



wwPDB EM Validation Summary Report ⓘ

Oct 2, 2025 – 07:05 PM JST

PDB ID : 9LE7 / pdb_00009le7
EMDB ID : EMD-63017
Title : Coordinates of Cryo-EM structure of the Arabidopsis thaliana C4S4M4-type PSII supercomplex
Authors : Chen, S.J.B.; Wu, C.; Wu, J.H.; Sui, S.F.; Zhang, L.X.
Deposited on : 2025-01-07
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

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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

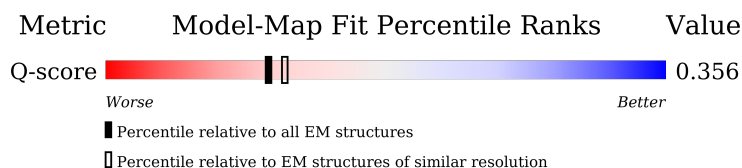
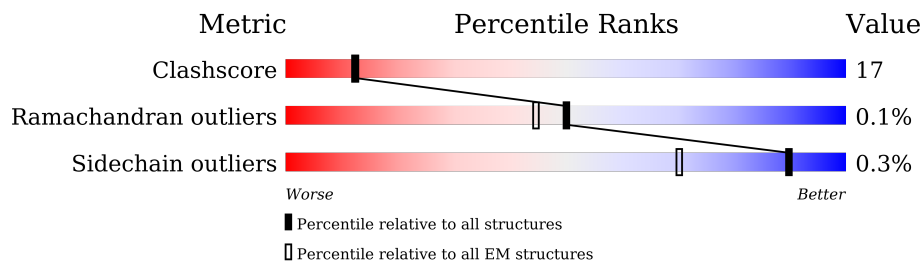
1 Overall quality at a glance

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.














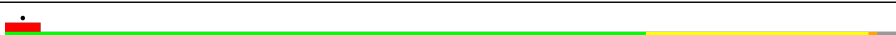

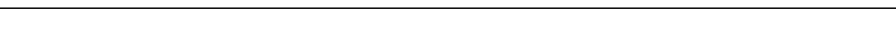
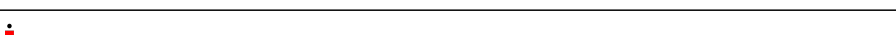
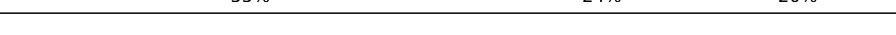

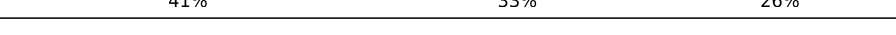







| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore | 210492 | 15764 | - |
| Ramachandran outliers | 207382 | 16835 | - |
| Sidechain outliers | 206894 | 16415 | - |
| 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 ≥ 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 | 5 | 266 | <div> <div>50%</div> <div>25%</div> <div>24%</div> </div> |
| 1 | 7 | 266 | <div> <div>49%</div> <div>26%</div> <div>24%</div> </div> |
| 1 | 9 | 266 | <div> <div>49%</div> <div>27%</div> <div>24%</div> </div> |
| 1 | AA | 266 | <div> <div>48%</div> <div>27%</div> <div>24%</div> </div> |



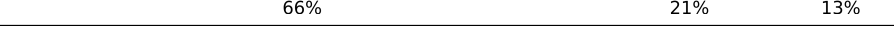
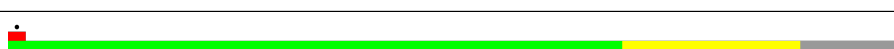



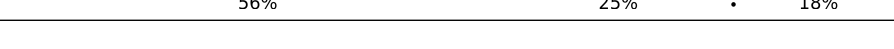



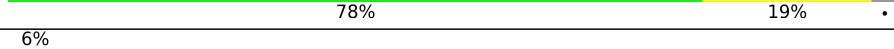

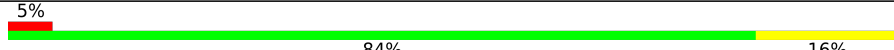


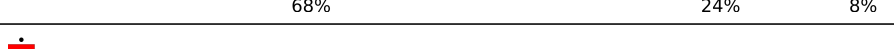







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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | 0 | 243 |  |
| 2 | 6 | 243 |  |
| 3 | 8 | 212 |  |
| 3 | AB | 212 |  |
| 4 | B | 508 |  |
| 4 | BE | 508 |  |
| 4 | b | 508 |  |
| 4 | v | 508 |  |
| 5 | 2 | 352 |  |
| 5 | BG | 352 |  |
| 5 | D | 352 |  |
| 5 | d | 352 |  |
| 6 | 3 | 83 |  |
| 6 | BH | 83 |  |
| 6 | E | 83 |  |
| 6 | e | 83 |  |
| 7 | 4 | 39 |  |
| 7 | BI | 39 |  |
| 7 | F | 39 |  |
| 7 | f | 39 |  |
| 8 | A2 | 232 |  |
| 8 | Au | 232 |  |
| 8 | BB | 232 |  |
| 8 | BJ | 232 |  |
| 8 | BQ | 232 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 8 | Ba | 232 |  |
| 8 | G | 232 |  |
| 8 | N | 232 |  |
| 8 | Y | 232 |  |
| 8 | g | 232 |  |
| 8 | n | 232 |  |
| 8 | y | 232 |  |
| 9 | Av | 72 |  |
| 9 | BK | 72 |  |
| 9 | H | 72 |  |
| 9 | h | 72 |  |
| 10 | Aw | 36 |  |
| 10 | BL | 36 |  |
| 10 | I | 36 |  |
| 10 | i | 36 |  |
| 11 | Ay | 37 |  |
| 11 | BN | 37 |  |
| 11 | K | 37 |  |
| 11 | k | 37 |  |
| 12 | Az | 38 |  |
| 12 | BO | 38 |  |
| 12 | L | 38 |  |
| 12 | l | 38 |  |
| 13 | A1 | 34 |  |
| 13 | BP | 34 | |

