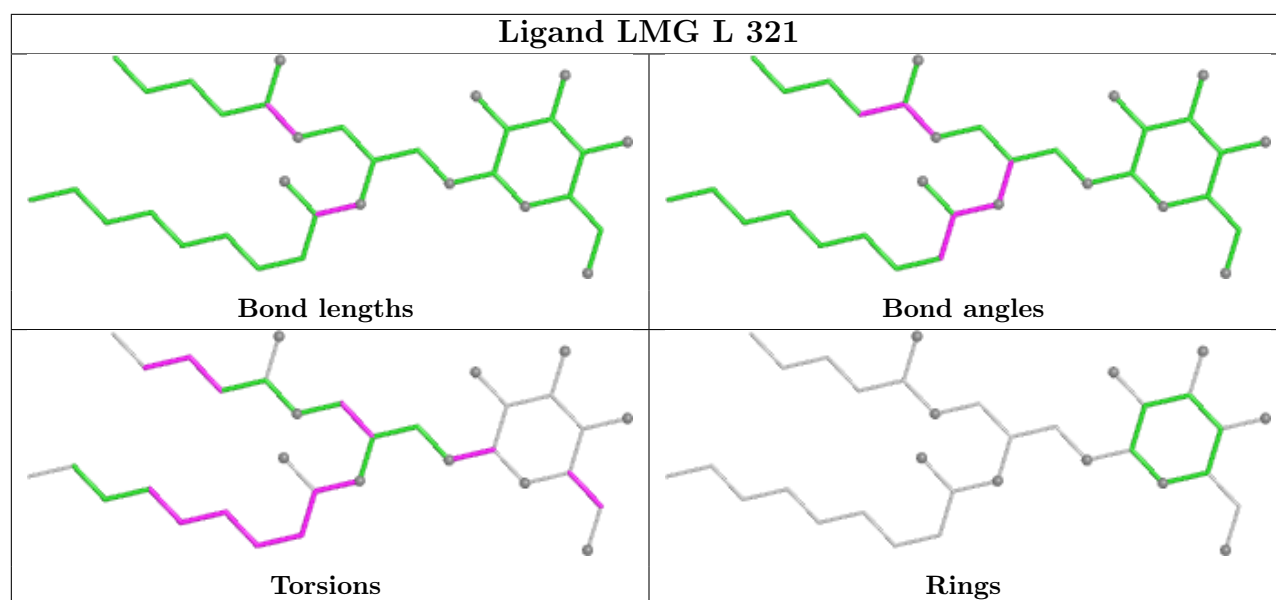




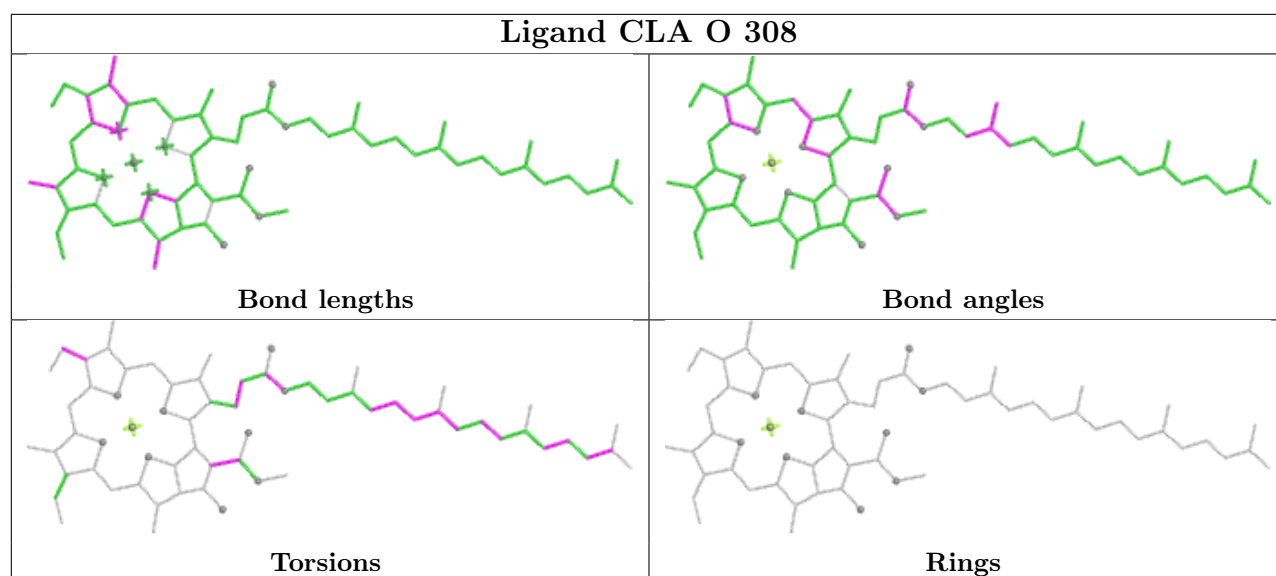
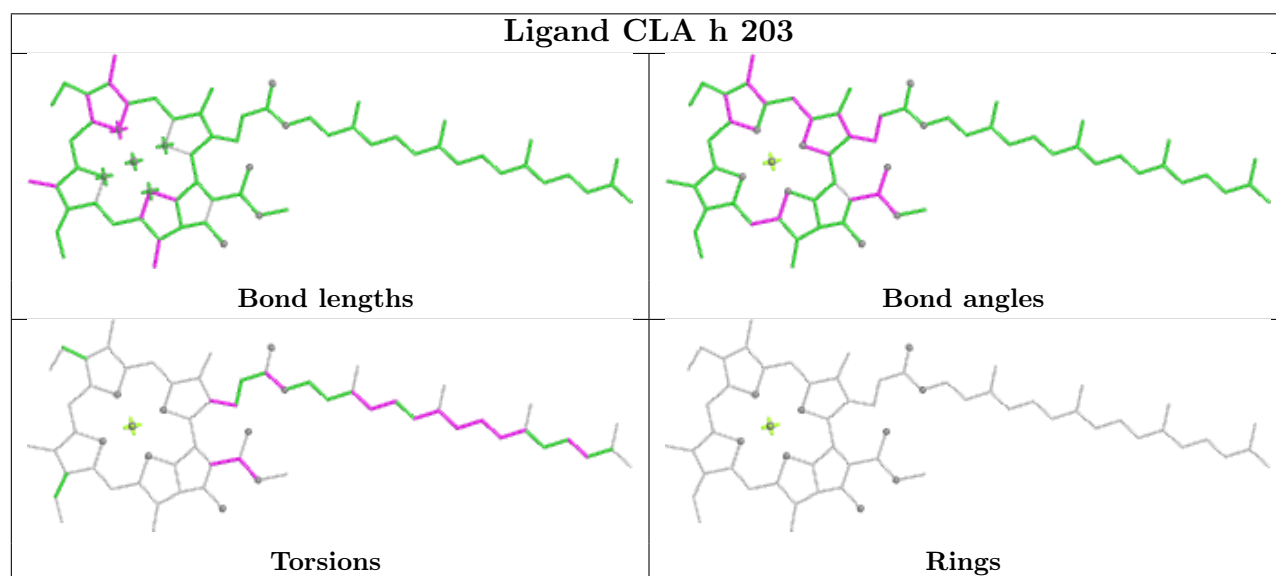
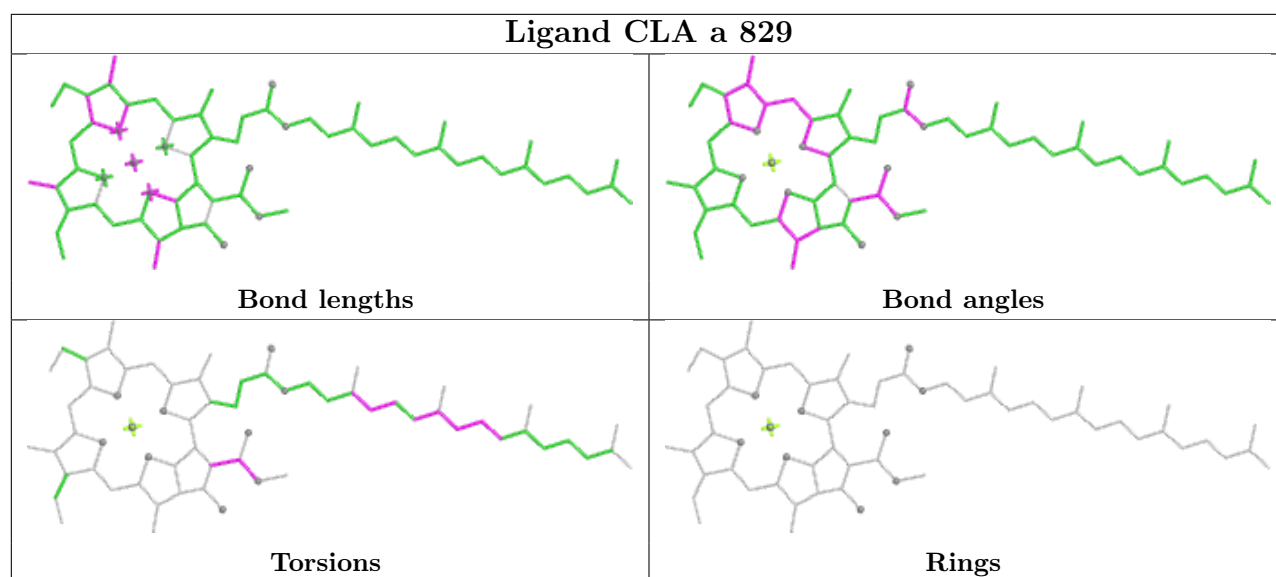


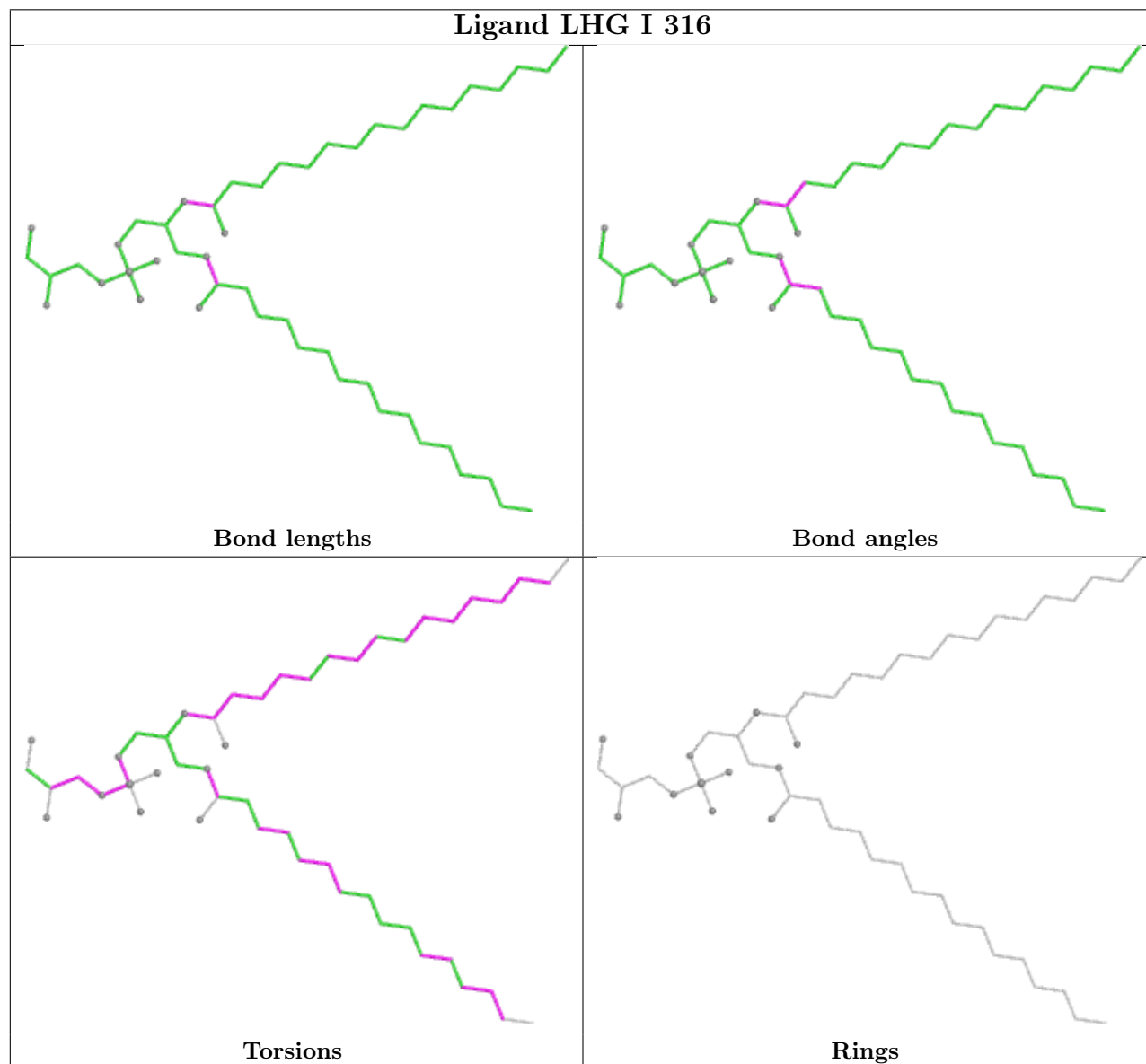
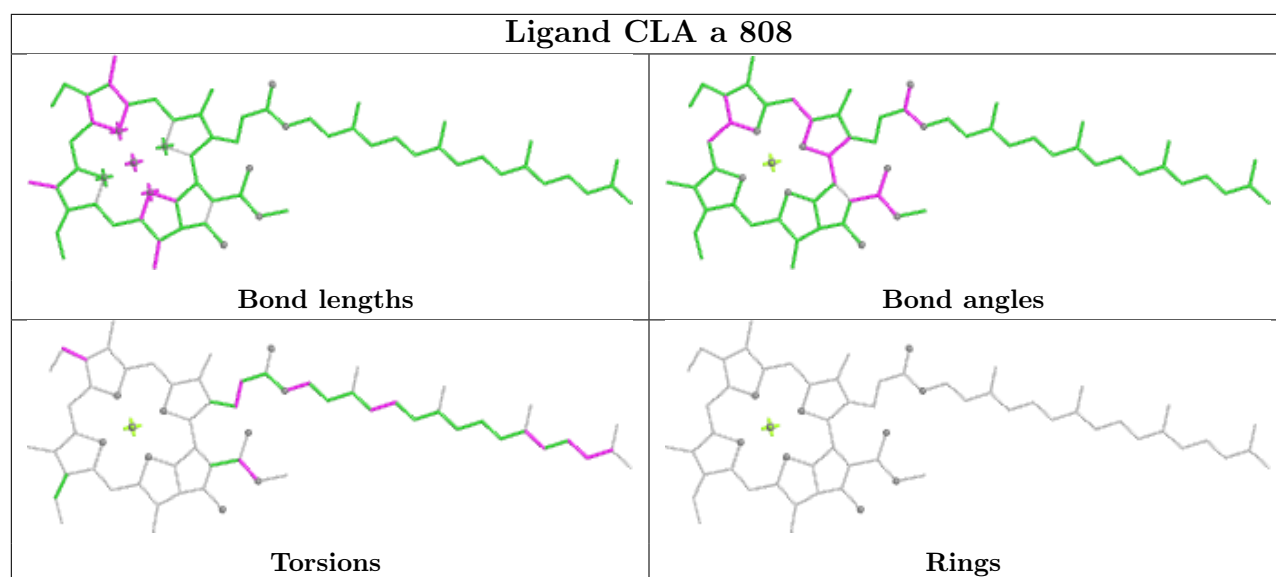


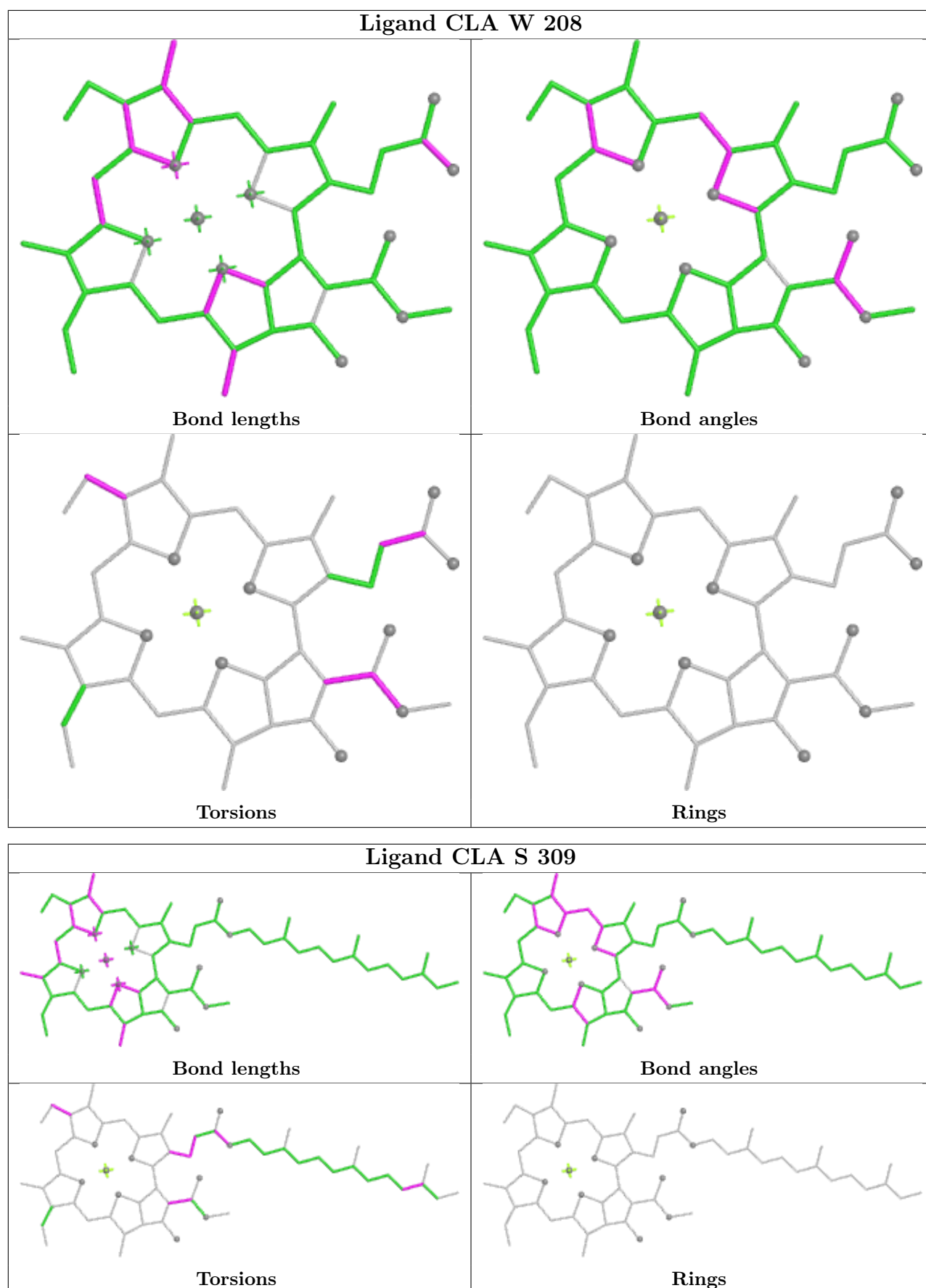


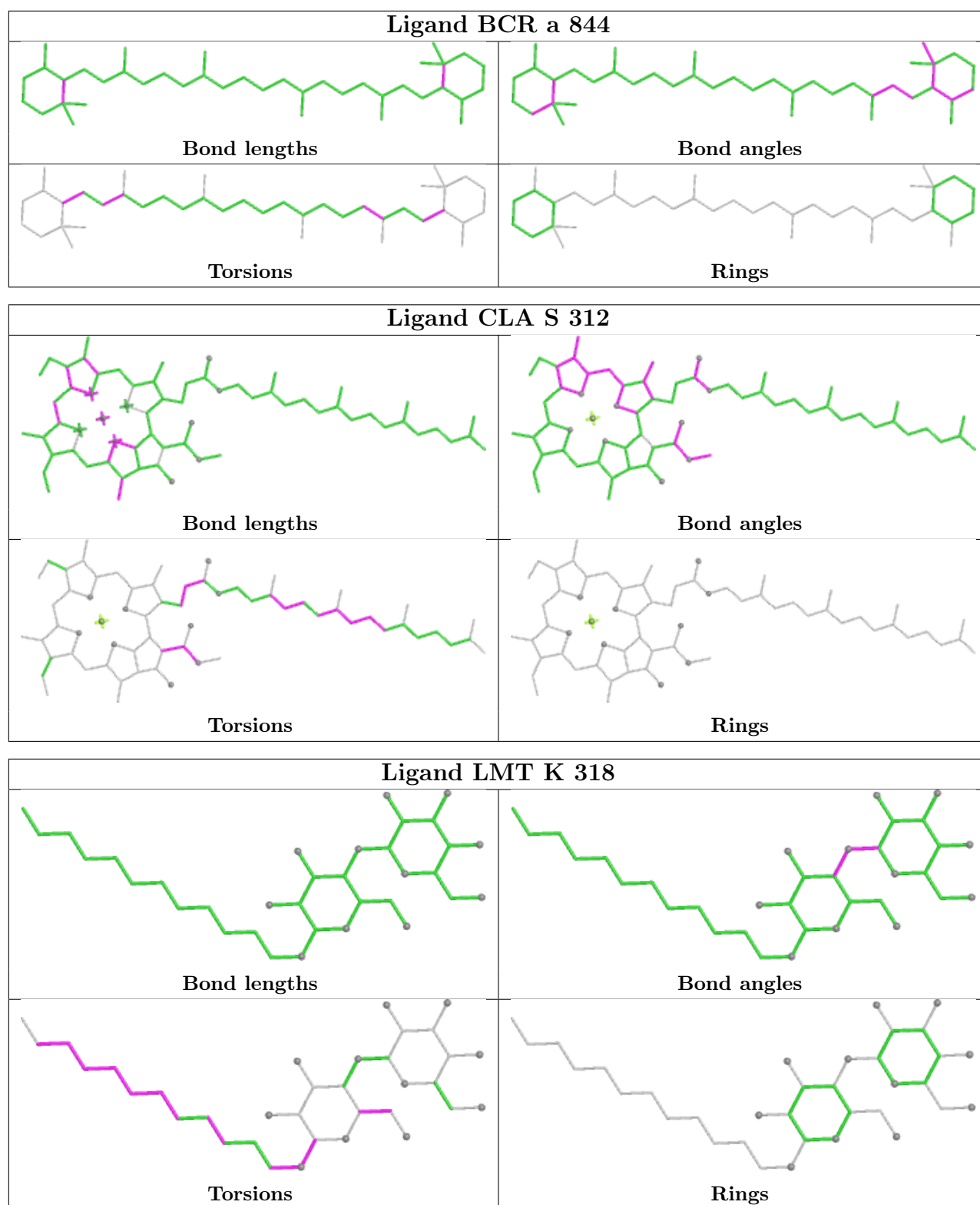


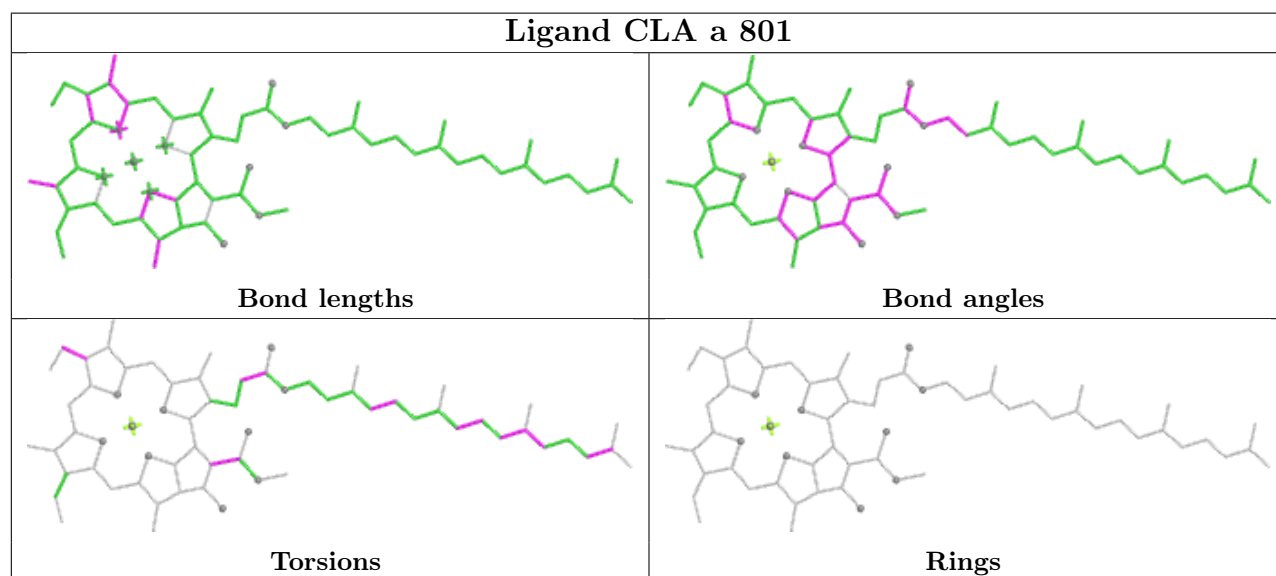
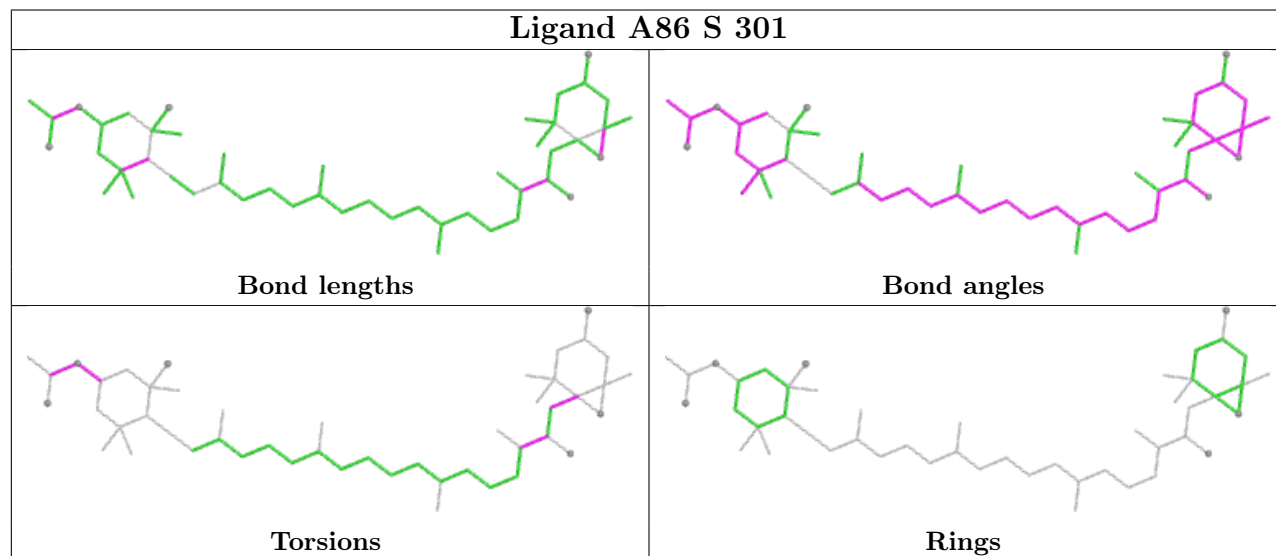
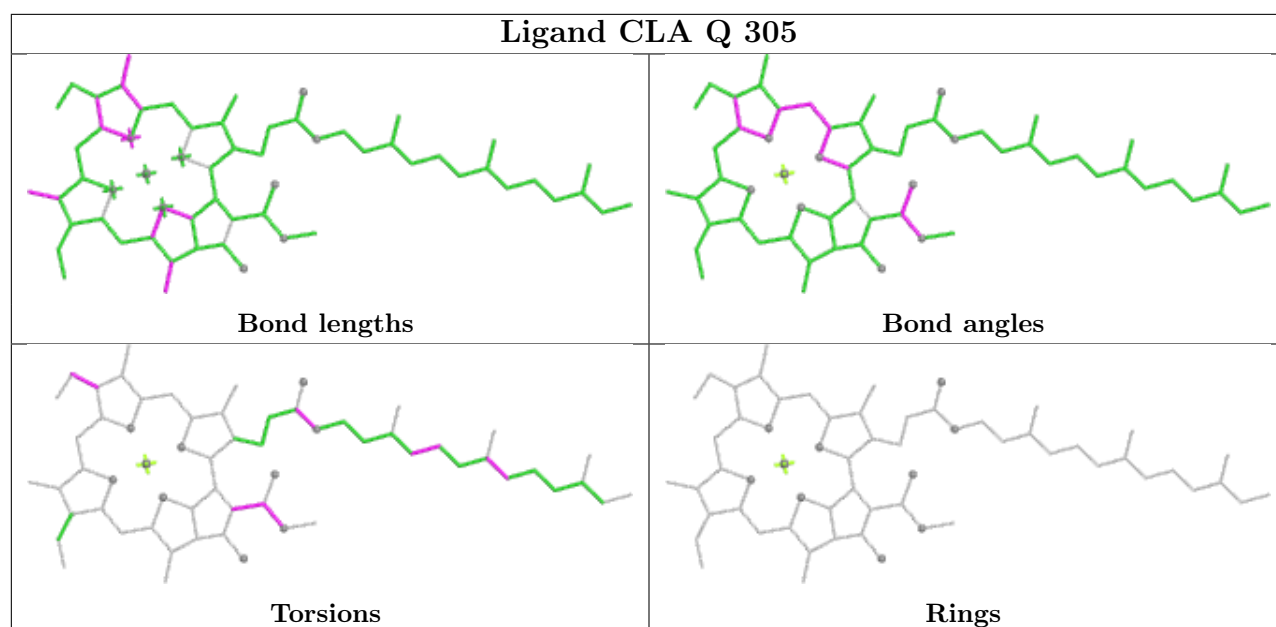


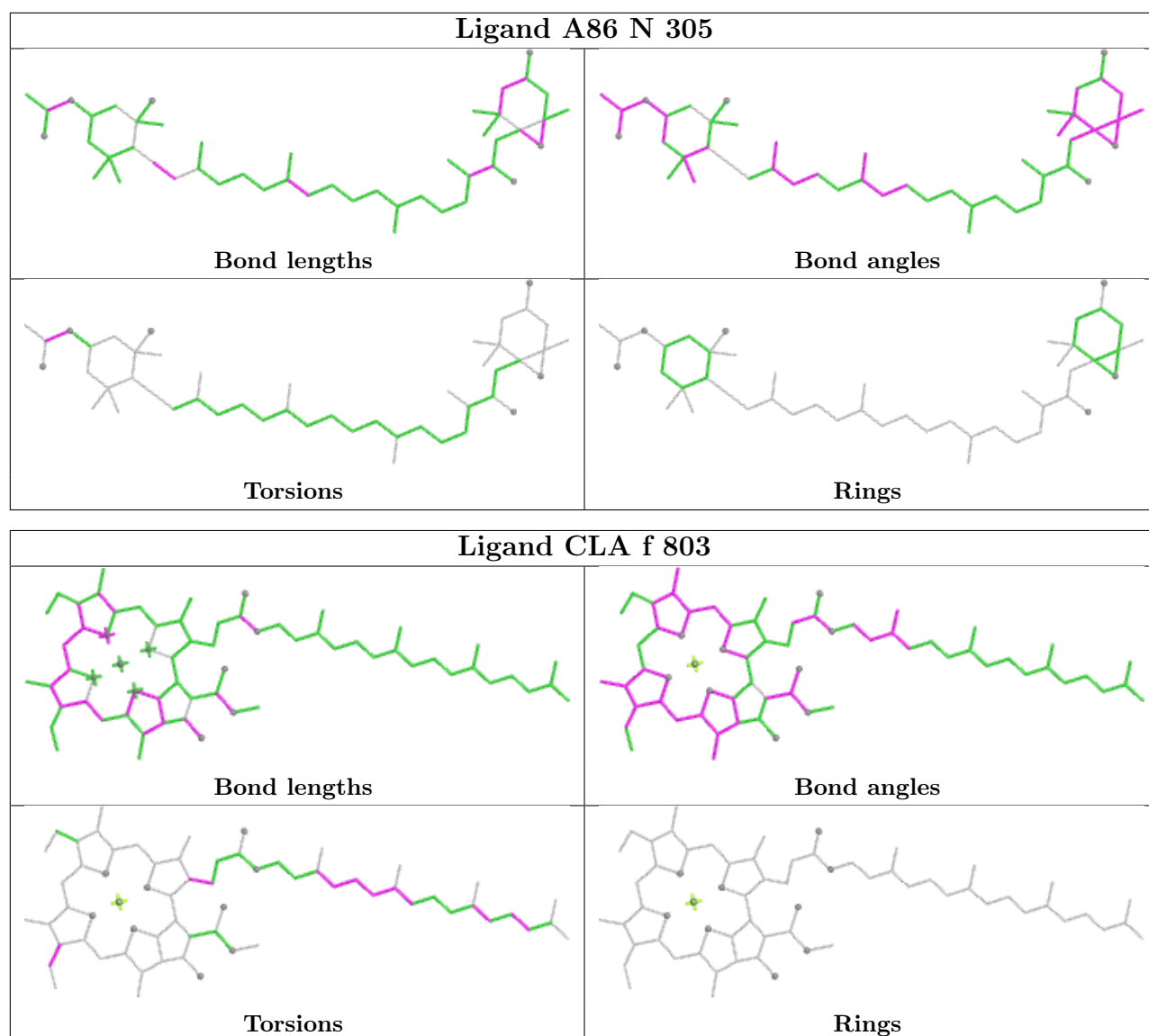




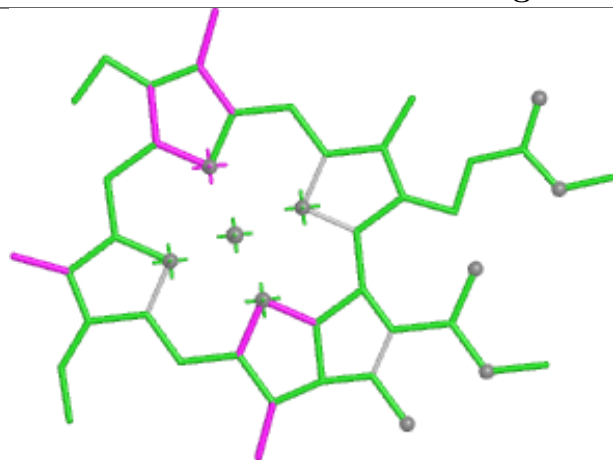




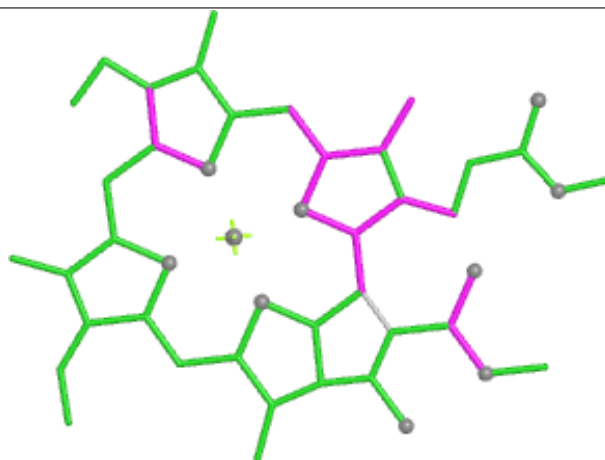




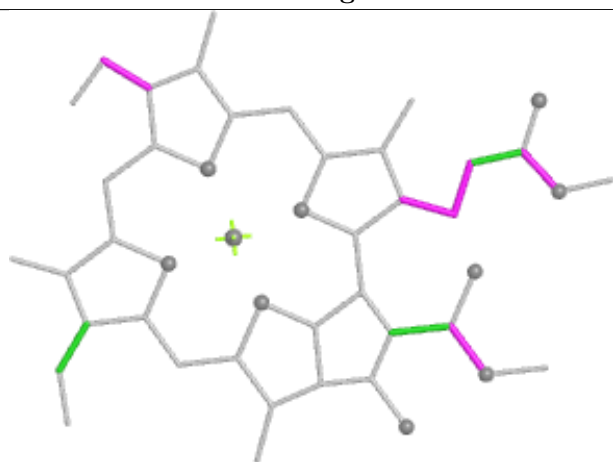
## Ligand CLA K 311



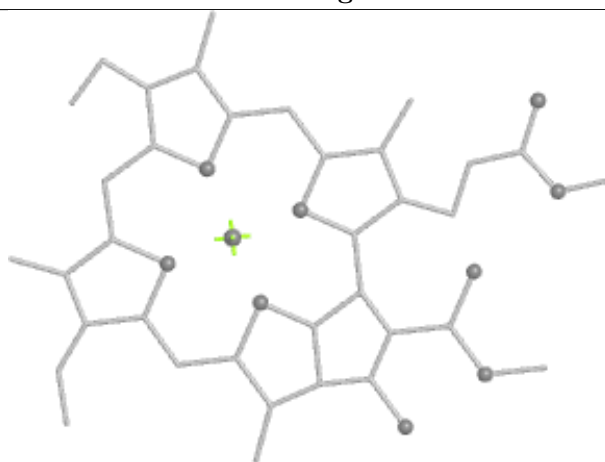
Bond lengths



Bond angles

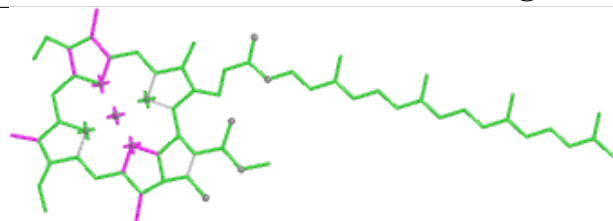


Torsions

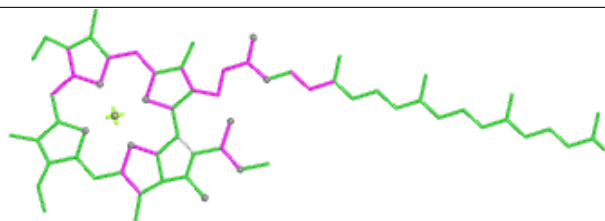


Rings

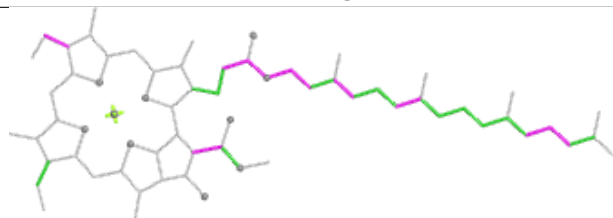
## Ligand CLA a 804



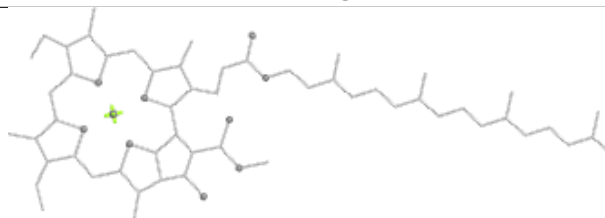
Bond lengths



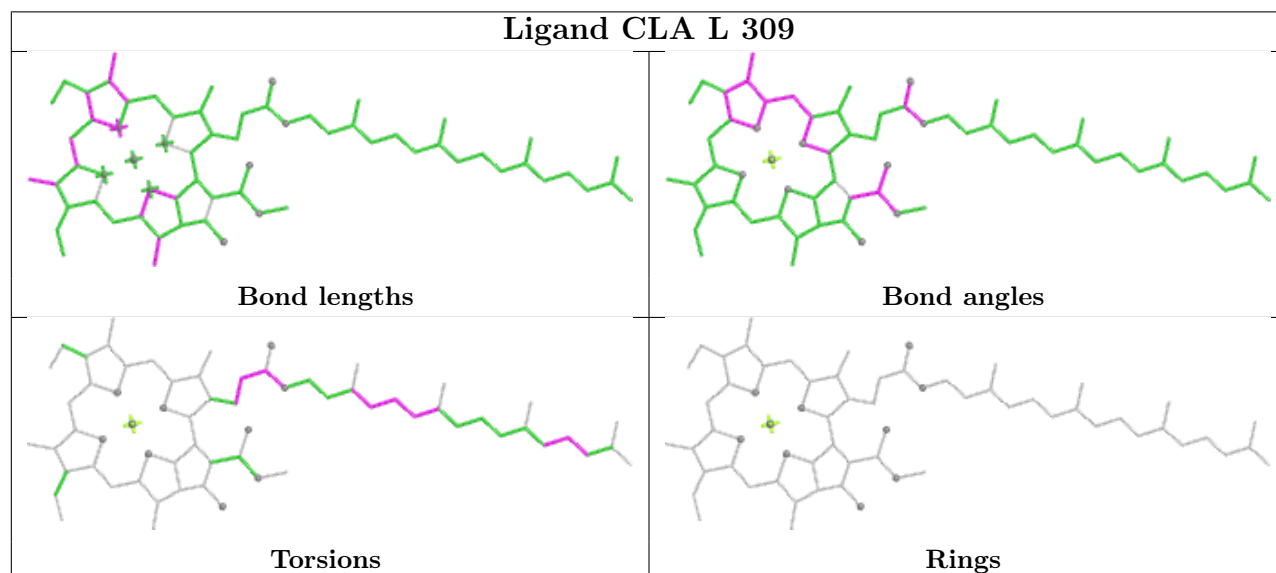
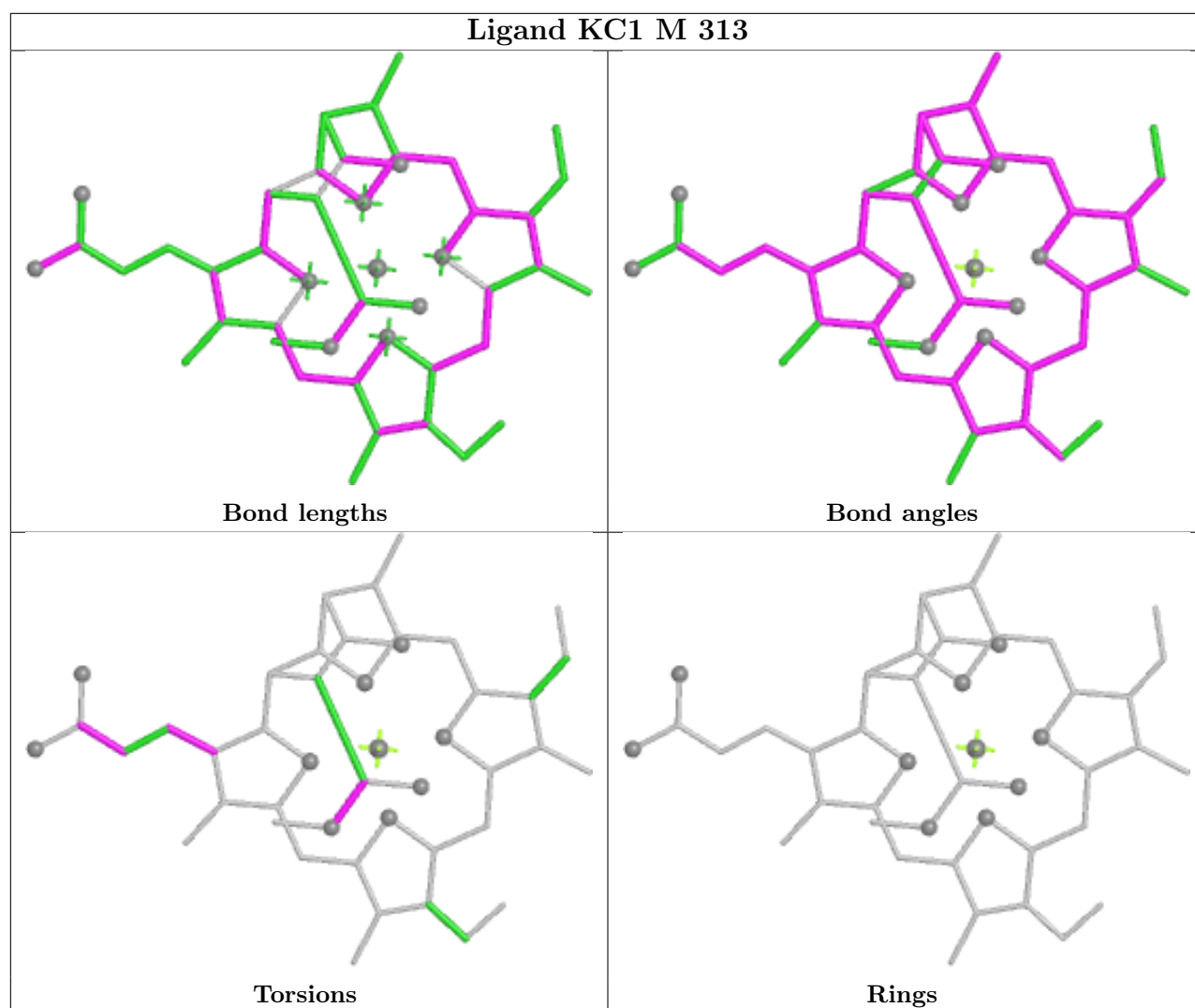
Bond angles



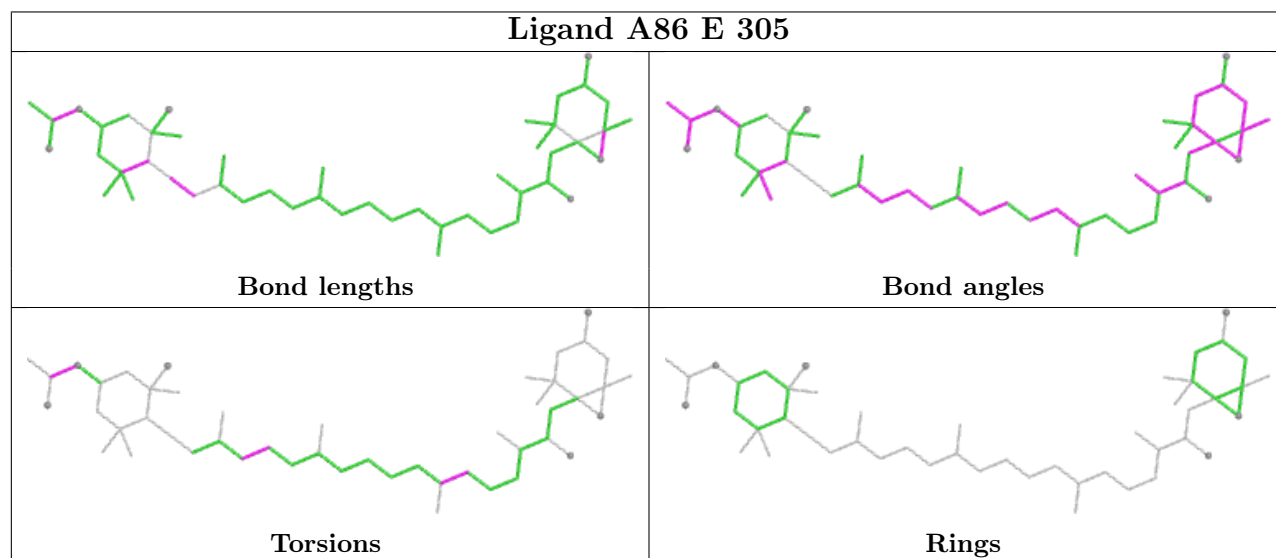
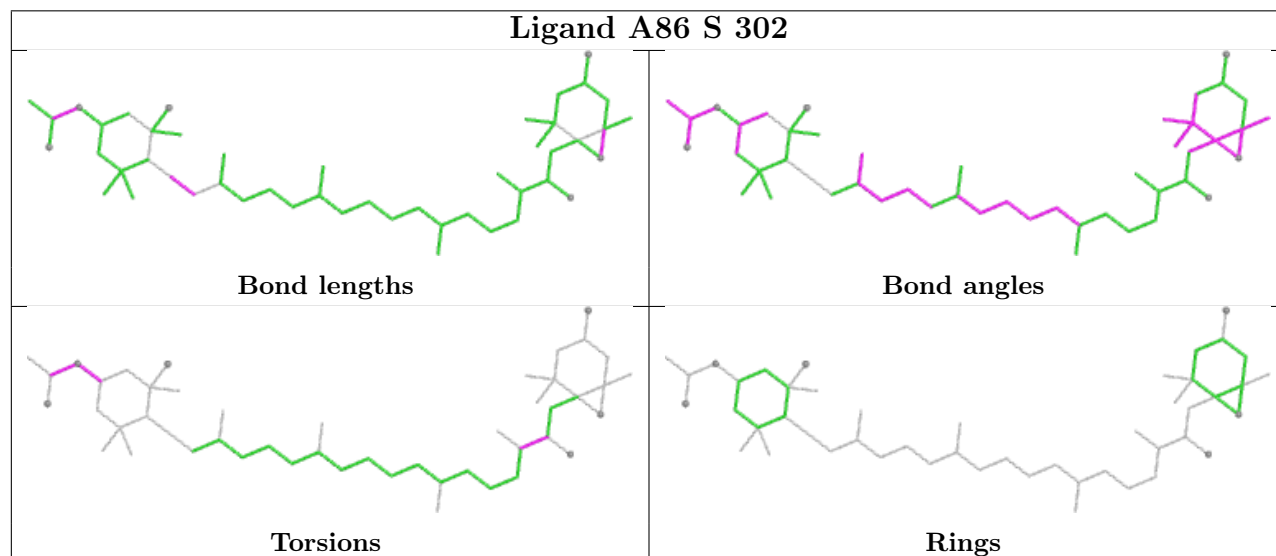
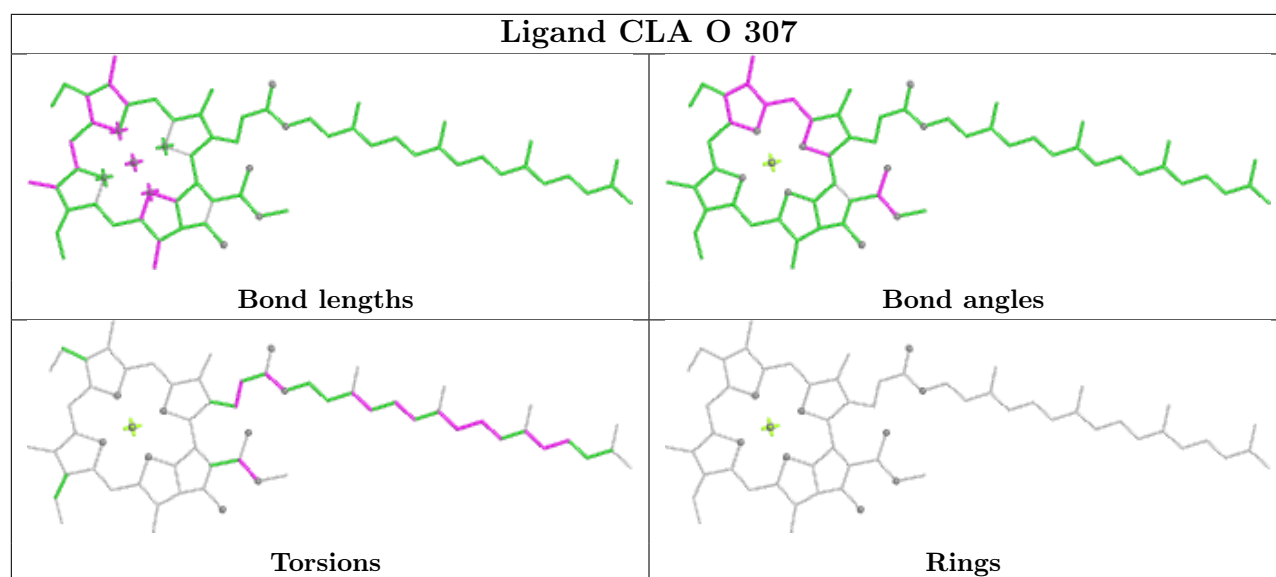
Torsions

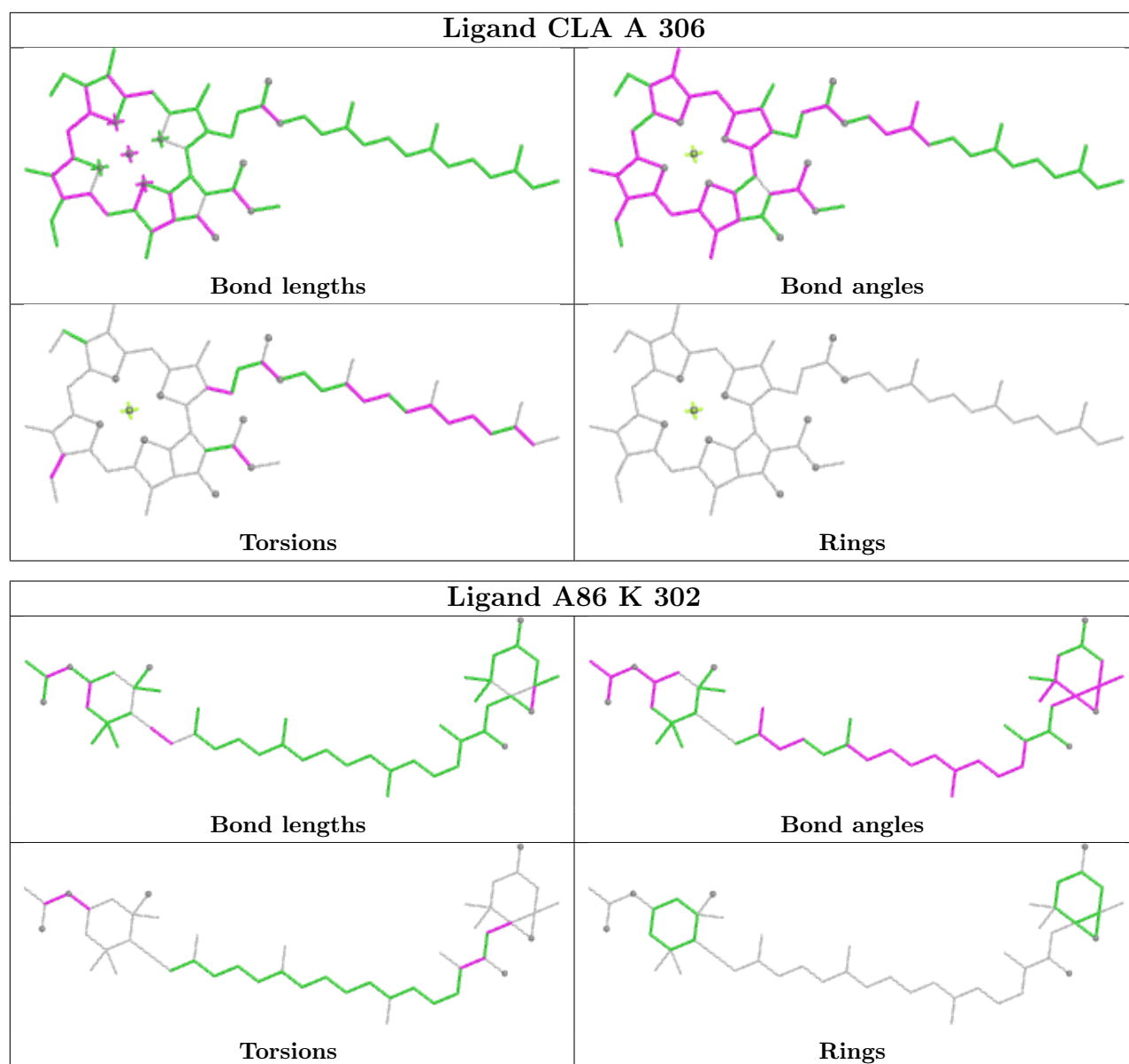


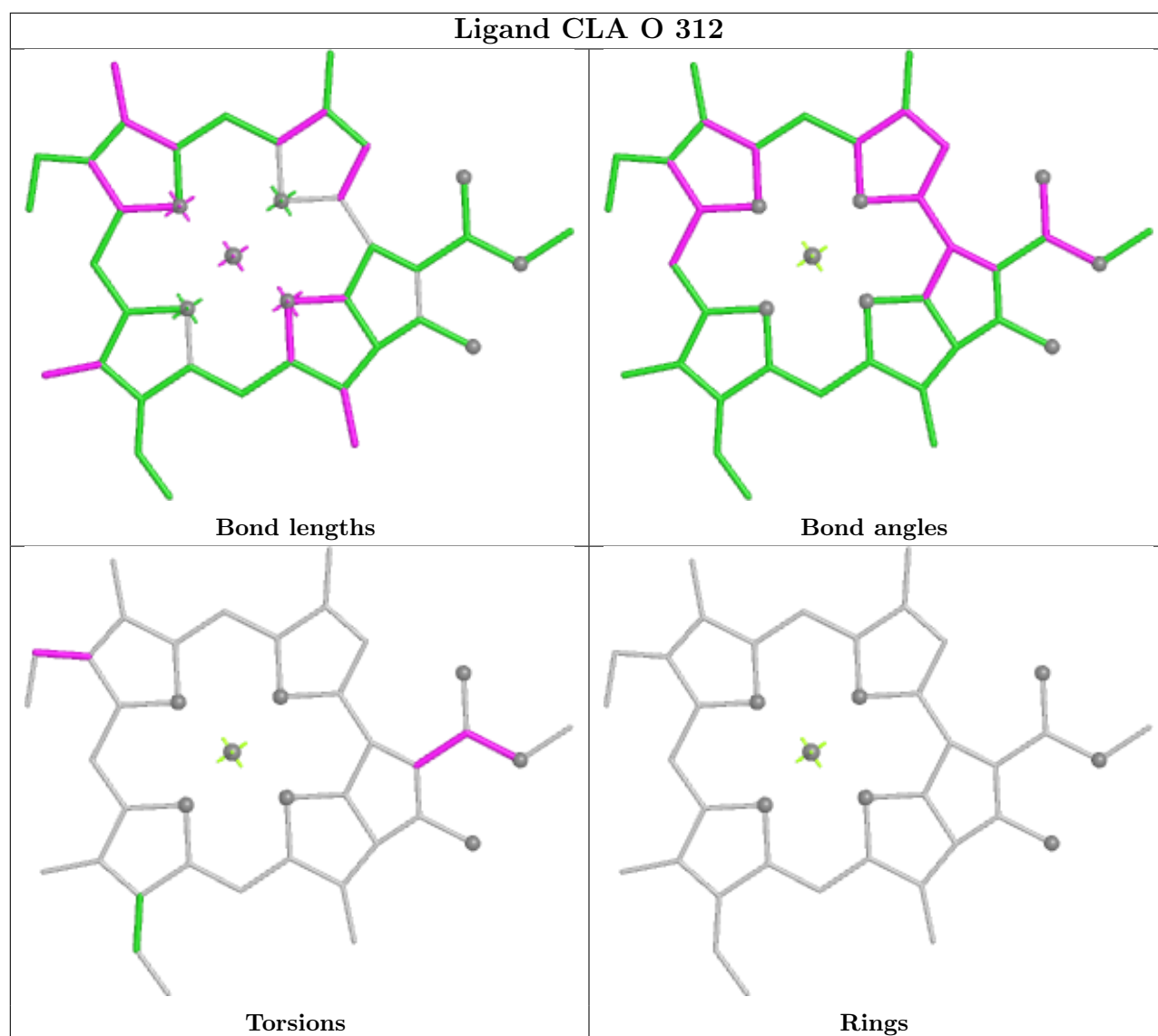
Rings



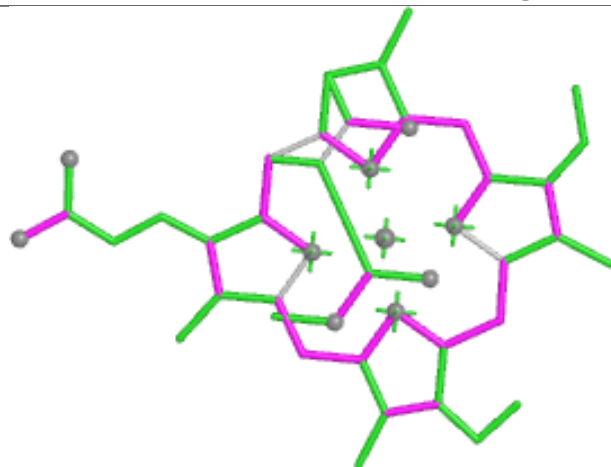




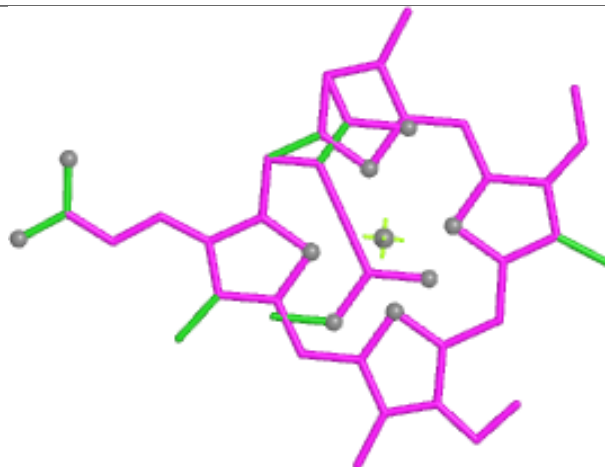




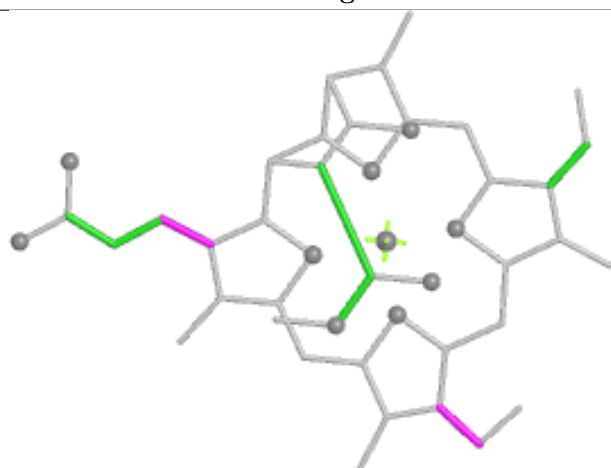
## Ligand KC1 P 317



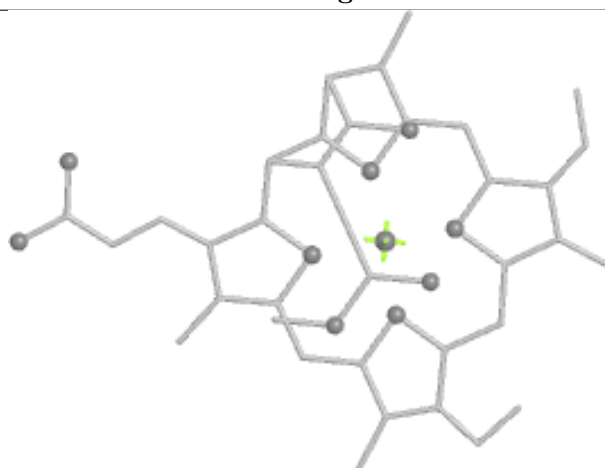
Bond lengths



Bond angles

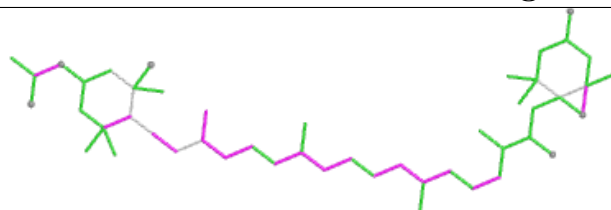


Torsions

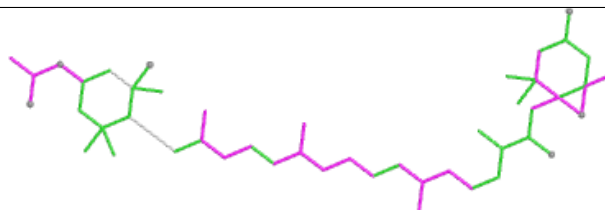


Rings

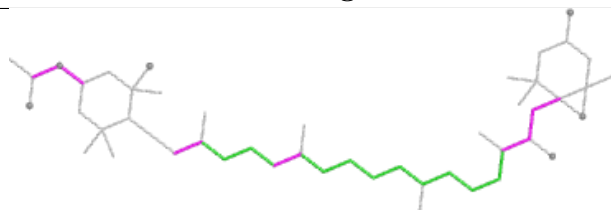
## Ligand A86 C 204



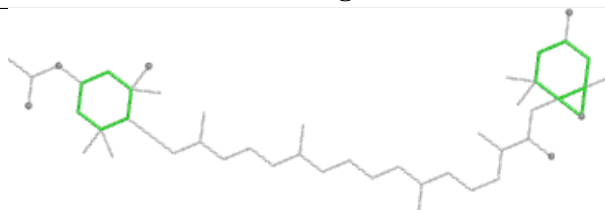
Bond lengths



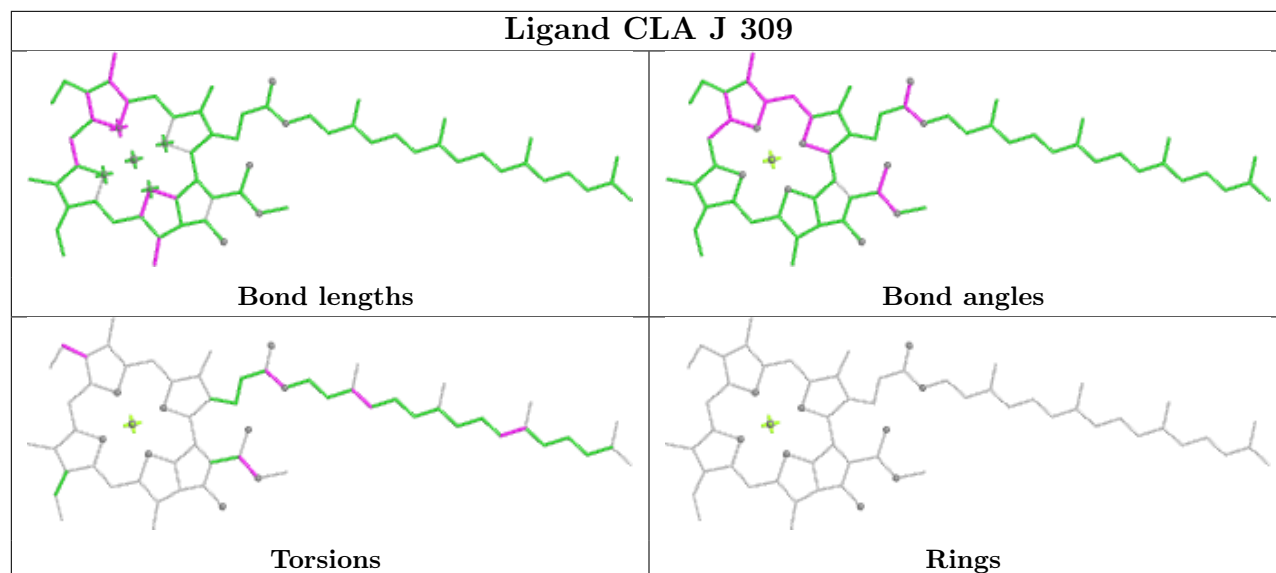
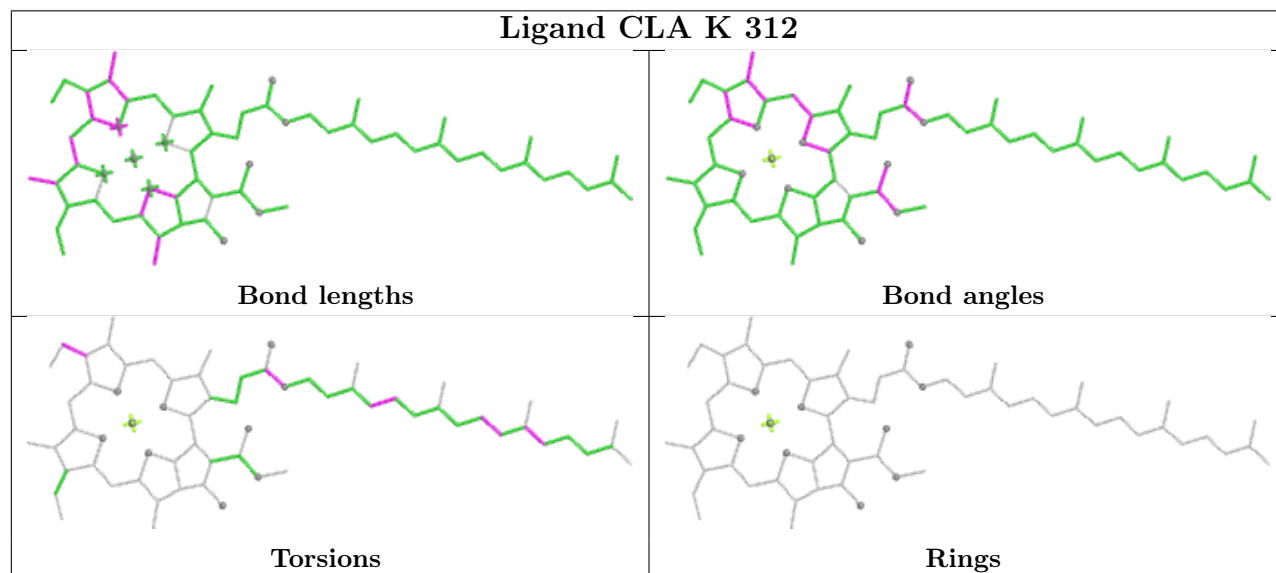
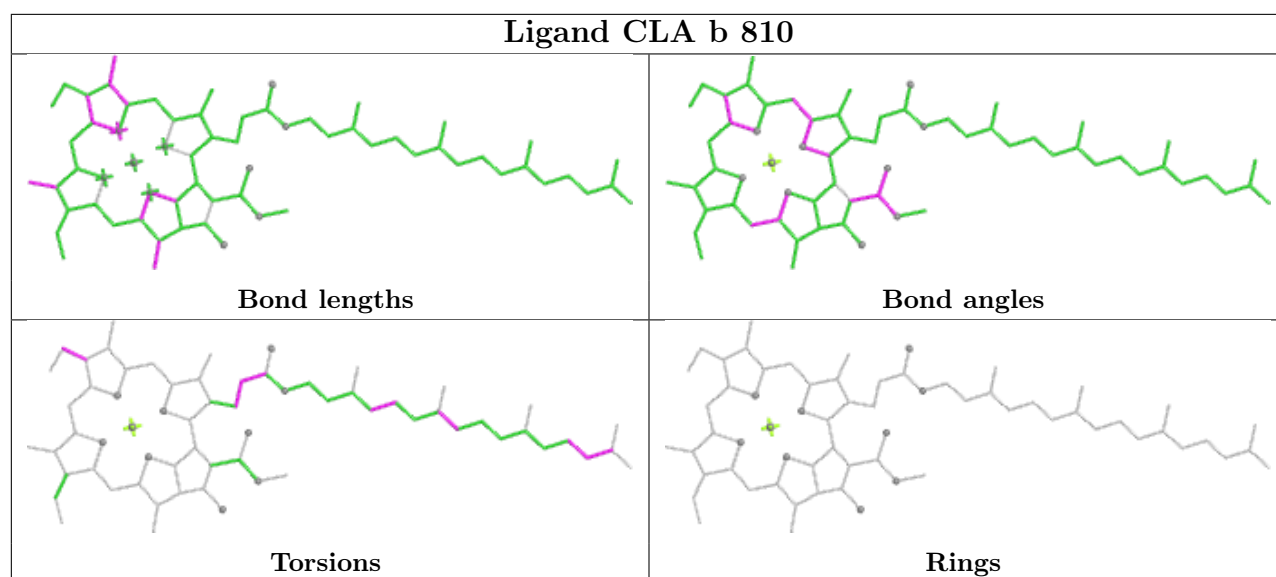
Bond angles



