



## wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 11:34 AM UTC

PDB ID : 6YP7 / pdb\_00006yp7  
EMDB ID : EMD-10865  
Title : PSII-LHCII C2S2 supercomplex from *Pisum sativum* grown in high light conditions  
Authors : Grinzato, A.; Albanese, P.; Zanotti, G.; Pagliano, C.  
Deposited on : 2020-04-15  
Resolution : 3.80 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>.

---

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
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) : 2.49

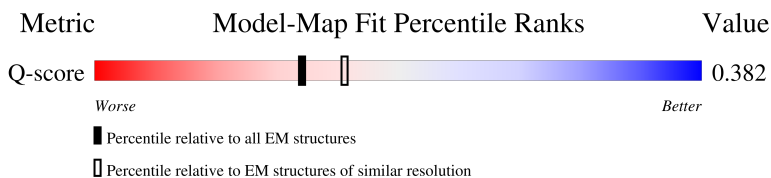
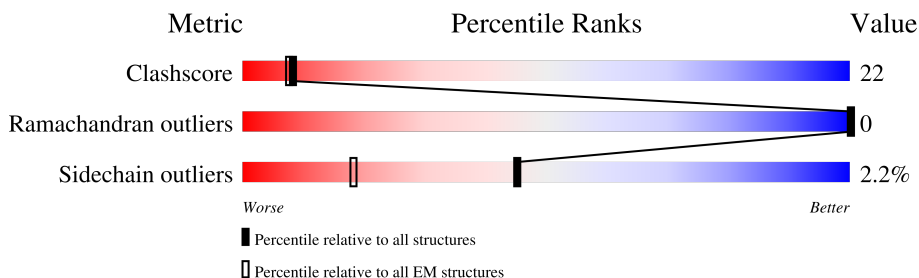
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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                       | 10198 ( 3.30 - 4.30 )                                    |

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   | G     | 219    | <div> <div>33%</div> <div>66%</div> <div>32%</div> </div> |
| 1   | N     | 219    | <div> <div>25%</div> <div>65%</div> <div>33%</div> </div> |
| 1   | Y     | 219    | <div> <div>13%</div> <div>64%</div> <div>35%</div> </div> |
| 1   | g     | 219    | <div> <div>34%</div> <div>65%</div> <div>33%</div> </div> |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | n     | 219    |                  |
| 1   | y     | 219    |                  |
| 2   | A     | 334    |                  |
| 2   | a     | 334    |                  |
| 3   | B     | 503    |                  |
| 3   | b     | 503    |                  |
| 4   | C     | 450    |                  |
| 4   | c     | 450    |                  |
| 5   | D     | 341    |                  |
| 5   | d     | 341    |                  |
| 6   | E     | 75     |                  |
| 6   | e     | 75     |                  |
| 7   | F     | 30     |                  |
| 7   | f     | 30     |                  |
| 8   | H     | 60     |                  |
| 8   | h     | 60     |                  |
| 9   | I     | 34     |                  |
| 9   | i     | 34     |                  |
| 10  | J     | 35     |                  |
| 10  | j     | 35     |                  |
| 11  | K     | 37     |                  |
| 11  | k     | 37     |                  |
| 12  | L     | 37     |                  |
| 12  | l     | 37     |                  |
| 13  | M     | 33     |                  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 13  | m     | 33     |                  |
| 14  | O     | 248    |                  |
| 14  | o     | 248    |                  |
| 15  | T     | 32     |                  |
| 15  | t     | 32     |                  |
| 16  | W     | 54     |                  |
| 16  | w     | 54     |                  |
| 17  | X     | 39     |                  |
| 17  | x     | 39     |                  |
| 18  | Z     | 62     |                  |
| 18  | z     | 62     |                  |
| 19  | R     | 222    |                  |
| 19  | r     | 222    |                  |
| 20  | S     | 218    |                  |
| 20  | s     | 218    |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 21  | CHL  | G     | 601 | X         | -        | X       | -                |
| 21  | CHL  | G     | 605 | X         | -        | -       | -                |
| 21  | CHL  | G     | 606 | X         | -        | X       | -                |
| 21  | CHL  | G     | 607 | X         | -        | X       | -                |
| 21  | CHL  | G     | 608 | X         | -        | X       | -                |
| 21  | CHL  | G     | 609 | X         | -        | X       | -                |
| 21  | CHL  | N     | 601 | X         | -        | X       | -                |
| 21  | CHL  | N     | 605 | X         | -        | X       | -                |
| 21  | CHL  | N     | 606 | X         | -        | X       | -                |
| 21  | CHL  | N     | 607 | X         | -        | X       | -                |
| 21  | CHL  | N     | 608 | X         | -        | X       | -                |
| 21  | CHL  | R     | 305 | X         | -        | X       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 21  | CHL  | R     | 306 | X         | -        | X       | -                |
| 21  | CHL  | R     | 307 | X         | -        | -       | -                |
| 21  | CHL  | S     | 301 | X         | -        | X       | -                |
| 21  | CHL  | S     | 302 | X         | -        | -       | -                |
| 21  | CHL  | S     | 306 | X         | -        | -       | -                |
| 21  | CHL  | S     | 307 | X         | -        | X       | -                |
| 21  | CHL  | Y     | 601 | X         | -        | X       | -                |
| 21  | CHL  | Y     | 605 | X         | -        | X       | -                |
| 21  | CHL  | Y     | 606 | X         | -        | X       | -                |
| 21  | CHL  | Y     | 607 | X         | -        | X       | -                |
| 21  | CHL  | Y     | 608 | X         | -        | X       | -                |
| 21  | CHL  | g     | 601 | X         | -        | X       | -                |
| 21  | CHL  | g     | 605 | X         | -        | -       | -                |
| 21  | CHL  | g     | 606 | X         | -        | X       | -                |
| 21  | CHL  | g     | 607 | X         | -        | X       | -                |
| 21  | CHL  | g     | 608 | X         | -        | X       | -                |
| 21  | CHL  | g     | 609 | X         | -        | X       | -                |
| 21  | CHL  | n     | 601 | X         | -        | X       | -                |
| 21  | CHL  | n     | 605 | X         | -        | X       | -                |
| 21  | CHL  | n     | 606 | X         | -        | -       | -                |
| 21  | CHL  | n     | 607 | X         | -        | X       | -                |
| 21  | CHL  | n     | 608 | X         | -        | X       | -                |
| 21  | CHL  | r     | 301 | X         | -        | X       | -                |
| 21  | CHL  | r     | 306 | X         | -        | X       | -                |
| 21  | CHL  | r     | 307 | X         | -        | X       | -                |
| 21  | CHL  | r     | 308 | X         | -        | -       | -                |
| 21  | CHL  | s     | 301 | X         | -        | X       | -                |
| 21  | CHL  | s     | 302 | X         | -        | -       | -                |
| 21  | CHL  | s     | 306 | X         | -        | -       | -                |
| 21  | CHL  | s     | 307 | X         | -        | X       | -                |
| 21  | CHL  | y     | 601 | X         | -        | X       | -                |
| 21  | CHL  | y     | 605 | X         | -        | X       | -                |
| 21  | CHL  | y     | 606 | X         | -        | X       | -                |
| 21  | CHL  | y     | 607 | X         | -        | -       | -                |
| 21  | CHL  | y     | 608 | X         | -        | X       | -                |
| 21  | CHL  | y     | 609 | X         | -        | X       | -                |
| 22  | CLA  | A     | 405 | X         | -        | -       | -                |
| 22  | CLA  | A     | 406 | X         | -        | -       | -                |
| 22  | CLA  | A     | 407 | X         | -        | -       | -                |
| 22  | CLA  | A     | 409 | X         | -        | -       | -                |
| 22  | CLA  | B     | 603 | X         | -        | -       | -                |
| 22  | CLA  | B     | 604 | X         | -        | -       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | B     | 605 | X         | -        | -       | -                |
| 22  | CLA  | B     | 606 | X         | -        | -       | -                |
| 22  | CLA  | B     | 607 | X         | -        | -       | -                |
| 22  | CLA  | B     | 608 | X         | -        | -       | -                |
| 22  | CLA  | B     | 609 | X         | -        | -       | -                |
| 22  | CLA  | B     | 610 | X         | -        | -       | -                |
| 22  | CLA  | B     | 611 | X         | -        | -       | -                |
| 22  | CLA  | B     | 612 | X         | -        | -       | -                |
| 22  | CLA  | B     | 613 | X         | -        | -       | -                |
| 22  | CLA  | B     | 614 | X         | -        | -       | -                |
| 22  | CLA  | B     | 615 | X         | -        | -       | -                |
| 22  | CLA  | B     | 616 | X         | -        | -       | -                |
| 22  | CLA  | B     | 617 | X         | -        | -       | -                |
| 22  | CLA  | B     | 618 | X         | -        | -       | -                |
| 22  | CLA  | C     | 503 | X         | -        | -       | -                |
| 22  | CLA  | C     | 504 | X         | -        | -       | -                |
| 22  | CLA  | C     | 505 | X         | -        | -       | -                |
| 22  | CLA  | C     | 506 | X         | -        | -       | -                |
| 22  | CLA  | C     | 507 | X         | -        | -       | -                |
| 22  | CLA  | C     | 508 | X         | -        | -       | -                |
| 22  | CLA  | C     | 509 | X         | -        | -       | -                |
| 22  | CLA  | C     | 510 | X         | -        | -       | -                |
| 22  | CLA  | C     | 511 | X         | -        | X       | -                |
| 22  | CLA  | C     | 512 | X         | -        | -       | -                |
| 22  | CLA  | C     | 513 | X         | -        | -       | -                |
| 22  | CLA  | C     | 514 | X         | -        | -       | -                |
| 22  | CLA  | C     | 515 | X         | -        | -       | -                |
| 22  | CLA  | D     | 404 | X         | -        | -       | -                |
| 22  | CLA  | D     | 405 | X         | -        | -       | -                |
| 22  | CLA  | G     | 602 | X         | -        | -       | -                |
| 22  | CLA  | G     | 603 | X         | -        | -       | -                |
| 22  | CLA  | G     | 604 | X         | -        | -       | -                |
| 22  | CLA  | G     | 610 | X         | -        | -       | -                |
| 22  | CLA  | G     | 611 | X         | -        | -       | -                |
| 22  | CLA  | G     | 612 | X         | -        | -       | -                |
| 22  | CLA  | G     | 613 | X         | -        | -       | -                |
| 22  | CLA  | G     | 614 | X         | -        | -       | -                |
| 22  | CLA  | N     | 602 | X         | -        | -       | -                |
| 22  | CLA  | N     | 603 | X         | -        | -       | -                |
| 22  | CLA  | N     | 604 | X         | -        | -       | -                |
| 22  | CLA  | N     | 609 | X         | -        | -       | -                |
| 22  | CLA  | N     | 610 | X         | -        | -       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | N     | 611 | X         | -        | -       | -                |
| 22  | CLA  | N     | 612 | X         | -        | -       | -                |
| 22  | CLA  | N     | 613 | X         | -        | -       | -                |
| 22  | CLA  | R     | 302 | X         | -        | -       | -                |
| 22  | CLA  | R     | 303 | X         | -        | -       | -                |
| 22  | CLA  | R     | 304 | X         | -        | -       | -                |
| 22  | CLA  | R     | 308 | X         | -        | -       | -                |
| 22  | CLA  | R     | 309 | X         | -        | -       | -                |
| 22  | CLA  | R     | 310 | X         | -        | -       | -                |
| 22  | CLA  | R     | 311 | X         | -        | -       | -                |
| 22  | CLA  | S     | 303 | X         | -        | -       | -                |
| 22  | CLA  | S     | 304 | X         | -        | -       | -                |
| 22  | CLA  | S     | 305 | X         | -        | -       | -                |
| 22  | CLA  | S     | 309 | X         | -        | -       | -                |
| 22  | CLA  | S     | 310 | X         | -        | -       | -                |
| 22  | CLA  | S     | 311 | X         | -        | -       | -                |
| 22  | CLA  | S     | 312 | X         | -        | -       | -                |
| 22  | CLA  | S     | 313 | X         | -        | -       | -                |
| 22  | CLA  | W     | 101 | X         | -        | -       | -                |
| 22  | CLA  | Y     | 602 | X         | -        | -       | -                |
| 22  | CLA  | Y     | 603 | X         | -        | -       | -                |
| 22  | CLA  | Y     | 604 | X         | -        | -       | -                |
| 22  | CLA  | Y     | 609 | X         | -        | -       | -                |
| 22  | CLA  | Y     | 610 | X         | -        | -       | -                |
| 22  | CLA  | Y     | 611 | X         | -        | X       | -                |
| 22  | CLA  | Y     | 612 | X         | -        | -       | -                |
| 22  | CLA  | a     | 404 | X         | -        | -       | -                |
| 22  | CLA  | a     | 405 | X         | -        | -       | -                |
| 22  | CLA  | a     | 406 | X         | -        | -       | -                |
| 22  | CLA  | a     | 408 | X         | -        | -       | -                |
| 22  | CLA  | b     | 601 | X         | -        | -       | -                |
| 22  | CLA  | b     | 602 | X         | -        | -       | -                |
| 22  | CLA  | b     | 603 | X         | -        | -       | -                |
| 22  | CLA  | b     | 604 | X         | -        | -       | -                |
| 22  | CLA  | b     | 605 | X         | -        | -       | -                |
| 22  | CLA  | b     | 606 | X         | -        | -       | -                |
| 22  | CLA  | b     | 607 | X         | -        | -       | -                |
| 22  | CLA  | b     | 608 | X         | -        | -       | -                |
| 22  | CLA  | b     | 609 | X         | -        | -       | -                |
| 22  | CLA  | b     | 610 | X         | -        | -       | -                |
| 22  | CLA  | b     | 611 | X         | -        | -       | -                |
| 22  | CLA  | b     | 612 | X         | -        | -       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | b     | 613 | X         | -        | -       | -                |
| 22  | CLA  | b     | 614 | X         | -        | -       | -                |
| 22  | CLA  | b     | 615 | X         | -        | -       | -                |
| 22  | CLA  | c     | 502 | X         | -        | -       | -                |
| 22  | CLA  | c     | 503 | X         | -        | -       | -                |
| 22  | CLA  | c     | 504 | X         | -        | -       | -                |
| 22  | CLA  | c     | 505 | X         | -        | -       | -                |
| 22  | CLA  | c     | 506 | X         | -        | -       | -                |
| 22  | CLA  | c     | 507 | X         | -        | -       | -                |
| 22  | CLA  | c     | 508 | X         | -        | -       | -                |
| 22  | CLA  | c     | 509 | X         | -        | -       | -                |
| 22  | CLA  | c     | 510 | X         | -        | X       | -                |
| 22  | CLA  | c     | 511 | X         | -        | -       | -                |
| 22  | CLA  | c     | 512 | X         | -        | -       | -                |
| 22  | CLA  | c     | 513 | X         | -        | -       | -                |
| 22  | CLA  | c     | 514 | X         | -        | -       | -                |
| 22  | CLA  | d     | 403 | X         | -        | -       | -                |
| 22  | CLA  | d     | 404 | X         | -        | -       | -                |
| 22  | CLA  | g     | 602 | X         | -        | -       | -                |
| 22  | CLA  | g     | 603 | X         | -        | -       | -                |
| 22  | CLA  | g     | 604 | X         | -        | -       | -                |
| 22  | CLA  | g     | 610 | X         | -        | -       | -                |
| 22  | CLA  | g     | 611 | X         | -        | -       | -                |
| 22  | CLA  | g     | 612 | X         | -        | -       | -                |
| 22  | CLA  | g     | 613 | X         | -        | -       | -                |
| 22  | CLA  | g     | 614 | X         | -        | -       | -                |
| 22  | CLA  | n     | 602 | X         | -        | -       | -                |
| 22  | CLA  | n     | 603 | X         | -        | -       | -                |
| 22  | CLA  | n     | 604 | X         | -        | -       | -                |
| 22  | CLA  | n     | 609 | X         | -        | -       | -                |
| 22  | CLA  | n     | 610 | X         | -        | -       | -                |
| 22  | CLA  | n     | 611 | X         | -        | -       | -                |
| 22  | CLA  | n     | 612 | X         | -        | -       | -                |
| 22  | CLA  | n     | 613 | X         | -        | -       | -                |
| 22  | CLA  | r     | 303 | X         | -        | -       | -                |
| 22  | CLA  | r     | 304 | X         | -        | -       | -                |
| 22  | CLA  | r     | 305 | X         | -        | -       | -                |
| 22  | CLA  | r     | 309 | X         | -        | -       | -                |
| 22  | CLA  | r     | 310 | X         | -        | -       | -                |
| 22  | CLA  | r     | 311 | X         | -        | -       | -                |
| 22  | CLA  | r     | 312 | X         | -        | -       | -                |
| 22  | CLA  | s     | 303 | X         | -        | -       | -                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | s     | 304 | X         | -        | -       | -                |
| 22  | CLA  | s     | 305 | X         | -        | -       | -                |
| 22  | CLA  | s     | 309 | X         | -        | -       | -                |
| 22  | CLA  | s     | 310 | X         | -        | -       | -                |
| 22  | CLA  | s     | 311 | X         | -        | -       | -                |
| 22  | CLA  | s     | 312 | X         | -        | -       | -                |
| 22  | CLA  | s     | 313 | X         | -        | -       | -                |
| 22  | CLA  | w     | 101 | X         | -        | -       | -                |
| 22  | CLA  | x     | 101 | X         | -        | -       | -                |
| 22  | CLA  | y     | 602 | X         | -        | -       | -                |
| 22  | CLA  | y     | 603 | X         | -        | -       | -                |
| 22  | CLA  | y     | 604 | X         | -        | -       | -                |
| 22  | CLA  | y     | 610 | X         | -        | -       | -                |
| 22  | CLA  | y     | 611 | X         | -        | -       | -                |
| 22  | CLA  | y     | 612 | X         | -        | X       | -                |
| 22  | CLA  | y     | 613 | X         | -        | -       | -                |
| 24  | XAT  | G     | 617 | X         | -        | -       | -                |
| 24  | XAT  | N     | 616 | X         | -        | -       | -                |
| 24  | XAT  | R     | 313 | X         | -        | -       | -                |
| 24  | XAT  | Y     | 615 | X         | -        | -       | -                |
| 24  | XAT  | g     | 617 | X         | -        | -       | -                |
| 24  | XAT  | n     | 615 | X         | -        | -       | -                |
| 24  | XAT  | r     | 314 | X         | -        | -       | -                |
| 24  | XAT  | y     | 615 | X         | -        | -       | -                |
| 25  | NEX  | N     | 617 | X         | -        | -       | -                |
| 25  | NEX  | Y     | 616 | X         | -        | -       | -                |
| 25  | NEX  | g     | 618 | X         | -        | -       | -                |
| 25  | NEX  | n     | 616 | X         | -        | -       | -                |
| 25  | NEX  | r     | 315 | X         | -        | -       | -                |
| 25  | NEX  | y     | 616 | X         | -        | -       | -                |
| 25  | NEX  | y     | 618 | X         | -        | -       | -                |
| 33  | SQD  | D     | 402 | X         | -        | -       | -                |
| 33  | SQD  | d     | 402 | X         | -        | -       | -                |
| 34  | BCT  | D     | 403 | -         | X        | X       | -                |
| 34  | BCT  | a     | 412 | -         | X        | X       | -                |
| 36  | LMG  | B     | 623 | -         | -        | X       | -                |
| 36  | LMG  | b     | 620 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 71784 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein 8, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | g     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1668  | 1081 | 270 | 312 | 5 |         |       |
| 1   | n     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1668  | 1081 | 270 | 312 | 5 |         |       |
| 1   | y     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1668  | 1081 | 270 | 312 | 5 |         |       |
| 1   | G     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1668  | 1081 | 270 | 312 | 5 |         |       |
| 1   | N     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1668  | 1081 | 270 | 312 | 5 |         |       |
| 1   | Y     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1668  | 1081 | 270 | 312 | 5 |         |       |

- Molecule 2 is a protein called Photosystem II protein D1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | a     | 334      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2616  | 1708 | 431 | 464 | 13 |         |       |
| 2   | A     | 334      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2616  | 1708 | 431 | 464 | 13 |         |       |

- Molecule 3 is a protein called Photosystem II CP47 reaction center protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | b     | 503      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3948  | 2581 | 669 | 686 | 12 |         |       |
| 3   | B     | 503      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3948  | 2581 | 669 | 686 | 12 |         |       |

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | c     | 450      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3497  | 2300 | 583 | 604 | 10 |         |       |
| 4   | C     | 450      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3497  | 2300 | 583 | 604 | 10 |         |       |

- Molecule 5 is a protein called Photosystem II D2 protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | d     | 341      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2712  | 1790 | 444 | 466 | 12 |         |       |
| 5   | D     | 341      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2712  | 1790 | 444 | 466 | 12 |         |       |

- Molecule 6 is a protein called Cytochrome b559 subunit alpha.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 6   | e     | 75       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 612   | 400 | 100 | 112 |         |       |
| 6   | E     | 75       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 612   | 400 | 100 | 112 |         |       |

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | f     | 30       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 241   | 162 | 41 | 37 | 1 |         |       |
| 7   | F     | 30       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 241   | 162 | 41 | 37 | 1 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| f     | 26      | PHE      | SER    | conflict | UNP P62096 |
| F     | 26      | PHE      | SER    | conflict | UNP P62096 |

- Molecule 8 is a protein called Photosystem II reaction center protein H.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | h     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 452   | 296 | 72 | 81 | 3 |         |       |
| 8   | H     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 452   | 296 | 72 | 81 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | i     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 278   | 191 | 43 | 43 | 1 |         |       |
| 9   | I     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 278   | 191 | 43 | 43 | 1 |         |       |

- Molecule 10 is a protein called Photosystem II reaction center protein J.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10  | j     | 35       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 256   | 174 | 39 | 43 |         |       |
| 10  | J     | 35       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 256   | 174 | 39 | 43 |         |       |

- Molecule 11 is a protein called Photosystem II reaction center protein K.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11  | k     | 37       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 306   | 215 | 44 | 46 | 1 |         |       |
| 11  | K     | 37       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 306   | 215 | 44 | 46 | 1 |         |       |

- Molecule 12 is a protein called Photosystem II reaction center protein L.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 12  | l     | 37       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 311   | 205 | 49 | 57 |         |       |
| 12  | L     | 37       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 311   | 205 | 49 | 57 |         |       |

- Molecule 13 is a protein called Photosystem II reaction center protein M.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 13  | m     | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 256   | 176 | 36 | 43 | 1 |         |       |
| 13  | M     | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 256   | 176 | 36 | 43 | 1 |         |       |

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | o     | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1870  | 1179 | 306 | 382 | 3 |         |       |
| 14  | O     | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1870  | 1179 | 306 | 382 | 3 |         |       |

- Molecule 15 is a protein called Photosystem II reaction center protein T.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 15  | t     | 32       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 261   | 182 | 37 | 41 | 1 |         |       |
| 15  | T     | 32       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 261   | 182 | 37 | 41 | 1 |         |       |

- Molecule 16 is a protein called Photosystem II reaction center protein W.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 16  | w     | 54       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 419   | 275 | 61 | 82 | 1 |         |       |
| 16  | W     | 54       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 419   | 275 | 61 | 82 | 1 |         |       |

- Molecule 17 is a protein called Ultraviolet-B-repressible protein.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 17  | x     | 39       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 276   | 180 | 46 | 50 |         |       |
| 17  | X     | 39       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 276   | 180 | 46 | 50 |         |       |

- Molecule 18 is a protein called Photosystem II reaction center protein Z.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 18  | z     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 464   | 312 | 69 | 82 | 1 |         |       |
| 18  | Z     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 464   | 312 | 69 | 82 | 1 |         |       |

- Molecule 19 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb4.3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 19  | r     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1732  | 1133 | 281 | 314 | 4 |         |       |

*Continued on next page...*

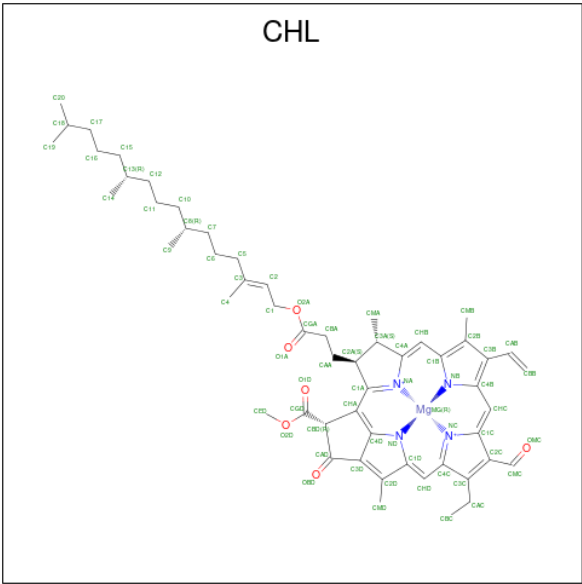
Continued from previous page...

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 19  | R     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1732  | 1133 | 281 | 314 | 4 |         |       |

- Molecule 20 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20  | s     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1688  | 1105 | 271 | 308 | 4 |         |       |
| 20  | S     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1688  | 1105 | 271 | 308 | 4 |         |       |

- Molecule 21 is CHLOROPHYLL B (CCD ID: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 21  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 21  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 21  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 39 | 1  | 4 | 6 |         |
| 21  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 21  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 21  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |

Continued on next page...

*Continued from previous page...*

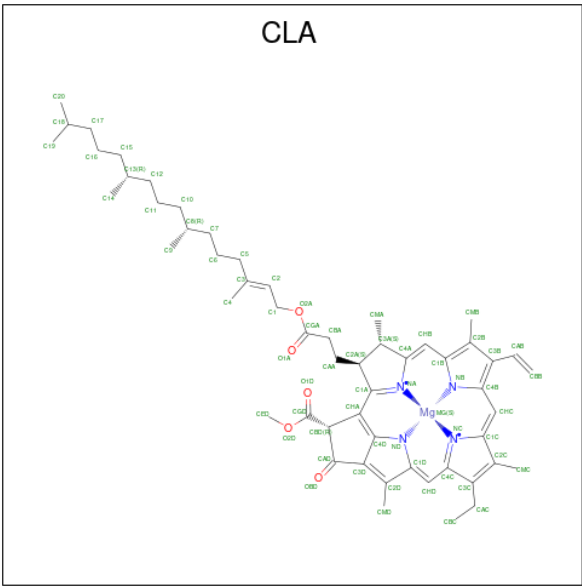
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 21  | n     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | n     | 1        | Total<br>50 | C<br>39 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | n     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | n     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | n     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | y     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | y     | 1        | Total<br>48 | C<br>37 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | y     | 1        | Total<br>50 | C<br>39 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | y     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | y     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | y     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | G     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | G     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | G     | 1        | Total<br>50 | C<br>39 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | G     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | G     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | G     | 1        | Total<br>61 | C<br>50 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | N     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | N     | 1        | Total<br>50 | C<br>39 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | N     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | N     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 21  | N     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | Y     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | Y     | 1        | Total<br>50 | C<br>39 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | Y     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | Y     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | Y     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | r     | 1        | Total<br>48 | C<br>37 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | r     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | r     | 1        | Total<br>56 | C<br>45 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | r     | 1        | Total<br>61 | C<br>50 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | s     | 1        | Total<br>48 | C<br>37 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | s     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | s     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | s     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | S     | 1        | Total<br>48 | C<br>37 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | S     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | S     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | S     | 1        | Total<br>46 | C<br>35 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | R     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | R     | 1        | Total<br>56 | C<br>45 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 21  | R     | 1        | Total<br>61 | C<br>50 | Mg<br>1 | N<br>4 | O<br>6 | 0       |

- Molecule 22 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 |
|-----|-------|----------|-------|----|----|---|---|---------|
| 22  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 64    | 54 | 1  | 4 | 5 |         |
| 22  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 38 | 1  | 4 | 5 |         |
| 22  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | n     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | n     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | n     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | y     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | y     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | y     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | y     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>64 | C<br>54 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | N     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | N     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | N     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | N     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | N     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | N     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | N     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | N     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Y     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Y     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Y     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Y     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Y     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | a     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | d     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | d     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | w     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | x     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | W     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

*Continued on next page...*

*Continued from previous page...*

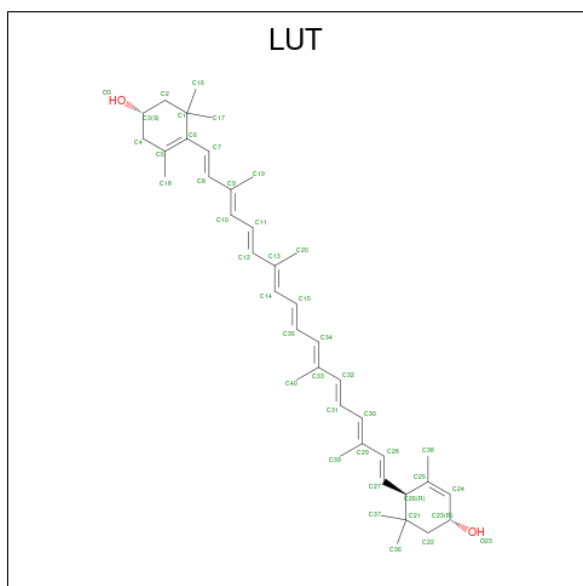
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | r     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | r     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | r     | 1        | Total<br>48 | C<br>38 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | r     | 1        | Total<br>58 | C<br>48 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | r     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | r     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | r     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | s     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | S     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | S     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | S     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | S     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | S     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

*Continued on next page...*

*Continued from previous page...*

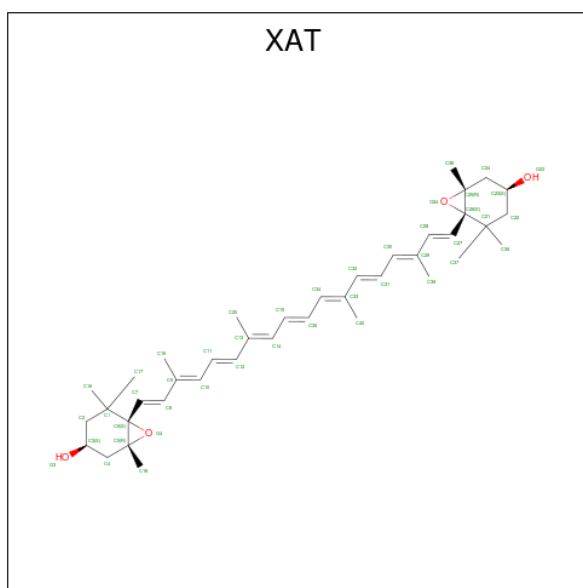
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 22  | S     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | S     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 22  | S     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 22  | S     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 38 | 1  | 4 | 5 |         |
| 22  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |
| 22  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 22  | R     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |

- Molecule 23 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



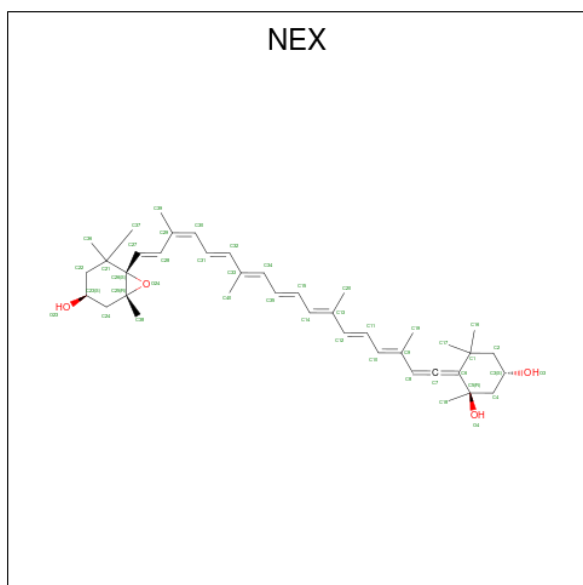
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 23  | g     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | g     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | n     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | y     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | G     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | G     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | Y     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | Y     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | r     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 23  | R     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

- Molecule 24 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 24  | g     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 24  | n     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 24  | y     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 24  | G     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 24  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 24  | Y     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 24  | r     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 24  | R     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

- Molecule 25 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



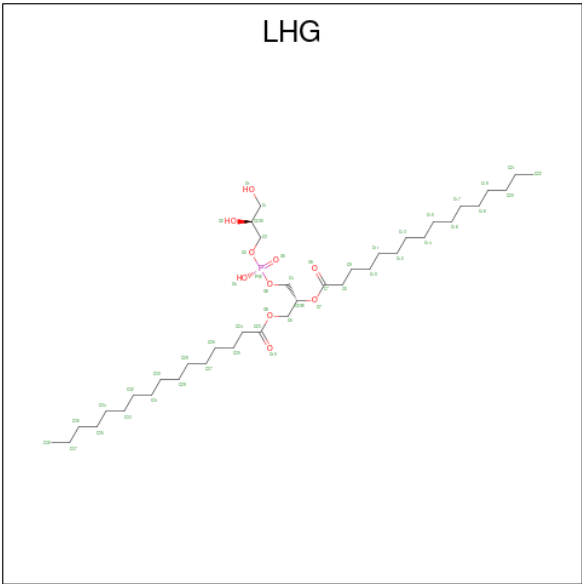
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 25  | g     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 25  | n     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 25  | y     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 25  | y     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 25  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 25  | Y     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |
| 25  | r     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



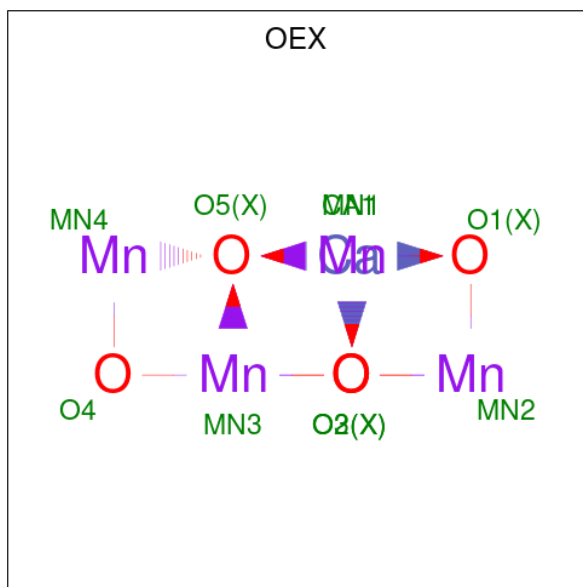
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 26  | g     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | n     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | y     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | G     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | N     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | Y     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         |         |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|
| 26  | b     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 26  | c     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 26  | c     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 26  | c     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 26  | d     | 1        | Total<br>46 | C<br>35 | O<br>10 | P<br>1 | 0       |
| 26  | d     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 26  | d     | 1        | Total<br>43 | C<br>32 | O<br>10 | P<br>1 | 0       |
| 26  | l     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 26  | B     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 26  | C     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 26  | C     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 26  | C     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 26  | D     | 1        | Total<br>46 | C<br>35 | O<br>10 | P<br>1 | 0       |
| 26  | D     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 26  | D     | 1        | Total<br>43 | C<br>32 | O<br>10 | P<br>1 | 0       |
| 26  | L     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 26  | r     | 1        | Total<br>47 | C<br>36 | O<br>10 | P<br>1 | 0       |
| 26  | s     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 26  | S     | 1        | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0       |
| 26  | R     | 1        | Total<br>47 | C<br>36 | O<br>10 | P<br>1 | 0       |

- Molecule 27 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 27  | a     | 1        | Total | Ca | Mn | O | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |
| 27  | A     | 1        | Total | Ca | Mn | O | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |

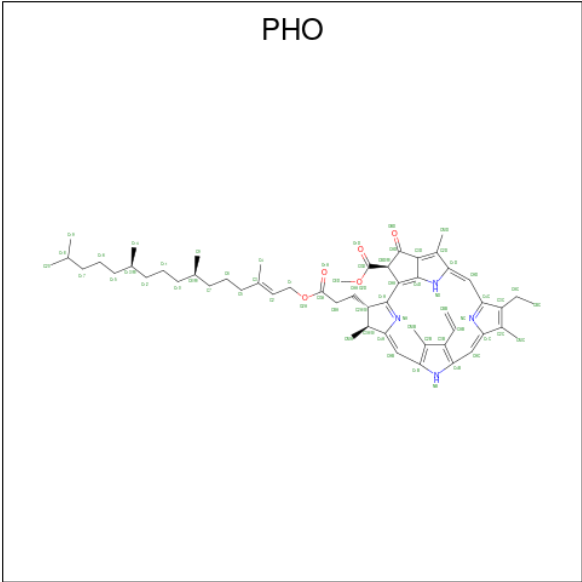
- Molecule 28 is FE (II) ION (CCD ID: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 28  | a     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 28  | A     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 29 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

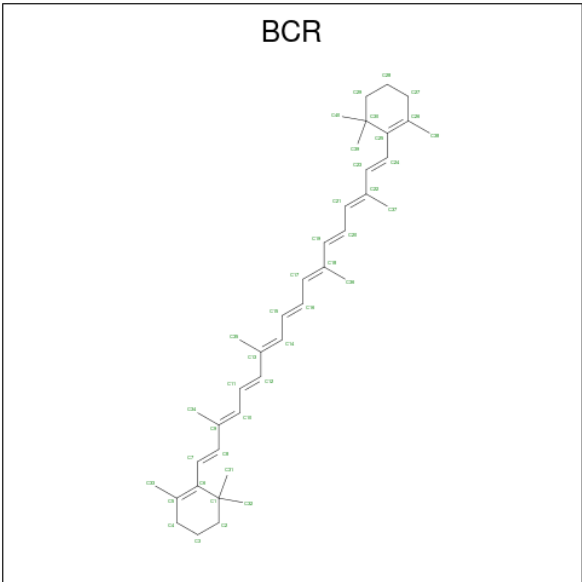
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 29  | a     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |
| 29  | c     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |
| 29  | A     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |
| 29  | C     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 30 is PHEOPHYTIN A (CCD ID: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



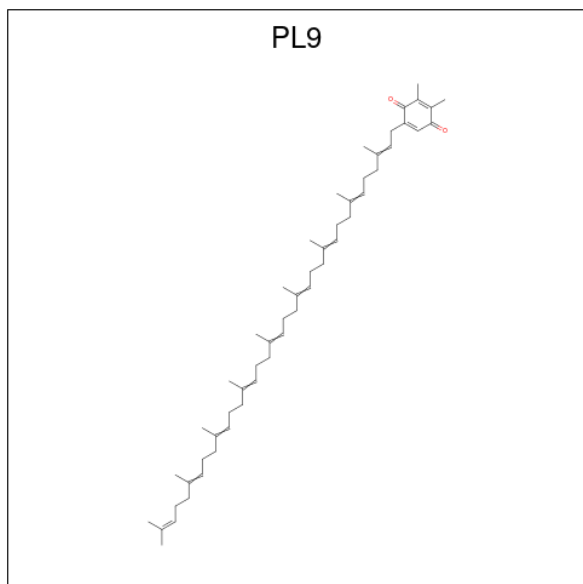
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 30  | a     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 30  | d     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 30  | A     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 30  | D     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



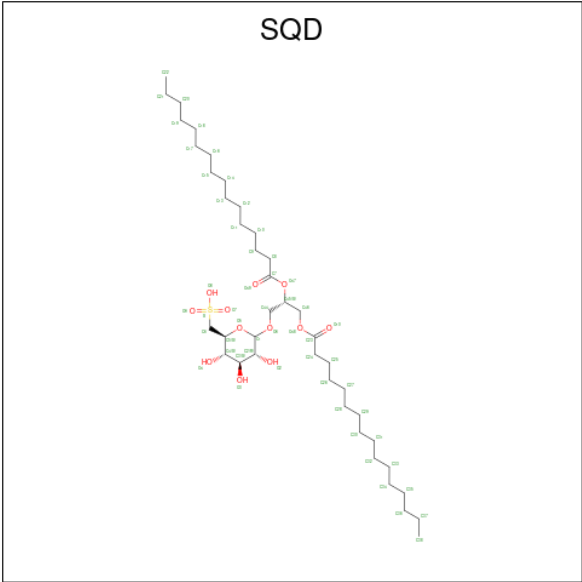
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 31  | a     | 1        | Total C<br>40 40 | 0       |
| 31  | b     | 1        | Total C<br>40 40 | 0       |
| 31  | b     | 1        | Total C<br>40 40 | 0       |
| 31  | b     | 1        | Total C<br>40 40 | 0       |
| 31  | c     | 1        | Total C<br>40 40 | 0       |
| 31  | c     | 1        | Total C<br>40 40 | 0       |
| 31  | d     | 1        | Total C<br>40 40 | 0       |
| 31  | h     | 1        | Total C<br>40 40 | 0       |
| 31  | k     | 1        | Total C<br>40 40 | 0       |
| 31  | k     | 1        | Total C<br>40 40 | 0       |
| 31  | A     | 1        | Total C<br>40 40 | 0       |
| 31  | B     | 1        | Total C<br>40 40 | 0       |
| 31  | B     | 1        | Total C<br>40 40 | 0       |
| 31  | B     | 1        | Total C<br>40 40 | 0       |
| 31  | B     | 1        | Total C<br>40 40 | 0       |
| 31  | C     | 1        | Total C<br>40 40 | 0       |
| 31  | C     | 1        | Total C<br>40 40 | 0       |
| 31  | D     | 1        | Total C<br>40 40 | 0       |
| 31  | H     | 1        | Total C<br>40 40 | 0       |
| 31  | K     | 1        | Total C<br>40 40 | 0       |
| 31  | K     | 1        | Total C<br>40 40 | 0       |
| 31  | T     | 1        | Total C<br>40 40 | 0       |

- Molecule 32 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula:  $C_{53}H_{80}O_2$ ).



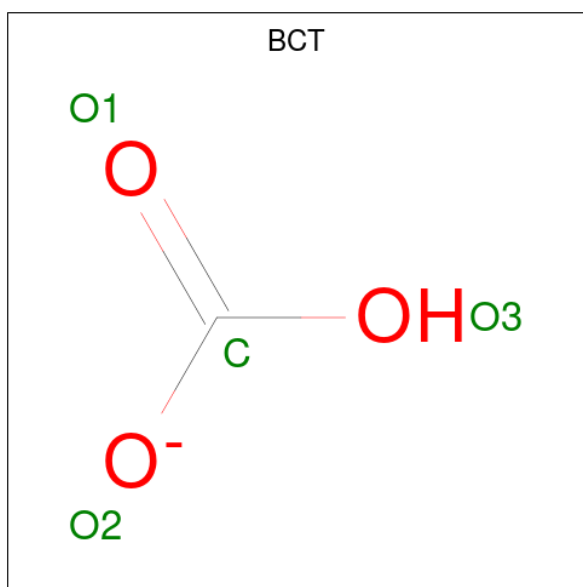
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 32  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 13    | 11 | 2 |         |
| 32  | d     | 1        | Total | C  | O | 0       |
|     |       |          | 55    | 53 | 2 |         |
| 32  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 13    | 11 | 2 |         |
| 32  | D     | 1        | Total | C  | O | 0       |
|     |       |          | 55    | 53 | 2 |         |

- Molecule 33 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



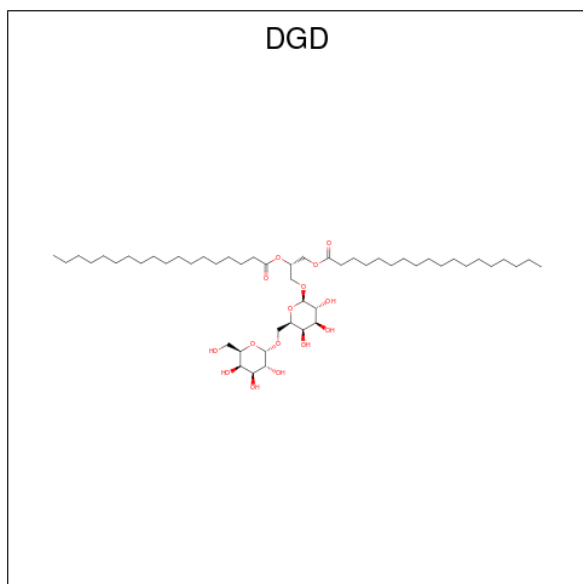
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 33  | a     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 33  | d     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 50    | 37 | 12 | 1 |         |
| 33  | l     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 42    | 29 | 12 | 1 |         |
| 33  | l     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 33  | A     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 33  | D     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 50    | 37 | 12 | 1 |         |
| 33  | L     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 33  | L     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 42    | 29 | 12 | 1 |         |

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 34  | a     | 1        | Total | C | O | 0       |
|     |       |          | 4     | 1 | 3 |         |
| 34  | D     | 1        | Total | C | O | 0       |
|     |       |          | 4     | 1 | 3 |         |

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



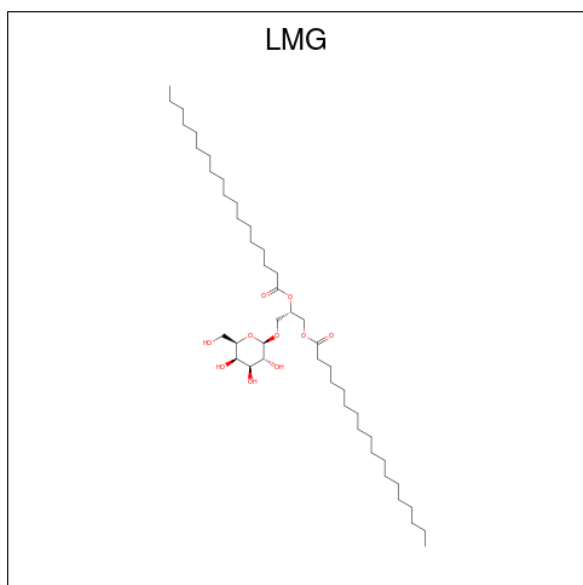
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 35  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 59    | 44 | 15 |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 35  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 40 | 15 |         |
| 35  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 15 |         |
| 35  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 60    | 45 | 15 |         |
| 35  | h     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 15 |         |
| 35  | A     | 1        | Total | C  | O  | 0       |
|     |       |          | 59    | 44 | 15 |         |
| 35  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 40 | 15 |         |
| 35  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 15 |         |
| 35  | H     | 1        | Total | C  | O  | 0       |
|     |       |          | 62    | 47 | 15 |         |
| 35  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 60    | 45 | 15 |         |

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 36  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |
| 36  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 51    | 41 | 10 |         |

*Continued on next page...*

| Mol | Chain | Residues | Atoms       |         |         | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 36  | d     | 1        | Total<br>46 | C<br>36 | O<br>10 | 0       |
| 36  | k     | 1        | Total<br>51 | C<br>41 | O<br>10 | 0       |
| 36  | w     | 1        | Total<br>48 | C<br>38 | O<br>10 | 0       |
| 36  | B     | 1        | Total<br>40 | C<br>30 | O<br>10 | 0       |
| 36  | B     | 1        | Total<br>55 | C<br>45 | O<br>10 | 0       |
| 36  | C     | 1        | Total<br>48 | C<br>38 | O<br>10 | 0       |
| 36  | C     | 1        | Total<br>51 | C<br>41 | O<br>10 | 0       |
| 36  | D     | 1        | Total<br>46 | C<br>36 | O<br>10 | 0       |
| 36  | I     | 1        | Total<br>40 | C<br>30 | O<br>10 | 0       |
| 36  | K     | 1        | Total<br>51 | C<br>41 | O<br>10 | 0       |
| 36  | M     | 1        | Total<br>51 | C<br>41 | O<br>10 | 0       |
| 36  | T     | 1        | Total<br>51 | C<br>41 | O<br>10 | 0       |

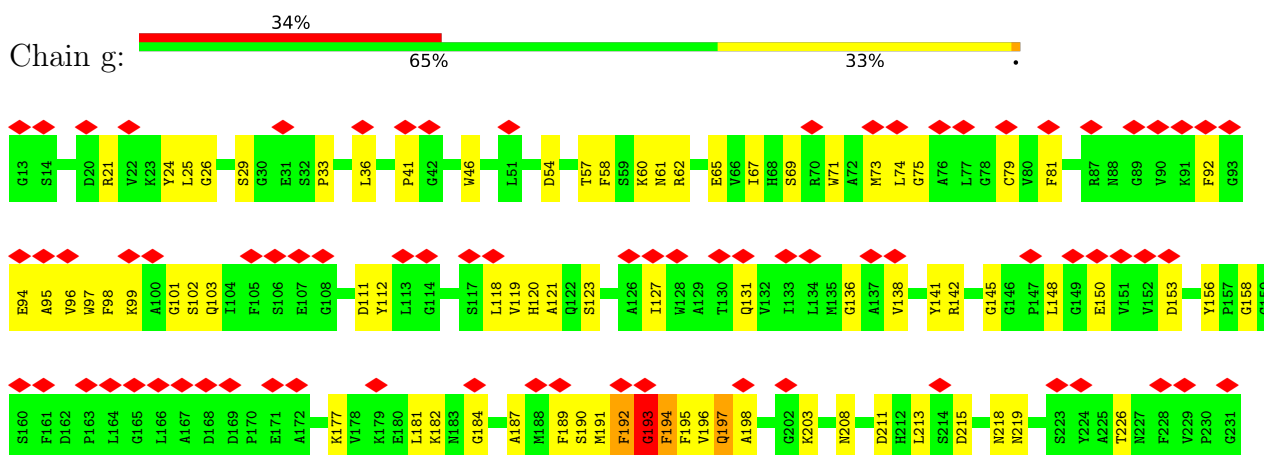
- # HEM

| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 37  | f     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 37  | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |

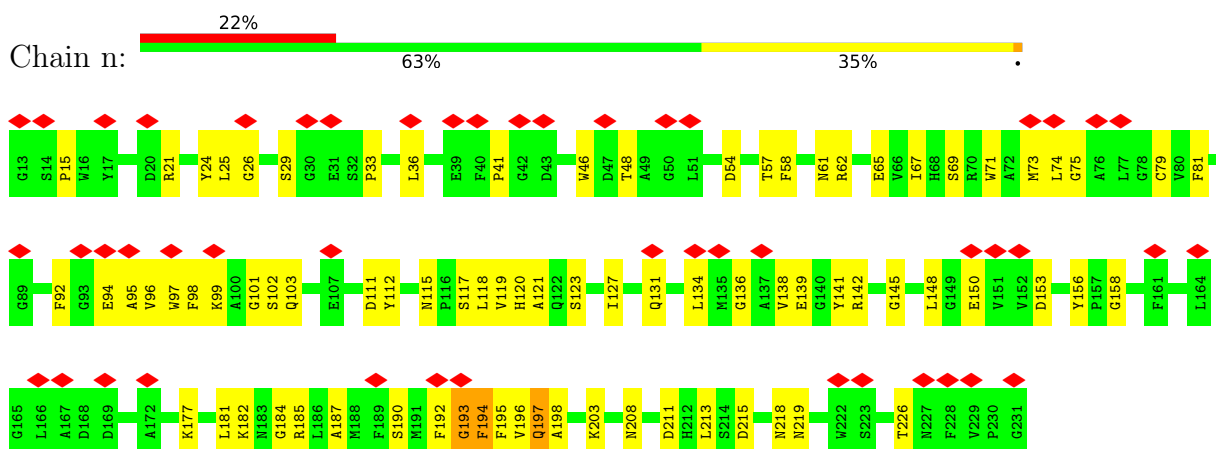
### 3 Residue-property plots

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.

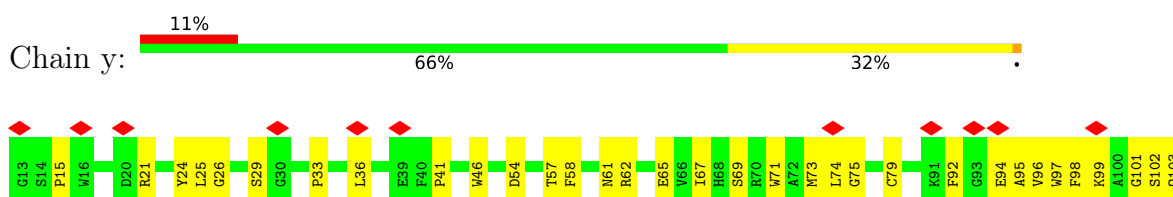
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

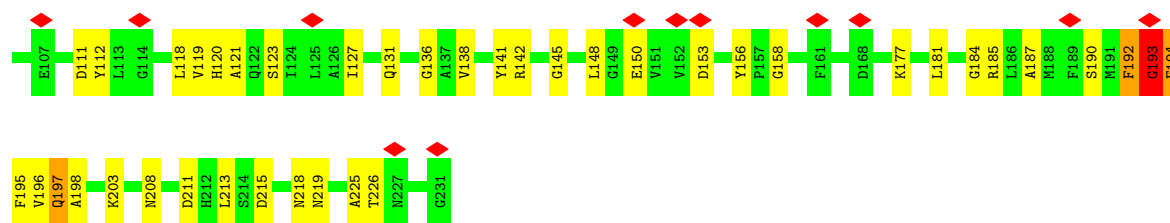


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

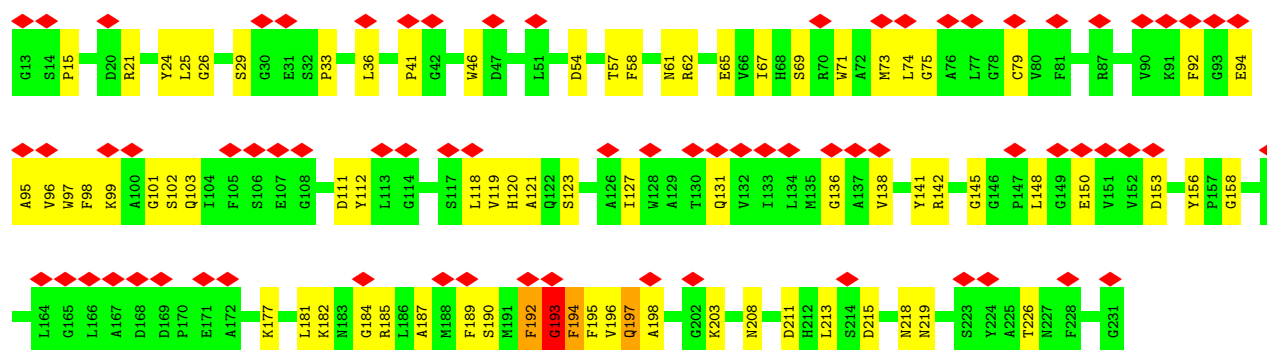


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

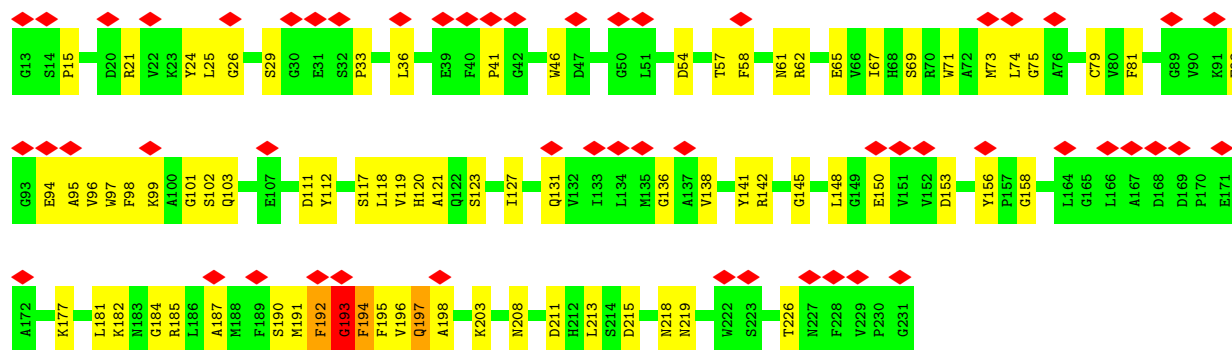




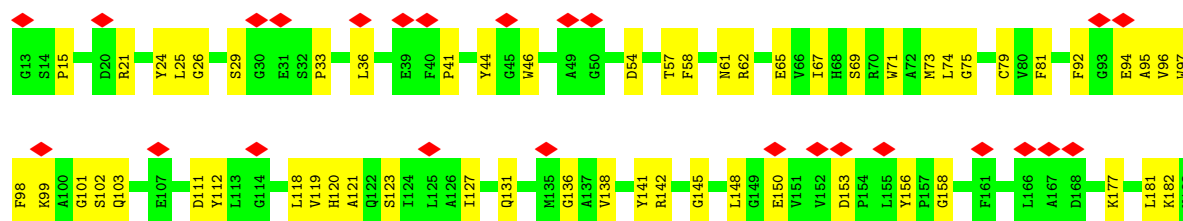
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

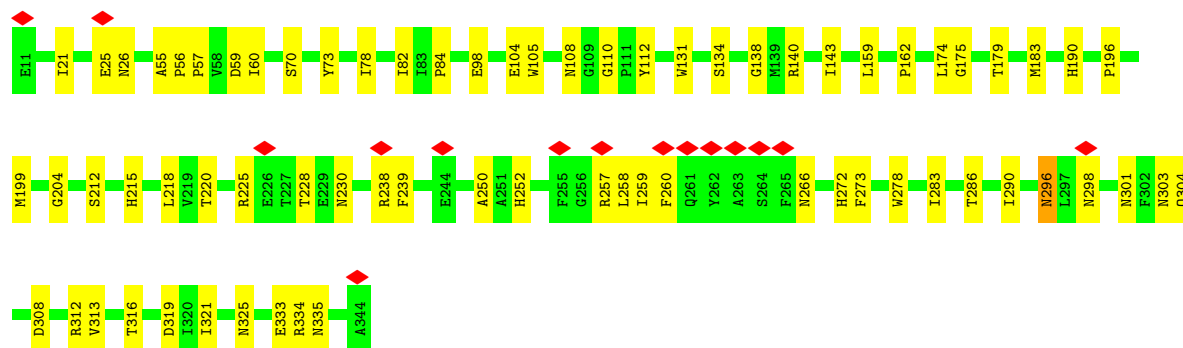
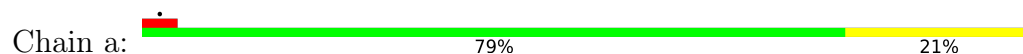


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

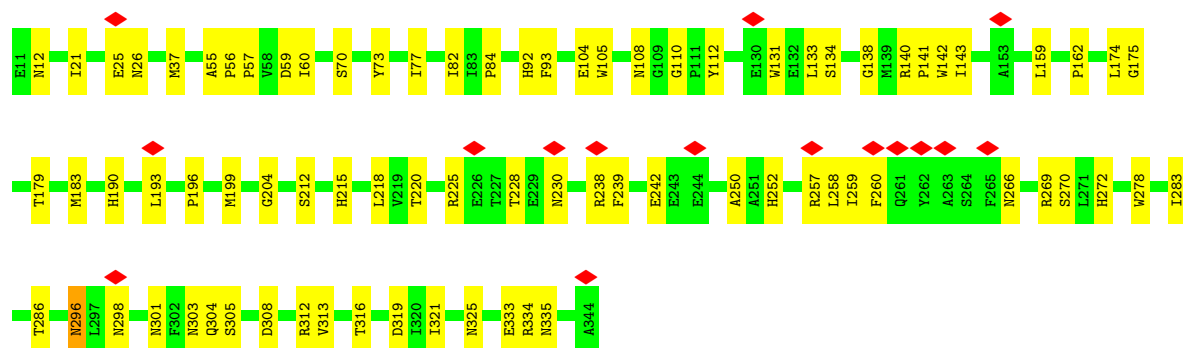
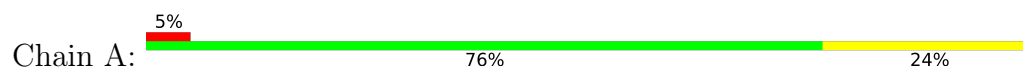




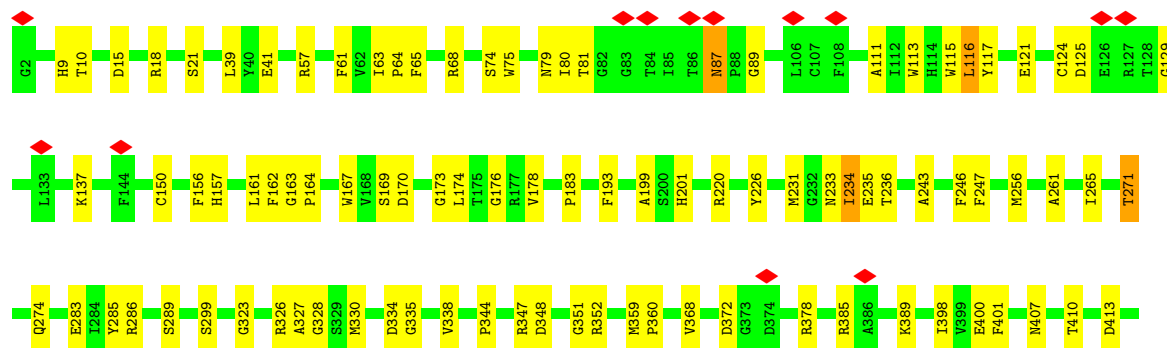
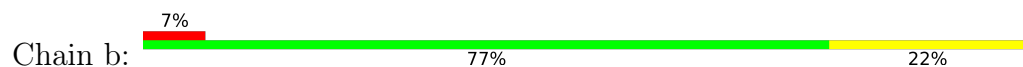
• Molecule 2: Photosystem II protein D1

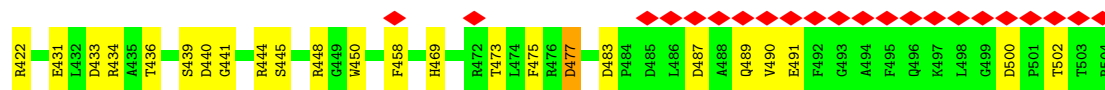


• Molecule 2: Photosystem II protein D1

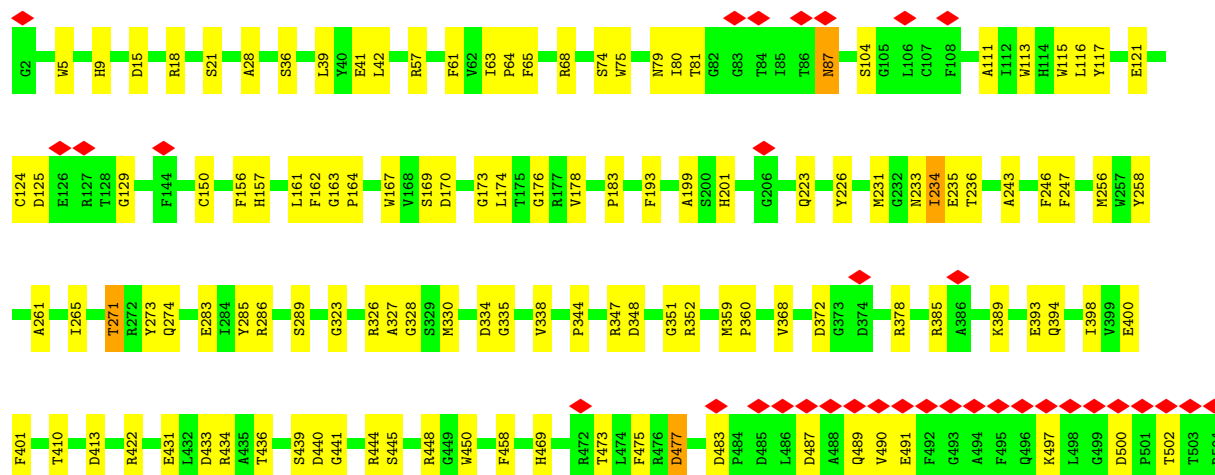
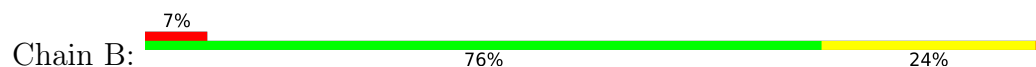


• Molecule 3: Photosystem II CP47 reaction center protein

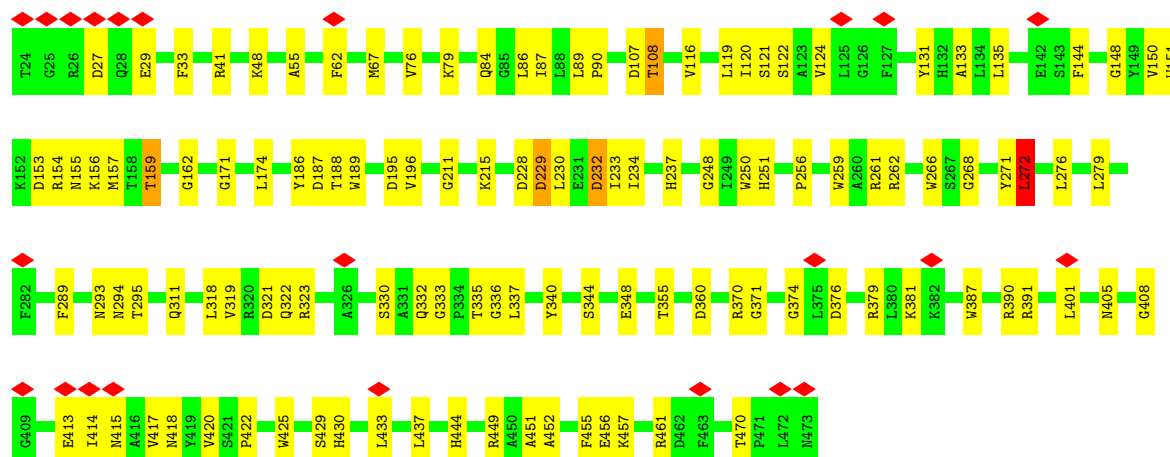




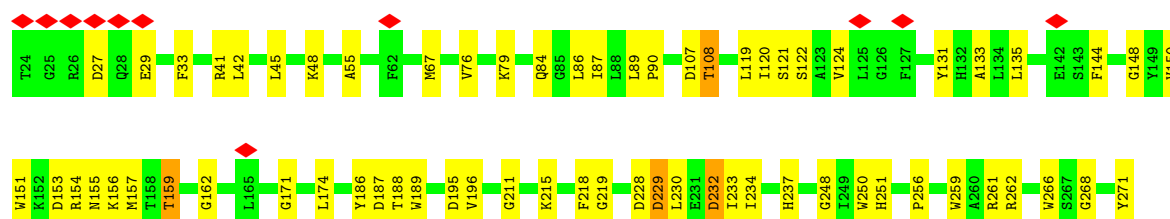
• Molecule 3: Photosystem II CP47 reaction center protein

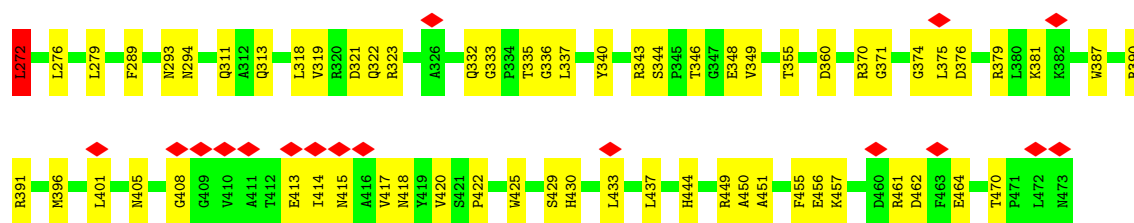


• Molecule 4: Photosystem II CP43 reaction center protein

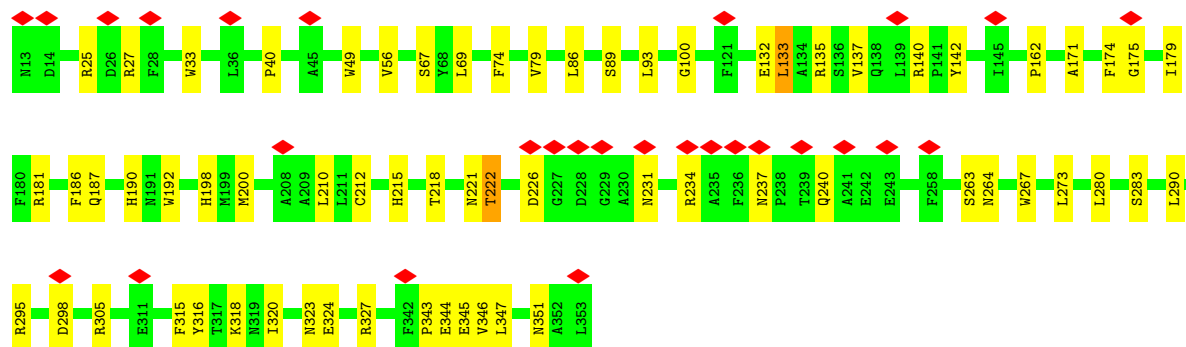
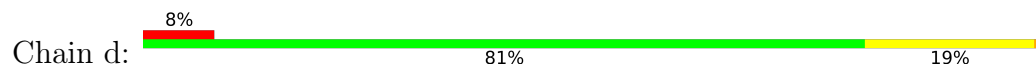


• Molecule 4: Photosystem II CP43 reaction center protein

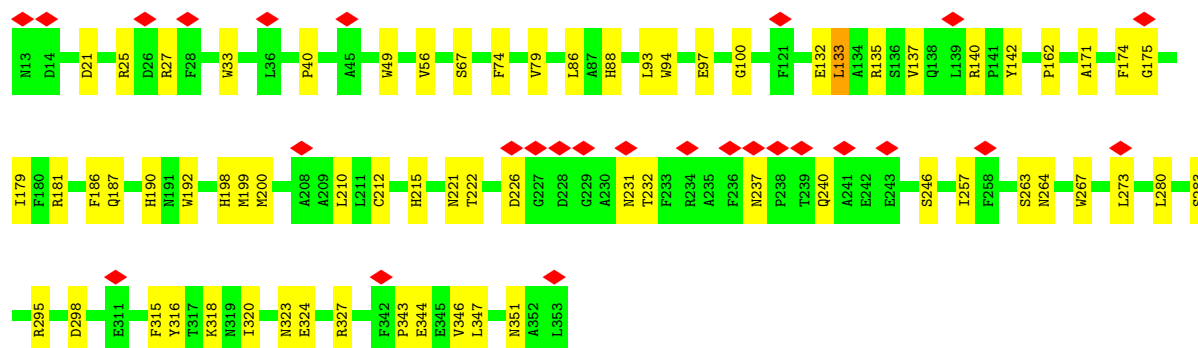
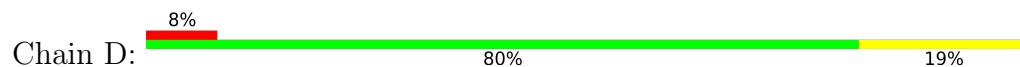




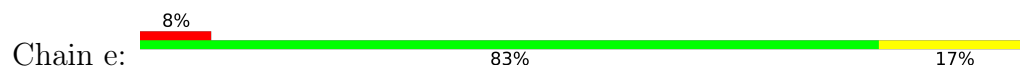
• Molecule 5: Photosystem II D2 protein



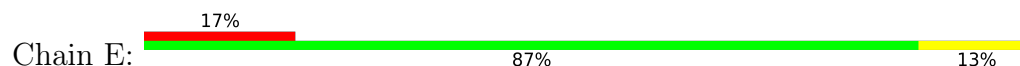
• Molecule 5: Photosystem II D2 protein

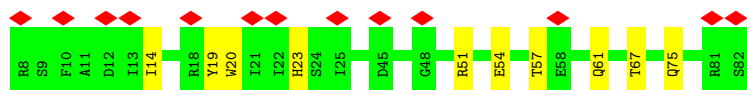


• Molecule 6: Cytochrome b559 subunit alpha

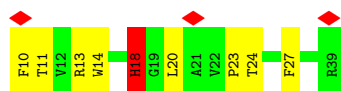


• Molecule 6: Cytochrome b559 subunit alpha

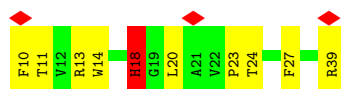




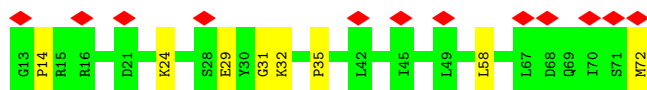
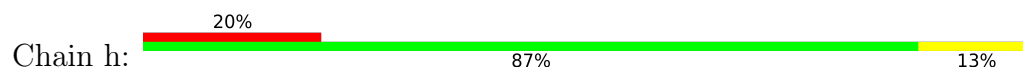
- Molecule 7: Cytochrome b559 subunit beta



- Molecule 7: Cytochrome b559 subunit beta



- Molecule 8: Photosystem II reaction center protein H



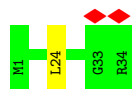
- Molecule 8: Photosystem II reaction center protein H



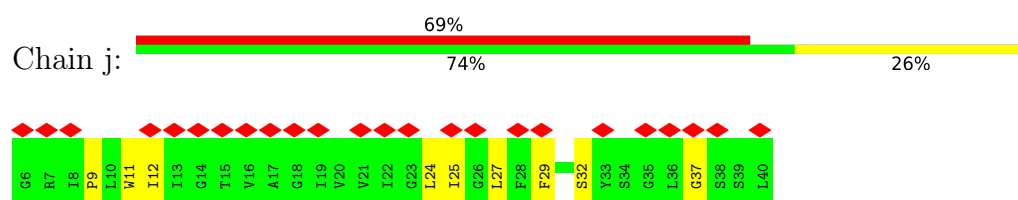
- Molecule 9: Photosystem II reaction center protein I



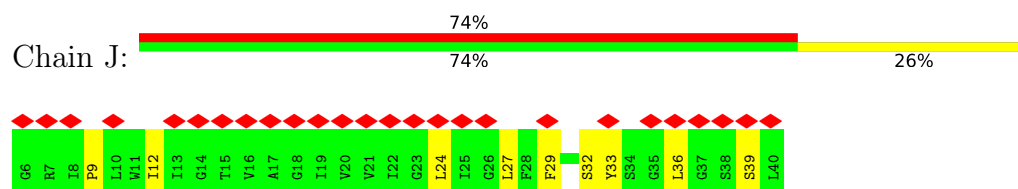
- Molecule 9: Photosystem II reaction center protein I



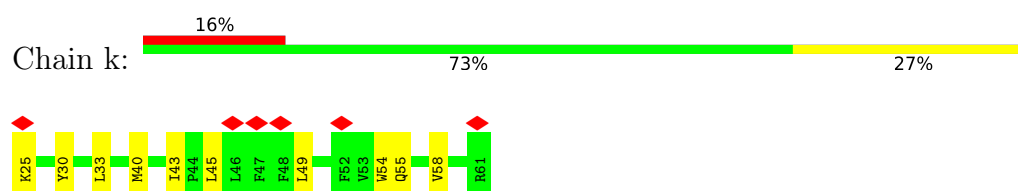
- Molecule 10: Photosystem II reaction center protein J



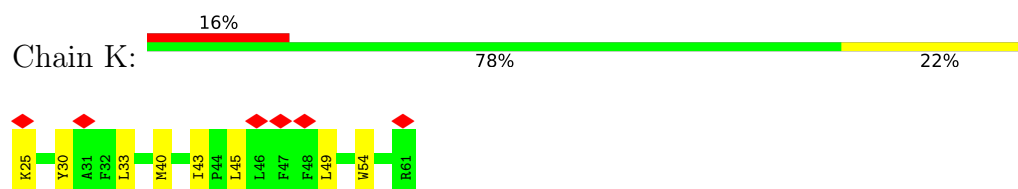
- Molecule 10: Photosystem II reaction center protein J



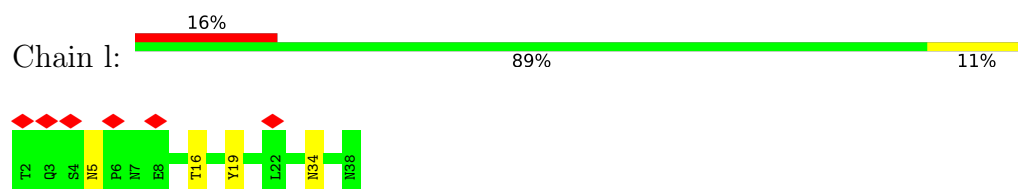
- Molecule 11: Photosystem II reaction center protein K



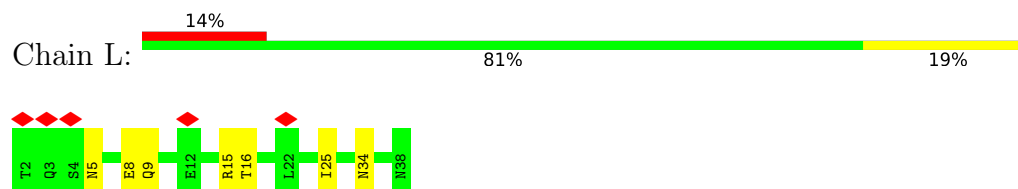
- Molecule 11: Photosystem II reaction center protein K



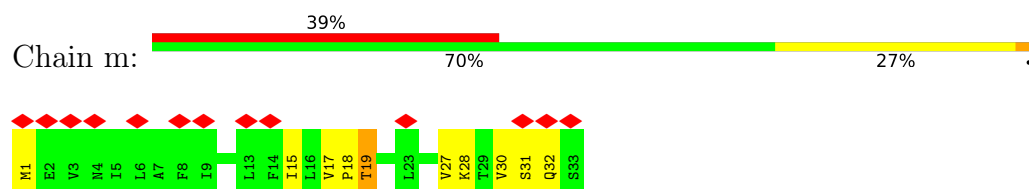
- Molecule 12: Photosystem II reaction center protein L



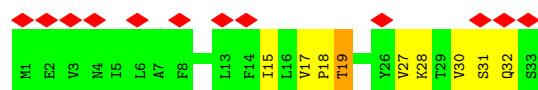
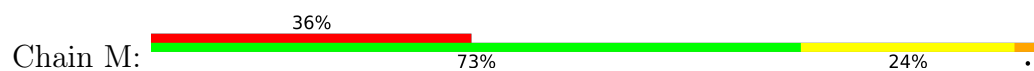
- Molecule 12: Photosystem II reaction center protein L



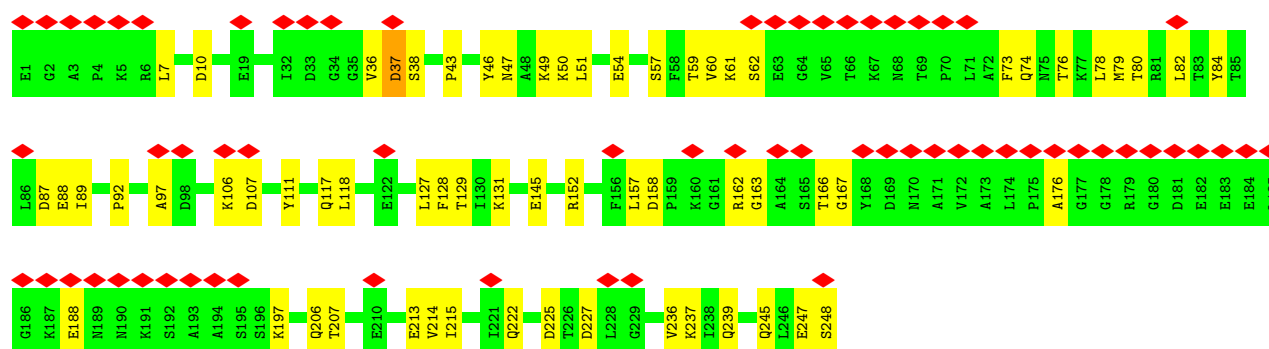
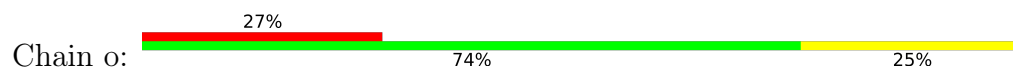
- Molecule 13: Photosystem II reaction center protein M



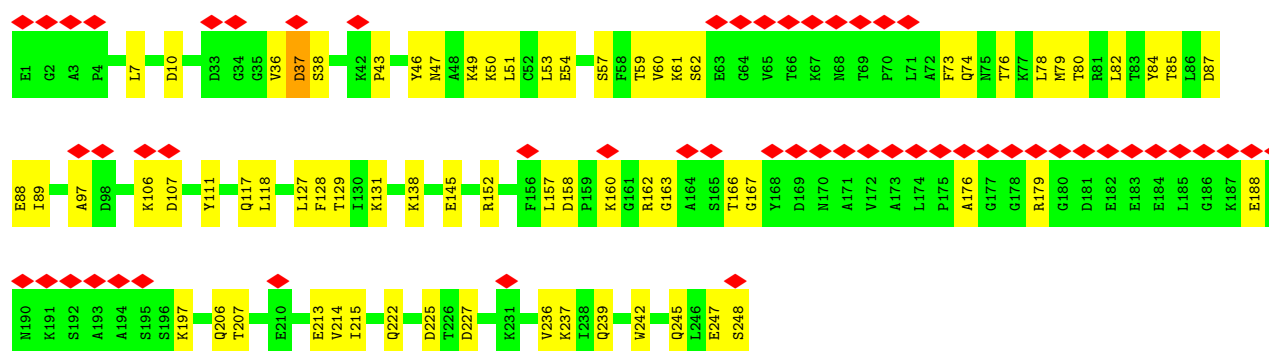
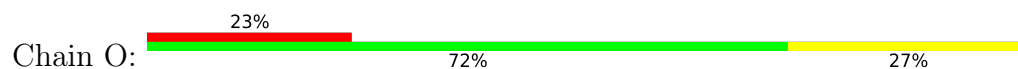
- Molecule 13: Photosystem II reaction center protein M



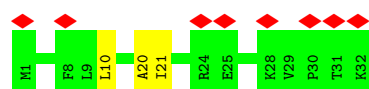
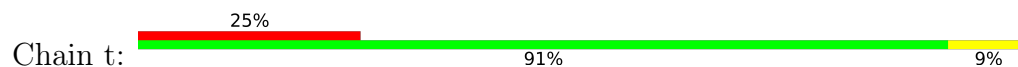
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic



- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic



- Molecule 15: Photosystem II reaction center protein T

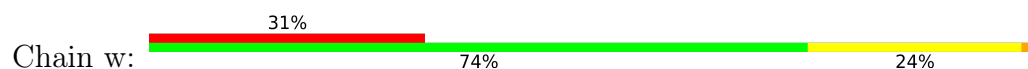


- Molecule 15: Photosystem II reaction center protein T

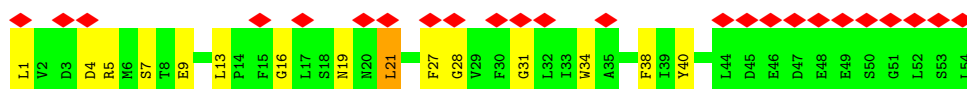




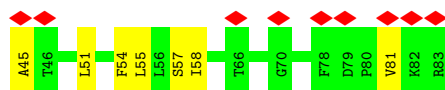
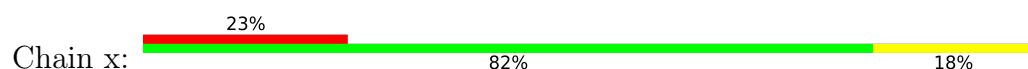
- Molecule 16: Photosystem II reaction center protein W



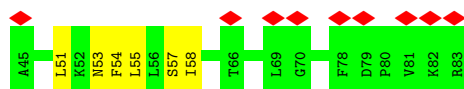
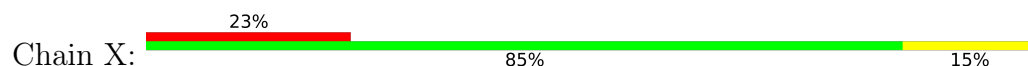
- Molecule 16: Photosystem II reaction center protein W



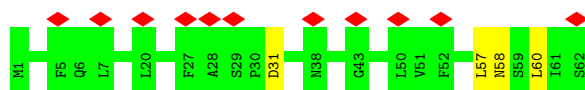
- Molecule 17: Ultraviolet-B-repressible protein



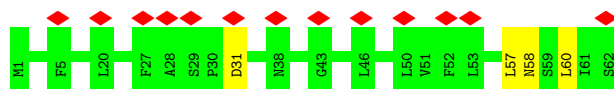
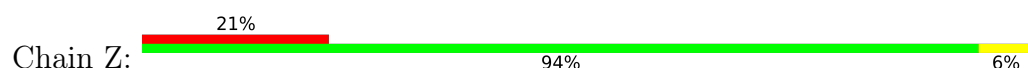
- Molecule 17: Ultraviolet-B-repressible protein



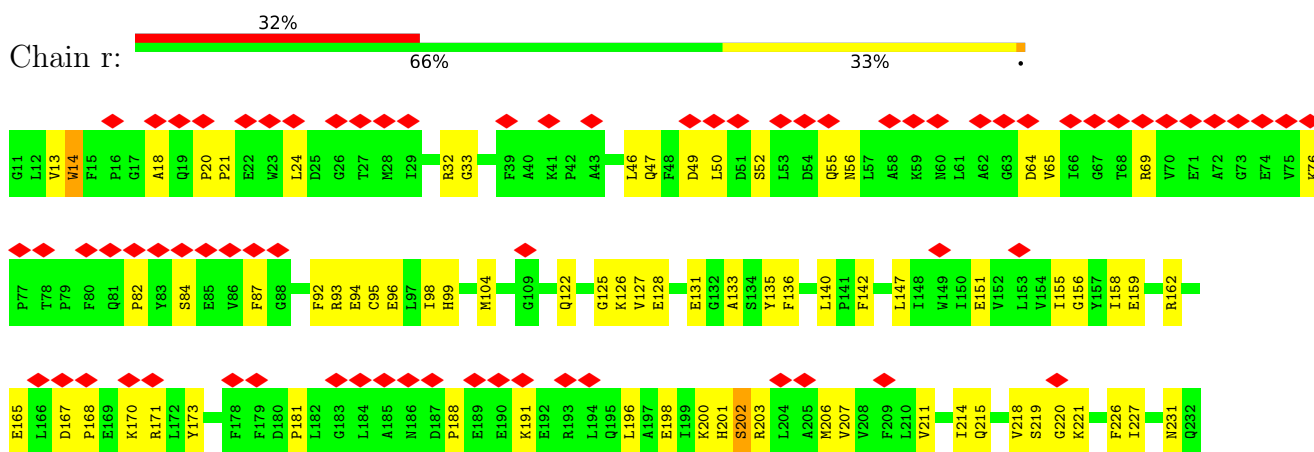
- Molecule 18: Photosystem II reaction center protein Z



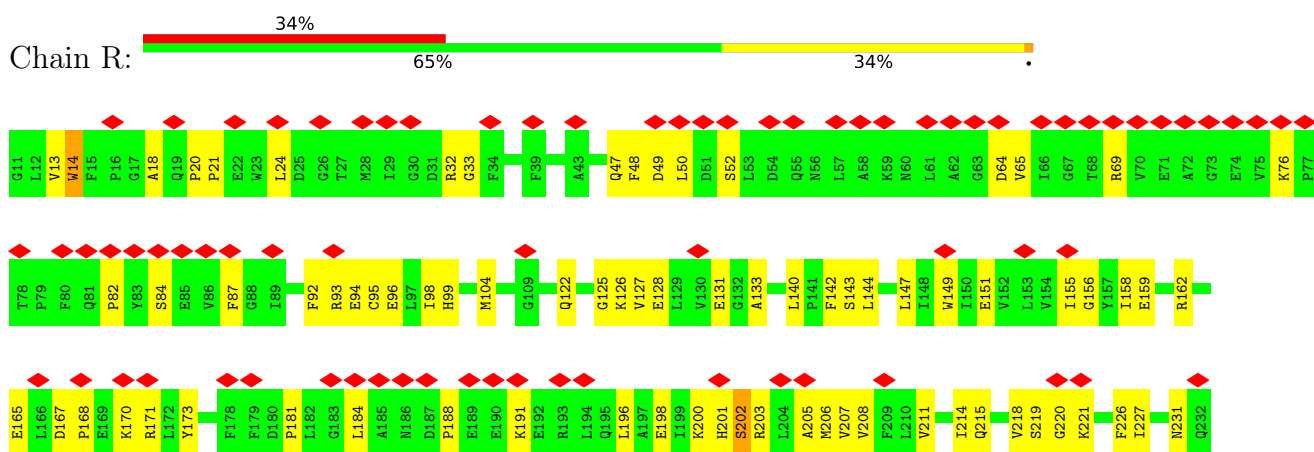
- Molecule 18: Photosystem II reaction center protein Z



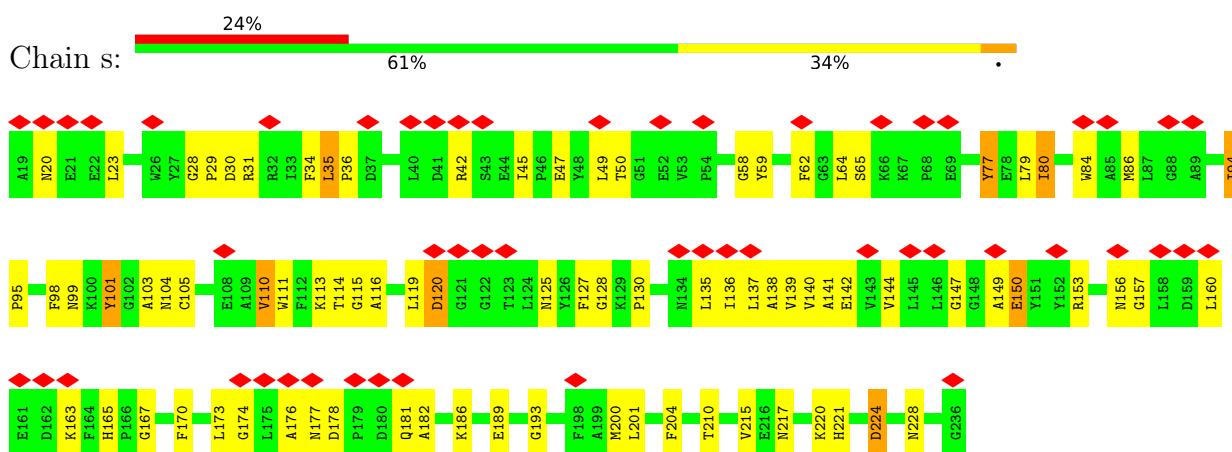
- Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4.3



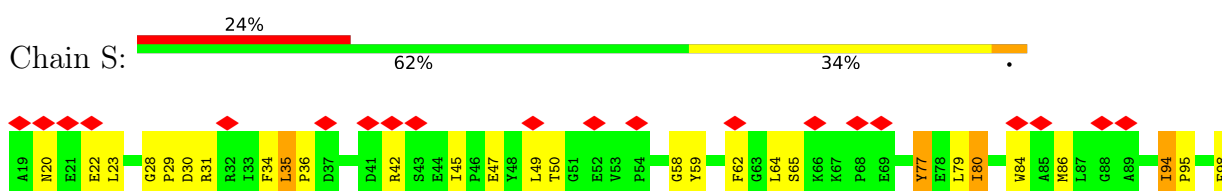
• Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4.3

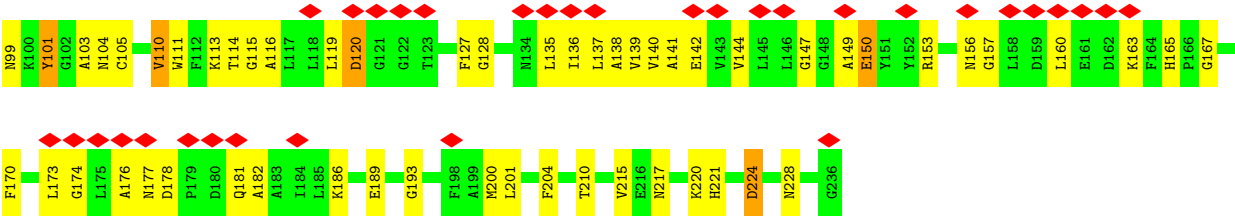


• Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26



• Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26





## 4 Experimental information

| Property                             | Value                                            | Source    |
|--------------------------------------|--------------------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                                  | Depositor |
| Imposed symmetry                     | POINT, C2                                        | Depositor |
| Number of particles used             | 27942                                            | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                                | Depositor |
| CTF correction method                | NONE                                             | Depositor |
| Microscope                           | FEI TITAN KRIOS                                  | Depositor |
| Voltage (kV)                         | 300                                              | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40, 40                                           | Depositor |
| Minimum defocus (nm)                 | Not provided                                     |           |
| Maximum defocus (nm)                 | Not provided                                     |           |
| Magnification                        | Not provided                                     |           |
| Image detector                       | GATAN K2 BASE (4k x 4k), GATAN K2 BASE (4k x 4k) | Depositor |
| Maximum map value                    | 1.923                                            | Depositor |
| Minimum map value                    | -0.630                                           | Depositor |
| Average map value                    | 0.055                                            | Depositor |
| Map value standard deviation         | 0.166                                            | Depositor |
| Recommended contour level            | 0.85                                             | Depositor |
| Map size (Å)                         | 374.0, 374.0, 374.0                              | wwPDB     |
| Map dimensions                       | 340, 340, 340                                    | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                                 | wwPDB     |
| Pixel spacing (Å)                    | 1.1, 1.1, 1.1                                    | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, LHG, OEX, LMG, CLA, BCT, NEX, PL9, BCR, CHL, XAT, FE2, CL, LUT, PHO, SQD, HEM

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   | G     | 0.22         | 0/1720        | 0.47        | 3/2342 (0.1%) |
| 1   | N     | 0.22         | 0/1720        | 0.47        | 3/2342 (0.1%) |
| 1   | Y     | 0.22         | 0/1720        | 0.47        | 3/2342 (0.1%) |
| 1   | g     | 0.22         | 0/1720        | 0.47        | 3/2342 (0.1%) |
| 1   | n     | 0.22         | 0/1720        | 0.47        | 3/2342 (0.1%) |
| 1   | y     | 0.22         | 0/1720        | 0.47        | 3/2342 (0.1%) |
| 2   | A     | 0.22         | 0/2697        | 0.39        | 0/3677        |
| 2   | a     | 0.22         | 0/2697        | 0.39        | 0/3677        |
| 3   | B     | 0.21         | 0/4081        | 0.36        | 0/5556        |
| 3   | b     | 0.21         | 0/4081        | 0.36        | 0/5556        |
| 4   | C     | 0.88         | 1/3614 (0.0%) | 0.40        | 2/4922 (0.0%) |
| 4   | c     | 0.88         | 1/3614 (0.0%) | 0.40        | 2/4922 (0.0%) |
| 5   | D     | 0.21         | 0/2804        | 0.36        | 0/3823        |
| 5   | d     | 0.21         | 0/2804        | 0.36        | 0/3823        |
| 6   | E     | 0.17         | 0/630         | 0.34        | 0/857         |
| 6   | e     | 0.17         | 0/630         | 0.34        | 0/857         |
| 7   | F     | 0.66         | 1/248 (0.4%)  | 0.58        | 0/335         |
| 7   | f     | 0.66         | 1/248 (0.4%)  | 0.58        | 0/335         |
| 8   | H     | 0.19         | 0/461         | 0.37        | 0/626         |
| 8   | h     | 0.19         | 0/461         | 0.36        | 0/626         |
| 9   | I     | 0.25         | 0/286         | 0.39        | 0/386         |
| 9   | i     | 0.24         | 0/286         | 0.39        | 0/386         |
| 10  | J     | 0.13         | 0/262         | 0.34        | 0/354         |
| 10  | j     | 0.14         | 0/262         | 0.34        | 0/354         |
| 11  | K     | 0.21         | 0/318         | 0.46        | 0/434         |
| 11  | k     | 0.21         | 0/318         | 0.46        | 0/434         |
| 12  | L     | 0.21         | 0/319         | 0.37        | 0/434         |
| 12  | l     | 0.21         | 0/319         | 0.37        | 0/434         |
| 13  | M     | 0.20         | 0/260         | 0.37        | 0/355         |
| 13  | m     | 0.20         | 0/260         | 0.37        | 0/355         |
| 14  | O     | 0.17         | 0/1906        | 0.33        | 0/2575        |

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 14  | o     | 0.17         | 0/1906         | 0.33        | 0/2575          |
| 15  | T     | 0.25         | 0/269          | 0.35        | 0/365           |
| 15  | t     | 0.25         | 0/269          | 0.35        | 0/365           |
| 16  | W     | 0.25         | 0/429          | 0.38        | 0/581           |
| 16  | w     | 0.25         | 0/429          | 0.38        | 0/581           |
| 17  | X     | 0.18         | 0/279          | 0.35        | 0/380           |
| 17  | x     | 0.19         | 0/279          | 0.35        | 0/380           |
| 18  | Z     | 0.17         | 0/474          | 0.26        | 0/648           |
| 18  | z     | 0.17         | 0/474          | 0.27        | 0/648           |
| 19  | R     | 0.17         | 0/1780         | 0.34        | 0/2417          |
| 19  | r     | 0.17         | 0/1780         | 0.34        | 0/2417          |
| 20  | S     | 0.20         | 0/1737         | 0.41        | 0/2361          |
| 20  | s     | 0.20         | 0/1737         | 0.41        | 0/2361          |
| All | All   | 0.37         | 4/56028 (0.0%) | 0.39        | 22/76224 (0.0%) |

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 |
|-----|-------|---------------------|---------------------|
| 1   | G     | 0                   | 2                   |
| 1   | N     | 0                   | 2                   |
| 1   | Y     | 0                   | 2                   |
| 1   | g     | 0                   | 2                   |
| 1   | n     | 0                   | 2                   |
| 1   | y     | 0                   | 2                   |
| All | All   | 0                   | 12                  |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | c     | 272 | LEU  | CG-CD1 | 50.99 | 3.20        | 1.52     |
| 4   | C     | 272 | LEU  | CG-CD1 | 50.99 | 3.20        | 1.52     |
| 7   | F     | 18  | HIS  | CB-CG  | 9.20  | 1.63        | 1.50     |
| 7   | f     | 18  | HIS  | CB-CG  | 9.17  | 1.62        | 1.50     |

The worst 5 of 22 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | n     | 194 | PHE  | N-CA-C | 8.26 | 121.89      | 111.24   |
| 1   | Y     | 194 | PHE  | N-CA-C | 8.25 | 121.88      | 111.24   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | g     | 194 | PHE  | N-CA-C | 8.24 | 121.87      | 111.24   |
| 1   | G     | 194 | PHE  | N-CA-C | 8.24 | 121.87      | 111.24   |
| 1   | y     | 194 | PHE  | N-CA-C | 8.22 | 121.85      | 111.24   |

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | g     | 193 | GLY  | Mainchain |
| 1   | g     | 197 | GLN  | Sidechain |
| 1   | n     | 193 | GLY  | Mainchain |
| 1   | n     | 197 | GLN  | Sidechain |
| 1   | y     | 193 | GLY  | Mainchain |

## 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   | G     | 1668  | 0        | 1596     | 144     | 0            |
| 1   | N     | 1668  | 0        | 1596     | 150     | 0            |
| 1   | Y     | 1668  | 0        | 1596     | 149     | 0            |
| 1   | g     | 1668  | 0        | 1596     | 146     | 0            |
| 1   | n     | 1668  | 0        | 1596     | 146     | 0            |
| 1   | y     | 1668  | 0        | 1596     | 148     | 0            |
| 2   | A     | 2616  | 0        | 2522     | 70      | 0            |
| 2   | a     | 2616  | 0        | 2522     | 60      | 0            |
| 3   | B     | 3948  | 0        | 3818     | 97      | 0            |
| 3   | b     | 3948  | 0        | 3818     | 93      | 0            |
| 4   | C     | 3497  | 0        | 3422     | 107     | 0            |
| 4   | c     | 3497  | 0        | 3422     | 105     | 0            |
| 5   | D     | 2712  | 0        | 2604     | 52      | 0            |
| 5   | d     | 2712  | 0        | 2604     | 47      | 0            |
| 6   | E     | 612   | 0        | 595      | 7       | 0            |
| 6   | e     | 612   | 0        | 595      | 8       | 0            |
| 7   | F     | 241   | 0        | 246      | 24      | 0            |
| 7   | f     | 241   | 0        | 246      | 23      | 0            |
| 8   | H     | 452   | 0        | 473      | 4       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8   | h     | 452   | 0        | 473      | 11      | 0            |
| 9   | I     | 278   | 0        | 291      | 1       | 0            |
| 9   | i     | 278   | 0        | 291      | 3       | 0            |
| 10  | J     | 256   | 0        | 269      | 7       | 0            |
| 10  | j     | 256   | 0        | 269      | 6       | 0            |
| 11  | K     | 306   | 0        | 313      | 4       | 0            |
| 11  | k     | 306   | 0        | 313      | 8       | 0            |
| 12  | L     | 311   | 0        | 298      | 10      | 0            |
| 12  | l     | 311   | 0        | 298      | 6       | 0            |
| 13  | M     | 256   | 0        | 284      | 7       | 0            |
| 13  | m     | 256   | 0        | 284      | 8       | 0            |
| 14  | O     | 1870  | 0        | 1851     | 47      | 0            |
| 14  | o     | 1870  | 0        | 1851     | 44      | 0            |
| 15  | T     | 261   | 0        | 280      | 2       | 0            |
| 15  | t     | 261   | 0        | 280      | 3       | 0            |
| 16  | W     | 419   | 0        | 402      | 19      | 0            |
| 16  | w     | 419   | 0        | 402      | 13      | 0            |
| 17  | X     | 276   | 0        | 301      | 4       | 0            |
| 17  | x     | 276   | 0        | 301      | 5       | 0            |
| 18  | Z     | 464   | 0        | 493      | 3       | 0            |
| 18  | z     | 464   | 0        | 493      | 2       | 0            |
| 19  | R     | 1732  | 0        | 1697     | 67      | 0            |
| 19  | r     | 1732  | 0        | 1697     | 71      | 0            |
| 20  | S     | 1688  | 0        | 1649     | 118     | 0            |
| 20  | s     | 1688  | 0        | 1650     | 120     | 0            |
| 21  | G     | 355   | 0        | 335      | 168     | 0            |
| 21  | N     | 314   | 0        | 317      | 147     | 0            |
| 21  | R     | 183   | 0        | 173      | 76      | 0            |
| 21  | S     | 186   | 0        | 124      | 104     | 0            |
| 21  | Y     | 314   | 0        | 317      | 145     | 0            |
| 21  | g     | 355   | 0        | 335      | 145     | 0            |
| 21  | n     | 314   | 0        | 317      | 142     | 0            |
| 21  | r     | 231   | 0        | 206      | 83      | 0            |
| 21  | s     | 186   | 0        | 124      | 107     | 0            |
| 21  | y     | 362   | 0        | 350      | 154     | 0            |
| 22  | A     | 240   | 0        | 242      | 10      | 0            |
| 22  | B     | 1040  | 0        | 1152     | 40      | 0            |
| 22  | C     | 845   | 0        | 935      | 64      | 0            |
| 22  | D     | 130   | 0        | 144      | 5       | 0            |
| 22  | G     | 477   | 0        | 471      | 55      | 0            |
| 22  | N     | 473   | 0        | 462      | 59      | 0            |
| 22  | R     | 400   | 0        | 373      | 29      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | S     | 471   | 0        | 389      | 34      | 0            |
| 22  | W     | 60    | 0        | 59       | 16      | 0            |
| 22  | Y     | 413   | 0        | 403      | 66      | 0            |
| 22  | a     | 240   | 0        | 242      | 12      | 0            |
| 22  | b     | 975   | 0        | 1080     | 37      | 0            |
| 22  | c     | 845   | 0        | 935      | 67      | 0            |
| 22  | d     | 130   | 0        | 144      | 7       | 0            |
| 22  | g     | 477   | 0        | 471      | 54      | 0            |
| 22  | n     | 473   | 0        | 462      | 54      | 0            |
| 22  | r     | 400   | 0        | 373      | 23      | 0            |
| 22  | s     | 471   | 0        | 389      | 30      | 0            |
| 22  | w     | 60    | 0        | 58       | 5       | 0            |
| 22  | x     | 65    | 0        | 72       | 2       | 0            |
| 22  | y     | 413   | 0        | 403      | 50      | 0            |
| 23  | G     | 84    | 0        | 112      | 21      | 0            |
| 23  | N     | 84    | 0        | 112      | 28      | 0            |
| 23  | R     | 42    | 0        | 55       | 2       | 0            |
| 23  | Y     | 84    | 0        | 112      | 25      | 0            |
| 23  | g     | 84    | 0        | 112      | 24      | 0            |
| 23  | n     | 42    | 0        | 56       | 12      | 0            |
| 23  | r     | 42    | 0        | 55       | 2       | 0            |
| 23  | y     | 42    | 0        | 56       | 11      | 0            |
| 24  | G     | 44    | 0        | 55       | 1       | 0            |
| 24  | N     | 44    | 0        | 55       | 2       | 0            |
| 24  | R     | 44    | 0        | 55       | 5       | 0            |
| 24  | Y     | 44    | 0        | 55       | 2       | 0            |
| 24  | g     | 44    | 0        | 55       | 0       | 0            |
| 24  | n     | 44    | 0        | 55       | 2       | 0            |
| 24  | r     | 44    | 0        | 55       | 5       | 0            |
| 24  | y     | 44    | 0        | 55       | 2       | 0            |
| 25  | N     | 44    | 0        | 56       | 9       | 0            |
| 25  | Y     | 44    | 0        | 56       | 9       | 0            |
| 25  | g     | 44    | 0        | 56       | 8       | 0            |
| 25  | n     | 44    | 0        | 56       | 12      | 0            |
| 25  | r     | 44    | 0        | 56       | 8       | 0            |
| 25  | y     | 88    | 0        | 112      | 16      | 0            |
| 26  | B     | 49    | 0        | 74       | 1       | 0            |
| 26  | C     | 147   | 0        | 220      | 14      | 0            |
| 26  | D     | 138   | 0        | 195      | 9       | 0            |
| 26  | G     | 49    | 0        | 74       | 13      | 0            |
| 26  | L     | 49    | 0        | 74       | 2       | 0            |
| 26  | N     | 49    | 0        | 74       | 9       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 26  | R     | 47    | 0        | 66       | 5       | 0            |
| 26  | S     | 49    | 0        | 74       | 6       | 0            |
| 26  | Y     | 49    | 0        | 74       | 10      | 0            |
| 26  | b     | 49    | 0        | 74       | 1       | 0            |
| 26  | c     | 147   | 0        | 220      | 8       | 0            |
| 26  | d     | 138   | 0        | 195      | 12      | 0            |
| 26  | g     | 49    | 0        | 74       | 6       | 0            |
| 26  | l     | 49    | 0        | 74       | 0       | 0            |
| 26  | n     | 49    | 0        | 74       | 10      | 0            |
| 26  | r     | 47    | 0        | 66       | 3       | 0            |
| 26  | s     | 49    | 0        | 74       | 7       | 0            |
| 26  | y     | 49    | 0        | 74       | 9       | 0            |
| 27  | A     | 10    | 0        | 0        | 0       | 0            |
| 27  | a     | 10    | 0        | 0        | 0       | 0            |
| 28  | A     | 1     | 0        | 0        | 0       | 0            |
| 28  | a     | 1     | 0        | 0        | 0       | 0            |
| 29  | A     | 1     | 0        | 0        | 1       | 0            |
| 29  | C     | 1     | 0        | 0        | 0       | 0            |
| 29  | a     | 1     | 0        | 0        | 1       | 0            |
| 29  | c     | 1     | 0        | 0        | 0       | 0            |
| 30  | A     | 64    | 0        | 74       | 4       | 0            |
| 30  | D     | 64    | 0        | 74       | 6       | 0            |
| 30  | a     | 64    | 0        | 74       | 5       | 0            |
| 30  | d     | 64    | 0        | 74       | 6       | 0            |
| 31  | A     | 40    | 0        | 56       | 2       | 0            |
| 31  | B     | 160   | 0        | 224      | 8       | 0            |
| 31  | C     | 80    | 0        | 112      | 8       | 0            |
| 31  | D     | 40    | 0        | 56       | 4       | 0            |
| 31  | H     | 40    | 0        | 56       | 3       | 0            |
| 31  | K     | 80    | 0        | 112      | 5       | 0            |
| 31  | T     | 40    | 0        | 56       | 2       | 0            |
| 31  | a     | 40    | 0        | 56       | 1       | 0            |
| 31  | b     | 120   | 0        | 168      | 8       | 0            |
| 31  | c     | 80    | 0        | 112      | 7       | 0            |
| 31  | d     | 40    | 0        | 56       | 4       | 0            |
| 31  | h     | 40    | 0        | 56       | 5       | 0            |
| 31  | k     | 80    | 0        | 112      | 5       | 0            |
| 32  | A     | 13    | 0        | 7        | 2       | 0            |
| 32  | D     | 55    | 0        | 80       | 3       | 0            |
| 32  | a     | 13    | 0        | 7        | 2       | 0            |
| 32  | d     | 55    | 0        | 80       | 3       | 0            |
| 33  | A     | 54    | 0        | 78       | 4       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 33  | D     | 50    | 0        | 66       | 3       | 0            |
| 33  | L     | 96    | 0        | 125      | 9       | 0            |
| 33  | a     | 54    | 0        | 78       | 4       | 0            |
| 33  | d     | 50    | 0        | 66       | 3       | 0            |
| 33  | l     | 96    | 0        | 125      | 7       | 0            |
| 34  | D     | 4     | 0        | 0        | 4       | 0            |
| 34  | a     | 4     | 0        | 0        | 4       | 0            |
| 35  | A     | 59    | 0        | 76       | 7       | 0            |
| 35  | C     | 117   | 0        | 150      | 10      | 0            |
| 35  | H     | 62    | 0        | 82       | 8       | 0            |
| 35  | J     | 60    | 0        | 78       | 6       | 0            |
| 35  | a     | 59    | 0        | 76       | 7       | 0            |
| 35  | c     | 177   | 0        | 228      | 14      | 0            |
| 35  | h     | 62    | 0        | 82       | 4       | 0            |
| 36  | B     | 95    | 0        | 134      | 58      | 0            |
| 36  | C     | 99    | 0        | 138      | 5       | 0            |
| 36  | D     | 46    | 0        | 62       | 2       | 0            |
| 36  | I     | 40    | 0        | 50       | 6       | 0            |
| 36  | K     | 51    | 0        | 72       | 1       | 0            |
| 36  | M     | 51    | 0        | 72       | 5       | 0            |
| 36  | T     | 51    | 0        | 72       | 5       | 0            |
| 36  | b     | 55    | 0        | 86       | 36      | 0            |
| 36  | c     | 51    | 0        | 72       | 3       | 0            |
| 36  | d     | 46    | 0        | 62       | 4       | 0            |
| 36  | k     | 51    | 0        | 72       | 1       | 0            |
| 36  | w     | 48    | 0        | 66       | 3       | 0            |
| 37  | F     | 43    | 0        | 30       | 17      | 0            |
| 37  | f     | 43    | 0        | 30       | 20      | 0            |
| All | All   | 71784 | 0        | 72432    | 3133    | 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 22.