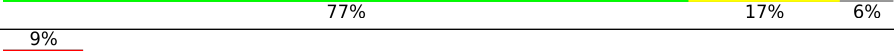
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 13 | M | 34 | |
| 13 | m | 34 | |
| 14 | A6 | 232 | |
| 14 | BV | 232 | |
| 14 | S | 232 | |
| 14 | s | 232 | |
| 15 | A7 | 33 | |
| 15 | BW | 33 | |
| 15 | T | 33 | |
| 15 | t | 33 | |
| 16 | A8 | 28 | |
| 16 | BX | 28 | |
| 16 | U | 28 | |
| 16 | u | 28 | |
| 17 | A0 | 54 | |
| 17 | BY | 54 | |
| 17 | W | 54 | |
| 17 | w | 54 | |
| 18 | BA | 42 | |
| 18 | BZ | 42 | |
| 18 | X | 42 | |
| 18 | x | 42 | |
| 19 | BC | 62 | |
| 19 | Bb | 62 | |
| 19 | Z | 62 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 19 | z | 62 |  |
| 20 | A | 352 |  |
| 20 | BD | 352 |  |
| 20 | R | 352 |  |
| 20 | a | 352 |  |
| 21 | 1 | 459 |  |
| 21 | BF | 459 |  |
| 21 | C | 459 |  |
| 21 | c | 459 |  |
| 22 | BU | 250 |  |
| 22 | r | 250 |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 23 | CHL | 0 | 601 | X | - | - | - |
| 23 | CHL | 0 | 605 | X | - | - | - |
| 23 | CHL | 0 | 606 | X | - | - | - |
| 23 | CHL | 0 | 607 | X | - | - | - |
| 23 | CHL | 0 | 608 | X | - | - | - |
| 23 | CHL | 0 | 609 | X | - | - | - |
| 23 | CHL | 5 | 601 | X | - | - | - |
| 23 | CHL | 5 | 605 | X | - | - | - |
| 23 | CHL | 5 | 606 | X | - | - | - |
| 23 | CHL | 5 | 607 | X | - | - | - |
| 23 | CHL | 5 | 608 | X | - | - | - |
| 23 | CHL | 5 | 609 | X | - | - | - |
| 23 | CHL | 6 | 601 | X | - | - | - |
| 23 | CHL | 6 | 605 | X | - | - | - |
| 23 | CHL | 6 | 606 | X | - | - | - |
| 23 | CHL | 6 | 607 | X | - | - | - |
| 23 | CHL | 6 | 608 | X | - | - | - |
| 23 | CHL | 6 | 609 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 23 | CHL | 7 | 302 | X | - | - | - |
| 23 | CHL | 7 | 306 | X | - | - | - |
| 23 | CHL | 7 | 307 | X | - | - | - |
| 23 | CHL | 7 | 308 | X | - | - | - |
| 23 | CHL | 7 | 309 | X | - | - | - |
| 23 | CHL | 7 | 310 | X | - | - | - |
| 23 | CHL | 8 | 304 | X | - | - | - |
| 23 | CHL | 8 | 305 | X | - | - | - |
| 23 | CHL | 8 | 306 | X | - | - | - |
| 23 | CHL | 8 | 307 | X | - | - | - |
| 23 | CHL | 9 | 601 | X | - | - | - |
| 23 | CHL | 9 | 605 | X | - | - | - |
| 23 | CHL | 9 | 606 | X | - | - | - |
| 23 | CHL | 9 | 607 | X | - | - | - |
| 23 | CHL | 9 | 608 | X | - | - | - |
| 23 | CHL | 9 | 609 | X | - | - | - |
| 23 | CHL | A2 | 601 | X | - | - | - |
| 23 | CHL | A2 | 605 | X | - | - | - |
| 23 | CHL | A2 | 606 | X | - | - | - |
| 23 | CHL | A2 | 607 | X | - | - | - |
| 23 | CHL | A2 | 608 | X | - | - | - |
| 23 | CHL | A2 | 609 | X | - | - | - |
| 23 | CHL | A6 | 601 | X | - | - | - |
| 23 | CHL | A6 | 605 | X | - | - | - |
| 23 | CHL | A6 | 606 | X | - | - | - |
| 23 | CHL | A6 | 607 | X | - | - | - |
| 23 | CHL | AA | 302 | X | - | - | - |
| 23 | CHL | AA | 306 | X | - | - | - |
| 23 | CHL | AA | 307 | X | - | - | - |
| 23 | CHL | AA | 308 | X | - | - | - |
| 23 | CHL | AA | 309 | X | - | - | - |
| 23 | CHL | AA | 310 | X | - | - | - |
| 23 | CHL | AB | 304 | X | - | - | - |
| 23 | CHL | AB | 305 | X | - | - | - |
| 23 | CHL | AB | 306 | X | - | - | - |
| 23 | CHL | AB | 307 | X | - | - | - |
| 23 | CHL | Au | 601 | X | - | - | - |
| 23 | CHL | Au | 605 | X | - | - | - |
| 23 | CHL | Au | 606 | X | - | - | - |
| 23 | CHL | Au | 607 | X | - | - | - |
| 23 | CHL | Au | 608 | X | - | - | - |
| 23 | CHL | Au | 609 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 23 | CHL | BB | 302 | X | - | - | - |
| 23 | CHL | BB | 306 | X | - | - | - |
| 23 | CHL | BB | 307 | X | - | - | - |
| 23 | CHL | BB | 308 | X | - | - | - |
| 23 | CHL | BB | 309 | X | - | - | - |
| 23 | CHL | BB | 310 | X | - | - | - |
| 23 | CHL | BH | 601 | X | - | - | - |
| 23 | CHL | BJ | 601 | X | - | - | - |
| 23 | CHL | BJ | 605 | X | - | - | - |
| 23 | CHL | BJ | 606 | X | - | - | - |
| 23 | CHL | BJ | 607 | X | - | - | - |
| 23 | CHL | BJ | 608 | X | - | - | - |
| 23 | CHL | BJ | 609 | X | - | - | - |
| 23 | CHL | BQ | 601 | X | - | - | - |
| 23 | CHL | BQ | 605 | X | - | - | - |
| 23 | CHL | BQ | 606 | X | - | - | - |
| 23 | CHL | BQ | 607 | X | - | - | - |
| 23 | CHL | BQ | 608 | X | - | - | - |
| 23 | CHL | BQ | 609 | X | - | - | - |
| 23 | CHL | BU | 605 | X | - | - | - |
| 23 | CHL | BU | 606 | X | - | - | - |