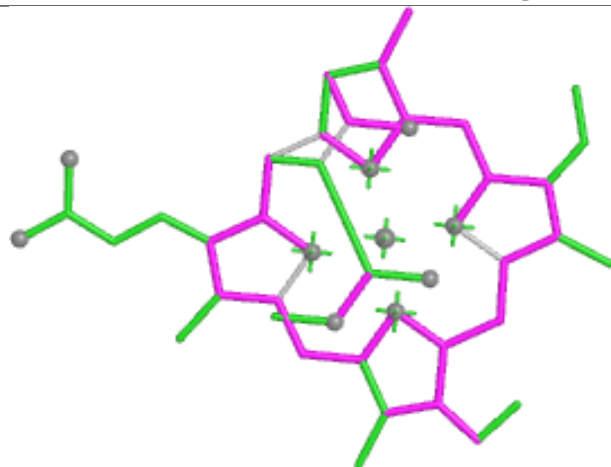
Torsions



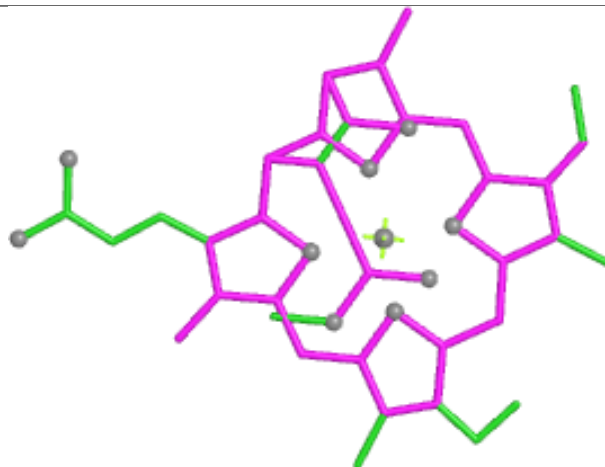
Rings



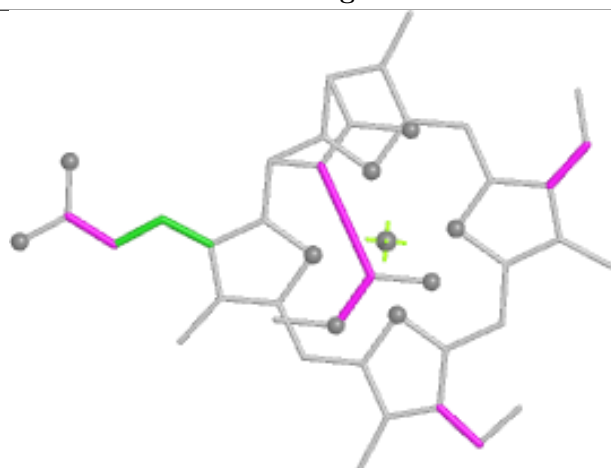
## Ligand KC1 T 310



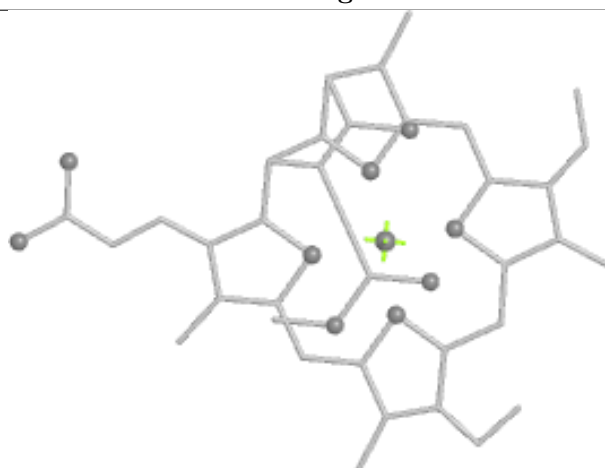
Bond lengths



Bond angles

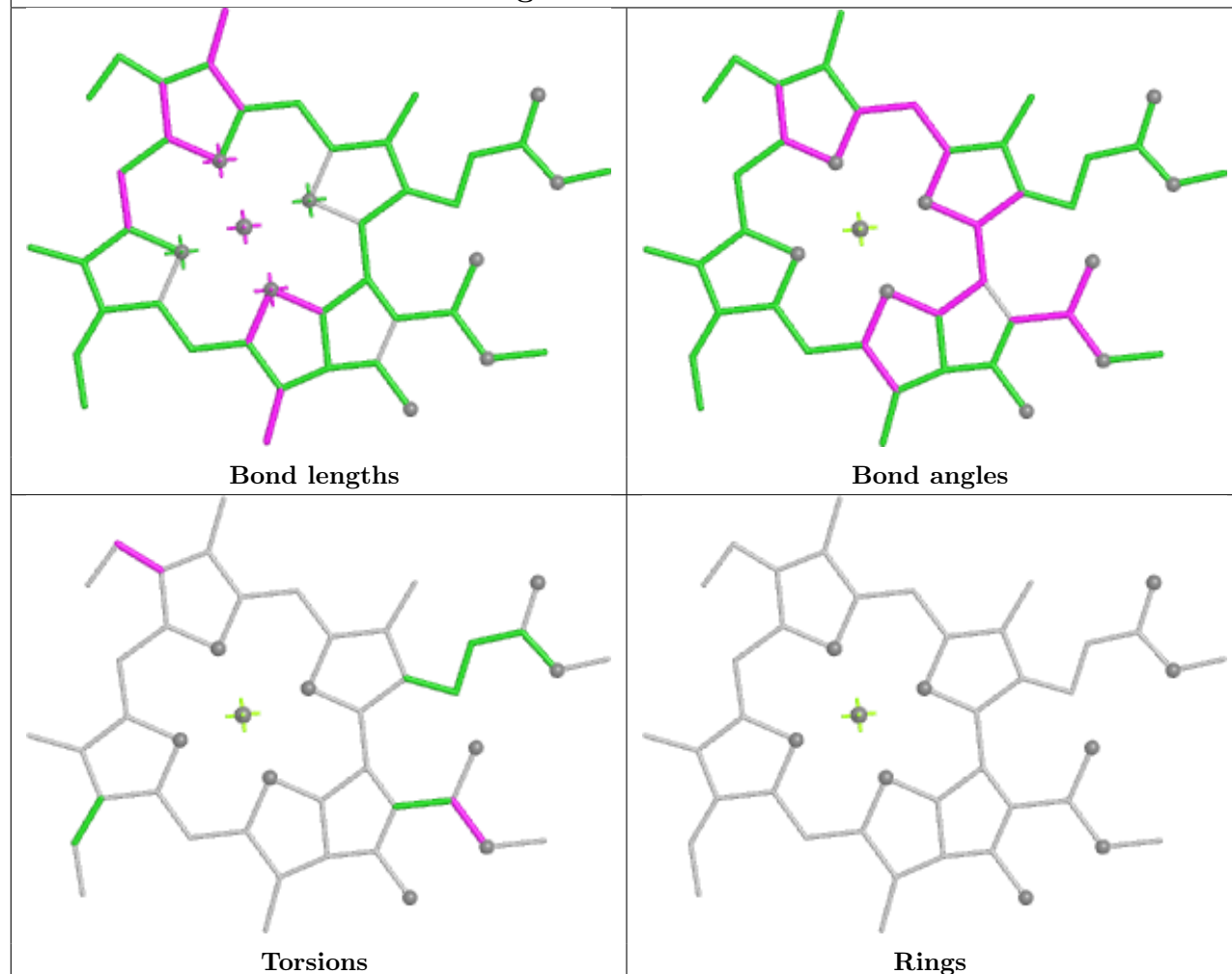


Torsions

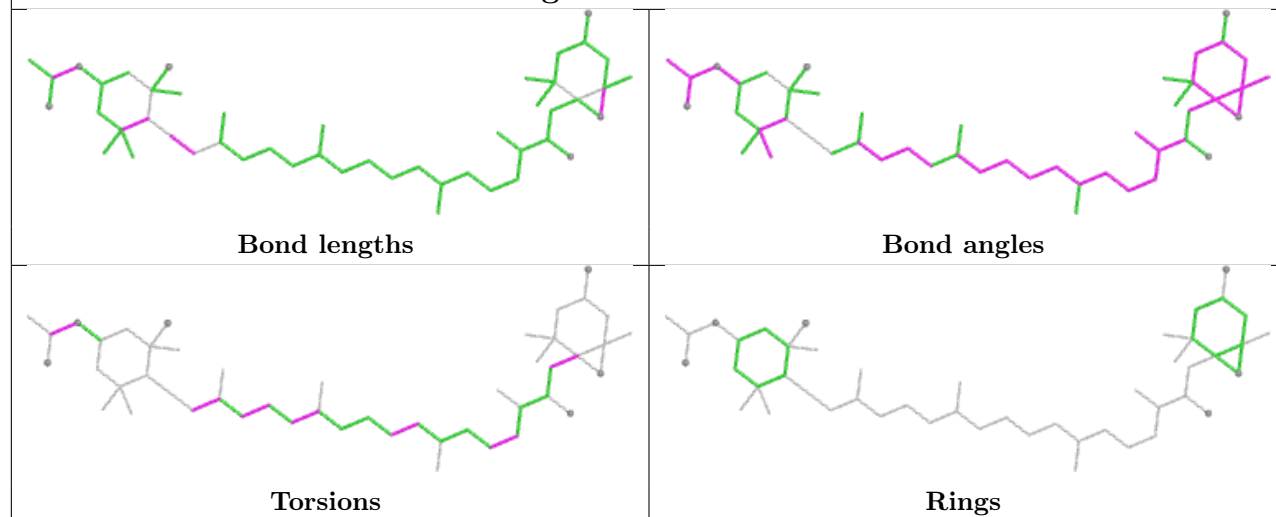


Rings

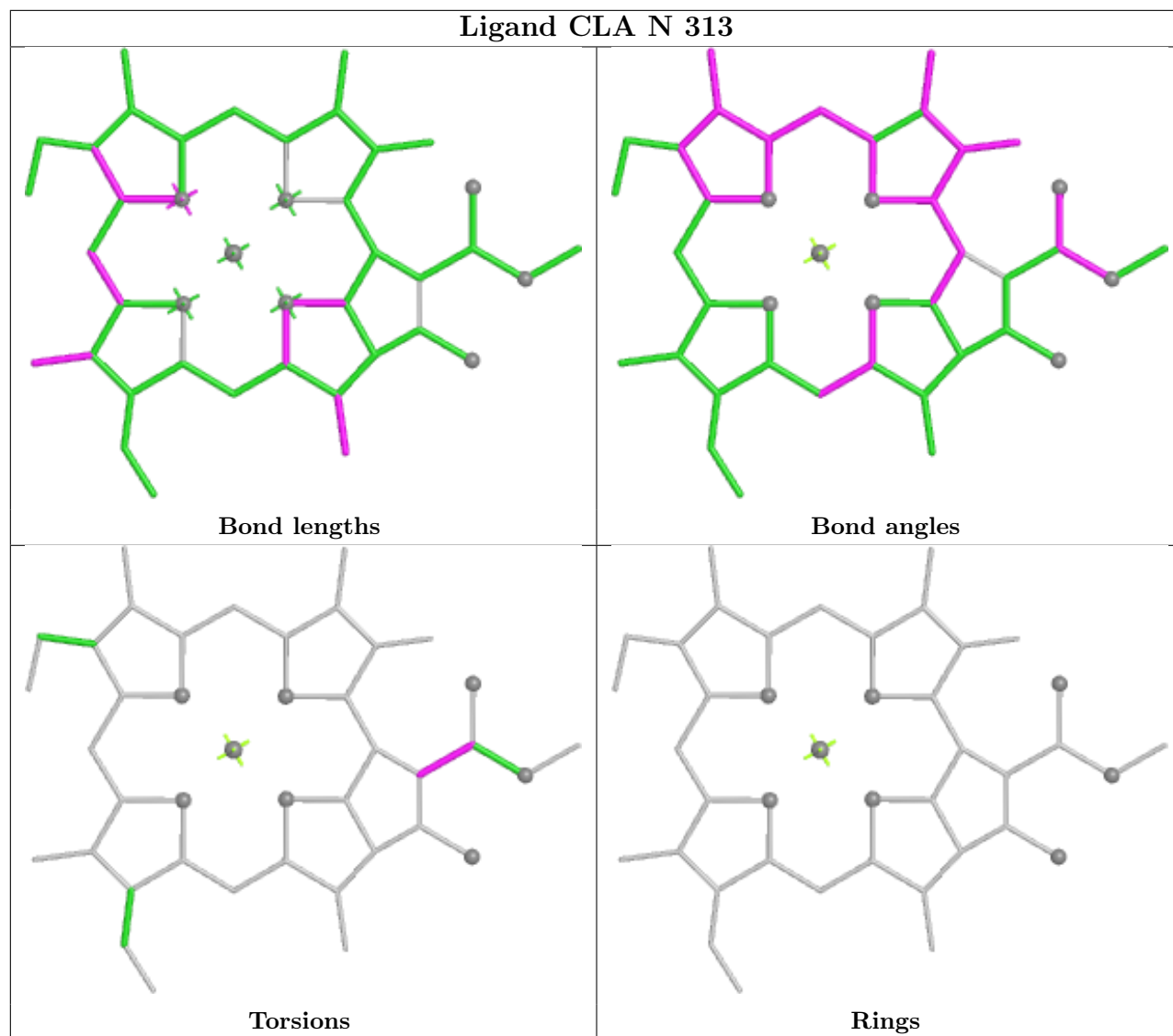
## Ligand CLA S 311



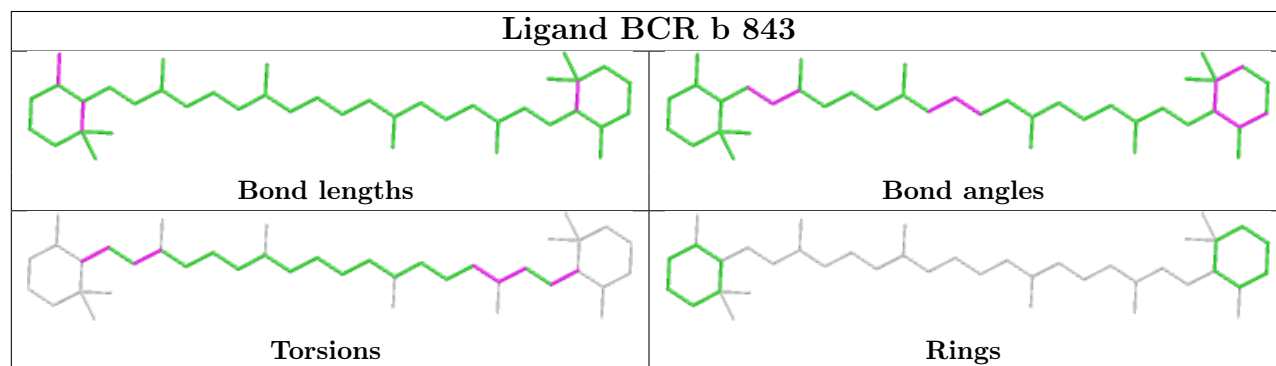
## Ligand A86 J 301



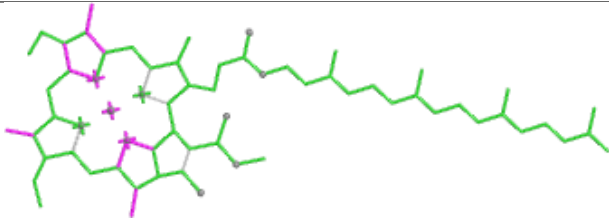
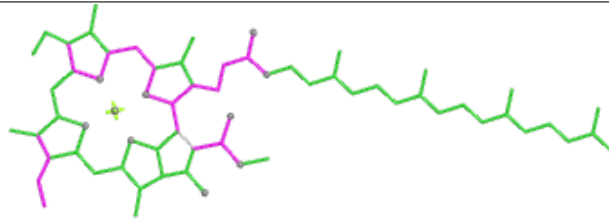
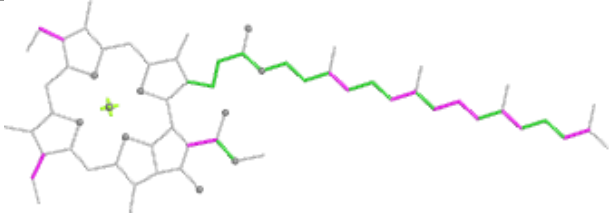
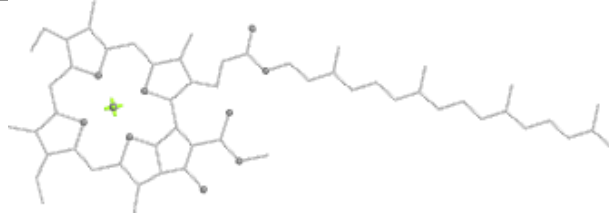
## Ligand CLA N 313

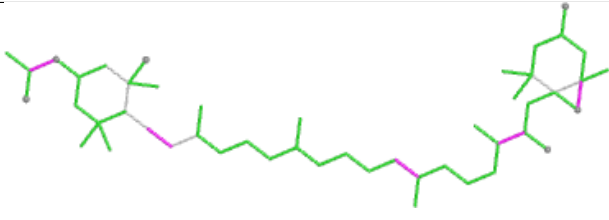
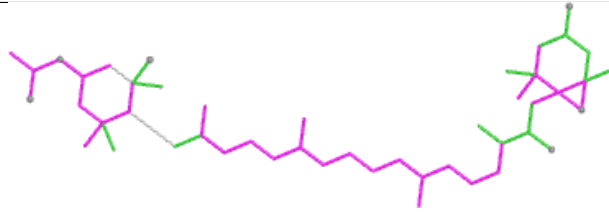
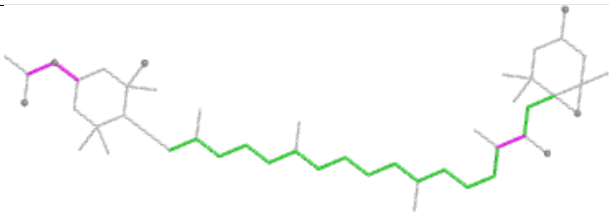
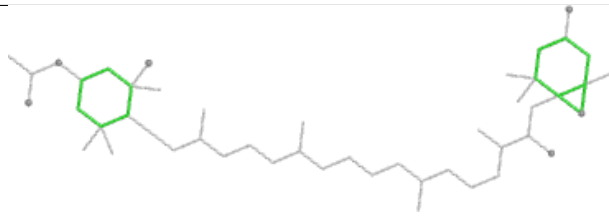


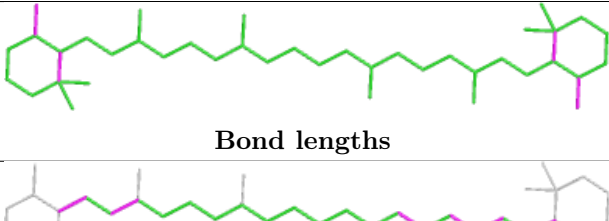
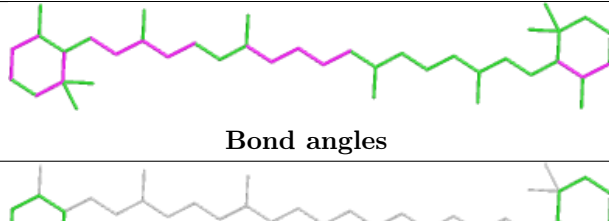
## Ligand BCR b 843



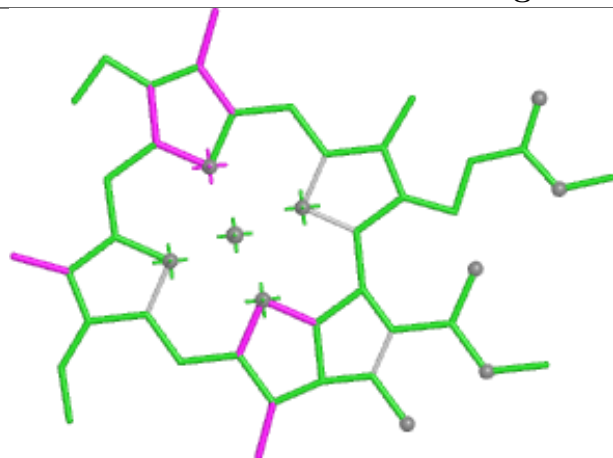


| Ligand CLA H 315                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

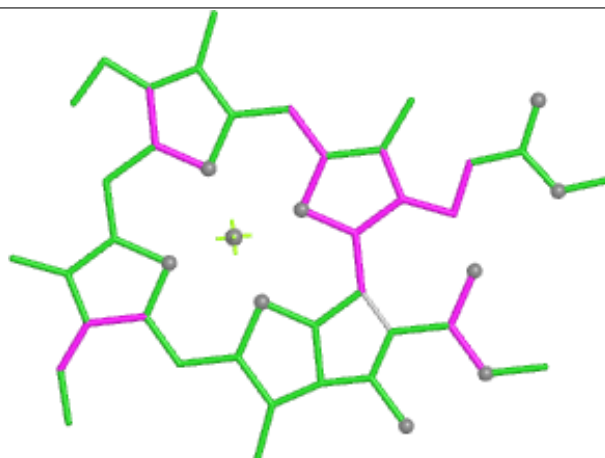
| Ligand A86 S 303                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

| Ligand BCR m 101                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

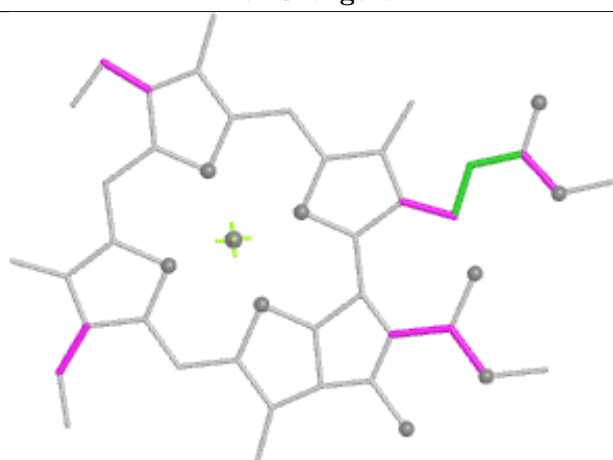
## Ligand CLA R 314



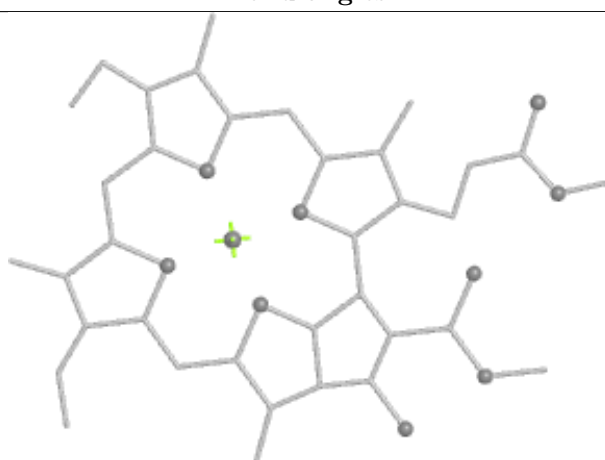
Bond lengths



Bond angles

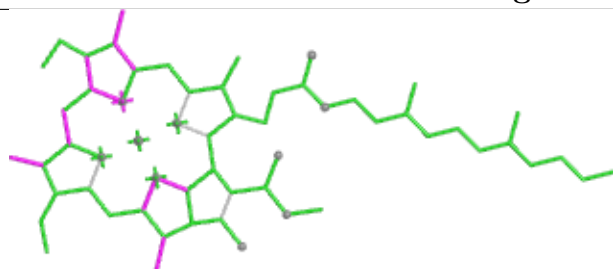


Torsions

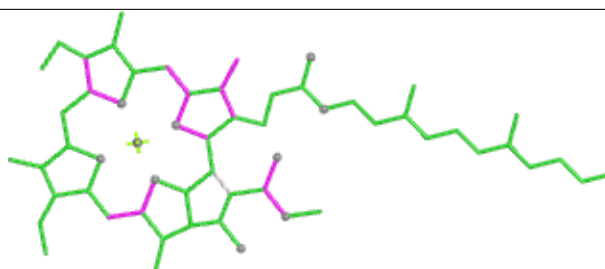


Rings

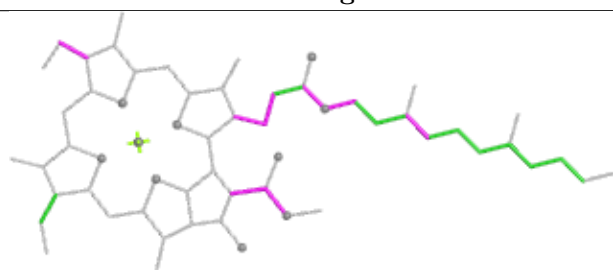
## Ligand CLA D 317



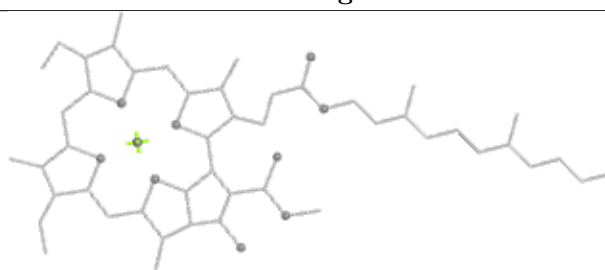
Bond lengths



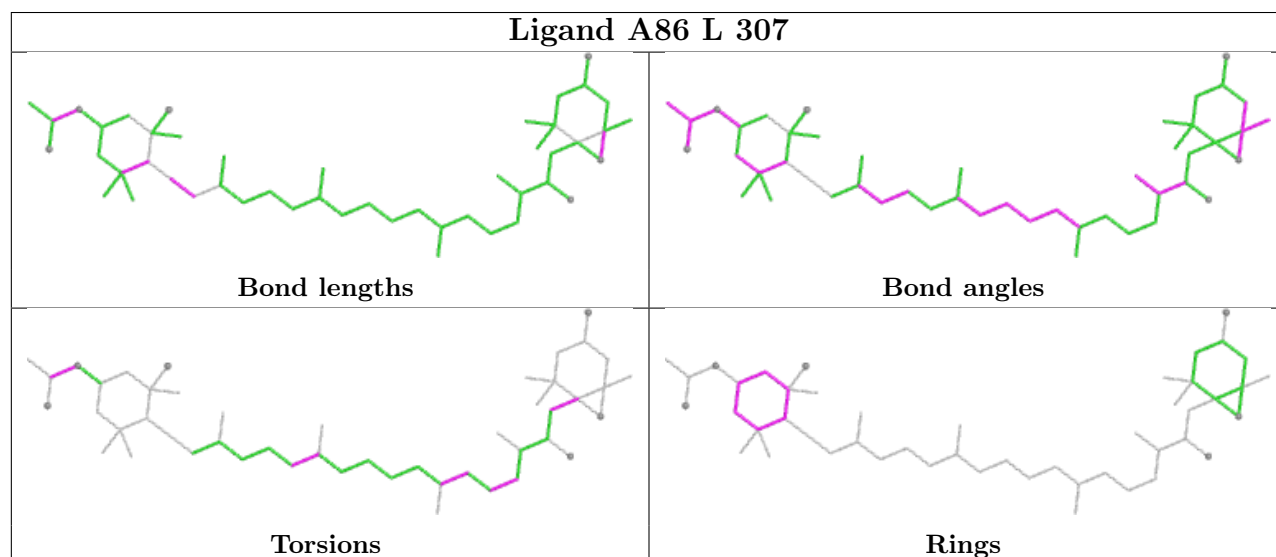
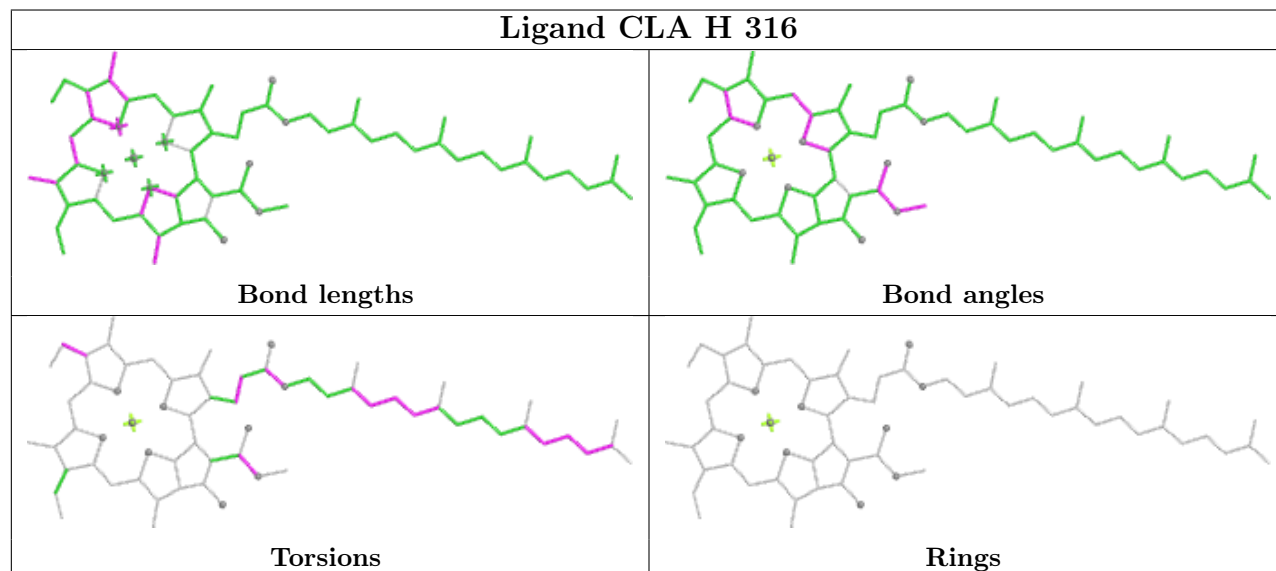
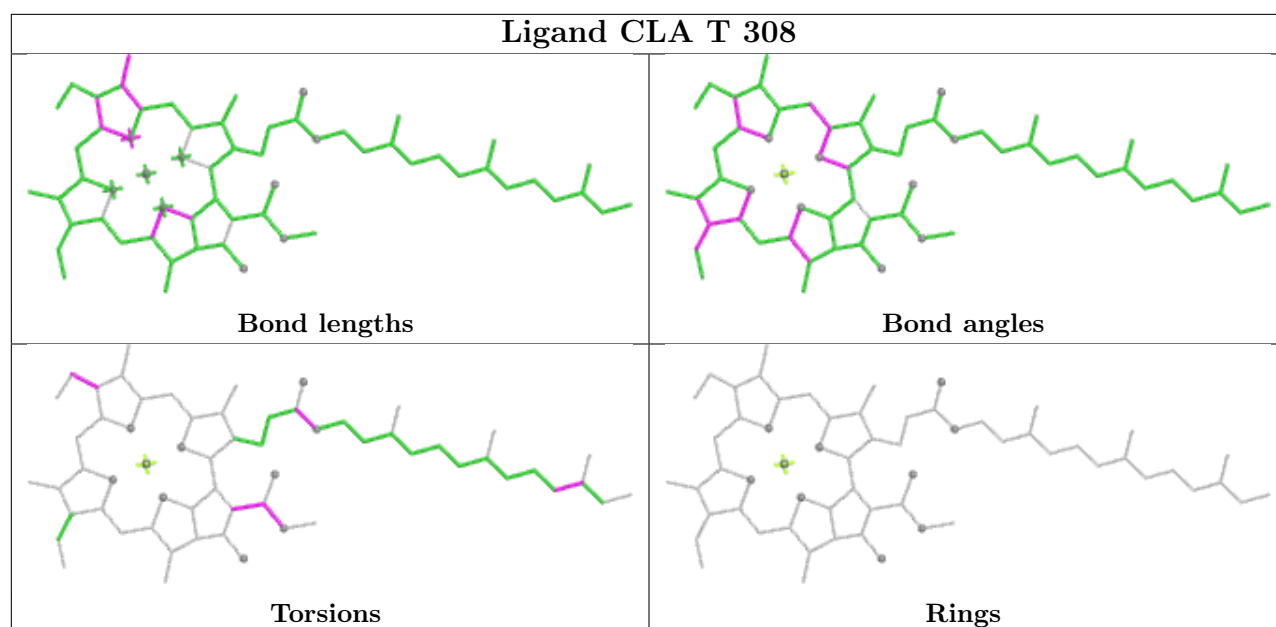
Bond angles

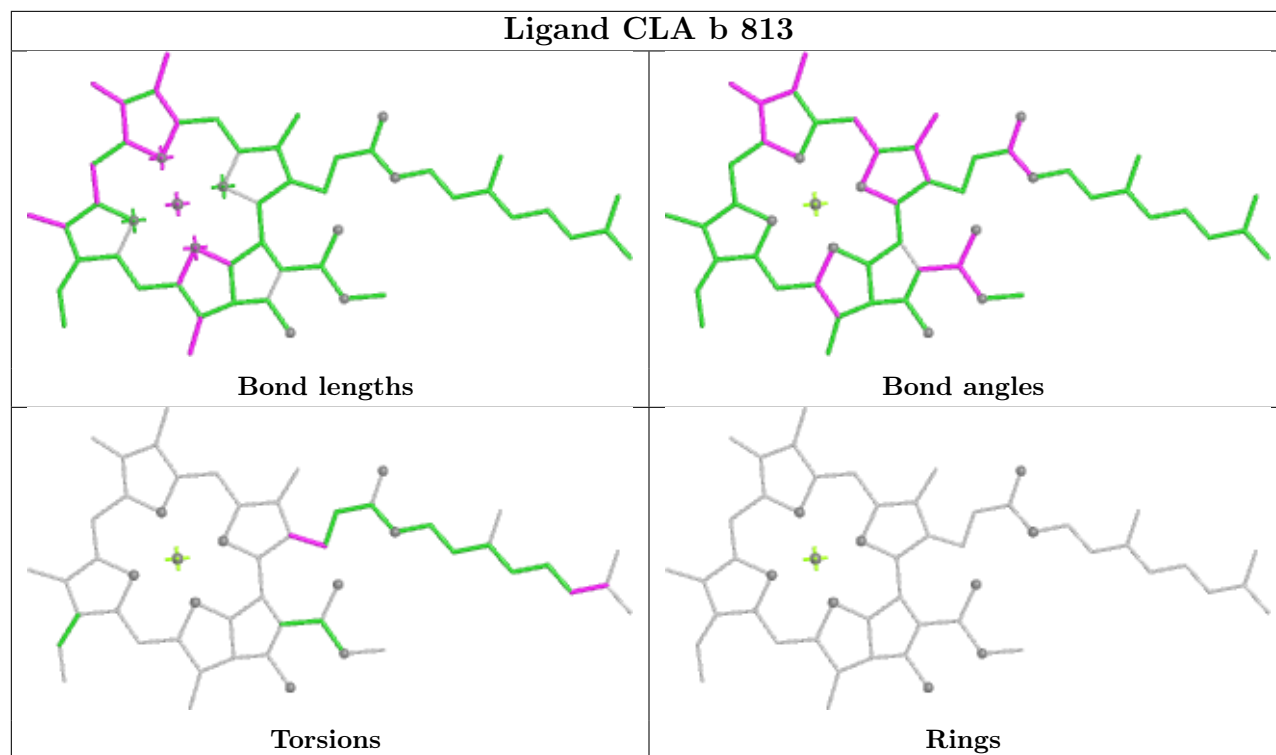
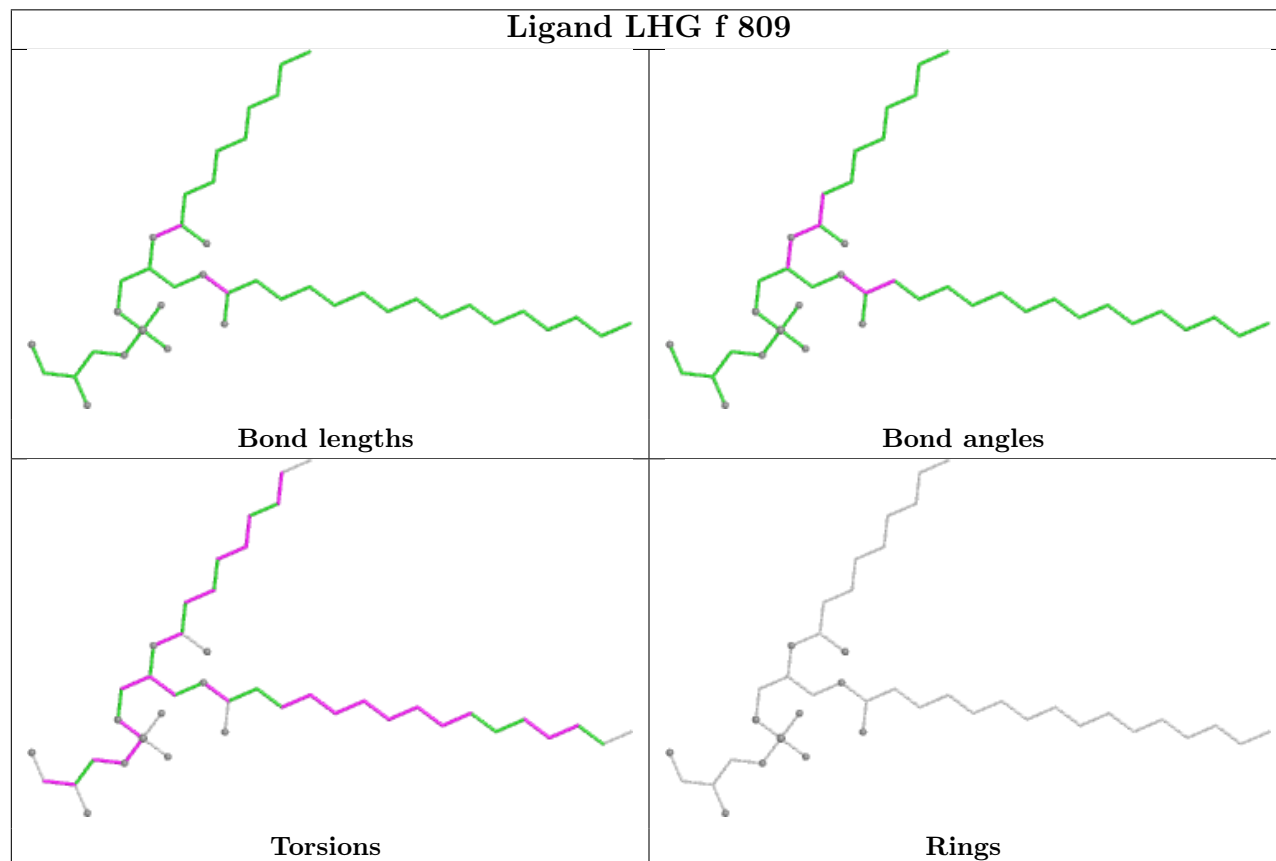


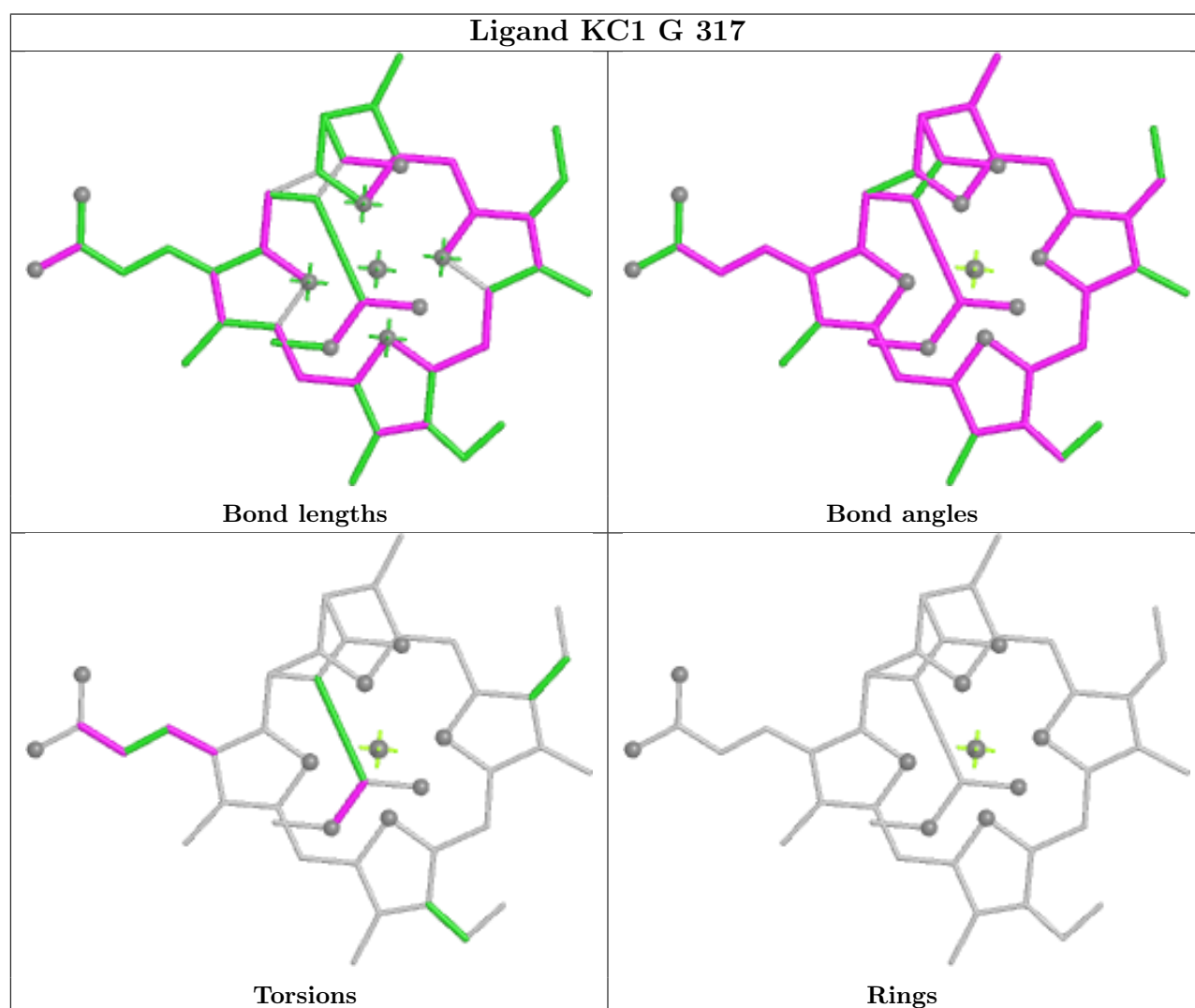
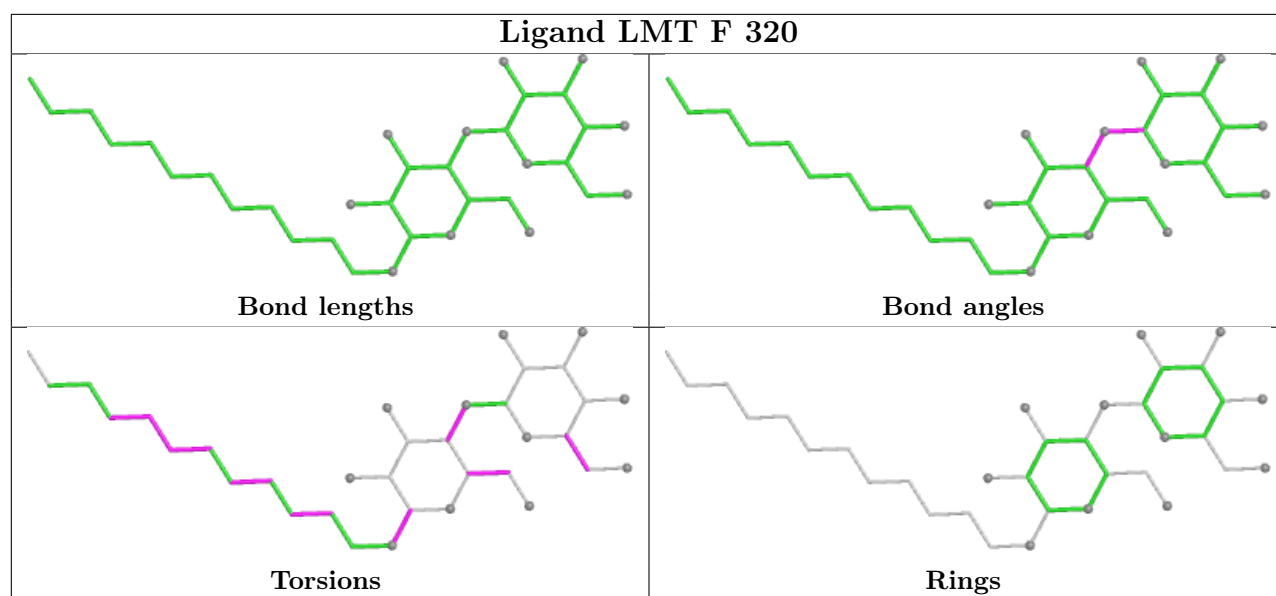
Torsions

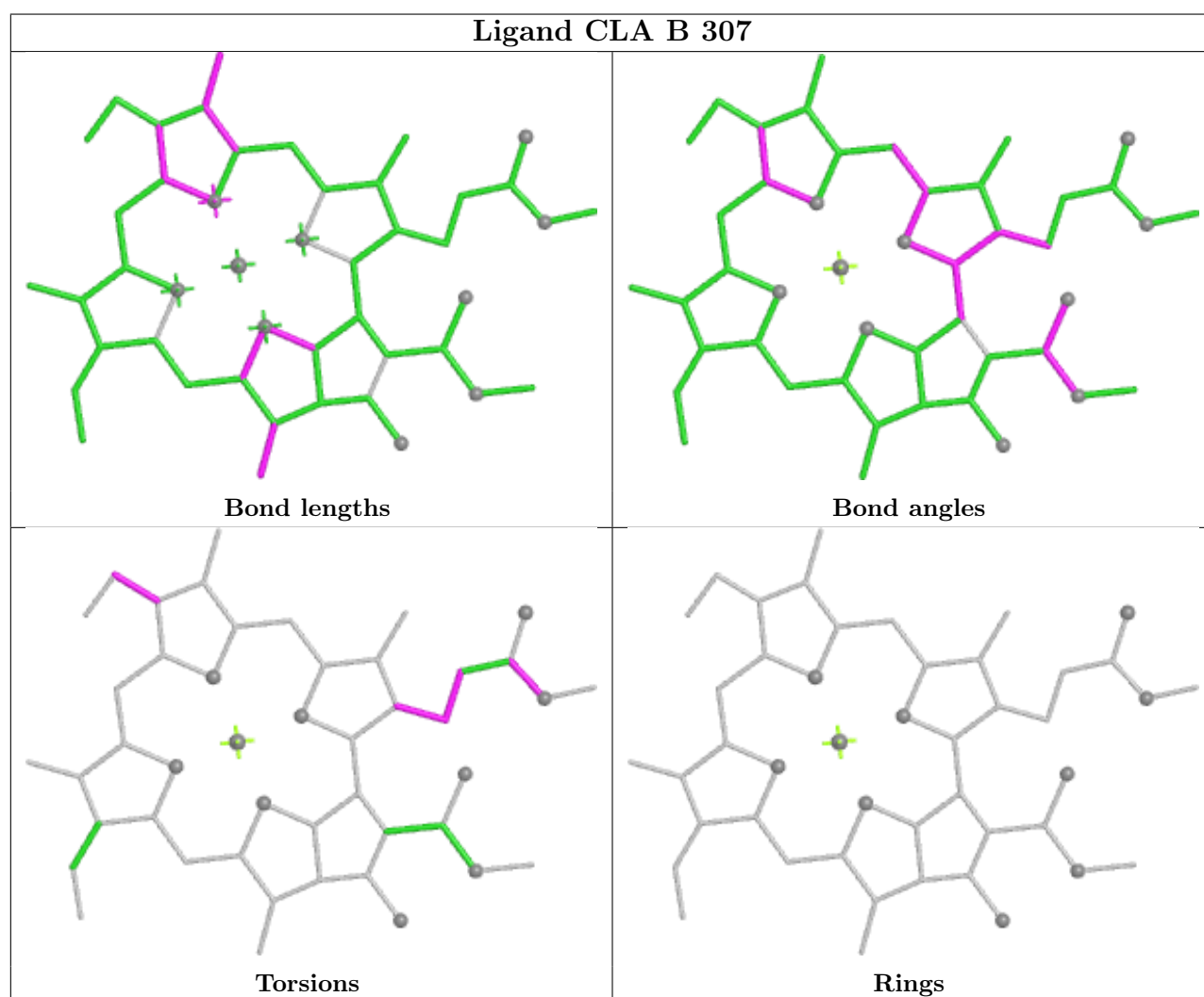
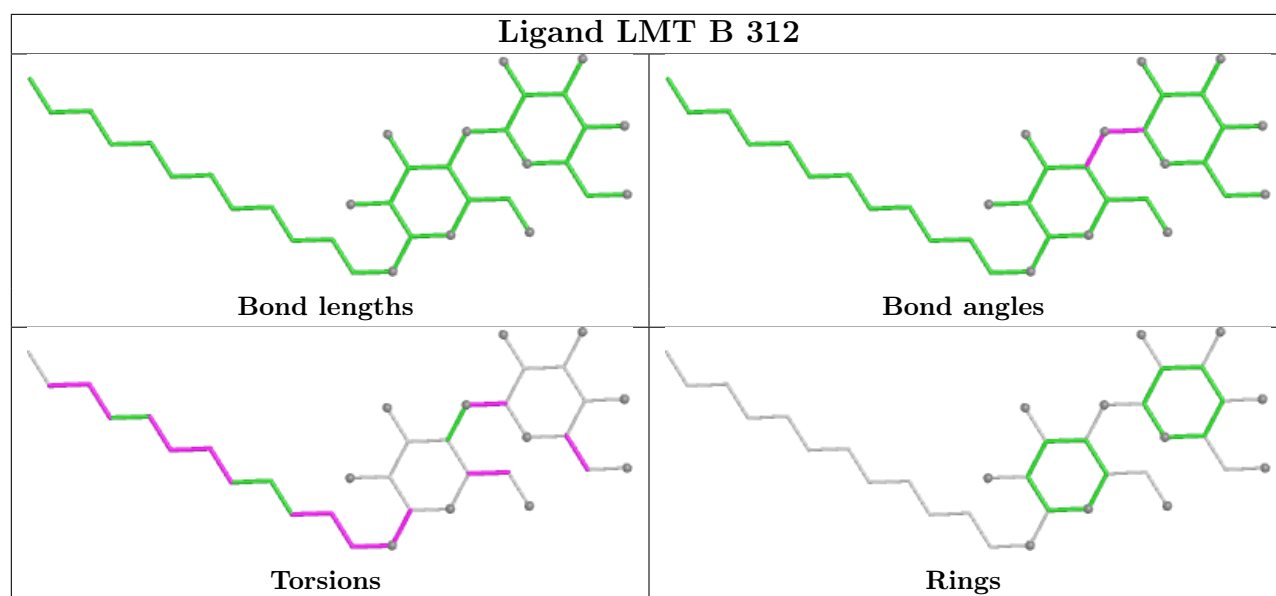


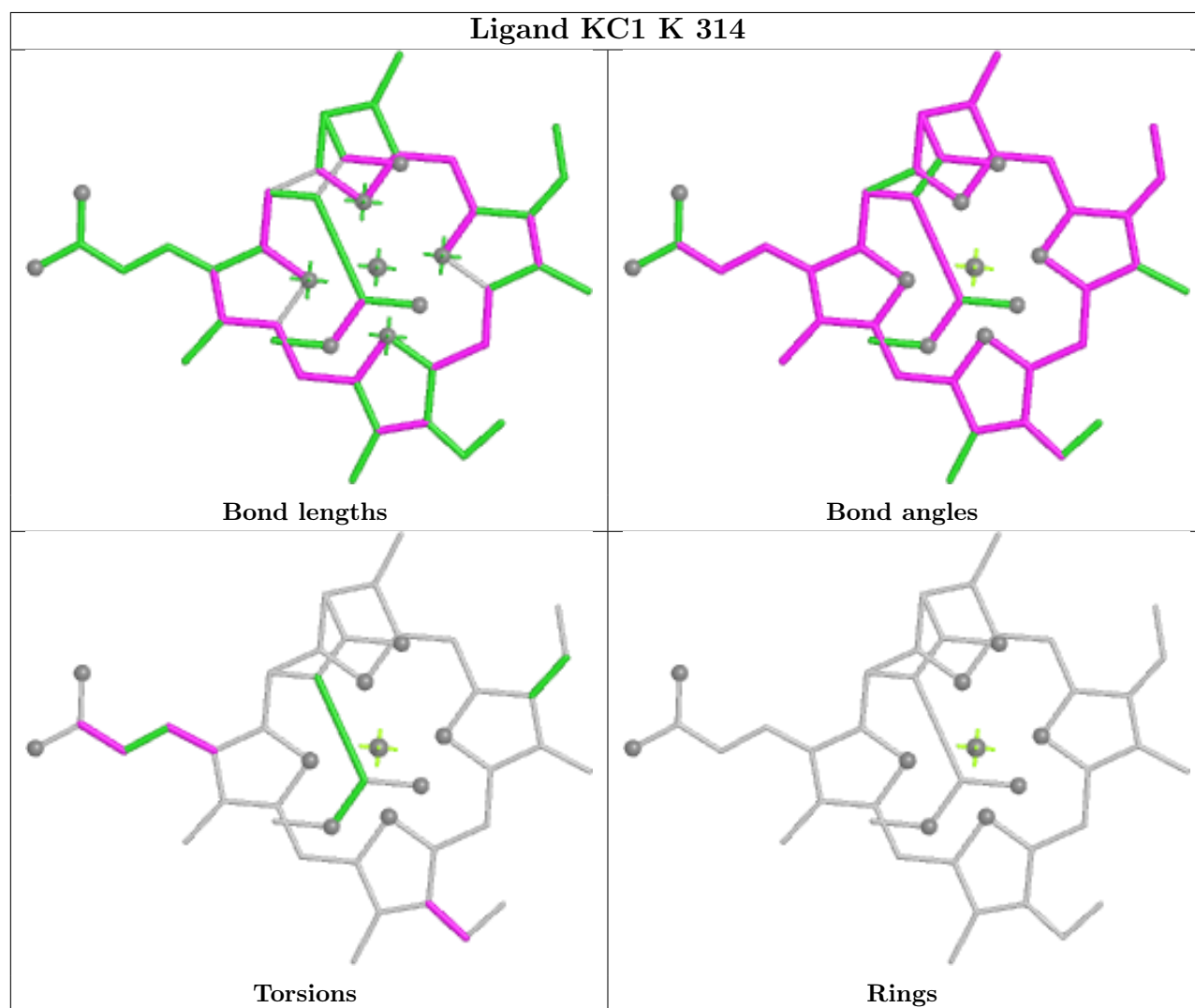
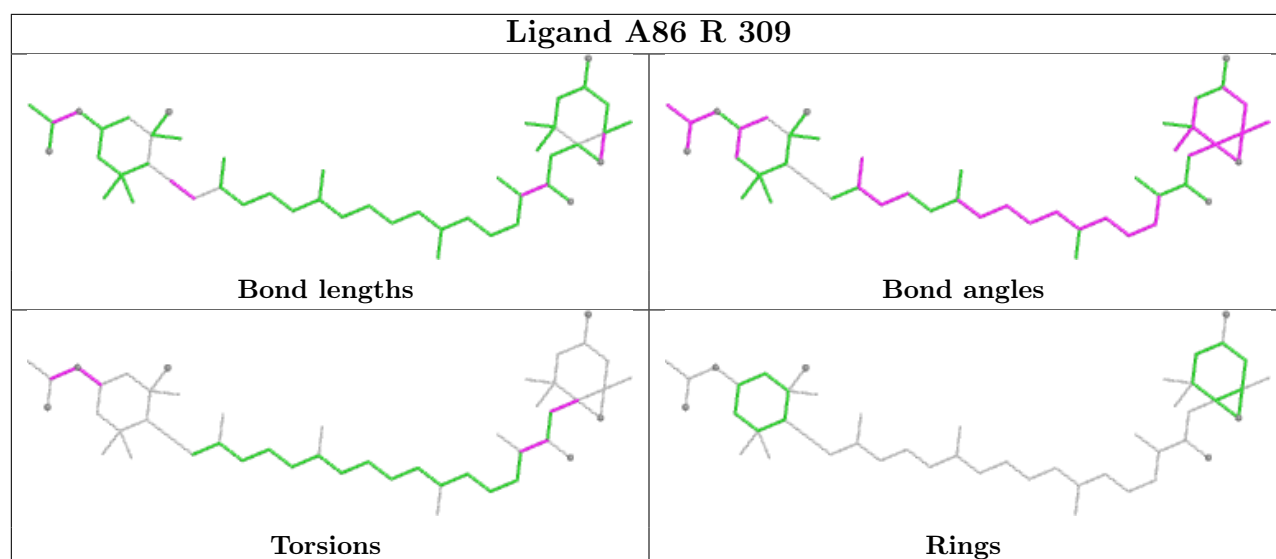
Rings