The worst 5 of 3133 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:y:121:ALA:CB   | 21:y:605:CHL:CB   | 1.79                     | 1.57              |
| 1:y:102:SER:CB   | 21:y:607:CHL:HED3 | 1.35                     | 1.56              |
| 20:S:101:TYR:CE1 | 21:S:301:CHL:CMA  | 1.87                     | 1.54              |
| 1:y:102:SER:HB3  | 21:y:607:CHL:CED  | 1.34                     | 1.53              |
| 1:g:102:SER:HB3  | 21:g:607:CHL:CED  | 1.34                     | 1.53              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | G     | 217/219 (99%)  | 202 (93%) | 15 (7%) | 0        | 100         | 100 |
| 1   | N     | 217/219 (99%)  | 202 (93%) | 15 (7%) | 0        | 100         | 100 |
| 1   | Y     | 217/219 (99%)  | 202 (93%) | 15 (7%) | 0        | 100         | 100 |
| 1   | g     | 217/219 (99%)  | 202 (93%) | 15 (7%) | 0        | 100         | 100 |
| 1   | n     | 217/219 (99%)  | 202 (93%) | 15 (7%) | 0        | 100         | 100 |
| 1   | y     | 217/219 (99%)  | 202 (93%) | 15 (7%) | 0        | 100         | 100 |
| 2   | A     | 332/334 (99%)  | 320 (96%) | 12 (4%) | 0        | 100         | 100 |
| 2   | a     | 332/334 (99%)  | 320 (96%) | 12 (4%) | 0        | 100         | 100 |
| 3   | B     | 501/503 (100%) | 485 (97%) | 16 (3%) | 0        | 100         | 100 |
| 3   | b     | 501/503 (100%) | 485 (97%) | 16 (3%) | 0        | 100         | 100 |
| 4   | C     | 448/450 (100%) | 428 (96%) | 20 (4%) | 0        | 100         | 100 |
| 4   | c     | 448/450 (100%) | 428 (96%) | 20 (4%) | 0        | 100         | 100 |
| 5   | D     | 339/341 (99%)  | 326 (96%) | 13 (4%) | 0        | 100         | 100 |
| 5   | d     | 339/341 (99%)  | 327 (96%) | 12 (4%) | 0        | 100         | 100 |
| 6   | E     | 73/75 (97%)    | 73 (100%) | 0       | 0        | 100         | 100 |
| 6   | e     | 73/75 (97%)    | 73 (100%) | 0       | 0        | 100         | 100 |
| 7   | F     | 28/30 (93%)    | 25 (89%)  | 3 (11%) | 0        | 100         | 100 |
| 7   | f     | 28/30 (93%)    | 25 (89%)  | 3 (11%) | 0        | 100         | 100 |
| 8   | H     | 58/60 (97%)    | 57 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 8   | h     | 58/60 (97%)    | 57 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 9   | I     | 32/34 (94%)    | 32 (100%) | 0       | 0        | 100         | 100 |
| 9   | i     | 32/34 (94%)    | 32 (100%) | 0       | 0        | 100         | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 10  | J     | 33/35 (94%)     | 33 (100%)  | 0        | 0        | 100         | 100 |
| 10  | j     | 33/35 (94%)     | 33 (100%)  | 0        | 0        | 100         | 100 |
| 11  | K     | 35/37 (95%)     | 32 (91%)   | 3 (9%)   | 0        | 100         | 100 |
| 11  | k     | 35/37 (95%)     | 32 (91%)   | 3 (9%)   | 0        | 100         | 100 |
| 12  | L     | 35/37 (95%)     | 34 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 12  | l     | 35/37 (95%)     | 34 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 13  | M     | 31/33 (94%)     | 31 (100%)  | 0        | 0        | 100         | 100 |
| 13  | m     | 31/33 (94%)     | 31 (100%)  | 0        | 0        | 100         | 100 |
| 14  | O     | 246/248 (99%)   | 230 (94%)  | 16 (6%)  | 0        | 100         | 100 |
| 14  | o     | 246/248 (99%)   | 230 (94%)  | 16 (6%)  | 0        | 100         | 100 |
| 15  | T     | 30/32 (94%)     | 29 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 15  | t     | 30/32 (94%)     | 29 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 16  | W     | 52/54 (96%)     | 48 (92%)   | 4 (8%)   | 0        | 100         | 100 |
| 16  | w     | 52/54 (96%)     | 48 (92%)   | 4 (8%)   | 0        | 100         | 100 |
| 17  | X     | 37/39 (95%)     | 37 (100%)  | 0        | 0        | 100         | 100 |
| 17  | x     | 37/39 (95%)     | 37 (100%)  | 0        | 0        | 100         | 100 |
| 18  | Z     | 60/62 (97%)     | 60 (100%)  | 0        | 0        | 100         | 100 |
| 18  | z     | 60/62 (97%)     | 60 (100%)  | 0        | 0        | 100         | 100 |
| 19  | R     | 220/222 (99%)   | 207 (94%)  | 13 (6%)  | 0        | 100         | 100 |
| 19  | r     | 220/222 (99%)   | 207 (94%)  | 13 (6%)  | 0        | 100         | 100 |
| 20  | S     | 216/218 (99%)   | 198 (92%)  | 18 (8%)  | 0        | 100         | 100 |
| 20  | s     | 216/218 (99%)   | 198 (92%)  | 18 (8%)  | 0        | 100         | 100 |
| All | All   | 6914/7002 (99%) | 6583 (95%) | 331 (5%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 1   | G     | 171/171 (100%) | 168 (98%) | 3 (2%)   | 51          | 67  |
| 1   | N     | 171/171 (100%) | 168 (98%) | 3 (2%)   | 51          | 67  |
| 1   | Y     | 171/171 (100%) | 168 (98%) | 3 (2%)   | 51          | 67  |
| 1   | g     | 171/171 (100%) | 168 (98%) | 3 (2%)   | 51          | 67  |
| 1   | n     | 171/171 (100%) | 168 (98%) | 3 (2%)   | 51          | 67  |
| 1   | y     | 171/171 (100%) | 168 (98%) | 3 (2%)   | 51          | 67  |
| 2   | A     | 270/270 (100%) | 266 (98%) | 4 (2%)   | 57          | 69  |
| 2   | a     | 270/270 (100%) | 266 (98%) | 4 (2%)   | 57          | 69  |
| 3   | B     | 400/400 (100%) | 394 (98%) | 6 (2%)   | 57          | 69  |
| 3   | b     | 400/400 (100%) | 394 (98%) | 6 (2%)   | 57          | 69  |
| 4   | C     | 352/352 (100%) | 341 (97%) | 11 (3%)  | 35          | 57  |
| 4   | c     | 352/352 (100%) | 342 (97%) | 10 (3%)  | 38          | 58  |
| 5   | D     | 275/275 (100%) | 271 (98%) | 4 (2%)   | 57          | 69  |
| 5   | d     | 275/275 (100%) | 271 (98%) | 4 (2%)   | 57          | 69  |
| 6   | E     | 67/67 (100%)   | 67 (100%) | 0        | 100         | 100 |
| 6   | e     | 67/67 (100%)   | 67 (100%) | 0        | 100         | 100 |
| 7   | F     | 25/25 (100%)   | 23 (92%)  | 2 (8%)   | 11          | 36  |
| 7   | f     | 25/25 (100%)   | 23 (92%)  | 2 (8%)   | 11          | 36  |
| 8   | H     | 49/49 (100%)   | 49 (100%) | 0        | 100         | 100 |
| 8   | h     | 49/49 (100%)   | 49 (100%) | 0        | 100         | 100 |
| 9   | I     | 31/31 (100%)   | 31 (100%) | 0        | 100         | 100 |
| 9   | i     | 31/31 (100%)   | 31 (100%) | 0        | 100         | 100 |
| 10  | J     | 26/26 (100%)   | 26 (100%) | 0        | 100         | 100 |
| 10  | j     | 26/26 (100%)   | 26 (100%) | 0        | 100         | 100 |
| 11  | K     | 32/32 (100%)   | 31 (97%)  | 1 (3%)   | 35          | 57  |
| 11  | k     | 32/32 (100%)   | 31 (97%)  | 1 (3%)   | 35          | 57  |
| 12  | L     | 35/35 (100%)   | 35 (100%) | 0        | 100         | 100 |
| 12  | l     | 35/35 (100%)   | 35 (100%) | 0        | 100         | 100 |
| 13  | M     | 29/29 (100%)   | 28 (97%)  | 1 (3%)   | 32          | 55  |
| 13  | m     | 29/29 (100%)   | 28 (97%)  | 1 (3%)   | 32          | 55  |
| 14  | O     | 204/204 (100%) | 201 (98%) | 3 (2%)   | 57          | 69  |
| 14  | o     | 204/204 (100%) | 201 (98%) | 3 (2%)   | 57          | 69  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 15  | T     | 29/29 (100%)     | 29 (100%)  | 0        | 100         | 100 |
| 15  | t     | 29/29 (100%)     | 29 (100%)  | 0        | 100         | 100 |
| 16  | W     | 44/44 (100%)     | 42 (96%)   | 2 (4%)   | 24          | 48  |
| 16  | w     | 44/44 (100%)     | 42 (96%)   | 2 (4%)   | 24          | 48  |
| 17  | X     | 32/32 (100%)     | 32 (100%)  | 0        | 100         | 100 |
| 17  | x     | 32/32 (100%)     | 32 (100%)  | 0        | 100         | 100 |
| 18  | Z     | 54/54 (100%)     | 53 (98%)   | 1 (2%)   | 50          | 66  |
| 18  | z     | 54/54 (100%)     | 53 (98%)   | 1 (2%)   | 50          | 66  |
| 19  | R     | 175/175 (100%)   | 171 (98%)  | 4 (2%)   | 44          | 63  |
| 19  | r     | 175/175 (100%)   | 171 (98%)  | 4 (2%)   | 44          | 63  |
| 20  | S     | 169/169 (100%)   | 156 (92%)  | 13 (8%)  | 12          | 37  |
| 20  | s     | 169/169 (100%)   | 156 (92%)  | 13 (8%)  | 12          | 37  |
| All | All   | 5622/5622 (100%) | 5501 (98%) | 121 (2%) | 45          | 63  |

5 of 121 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B     | 116 | LEU  |
| 20  | S     | 94  | ILE  |
| 4   | C     | 462 | ASP  |
| 20  | S     | 80  | ILE  |
| 19  | R     | 52  | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B     | 466 | HIS  |
| 12  | L     | 34  | ASN  |
| 4   | C     | 322 | GLN  |
| 5   | D     | 84  | ASN  |
| 18  | Z     | 58  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 325 ligands modelled in this entry, 6 are monoatomic - leaving 319 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 22  | CLA  | C     | 509 | -    | 69,73,73     | 1.15 | 8 (11%)     | 82,113,113  | 1.29 | 6 (7%)      |
| 25  | NEX  | Y     | 616 | 22   | 40,46,46     | 4.83 | 17 (42%)    | 50,70,70    | 9.76 | 28 (56%)    |
| 22  | CLA  | b     | 610 | -    | 69,73,73     | 1.16 | 9 (13%)     | 82,113,113  | 1.27 | 5 (6%)      |
| 25  | NEX  | y     | 616 | 22   | 40,46,46     | 4.84 | 16 (40%)    | 50,70,70    | 9.98 | 27 (54%)    |
| 22  | CLA  | b     | 603 | -    | 69,73,73     | 1.14 | 9 (13%)     | 82,113,113  | 1.27 | 5 (6%)      |
| 21  | CHL  | n     | 608 | -    | 60,74,74     | 3.62 | 18 (30%)    | 58,114,114  | 1.98 | 13 (22%)    |
| 21  | CHL  | R     | 305 | -    | 60,74,74     | 3.61 | 18 (30%)    | 58,114,114  | 1.98 | 13 (22%)    |
| 22  | CLA  | r     | 303 | -    | 64,68,73     | 1.21 | 9 (14%)     | 76,107,113  | 1.30 | 5 (6%)      |
| 21  | CHL  | y     | 609 | -    | 60,74,74     | 3.61 | 18 (30%)    | 58,114,114  | 1.98 | 13 (22%)    |
| 26  | LHG  | n     | 617 | 22   | 48,48,48     | 0.65 | 1 (2%)      | 51,54,54    | 1.31 | 7 (13%)     |
| 22  | CLA  | g     | 611 | -    | 64,68,73     | 1.20 | 9 (14%)     | 76,107,113  | 1.29 | 5 (6%)      |
| 22  | CLA  | c     | 507 | -    | 69,73,73     | 1.16 | 9 (13%)     | 82,113,113  | 1.29 | 6 (7%)      |
| 22  | CLA  | G     | 614 | -    | 52,56,73     | 1.32 | 9 (17%)     | 61,92,113   | 1.35 | 5 (8%)      |
| 22  | CLA  | C     | 512 | -    | 69,73,73     | 1.16 | 10 (14%)    | 82,113,113  | 1.26 | 6 (7%)      |
| 23  | LUT  | Y     | 613 | -    | 42,43,43     | 4.65 | 18 (42%)    | 51,60,60    | 5.32 | 26 (50%)    |
| 22  | CLA  | n     | 612 | 1    | 64,68,73     | 1.66 | 11 (17%)    | 76,107,113  | 1.86 | 17 (22%)    |
| 22  | CLA  | B     | 614 | -    | 69,73,73     | 1.15 | 9 (13%)     | 82,113,113  | 1.30 | 4 (4%)      |
| 22  | CLA  | y     | 610 | -    | 64,68,73     | 1.21 | 9 (14%)     | 76,107,113  | 1.32 | 5 (6%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 36  | LMG  | d     | 410 | -    | 46,46,55     | 0.81 | 3 (6%)   | 54,54,63    | 1.39 | 6 (11%)  |
| 22  | CLA  | y     | 603 | -    | 69,73,73     | 1.15 | 10 (14%) | 82,113,113  | 1.23 | 6 (7%)   |
| 32  | PL9  | a     | 410 | -    | 13,13,55     | 1.44 | 2 (15%)  | 17,17,69    | 1.79 | 4 (23%)  |
| 22  | CLA  | N     | 602 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 22  | CLA  | N     | 610 | -    | 64,68,73     | 1.19 | 9 (14%)  | 76,107,113  | 1.28 | 5 (6%)   |
| 31  | BCR  | C     | 517 | -    | 41,41,41     | 1.24 | 2 (4%)   | 56,56,56    | 1.30 | 7 (12%)  |
| 25  | NEX  | y     | 618 | -    | 40,46,46     | 5.03 | 17 (42%) | 50,70,70    | 8.52 | 27 (54%) |
| 22  | CLA  | y     | 613 | -    | 52,56,73     | 1.32 | 9 (17%)  | 61,92,113   | 1.34 | 5 (8%)   |
| 23  | LUT  | G     | 616 | -    | 42,43,43     | 4.83 | 19 (45%) | 51,60,60    | 4.79 | 24 (47%) |
| 22  | CLA  | G     | 612 | -    | 64,68,73     | 1.23 | 8 (12%)  | 76,107,113  | 1.28 | 4 (5%)   |
| 21  | CHL  | S     | 301 | -    | 42,56,74     | 4.31 | 18 (42%) | 36,92,114   | 2.30 | 11 (30%) |
| 21  | CHL  | y     | 607 | -    | 60,74,74     | 3.61 | 18 (30%) | 58,114,114  | 1.98 | 13 (22%) |
| 22  | CLA  | B     | 604 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 22  | CLA  | c     | 509 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.27 | 7 (8%)   |
| 22  | CLA  | n     | 613 | -    | 52,56,73     | 1.33 | 9 (17%)  | 61,92,113   | 1.35 | 5 (8%)   |
| 22  | CLA  | A     | 405 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.31 | 6 (7%)   |
| 31  | BCR  | B     | 621 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.25 | 3 (5%)   |
| 27  | OEX  | A     | 402 | 4,2  | 0,15,15      | -    | -        | -           | -    | -        |
| 22  | CLA  | g     | 613 | 1    | 69,73,73     | 1.61 | 12 (17%) | 82,113,113  | 1.81 | 17 (20%) |
| 22  | CLA  | b     | 604 | -    | 69,73,73     | 1.15 | 10 (14%) | 82,113,113  | 1.25 | 4 (4%)   |
| 22  | CLA  | B     | 611 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.28 | 5 (6%)   |
| 31  | BCR  | A     | 410 | -    | 41,41,41     | 1.25 | 3 (7%)   | 56,56,56    | 1.27 | 7 (12%)  |
| 22  | CLA  | B     | 606 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 22  | CLA  | S     | 304 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.34 | 4 (6%)   |
| 22  | CLA  | Y     | 612 | -    | 52,56,73     | 1.32 | 9 (17%)  | 61,92,113   | 1.34 | 5 (8%)   |
| 22  | CLA  | b     | 605 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 21  | CHL  | G     | 608 | -    | 60,74,74     | 3.61 | 18 (30%) | 58,114,114  | 1.98 | 13 (22%) |
| 31  | BCR  | k     | 102 | -    | 41,41,41     | 1.21 | 3 (7%)   | 56,56,56    | 1.26 | 7 (12%)  |
| 22  | CLA  | y     | 604 | 25   | 54,58,73     | 1.29 | 7 (12%)  | 64,95,113   | 1.45 | 6 (9%)   |
| 31  | BCR  | b     | 616 | -    | 41,41,41     | 1.25 | 2 (4%)   | 56,56,56    | 1.25 | 7 (12%)  |
| 26  | LHG  | N     | 618 | -    | 48,48,48     | 0.64 | 2 (4%)   | 51,54,54    | 1.25 | 7 (13%)  |
| 31  | BCR  | B     | 620 | -    | 41,41,41     | 1.21 | 2 (4%)   | 56,56,56    | 1.27 | 6 (10%)  |
| 21  | CHL  | r     | 308 | -    | 55,69,74     | 3.77 | 18 (32%) | 52,108,114  | 2.07 | 13 (25%) |
| 22  | CLA  | C     | 513 | 4    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.30 | 8 (9%)   |
| 26  | LHG  | c     | 520 | 22   | 48,48,48     | 0.81 | 4 (8%)   | 51,54,54    | 1.32 | 7 (13%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |       |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|-------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ  | # Z  > 2 |
| 22  | CLA  | C     | 507 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.26  | 5 (6%)   |
| 22  | CLA  | w     | 101 | -    | 64,68,73     | 1.22 | 9 (14%)  | 76,107,113  | 1.27  | 4 (5%)   |
| 24  | XAT  | g     | 617 | -    | 41,47,47     | 3.64 | 23 (56%) | 54,74,74    | 11.18 | 32 (59%) |
| 22  | CLA  | y     | 612 | 1    | 69,73,73     | 1.60 | 11 (15%) | 82,113,113  | 1.80  | 17 (20%) |
| 22  | CLA  | B     | 607 | -    | 69,73,73     | 1.15 | 10 (14%) | 82,113,113  | 1.26  | 4 (4%)   |
| 31  | BCR  | b     | 618 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.25  | 3 (5%)   |
| 22  | CLA  | B     | 613 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.27  | 5 (6%)   |
| 21  | CHL  | y     | 605 | -    | 42,56,74     | 4.31 | 18 (42%) | 36,92,114   | 2.29  | 11 (30%) |
| 22  | CLA  | N     | 609 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.30  | 5 (6%)   |
| 22  | CLA  | W     | 101 | -    | 64,68,73     | 1.22 | 8 (12%)  | 76,107,113  | 1.27  | 4 (5%)   |
| 22  | CLA  | B     | 603 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.24  | 5 (6%)   |
| 22  | CLA  | b     | 613 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.27  | 5 (6%)   |
| 22  | CLA  | d     | 403 | -    | 69,73,73     | 1.15 | 10 (14%) | 82,113,113  | 1.25  | 6 (7%)   |
| 22  | CLA  | n     | 603 | -    | 69,73,73     | 1.16 | 10 (14%) | 82,113,113  | 1.25  | 6 (7%)   |
| 21  | CHL  | y     | 608 | -    | 60,74,74     | 3.61 | 18 (30%) | 58,114,114  | 1.98  | 13 (22%) |
| 22  | CLA  | g     | 614 | -    | 52,56,73     | 1.32 | 9 (17%)  | 61,92,113   | 1.35  | 5 (8%)   |
| 21  | CHL  | N     | 605 | -    | 44,58,74     | 4.22 | 18 (40%) | 37,94,114   | 2.27  | 11 (29%) |
| 22  | CLA  | B     | 617 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.28  | 5 (6%)   |
| 22  | CLA  | R     | 310 | 23   | 53,57,73     | 1.35 | 7 (13%)  | 61,93,113   | 1.32  | 4 (6%)   |
| 22  | CLA  | c     | 514 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.32  | 6 (7%)   |
| 26  | LHG  | c     | 521 | -    | 48,48,48     | 0.62 | 1 (2%)   | 51,54,54    | 1.25  | 7 (13%)  |
| 22  | CLA  | b     | 606 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.31  | 6 (7%)   |
| 22  | CLA  | r     | 312 | -    | 64,68,73     | 1.21 | 9 (14%)  | 76,107,113  | 1.30  | 4 (5%)   |
| 22  | CLA  | S     | 303 | 20   | 65,69,73     | 1.19 | 8 (12%)  | 77,108,113  | 1.28  | 6 (7%)   |
| 26  | LHG  | C     | 521 | -    | 48,48,48     | 0.62 | 1 (2%)   | 51,54,54    | 1.25  | 7 (13%)  |
| 21  | CHL  | R     | 307 | -    | 55,69,74     | 3.77 | 18 (32%) | 52,108,114  | 2.08  | 13 (25%) |
| 22  | CLA  | C     | 503 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.25  | 4 (4%)   |
| 22  | CLA  | N     | 603 | -    | 69,73,73     | 1.16 | 10 (14%) | 82,113,113  | 1.25  | 6 (7%)   |
| 35  | DGD  | H     | 102 | -    | 63,63,67     | 0.95 | 3 (4%)   | 77,77,81    | 1.48  | 14 (18%) |
| 32  | PL9  | A     | 411 | -    | 13,13,55     | 1.46 | 2 (15%)  | 17,17,69    | 1.77  | 4 (23%)  |
| 22  | CLA  | C     | 504 | -    | 69,73,73     | 1.15 | 10 (14%) | 82,113,113  | 1.29  | 6 (7%)   |
| 22  | CLA  | n     | 602 | -    | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.26  | 6 (7%)   |
| 21  | CHL  | R     | 306 | -    | 50,64,74     | 3.95 | 18 (36%) | 46,102,114  | 2.18  | 13 (28%) |
| 21  | CHL  | s     | 302 | -    | 40,54,74     | 4.42 | 18 (45%) | 34,90,114   | 2.33  | 10 (29%) |
| 21  | CHL  | n     | 601 | 1    | 60,74,74     | 3.60 | 18 (30%) | 58,114,114  | 1.98  | 13 (22%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |       |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|-------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ  | # Z  > 2 |
| 21  | CHL  | N     | 606 | -    | 60,74,74     | 3.62 | 18 (30%) | 58,114,114  | 1.98  | 13 (22%) |
| 26  | LHG  | d     | 409 | -    | 42,42,48     | 0.69 | 1 (2%)   | 45,48,54    | 1.28  | 5 (11%)  |
| 22  | CLA  | c     | 513 | 22   | 69,73,73     | 1.16 | 10 (14%) | 82,113,113  | 1.21  | 4 (4%)   |
| 32  | PL9  | d     | 406 | -    | 55,55,55     | 1.31 | 4 (7%)   | 68,69,69    | 1.51  | 12 (17%) |
| 36  | LMG  | D     | 411 | -    | 46,46,55     | 0.81 | 3 (6%)   | 54,54,63    | 1.39  | 6 (11%)  |
| 22  | CLA  | B     | 605 | -    | 69,73,73     | 1.14 | 9 (13%)  | 82,113,113  | 1.29  | 6 (7%)   |
| 36  | LMG  | B     | 601 | -    | 40,40,55     | 0.84 | 1 (2%)   | 48,48,63    | 1.31  | 5 (10%)  |
| 26  | LHG  | Y     | 617 | 22   | 48,48,48     | 0.67 | 1 (2%)   | 51,54,54    | 1.28  | 7 (13%)  |
| 21  | CHL  | G     | 606 | -    | 44,58,74     | 4.22 | 18 (40%) | 37,94,114   | 2.28  | 11 (29%) |
| 21  | CHL  | Y     | 606 | -    | 60,74,74     | 3.61 | 18 (30%) | 58,114,114  | 1.97  | 13 (22%) |
| 33  | SQD  | L     | 102 | -    | 40,42,54     | 1.08 | 3 (7%)   | 50,53,65    | 1.54  | 10 (20%) |
| 25  | NEX  | n     | 616 | 22   | 40,46,46     | 4.86 | 17 (42%) | 50,70,70    | 10.00 | 26 (52%) |
| 22  | CLA  | n     | 604 | 25   | 54,58,73     | 1.29 | 6 (11%)  | 64,95,113   | 1.45  | 6 (9%)   |
| 21  | CHL  | Y     | 605 | -    | 44,58,74     | 4.21 | 18 (40%) | 37,94,114   | 2.27  | 11 (29%) |
| 22  | CLA  | Y     | 611 | 1    | 69,73,73     | 1.60 | 11 (15%) | 82,113,113  | 1.80  | 17 (20%) |
| 22  | CLA  | b     | 614 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.28  | 5 (6%)   |
| 23  | LUT  | g     | 616 | -    | 42,43,43     | 4.84 | 19 (45%) | 51,60,60    | 4.79  | 24 (47%) |
| 32  | PL9  | D     | 407 | -    | 55,55,55     | 1.32 | 5 (9%)   | 68,69,69    | 1.51  | 12 (17%) |
| 26  | LHG  | d     | 408 | -    | 48,48,48     | 0.65 | 1 (2%)   | 51,54,54    | 1.31  | 6 (11%)  |
| 22  | CLA  | Y     | 602 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.27  | 6 (7%)   |
| 22  | CLA  | N     | 613 | -    | 52,56,73     | 1.32 | 9 (17%)  | 61,92,113   | 1.34  | 5 (8%)   |
| 22  | CLA  | C     | 508 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.29  | 6 (7%)   |
| 26  | LHG  | S     | 314 | 22   | 48,48,48     | 0.63 | 1 (2%)   | 51,54,54    | 1.29  | 6 (11%)  |
| 23  | LUT  | Y     | 614 | -    | 42,43,43     | 4.79 | 20 (47%) | 51,60,60    | 4.75  | 23 (45%) |
| 22  | CLA  | g     | 612 | -    | 64,68,73     | 1.22 | 8 (12%)  | 76,107,113  | 1.28  | 4 (5%)   |
| 33  | SQD  | d     | 402 | -    | 48,50,54     | 1.01 | 3 (6%)   | 58,61,65    | 1.49  | 10 (17%) |
| 22  | CLA  | R     | 309 | 19   | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.27  | 6 (7%)   |
| 22  | CLA  | C     | 506 | -    | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.34  | 5 (6%)   |
| 22  | CLA  | s     | 313 | 22   | 59,63,73     | 1.24 | 9 (15%)  | 70,101,113  | 1.36  | 5 (7%)   |
| 31  | BCR  | c     | 516 | -    | 41,41,41     | 1.26 | 3 (7%)   | 56,56,56    | 1.29  | 7 (12%)  |
| 31  | BCR  | c     | 515 | -    | 41,41,41     | 1.26 | 3 (7%)   | 56,56,56    | 1.26  | 6 (10%)  |
| 27  | OEX  | a     | 401 | 4,2  | 0,15,15      | -    | -        | -           | -     | -        |
| 36  | LMG  | k     | 103 | -    | 51,51,55     | 0.73 | 0        | 59,59,63    | 1.34  | 6 (10%)  |
| 22  | CLA  | C     | 514 | 22   | 69,73,73     | 1.15 | 10 (14%) | 82,113,113  | 1.21  | 4 (4%)   |
| 22  | CLA  | B     | 616 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.27  | 5 (6%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |       |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|-------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ  | # Z  > 2 |
| 21  | CHL  | Y     | 607 | -    | 60,74,74     | 3.61 | 18 (30%) | 58,114,114  | 1.98  | 13 (22%) |
| 22  | CLA  | C     | 505 | -    | 69,73,73     | 1.14 | 8 (11%)  | 82,113,113  | 1.31  | 7 (8%)   |
| 26  | LHG  | c     | 522 | -    | 48,48,48     | 0.61 | 1 (2%)   | 51,54,54    | 1.31  | 8 (15%)  |
| 22  | CLA  | g     | 610 | -    | 68,72,73     | 1.18 | 9 (13%)  | 80,111,113  | 1.32  | 5 (6%)   |
| 23  | LUT  | G     | 615 | -    | 42,43,43     | 4.66 | 18 (42%) | 51,60,60    | 5.32  | 26 (50%) |
| 26  | LHG  | G     | 618 | -    | 48,48,48     | 0.66 | 1 (2%)   | 51,54,54    | 1.30  | 7 (13%)  |
| 21  | CHL  | n     | 607 | -    | 60,74,74     | 3.62 | 18 (30%) | 58,114,114  | 1.98  | 13 (22%) |
| 21  | CHL  | g     | 609 | -    | 55,69,74     | 3.78 | 18 (32%) | 52,108,114  | 2.07  | 13 (25%) |
| 21  | CHL  | r     | 306 | -    | 60,74,74     | 3.60 | 18 (30%) | 58,114,114  | 1.98  | 13 (22%) |
| 22  | CLA  | C     | 515 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.32  | 6 (7%)   |
| 35  | DGD  | J     | 101 | -    | 61,61,67     | 0.98 | 5 (8%)   | 75,75,81    | 1.52  | 11 (14%) |
| 22  | CLA  | s     | 310 | 26   | 59,63,73     | 1.25 | 9 (15%)  | 70,101,113  | 1.32  | 5 (7%)   |
| 26  | LHG  | C     | 522 | -    | 48,48,48     | 0.61 | 1 (2%)   | 51,54,54    | 1.31  | 8 (15%)  |
| 22  | CLA  | c     | 508 | -    | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.28  | 5 (6%)   |
| 36  | LMG  | C     | 502 | -    | 48,48,55     | 0.79 | 2 (4%)   | 56,56,63    | 1.42  | 8 (14%)  |
| 22  | CLA  | G     | 611 | -    | 64,68,73     | 1.20 | 9 (14%)  | 76,107,113  | 1.29  | 5 (6%)   |
| 22  | CLA  | b     | 611 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.30  | 4 (4%)   |
| 26  | LHG  | b     | 619 | -    | 48,48,48     | 0.62 | 2 (4%)   | 51,54,54    | 1.28  | 6 (11%)  |
| 30  | PHO  | D     | 401 | -    | 58,69,69     | 2.12 | 11 (18%) | 55,99,99    | 1.50  | 7 (12%)  |
| 22  | CLA  | y     | 602 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.27  | 6 (7%)   |
| 37  | HEM  | f     | 101 | -    | 50,50,50     | 7.20 | 11 (22%) | 67,82,82    | 3.51  | 31 (46%) |
| 22  | CLA  | b     | 612 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.25  | 4 (4%)   |
| 22  | CLA  | c     | 511 | -    | 69,73,73     | 1.16 | 10 (14%) | 82,113,113  | 1.26  | 6 (7%)   |
| 35  | DGD  | C     | 518 | -    | 56,56,67     | 1.00 | 4 (7%)   | 70,70,81    | 1.55  | 12 (17%) |
| 21  | CHL  | S     | 306 | 20   | 40,54,74     | 4.42 | 18 (45%) | 34,90,114   | 2.33  | 10 (29%) |
| 26  | LHG  | D     | 410 | -    | 42,42,48     | 0.69 | 1 (2%)   | 45,48,54    | 1.28  | 5 (11%)  |
| 22  | CLA  | C     | 510 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.27  | 7 (8%)   |
| 30  | PHO  | A     | 408 | -    | 58,69,69     | 2.10 | 12 (20%) | 55,99,99    | 1.43  | 6 (10%)  |
| 26  | LHG  | r     | 302 | -    | 46,46,48     | 0.65 | 2 (4%)   | 49,52,54    | 1.30  | 7 (14%)  |
| 36  | LMG  | C     | 523 | -    | 51,51,55     | 0.73 | 1 (1%)   | 59,59,63    | 1.38  | 8 (13%)  |
| 22  | CLA  | R     | 308 | -    | 62,66,73     | 1.23 | 9 (14%)  | 73,104,113  | 1.32  | 5 (6%)   |
| 24  | XAT  | R     | 313 | -    | 41,47,47     | 3.57 | 22 (53%) | 54,74,74    | 11.15 | 27 (50%) |
| 22  | CLA  | a     | 406 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.38  | 6 (9%)   |
| 31  | BCR  | k     | 101 | -    | 41,41,41     | 1.19 | 2 (4%)   | 56,56,56    | 1.25  | 7 (12%)  |
| 21  | CHL  | s     | 301 | -    | 42,56,74     | 4.31 | 18 (42%) | 36,92,114   | 2.30  | 11 (30%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |       |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|-------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ  | # Z  > 2 |
| 22  | CLA  | D     | 404 | -    | 69,73,73     | 1.15 | 10 (14%) | 82,113,113  | 1.25  | 6 (7%)   |
| 26  | LHG  | s     | 314 | 22   | 48,48,48     | 0.63 | 1 (2%)   | 51,54,54    | 1.29  | 6 (11%)  |
| 22  | CLA  | S     | 308 | -    | 49,53,73     | 1.37 | 7 (14%)  | 58,89,113   | 1.33  | 3 (5%)   |
| 22  | CLA  | b     | 601 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.26  | 5 (6%)   |
| 22  | CLA  | g     | 604 | 25   | 54,58,73     | 1.29 | 7 (12%)  | 64,95,113   | 1.44  | 6 (9%)   |
| 22  | CLA  | c     | 510 | -    | 69,73,73     | 3.21 | 14 (20%) | 82,113,113  | 2.26  | 20 (24%) |
| 22  | CLA  | c     | 512 | 4    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.30  | 7 (8%)   |
| 22  | CLA  | r     | 310 | 19   | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.28  | 6 (7%)   |
| 21  | CHL  | G     | 609 | -    | 55,69,74     | 3.77 | 18 (32%) | 52,108,114  | 2.07  | 13 (25%) |
| 21  | CHL  | G     | 601 | 1    | 60,74,74     | 3.61 | 18 (30%) | 58,114,114  | 1.98  | 13 (22%) |
| 22  | CLA  | c     | 505 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.35  | 5 (6%)   |
| 36  | LMG  | K     | 103 | -    | 51,51,55     | 0.72 | 0        | 59,59,63    | 1.34  | 6 (10%)  |
| 21  | CHL  | n     | 605 | -    | 44,58,74     | 4.22 | 18 (40%) | 37,94,114   | 2.28  | 11 (29%) |
| 22  | CLA  | b     | 615 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.25  | 5 (6%)   |
| 22  | CLA  | A     | 407 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.38  | 6 (9%)   |
| 22  | CLA  | S     | 313 | 22   | 59,63,73     | 1.25 | 9 (15%)  | 70,101,113  | 1.35  | 5 (7%)   |
| 31  | BCR  | B     | 619 | -    | 41,41,41     | 1.25 | 2 (4%)   | 56,56,56    | 1.25  | 7 (12%)  |
| 22  | CLA  | S     | 305 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.44  | 6 (9%)   |
| 33  | SQD  | l     | 101 | -    | 40,42,54     | 1.09 | 3 (7%)   | 50,53,65    | 1.54  | 10 (20%) |
| 36  | LMG  | I     | 101 | -    | 40,40,55     | 0.84 | 0        | 48,48,63    | 1.31  | 5 (10%)  |
| 22  | CLA  | x     | 101 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.25  | 5 (6%)   |
| 22  | CLA  | B     | 612 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.29  | 6 (7%)   |
| 22  | CLA  | s     | 311 | 22   | 60,64,73     | 1.24 | 9 (15%)  | 71,102,113  | 1.28  | 6 (8%)   |
| 22  | CLA  | R     | 304 | -    | 52,56,73     | 1.32 | 8 (15%)  | 61,92,113   | 1.38  | 5 (8%)   |
| 24  | XAT  | Y     | 615 | -    | 41,47,47     | 3.67 | 23 (56%) | 54,74,74    | 11.16 | 31 (57%) |
| 21  | CHL  | Y     | 601 | 1    | 60,74,74     | 3.61 | 18 (30%) | 58,114,114  | 1.98  | 13 (22%) |
| 23  | LUT  | R     | 312 | 22   | 42,43,43     | 4.71 | 19 (45%) | 51,60,60    | 5.05  | 29 (56%) |
| 21  | CHL  | r     | 301 | -    | 42,56,74     | 4.32 | 18 (42%) | 36,92,114   | 2.30  | 11 (30%) |
| 21  | CHL  | y     | 601 | 1    | 60,74,74     | 3.61 | 18 (30%) | 58,114,114  | 1.98  | 13 (22%) |
| 33  | SQD  | L     | 101 | -    | 52,54,54     | 0.97 | 4 (7%)   | 62,65,65    | 1.54  | 11 (17%) |
| 22  | CLA  | G     | 602 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.27  | 6 (7%)   |
| 35  | DGD  | h     | 102 | -    | 63,63,67     | 0.95 | 3 (4%)   | 77,77,81    | 1.48  | 14 (18%) |
| 35  | DGD  | c     | 518 | -    | 63,63,67     | 0.93 | 4 (6%)   | 77,77,81    | 1.46  | 10 (12%) |
| 22  | CLA  | Y     | 609 | -    | 64,68,73     | 1.20 | 9 (14%)  | 76,107,113  | 1.32  | 5 (6%)   |
| 26  | LHG  | C     | 520 | 22   | 48,48,48     | 0.81 | 4 (8%)   | 51,54,54    | 1.32  | 7 (13%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | C     | 511 | -    | 69,73,73     | 3.21 | 14 (20%) | 82,113,113  | 2.26 | 19 (23%) |
| 36  | LMG  | c     | 523 | -    | 51,51,55     | 0.72 | 1 (1%)   | 59,59,63    | 1.39 | 8 (13%)  |
| 22  | CLA  | G     | 610 | -    | 68,72,73     | 1.17 | 8 (11%)  | 80,111,113  | 1.33 | 6 (7%)   |
| 22  | CLA  | G     | 603 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 21  | CHL  | s     | 306 | 20   | 40,54,74     | 4.42 | 18 (45%) | 34,90,114   | 2.33 | 10 (29%) |
| 21  | CHL  | g     | 601 | 1    | 60,74,74     | 3.61 | 18 (30%) | 58,114,114  | 1.98 | 13 (22%) |
| 31  | BCR  | K     | 101 | -    | 41,41,41     | 1.19 | 2 (4%)   | 56,56,56    | 1.25 | 7 (12%)  |
| 22  | CLA  | S     | 311 | 22   | 60,64,73     | 1.25 | 9 (15%)  | 71,102,113  | 1.29 | 6 (8%)   |
| 21  | CHL  | N     | 607 | -    | 60,74,74     | 3.62 | 18 (30%) | 58,114,114  | 1.98 | 13 (22%) |
| 31  | BCR  | h     | 101 | -    | 41,41,41     | 1.20 | 2 (4%)   | 56,56,56    | 1.31 | 6 (10%)  |
| 22  | CLA  | g     | 603 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 22  | CLA  | y     | 611 | -    | 64,68,73     | 1.20 | 9 (14%)  | 76,107,113  | 1.28 | 5 (6%)   |
| 21  | CHL  | n     | 606 | -    | 60,74,74     | 3.61 | 18 (30%) | 58,114,114  | 1.98 | 13 (22%) |
| 22  | CLA  | r     | 305 | -    | 52,56,73     | 1.33 | 7 (13%)  | 61,92,113   | 1.38 | 5 (8%)   |
| 22  | CLA  | d     | 404 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.29 | 6 (7%)   |
| 22  | CLA  | S     | 310 | 26   | 59,63,73     | 1.25 | 9 (15%)  | 70,101,113  | 1.32 | 5 (7%)   |
| 22  | CLA  | R     | 303 | -    | 64,68,73     | 1.21 | 9 (14%)  | 76,107,113  | 1.31 | 5 (6%)   |
| 31  | BCR  | H     | 101 | -    | 41,41,41     | 1.22 | 3 (7%)   | 56,56,56    | 1.30 | 6 (10%)  |
| 22  | CLA  | r     | 309 | -    | 62,66,73     | 1.23 | 9 (14%)  | 73,104,113  | 1.31 | 5 (6%)   |
| 22  | CLA  | a     | 404 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.31 | 6 (7%)   |
| 23  | LUT  | y     | 614 | -    | 42,43,43     | 4.66 | 18 (42%) | 51,60,60    | 5.32 | 26 (50%) |
| 22  | CLA  | n     | 611 | -    | 64,68,73     | 1.23 | 8 (12%)  | 76,107,113  | 1.27 | 4 (5%)   |
| 21  | CHL  | g     | 606 | -    | 44,58,74     | 4.22 | 18 (40%) | 37,94,114   | 2.28 | 11 (29%) |
| 22  | CLA  | Y     | 610 | 26   | 64,68,73     | 1.20 | 9 (14%)  | 76,107,113  | 1.28 | 5 (6%)   |
| 22  | CLA  | s     | 308 | -    | 49,53,73     | 1.37 | 8 (16%)  | 58,89,113   | 1.34 | 3 (5%)   |
| 26  | LHG  | y     | 617 | -    | 48,48,48     | 0.66 | 1 (2%)   | 51,54,54    | 1.31 | 7 (13%)  |
| 25  | NEX  | N     | 617 | 22   | 40,46,46     | 4.99 | 17 (42%) | 50,70,70    | 9.45 | 27 (54%) |
| 22  | CLA  | Y     | 603 | -    | 69,73,73     | 1.16 | 10 (14%) | 82,113,113  | 1.24 | 6 (7%)   |
| 21  | CHL  | y     | 606 | -    | 44,58,74     | 4.22 | 18 (40%) | 37,94,114   | 2.28 | 11 (29%) |
| 22  | CLA  | A     | 406 | -    | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.26 | 4 (4%)   |
| 36  | LMG  | T     | 101 | -    | 51,51,55     | 0.74 | 1 (1%)   | 59,59,63    | 1.36 | 6 (10%)  |
| 22  | CLA  | B     | 610 | -    | 69,73,73     | 1.14 | 9 (13%)  | 82,113,113  | 1.29 | 8 (9%)   |
| 35  | DGD  | a     | 413 | -    | 60,60,67     | 0.88 | 2 (3%)   | 74,74,81    | 1.44 | 11 (14%) |
| 22  | CLA  | s     | 312 | 20   | 53,57,73     | 1.31 | 8 (15%)  | 61,93,113   | 1.36 | 5 (8%)   |
| 22  | CLA  | N     | 604 | 25   | 54,58,73     | 1.29 | 6 (11%)  | 64,95,113   | 1.46 | 6 (9%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |       |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|-------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ  | # Z  > 2 |
| 26  | LHG  | L     | 103 | -    | 48,48,48     | 0.65 | 1 (2%)   | 51,54,54    | 1.31  | 7 (13%)  |
| 21  | CHL  | s     | 307 | -    | 40,54,74     | 4.42 | 18 (45%) | 34,90,114   | 2.33  | 10 (29%) |
| 33  | SQD  | D     | 402 | -    | 48,50,54     | 1.01 | 5 (10%)  | 58,61,65    | 1.50  | 10 (17%) |
| 22  | CLA  | c     | 502 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.25  | 5 (6%)   |
| 22  | CLA  | N     | 612 | 1    | 64,68,73     | 1.67 | 11 (17%) | 76,107,113  | 1.86  | 17 (22%) |
| 31  | BCR  | B     | 602 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.24  | 6 (10%)  |
| 22  | CLA  | B     | 615 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.26  | 4 (4%)   |
| 35  | DGD  | c     | 517 | -    | 56,56,67     | 1.00 | 4 (7%)   | 70,70,81    | 1.55  | 12 (17%) |
| 22  | CLA  | G     | 604 | -    | 54,58,73     | 1.29 | 6 (11%)  | 64,95,113   | 1.44  | 6 (9%)   |
| 22  | CLA  | B     | 608 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.27  | 5 (6%)   |
| 24  | XAT  | r     | 314 | -    | 41,47,47     | 3.57 | 22 (53%) | 54,74,74    | 11.15 | 27 (50%) |
| 23  | LUT  | g     | 615 | -    | 42,43,43     | 4.65 | 18 (42%) | 51,60,60    | 5.32  | 26 (50%) |
| 22  | CLA  | b     | 608 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.27  | 5 (6%)   |
| 36  | LMG  | B     | 623 | -    | 55,55,55     | 0.89 | 3 (5%)   | 63,63,63    | 1.36  | 8 (12%)  |
| 31  | BCR  | b     | 617 | -    | 41,41,41     | 1.21 | 2 (4%)   | 56,56,56    | 1.27  | 6 (10%)  |
| 21  | CHL  | g     | 607 | -    | 60,74,74     | 3.61 | 18 (30%) | 58,114,114  | 1.98  | 13 (22%) |
| 33  | SQD  | a     | 411 | -    | 52,54,54     | 0.97 | 3 (5%)   | 62,65,65    | 1.54  | 12 (19%) |
| 30  | PHO  | a     | 407 | -    | 58,69,69     | 2.09 | 12 (20%) | 55,99,99    | 1.42  | 6 (10%)  |
| 21  | CHL  | S     | 307 | -    | 40,54,74     | 4.43 | 18 (45%) | 34,90,114   | 2.33  | 10 (29%) |
| 22  | CLA  | g     | 602 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.27  | 6 (7%)   |
| 22  | CLA  | c     | 503 | -    | 69,73,73     | 1.15 | 10 (14%) | 82,113,113  | 1.29  | 6 (7%)   |
| 23  | LUT  | N     | 614 | -    | 42,43,43     | 4.66 | 18 (42%) | 51,60,60    | 5.32  | 26 (50%) |
| 35  | DGD  | c     | 519 | -    | 61,61,67     | 0.98 | 5 (8%)   | 75,75,81    | 1.52  | 11 (14%) |
| 31  | BCR  | d     | 405 | -    | 41,41,41     | 1.23 | 3 (7%)   | 56,56,56    | 1.26  | 7 (12%)  |
| 22  | CLA  | s     | 304 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.34  | 4 (6%)   |
| 22  | CLA  | R     | 302 | -    | 64,68,73     | 1.20 | 9 (14%)  | 76,107,113  | 1.30  | 5 (6%)   |
| 23  | LUT  | r     | 313 | 22   | 42,43,43     | 4.70 | 19 (45%) | 51,60,60    | 5.04  | 29 (56%) |
| 33  | SQD  | A     | 412 | -    | 52,54,54     | 0.97 | 3 (5%)   | 62,65,65    | 1.54  | 12 (19%) |
| 21  | CHL  | S     | 302 | -    | 40,54,74     | 4.43 | 18 (45%) | 34,90,114   | 2.33  | 10 (29%) |
| 22  | CLA  | c     | 504 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.30  | 7 (8%)   |
| 22  | CLA  | Y     | 604 | 25   | 54,58,73     | 1.29 | 7 (12%)  | 64,95,113   | 1.45  | 6 (9%)   |
| 22  | CLA  | B     | 618 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.25  | 5 (6%)   |
| 24  | XAT  | G     | 617 | -    | 41,47,47     | 3.63 | 22 (53%) | 54,74,74    | 11.18 | 32 (59%) |
| 22  | CLA  | D     | 405 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.29  | 6 (7%)   |
| 21  | CHL  | G     | 605 | -    | 40,54,74     | 4.42 | 18 (45%) | 34,90,114   | 2.32  | 10 (29%) |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |       |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|-------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ  | # Z  > 2 |
| 23  | LUT  | N     | 615 | -     | 42,43,43     | 4.84 | 20 (47%) | 51,60,60    | 4.51  | 28 (54%) |
| 22  | CLA  | B     | 609 | -     | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.30  | 5 (6%)   |
| 22  | CLA  | S     | 309 | 20,22 | 59,63,73     | 1.25 | 8 (13%)  | 70,101,113  | 1.38  | 6 (8%)   |
| 22  | CLA  | n     | 609 | -     | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.29  | 5 (6%)   |
| 22  | CLA  | s     | 305 | -     | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.43  | 6 (9%)   |
| 22  | CLA  | c     | 506 | -     | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.26  | 5 (6%)   |
| 34  | BCT  | a     | 412 | -     | 3,3,3        | 3.21 | 1 (33%)  | 2,3,3       | 2.84  | 2 (100%) |
| 22  | CLA  | r     | 304 | -     | 64,68,73     | 1.21 | 9 (14%)  | 76,107,113  | 1.31  | 5 (6%)   |
| 25  | NEX  | g     | 618 | 22    | 40,46,46     | 4.81 | 16 (40%) | 50,70,70    | 9.98  | 27 (54%) |
| 26  | LHG  | B     | 622 | -     | 48,48,48     | 0.62 | 2 (4%)   | 51,54,54    | 1.28  | 6 (11%)  |
| 22  | CLA  | r     | 311 | 23    | 53,57,73     | 1.35 | 7 (13%)  | 61,93,113   | 1.32  | 4 (6%)   |
| 21  | CHL  | N     | 601 | 1     | 60,74,74     | 3.61 | 18 (30%) | 58,114,114  | 1.99  | 13 (22%) |
| 26  | LHG  | R     | 301 | -     | 46,46,48     | 0.65 | 2 (4%)   | 49,52,54    | 1.30  | 7 (14%)  |
| 22  | CLA  | b     | 607 | -     | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.29  | 8 (9%)   |
| 26  | LHG  | l     | 102 | -     | 48,48,48     | 0.65 | 1 (2%)   | 51,54,54    | 1.31  | 7 (13%)  |
| 22  | CLA  | G     | 613 | 1     | 69,73,73     | 1.60 | 11 (15%) | 82,113,113  | 1.80  | 17 (20%) |
| 34  | BCT  | D     | 403 | -     | 3,3,3        | 3.20 | 1 (33%)  | 2,3,3       | 2.83  | 2 (100%) |
| 31  | BCR  | T     | 102 | -     | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.24  | 6 (10%)  |
| 26  | LHG  | D     | 409 | -     | 48,48,48     | 0.65 | 1 (2%)   | 51,54,54    | 1.31  | 6 (11%)  |
| 36  | LMG  | w     | 102 | -     | 48,48,55     | 0.79 | 2 (4%)   | 56,56,63    | 1.42  | 8 (14%)  |
| 36  | LMG  | M     | 101 | -     | 51,51,55     | 0.75 | 1 (1%)   | 59,59,63    | 1.36  | 6 (10%)  |
| 24  | XAT  | N     | 616 | -     | 41,47,47     | 3.59 | 22 (53%) | 54,74,74    | 11.35 | 32 (59%) |
| 31  | BCR  | C     | 516 | -     | 41,41,41     | 1.26 | 2 (4%)   | 56,56,56    | 1.28  | 7 (12%)  |
| 33  | SQD  | l     | 103 | -     | 52,54,54     | 0.97 | 3 (5%)   | 62,65,65    | 1.54  | 11 (17%) |
| 26  | LHG  | g     | 619 | -     | 48,48,48     | 0.63 | 1 (2%)   | 51,54,54    | 1.33  | 8 (15%)  |
| 22  | CLA  | A     | 409 | -     | 64,68,73     | 1.21 | 9 (14%)  | 76,107,113  | 1.34  | 6 (7%)   |
| 21  | CHL  | N     | 608 | -     | 60,74,74     | 3.61 | 18 (30%) | 58,114,114  | 1.98  | 13 (22%) |
| 30  | PHO  | d     | 401 | -     | 58,69,69     | 2.12 | 11 (18%) | 55,99,99    | 1.50  | 7 (12%)  |
| 23  | LUT  | n     | 614 | -     | 42,43,43     | 4.66 | 19 (45%) | 51,60,60    | 5.32  | 26 (50%) |
| 22  | CLA  | s     | 303 | 20    | 65,69,73     | 1.19 | 8 (12%)  | 77,108,113  | 1.28  | 7 (9%)   |
| 22  | CLA  | a     | 408 | -     | 64,68,73     | 1.21 | 8 (12%)  | 76,107,113  | 1.33  | 6 (7%)   |
| 21  | CHL  | G     | 607 | -     | 60,74,74     | 3.61 | 18 (30%) | 58,114,114  | 1.99  | 13 (22%) |
| 26  | LHG  | D     | 408 | -     | 45,45,48     | 0.66 | 1 (2%)   | 48,51,54    | 1.26  | 4 (8%)   |
| 35  | DGD  | A     | 401 | -     | 60,60,67     | 0.88 | 2 (3%)   | 74,74,81    | 1.44  | 11 (14%) |
| 22  | CLA  | n     | 610 | 26    | 64,68,73     | 1.20 | 9 (14%)  | 76,107,113  | 1.28  | 5 (6%)   |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |       |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|-------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ  | # Z  > 2 |
| 21  | CHL  | g     | 605 | -     | 40,54,74     | 4.42 | 18 (45%) | 34,90,114   | 2.33  | 10 (29%) |
| 21  | CHL  | Y     | 608 | -     | 60,74,74     | 3.61 | 18 (30%) | 58,114,114  | 1.98  | 13 (22%) |
| 22  | CLA  | b     | 609 | -     | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.28  | 6 (7%)   |
| 22  | CLA  | s     | 309 | 20,22 | 59,63,73     | 1.25 | 8 (13%)  | 70,101,113  | 1.38  | 6 (8%)   |
| 37  | HEM  | F     | 101 | -     | 50,50,50     | 7.20 | 12 (24%) | 67,82,82    | 3.51  | 31 (46%) |
| 24  | XAT  | y     | 615 | -     | 41,47,47     | 3.65 | 23 (56%) | 54,74,74    | 11.15 | 31 (57%) |
| 21  | CHL  | r     | 307 | -     | 50,64,74     | 3.95 | 18 (36%) | 46,102,114  | 2.18  | 13 (28%) |
| 22  | CLA  | R     | 311 | -     | 64,68,73     | 1.20 | 8 (12%)  | 76,107,113  | 1.28  | 4 (5%)   |
| 22  | CLA  | N     | 611 | -     | 64,68,73     | 1.23 | 8 (12%)  | 76,107,113  | 1.28  | 4 (5%)   |
| 35  | DGD  | C     | 519 | -     | 63,63,67     | 0.93 | 4 (6%)   | 77,77,81    | 1.46  | 10 (12%) |
| 22  | CLA  | a     | 405 | -     | 69,73,73     | 1.15 | 10 (14%) | 82,113,113  | 1.25  | 4 (4%)   |
| 25  | NEX  | r     | 315 | -     | 40,46,46     | 5.01 | 17 (42%) | 50,70,70    | 8.52  | 28 (56%) |
| 26  | LHG  | d     | 407 | -     | 45,45,48     | 0.66 | 1 (2%)   | 48,51,54    | 1.26  | 5 (10%)  |
| 21  | CHL  | g     | 608 | -     | 60,74,74     | 3.61 | 18 (30%) | 58,114,114  | 1.98  | 13 (22%) |
| 22  | CLA  | b     | 602 | -     | 69,73,73     | 1.14 | 9 (13%)  | 82,113,113  | 1.30  | 6 (7%)   |
| 31  | BCR  | D     | 406 | -     | 41,41,41     | 1.22 | 3 (7%)   | 56,56,56    | 1.25  | 7 (12%)  |
| 36  | LMG  | b     | 620 | -     | 55,55,55     | 0.88 | 3 (5%)   | 63,63,63    | 1.36  | 9 (14%)  |
| 24  | XAT  | n     | 615 | -     | 41,47,47     | 3.61 | 21 (51%) | 54,74,74    | 11.31 | 32 (59%) |
| 31  | BCR  | a     | 409 | -     | 41,41,41     | 1.25 | 3 (7%)   | 56,56,56    | 1.27  | 7 (12%)  |
| 31  | BCR  | K     | 102 | -     | 41,41,41     | 1.21 | 3 (7%)   | 56,56,56    | 1.27  | 7 (12%)  |
| 22  | CLA  | S     | 312 | 20    | 53,57,73     | 1.31 | 7 (13%)  | 61,93,113   | 1.35  | 5 (8%)   |

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   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22  | CLA  | C     | 509 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 25  | NEX  | Y     | 616 | 22   | 2/2/12/25 | 16/27/83/83   | 0/3/3/3 |
| 22  | CLA  | b     | 610 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 25  | NEX  | y     | 616 | 22   | 2/2/12/25 | 15/27/83/83   | 0/3/3/3 |
| 22  | CLA  | b     | 603 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 21  | CHL  | n     | 608 | -    | 4/4/20/26 | 15/39/137/137 | -       |
| 21  | CHL  | R     | 305 | -    | 4/4/20/26 | 18/39/137/137 | -       |
| 22  | CLA  | r     | 303 | -    | 1/1/14/20 | 10/33/109/115 | -       |

Continued on next page...

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 21  | CHL  | y     | 609 | -    | 4/4/20/26 | 14/39/137/137 | -       |
| 26  | LHG  | n     | 617 | 22   | -         | 25/53/53/53   | -       |
| 22  | CLA  | g     | 611 | -    | 1/1/14/20 | 10/33/109/115 | -       |
| 22  | CLA  | c     | 507 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 22  | CLA  | G     | 614 | -    | 1/1/11/20 | 11/19/95/115  | -       |
| 22  | CLA  | C     | 512 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 23  | LUT  | Y     | 613 | -    | -         | 17/29/67/67   | 0/2/2/2 |
| 22  | CLA  | n     | 612 | 1    | 1/1/14/20 | 15/33/109/115 | -       |
| 22  | CLA  | B     | 614 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | y     | 610 | -    | 1/1/14/20 | 16/33/109/115 | -       |
| 36  | LMG  | d     | 410 | -    | -         | 11/41/61/70   | 0/1/1/1 |
| 22  | CLA  | y     | 603 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 32  | PL9  | a     | 410 | -    | -         | 3/5/18/73     | 0/1/1/1 |
| 22  | CLA  | N     | 602 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 22  | CLA  | N     | 610 | -    | 1/1/14/20 | 11/33/109/115 | -       |
| 31  | BCR  | C     | 517 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 25  | NEX  | y     | 618 | -    | 2/2/12/25 | 15/27/83/83   | 0/3/3/3 |
| 22  | CLA  | y     | 613 | -    | 1/1/11/20 | 11/19/95/115  | -       |
| 23  | LUT  | G     | 616 | -    | -         | 16/29/67/67   | 0/2/2/2 |
| 22  | CLA  | G     | 612 | -    | 1/1/14/20 | 13/33/109/115 | -       |
| 21  | CHL  | S     | 301 | -    | 3/3/16/26 | 11/18/116/137 | -       |
| 21  | CHL  | y     | 607 | -    | 4/4/20/26 | 20/39/137/137 | -       |
| 22  | CLA  | B     | 604 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | c     | 509 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | n     | 613 | -    | 1/1/11/20 | 11/19/95/115  | -       |
| 22  | CLA  | A     | 405 | -    | 1/1/15/20 | 3/39/115/115  | -       |
| 31  | BCR  | B     | 621 | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 22  | CLA  | g     | 613 | 1    | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | b     | 604 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | B     | 611 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 31  | BCR  | A     | 410 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 22  | CLA  | B     | 606 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 22  | CLA  | S     | 304 | -    | 1/1/11/20 | 8/15/91/115   | -       |
| 22  | CLA  | Y     | 612 | -    | 1/1/11/20 | 11/19/95/115  | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22  | CLA  | b     | 605 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 21  | CHL  | G     | 608 | -    | 4/4/20/26 | 22/39/137/137 | -       |
| 31  | BCR  | k     | 102 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 22  | CLA  | y     | 604 | 25   | 1/1/12/20 | 7/21/97/115   | -       |
| 31  | BCR  | b     | 616 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 26  | LHG  | N     | 618 | -    | -         | 29/53/53/53   | -       |
| 31  | BCR  | B     | 620 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 21  | CHL  | r     | 308 | -    | 4/4/19/26 | 19/33/131/137 | -       |
| 22  | CLA  | C     | 513 | 4    | 1/1/15/20 | 11/39/115/115 | -       |
| 26  | LHG  | c     | 520 | 22   | -         | 29/53/53/53   | -       |
| 22  | CLA  | C     | 507 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | w     | 101 | -    | 1/1/14/20 | 13/33/109/115 | -       |
| 24  | XAT  | g     | 617 | -    | 2/2/12/26 | 17/31/93/93   | 0/4/4/4 |
| 22  | CLA  | y     | 612 | 1    | 1/1/15/20 | 19/39/115/115 | -       |
| 22  | CLA  | B     | 607 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 31  | BCR  | b     | 618 | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 22  | CLA  | B     | 613 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 21  | CHL  | y     | 605 | -    | 3/3/16/26 | 12/18/116/137 | -       |
| 22  | CLA  | N     | 609 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | W     | 101 | -    | 1/1/14/20 | 13/33/109/115 | -       |
| 22  | CLA  | B     | 603 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | b     | 613 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 22  | CLA  | d     | 403 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 22  | CLA  | n     | 603 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 21  | CHL  | y     | 608 | -    | 4/4/20/26 | 22/39/137/137 | -       |
| 22  | CLA  | g     | 614 | -    | 1/1/11/20 | 11/19/95/115  | -       |
| 21  | CHL  | N     | 605 | -    | 3/3/16/26 | 12/20/118/137 | -       |
| 22  | CLA  | B     | 617 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 22  | CLA  | R     | 310 | 23   | 1/1/11/20 | 13/20/96/115  | -       |
| 22  | CLA  | c     | 514 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 26  | LHG  | c     | 521 | -    | -         | 21/53/53/53   | -       |
| 22  | CLA  | b     | 606 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 22  | CLA  | r     | 312 | -    | 1/1/14/20 | 14/33/109/115 | -       |
| 22  | CLA  | S     | 303 | 20   | 1/1/14/20 | 14/35/111/115 | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 26  | LHG  | C     | 521 | -    | -         | 21/53/53/53   | -       |
| 21  | CHL  | R     | 307 | -    | 4/4/19/26 | 19/33/131/137 | -       |
| 22  | CLA  | C     | 503 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | N     | 603 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 35  | DGD  | H     | 102 | -    | -         | 20/51/91/95   | 0/2/2/2 |
| 32  | PL9  | A     | 411 | -    | -         | 3/5/18/73     | 0/1/1/1 |
| 22  | CLA  | C     | 504 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | n     | 602 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 21  | CHL  | R     | 306 | -    | 4/4/18/26 | 15/27/125/137 | -       |
| 21  | CHL  | s     | 302 | -    | 3/3/16/26 | 8/15/113/137  | -       |
| 21  | CHL  | n     | 601 | 1    | 4/4/20/26 | 23/39/137/137 | -       |
| 21  | CHL  | N     | 606 | -    | 4/4/20/26 | 20/39/137/137 | -       |
| 26  | LHG  | d     | 409 | -    | -         | 18/47/47/53   | -       |
| 22  | CLA  | c     | 513 | 22   | 1/1/15/20 | 18/39/115/115 | -       |
| 32  | PL9  | d     | 406 | -    | -         | 17/53/73/73   | 0/1/1/1 |
| 36  | LMG  | D     | 411 | -    | -         | 11/41/61/70   | 0/1/1/1 |
| 22  | CLA  | B     | 605 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 36  | LMG  | B     | 601 | -    | -         | 18/35/55/70   | 0/1/1/1 |
| 26  | LHG  | Y     | 617 | 22   | -         | 28/53/53/53   | -       |
| 21  | CHL  | G     | 606 | -    | 3/3/16/26 | 12/20/118/137 | -       |
| 21  | CHL  | Y     | 606 | -    | 4/4/20/26 | 20/39/137/137 | -       |
| 33  | SQD  | L     | 102 | -    | -         | 13/37/57/69   | 0/1/1/1 |
| 25  | NEX  | n     | 616 | 22   | 2/2/12/25 | 16/27/83/83   | 0/3/3/3 |
| 22  | CLA  | n     | 604 | 25   | 1/1/12/20 | 7/21/97/115   | -       |
| 21  | CHL  | Y     | 605 | -    | 3/3/16/26 | 12/20/118/137 | -       |
| 22  | CLA  | Y     | 611 | 1    | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | b     | 614 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 23  | LUT  | g     | 616 | -    | -         | 15/29/67/67   | 0/2/2/2 |
| 32  | PL9  | D     | 407 | -    | -         | 17/53/73/73   | 0/1/1/1 |
| 26  | LHG  | d     | 408 | -    | -         | 18/53/53/53   | -       |
| 22  | CLA  | Y     | 602 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 22  | CLA  | N     | 613 | -    | 1/1/11/20 | 11/19/95/115  | -       |
| 22  | CLA  | C     | 508 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 26  | LHG  | S     | 314 | 22   | -         | 29/53/53/53   | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 23  | LUT  | Y     | 614 | -    | -         | 14/29/67/67   | 0/2/2/2 |
| 22  | CLA  | g     | 612 | -    | 1/1/14/20 | 13/33/109/115 | -       |
| 33  | SQD  | d     | 402 | -    | 1/1/9/9   | 18/45/65/69   | 0/1/1/1 |
| 22  | CLA  | R     | 309 | 19   | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | C     | 506 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 22  | CLA  | s     | 313 | 22   | 1/1/13/20 | 11/27/103/115 | -       |
| 31  | BCR  | c     | 516 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 31  | BCR  | c     | 515 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 36  | LMG  | k     | 103 | -    | -         | 26/46/66/70   | 0/1/1/1 |
| 22  | CLA  | C     | 514 | 22   | 1/1/15/20 | 18/39/115/115 | -       |
| 22  | CLA  | B     | 616 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 21  | CHL  | Y     | 607 | -    | 4/4/20/26 | 22/39/137/137 | -       |
| 22  | CLA  | C     | 505 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 26  | LHG  | c     | 522 | -    | -         | 22/53/53/53   | -       |
| 22  | CLA  | g     | 610 | -    | 1/1/14/20 | 16/38/114/115 | -       |
| 23  | LUT  | G     | 615 | -    | -         | 17/29/67/67   | 0/2/2/2 |
| 26  | LHG  | G     | 618 | -    | -         | 28/53/53/53   | -       |
| 21  | CHL  | n     | 607 | -    | 4/4/20/26 | 22/39/137/137 | -       |
| 21  | CHL  | g     | 609 | -    | 4/4/19/26 | 10/33/131/137 | -       |
| 21  | CHL  | r     | 306 | -    | 4/4/20/26 | 18/39/137/137 | -       |
| 22  | CLA  | C     | 515 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 35  | DGD  | J     | 101 | -    | -         | 17/49/89/95   | 0/2/2/2 |
| 22  | CLA  | s     | 310 | 26   | 1/1/13/20 | 14/27/103/115 | -       |
| 26  | LHG  | C     | 522 | -    | -         | 22/53/53/53   | -       |
| 22  | CLA  | c     | 508 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 36  | LMG  | C     | 502 | -    | -         | 16/43/63/70   | 0/1/1/1 |
| 22  | CLA  | G     | 611 | -    | 1/1/14/20 | 10/33/109/115 | -       |
| 22  | CLA  | b     | 611 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 26  | LHG  | b     | 619 | -    | -         | 27/53/53/53   | -       |
| 30  | PHO  | D     | 401 | -    | -         | 15/37/103/103 | 0/5/6/6 |
| 22  | CLA  | y     | 602 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 37  | HEM  | f     | 101 | -    | -         | 5/14/54/54    | -       |
| 22  | CLA  | b     | 612 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 22  | CLA  | c     | 511 | -    | 1/1/15/20 | 14/39/115/115 | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 35  | DGD  | C     | 518 | -    | -         | 18/44/84/95   | 0/2/2/2 |
| 21  | CHL  | S     | 306 | 20   | 3/3/16/26 | 9/15/113/137  | -       |
| 26  | LHG  | D     | 410 | -    | -         | 18/47/47/53   | -       |
| 22  | CLA  | C     | 510 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 30  | PHO  | A     | 408 | -    | -         | 12/37/103/103 | 0/5/6/6 |
| 26  | LHG  | r     | 302 | -    | -         | 24/51/51/53   | -       |
| 36  | LMG  | C     | 523 | -    | -         | 20/46/66/70   | 0/1/1/1 |
| 22  | CLA  | R     | 308 | -    | 1/1/13/20 | 11/31/107/115 | -       |
| 24  | XAT  | R     | 313 | -    | 1/1/12/26 | 14/31/93/93   | 0/4/4/4 |
| 22  | CLA  | a     | 406 | -    | 1/1/12/20 | 8/21/97/115   | -       |
| 31  | BCR  | k     | 101 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 21  | CHL  | s     | 301 | -    | 3/3/16/26 | 12/18/116/137 | -       |
| 22  | CLA  | D     | 404 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 26  | LHG  | s     | 314 | 22   | -         | 29/53/53/53   | -       |
| 22  | CLA  | S     | 308 | -    | -         | 9/15/91/115   | -       |
| 22  | CLA  | b     | 601 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | g     | 604 | 25   | 1/1/12/20 | 7/21/97/115   | -       |
| 22  | CLA  | c     | 510 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 22  | CLA  | c     | 512 | 4    | 1/1/15/20 | 11/39/115/115 | -       |
| 22  | CLA  | r     | 310 | 19   | 1/1/15/20 | 15/39/115/115 | -       |
| 21  | CHL  | G     | 609 | -    | 4/4/19/26 | 10/33/131/137 | -       |
| 21  | CHL  | G     | 601 | 1    | 4/4/20/26 | 23/39/137/137 | -       |
| 22  | CLA  | c     | 505 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 36  | LMG  | K     | 103 | -    | -         | 26/46/66/70   | 0/1/1/1 |
| 21  | CHL  | n     | 605 | -    | 3/3/16/26 | 12/20/118/137 | -       |
| 22  | CLA  | b     | 615 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 22  | CLA  | A     | 407 | -    | 1/1/12/20 | 8/21/97/115   | -       |
| 22  | CLA  | S     | 313 | 22   | 1/1/13/20 | 11/27/103/115 | -       |
| 31  | BCR  | B     | 619 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 22  | CLA  | S     | 305 | -    | 1/1/12/20 | 10/21/97/115  | -       |
| 33  | SQD  | l     | 101 | -    | -         | 13/37/57/69   | 0/1/1/1 |
| 36  | LMG  | I     | 101 | -    | -         | 18/35/55/70   | 0/1/1/1 |
| 22  | CLA  | x     | 101 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | B     | 612 | -    | 1/1/15/20 | 9/39/115/115  | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22  | CLA  | s     | 311 | 22   | 1/1/13/20 | 10/29/105/115 | -       |
| 22  | CLA  | R     | 304 | -    | 1/1/11/20 | 8/19/95/115   | -       |
| 24  | XAT  | Y     | 615 | -    | 2/2/12/26 | 18/31/93/93   | 0/4/4/4 |
| 21  | CHL  | Y     | 601 | 1    | 4/4/20/26 | 23/39/137/137 | -       |
| 23  | LUT  | R     | 312 | 22   | -         | 18/29/67/67   | 0/2/2/2 |
| 21  | CHL  | r     | 301 | -    | 3/3/16/26 | 8/18/116/137  | -       |
| 21  | CHL  | y     | 601 | 1    | 4/4/20/26 | 23/39/137/137 | -       |
| 33  | SQD  | L     | 101 | -    | -         | 18/49/69/69   | 0/1/1/1 |
| 22  | CLA  | G     | 602 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 35  | DGD  | h     | 102 | -    | -         | 20/51/91/95   | 0/2/2/2 |
| 35  | DGD  | c     | 518 | -    | -         | 26/51/91/95   | 0/2/2/2 |
| 22  | CLA  | Y     | 609 | -    | 1/1/14/20 | 16/33/109/115 | -       |
| 26  | LHG  | C     | 520 | 22   | -         | 29/53/53/53   | -       |
| 22  | CLA  | C     | 511 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 36  | LMG  | c     | 523 | -    | -         | 20/46/66/70   | 0/1/1/1 |
| 22  | CLA  | G     | 610 | -    | 1/1/14/20 | 19/38/114/115 | -       |
| 22  | CLA  | G     | 603 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 21  | CHL  | s     | 306 | 20   | 3/3/16/26 | 9/15/113/137  | -       |
| 21  | CHL  | g     | 601 | 1    | 4/4/20/26 | 23/39/137/137 | -       |
| 31  | BCR  | K     | 101 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 22  | CLA  | S     | 311 | 22   | 1/1/13/20 | 10/29/105/115 | -       |
| 21  | CHL  | N     | 607 | -    | 4/4/20/26 | 22/39/137/137 | -       |
| 31  | BCR  | h     | 101 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 22  | CLA  | g     | 603 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | y     | 611 | -    | 1/1/14/20 | 11/33/109/115 | -       |
| 21  | CHL  | n     | 606 | -    | 4/4/20/26 | 20/39/137/137 | -       |
| 22  | CLA  | r     | 305 | -    | 1/1/11/20 | 8/19/95/115   | -       |
| 22  | CLA  | d     | 404 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 22  | CLA  | S     | 310 | 26   | 1/1/13/20 | 14/27/103/115 | -       |
| 22  | CLA  | R     | 303 | -    | 1/1/14/20 | 11/33/109/115 | -       |
| 31  | BCR  | H     | 101 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 22  | CLA  | r     | 309 | -    | 1/1/13/20 | 11/31/107/115 | -       |
| 22  | CLA  | a     | 404 | -    | 1/1/15/20 | 3/39/115/115  | -       |
| 23  | LUT  | y     | 614 | -    | -         | 17/29/67/67   | 0/2/2/2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22  | CLA  | n     | 611 | -    | 1/1/14/20 | 13/33/109/115 | -       |
| 21  | CHL  | g     | 606 | -    | 3/3/16/26 | 12/20/118/137 | -       |
| 22  | CLA  | Y     | 610 | 26   | 1/1/14/20 | 10/33/109/115 | -       |
| 22  | CLA  | s     | 308 | -    | -         | 9/15/91/115   | -       |
| 26  | LHG  | y     | 617 | -    | -         | 22/53/53/53   | -       |
| 25  | NEX  | N     | 617 | 22   | 2/2/12/25 | 15/27/83/83   | 0/3/3/3 |
| 22  | CLA  | Y     | 603 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 21  | CHL  | y     | 606 | -    | 3/3/16/26 | 12/20/118/137 | -       |
| 22  | CLA  | A     | 406 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 36  | LMG  | T     | 101 | -    | -         | 23/46/66/70   | 0/1/1/1 |
| 22  | CLA  | B     | 610 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 35  | DGD  | a     | 413 | -    | -         | 21/48/88/95   | 0/2/2/2 |
| 22  | CLA  | s     | 312 | 20   | 1/1/11/20 | 9/20/96/115   | -       |
| 22  | CLA  | N     | 604 | 25   | 1/1/12/20 | 7/21/97/115   | -       |
| 26  | LHG  | L     | 103 | -    | -         | 18/53/53/53   | -       |
| 21  | CHL  | s     | 307 | -    | 3/3/16/26 | 9/15/113/137  | -       |
| 33  | SQD  | D     | 402 | -    | 1/1/9/9   | 18/45/65/69   | 0/1/1/1 |
| 22  | CLA  | c     | 502 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | N     | 612 | 1    | 1/1/14/20 | 15/33/109/115 | -       |
| 31  | BCR  | B     | 602 | -    | -         | 19/29/63/63   | 0/2/2/2 |
| 22  | CLA  | B     | 615 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 35  | DGD  | c     | 517 | -    | -         | 18/44/84/95   | 0/2/2/2 |
| 22  | CLA  | G     | 604 | -    | 1/1/12/20 | 7/21/97/115   | -       |
| 22  | CLA  | B     | 608 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 24  | XAT  | r     | 314 | -    | 1/1/12/26 | 14/31/93/93   | 0/4/4/4 |
| 23  | LUT  | g     | 615 | -    | -         | 17/29/67/67   | 0/2/2/2 |
| 22  | CLA  | b     | 608 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 36  | LMG  | B     | 623 | -    | -         | 21/50/70/70   | 0/1/1/1 |
| 31  | BCR  | b     | 617 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 21  | CHL  | g     | 607 | -    | 4/4/20/26 | 20/39/137/137 | -       |
| 33  | SQD  | a     | 411 | -    | -         | 23/49/69/69   | 0/1/1/1 |
| 30  | PHO  | a     | 407 | -    | -         | 12/37/103/103 | 0/5/6/6 |
| 21  | CHL  | S     | 307 | -    | 3/3/16/26 | 10/15/113/137 | -       |
| 22  | CLA  | g     | 602 | -    | 1/1/15/20 | 14/39/115/115 | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 22  | CLA  | c     | 503 | -     | 1/1/15/20 | 13/39/115/115 | -       |
| 23  | LUT  | N     | 614 | -     | -         | 17/29/67/67   | 0/2/2/2 |
| 35  | DGD  | c     | 519 | -     | -         | 16/49/89/95   | 0/2/2/2 |
| 31  | BCR  | d     | 405 | -     | -         | 8/29/63/63    | 0/2/2/2 |
| 22  | CLA  | s     | 304 | -     | 1/1/11/20 | 8/15/91/115   | -       |
| 22  | CLA  | R     | 302 | -     | 1/1/14/20 | 10/33/109/115 | -       |
| 23  | LUT  | r     | 313 | 22    | -         | 18/29/67/67   | 0/2/2/2 |
| 33  | SQD  | A     | 412 | -     | -         | 23/49/69/69   | 0/1/1/1 |
| 21  | CHL  | S     | 302 | -     | 3/3/16/26 | 8/15/113/137  | -       |
| 22  | CLA  | c     | 504 | -     | 1/1/15/20 | 12/39/115/115 | -       |
| 22  | CLA  | Y     | 604 | 25    | 1/1/12/20 | 7/21/97/115   | -       |
| 22  | CLA  | B     | 618 | -     | 1/1/15/20 | 12/39/115/115 | -       |
| 24  | XAT  | G     | 617 | -     | 3/3/12/26 | 17/31/93/93   | 0/4/4/4 |
| 22  | CLA  | D     | 405 | -     | 1/1/15/20 | 14/39/115/115 | -       |
| 21  | CHL  | G     | 605 | -     | 3/3/16/26 | 11/15/113/137 | -       |
| 23  | LUT  | N     | 615 | -     | -         | 14/29/67/67   | 0/2/2/2 |
| 22  | CLA  | B     | 609 | -     | 1/1/15/20 | 7/39/115/115  | -       |
| 22  | CLA  | S     | 309 | 20,22 | 1/1/13/20 | 9/27/103/115  | -       |
| 22  | CLA  | n     | 609 | -     | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | s     | 305 | -     | 1/1/12/20 | 10/21/97/115  | -       |
| 22  | CLA  | c     | 506 | -     | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | r     | 304 | -     | 1/1/14/20 | 11/33/109/115 | -       |
| 25  | NEX  | g     | 618 | 22    | 2/2/12/25 | 15/27/83/83   | 0/3/3/3 |
| 26  | LHG  | B     | 622 | -     | -         | 27/53/53/53   | -       |
| 22  | CLA  | r     | 311 | 23    | 1/1/11/20 | 13/20/96/115  | -       |
| 21  | CHL  | N     | 601 | 1     | 4/4/20/26 | 22/39/137/137 | -       |
| 26  | LHG  | R     | 301 | -     | -         | 24/51/51/53   | -       |
| 22  | CLA  | b     | 607 | -     | 1/1/15/20 | 12/39/115/115 | -       |
| 26  | LHG  | l     | 102 | -     | -         | 18/53/53/53   | -       |
| 22  | CLA  | G     | 613 | 1     | 1/1/15/20 | 19/39/115/115 | -       |
| 31  | BCR  | T     | 102 | -     | -         | 19/29/63/63   | 0/2/2/2 |
| 26  | LHG  | D     | 409 | -     | -         | 19/53/53/53   | -       |
| 36  | LMG  | w     | 102 | -     | -         | 16/43/63/70   | 0/1/1/1 |
| 36  | LMG  | M     | 101 | -     | -         | 23/46/66/70   | 0/1/1/1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 24  | XAT  | N     | 616 | -     | 2/2/12/26 | 17/31/93/93   | 0/4/4/4 |
| 31  | BCR  | C     | 516 | -     | -         | 6/29/63/63    | 0/2/2/2 |
| 33  | SQD  | l     | 103 | -     | -         | 18/49/69/69   | 0/1/1/1 |
| 26  | LHG  | g     | 619 | -     | -         | 23/53/53/53   | -       |
| 22  | CLA  | A     | 409 | -     | 1/1/14/20 | 1/33/109/115  | -       |
| 21  | CHL  | N     | 608 | -     | 4/4/20/26 | 15/39/137/137 | -       |
| 30  | PHO  | d     | 401 | -     | -         | 15/37/103/103 | 0/5/6/6 |
| 23  | LUT  | n     | 614 | -     | -         | 17/29/67/67   | 0/2/2/2 |
| 22  | CLA  | s     | 303 | 20    | 1/1/14/20 | 14/35/111/115 | -       |
| 22  | CLA  | a     | 408 | -     | 1/1/14/20 | 2/33/109/115  | -       |
| 21  | CHL  | G     | 607 | -     | 4/4/20/26 | 20/39/137/137 | -       |
| 26  | LHG  | D     | 408 | -     | -         | 24/50/50/53   | -       |
| 35  | DGD  | A     | 401 | -     | -         | 21/48/88/95   | 0/2/2/2 |
| 22  | CLA  | n     | 610 | 26    | 1/1/14/20 | 11/33/109/115 | -       |
| 21  | CHL  | g     | 605 | -     | 3/3/16/26 | 11/15/113/137 | -       |
| 21  | CHL  | Y     | 608 | -     | 4/4/20/26 | 12/39/137/137 | -       |
| 22  | CLA  | b     | 609 | -     | 1/1/15/20 | 9/39/115/115  | -       |
| 22  | CLA  | s     | 309 | 20,22 | 1/1/13/20 | 9/27/103/115  | -       |
| 37  | HEM  | F     | 101 | -     | -         | 5/14/54/54    | -       |
| 24  | XAT  | y     | 615 | -     | 2/2/12/26 | 18/31/93/93   | 0/4/4/4 |
| 21  | CHL  | r     | 307 | -     | 4/4/18/26 | 15/27/125/137 | -       |
| 22  | CLA  | R     | 311 | -     | 1/1/14/20 | 14/33/109/115 | -       |
| 22  | CLA  | N     | 611 | -     | 1/1/14/20 | 13/33/109/115 | -       |
| 35  | DGD  | C     | 519 | -     | -         | 26/51/91/95   | 0/2/2/2 |
| 22  | CLA  | a     | 405 | -     | 1/1/15/20 | 15/39/115/115 | -       |
| 25  | NEX  | r     | 315 | -     | 2/2/12/25 | 15/27/83/83   | 0/3/3/3 |
| 26  | LHG  | d     | 407 | -     | -         | 23/50/50/53   | -       |
| 21  | CHL  | g     | 608 | -     | 4/4/20/26 | 22/39/137/137 | -       |
| 22  | CLA  | b     | 602 | -     | 1/1/15/20 | 11/39/115/115 | -       |
| 31  | BCR  | D     | 406 | -     | -         | 8/29/63/63    | 0/2/2/2 |
| 36  | LMG  | b     | 620 | -     | -         | 21/50/70/70   | 0/1/1/1 |
| 24  | XAT  | n     | 615 | -     | 2/2/12/26 | 16/31/93/93   | 0/4/4/4 |
| 31  | BCR  | a     | 409 | -     | -         | 5/29/63/63    | 0/2/2/2 |
| 31  | BCR  | K     | 102 | -     | -         | 6/29/63/63    | 0/2/2/2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions    | Rings |
|-----|------|-------|-----|------|-----------|-------------|-------|
| 22  | CLA  | S     | 312 | 20   | 1/1/11/20 | 9/20/96/115 | -     |

The worst 5 of 2975 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 37  | f     | 101 | HEM  | FE-NB | 41.17 | 3.21        | 1.94     |
| 37  | F     | 101 | HEM  | FE-NB | 41.15 | 3.21        | 1.94     |
| 25  | y     | 618 | NEX  | C7-C6 | 22.94 | 1.57        | 1.30     |
| 25  | r     | 315 | NEX  | C7-C6 | 22.84 | 1.57        | 1.30     |
| 25  | N     | 617 | NEX  | C7-C6 | 22.54 | 1.56        | 1.30     |

The worst 5 of 2953 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 24  | G     | 617 | XAT  | O24-C25-C24 | -62.78 | 54.66       | 113.49   |
| 24  | N     | 616 | XAT  | O24-C25-C24 | -62.64 | 54.78       | 113.49   |
| 24  | R     | 313 | XAT  | O24-C25-C24 | -62.35 | 55.06       | 113.49   |
| 24  | r     | 314 | XAT  | O24-C25-C24 | -62.32 | 55.08       | 113.49   |
| 24  | g     | 617 | XAT  | O24-C25-C24 | -62.20 | 55.19       | 113.49   |

5 of 353 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 21  | g     | 601 | CHL  | ND   |
| 21  | g     | 601 | CHL  | C8   |
| 21  | g     | 601 | CHL  | NC   |
| 21  | g     | 601 | CHL  | NA   |
| 21  | g     | 605 | CHL  | ND   |

5 of 4526 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | g     | 601 | CHL  | C1C-C2C-CMC-OMC |
| 21  | g     | 601 | CHL  | C3C-C2C-CMC-OMC |
| 21  | g     | 601 | CHL  | C4C-C3C-CAC-CBC |
| 21  | g     | 605 | CHL  | C1C-C2C-CMC-OMC |
| 21  | g     | 605 | CHL  | C3C-C2C-CMC-OMC |

There are no ring outliers.

311 monomers are involved in 2203 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | C     | 509 | CLA  | 2       | 0            |
| 25  | Y     | 616 | NEX  | 9       | 0            |
| 22  | b     | 610 | CLA  | 1       | 0            |
| 25  | y     | 616 | NEX  | 7       | 0            |
| 22  | b     | 603 | CLA  | 6       | 0            |
| 21  | n     | 608 | CHL  | 28      | 0            |
| 21  | R     | 305 | CHL  | 33      | 0            |
| 22  | r     | 303 | CLA  | 2       | 0            |
| 21  | y     | 609 | CHL  | 26      | 0            |
| 26  | n     | 617 | LHG  | 10      | 0            |
| 22  | g     | 611 | CLA  | 2       | 0            |
| 22  | c     | 507 | CLA  | 1       | 0            |
| 22  | G     | 614 | CLA  | 3       | 0            |
| 22  | C     | 512 | CLA  | 5       | 0            |
| 23  | Y     | 613 | LUT  | 16      | 0            |
| 22  | n     | 612 | CLA  | 18      | 0            |
| 22  | B     | 614 | CLA  | 4       | 0            |
| 22  | y     | 610 | CLA  | 6       | 0            |
| 36  | d     | 410 | LMG  | 4       | 0            |
| 22  | y     | 603 | CLA  | 3       | 0            |
| 32  | a     | 410 | PL9  | 2       | 0            |
| 22  | N     | 602 | CLA  | 4       | 0            |
| 22  | N     | 610 | CLA  | 2       | 0            |
| 31  | C     | 517 | BCR  | 2       | 0            |
| 25  | y     | 618 | NEX  | 9       | 0            |
| 22  | y     | 613 | CLA  | 3       | 0            |
| 23  | G     | 616 | LUT  | 11      | 0            |
| 22  | G     | 612 | CLA  | 6       | 0            |
| 21  | S     | 301 | CHL  | 48      | 0            |
| 21  | y     | 607 | CHL  | 19      | 0            |
| 22  | B     | 604 | CLA  | 3       | 0            |
| 22  | c     | 509 | CLA  | 3       | 0            |
| 22  | n     | 613 | CLA  | 1       | 0            |
| 22  | A     | 405 | CLA  | 3       | 0            |
| 31  | B     | 621 | BCR  | 1       | 0            |
| 22  | g     | 613 | CLA  | 18      | 0            |
| 22  | b     | 604 | CLA  | 2       | 0            |
| 22  | B     | 611 | CLA  | 1       | 0            |
| 31  | A     | 410 | BCR  | 2       | 0            |
| 22  | B     | 606 | CLA  | 6       | 0            |
| 22  | S     | 304 | CLA  | 1       | 0            |
| 22  | Y     | 612 | CLA  | 3       | 0            |
| 22  | b     | 605 | CLA  | 2       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 21  | G     | 608 | CHL  | 35      | 0            |
| 31  | k     | 102 | BCR  | 4       | 0            |
| 22  | y     | 604 | CLA  | 13      | 0            |
| 31  | b     | 616 | BCR  | 4       | 0            |
| 26  | N     | 618 | LHG  | 9       | 0            |
| 31  | B     | 620 | BCR  | 2       | 0            |
| 21  | r     | 308 | CHL  | 4       | 0            |
| 22  | C     | 513 | CLA  | 4       | 0            |
| 26  | c     | 520 | LHG  | 4       | 0            |
| 22  | C     | 507 | CLA  | 4       | 0            |
| 22  | w     | 101 | CLA  | 5       | 0            |
| 22  | y     | 612 | CLA  | 21      | 0            |
| 22  | B     | 607 | CLA  | 4       | 0            |
| 31  | b     | 618 | BCR  | 3       | 0            |
| 22  | B     | 613 | CLA  | 1       | 0            |
| 21  | y     | 605 | CHL  | 26      | 0            |
| 22  | N     | 609 | CLA  | 7       | 0            |
| 22  | W     | 101 | CLA  | 16      | 0            |
| 22  | B     | 603 | CLA  | 2       | 0            |
| 22  | b     | 613 | CLA  | 3       | 0            |
| 22  | d     | 403 | CLA  | 4       | 0            |
| 22  | n     | 603 | CLA  | 3       | 0            |
| 21  | y     | 608 | CHL  | 37      | 0            |
| 22  | g     | 614 | CLA  | 1       | 0            |
| 21  | N     | 605 | CHL  | 24      | 0            |
| 22  | B     | 617 | CLA  | 3       | 0            |
| 22  | R     | 310 | CLA  | 3       | 0            |
| 22  | c     | 514 | CLA  | 7       | 0            |
| 26  | c     | 521 | LHG  | 2       | 0            |
| 22  | b     | 606 | CLA  | 3       | 0            |
| 22  | r     | 312 | CLA  | 4       | 0            |
| 22  | S     | 303 | CLA  | 3       | 0            |
| 26  | C     | 521 | LHG  | 5       | 0            |
| 21  | R     | 307 | CHL  | 4       | 0            |
| 22  | C     | 503 | CLA  | 4       | 0            |
| 22  | N     | 603 | CLA  | 9       | 0            |
| 35  | H     | 102 | DGD  | 8       | 0            |
| 32  | A     | 411 | PL9  | 2       | 0            |
| 22  | C     | 504 | CLA  | 3       | 0            |
| 22  | n     | 602 | CLA  | 4       | 0            |
| 21  | R     | 306 | CHL  | 39      | 0            |
| 21  | s     | 302 | CHL  | 19      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 21  | n     | 601 | CHL  | 28      | 0            |
| 21  | N     | 606 | CHL  | 23      | 0            |
| 26  | d     | 409 | LHG  | 5       | 0            |
| 22  | c     | 513 | CLA  | 4       | 0            |
| 32  | d     | 406 | PL9  | 3       | 0            |
| 36  | D     | 411 | LMG  | 2       | 0            |
| 22  | B     | 605 | CLA  | 7       | 0            |
| 36  | B     | 601 | LMG  | 5       | 0            |
| 26  | Y     | 617 | LHG  | 10      | 0            |
| 21  | G     | 606 | CHL  | 23      | 0            |
| 21  | Y     | 606 | CHL  | 24      | 0            |
| 33  | L     | 102 | SQD  | 5       | 0            |
| 25  | n     | 616 | NEX  | 12      | 0            |
| 22  | n     | 604 | CLA  | 16      | 0            |
| 21  | Y     | 605 | CHL  | 29      | 0            |
| 22  | Y     | 611 | CLA  | 21      | 0            |
| 22  | b     | 614 | CLA  | 3       | 0            |
| 23  | g     | 616 | LUT  | 13      | 0            |
| 32  | D     | 407 | PL9  | 3       | 0            |
| 26  | d     | 408 | LHG  | 7       | 0            |
| 22  | Y     | 602 | CLA  | 5       | 0            |
| 22  | N     | 613 | CLA  | 3       | 0            |
| 22  | C     | 508 | CLA  | 1       | 0            |
| 26  | S     | 314 | LHG  | 6       | 0            |
| 23  | Y     | 614 | LUT  | 14      | 0            |
| 22  | g     | 612 | CLA  | 7       | 0            |
| 33  | d     | 402 | SQD  | 3       | 0            |
| 22  | R     | 309 | CLA  | 5       | 0            |
| 22  | C     | 506 | CLA  | 6       | 0            |
| 22  | s     | 313 | CLA  | 5       | 0            |
| 31  | c     | 515 | BCR  | 7       | 0            |
| 36  | k     | 103 | LMG  | 1       | 0            |
| 22  | C     | 514 | CLA  | 5       | 0            |
| 22  | B     | 616 | CLA  | 3       | 0            |
| 21  | Y     | 607 | CHL  | 37      | 0            |
| 22  | C     | 505 | CLA  | 5       | 0            |
| 26  | c     | 522 | LHG  | 3       | 0            |
| 22  | g     | 610 | CLA  | 6       | 0            |
| 23  | G     | 615 | LUT  | 14      | 0            |
| 26  | G     | 618 | LHG  | 13      | 0            |
| 21  | n     | 607 | CHL  | 38      | 0            |
| 21  | g     | 609 | CHL  | 25      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 21  | r     | 306 | CHL  | 25      | 0            |
| 22  | C     | 515 | CLA  | 8       | 0            |
| 35  | J     | 101 | DGD  | 6       | 0            |
| 22  | s     | 310 | CLA  | 6       | 0            |
| 26  | C     | 522 | LHG  | 3       | 0            |
| 22  | c     | 508 | CLA  | 4       | 0            |
| 36  | C     | 502 | LMG  | 2       | 0            |
| 22  | G     | 611 | CLA  | 2       | 0            |
| 22  | b     | 611 | CLA  | 3       | 0            |
| 26  | b     | 619 | LHG  | 1       | 0            |
| 30  | D     | 401 | PHO  | 6       | 0            |
| 22  | y     | 602 | CLA  | 3       | 0            |
| 37  | f     | 101 | HEM  | 20      | 0            |
| 22  | b     | 612 | CLA  | 3       | 0            |
| 22  | c     | 511 | CLA  | 5       | 0            |
| 35  | C     | 518 | DGD  | 1       | 0            |
| 21  | S     | 306 | CHL  | 16      | 0            |
| 26  | D     | 410 | LHG  | 4       | 0            |
| 22  | C     | 510 | CLA  | 4       | 0            |
| 30  | A     | 408 | PHO  | 4       | 0            |
| 26  | r     | 302 | LHG  | 3       | 0            |
| 36  | C     | 523 | LMG  | 3       | 0            |
| 22  | R     | 308 | CLA  | 8       | 0            |
| 24  | R     | 313 | XAT  | 5       | 0            |
| 22  | a     | 406 | CLA  | 2       | 0            |
| 31  | k     | 101 | BCR  | 2       | 0            |
| 21  | s     | 301 | CHL  | 51      | 0            |
| 22  | D     | 404 | CLA  | 2       | 0            |
| 26  | s     | 314 | LHG  | 7       | 0            |
| 22  | S     | 308 | CLA  | 2       | 0            |
| 22  | b     | 601 | CLA  | 6       | 0            |
| 22  | g     | 604 | CLA  | 13      | 0            |
| 22  | c     | 510 | CLA  | 21      | 0            |
| 22  | c     | 512 | CLA  | 5       | 0            |
| 22  | r     | 310 | CLA  | 3       | 0            |
| 21  | G     | 609 | CHL  | 34      | 0            |
| 21  | G     | 601 | CHL  | 42      | 0            |
| 22  | c     | 505 | CLA  | 6       | 0            |
| 36  | K     | 103 | LMG  | 1       | 0            |
| 21  | n     | 605 | CHL  | 31      | 0            |
| 22  | b     | 615 | CLA  | 1       | 0            |
| 22  | A     | 407 | CLA  | 2       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | S     | 313 | CLA  | 5       | 0            |
| 31  | B     | 619 | BCR  | 4       | 0            |
| 22  | S     | 305 | CLA  | 9       | 0            |
| 33  | l     | 101 | SQD  | 3       | 0            |
| 36  | I     | 101 | LMG  | 6       | 0            |
| 22  | x     | 101 | CLA  | 2       | 0            |
| 22  | B     | 612 | CLA  | 3       | 0            |
| 22  | s     | 311 | CLA  | 2       | 0            |
| 22  | R     | 304 | CLA  | 3       | 0            |
| 24  | Y     | 615 | XAT  | 2       | 0            |
| 21  | Y     | 601 | CHL  | 23      | 0            |
| 23  | R     | 312 | LUT  | 2       | 0            |
| 21  | r     | 301 | CHL  | 26      | 0            |
| 21  | y     | 601 | CHL  | 26      | 0            |
| 33  | L     | 101 | SQD  | 4       | 0            |
| 22  | G     | 602 | CLA  | 4       | 0            |
| 35  | h     | 102 | DGD  | 4       | 0            |
| 35  | c     | 518 | DGD  | 10      | 0            |
| 22  | Y     | 609 | CLA  | 6       | 0            |
| 26  | C     | 520 | LHG  | 7       | 0            |
| 22  | C     | 511 | CLA  | 21      | 0            |
| 36  | c     | 523 | LMG  | 3       | 0            |
| 22  | G     | 610 | CLA  | 7       | 0            |
| 22  | G     | 603 | CLA  | 6       | 0            |
| 21  | s     | 306 | CHL  | 15      | 0            |
| 21  | g     | 601 | CHL  | 23      | 0            |
| 31  | K     | 101 | BCR  | 2       | 0            |
| 22  | S     | 311 | CLA  | 3       | 0            |
| 21  | N     | 607 | CHL  | 41      | 0            |
| 31  | h     | 101 | BCR  | 5       | 0            |
| 22  | g     | 603 | CLA  | 7       | 0            |
| 22  | y     | 611 | CLA  | 2       | 0            |
| 21  | n     | 606 | CHL  | 17      | 0            |
| 22  | r     | 305 | CLA  | 2       | 0            |
| 22  | d     | 404 | CLA  | 3       | 0            |
| 22  | S     | 310 | CLA  | 8       | 0            |
| 22  | R     | 303 | CLA  | 5       | 0            |
| 31  | H     | 101 | BCR  | 3       | 0            |
| 22  | r     | 309 | CLA  | 6       | 0            |
| 22  | a     | 404 | CLA  | 4       | 0            |
| 23  | y     | 614 | LUT  | 11      | 0            |
| 22  | n     | 611 | CLA  | 7       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 21  | g     | 606 | CHL  | 28      | 0            |
| 22  | Y     | 610 | CLA  | 4       | 0            |
| 22  | s     | 308 | CLA  | 2       | 0            |
| 26  | y     | 617 | LHG  | 9       | 0            |
| 25  | N     | 617 | NEX  | 9       | 0            |
| 22  | Y     | 603 | CLA  | 14      | 0            |
| 21  | y     | 606 | CHL  | 28      | 0            |
| 22  | A     | 406 | CLA  | 3       | 0            |
| 36  | T     | 101 | LMG  | 5       | 0            |
| 22  | B     | 610 | CLA  | 2       | 0            |
| 35  | a     | 413 | DGD  | 7       | 0            |
| 22  | N     | 604 | CLA  | 13      | 0            |
| 26  | L     | 103 | LHG  | 2       | 0            |
| 21  | s     | 307 | CHL  | 24      | 0            |
| 33  | D     | 402 | SQD  | 3       | 0            |
| 22  | c     | 502 | CLA  | 7       | 0            |
| 22  | N     | 612 | CLA  | 17      | 0            |
| 31  | B     | 602 | BCR  | 2       | 0            |
| 22  | B     | 615 | CLA  | 3       | 0            |
| 35  | c     | 517 | DGD  | 1       | 0            |
| 22  | G     | 604 | CLA  | 12      | 0            |
| 22  | B     | 608 | CLA  | 2       | 0            |
| 24  | r     | 314 | XAT  | 5       | 0            |
| 23  | g     | 615 | LUT  | 16      | 0            |
| 22  | b     | 608 | CLA  | 3       | 0            |
| 36  | B     | 623 | LMG  | 53      | 0            |
| 31  | b     | 617 | BCR  | 1       | 0            |
| 21  | g     | 607 | CHL  | 22      | 0            |
| 33  | a     | 411 | SQD  | 4       | 0            |
| 30  | a     | 407 | PHO  | 5       | 0            |
| 21  | S     | 307 | CHL  | 25      | 0            |
| 22  | g     | 602 | CLA  | 3       | 0            |
| 22  | c     | 503 | CLA  | 3       | 0            |
| 23  | N     | 614 | LUT  | 16      | 0            |
| 35  | c     | 519 | DGD  | 4       | 0            |
| 31  | d     | 405 | BCR  | 4       | 0            |
| 22  | s     | 304 | CLA  | 1       | 0            |
| 22  | R     | 302 | CLA  | 2       | 0            |
| 23  | r     | 313 | LUT  | 2       | 0            |
| 33  | A     | 412 | SQD  | 4       | 0            |
| 21  | S     | 302 | CHL  | 17      | 0            |
| 22  | c     | 504 | CLA  | 5       | 0            |

*Continued on next page...*

*Continued from previous page...*

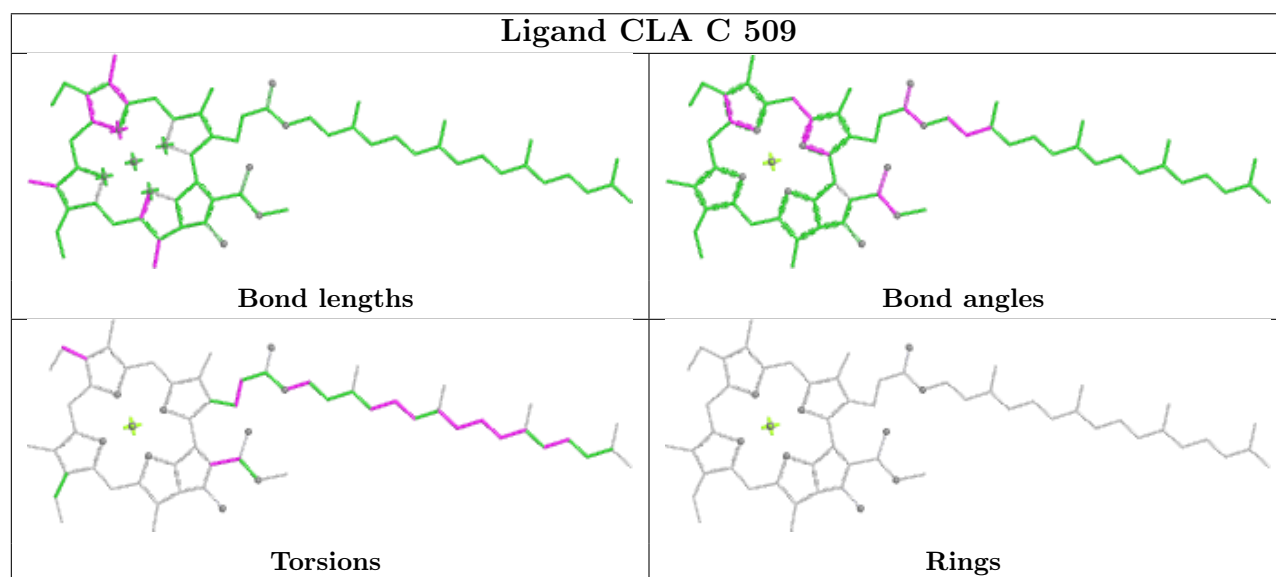
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | Y     | 604 | CLA  | 14      | 0            |
| 22  | B     | 618 | CLA  | 3       | 0            |
| 24  | G     | 617 | XAT  | 1       | 0            |
| 22  | D     | 405 | CLA  | 3       | 0            |
| 21  | G     | 605 | CHL  | 20      | 0            |
| 23  | N     | 615 | LUT  | 17      | 0            |
| 22  | B     | 609 | CLA  | 2       | 0            |
| 22  | S     | 309 | CLA  | 3       | 0            |
| 22  | n     | 609 | CLA  | 6       | 0            |
| 22  | s     | 305 | CLA  | 8       | 0            |
| 22  | c     | 506 | CLA  | 5       | 0            |
| 34  | a     | 412 | BCT  | 4       | 0            |
| 22  | r     | 304 | CLA  | 5       | 0            |
| 25  | g     | 618 | NEX  | 8       | 0            |
| 26  | B     | 622 | LHG  | 1       | 0            |
| 22  | r     | 311 | CLA  | 3       | 0            |
| 21  | N     | 601 | CHL  | 32      | 0            |
| 26  | R     | 301 | LHG  | 5       | 0            |
| 22  | b     | 607 | CLA  | 2       | 0            |
| 22  | G     | 613 | CLA  | 18      | 0            |
| 34  | D     | 403 | BCT  | 4       | 0            |
| 31  | T     | 102 | BCR  | 2       | 0            |
| 26  | D     | 409 | LHG  | 4       | 0            |
| 36  | w     | 102 | LMG  | 3       | 0            |
| 36  | M     | 101 | LMG  | 5       | 0            |
| 24  | N     | 616 | XAT  | 2       | 0            |
| 31  | C     | 516 | BCR  | 6       | 0            |
| 33  | l     | 103 | SQD  | 4       | 0            |
| 26  | g     | 619 | LHG  | 6       | 0            |
| 22  | A     | 409 | CLA  | 2       | 0            |
| 21  | N     | 608 | CHL  | 27      | 0            |
| 30  | d     | 401 | PHO  | 6       | 0            |
| 23  | n     | 614 | LUT  | 12      | 0            |
| 22  | s     | 303 | CLA  | 4       | 0            |
| 22  | a     | 408 | CLA  | 3       | 0            |
| 21  | G     | 607 | CHL  | 22      | 0            |
| 26  | D     | 408 | LHG  | 1       | 0            |
| 35  | A     | 401 | DGD  | 7       | 0            |
| 22  | n     | 610 | CLA  | 2       | 0            |
| 21  | g     | 605 | CHL  | 20      | 0            |
| 21  | Y     | 608 | CHL  | 32      | 0            |
| 22  | b     | 609 | CLA  | 3       | 0            |

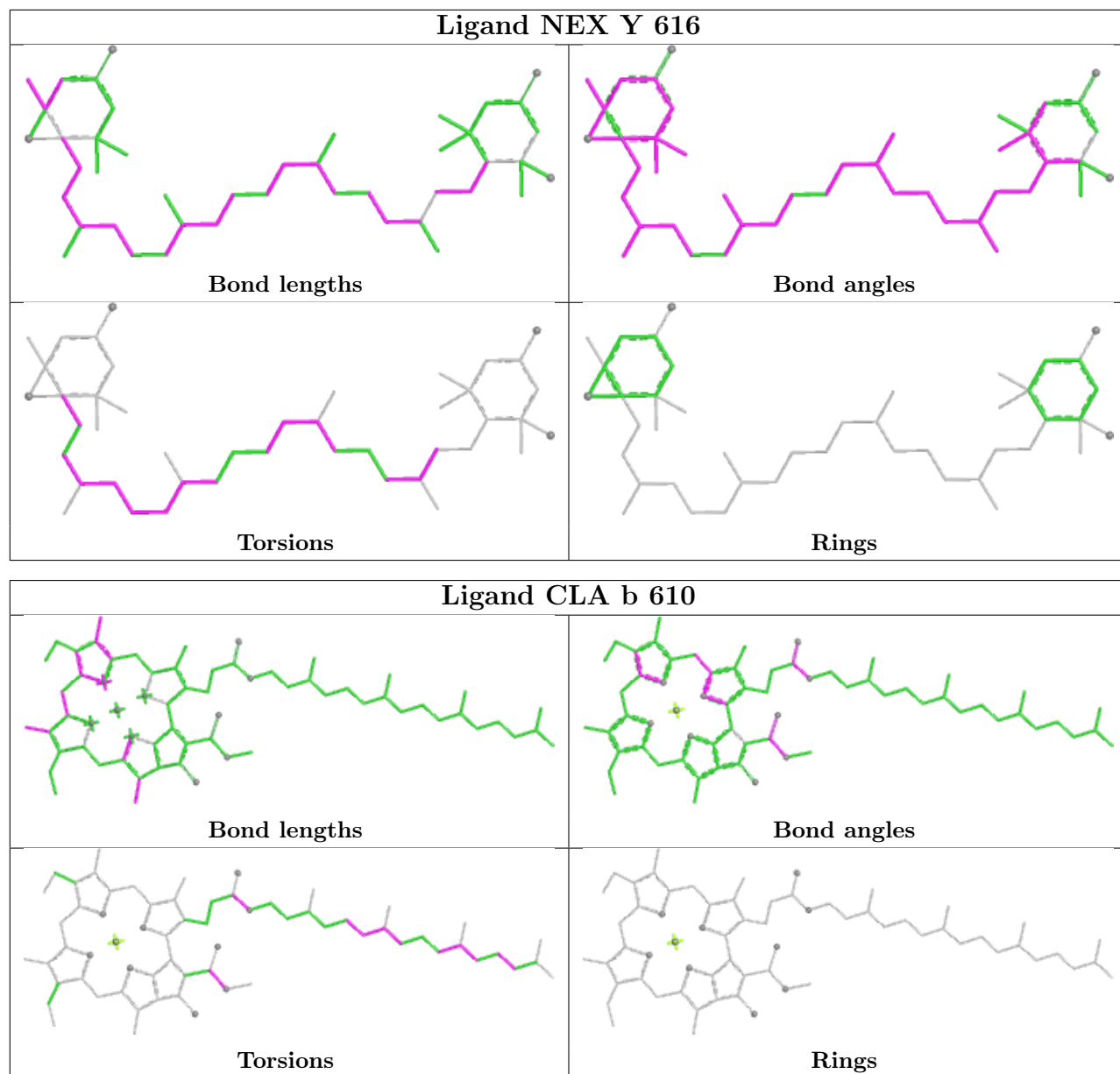
*Continued on next page...*

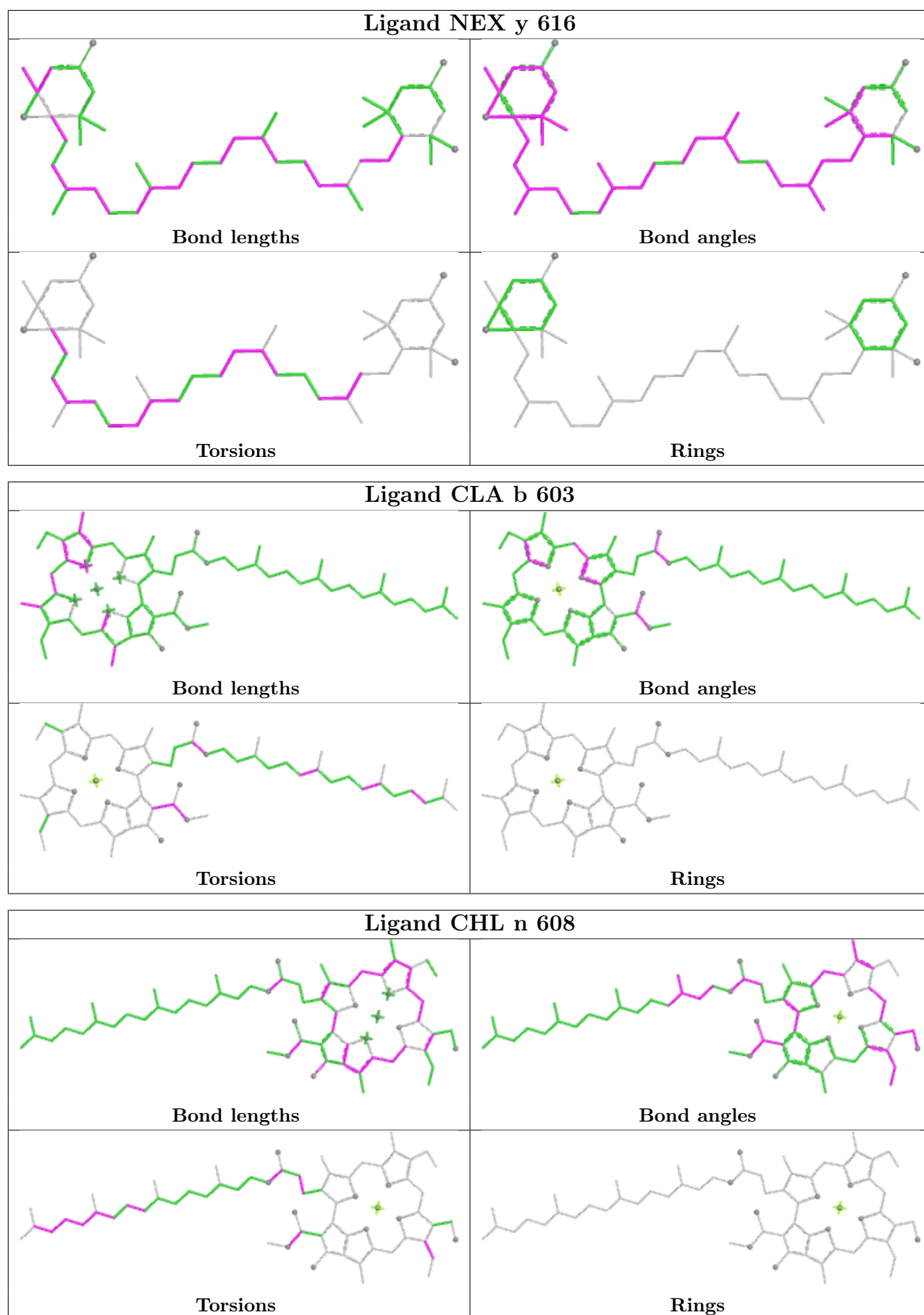
*Continued from previous page...*

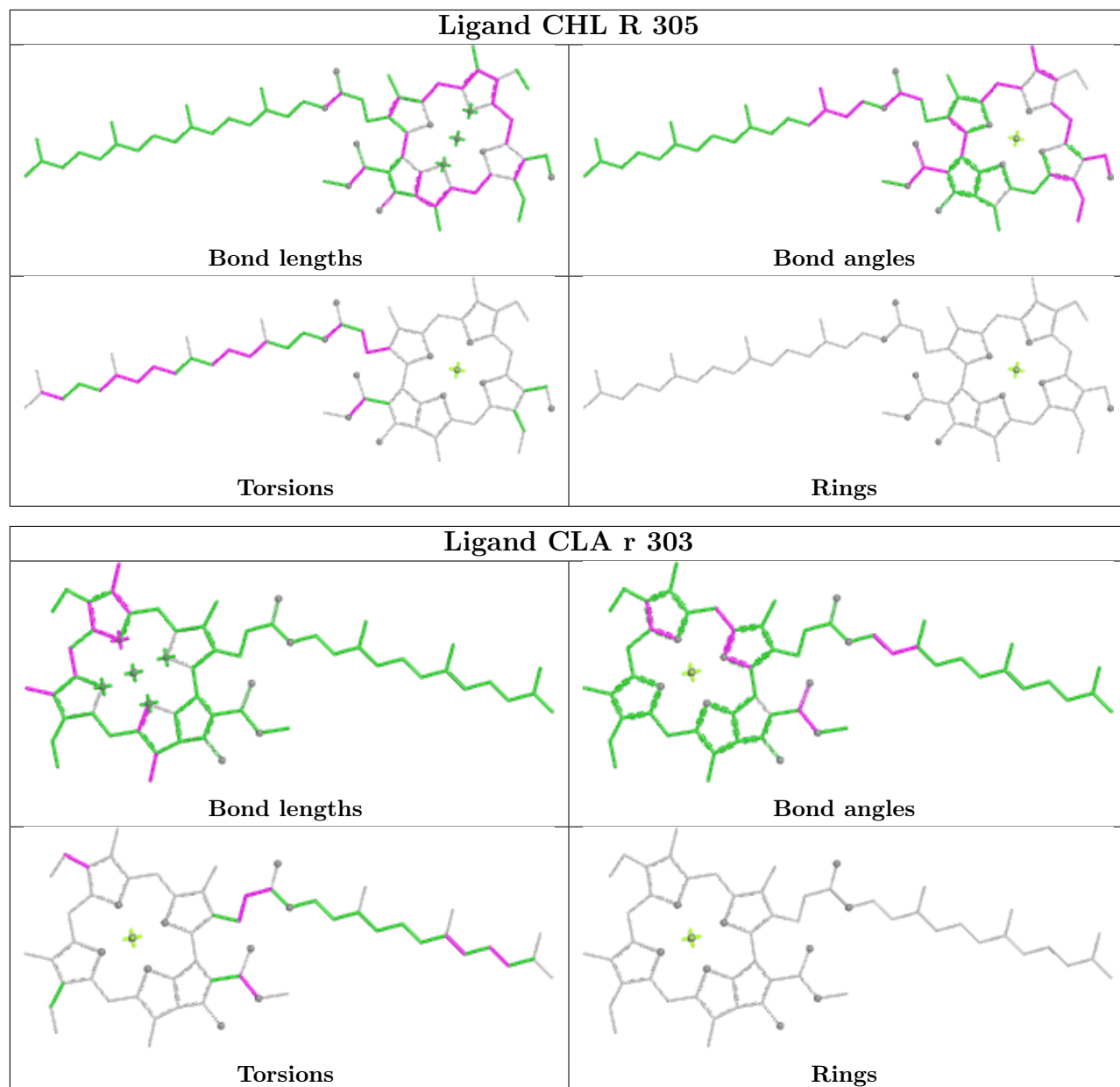
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | s     | 309 | CLA  | 2       | 0            |
| 37  | F     | 101 | HEM  | 17      | 0            |
| 24  | y     | 615 | XAT  | 2       | 0            |
| 21  | r     | 307 | CHL  | 28      | 0            |
| 22  | R     | 311 | CLA  | 5       | 0            |
| 22  | N     | 611 | CLA  | 8       | 0            |
| 35  | C     | 519 | DGD  | 9       | 0            |
| 22  | a     | 405 | CLA  | 3       | 0            |
| 25  | r     | 315 | NEX  | 8       | 0            |
| 21  | g     | 608 | CHL  | 35      | 0            |
| 22  | b     | 602 | CLA  | 5       | 0            |
| 31  | D     | 406 | BCR  | 4       | 0            |
| 36  | b     | 620 | LMG  | 36      | 0            |
| 24  | n     | 615 | XAT  | 2       | 0            |
| 31  | a     | 409 | BCR  | 1       | 0            |
| 31  | K     | 102 | BCR  | 4       | 0            |

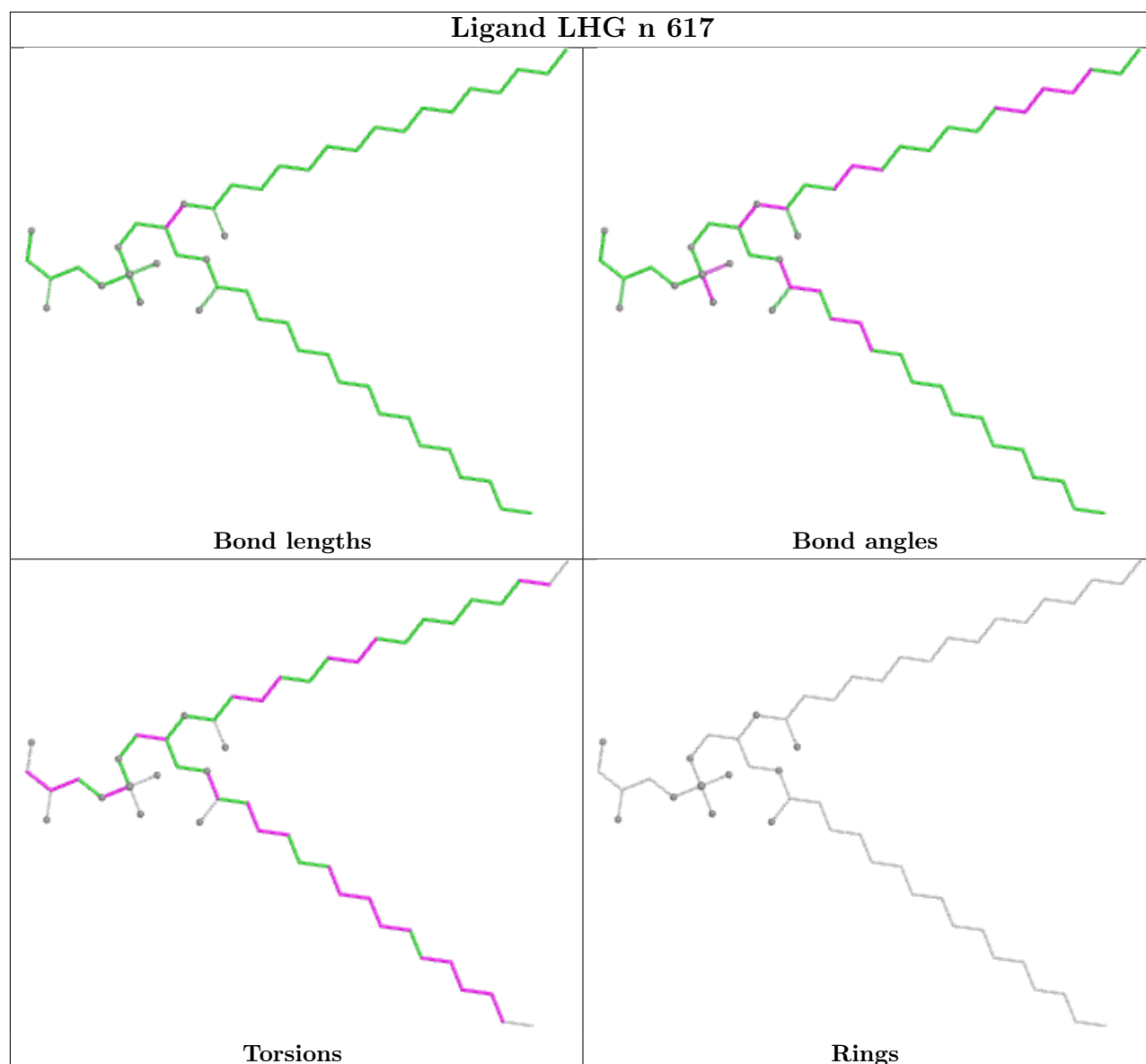
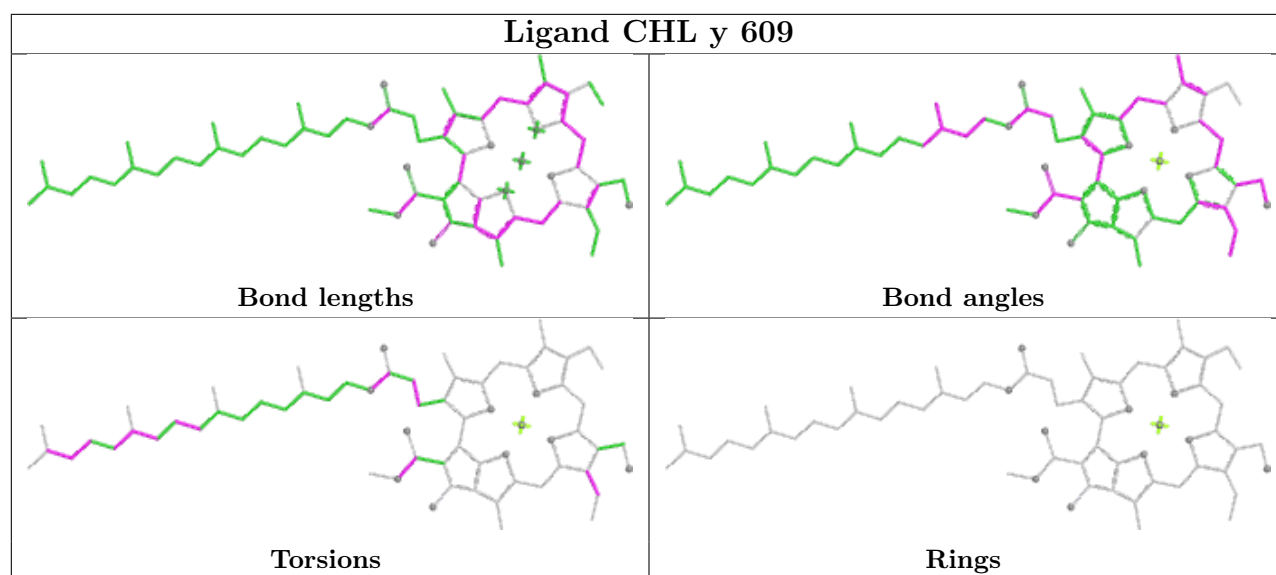
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

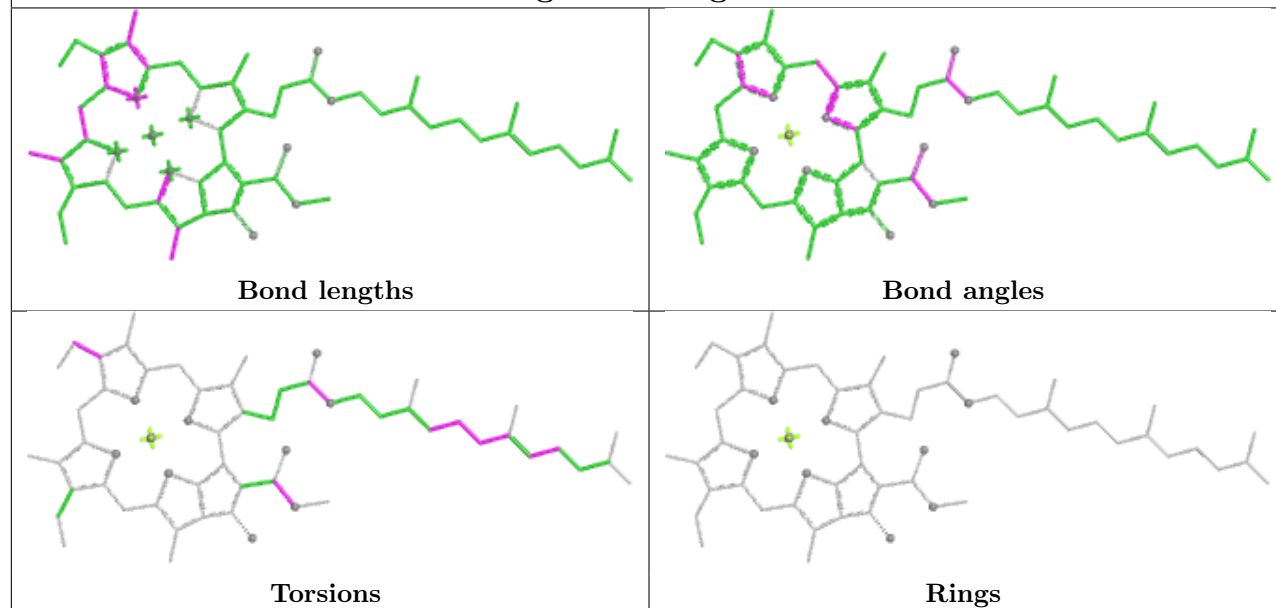
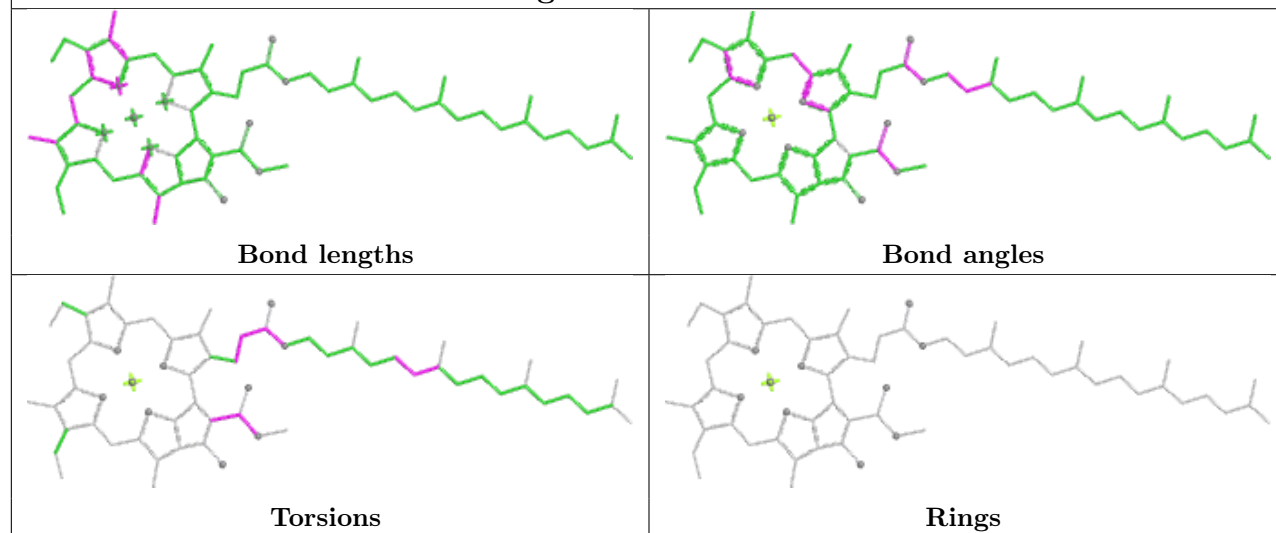