| 23 | CHL | BU | 607 | X | - | - | - |
| 23 | CHL | BU | 613 | X | - | - | - |
| 23 | CHL | BV | 601 | X | - | - | - |
| 23 | CHL | BV | 605 | X | - | - | - |
| 23 | CHL | BV | 606 | X | - | - | - |
| 23 | CHL | BV | 607 | X | - | - | - |
| 23 | CHL | Ba | 302 | X | - | - | - |
| 23 | CHL | Ba | 306 | X | - | - | - |
| 23 | CHL | Ba | 307 | X | - | - | - |
| 23 | CHL | Ba | 308 | X | - | - | - |
| 23 | CHL | Ba | 309 | X | - | - | - |
| 23 | CHL | Ba | 310 | X | - | - | - |
| 23 | CHL | G | 601 | X | - | - | - |
| 23 | CHL | G | 605 | X | - | - | - |
| 23 | CHL | G | 606 | X | - | - | - |
| 23 | CHL | G | 607 | X | - | - | - |
| 23 | CHL | G | 608 | X | - | - | - |
| 23 | CHL | G | 609 | X | - | - | - |
| 23 | CHL | N | 601 | X | - | - | - |
| 23 | CHL | N | 605 | X | - | - | - |
| 23 | CHL | N | 606 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 23 | CHL | N | 607 | X | - | - | - |
| 23 | CHL | N | 608 | X | - | - | - |
| 23 | CHL | N | 609 | X | - | - | - |
| 23 | CHL | S | 601 | X | - | - | - |
| 23 | CHL | S | 605 | X | - | - | - |
| 23 | CHL | S | 606 | X | - | - | - |
| 23 | CHL | S | 607 | X | - | - | - |
| 23 | CHL | Y | 302 | X | - | - | - |
| 23 | CHL | Y | 306 | X | - | - | - |
| 23 | CHL | Y | 307 | X | - | - | - |
| 23 | CHL | Y | 308 | X | - | - | - |
| 23 | CHL | Y | 309 | X | - | - | - |
| 23 | CHL | Y | 310 | X | - | - | - |
| 23 | CHL | e | 601 | X | - | - | - |
| 23 | CHL | g | 601 | X | - | - | - |
| 23 | CHL | g | 605 | X | - | - | - |
| 23 | CHL | g | 606 | X | - | - | - |
| 23 | CHL | g | 607 | X | - | - | - |
| 23 | CHL | g | 608 | X | - | - | - |
| 23 | CHL | g | 609 | X | - | - | - |
| 23 | CHL | n | 601 | X | - | - | - |
| 23 | CHL | n | 605 | X | - | - | - |
| 23 | CHL | n | 606 | X | - | - | - |
| 23 | CHL | n | 607 | X | - | - | - |
| 23 | CHL | n | 608 | X | - | - | - |
| 23 | CHL | n | 609 | X | - | - | - |
| 23 | CHL | r | 605 | X | - | - | - |
| 23 | CHL | r | 606 | X | - | - | - |
| 23 | CHL | r | 607 | X | - | - | - |
| 23 | CHL | r | 613 | X | - | - | - |
| 23 | CHL | s | 601 | X | - | - | - |
| 23 | CHL | s | 605 | X | - | - | - |
| 23 | CHL | s | 606 | X | - | - | - |
| 23 | CHL | s | 607 | X | - | - | - |
| 23 | CHL | y | 302 | X | - | - | - |
| 23 | CHL | y | 306 | X | - | - | - |
| 23 | CHL | y | 307 | X | - | - | - |
| 23 | CHL | y | 308 | X | - | - | - |
| 23 | CHL | y | 309 | X | - | - | - |
| 23 | CHL | y | 310 | X | - | - | - |
| 24 | CLA | 0 | 602 | X | - | - | - |
| 24 | CLA | 0 | 603 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24 | CLA | 0 | 604 | X | - | - | - |
| 24 | CLA | 0 | 610 | X | - | - | - |
| 24 | CLA | 0 | 611 | X | - | - | - |
| 24 | CLA | 0 | 612 | X | - | - | - |
| 24 | CLA | 0 | 613 | X | - | - | - |
| 24 | CLA | 0 | 614 | X | - | - | - |
| 24 | CLA | 1 | 502 | X | - | - | - |
| 24 | CLA | 1 | 503 | X | - | - | - |
| 24 | CLA | 1 | 504 | X | - | - | - |
| 24 | CLA | 1 | 505 | X | - | - | - |
| 24 | CLA | 1 | 506 | X | - | - | - |
| 24 | CLA | 1 | 507 | X | - | - | - |
| 24 | CLA | 1 | 508 | X | - | - | - |
| 24 | CLA | 1 | 509 | X | - | - | - |
| 24 | CLA | 1 | 510 | X | - | - | - |
| 24 | CLA | 1 | 511 | X | - | - | - |
| 24 | CLA | 1 | 512 | X | - | - | - |
| 24 | CLA | 1 | 513 | X | - | - | - |
| 24 | CLA | 2 | 402 | X | - | - | - |
| 24 | CLA | 2 | 403 | X | - | - | - |
| 24 | CLA | 5 | 602 | X | - | - | - |
| 24 | CLA | 5 | 603 | X | - | - | - |
| 24 | CLA | 5 | 604 | X | - | - | - |
| 24 | CLA | 5 | 610 | X | - | - | - |
| 24 | CLA | 5 | 611 | X | - | - | - |
| 24 | CLA | 5 | 612 | X | - | - | - |
| 24 | CLA | 5 | 613 | X | - | - | - |
| 24 | CLA | 5 | 614 | X | - | - | - |
| 24 | CLA | 6 | 602 | X | - | - | - |
| 24 | CLA | 6 | 603 | X | - | - | - |
| 24 | CLA | 6 | 604 | X | - | - | - |
| 24 | CLA | 6 | 610 | X | - | - | - |
| 24 | CLA | 6 | 611 | X | - | - | - |
| 24 | CLA | 6 | 612 | X | - | - | - |
| 24 | CLA | 6 | 613 | X | - | - | - |
| 24 | CLA | 6 | 614 | X | - | - | - |
| 24 | CLA | 7 | 303 | X | - | - | - |
| 24 | CLA | 7 | 304 | X | - | - | - |
| 24 | CLA | 7 | 305 | X | - | - | - |
| 24 | CLA | 7 | 311 | X | - | - | - |
| 24 | CLA | 7 | 312 | X | - | - | - |