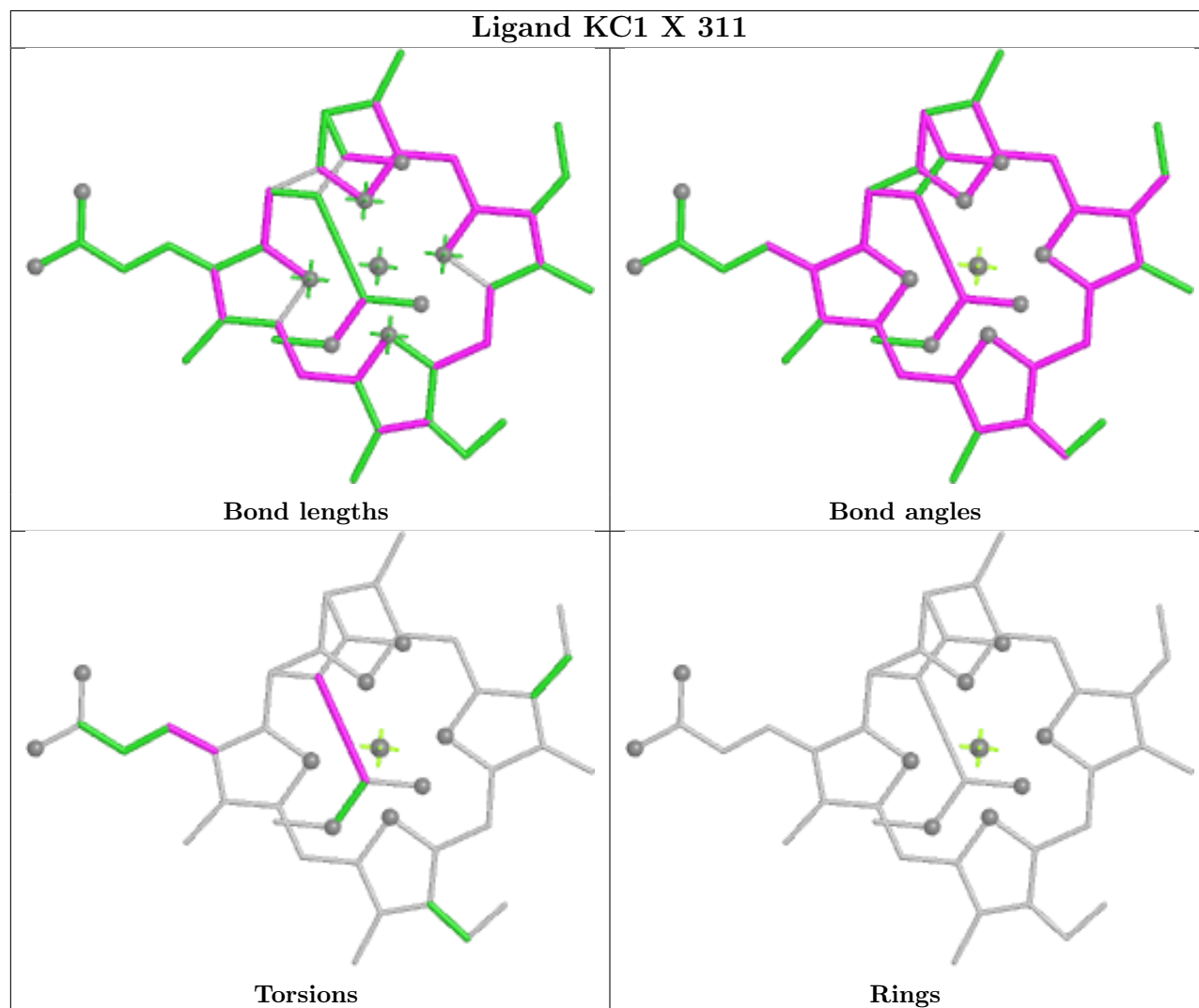
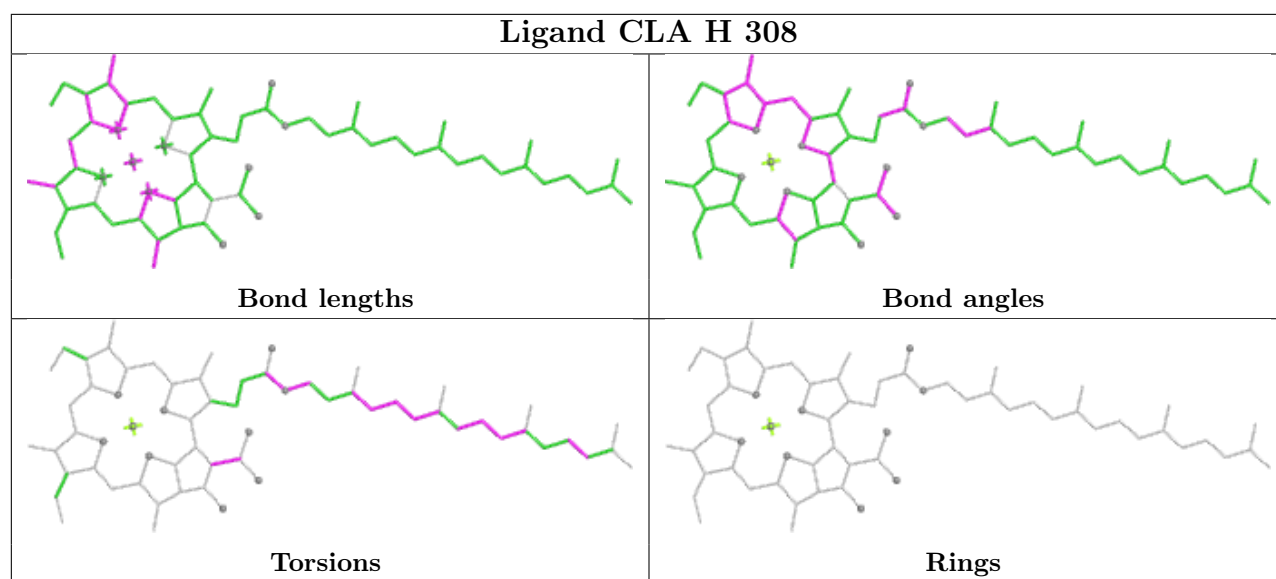


**Ligand CLA b 813****Ligand LHG f 809**

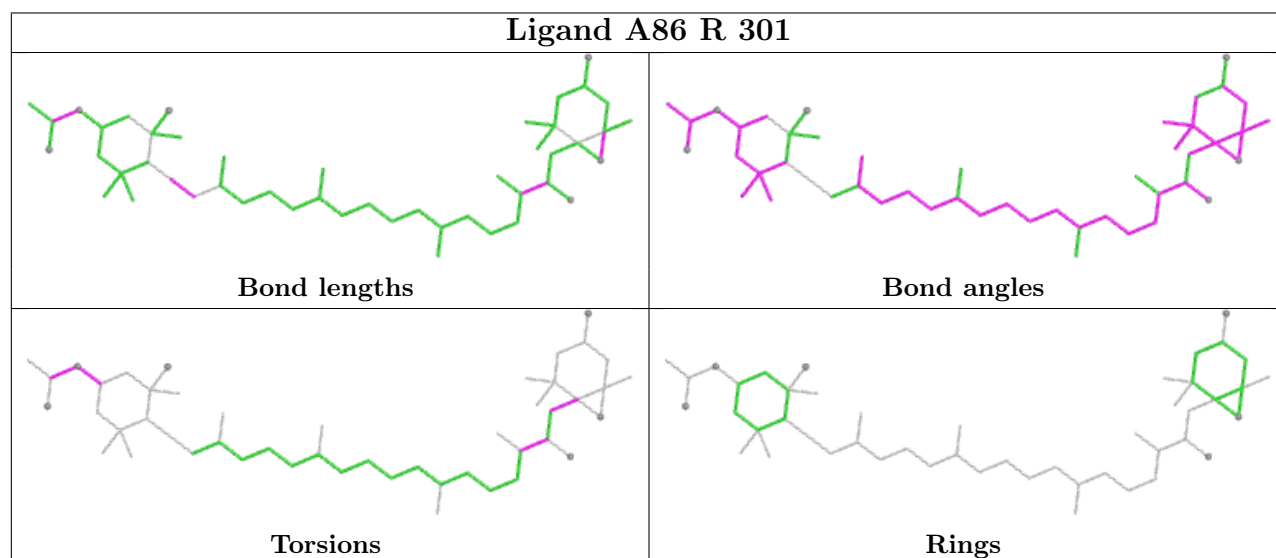
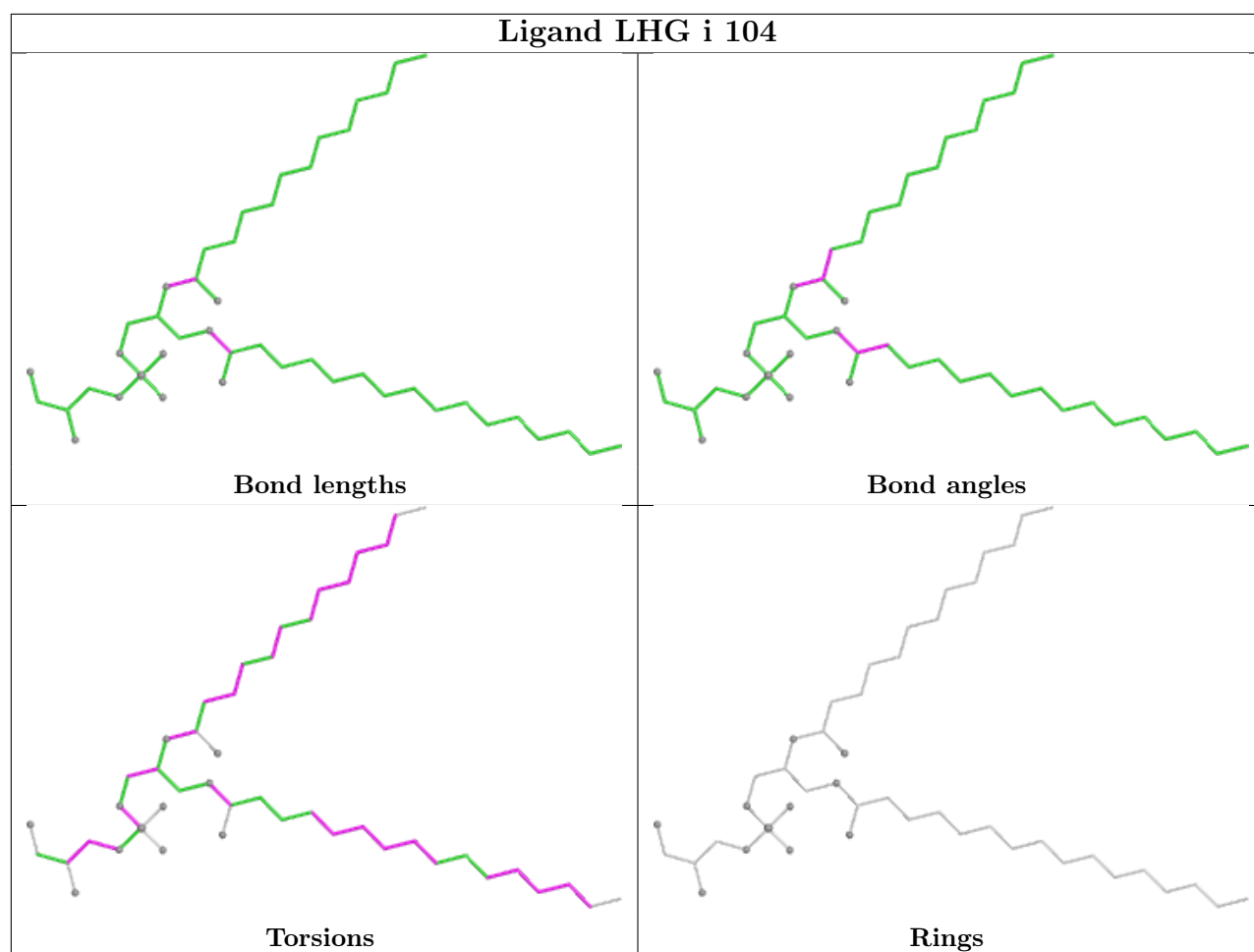




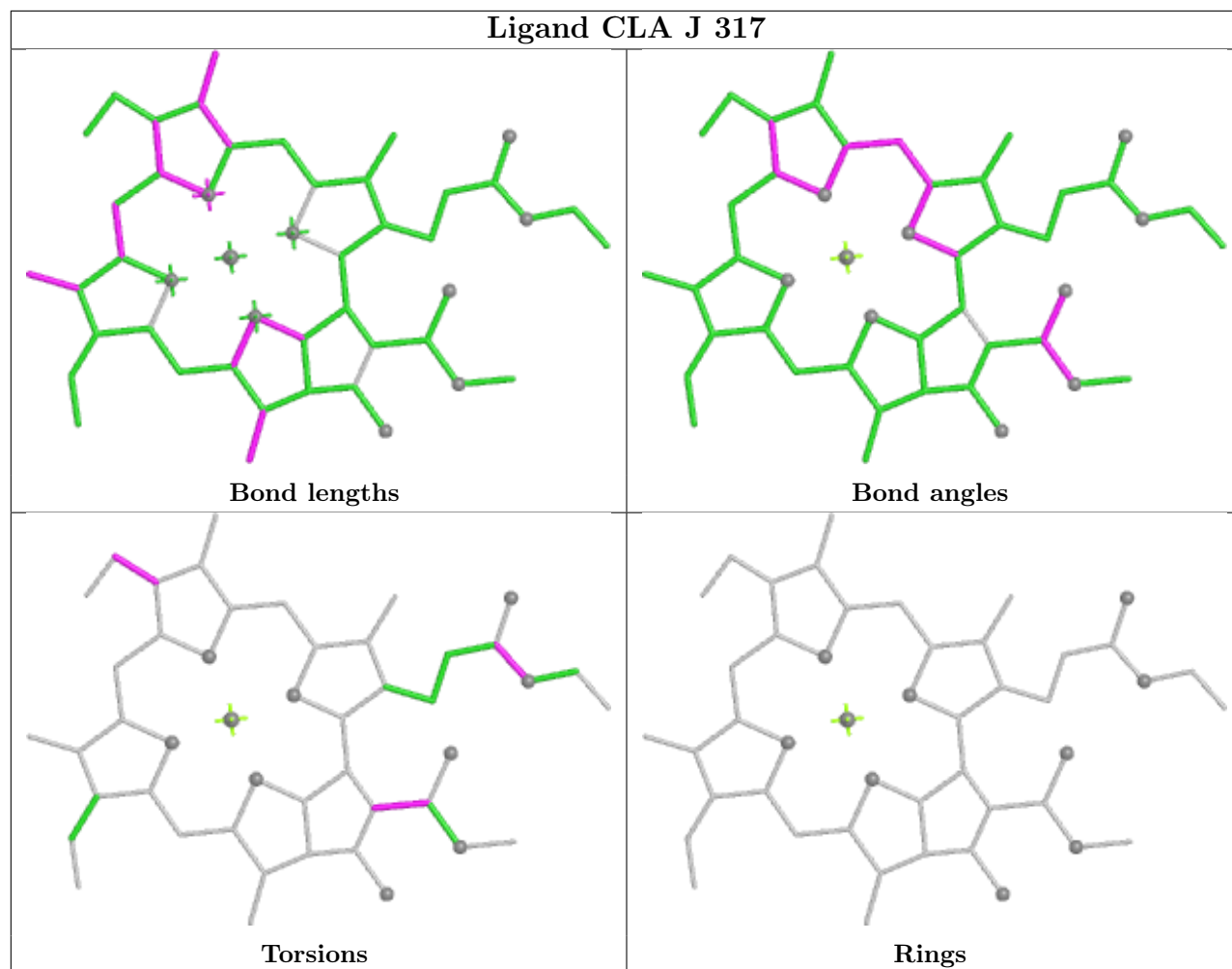




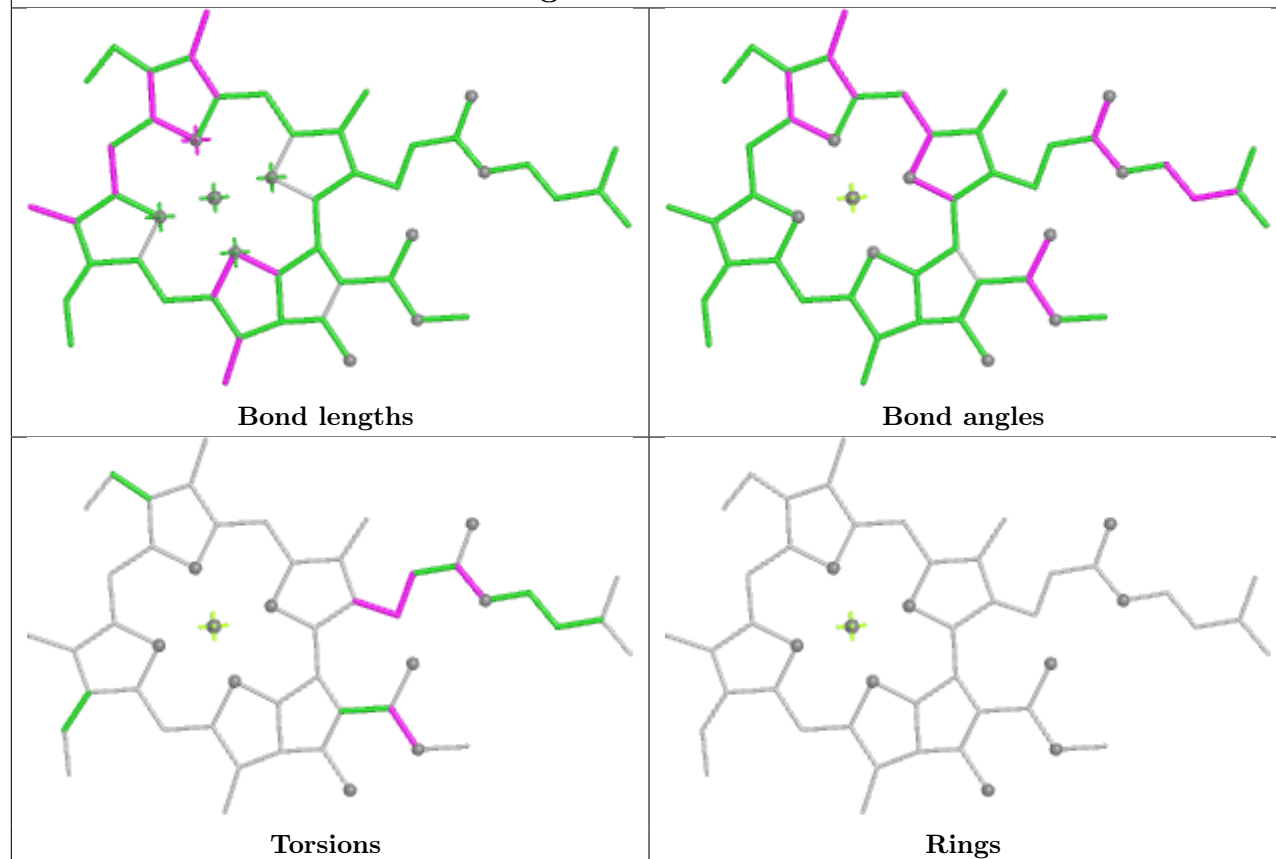




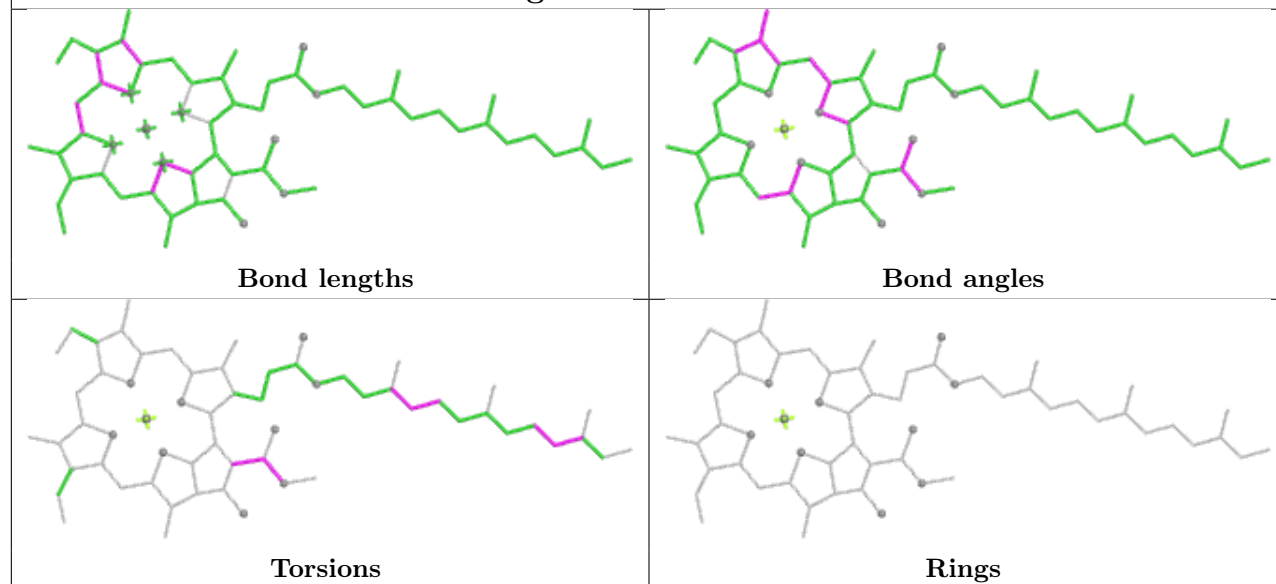
## Ligand CLA J 317

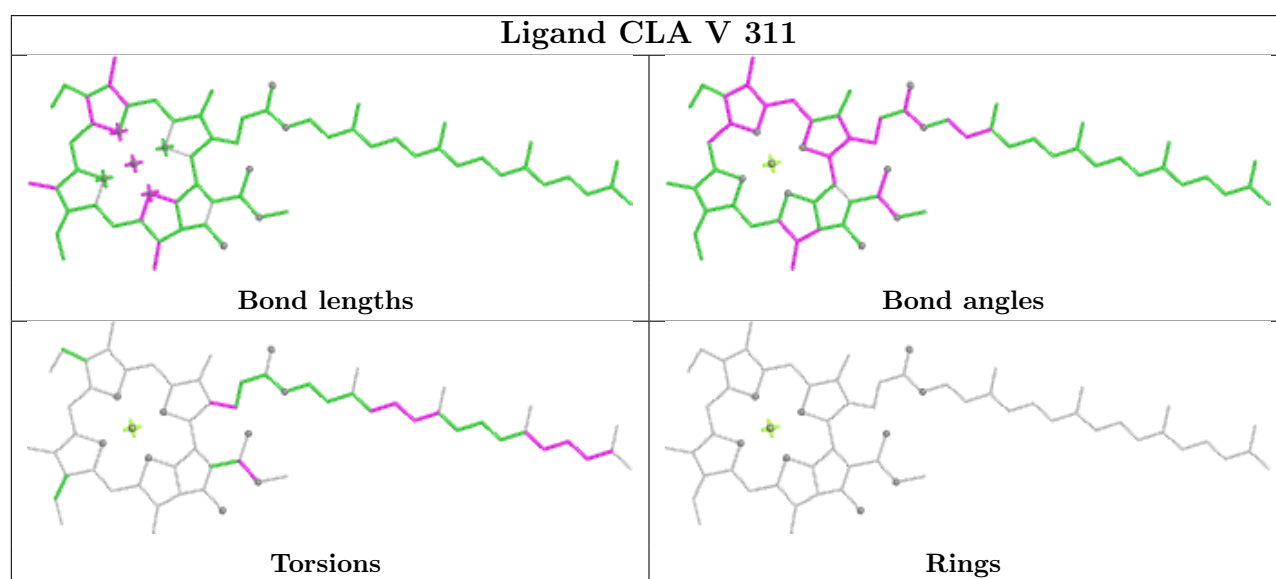
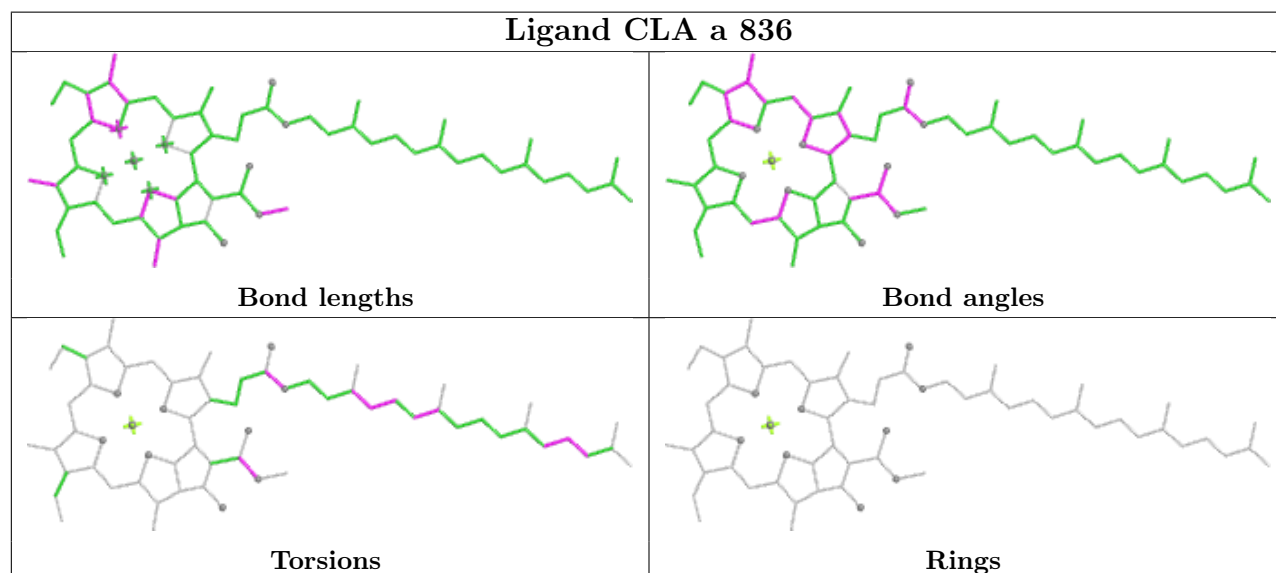
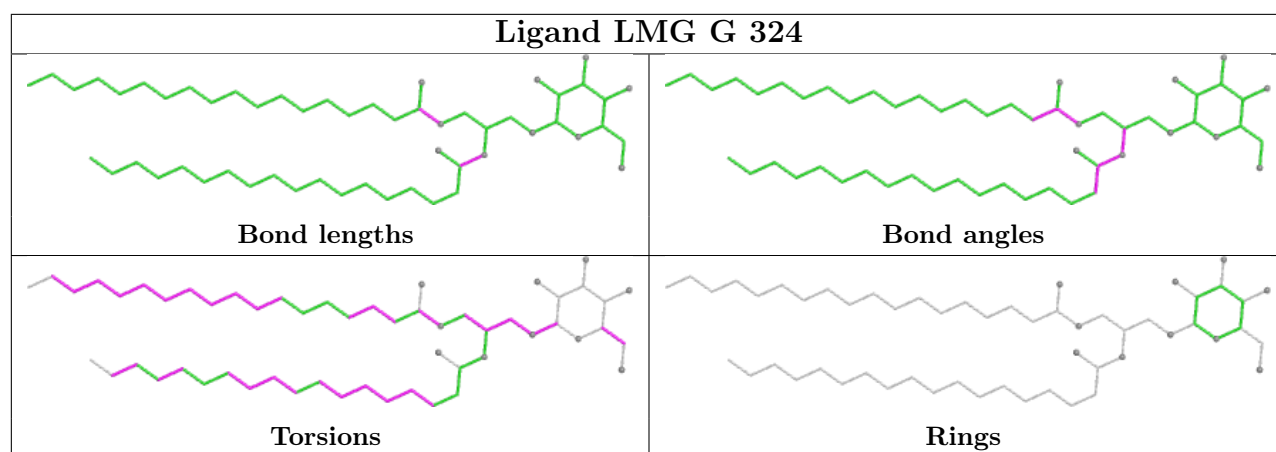


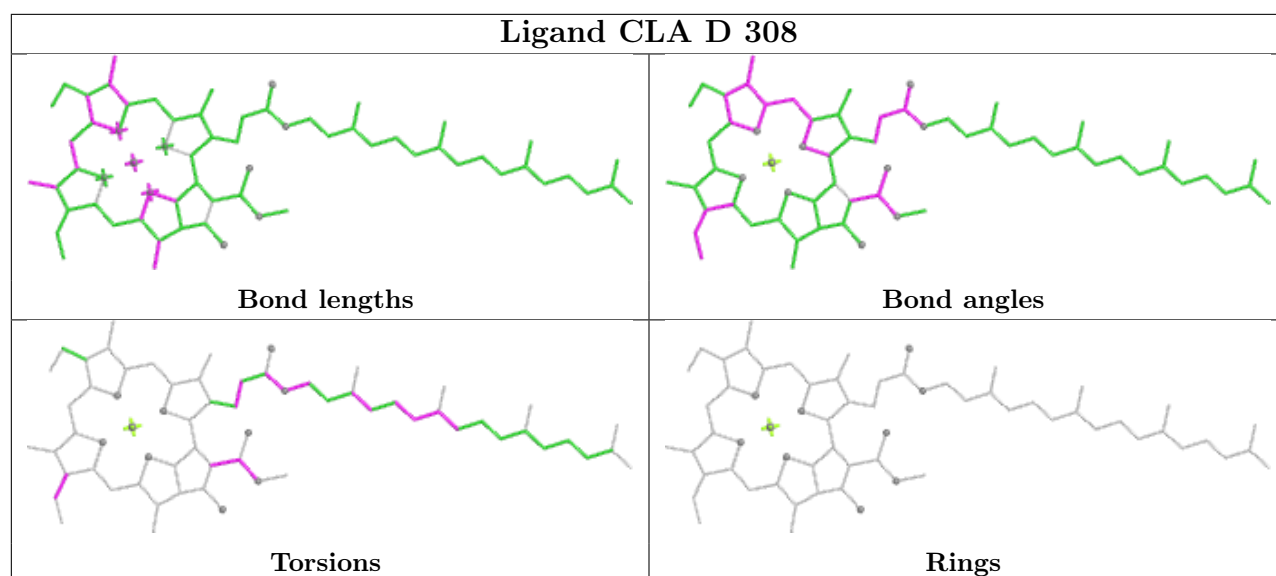
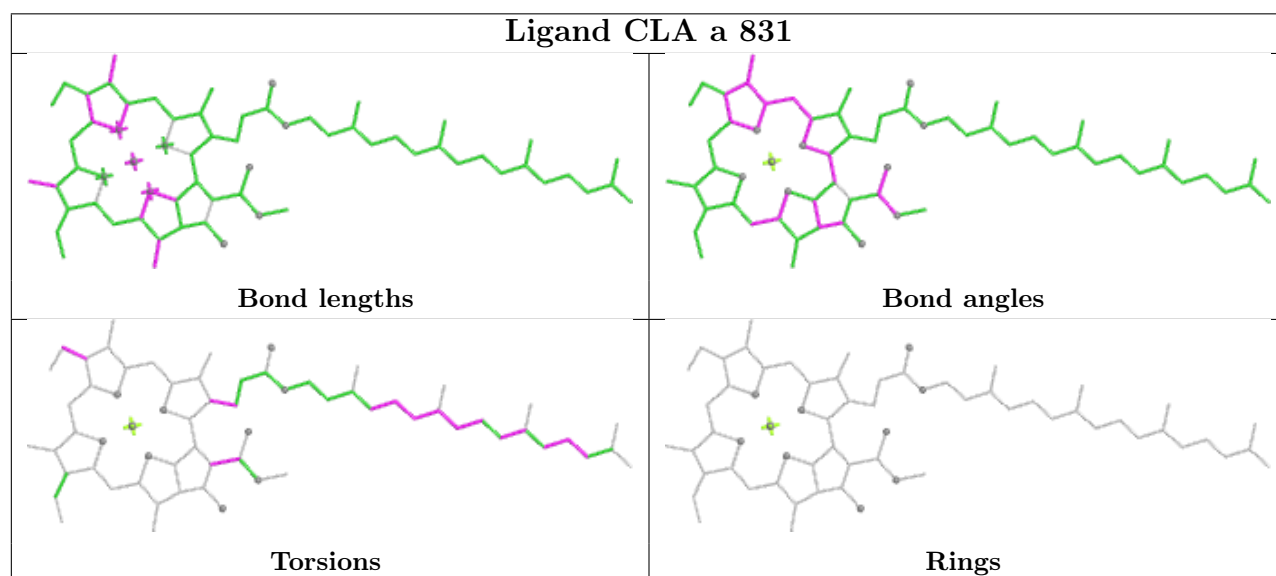
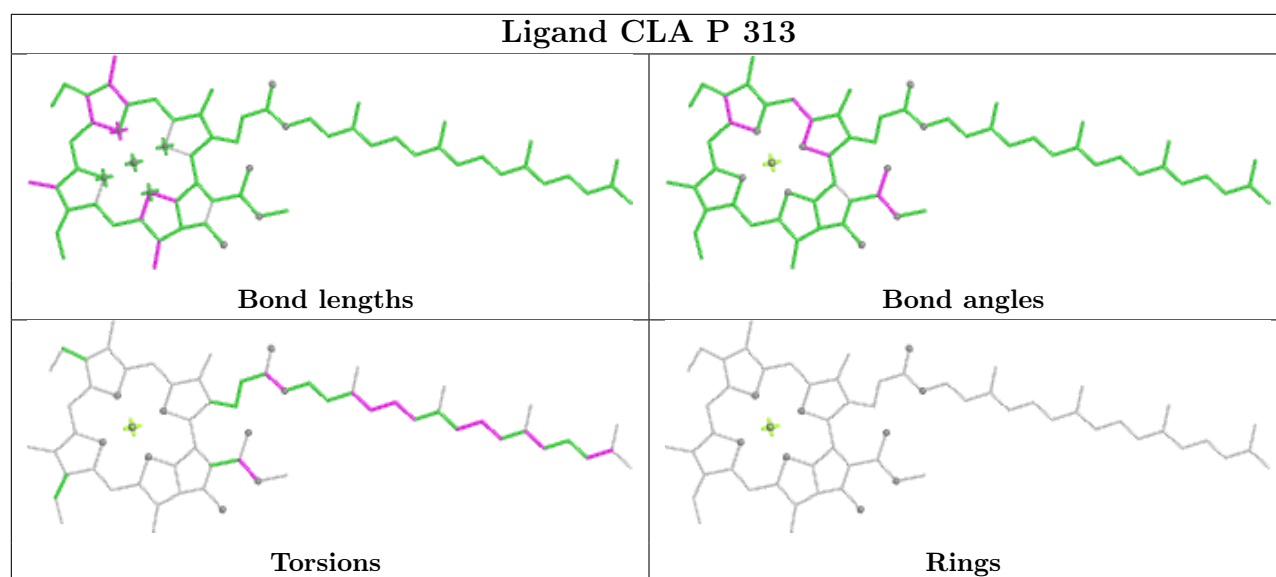
## Ligand CLA I 206



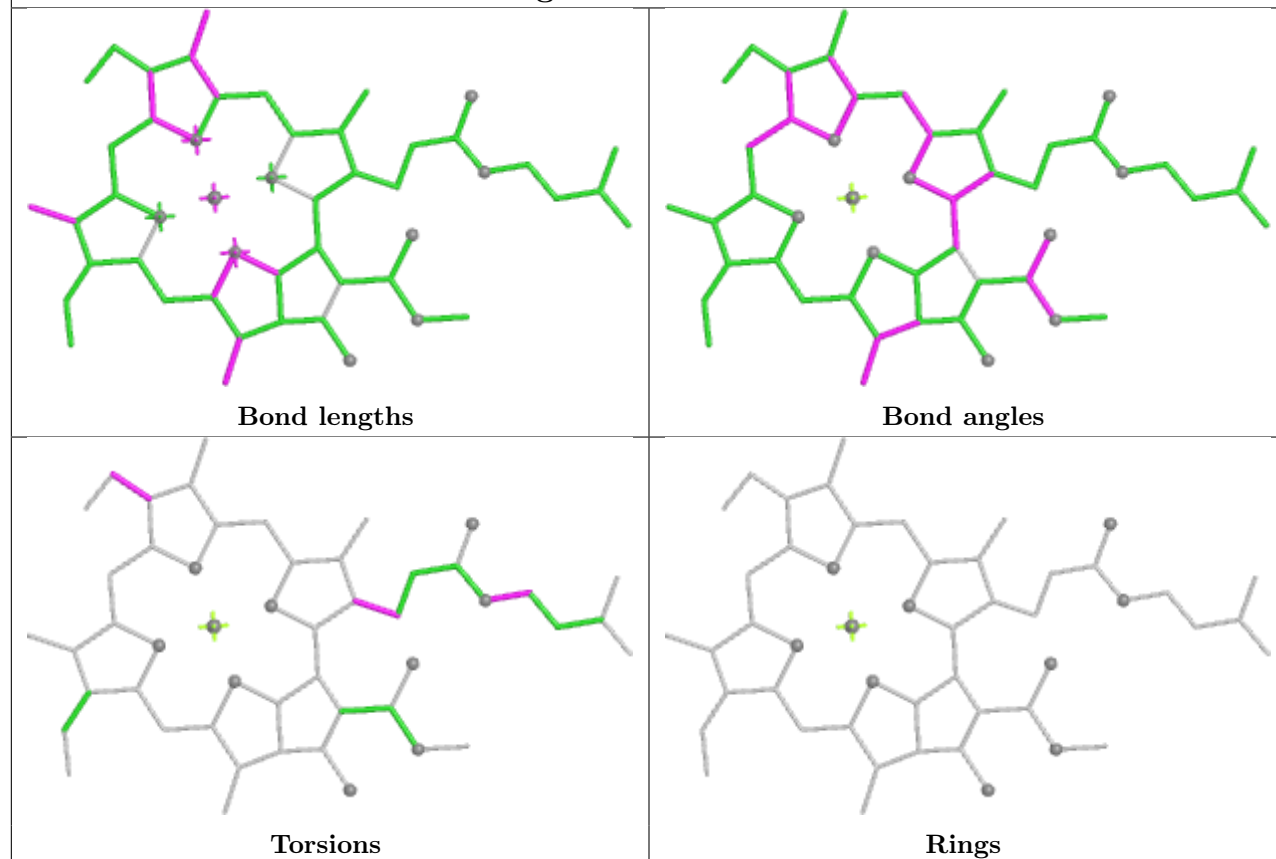
## Ligand CLA W 206



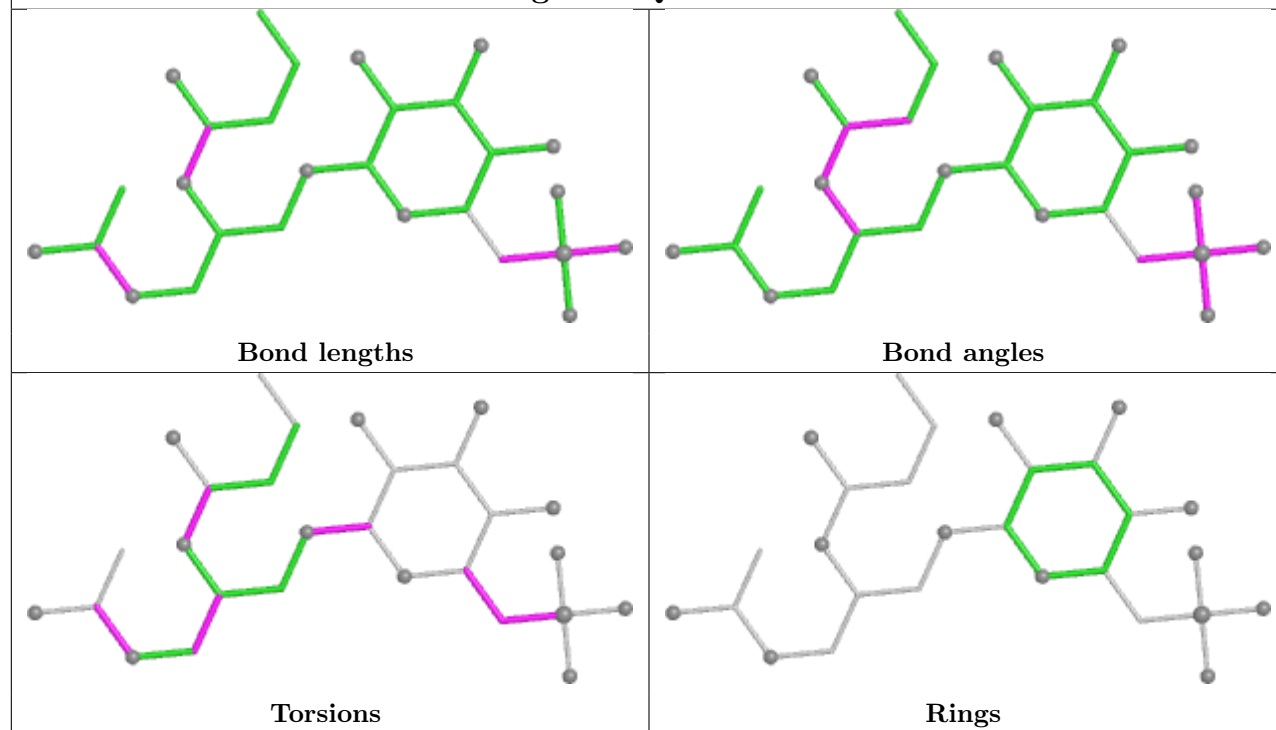


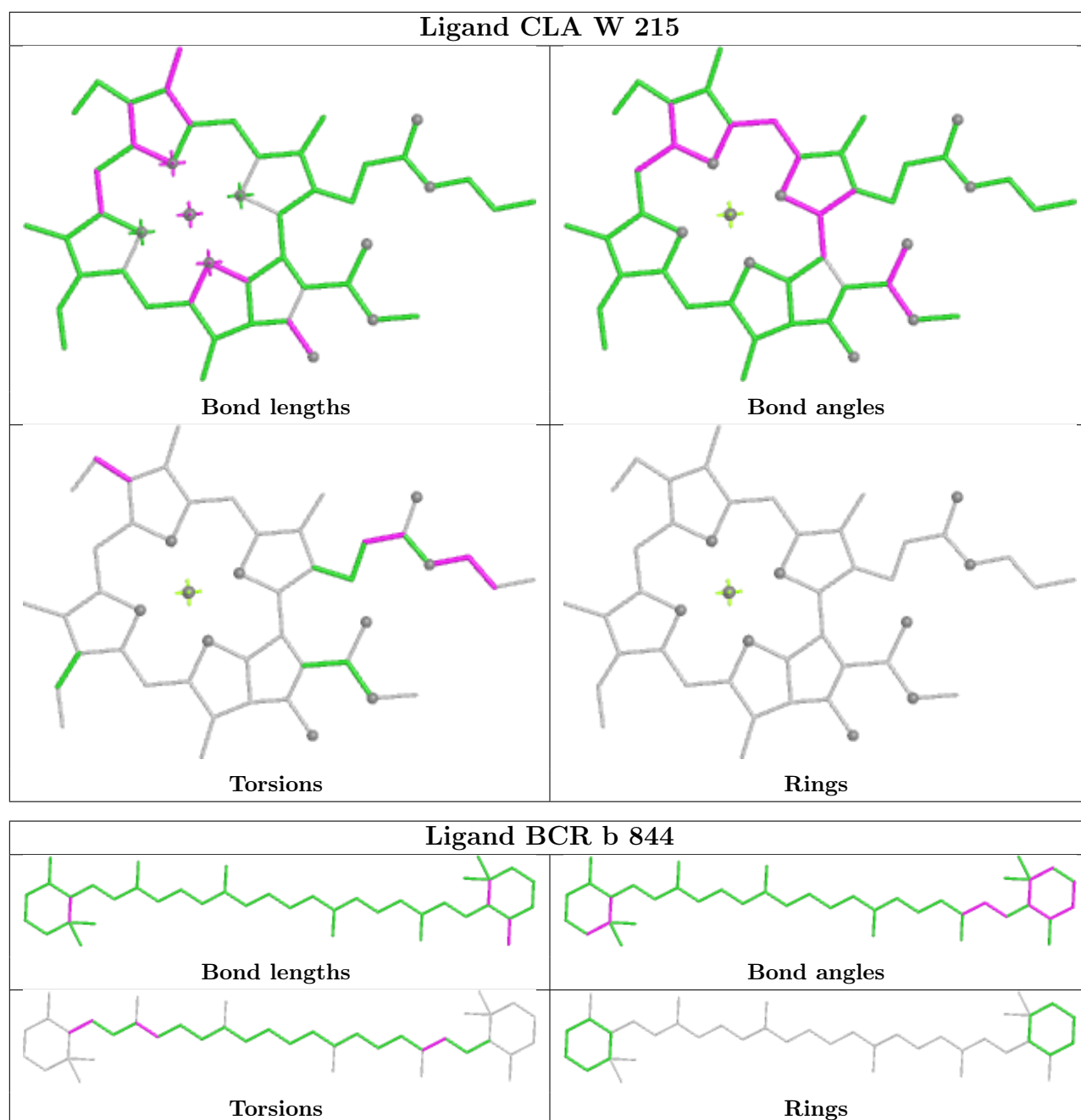


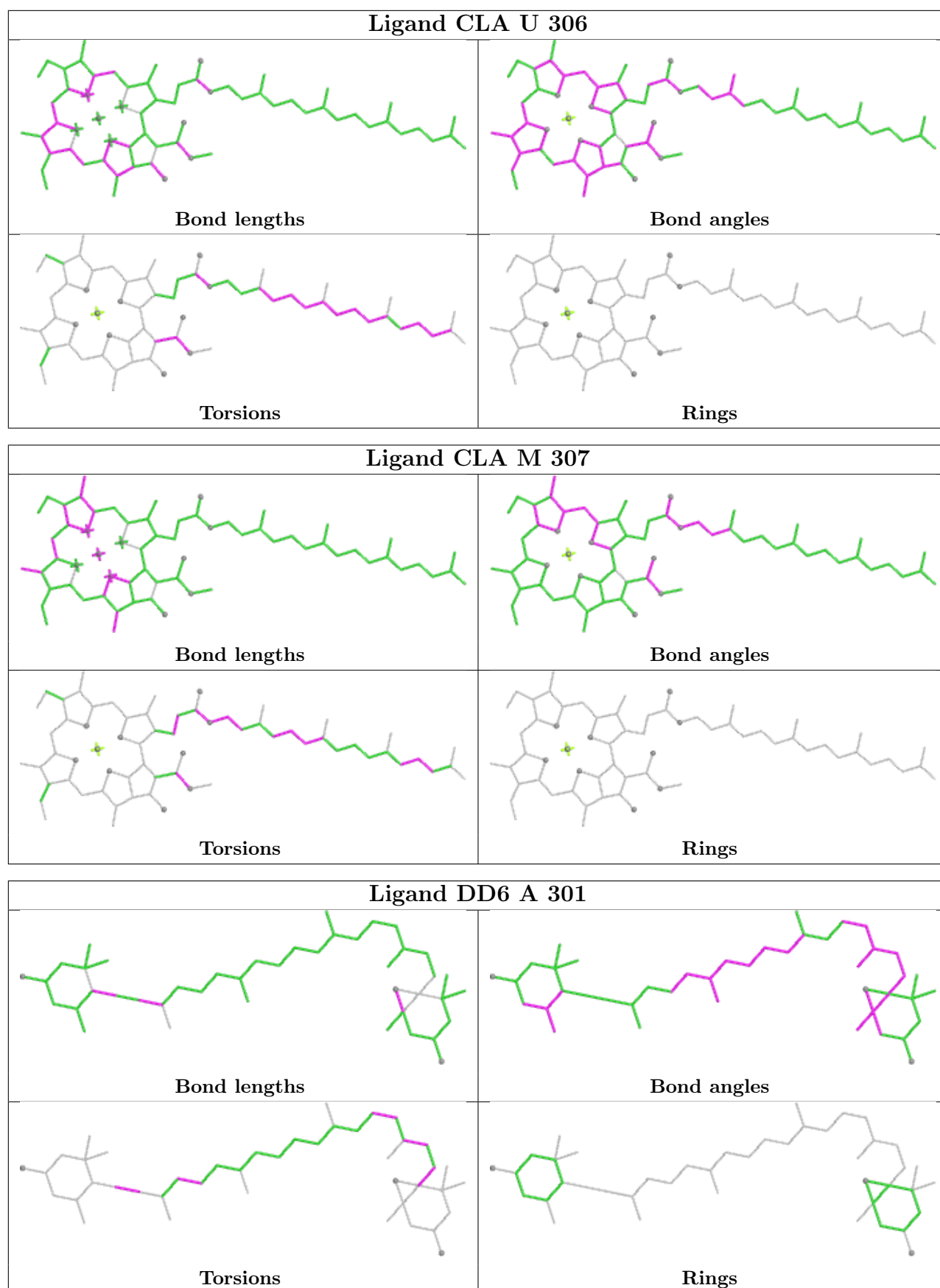
## Ligand CLA a 833



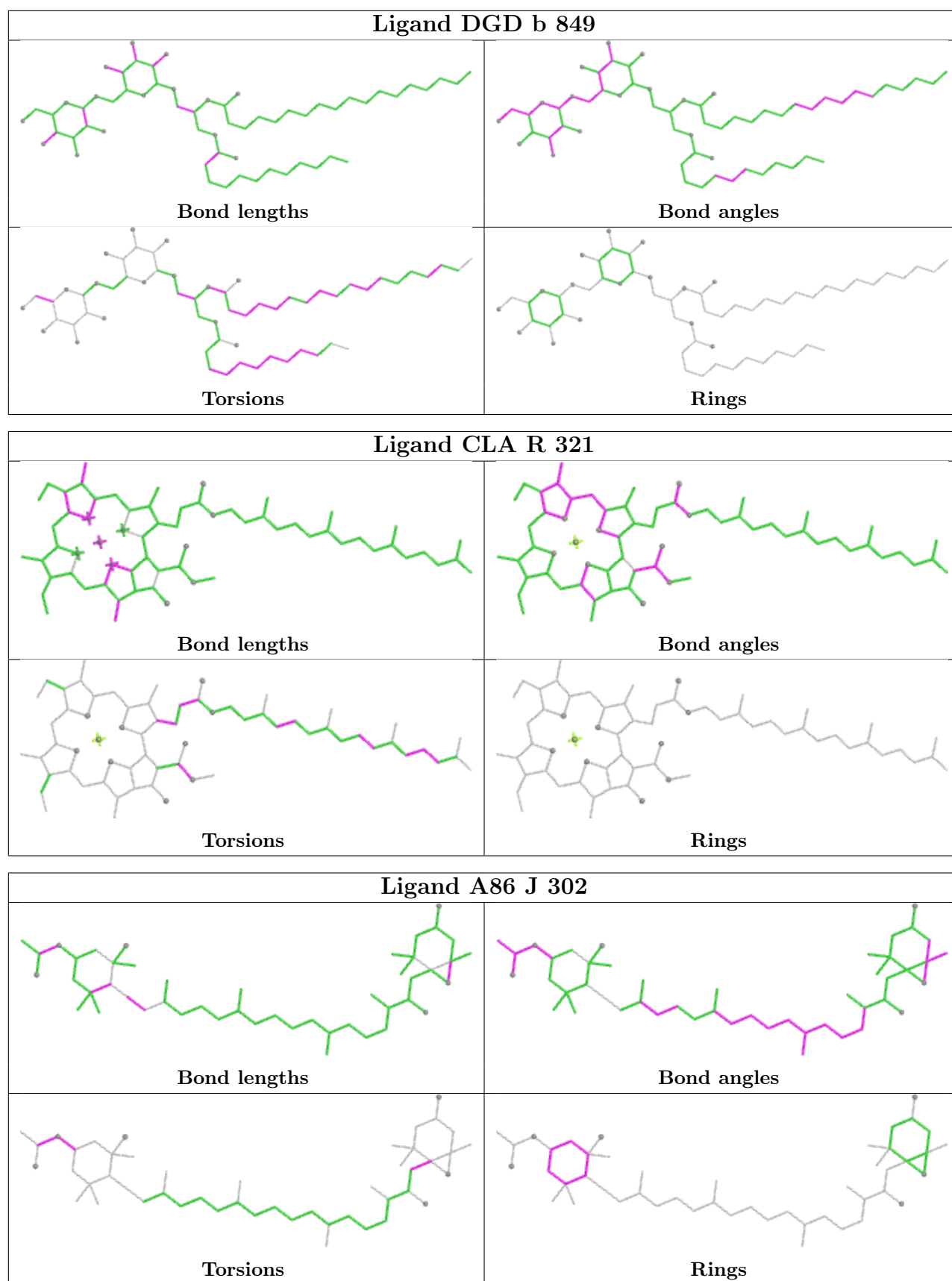
## Ligand SQD A 315



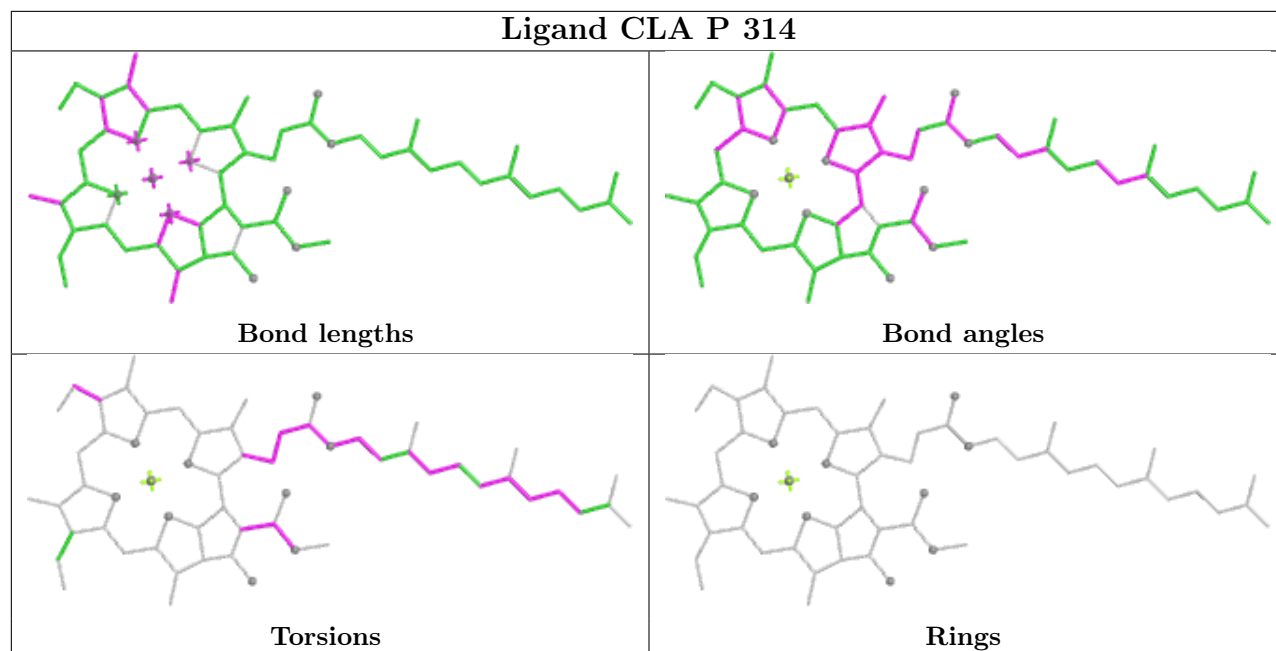




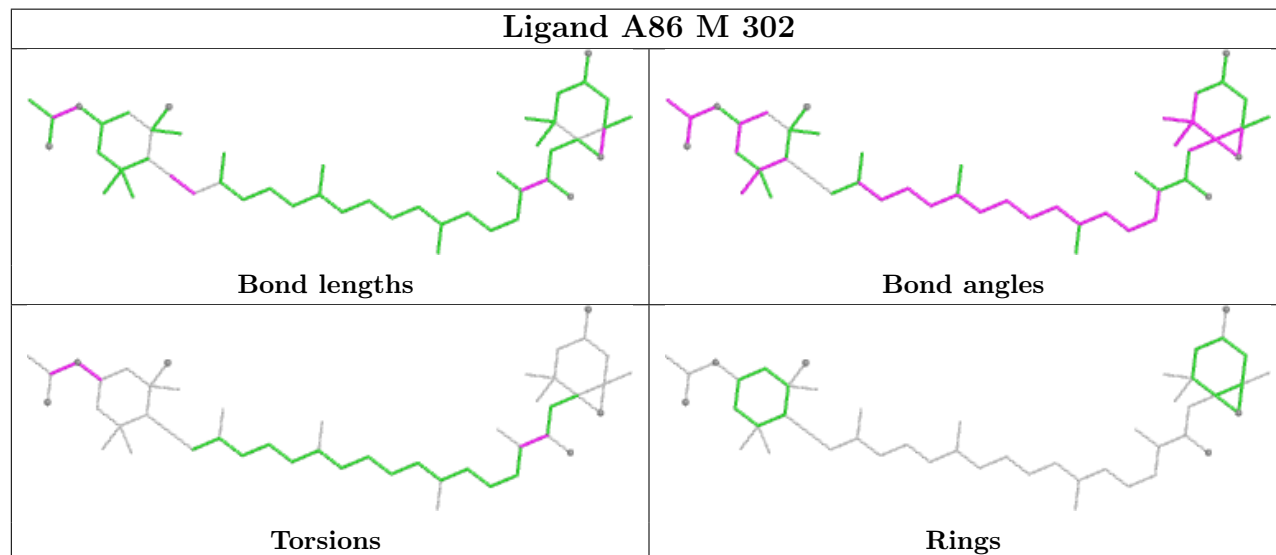


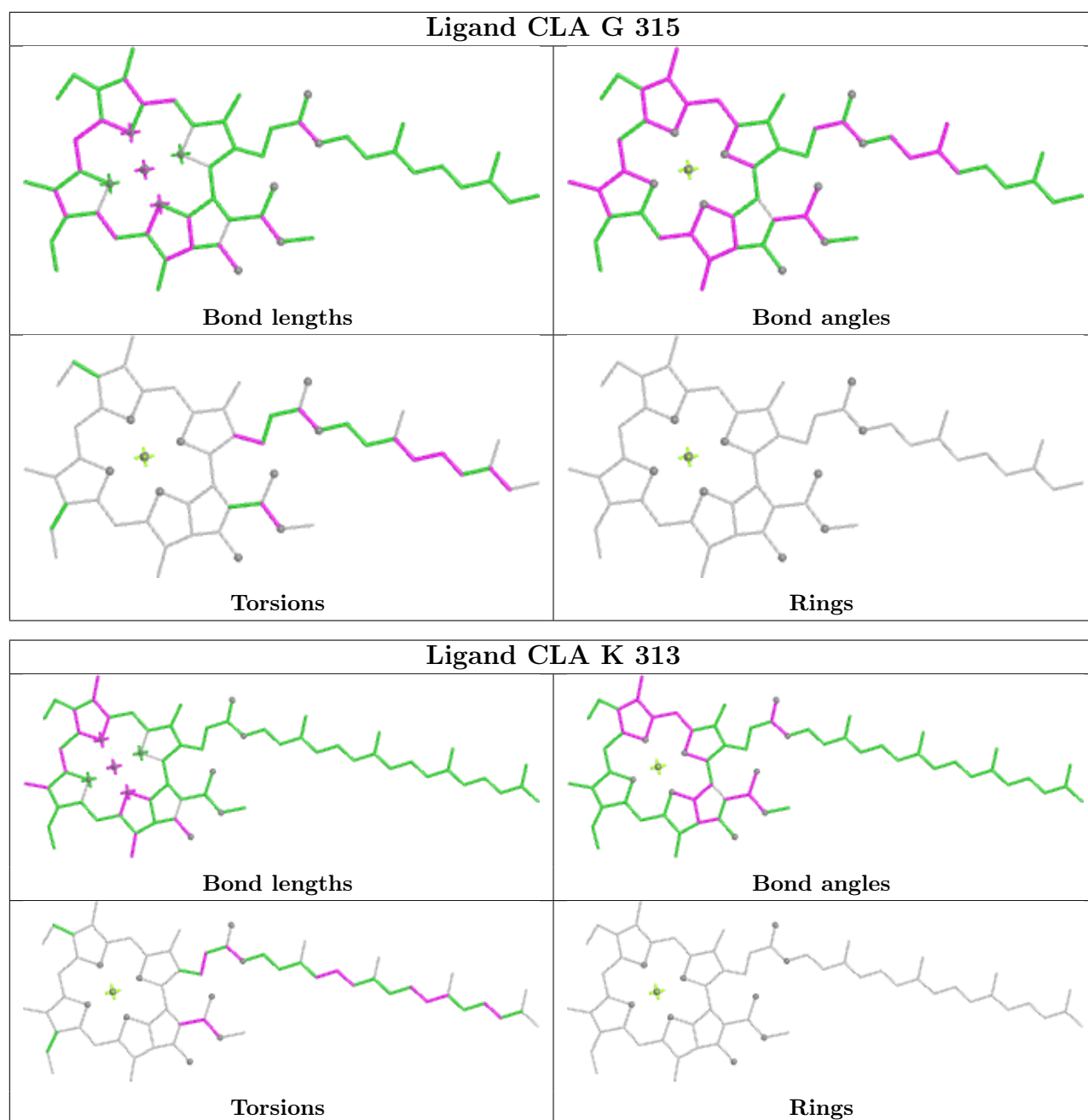


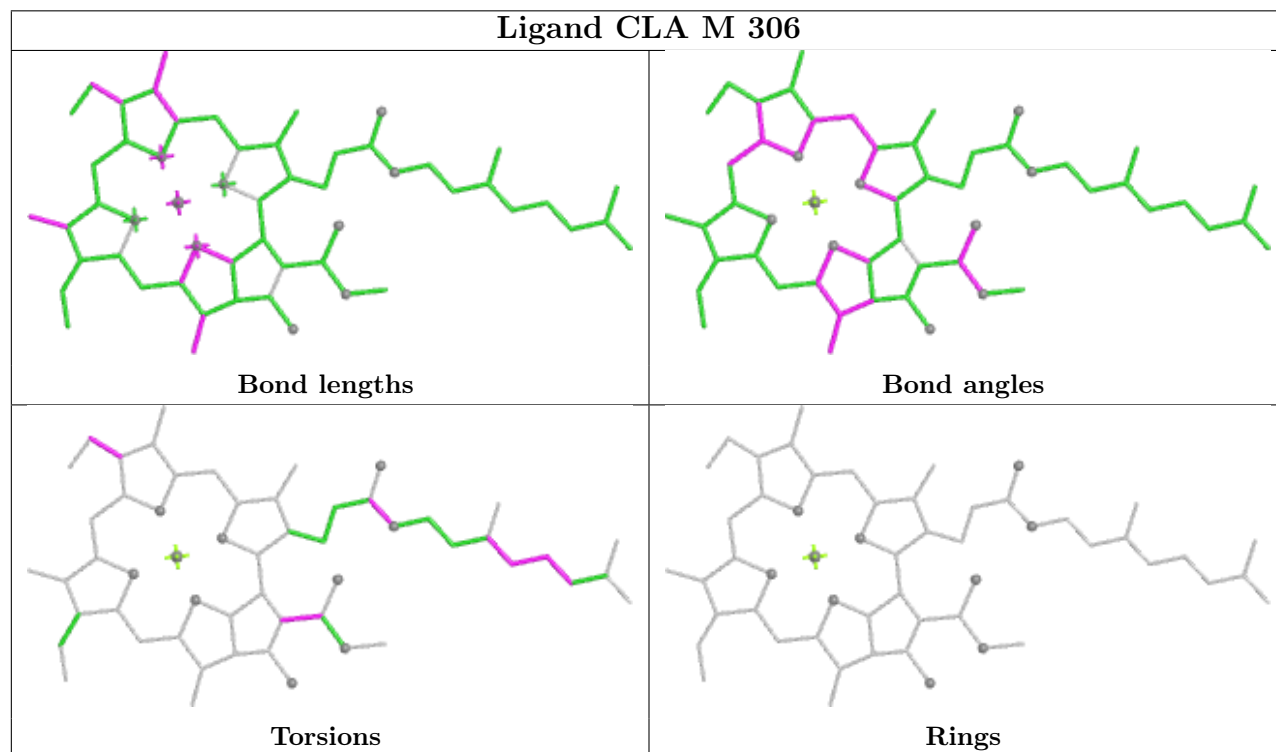
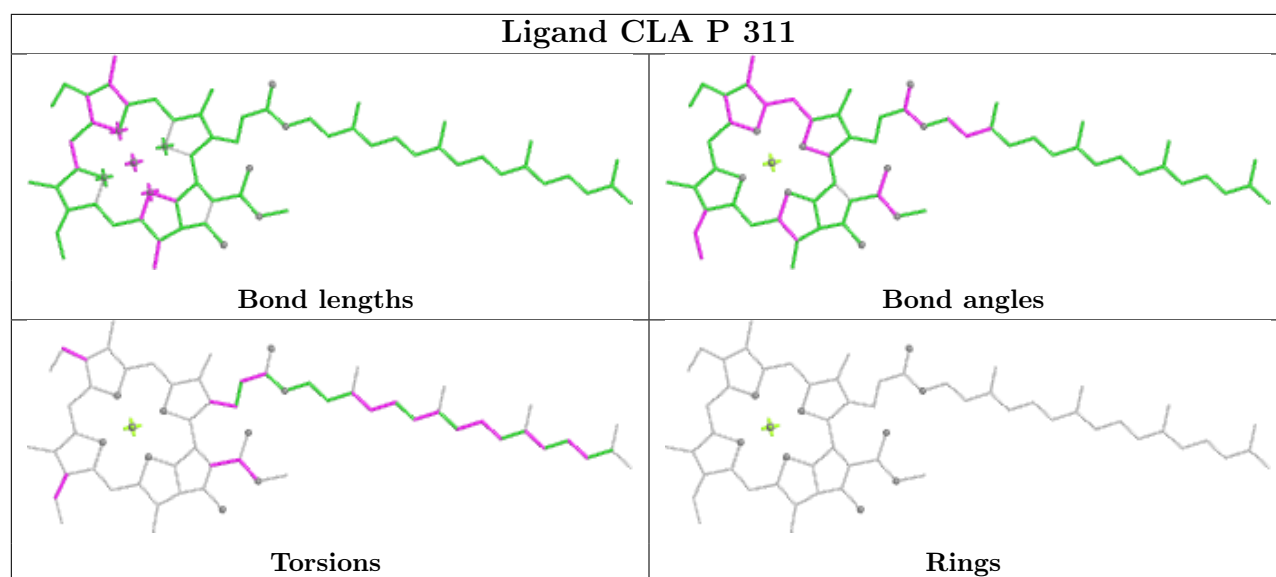
## Ligand CLA P 314