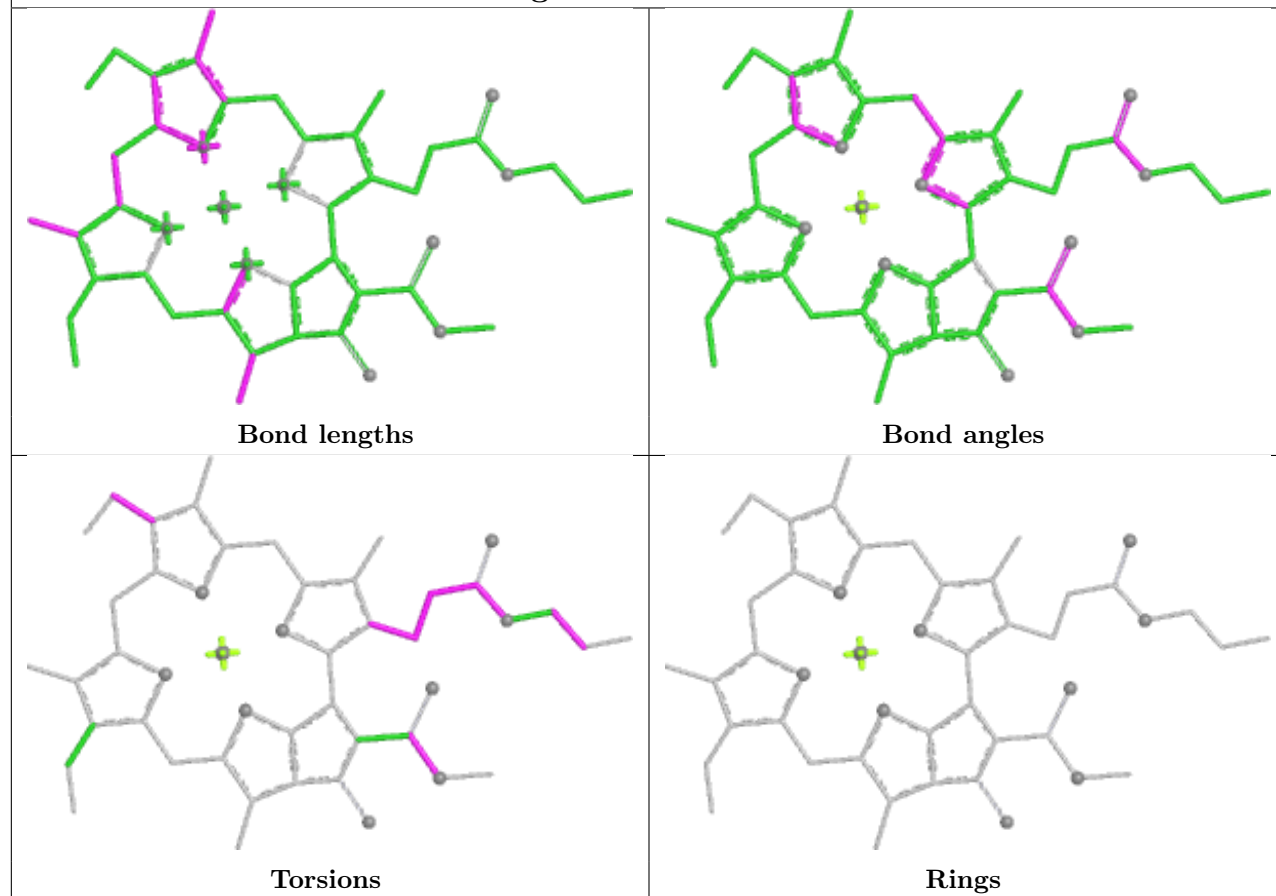




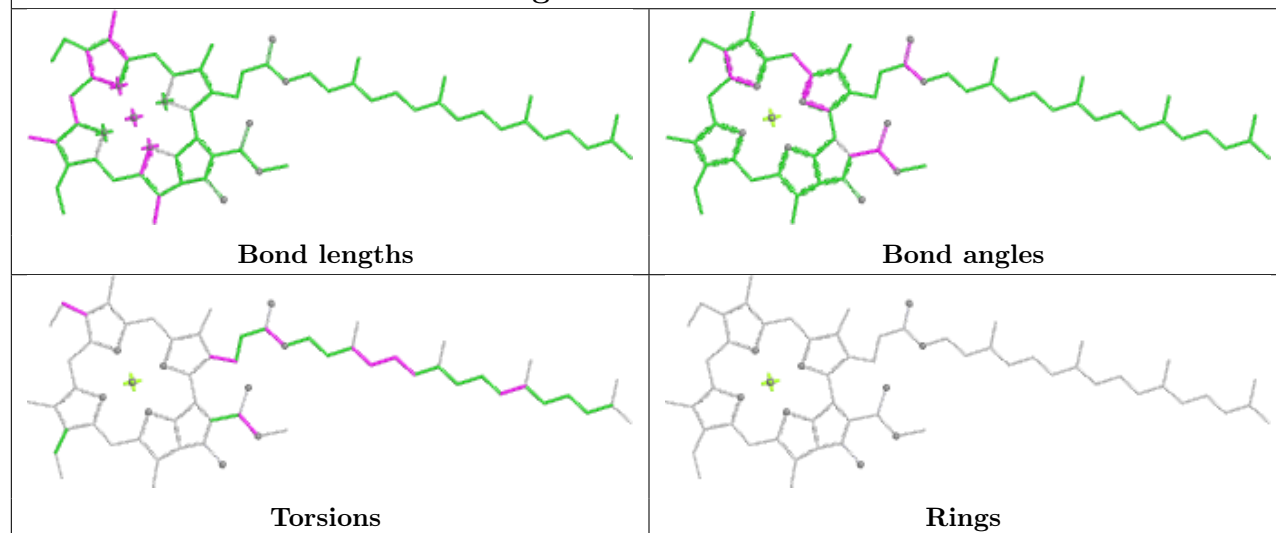


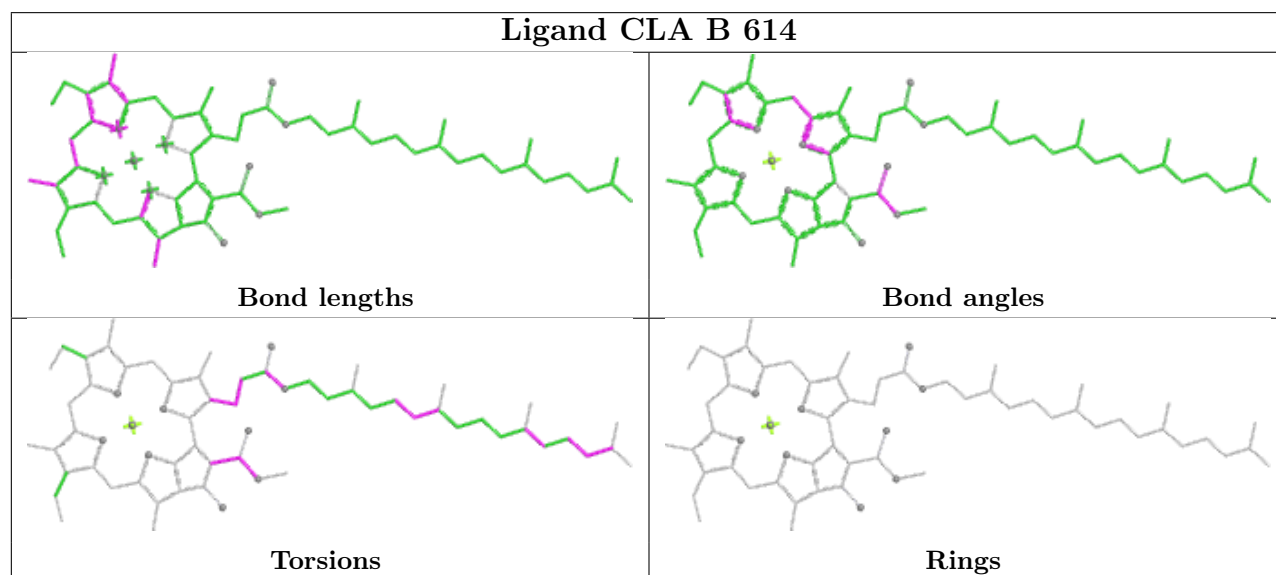
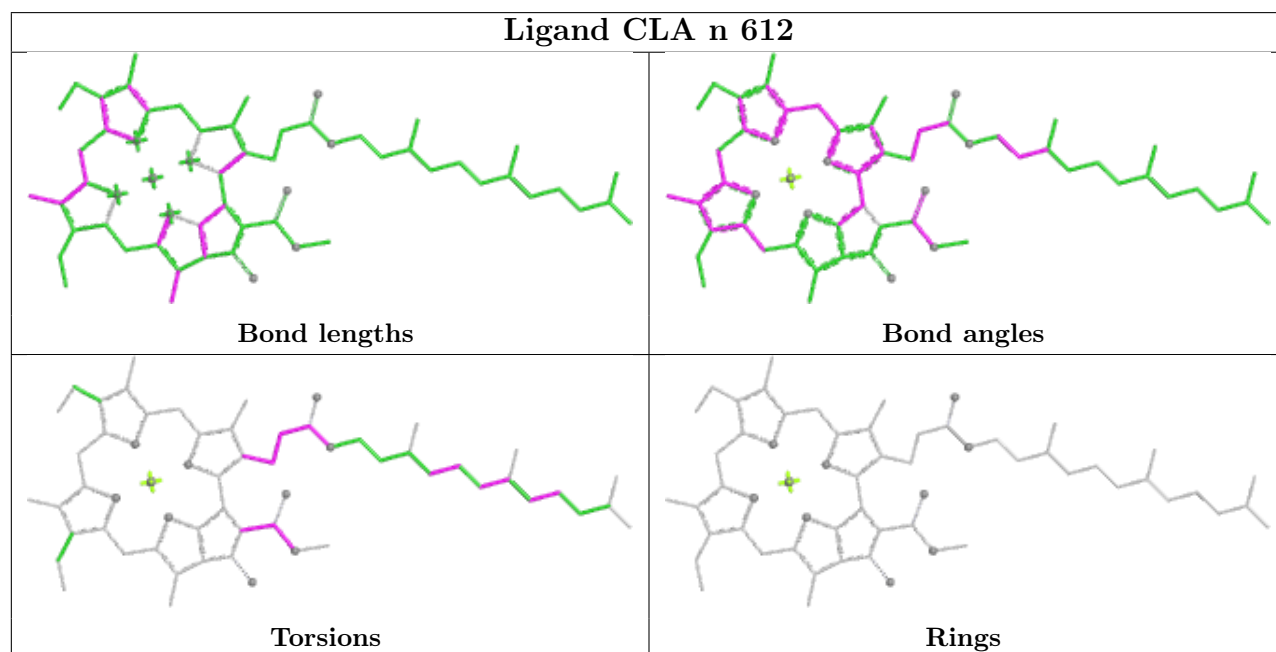
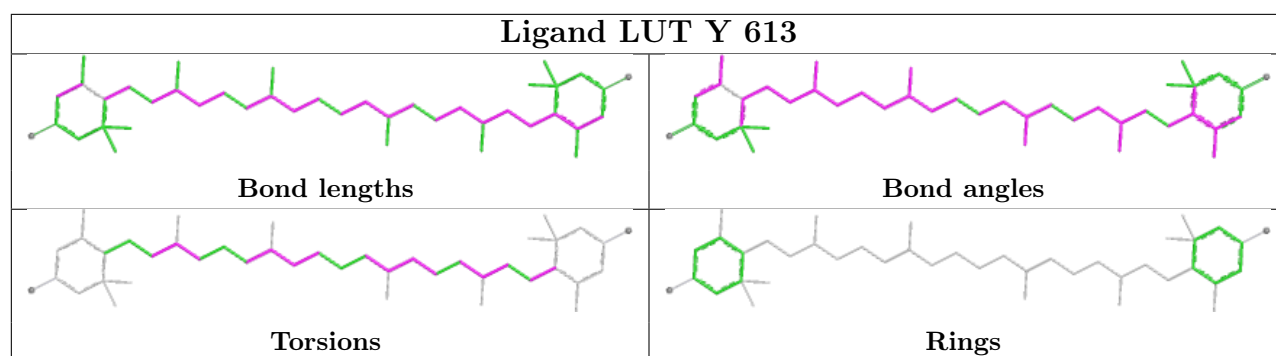
**Ligand CLA g 611****Ligand CLA c 507**

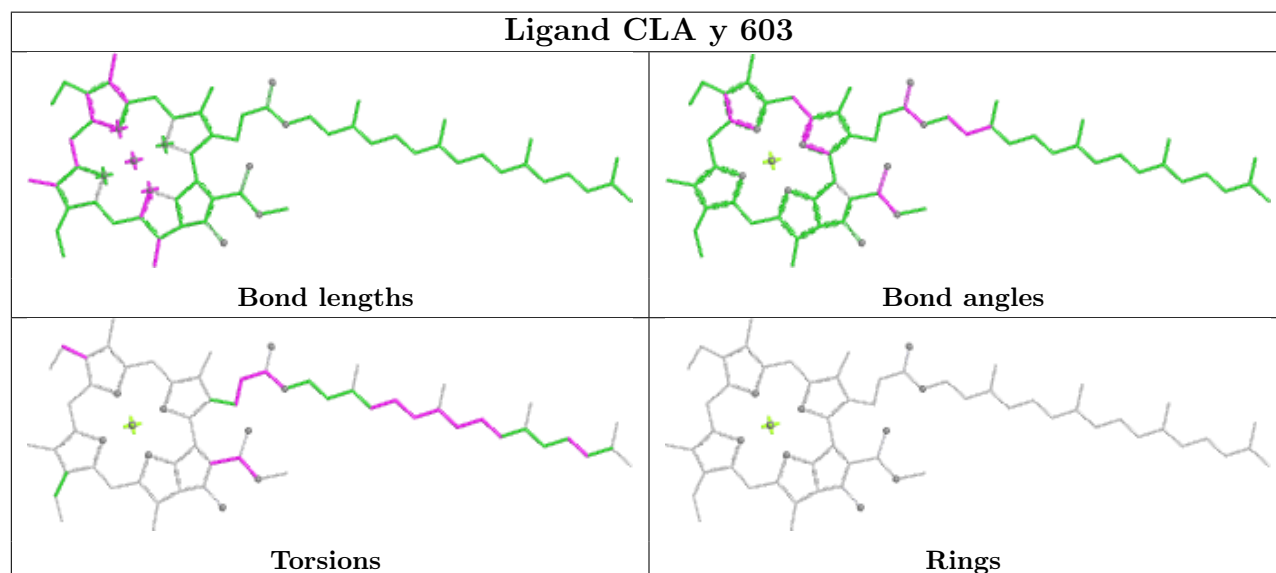
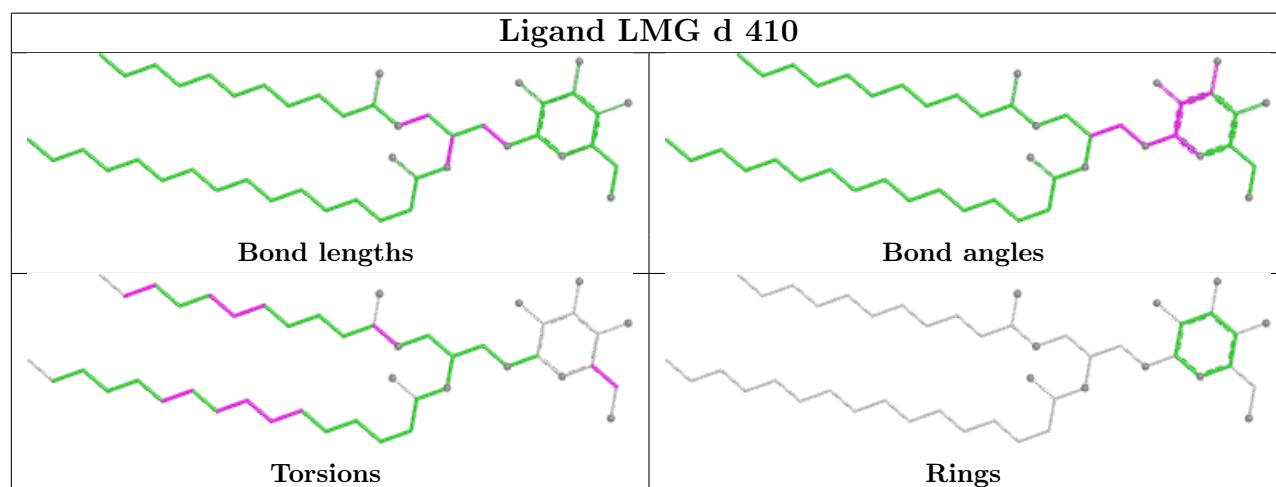
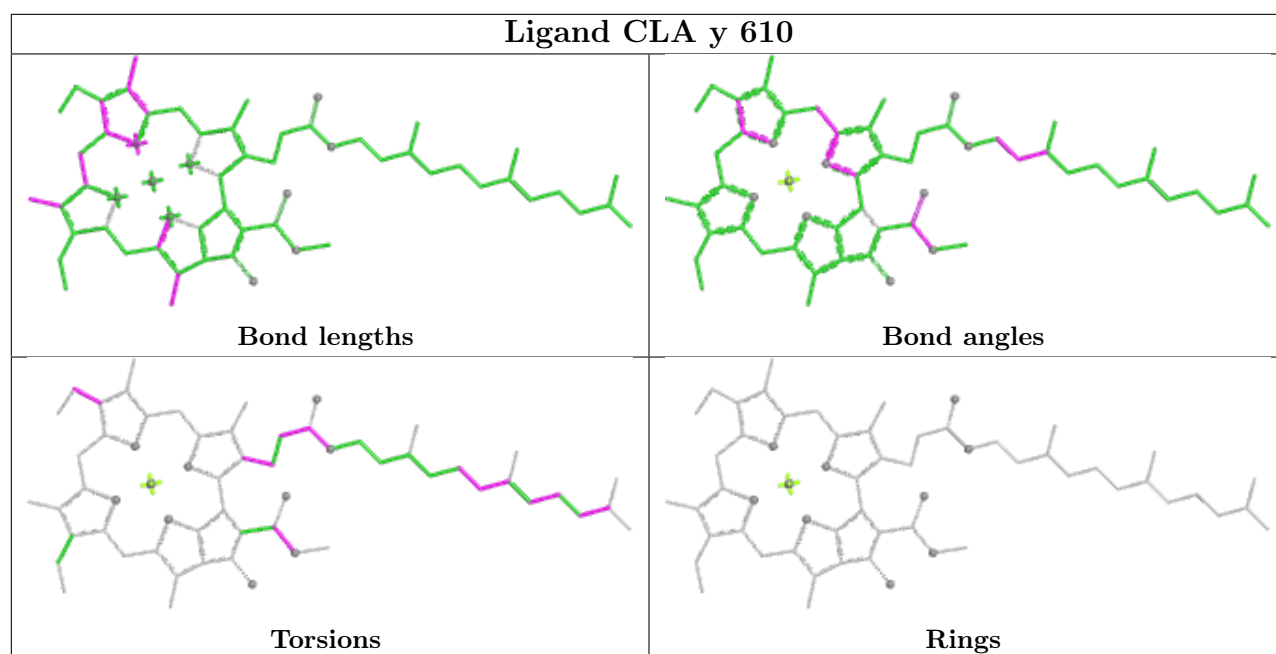
## Ligand CLA G 614

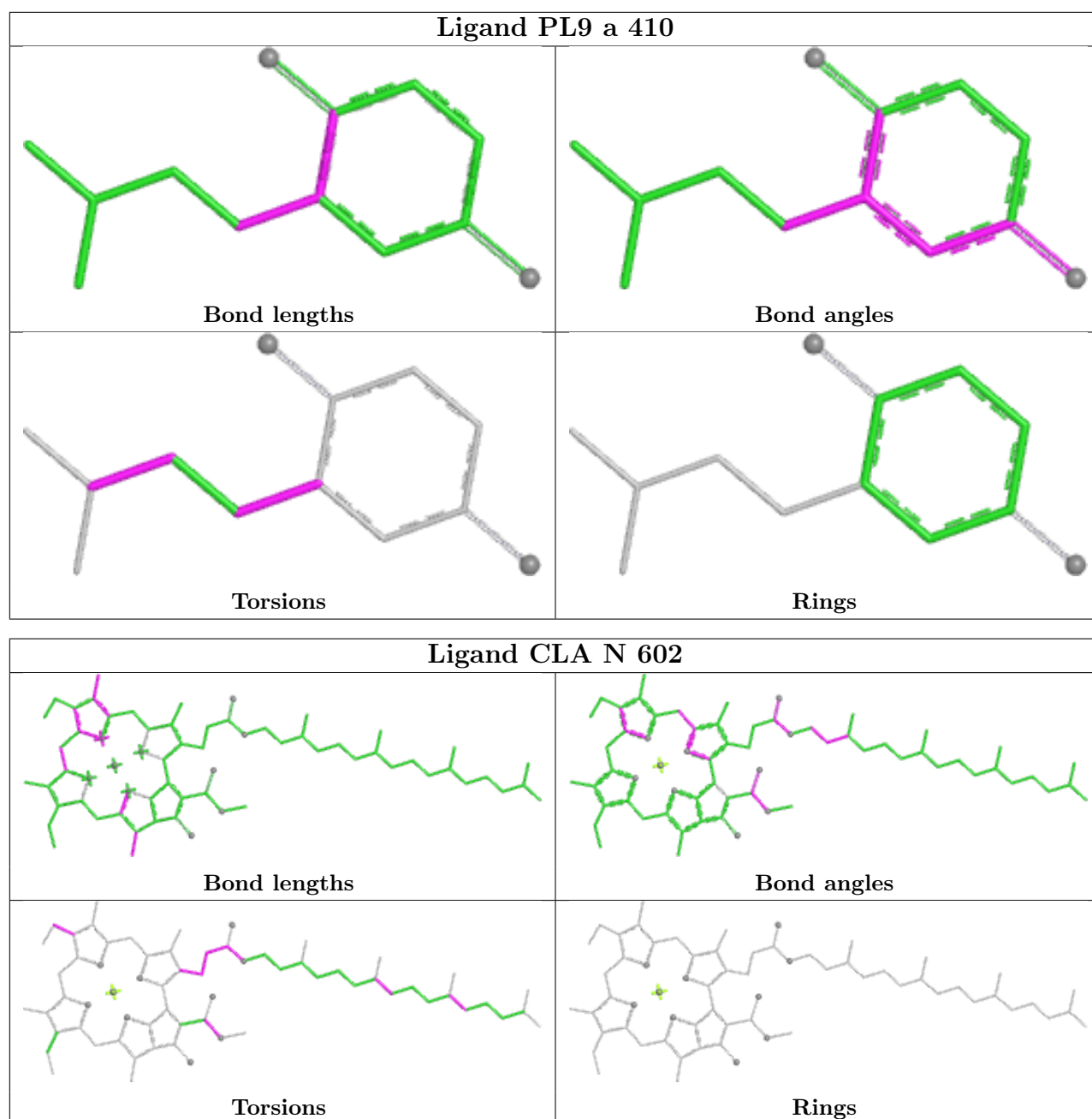


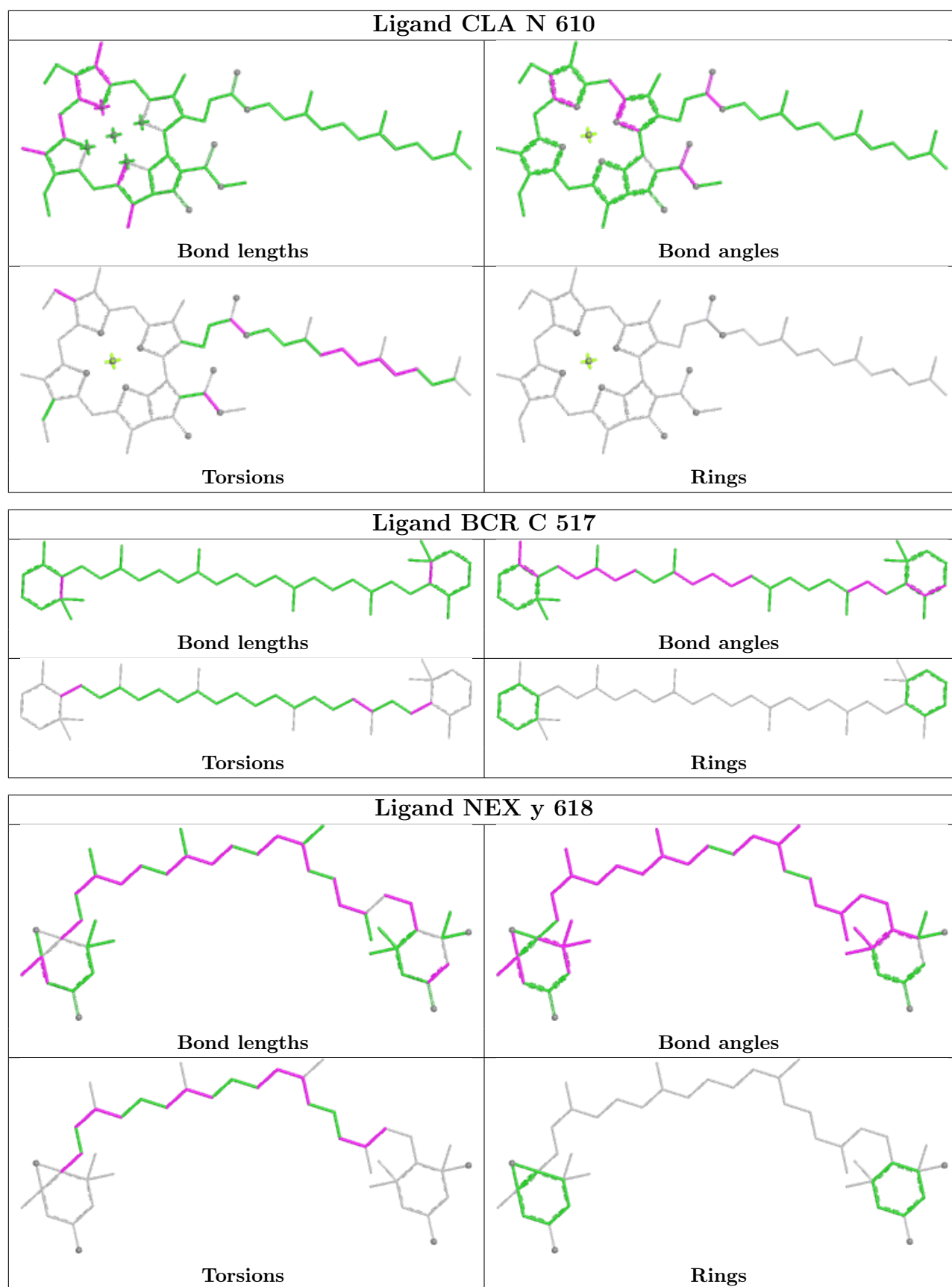
## Ligand CLA C 512

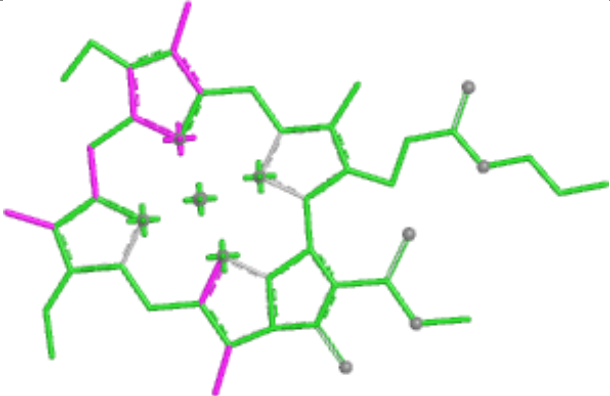
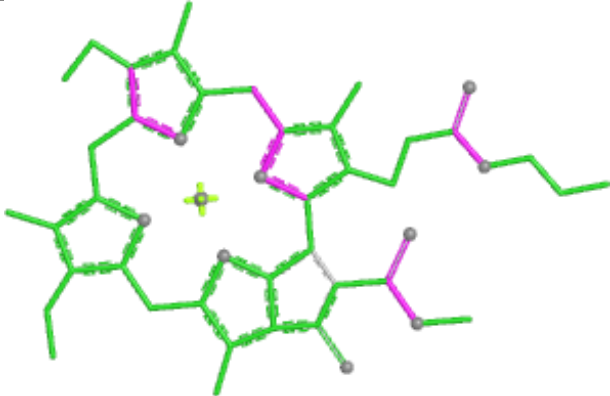
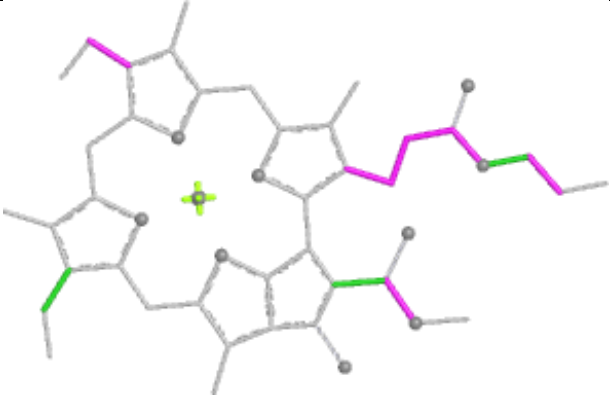
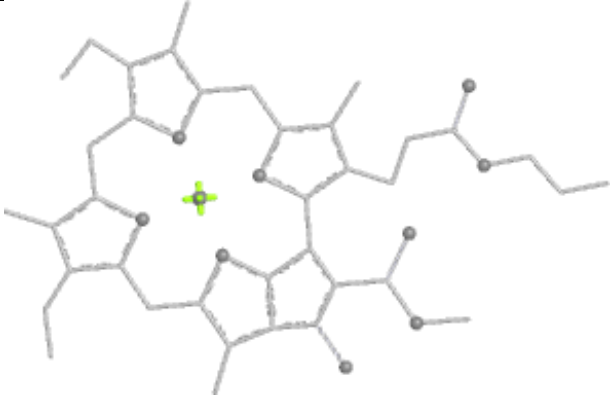


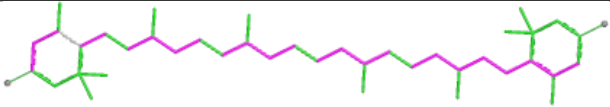
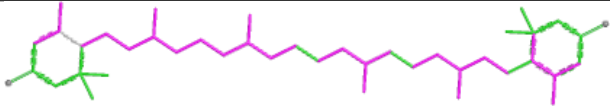
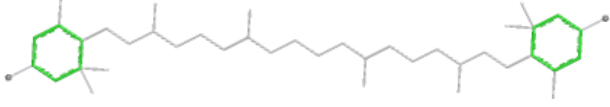


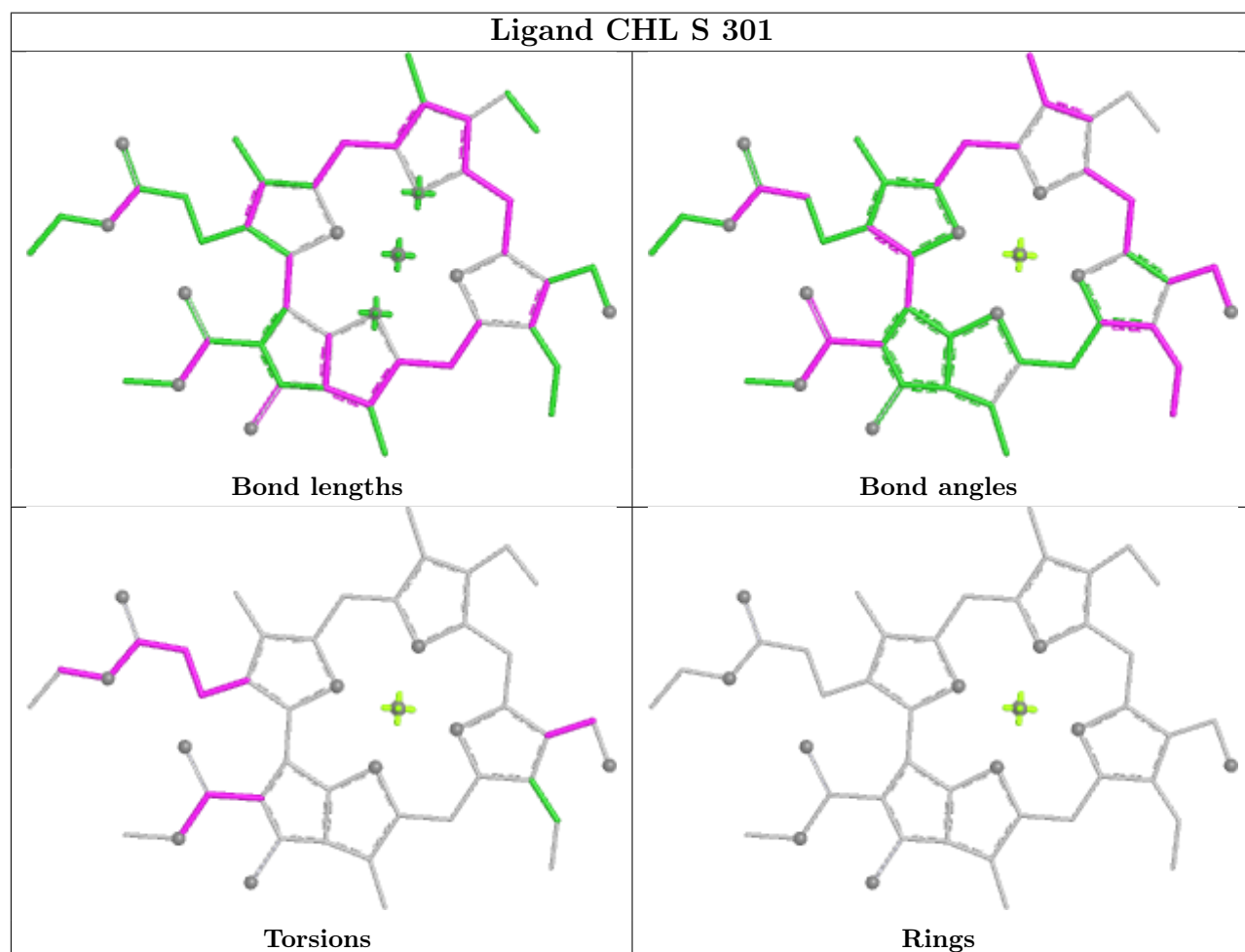
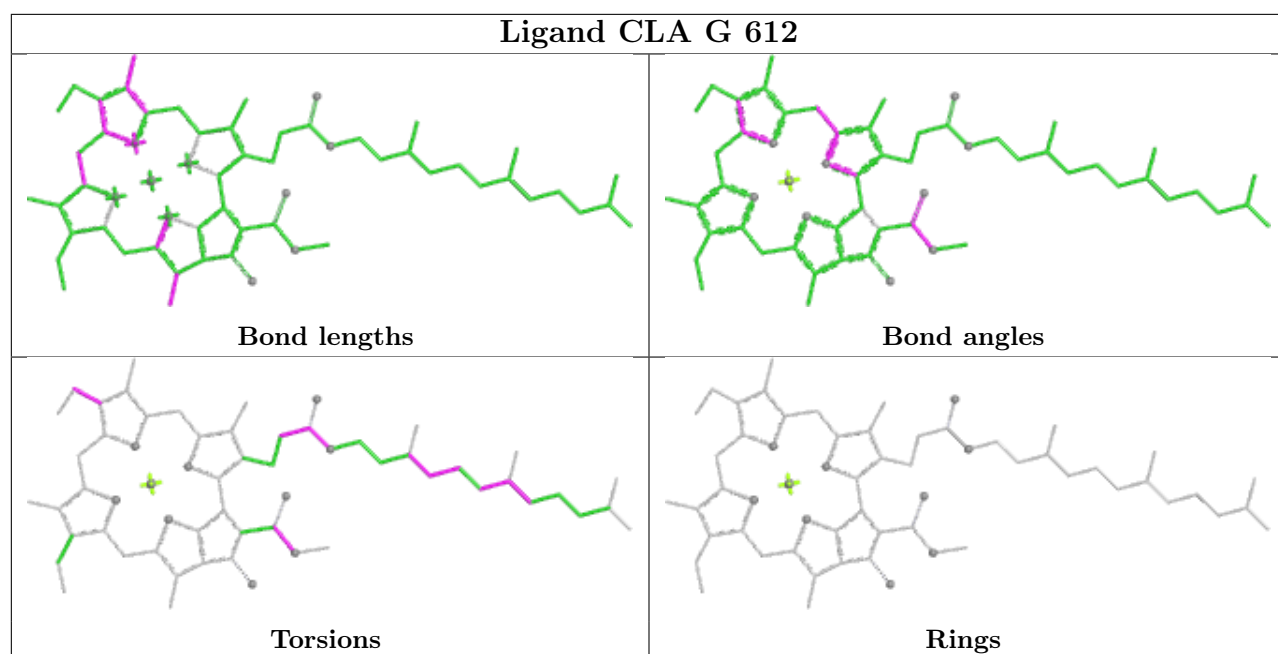


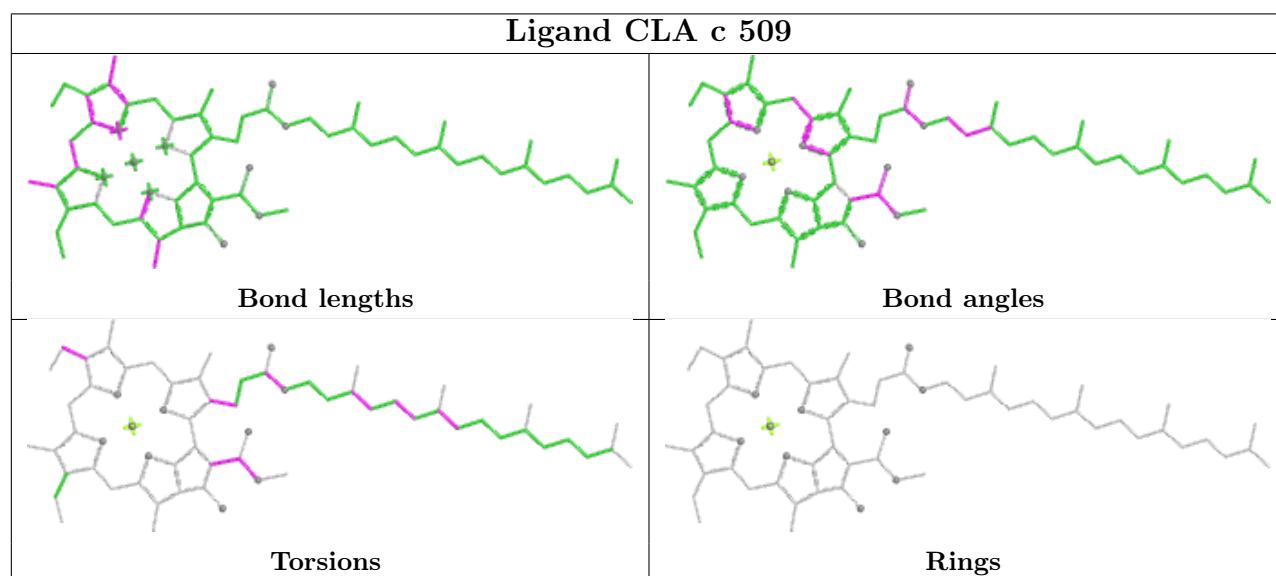
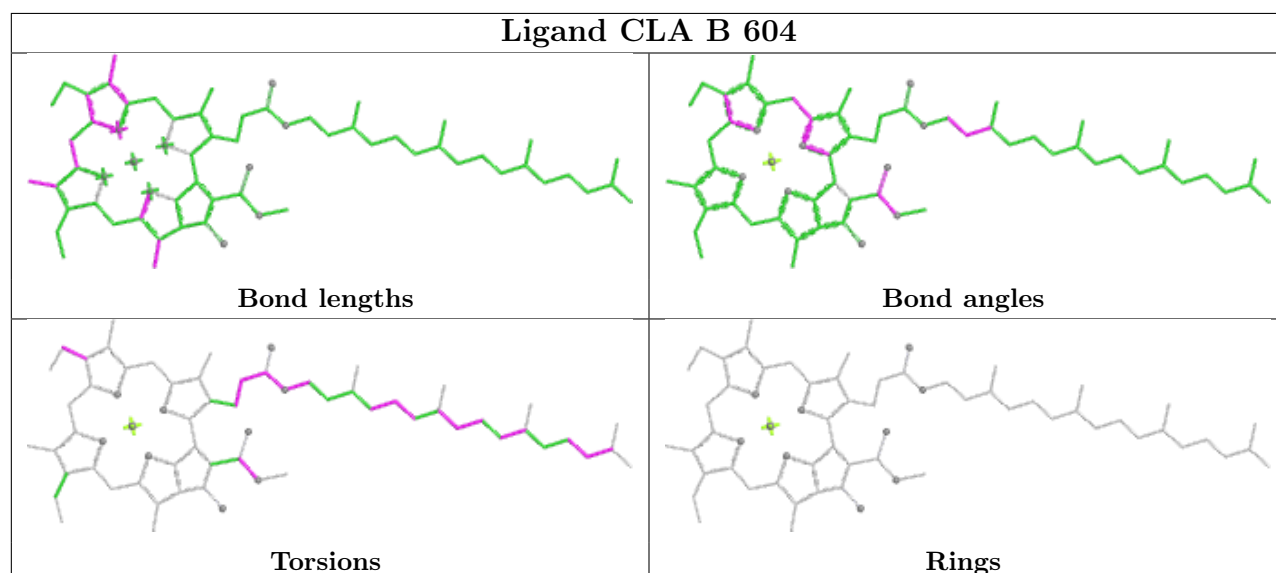
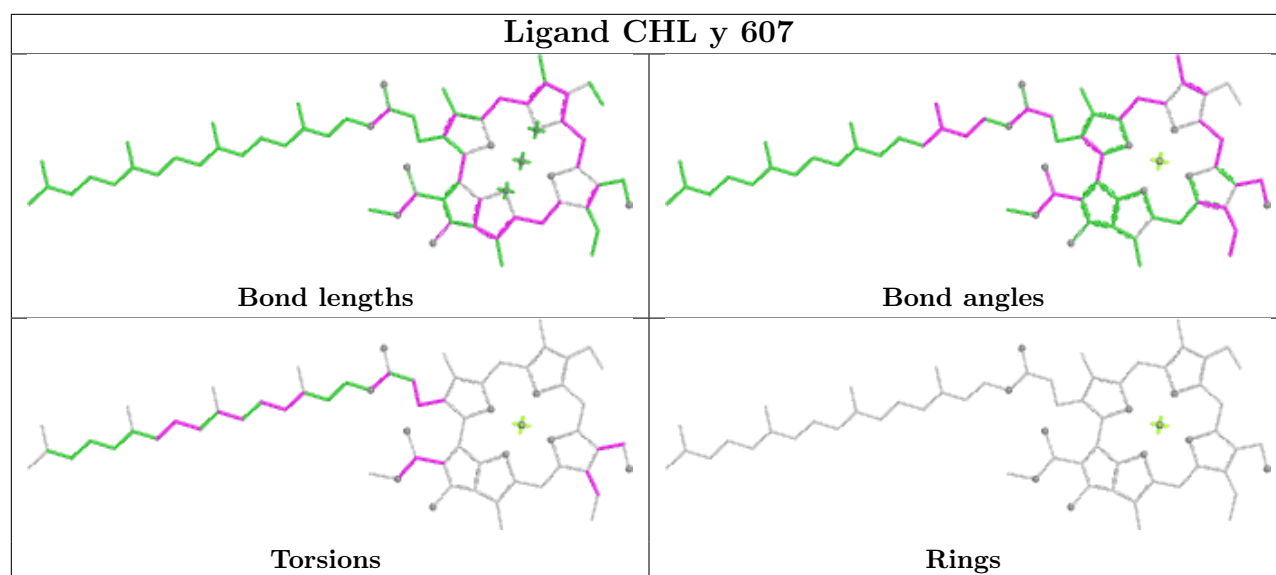




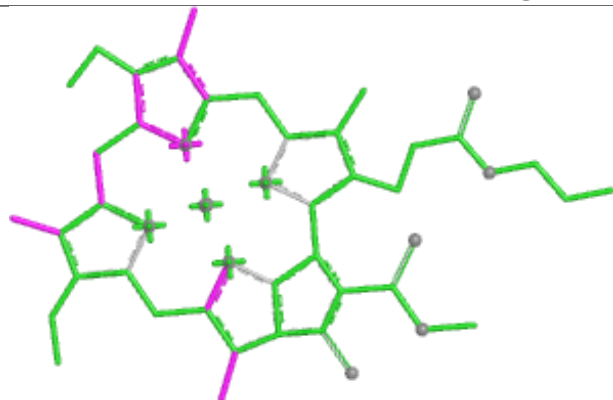
| Ligand CLA y 613                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

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

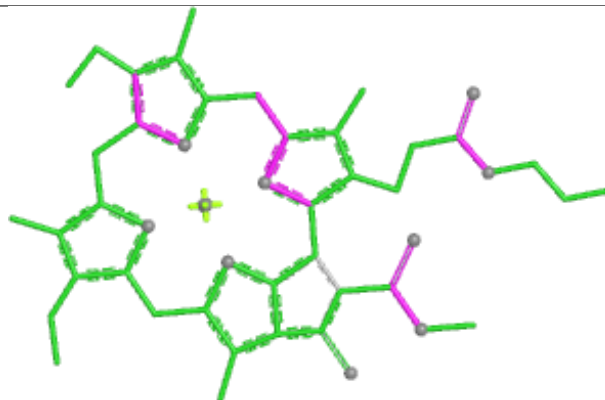




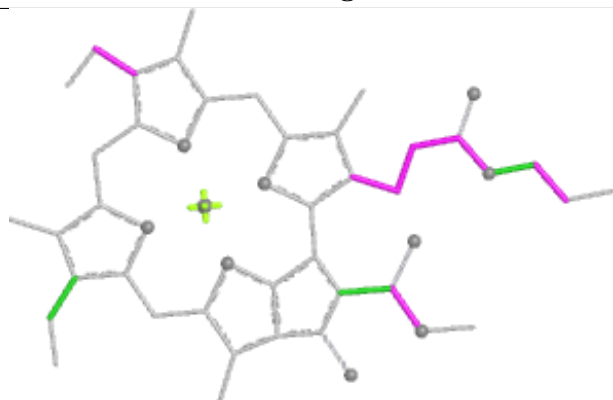
## Ligand CLA n 613



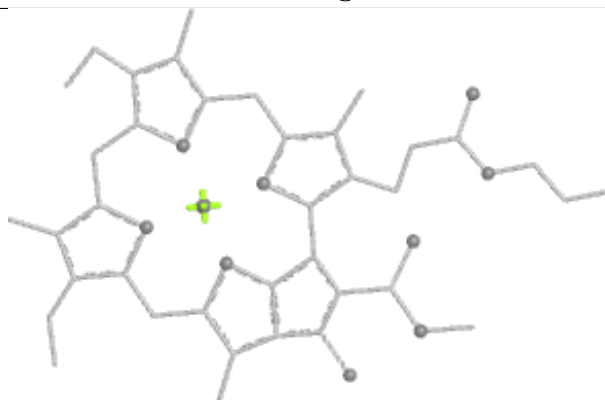
Bond lengths



Bond angles

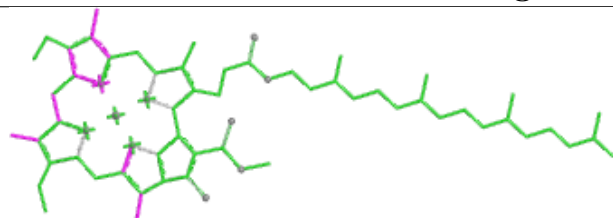


Torsions

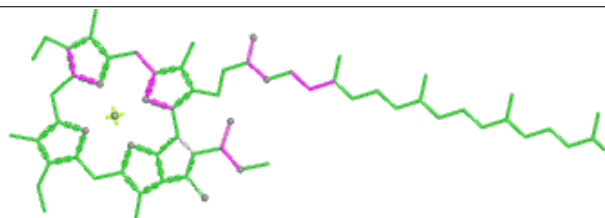


Rings

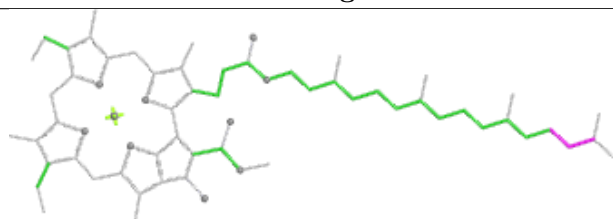
## Ligand CLA A 405



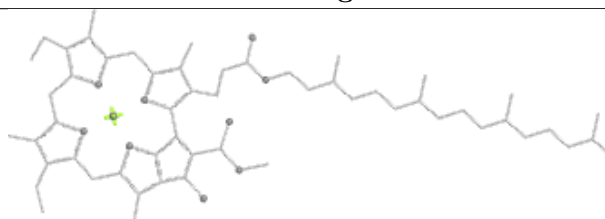
Bond lengths



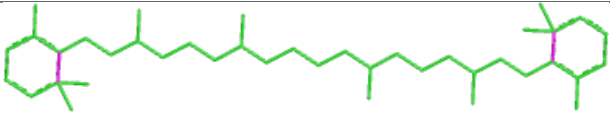
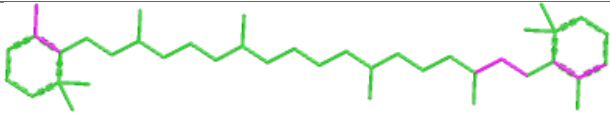
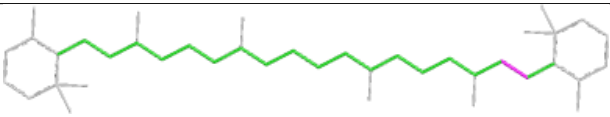
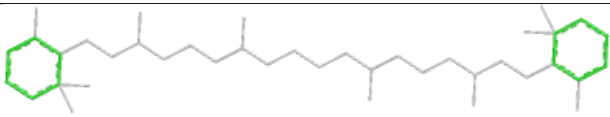
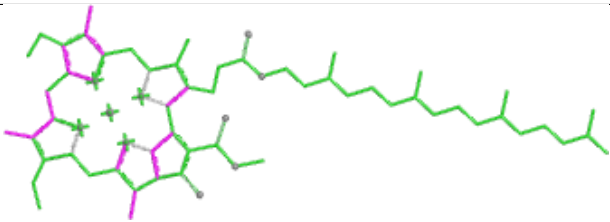
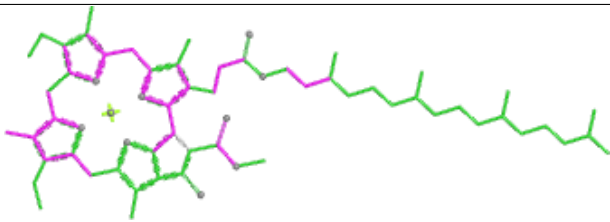
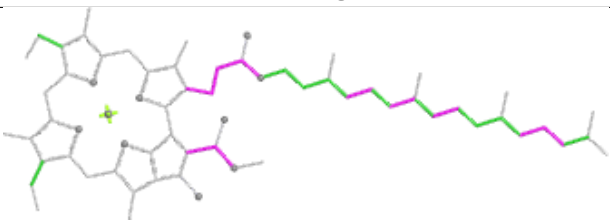
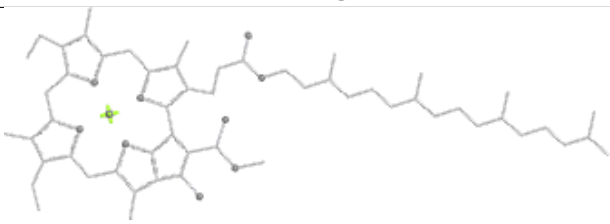
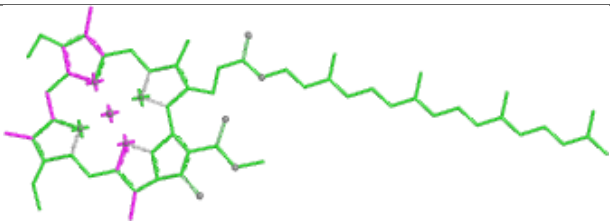
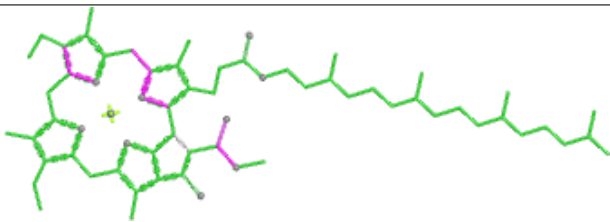
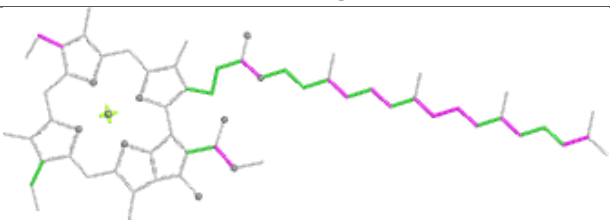
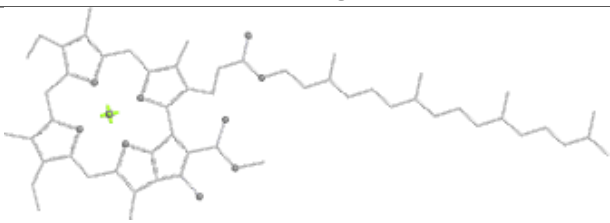
Bond angles

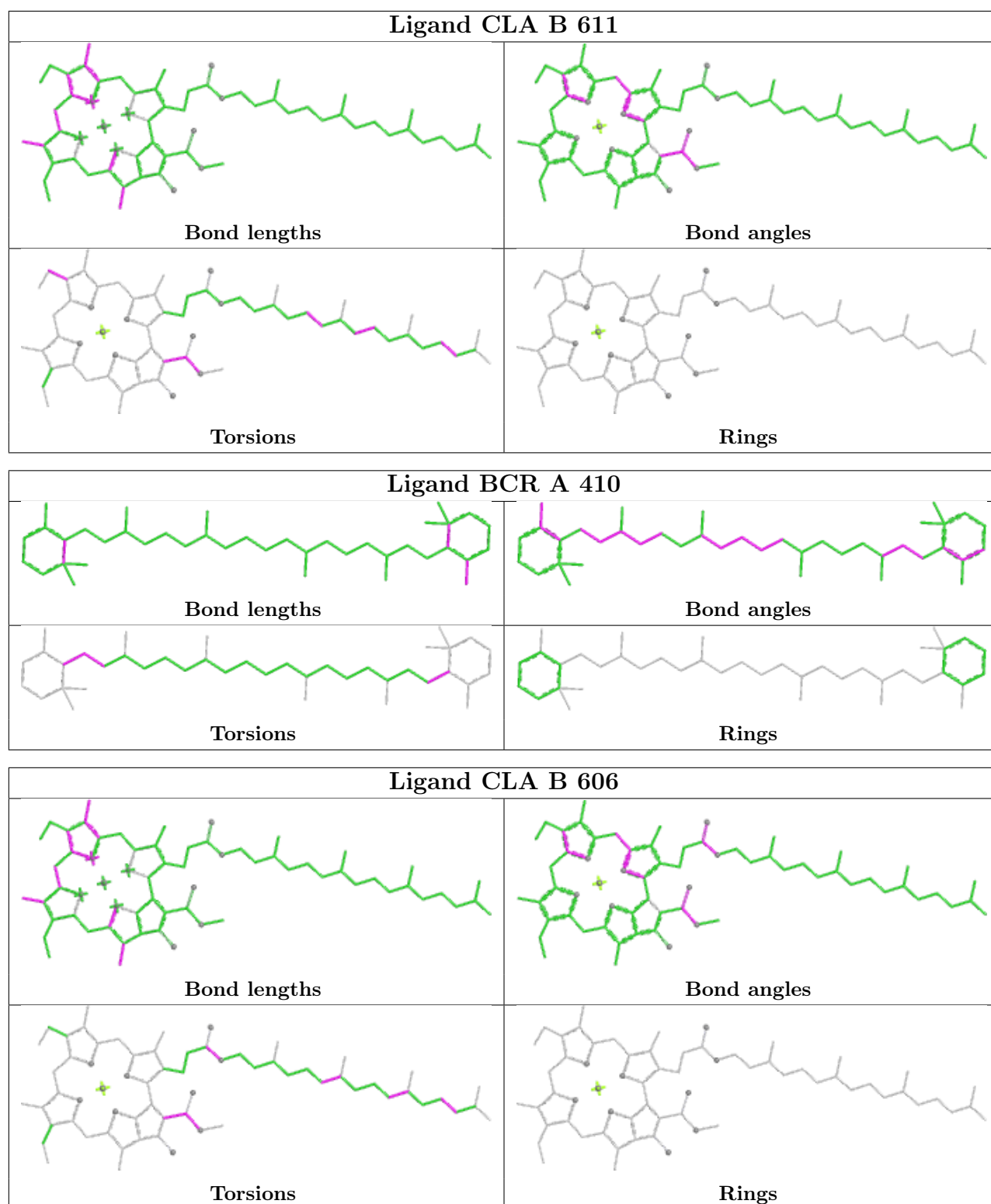


Torsions

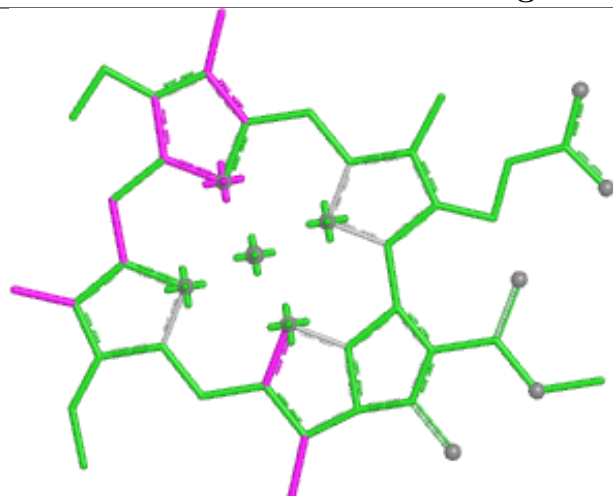


Rings

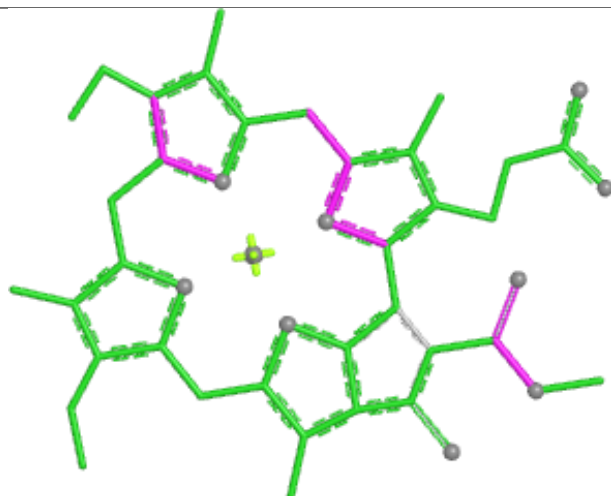
| Ligand BCR B 621                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand CLA g 613                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand CLA b 604                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |



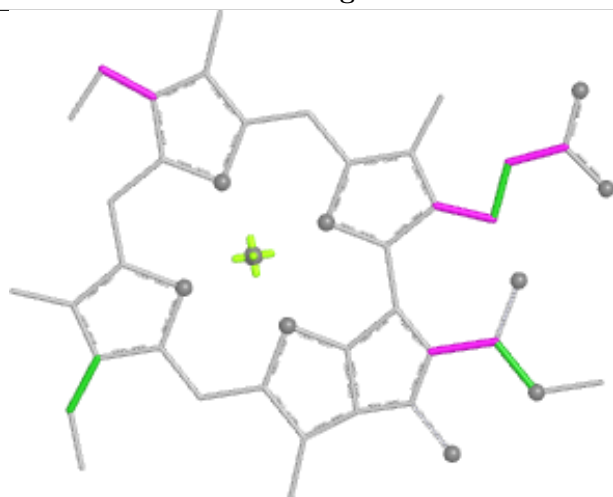
## Ligand CLA S 304



Bond lengths



Bond angles

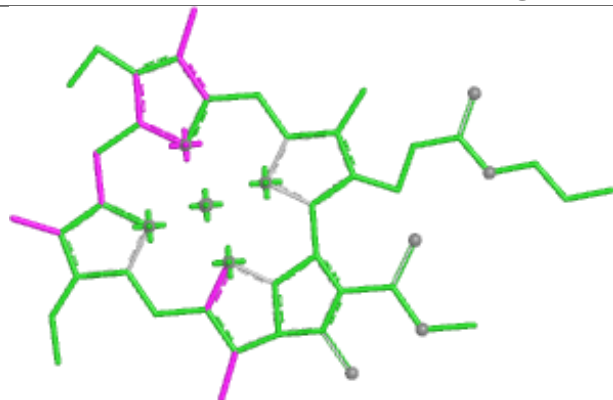


Torsions

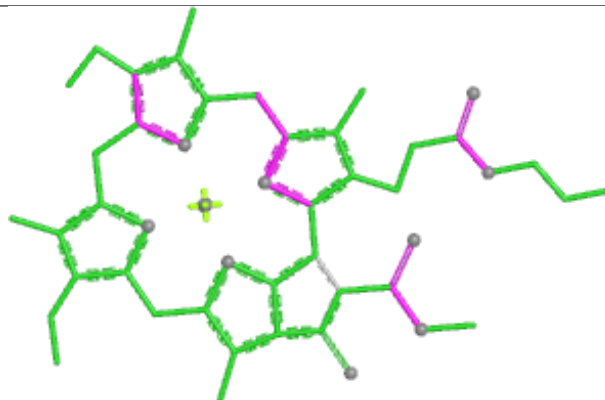


Rings

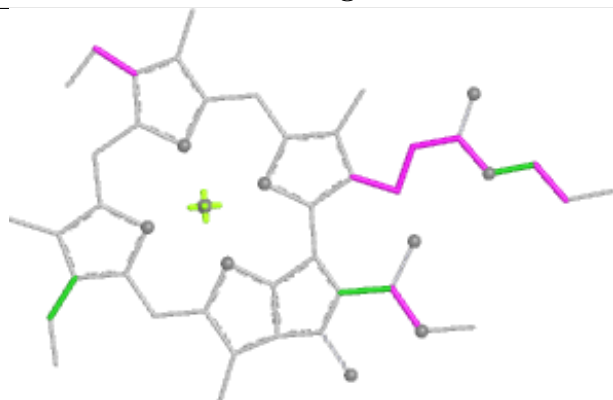
## Ligand CLA Y 612



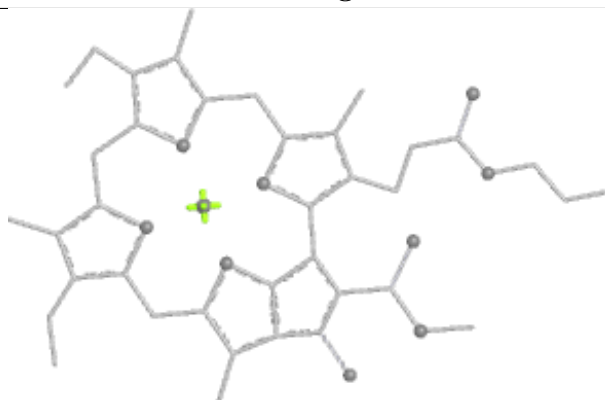
Bond lengths



Bond angles

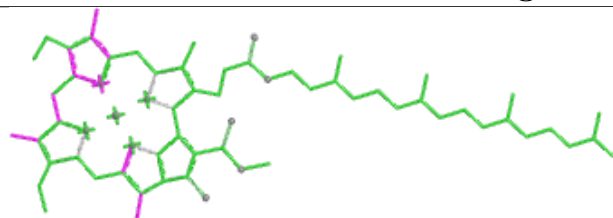


Torsions

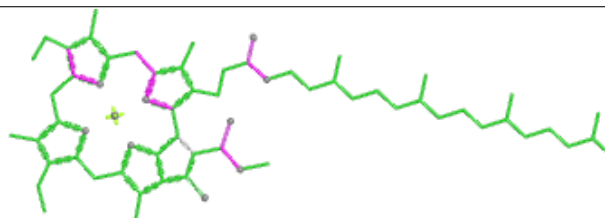


Rings

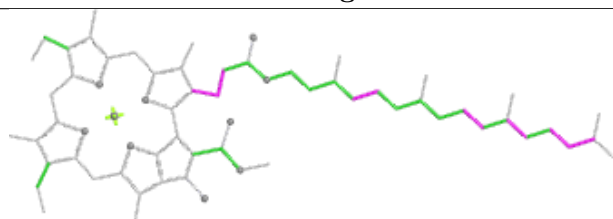
## Ligand CLA b 605



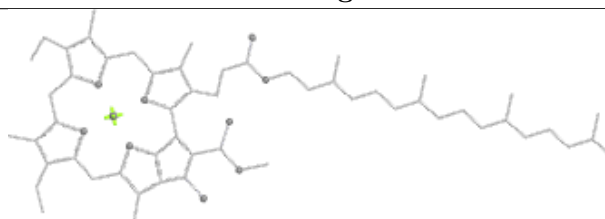
Bond lengths



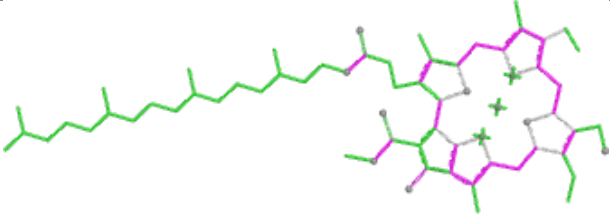
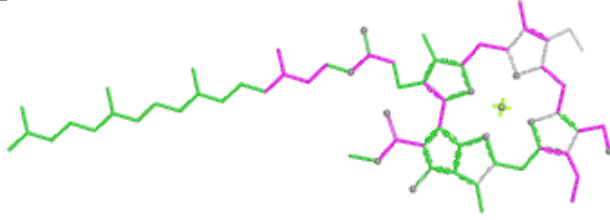
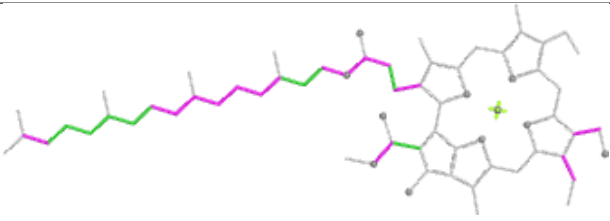
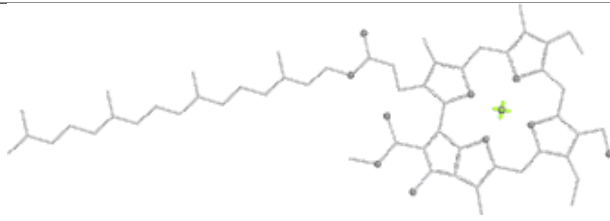
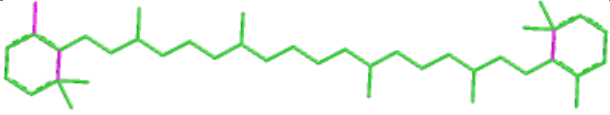
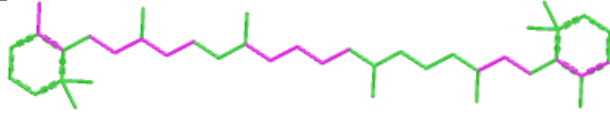
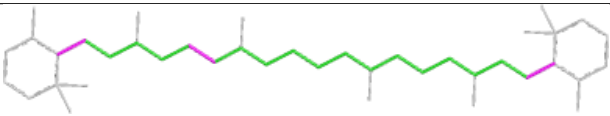
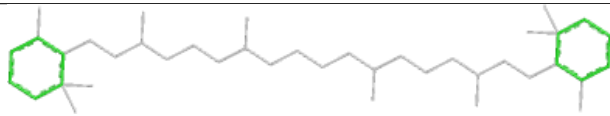
Bond angles



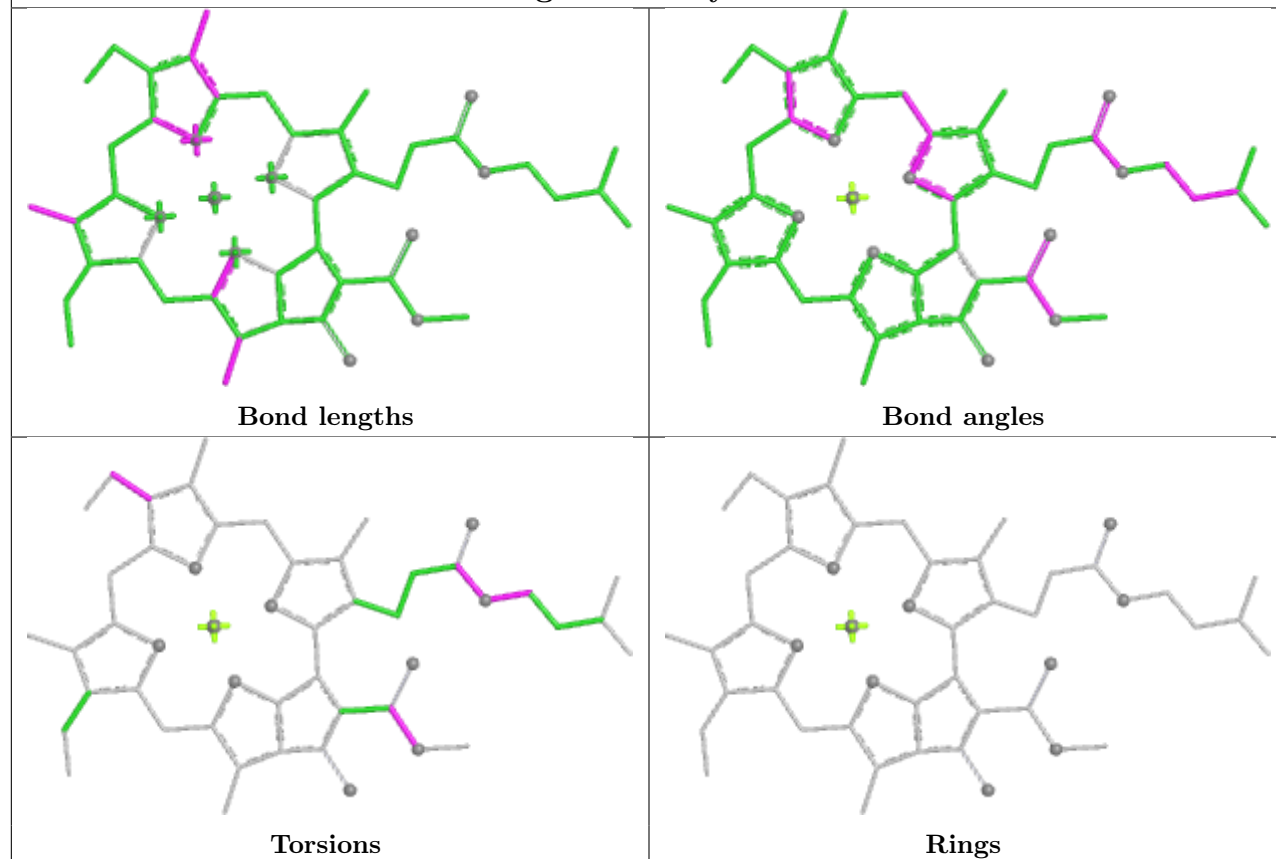
Torsions



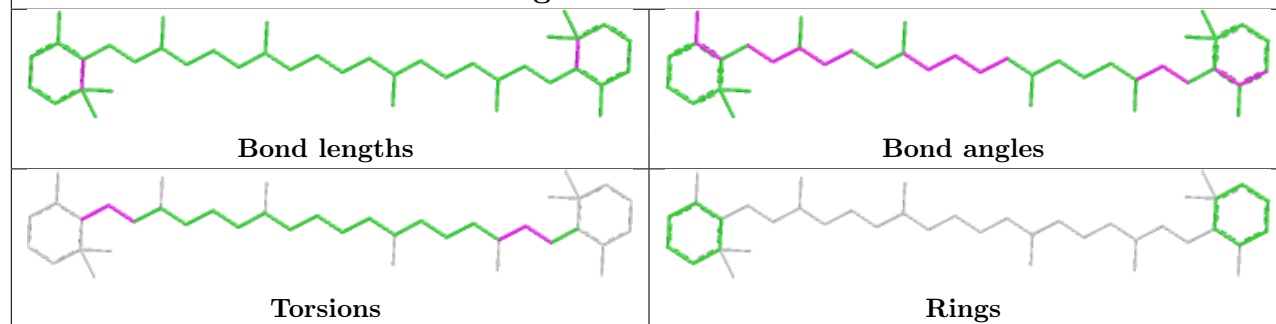
Rings

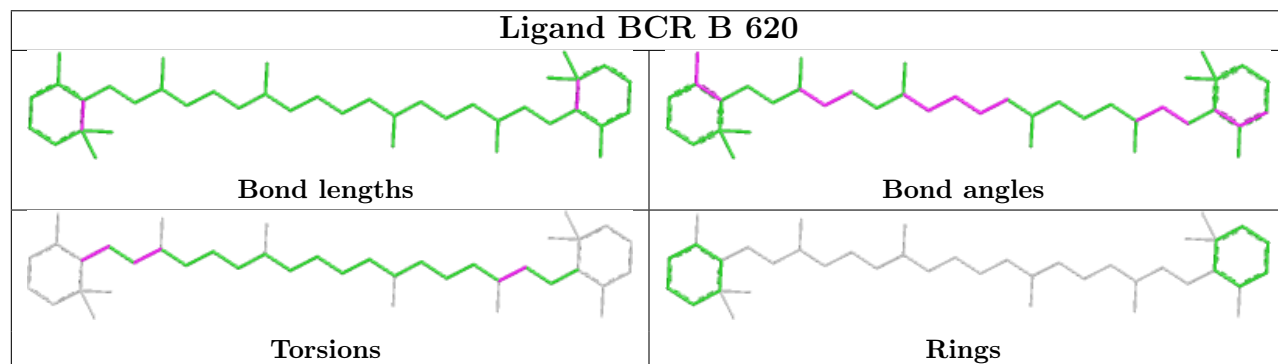
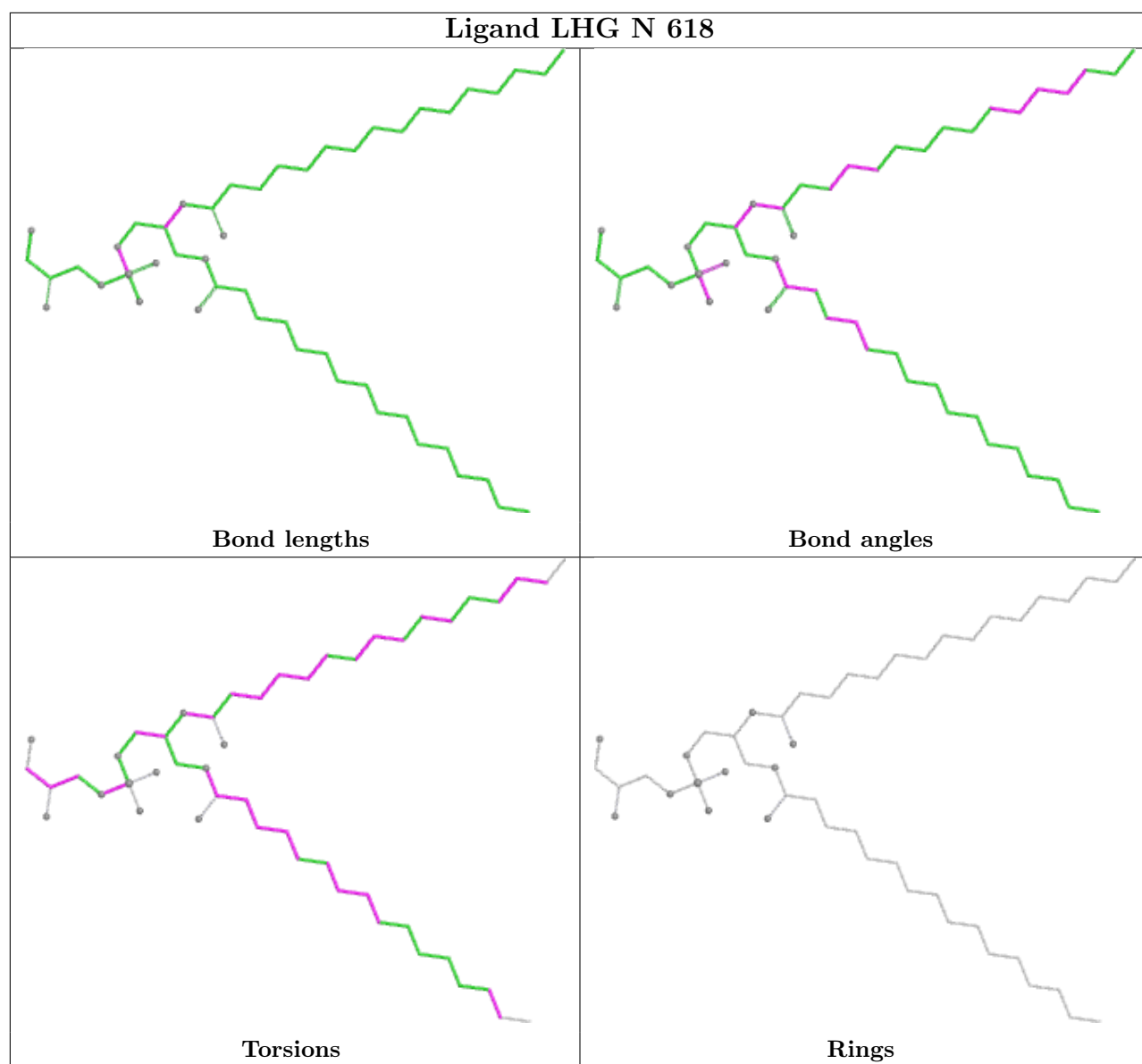
| Ligand CHL G 608                                                                                      |                                                                                                       |
|-------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand BCR k 102                                                                                      |                                                                                                       |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>    |  <p>Rings</p>      |

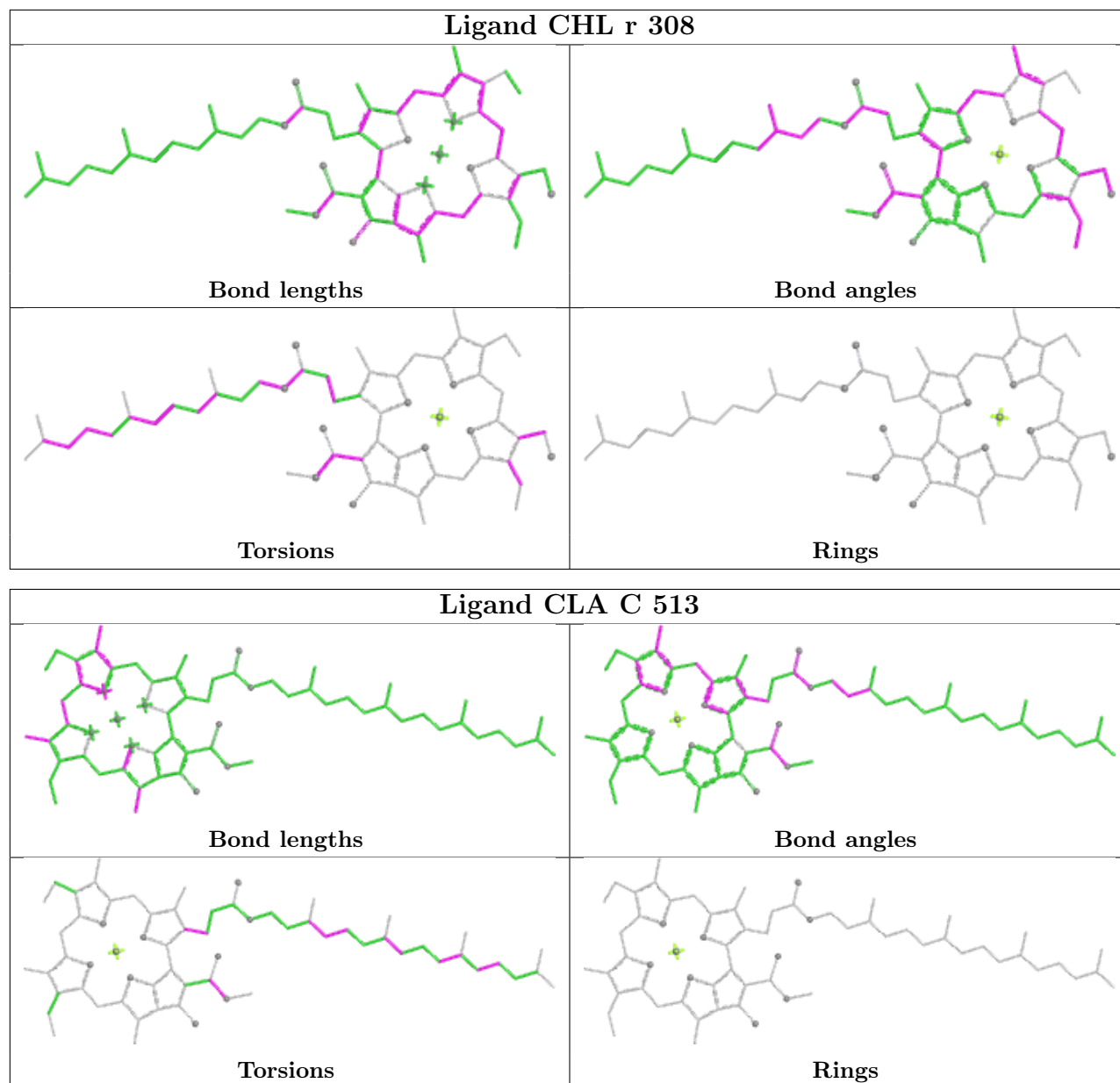
## Ligand CLA y 604

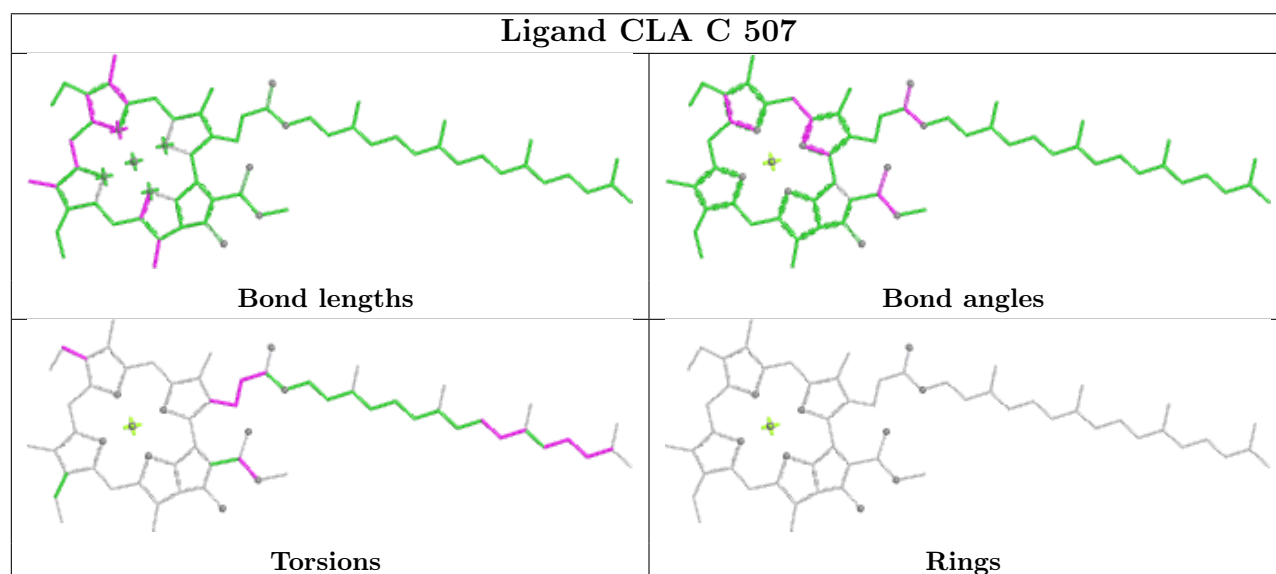
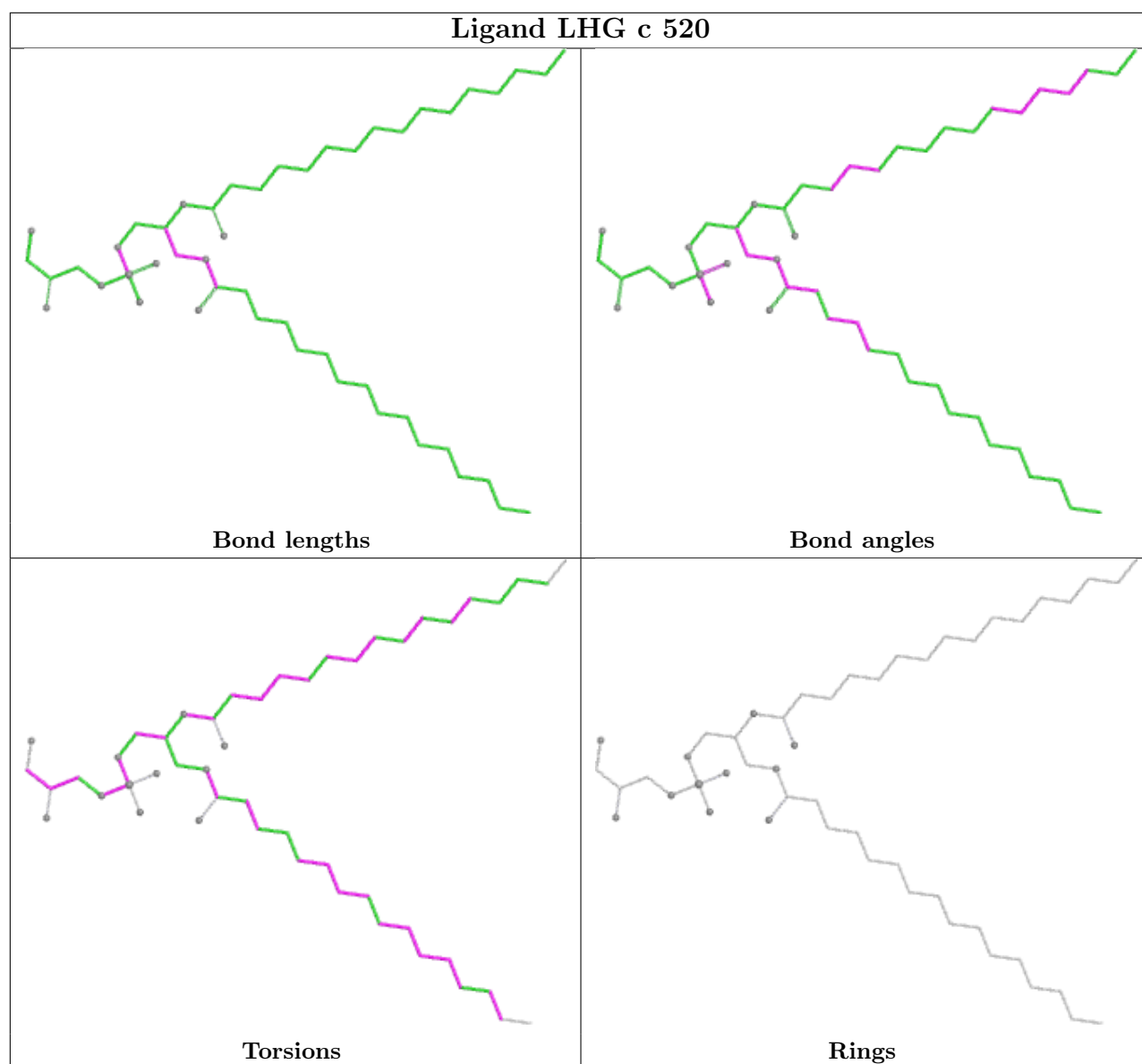


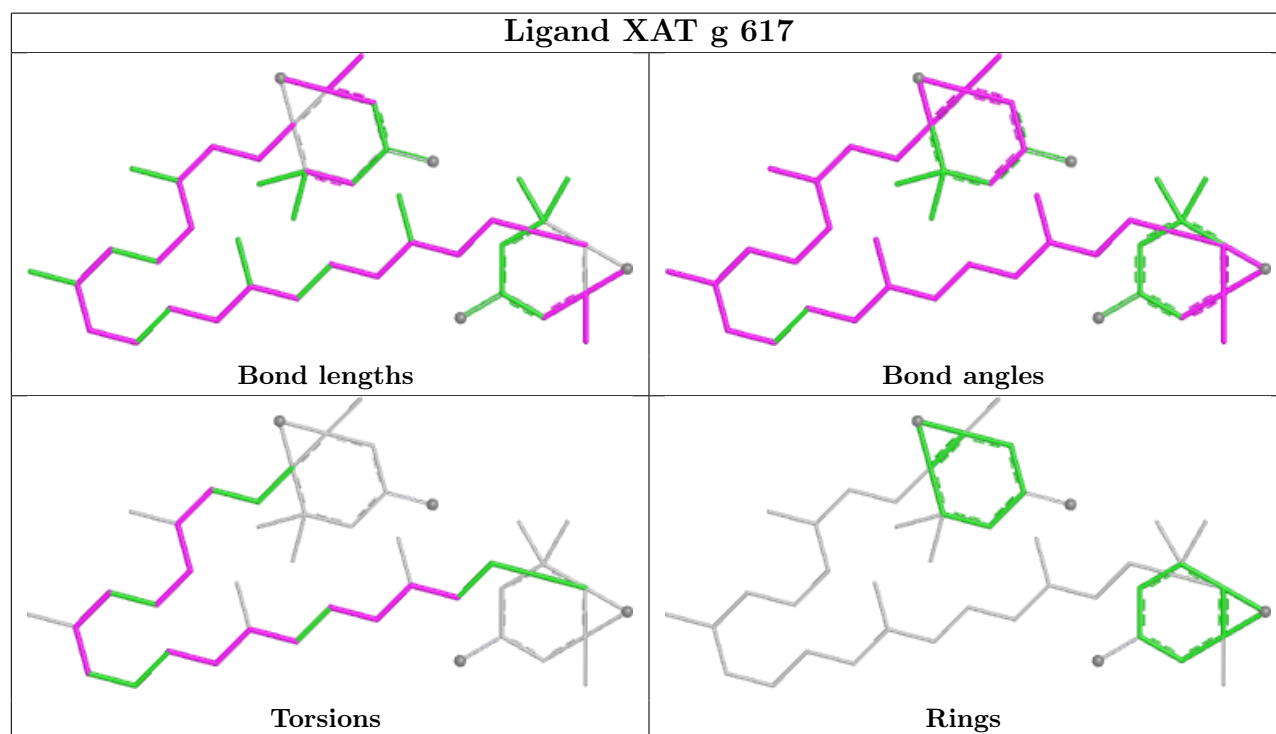
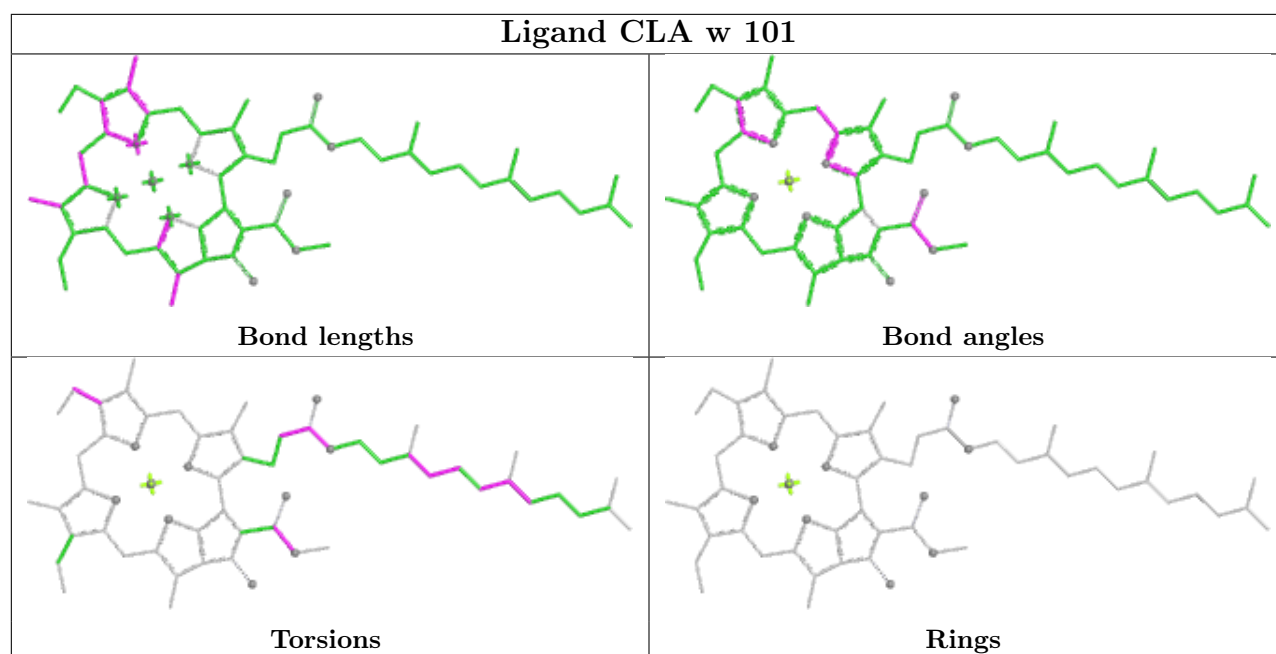
## Ligand BCR b 616

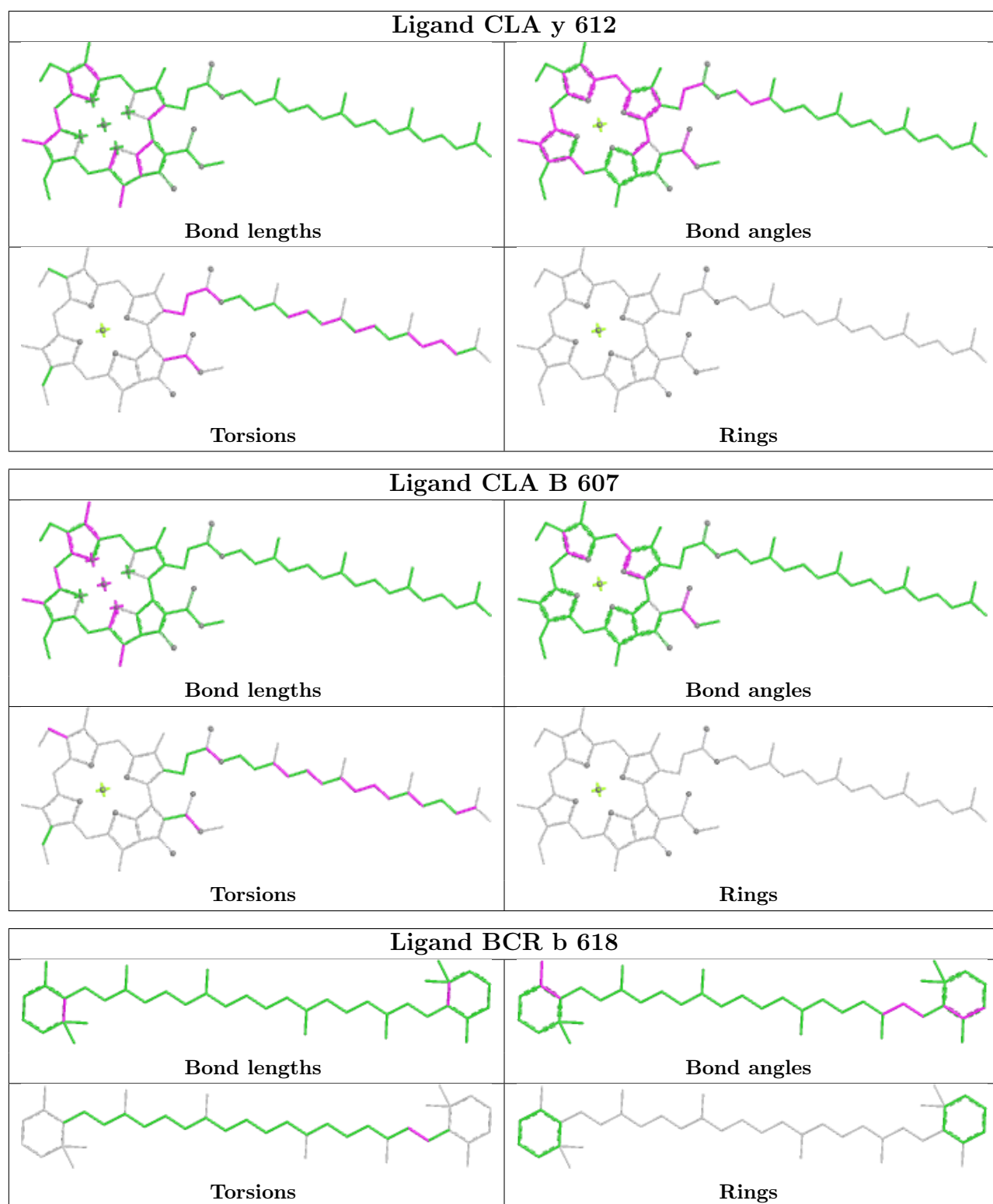


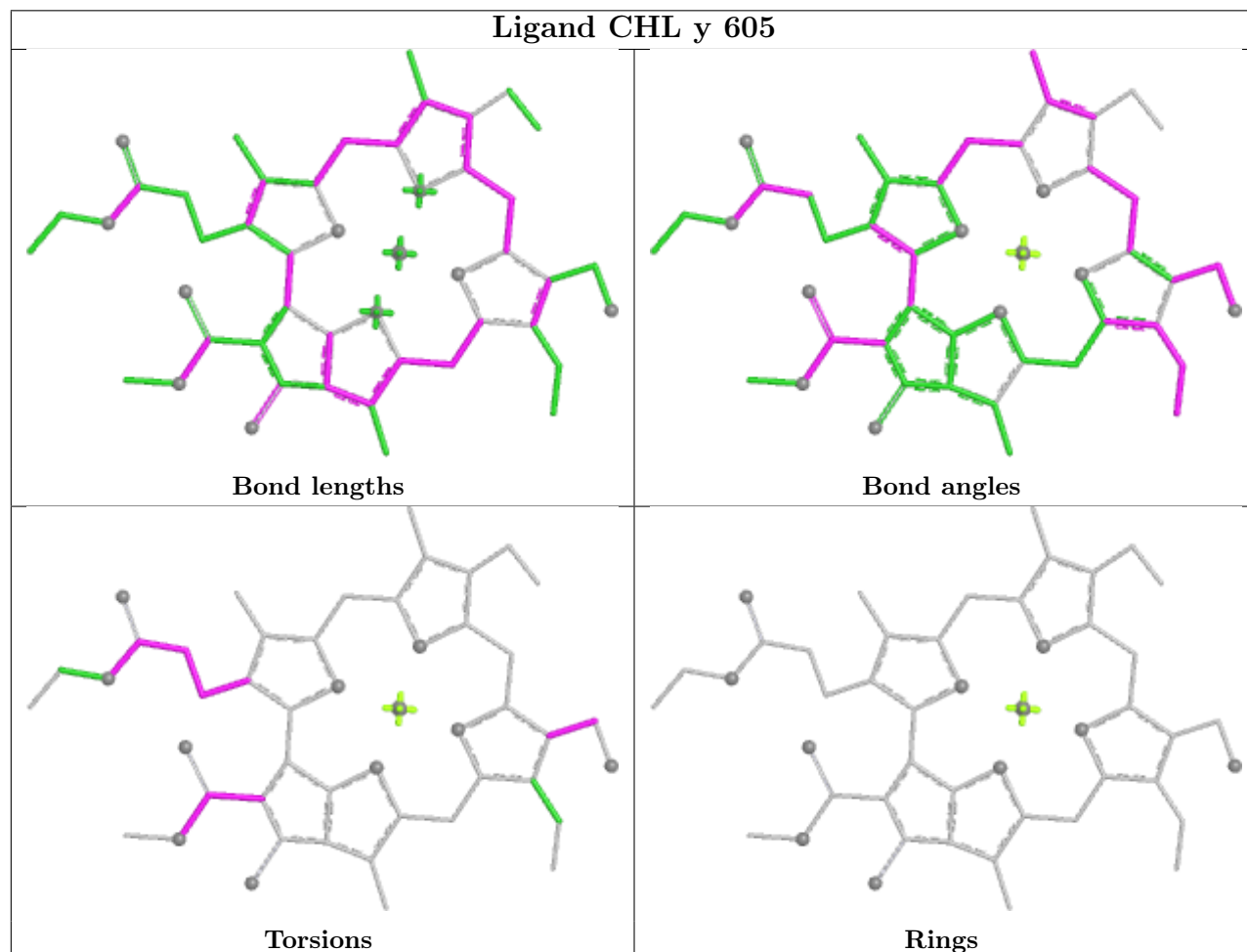
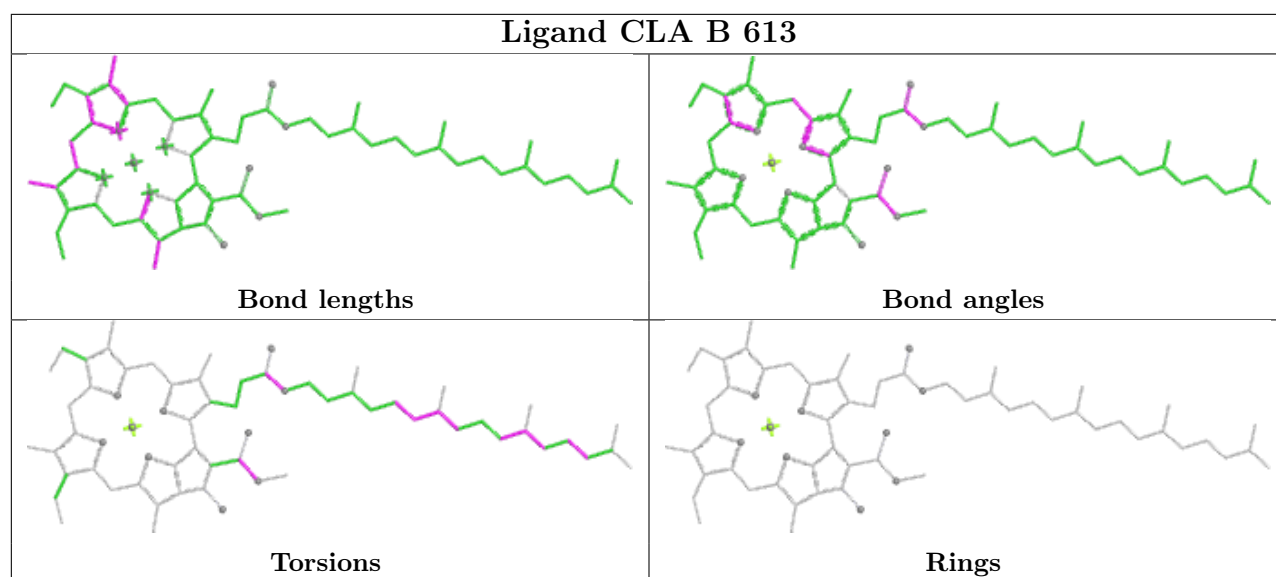


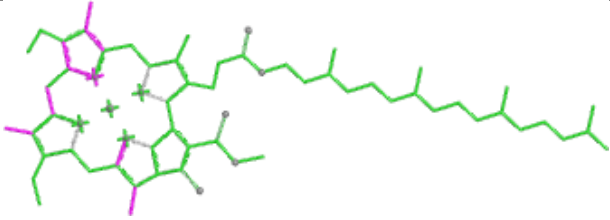
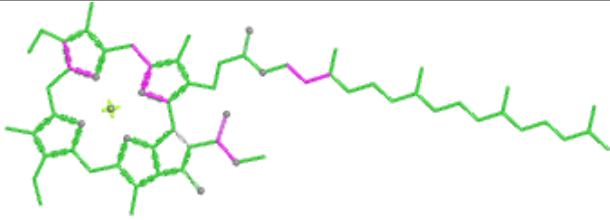
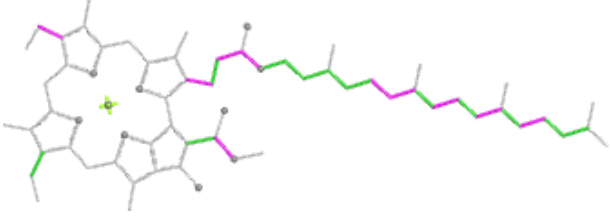
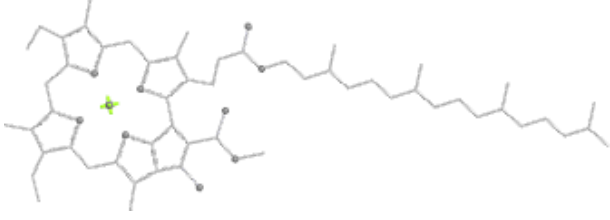
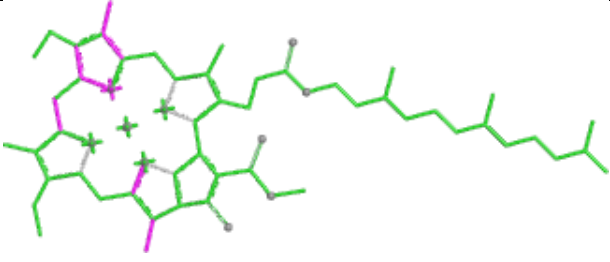
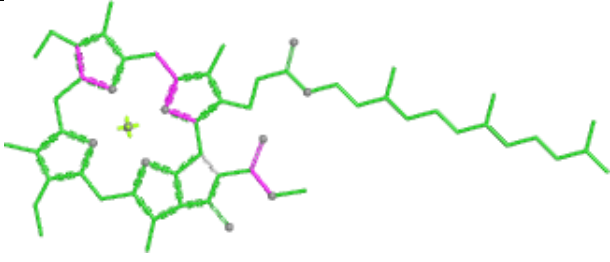
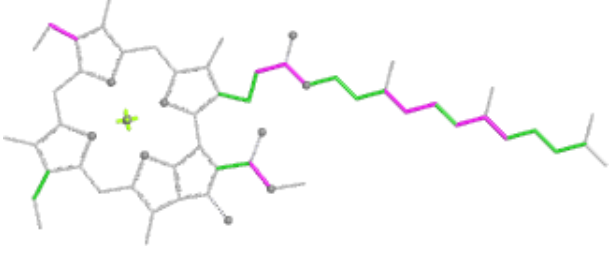
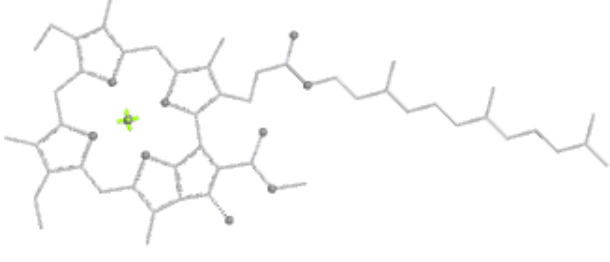


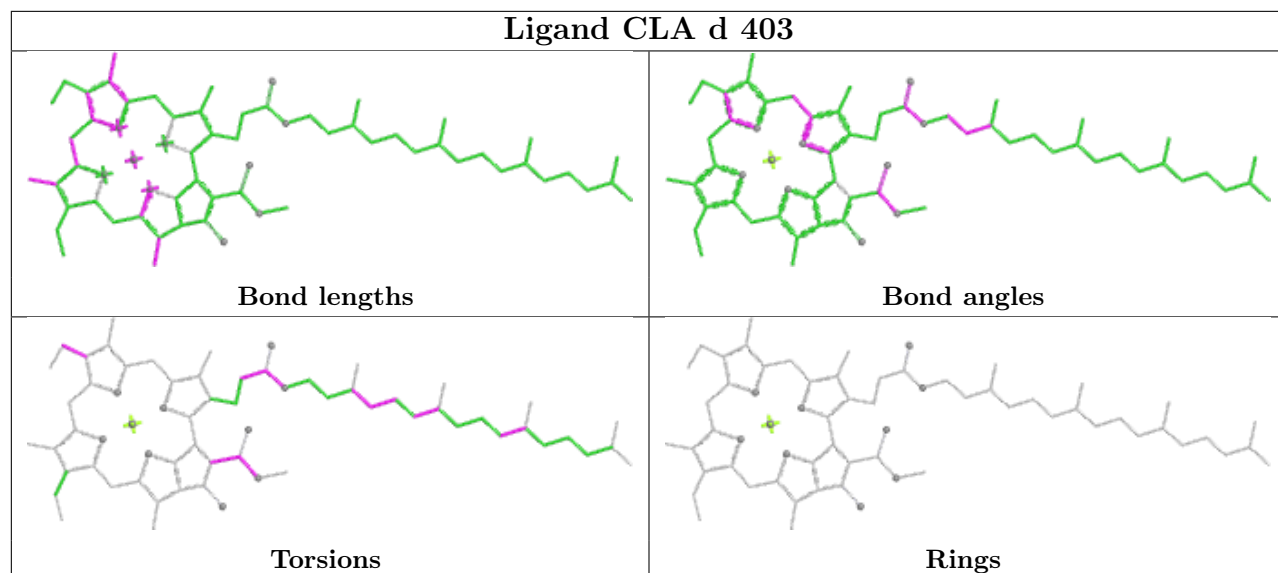
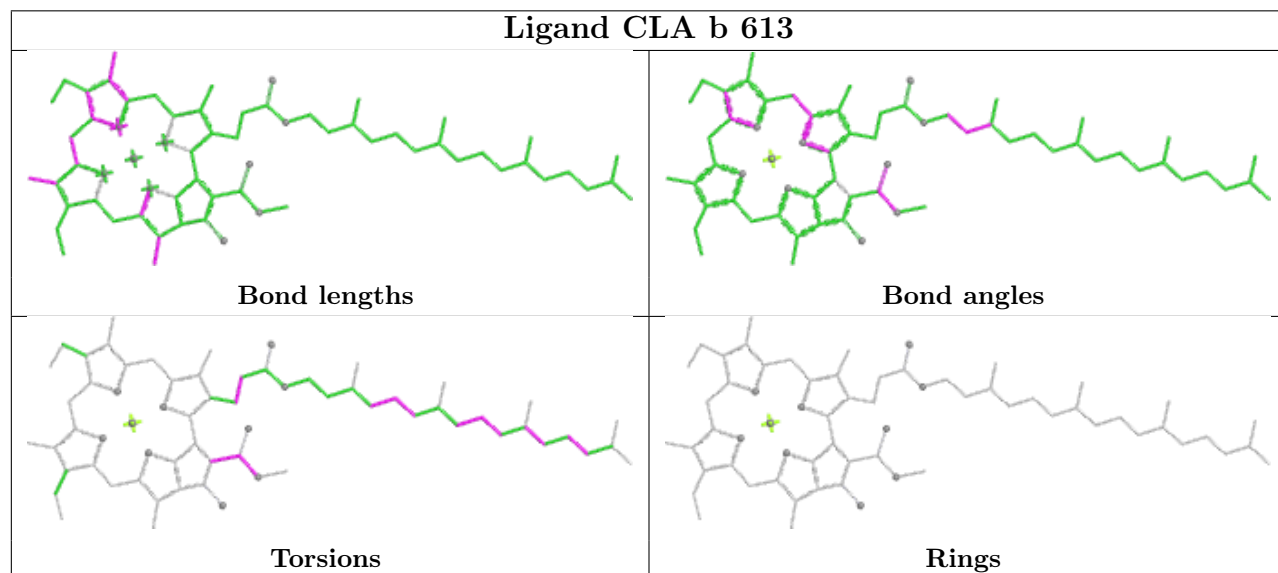
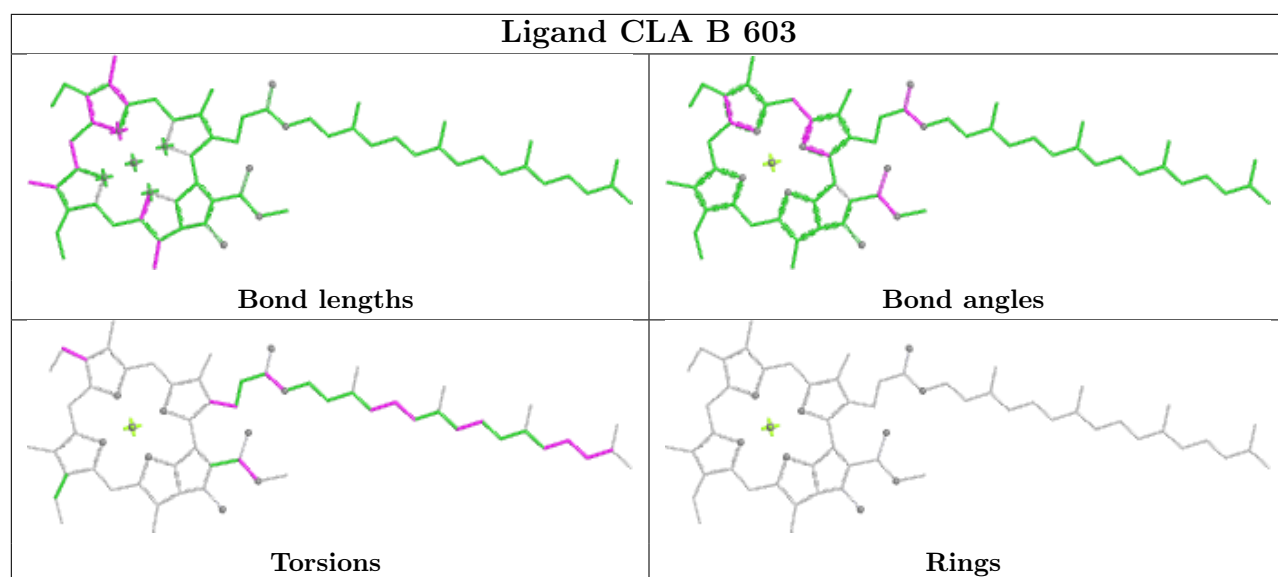


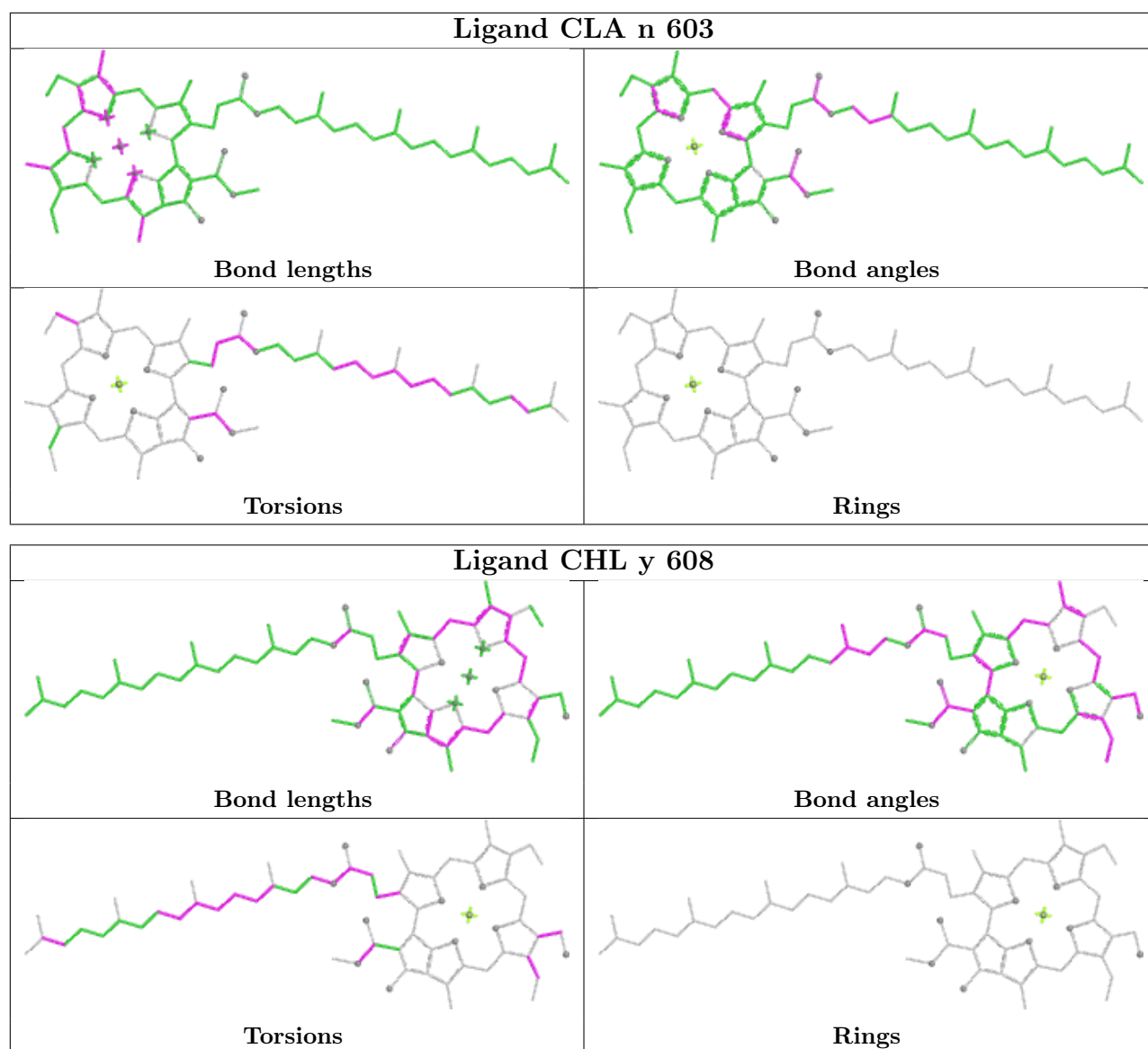


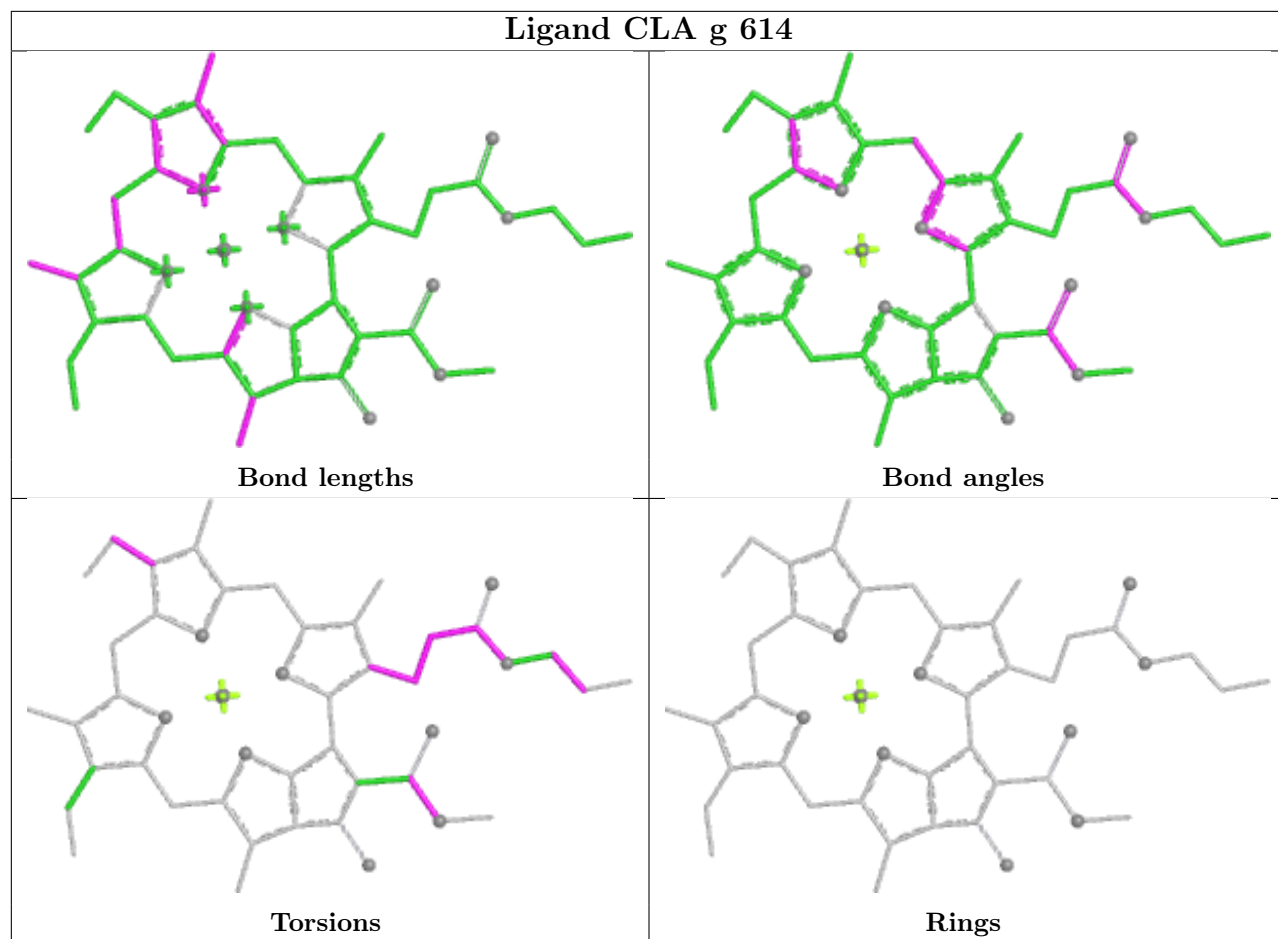


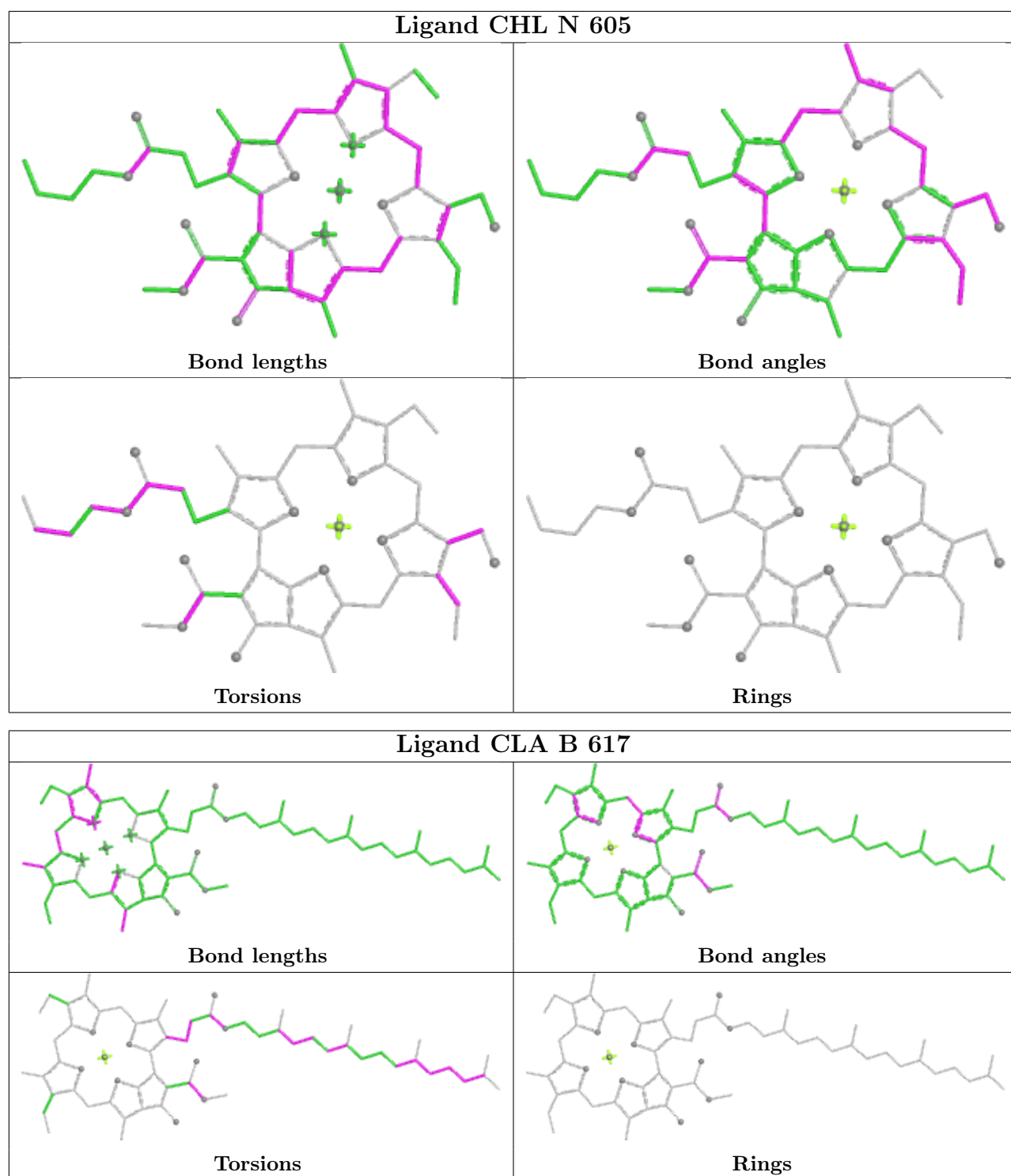


| Ligand CLA N 609                                                                                       |                                                                                                        |
|--------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>  |  <p>Bond angles</p>  |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand CLA W 101                                                                                       |                                                                                                        |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>    |  <p>Rings</p>      |