| 24 | CLA | 7 | 313 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24 | CLA | 7 | 314 | X | - | - | - |
| 24 | CLA | 7 | 315 | X | - | - | - |
| 24 | CLA | 8 | 301 | X | - | - | - |
| 24 | CLA | 8 | 302 | X | - | - | - |
| 24 | CLA | 8 | 303 | X | - | - | - |
| 24 | CLA | 8 | 308 | X | - | - | - |
| 24 | CLA | 8 | 309 | X | - | - | - |
| 24 | CLA | 8 | 310 | X | - | - | - |
| 24 | CLA | 9 | 602 | X | - | - | - |
| 24 | CLA | 9 | 603 | X | - | - | - |
| 24 | CLA | 9 | 604 | X | - | - | - |
| 24 | CLA | 9 | 610 | X | - | - | - |
| 24 | CLA | 9 | 611 | X | - | - | - |
| 24 | CLA | 9 | 612 | X | - | - | - |
| 24 | CLA | 9 | 613 | X | - | - | - |
| 24 | CLA | 9 | 614 | X | - | - | - |
| 24 | CLA | A | 405 | X | - | - | - |
| 24 | CLA | A | 406 | X | - | - | - |
| 24 | CLA | A | 407 | X | - | - | - |
| 24 | CLA | A | 410 | X | - | - | - |
| 24 | CLA | A2 | 602 | X | - | - | - |
| 24 | CLA | A2 | 603 | X | - | - | - |
| 24 | CLA | A2 | 604 | X | - | - | - |
| 24 | CLA | A2 | 610 | X | - | - | - |
| 24 | CLA | A2 | 611 | X | - | - | - |
| 24 | CLA | A2 | 612 | X | - | - | - |
| 24 | CLA | A2 | 613 | X | - | - | - |
| 24 | CLA | A2 | 614 | X | - | - | - |
| 24 | CLA | A6 | 602 | X | - | - | - |
| 24 | CLA | A6 | 603 | X | - | - | - |
| 24 | CLA | A6 | 604 | X | - | - | - |
| 24 | CLA | A6 | 608 | X | - | - | - |
| 24 | CLA | A6 | 609 | X | - | - | - |
| 24 | CLA | A6 | 610 | X | - | - | - |
| 24 | CLA | A6 | 611 | X | - | - | - |
| 24 | CLA | A6 | 612 | X | - | - | - |
| 24 | CLA | A6 | 613 | X | - | - | - |
| 24 | CLA | AA | 303 | X | - | - | - |
| 24 | CLA | AA | 304 | X | - | - | - |
| 24 | CLA | AA | 305 | X | - | - | - |
| 24 | CLA | AA | 311 | X | - | - | - |
| 24 | CLA | AA | 312 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24 | CLA | AA | 313 | X | - | - | - |
| 24 | CLA | AA | 314 | X | - | - | - |
| 24 | CLA | AA | 315 | X | - | - | - |
| 24 | CLA | AB | 301 | X | - | - | - |
| 24 | CLA | AB | 302 | X | - | - | - |
| 24 | CLA | AB | 303 | X | - | - | - |
| 24 | CLA | AB | 308 | X | - | - | - |
| 24 | CLA | AB | 309 | X | - | - | - |
| 24 | CLA | AB | 310 | X | - | - | - |
| 24 | CLA | Au | 602 | X | - | - | - |
| 24 | CLA | Au | 603 | X | - | - | - |
| 24 | CLA | Au | 604 | X | - | - | - |
| 24 | CLA | Au | 610 | X | - | - | - |
| 24 | CLA | Au | 611 | X | - | - | - |
| 24 | CLA | Au | 612 | X | - | - | - |
| 24 | CLA | Au | 613 | X | - | - | - |
| 24 | CLA | Au | 614 | X | - | - | - |
| 24 | CLA | Aw | 102 | X | - | - | - |
| 24 | CLA | B | 601 | X | - | - | - |
| 24 | CLA | B | 602 | X | - | - | - |
| 24 | CLA | B | 603 | X | - | - | - |
| 24 | CLA | B | 604 | X | - | - | - |
| 24 | CLA | B | 605 | X | - | - | - |
| 24 | CLA | B | 606 | X | - | - | - |
| 24 | CLA | B | 607 | X | - | - | - |
| 24 | CLA | B | 608 | X | - | - | - |
| 24 | CLA | B | 609 | X | - | - | - |
| 24 | CLA | B | 610 | X | - | - | - |
| 24 | CLA | B | 611 | X | - | - | - |
| 24 | CLA | B | 612 | X | - | - | - |
| 24 | CLA | B | 613 | X | - | - | - |
| 24 | CLA | B | 614 | X | - | - | - |
| 24 | CLA | B | 615 | X | - | - | - |
| 24 | CLA | B | 616 | X | - | - | - |
| 24 | CLA | BB | 303 | X | - | - | - |
| 24 | CLA | BB | 304 | X | - | - | - |
| 24 | CLA | BB | 305 | X | - | - | - |
| 24 | CLA | BB | 311 | X | - | - | - |
| 24 | CLA | BB | 312 | X | - | - | - |
| 24 | CLA | BB | 313 | X | - | - | - |
| 24 | CLA | BB | 314 | X | - | - | - |
| 24 | CLA | BB | 315 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24 | CLA | BD | 405 | X | - | - | - |
| 24 | CLA | BD | 406 | X | - | - | - |
| 24 | CLA | BD | 407 | X | - | - | - |
| 24 | CLA | BD | 410 | X | - | - | - |
| 24 | CLA | BE | 602 | X | - | - | - |
| 24 | CLA | BE | 603 | X | - | - | - |
| 24 | CLA | BE | 604 | X | - | - | - |
| 24 | CLA | BE | 605 | X | - | - | - |
| 24 | CLA | BE | 606 | X | - | - | - |
| 24 | CLA | BE | 607 | X | - | - | - |
| 24 | CLA | BE | 608 | X | - | - | - |
| 24 | CLA | BE | 609 | X | - | - | - |
| 24 | CLA | BE | 610 | X | - | - | - |
| 24 | CLA | BE | 611 | X | - | - | - |
| 24 | CLA | BE | 612 | X | - | - | - |
| 24 | CLA | BE | 613 | X | - | - | - |
| 24 | CLA | BE | 614 | X | - | - | - |