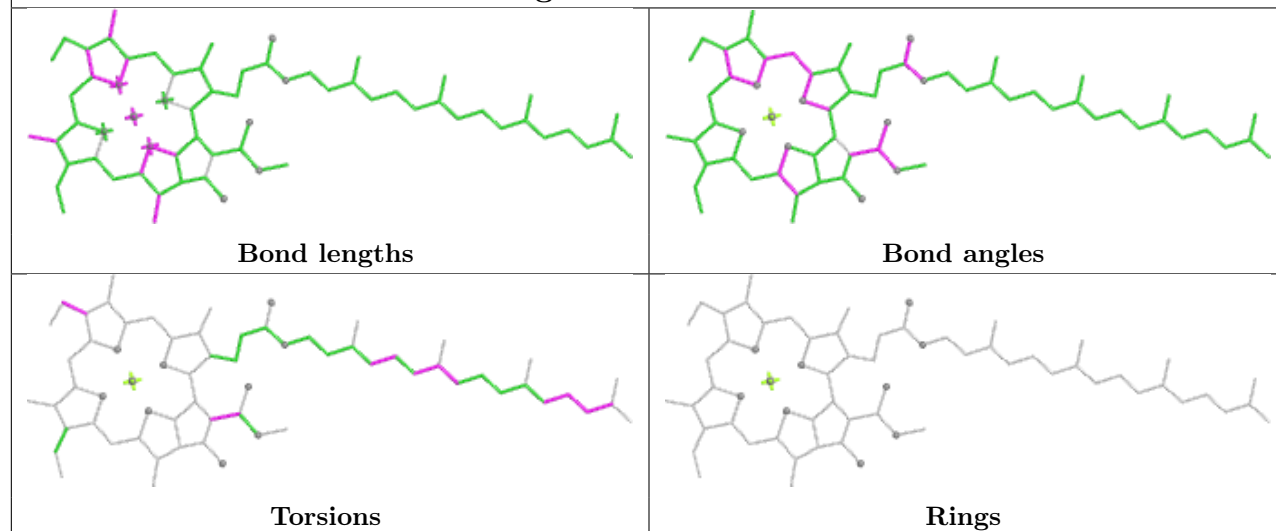
## Ligand A86 M 302



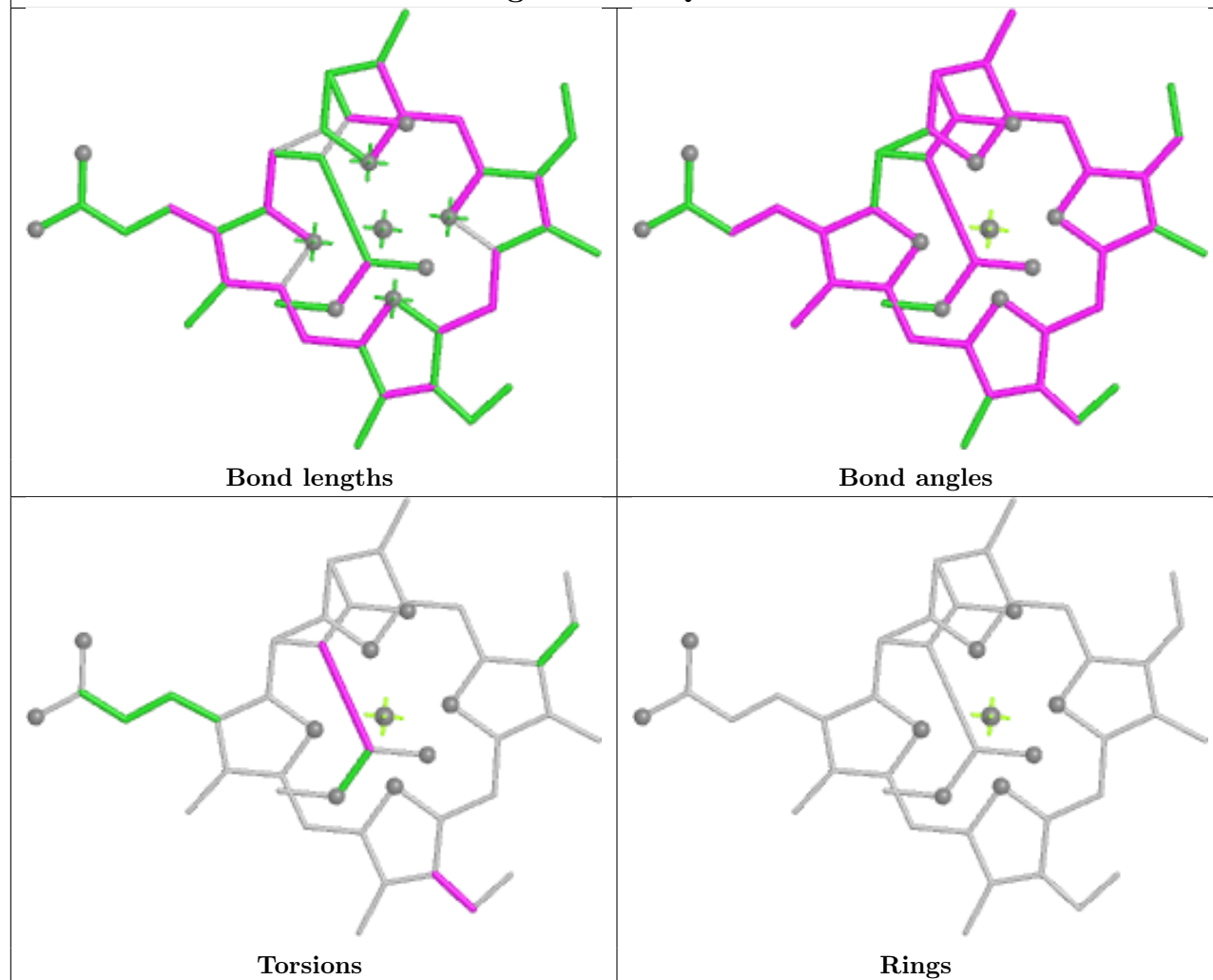


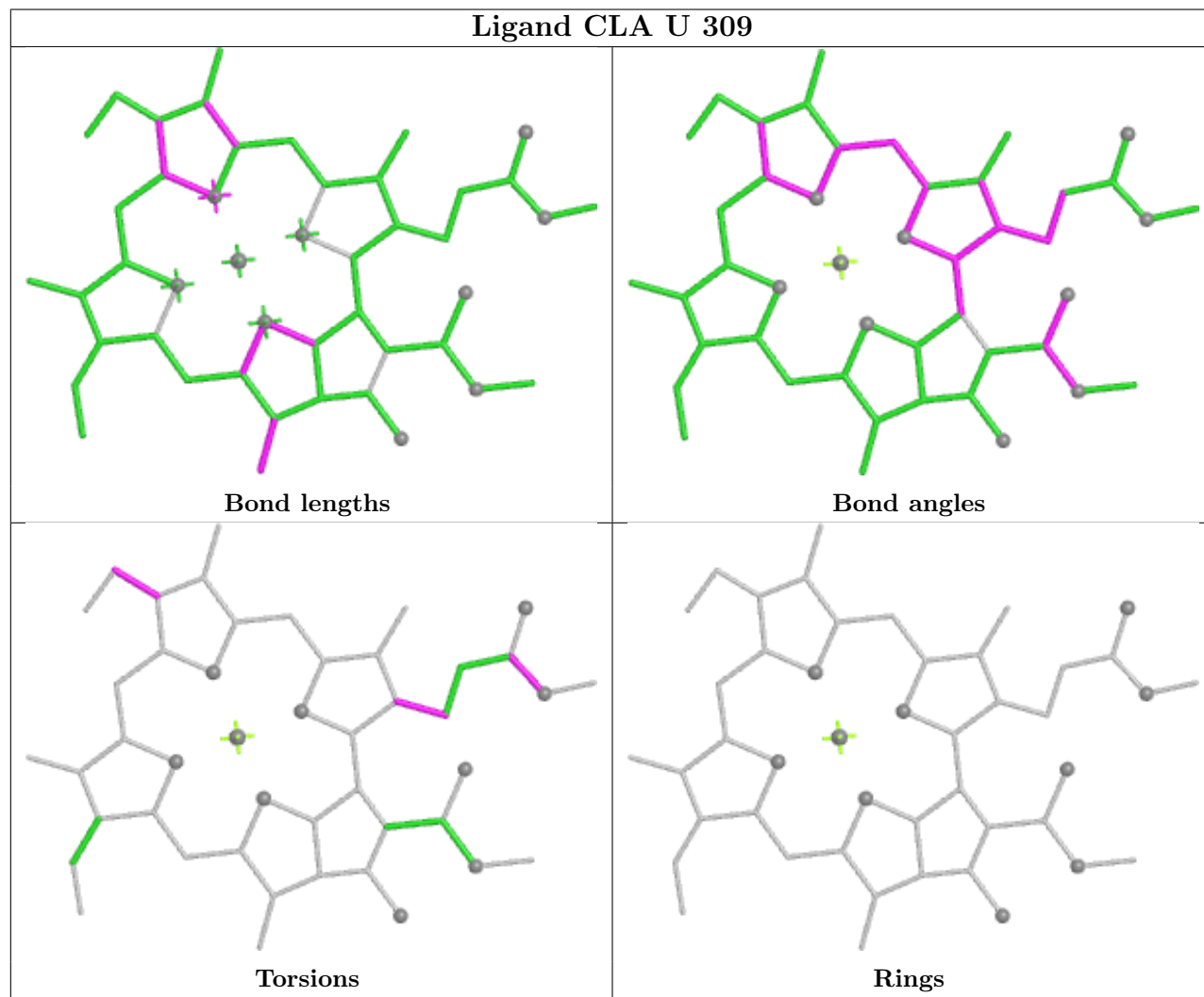
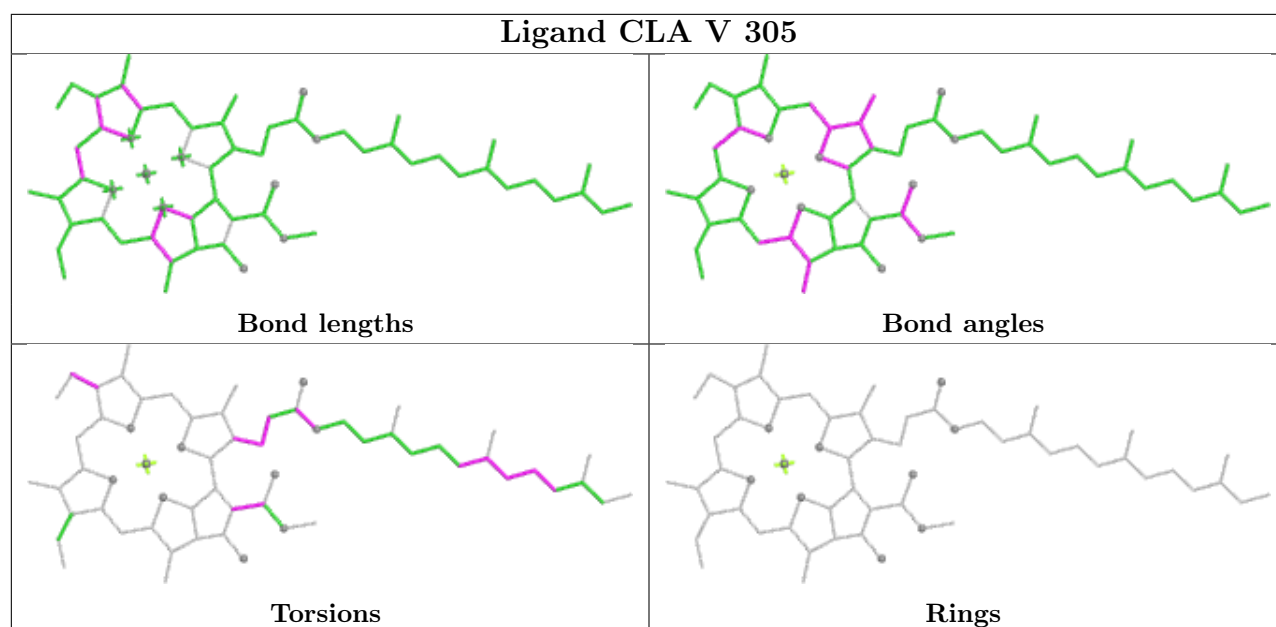


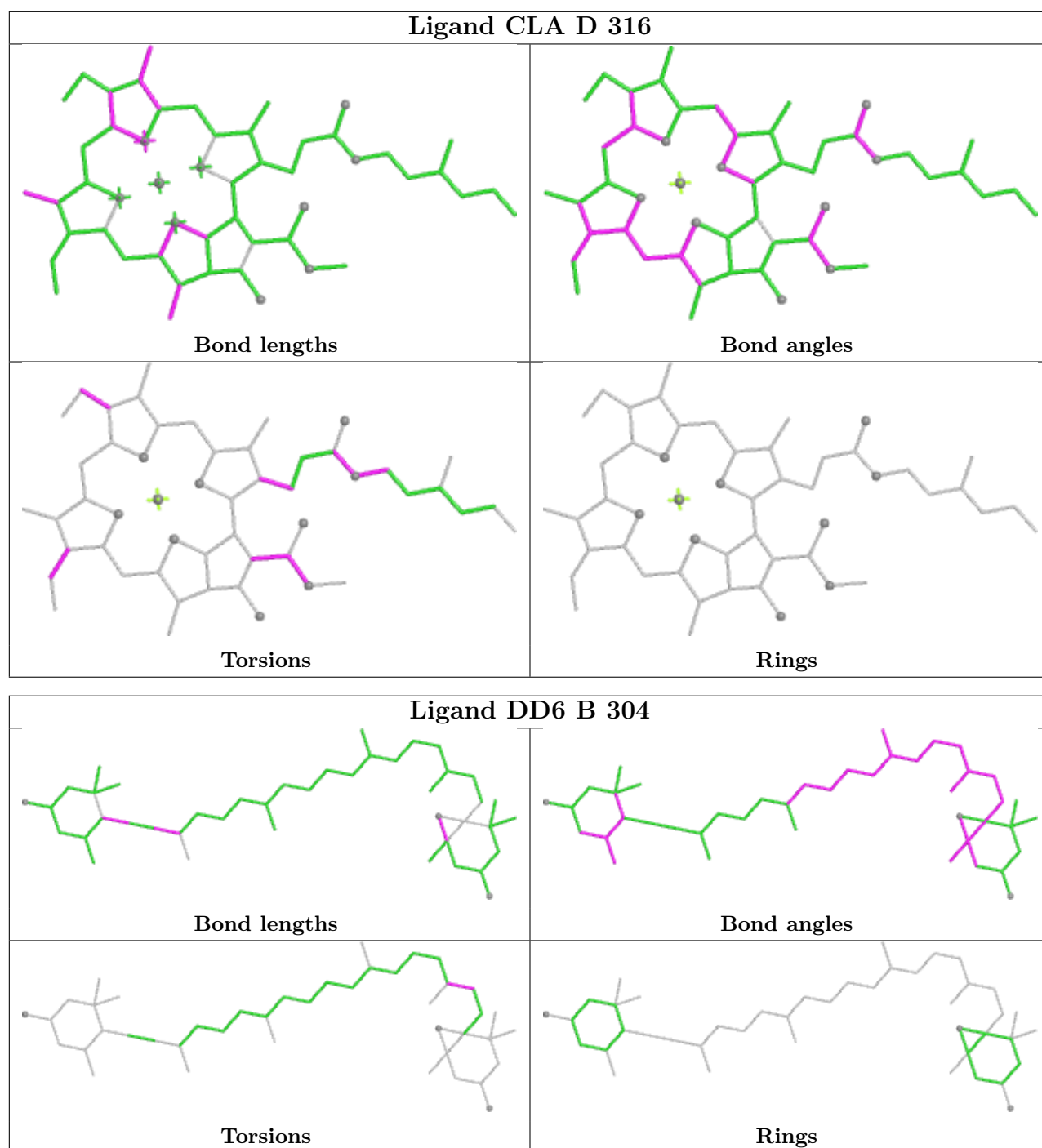
## Ligand CLA b 821

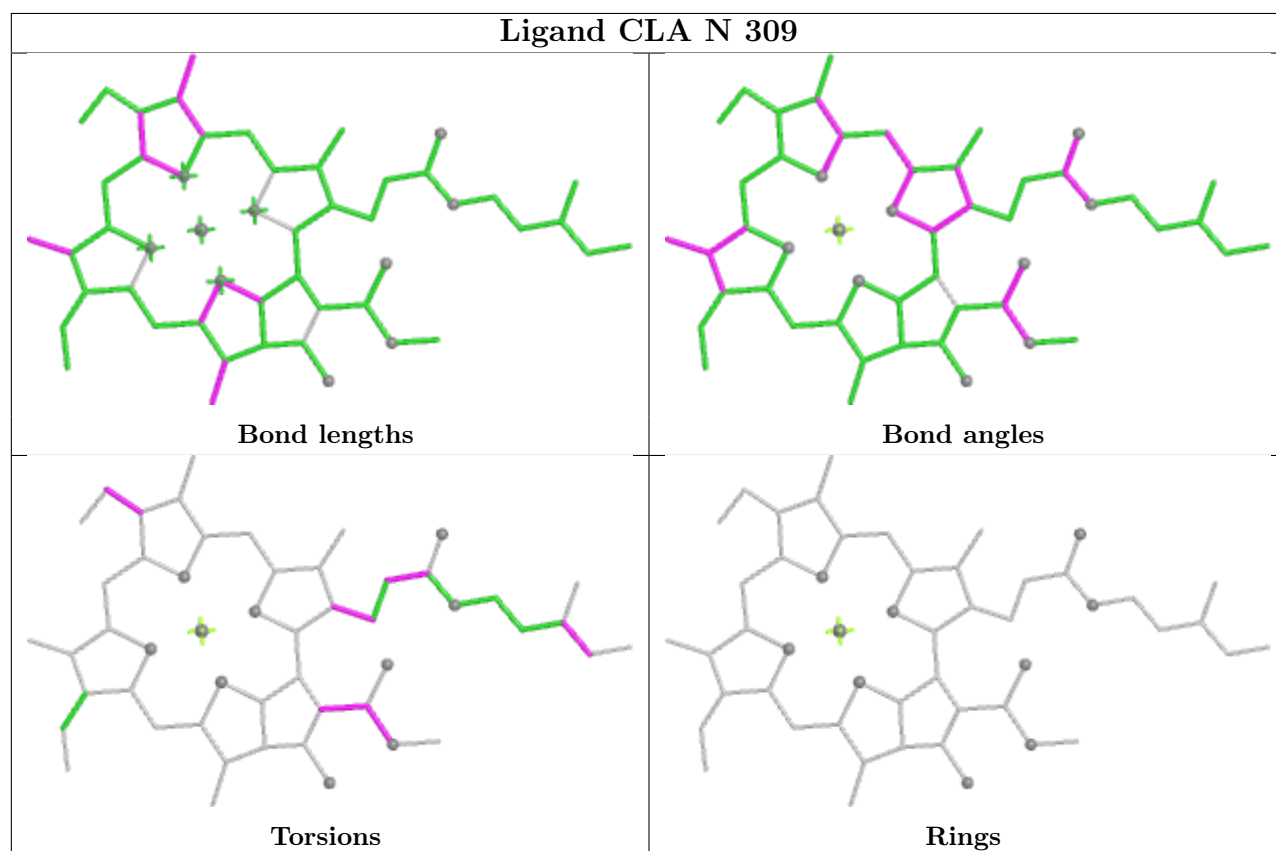
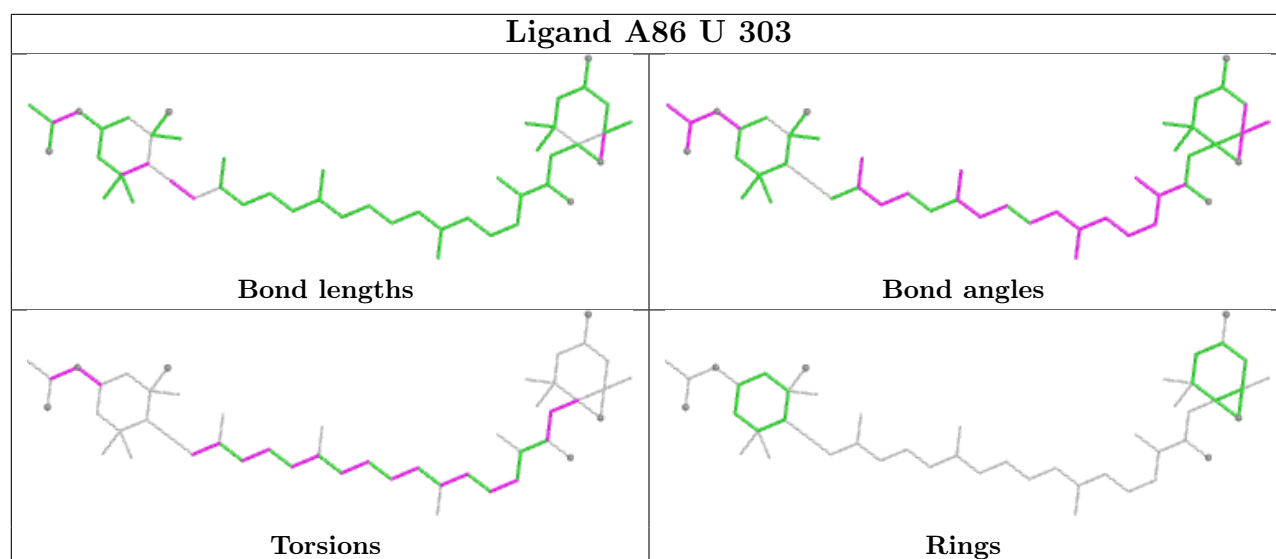


## Ligand KC1 Q 313

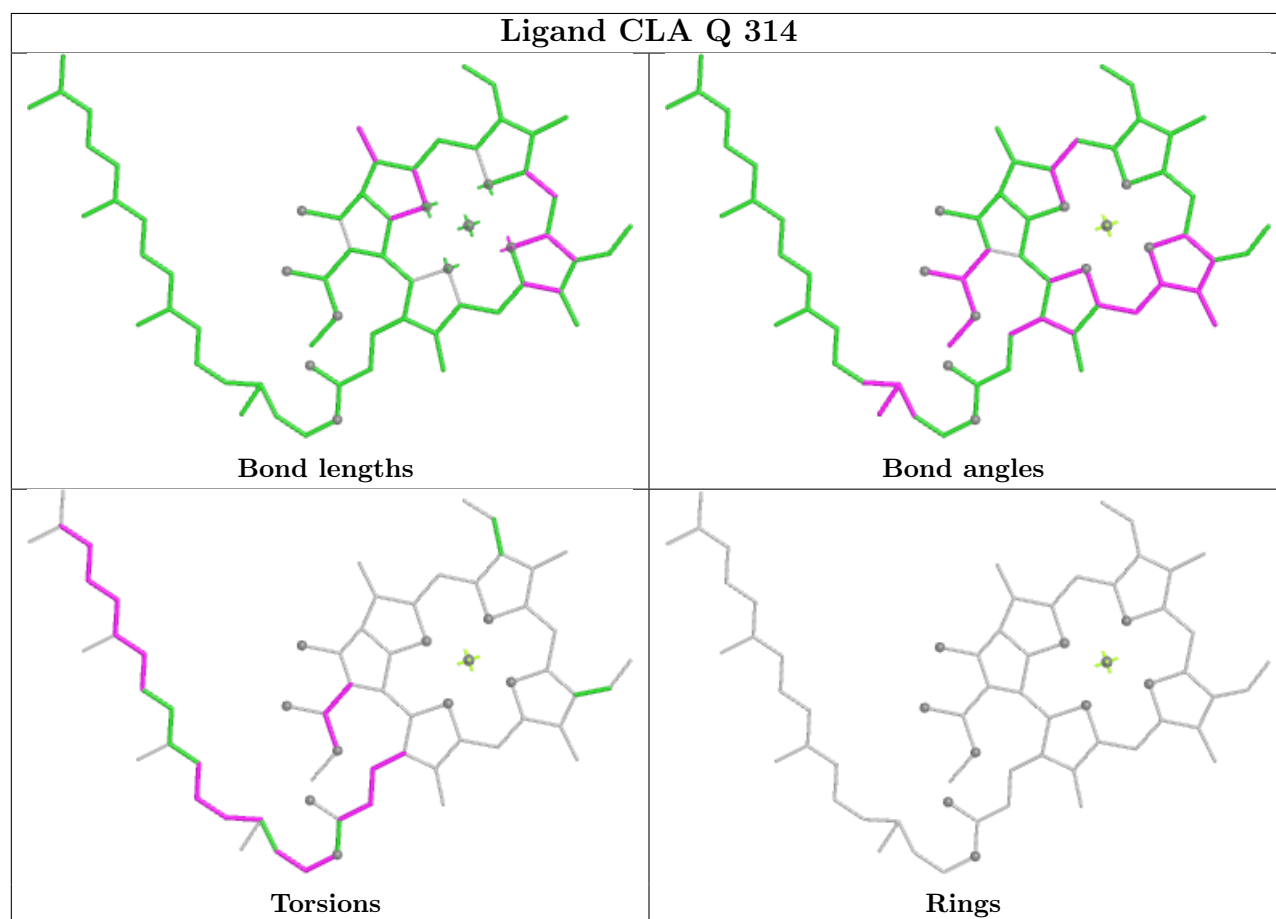
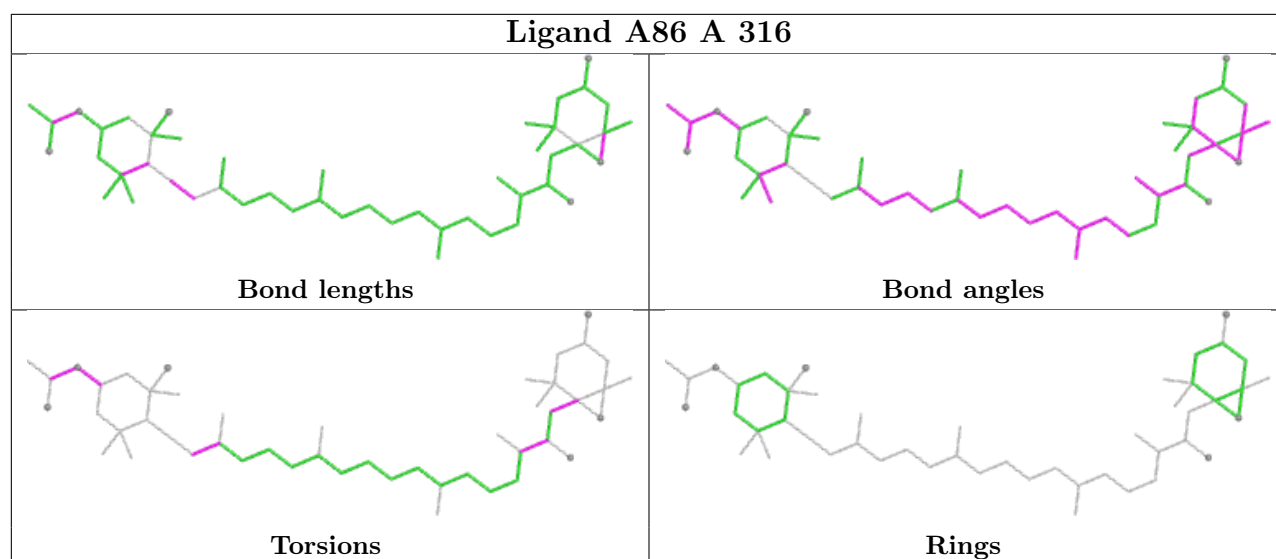


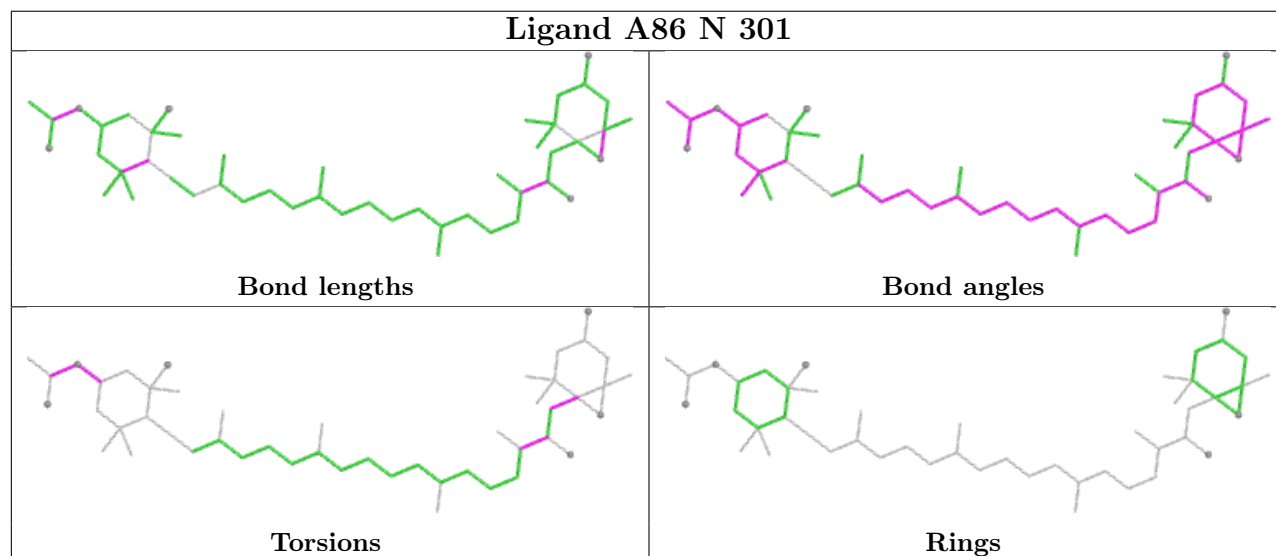
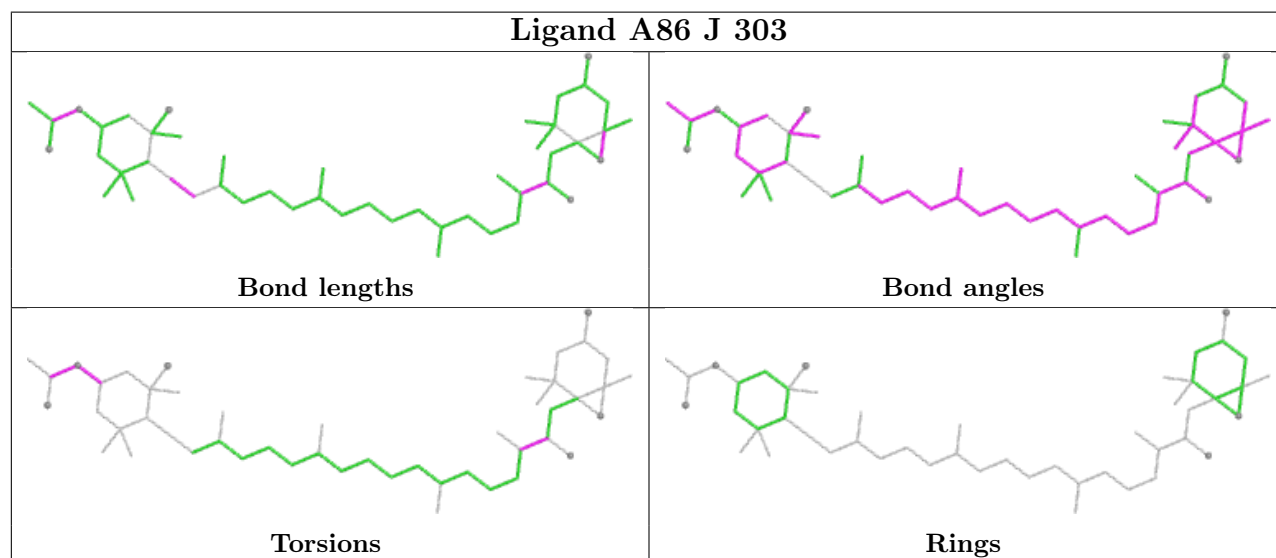
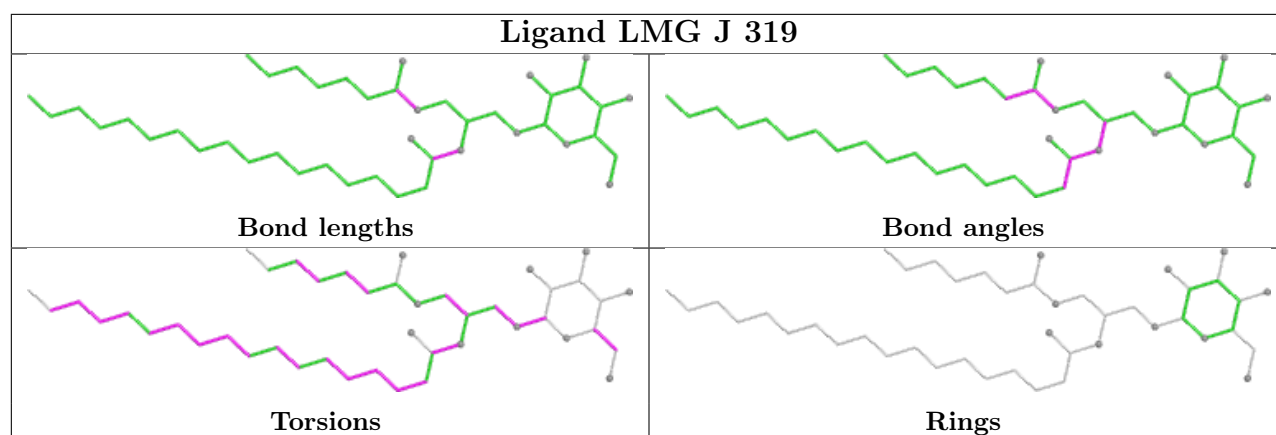


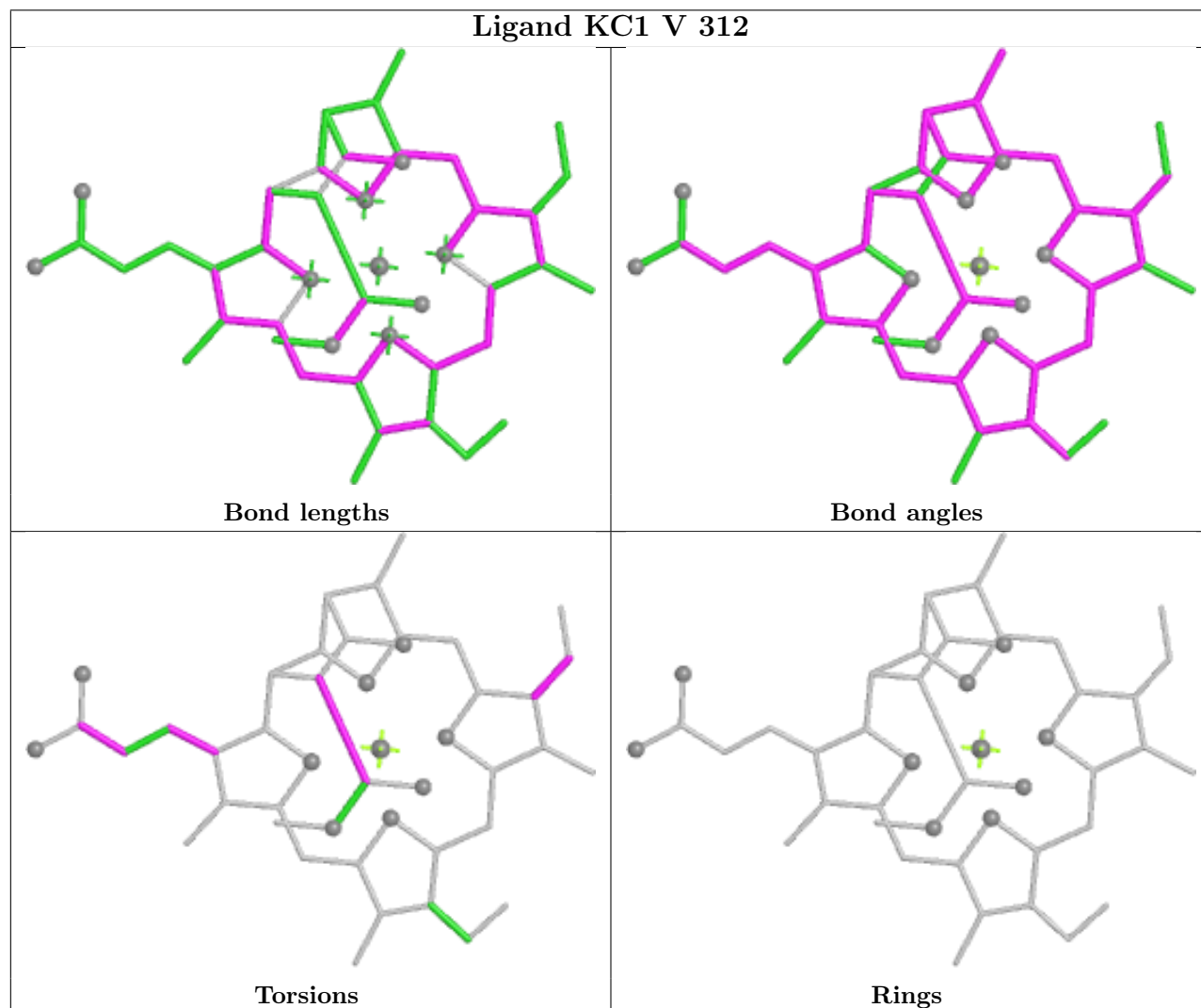
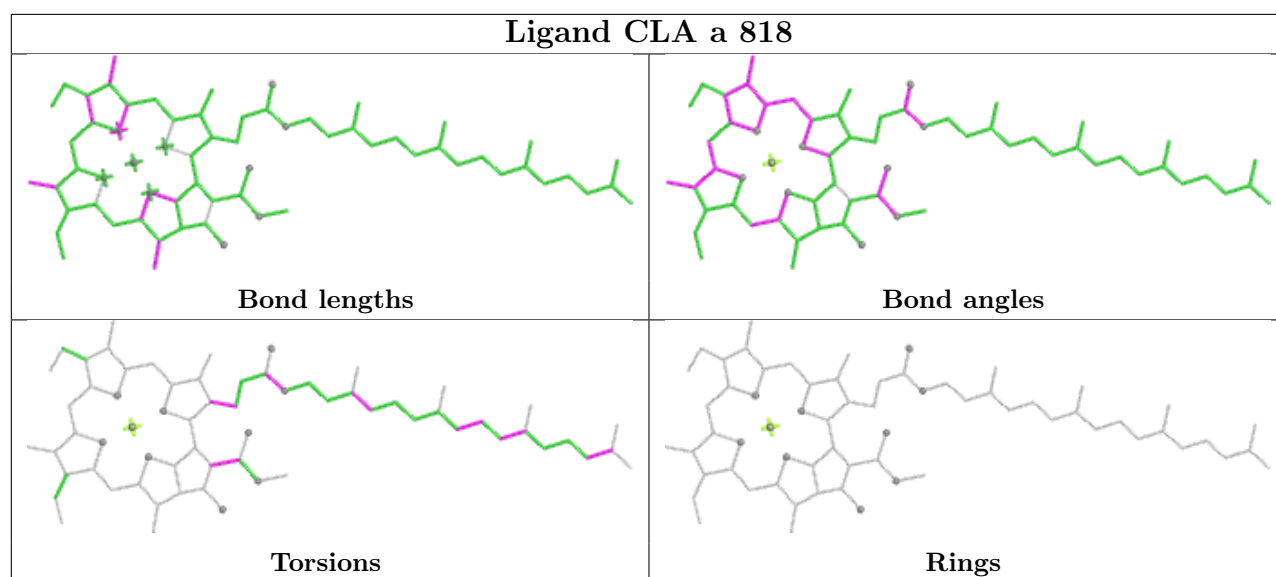


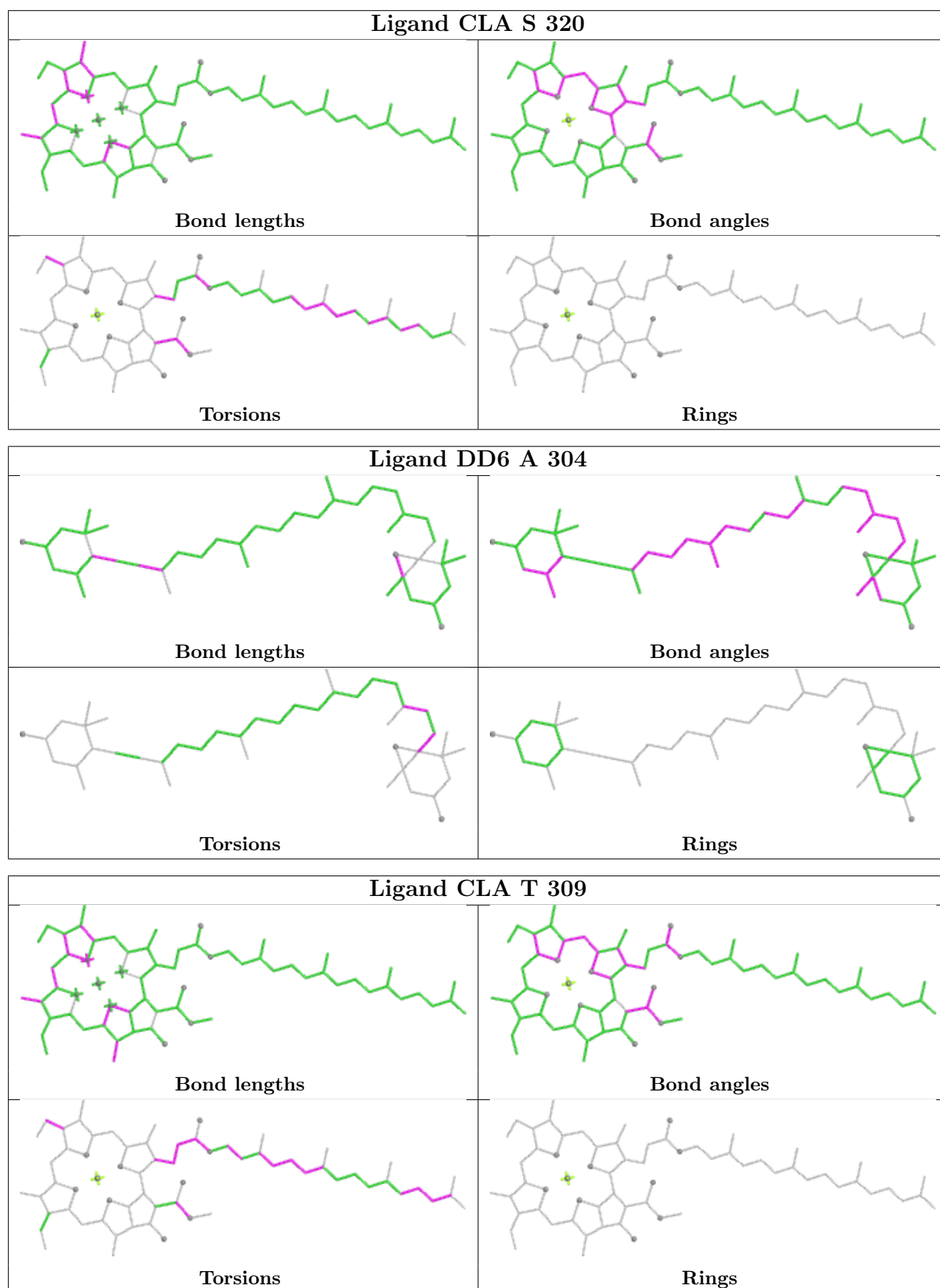


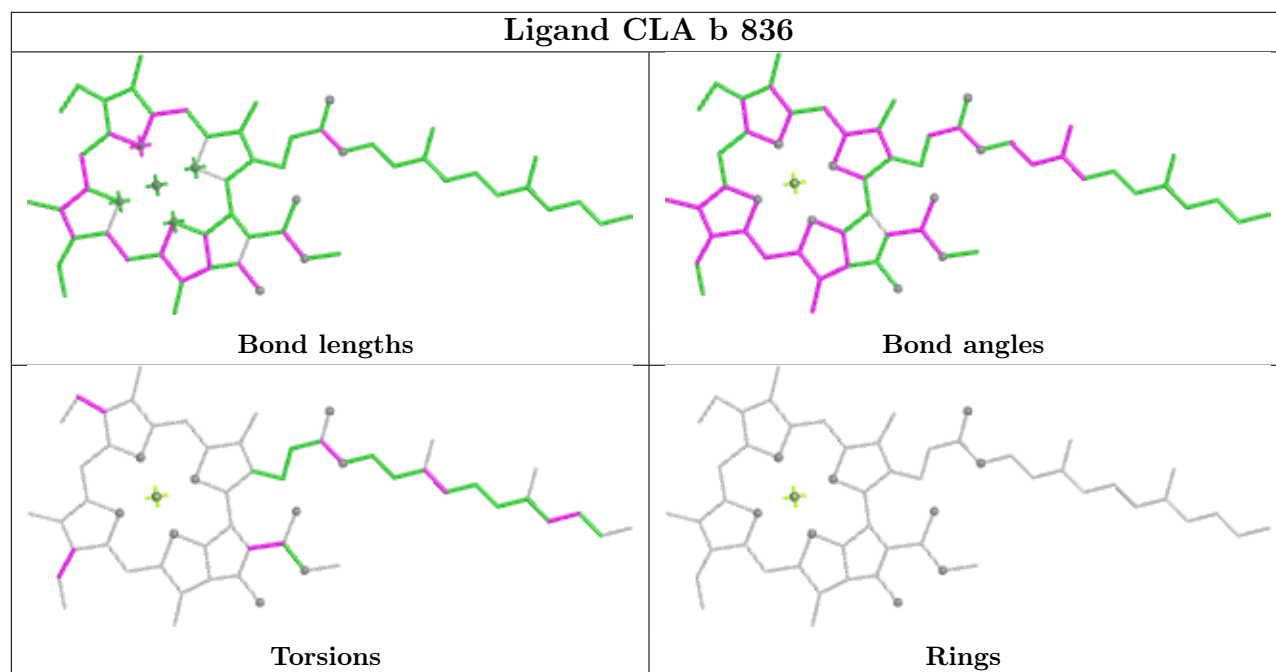
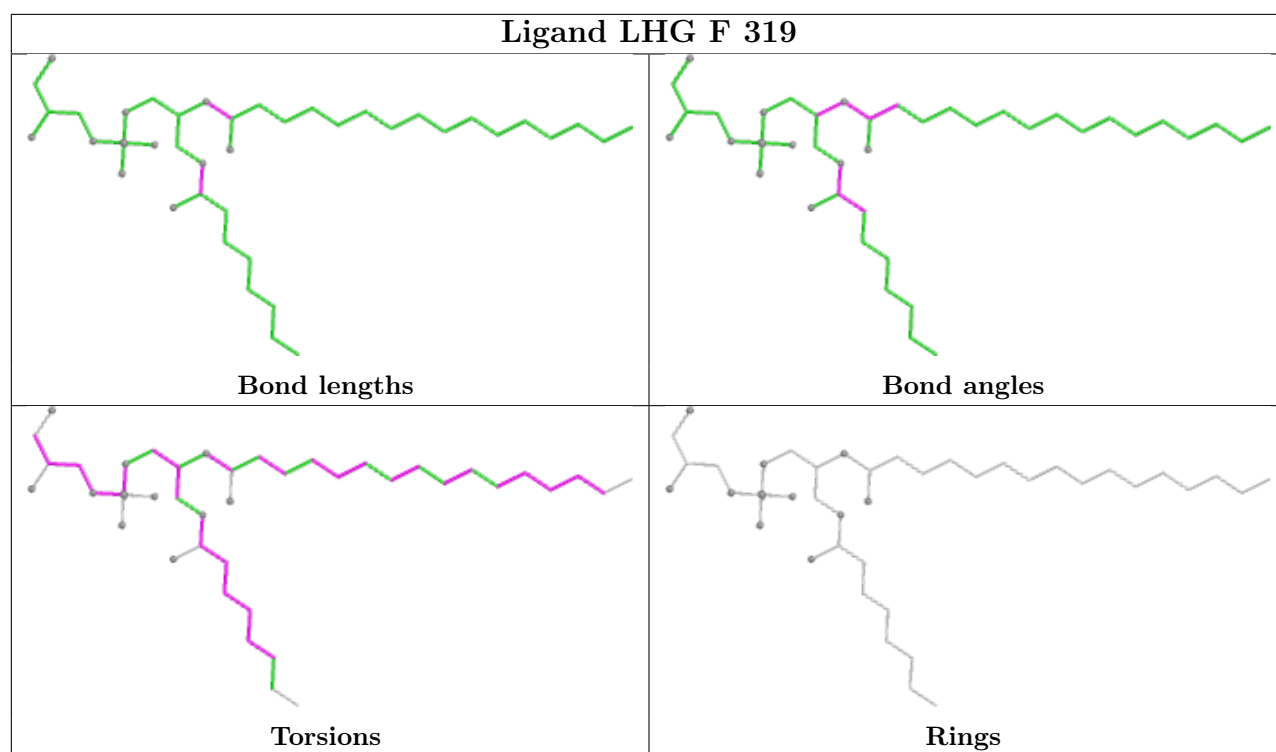




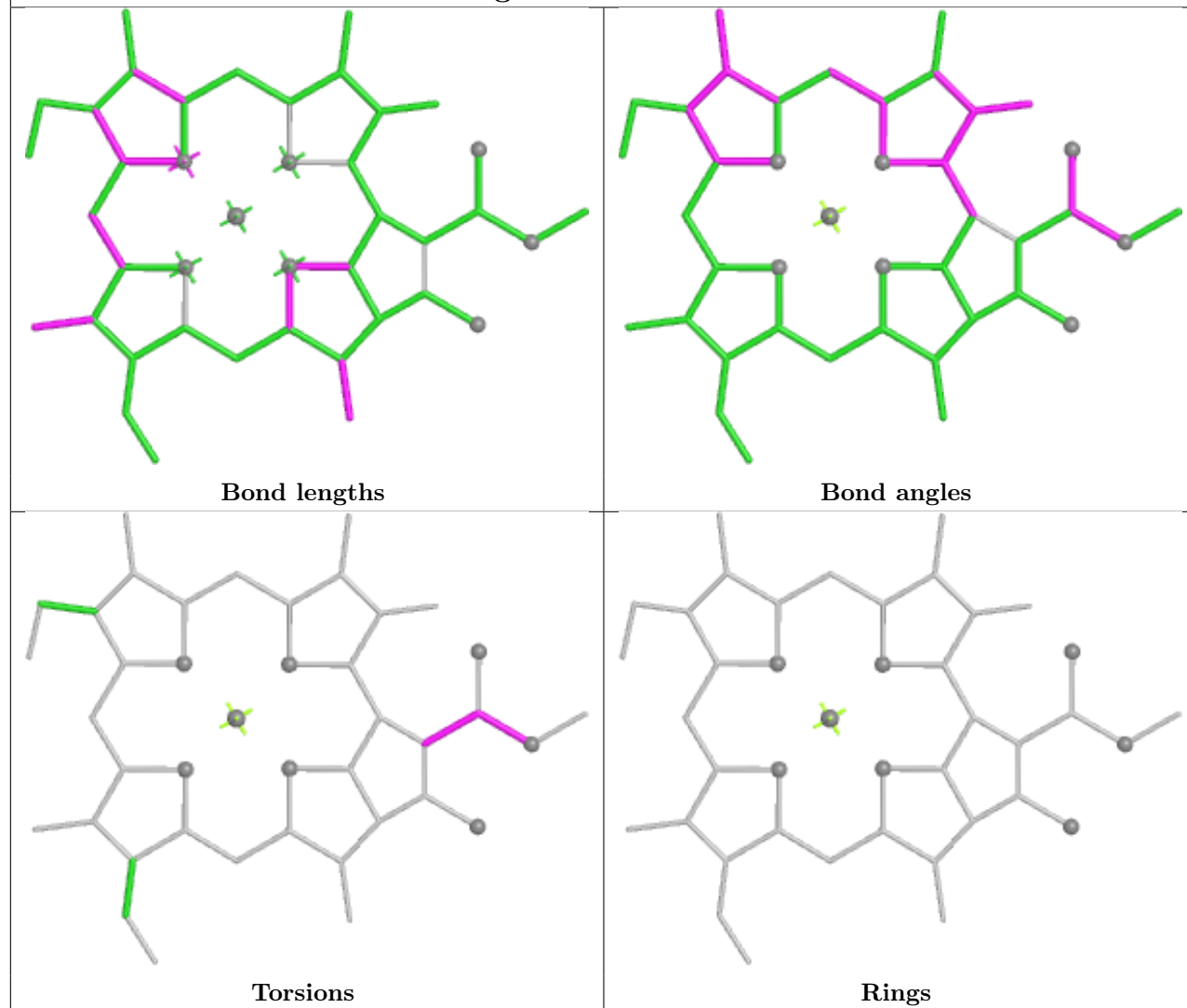




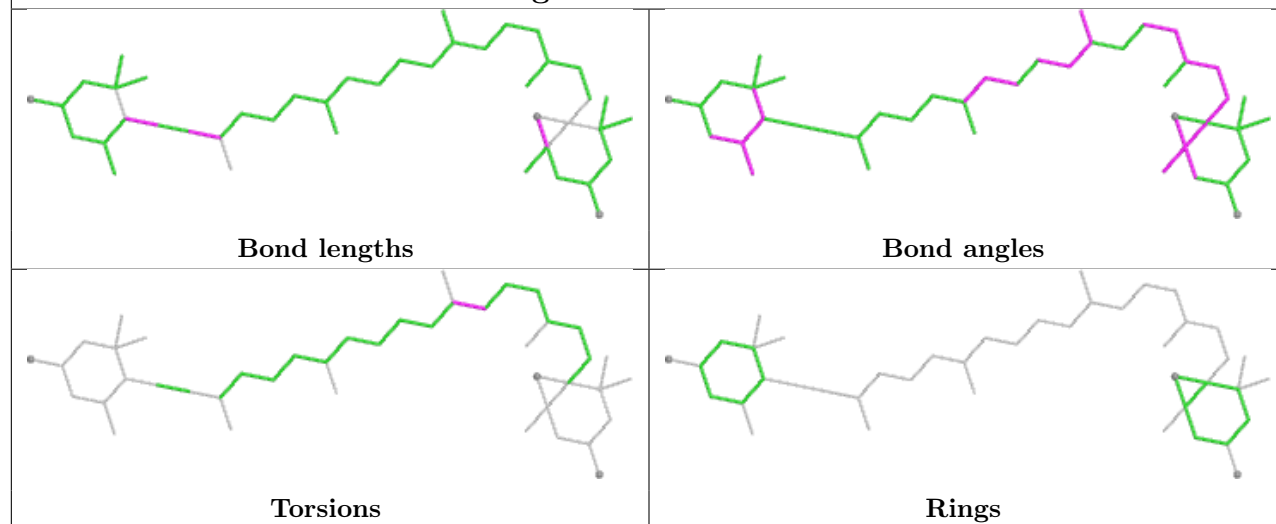


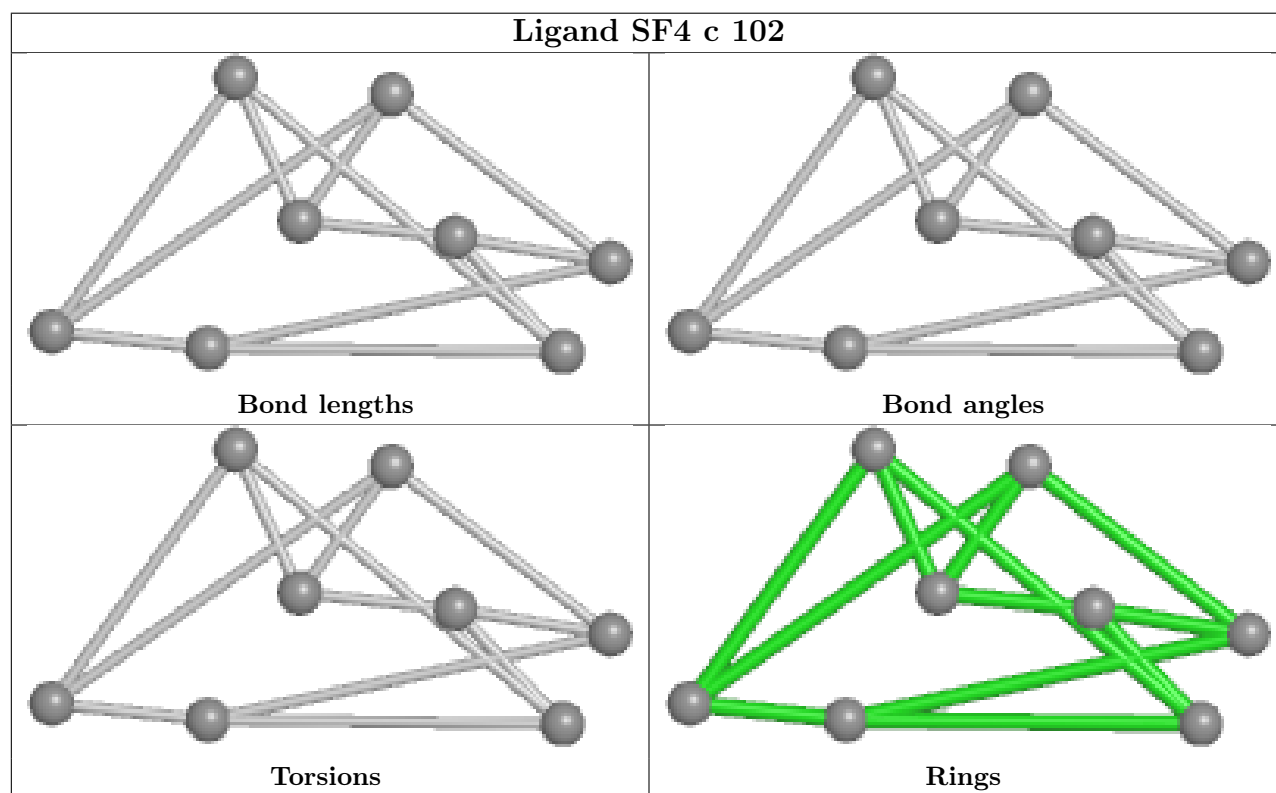
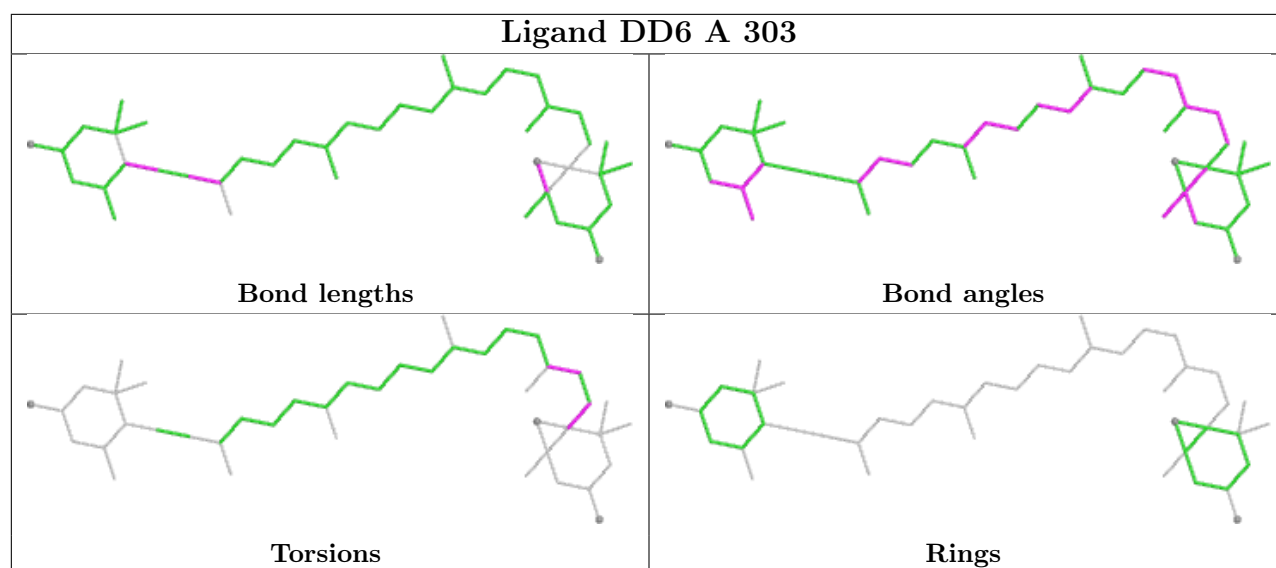