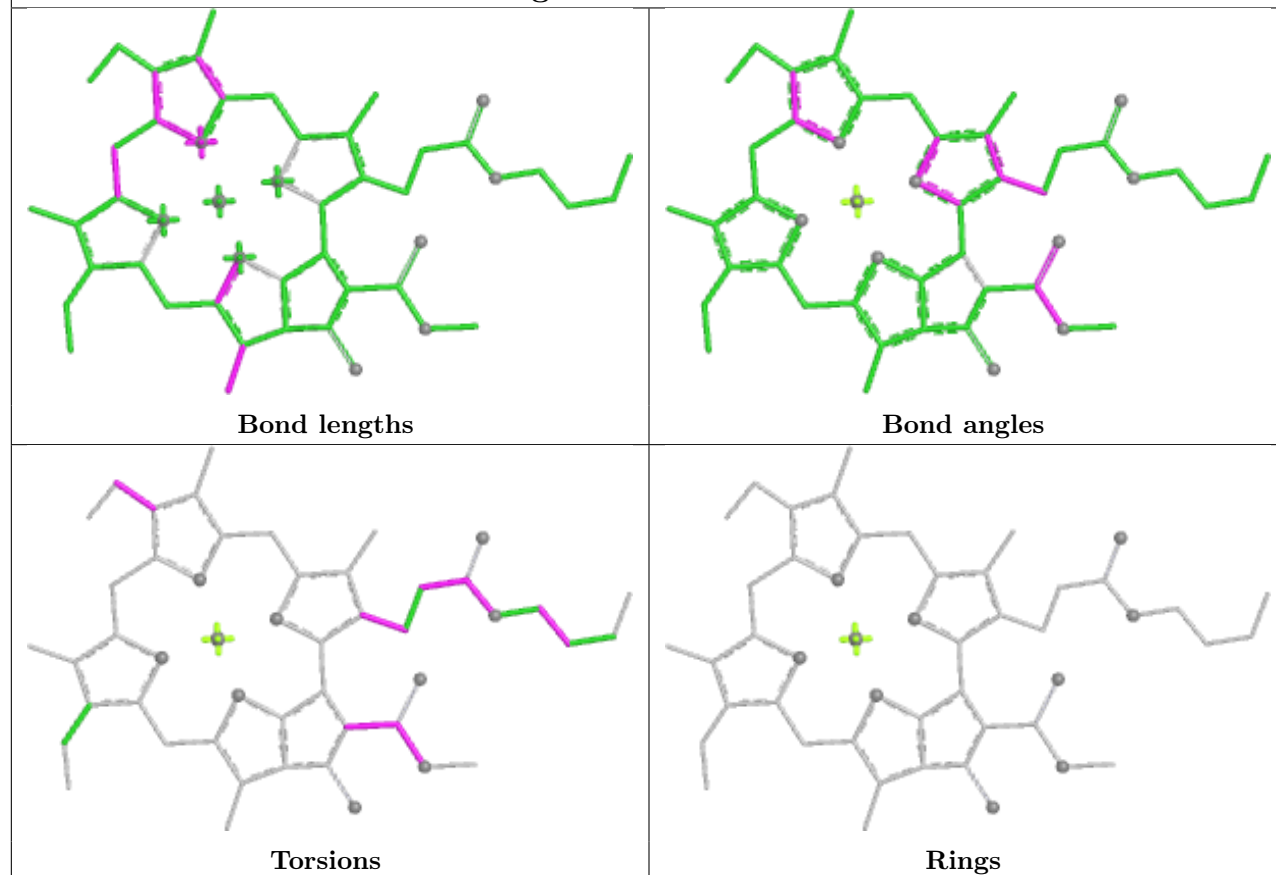




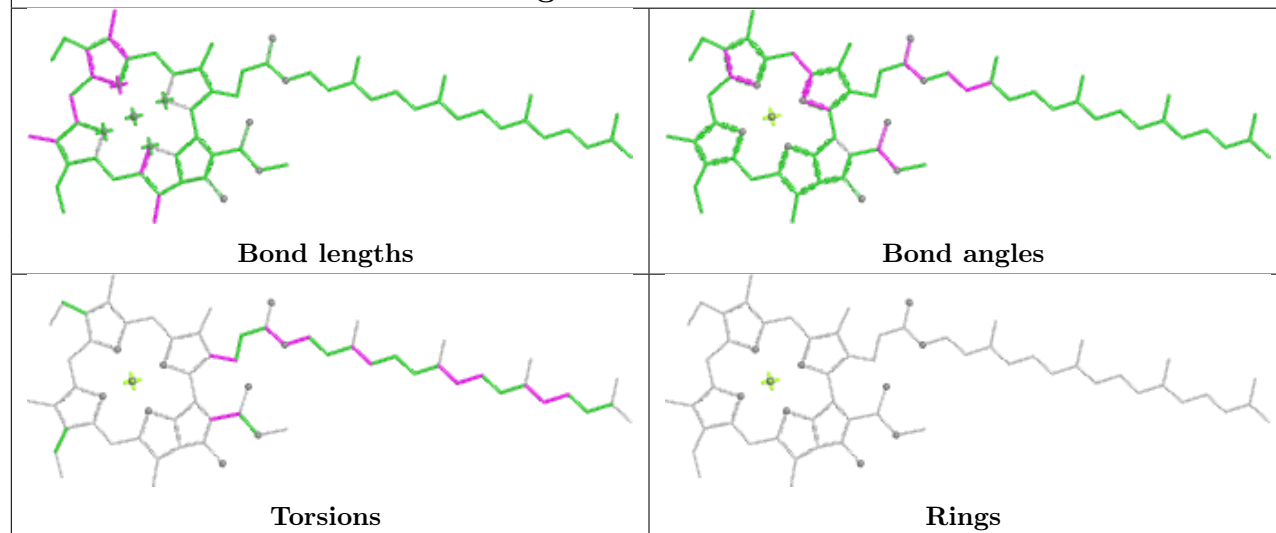


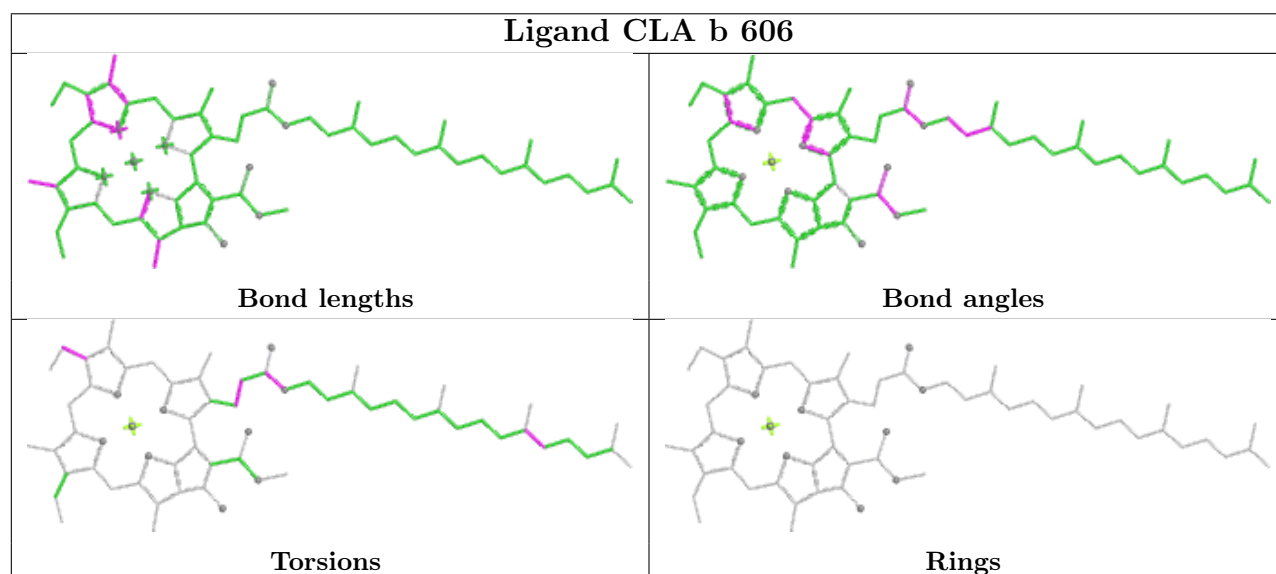
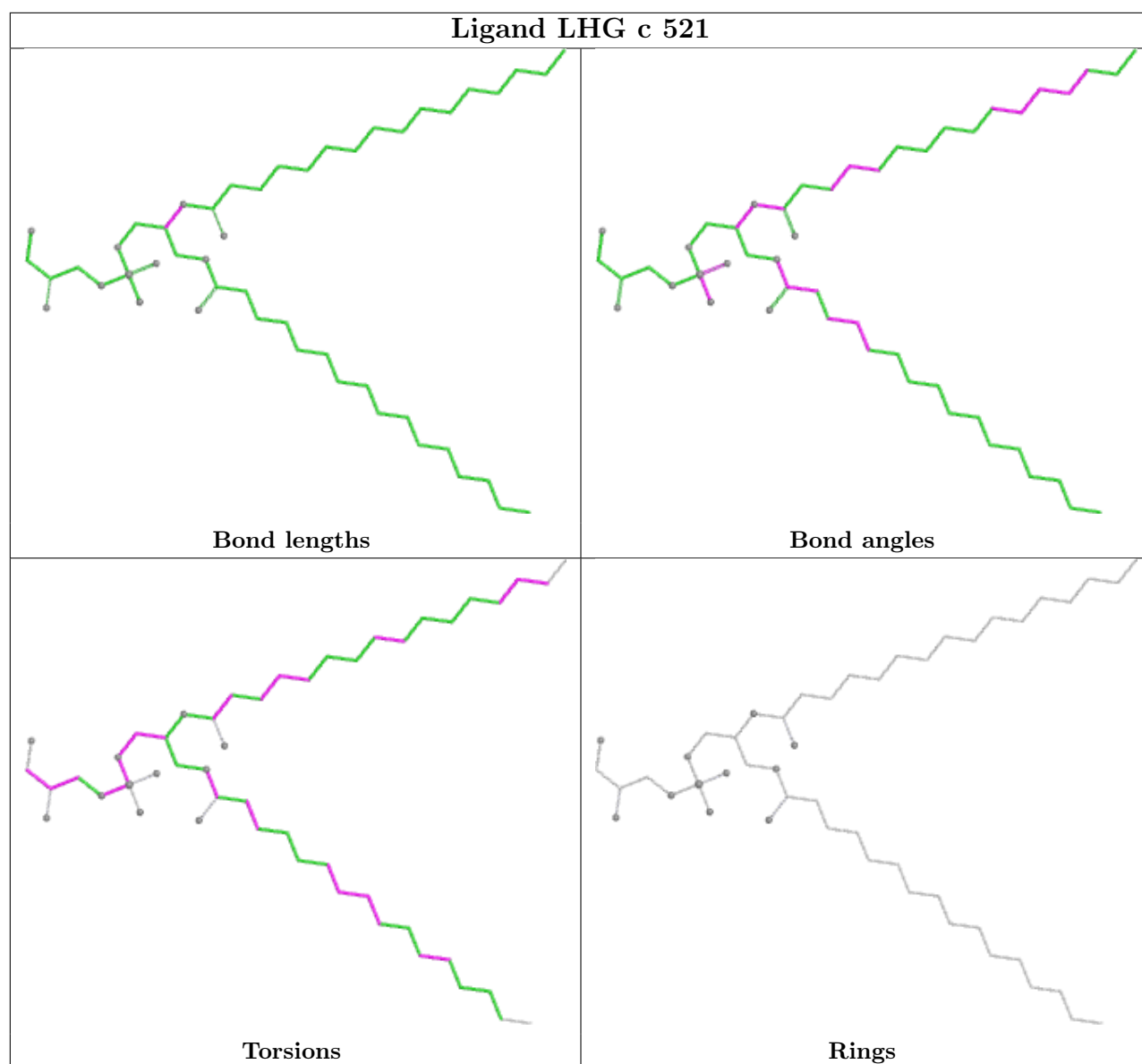


## Ligand CLA R 310

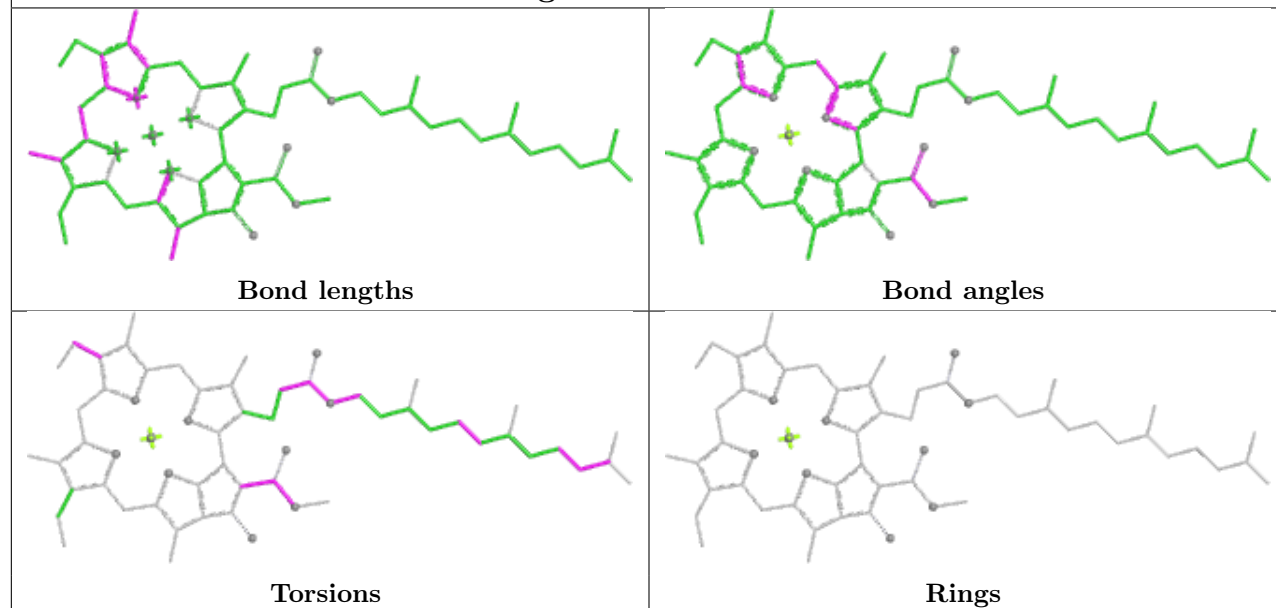


## Ligand CLA c 514

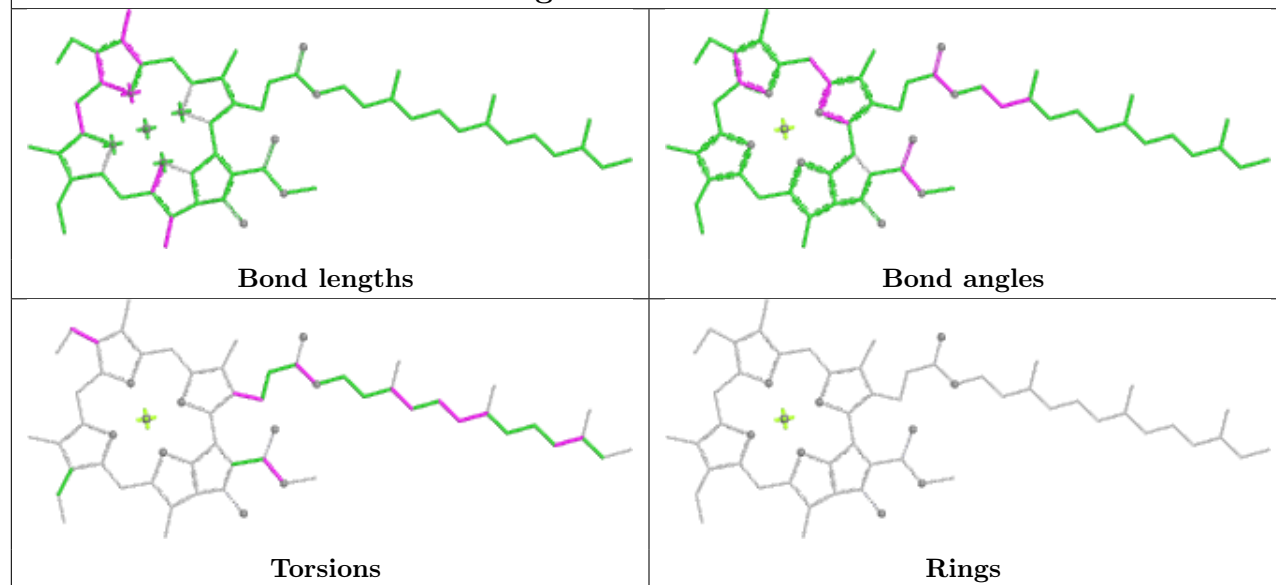


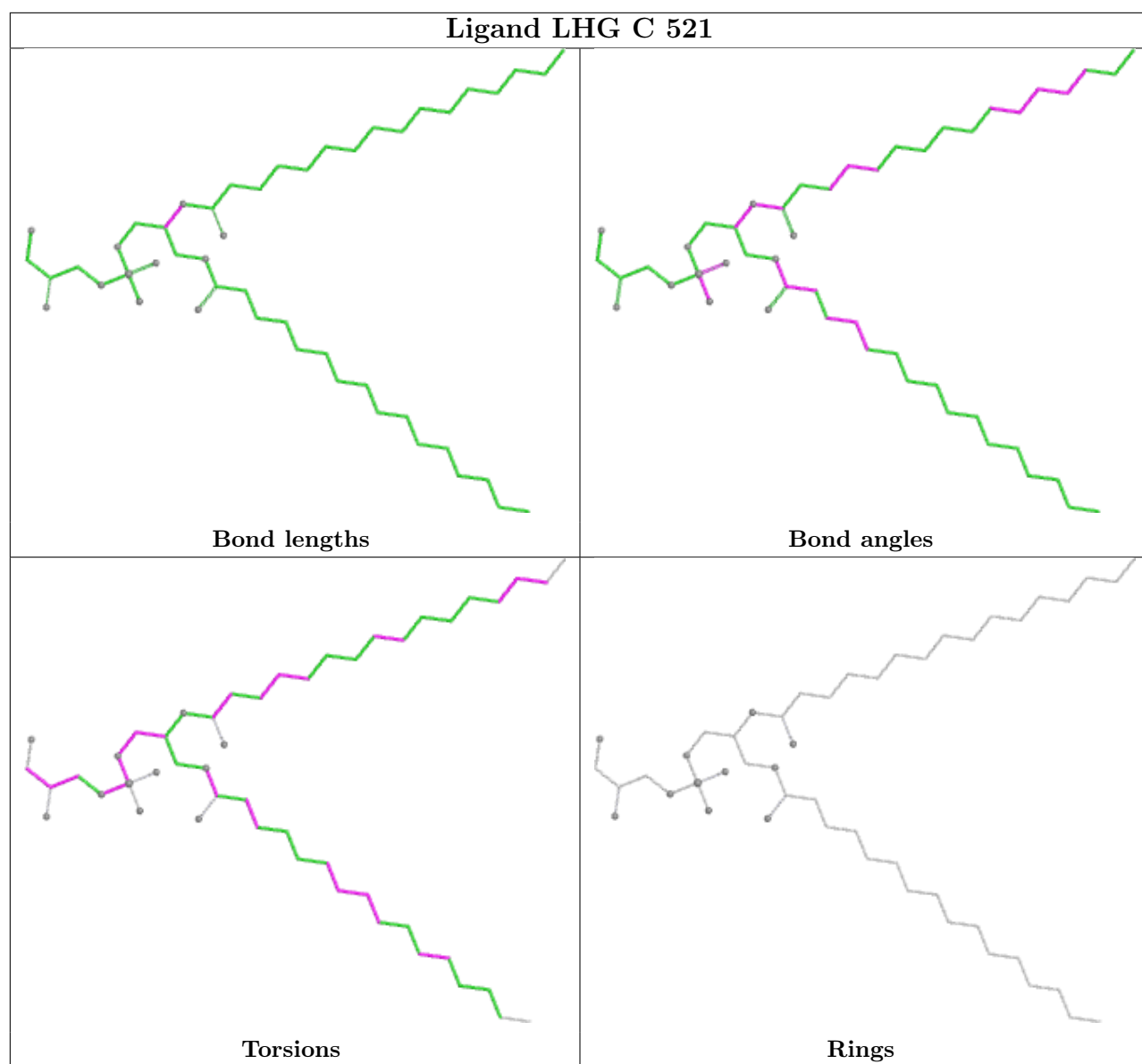


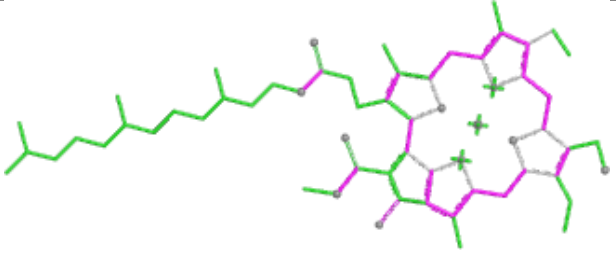
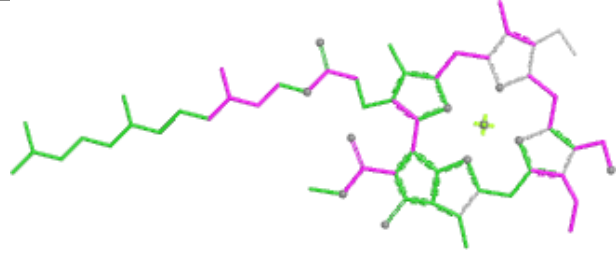
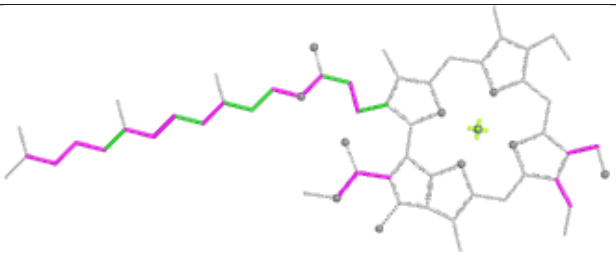
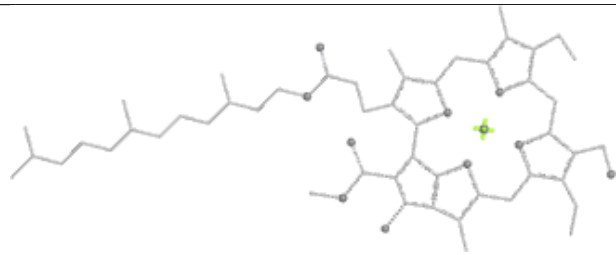
## Ligand CLA r 312

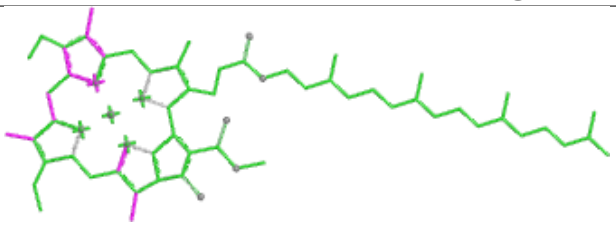
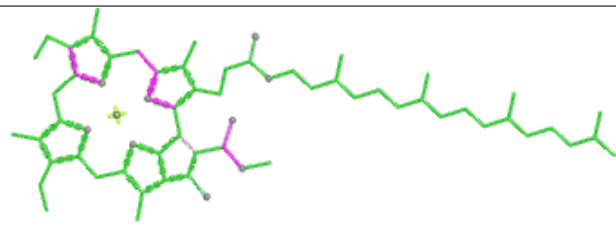
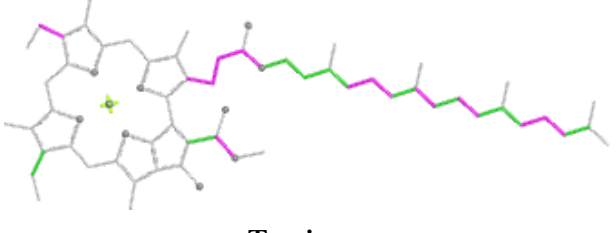
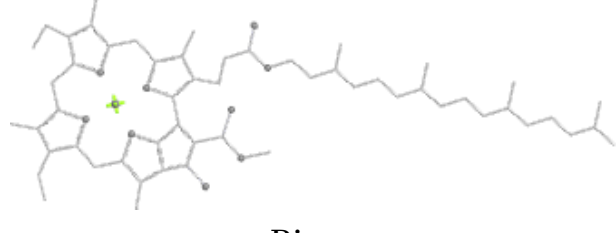


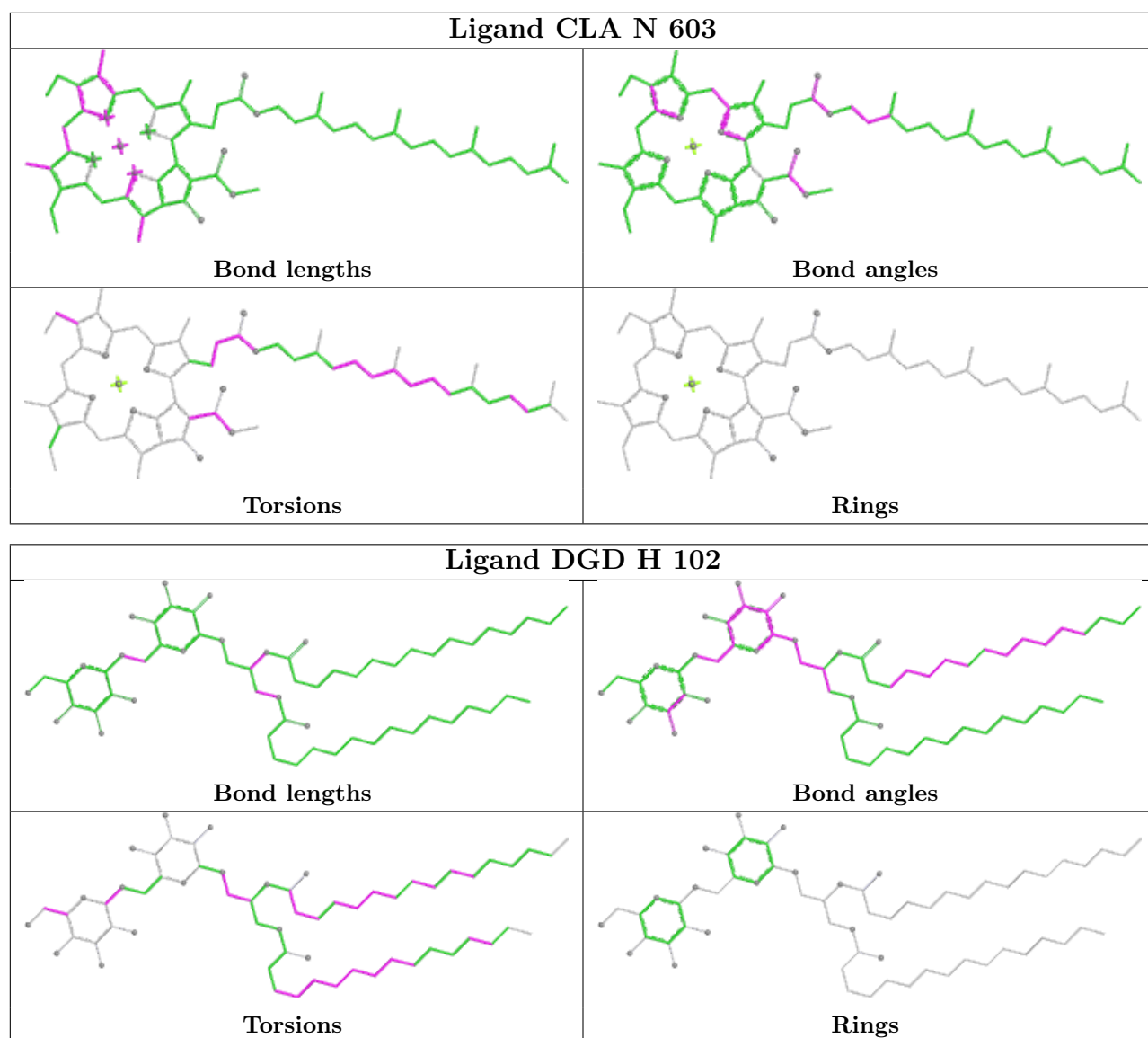
## Ligand CLA S 303

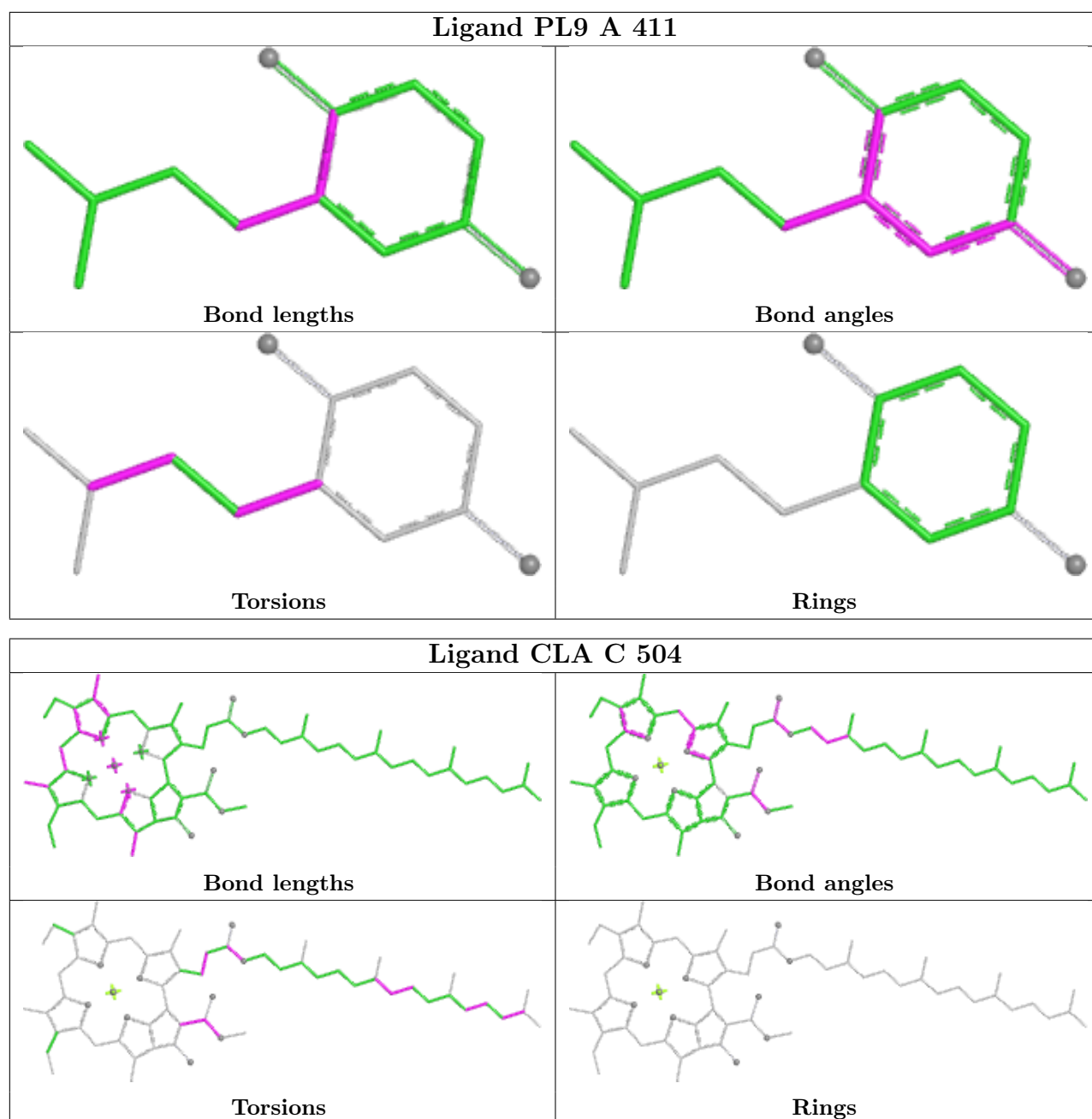


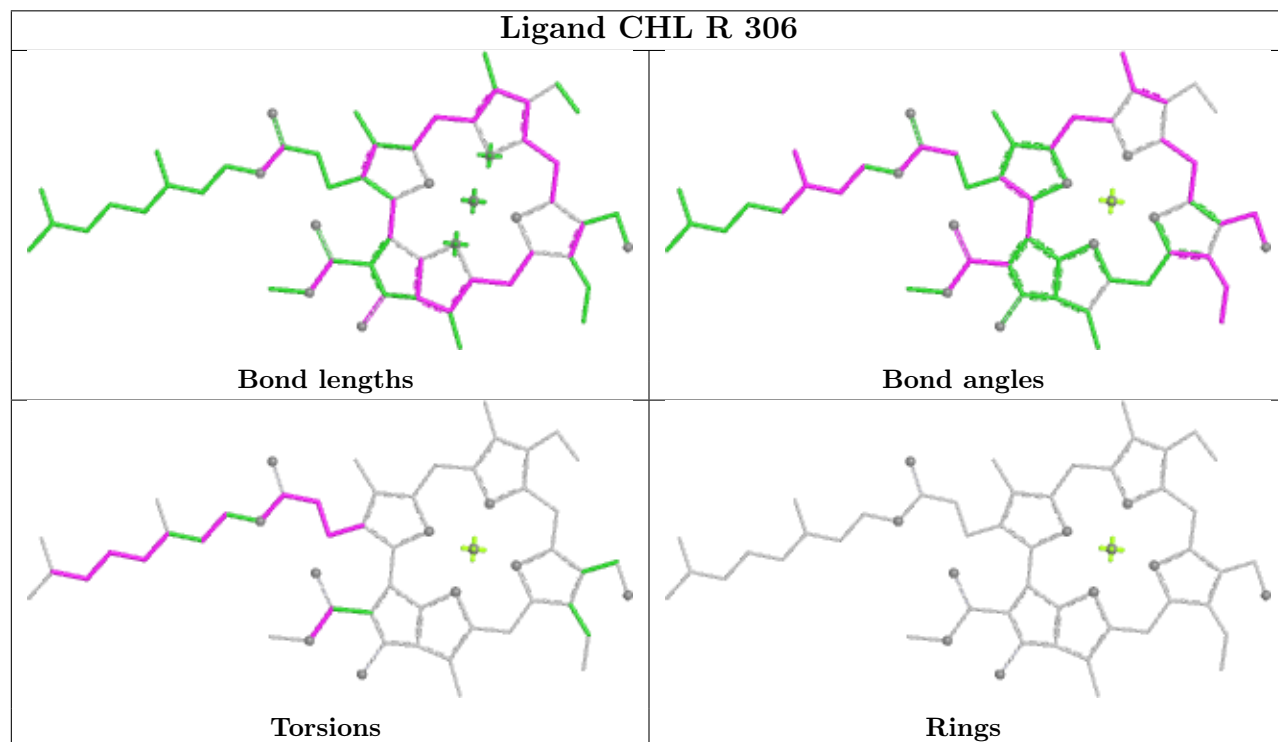
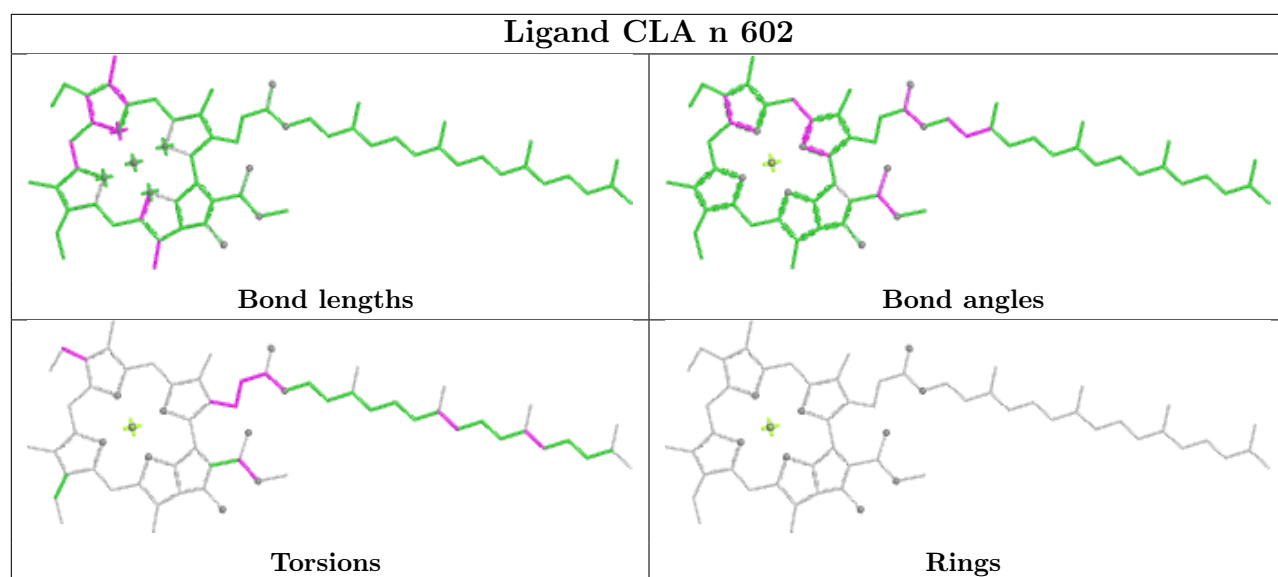


| Ligand CHL R 307                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

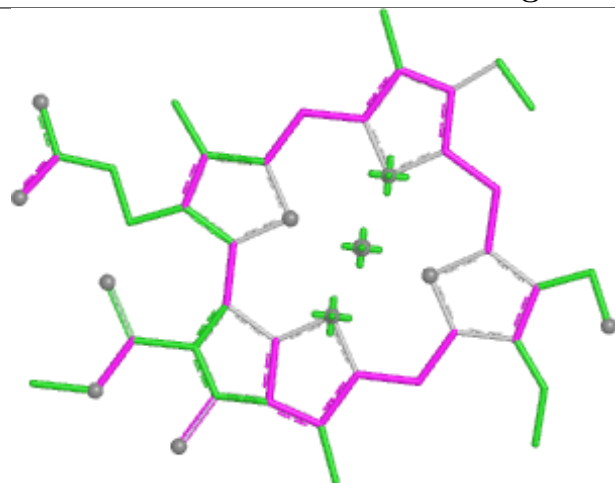
| Ligand CLA C 503                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



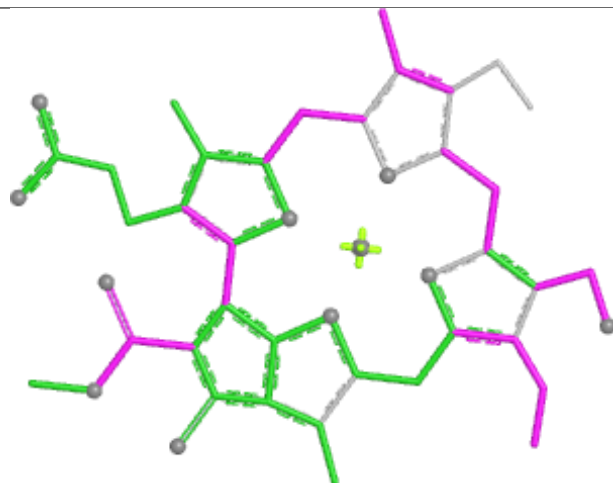




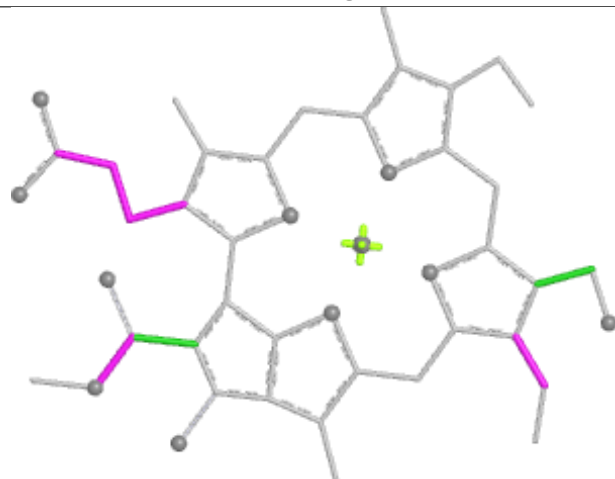
## Ligand CHL s 302



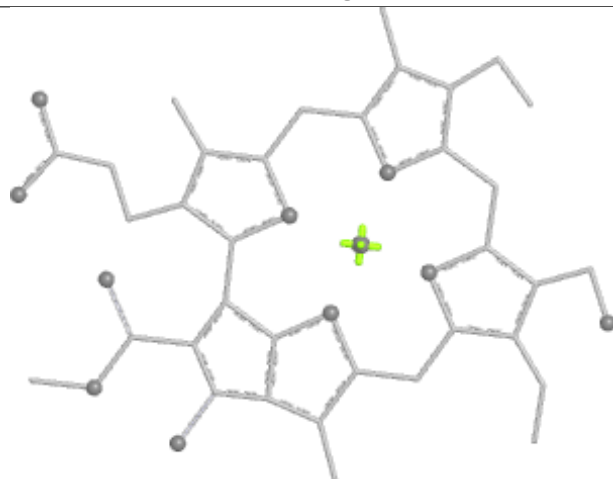
Bond lengths



Bond angles

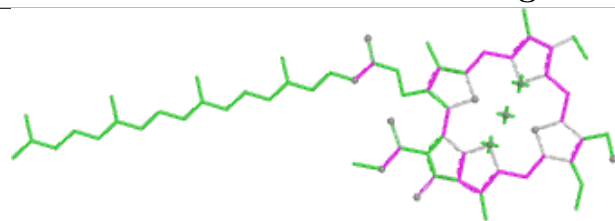


Torsions

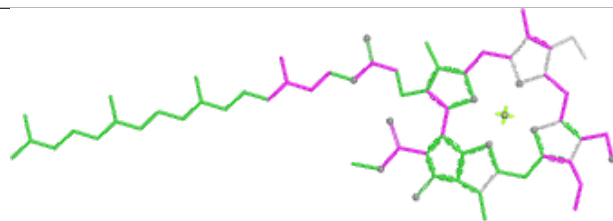


Rings

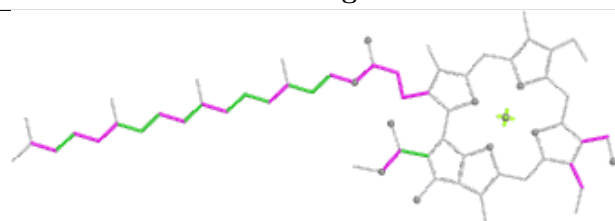
## Ligand CHL n 601



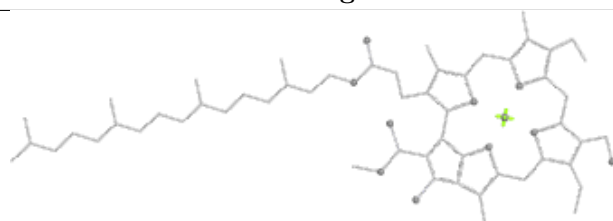
Bond lengths



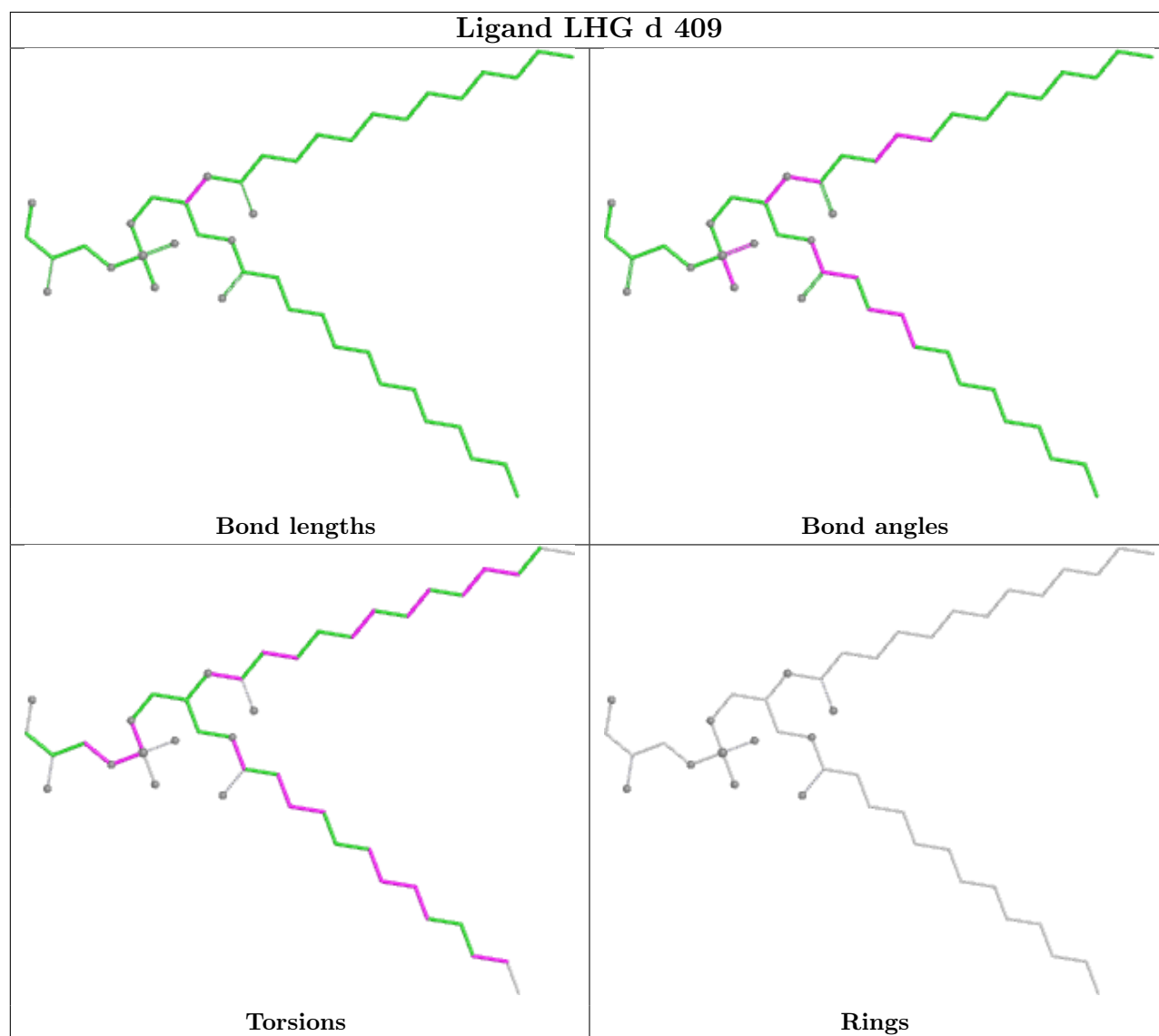
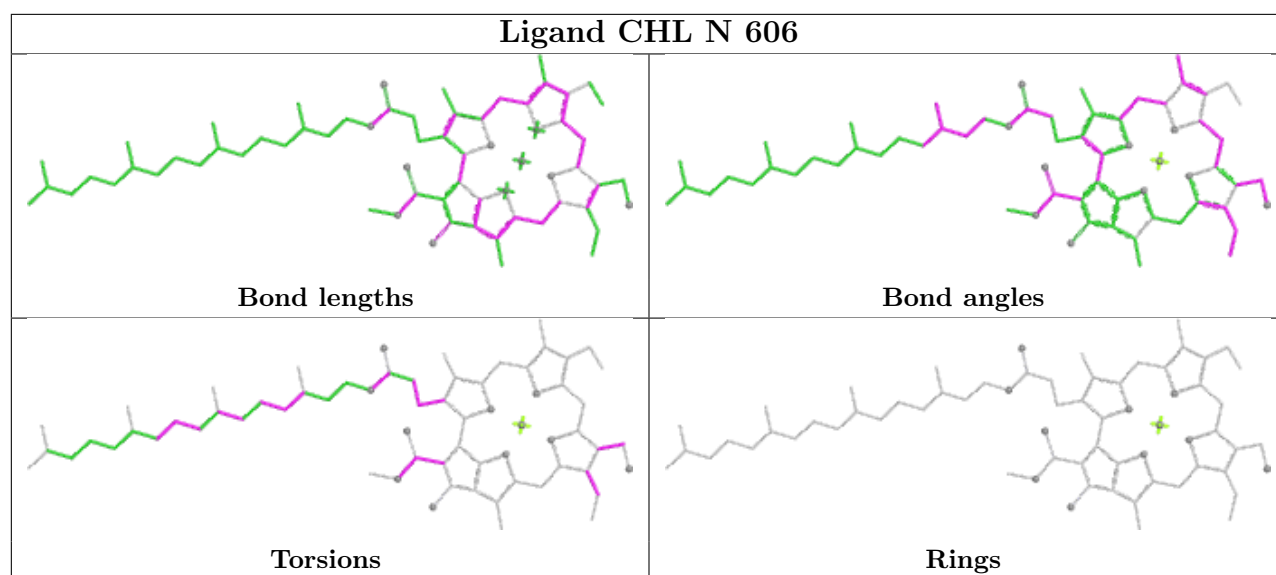
Bond angles

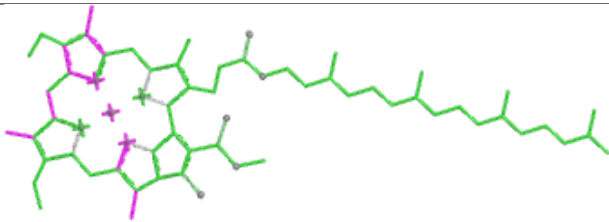
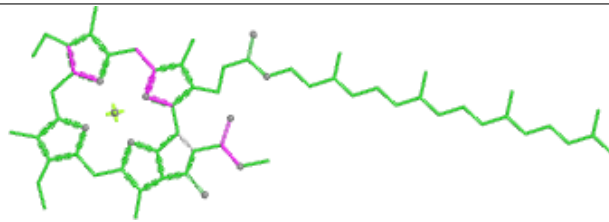
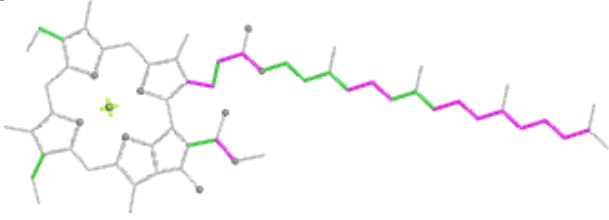
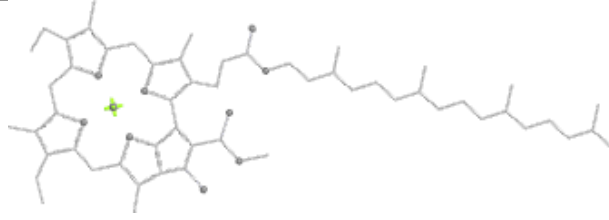


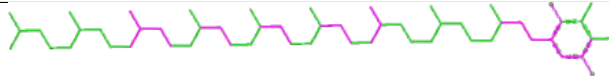
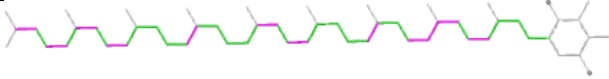
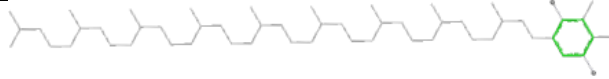
Torsions

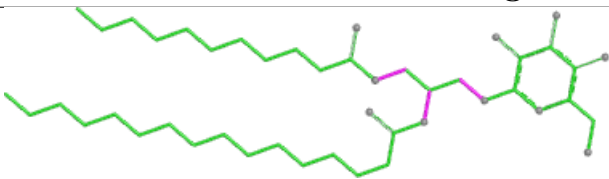
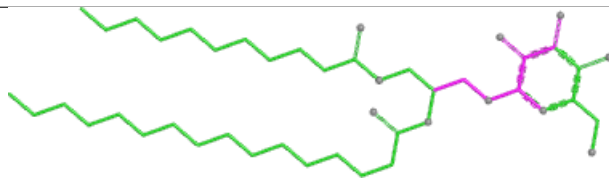
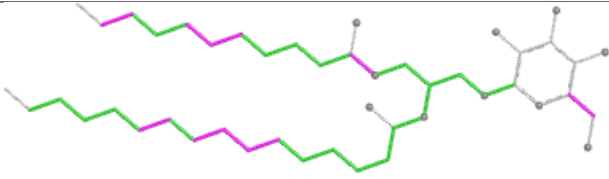
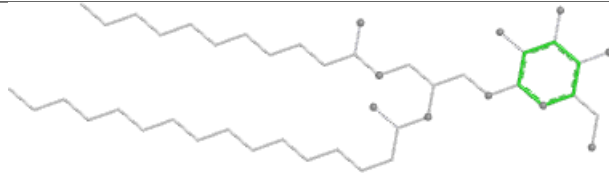


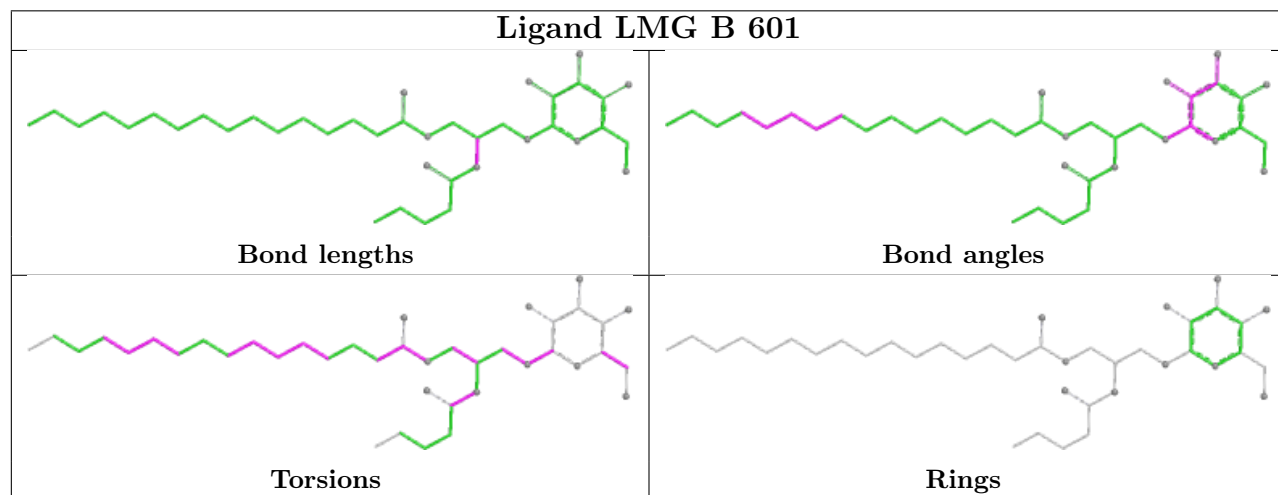
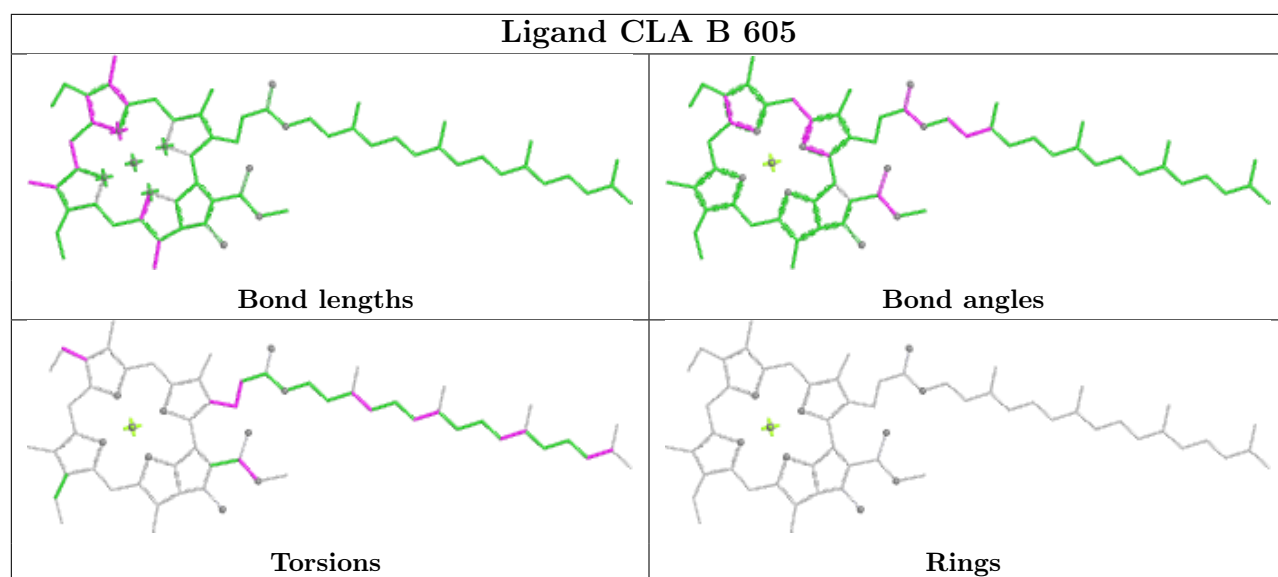
Rings

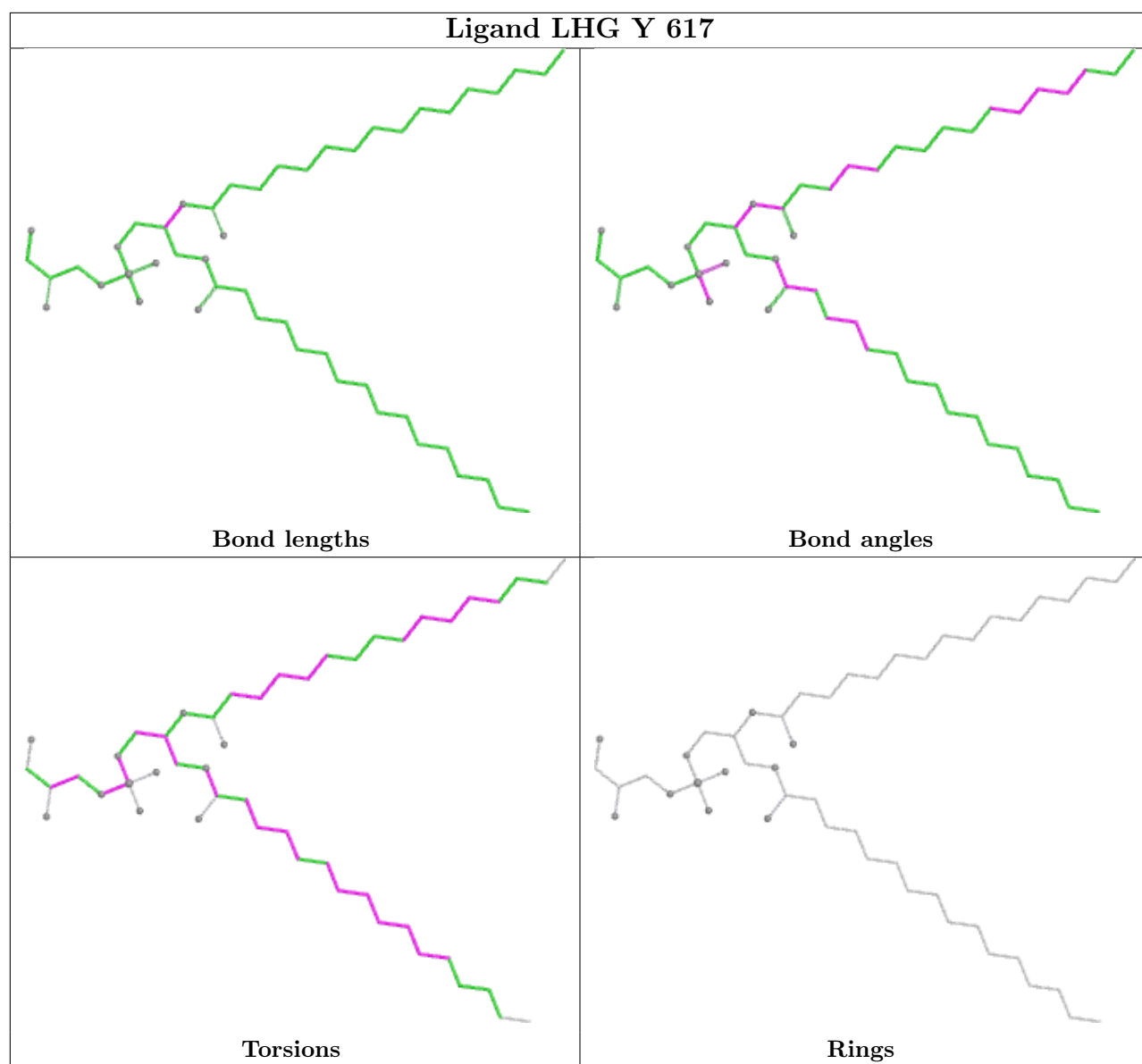


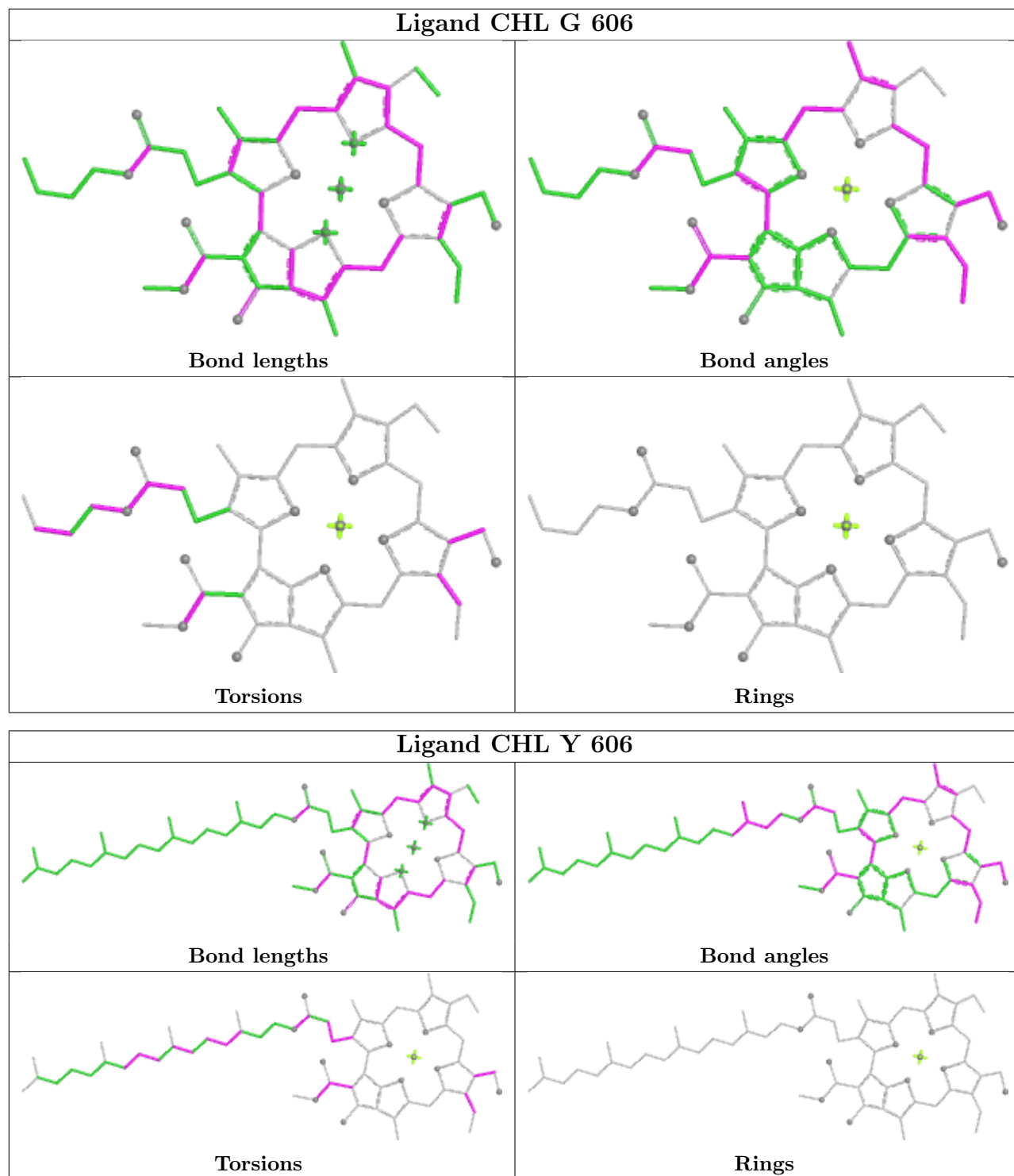
| Ligand CLA c 513                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

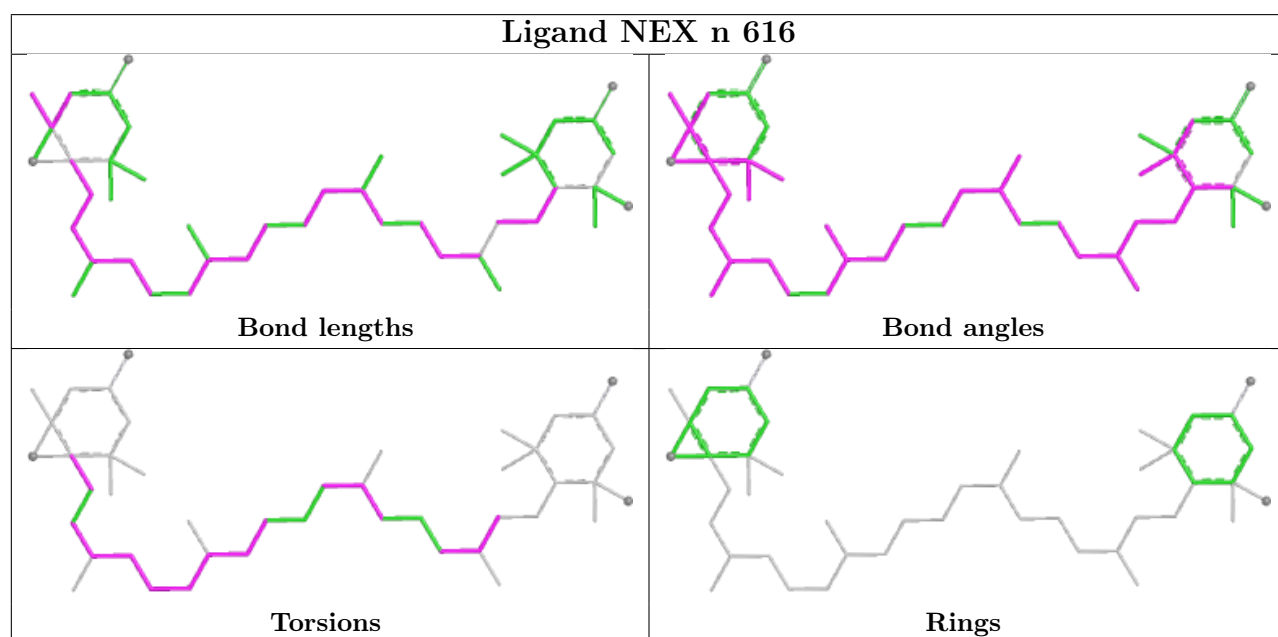
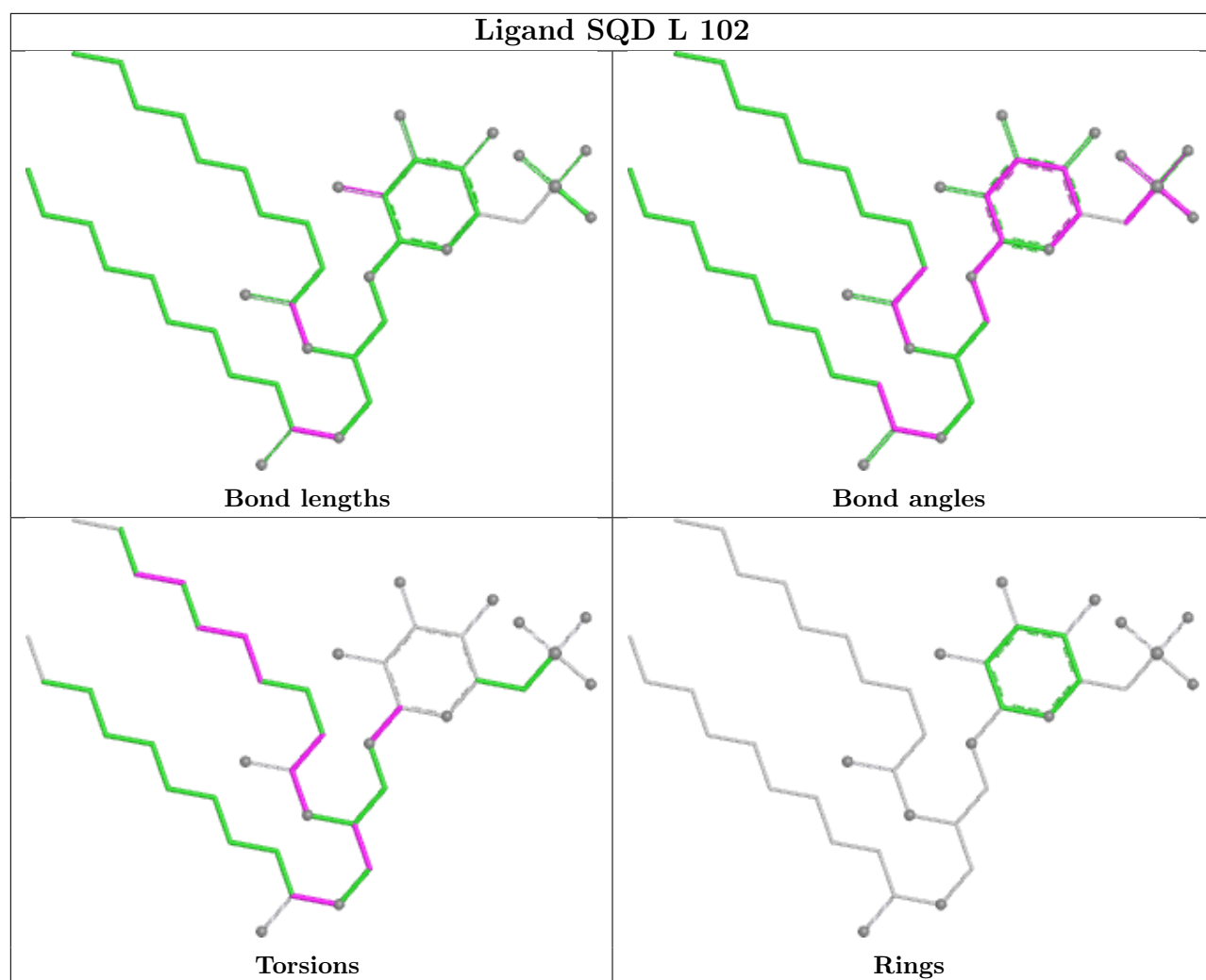
| Ligand PL9 d 406                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand LMG D 411                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

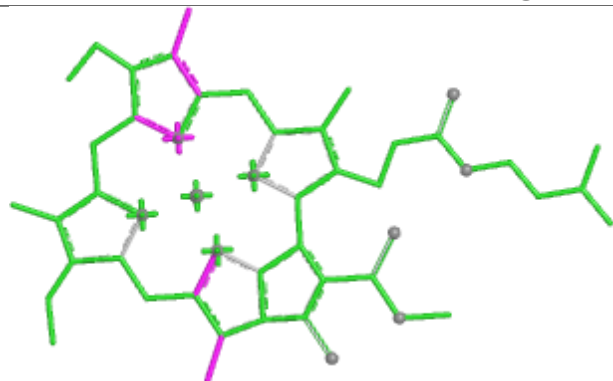




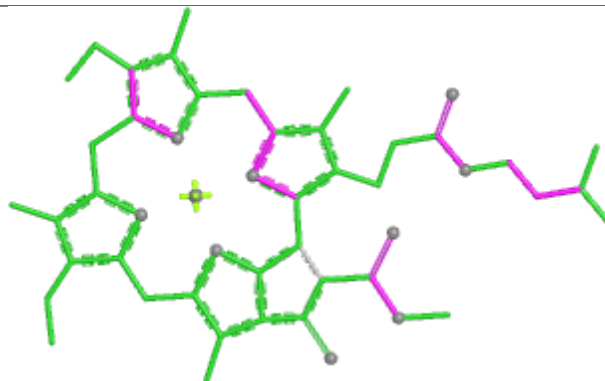




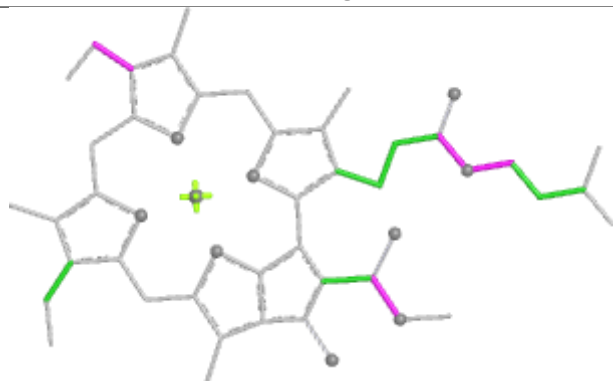
## Ligand CLA n 604



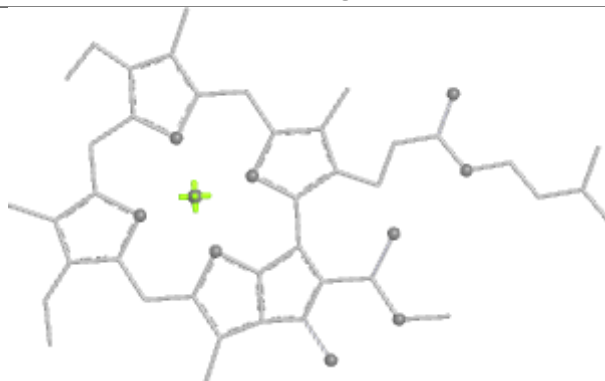
Bond lengths



Bond angles

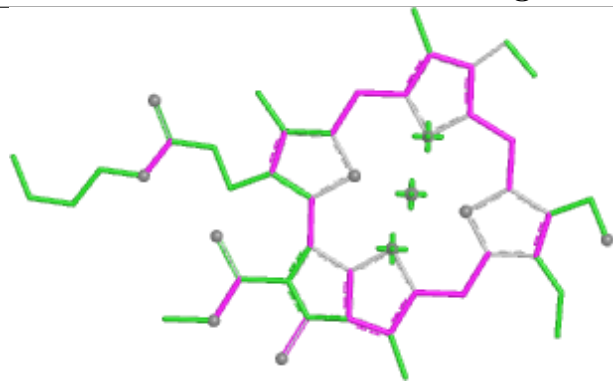


Torsions

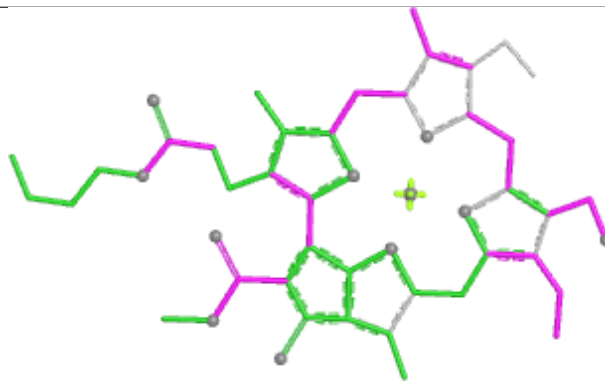


Rings

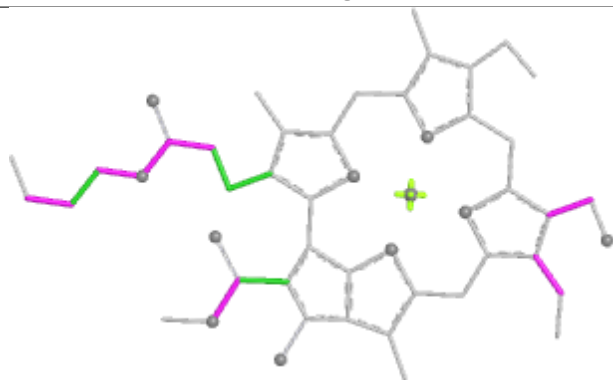
## Ligand CHL Y 605



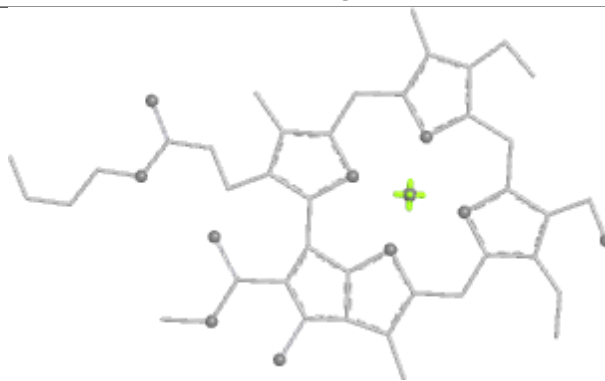
Bond lengths



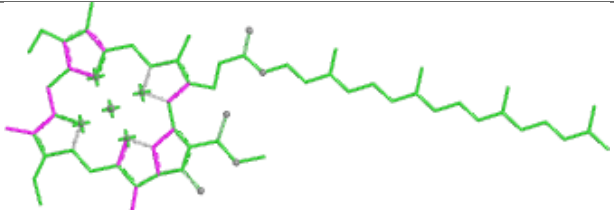
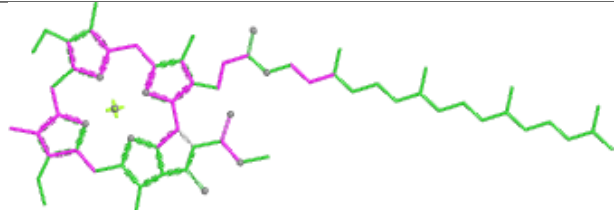
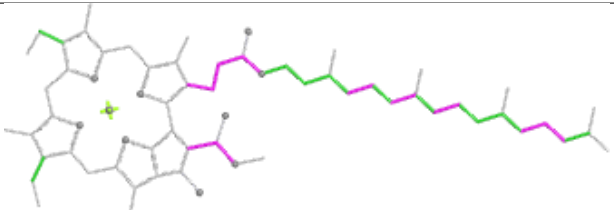
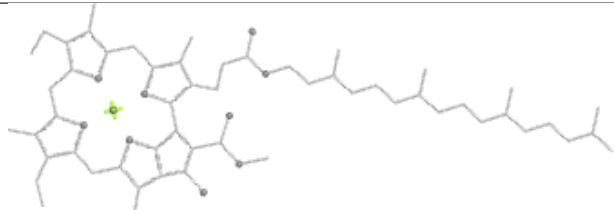
Bond angles

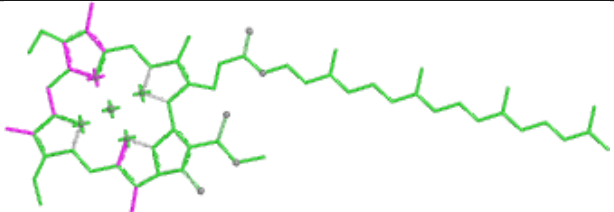
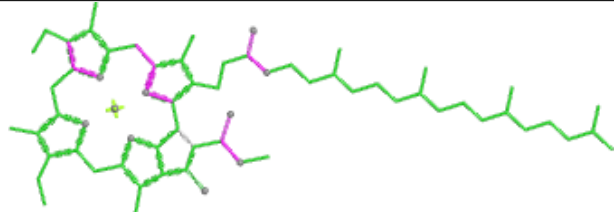
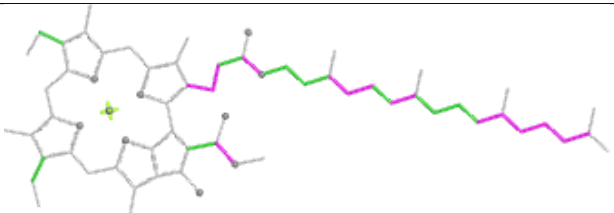
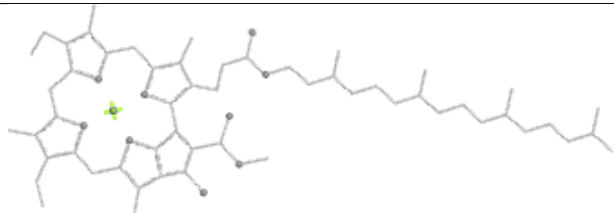


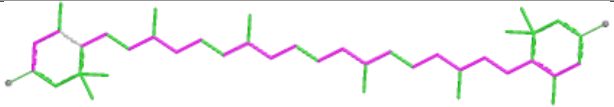
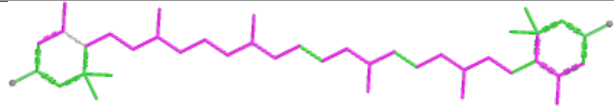
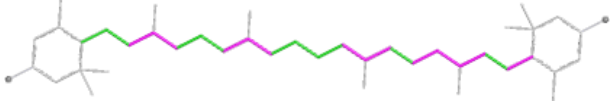
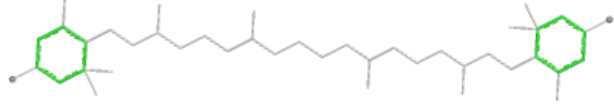
Torsions

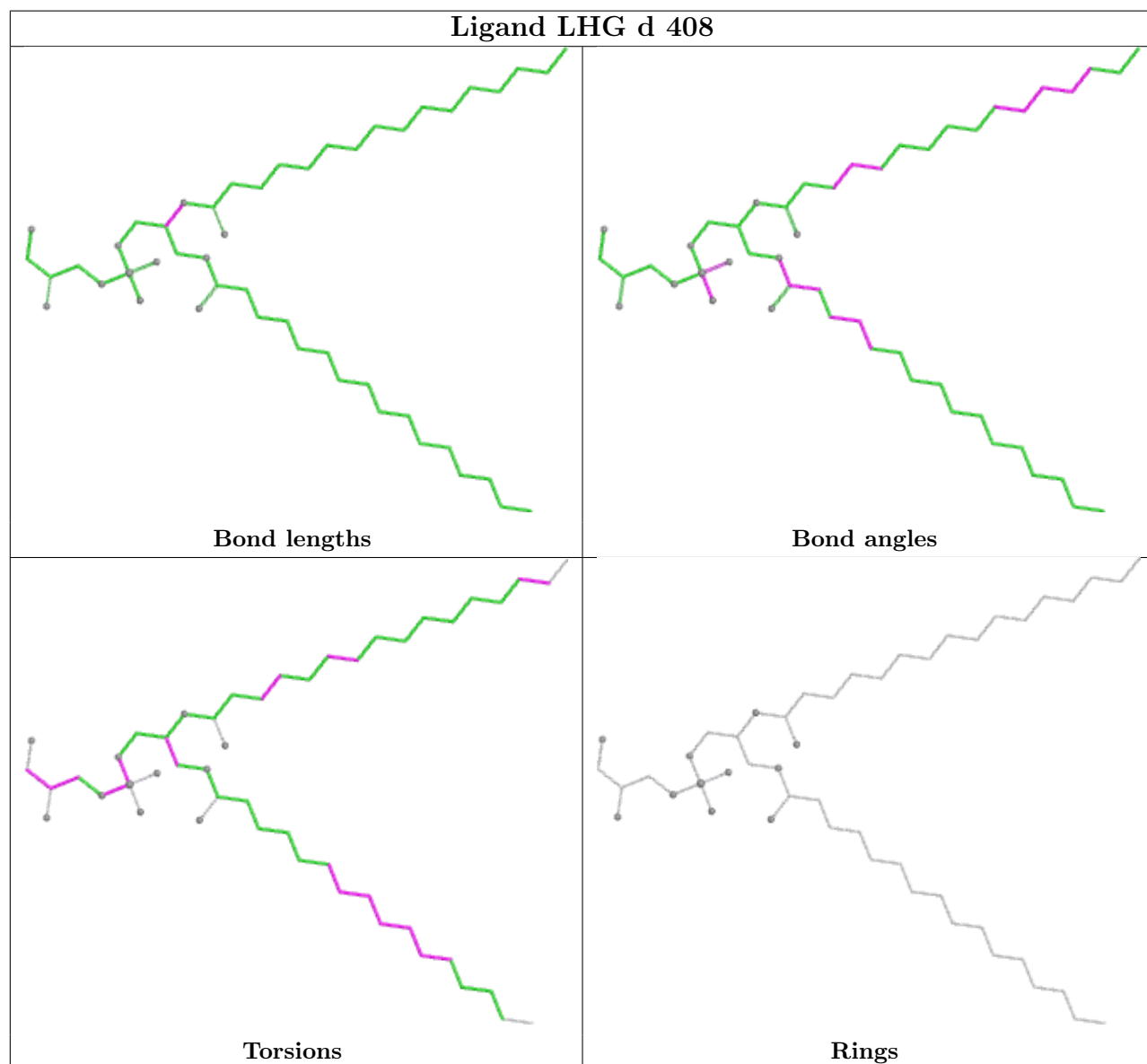
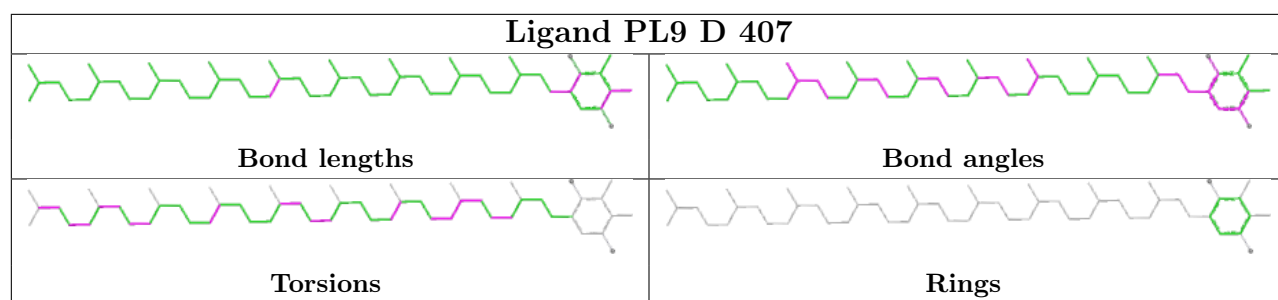


Rings

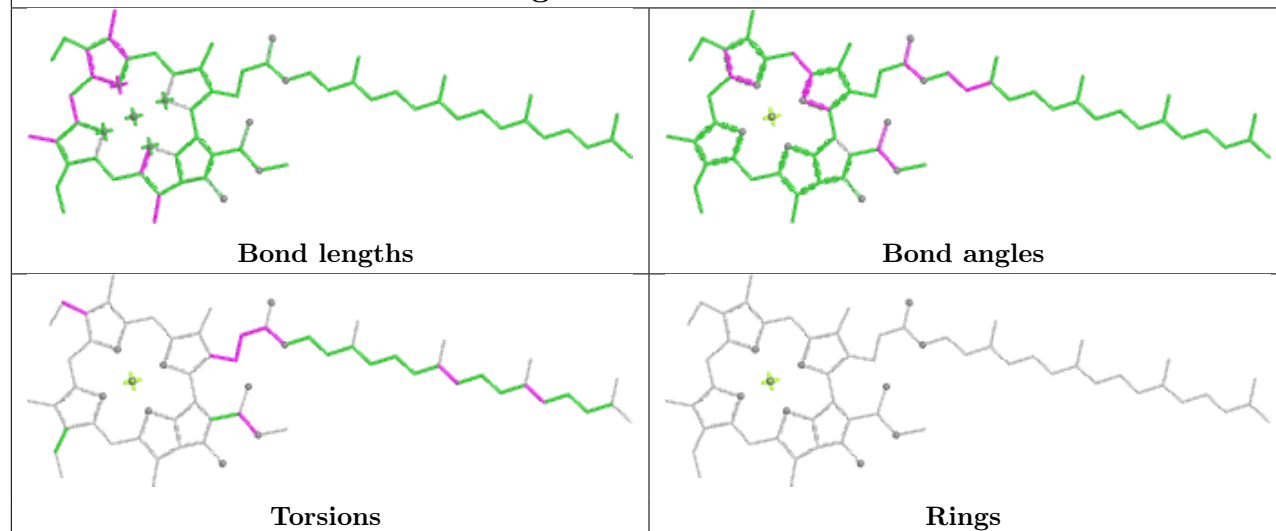
| Ligand CLA Y 611                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand CLA b 614                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|    |    |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

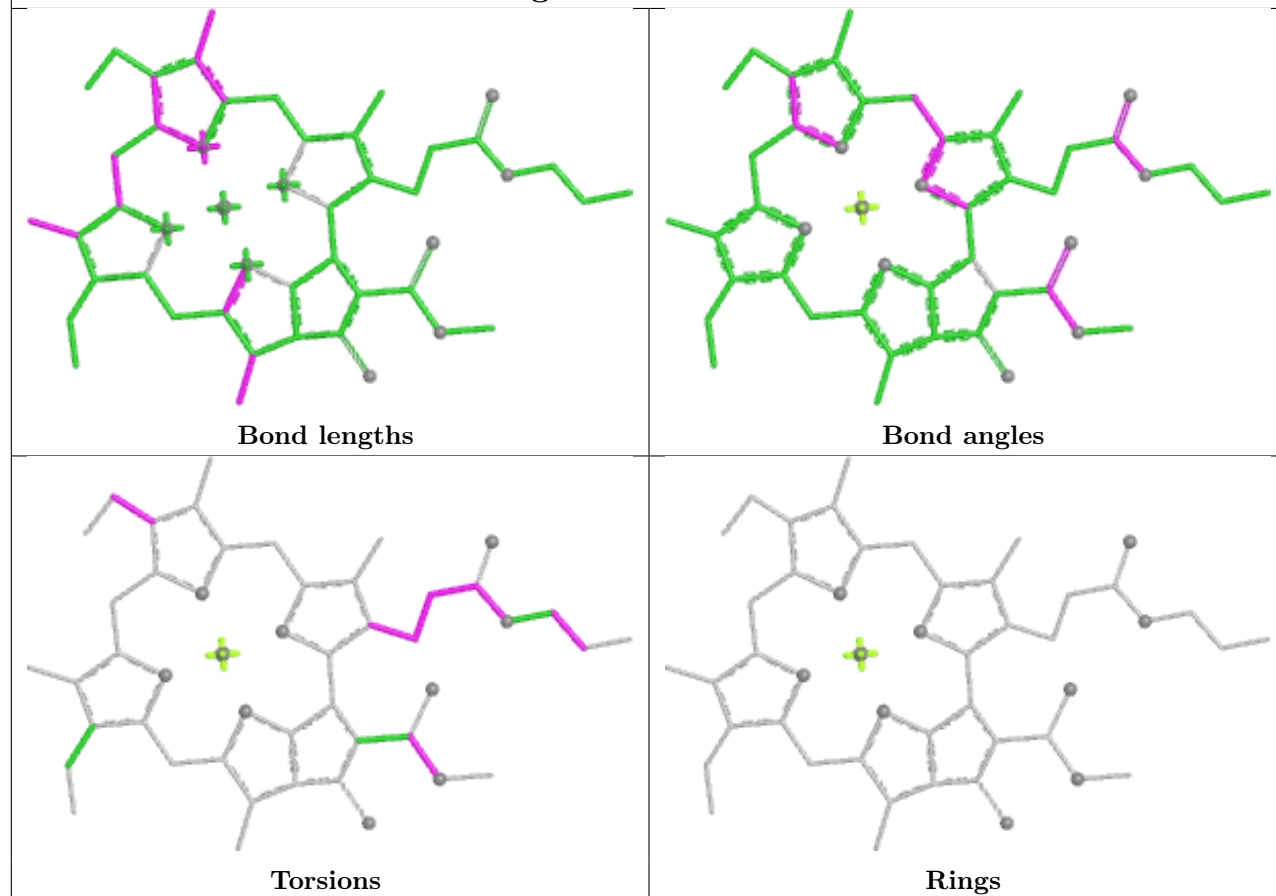
| Ligand LUT g 616                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|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

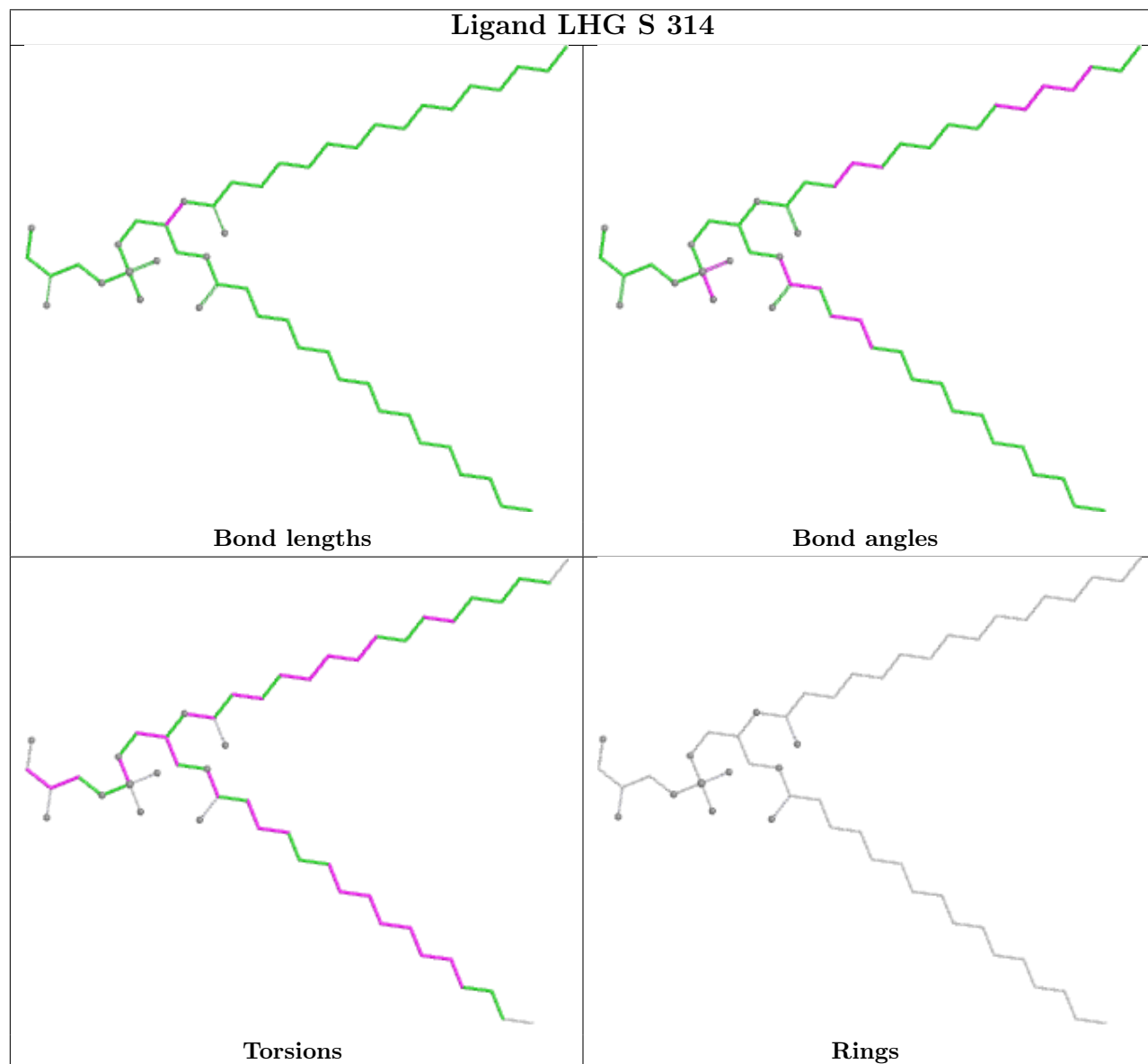
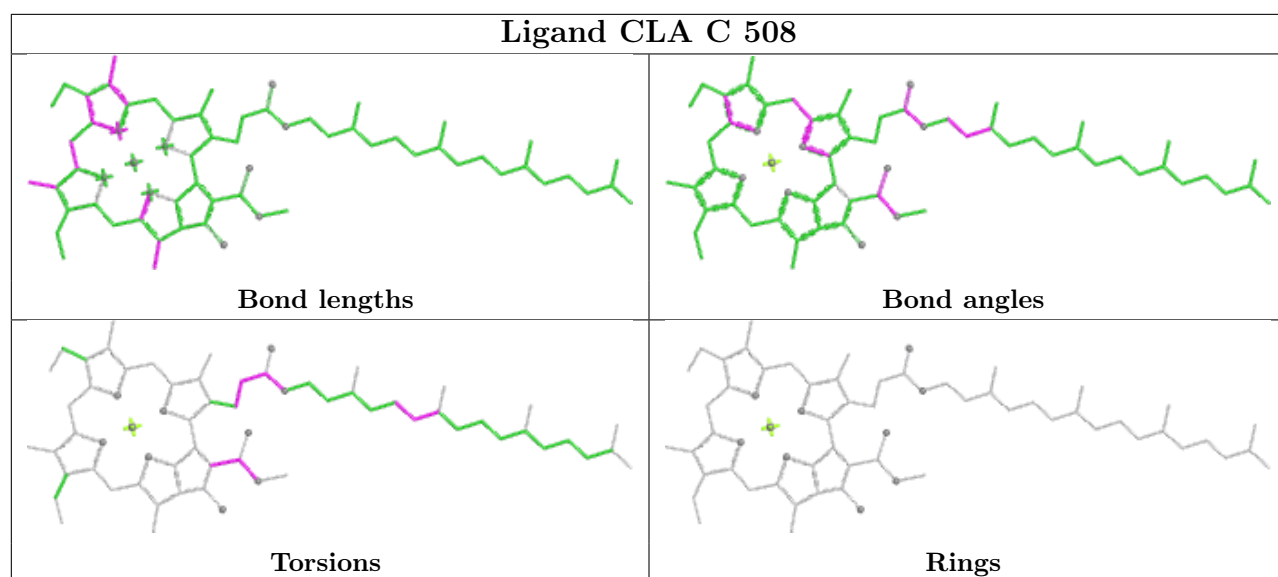


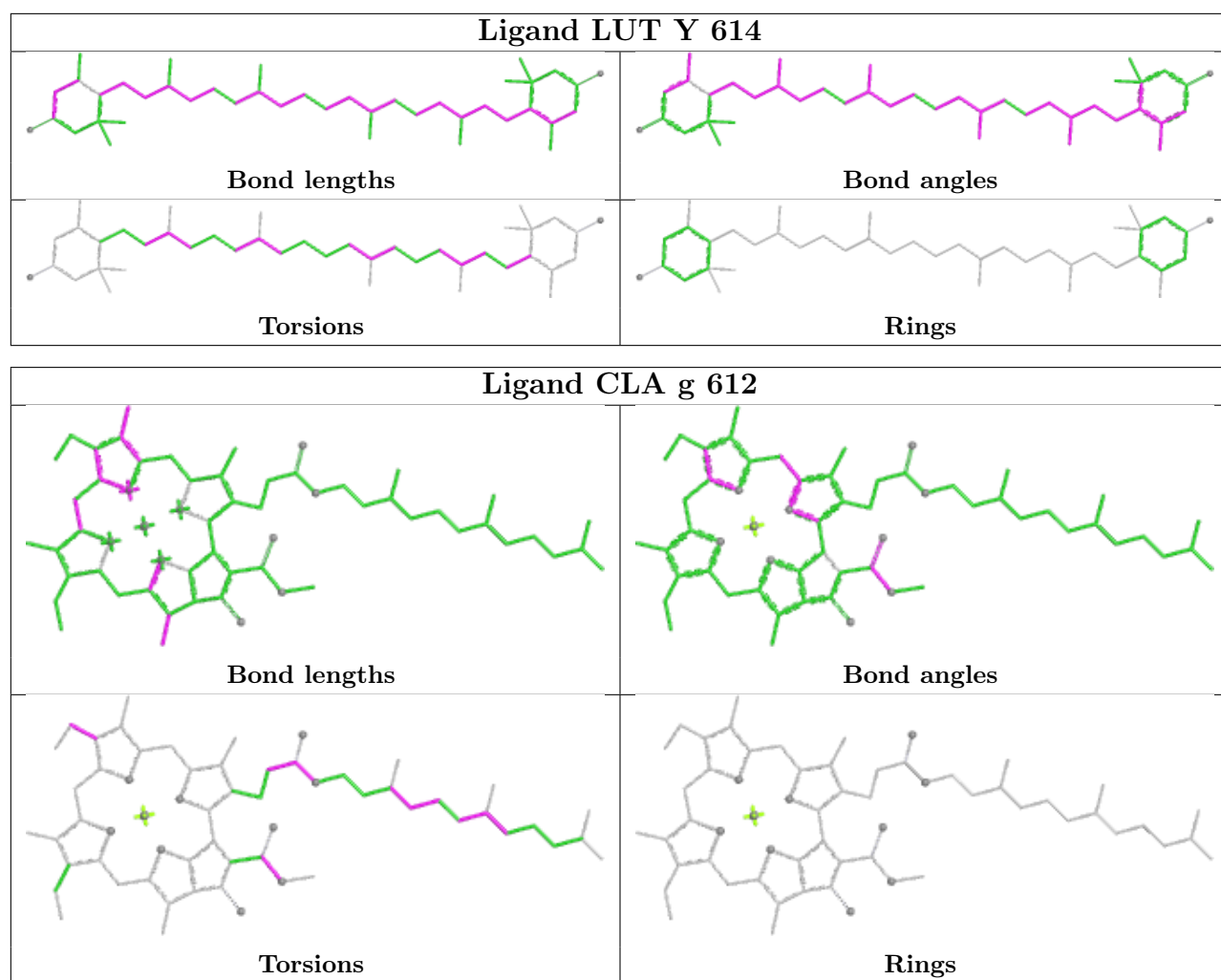
## Ligand CLA Y 602

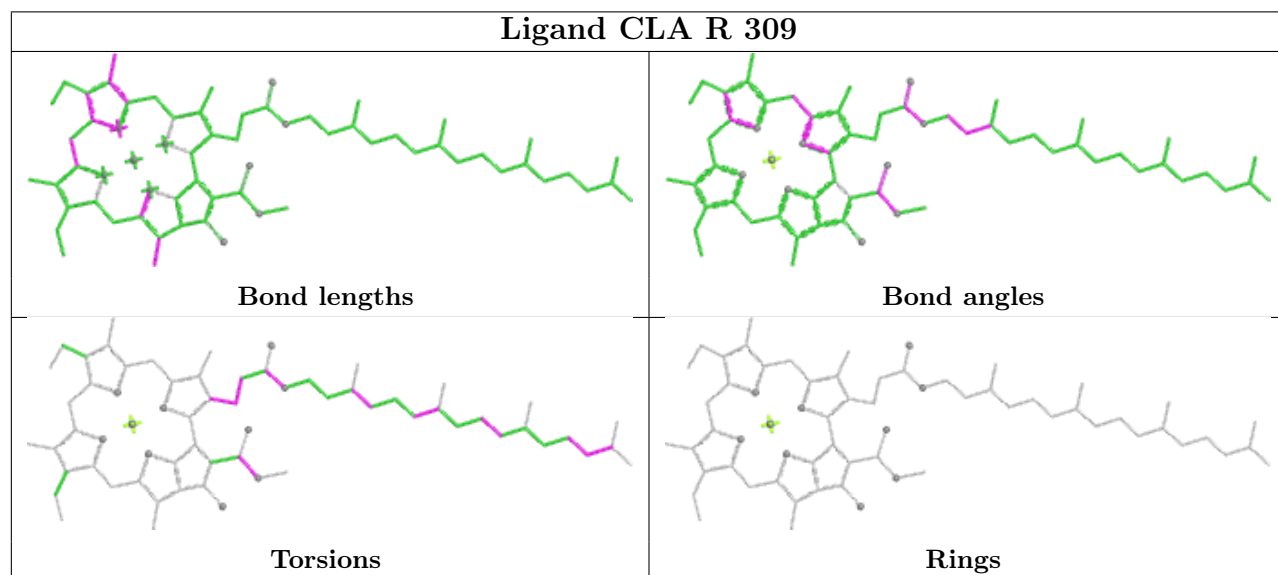
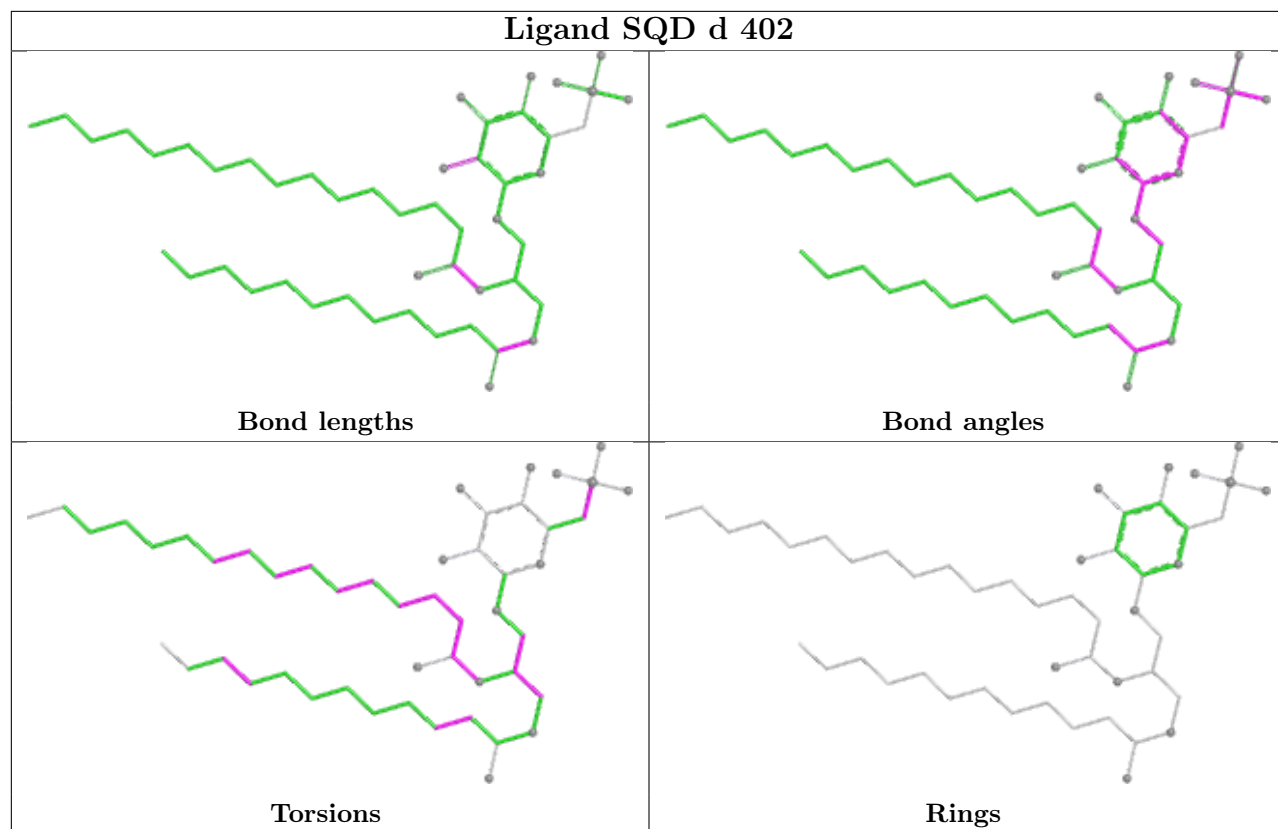


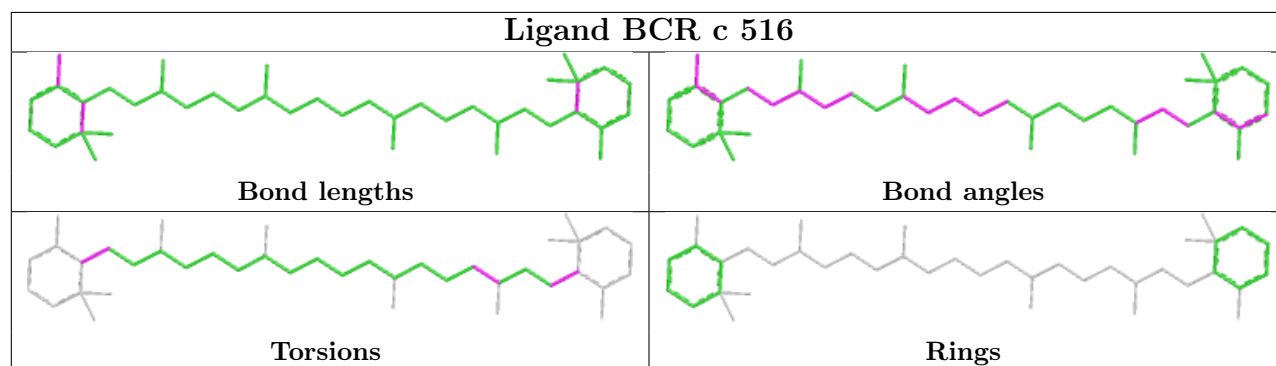
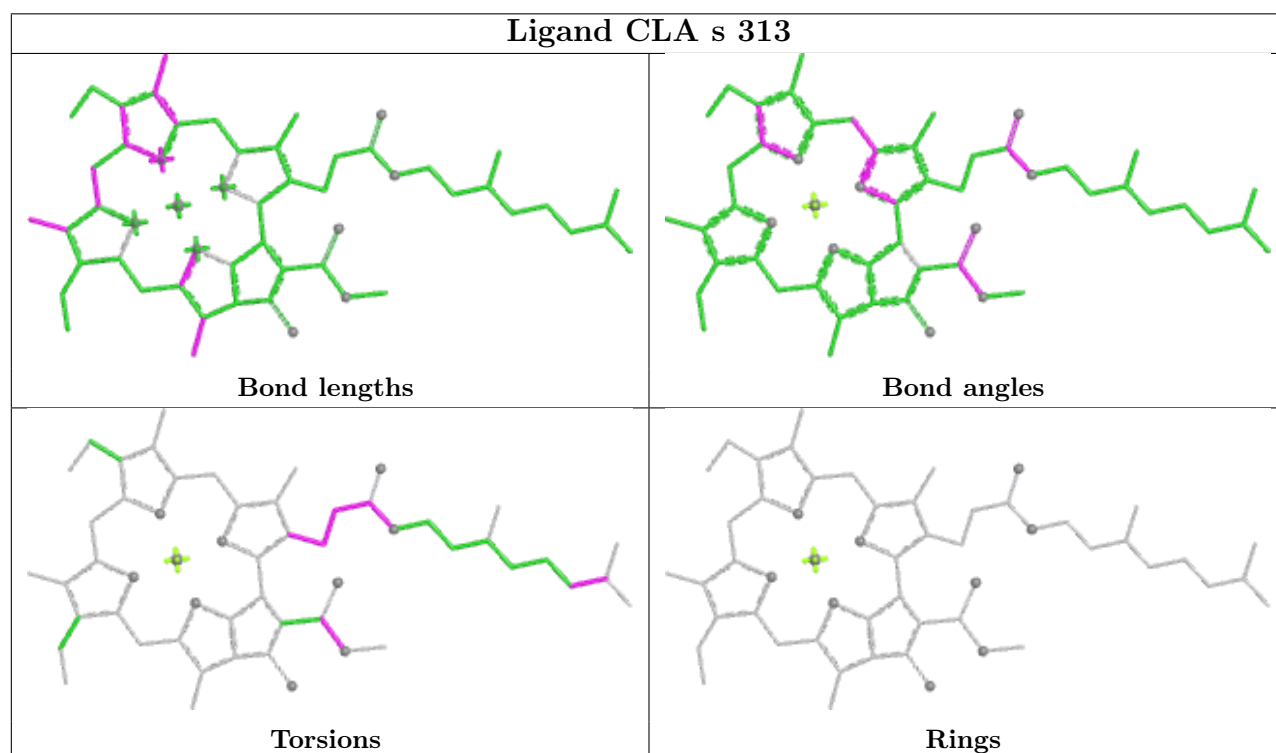
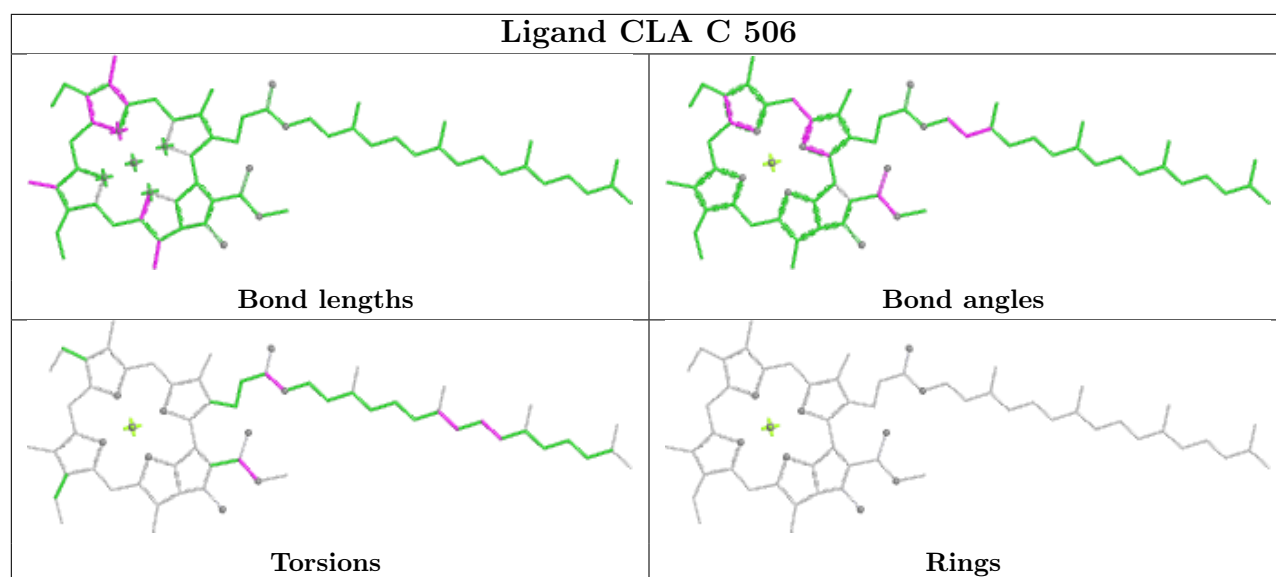
## Ligand CLA N 613