| 24 | CLA | BE | 615 | X | - | - | - |
| 24 | CLA | BE | 616 | X | - | - | - |
| 24 | CLA | BE | 617 | X | - | - | - |
| 24 | CLA | BF | 502 | X | - | - | - |
| 24 | CLA | BF | 503 | X | - | - | - |
| 24 | CLA | BF | 504 | X | - | - | - |
| 24 | CLA | BF | 505 | X | - | - | - |
| 24 | CLA | BF | 506 | X | - | - | - |
| 24 | CLA | BF | 507 | X | - | - | - |
| 24 | CLA | BF | 508 | X | - | - | - |
| 24 | CLA | BF | 509 | X | - | - | - |
| 24 | CLA | BF | 510 | X | - | - | - |
| 24 | CLA | BF | 511 | X | - | - | - |
| 24 | CLA | BF | 512 | X | - | - | - |
| 24 | CLA | BF | 513 | X | - | - | - |
| 24 | CLA | BF | 514 | X | - | - | - |
| 24 | CLA | BG | 401 | X | - | - | - |
| 24 | CLA | BG | 402 | X | - | - | - |
| 24 | CLA | BJ | 602 | X | - | - | - |
| 24 | CLA | BJ | 603 | X | - | - | - |
| 24 | CLA | BJ | 604 | X | - | - | - |
| 24 | CLA | BJ | 610 | X | - | - | - |
| 24 | CLA | BJ | 611 | X | - | - | - |
| 24 | CLA | BJ | 612 | X | - | - | - |
| 24 | CLA | BJ | 613 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24 | CLA | BJ | 614 | X | - | - | - |
| 24 | CLA | BQ | 602 | X | - | - | - |
| 24 | CLA | BQ | 603 | X | - | - | - |
| 24 | CLA | BQ | 604 | X | - | - | - |
| 24 | CLA | BQ | 610 | X | - | - | - |
| 24 | CLA | BQ | 611 | X | - | - | - |
| 24 | CLA | BQ | 612 | X | - | - | - |
| 24 | CLA | BQ | 613 | X | - | - | - |
| 24 | CLA | BQ | 614 | X | - | - | - |
| 24 | CLA | BU | 601 | X | - | - | - |
| 24 | CLA | BU | 602 | X | - | - | - |
| 24 | CLA | BU | 603 | X | - | - | - |
| 24 | CLA | BU | 604 | X | - | - | - |
| 24 | CLA | BU | 608 | X | - | - | - |
| 24 | CLA | BU | 609 | X | - | - | - |
| 24 | CLA | BU | 610 | X | - | - | - |
| 24 | CLA | BU | 611 | X | - | - | - |
| 24 | CLA | BU | 612 | X | - | - | - |
| 24 | CLA | BU | 614 | X | - | - | - |
| 24 | CLA | BV | 602 | X | - | - | - |
| 24 | CLA | BV | 603 | X | - | - | - |
| 24 | CLA | BV | 604 | X | - | - | - |
| 24 | CLA | BV | 608 | X | - | - | - |
| 24 | CLA | BV | 609 | X | - | - | - |
| 24 | CLA | BV | 610 | X | - | - | - |
| 24 | CLA | BV | 611 | X | - | - | - |
| 24 | CLA | BV | 612 | X | - | - | - |
| 24 | CLA | BV | 613 | X | - | - | - |
| 24 | CLA | Ba | 303 | X | - | - | - |
| 24 | CLA | Ba | 304 | X | - | - | - |
| 24 | CLA | Ba | 305 | X | - | - | - |
| 24 | CLA | Ba | 311 | X | - | - | - |
| 24 | CLA | Ba | 312 | X | - | - | - |
| 24 | CLA | Ba | 313 | X | - | - | - |
| 24 | CLA | Ba | 314 | X | - | - | - |
| 24 | CLA | Ba | 315 | X | - | - | - |
| 24 | CLA | C | 502 | X | - | - | - |
| 24 | CLA | C | 503 | X | - | - | - |
| 24 | CLA | C | 504 | X | - | - | - |
| 24 | CLA | C | 505 | X | - | - | - |
| 24 | CLA | C | 506 | X | - | - | - |
| 24 | CLA | C | 507 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24 | CLA | C | 508 | X | - | - | - |
| 24 | CLA | C | 509 | X | - | - | - |
| 24 | CLA | C | 510 | X | - | - | - |
| 24 | CLA | C | 511 | X | - | - | - |
| 24 | CLA | C | 512 | X | - | - | - |
| 24 | CLA | C | 513 | X | - | - | - |
| 24 | CLA | D | 401 | X | - | - | - |
| 24 | CLA | D | 402 | X | - | - | - |
| 24 | CLA | G | 602 | X | - | - | - |
| 24 | CLA | G | 603 | X | - | - | - |
| 24 | CLA | G | 604 | X | - | - | - |
| 24 | CLA | G | 610 | X | - | - | - |
| 24 | CLA | G | 611 | X | - | - | - |
| 24 | CLA | G | 612 | X | - | - | - |
| 24 | CLA | G | 613 | X | - | - | - |
| 24 | CLA | G | 614 | X | - | - | - |
| 24 | CLA | I | 102 | X | - | - | - |
| 24 | CLA | N | 602 | X | - | - | - |
| 24 | CLA | N | 603 | X | - | - | - |
| 24 | CLA | N | 604 | X | - | - | - |
| 24 | CLA | N | 610 | X | - | - | - |
| 24 | CLA | N | 611 | X | - | - | - |
| 24 | CLA | N | 612 | X | - | - | - |
| 24 | CLA | N | 613 | X | - | - | - |
| 24 | CLA | N | 614 | X | - | - | - |
| 24 | CLA | R | 404 | X | - | - | - |
| 24 | CLA | R | 405 | X | - | - | - |
| 24 | CLA | R | 406 | X | - | - | - |
| 24 | CLA | R | 409 | X | - | - | - |
| 24 | CLA | S | 602 | X | - | - | - |
| 24 | CLA | S | 603 | X | - | - | - |
| 24 | CLA | S | 604 | X | - | - | - |
| 24 | CLA | S | 608 | X | - | - | - |
| 24 | CLA | S | 609 | X | - | - | - |
| 24 | CLA | S | 610 | X | - | - | - |
| 24 | CLA | S | 611 | X | - | - | - |