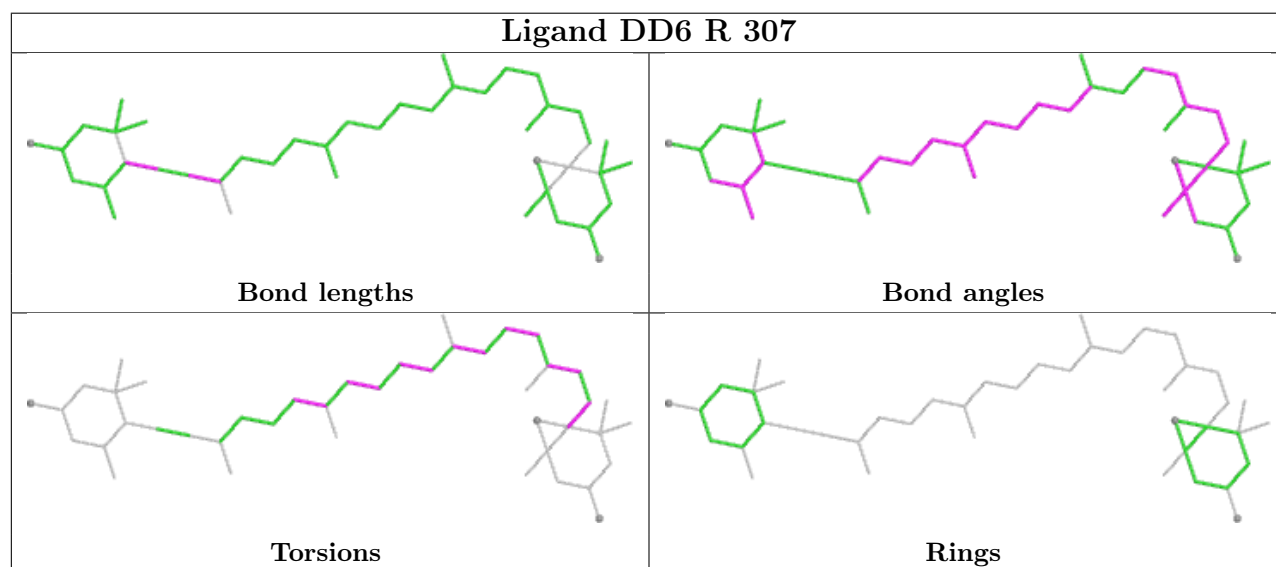
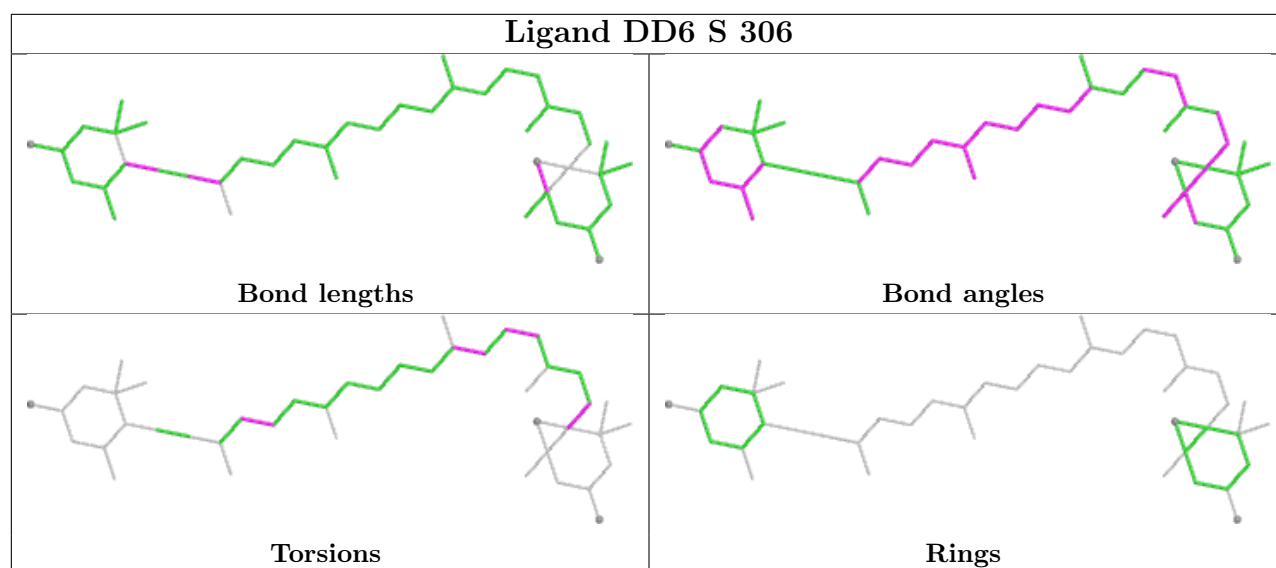
## Ligand CLA X 312



## Ligand DD6 K 304

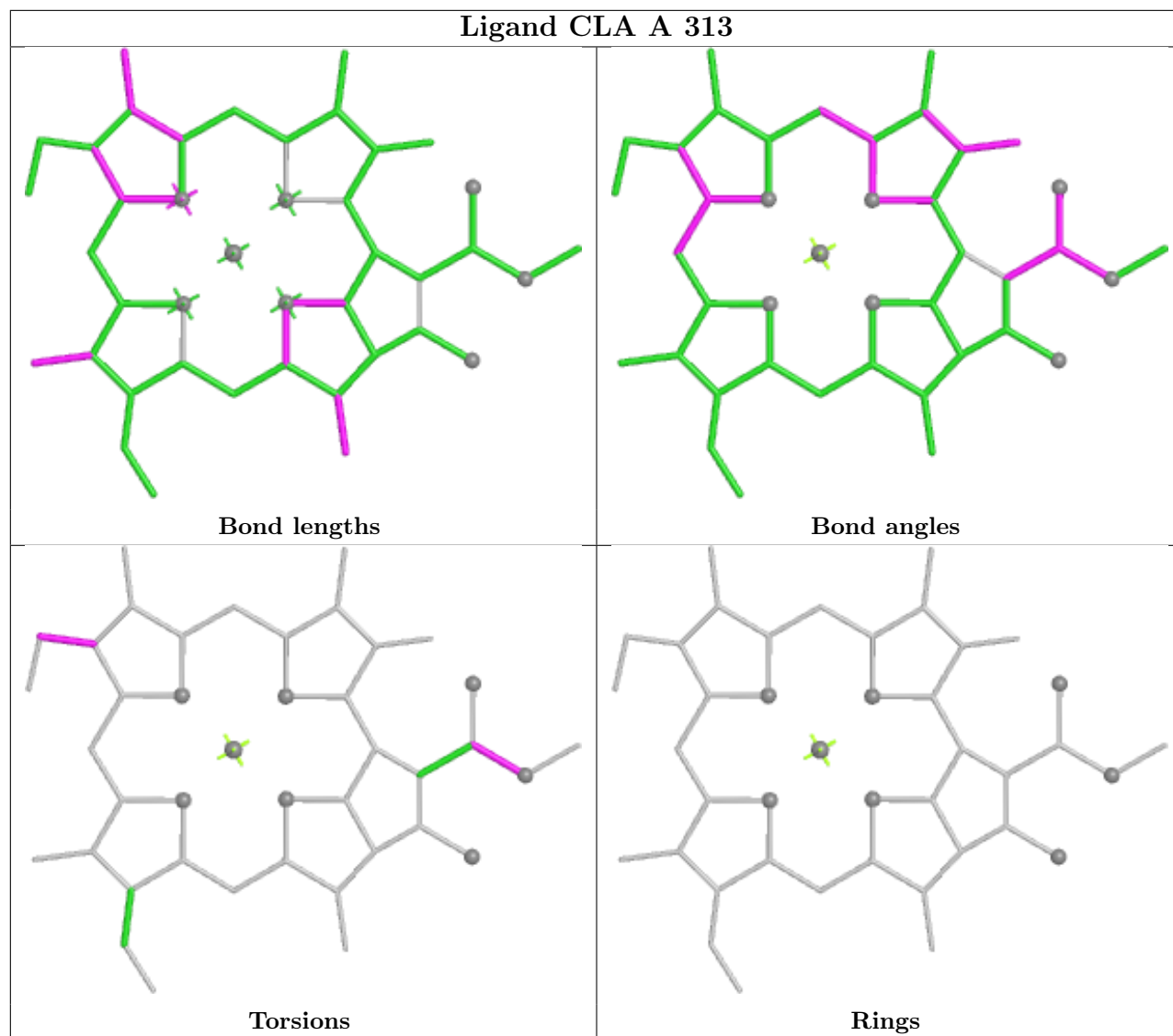




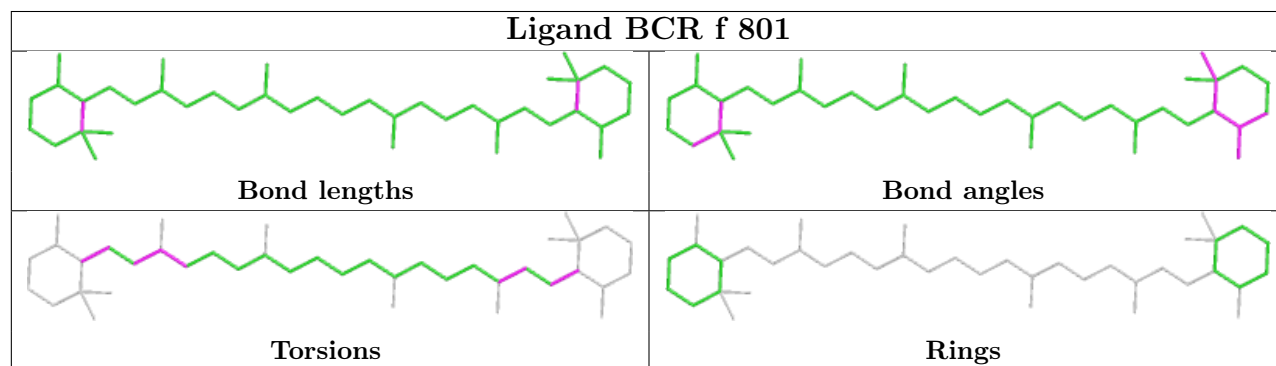


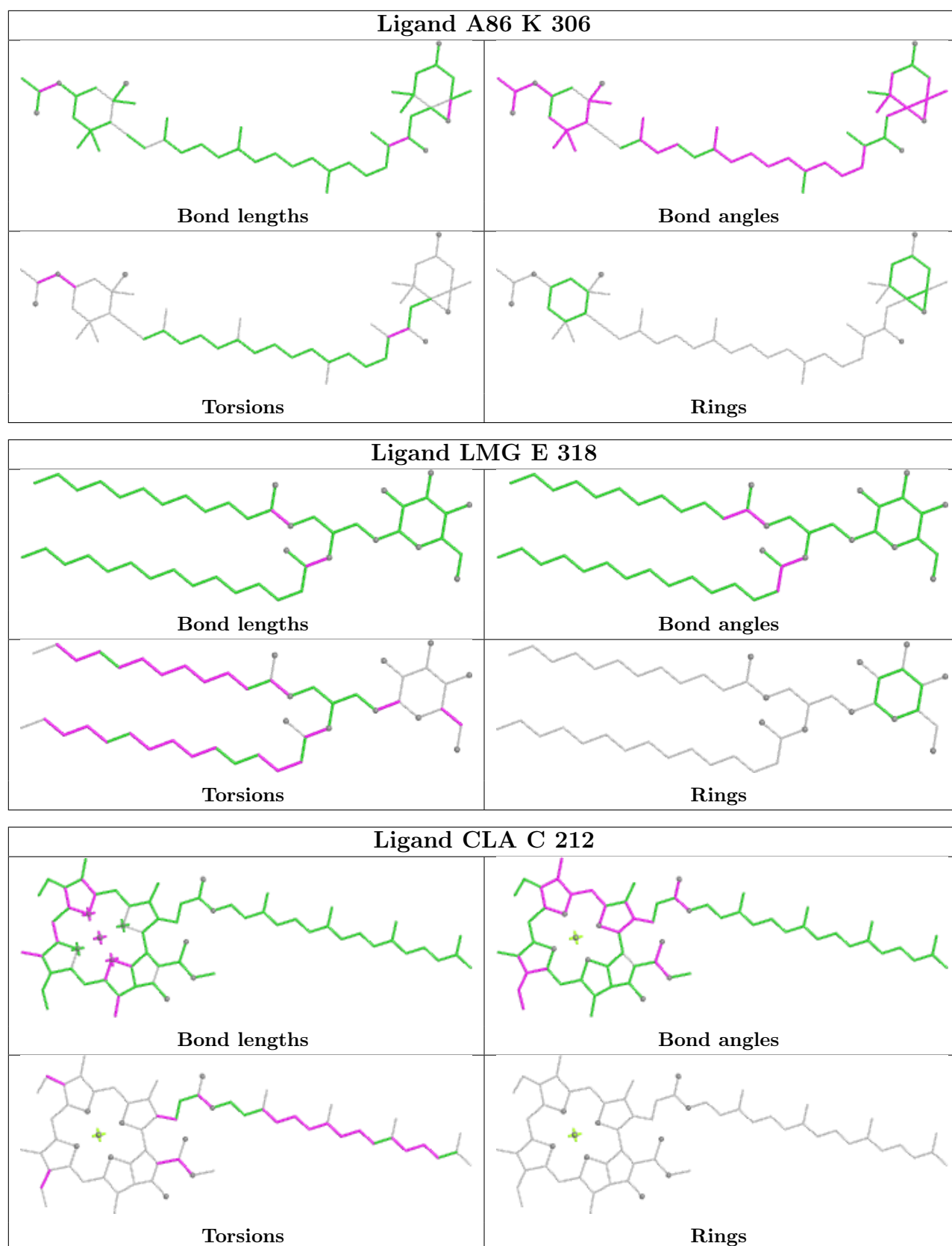


## Ligand CLA A 313

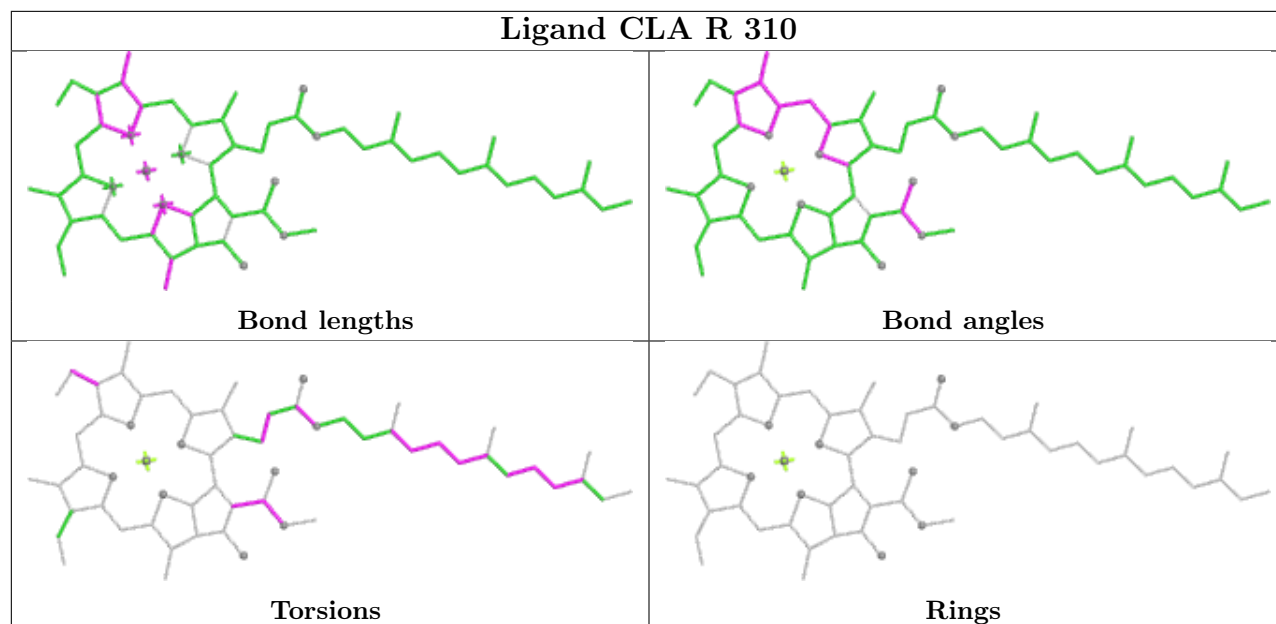


## Ligand BCR f 801

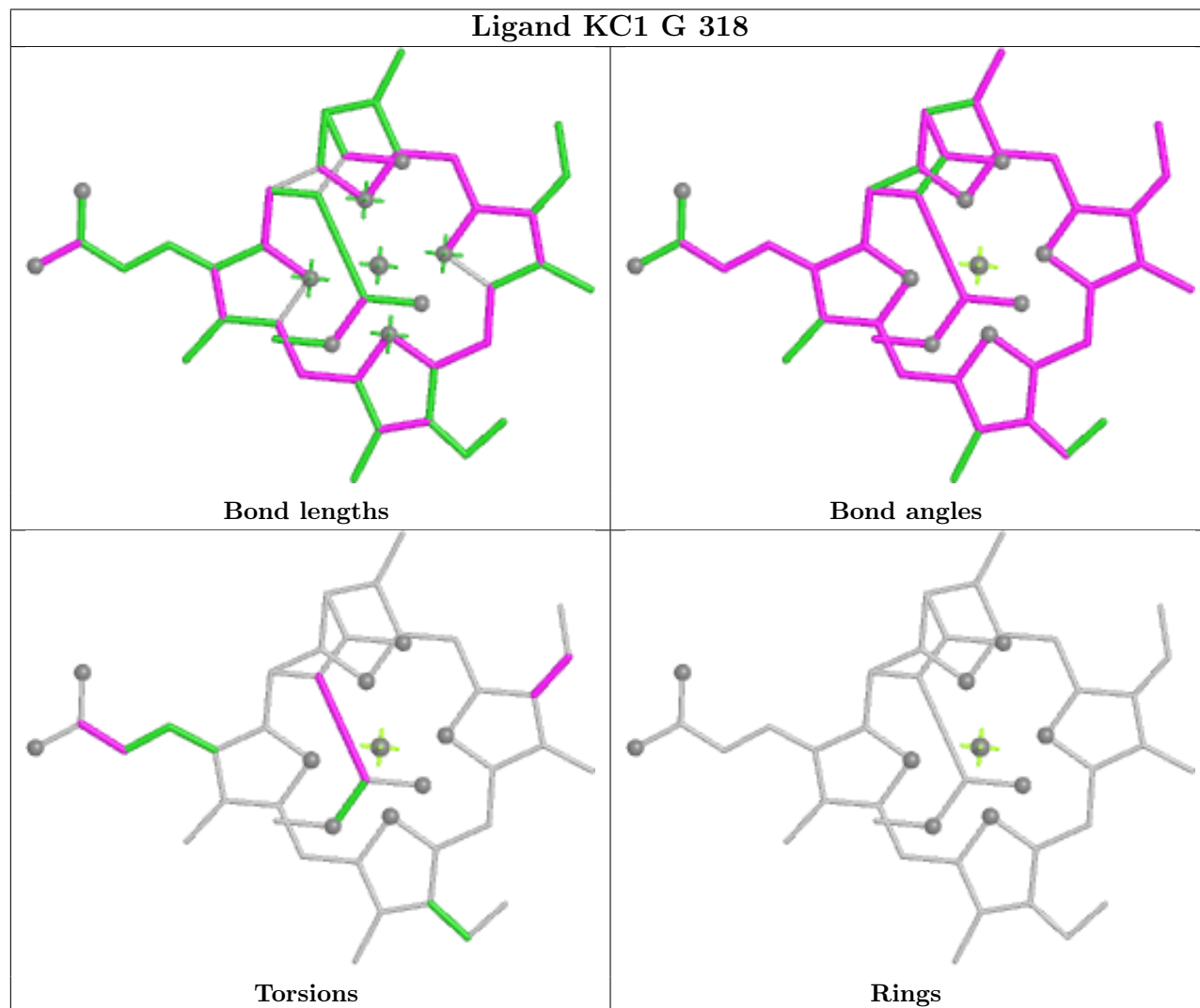


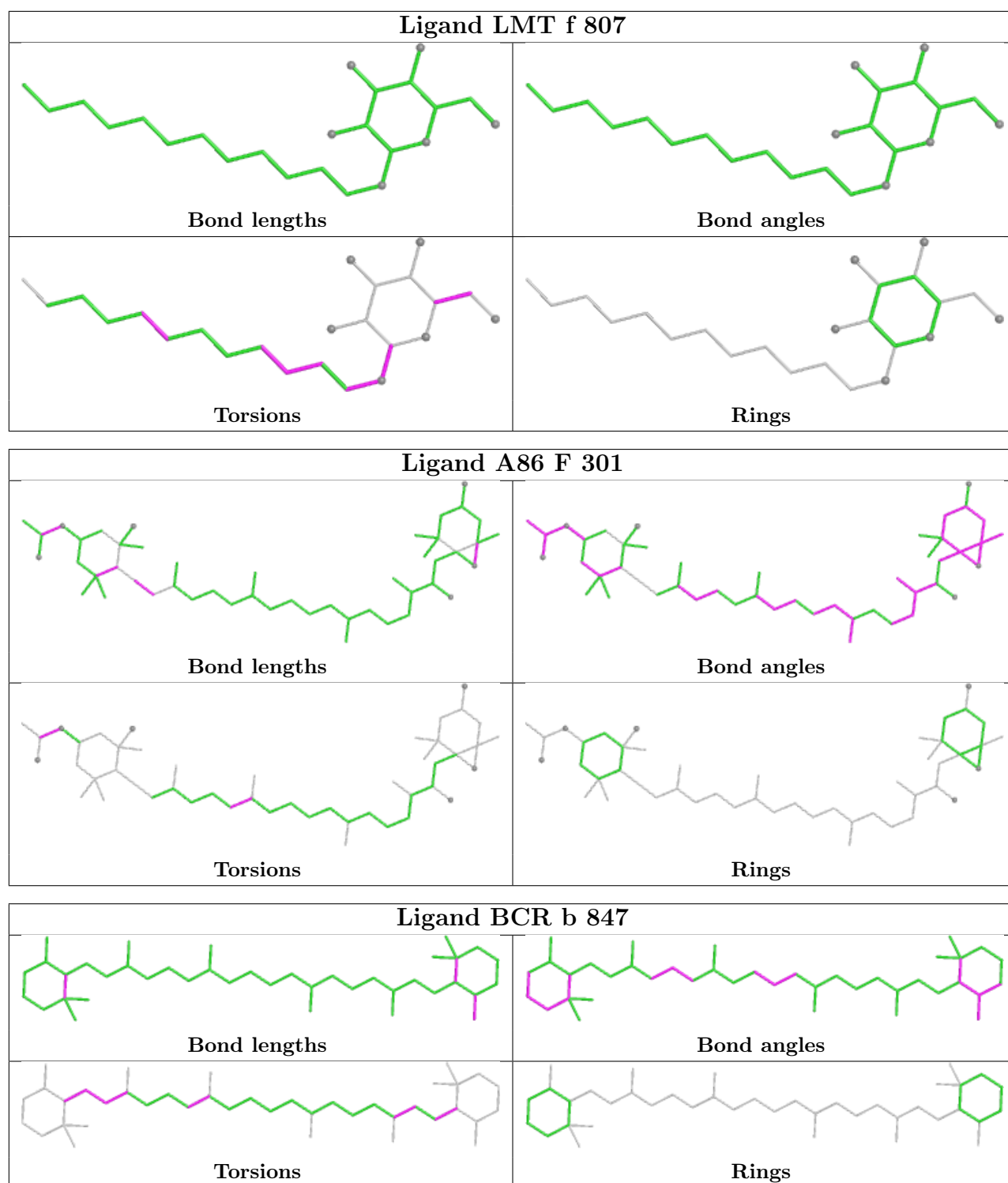


## Ligand CLA R 310

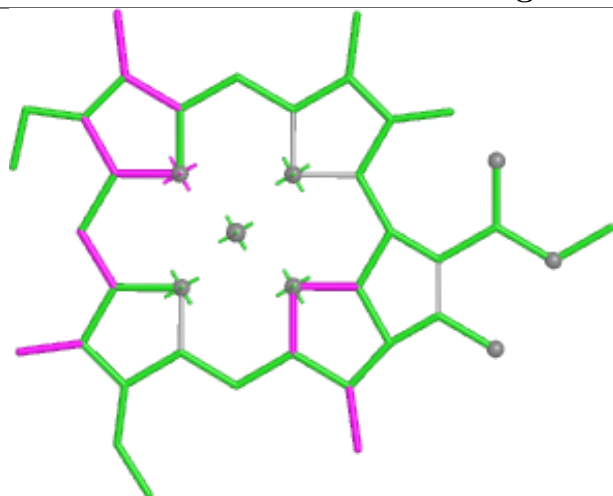


## Ligand KC1 G 318





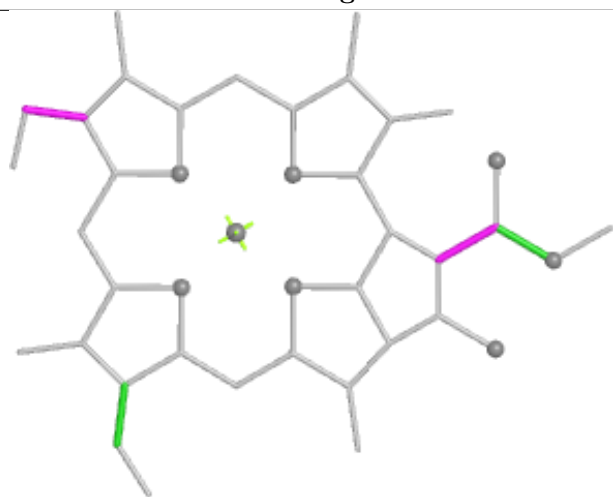
## Ligand CLA F 316



Bond lengths



Bond angles

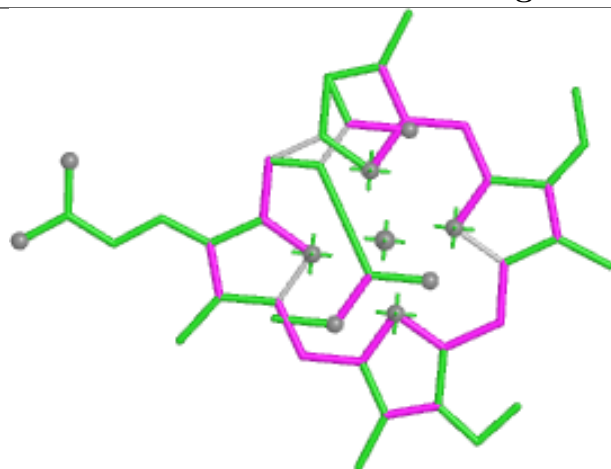


Torsions

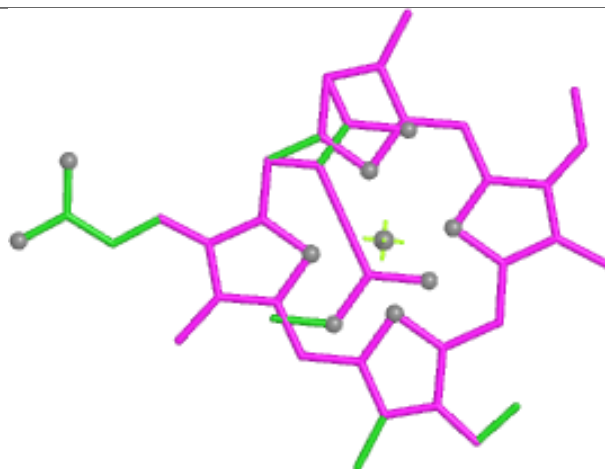


Rings

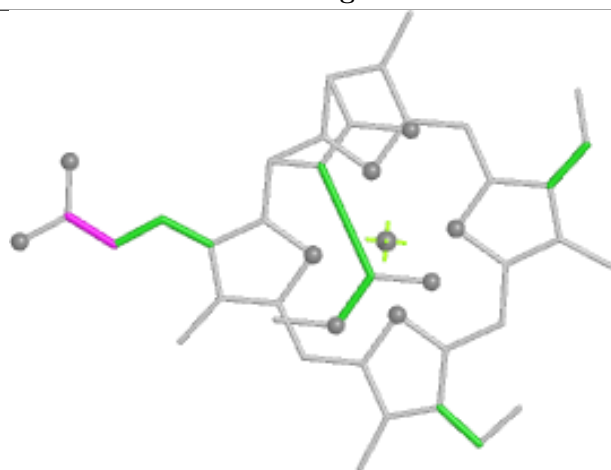
## Ligand KC1 A 312



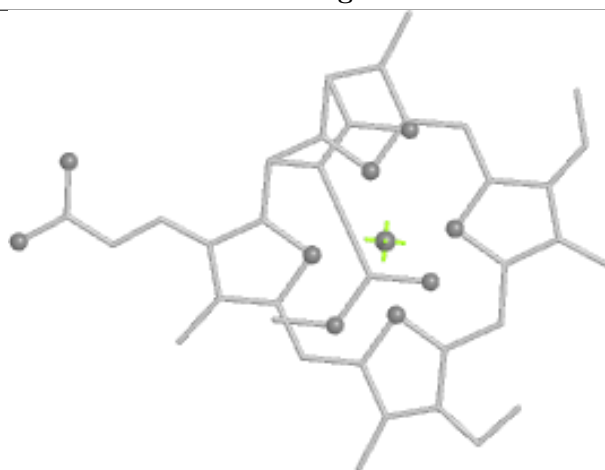
Bond lengths



Bond angles

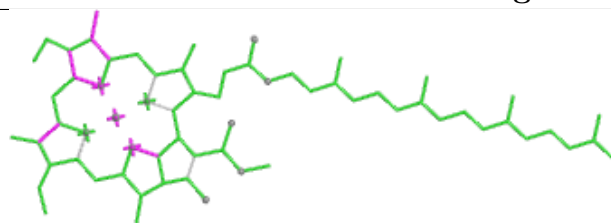


Torsions

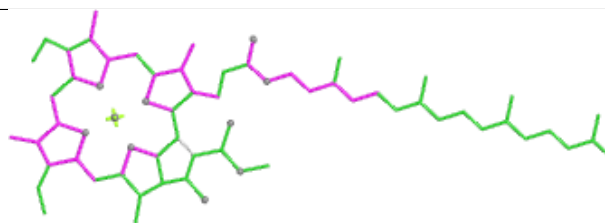


Rings

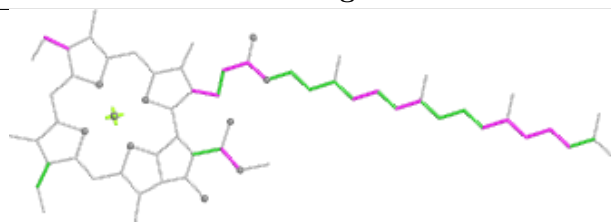
## Ligand CLA N 308



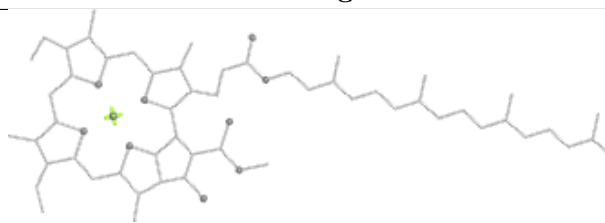
Bond lengths



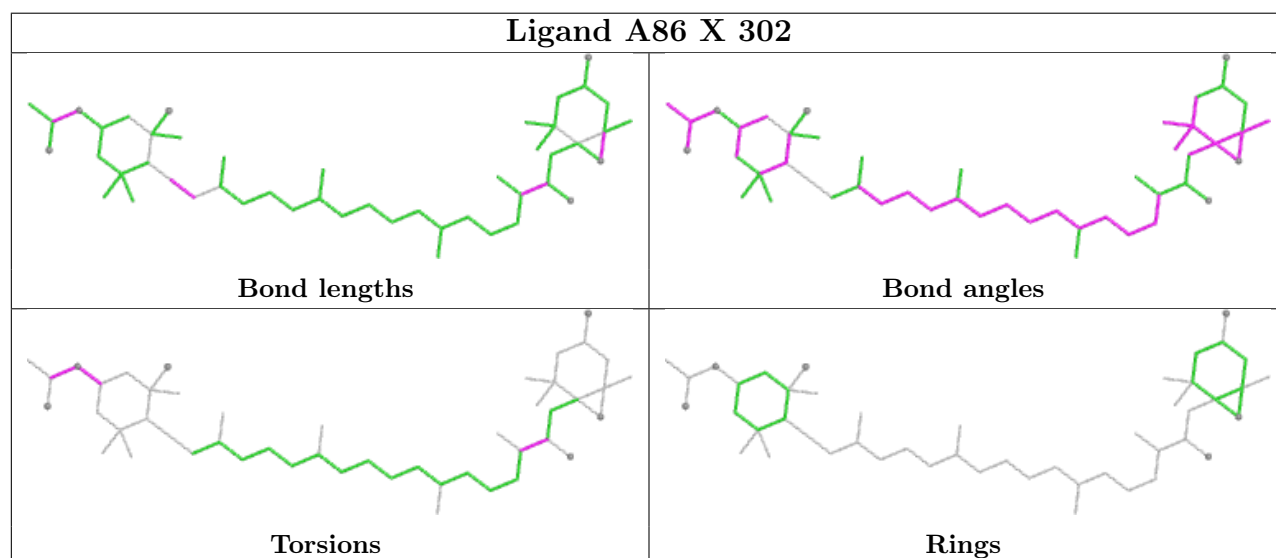
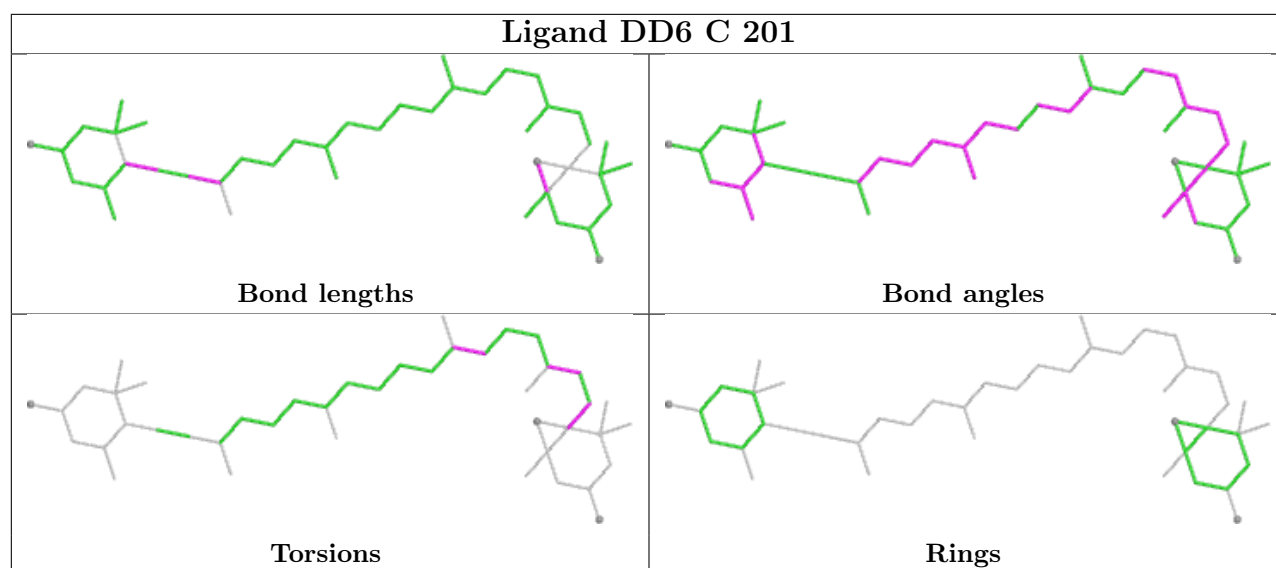
Bond angles



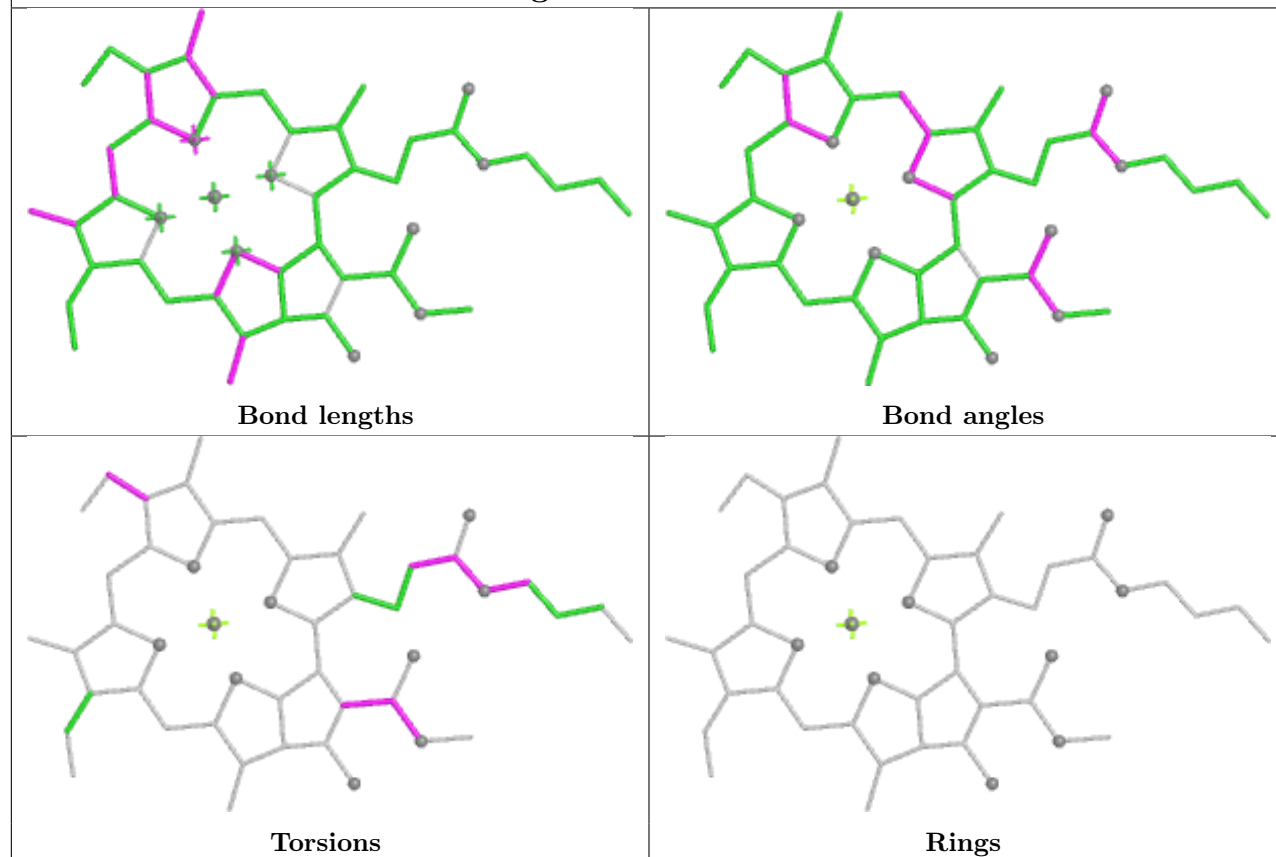
Torsions



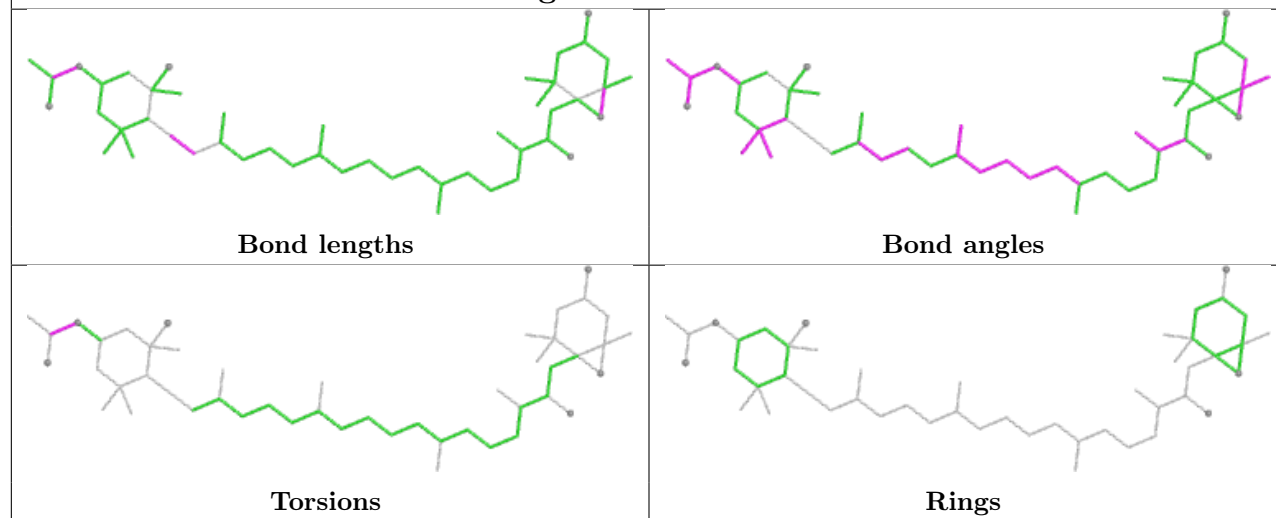
Rings



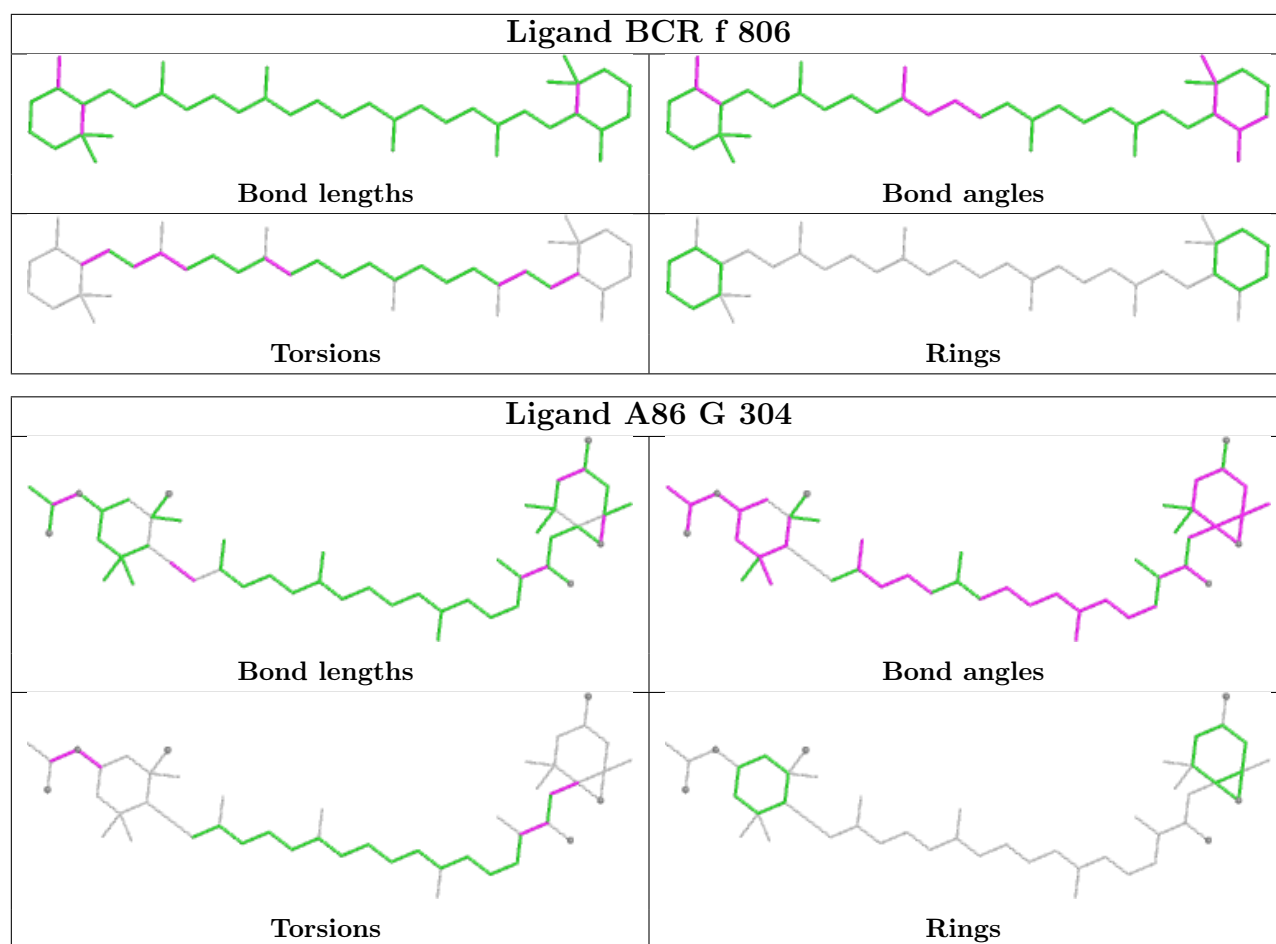
## Ligand CLA G 316

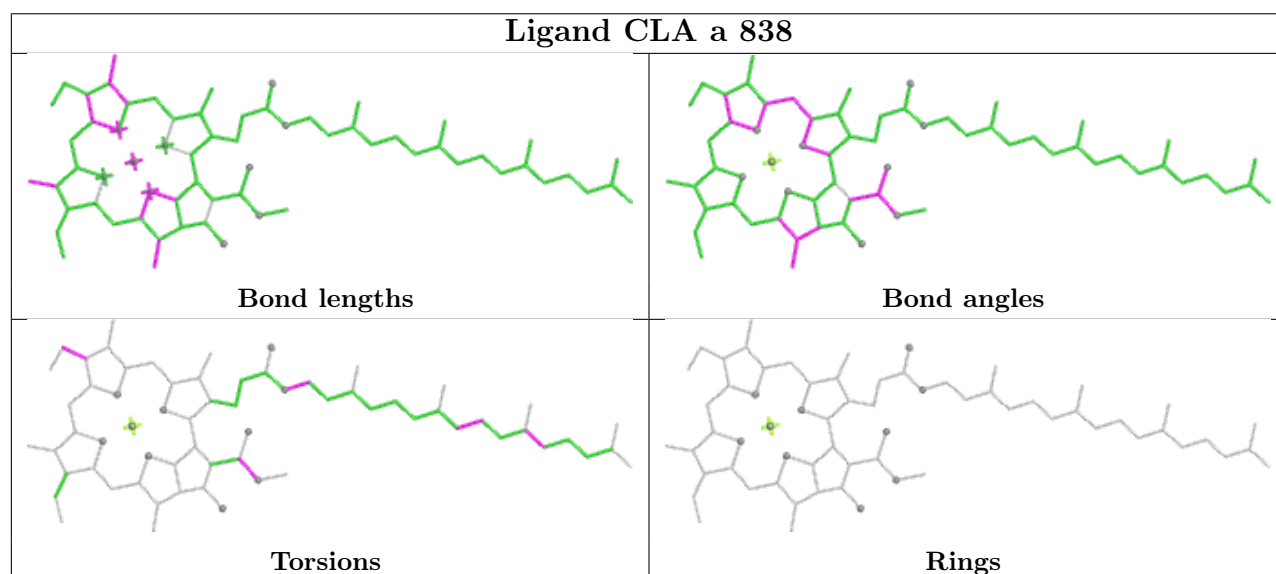
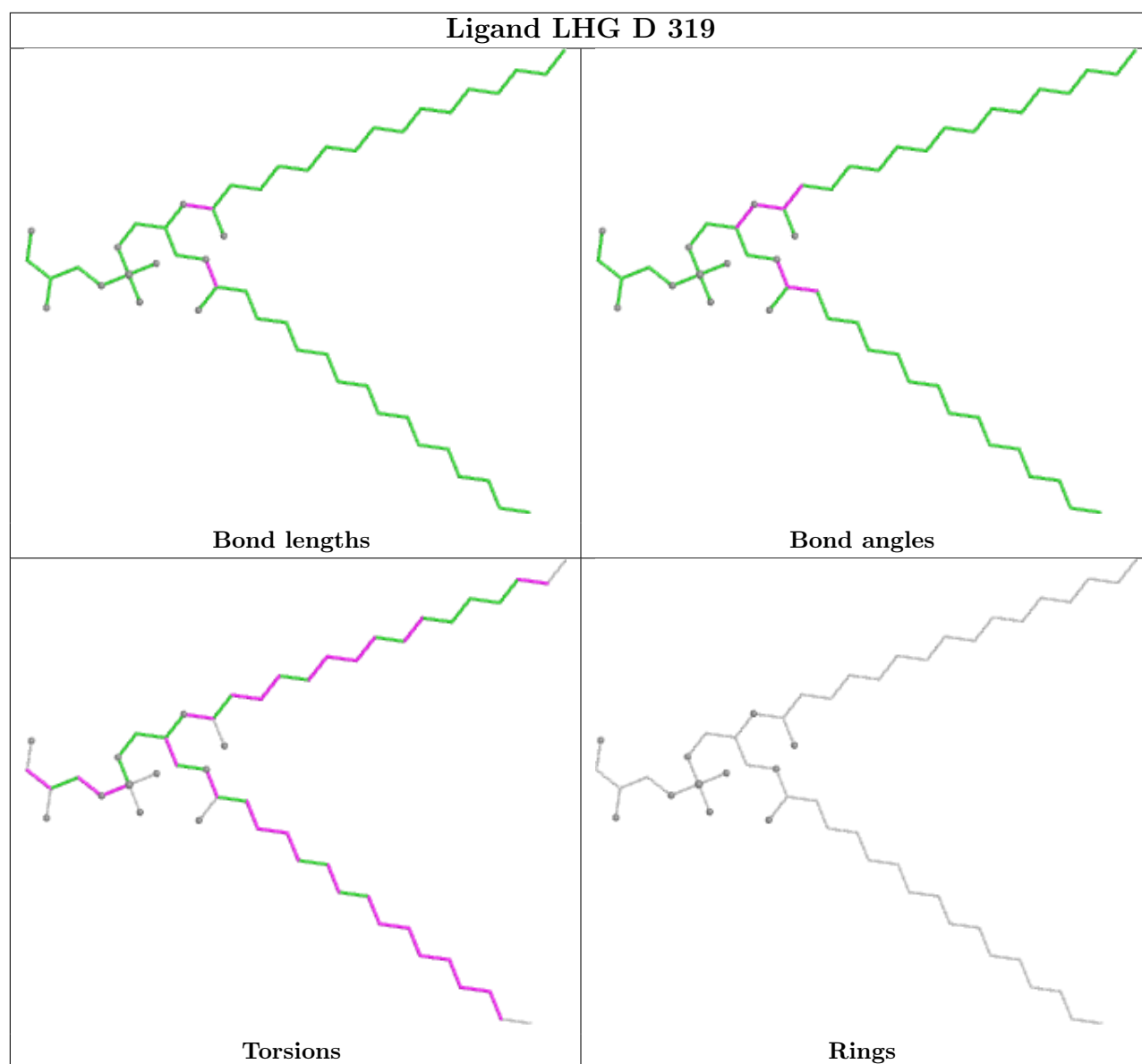


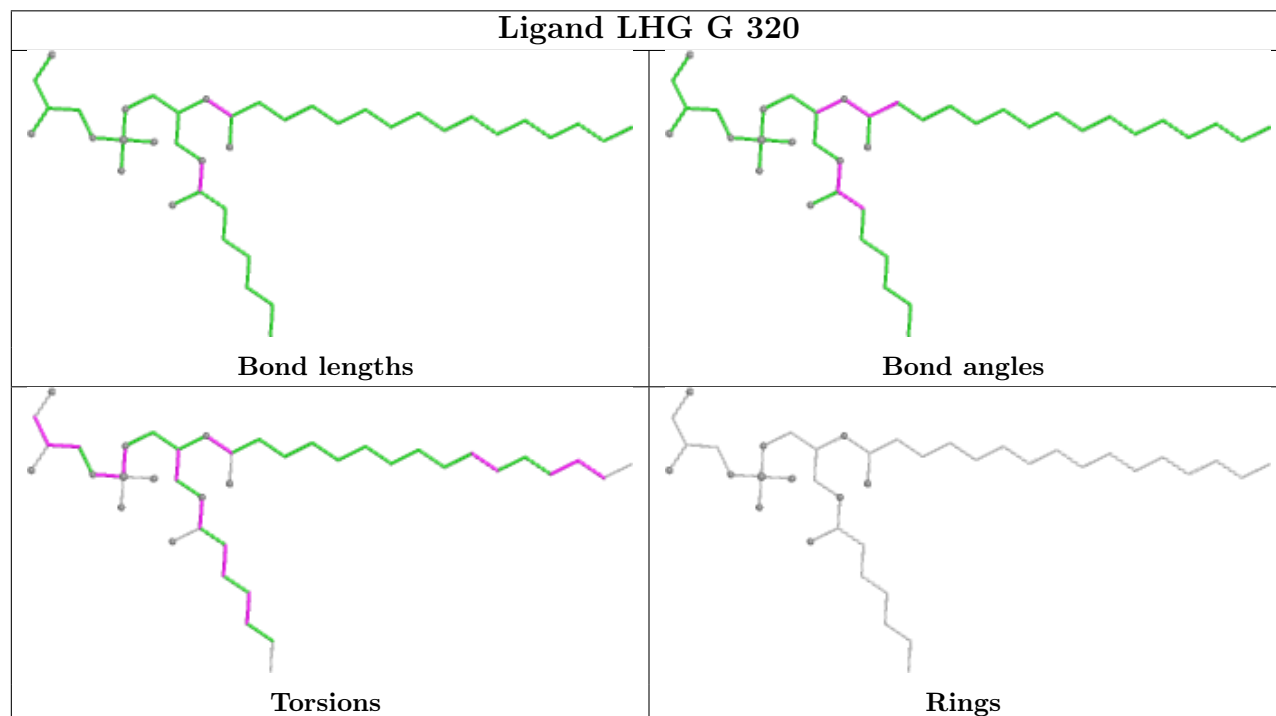
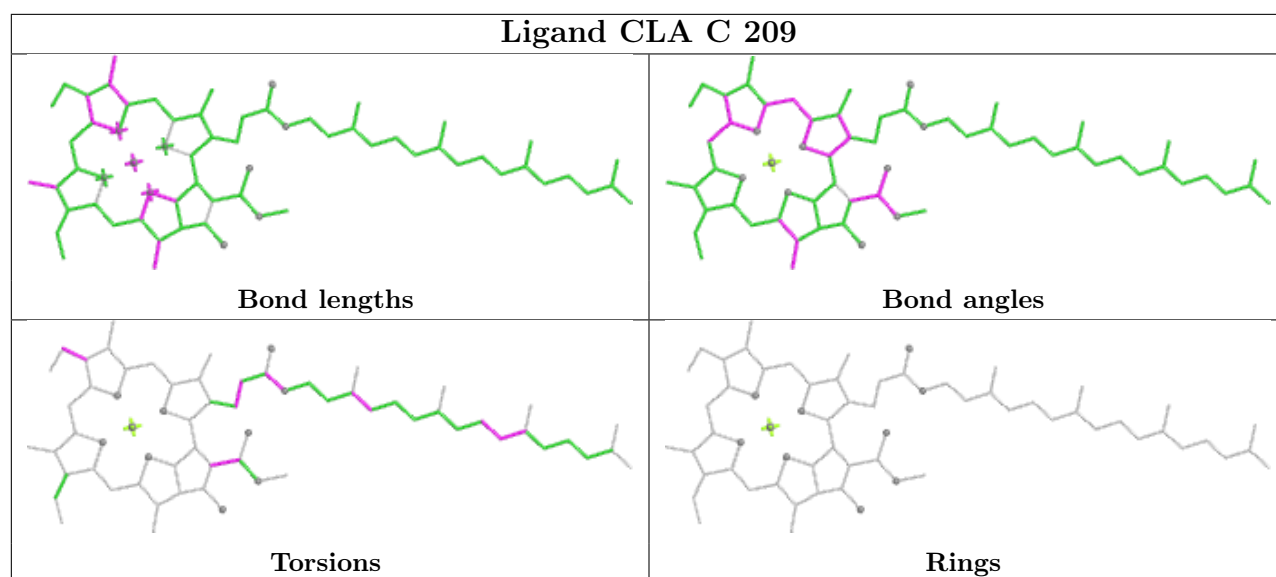
## Ligand A86 P 307



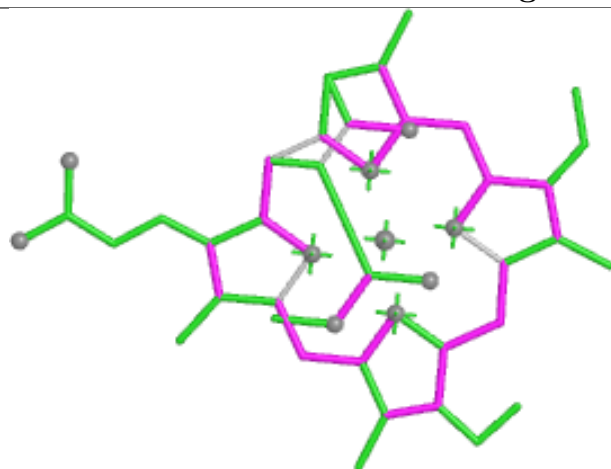




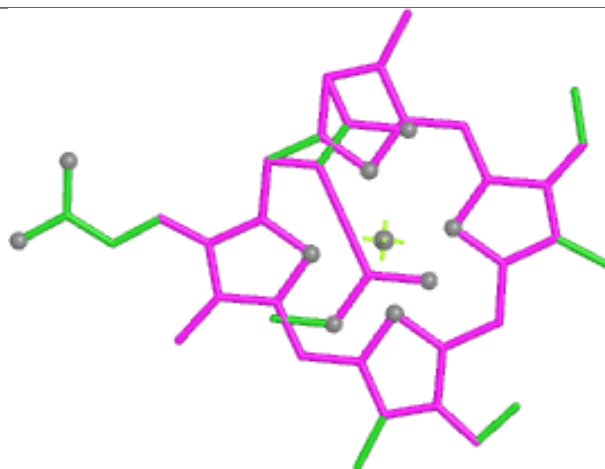




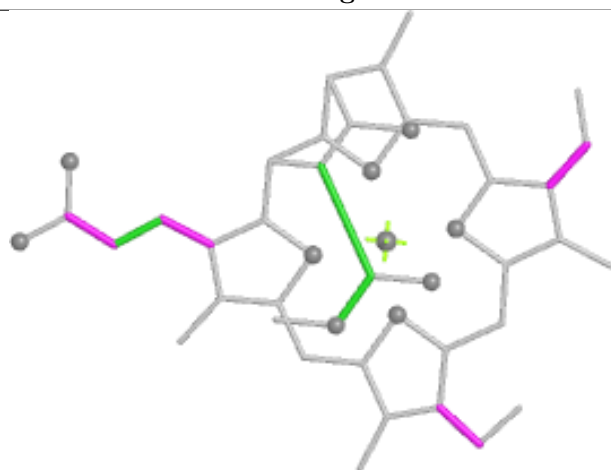
## Ligand KC1 S 316



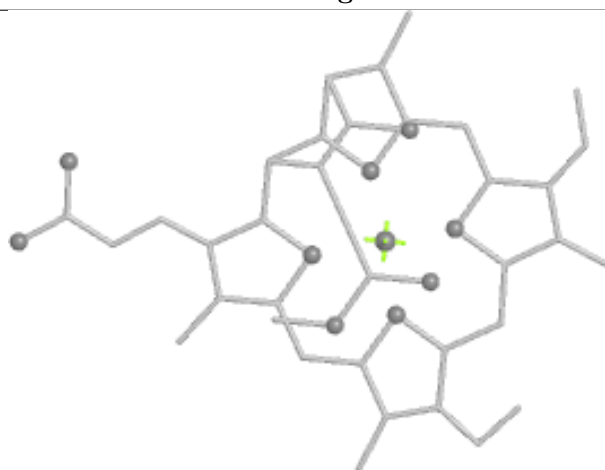
Bond lengths



Bond angles

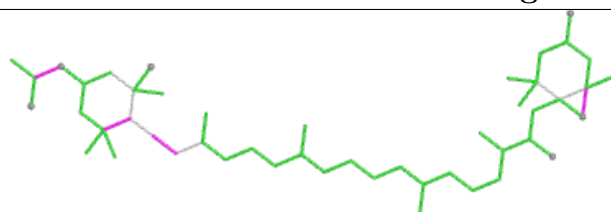


Torsions

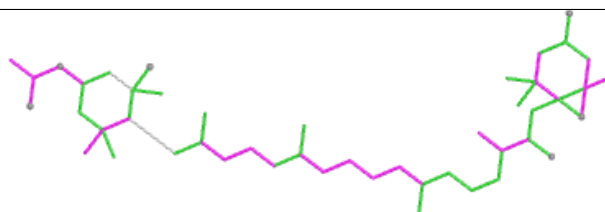


Rings

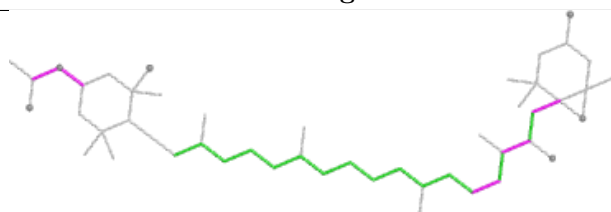
## Ligand A86 B 301



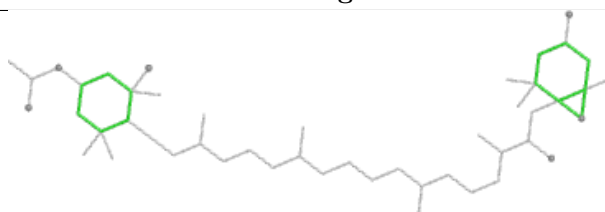
Bond lengths



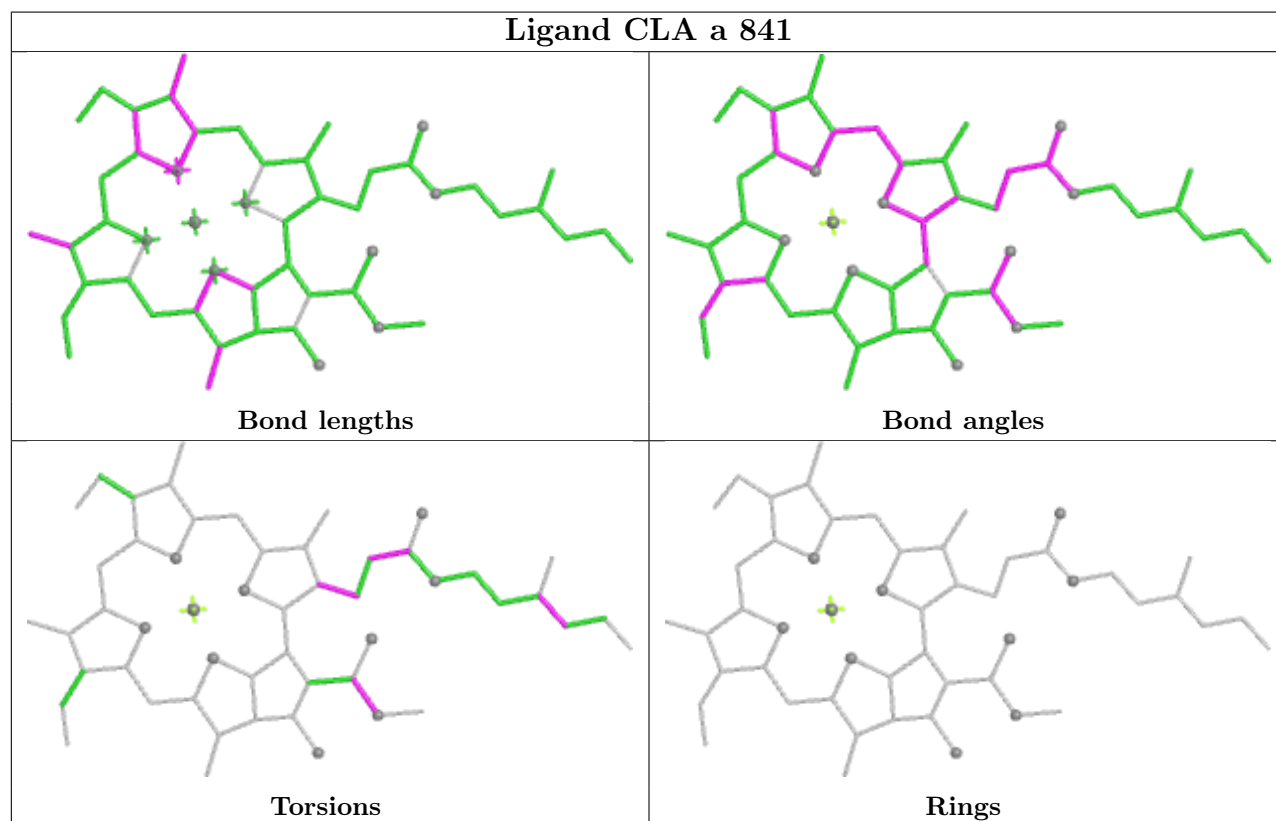
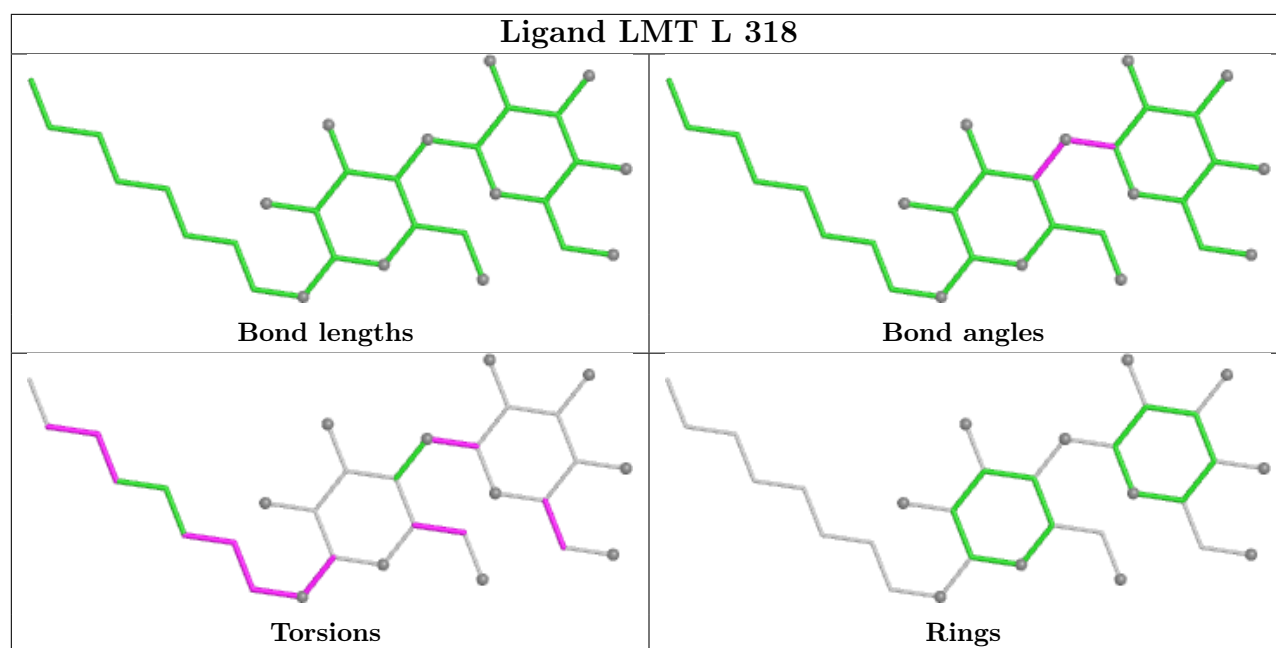
Bond angles