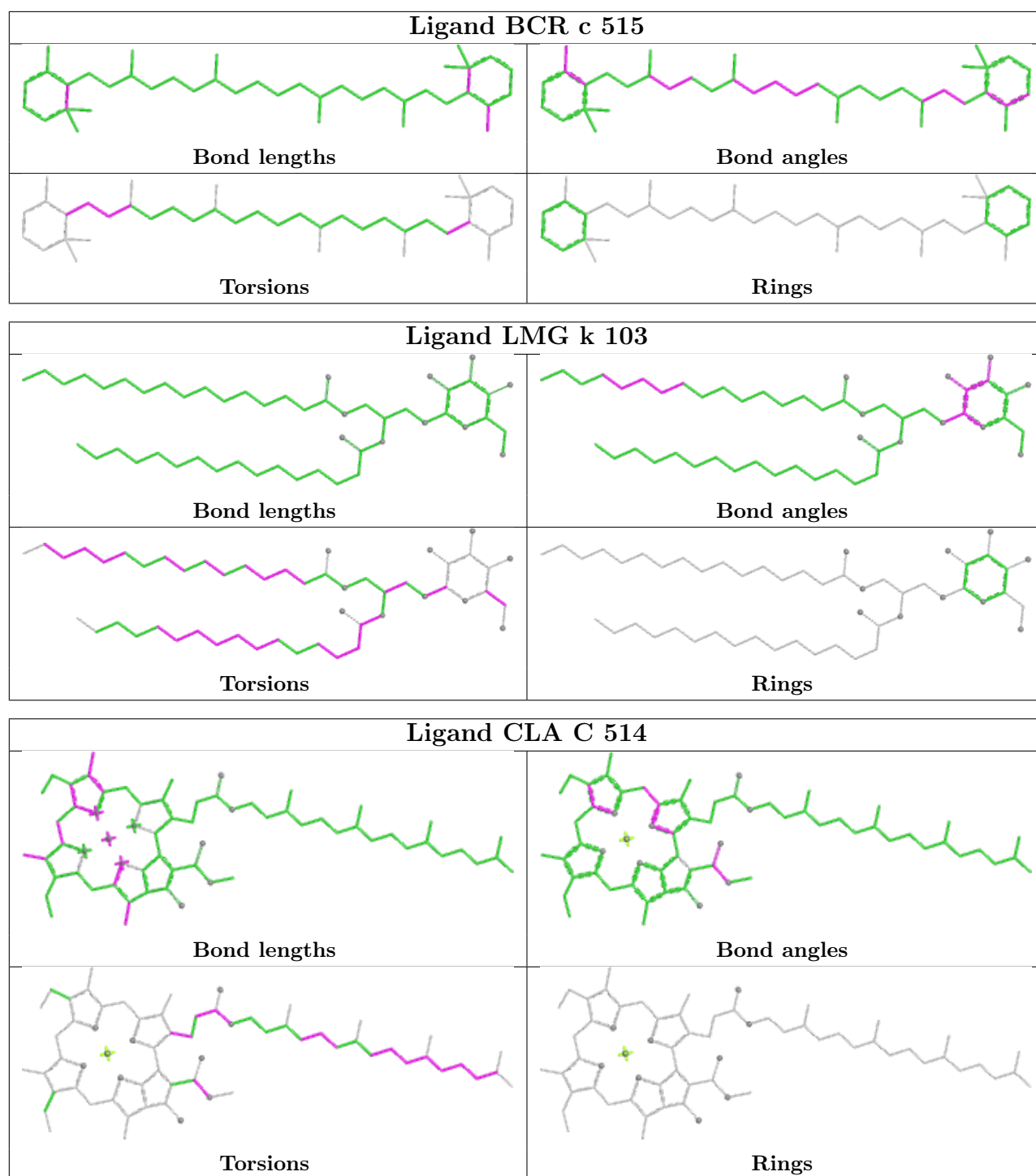


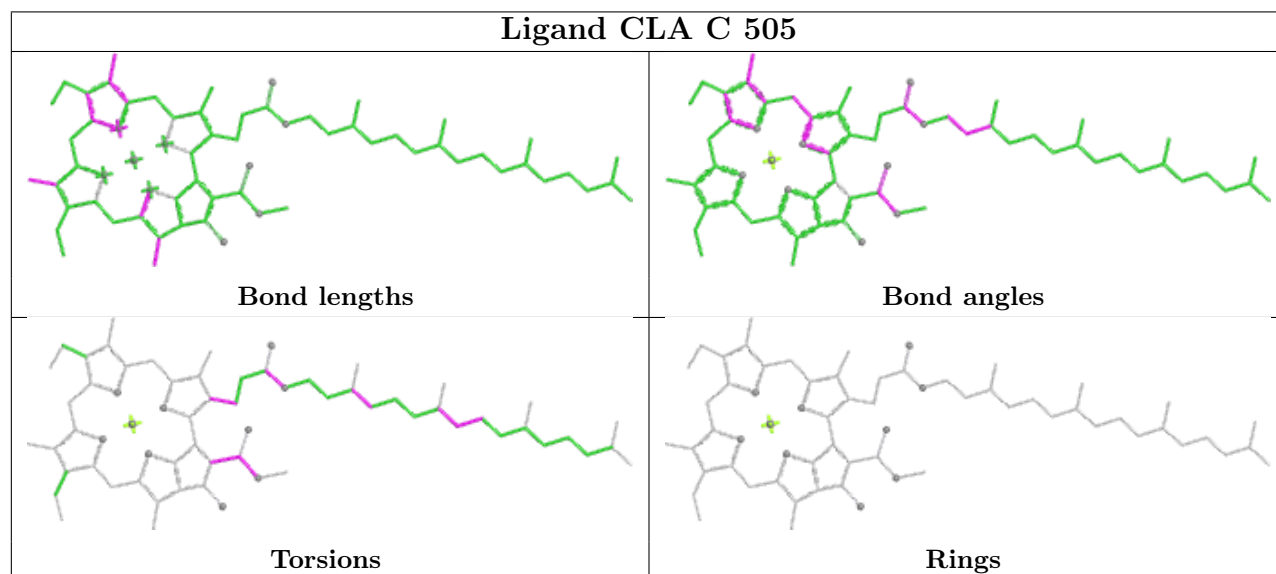
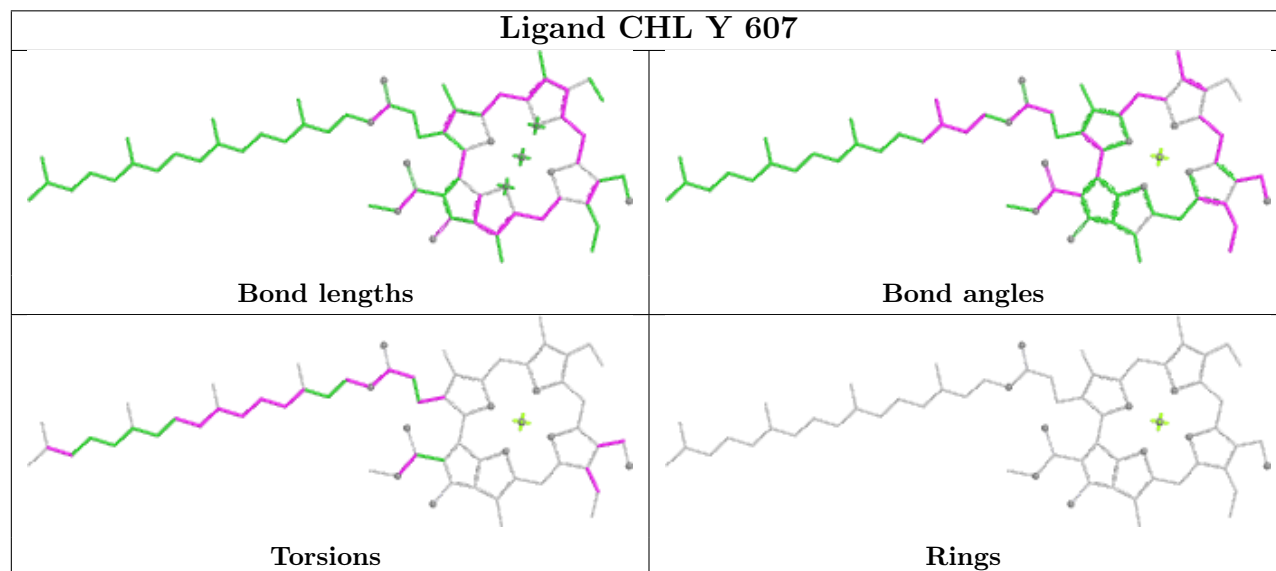
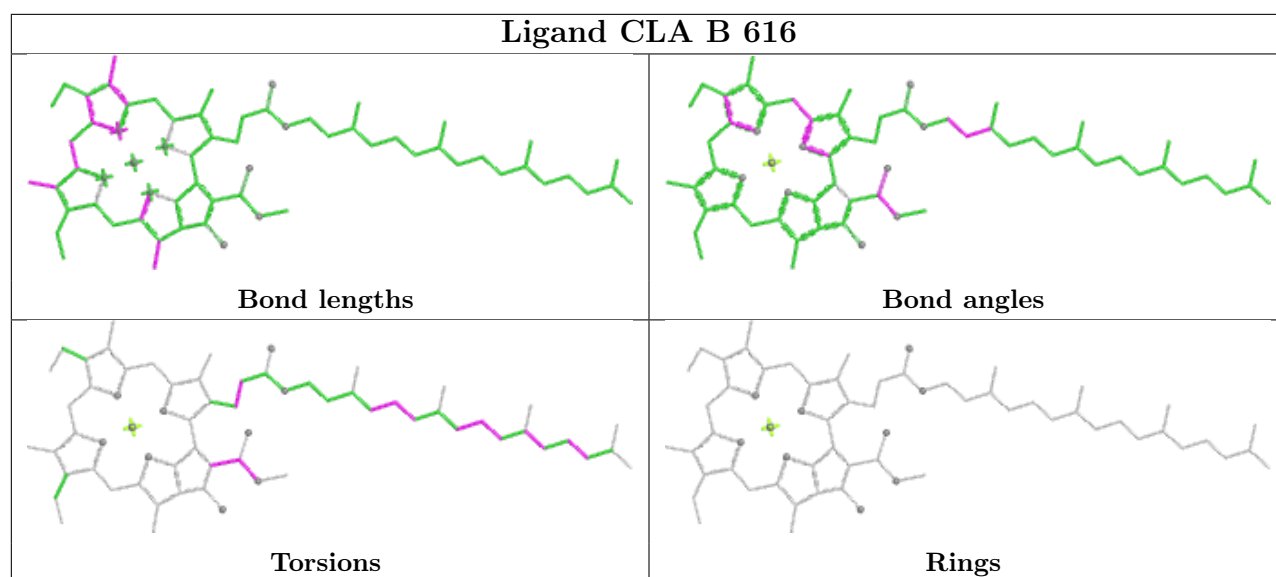


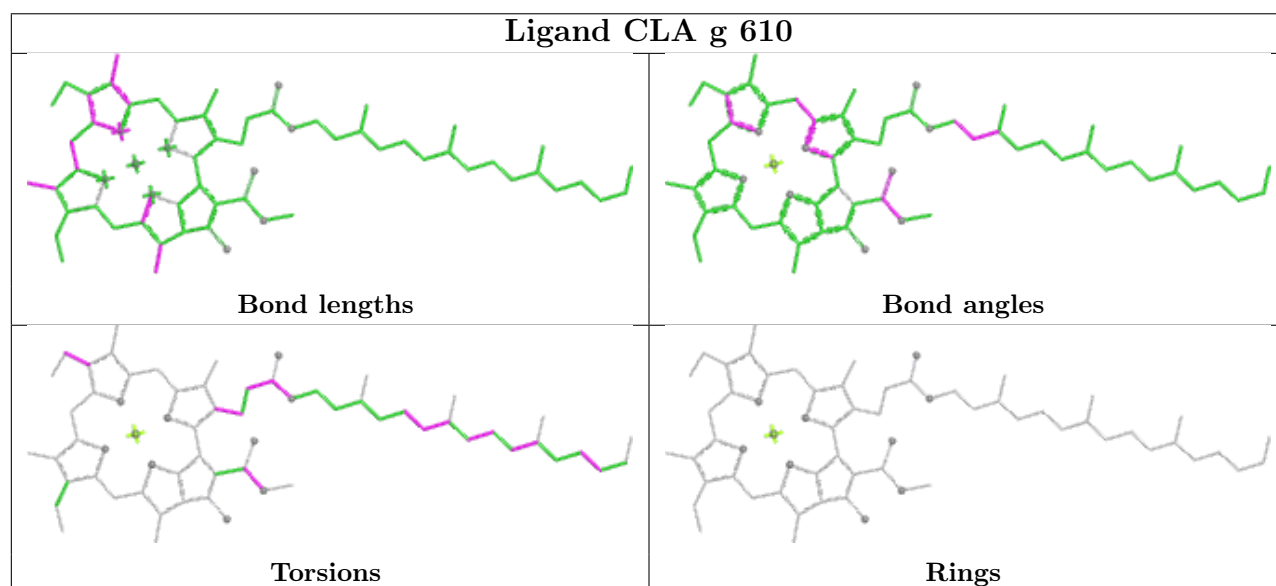
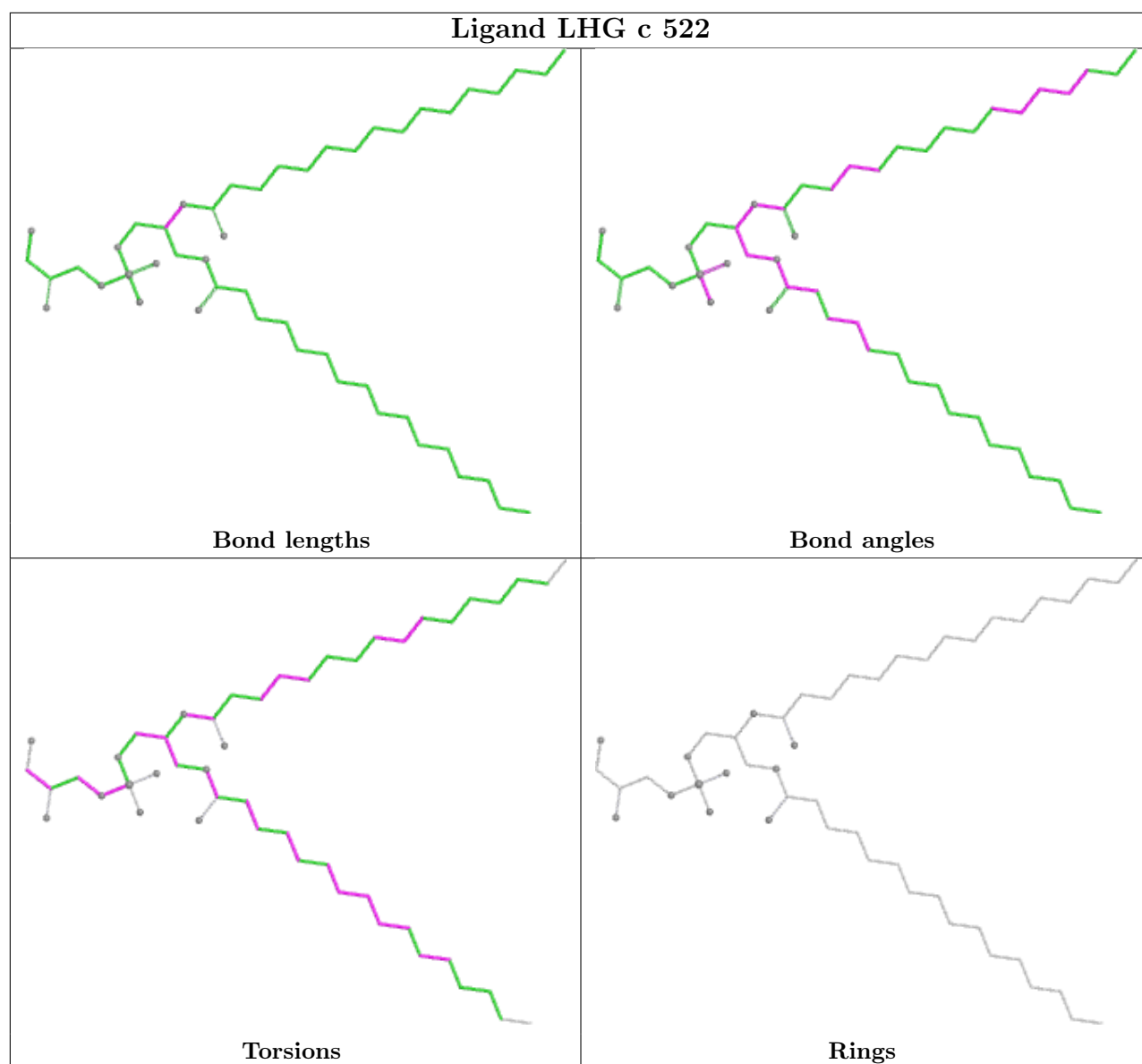


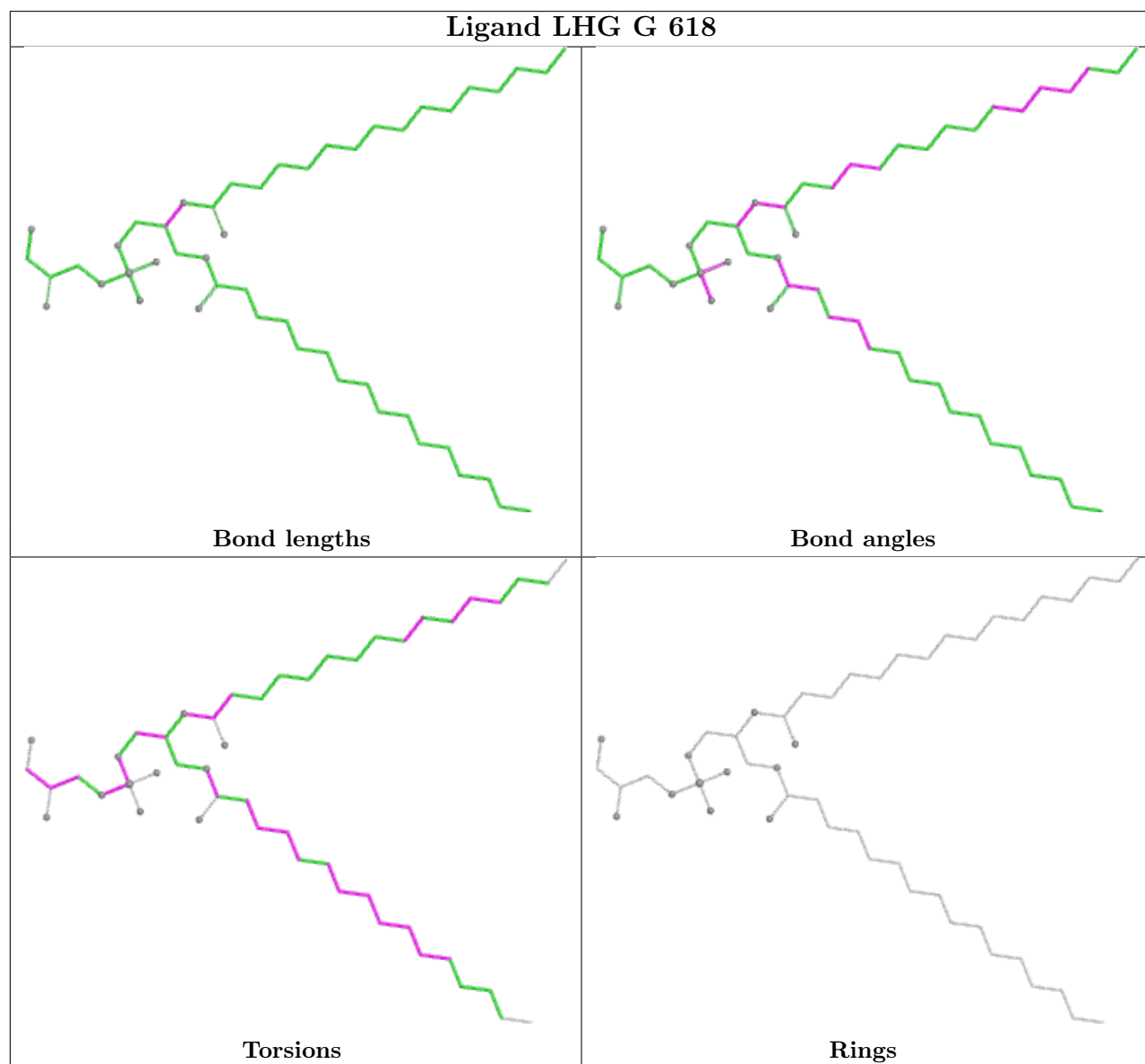
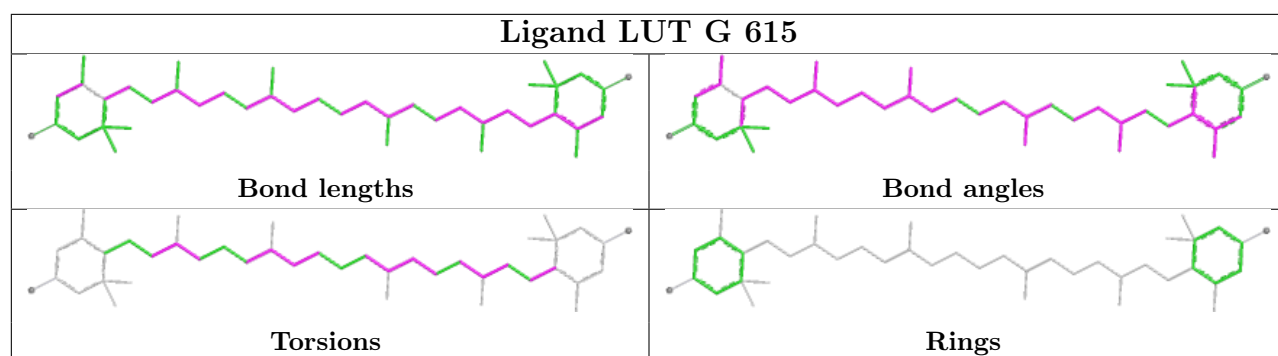


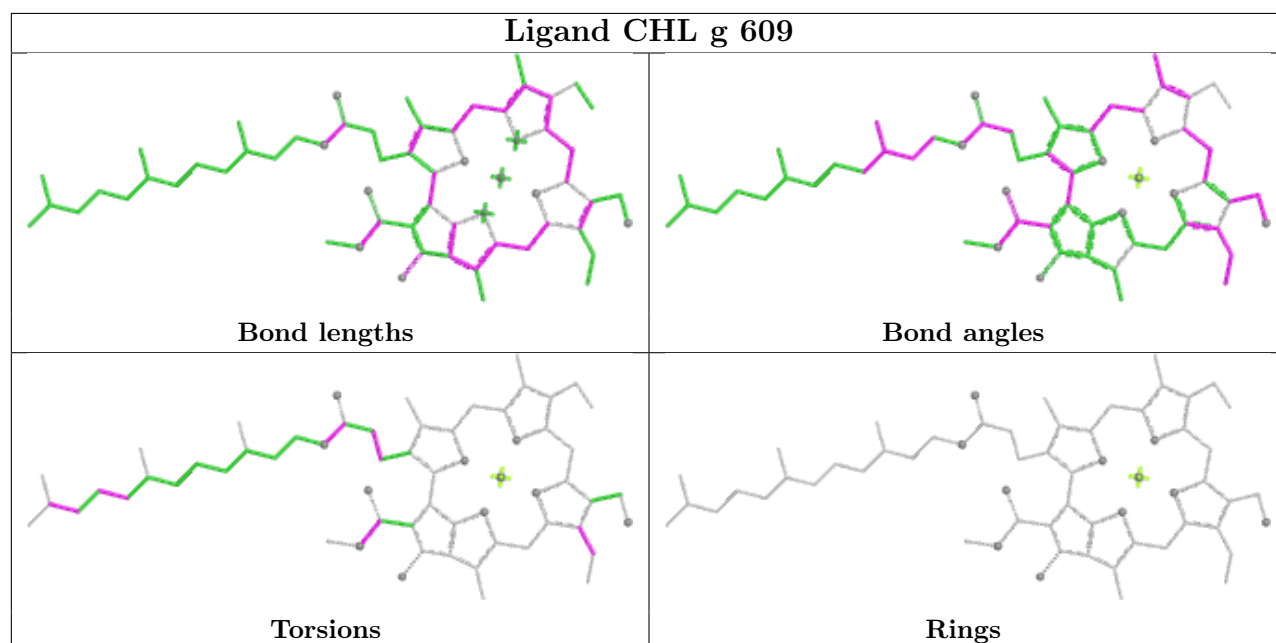
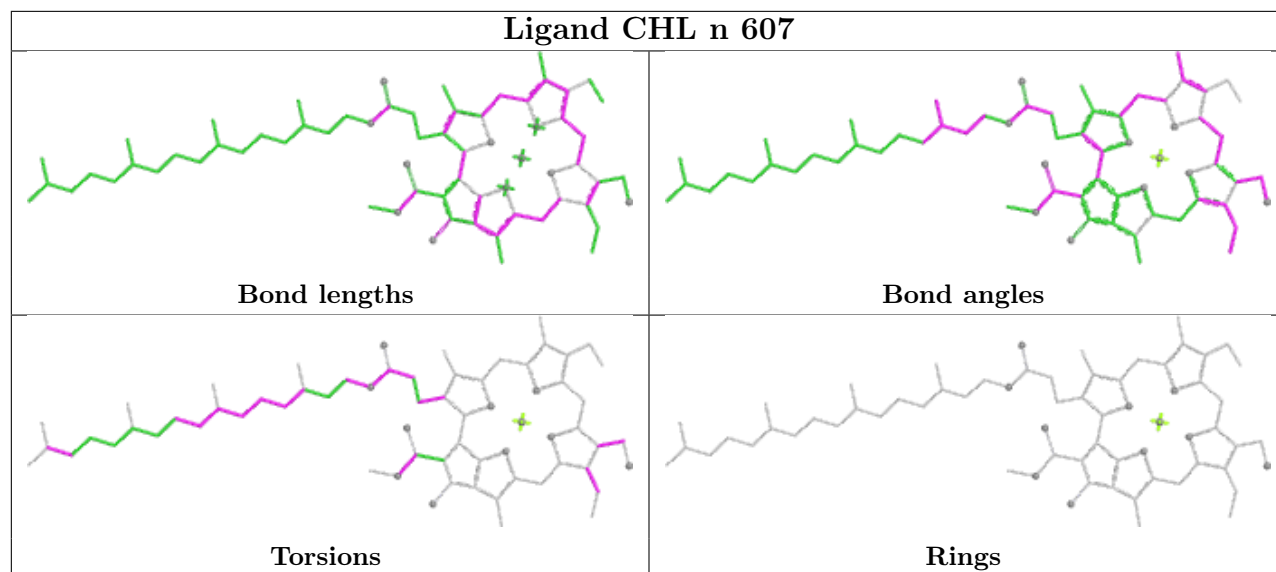


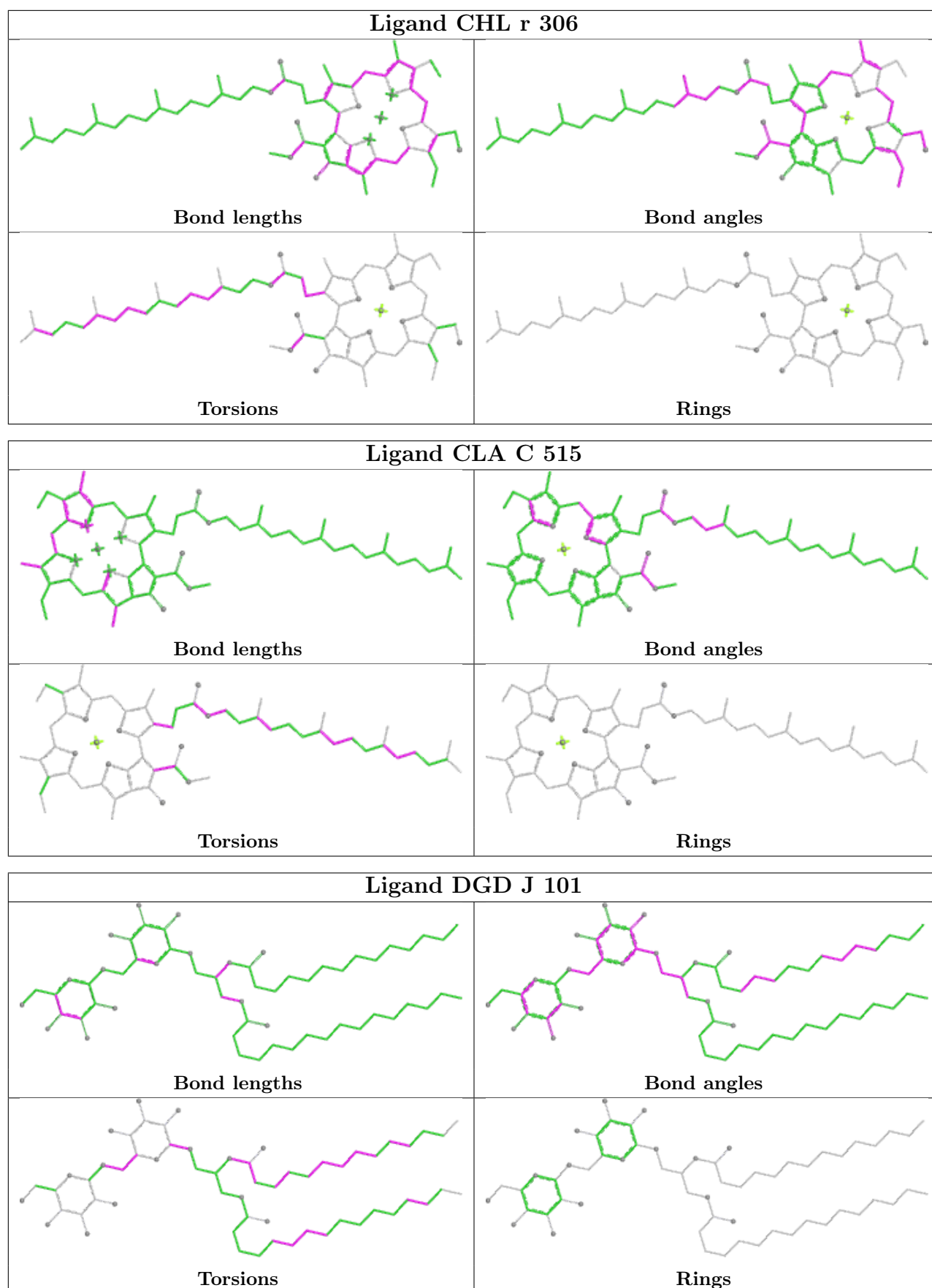


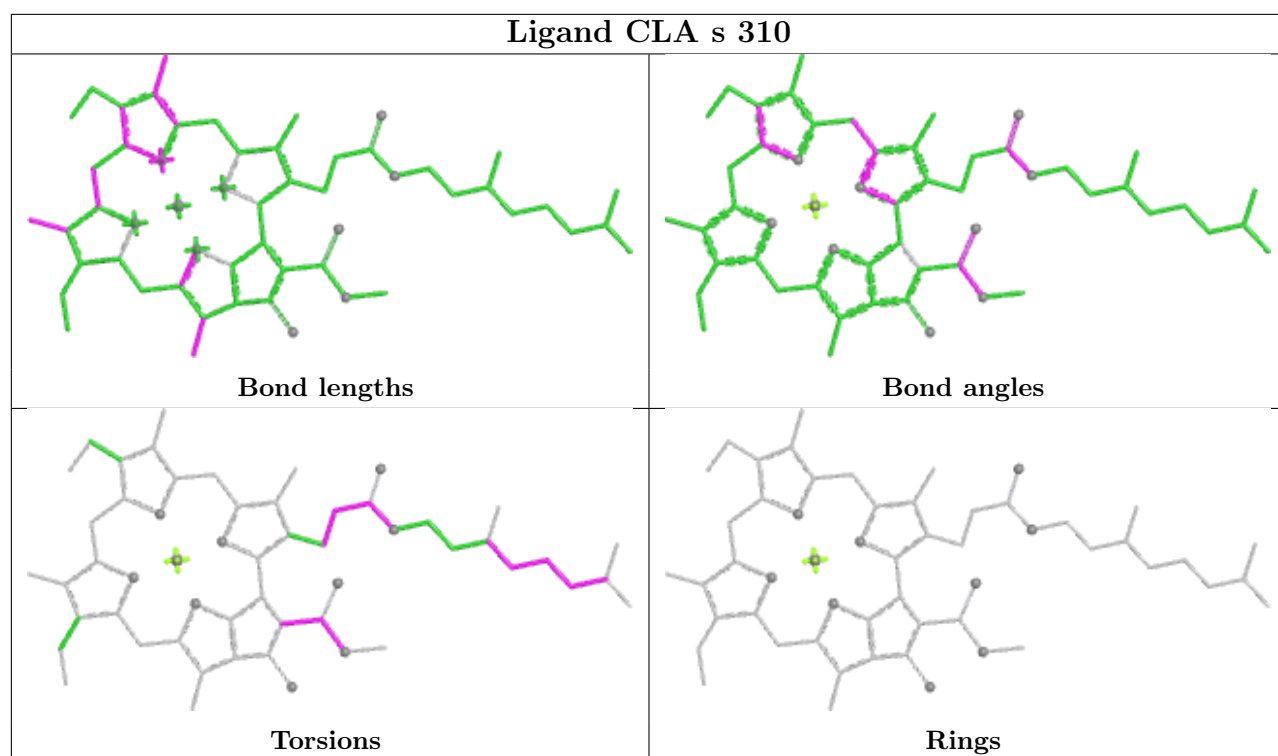


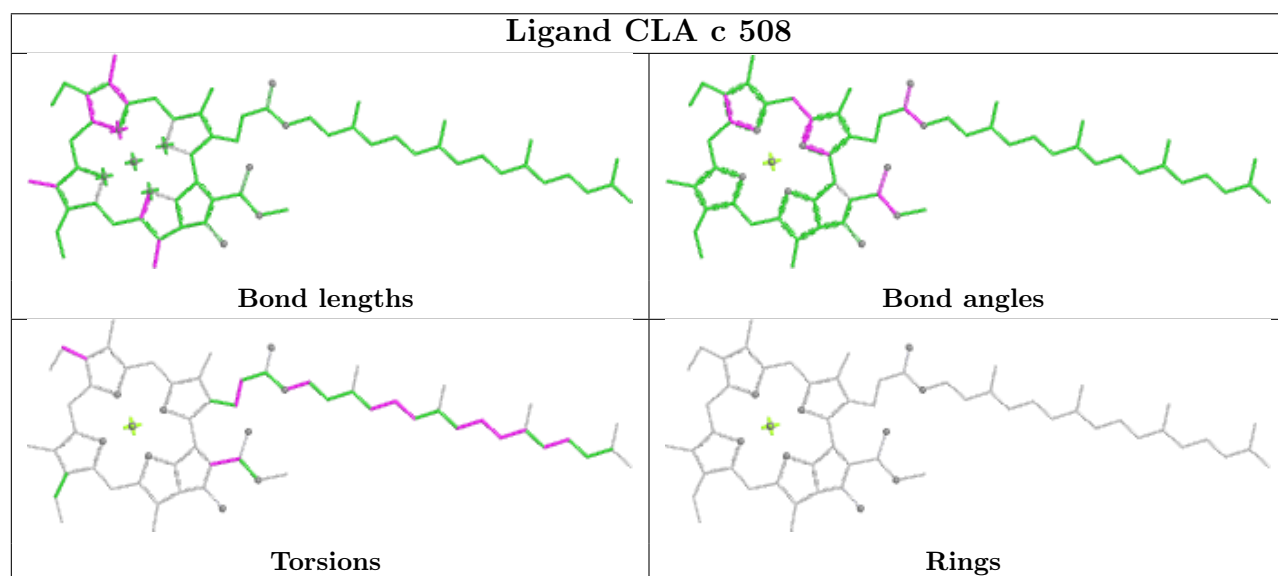
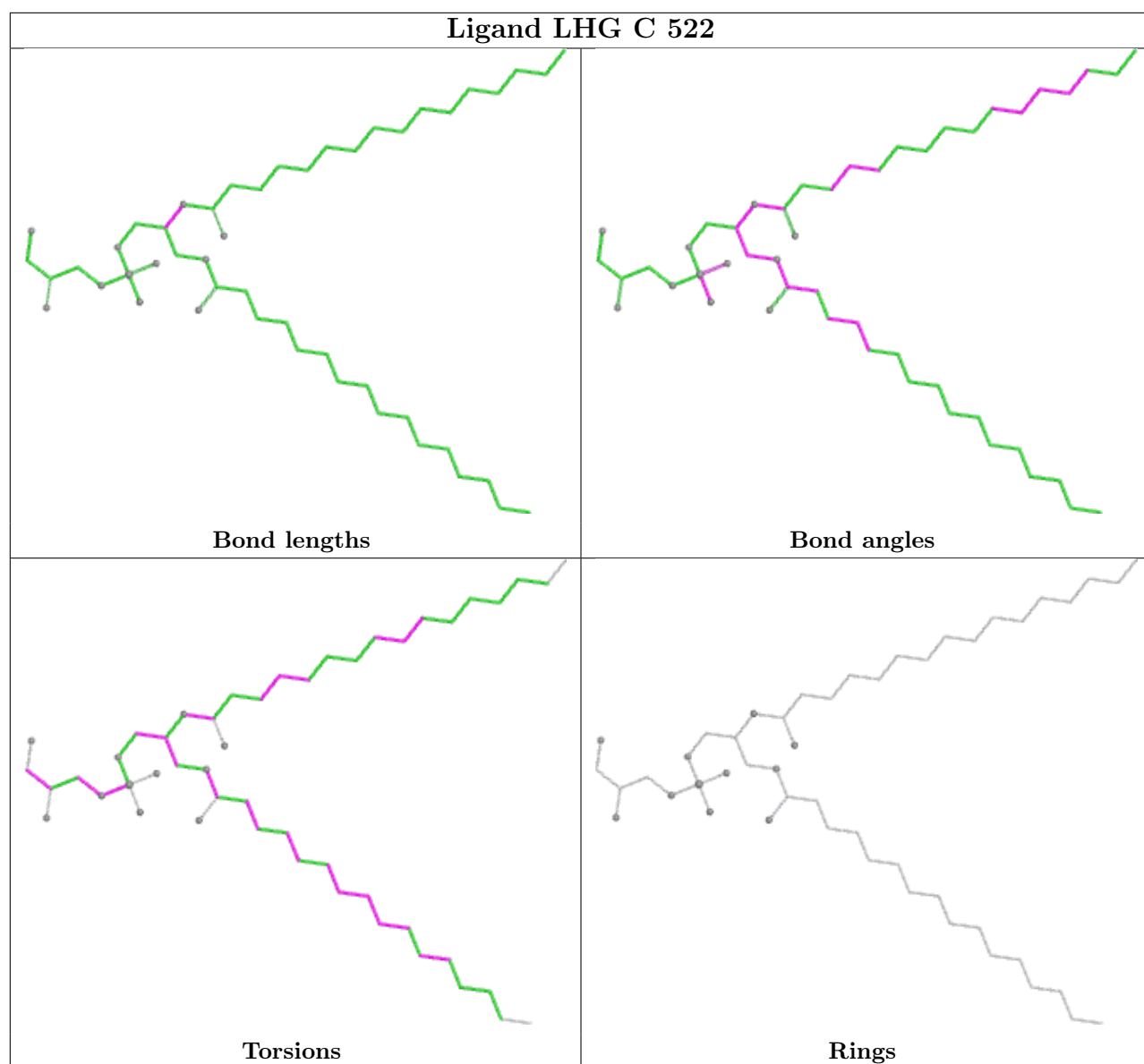


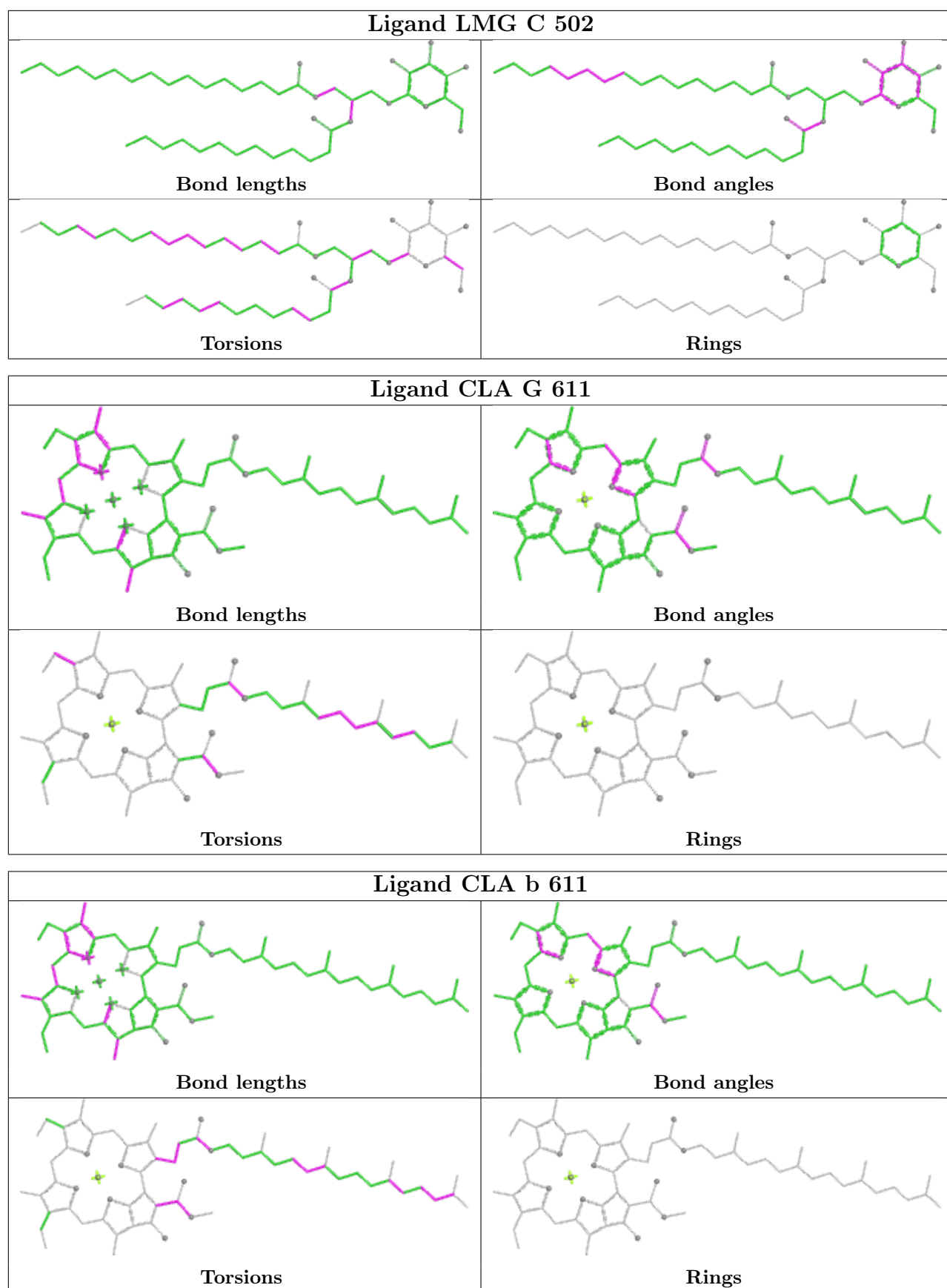


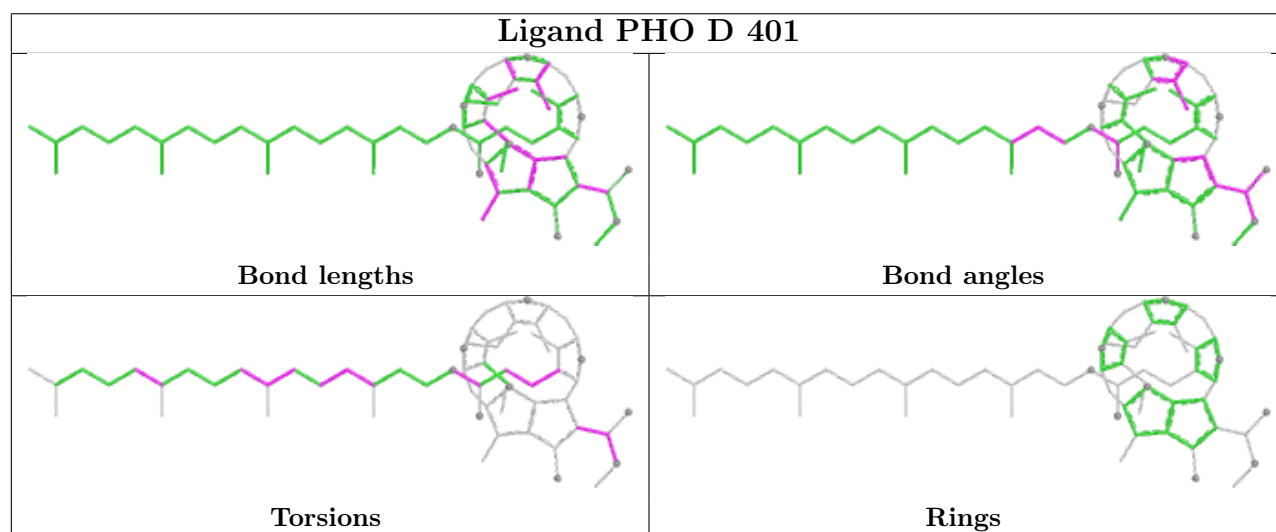
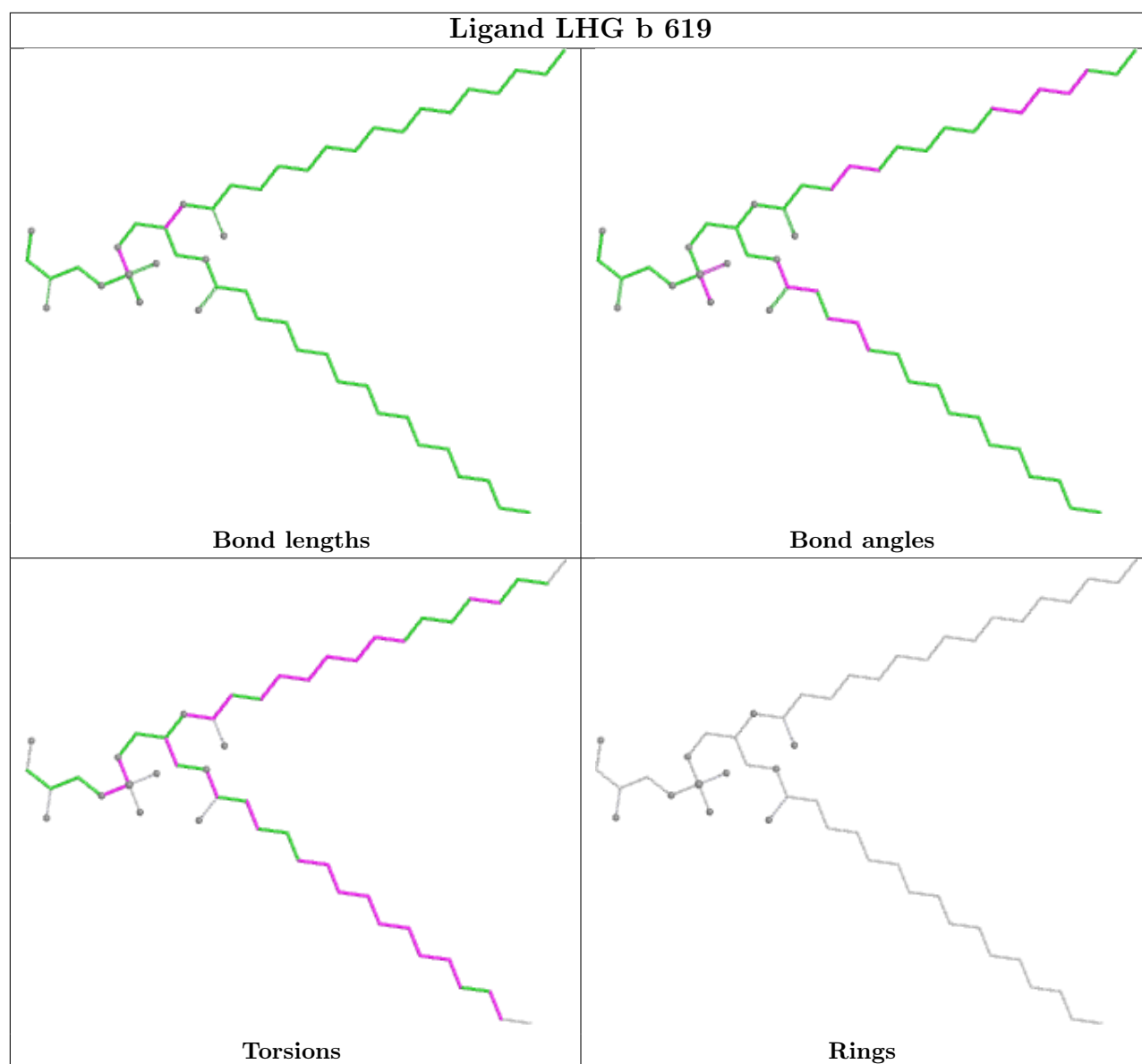




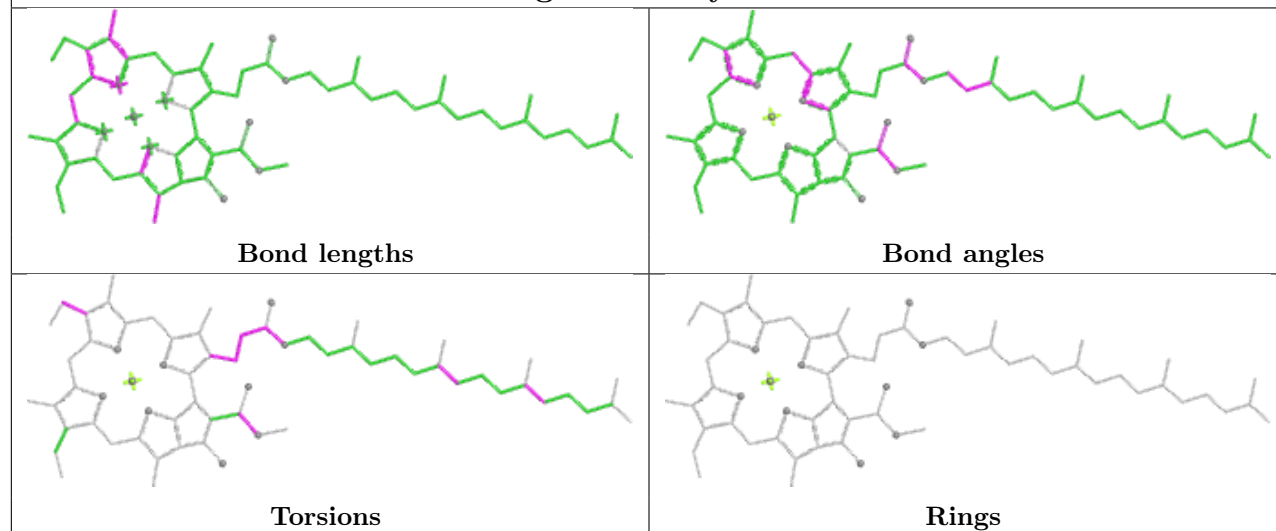




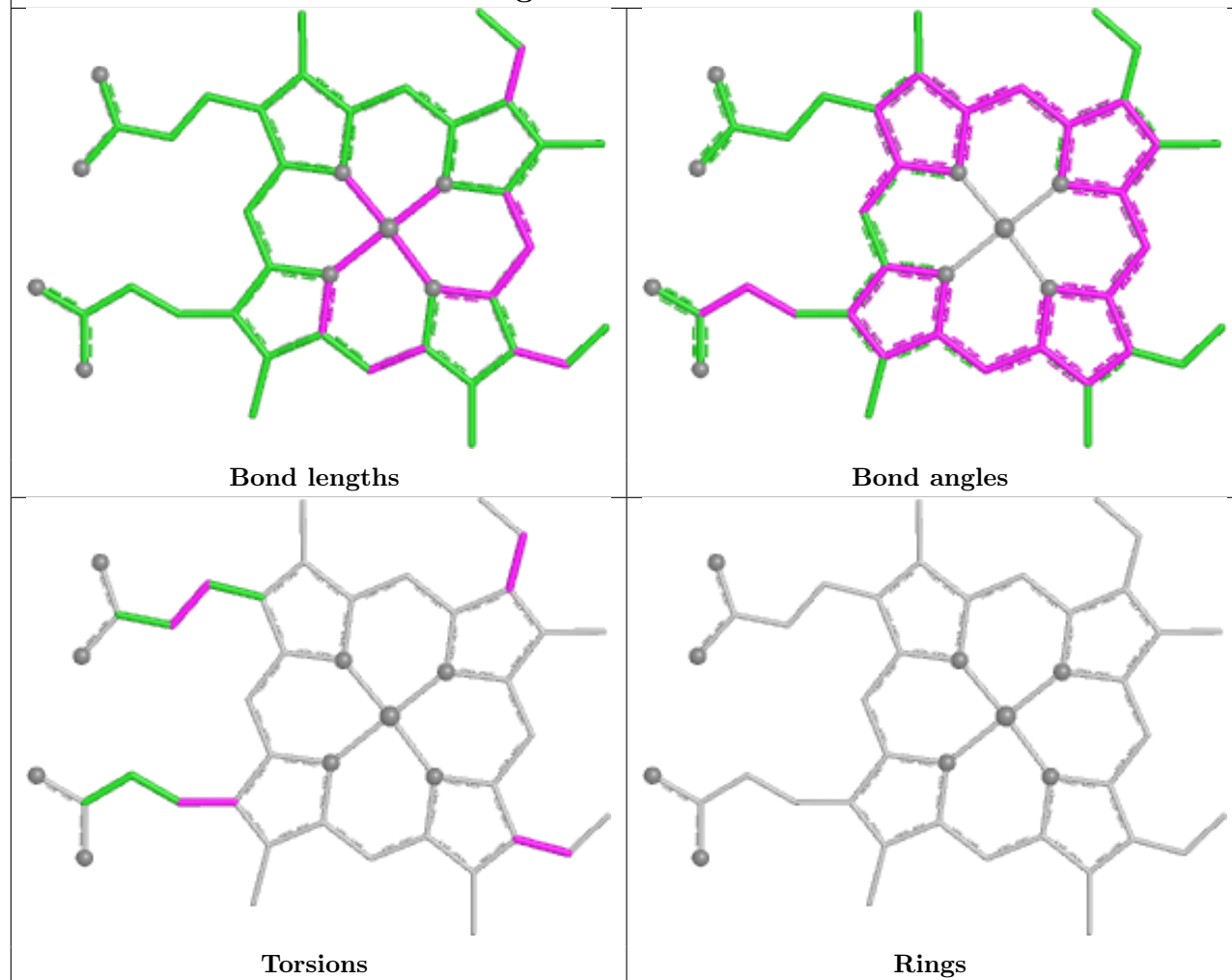


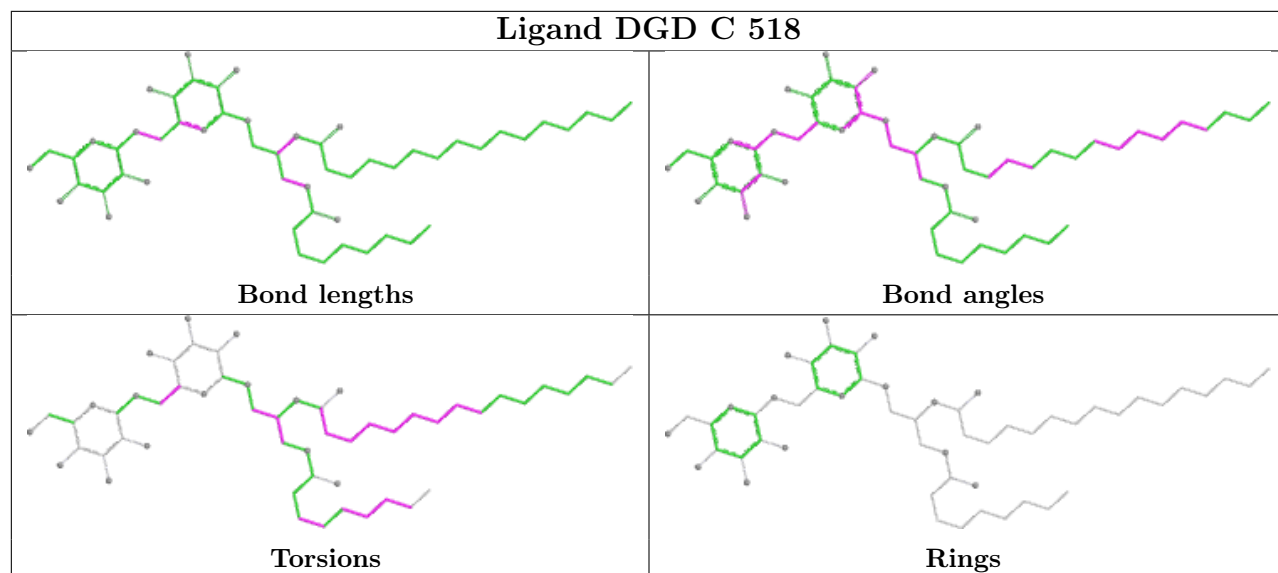
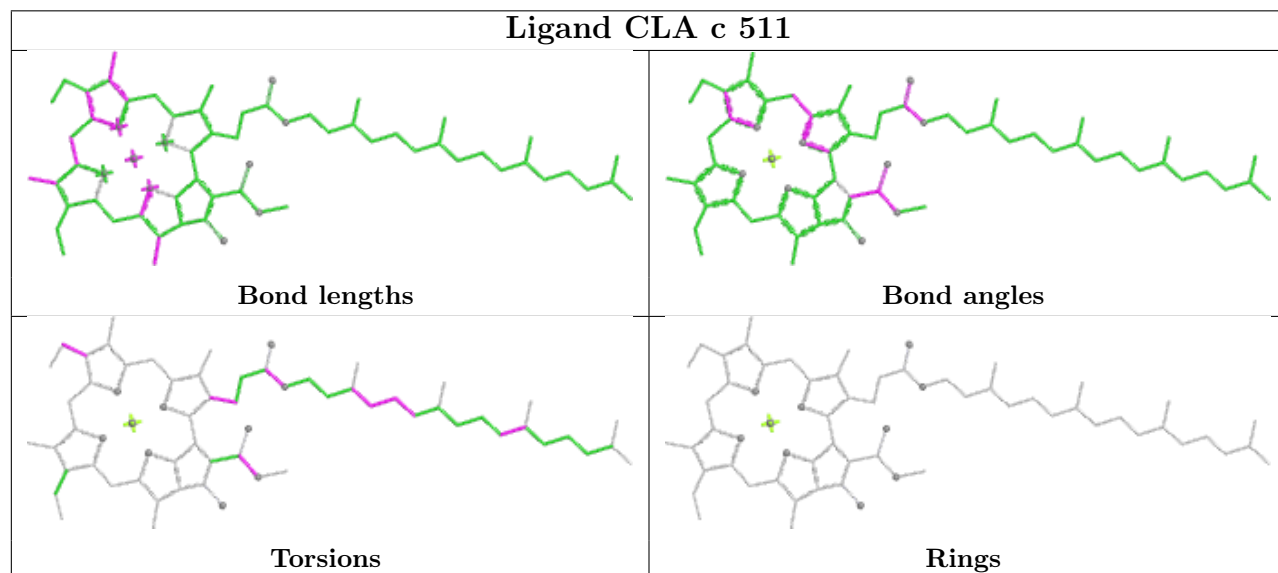
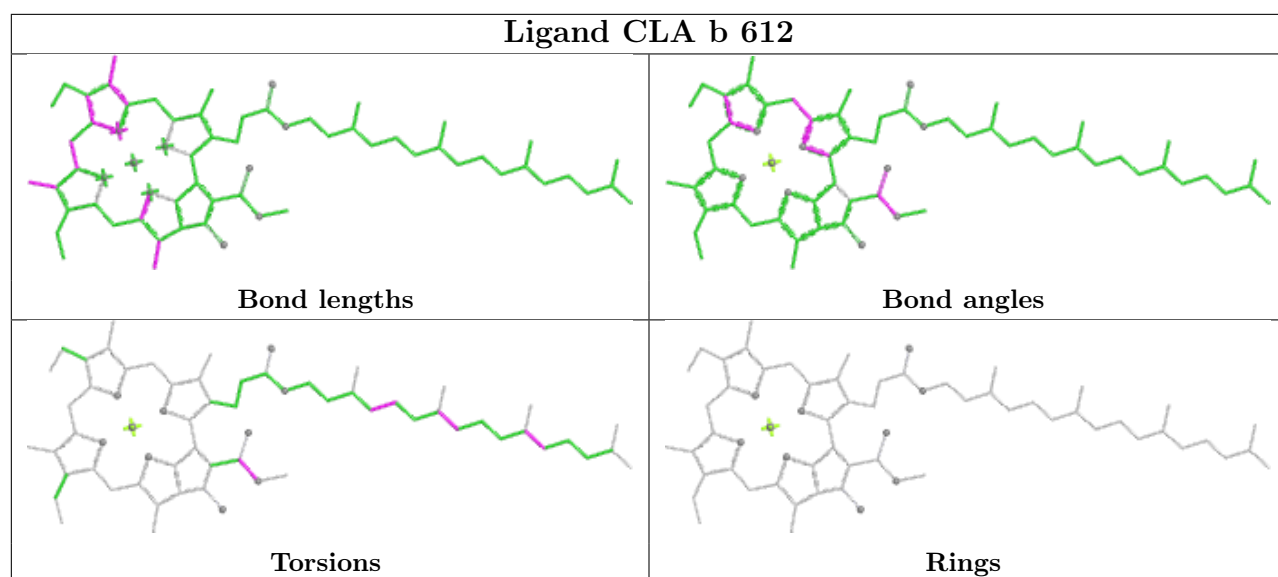


## Ligand CLA y 602

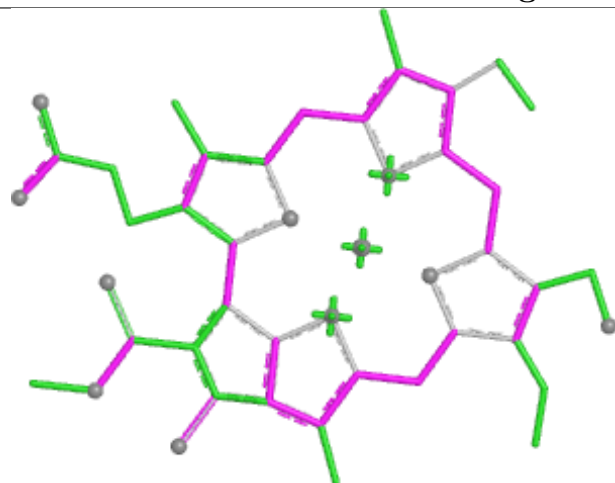


## Ligand HEM f 101

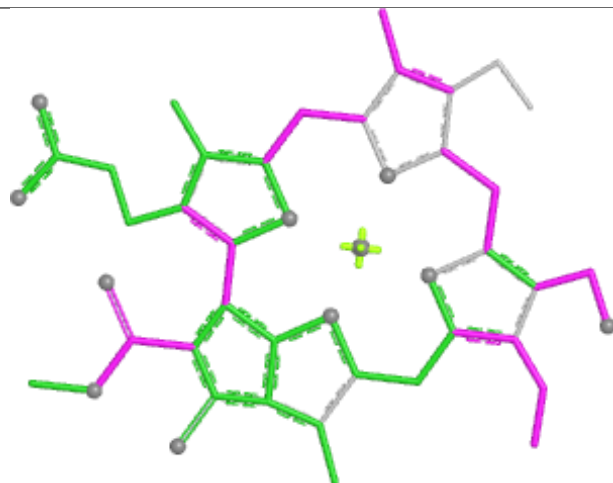




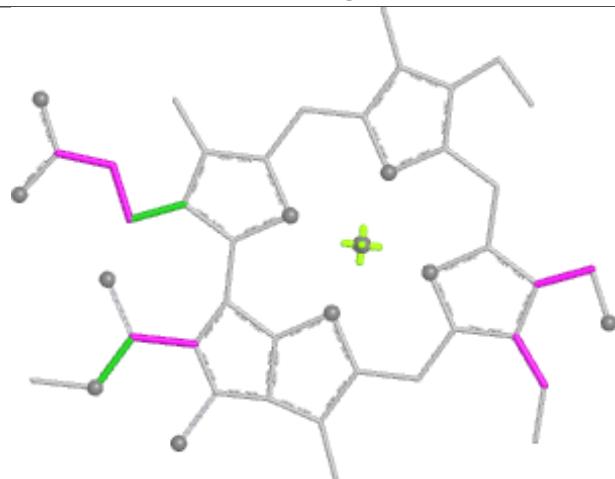
## Ligand CHL S 306



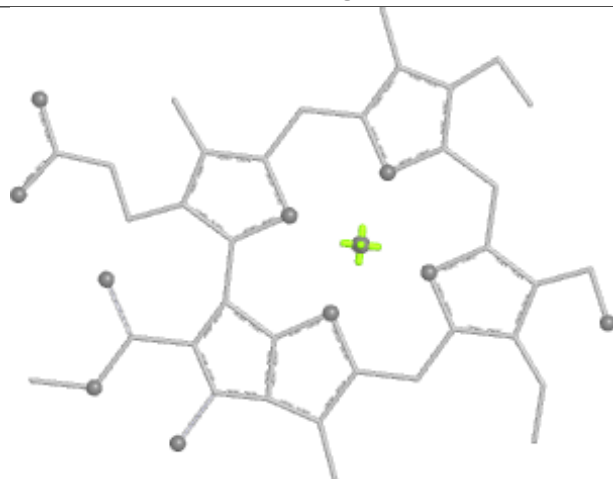
Bond lengths



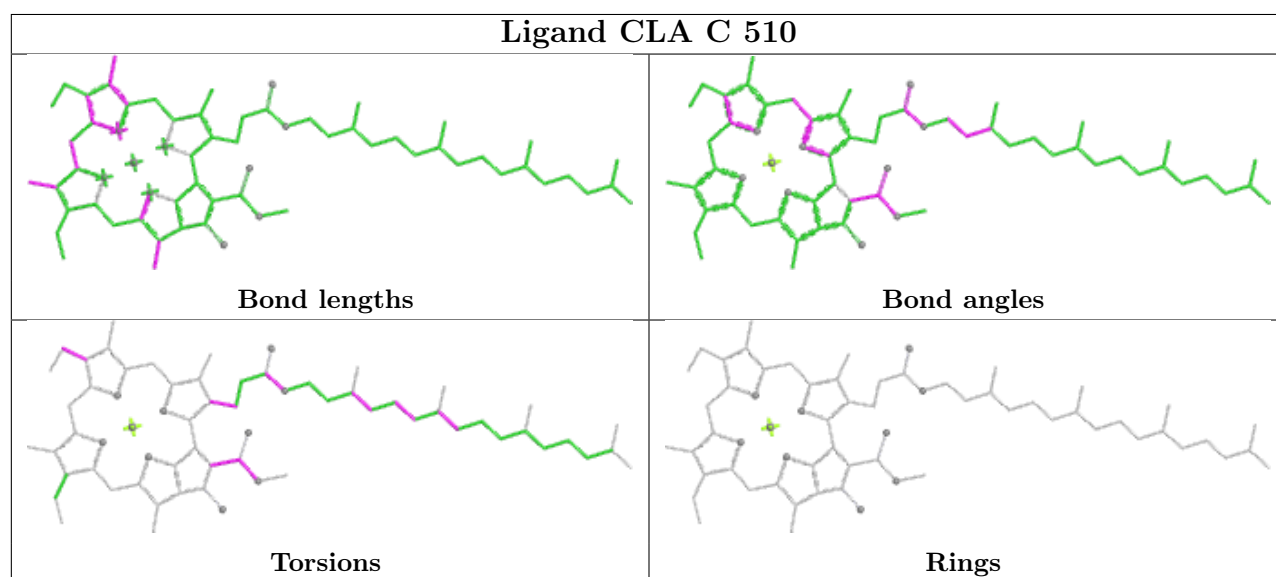
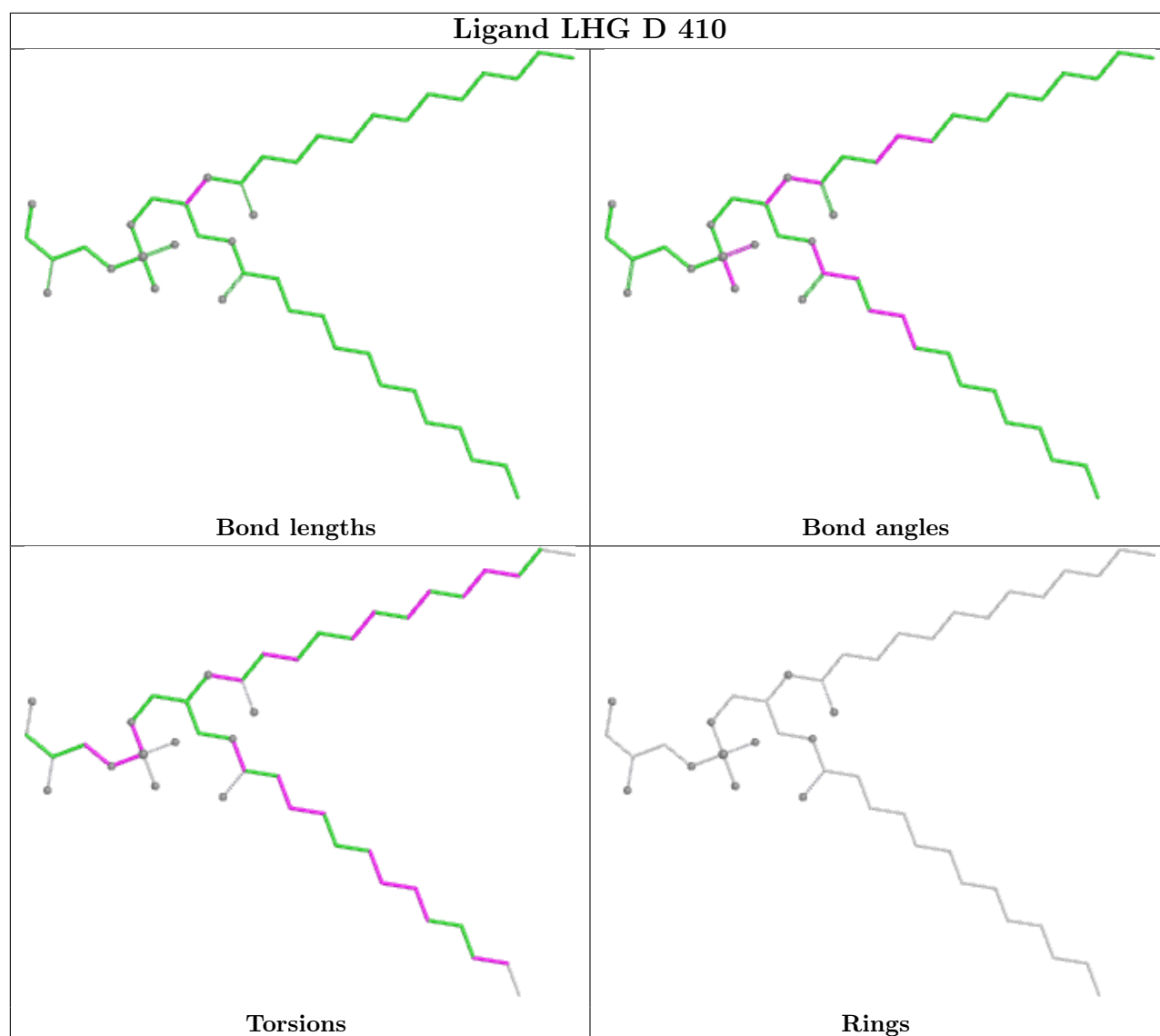
Bond angles

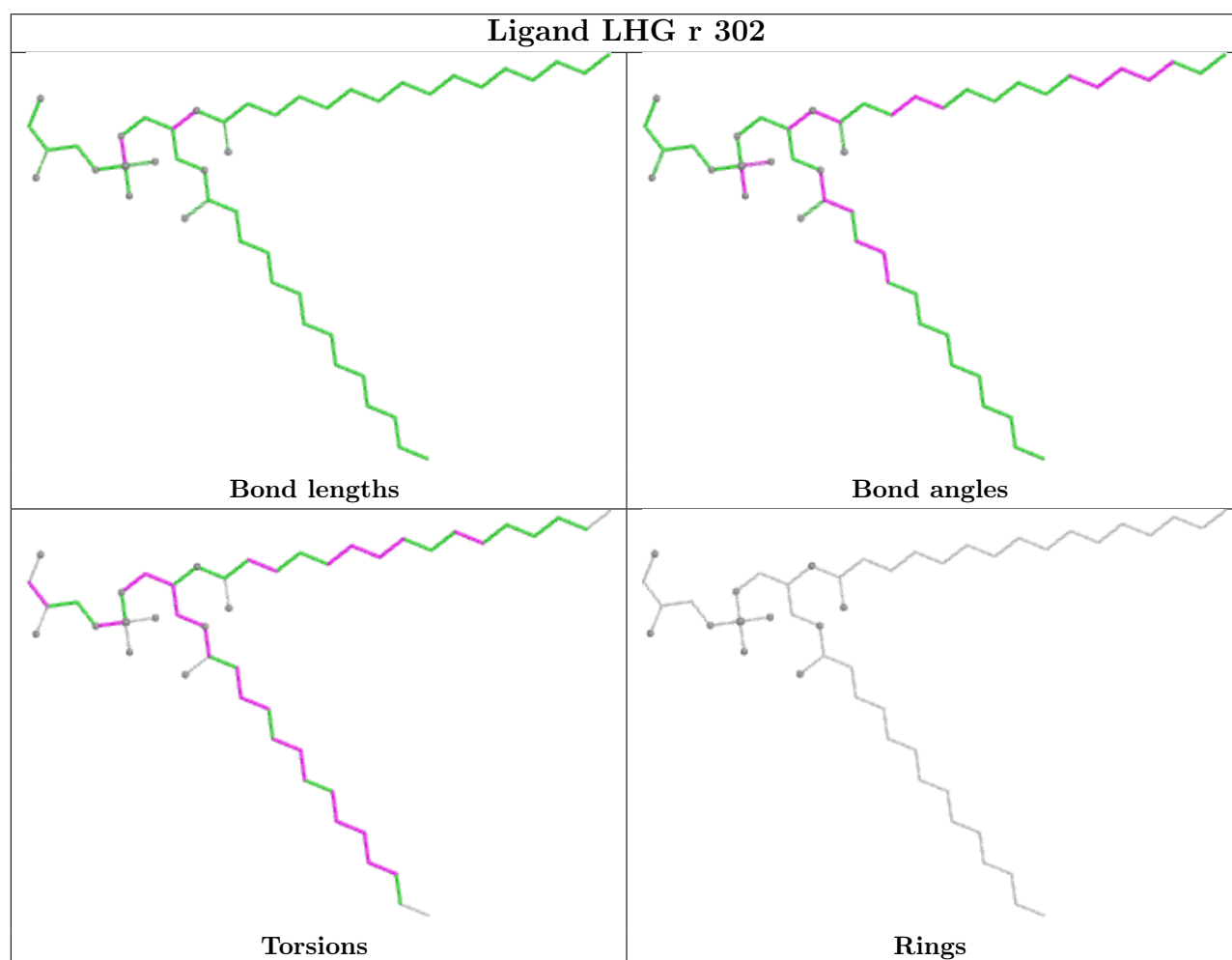
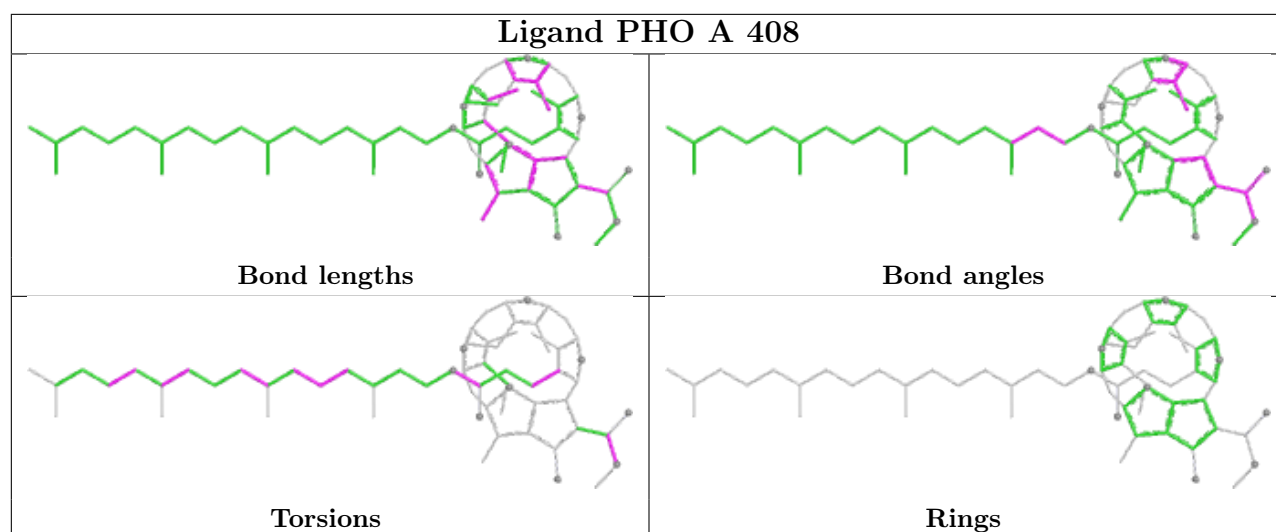


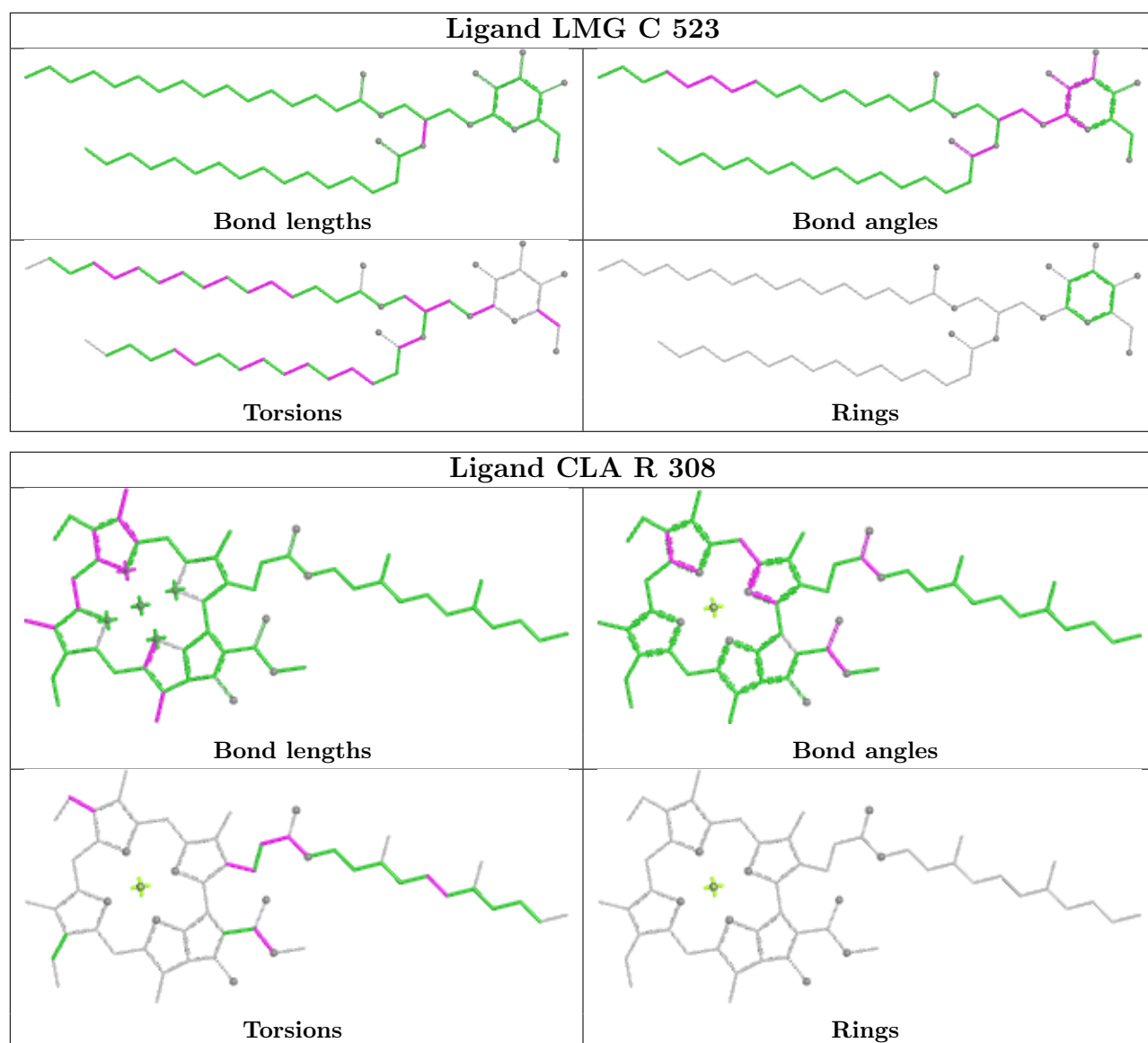
Torsions



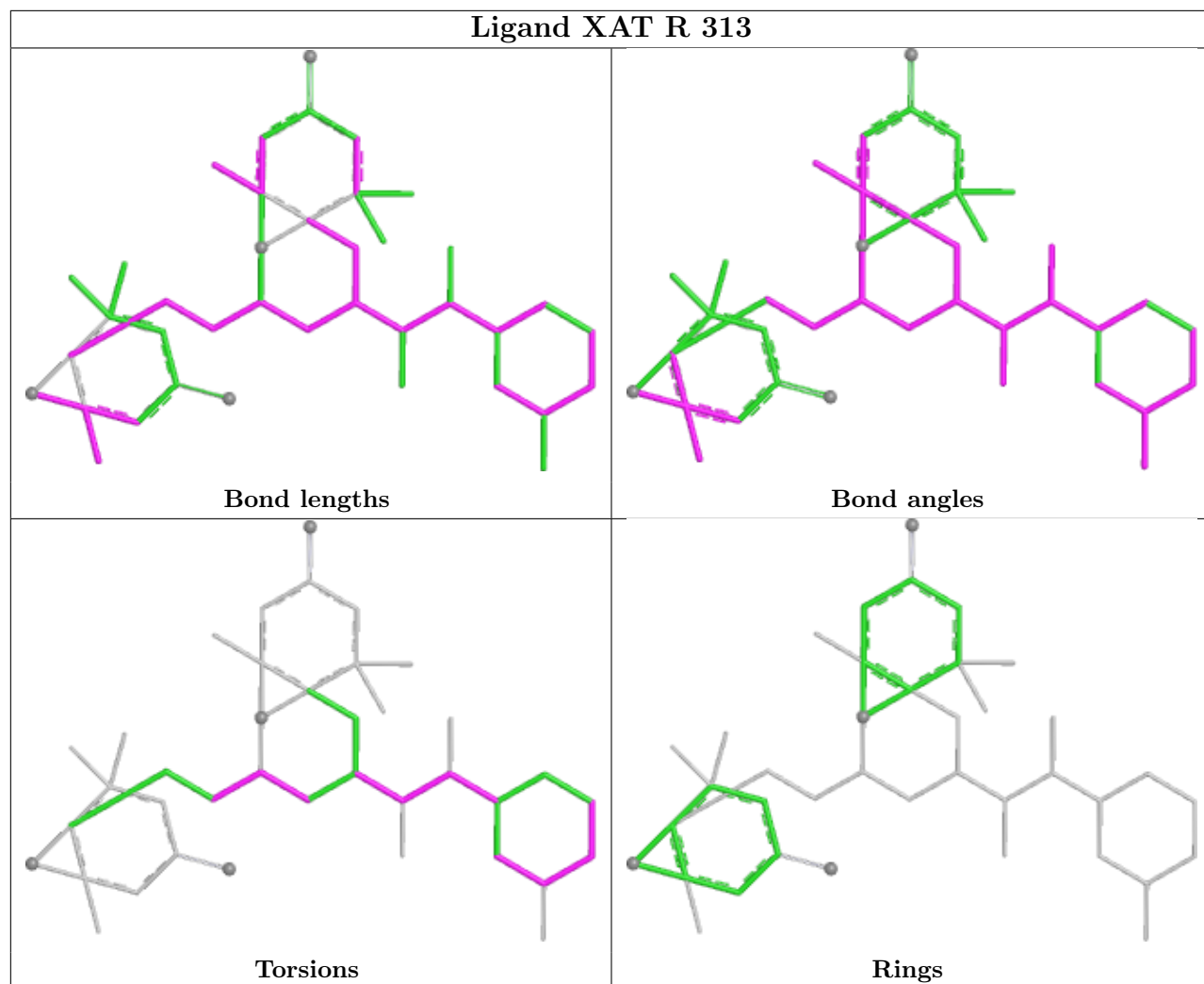
Rings



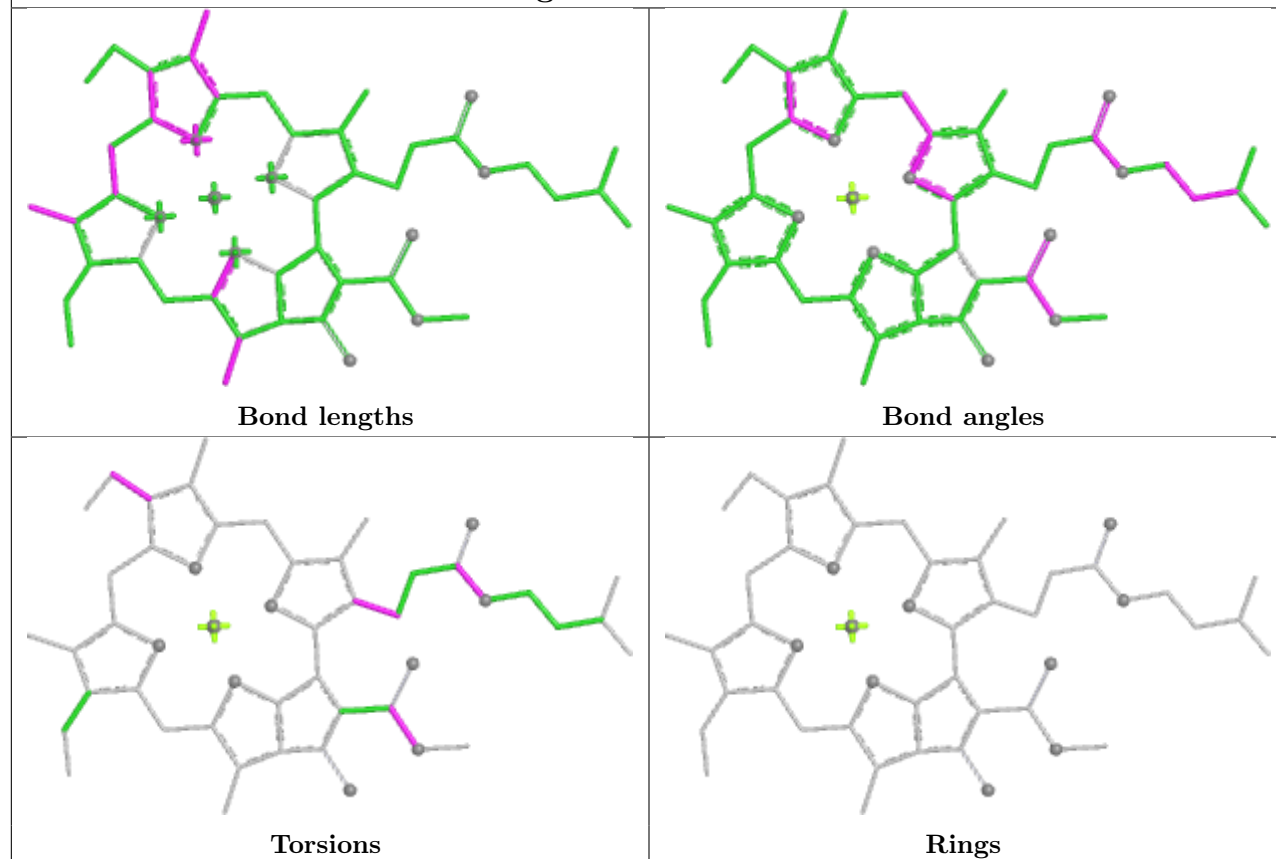




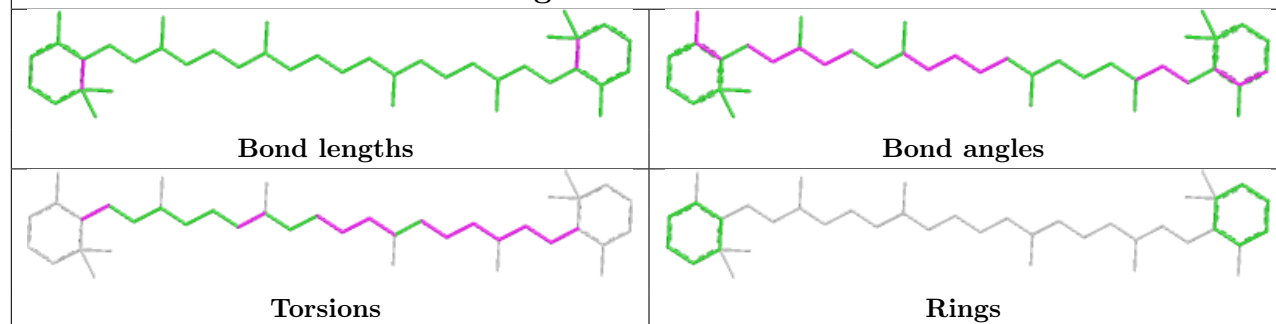
## Ligand XAT R 313



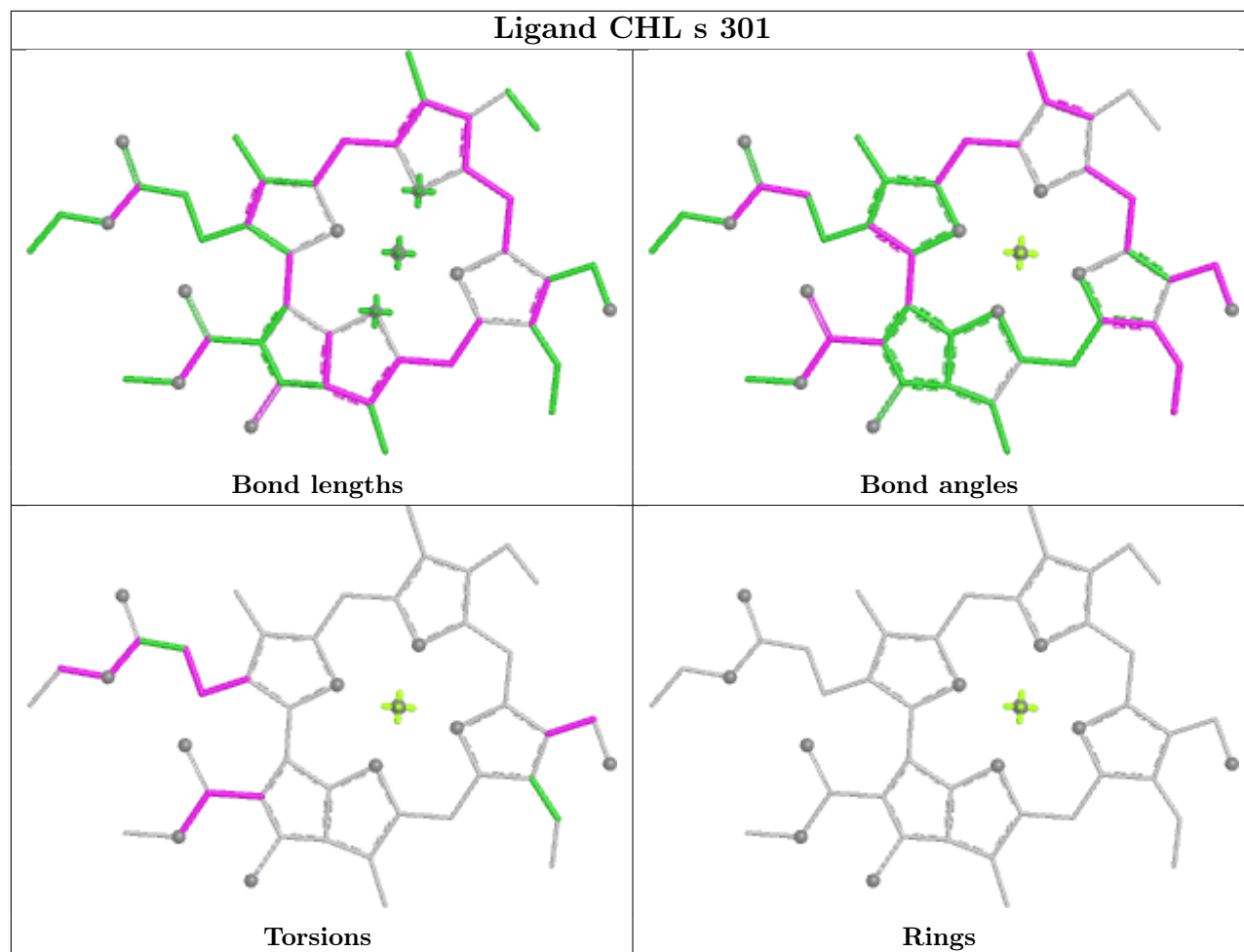
## Ligand CLA a 406



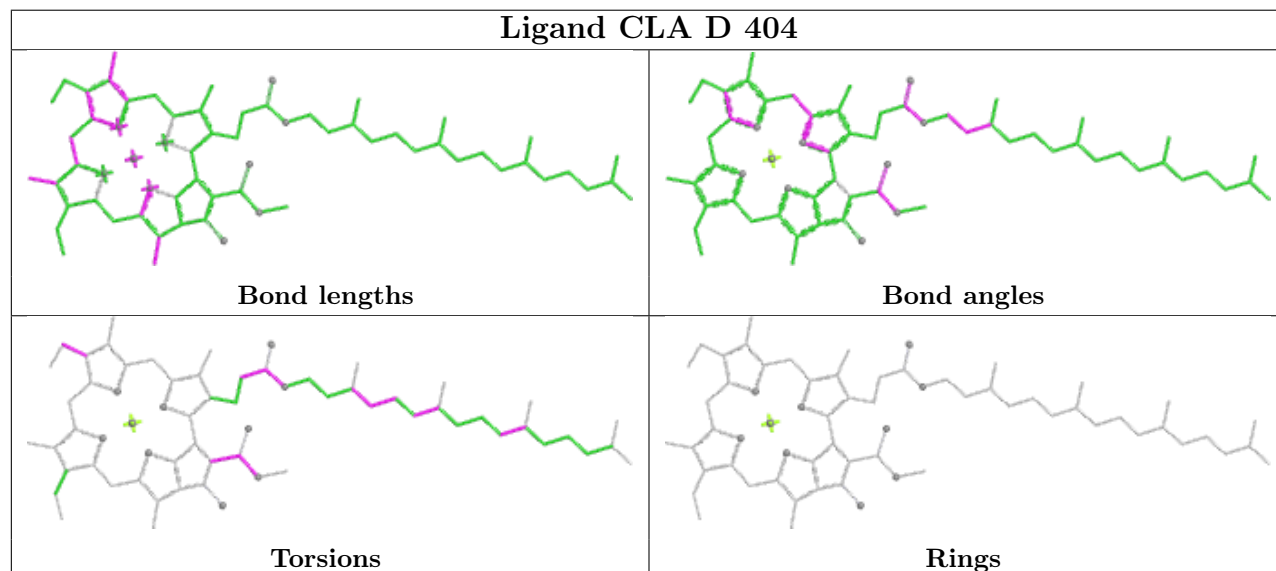
## Ligand BCR k 101

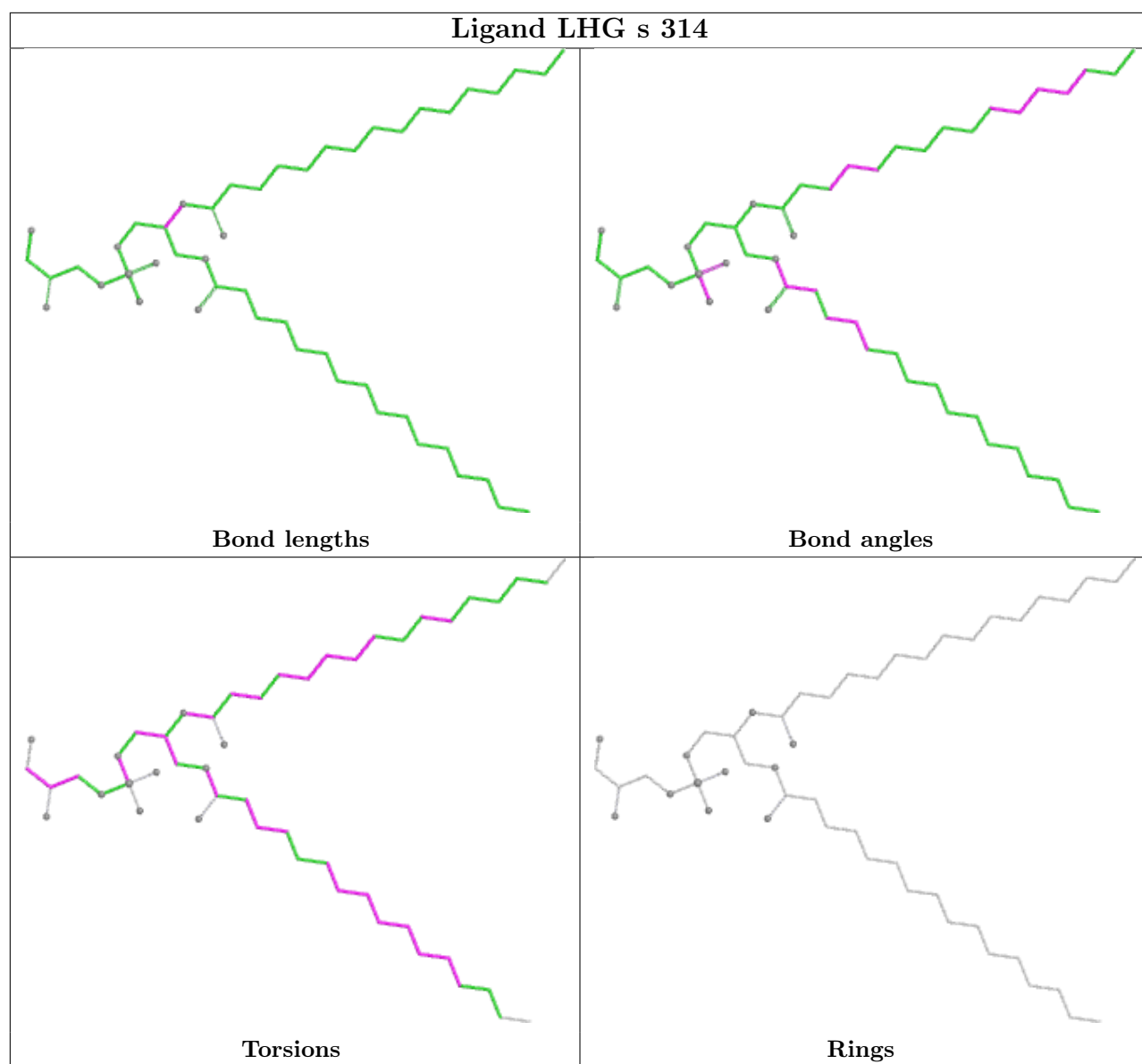


## Ligand CHL s 301

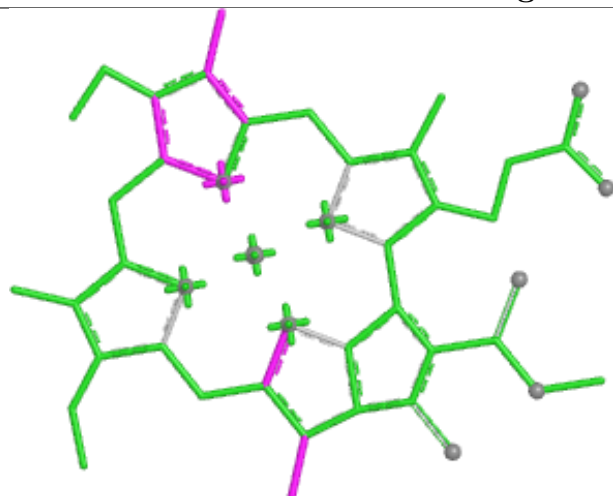


## Ligand CLA D 404

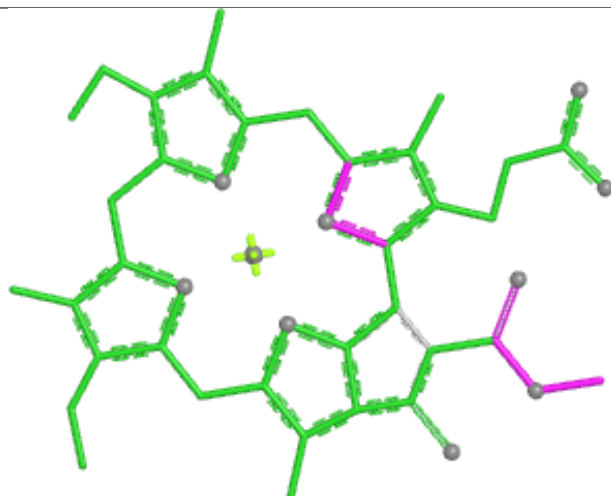




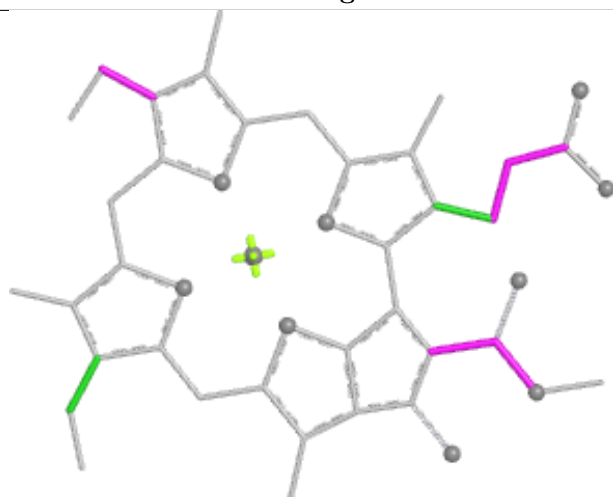
## Ligand CLA S 308



Bond lengths



Bond angles

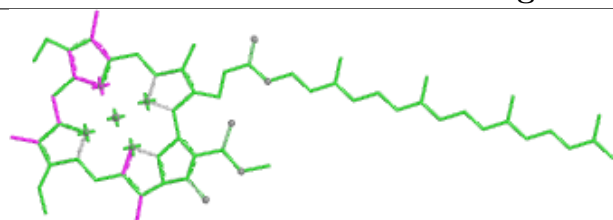


Torsions

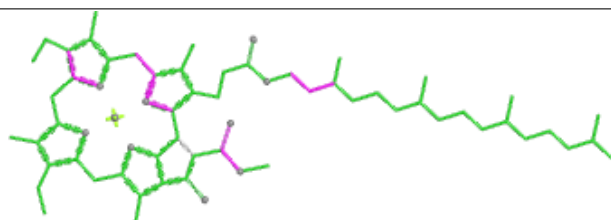


Rings

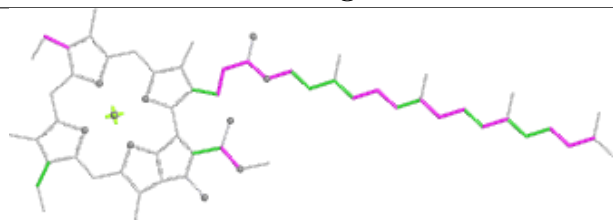
## Ligand CLA b 601



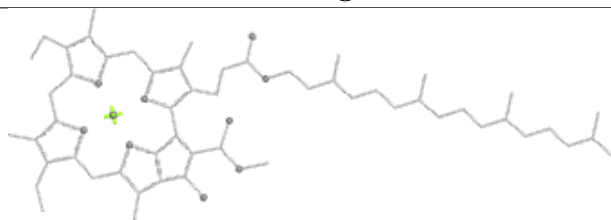
Bond lengths



Bond angles

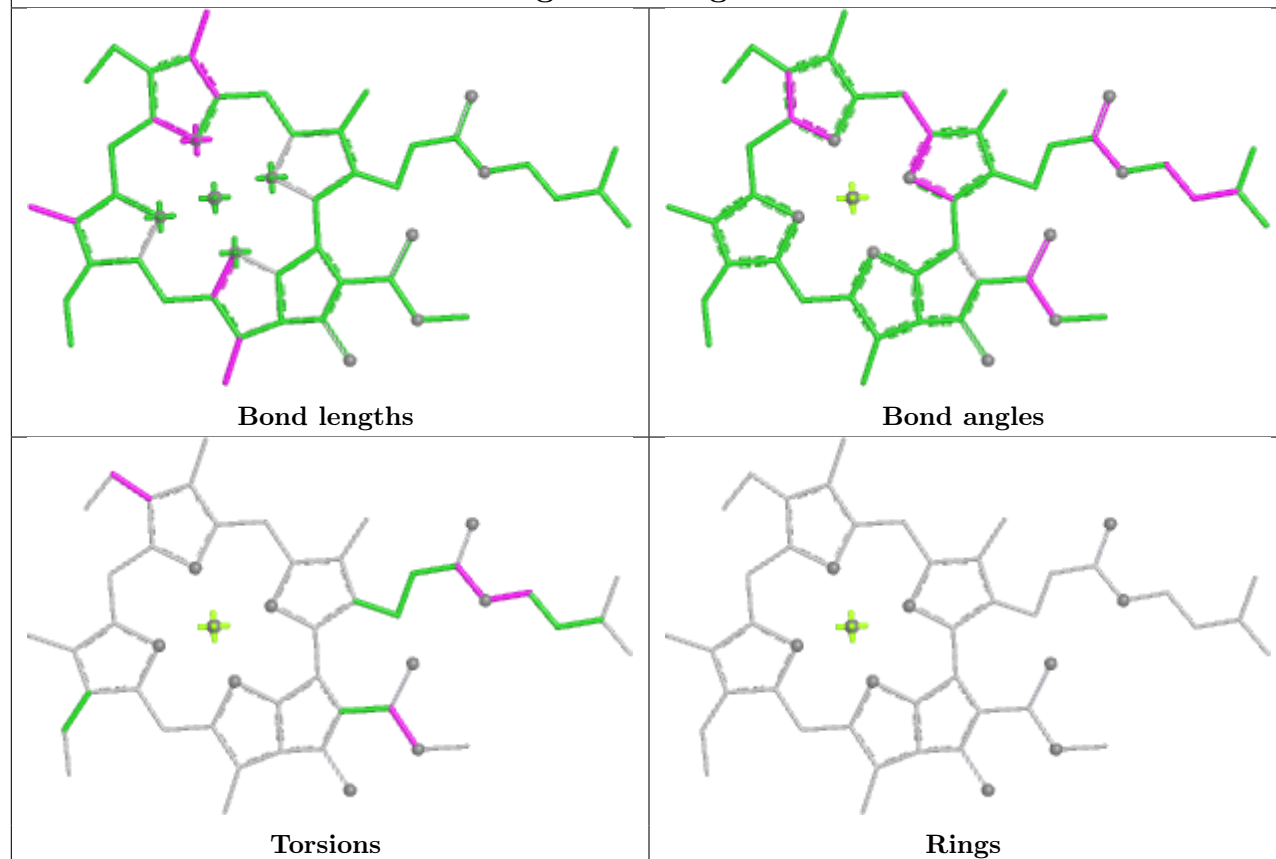


Torsions

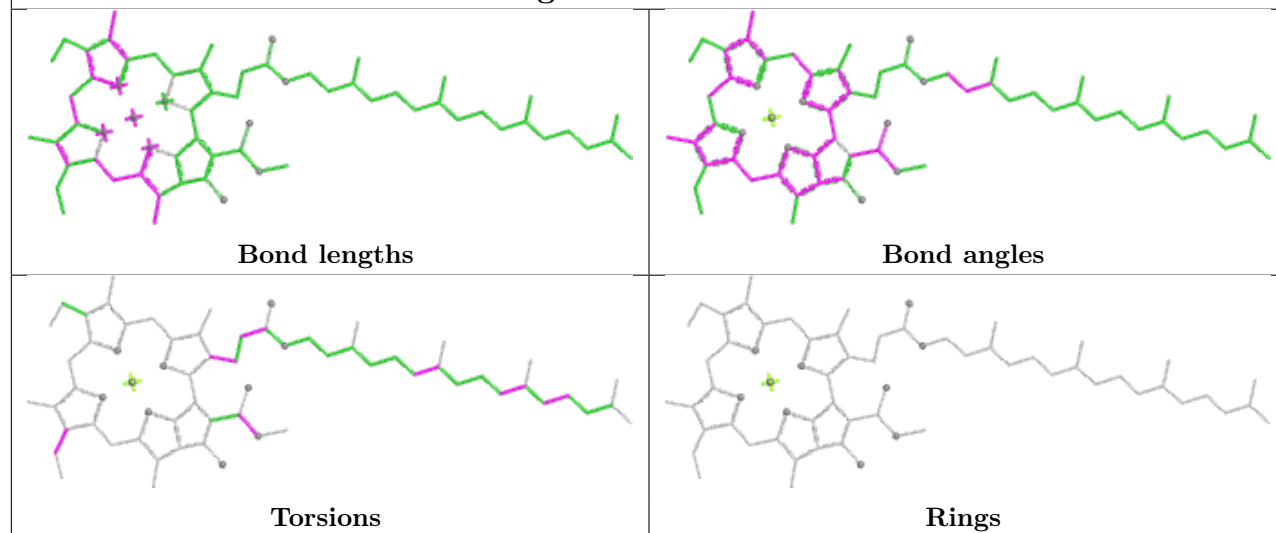


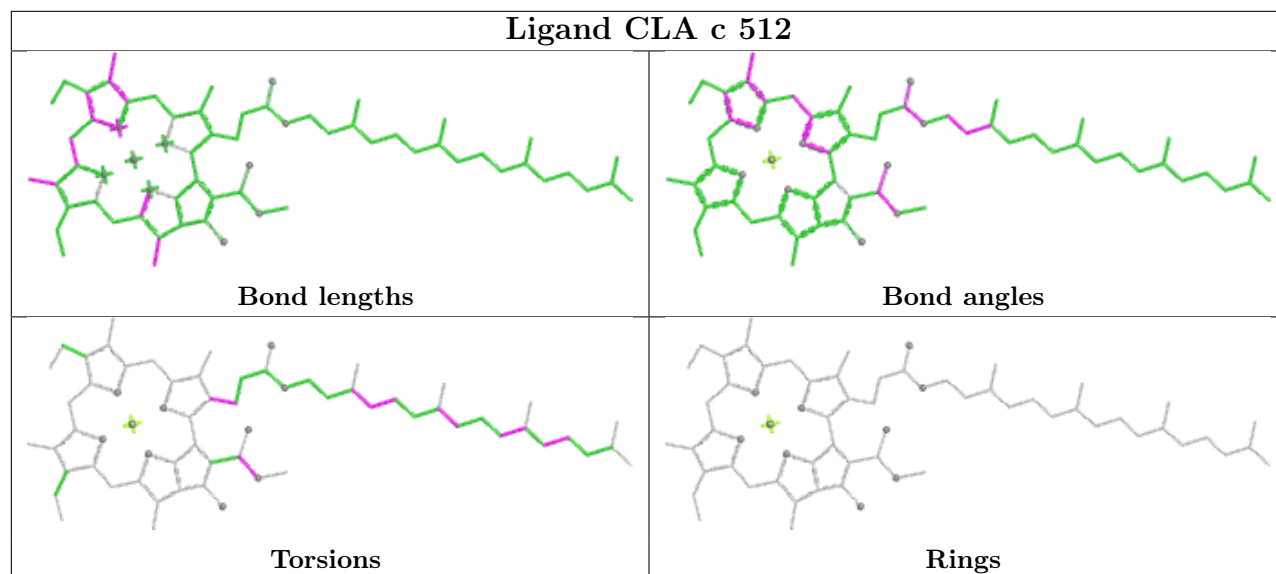
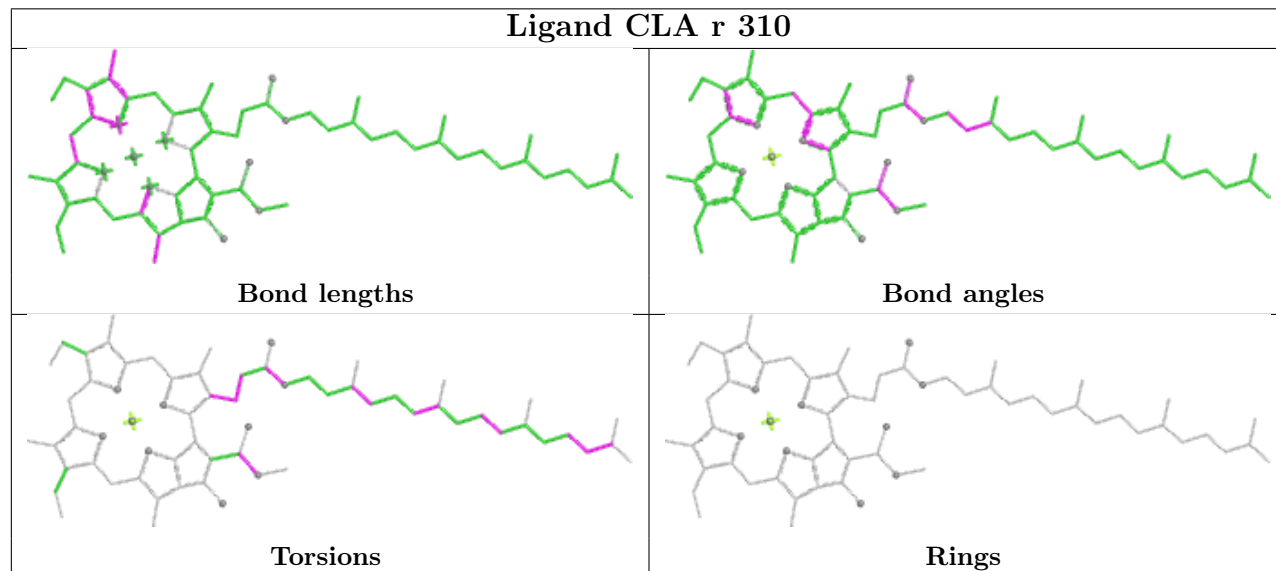
Rings

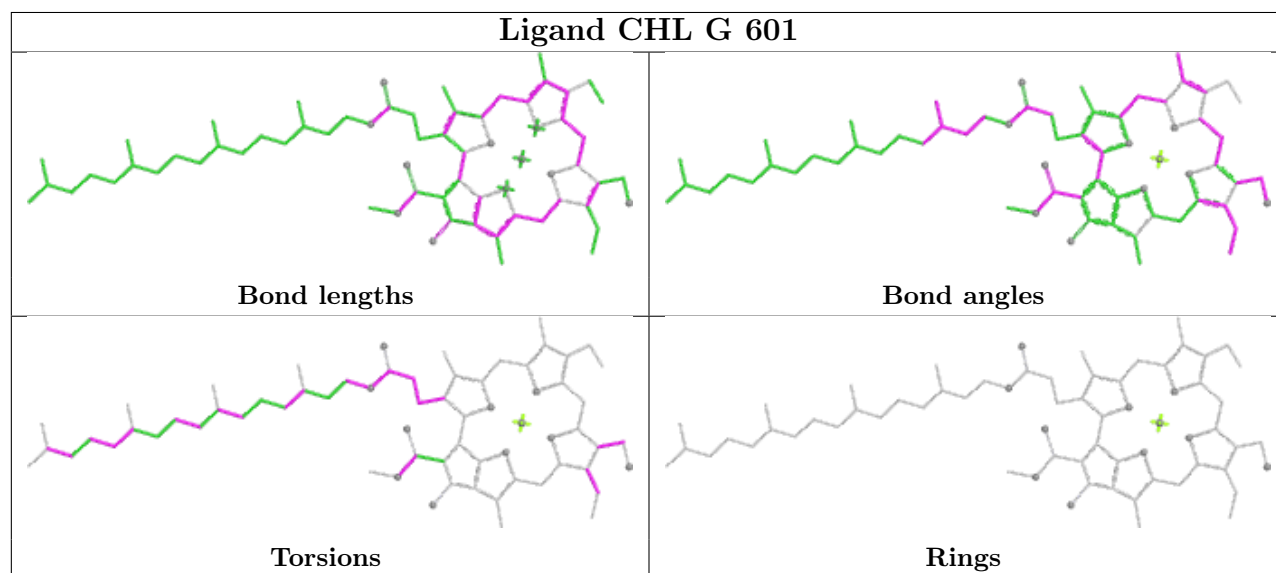
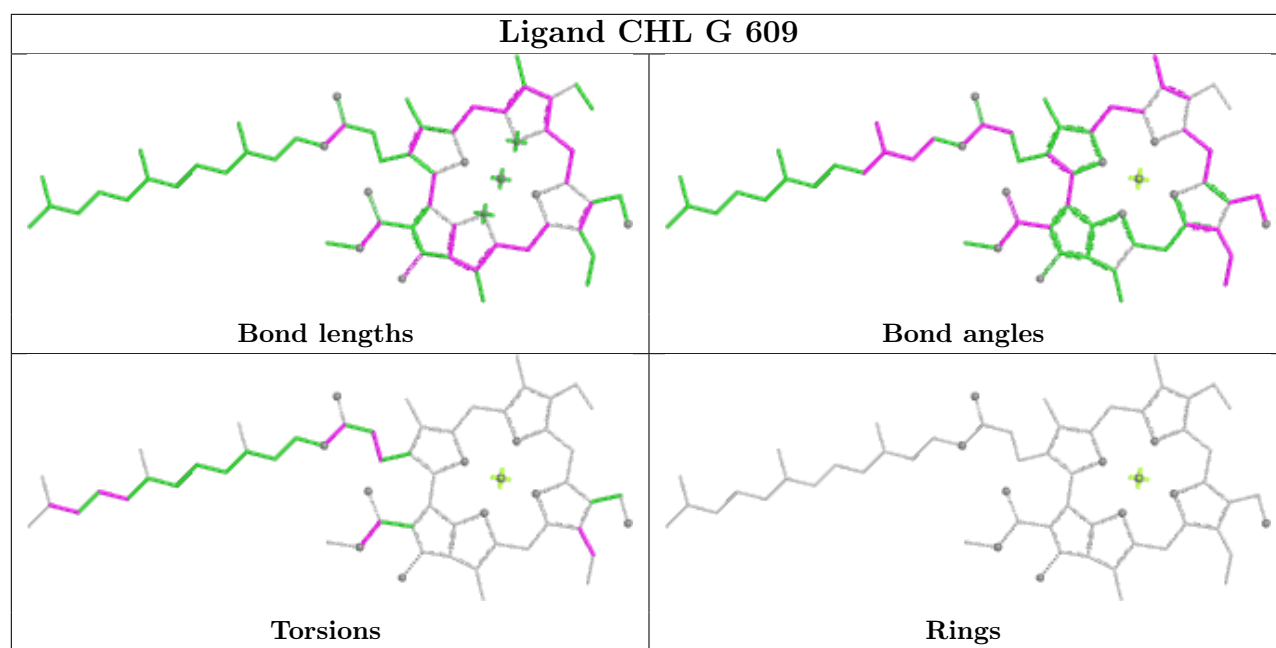
## Ligand CLA g 604

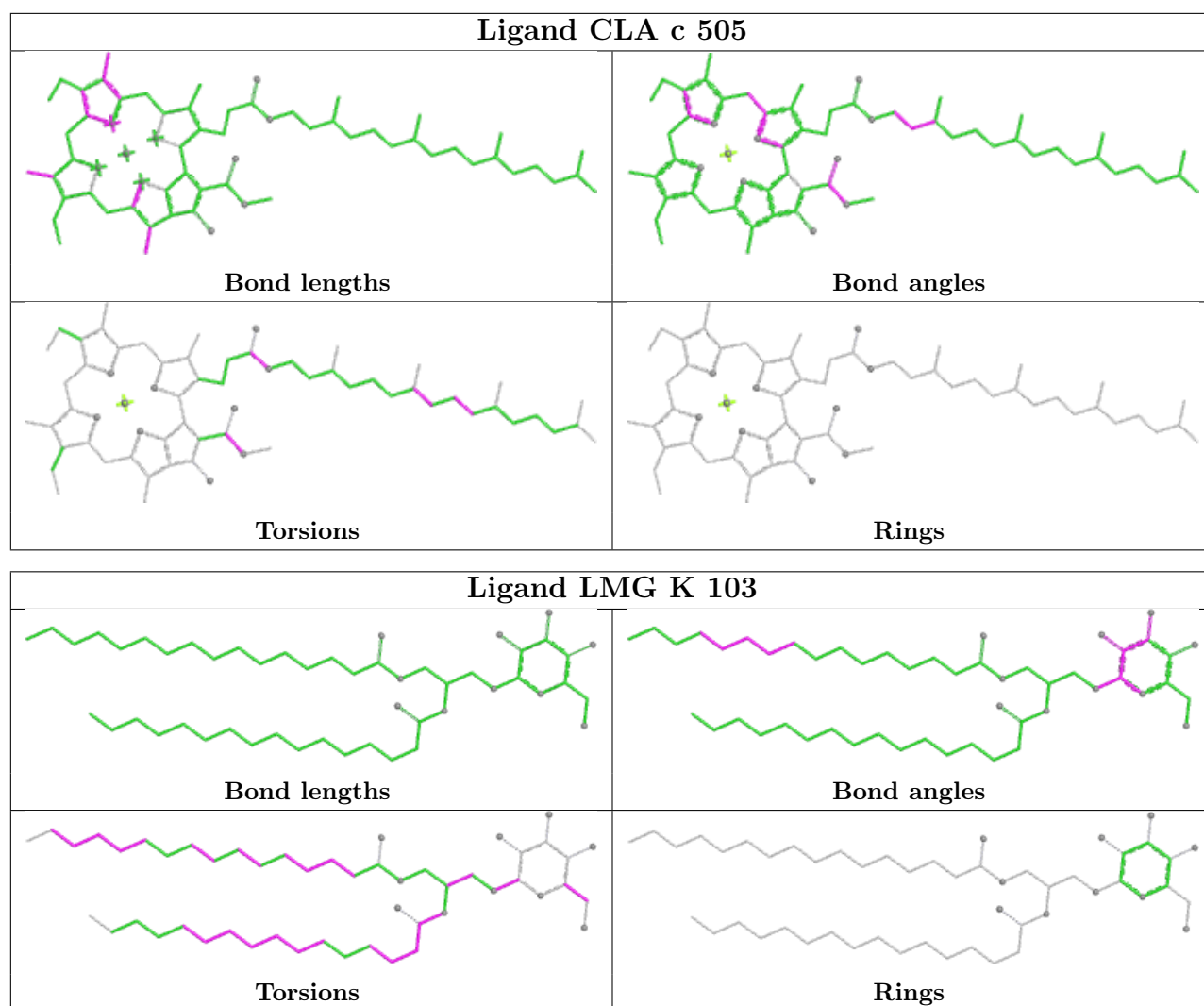


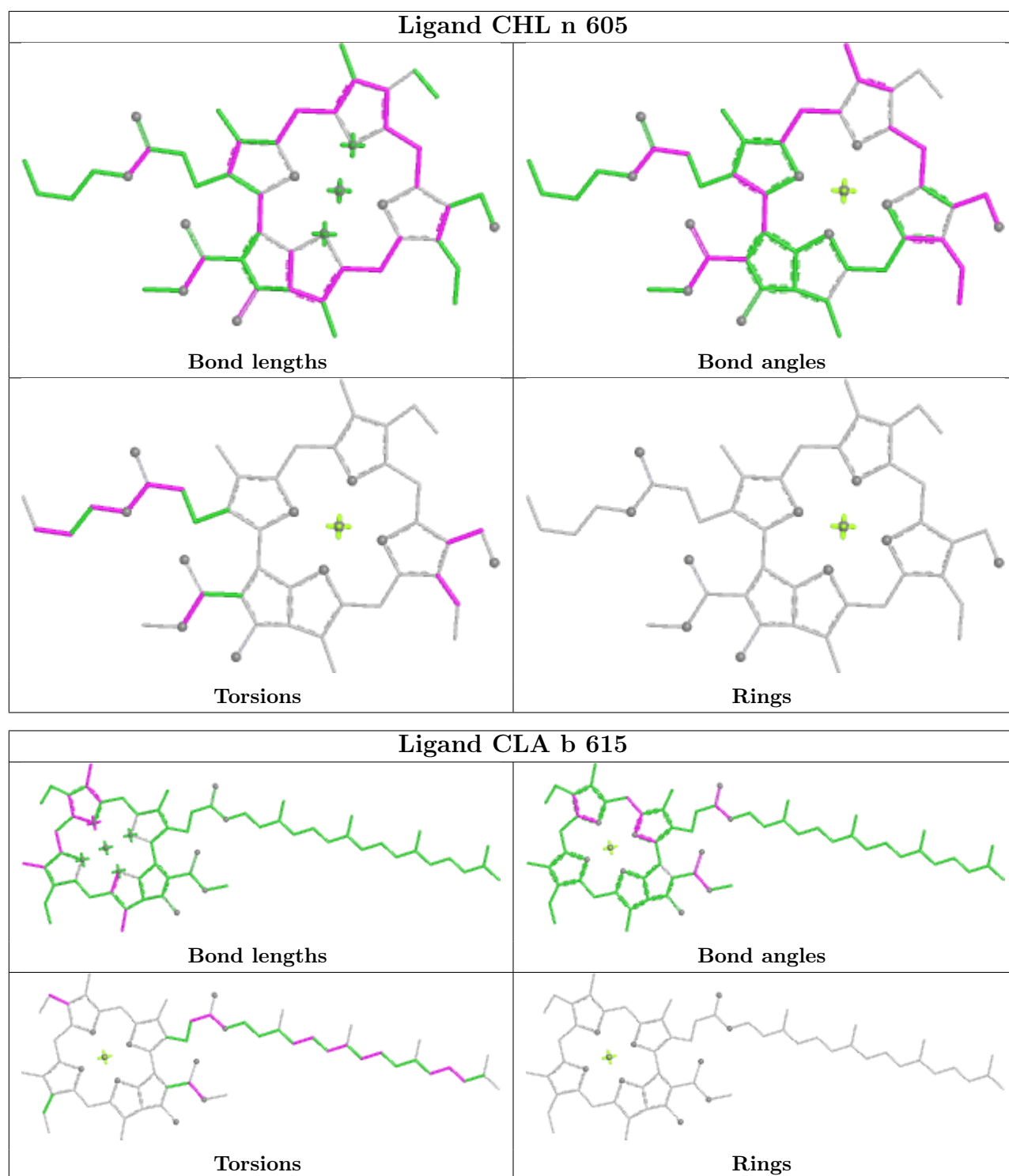
## Ligand CLA c 510



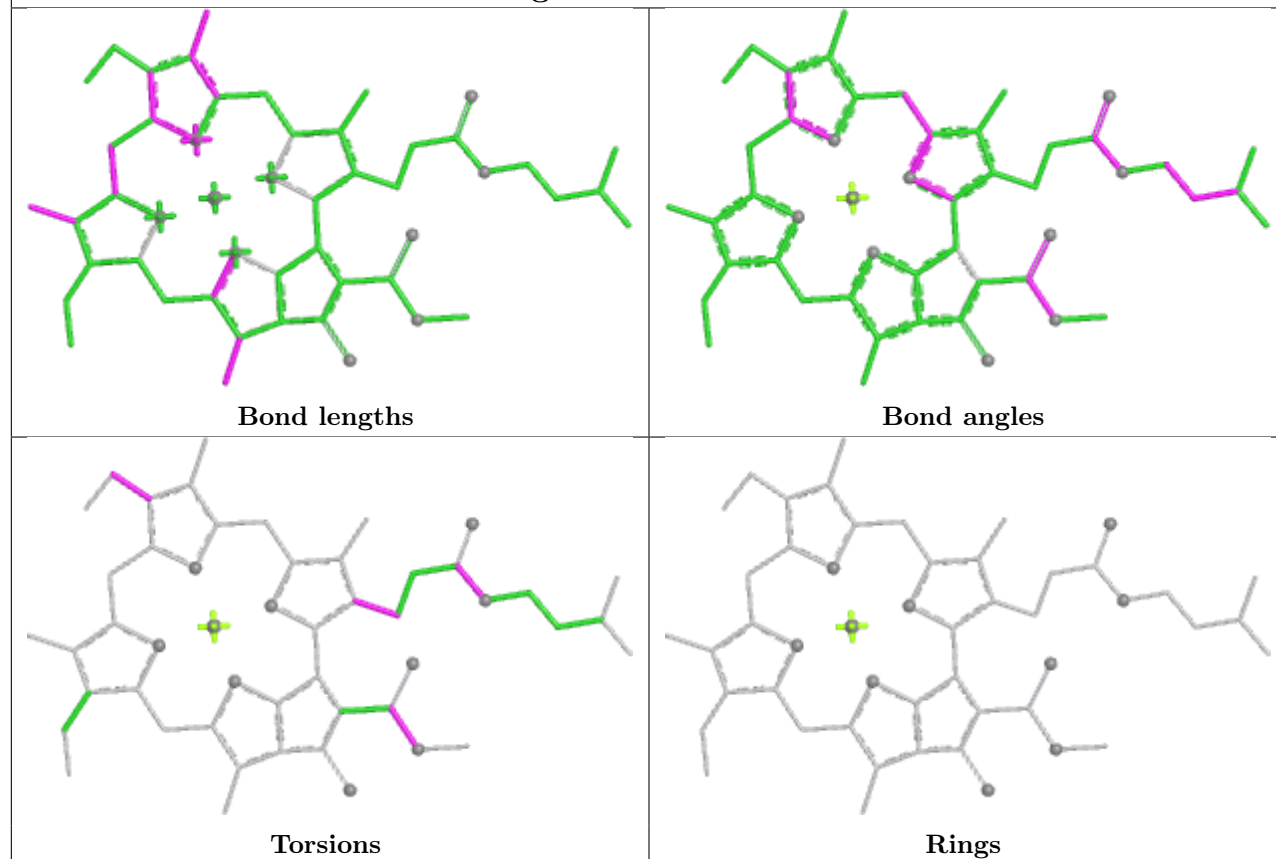
**Ligand CLA c 512****Ligand CLA r 310**