| 24 | CLA | S | 612 | X | - | - | - |
| 24 | CLA | S | 613 | X | - | - | - |
| 24 | CLA | Y | 303 | X | - | - | - |
| 24 | CLA | Y | 304 | X | - | - | - |
| 24 | CLA | Y | 305 | X | - | - | - |
| 24 | CLA | Y | 311 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24 | CLA | Y | 312 | X | - | - | - |
| 24 | CLA | Y | 313 | X | - | - | - |
| 24 | CLA | Y | 314 | X | - | - | - |
| 24 | CLA | Y | 315 | X | - | - | - |
| 24 | CLA | a | 405 | X | - | - | - |
| 24 | CLA | a | 406 | X | - | - | - |
| 24 | CLA | a | 407 | X | - | - | - |
| 24 | CLA | a | 410 | X | - | - | - |
| 24 | CLA | b | 602 | X | - | - | - |
| 24 | CLA | b | 603 | X | - | - | - |
| 24 | CLA | b | 604 | X | - | - | - |
| 24 | CLA | b | 605 | X | - | - | - |
| 24 | CLA | b | 606 | X | - | - | - |
| 24 | CLA | b | 607 | X | - | - | - |
| 24 | CLA | b | 608 | X | - | - | - |
| 24 | CLA | b | 609 | X | - | - | - |
| 24 | CLA | b | 610 | X | - | - | - |
| 24 | CLA | b | 611 | X | - | - | - |
| 24 | CLA | b | 612 | X | - | - | - |
| 24 | CLA | b | 613 | X | - | - | - |
| 24 | CLA | b | 614 | X | - | - | - |
| 24 | CLA | b | 615 | X | - | - | - |
| 24 | CLA | b | 616 | X | - | - | - |
| 24 | CLA | b | 617 | X | - | - | - |
| 24 | CLA | c | 502 | X | - | - | - |
| 24 | CLA | c | 503 | X | - | - | - |
| 24 | CLA | c | 504 | X | - | - | - |
| 24 | CLA | c | 505 | X | - | - | - |
| 24 | CLA | c | 506 | X | - | - | - |
| 24 | CLA | c | 507 | X | - | - | - |
| 24 | CLA | c | 508 | X | - | - | - |
| 24 | CLA | c | 509 | X | - | - | - |
| 24 | CLA | c | 510 | X | - | - | - |
| 24 | CLA | c | 511 | X | - | - | - |
| 24 | CLA | c | 512 | X | - | - | - |
| 24 | CLA | c | 513 | X | - | - | - |
| 24 | CLA | c | 514 | X | - | - | - |
| 24 | CLA | d | 401 | X | - | - | - |
| 24 | CLA | d | 402 | X | - | - | - |
| 24 | CLA | g | 602 | X | - | - | - |
| 24 | CLA | g | 603 | X | - | - | - |
| 24 | CLA | g | 604 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24 | CLA | g | 610 | X | - | - | - |
| 24 | CLA | g | 611 | X | - | - | - |
| 24 | CLA | g | 612 | X | - | - | - |
| 24 | CLA | g | 613 | X | - | - | - |
| 24 | CLA | g | 614 | X | - | - | - |
| 24 | CLA | n | 602 | X | - | - | - |
| 24 | CLA | n | 603 | X | - | - | - |
| 24 | CLA | n | 604 | X | - | - | - |
| 24 | CLA | n | 610 | X | - | - | - |
| 24 | CLA | n | 611 | X | - | - | - |
| 24 | CLA | n | 612 | X | - | - | - |
| 24 | CLA | n | 613 | X | - | - | - |
| 24 | CLA | n | 614 | X | - | - | - |
| 24 | CLA | r | 601 | X | - | - | - |
| 24 | CLA | r | 602 | X | - | - | - |
| 24 | CLA | r | 603 | X | - | - | - |
| 24 | CLA | r | 604 | X | - | - | - |
| 24 | CLA | r | 608 | X | - | - | - |
| 24 | CLA | r | 609 | X | - | - | - |
| 24 | CLA | r | 610 | X | - | - | - |
| 24 | CLA | r | 611 | X | - | - | - |
| 24 | CLA | r | 612 | X | - | - | - |
| 24 | CLA | r | 614 | X | - | - | - |
| 24 | CLA | s | 602 | X | - | - | - |
| 24 | CLA | s | 603 | X | - | - | - |
| 24 | CLA | s | 604 | X | - | - | - |
| 24 | CLA | s | 608 | X | - | - | - |
| 24 | CLA | s | 609 | X | - | - | - |
| 24 | CLA | s | 610 | X | - | - | - |
| 24 | CLA | s | 611 | X | - | - | - |
| 24 | CLA | s | 612 | X | - | - | - |
| 24 | CLA | s | 613 | X | - | - | - |
| 24 | CLA | v | 601 | X | - | - | - |
| 24 | CLA | v | 602 | X | - | - | - |
| 24 | CLA | v | 603 | X | - | - | - |
| 24 | CLA | v | 604 | X | - | - | - |
| 24 | CLA | v | 605 | X | - | - | - |
| 24 | CLA | v | 606 | X | - | - | - |
| 24 | CLA | v | 607 | X | - | - | - |
| 24 | CLA | v | 608 | X | - | - | - |
| 24 | CLA | v | 609 | X | - | - | - |
| 24 | CLA | v | 610 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24 | CLA | v | 611 | X | - | - | - |
| 24 | CLA | v | 612 | X | - | - | - |
| 24 | CLA | v | 613 | X | - | - | - |
| 24 | CLA | v | 614 | X | - | - | - |
| 24 | CLA | v | 615 | X | - | - | - |
| 24 | CLA | v | 616 | X | - | - | - |
| 24 | CLA | y | 303 | X | - | - | - |
| 24 | CLA | y | 304 | X | - | - | - |
| 24 | CLA | y | 305 | X | - | - | - |
| 24 | CLA | y | 311 | X | - | - | - |
| 24 | CLA | y | 312 | X | - | - | - |
| 24 | CLA | y | 313 | X | - | - | - |
| 24 | CLA | y | 314 | X | - | - | - |
| 24 | CLA | y | 315 | X | - | - | - |