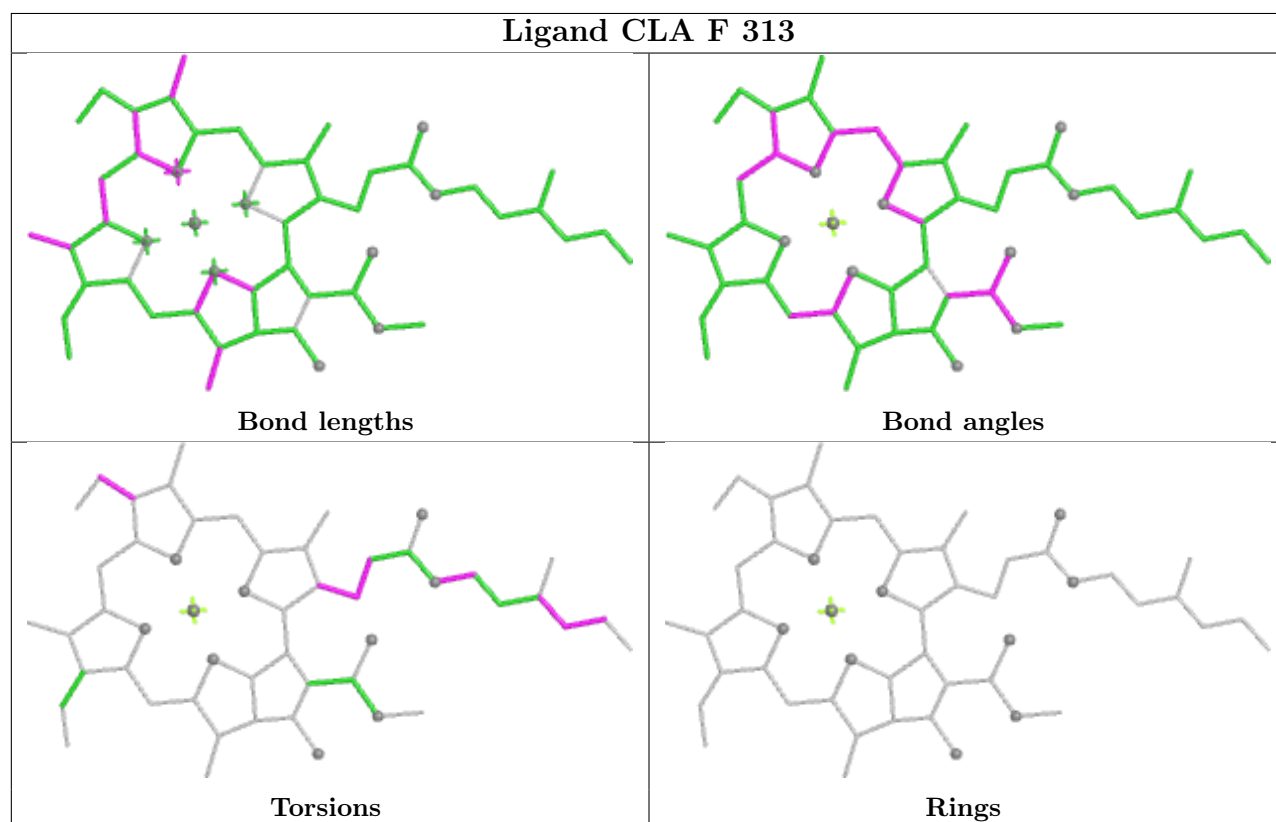
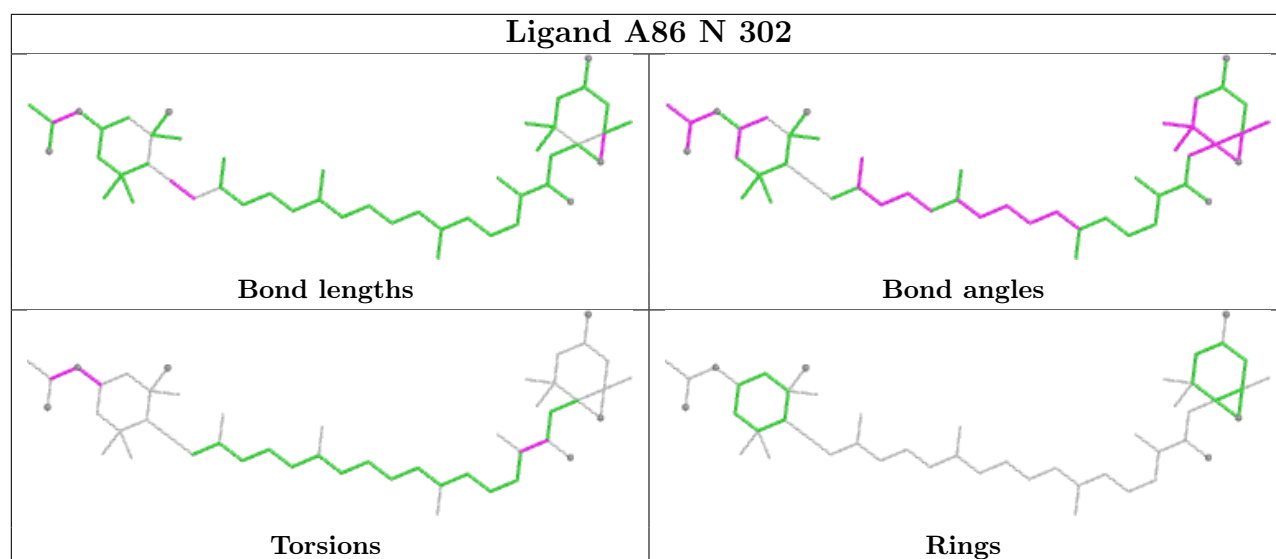


Torsions

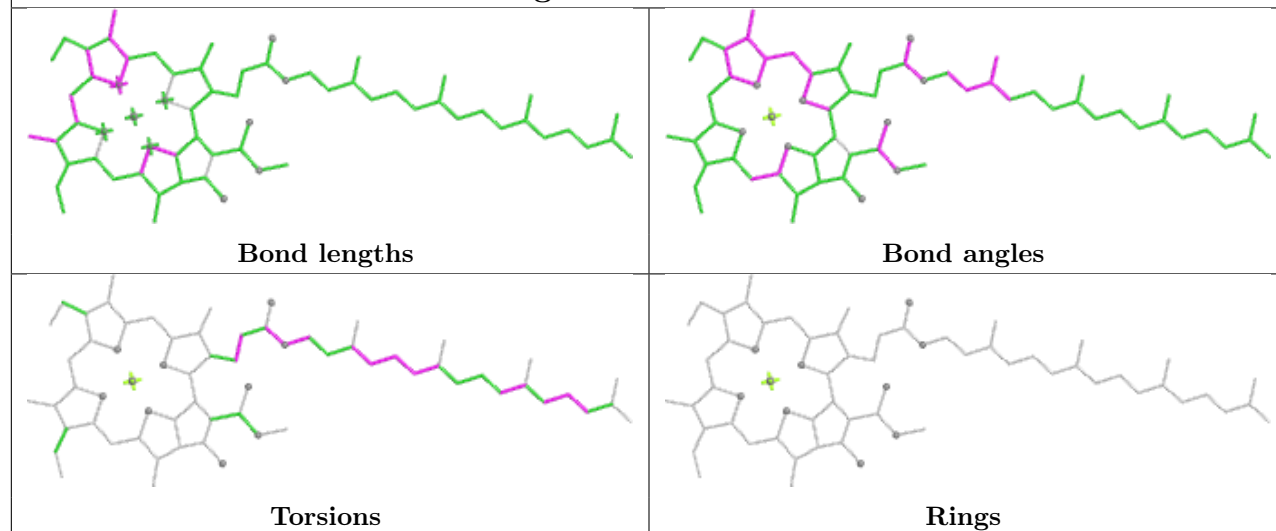


Rings

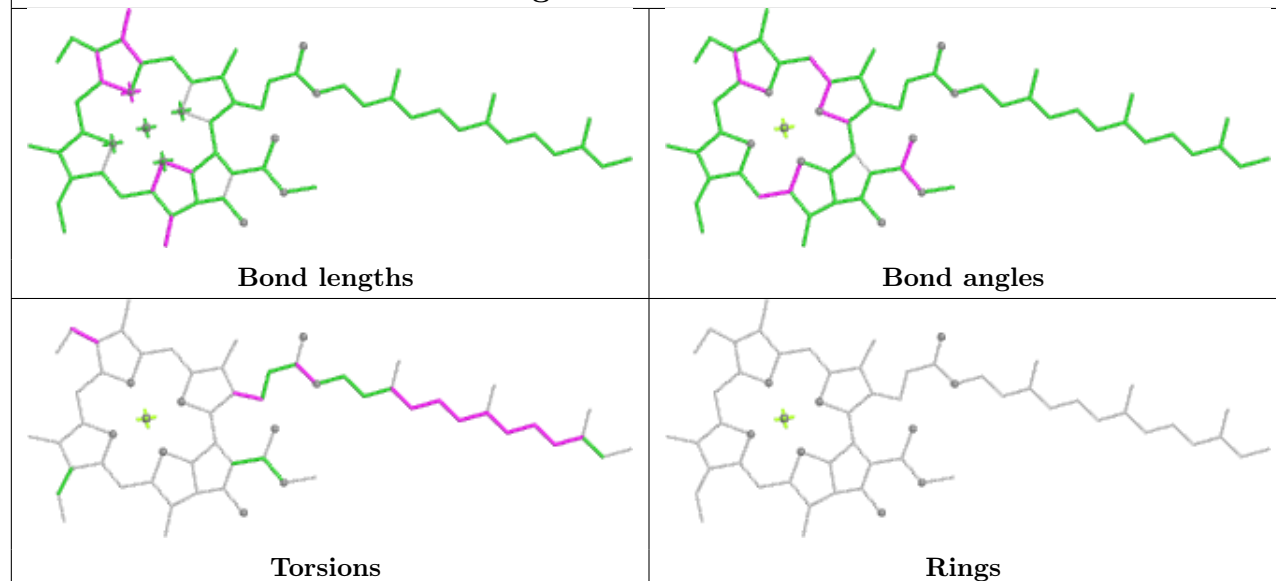




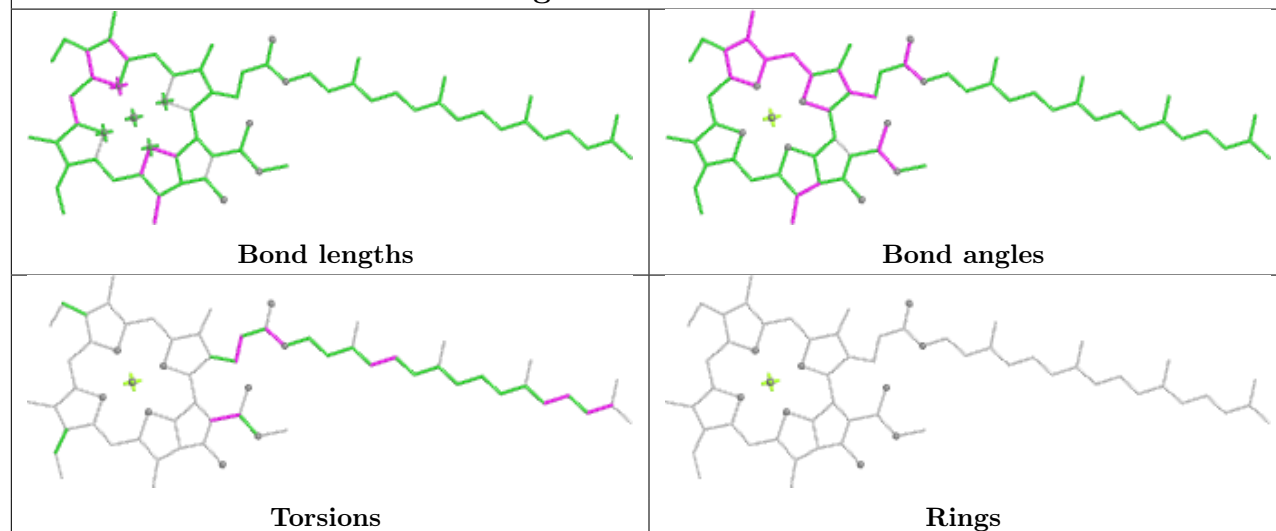
## Ligand CLA F 309

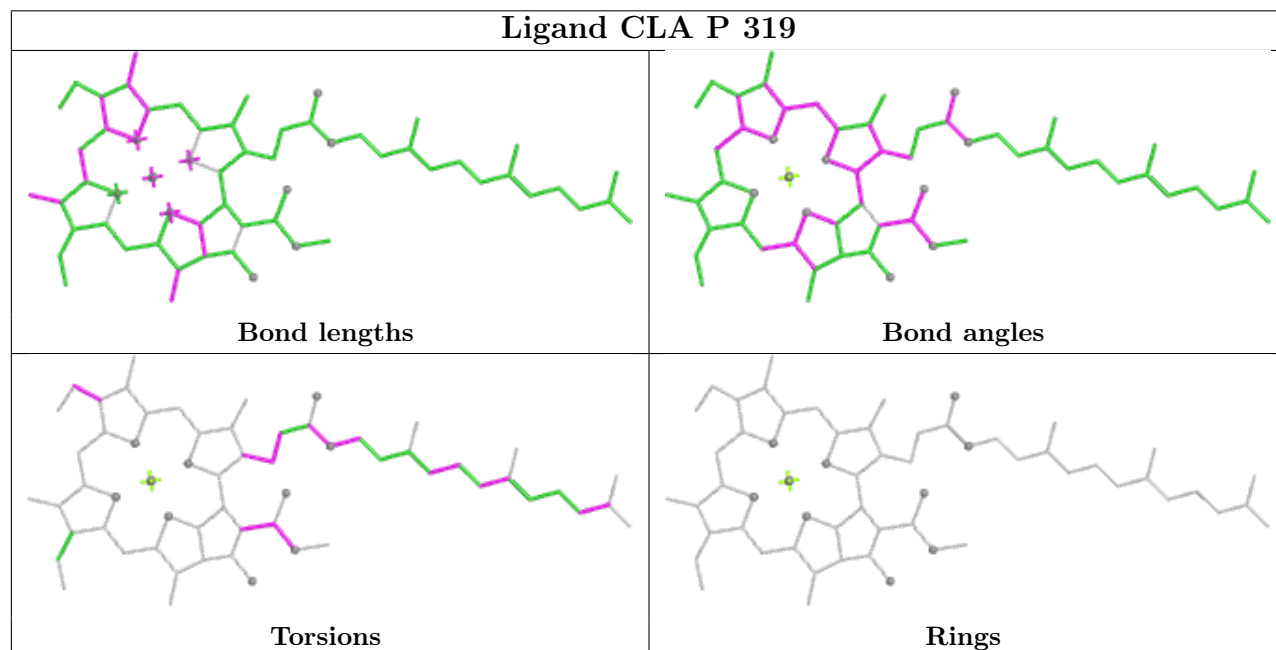
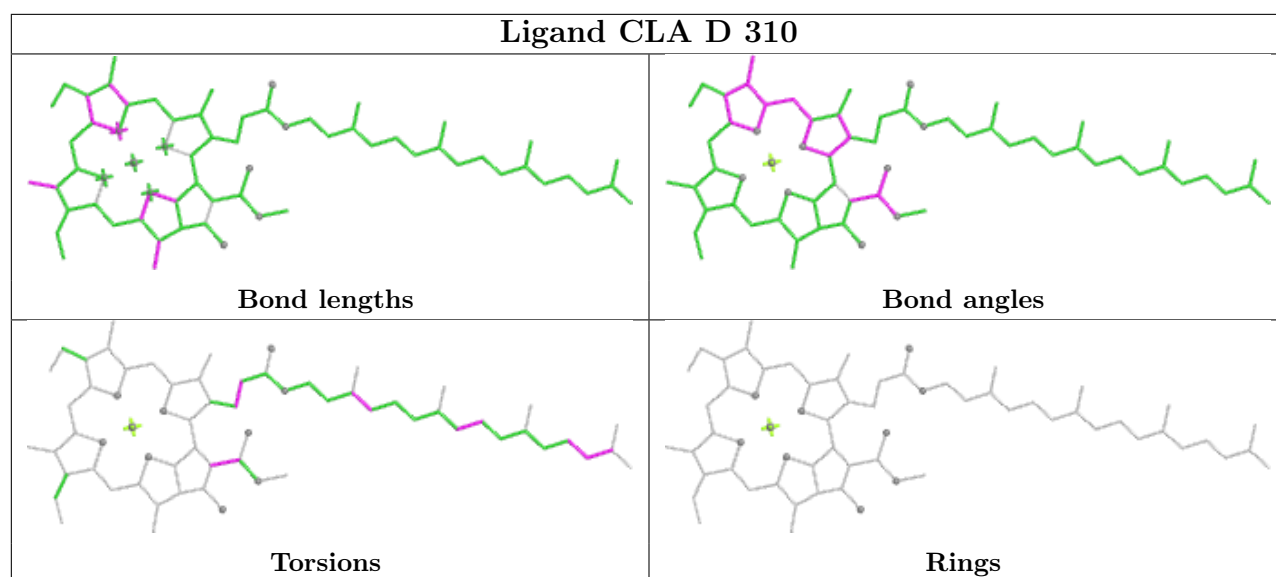


## Ligand CLA C 206

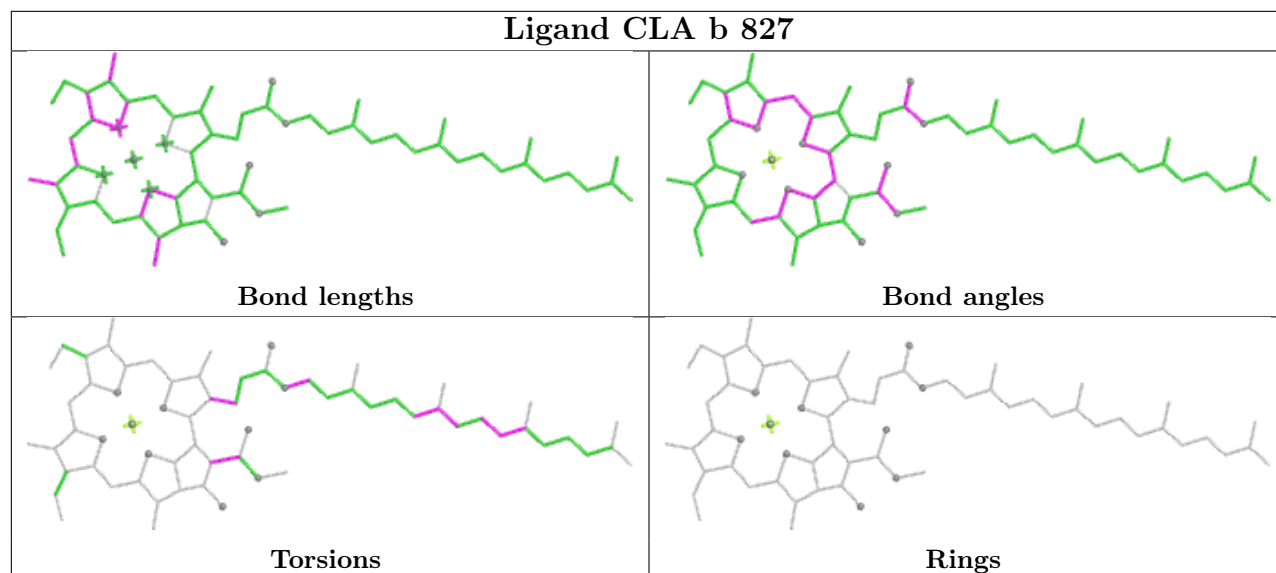
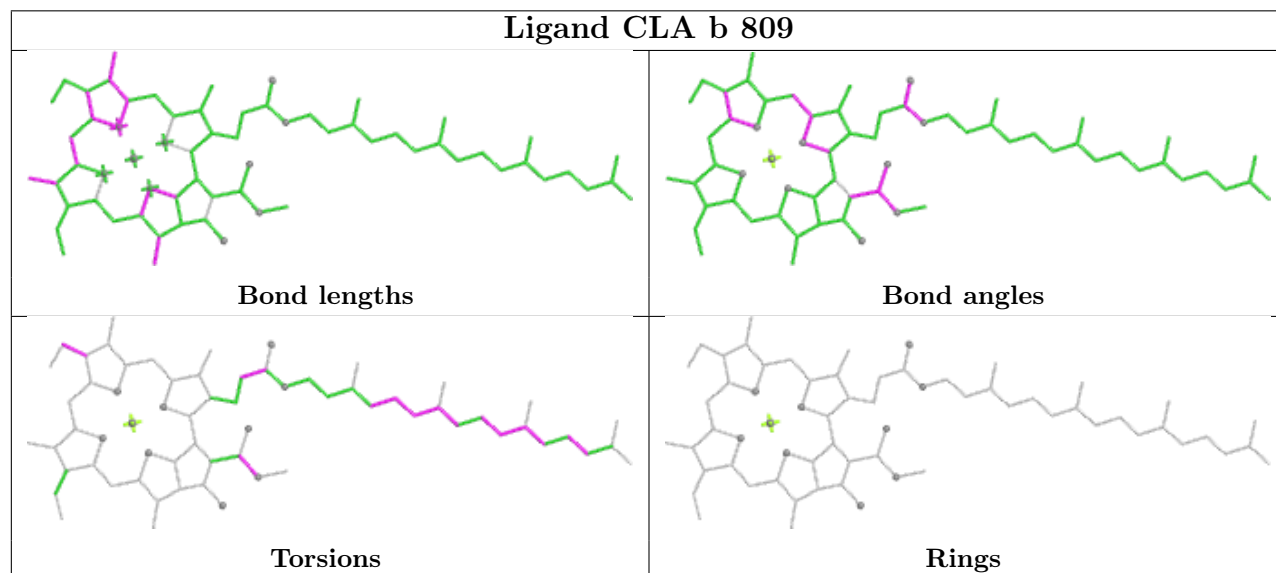
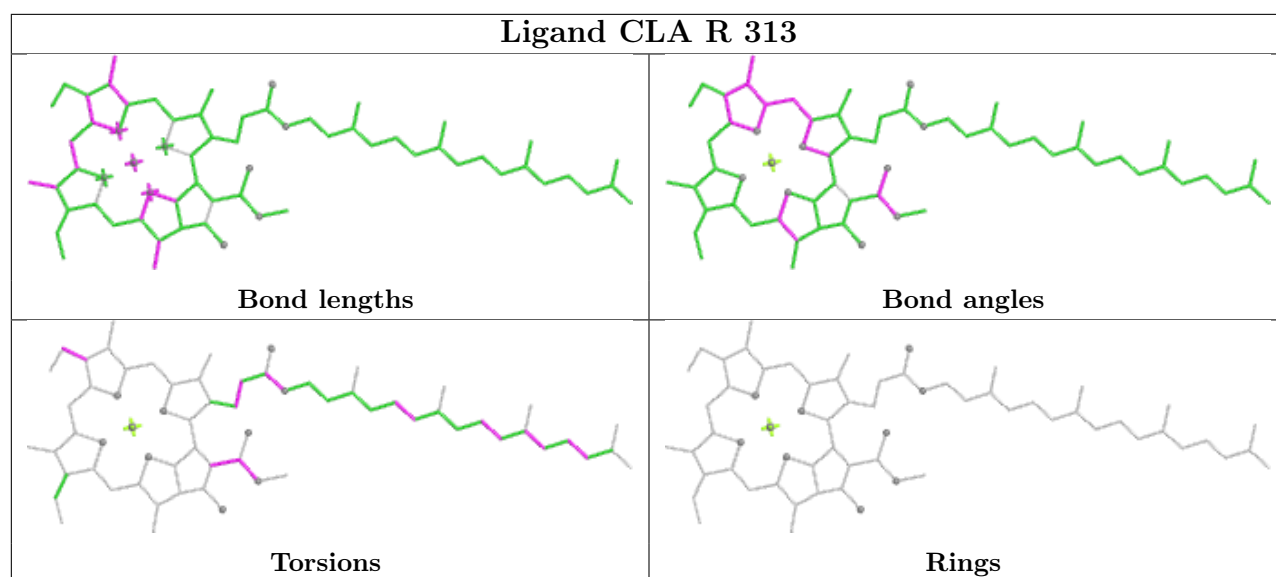


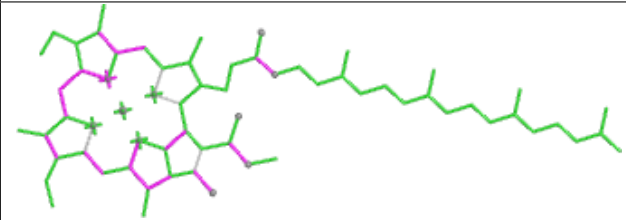
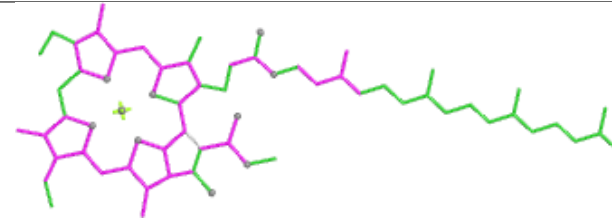
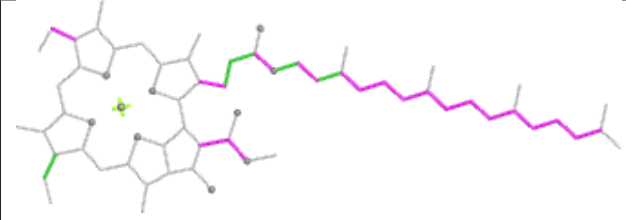
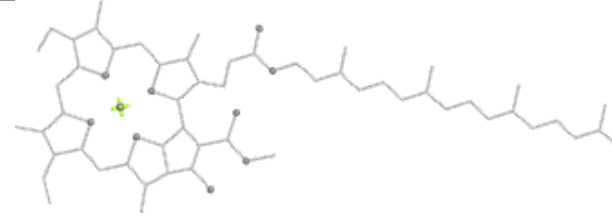
## Ligand CLA E 310

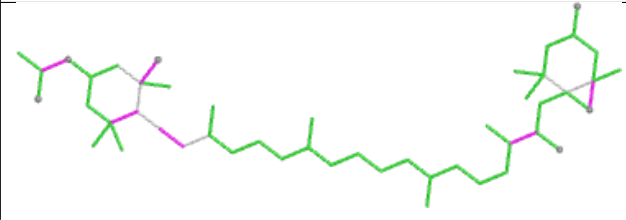
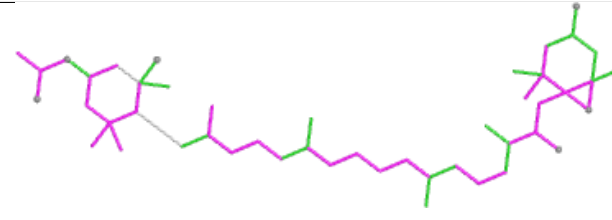
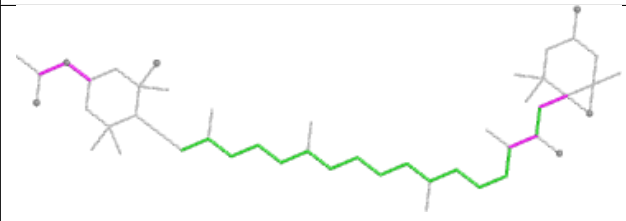
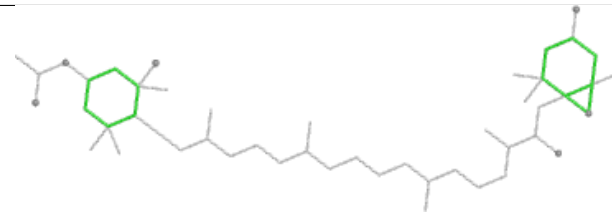


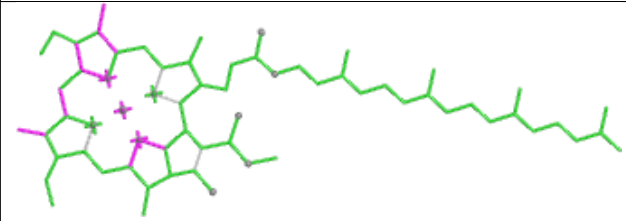
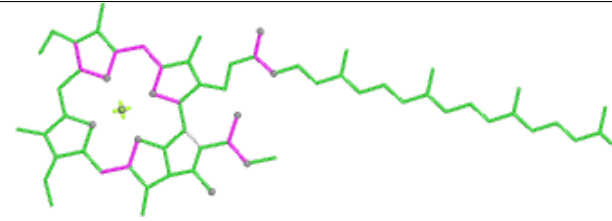
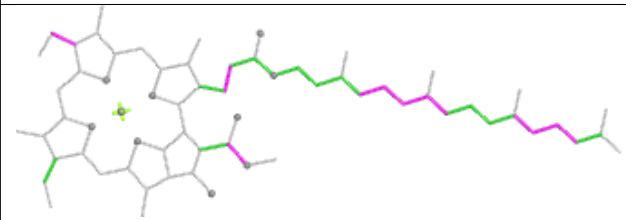
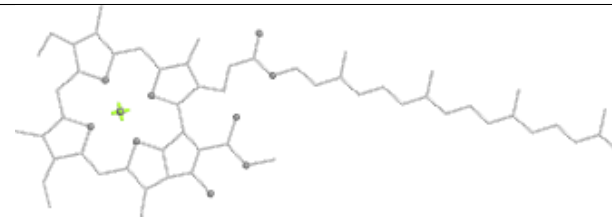


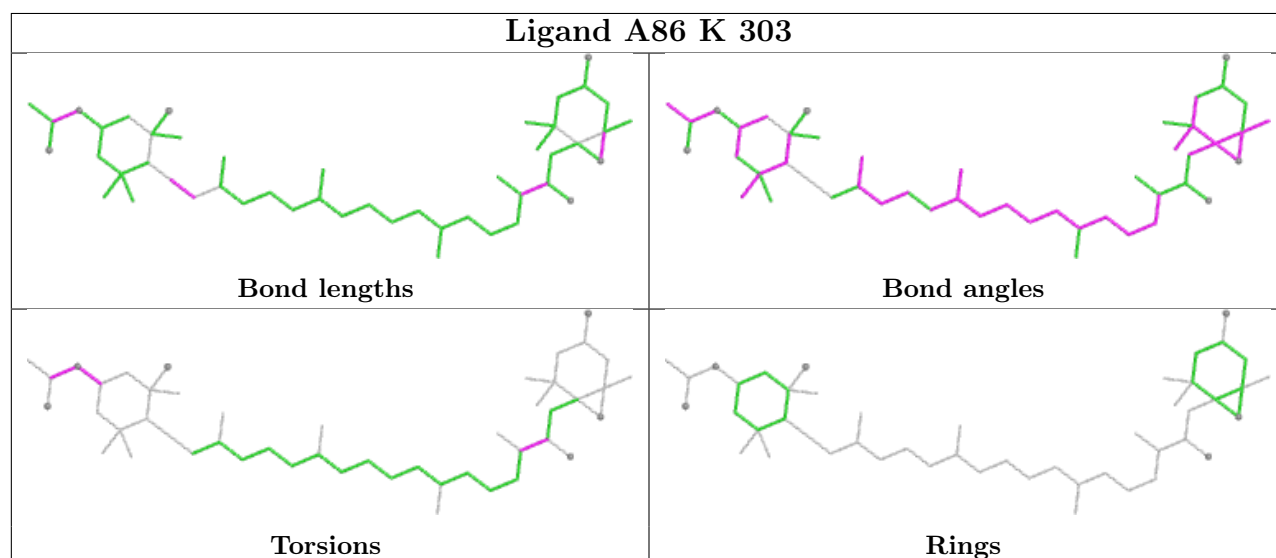
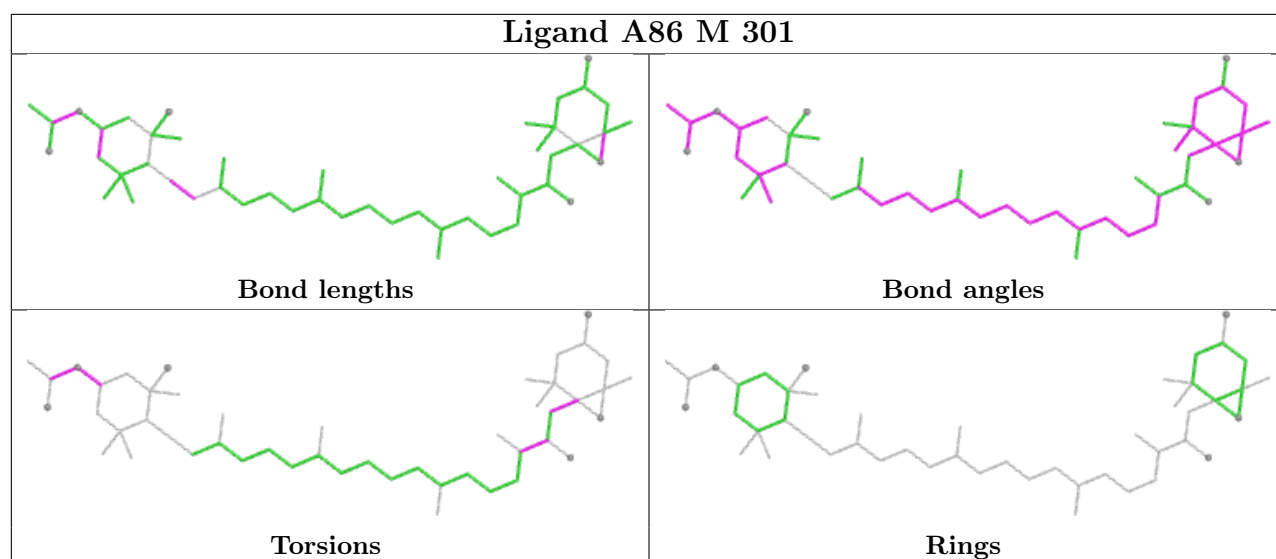




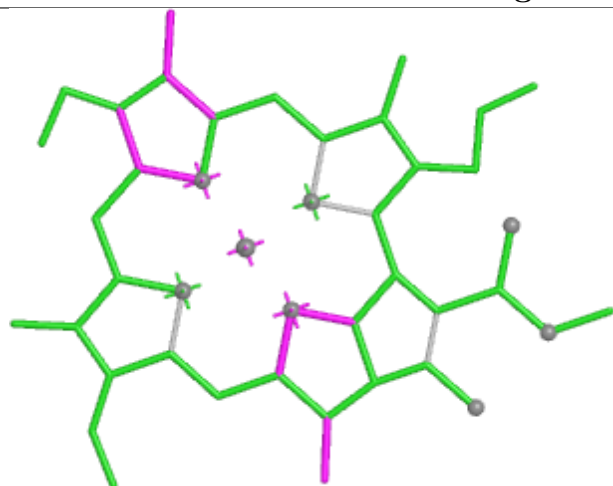
| Ligand CLA O 316                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand A86 F 305                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

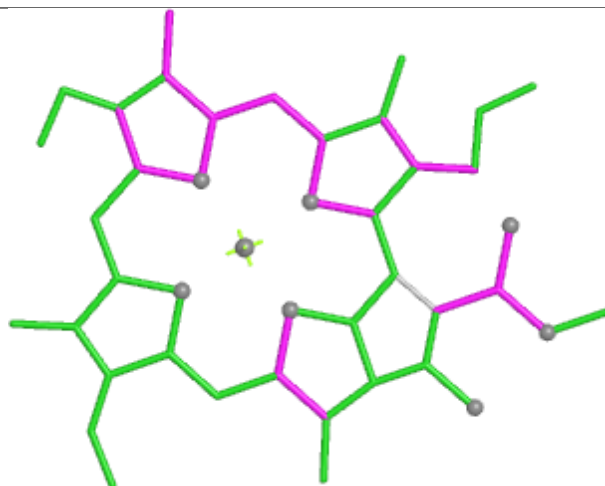
| Ligand CLA J 313                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



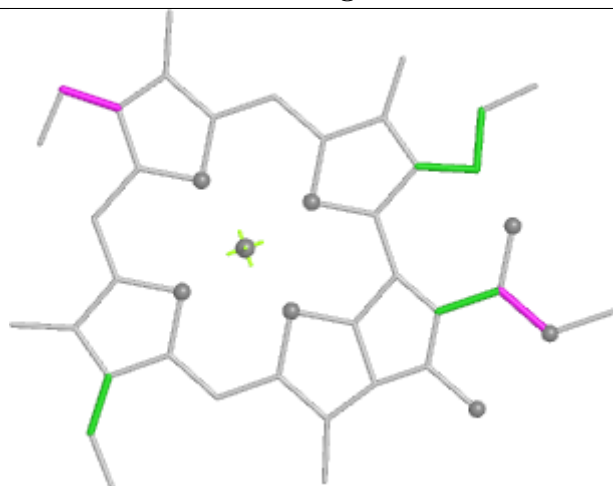
## Ligand CLA C 205



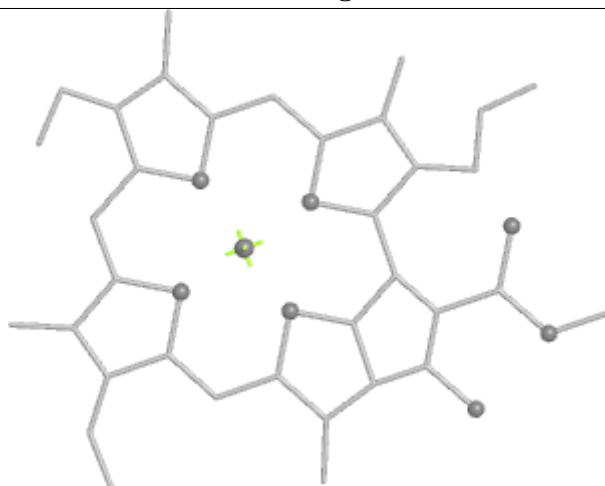
Bond lengths



Bond angles

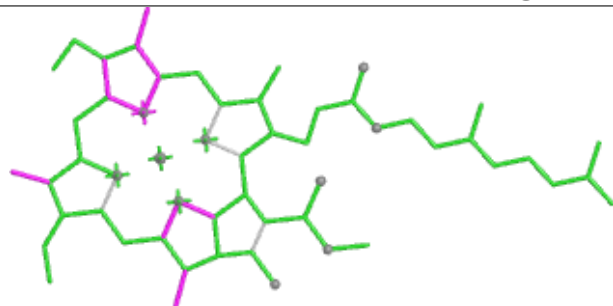


Torsions

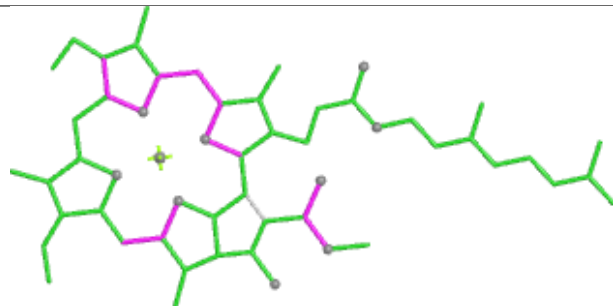


Rings

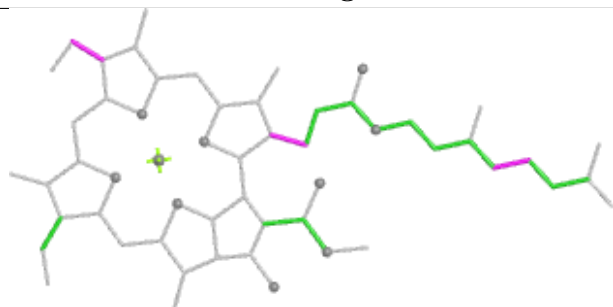
## Ligand CLA b 814



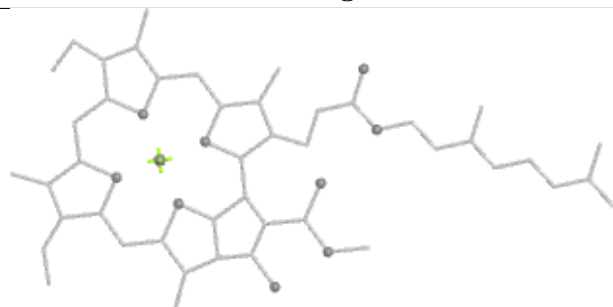
Bond lengths



Bond angles

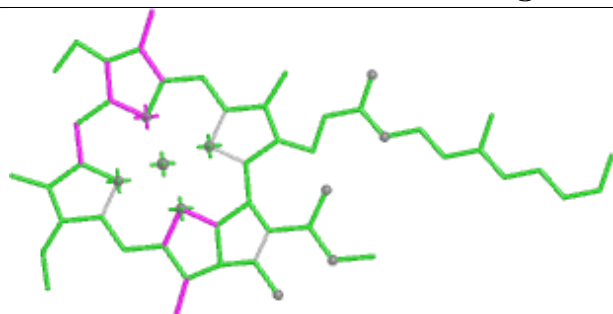


Torsions

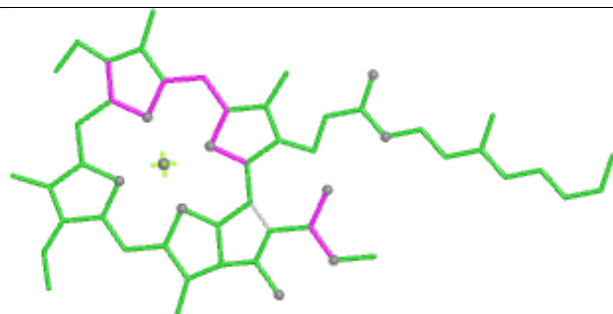


Rings

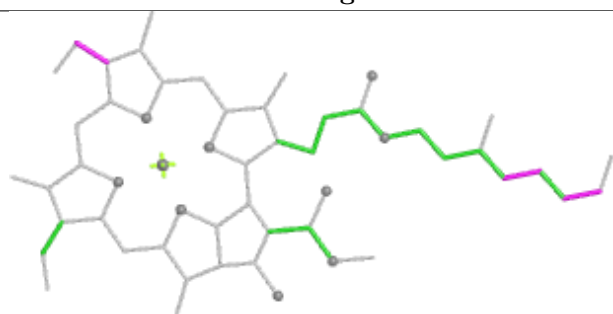
## Ligand CLA L 310



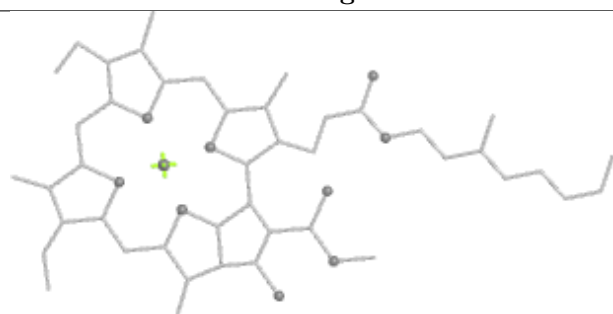
Bond lengths



Bond angles

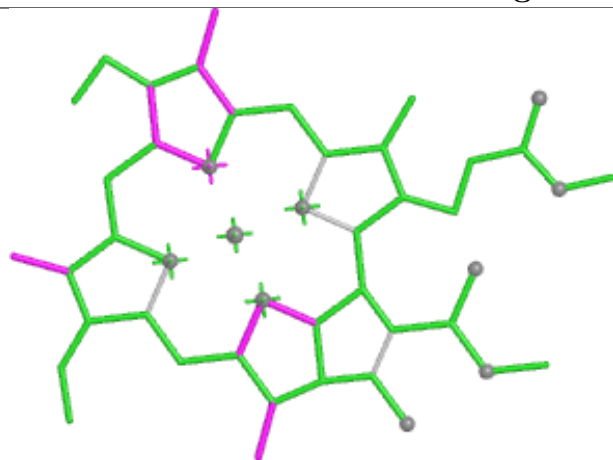


Torsions

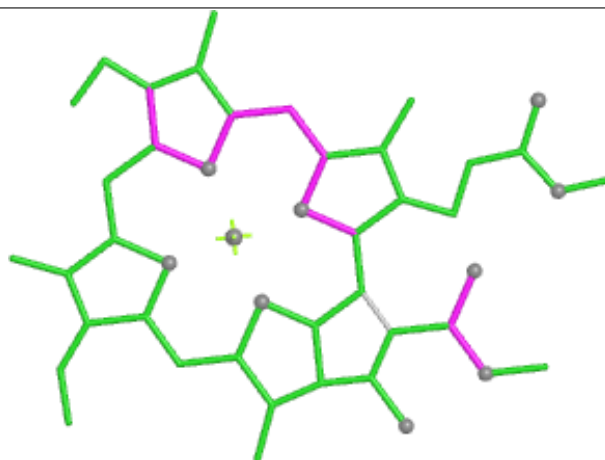


Rings

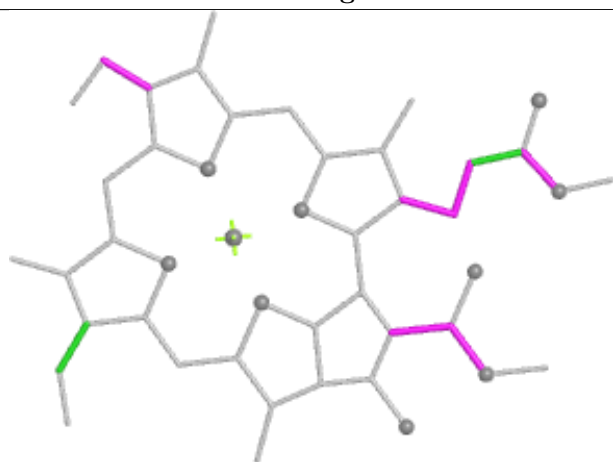
## Ligand CLA A 309



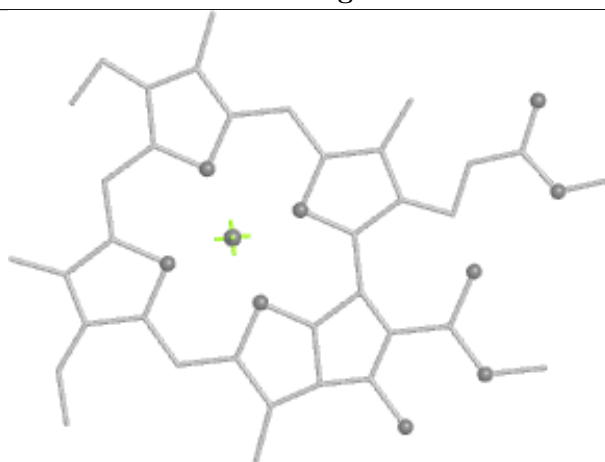
Bond lengths



Bond angles

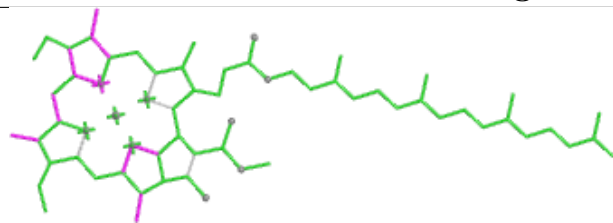


Torsions

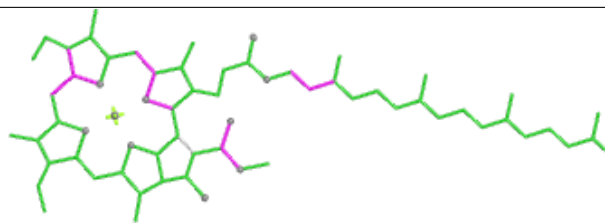


Rings

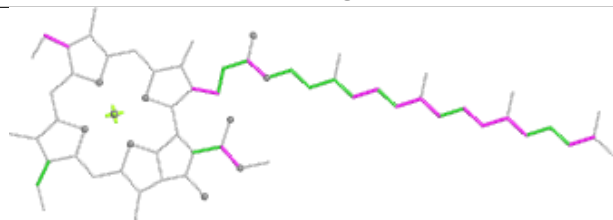
## Ligand CLA A 311



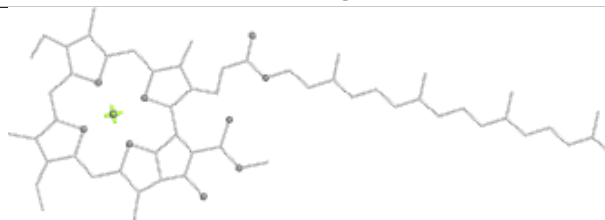
Bond lengths



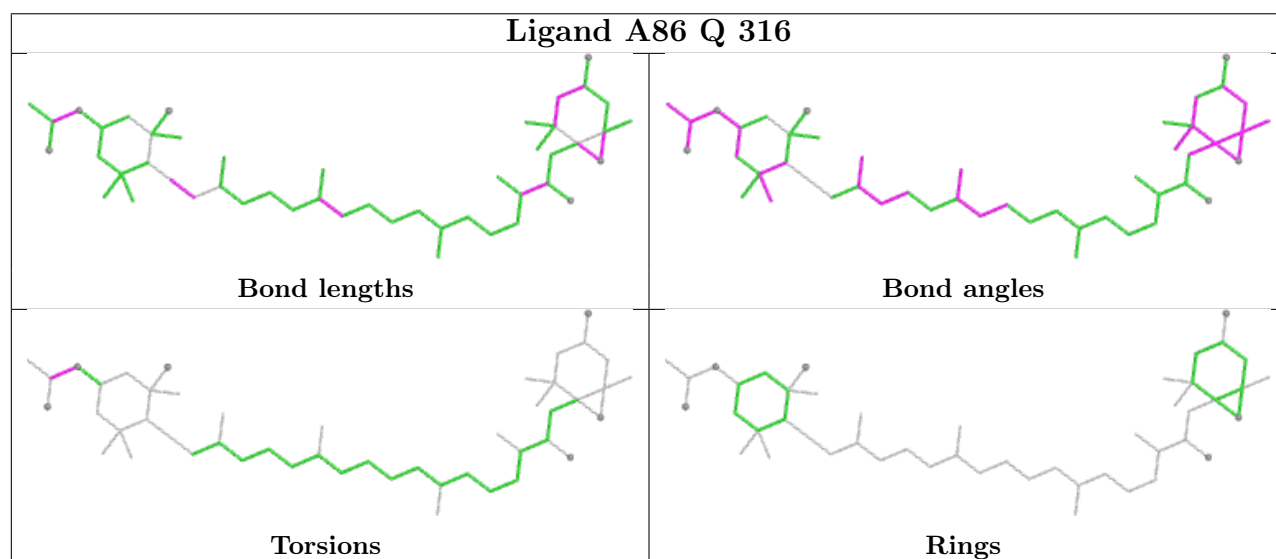
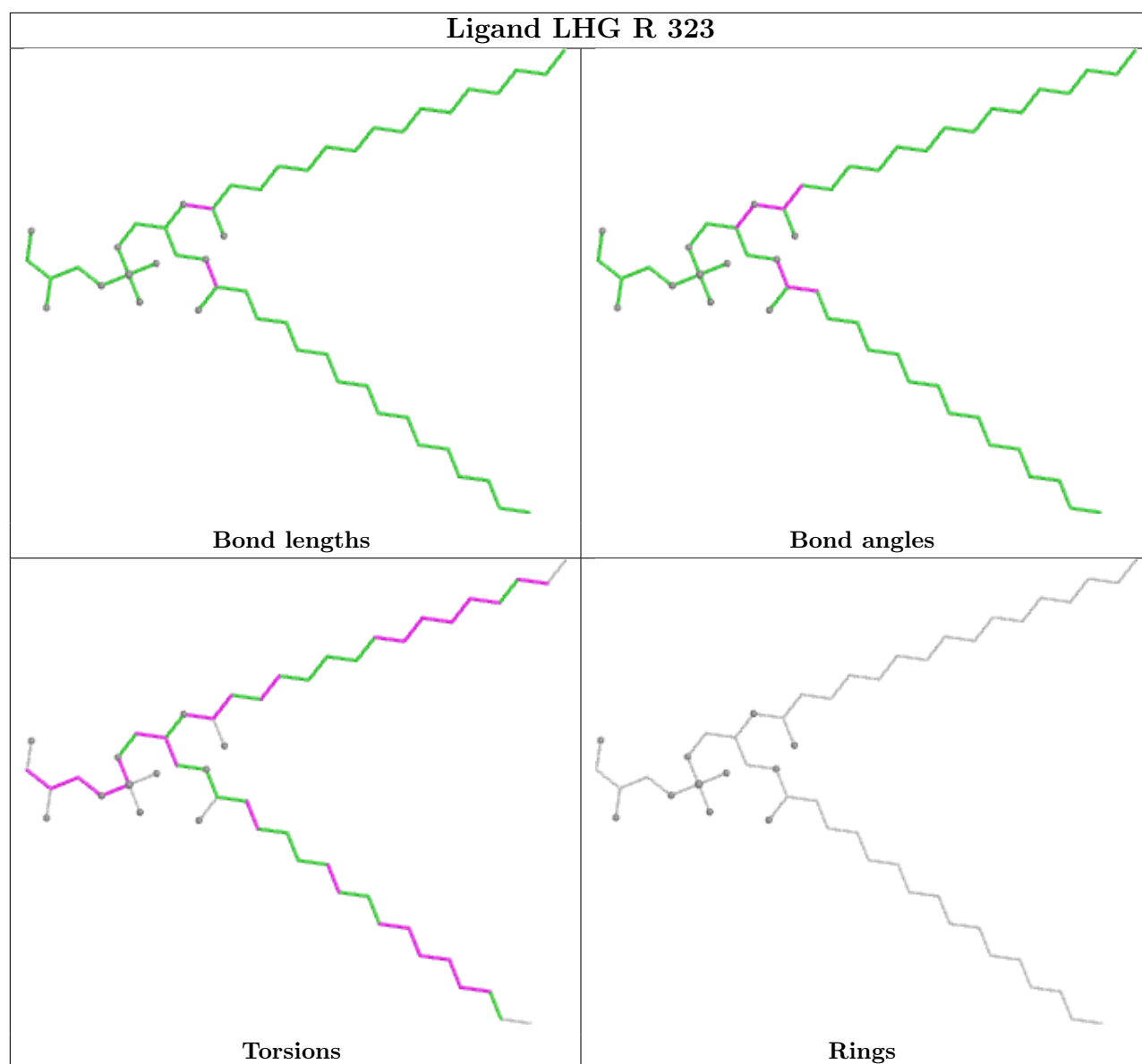
Bond angles