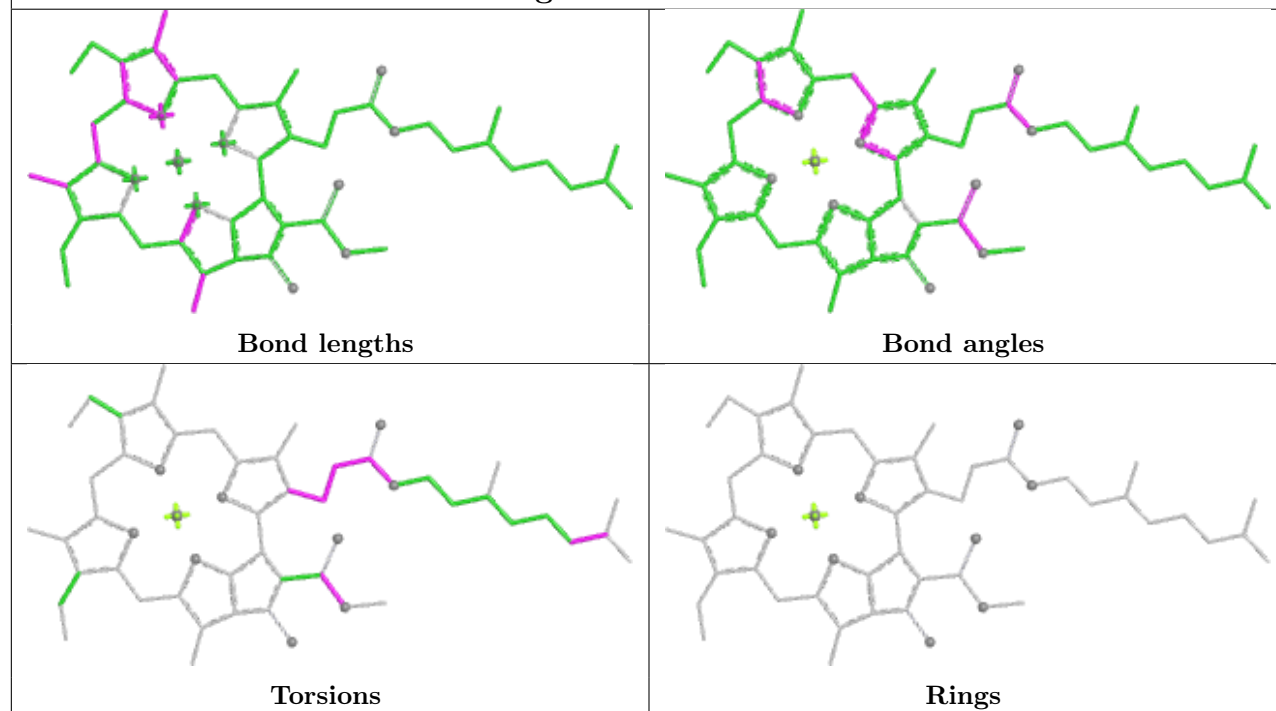


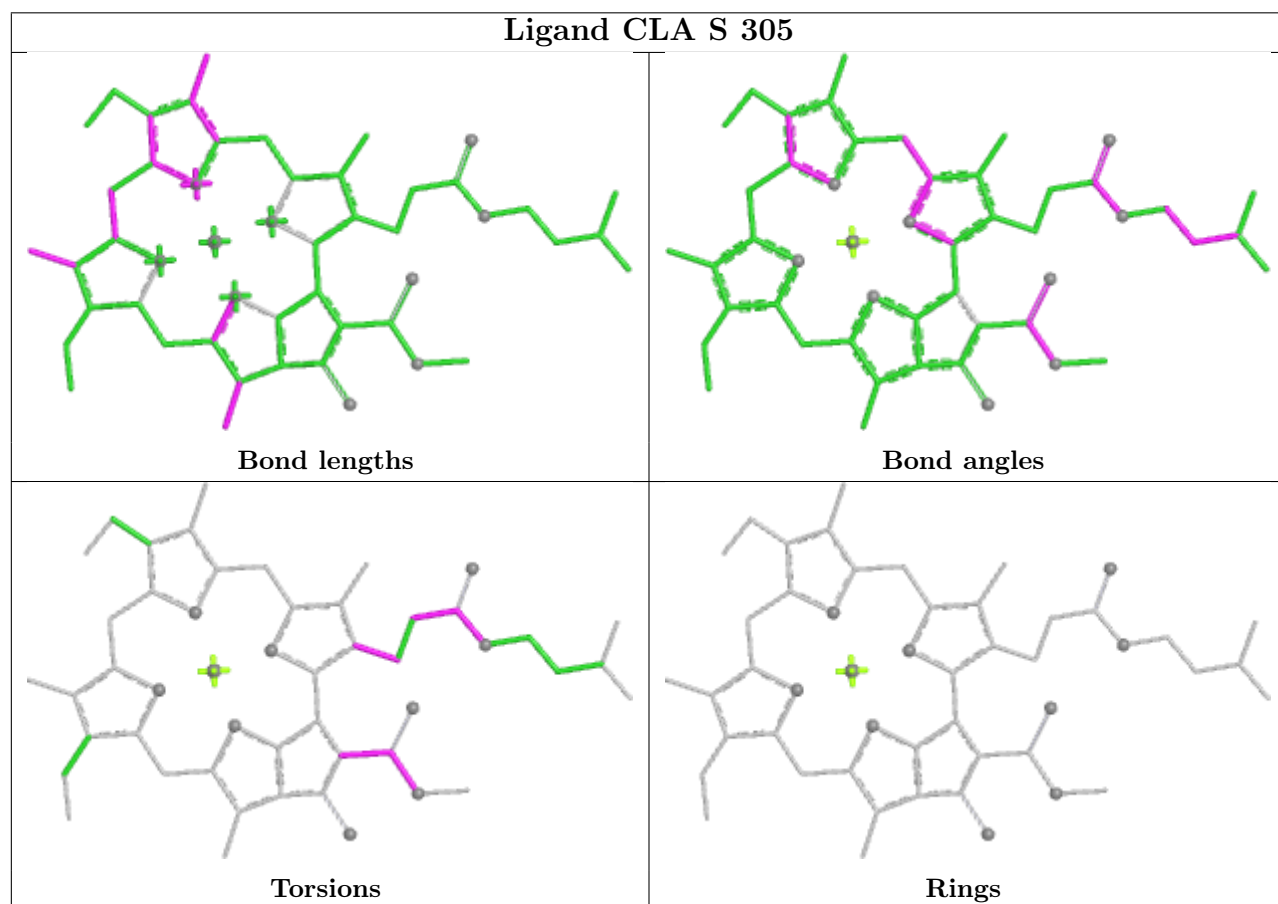
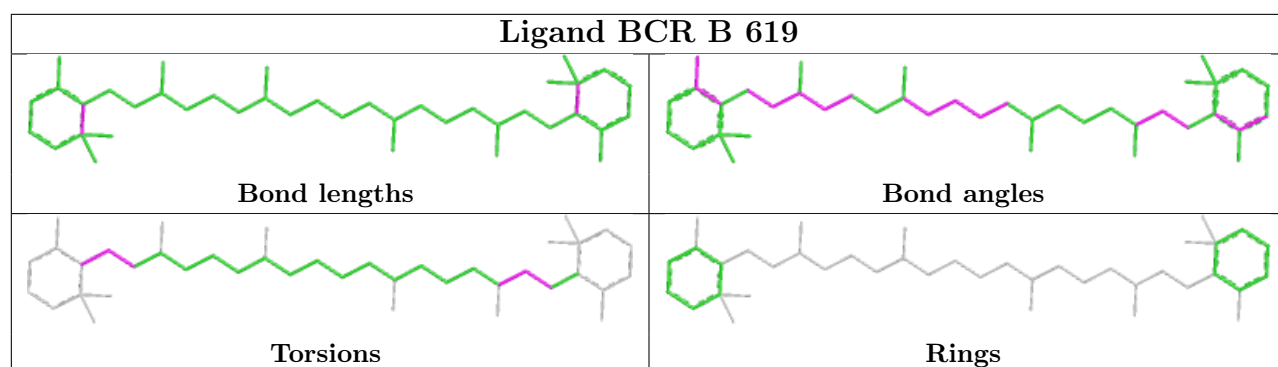


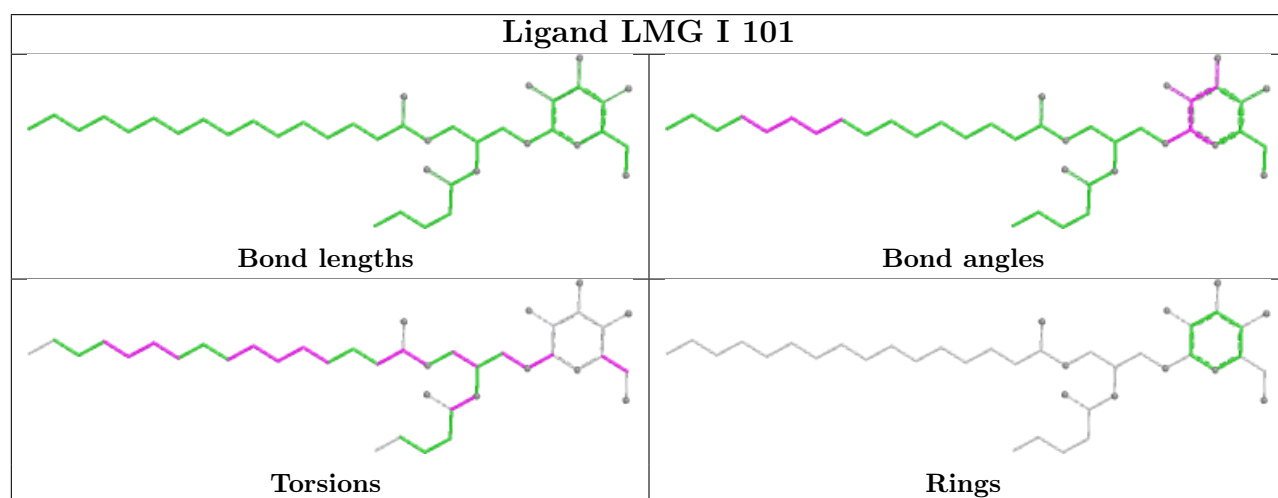
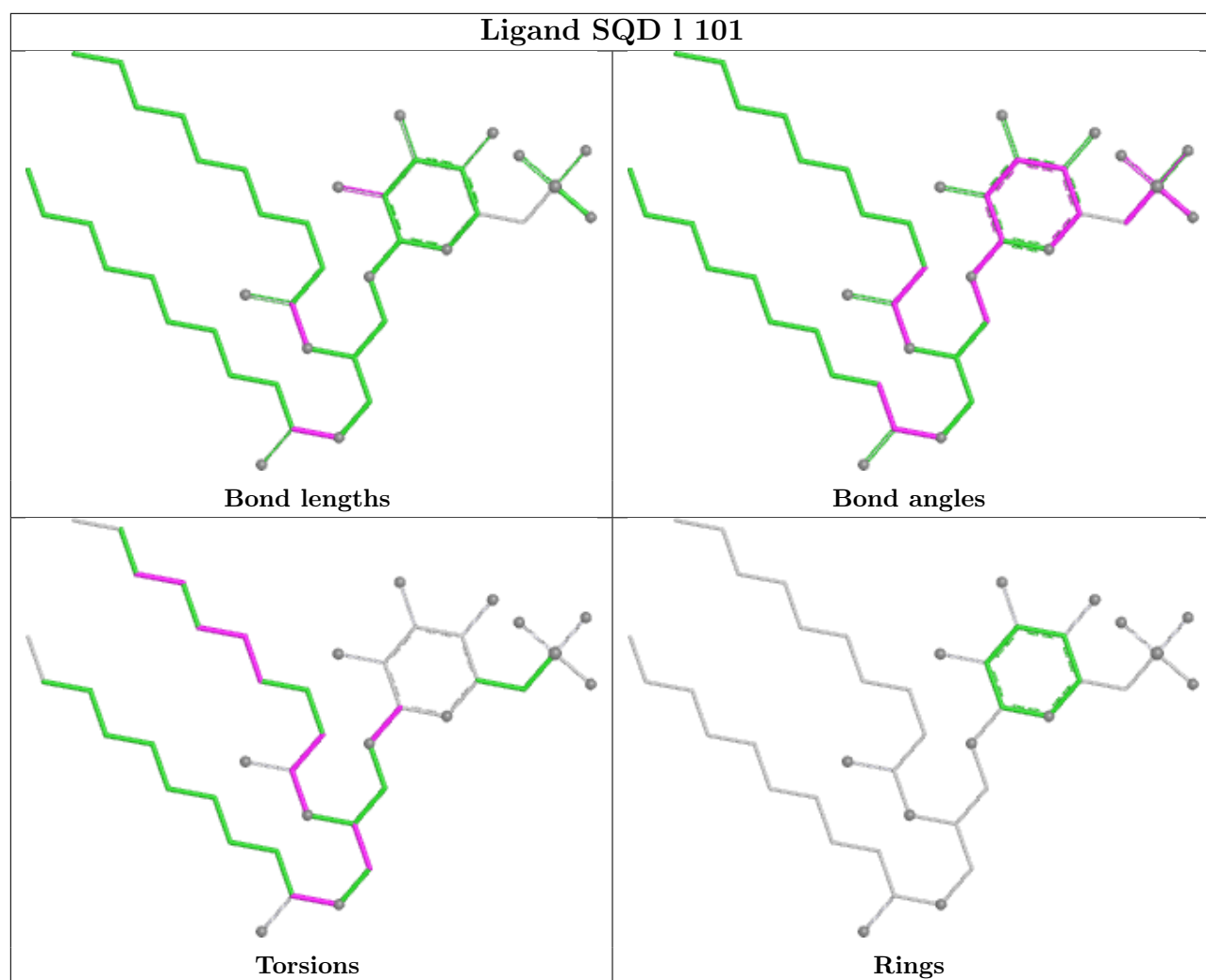
## Ligand CLA A 407

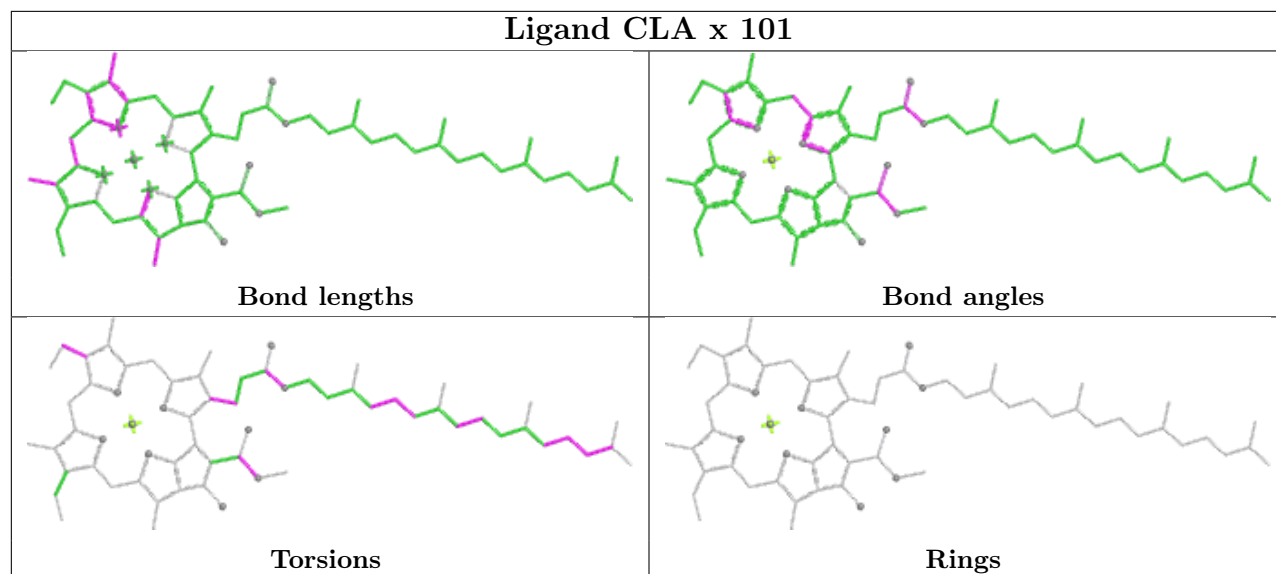
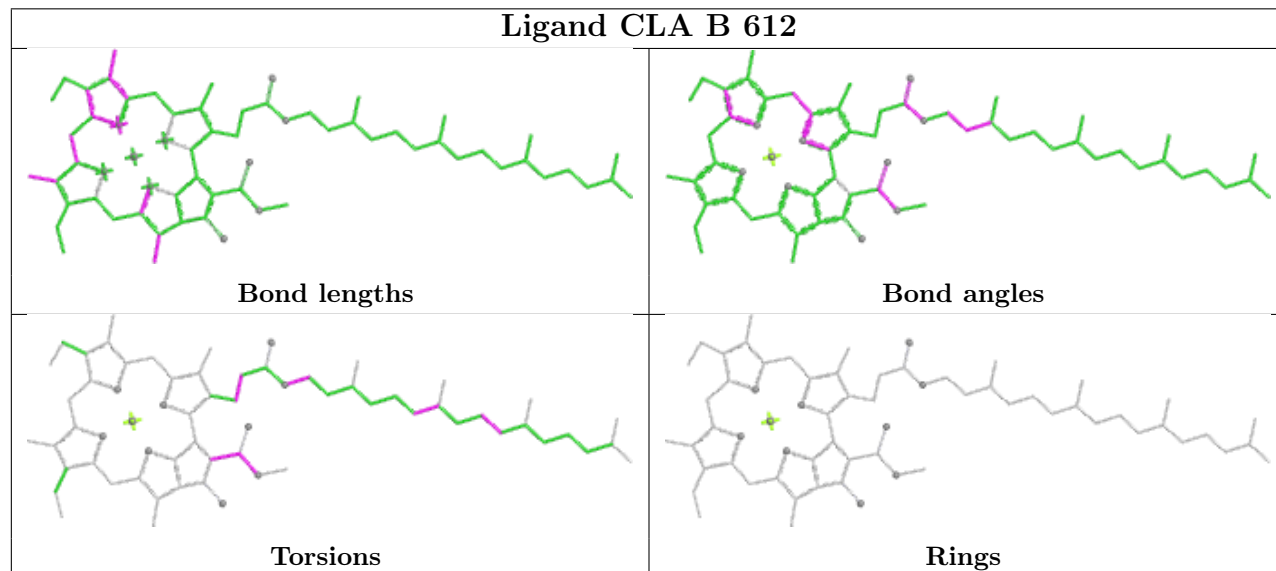


## Ligand CLA S 313

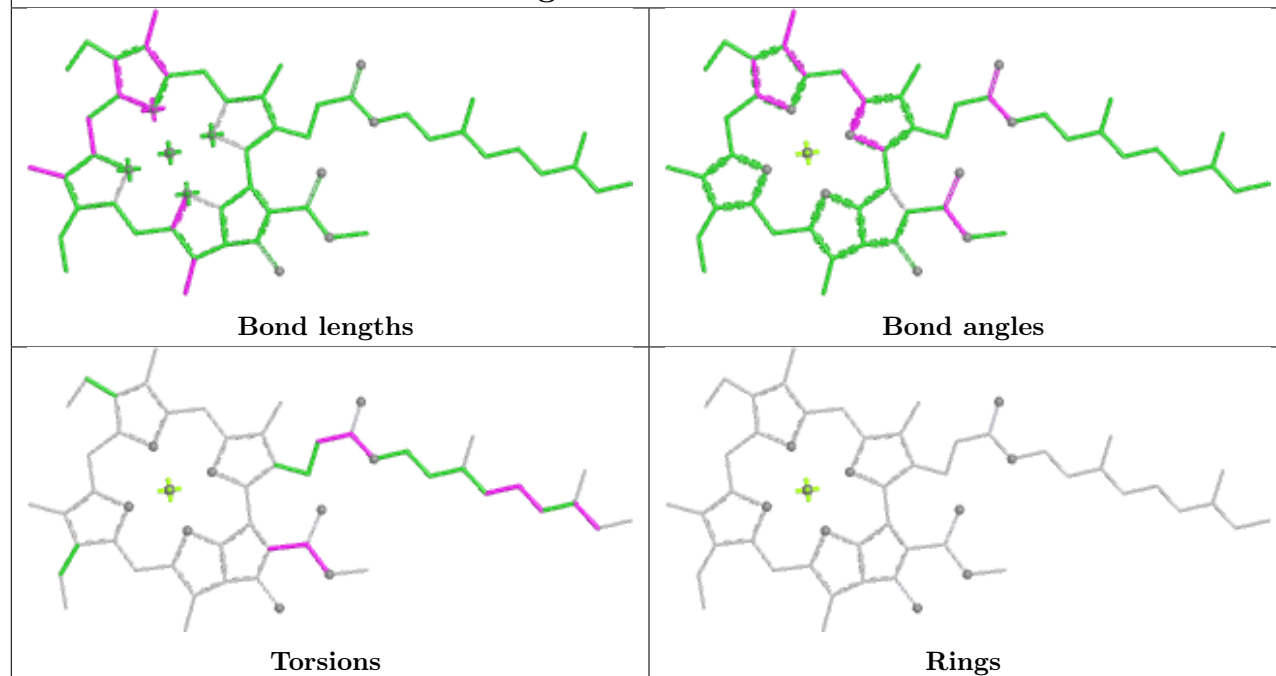




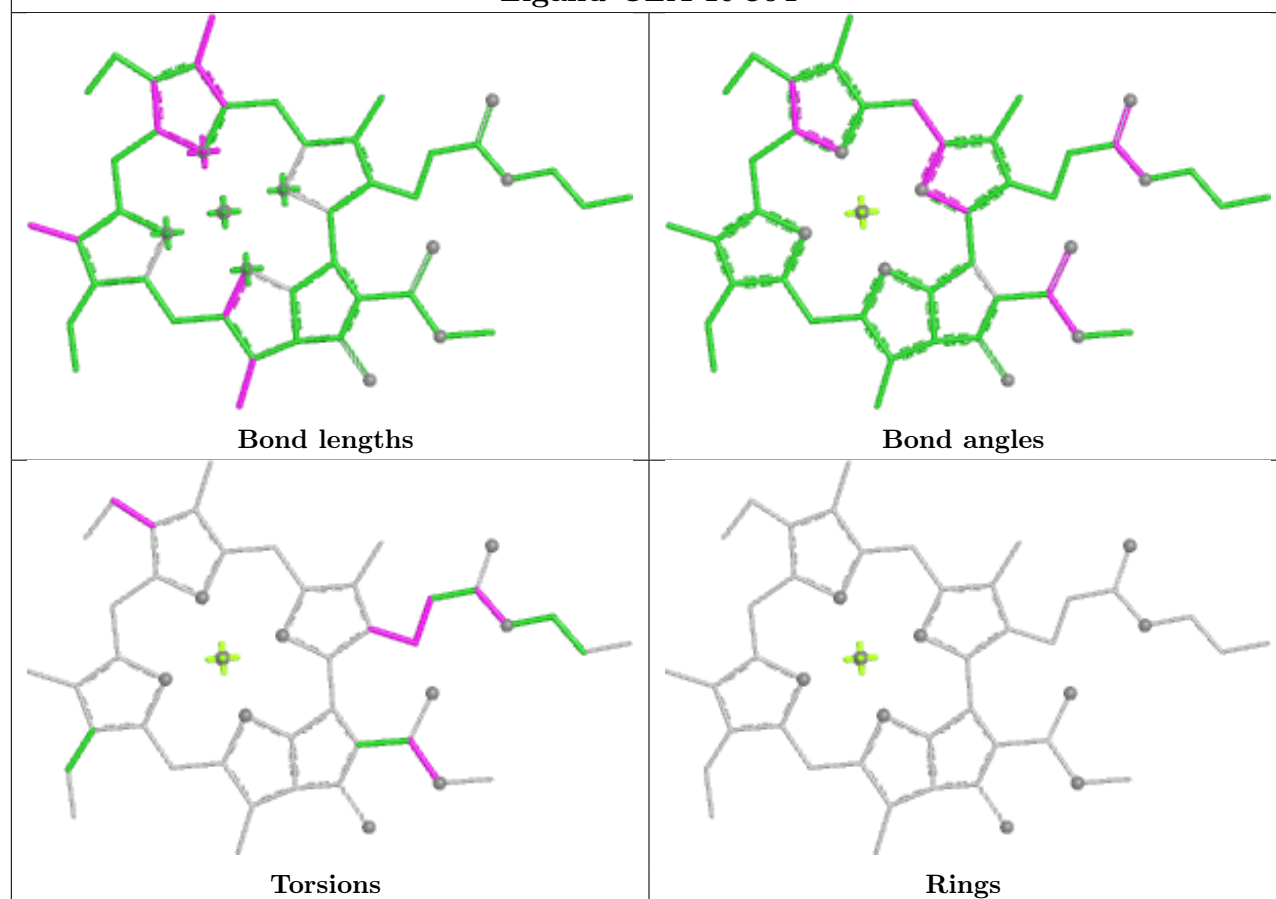


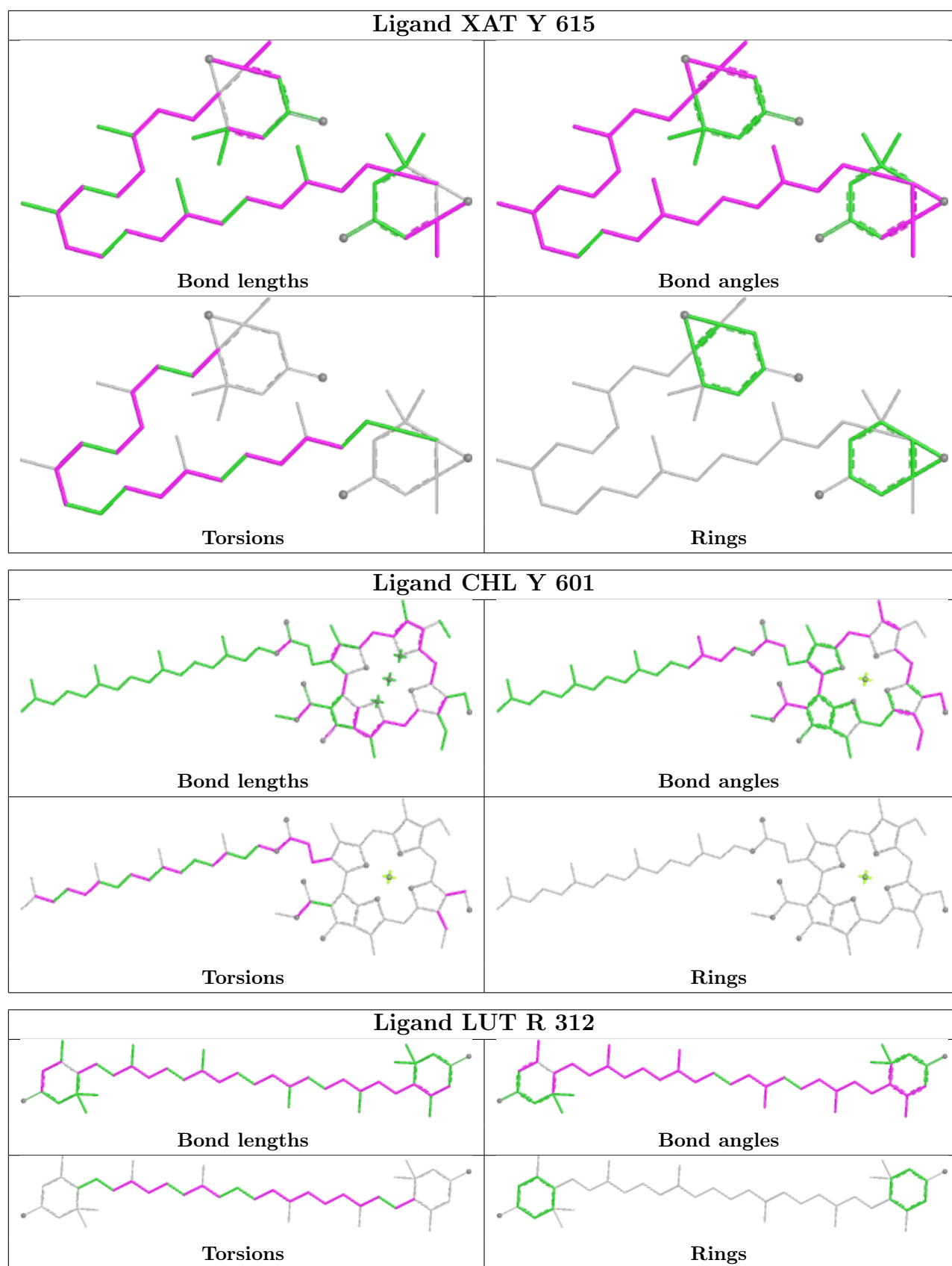
**Ligand CLA x 101****Ligand CLA B 612**

## Ligand CLA s 311

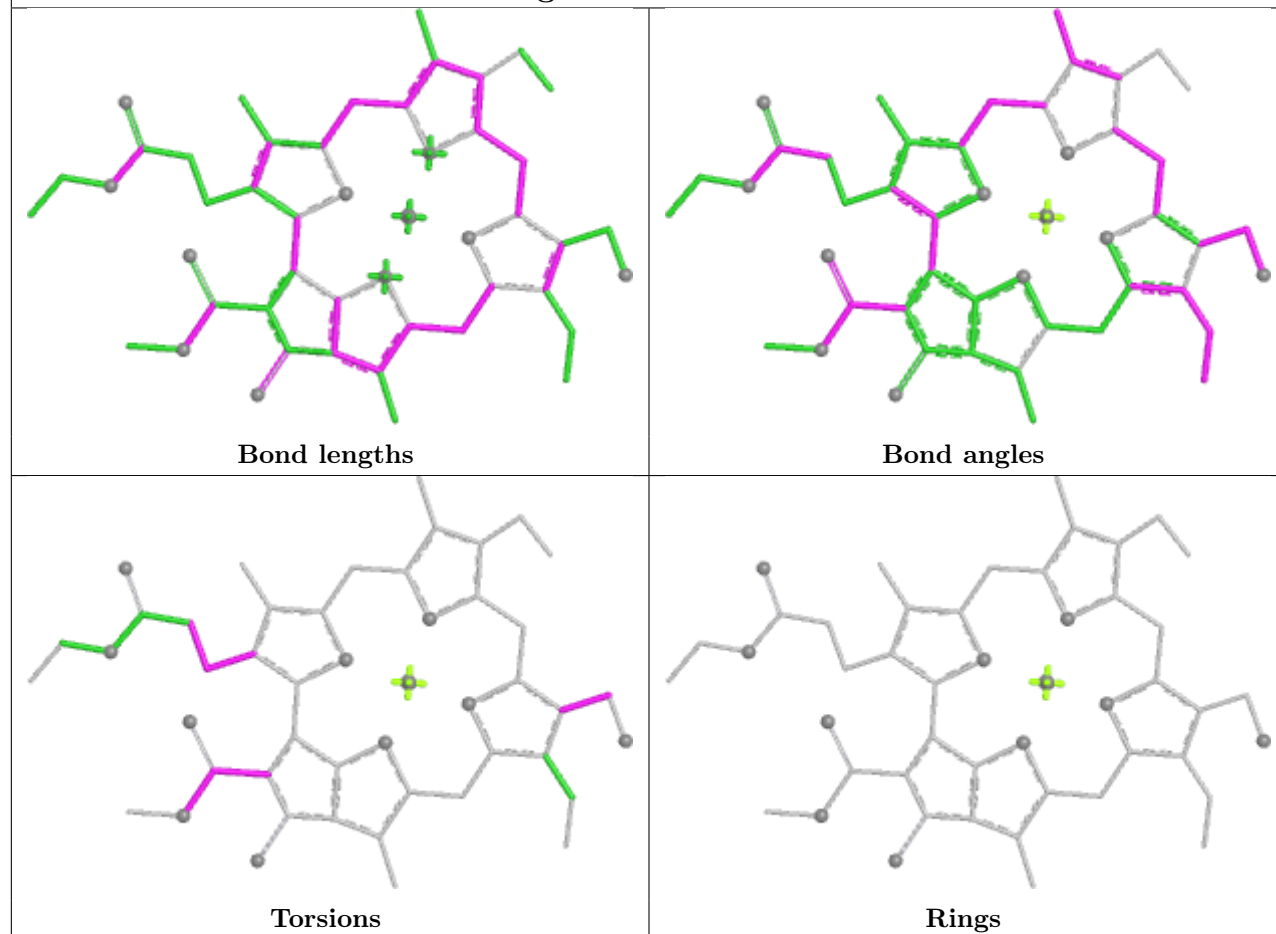


## Ligand CLA R 304

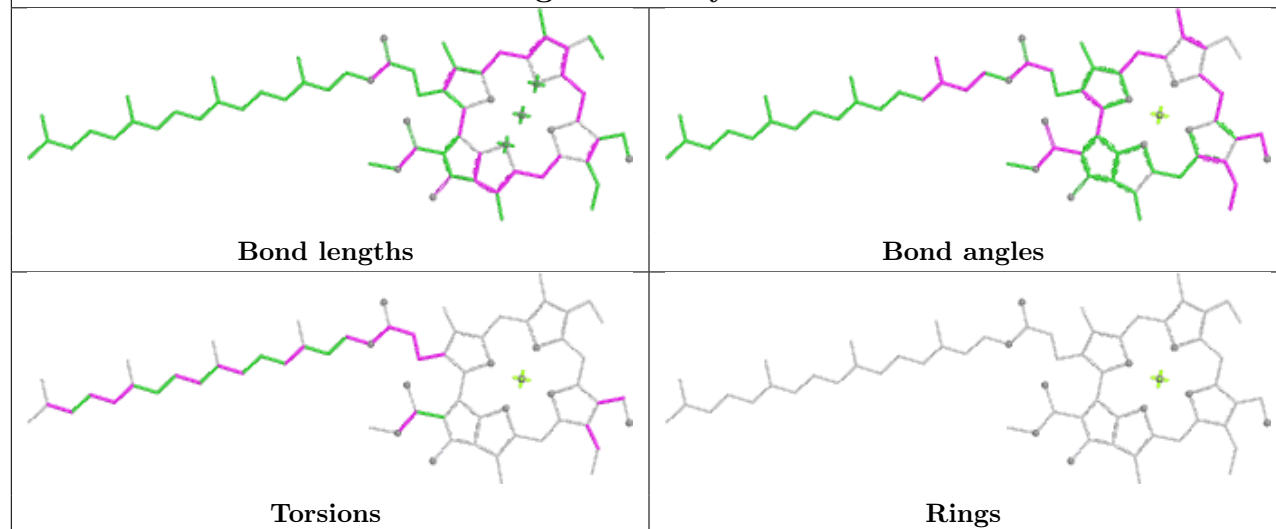


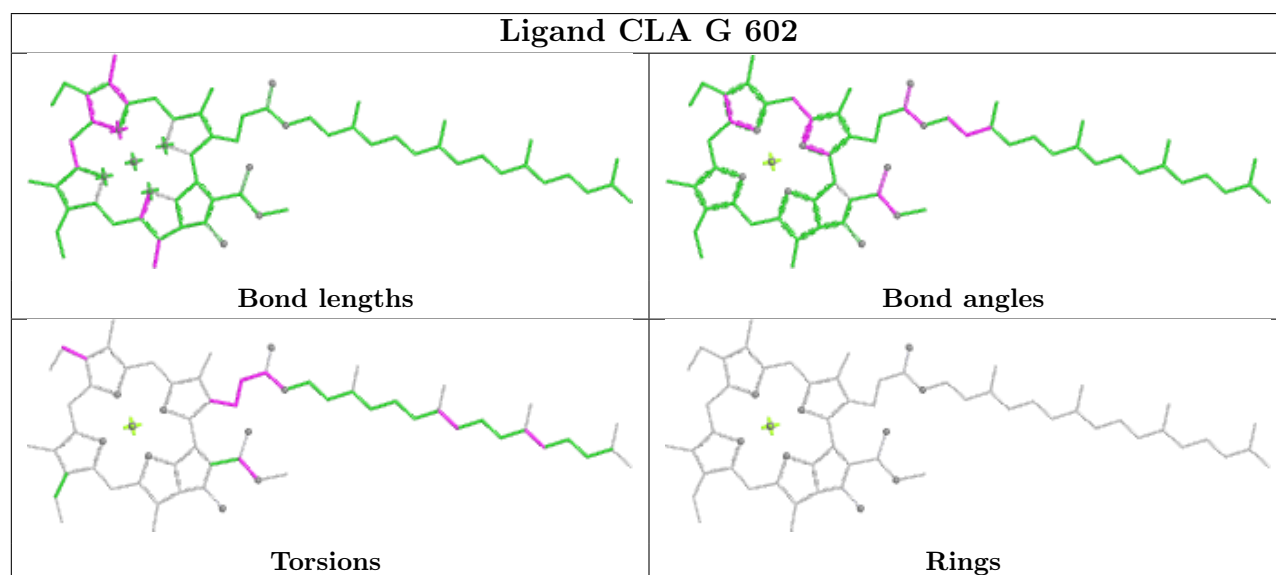
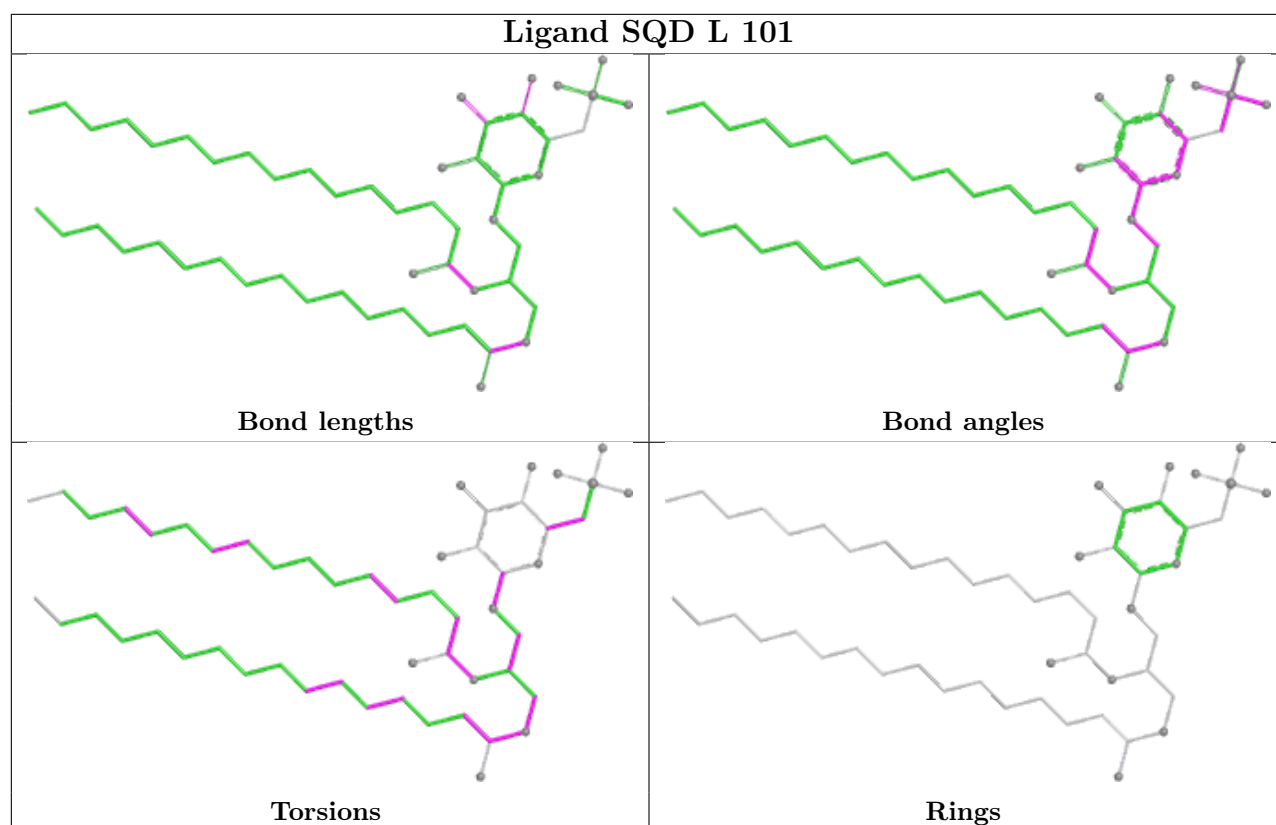


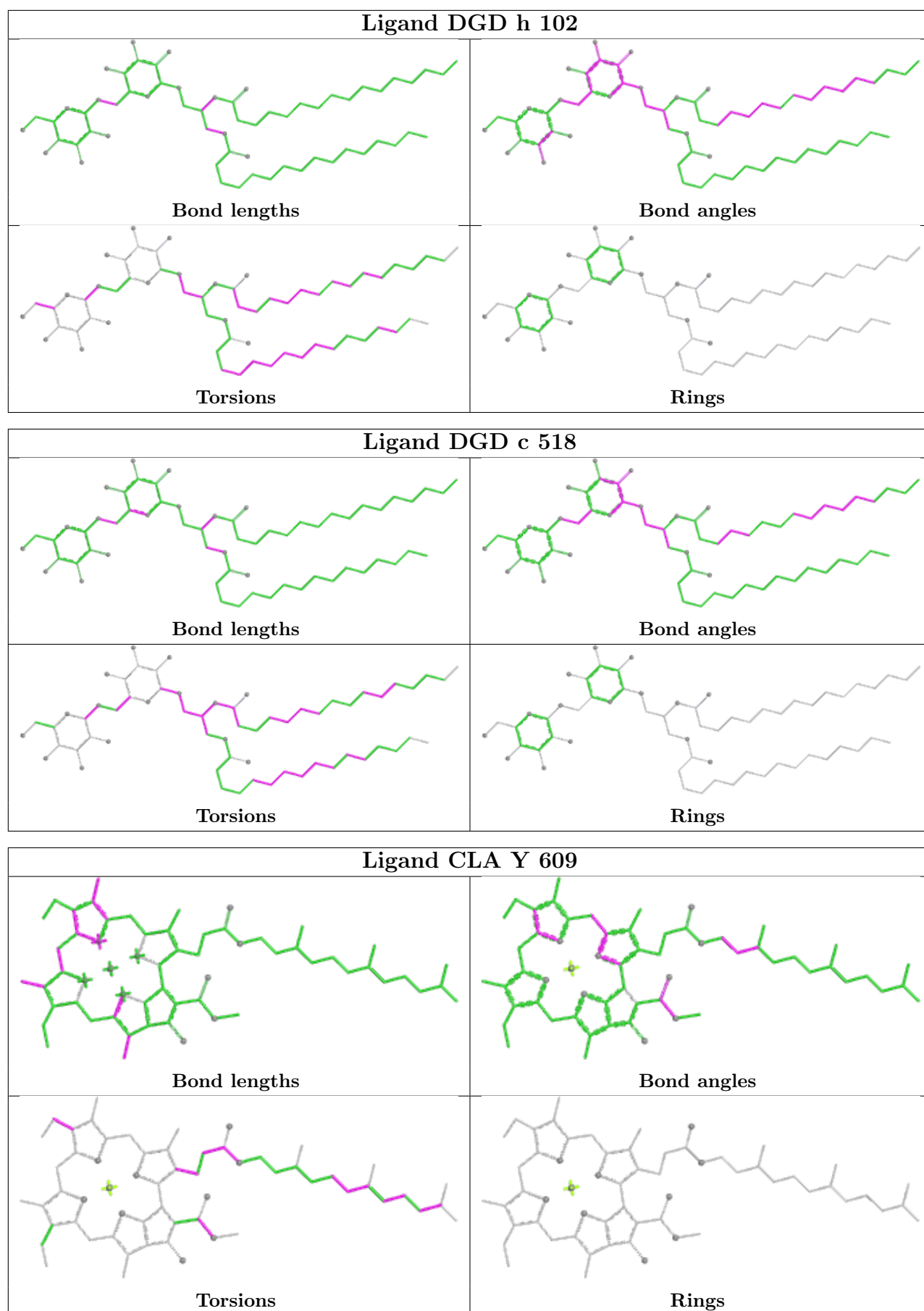
## Ligand CHL r 301

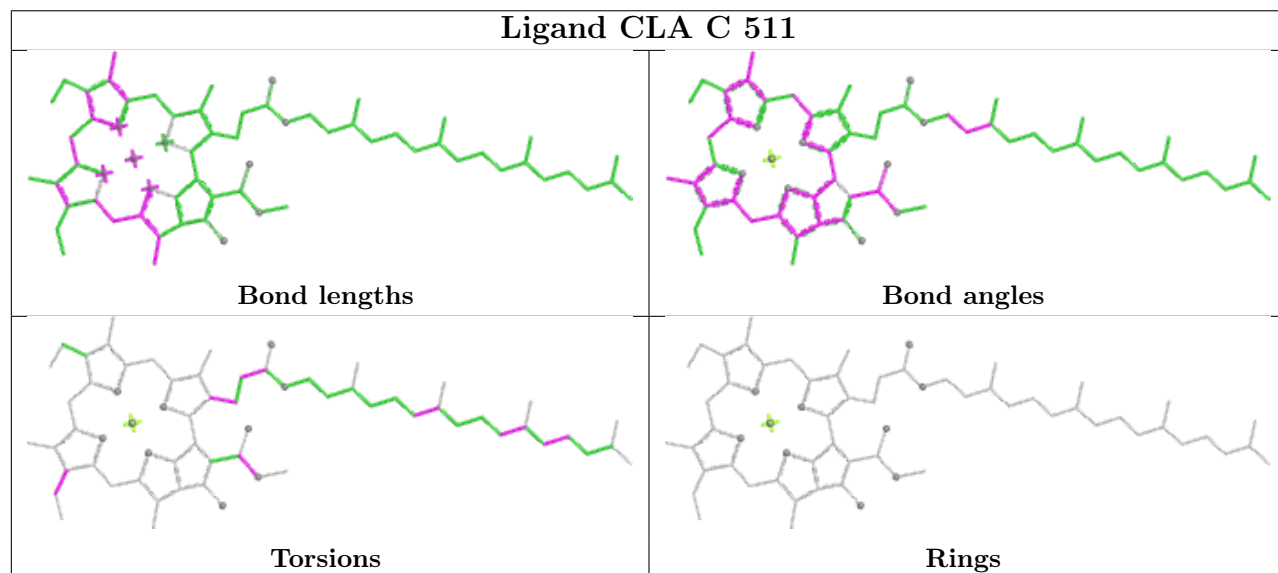
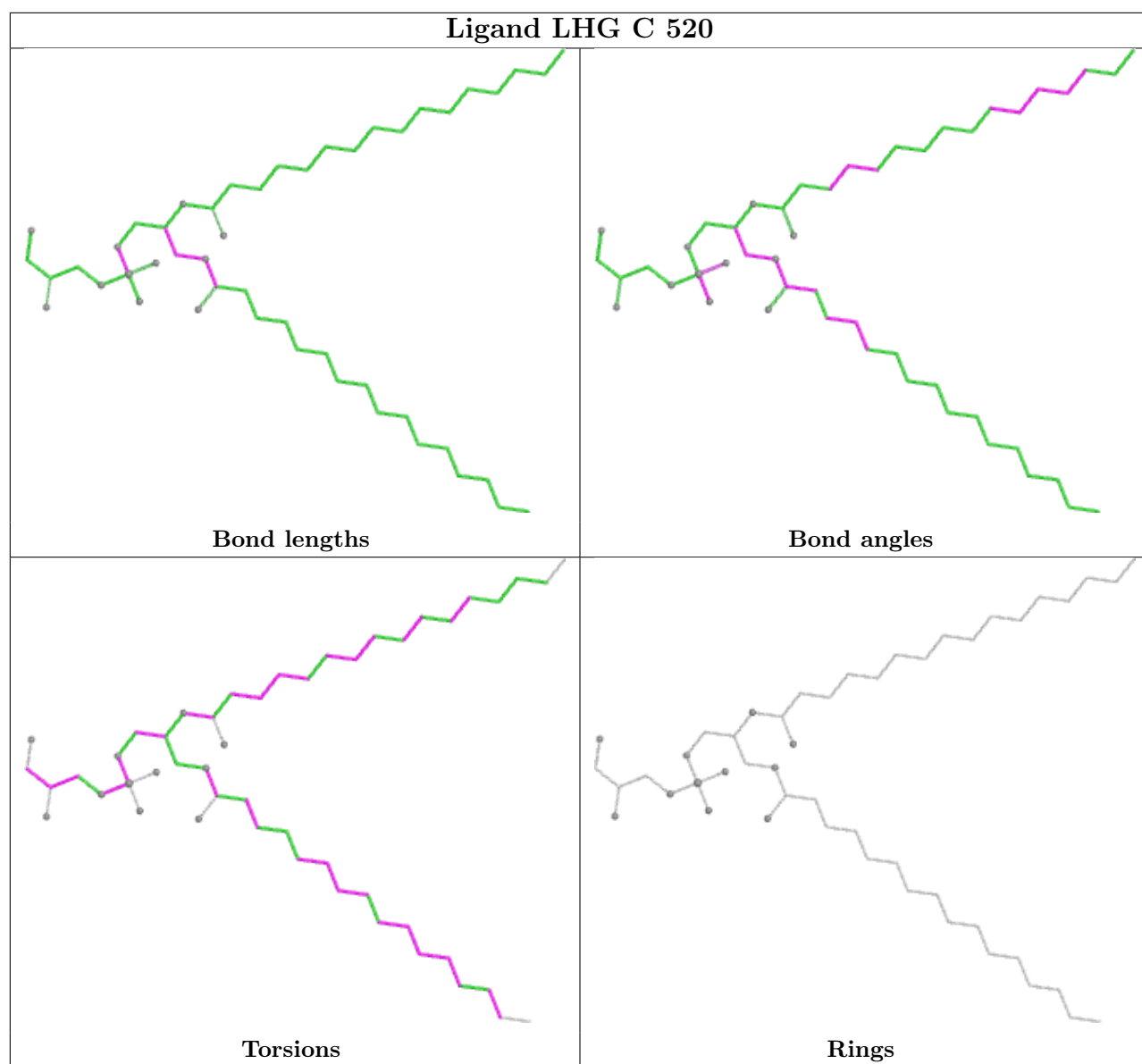


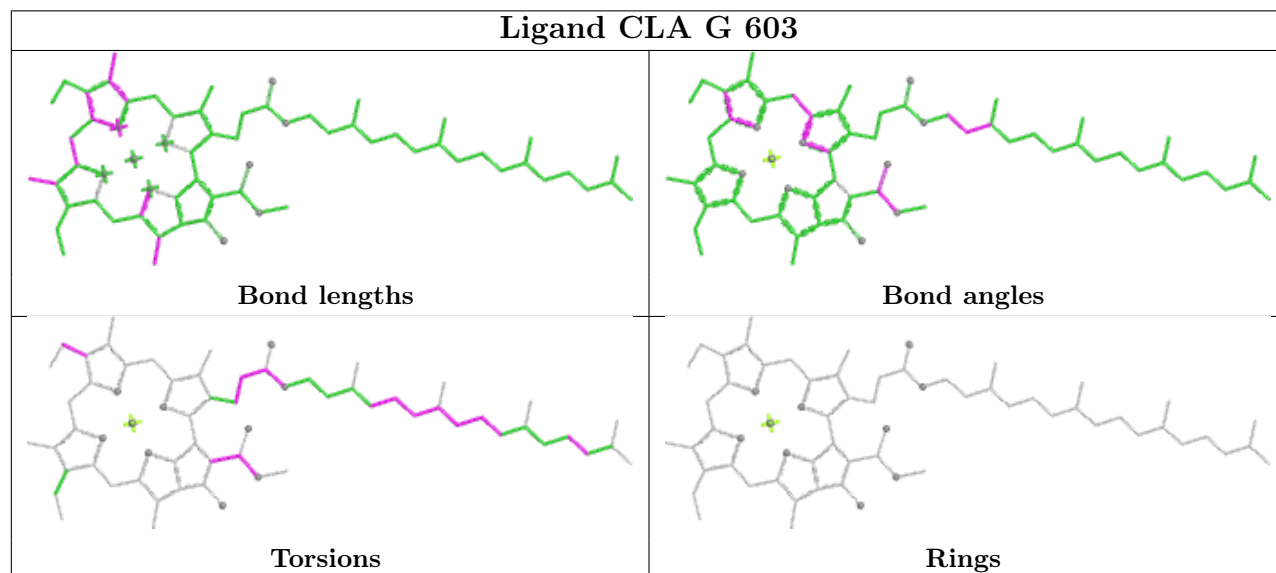
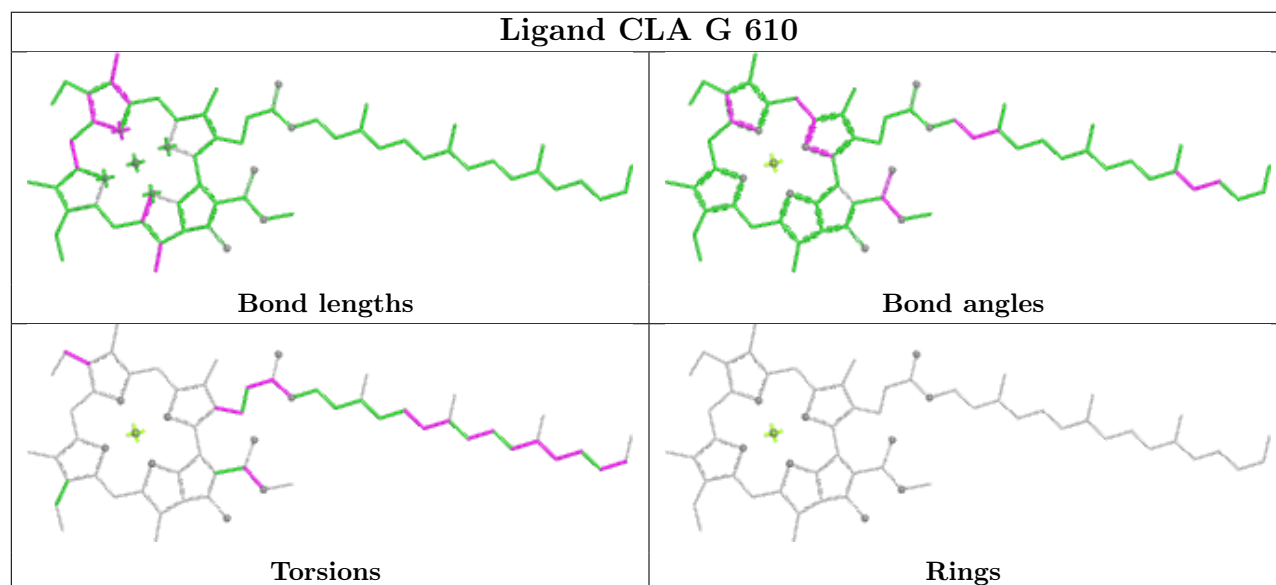
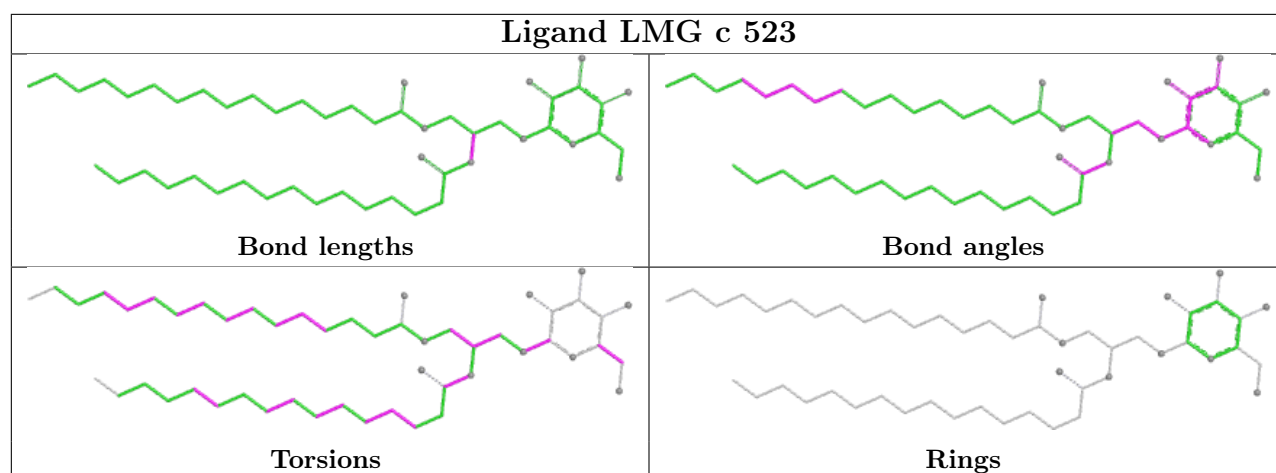
## Ligand CHL y 601



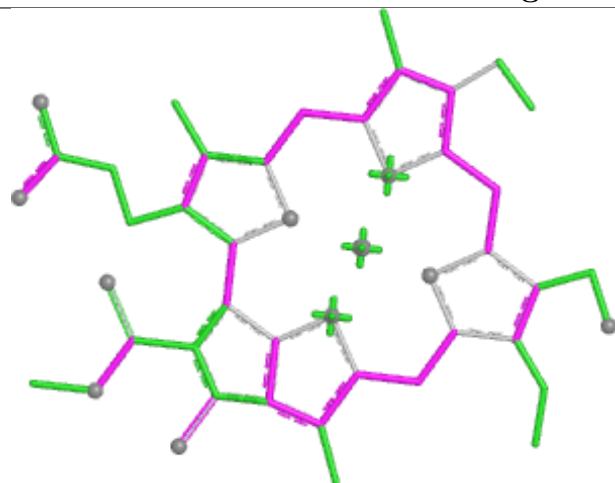




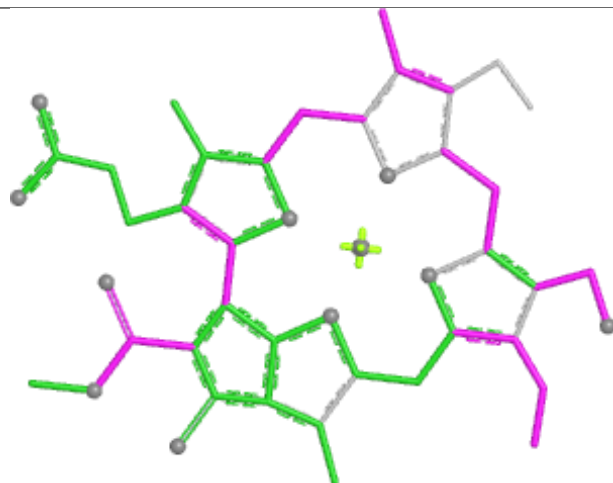




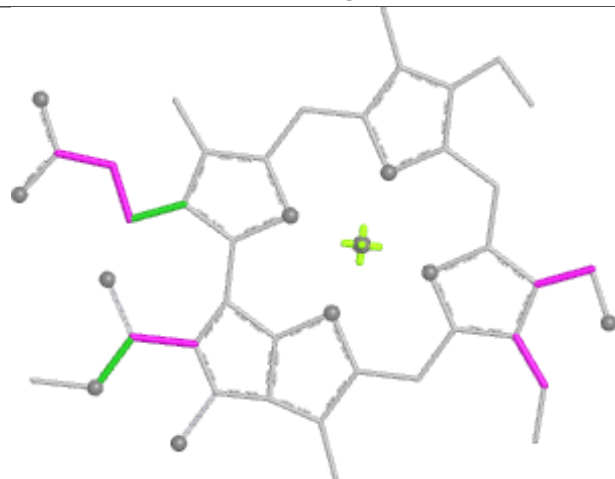
## Ligand CHL s 306



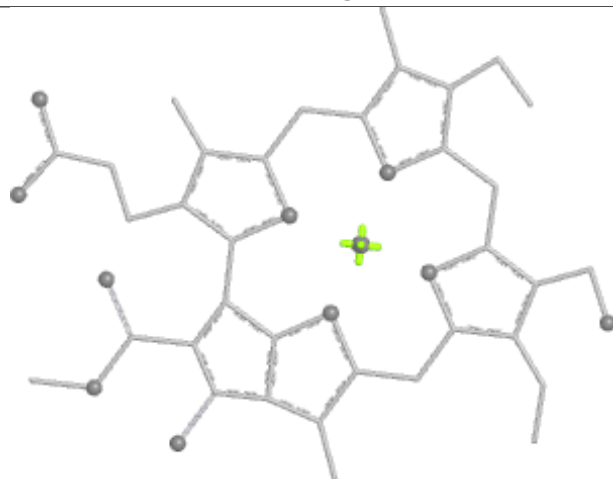
Bond lengths



Bond angles

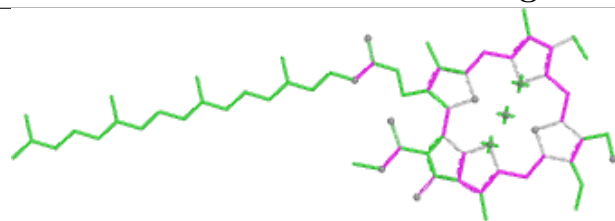


Torsions

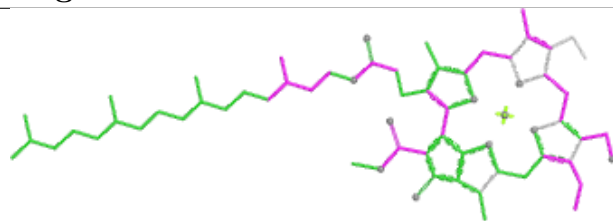


Rings

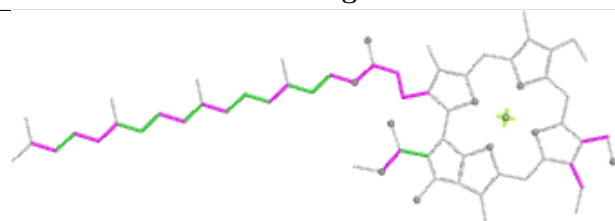
## Ligand CHL g 601



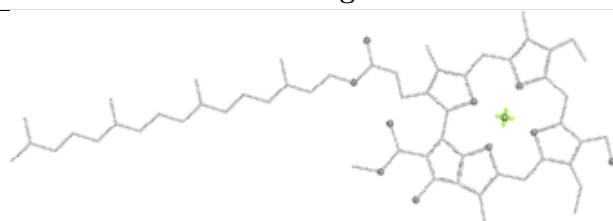
Bond lengths



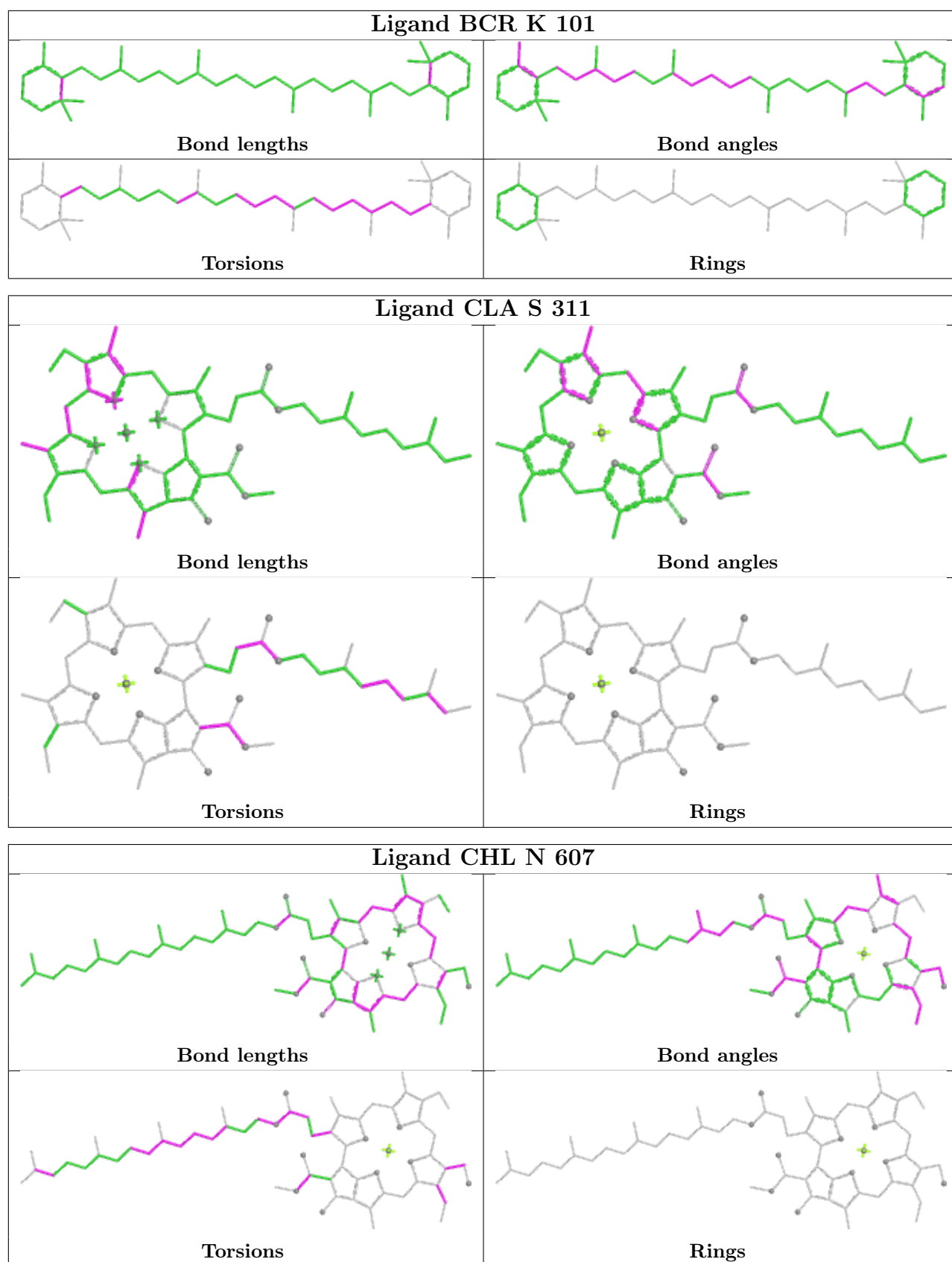
Bond angles

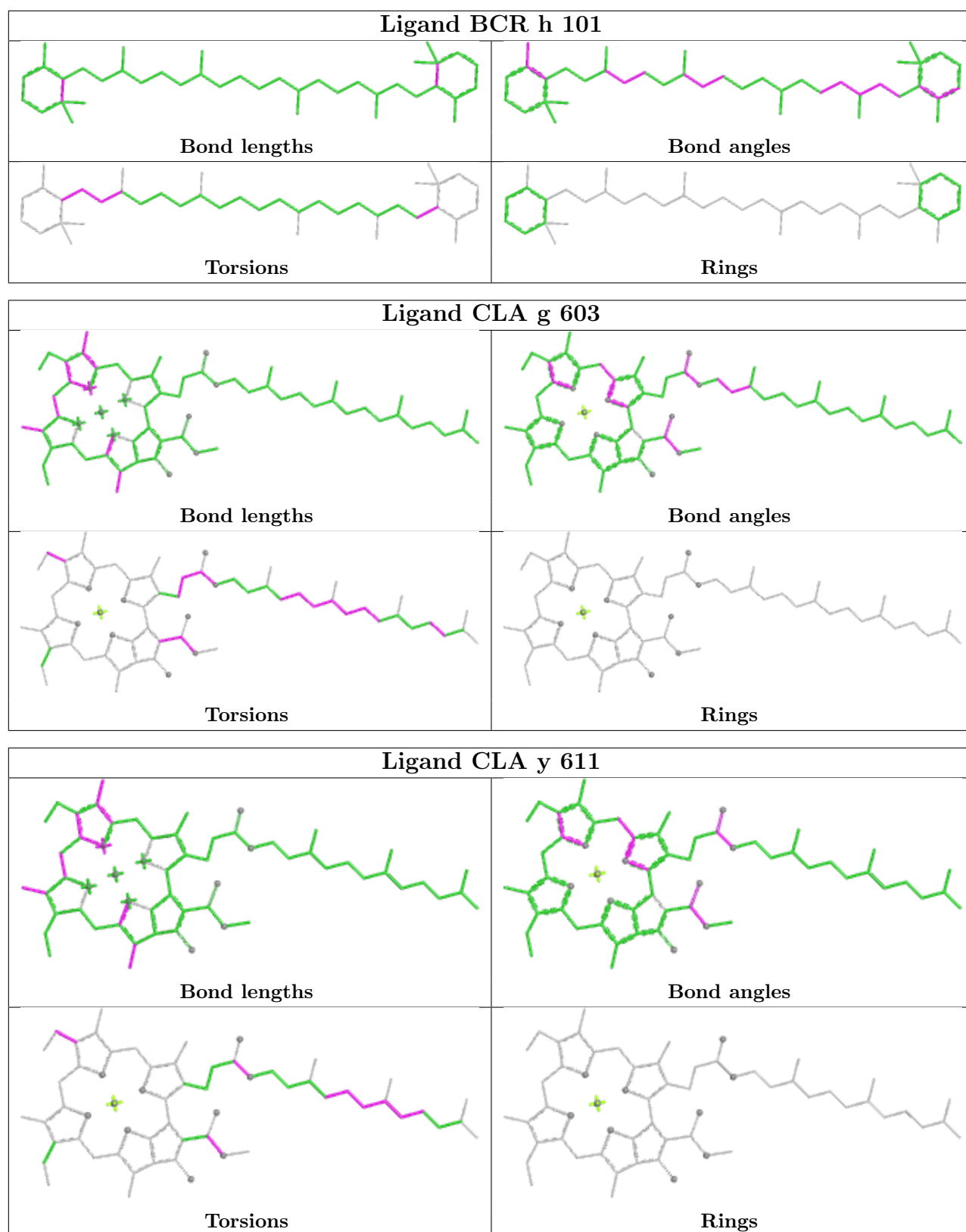


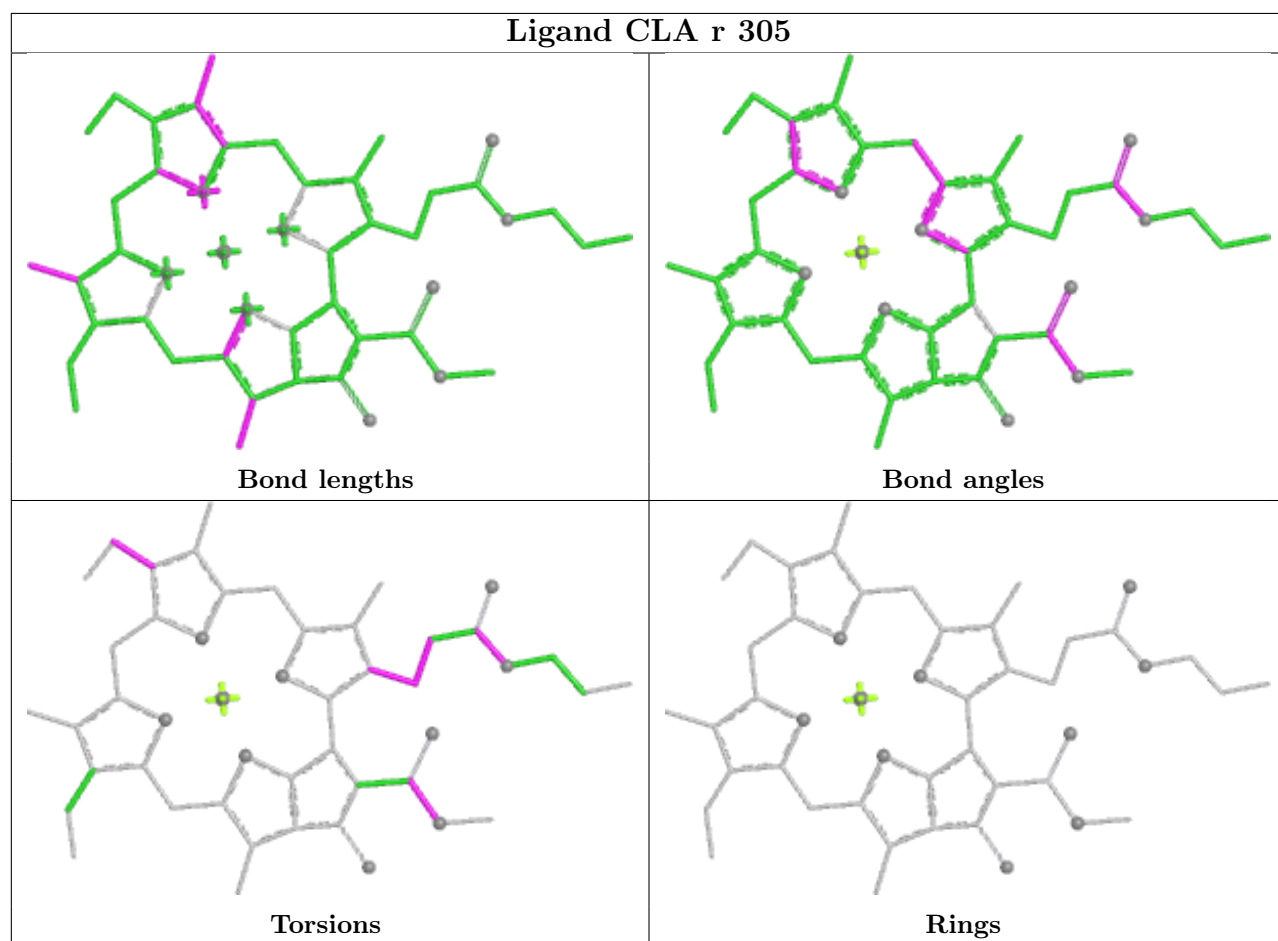
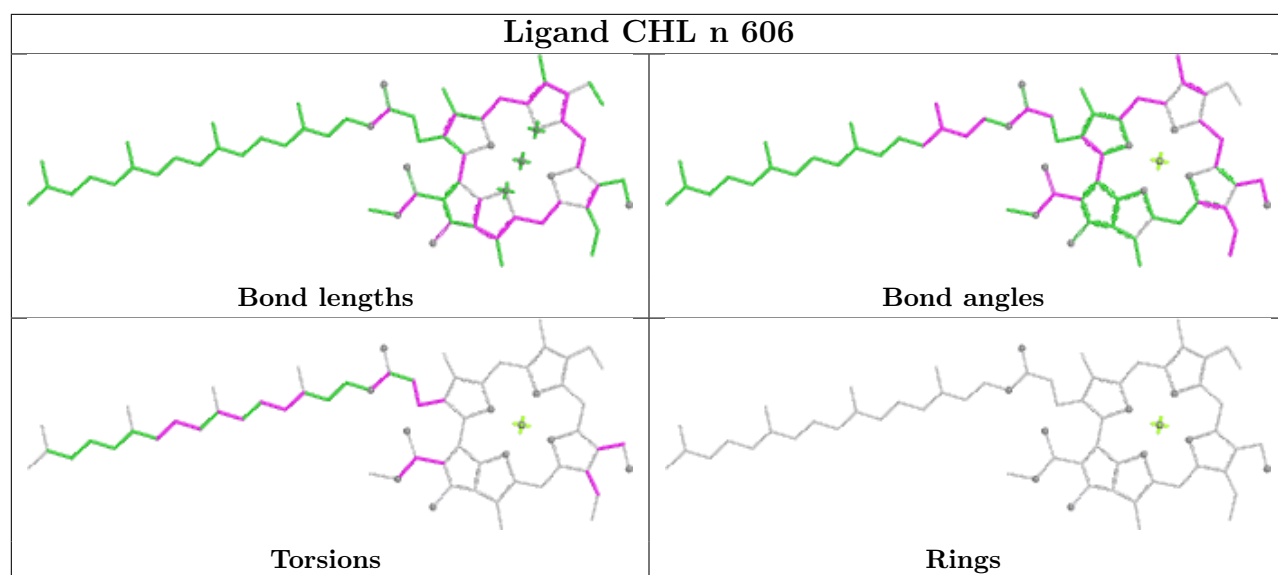
Torsions

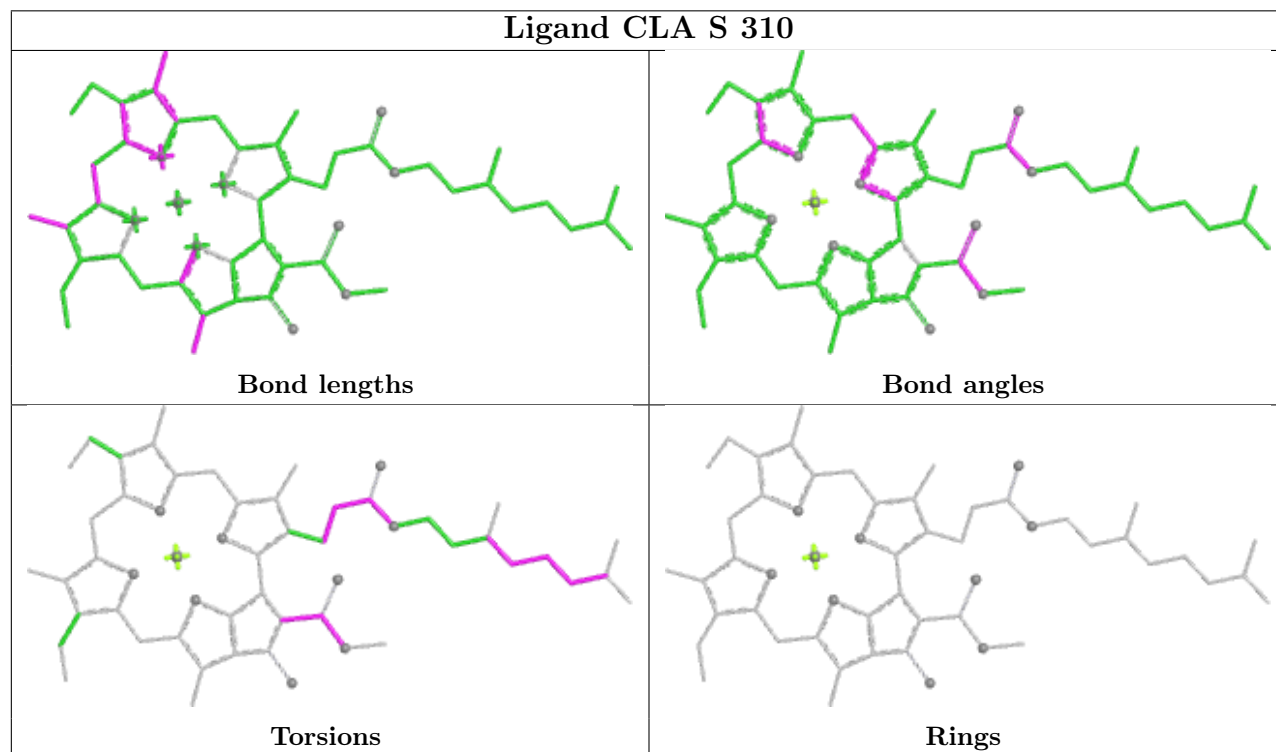
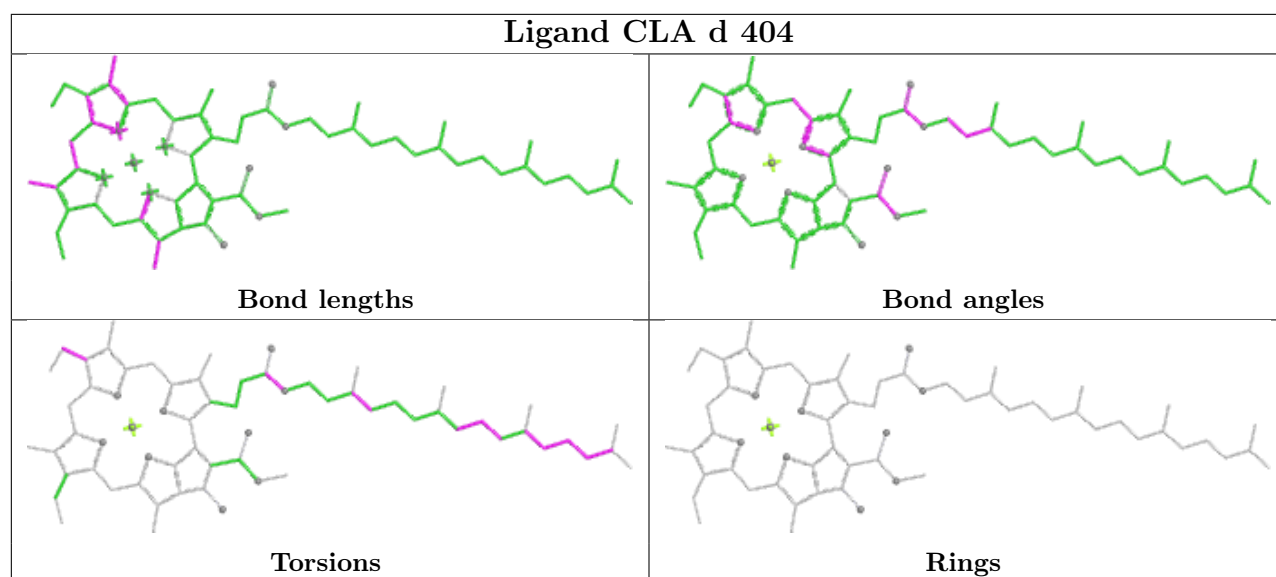


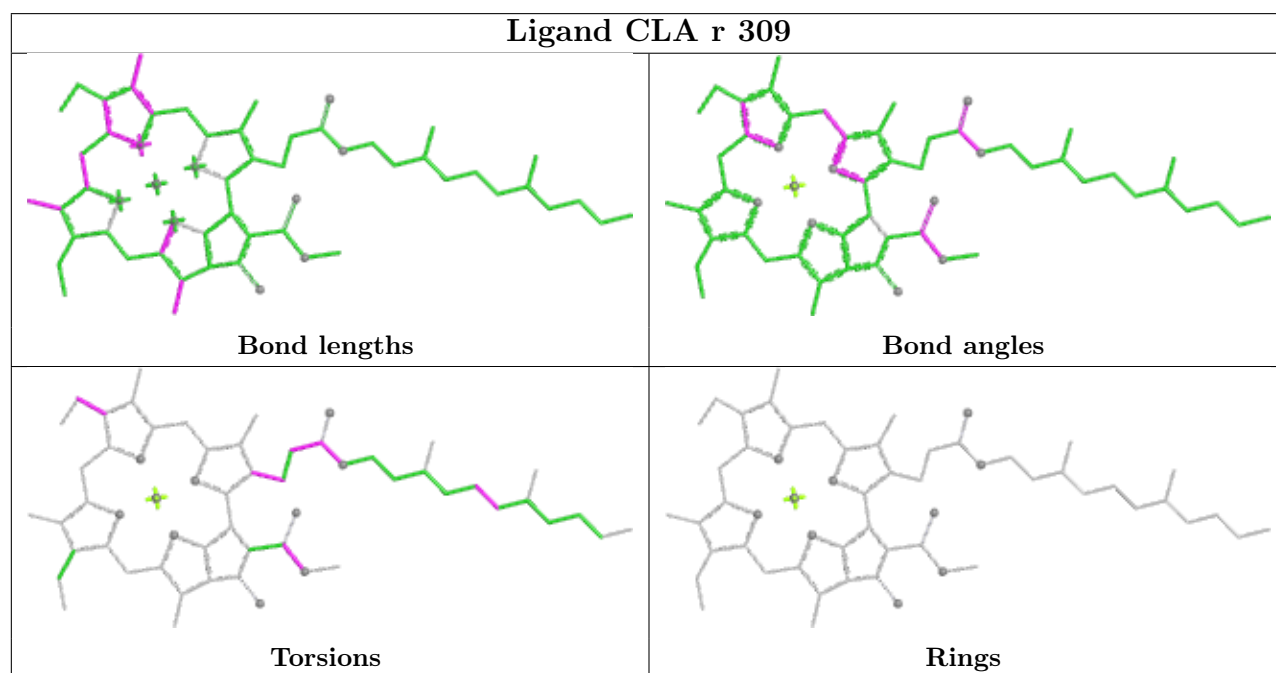
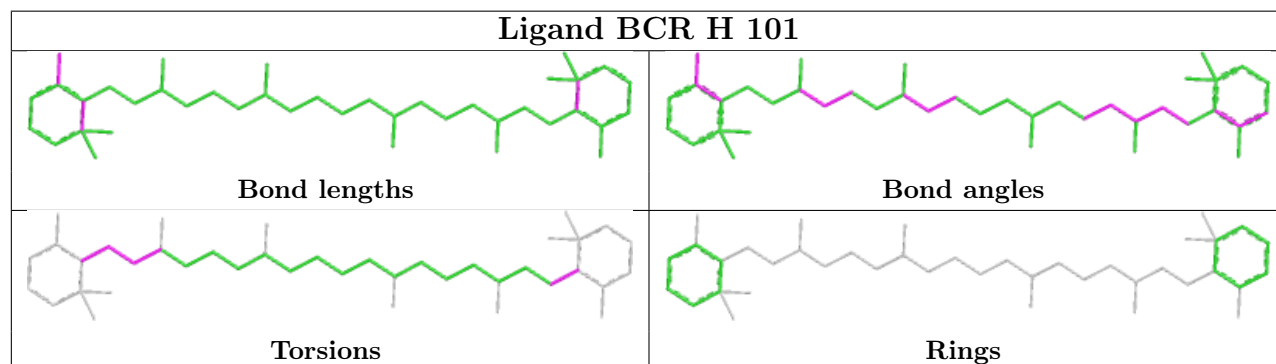
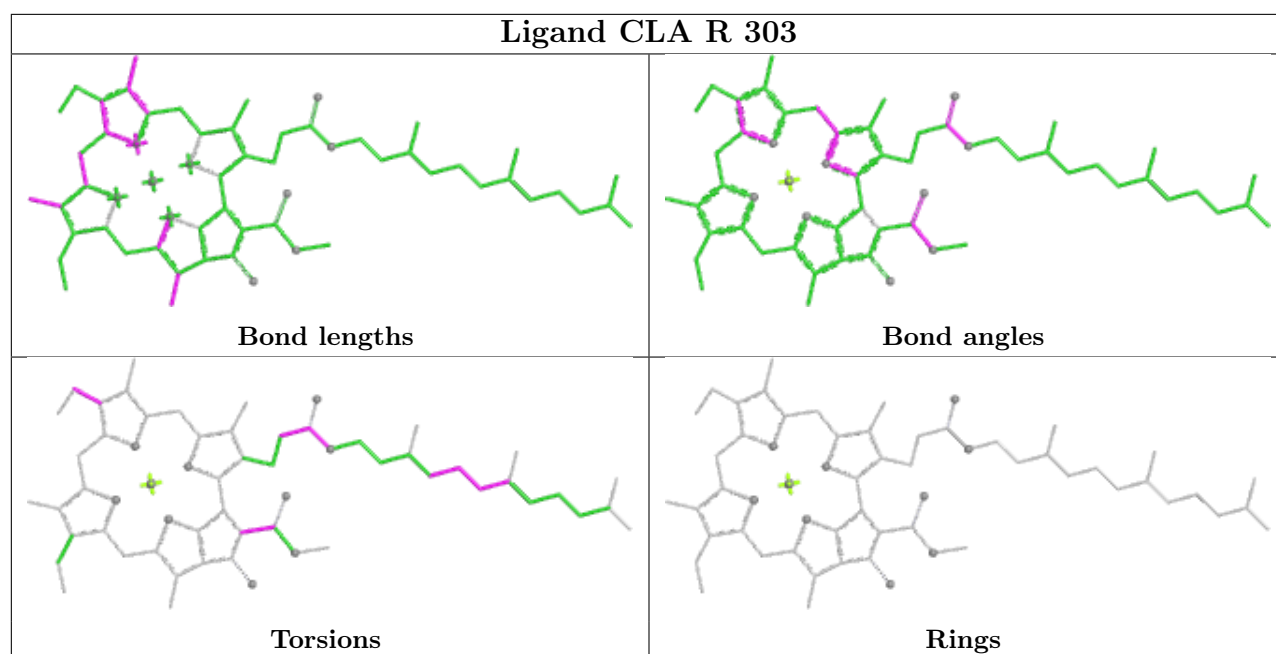
Rings

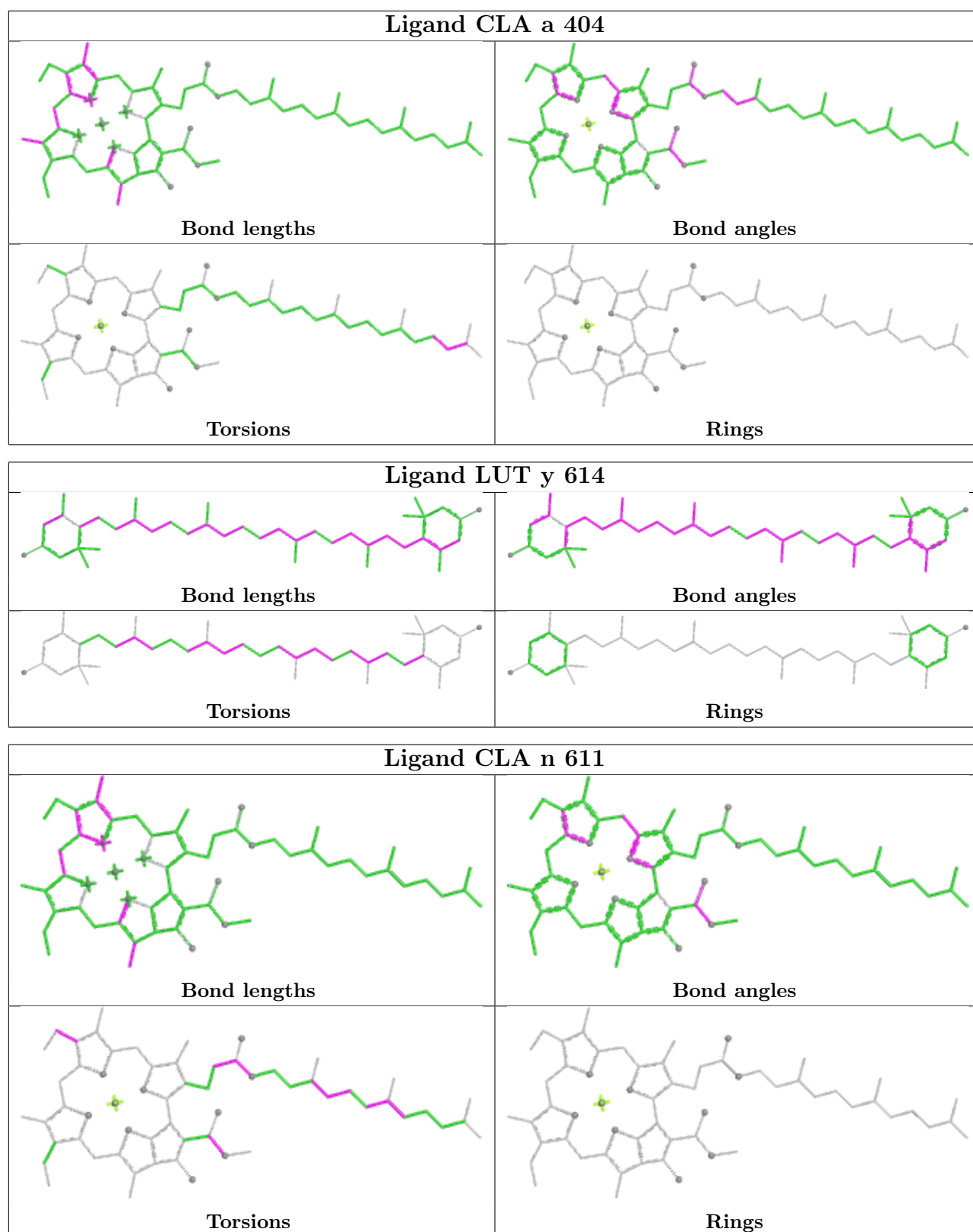


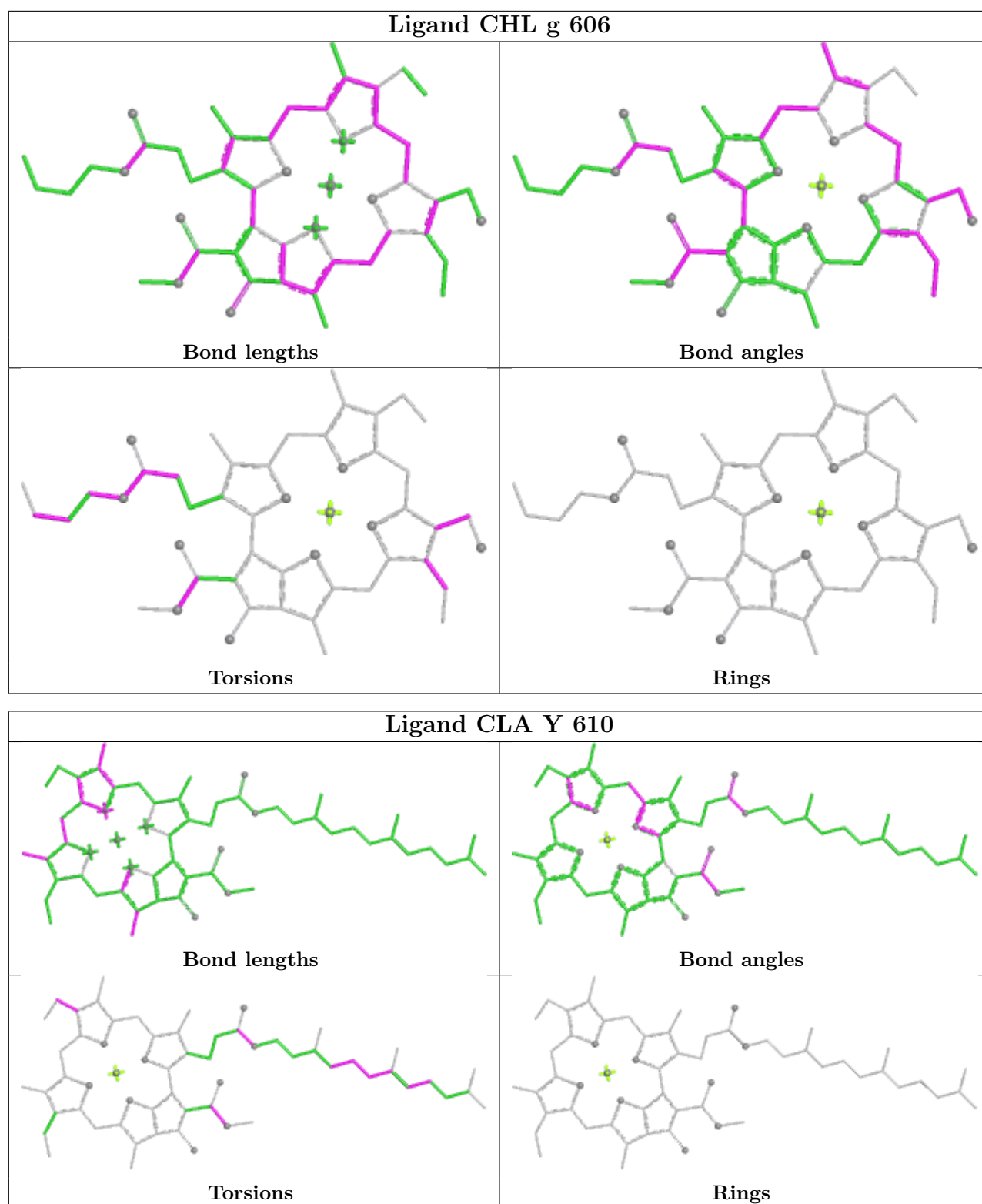




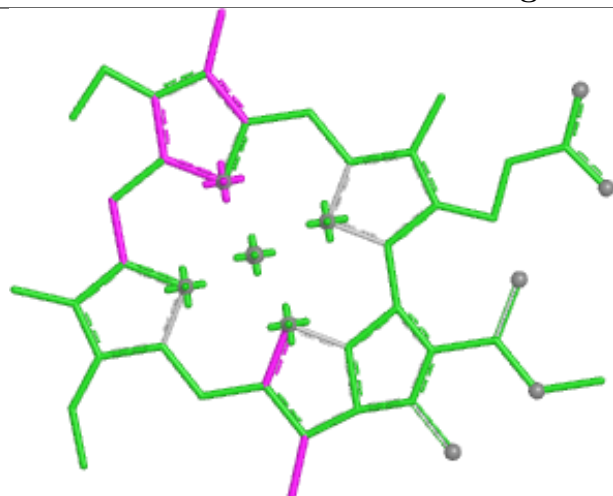




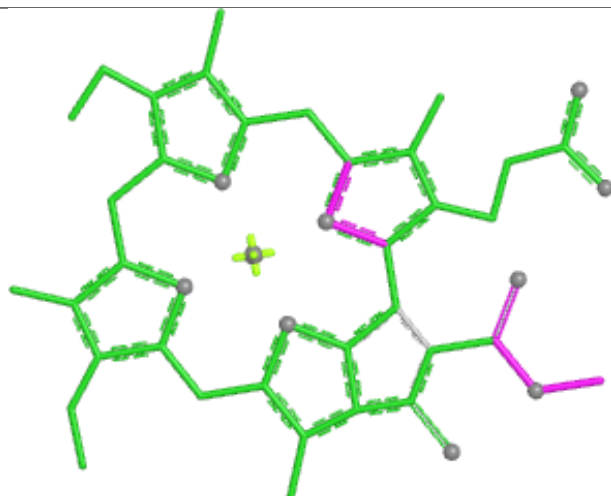




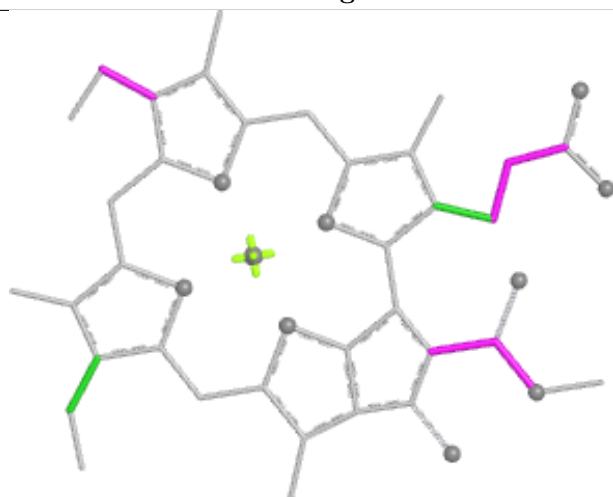
## Ligand CLA s 308



Bond lengths



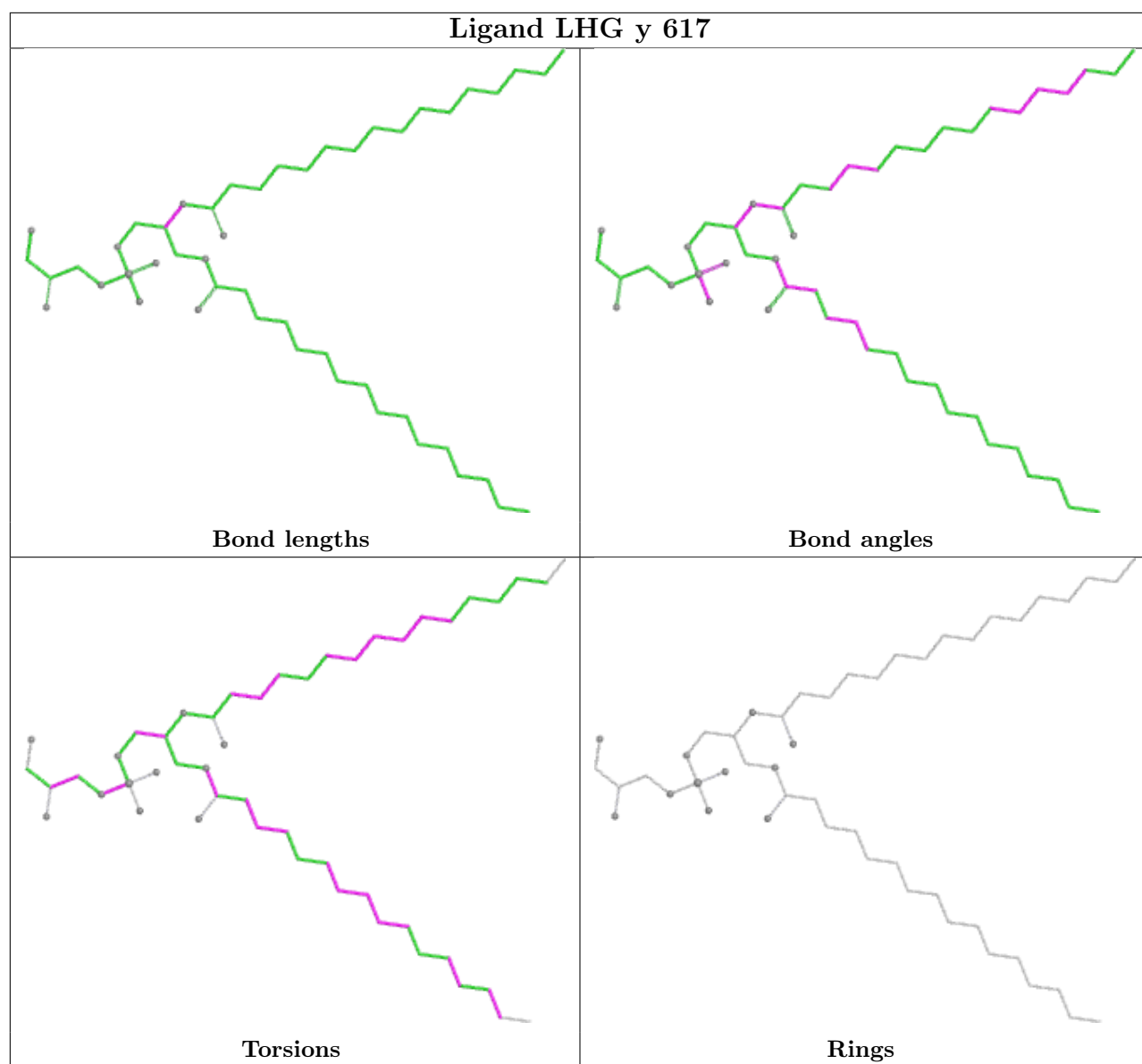
Bond angles

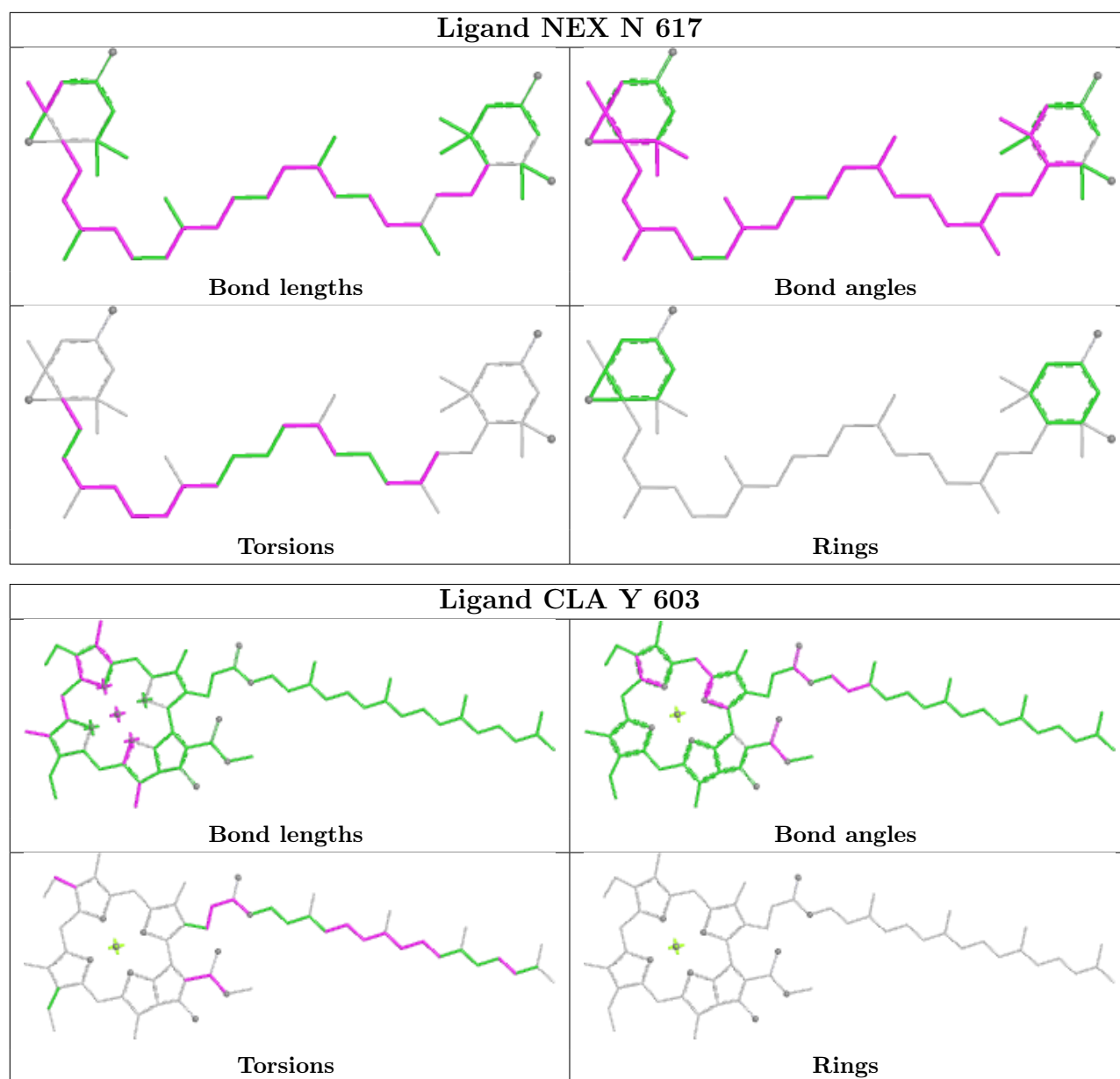


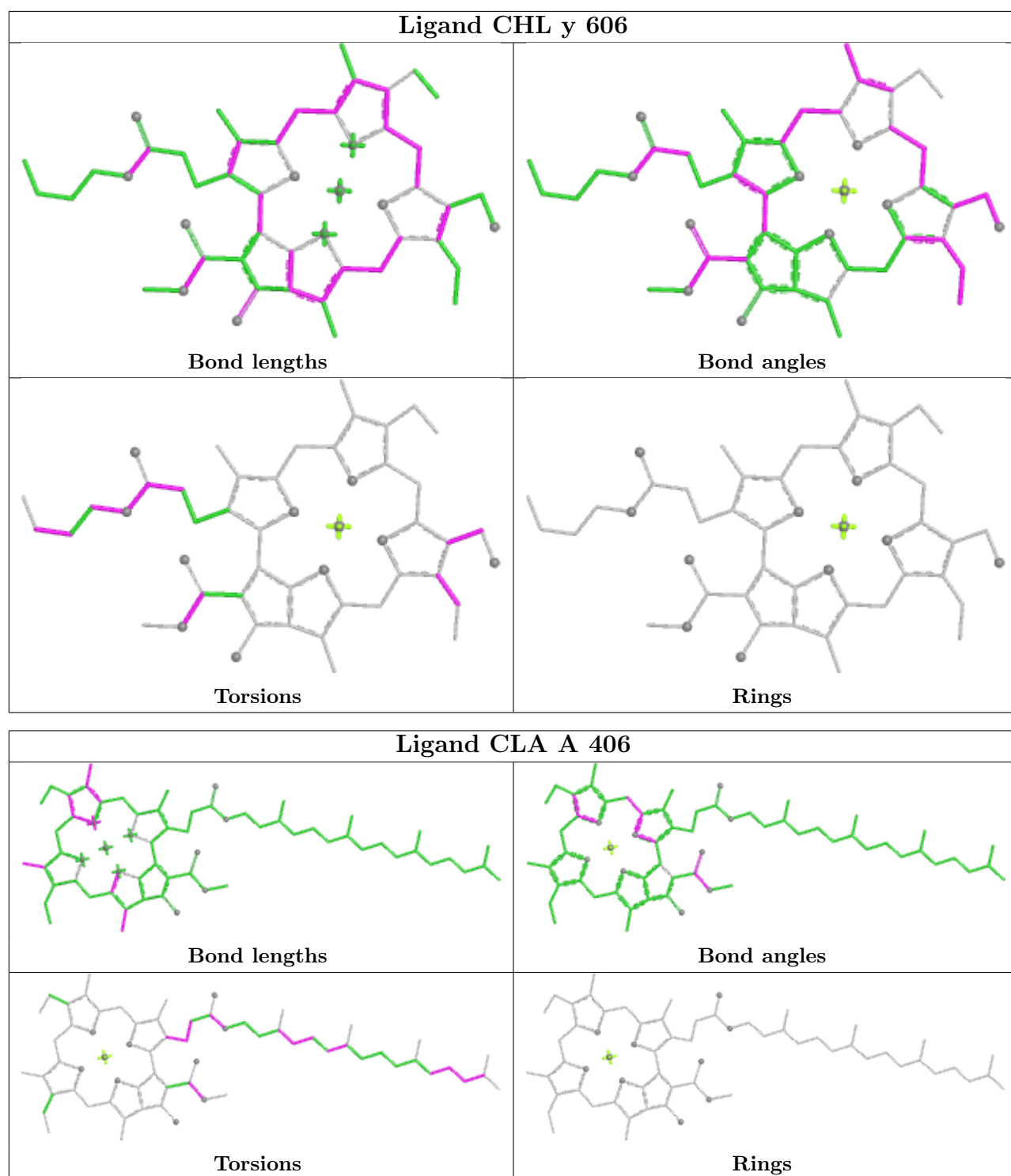
Torsions

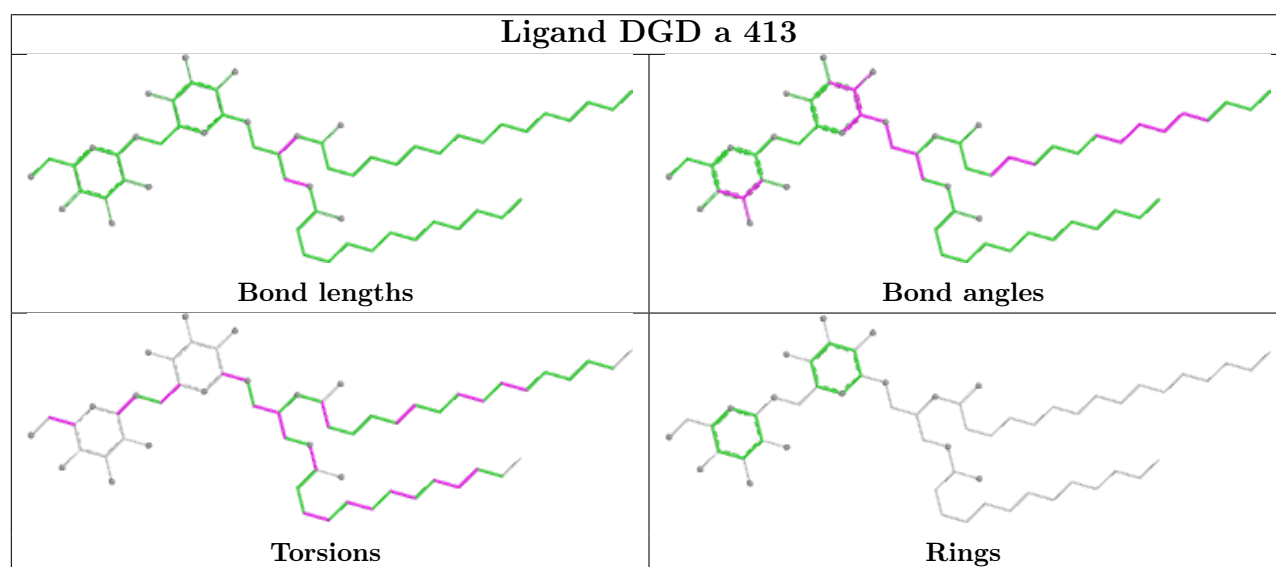
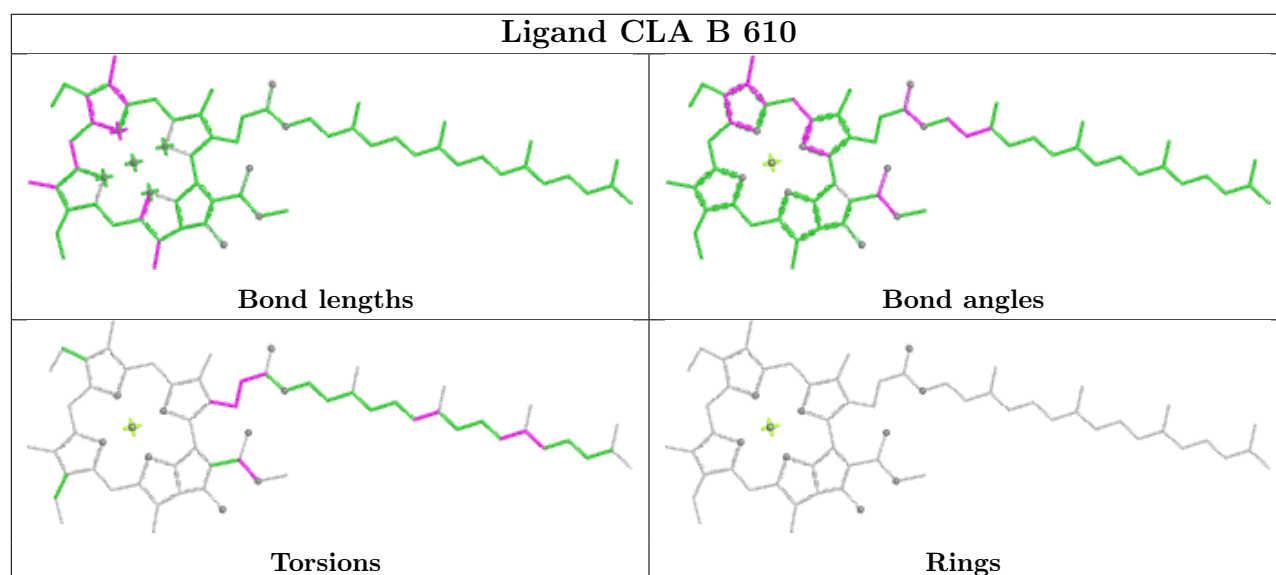
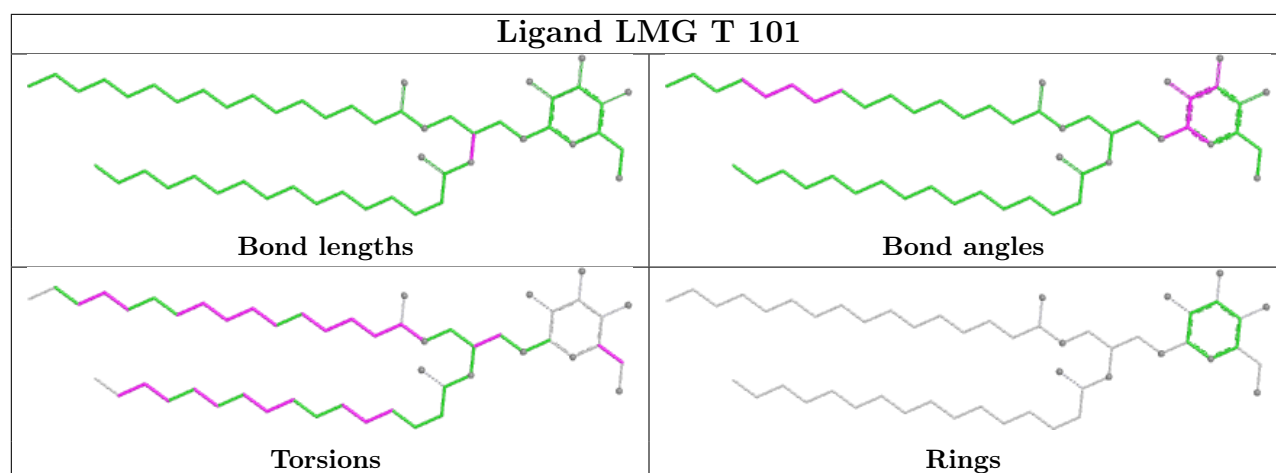