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 146846 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, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1 | 5 | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1529 | 991 | 249 | 285 | 4 | | |
| 1 | 7 | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1530 | 991 | 249 | 285 | 5 | | |
| 1 | 9 | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1529 | 991 | 249 | 285 | 4 | | |
| 1 | AA | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1530 | 991 | 249 | 285 | 5 | | |

- Molecule 2 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2 | 6 | 222 | Total | C | N | O | S | 0 | 0 |
| | | | 1716 | 1120 | 280 | 311 | 5 | | |
| 2 | 0 | 222 | Total | C | N | O | S | 0 | 0 |
| | | | 1716 | 1120 | 280 | 311 | 5 | | |

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | 8 | 192 | Total | C | N | O | S | 0 | 0 |
| | | | 1512 | 993 | 245 | 270 | 4 | | |
| 3 | AB | 192 | Total | C | N | O | S | 0 | 0 |
| | | | 1512 | 993 | 245 | 270 | 4 | | |

- Molecule 4 is a protein called Photosystem II CP47 reaction center protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4 | B | 479 | Total | C | N | O | S | 0 | 0 |
| | | | 3757 | 2462 | 636 | 647 | 12 | | |
| 4 | b | 479 | Total | C | N | O | S | 0 | 0 |
| | | | 3757 | 2462 | 636 | 647 | 12 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4 | v | 479 | Total | C | N | O | S | 0 | 0 |
| | | | 3757 | 2462 | 636 | 647 | 12 | | |
| 4 | BE | 479 | Total | C | N | O | S | 0 | 0 |
| | | | 3757 | 2462 | 636 | 647 | 12 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5 | D | 342 | Total | C | N | O | S | 0 | 0 |
| | | | 2723 | 1800 | 445 | 466 | 12 | | |
| 5 | d | 342 | Total | C | N | O | S | 0 | 0 |
| | | | 2723 | 1800 | 445 | 466 | 12 | | |
| 5 | 2 | 342 | Total | C | N | O | S | 0 | 0 |
| | | | 2723 | 1800 | 445 | 466 | 12 | | |
| 5 | BG | 342 | Total | C | N | O | S | 0 | 0 |
| | | | 2723 | 1800 | 445 | 466 | 12 | | |