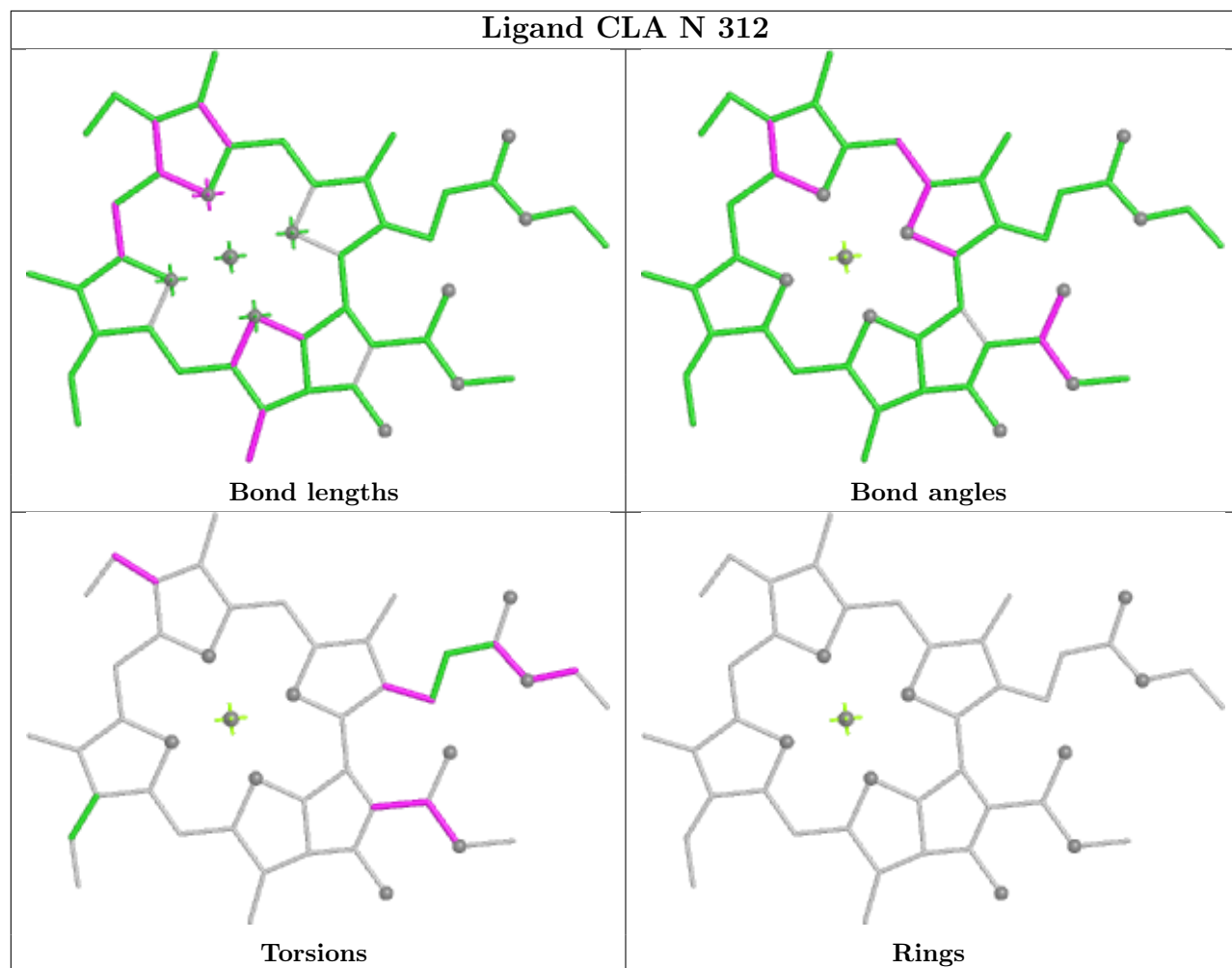
Torsions



Rings

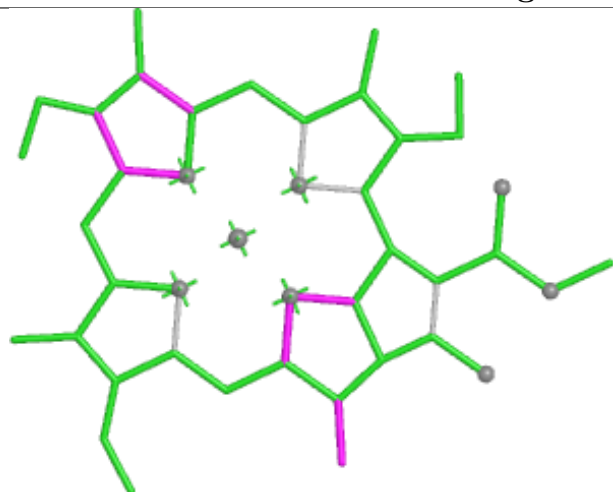


## Ligand CLA N 312

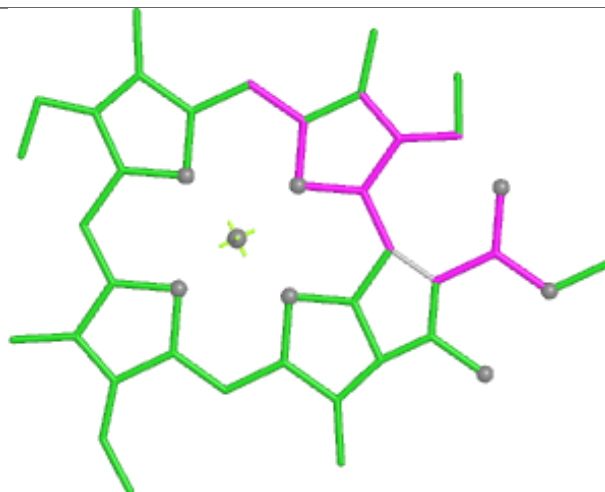




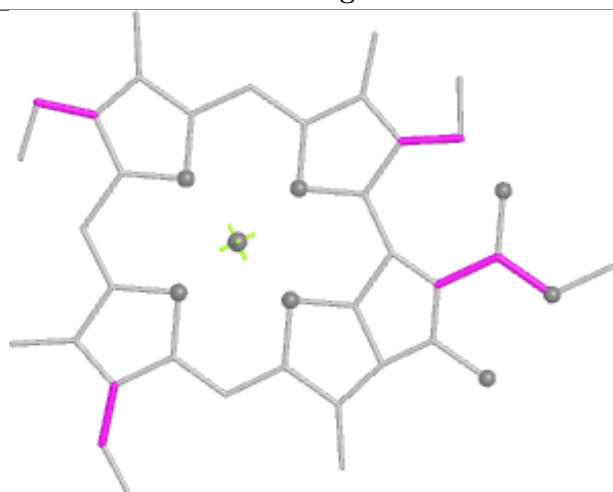
## Ligand CLA S 318



Bond lengths



Bond angles

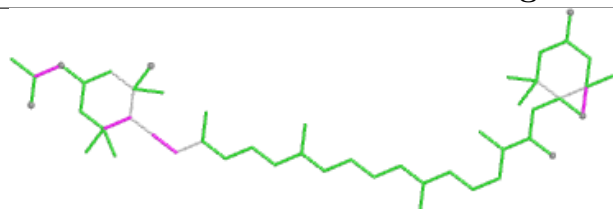


Torsions

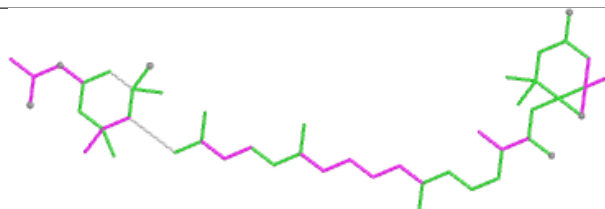


Rings

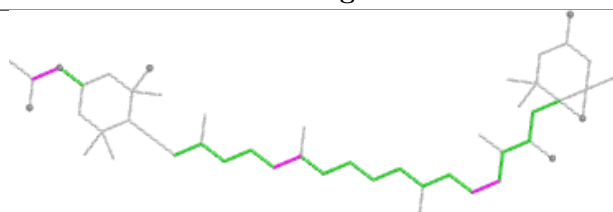
## Ligand A86 R 305



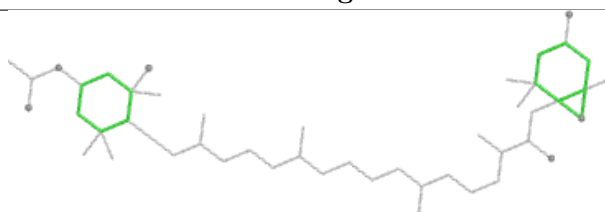
Bond lengths



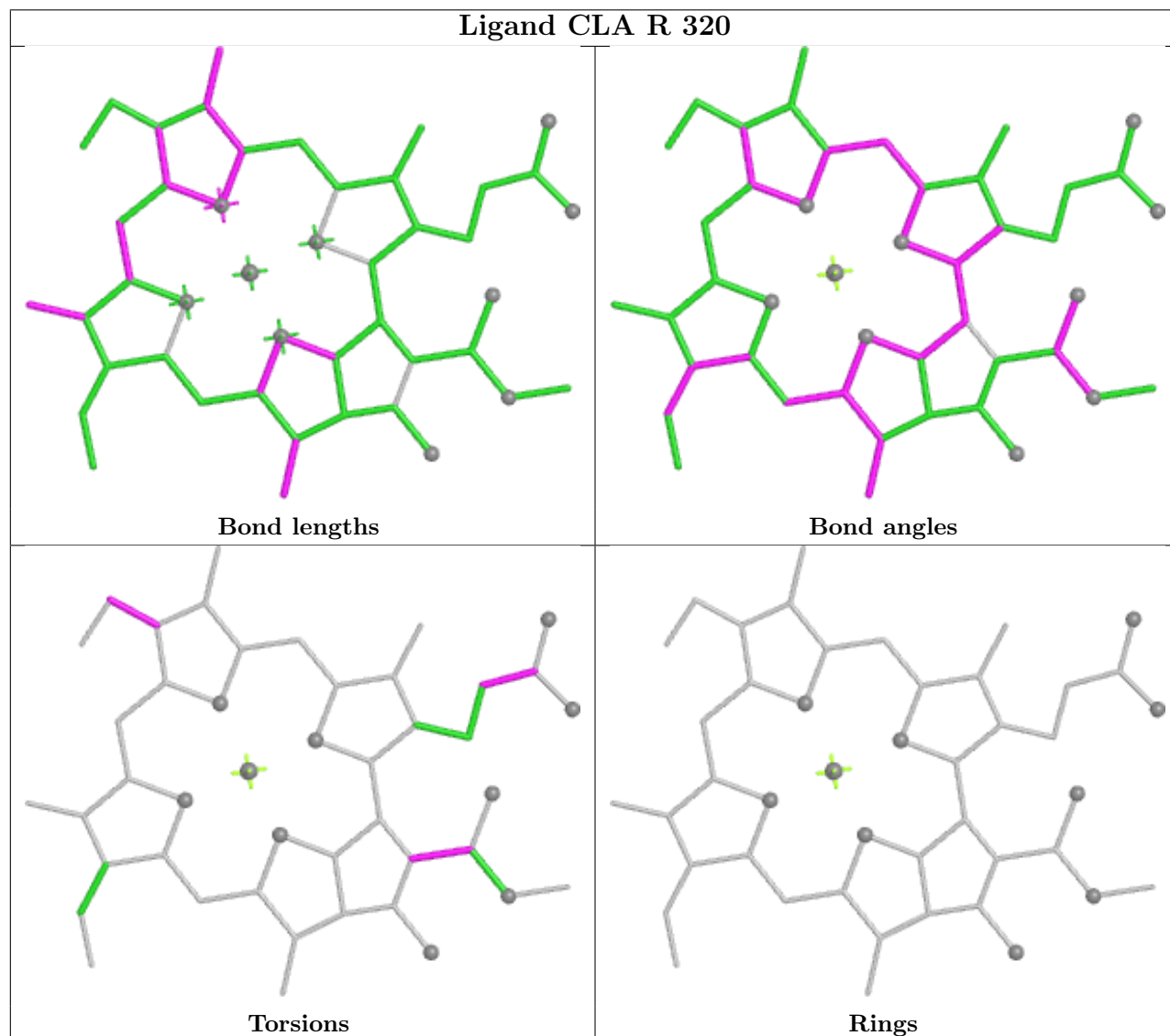
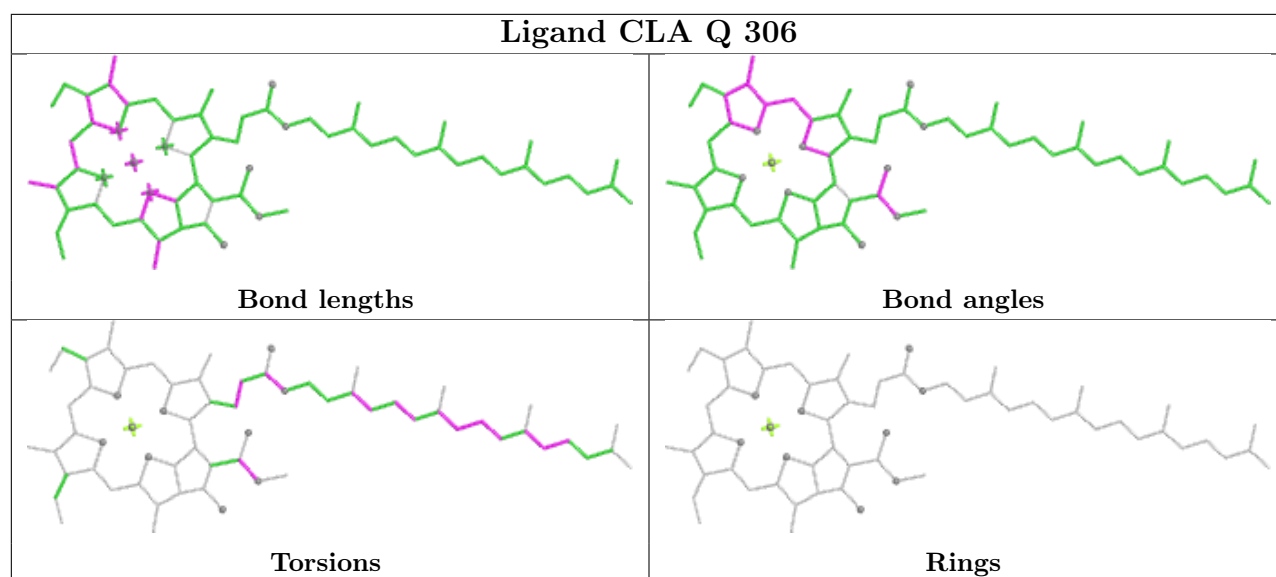
Bond angles



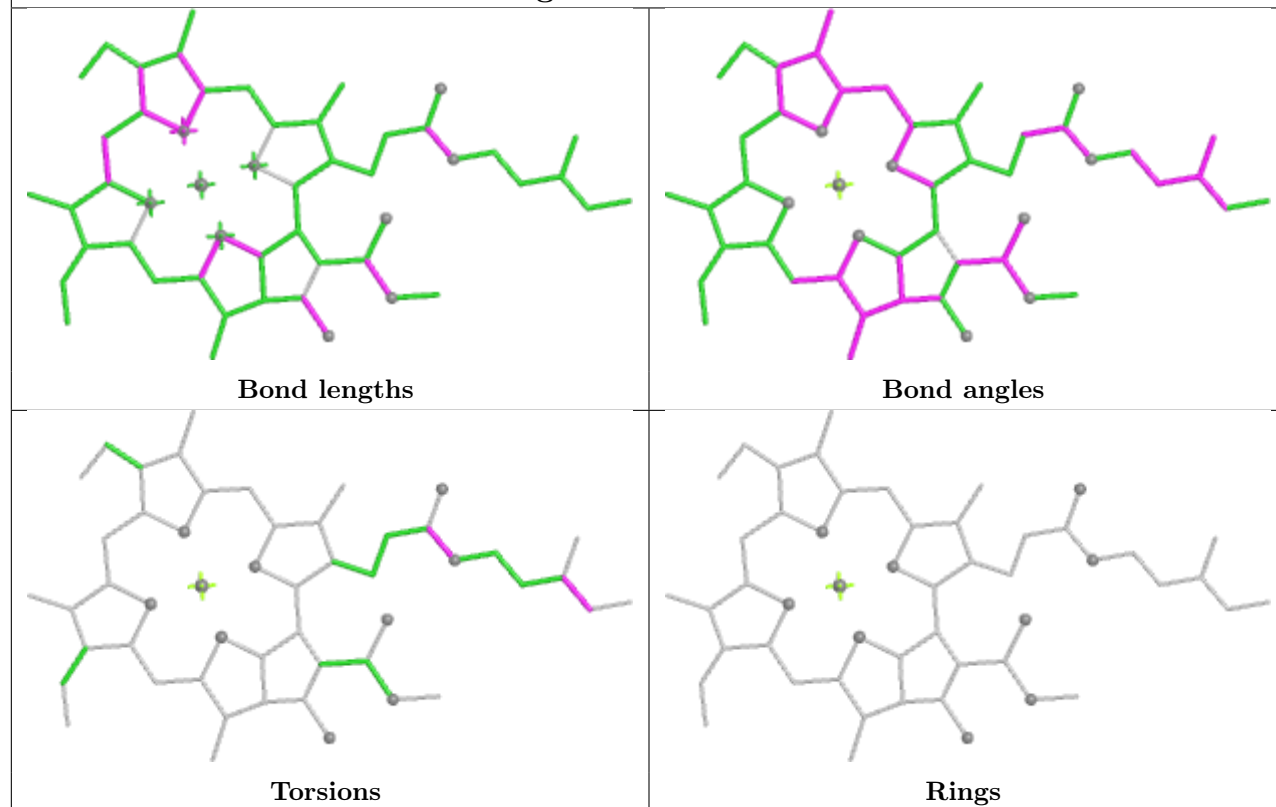
Torsions



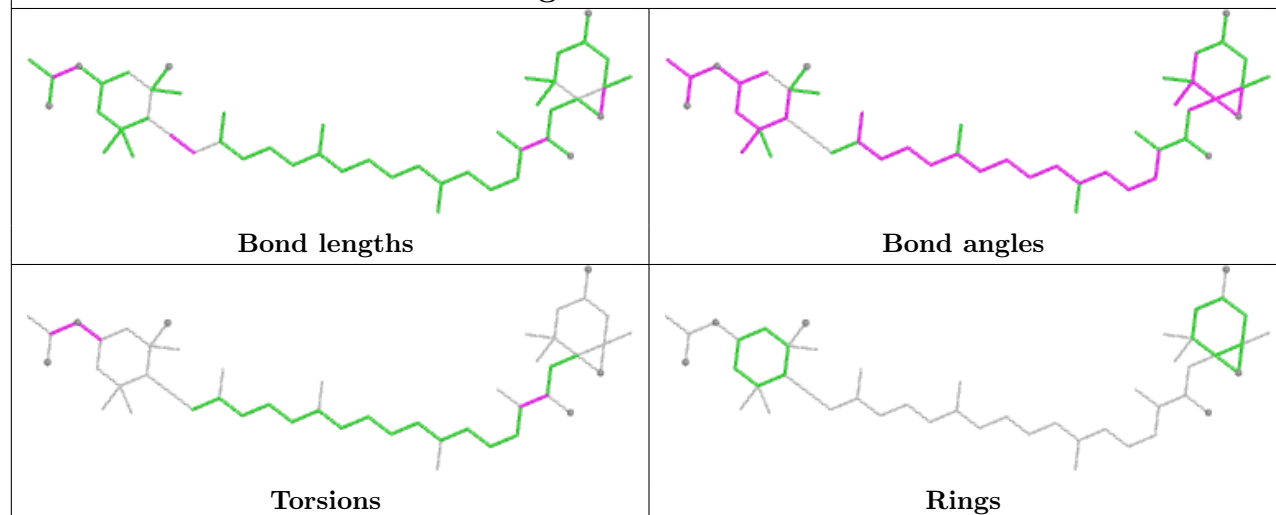
Rings

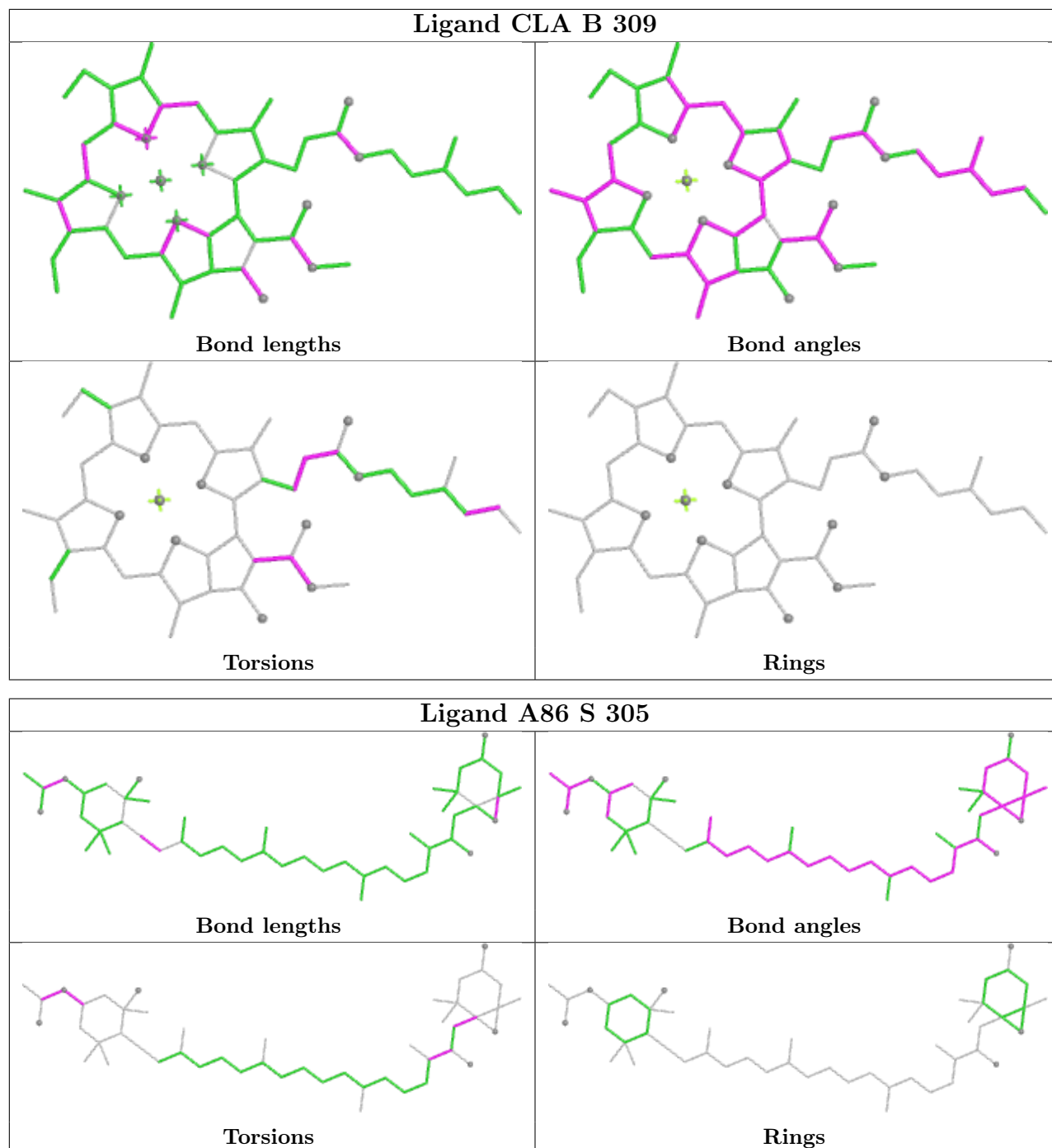


## Ligand CLA a 822

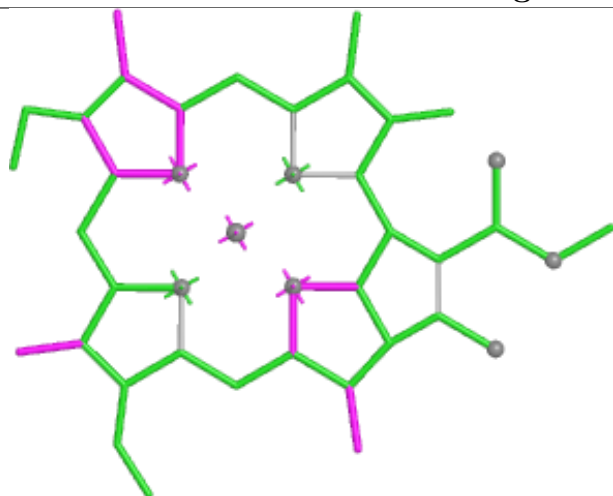


## Ligand A86 T 303

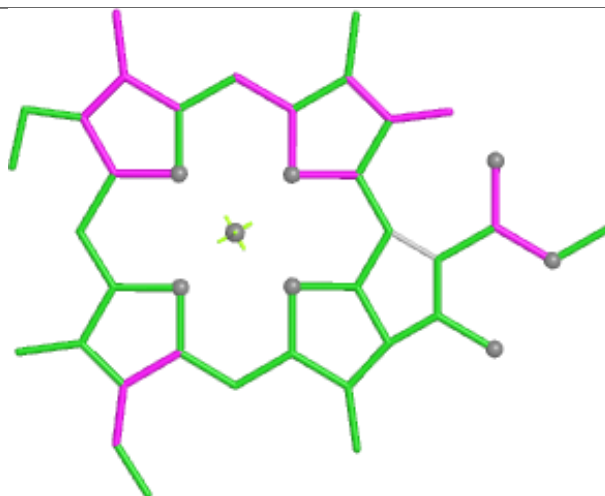




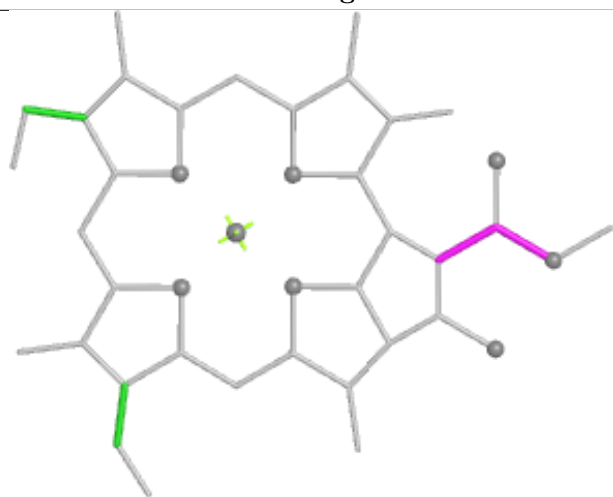
## Ligand CLA H 314



Bond lengths



Bond angles

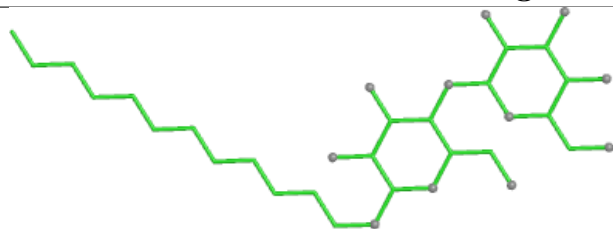


Torsions

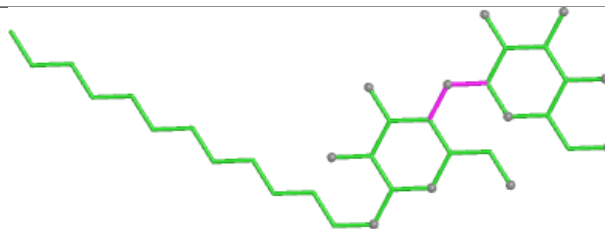


Rings

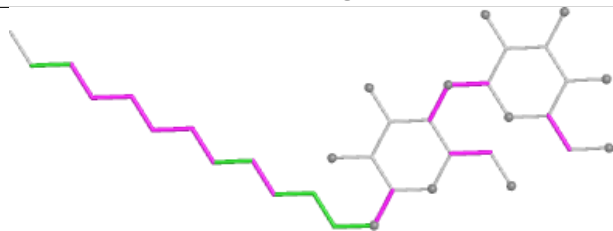
## Ligand LMT a 851



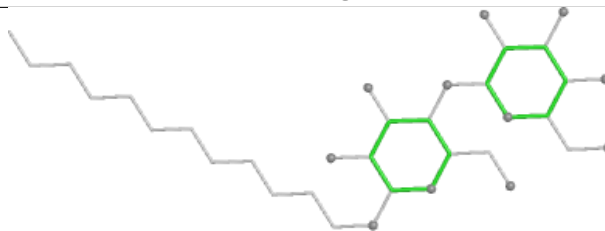
Bond lengths



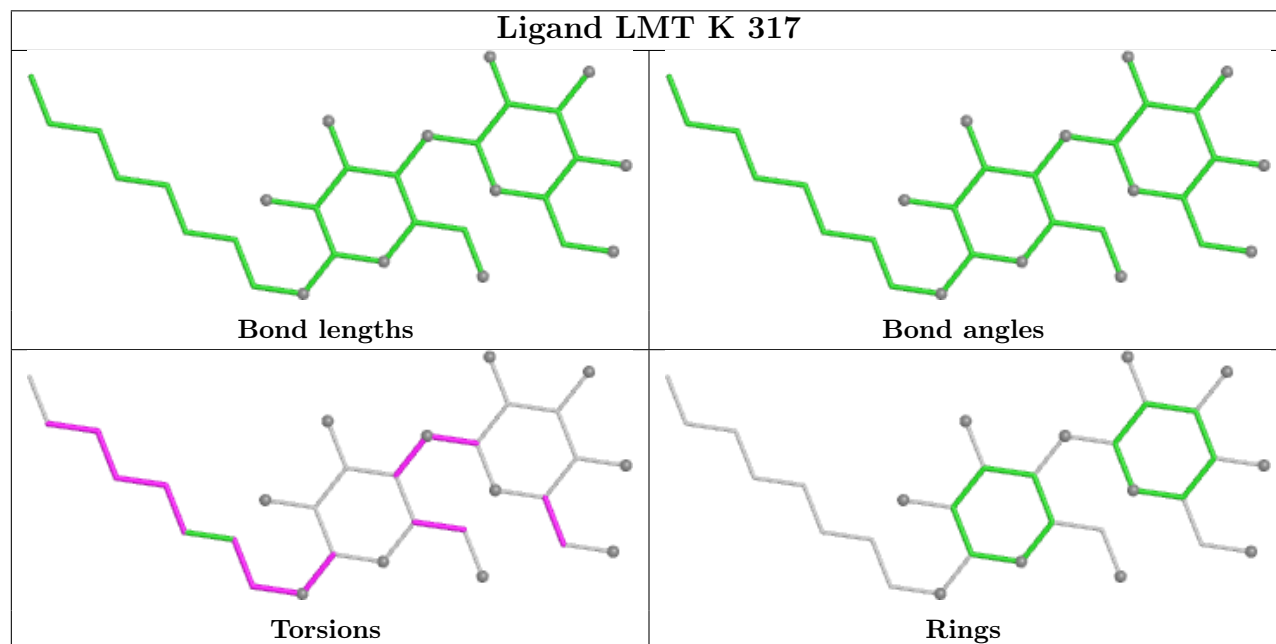
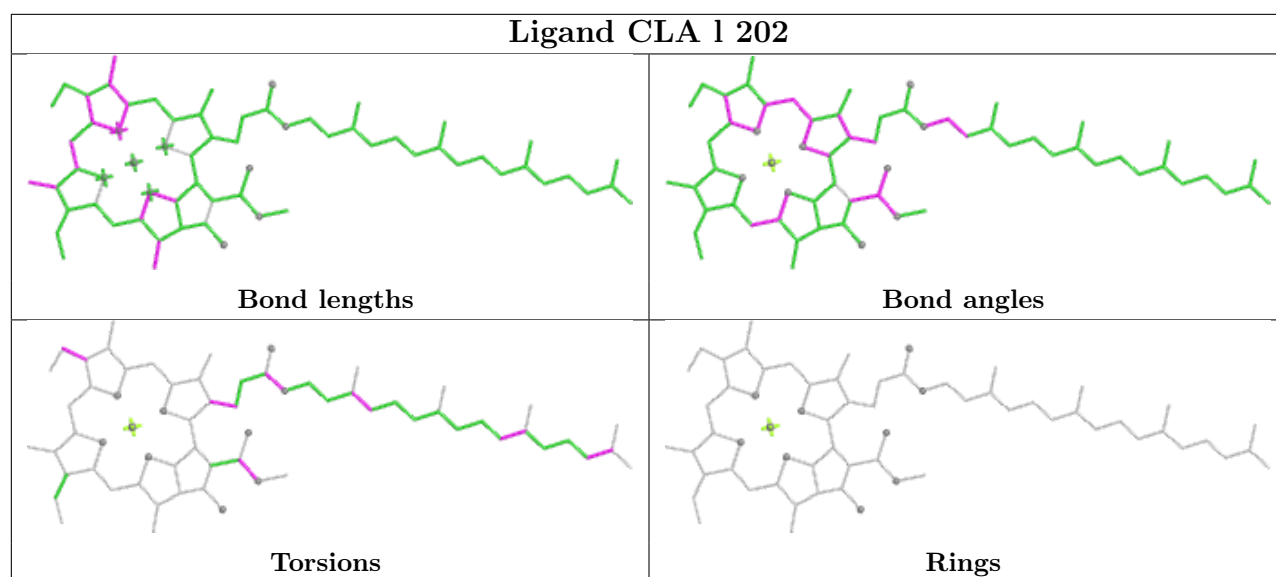
Bond angles

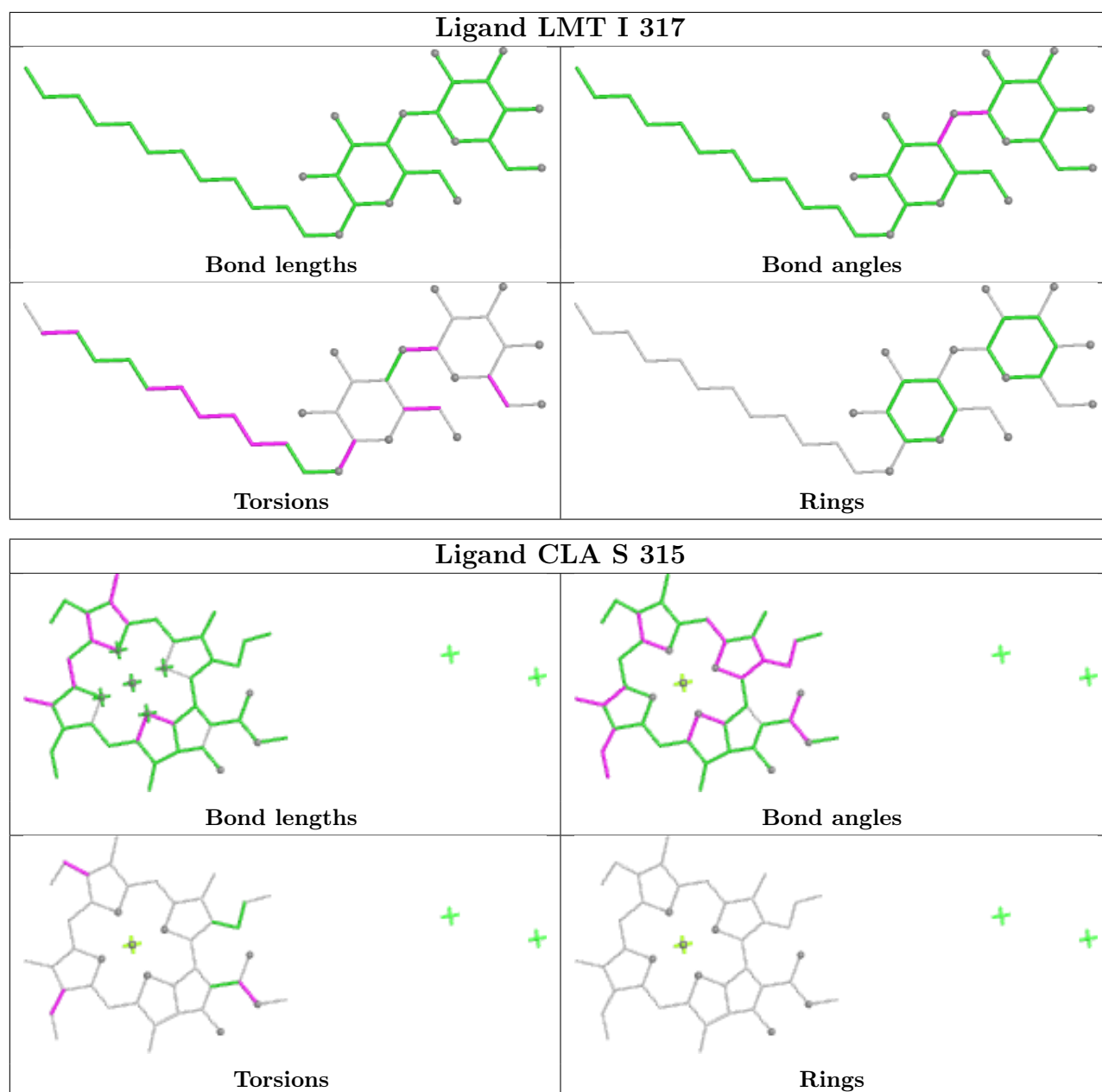


Torsions

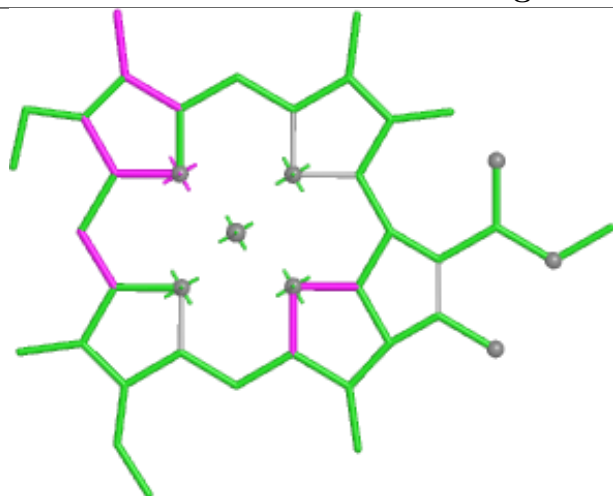


Rings





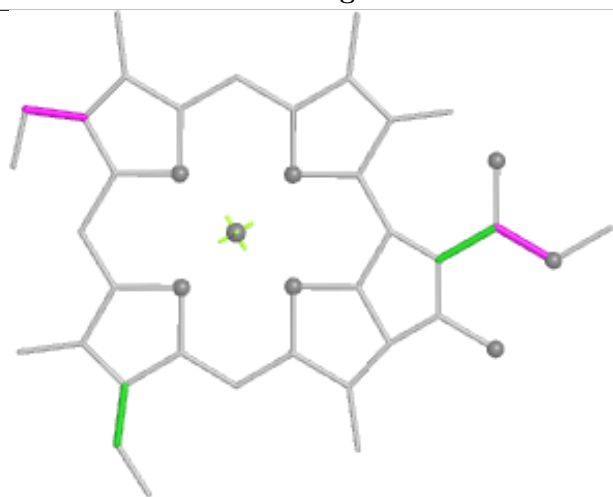
## Ligand CLA X 310



Bond lengths



Bond angles



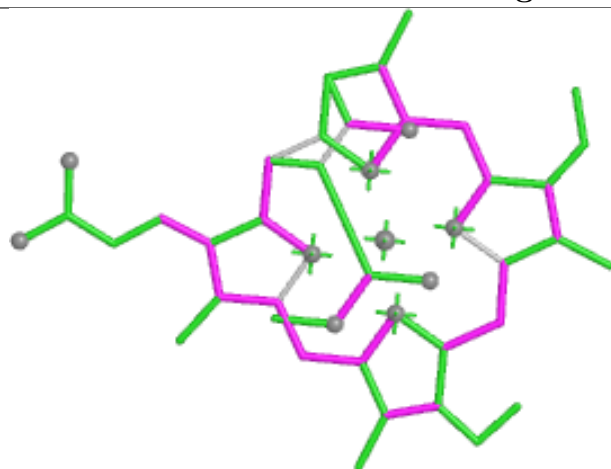
Torsions



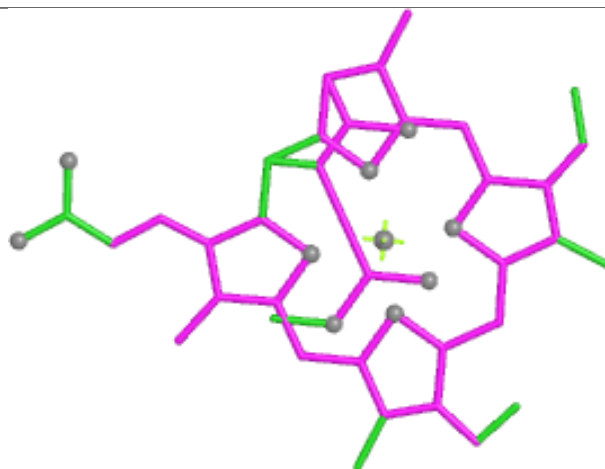
Rings



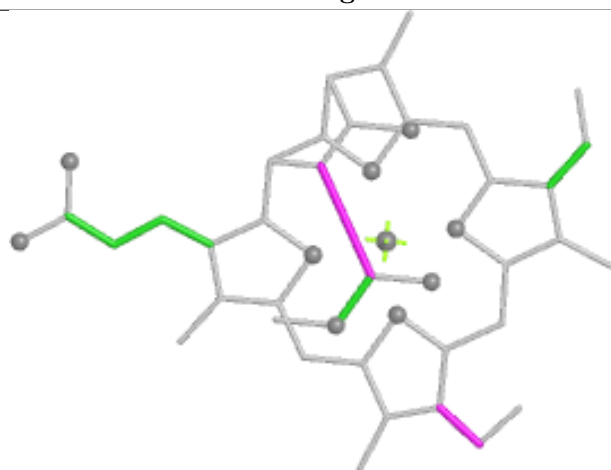
## Ligand KC1 O 315



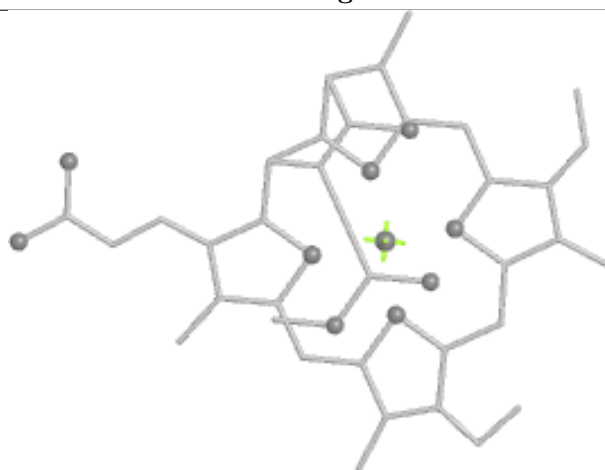
Bond lengths



Bond angles

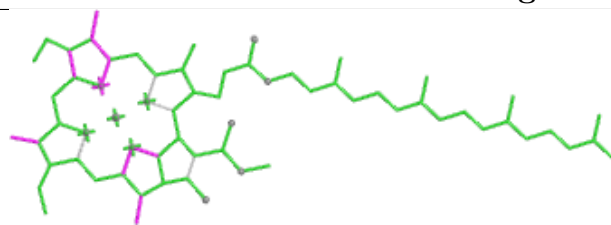


Torsions

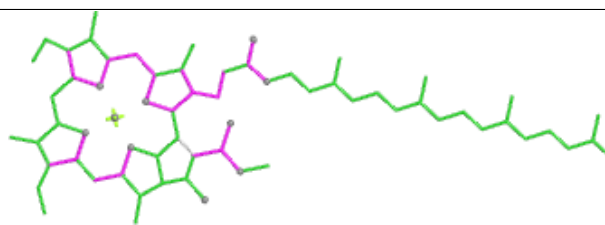


Rings

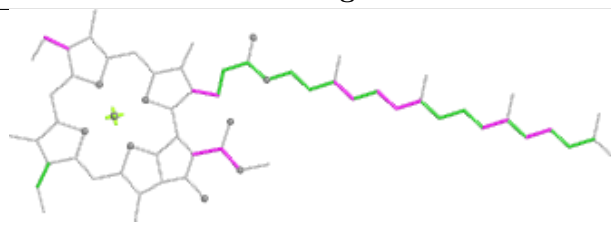
## Ligand CLA a 832



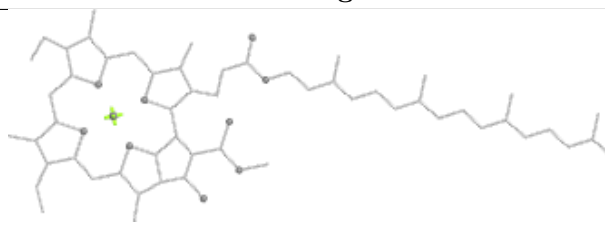
Bond lengths



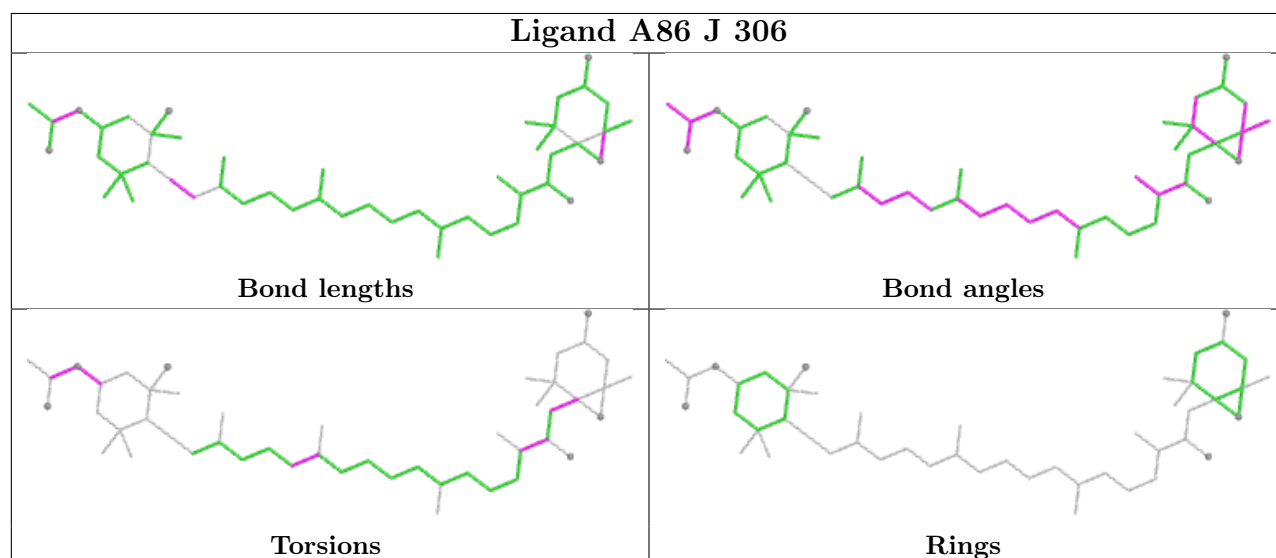
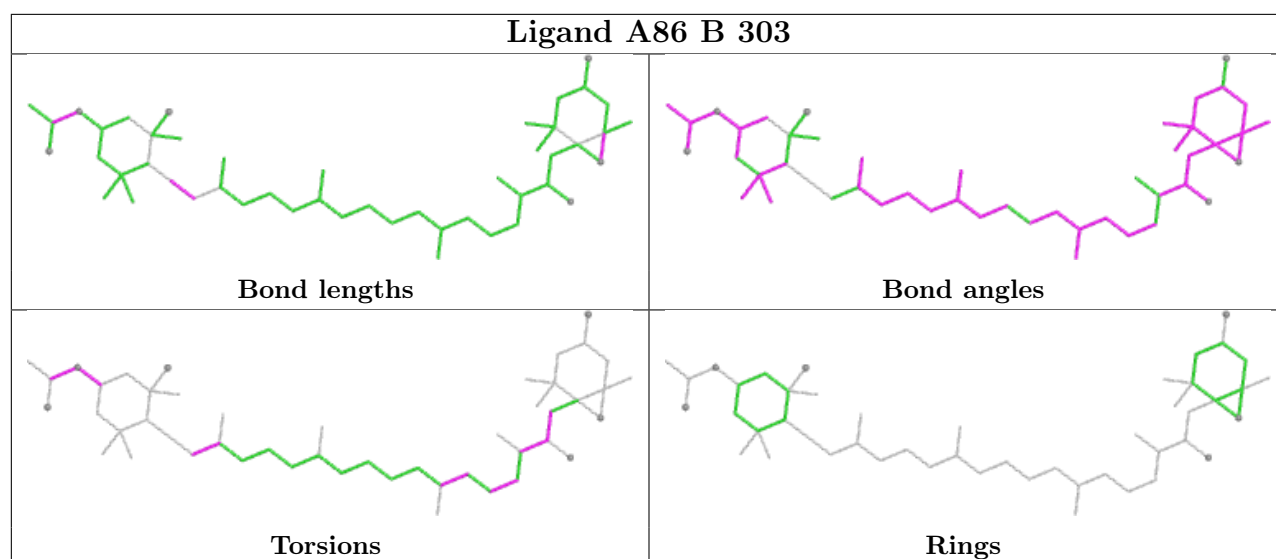
Bond angles

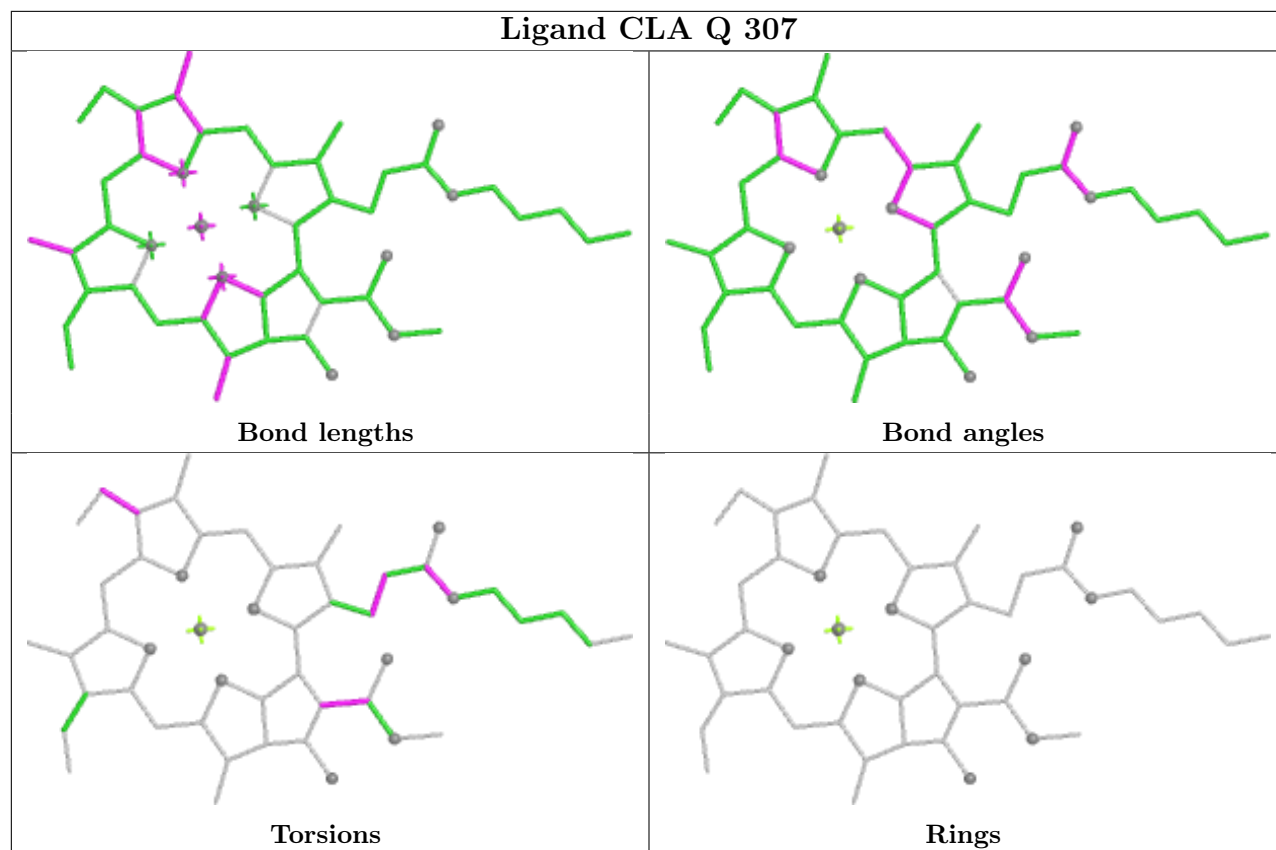


Torsions

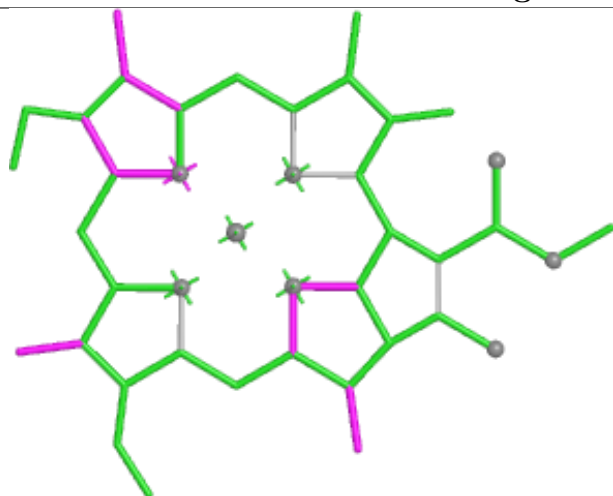


Rings

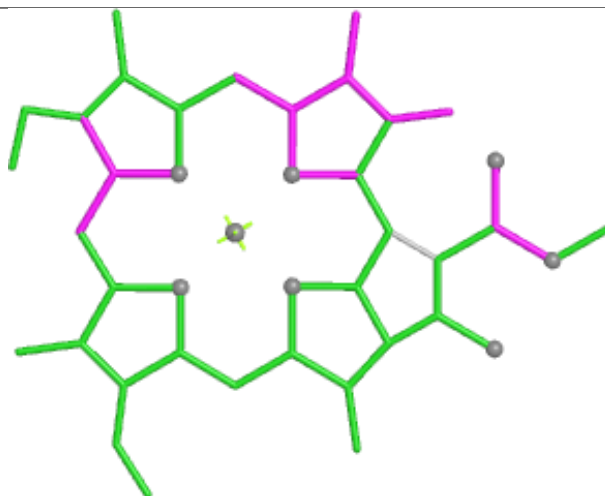




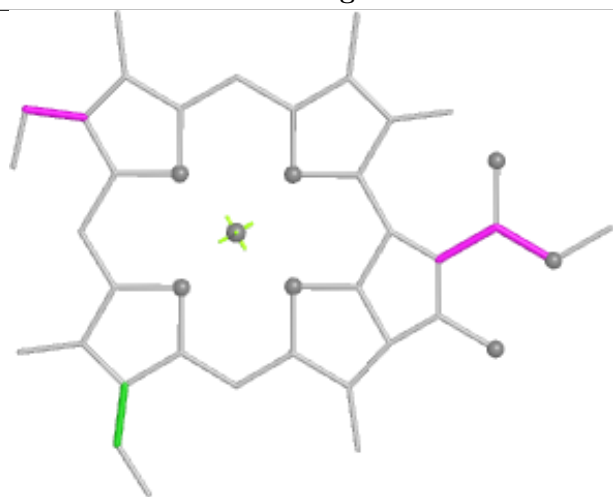
## Ligand CLA O 314



Bond lengths



Bond angles

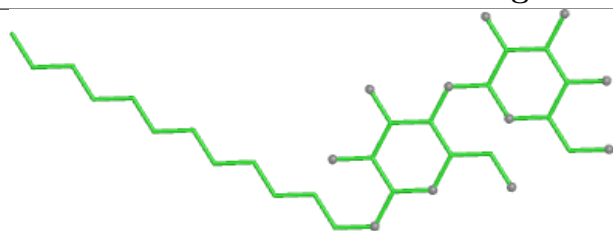


Torsions

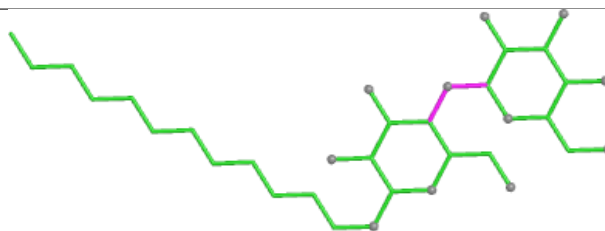


Rings

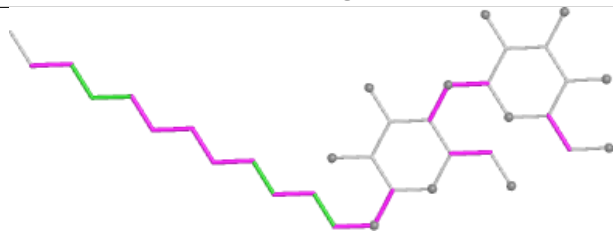
## Ligand LMT B 313



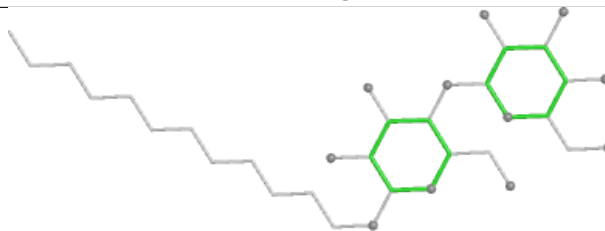
Bond lengths



Bond angles

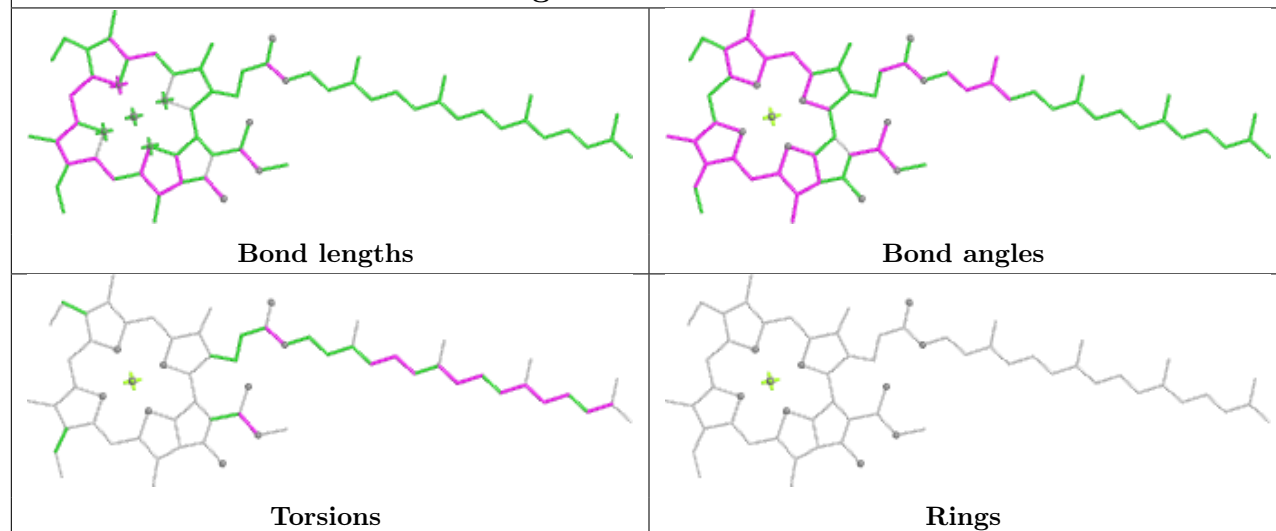


Torsions

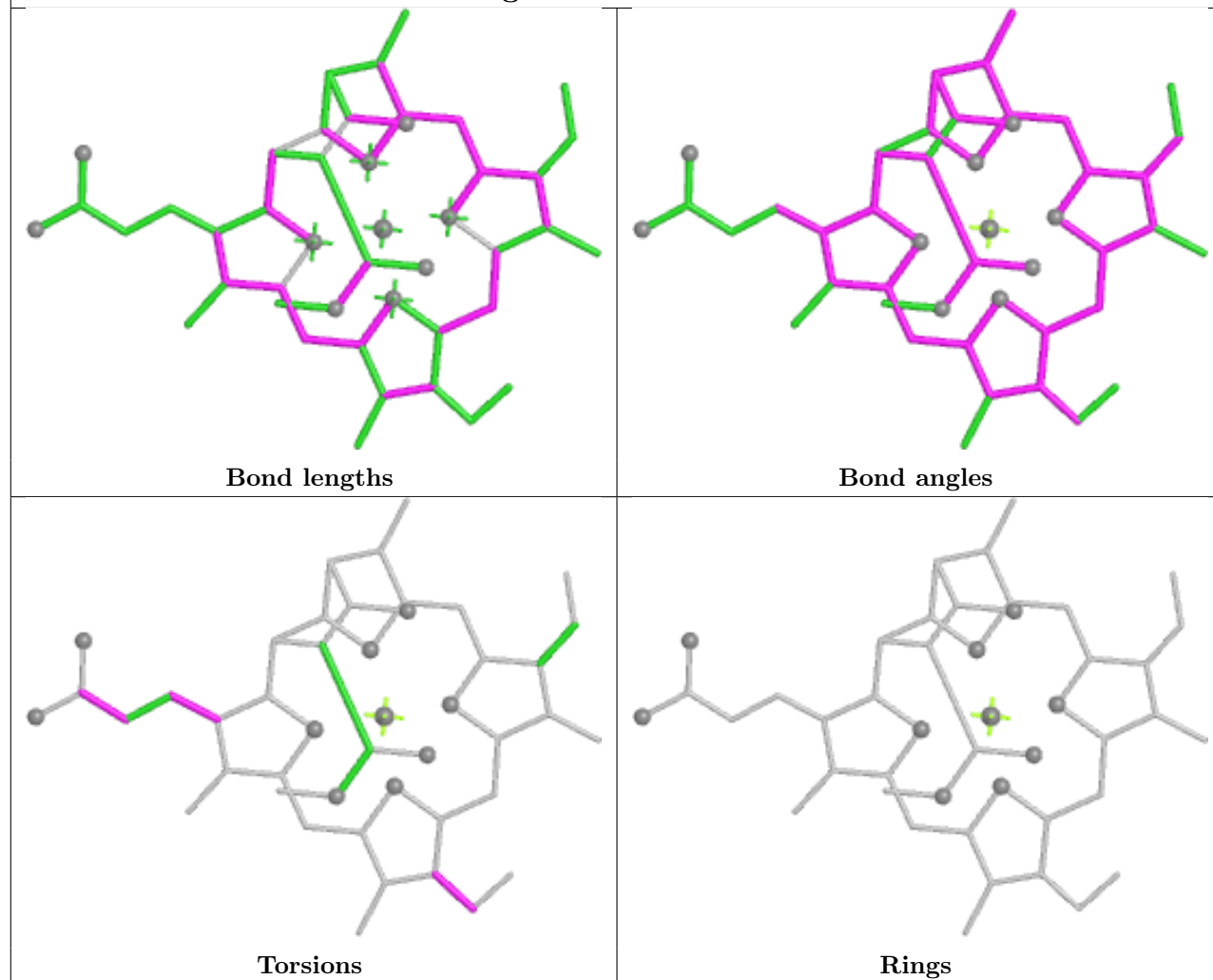


Rings

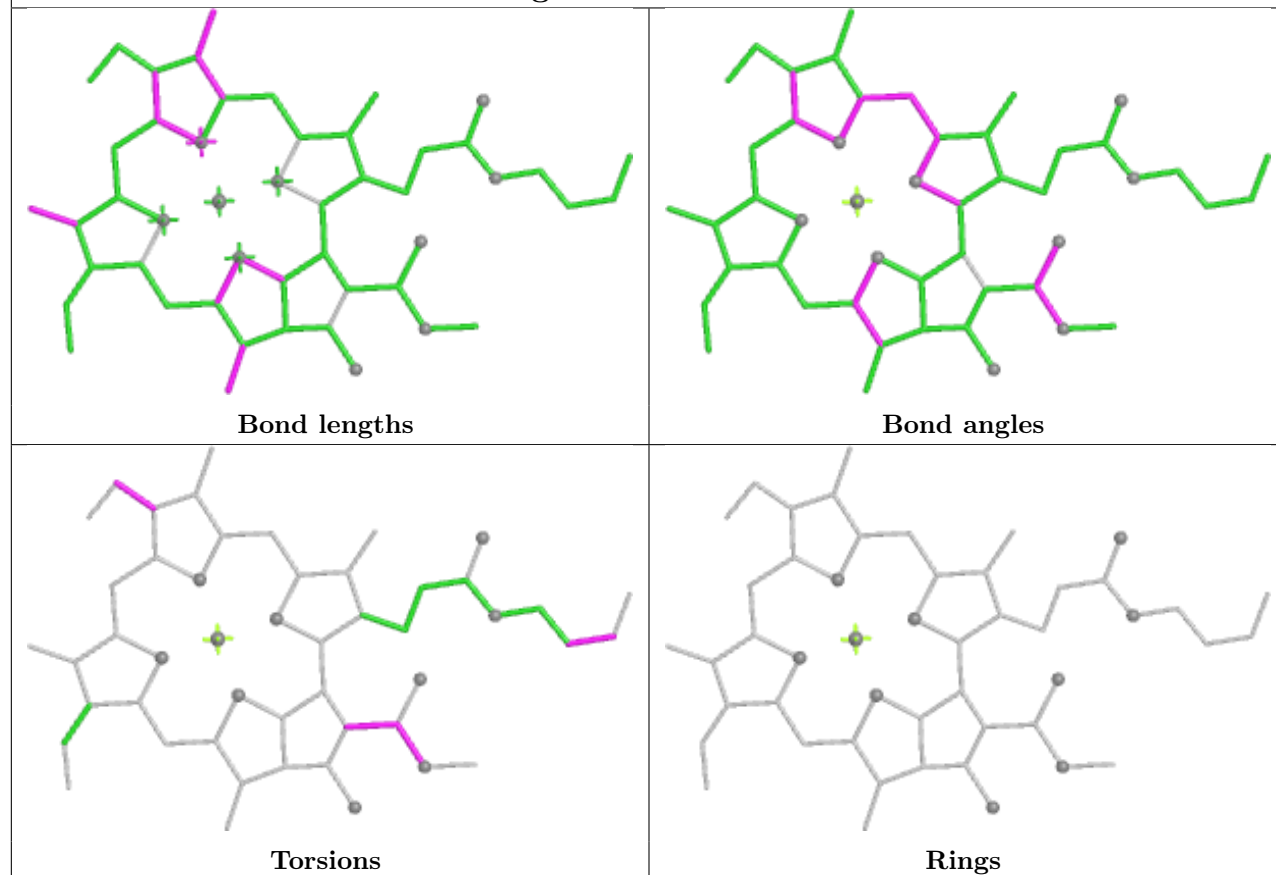
## Ligand CLA C 207



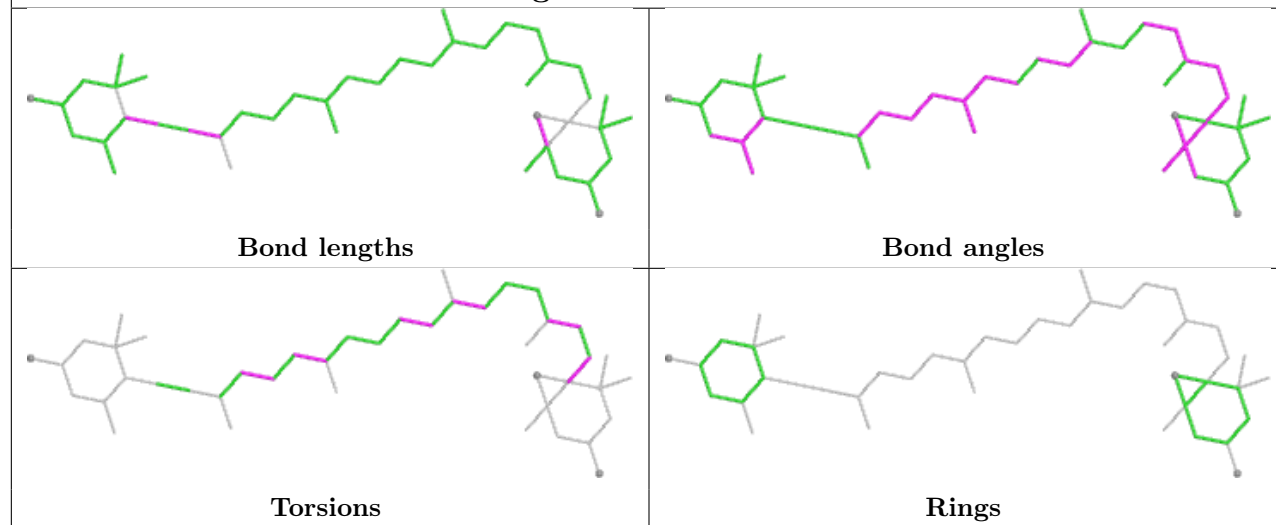
## Ligand KC1 W 213

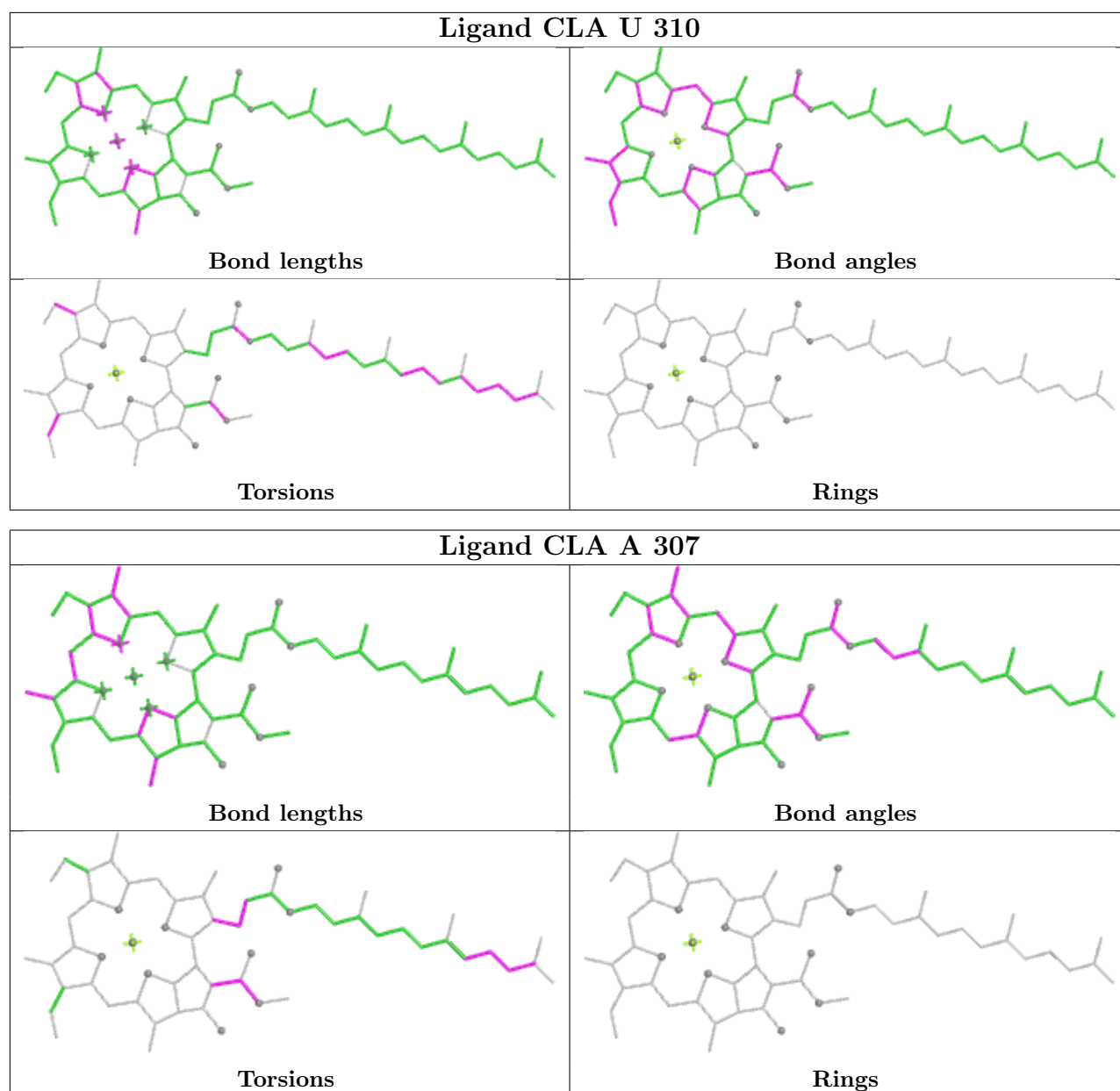


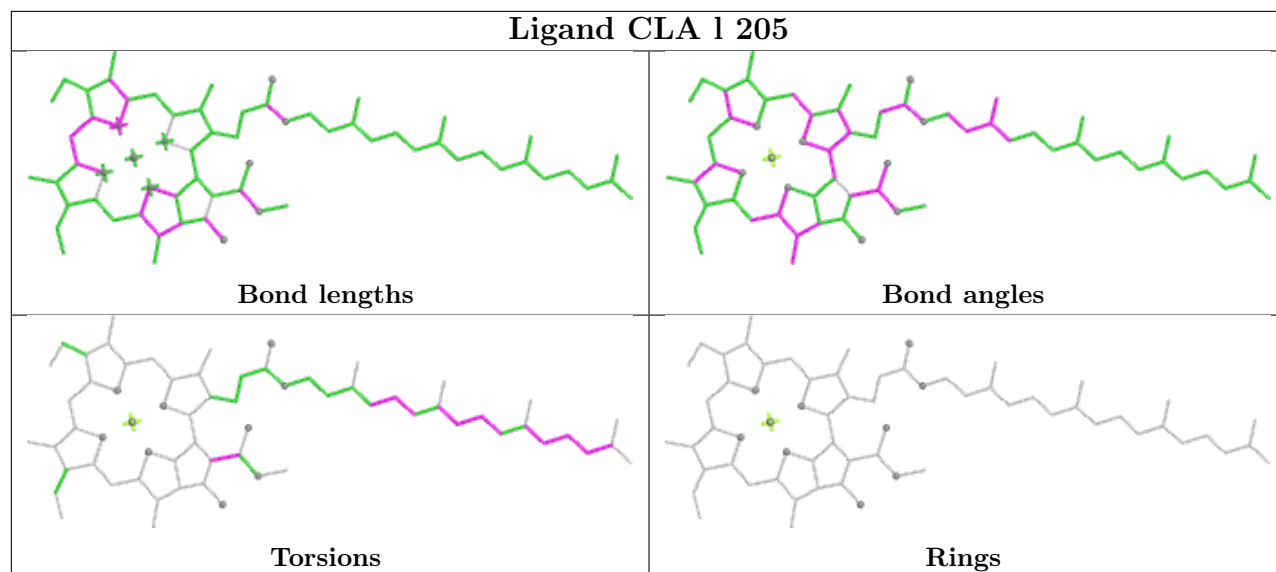
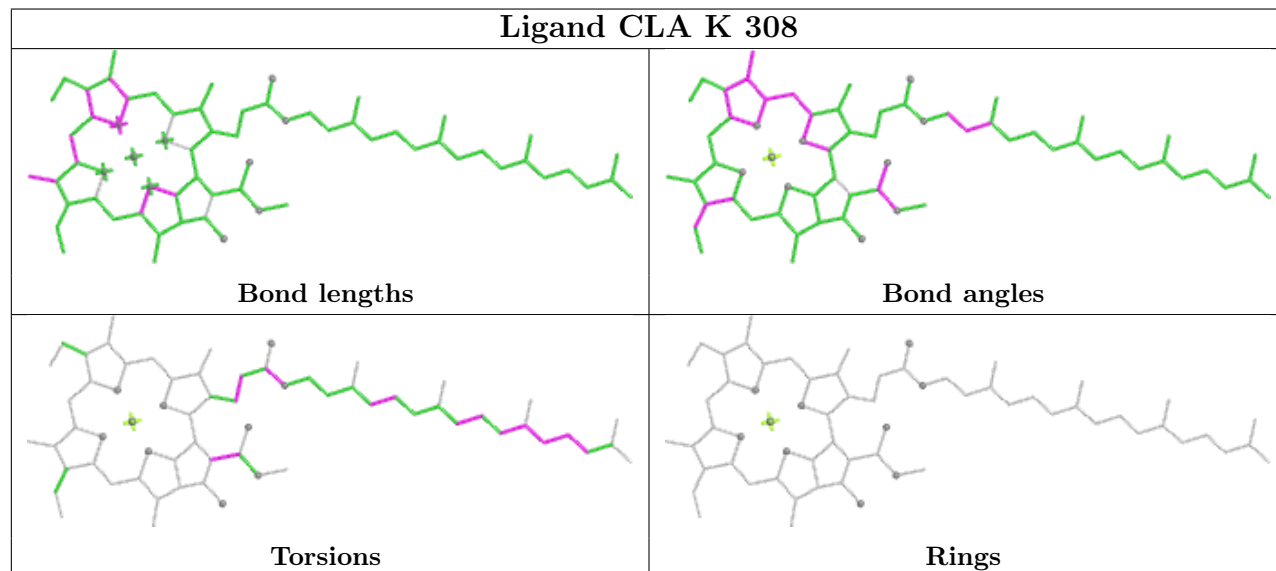
## Ligand CLA A 305