Rings

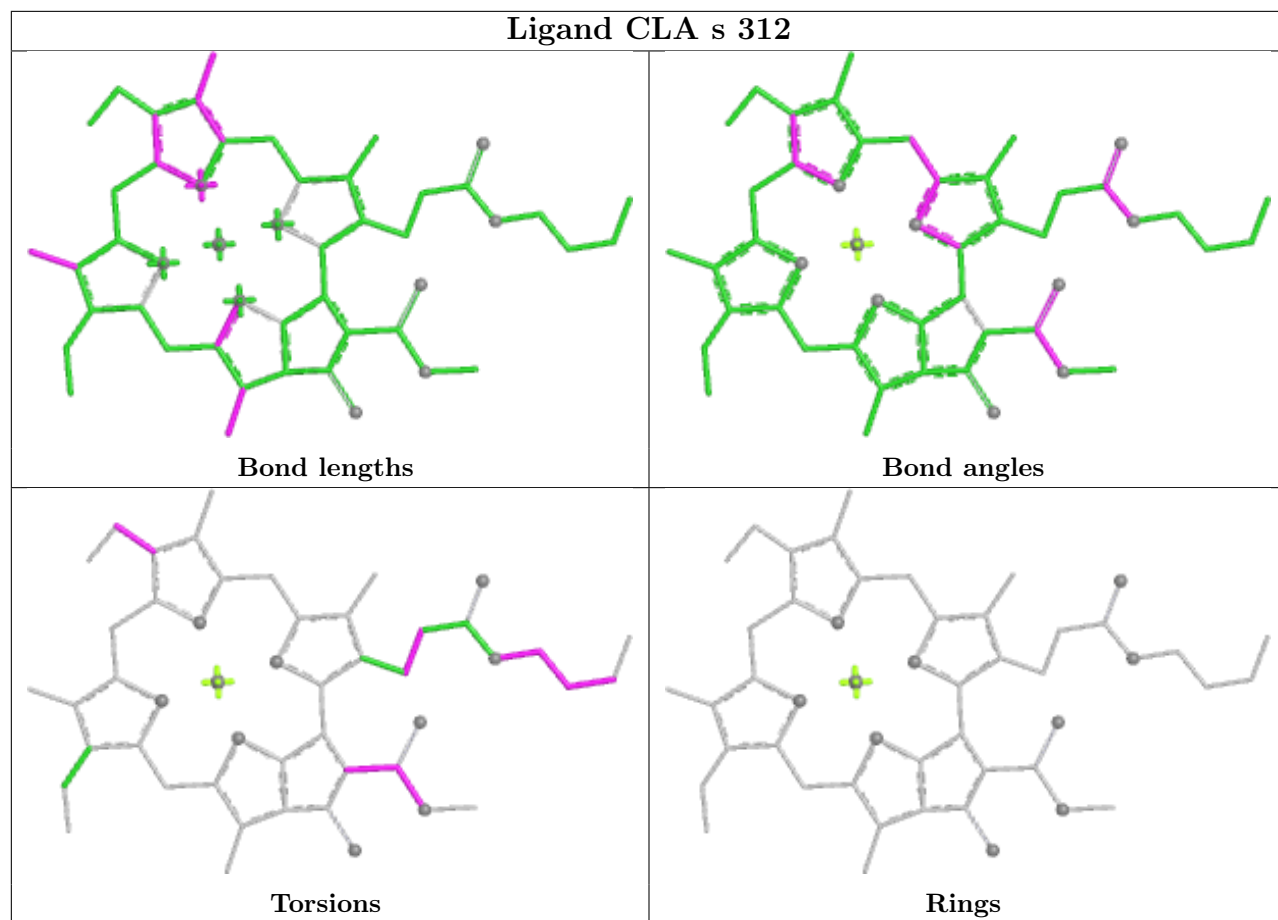


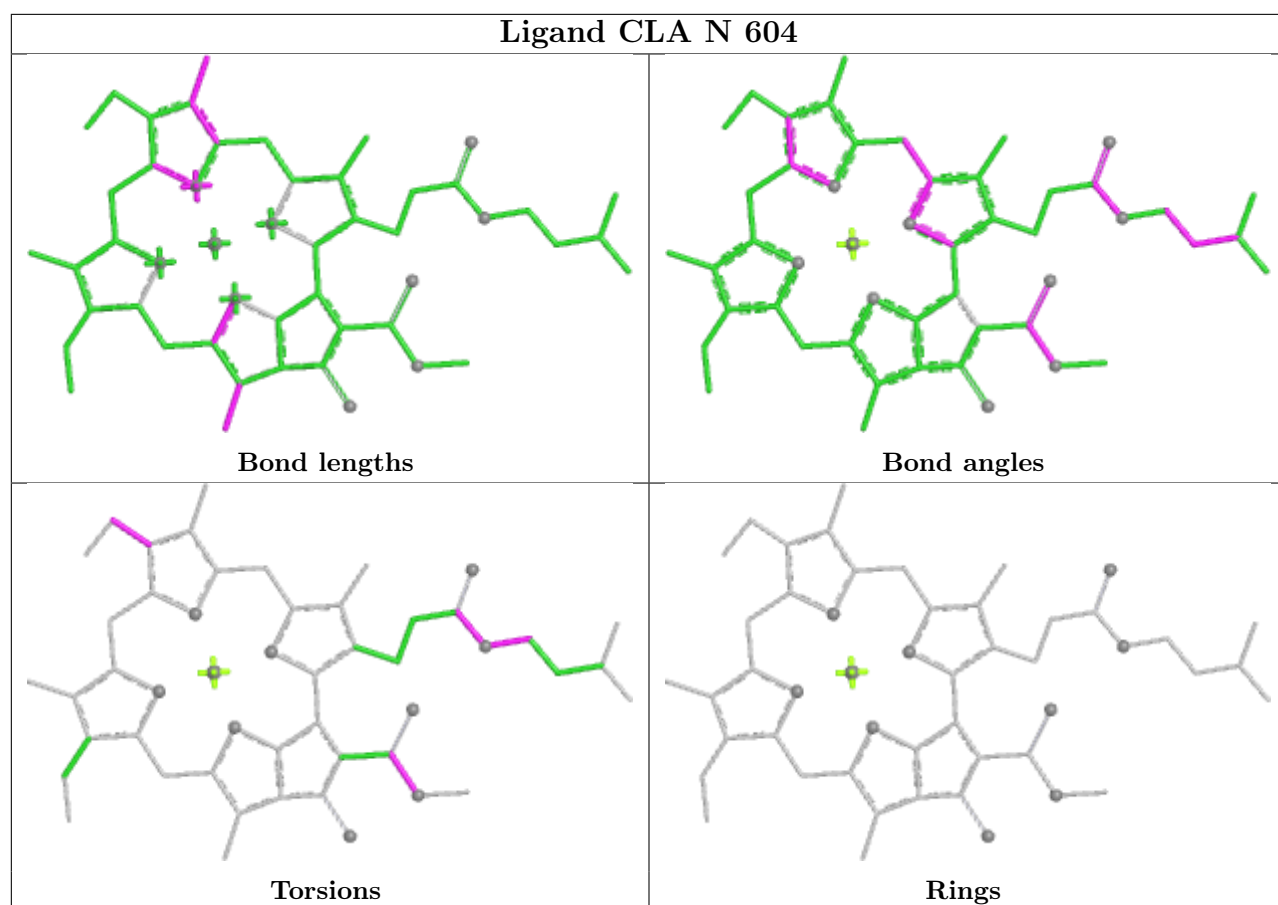


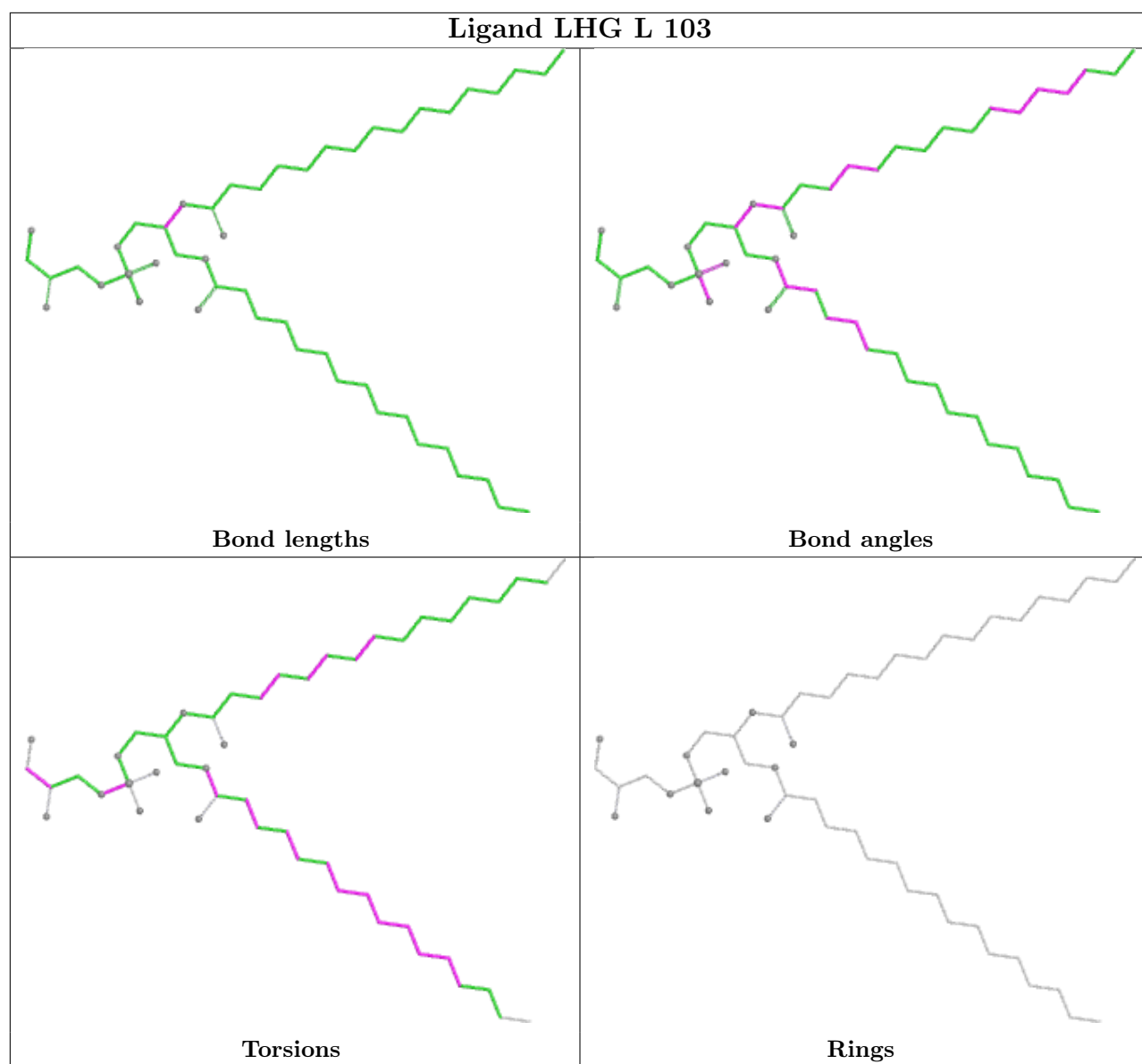




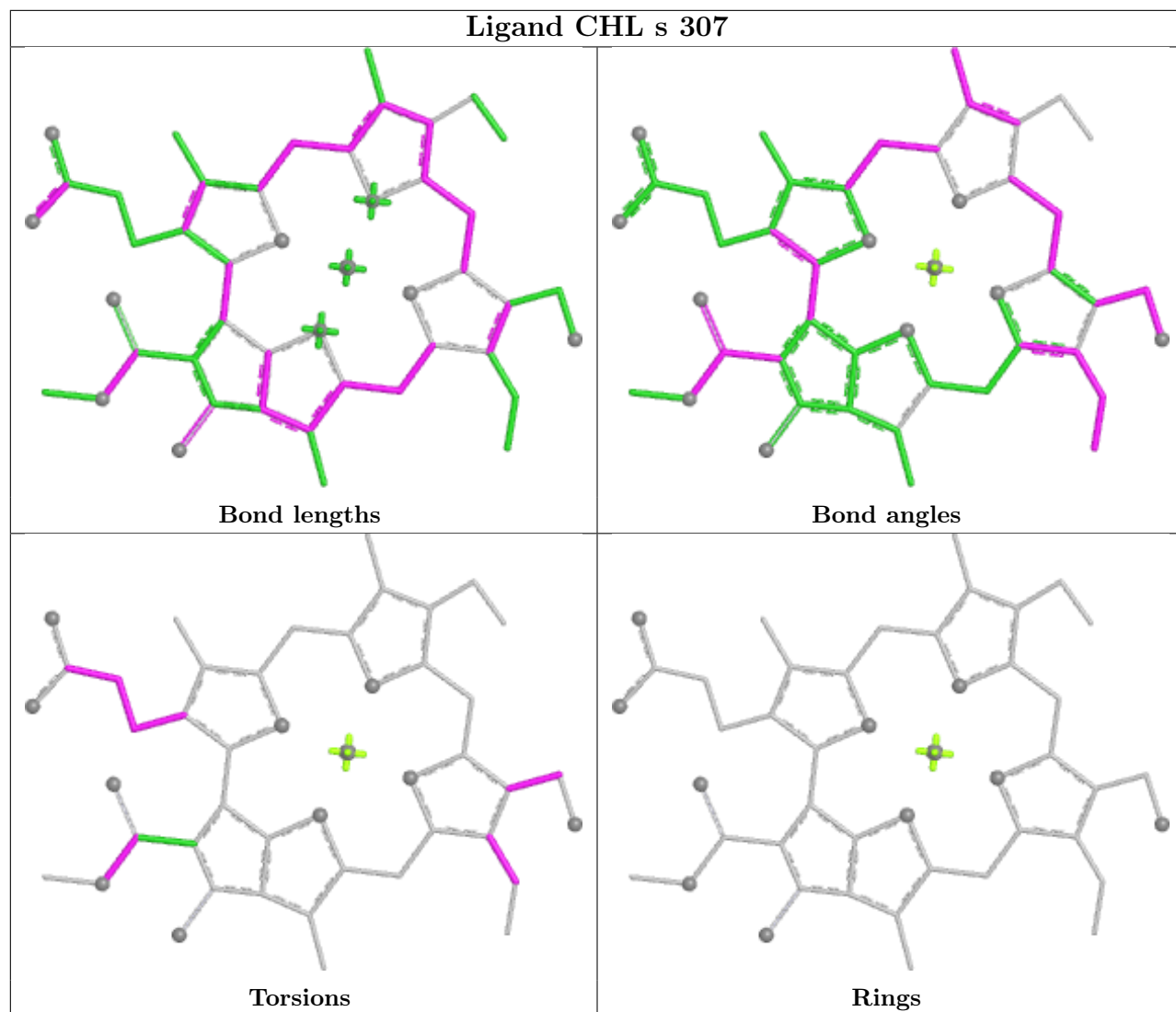
## Ligand CLA s 312

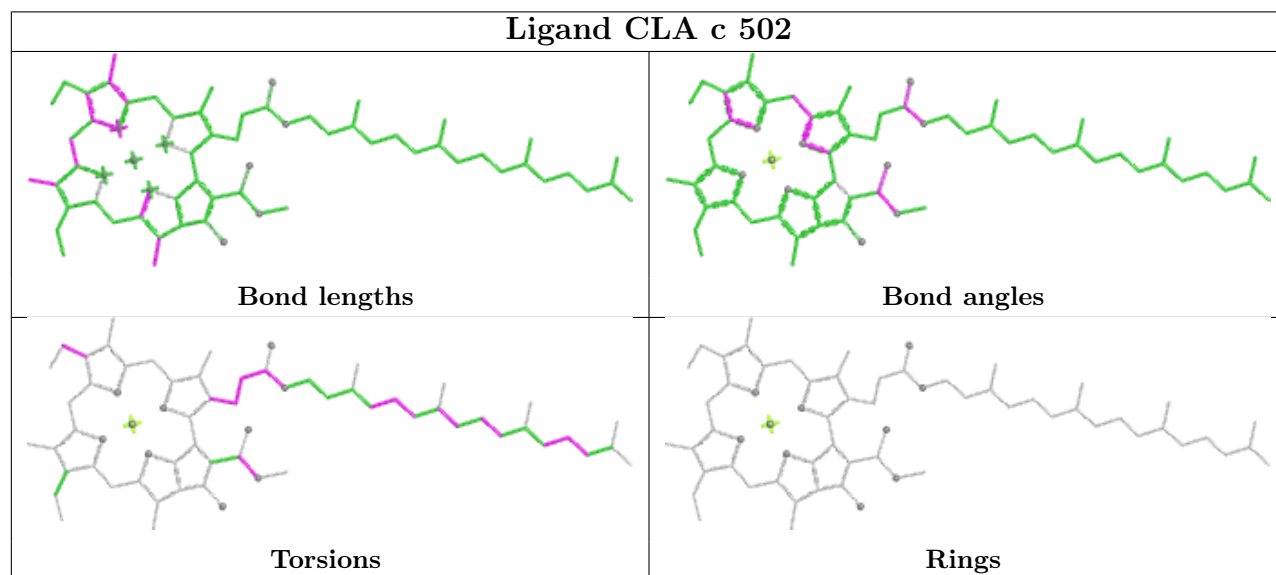
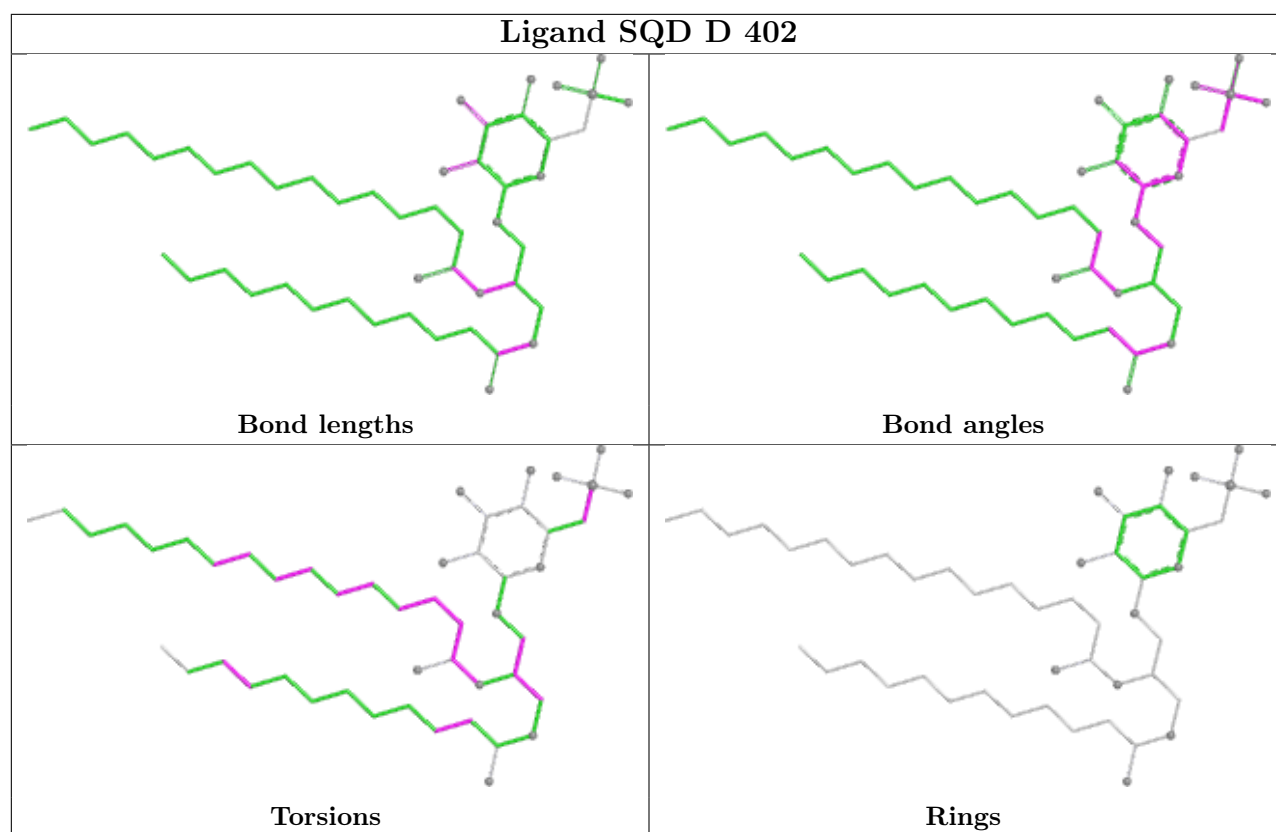


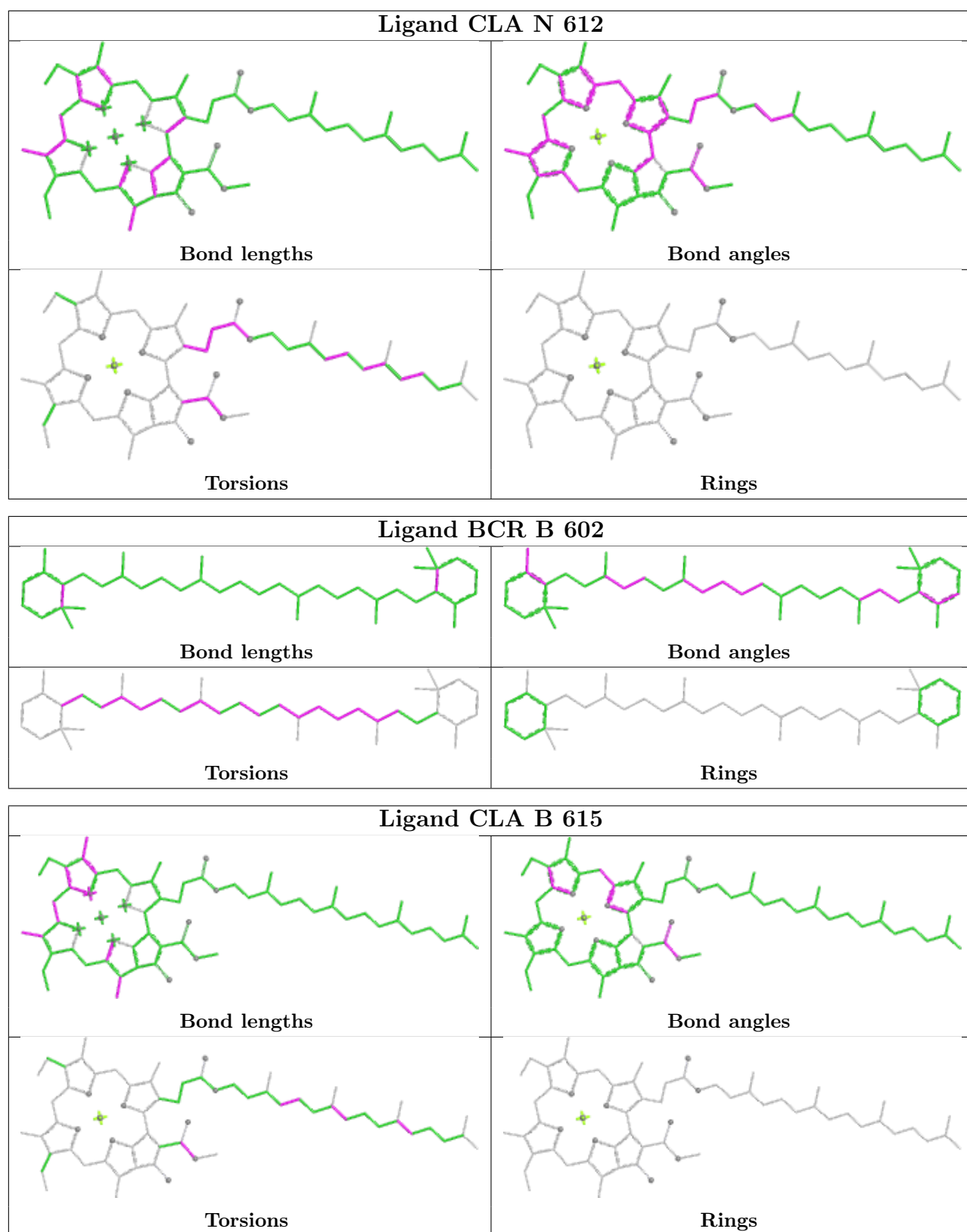


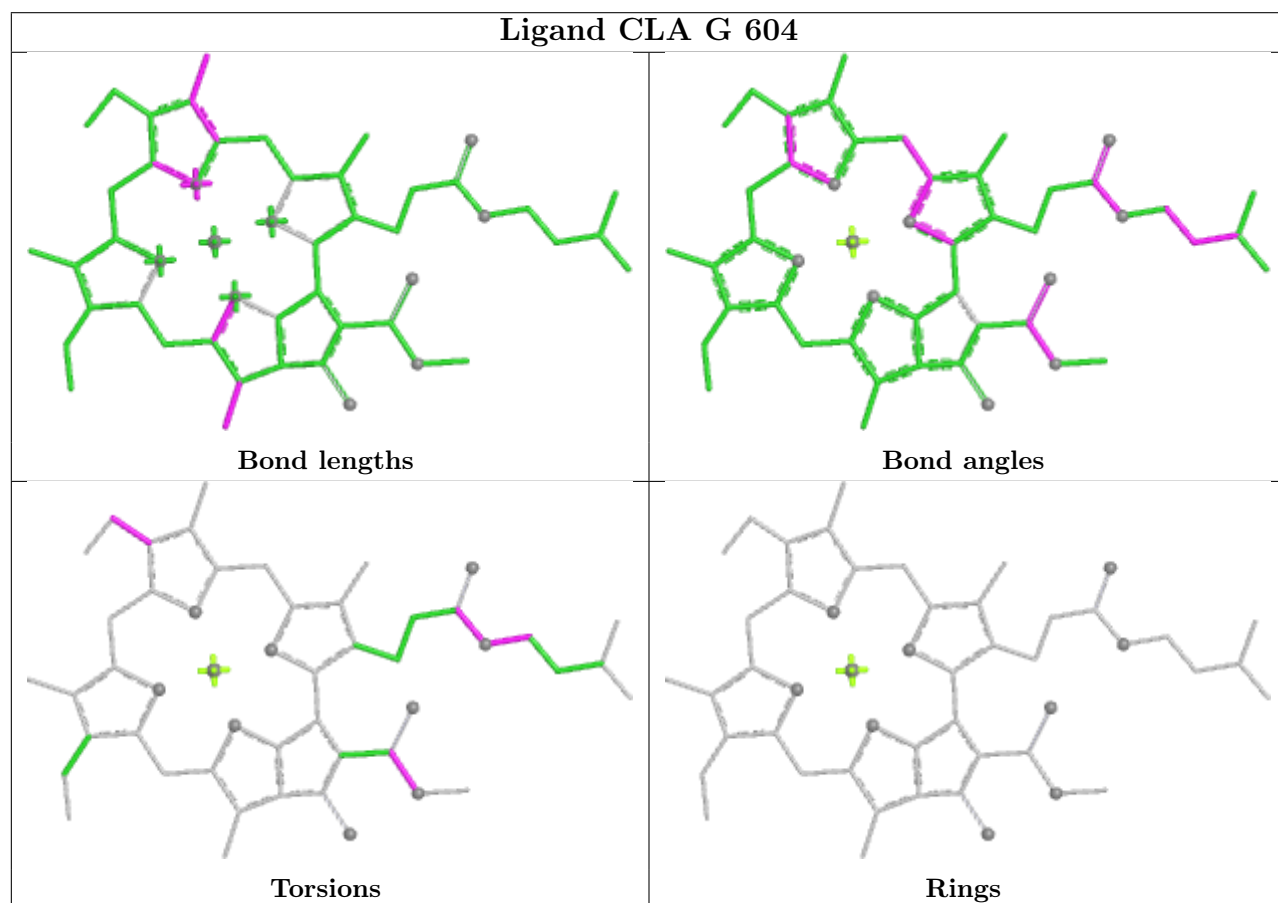
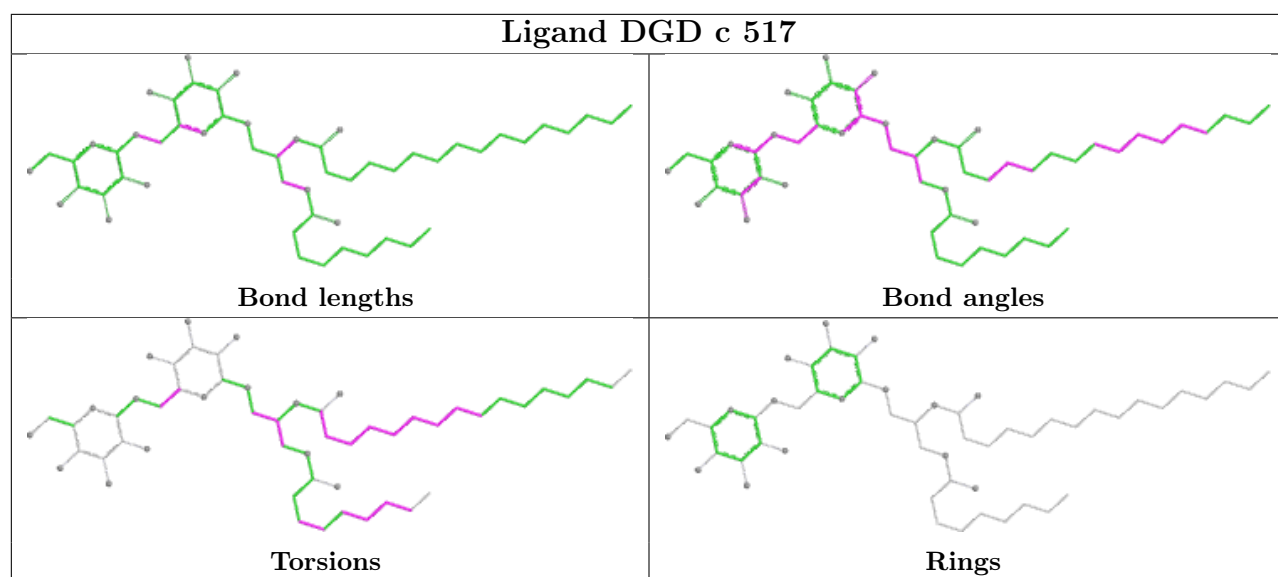


## Ligand CHL s 307

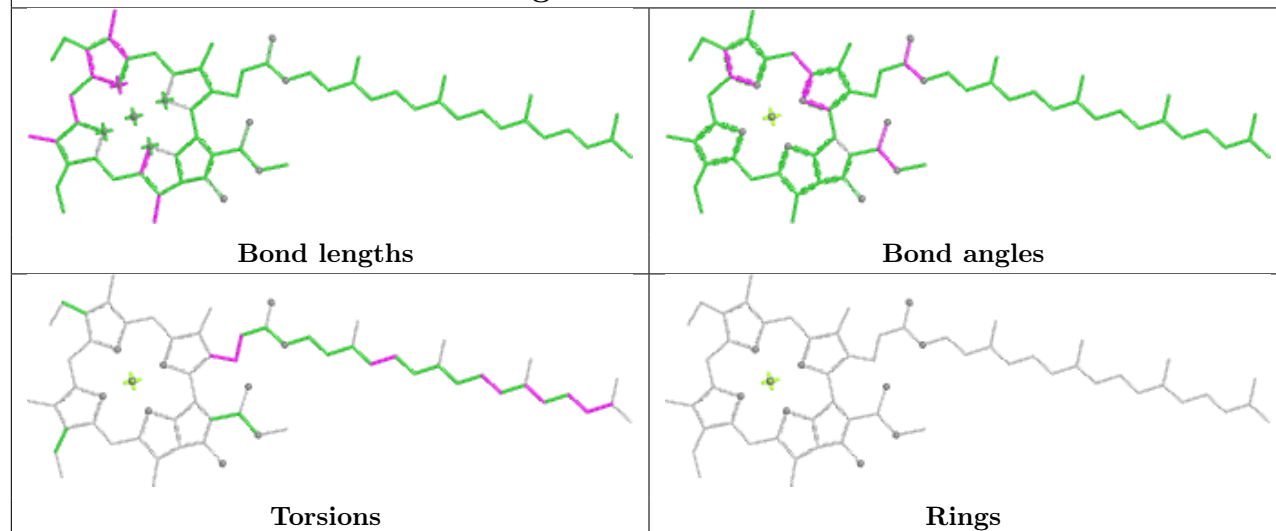




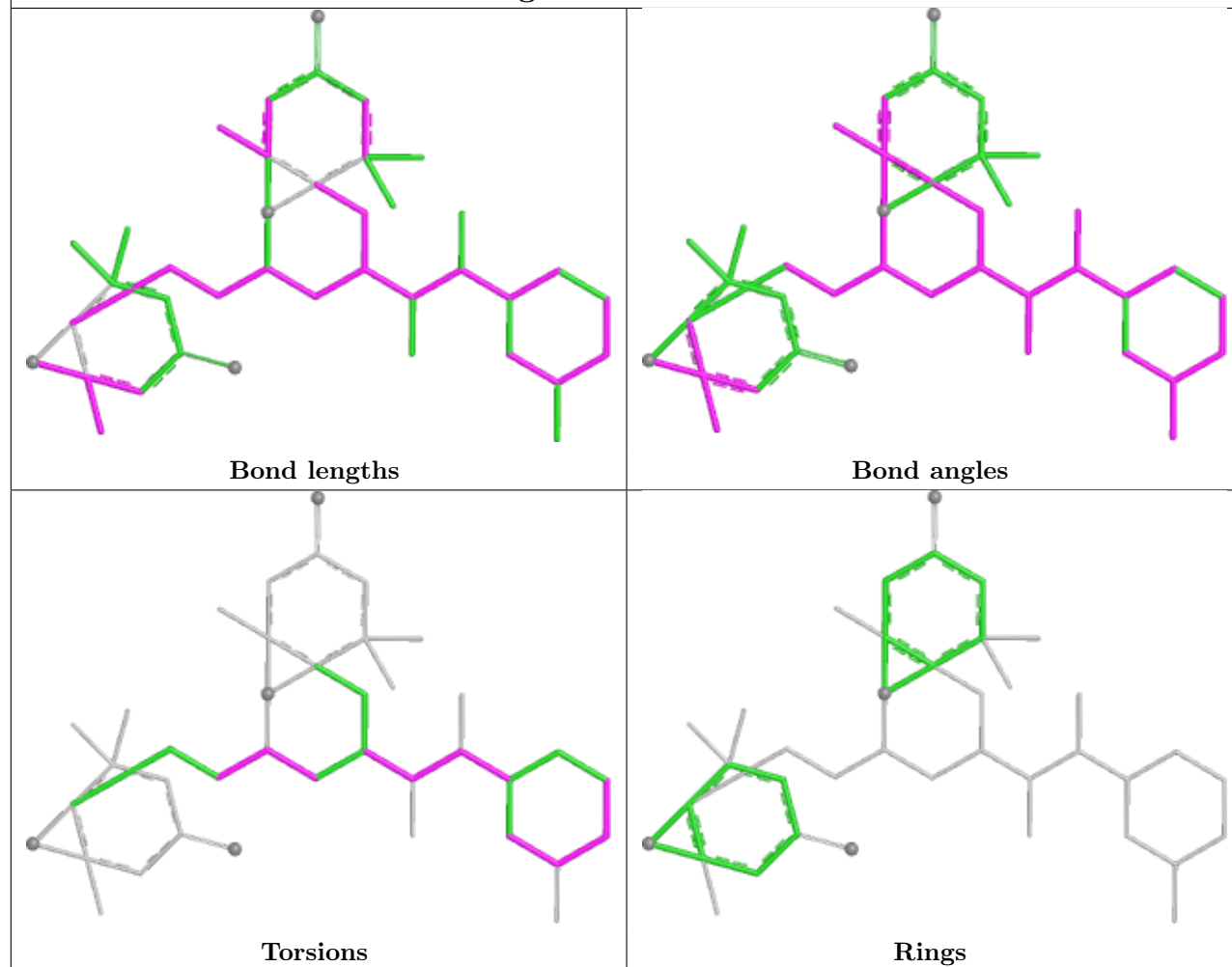


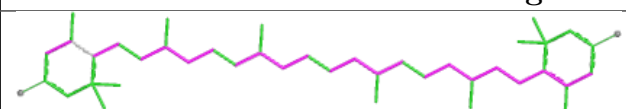
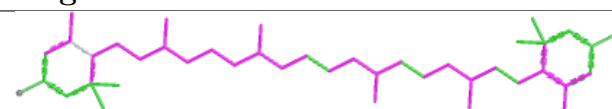
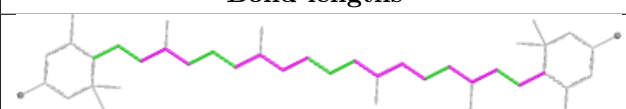
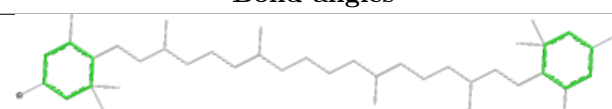


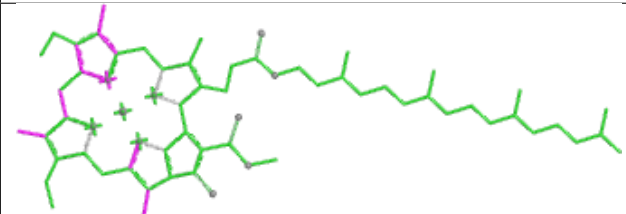
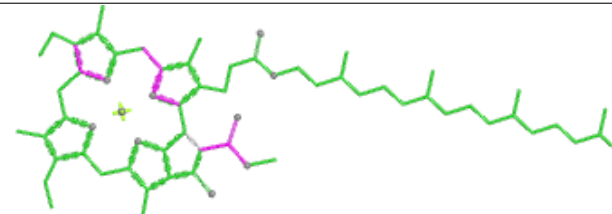
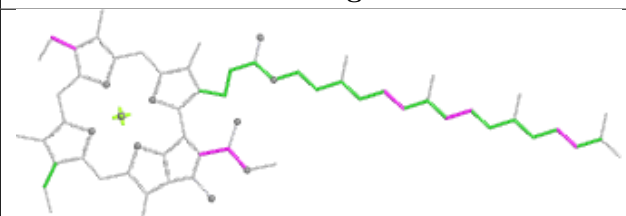
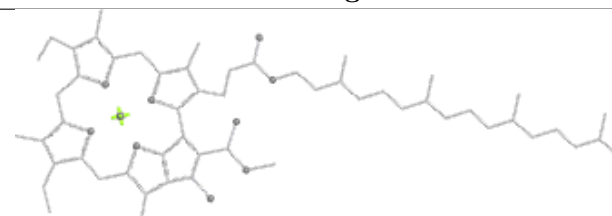
## Ligand CLA B 608

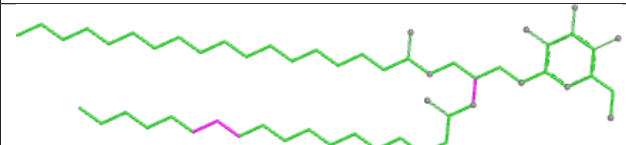
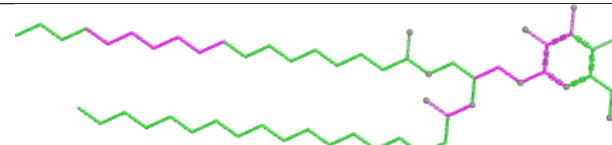
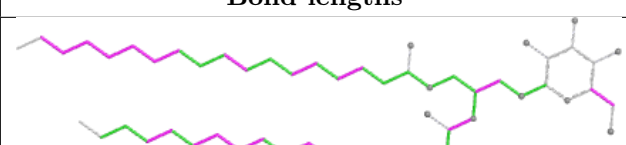
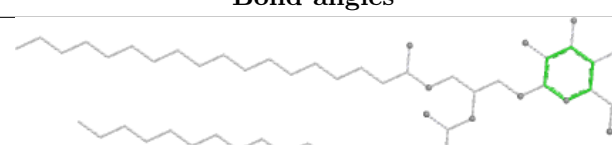


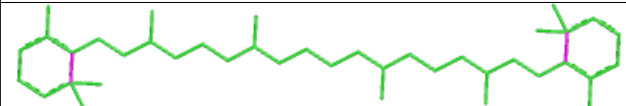
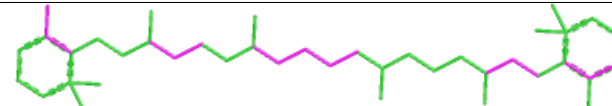
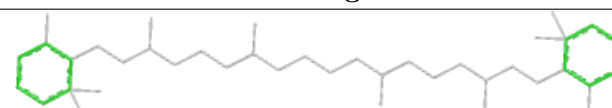
## Ligand XAT r 314

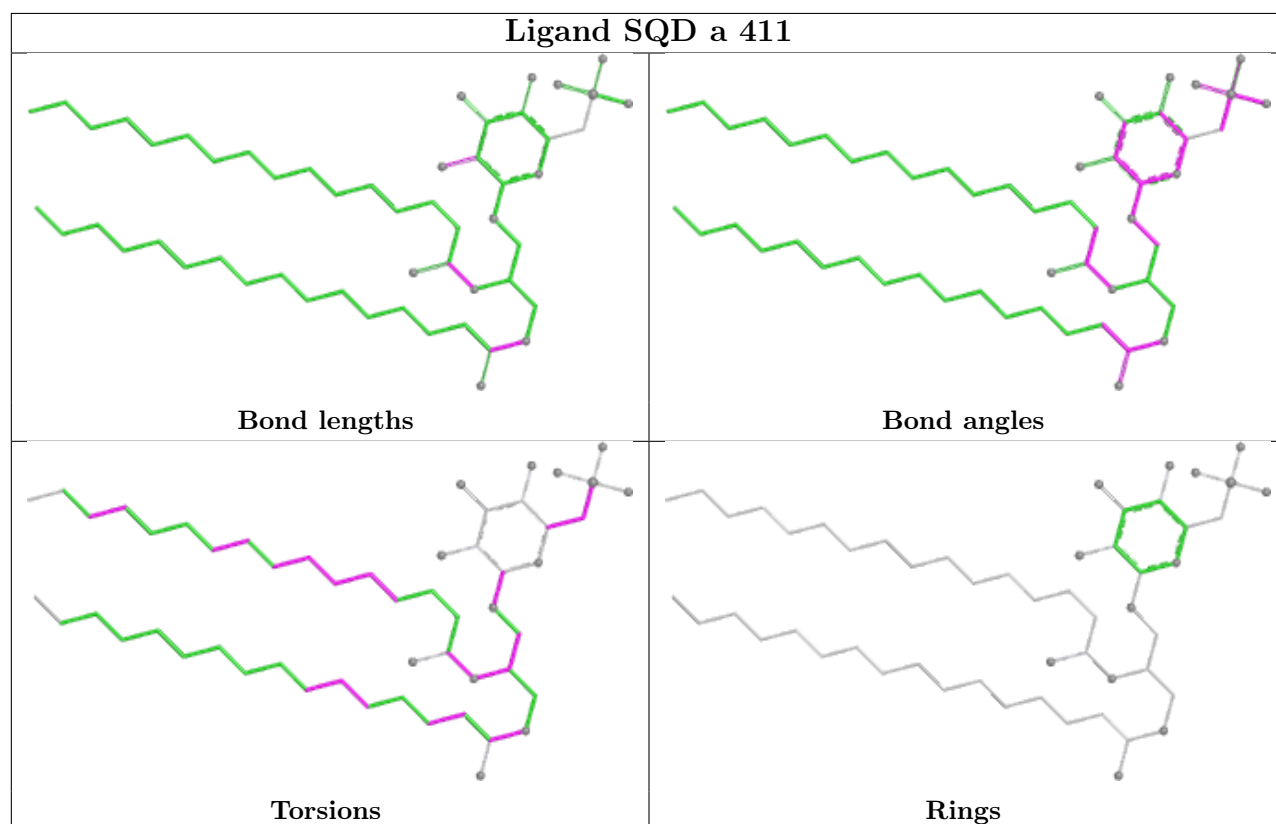
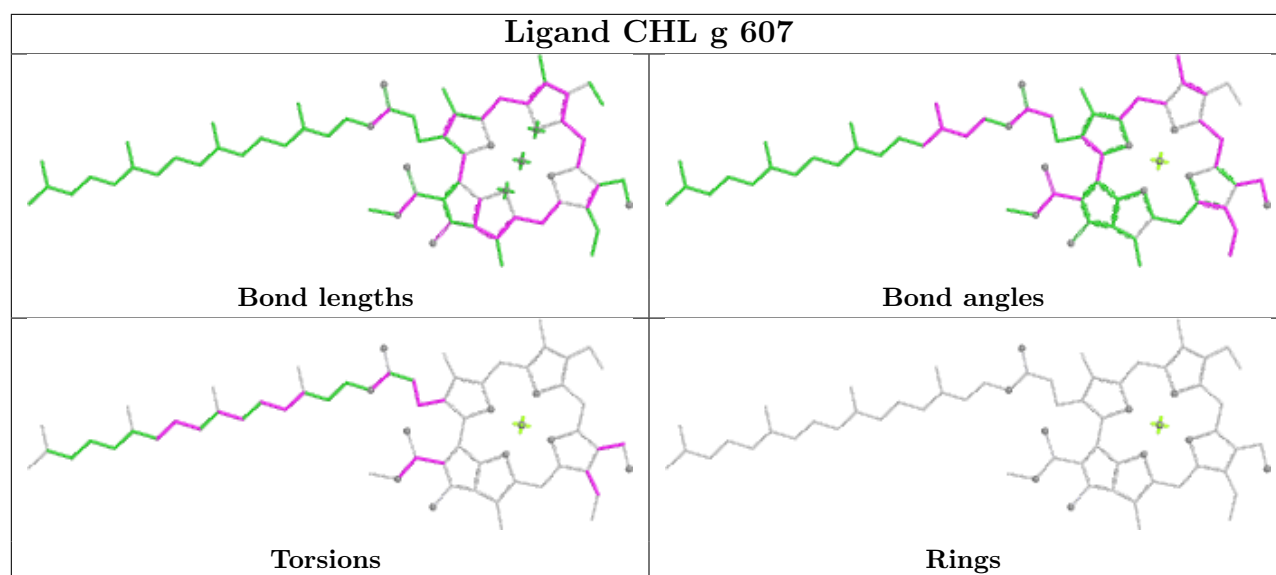


| Ligand LUT g 615                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

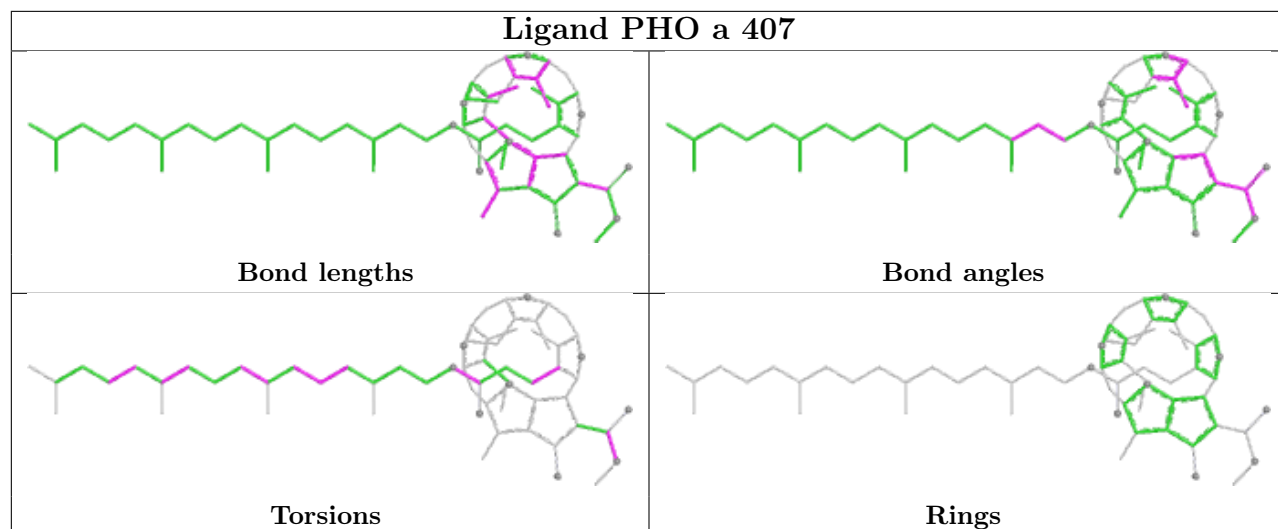
| Ligand CLA b 608                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

| Ligand LMG B 623                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

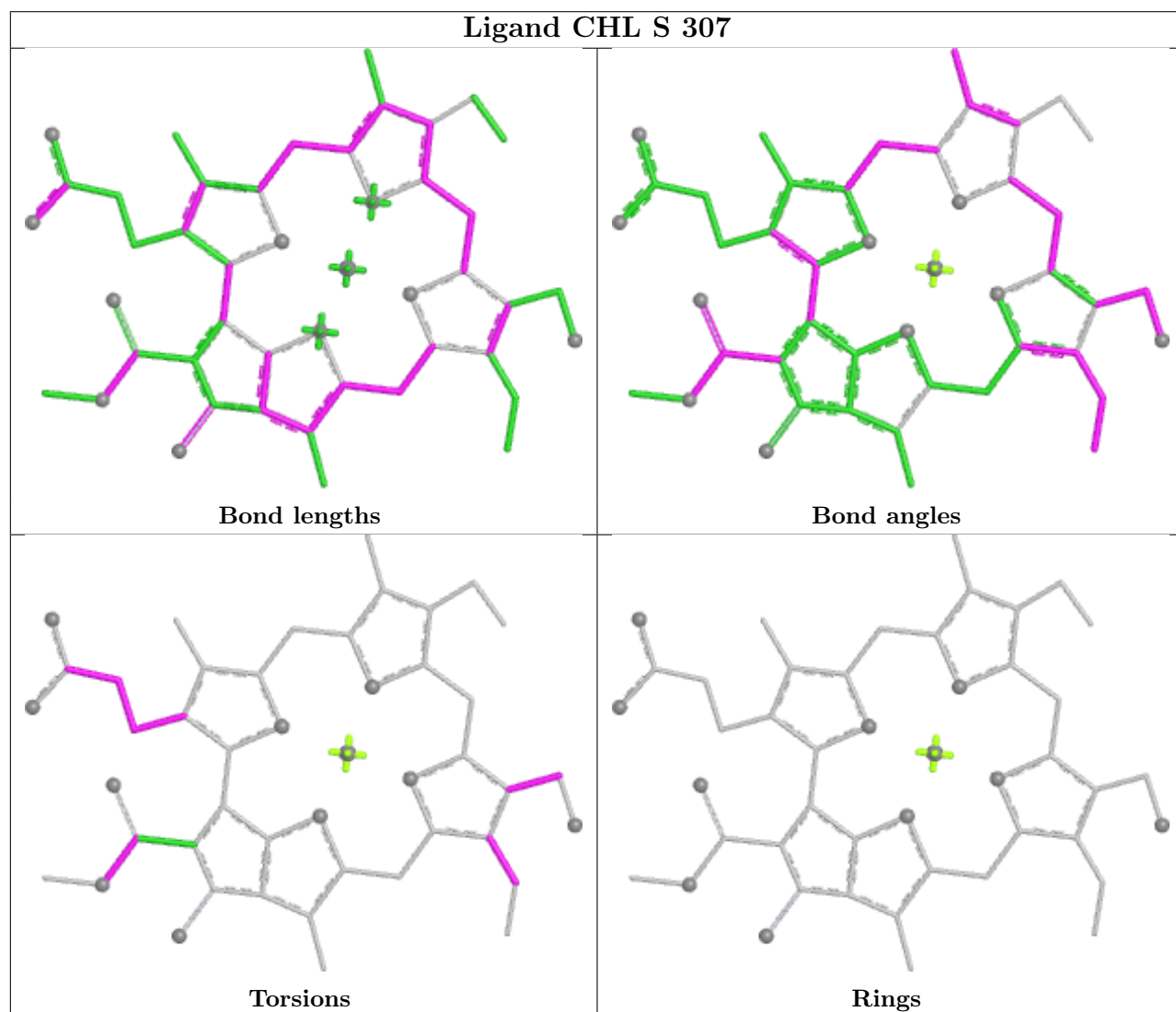
| Ligand BCR b 617                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

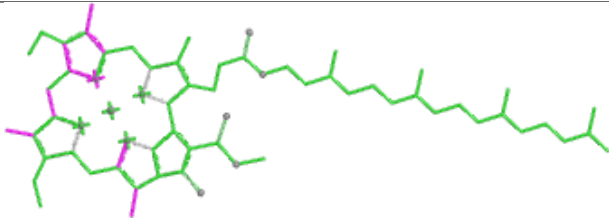
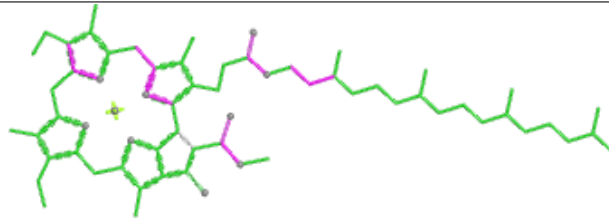
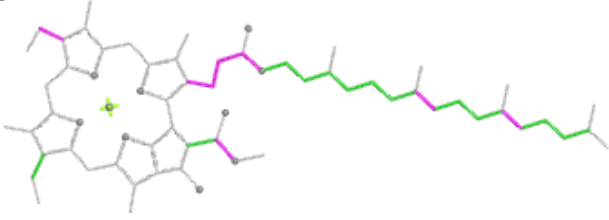
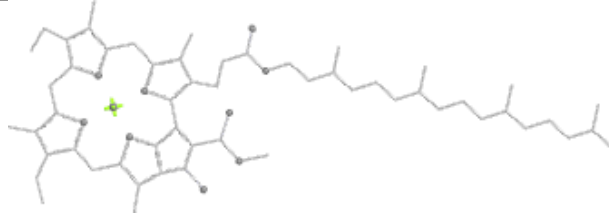


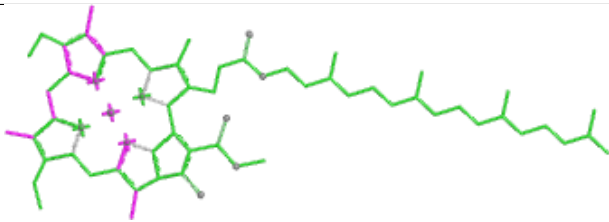
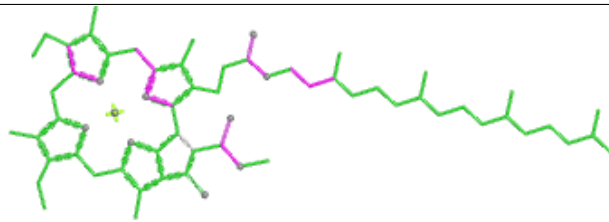
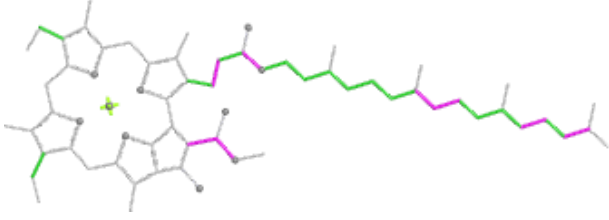
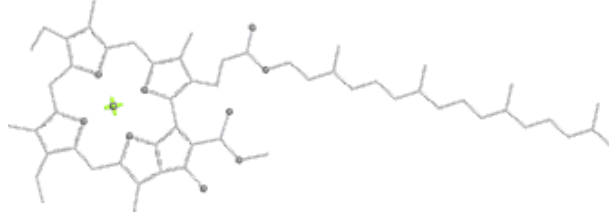
## Ligand PHO a 407

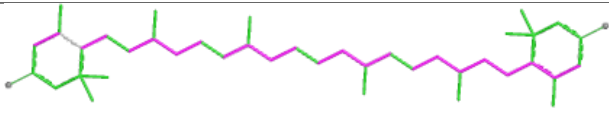
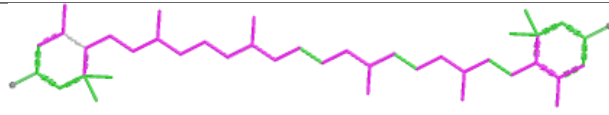
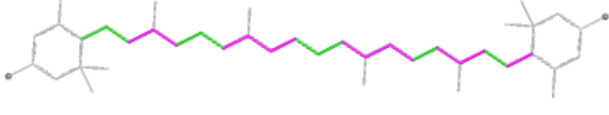
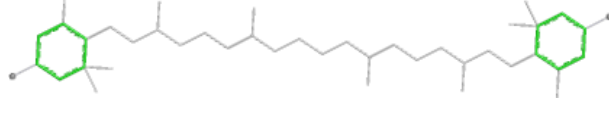


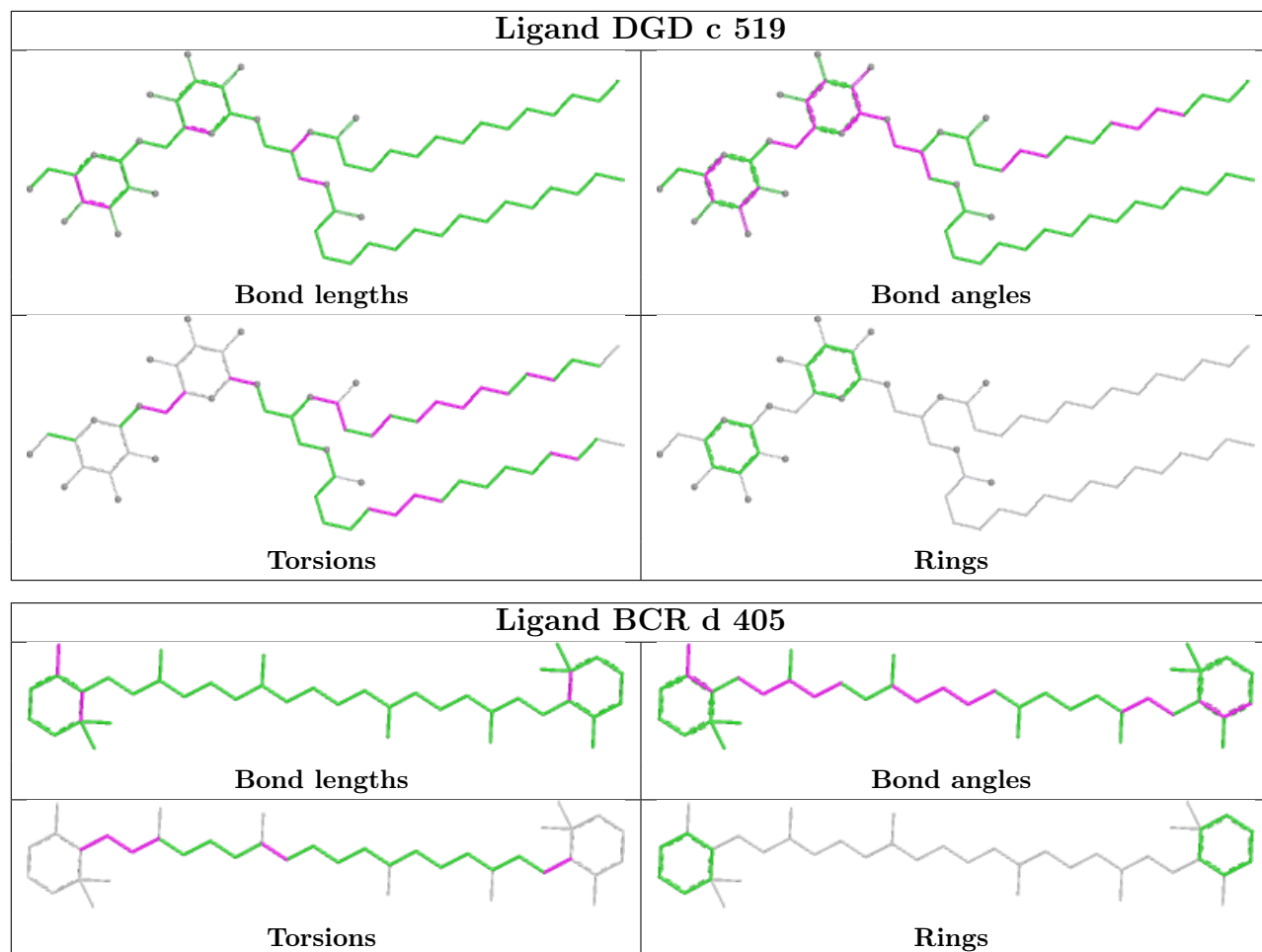
## Ligand CHL S 307



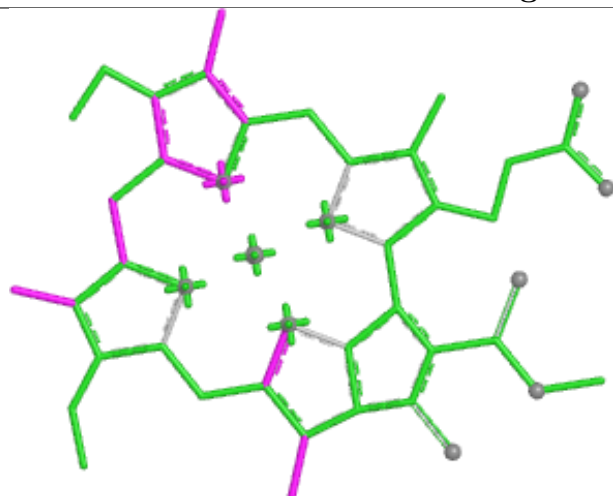
| Ligand CLA g 602                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand CLA c 503                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

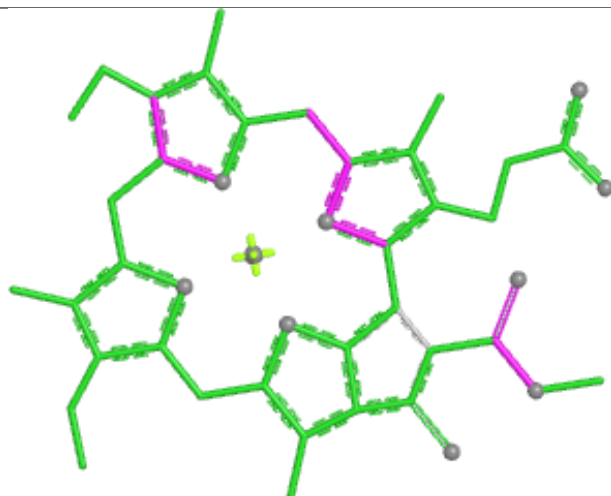
| Ligand LUT N 614                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



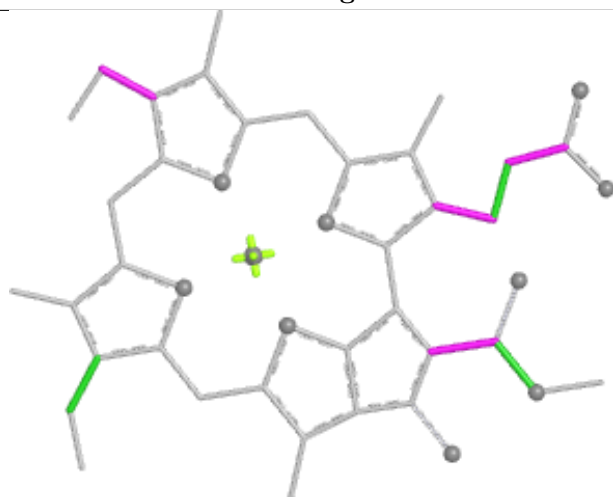
## Ligand CLA s 304



Bond lengths



Bond angles

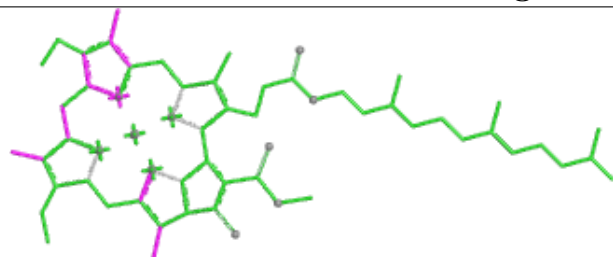


Torsions

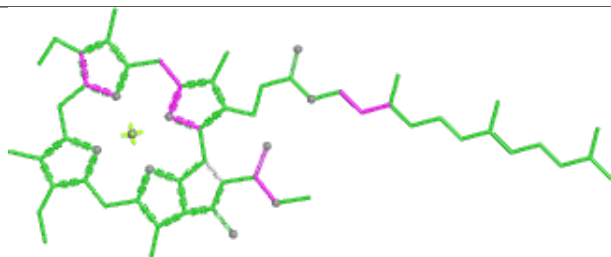


Rings

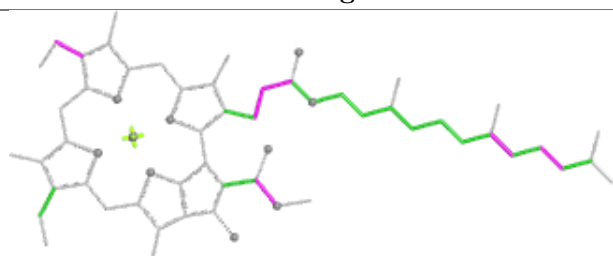
## Ligand CLA R 302



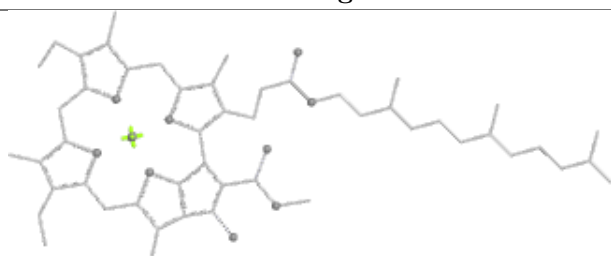
Bond lengths



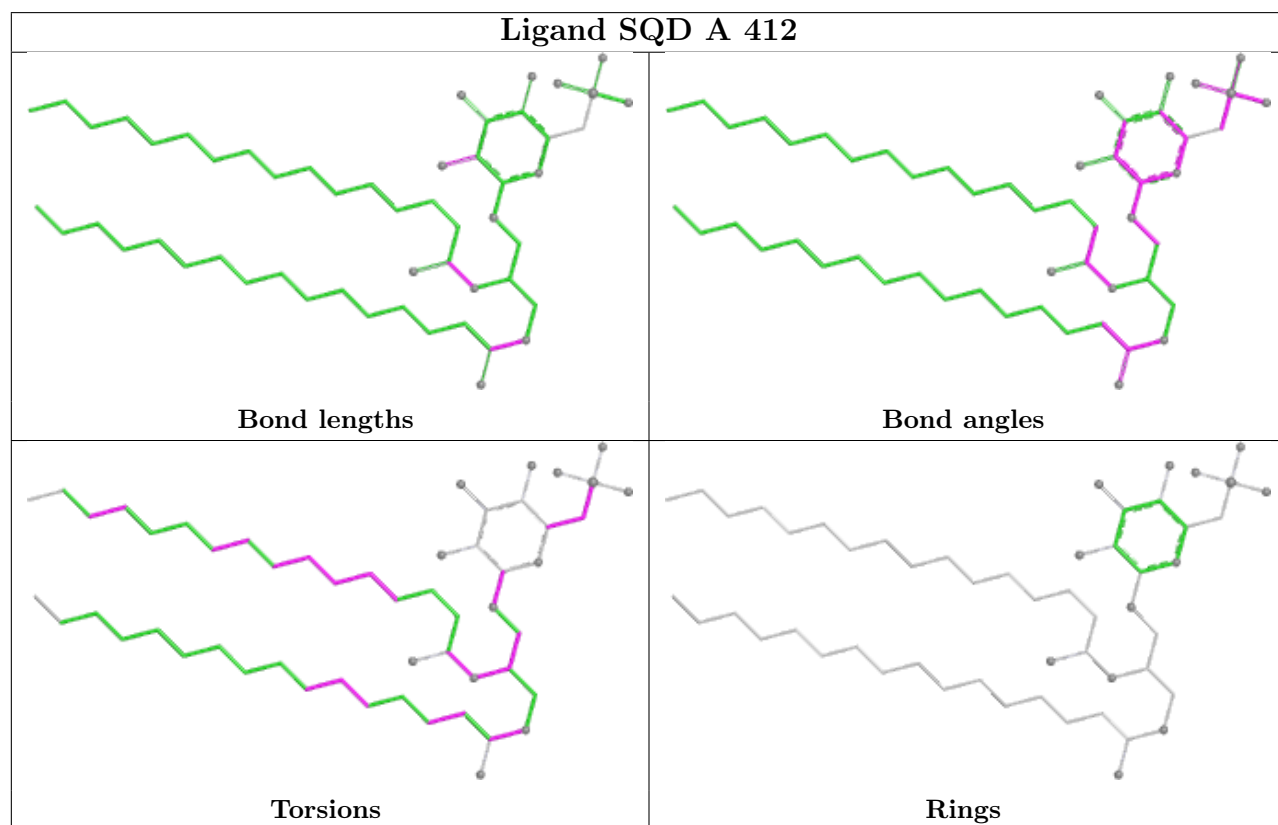
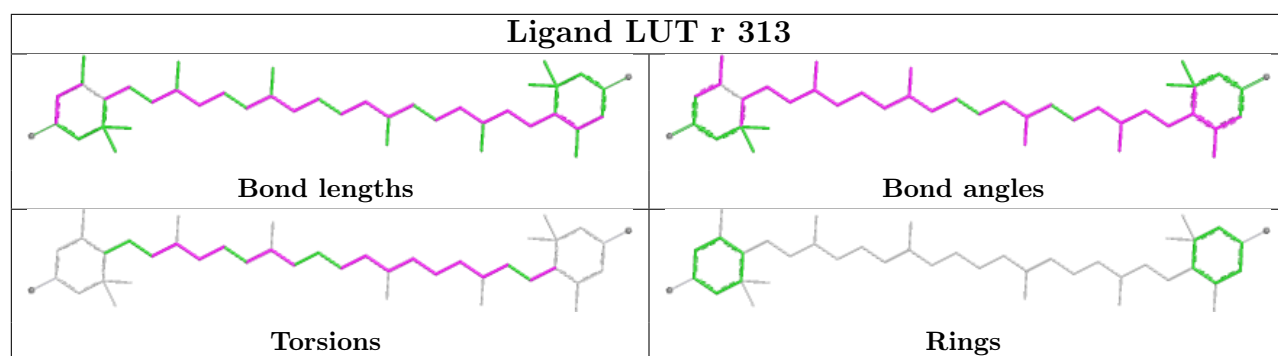
Bond angles



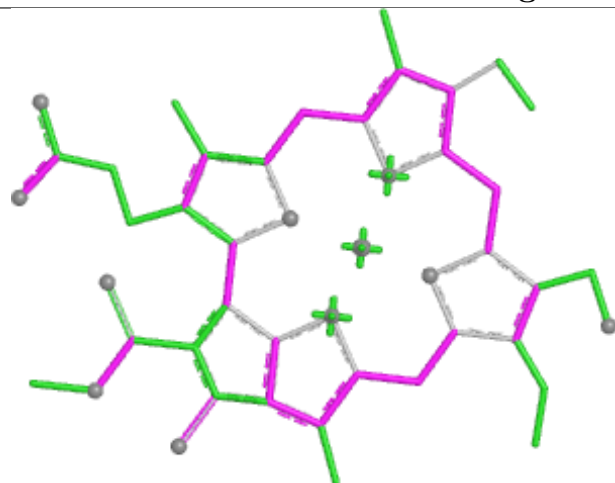
Torsions



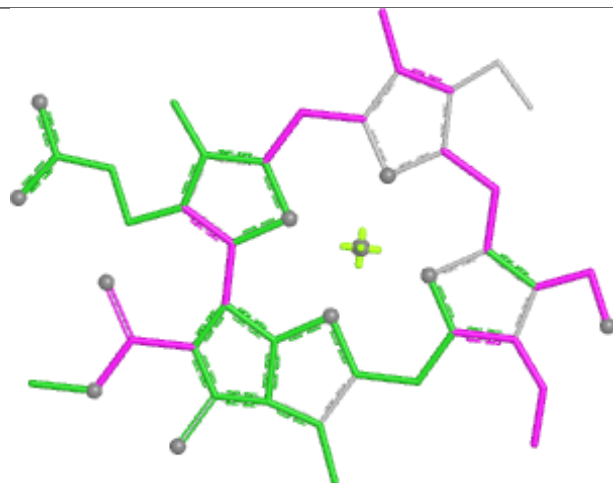
Rings



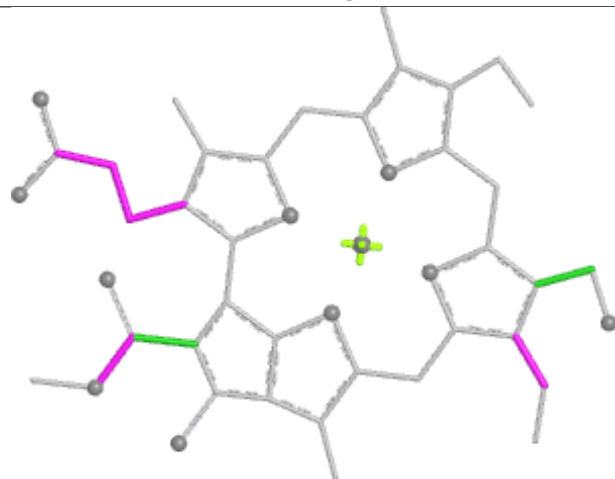
## Ligand CHL S 302



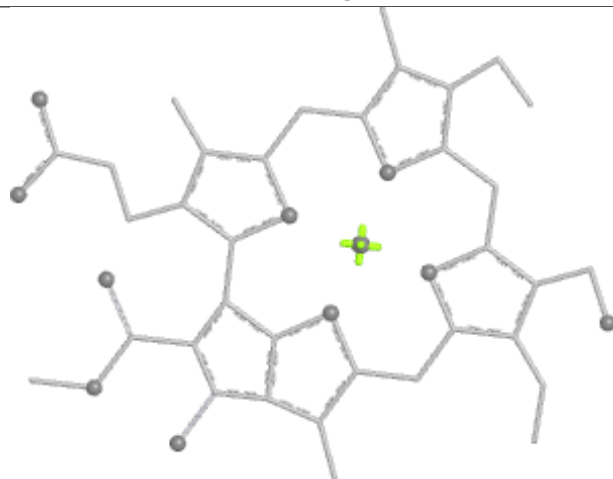
Bond lengths



Bond angles

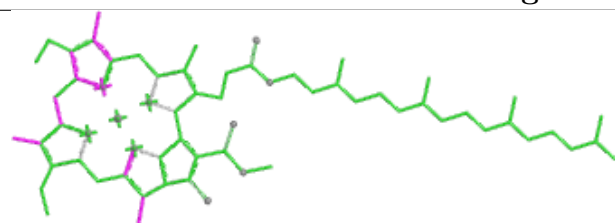


Torsions

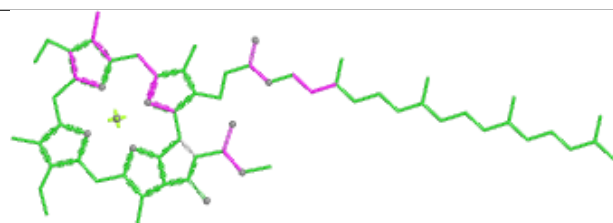


Rings

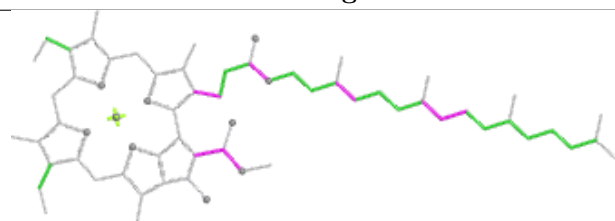
## Ligand CLA c 504



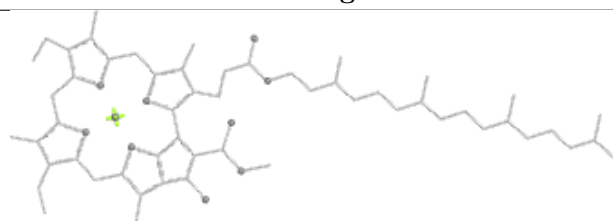
Bond lengths



Bond angles

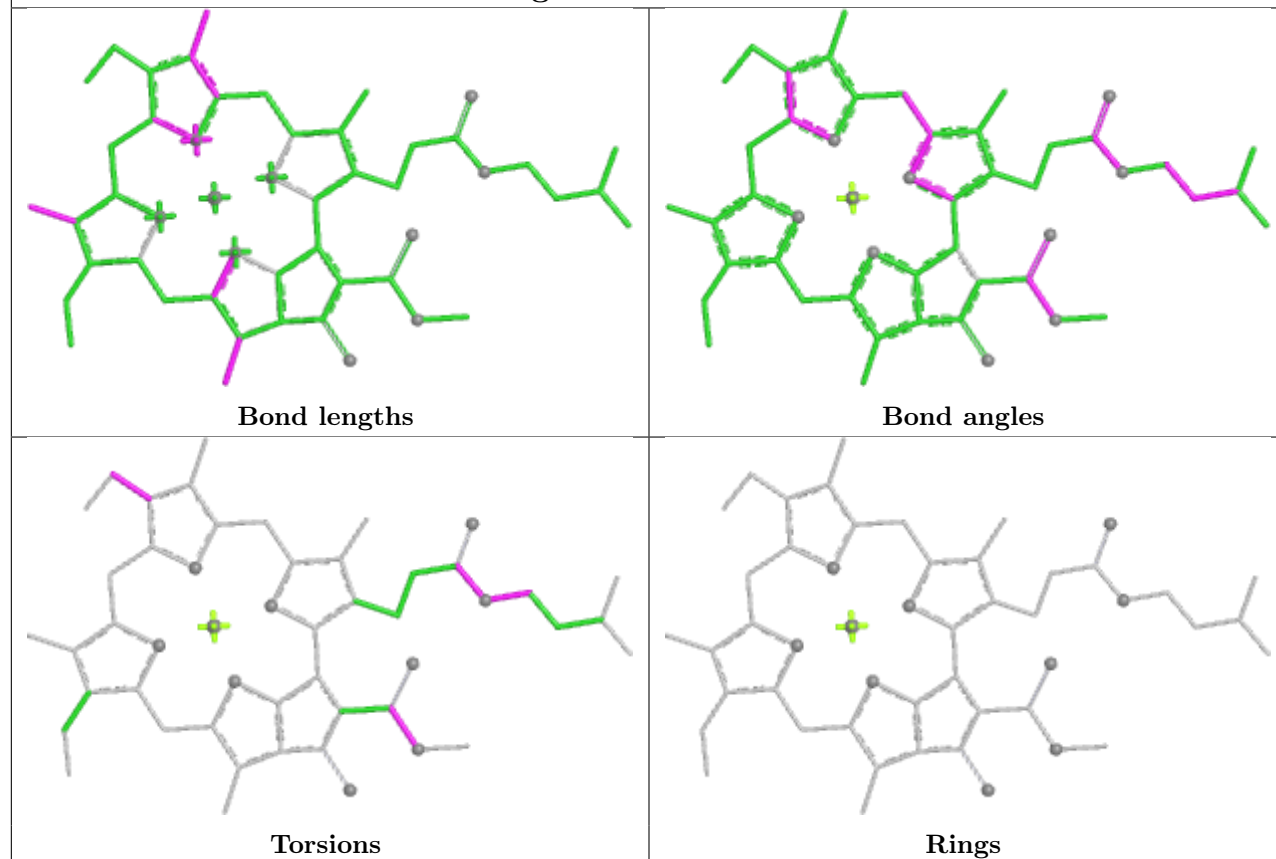


Torsions

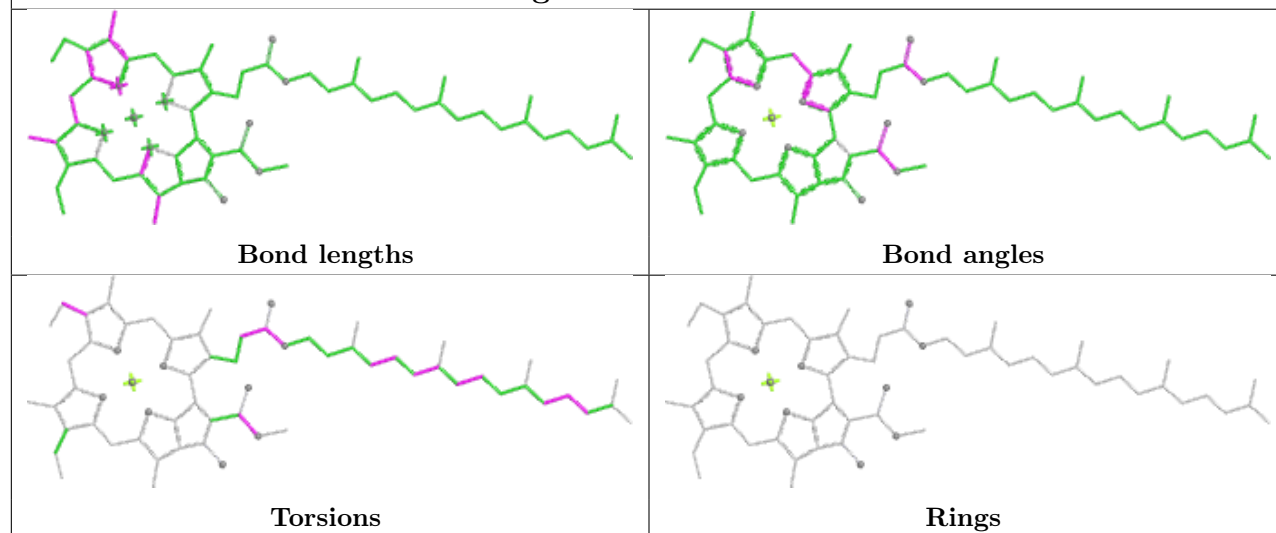


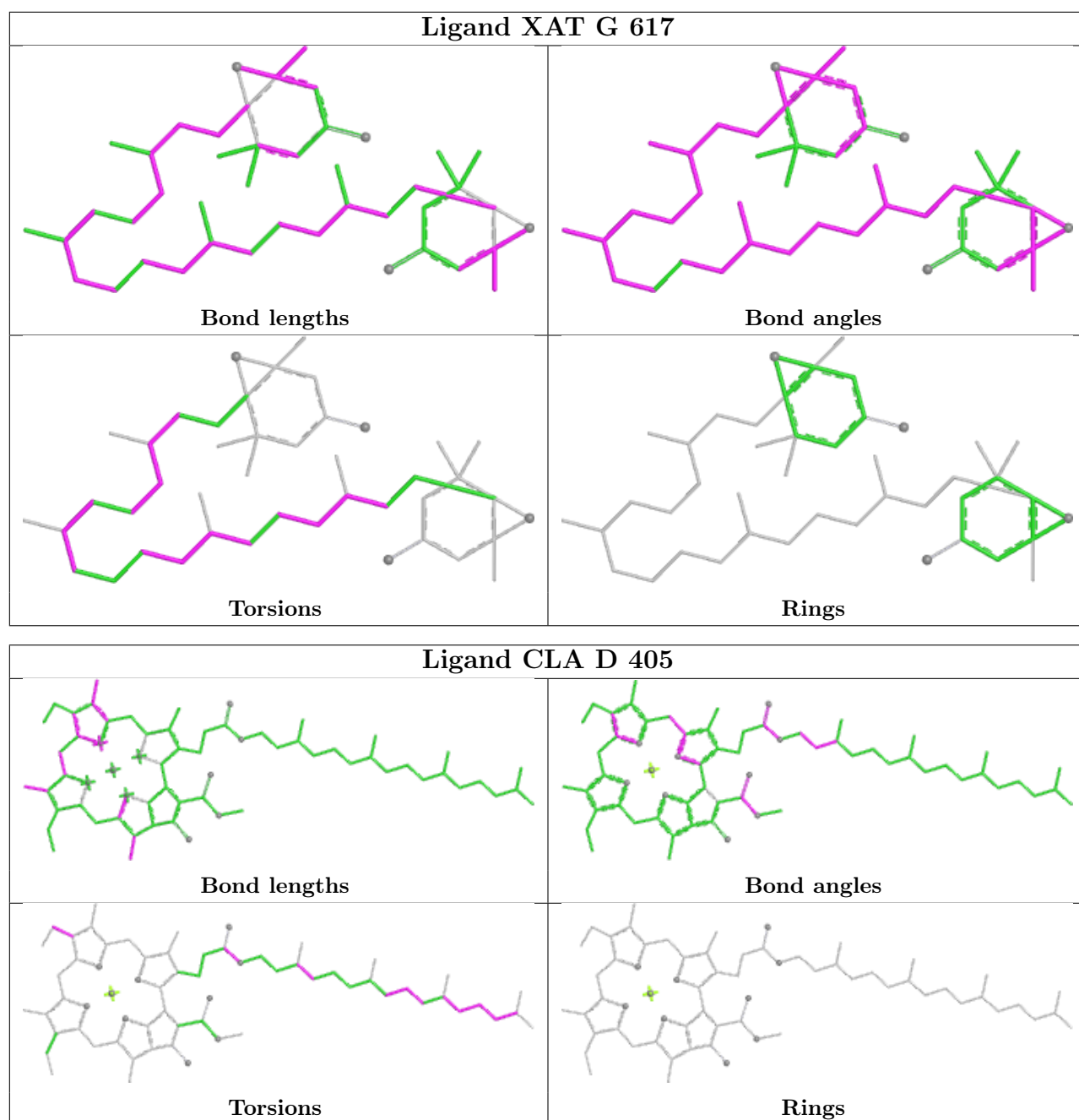
Rings

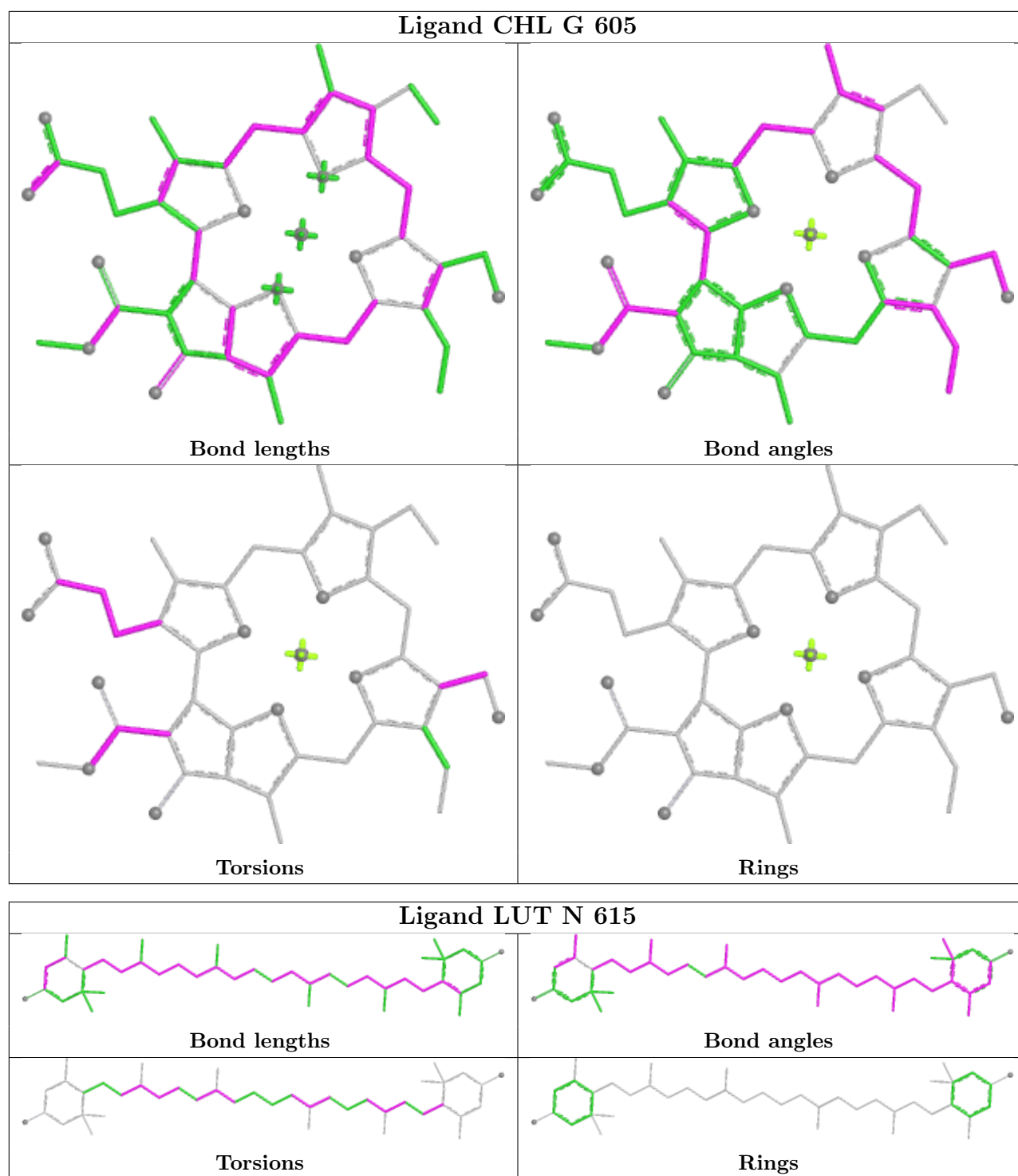
## Ligand CLA Y 604

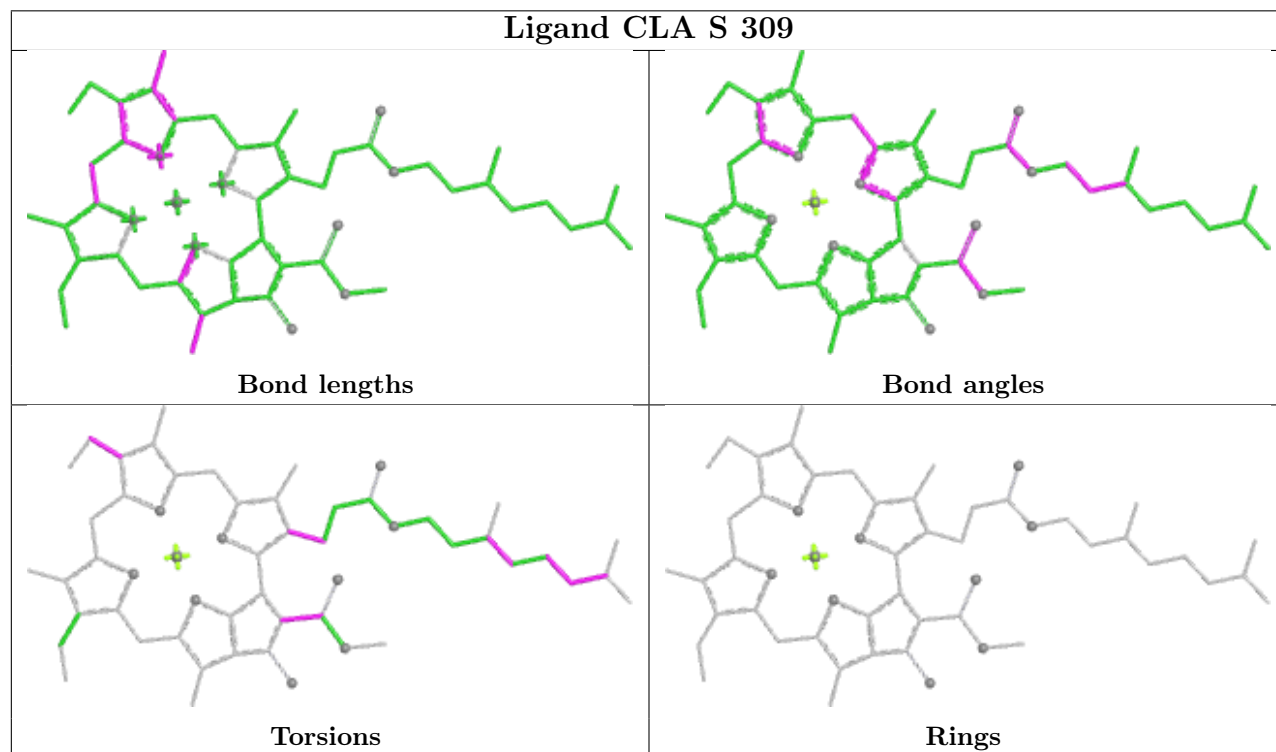
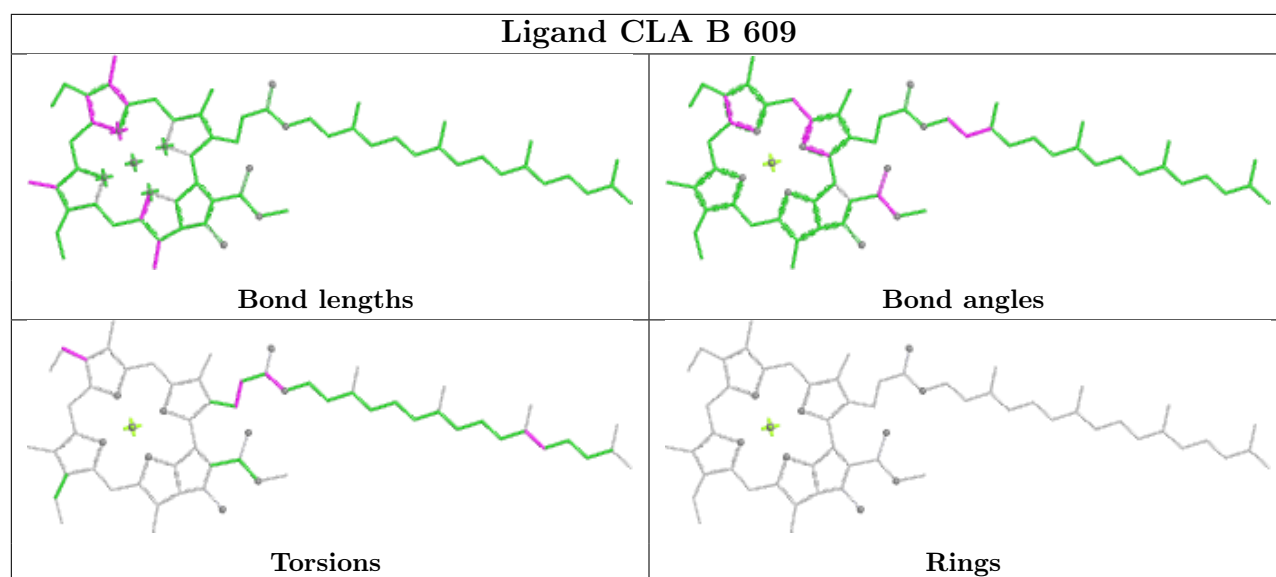


## Ligand CLA B 618

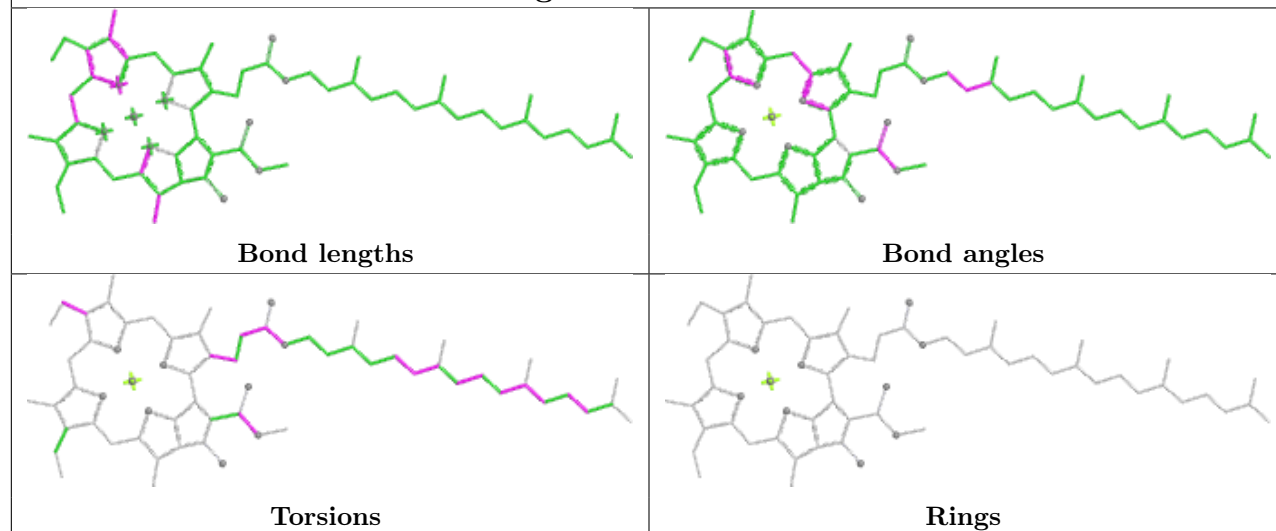




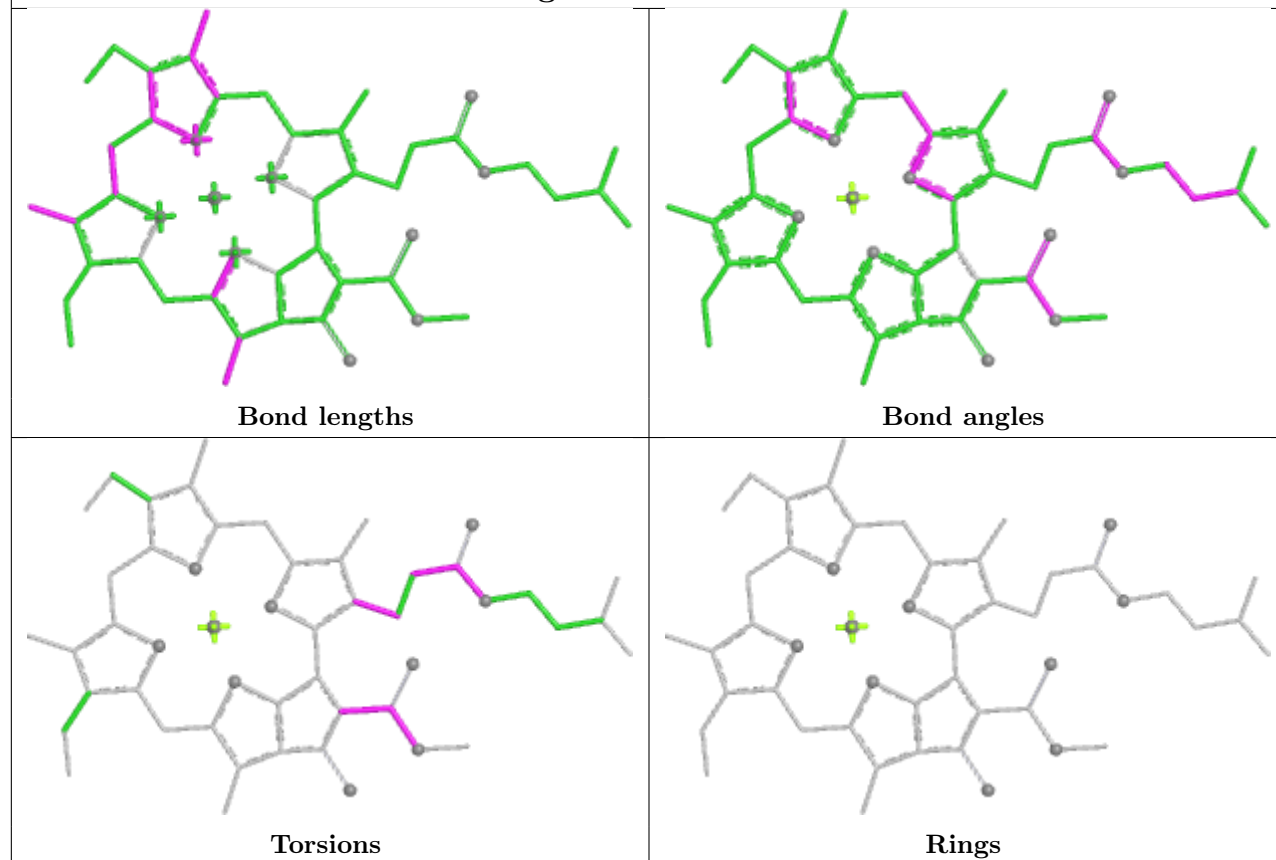


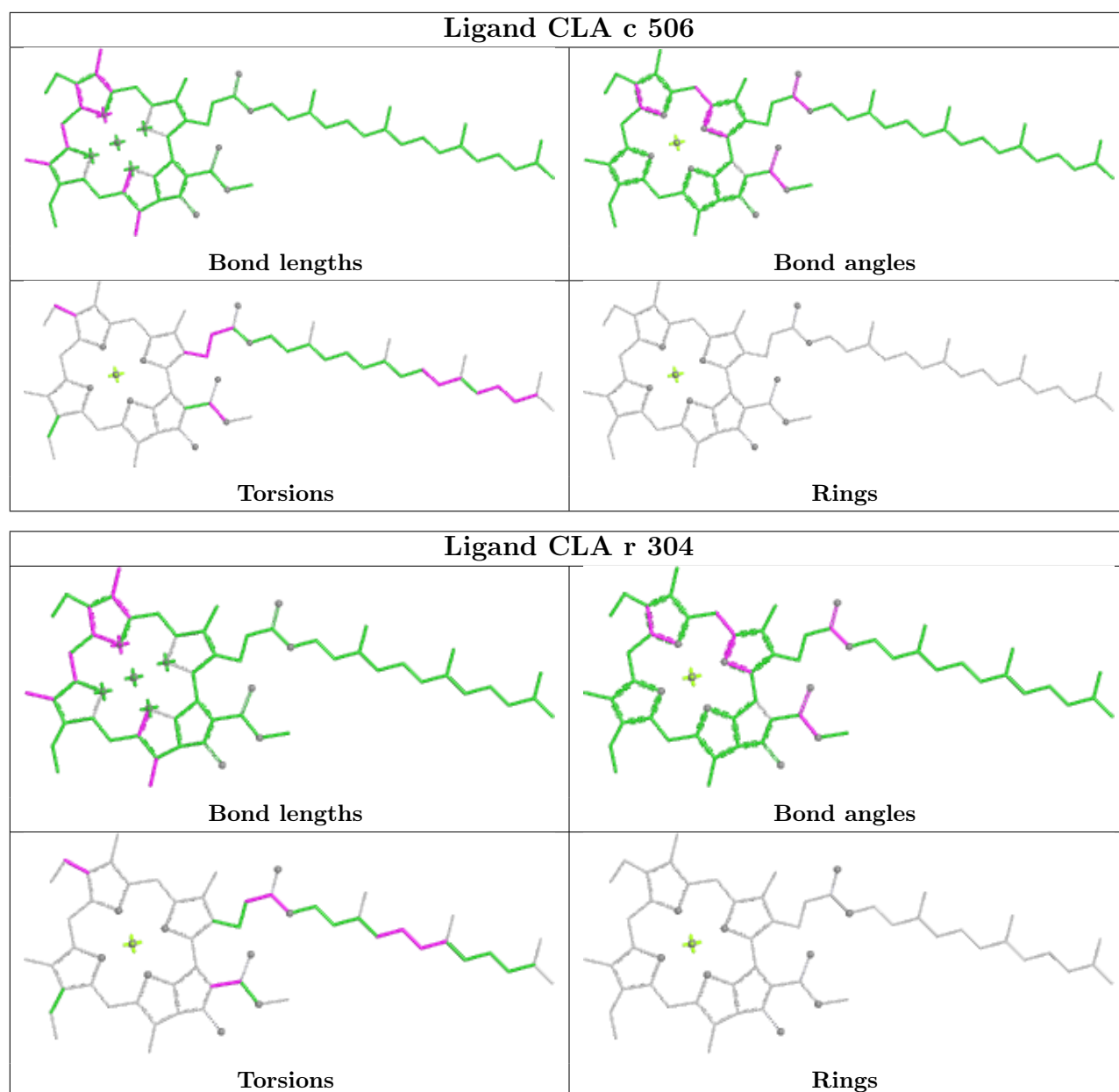


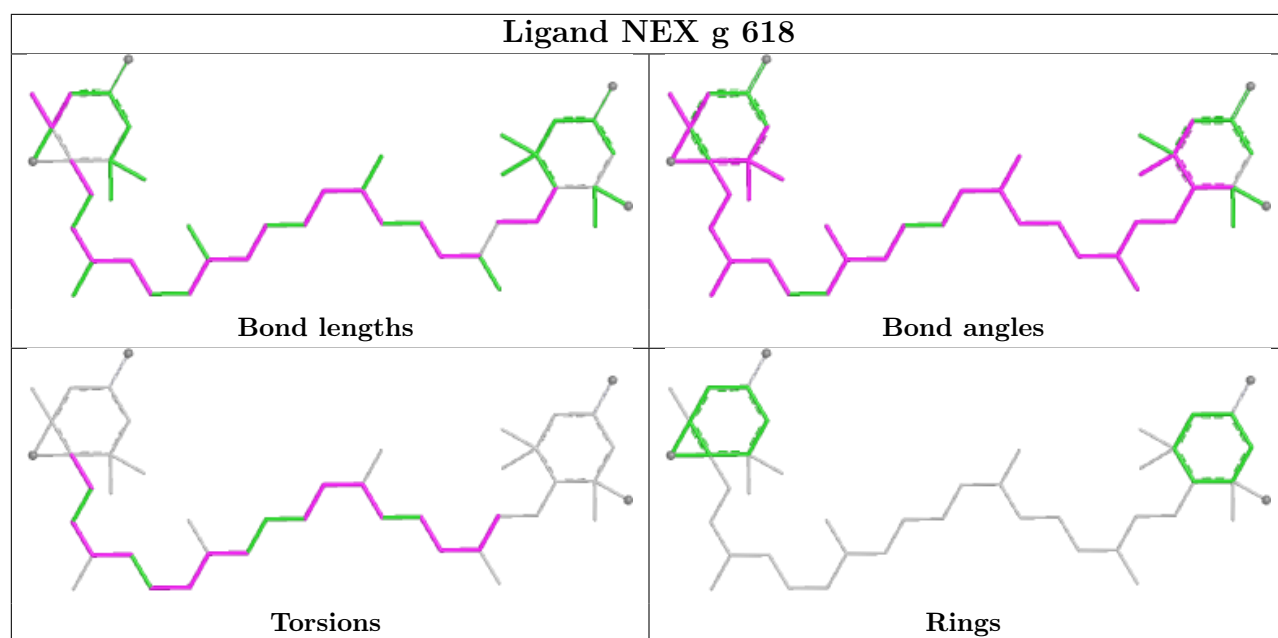
## Ligand CLA n 609

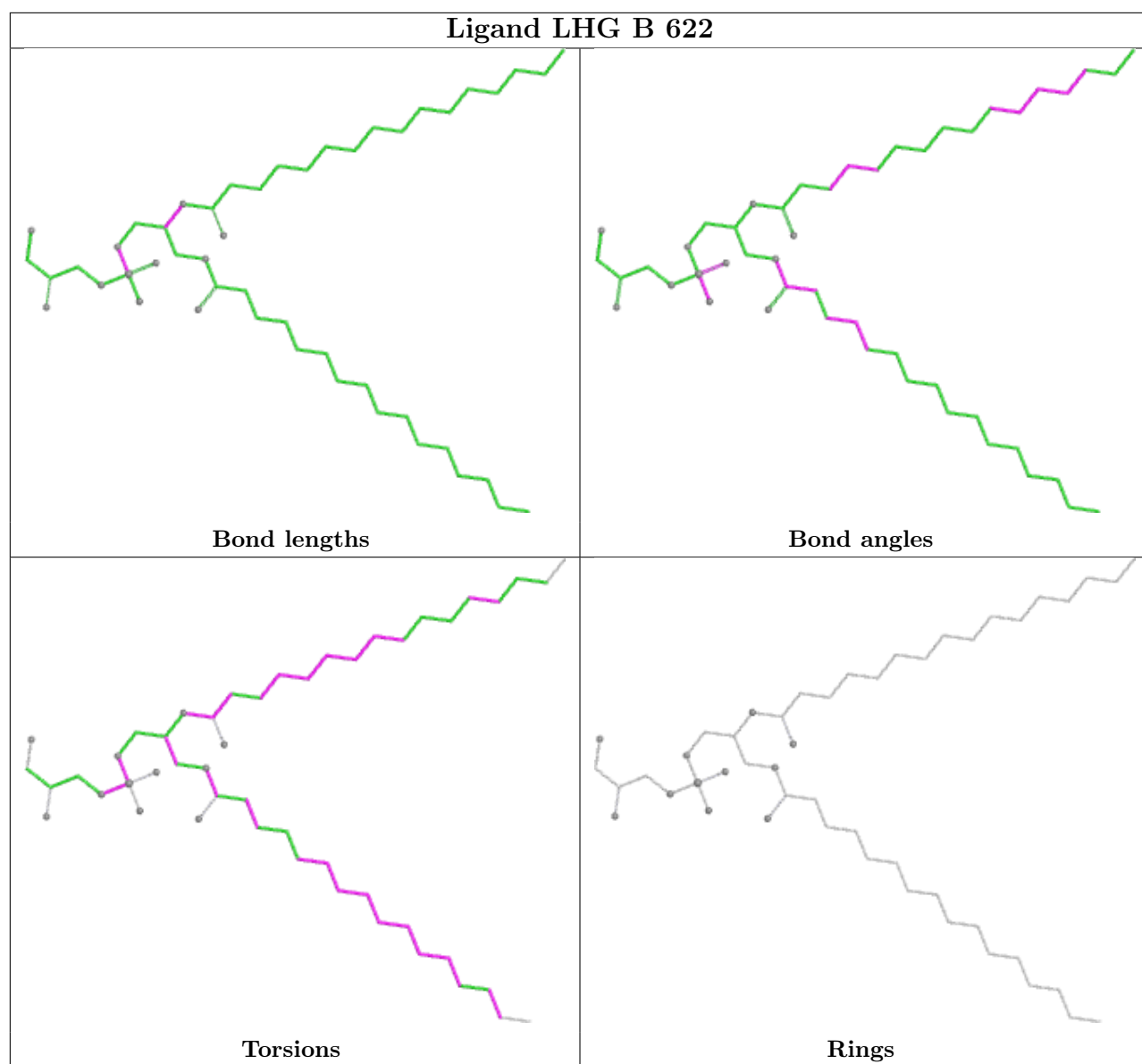


## Ligand CLA s 305

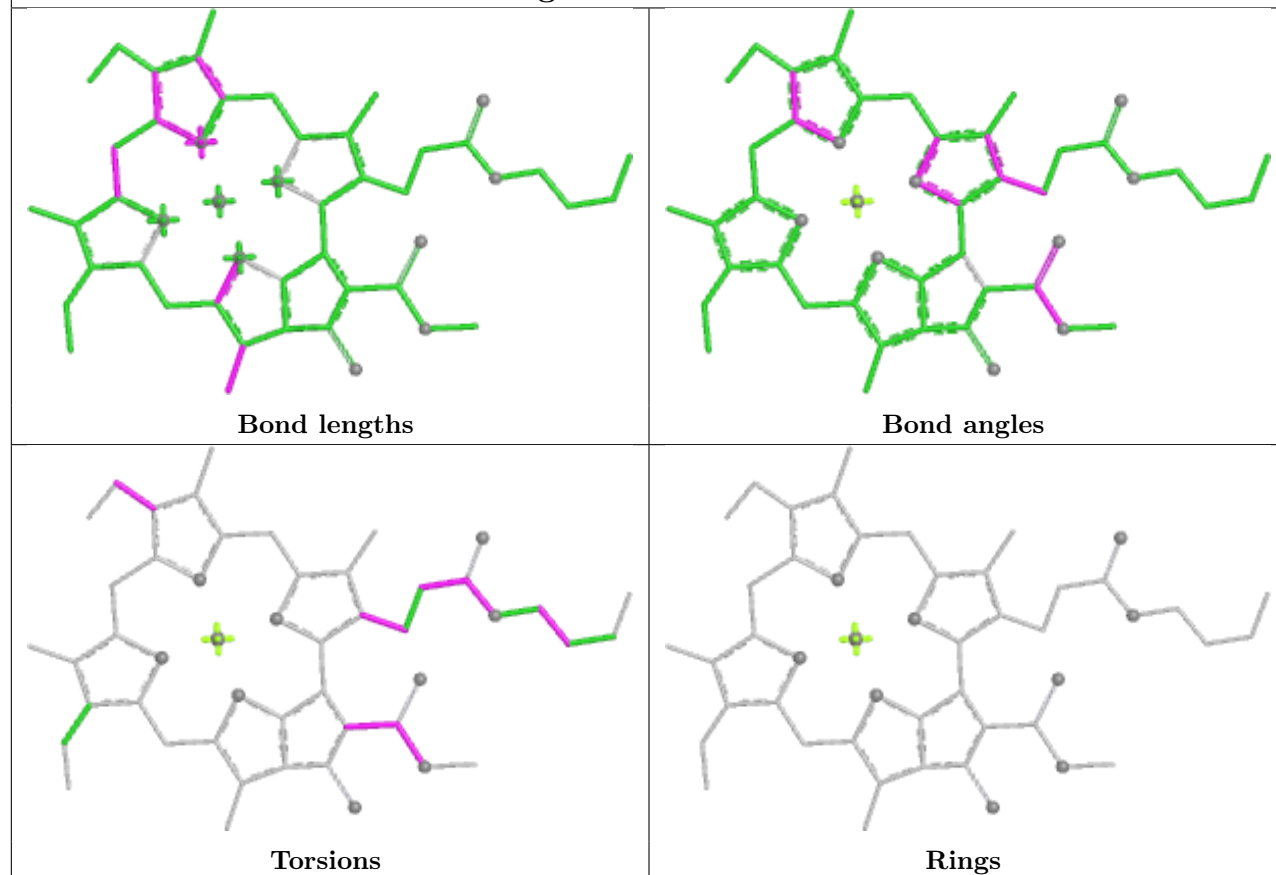




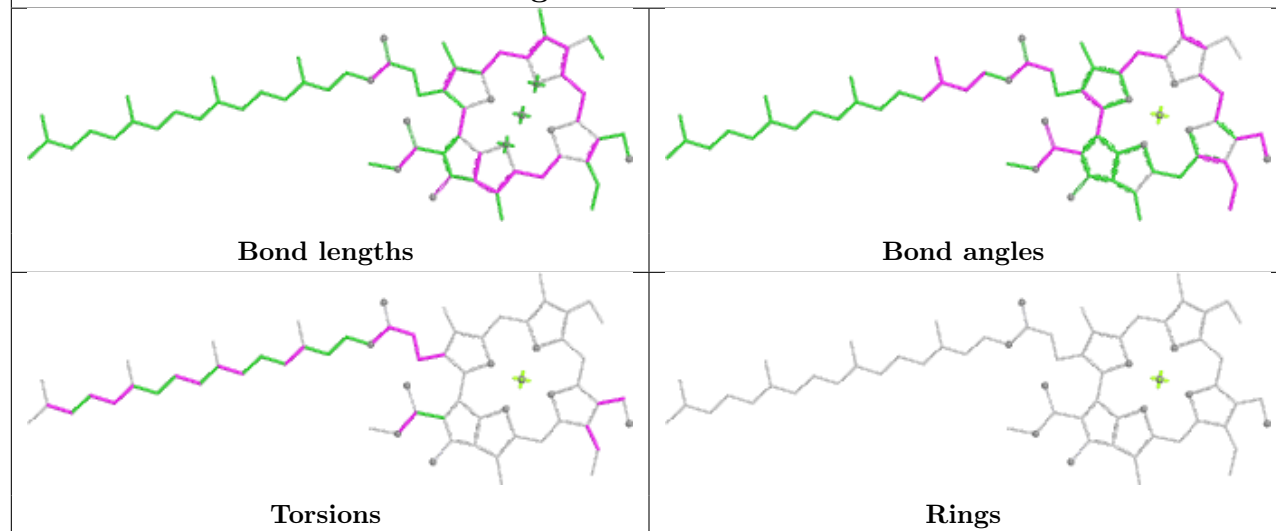


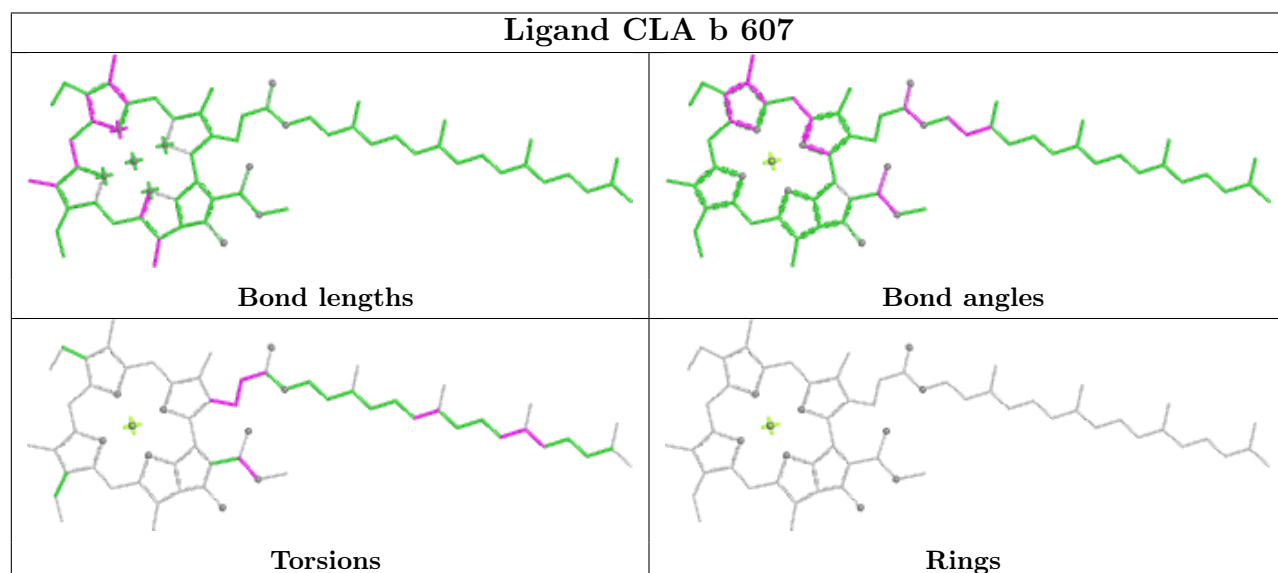
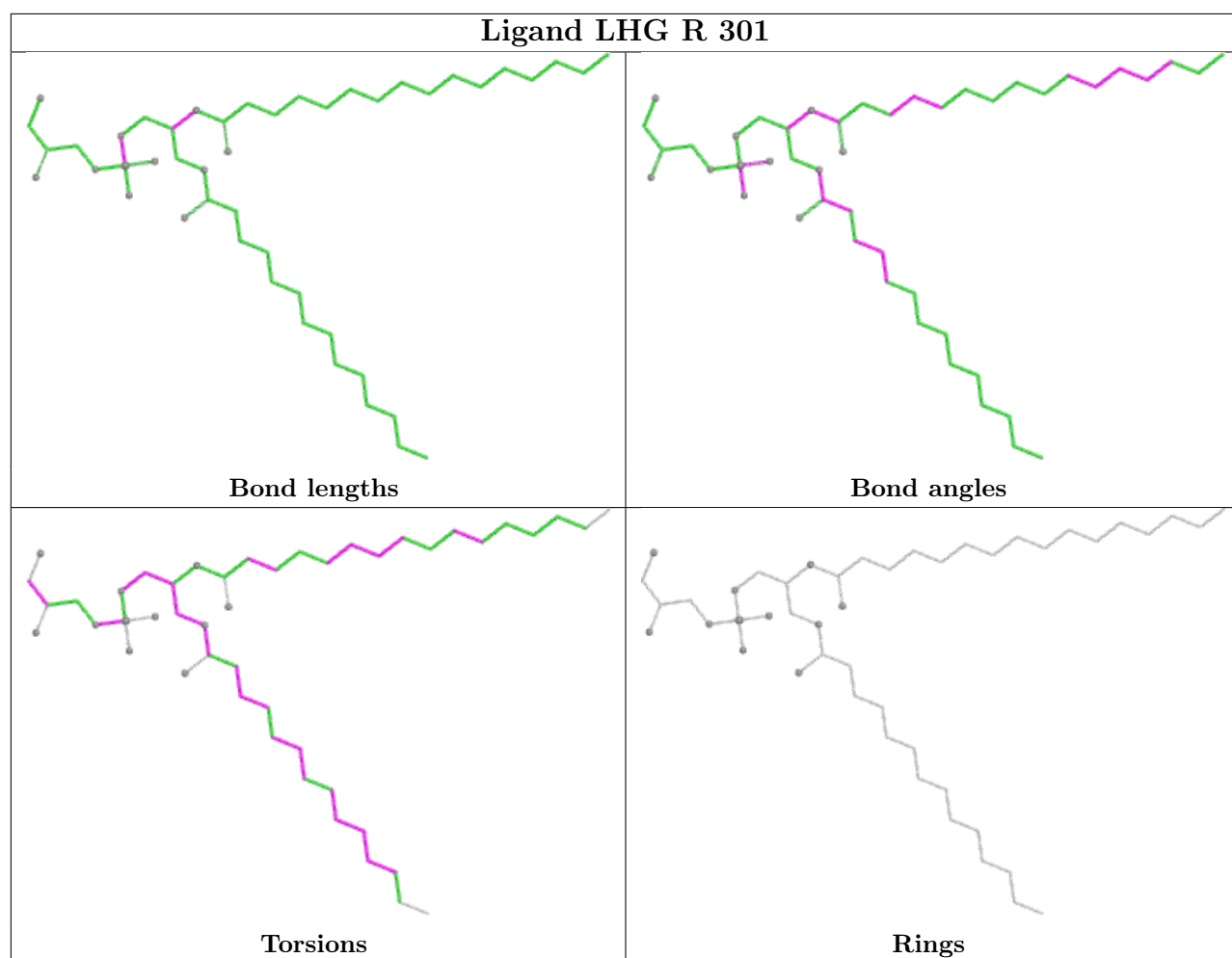


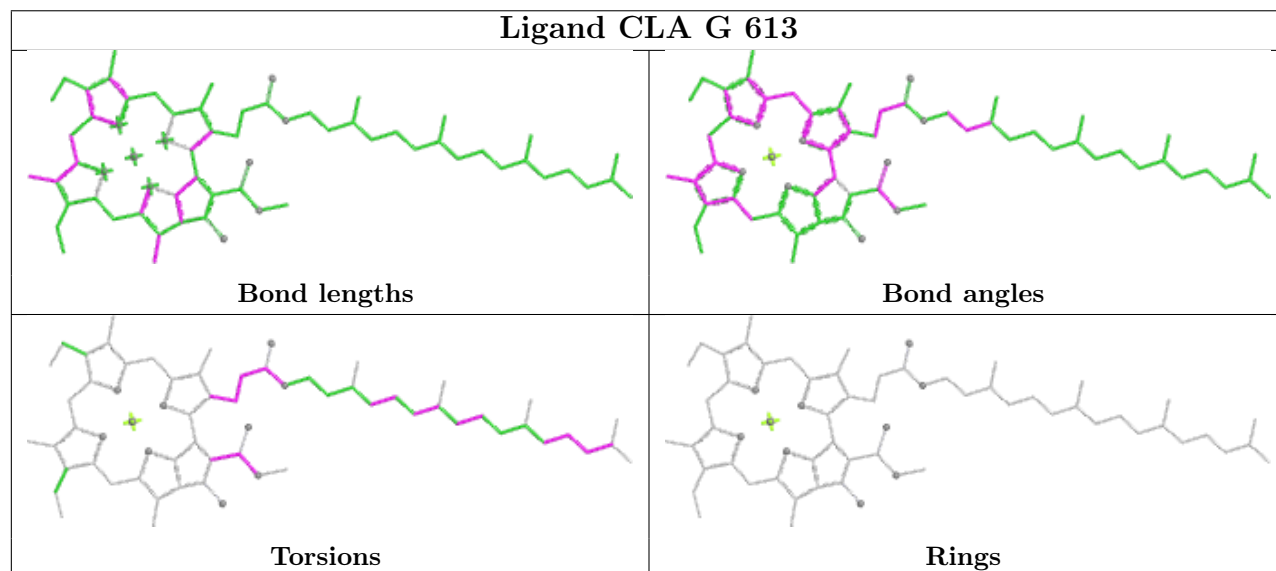
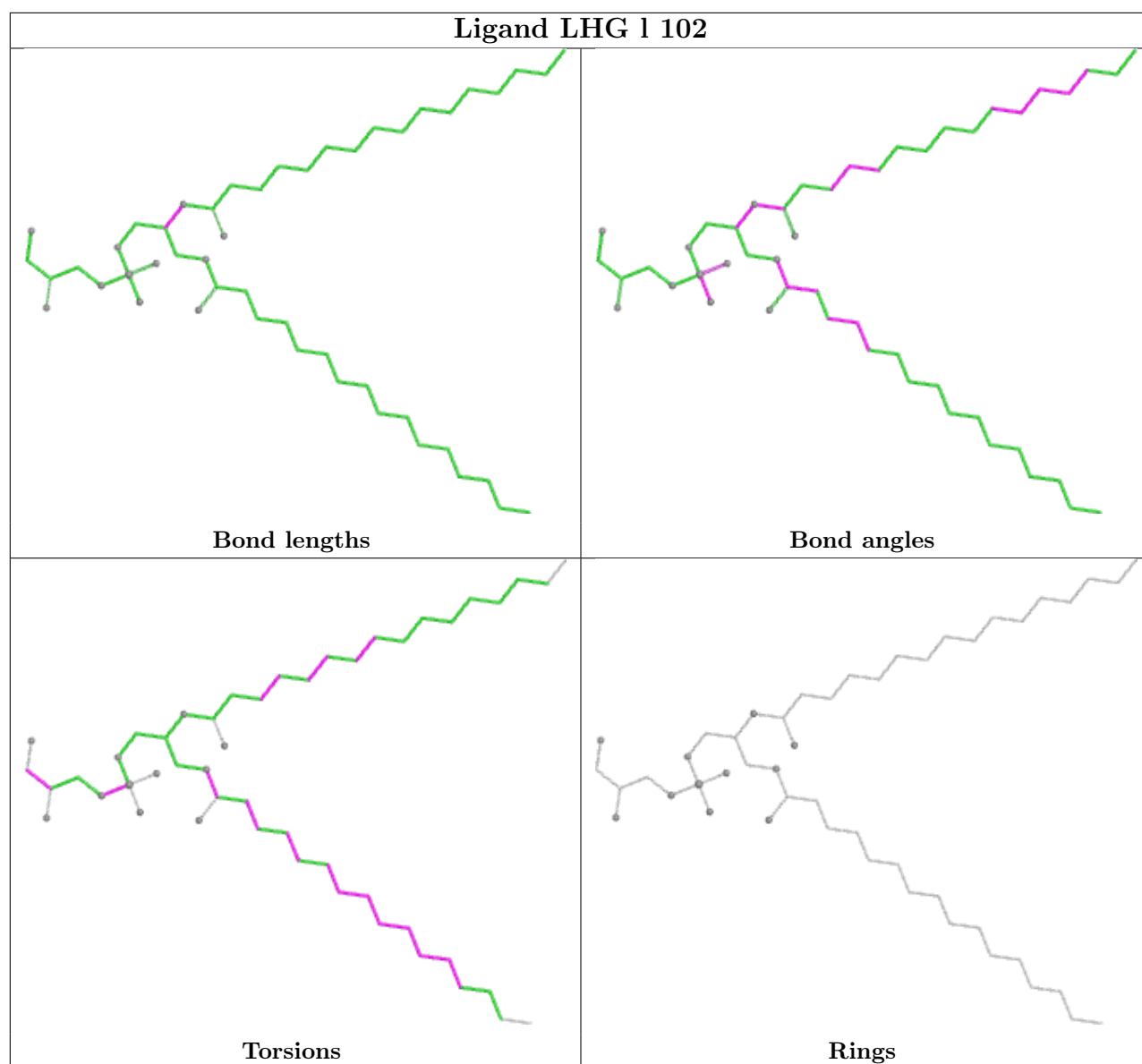
## Ligand CLA r 311

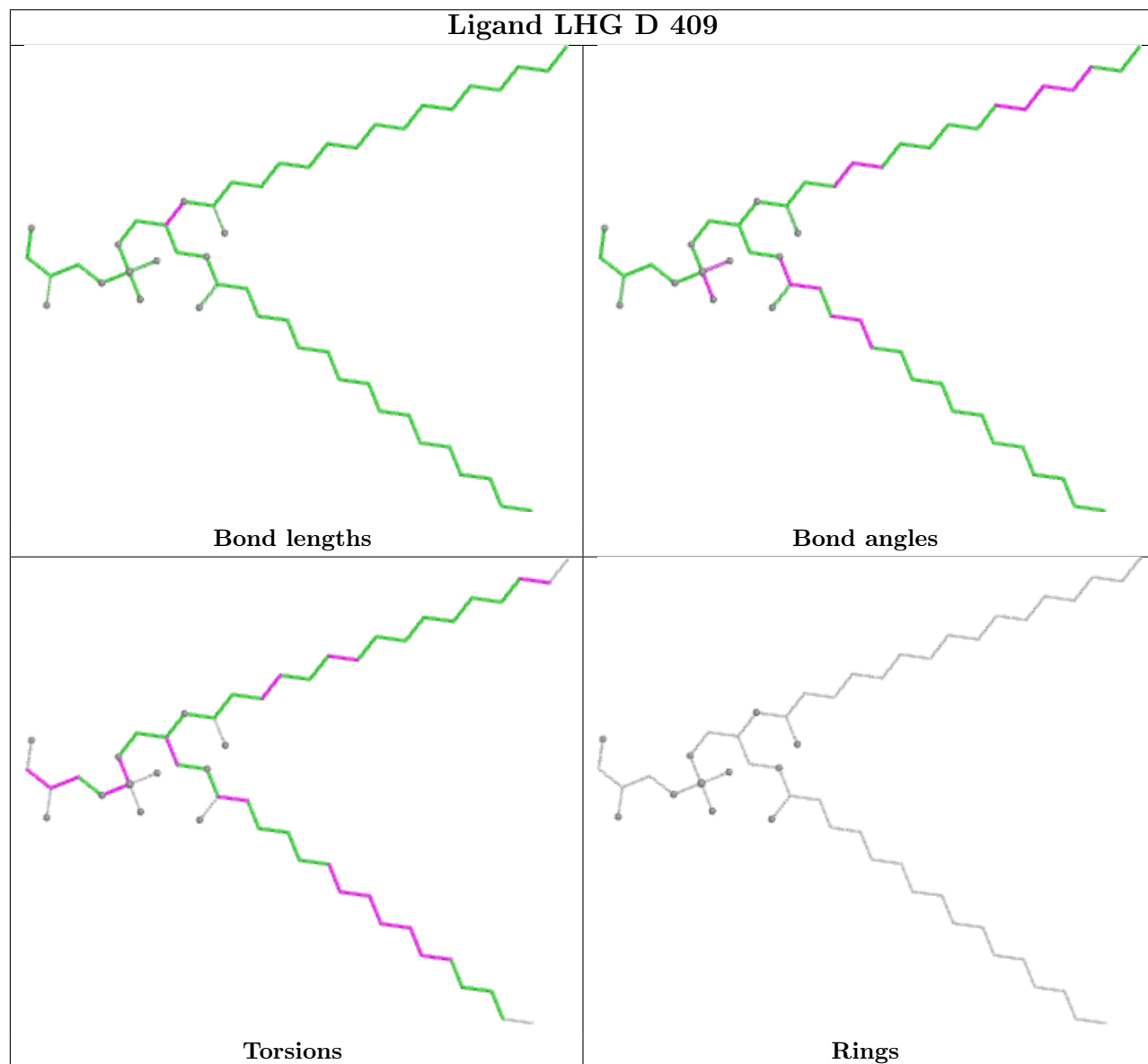
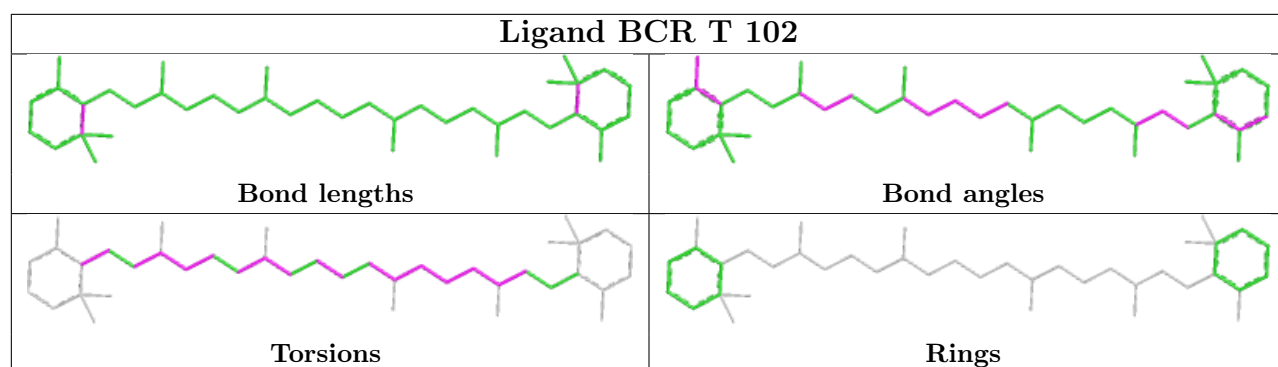


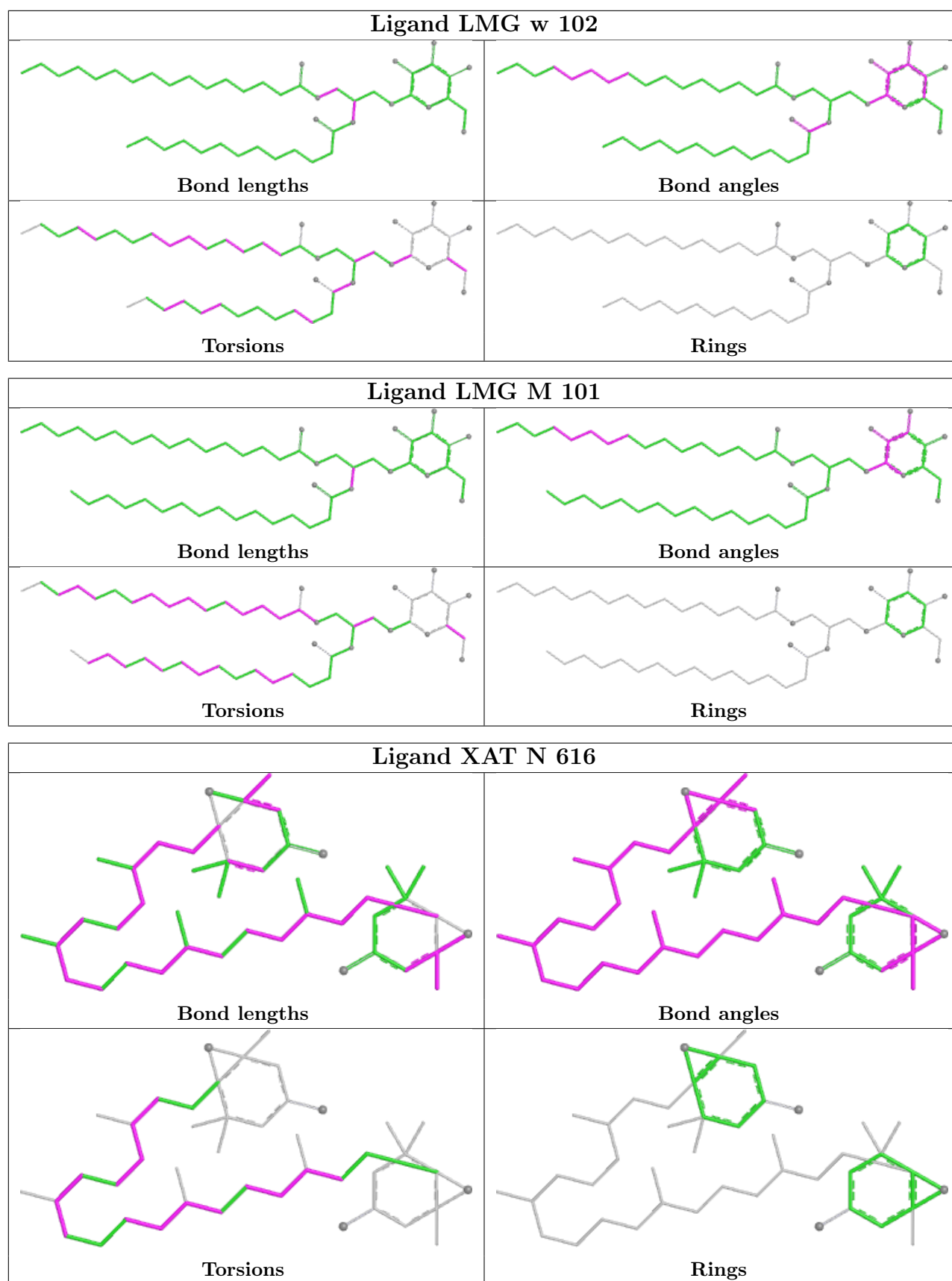
## Ligand CHL N 601

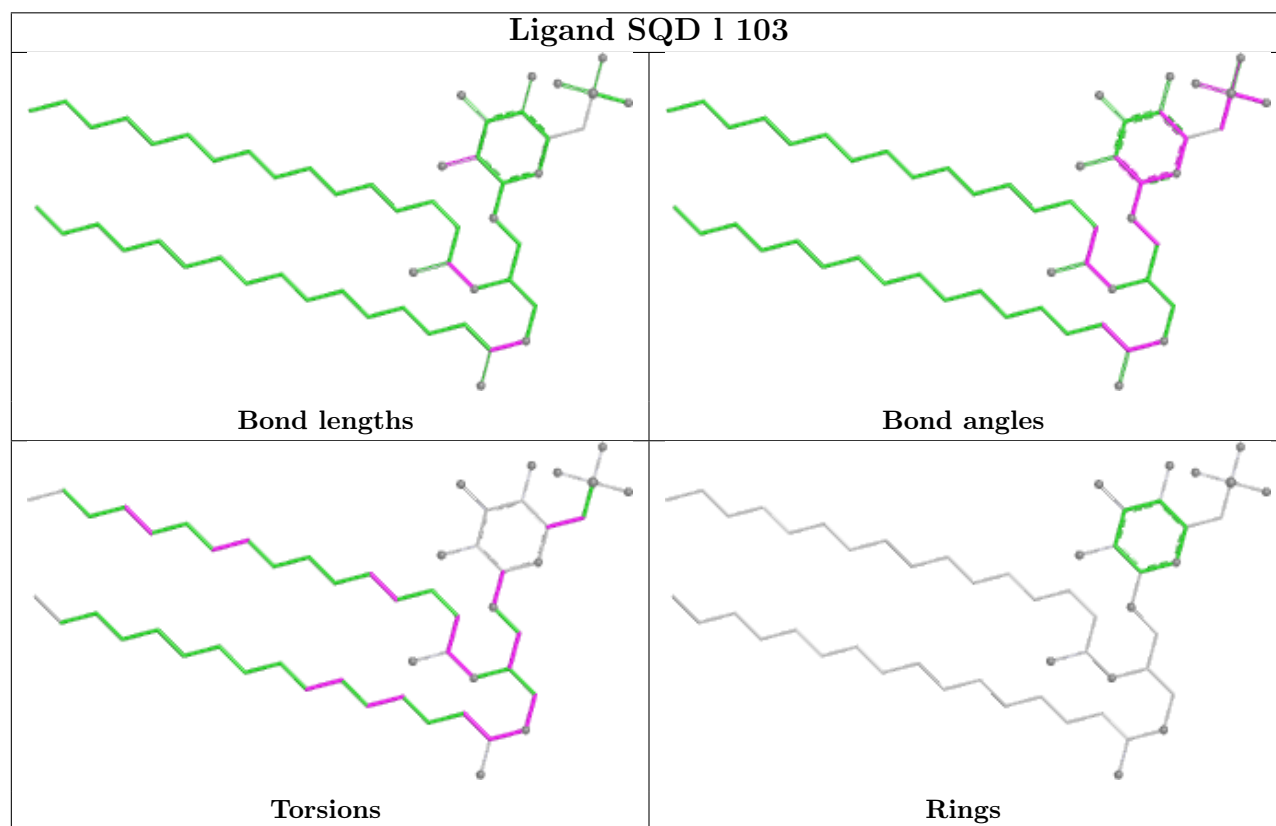
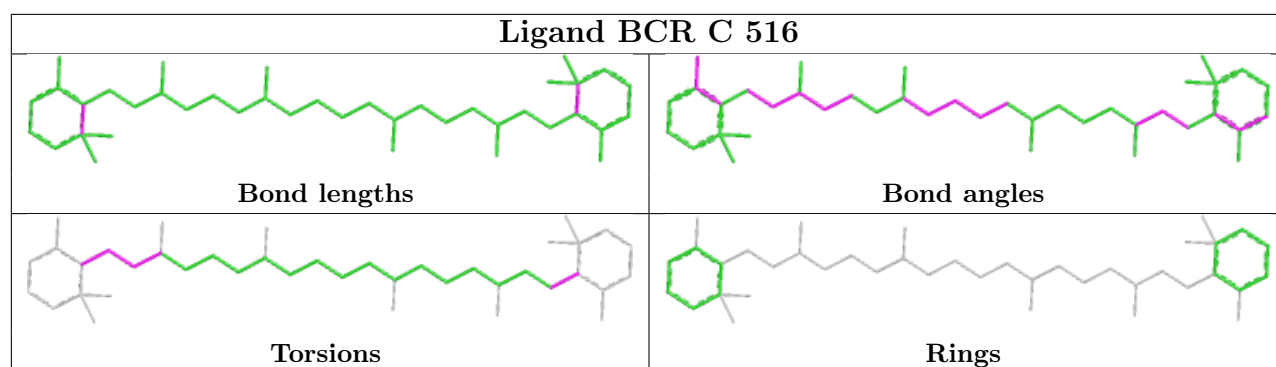


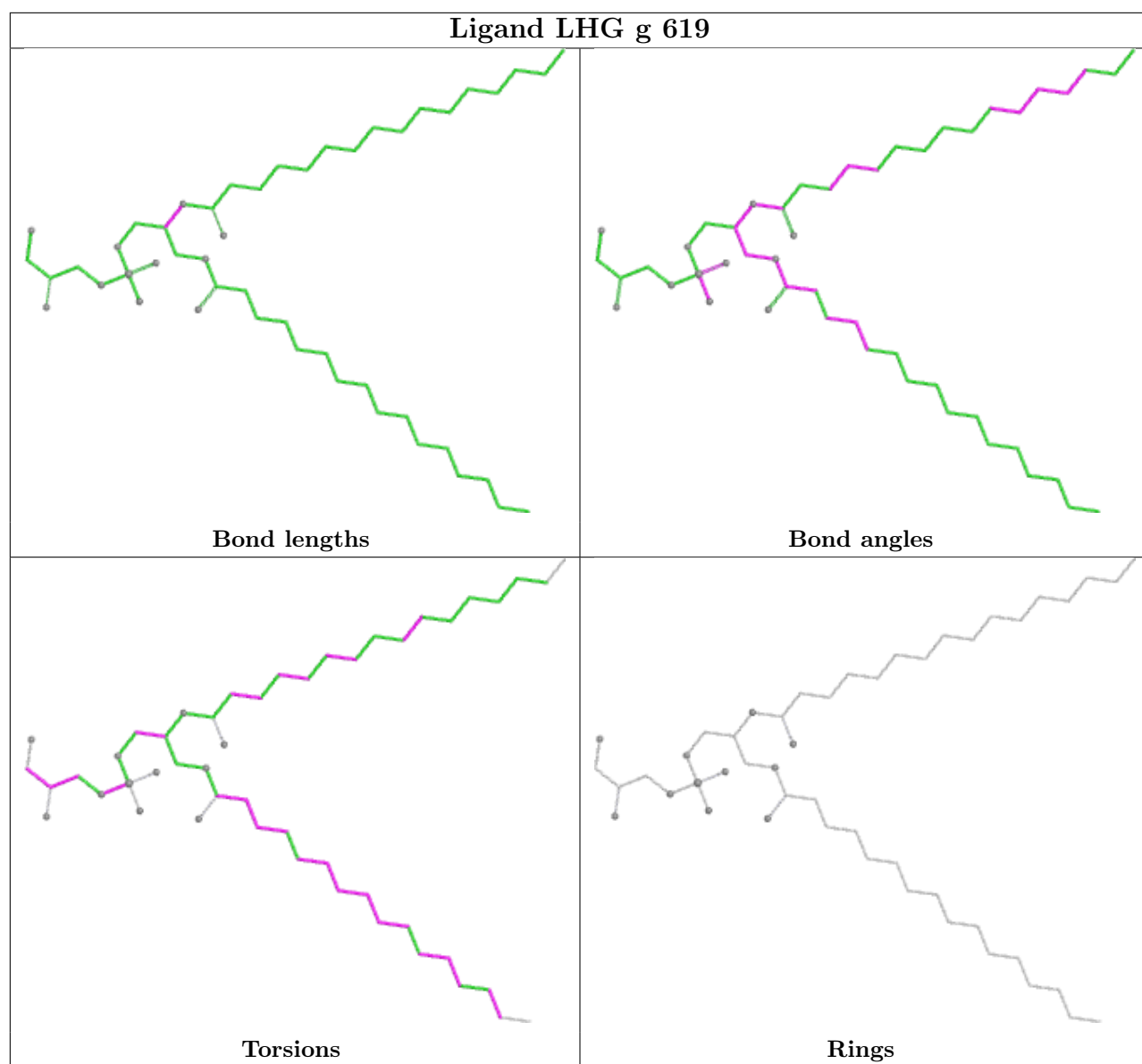


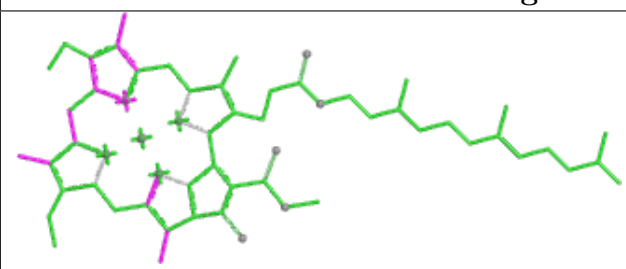
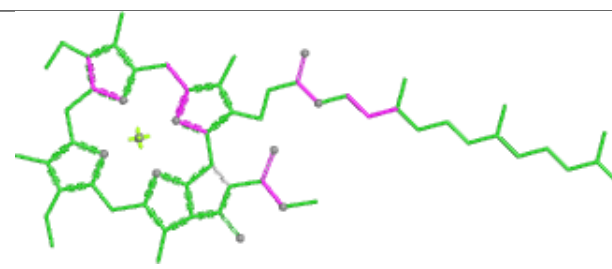
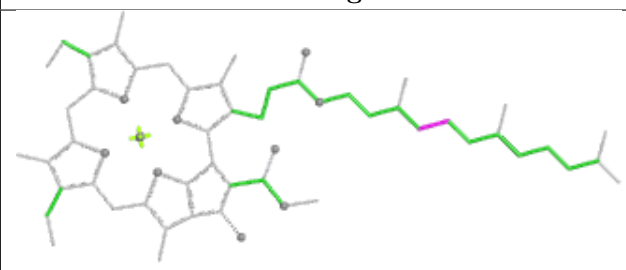
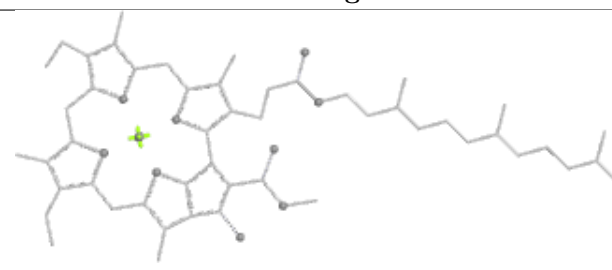


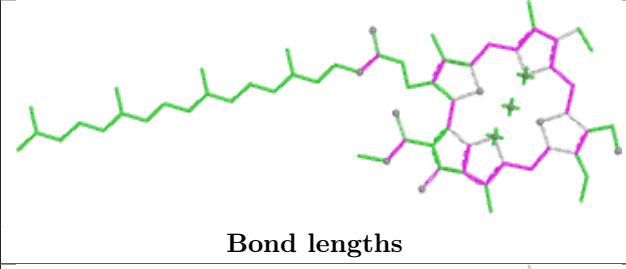
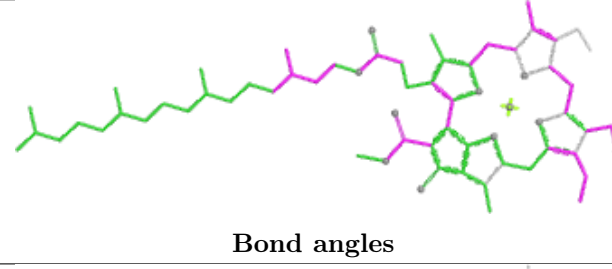
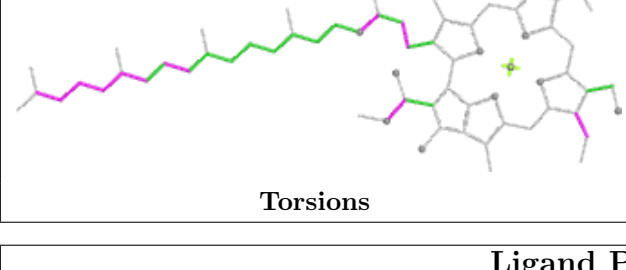
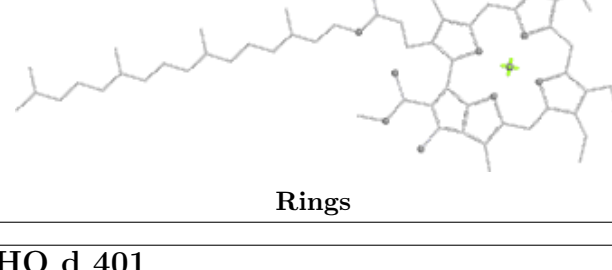


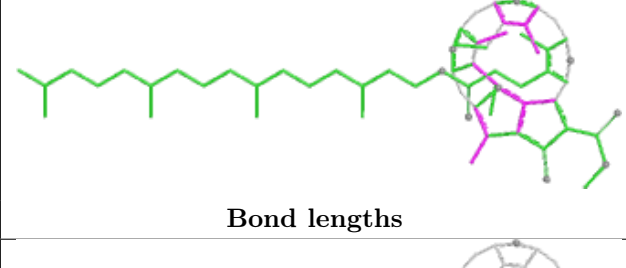
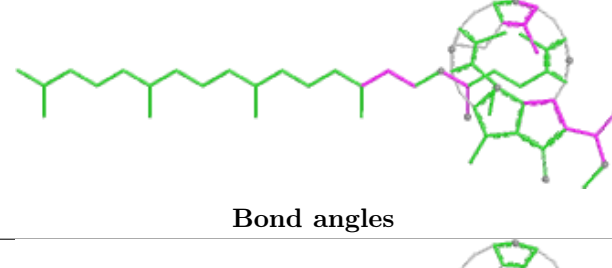
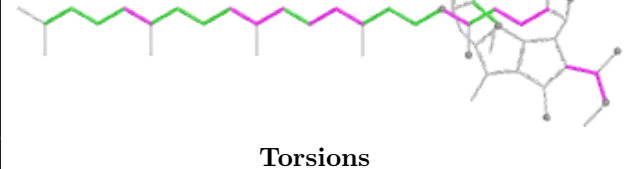
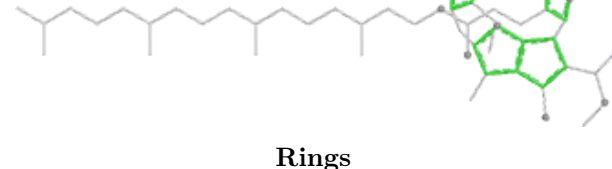


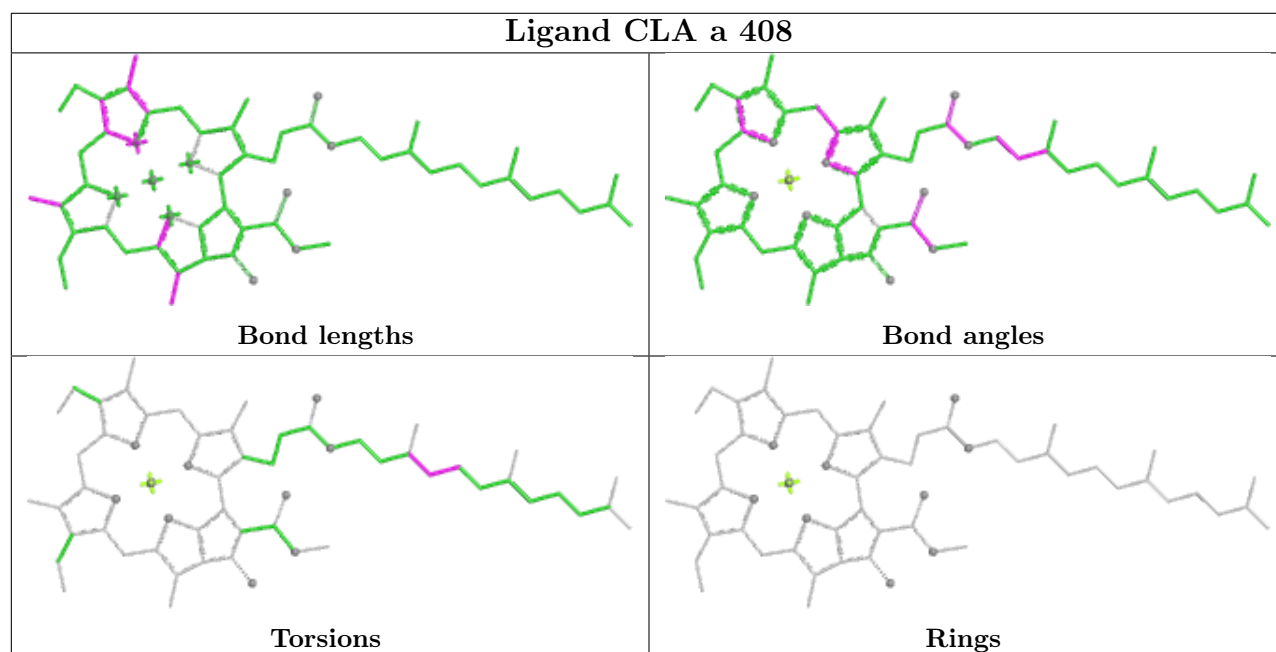
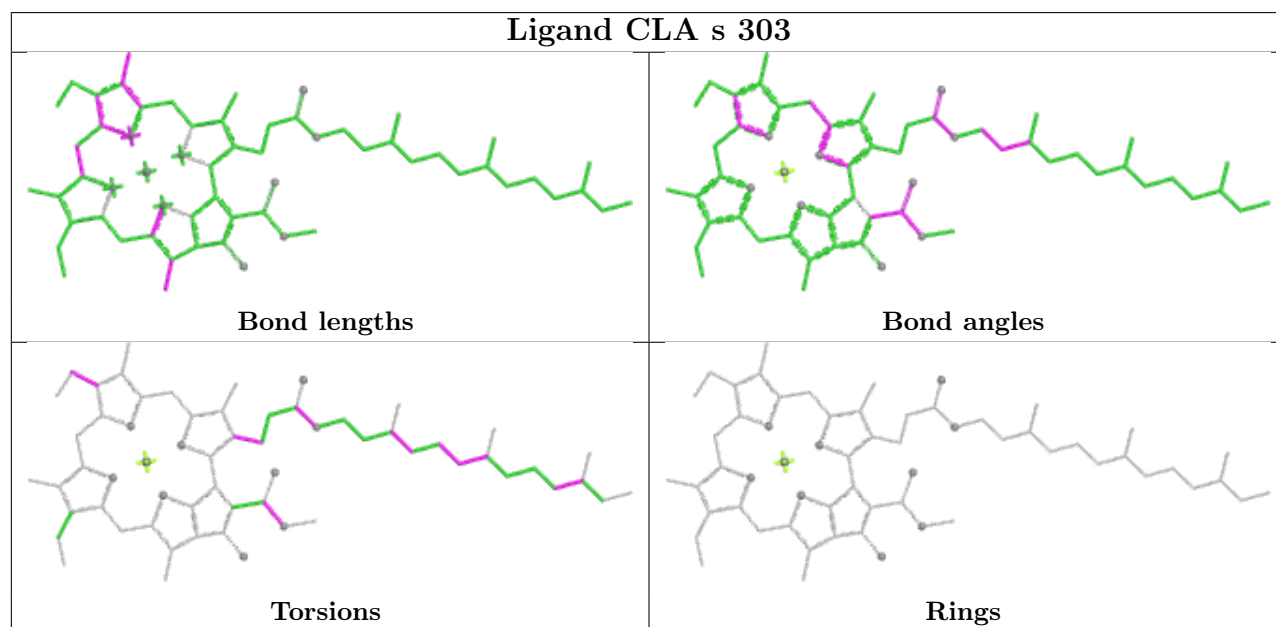
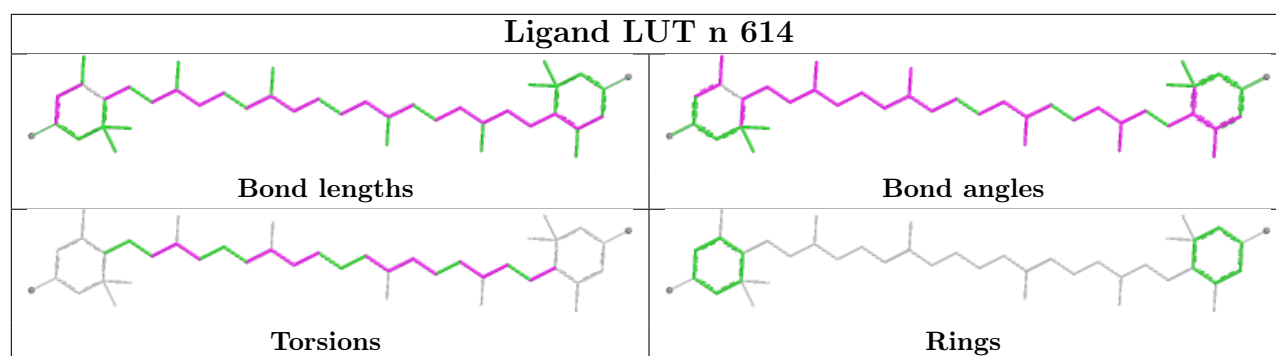


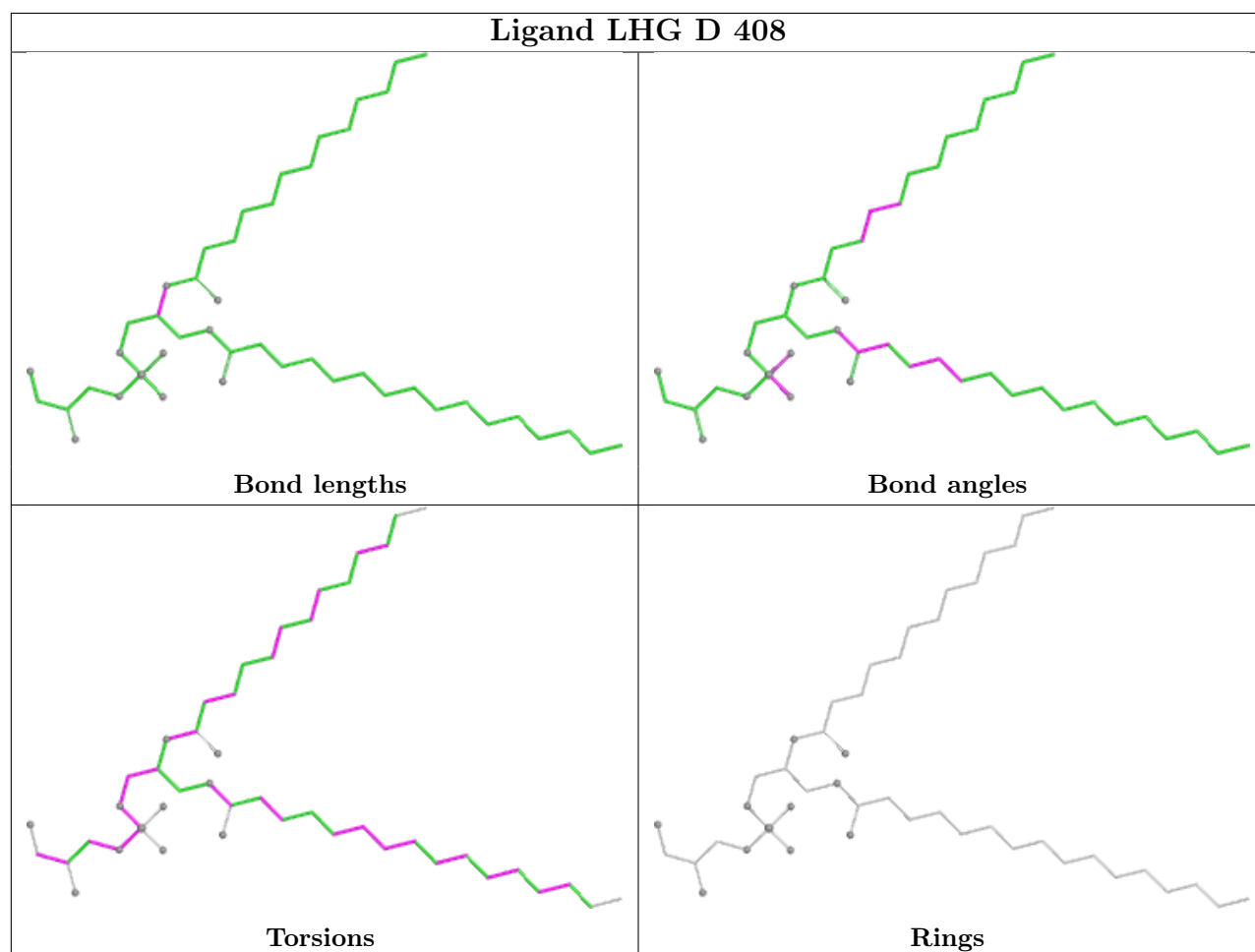
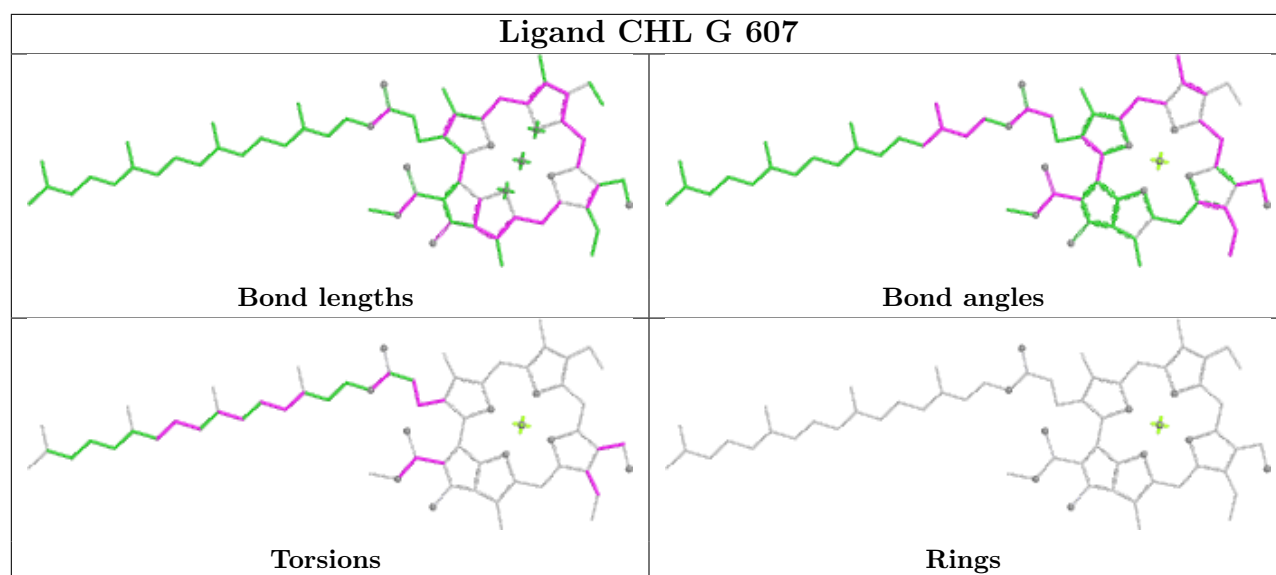


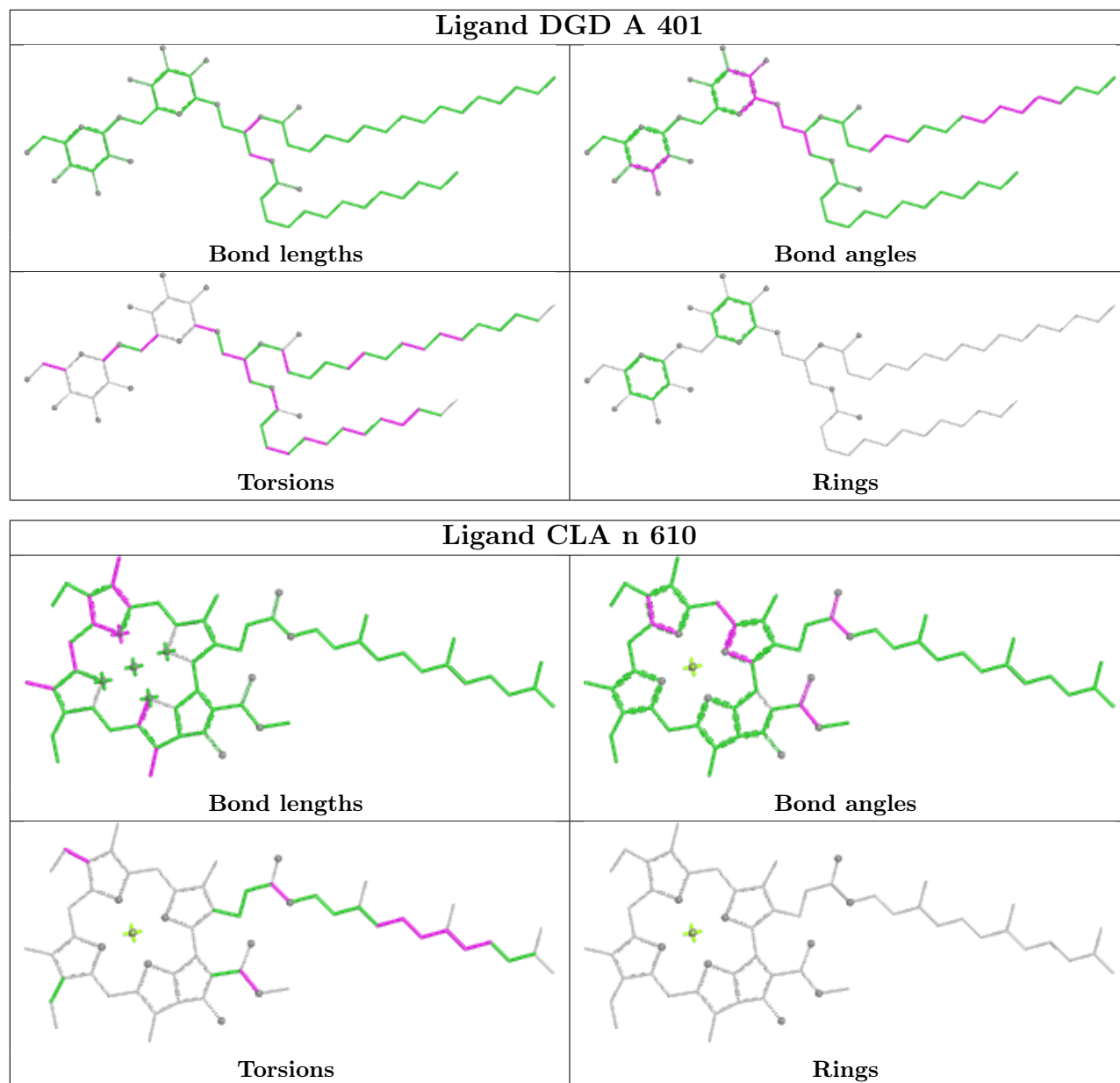
| Ligand CLA A 409                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

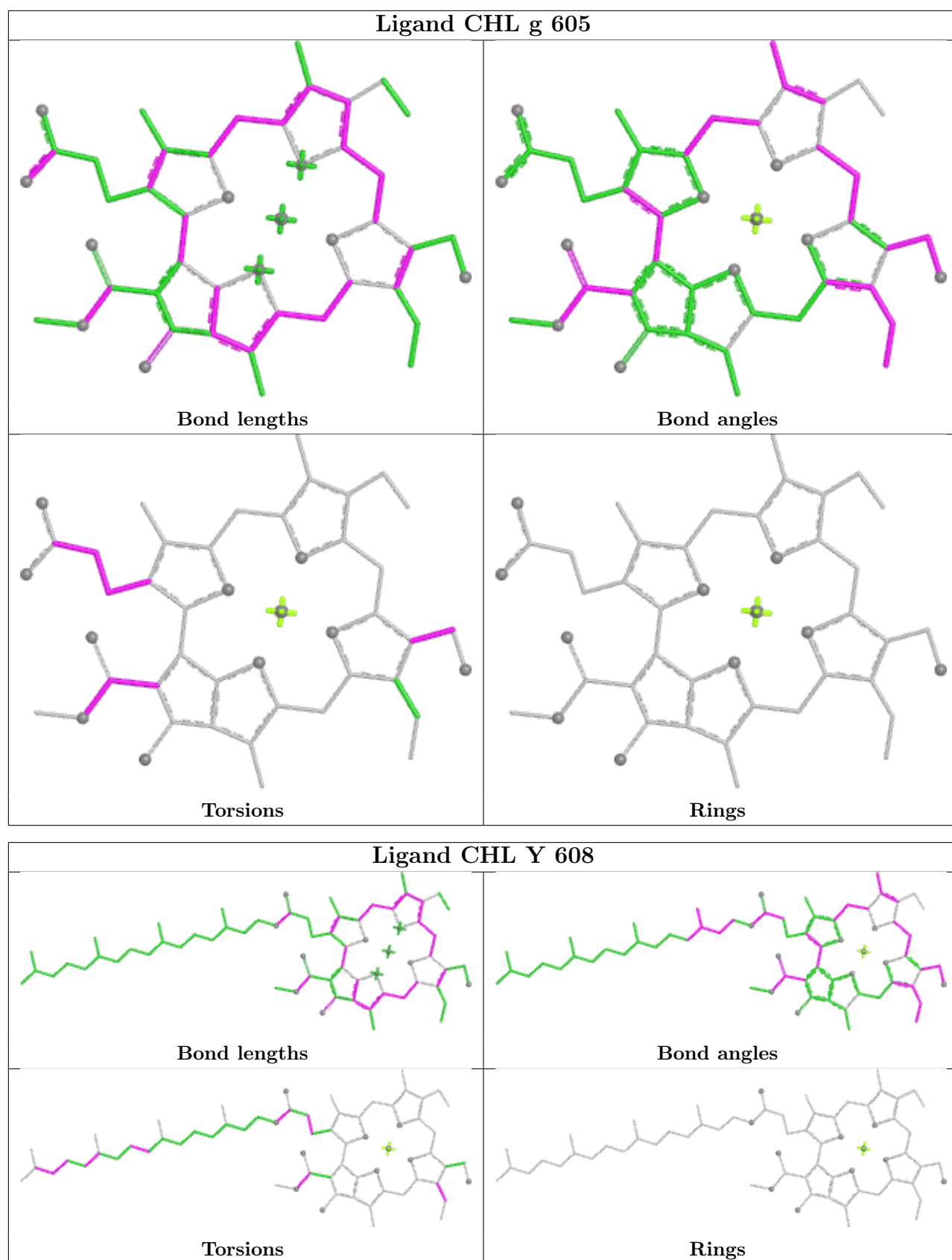
| Ligand CHL N 608                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

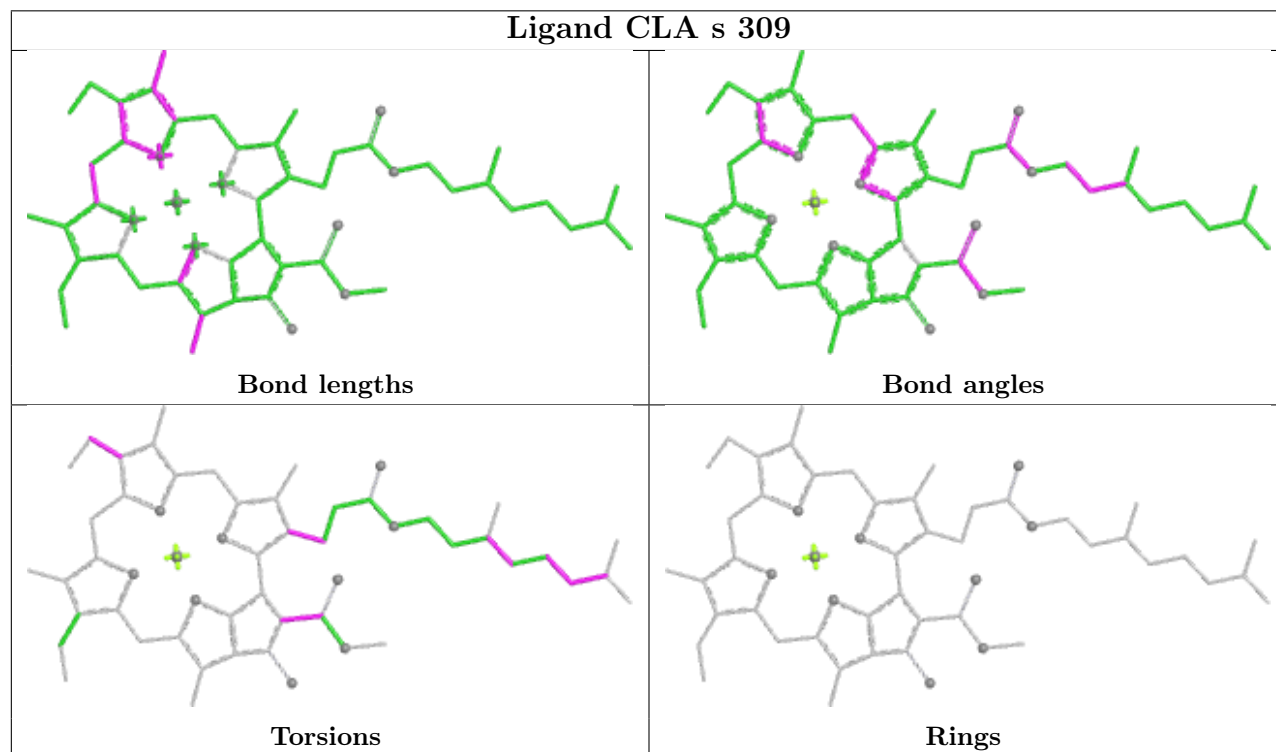
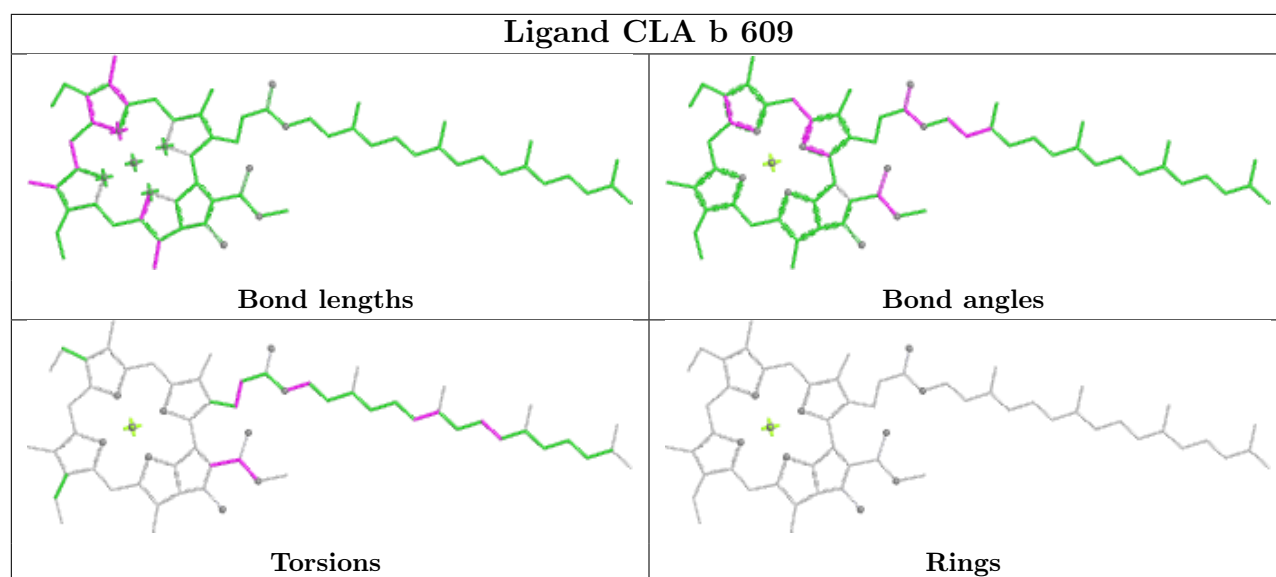
| Ligand PHO d 401                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

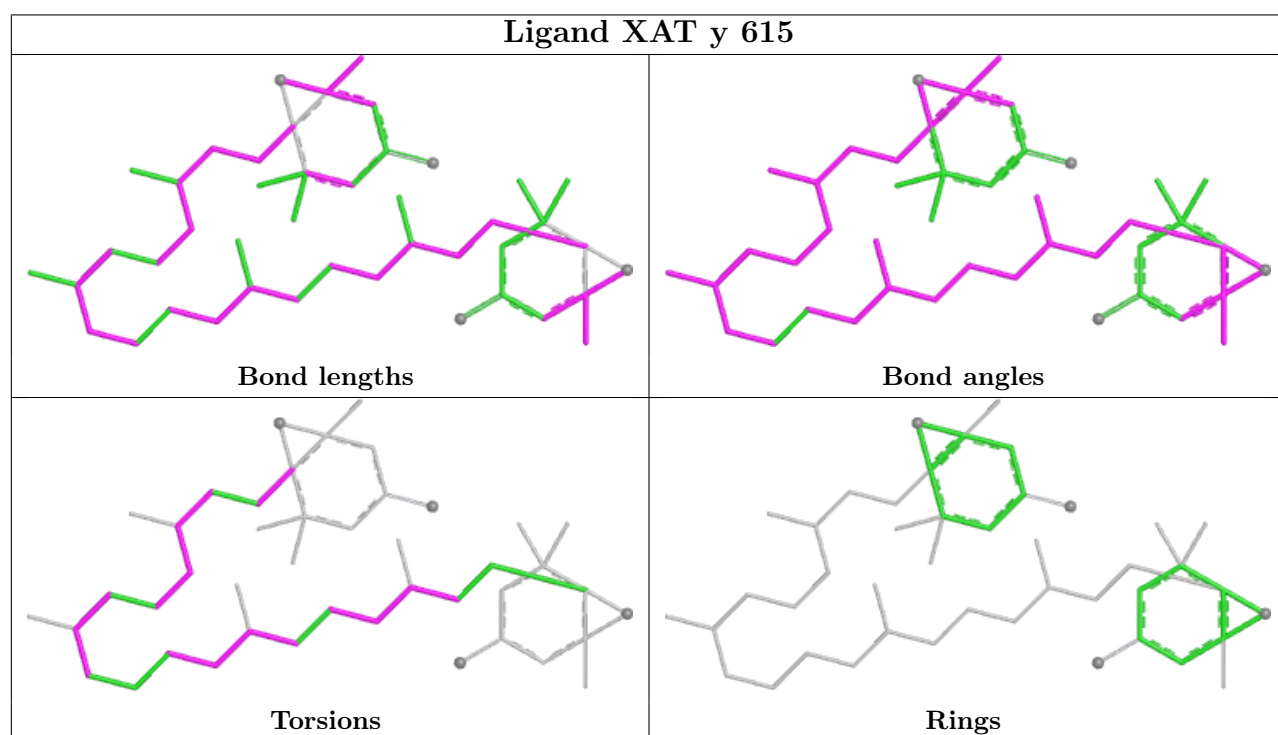
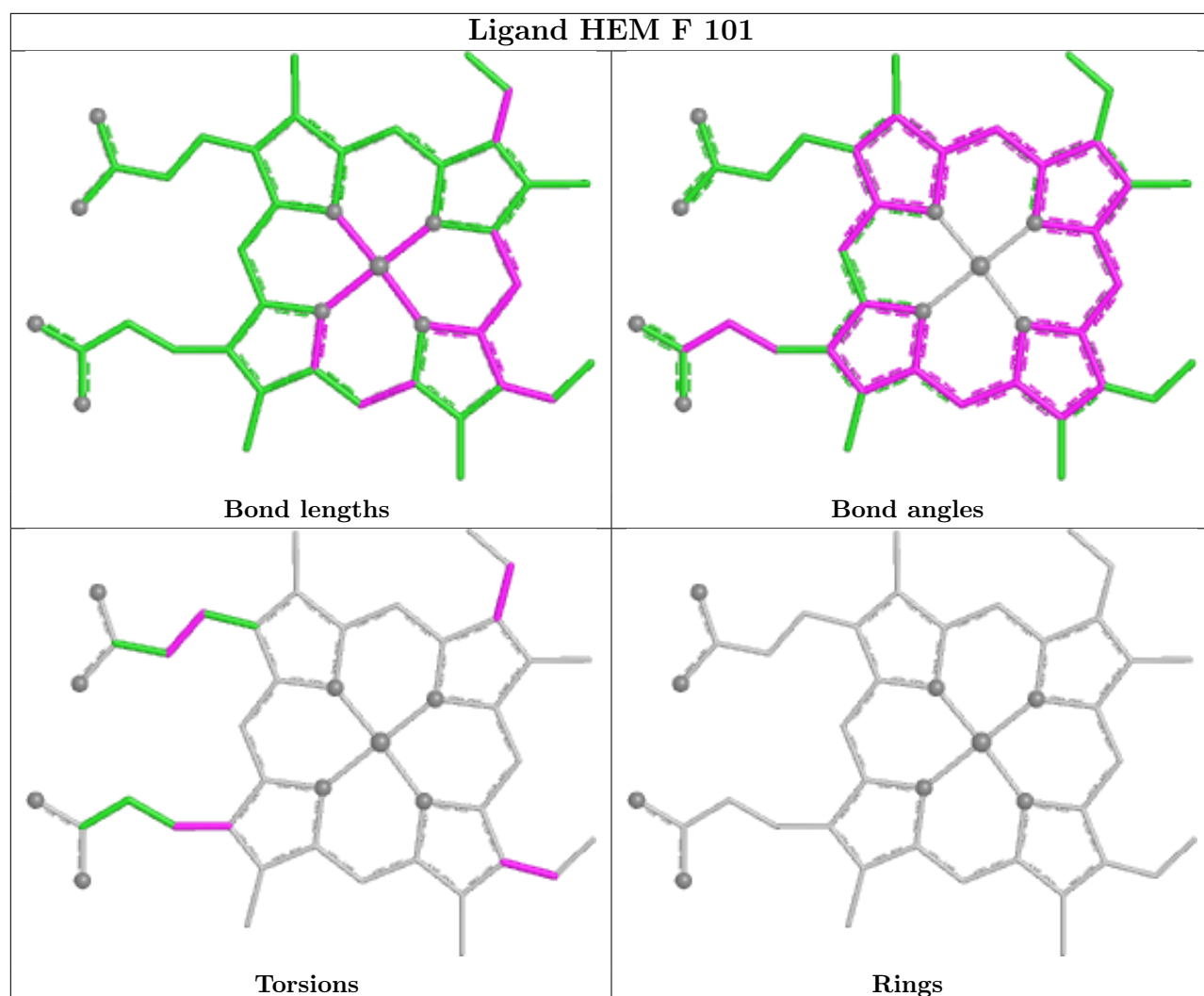


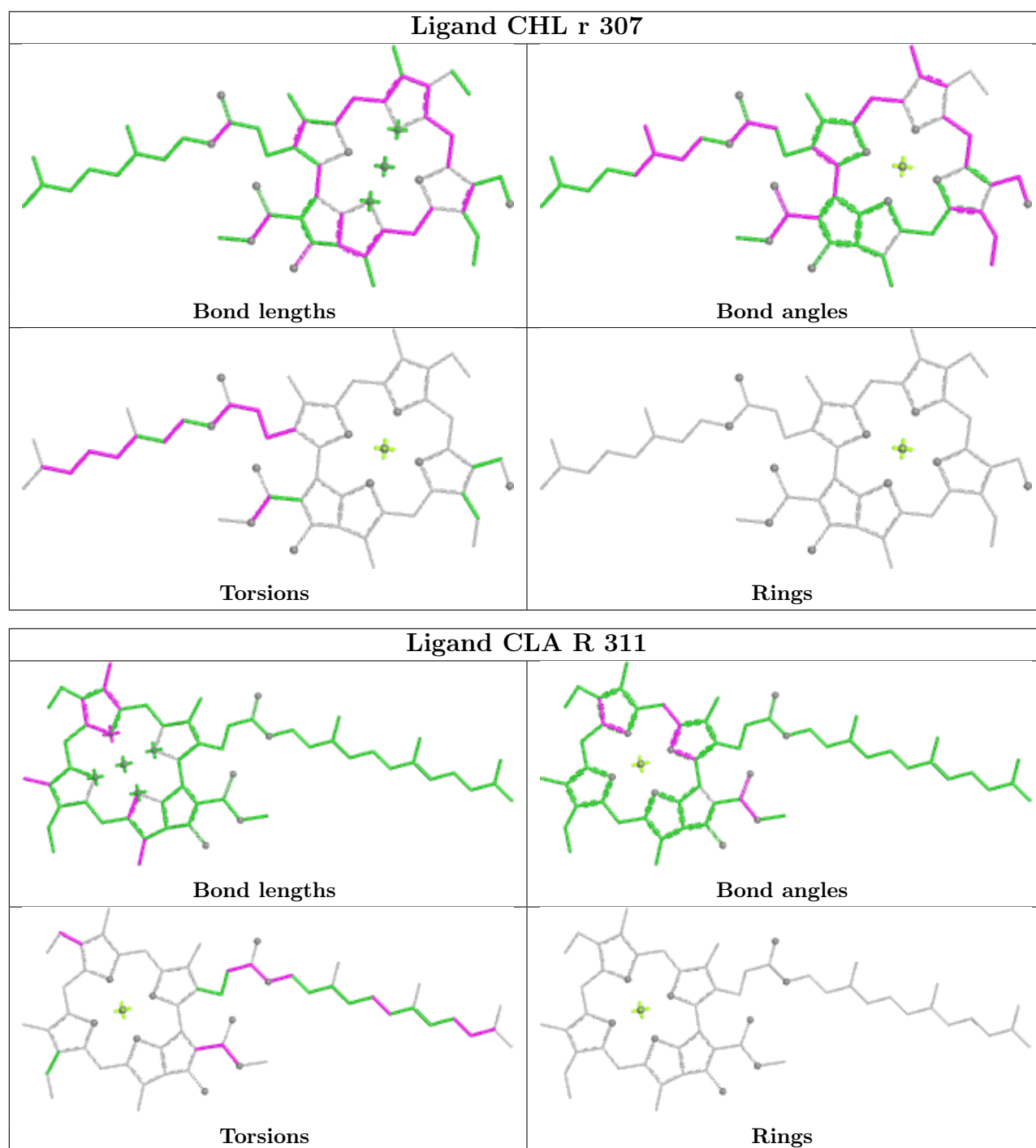


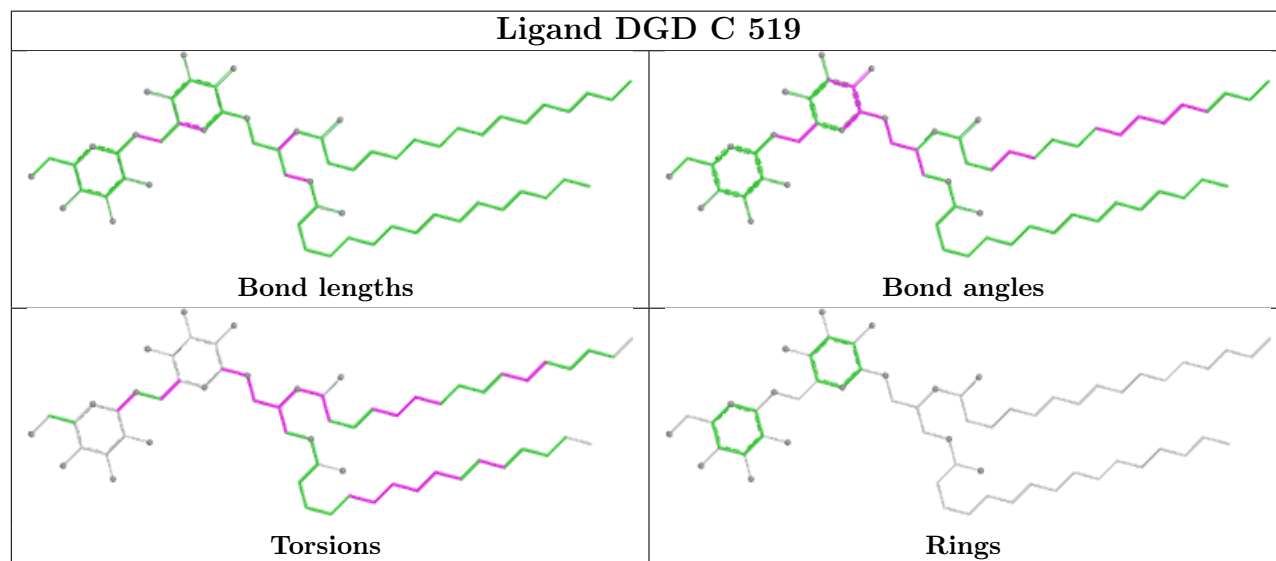
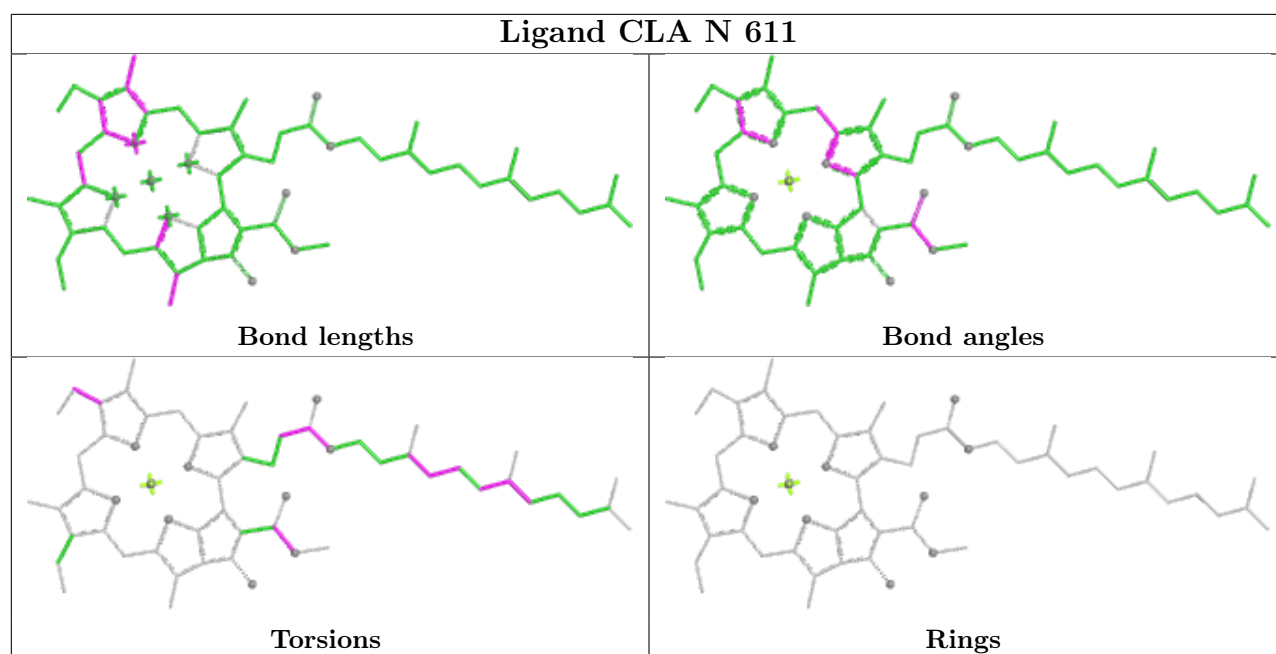


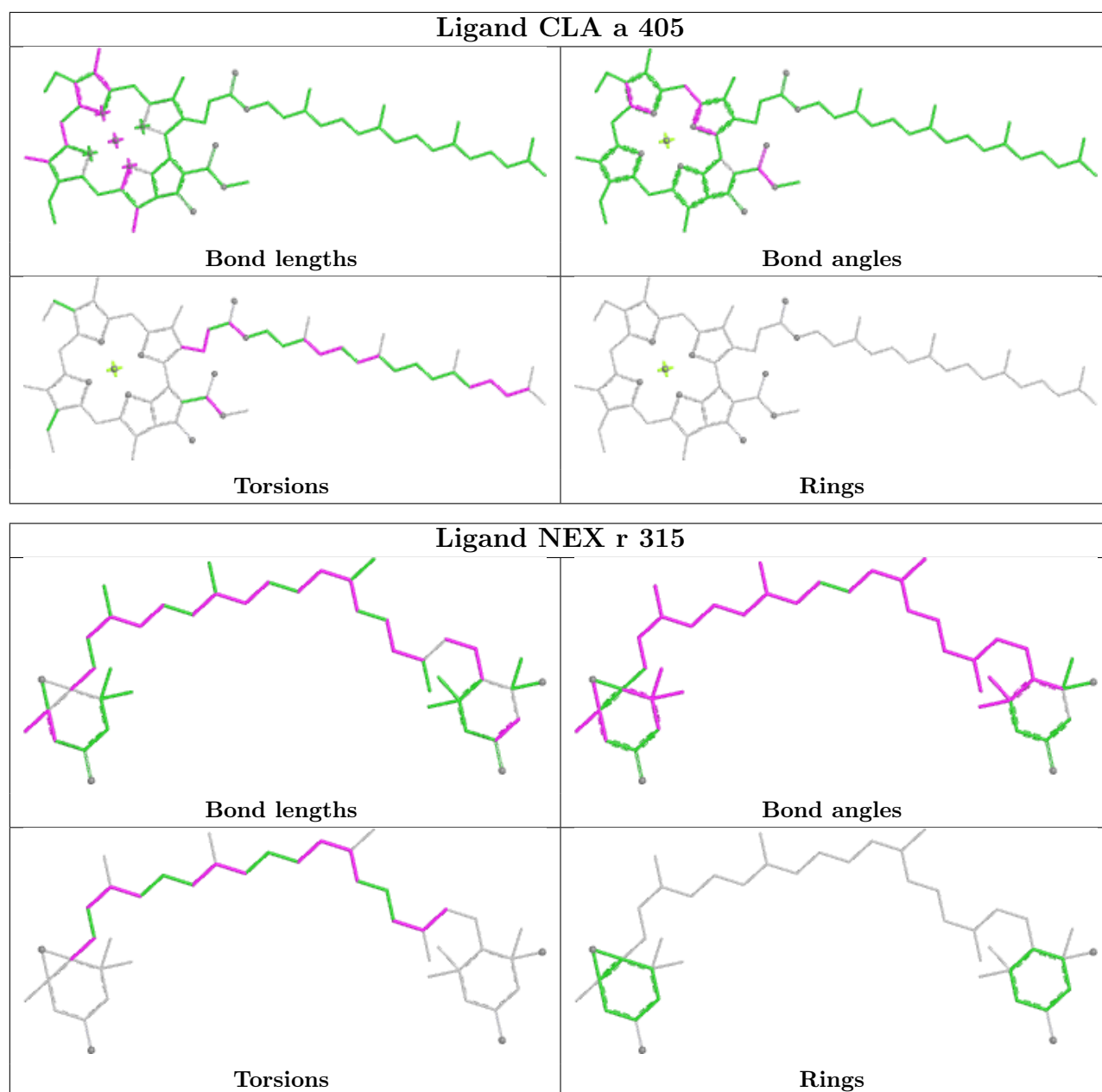


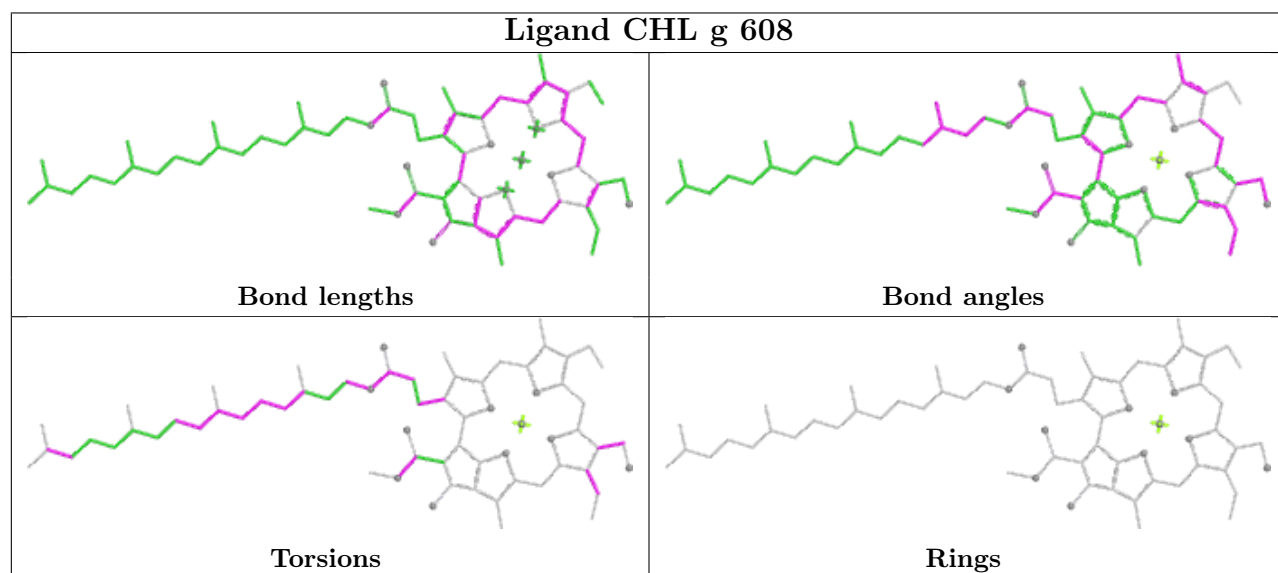
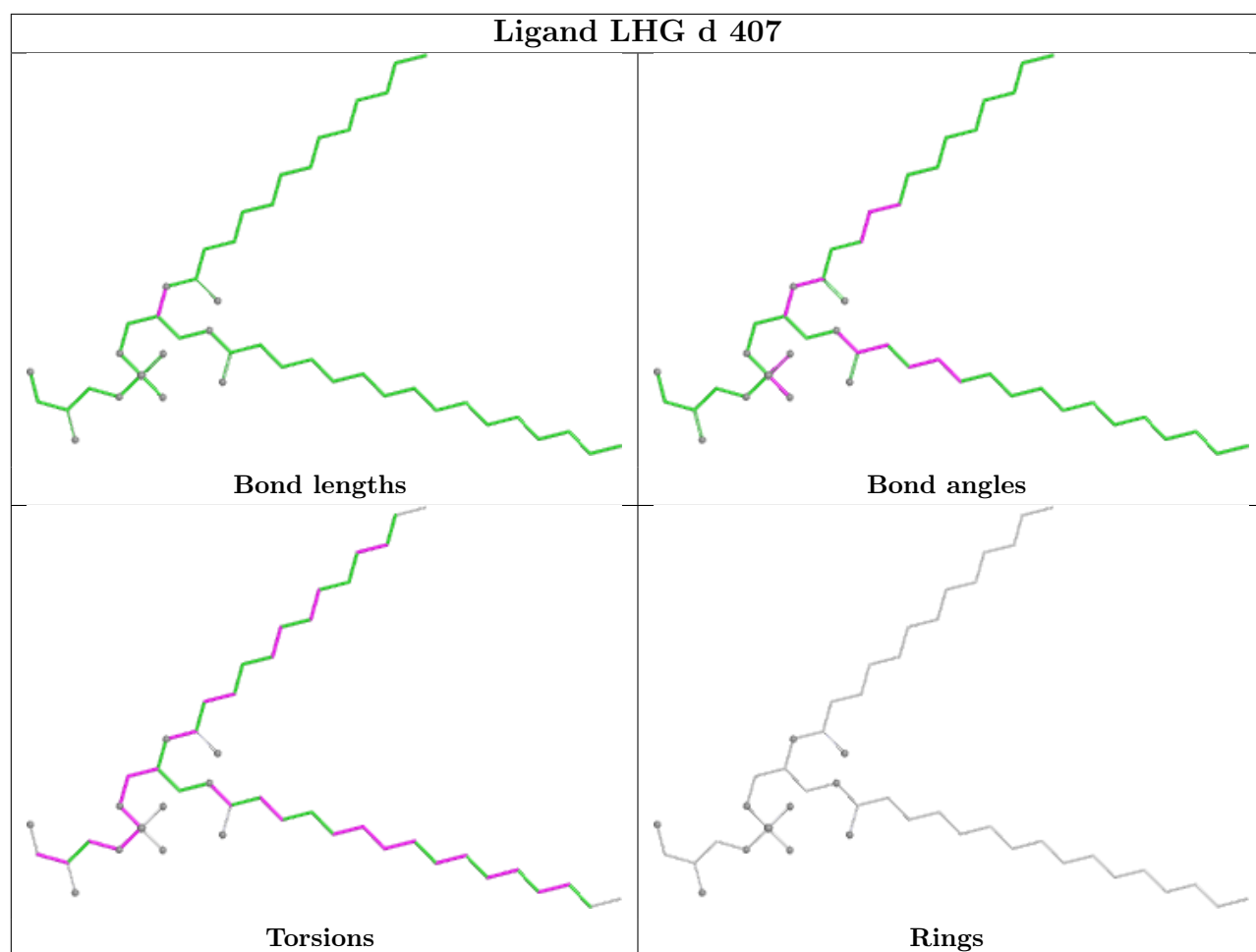


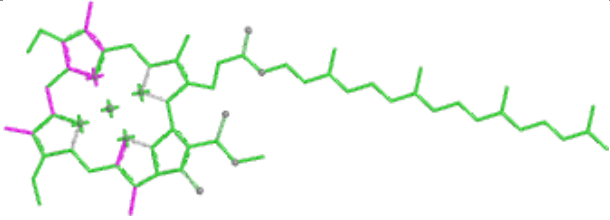
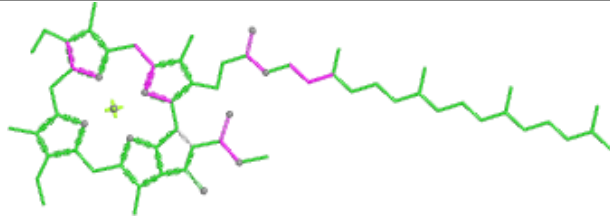
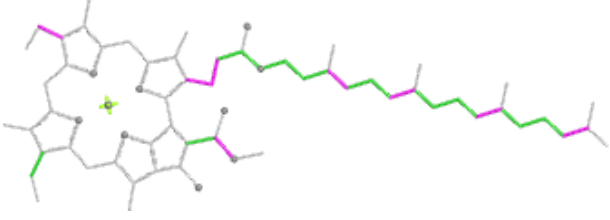
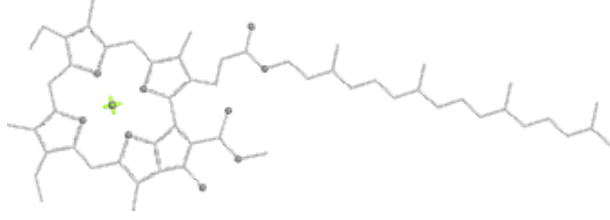
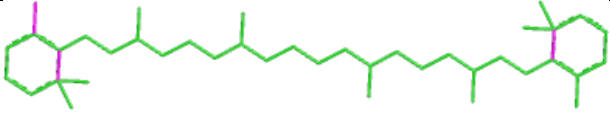
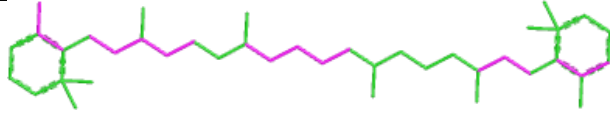
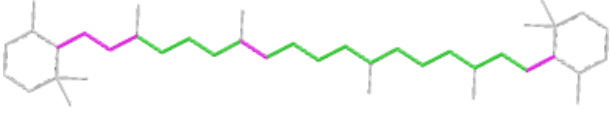
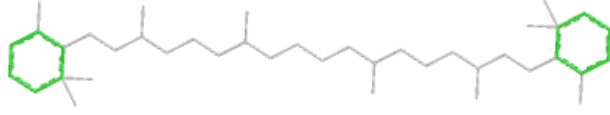
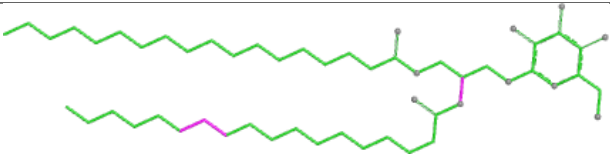
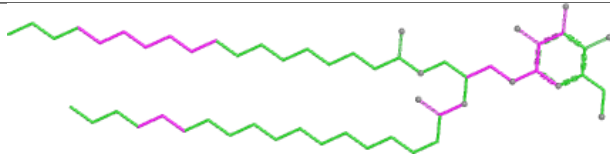
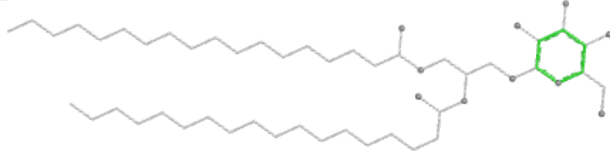


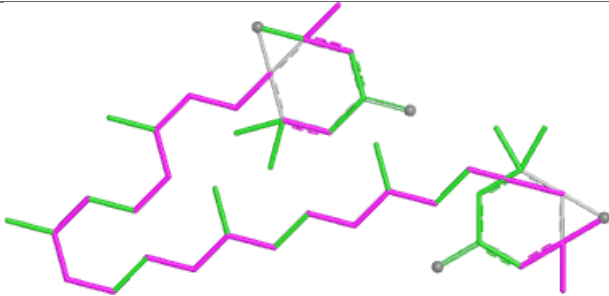
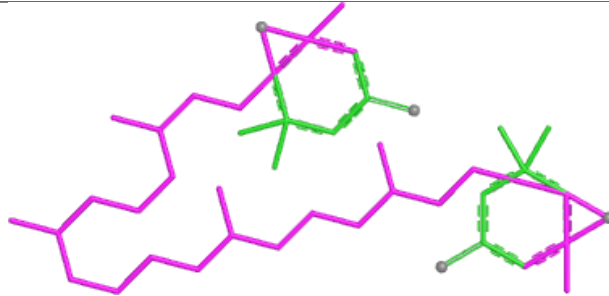
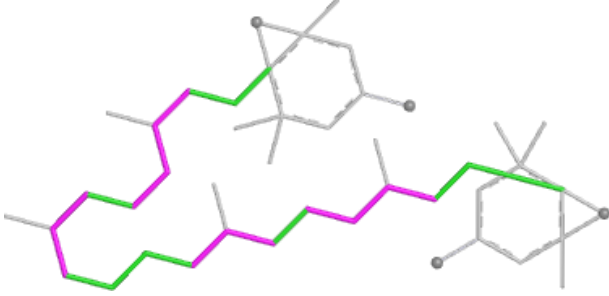
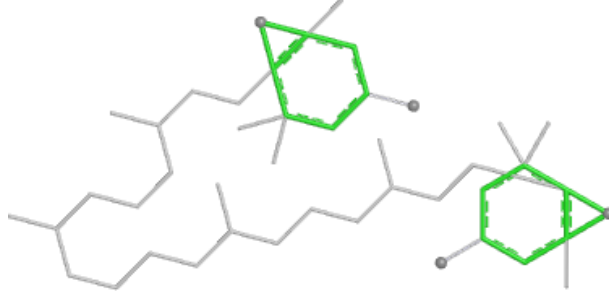


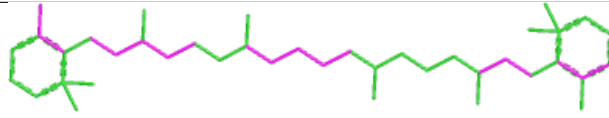
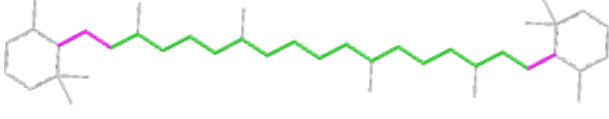
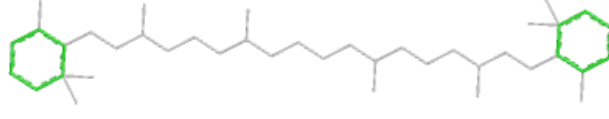


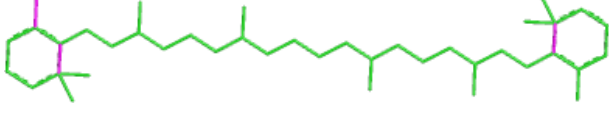
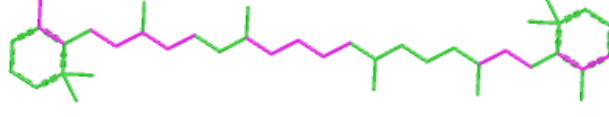
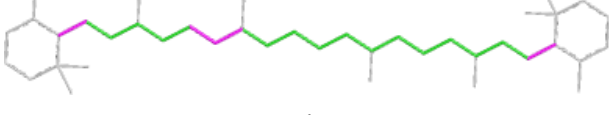
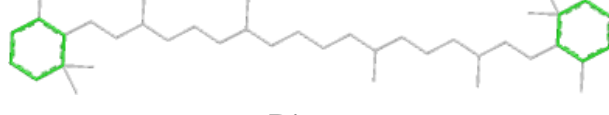


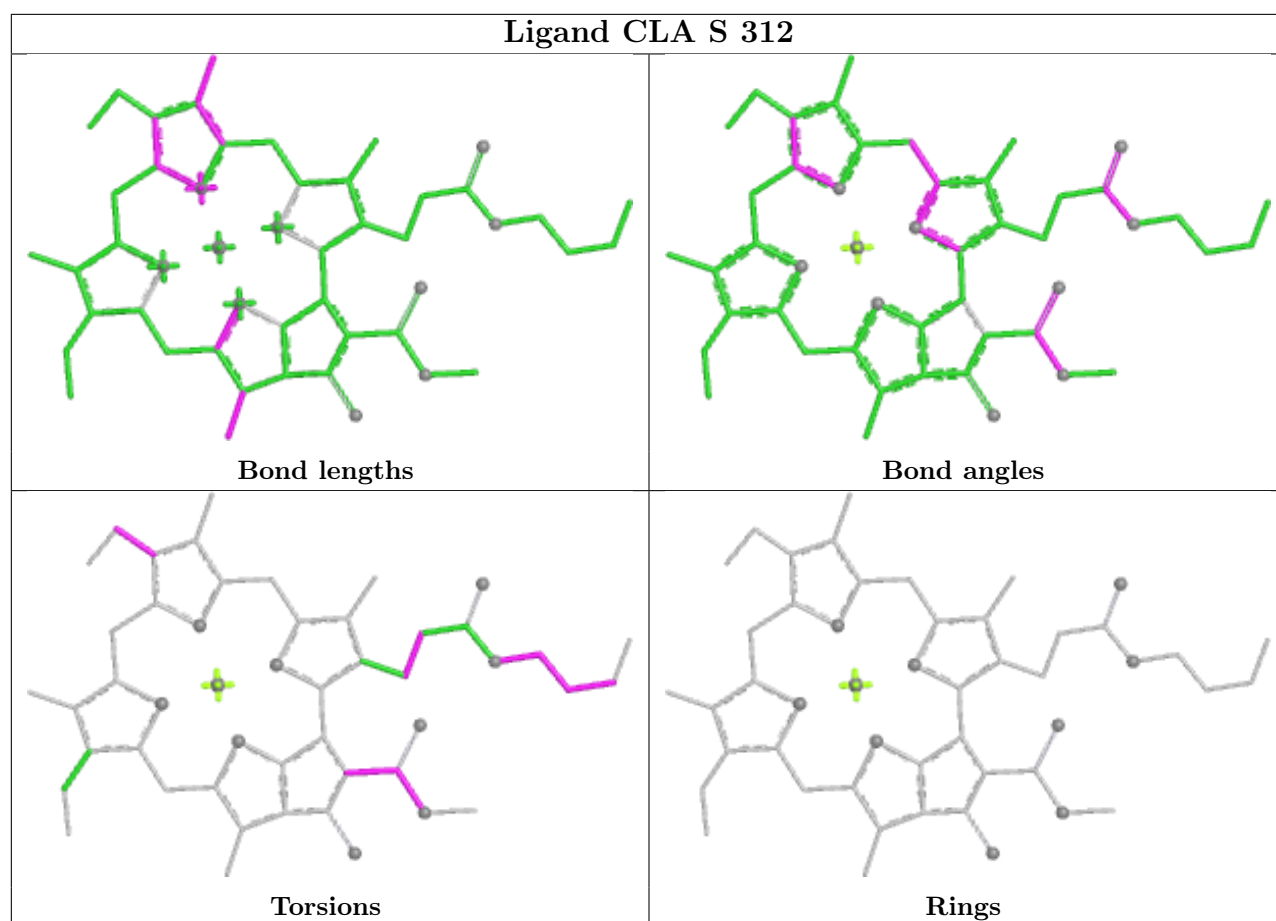


| Ligand CLA b 602                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand BCR D 406                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand LMG b 620                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

| Ligand XAT n 615                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand BCR a 409                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

| Ligand BCR K 102                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

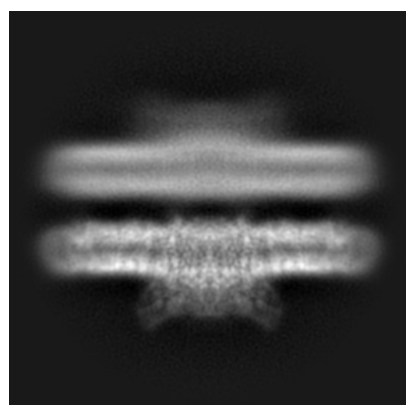
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10865. These allow visual inspection of the internal detail of the map and identification of artifacts.

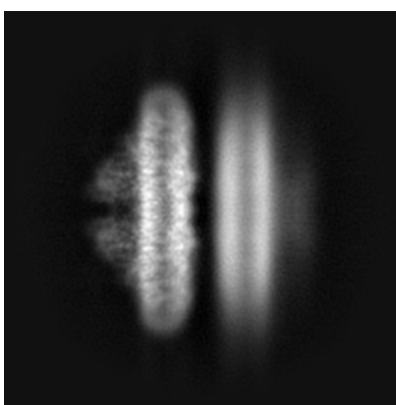
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

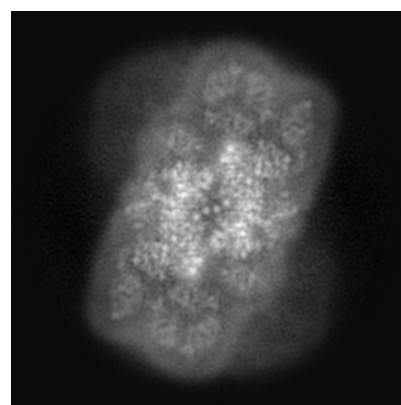
#### 6.1.1 Primary map



X



Y

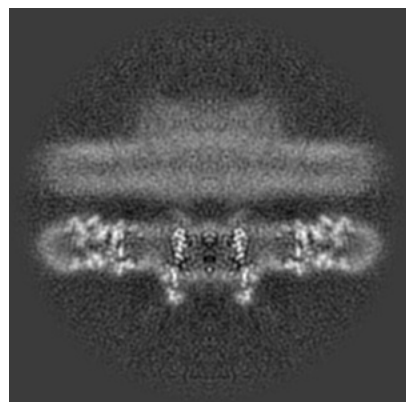


Z

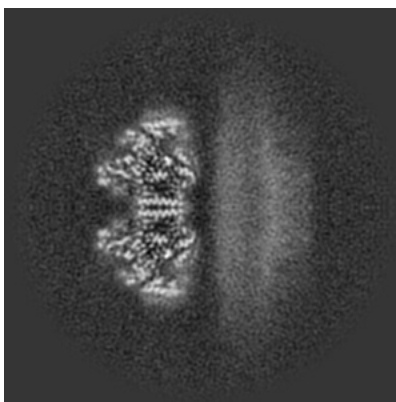
The images above show the map projected in three orthogonal directions.

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

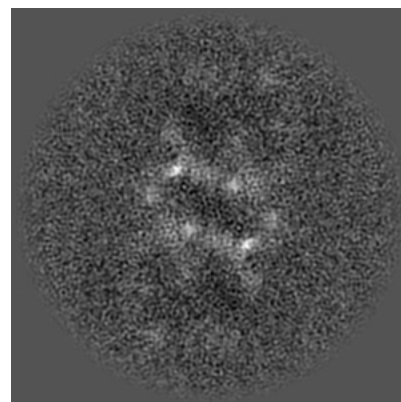
#### 6.2.1 Primary map



X Index: 170



Y Index: 170

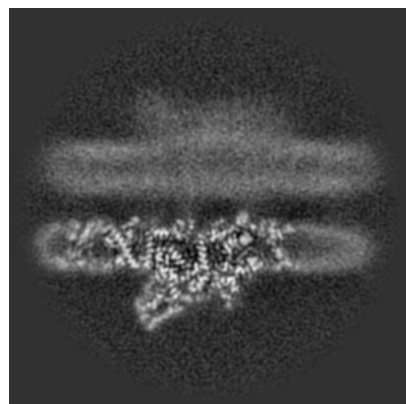


Z Index: 170

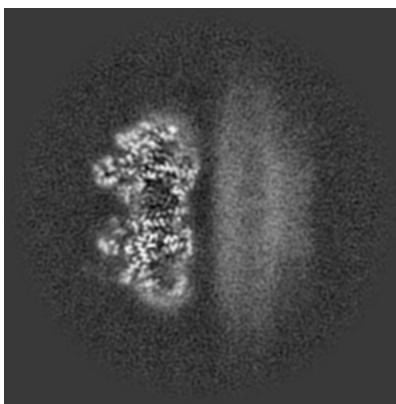
The images above show central slices of the map in three orthogonal directions.

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

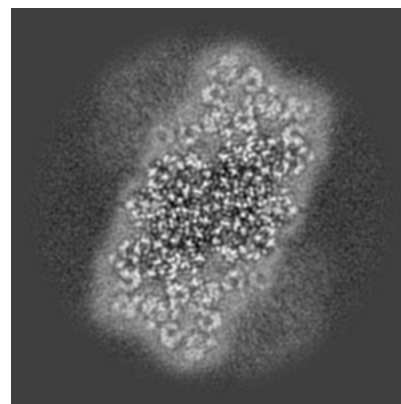
### 6.3.1 Primary map



X Index: 156



Y Index: 166

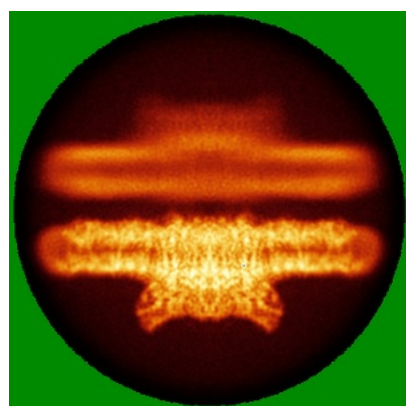


Z Index: 121

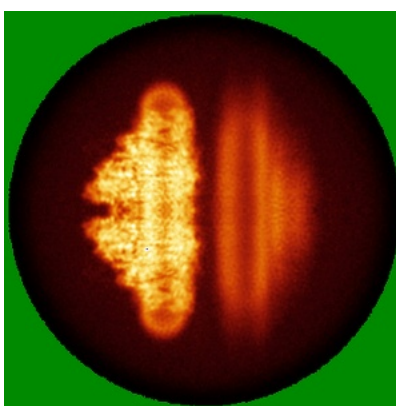
The images above show the largest variance slices of the map in three orthogonal directions.

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

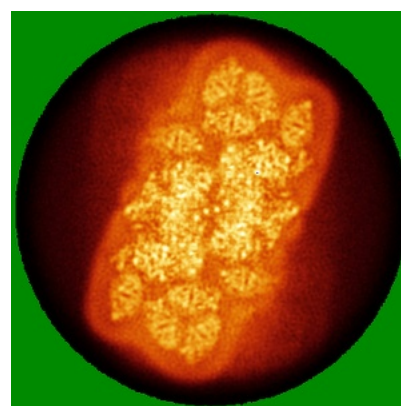
### 6.4.1 Primary map



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

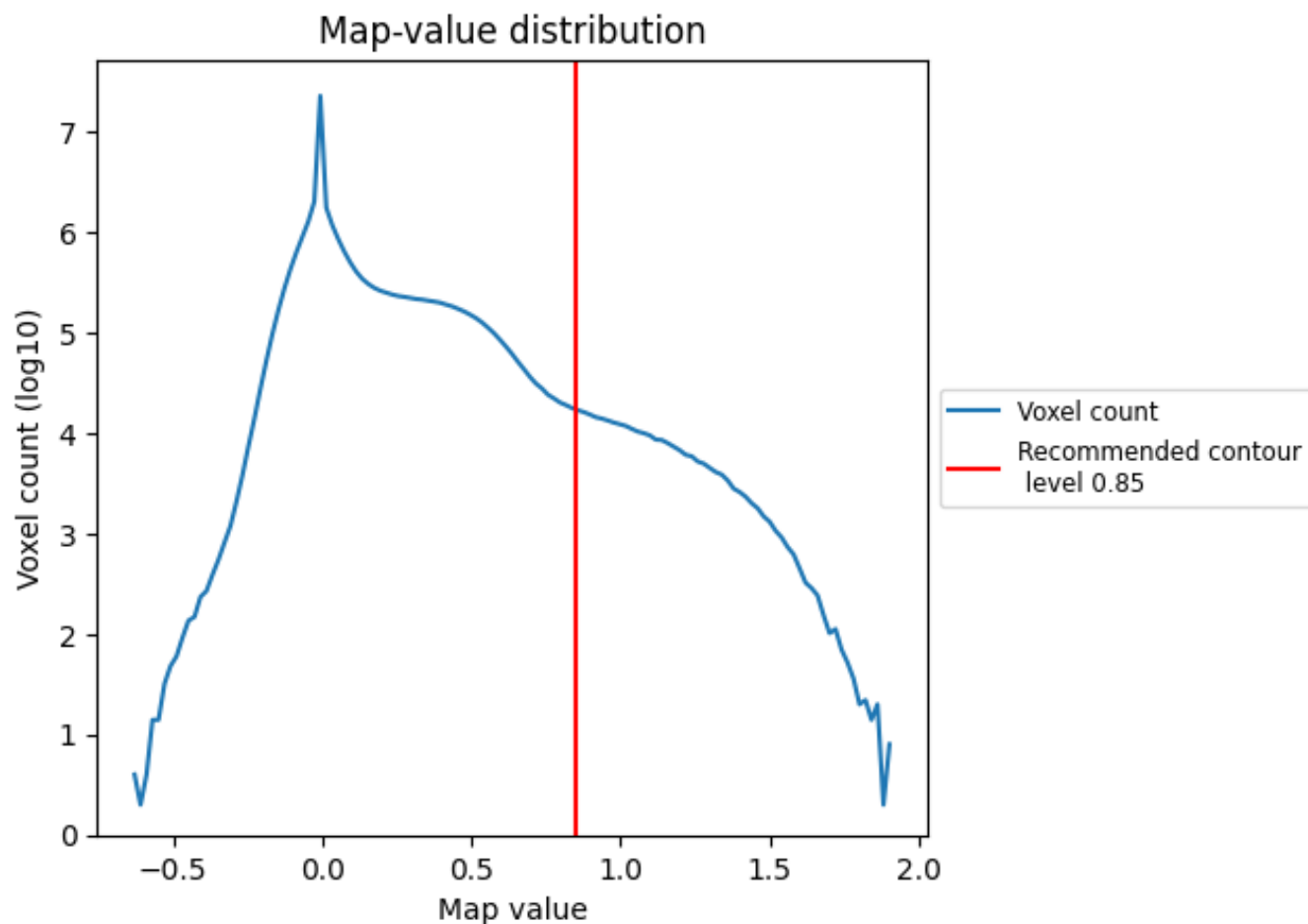
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

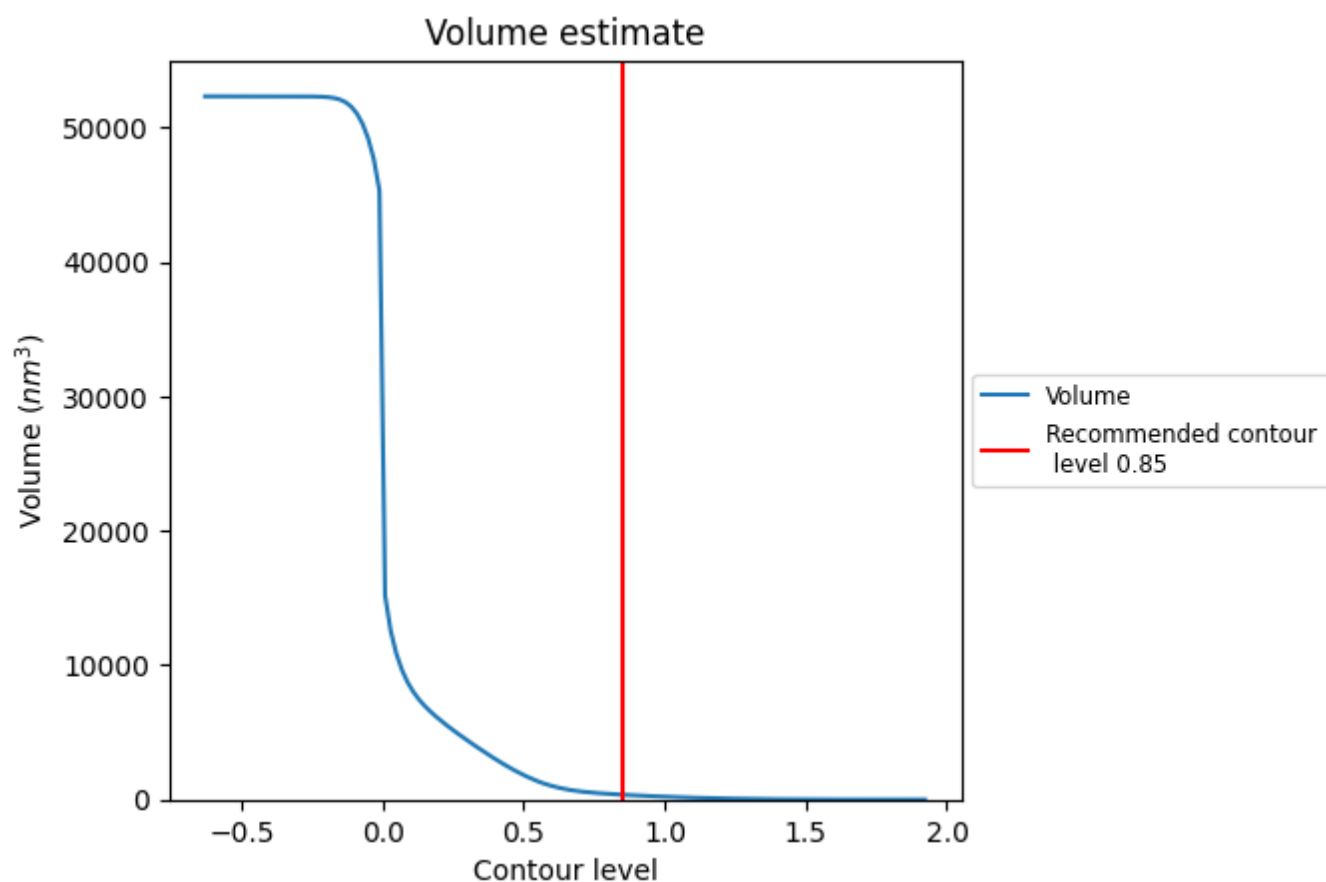
This section contains the results of statistical analysis of the map.

### 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.

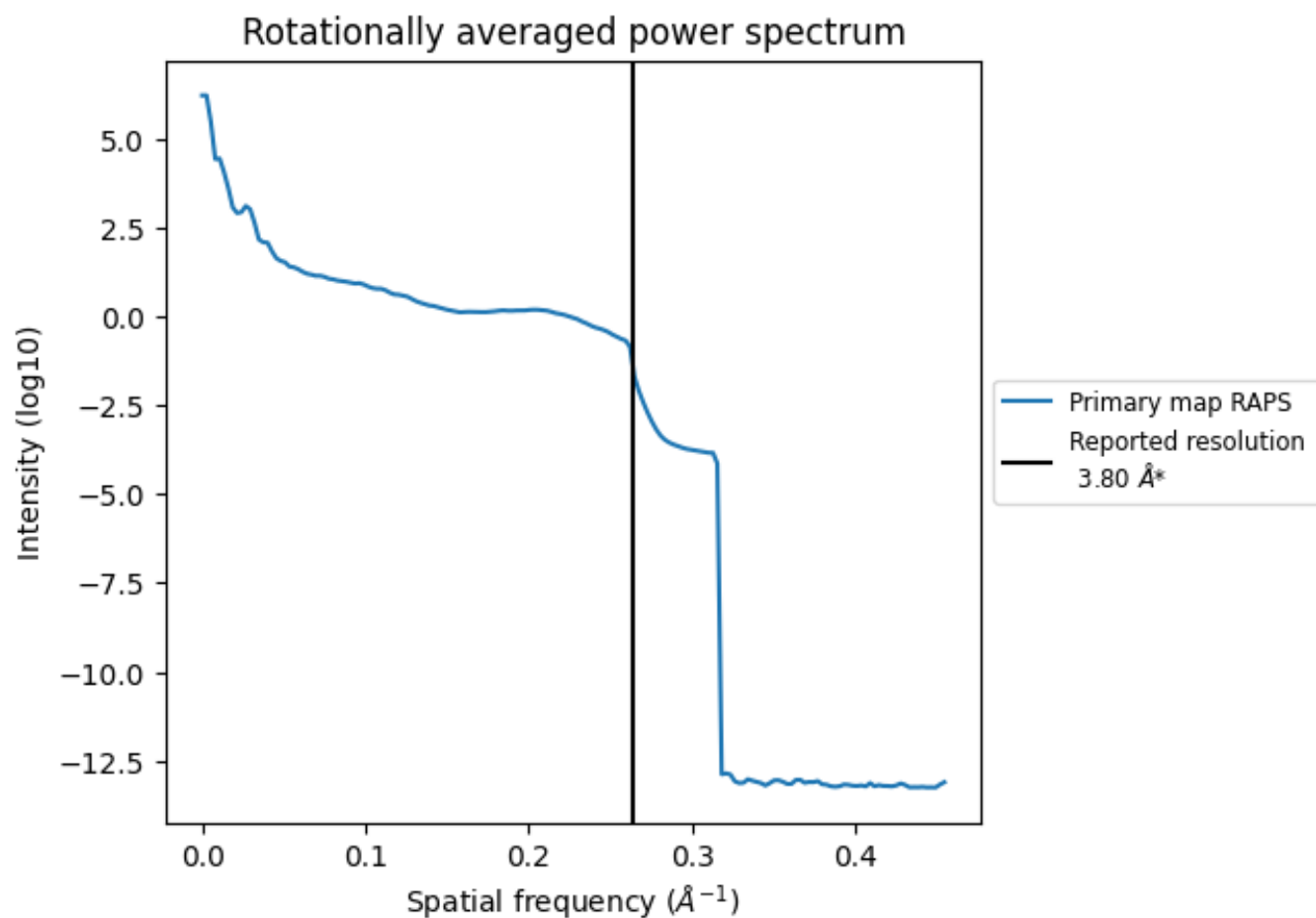
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 360 nm<sup>3</sup>; this corresponds to an approximate mass of 325 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 0.263  $\text{\AA}^{-1}$

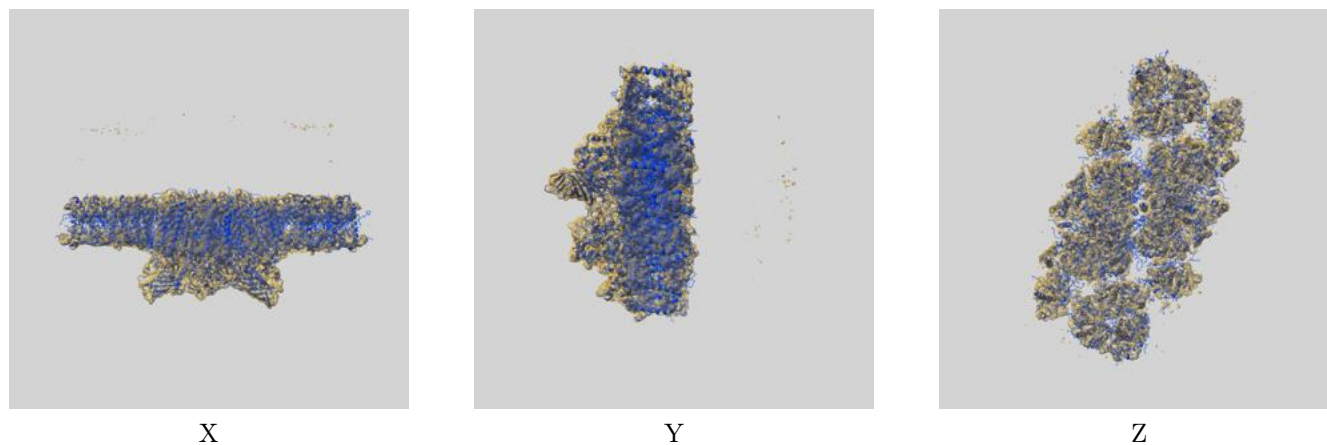
## 8 Fourier-Shell correlation

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

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

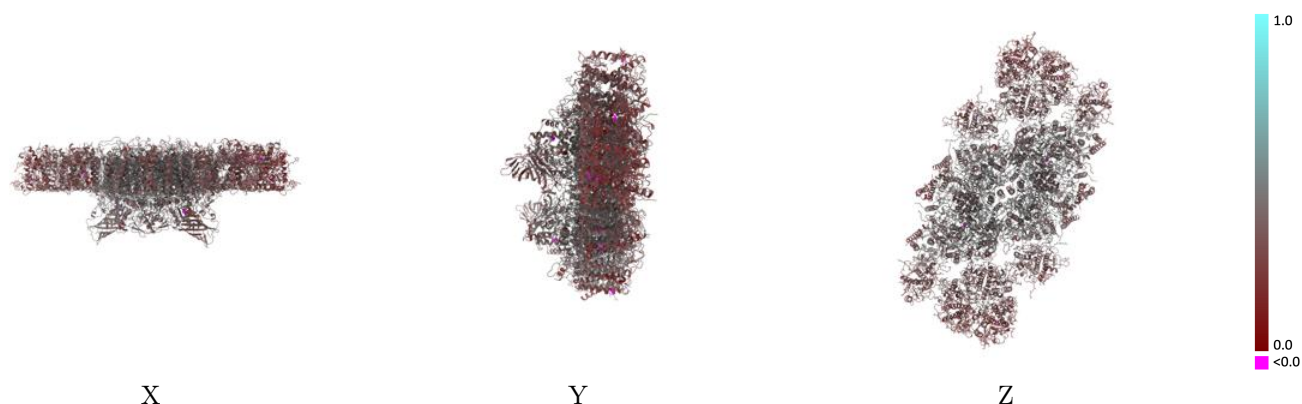
This section contains information regarding the fit between EMDB map EMD-10865 and PDB model 6YP7. Per-residue inclusion information can be found in section [3](#) on page [38](#).

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



The images above show the 3D surface view of the map at the recommended contour level 0.85 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](#)

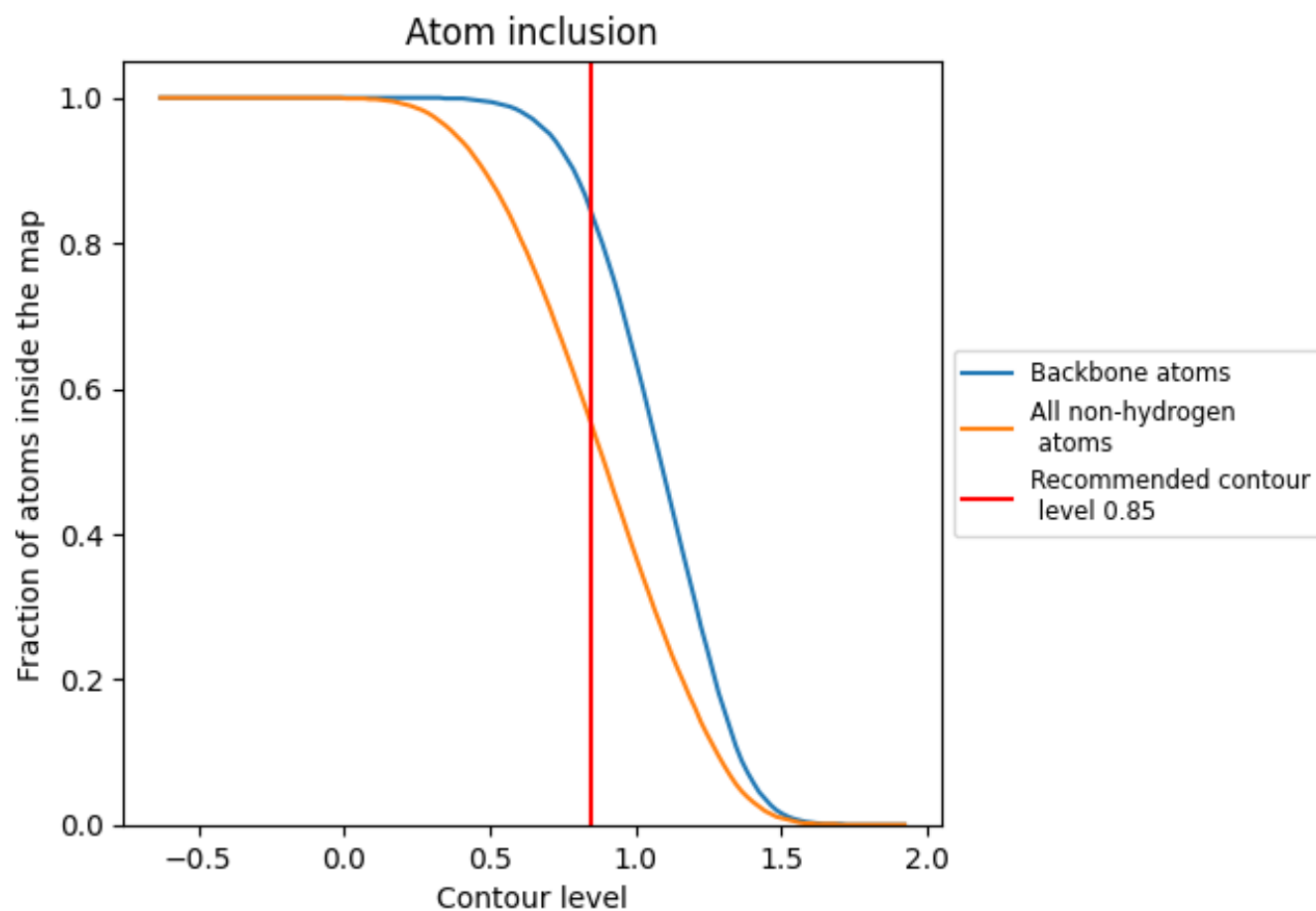


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 55% 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 (0.85) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.5490   |  0.3820   |
| A     |  0.6070   |  0.4440   |
| B     |  0.6110   |  0.4330   |
| C     |  0.6010   |  0.4200   |
| D     |  0.5870   |  0.4380   |
| E     |  0.6390   |  0.3060   |
| F     |  0.5960   |  0.3180   |
| G     |  0.4520   |  0.2780   |
| H     |  0.5190   |  0.3920   |
| I     |  0.5270   |  0.4460   |
| J     |  0.2670   |  0.3740   |
| K     |  0.4340   |  0.4020   |
| L     |  0.4010   |  0.4420   |
| M     |  0.3530   |  0.3940   |
| N     |  0.4790  |  0.2880  |
| O     |  0.5690 |  0.4020 |
| R     |  0.4710 |  0.3470 |
| S     |  0.5430 |  0.3340 |
| T     |  0.3670 |  0.4390 |
| W     |  0.4440 |  0.3460 |
| X     |  0.5220 |  0.3380 |
| Y     |  0.5450 |  0.3440 |
| Z     |  0.5280 |  0.3270 |
| a     |  0.6190 |  0.4440 |
| b     |  0.6220 |  0.4350 |
| c     |  0.6050 |  0.4220 |
| d     |  0.5890 |  0.4410 |
| e     |  0.6740 |  0.3500 |
| f     |  0.5960 |  0.3260 |
| g     |  0.4420 |  0.2710 |
| h     |  0.5360 |  0.4140 |
| i     |  0.6040 |  0.4440 |
| j     |  0.2790 |  0.3520 |
| k     |  0.4300 |  0.4000 |
| l     |  0.3950 |  0.4490 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| m     |  0.4160 |  0.3850 |
| n     |  0.4890 |  0.2920 |
| o     |  0.5420 |  0.3560 |
| r     |  0.4680 |  0.3520 |
| s     |  0.5430 |  0.3330 |
| t     |  0.4960 |  0.4360 |
| w     |  0.4700 |  0.4050 |
| x     |  0.5250 |  0.3640 |
| y     |  0.5440 |  0.3470 |
| z     |  0.5410 |  0.3310 |