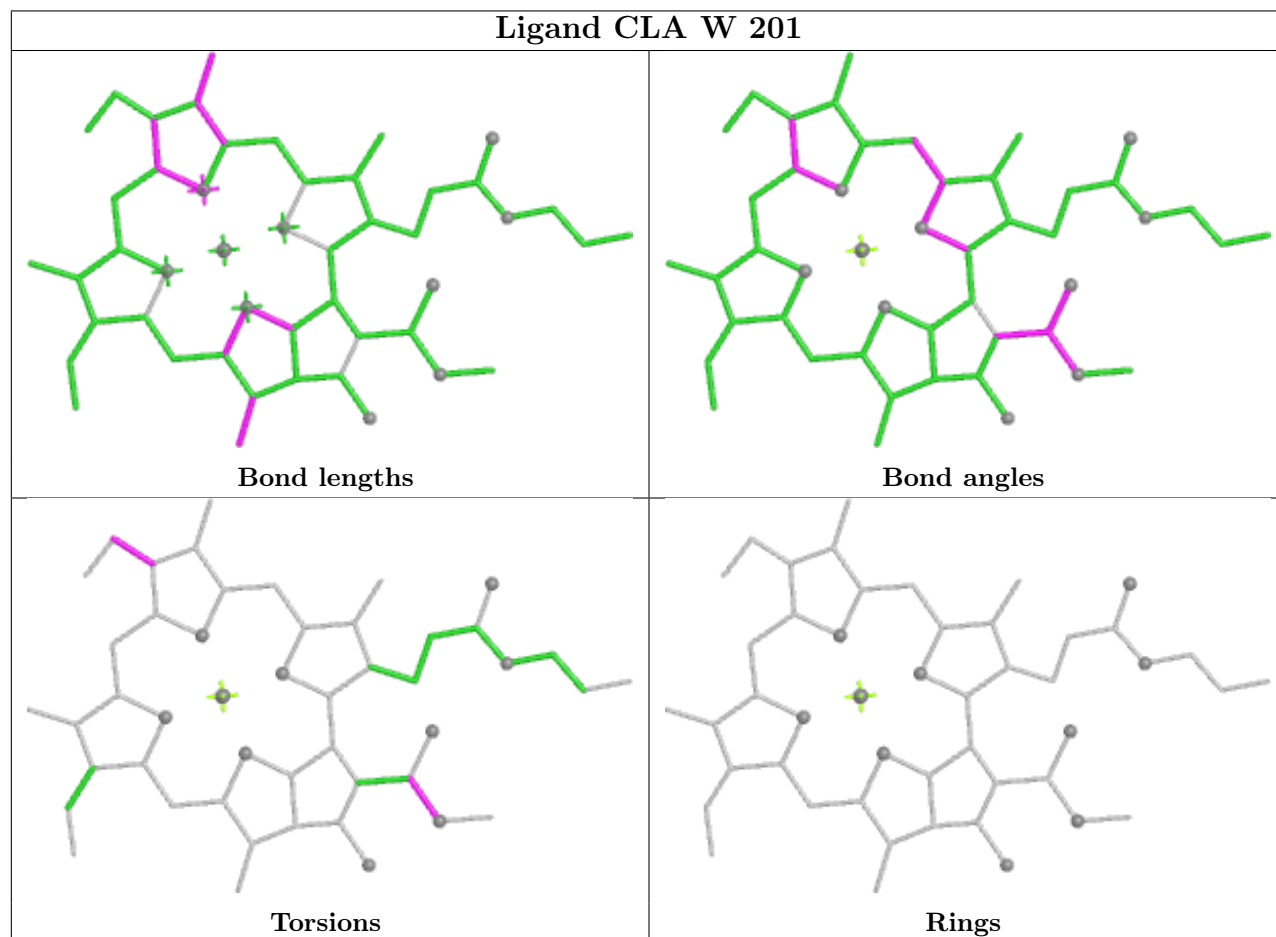
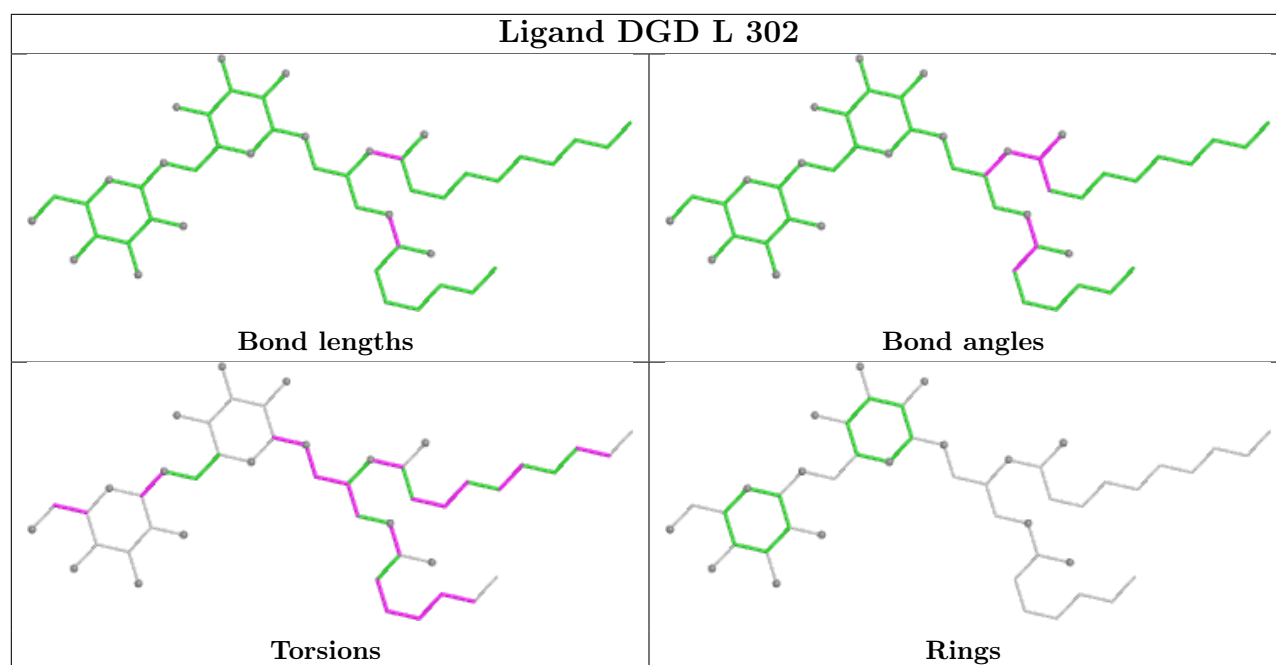
## Ligand DD6 D 301

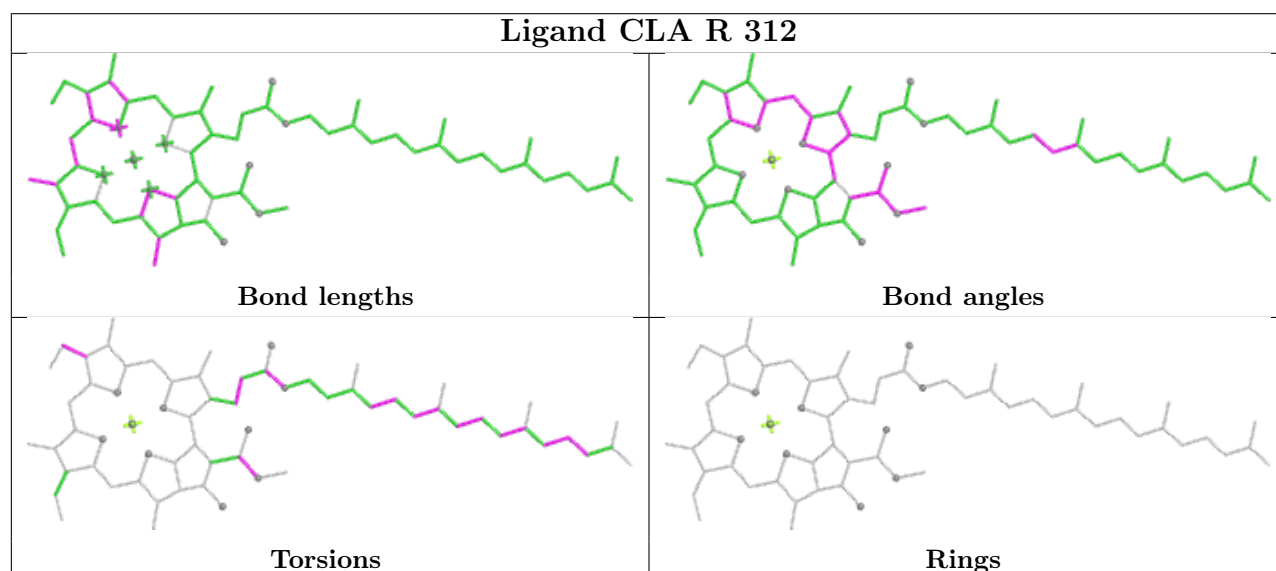
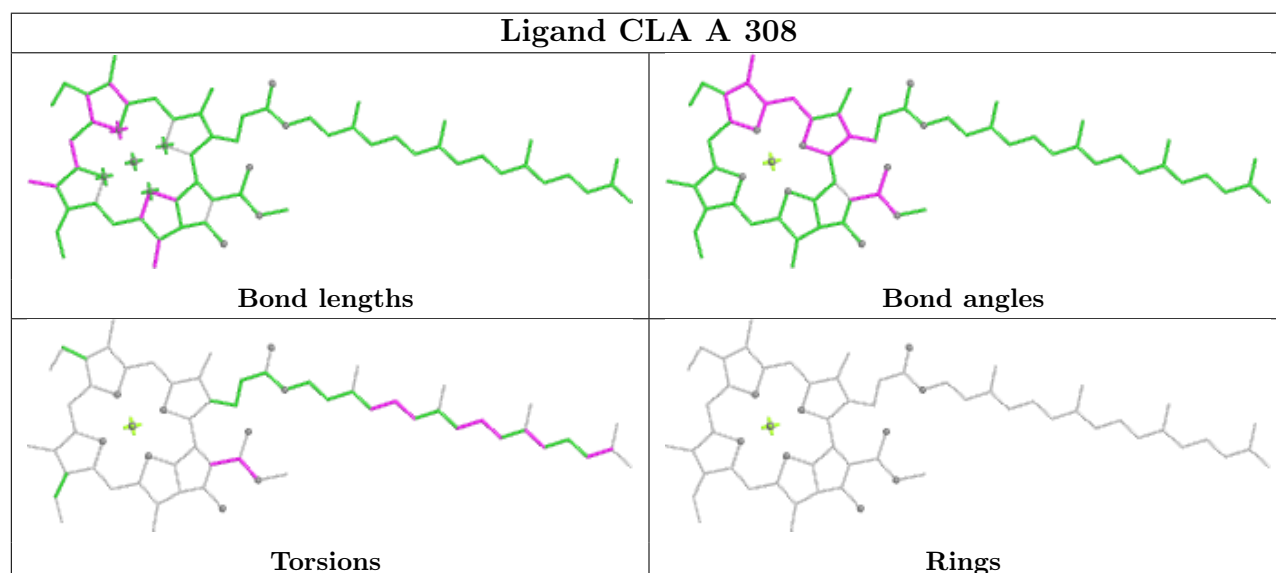
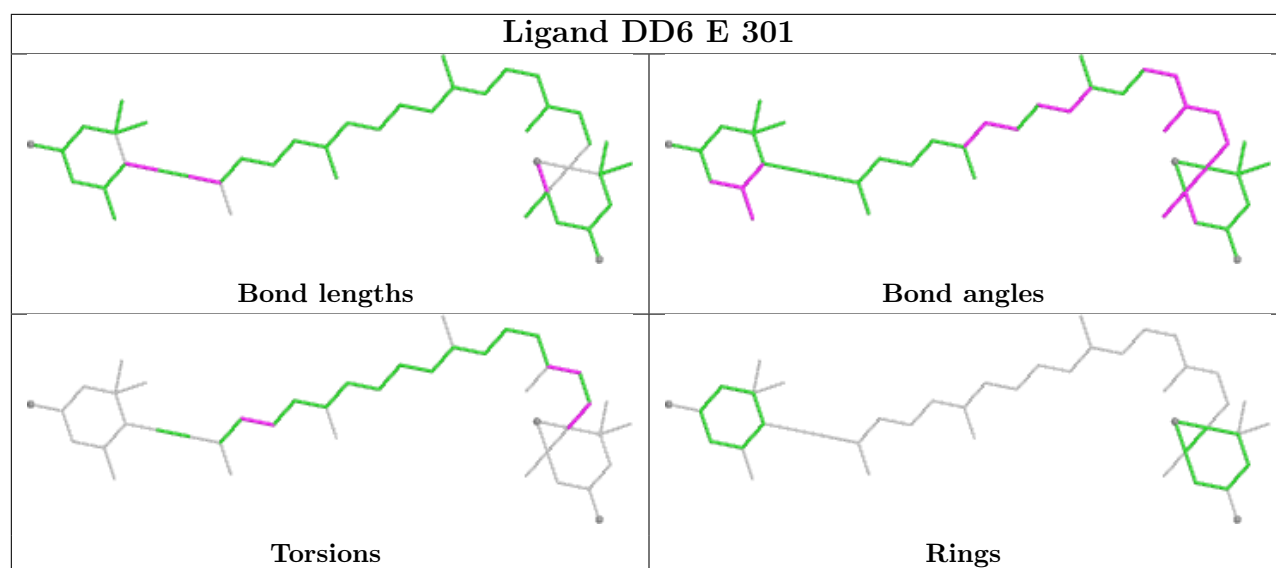


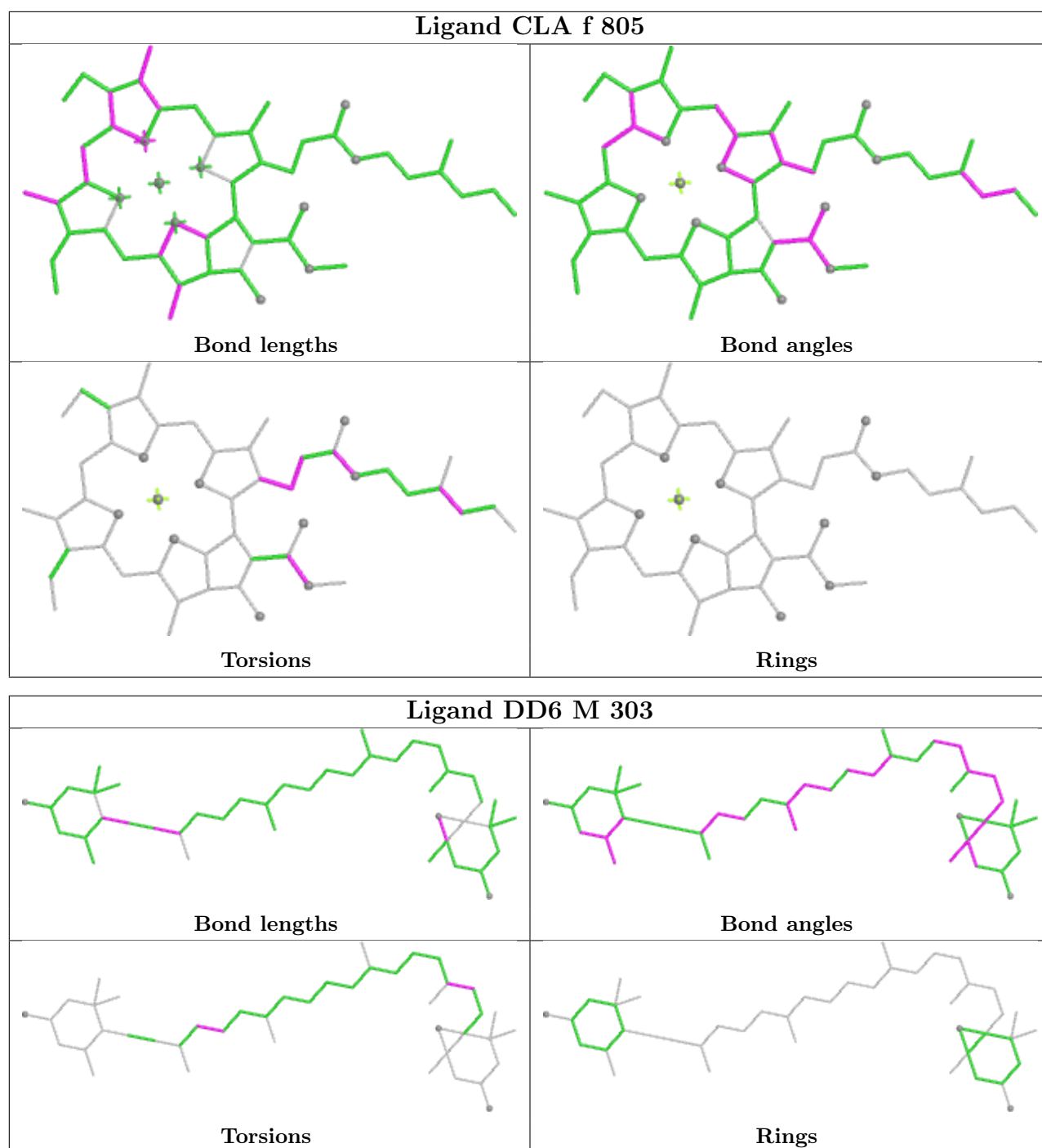


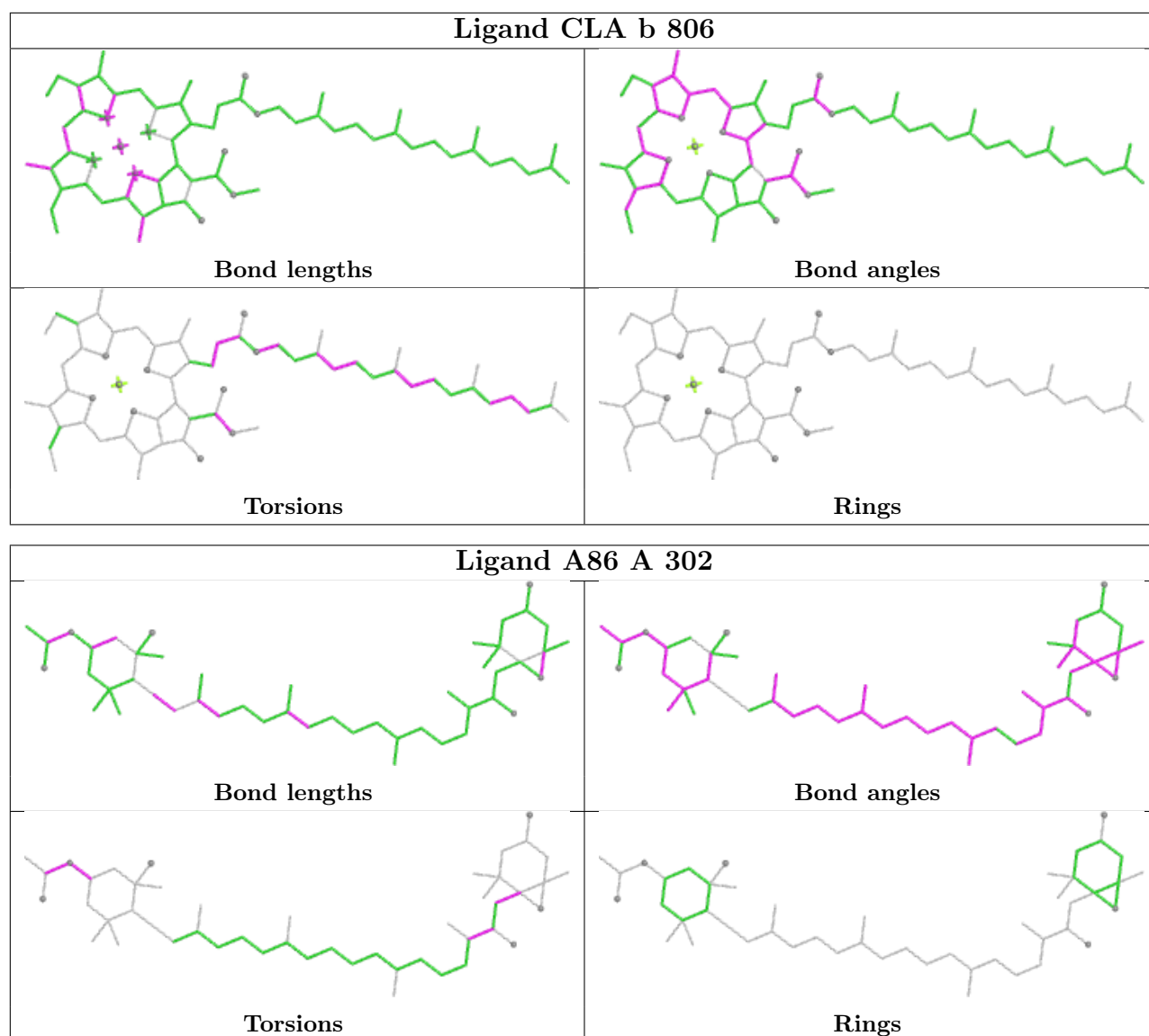
**Ligand CLA I 205****Ligand CLA K 308**

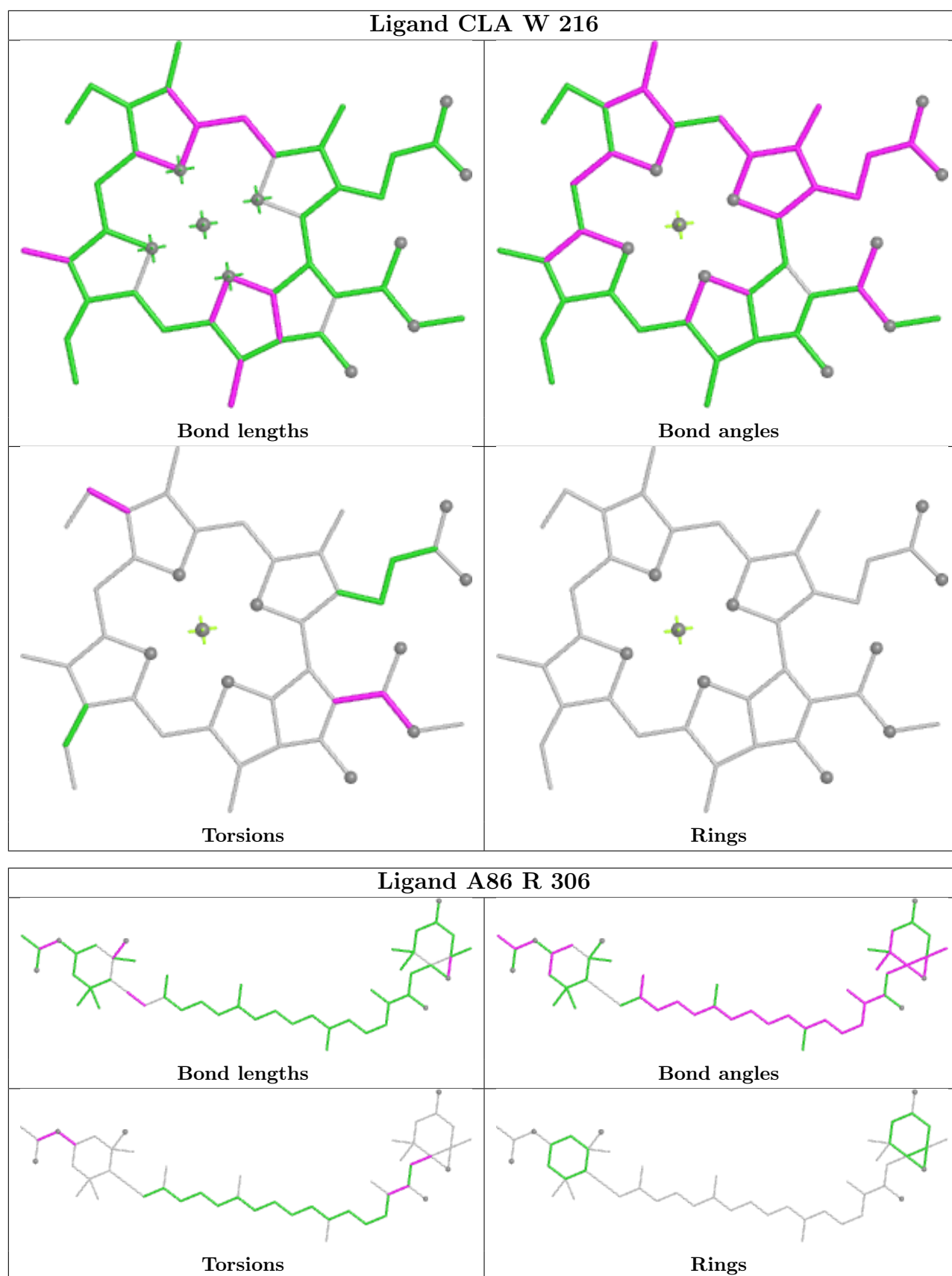












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

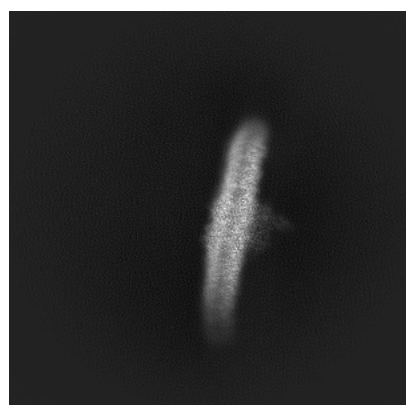
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30012. These allow visual inspection of the internal detail of the map and identification of artifacts.

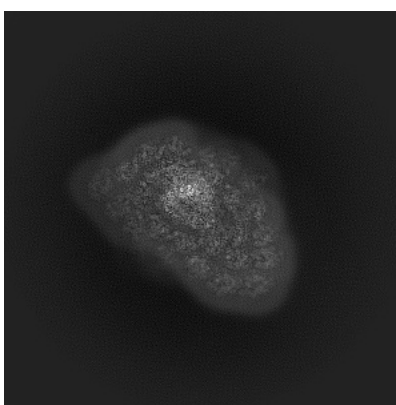
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

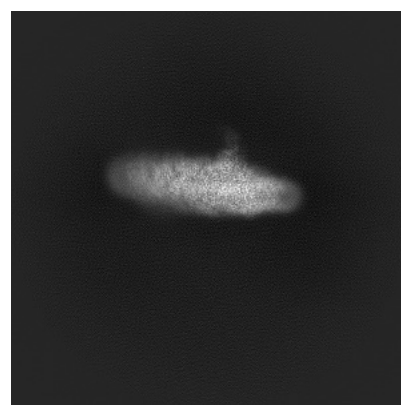
#### 6.1.1 Primary map



X



Y

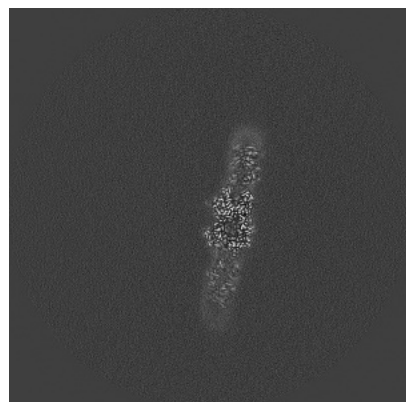


Z

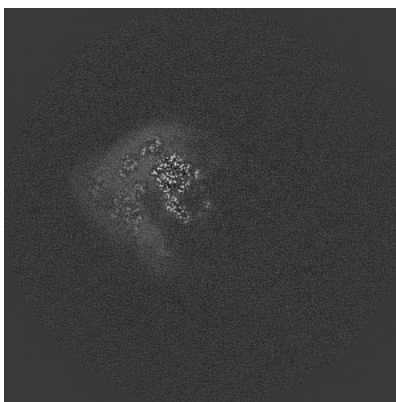
The images above show the map projected in three orthogonal directions.

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

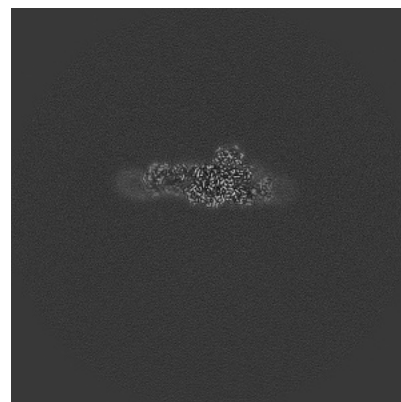
#### 6.2.1 Primary map



X Index: 260



Y Index: 260



Z Index: 260

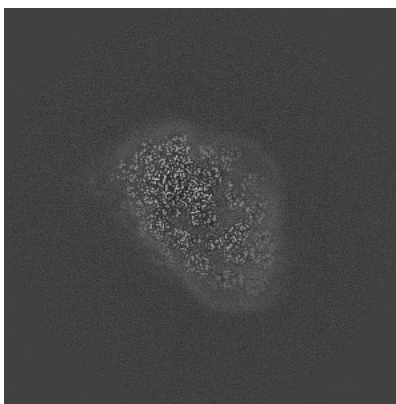
The images above show central slices of the map in three orthogonal directions.

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

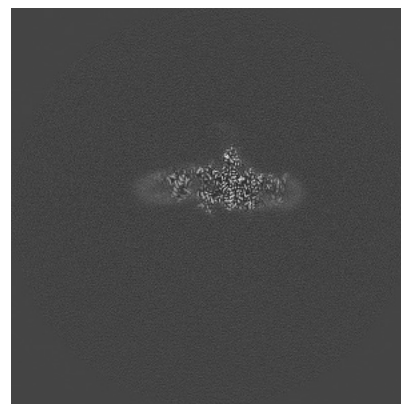
### 6.3.1 Primary map



X Index: 278



Y Index: 294

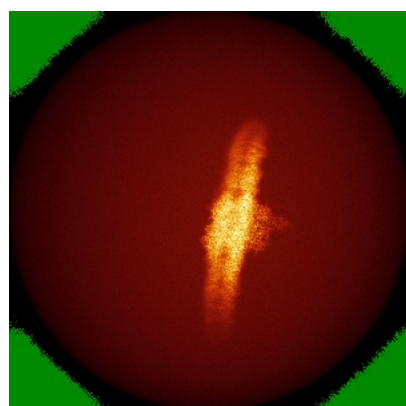


Z Index: 231

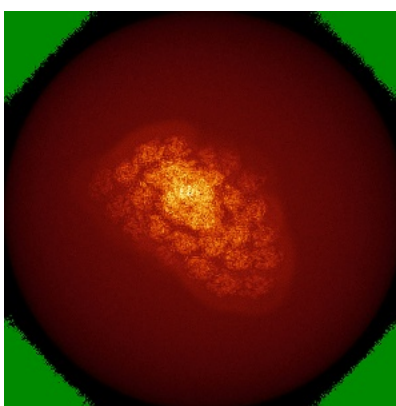
The images above show the largest variance slices of the map in three orthogonal directions.

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

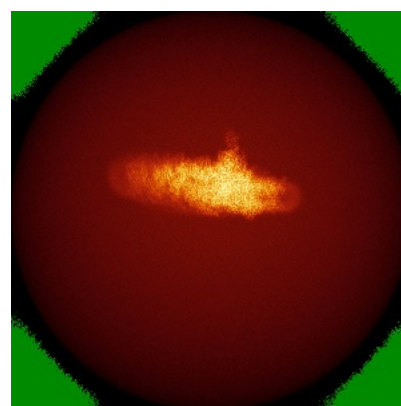
### 6.4.1 Primary map



X



Y



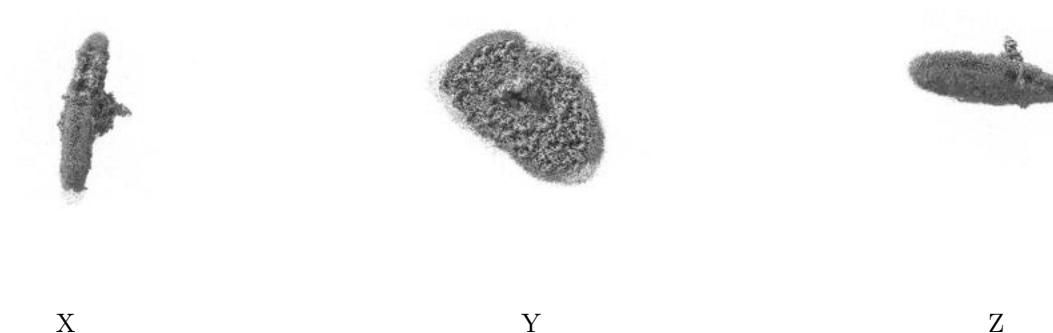
Z

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

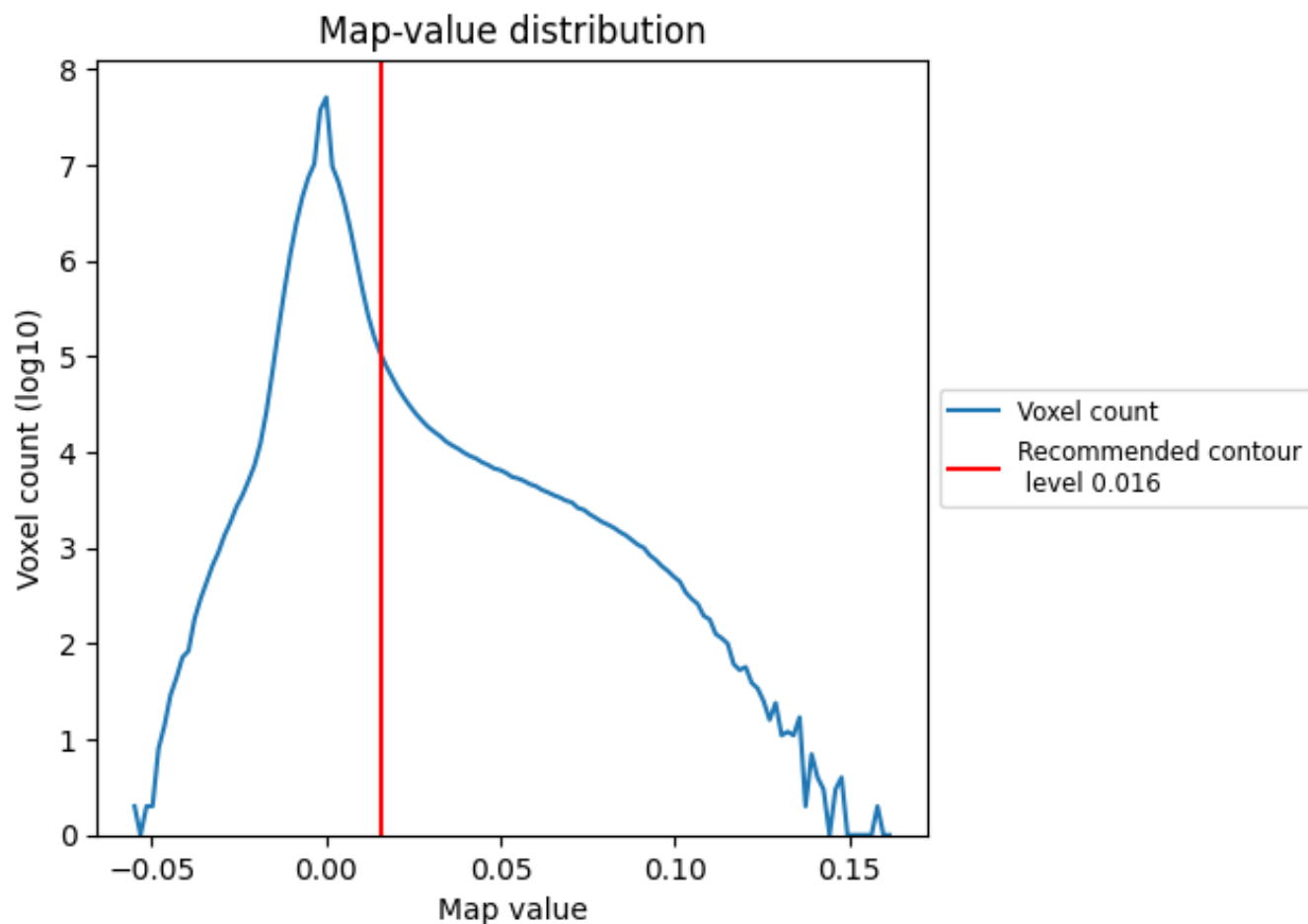
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

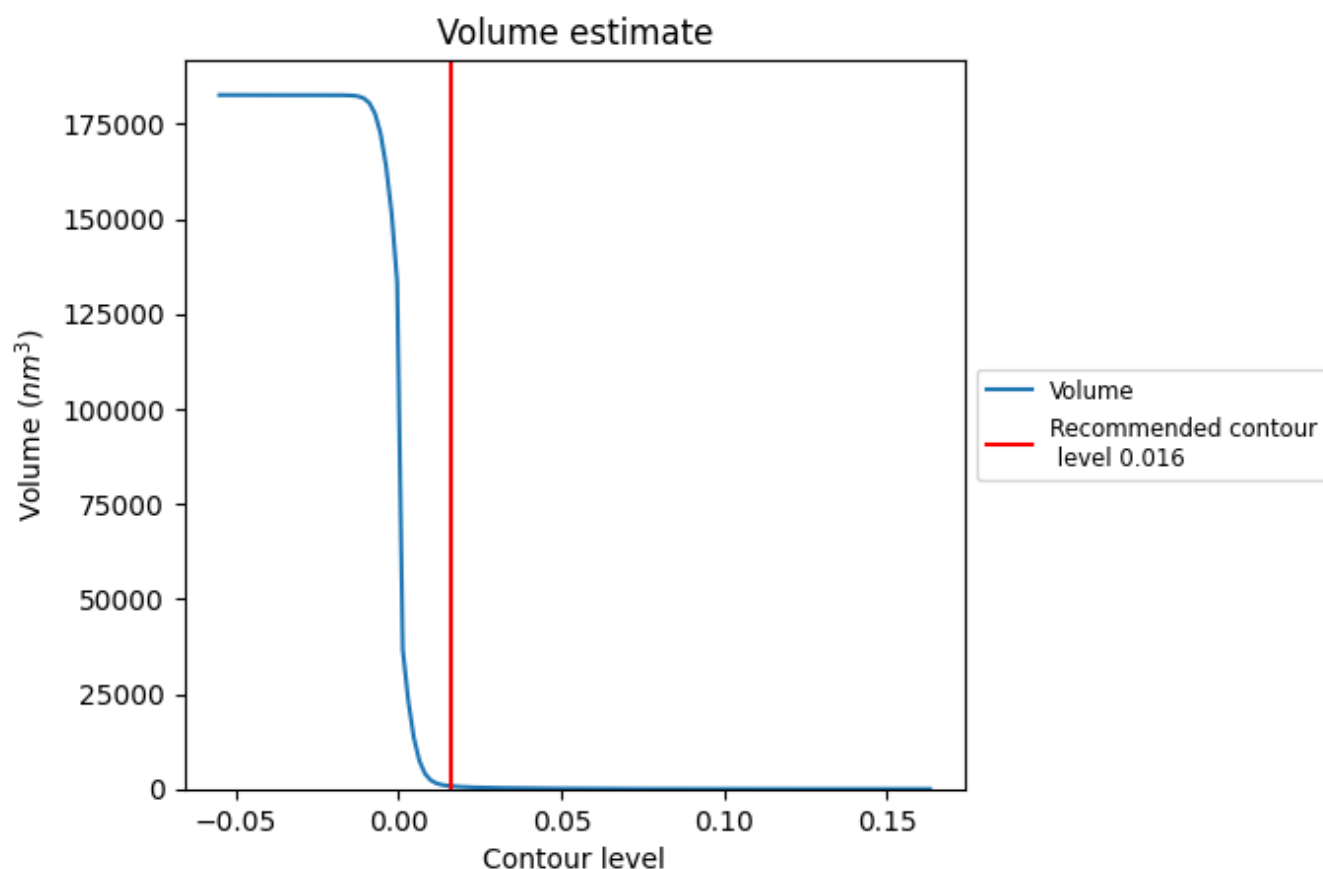
This section contains the results of statistical analysis of the map.

### 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.

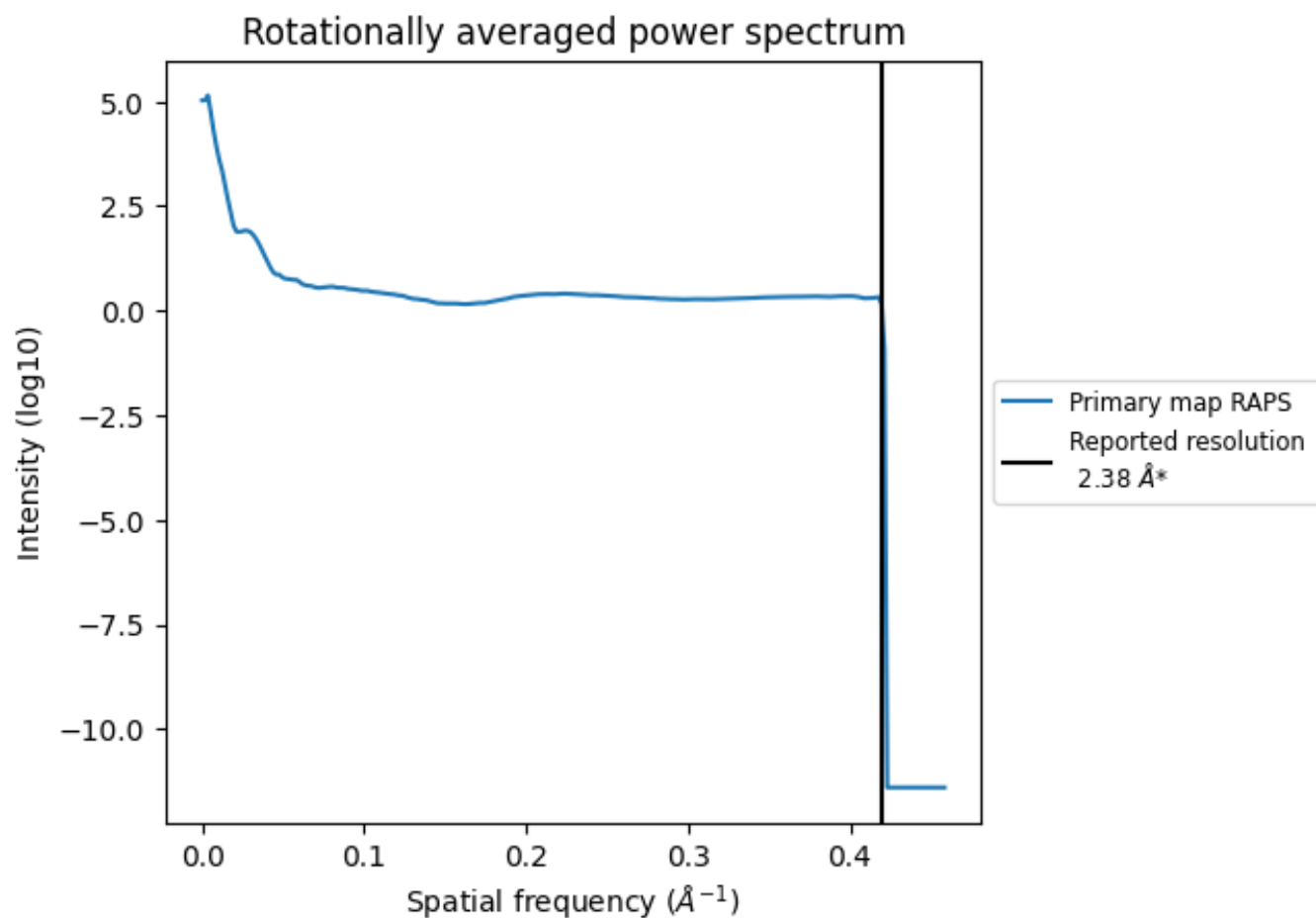
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $778 \text{ nm}^3$ ; this corresponds to an approximate mass of 703 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 0.420  $\text{\AA}^{-1}$

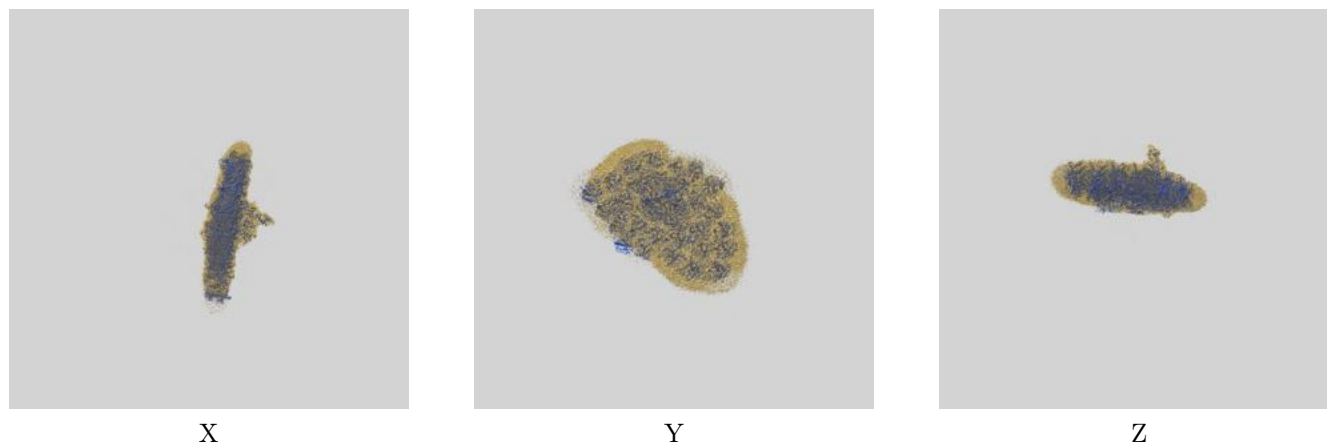
## 8 Fourier-Shell correlation

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

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

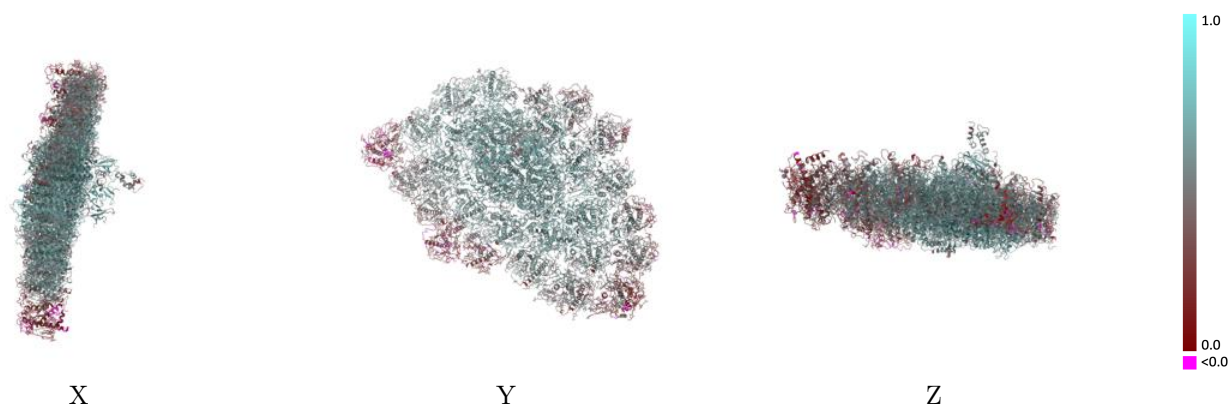
This section contains information regarding the fit between EMDB map EMD-30012 and PDB model 6LY5. Per-residue inclusion information can be found in [section 3](#) on [page 46](#).

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



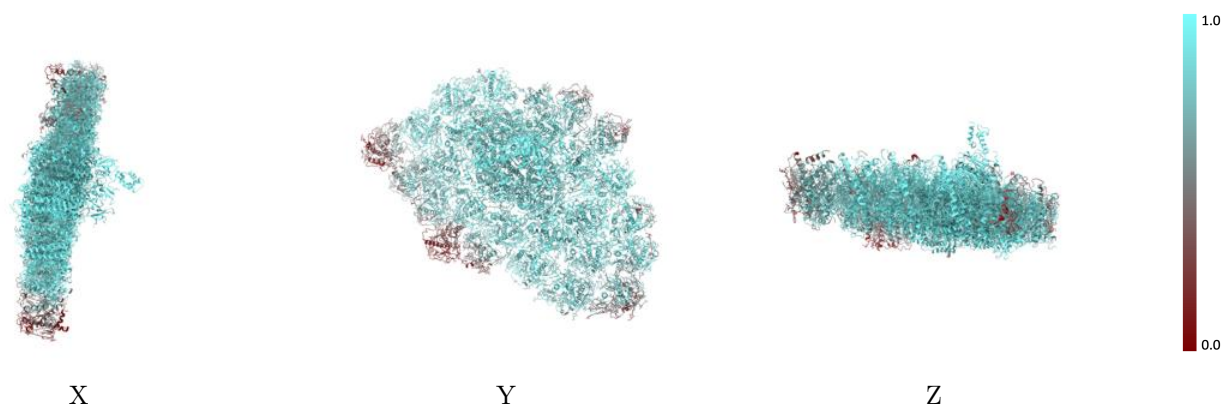
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



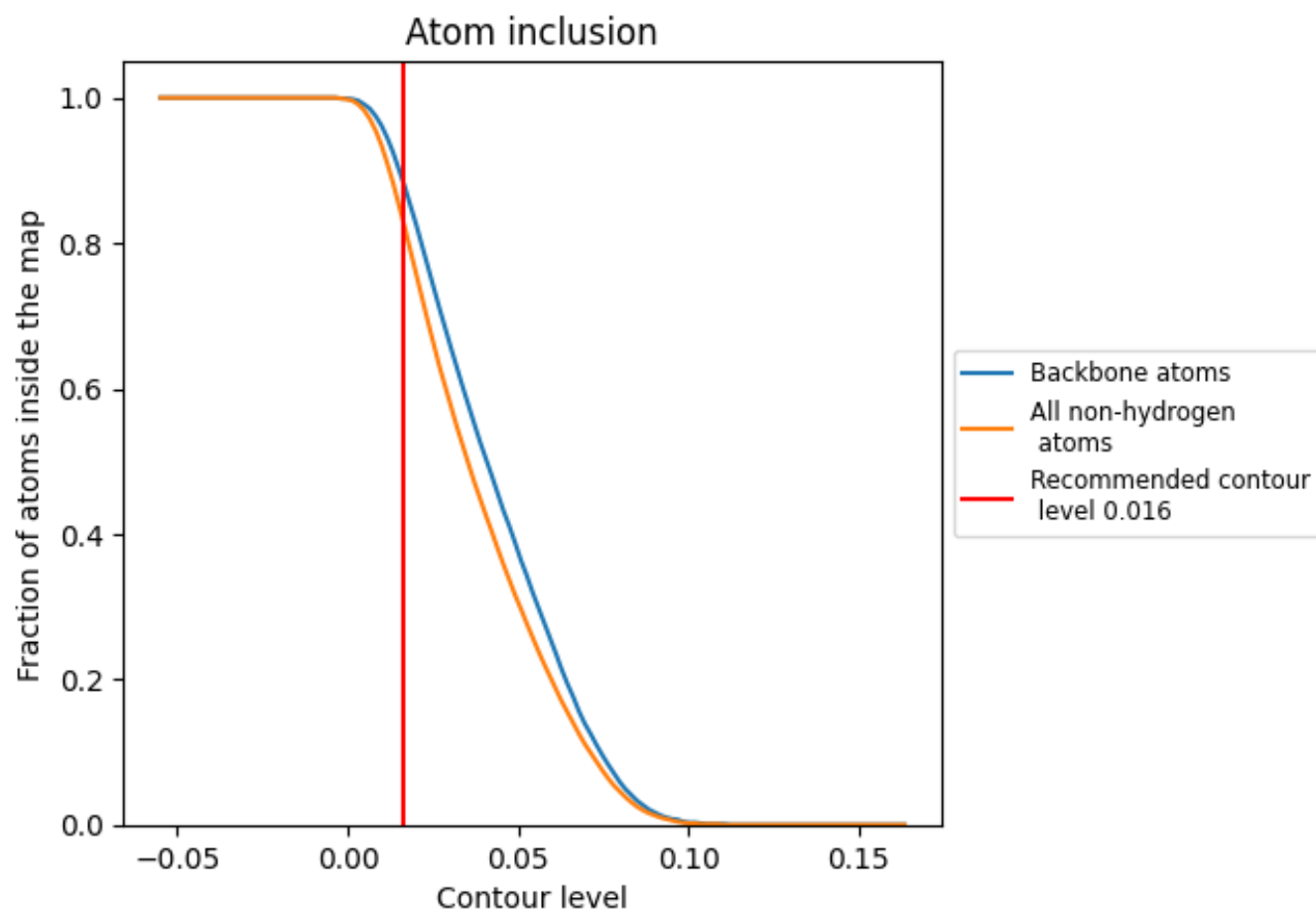
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.016) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8350   |  0.5170   |
| A     |  0.9410   |  0.5810   |
| B     |  0.8370   |  0.4930   |
| C     |  0.8980   |  0.5340   |
| D     |  0.9340   |  0.5870   |
| E     |  0.9530   |  0.6050   |
| F     |  0.9430   |  0.5960   |
| G     |  0.9570   |  0.6150   |
| H     |  0.8900   |  0.5450   |
| I     |  0.9240   |  0.5640   |
| J     |  0.9060   |  0.5400   |
| K     |  0.8890   |  0.5170   |
| L     |  0.8050   |  0.4220   |
| M     |  0.8700   |  0.4820   |
| N     |  0.3040  |  0.1740  |
| O     |  0.6670 |  0.4100 |
| P     |  0.8980 |  0.5260 |
| Q     |  0.7760 |  0.3880 |
| R     |  0.7930 |  0.4220 |
| S     |  0.5670 |  0.2610 |
| T     |  0.6280 |  0.3920 |
| U     |  0.6600 |  0.3880 |
| V     |  0.7550 |  0.4470 |
| W     |  0.4970 |  0.2640 |
| X     |  0.1530 |  0.1400 |
| a     |  0.9830 |  0.6690 |
| b     |  0.9910 |  0.6730 |
| c     |  0.9770 |  0.6620 |
| d     |  0.9460 |  0.6200 |
| e     |  0.9210 |  0.5940 |
| f     |  0.9320 |  0.6150 |
| g     |  0.8870 |  0.4480 |
| h     |  0.9690 |  0.6040 |
| i     |  0.9430 |  0.6250 |
| j     |  0.9380 |  0.6250 |



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*Continued from previous page...*

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| l     |  0.9580 |  0.6310 |
| m     |  0.9420 |  0.6140 |