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

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 6 | E | 66 | Total | C | N | O | 0 | 0 |
| | | | 544 | 357 | 88 | 99 | | |
| 6 | e | 66 | Total | C | N | O | 0 | 0 |
| | | | 544 | 357 | 88 | 99 | | |
| 6 | 3 | 66 | Total | C | N | O | 0 | 0 |
| | | | 544 | 357 | 88 | 99 | | |
| 6 | BH | 66 | Total | C | N | O | 0 | 0 |
| | | | 544 | 357 | 88 | 99 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7 | F | 29 | Total | C | N | O | S | 0 | 0 |
| | | | 225 | 147 | 40 | 37 | 1 | | |
| 7 | f | 29 | Total | C | N | O | S | 0 | 0 |
| | | | 225 | 147 | 40 | 37 | 1 | | |
| 7 | 4 | 29 | Total | C | N | O | S | 0 | 0 |
| | | | 225 | 147 | 40 | 37 | 1 | | |
| 7 | BI | 29 | Total | C | N | O | S | 0 | 0 |
| | | | 225 | 147 | 40 | 37 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8 | G | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1562 | 1010 | 255 | 292 | 5 | | |
| 8 | N | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1536 | 994 | 251 | 286 | 5 | | |
| 8 | Y | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1621 | 1048 | 266 | 302 | 5 | | |
| 8 | g | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1562 | 1010 | 255 | 292 | 5 | | |
| 8 | n | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1536 | 994 | 251 | 286 | 5 | | |
| 8 | y | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1621 | 1048 | 266 | 302 | 5 | | |
| 8 | Au | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1562 | 1010 | 255 | 292 | 5 | | |
| 8 | A2 | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1536 | 994 | 251 | 286 | 5 | | |
| 8 | BB | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1621 | 1048 | 266 | 302 | 5 | | |
| 8 | BJ | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1562 | 1010 | 255 | 292 | 5 | | |
| 8 | BQ | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1536 | 994 | 251 | 286 | 5 | | |
| 8 | Ba | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1621 | 1048 | 266 | 302 | 5 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9 | H | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 438 | 289 | 68 | 79 | 2 | | |
| 9 | h | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 438 | 289 | 68 | 79 | 2 | | |
| 9 | Av | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 438 | 289 | 68 | 79 | 2 | | |
| 9 | BK | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 438 | 289 | 68 | 79 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10 | I | 35 | Total | C | N | O | S | 0 | 0 |
| | | | 286 | 195 | 44 | 46 | 1 | | |
| 10 | i | 35 | Total | C | N | O | S | 0 | 0 |
| | | | 286 | 195 | 44 | 46 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10 | Aw | 35 | Total | C | N | O | S | 0 | 0 |
| | | | 286 | 195 | 44 | 46 | 1 | | |
| 10 | BL | 35 | Total | C | N | O | S | 0 | 0 |
| | | | 286 | 195 | 44 | 46 | 1 | | |

- 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 |
| | | | 302 | 211 | 44 | 46 | 1 | | |
| 11 | k | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 302 | 211 | 44 | 46 | 1 | | |
| 11 | Ay | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 302 | 211 | 44 | 46 | 1 | | |
| 11 | BN | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 302 | 211 | 44 | 46 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 12 | L | 35 | Total | C | N | O | | 0 | 0 |
| | | | 293 | 195 | 45 | 53 | | | |
| 12 | l | 35 | Total | C | N | O | | 0 | 0 |
| | | | 293 | 195 | 45 | 53 | | | |
| 12 | Az | 35 | Total | C | N | O | | 0 | 0 |
| | | | 293 | 195 | 45 | 53 | | | |
| 12 | BO | 35 | Total | C | N | O | | 0 | 0 |
| | | | 293 | 195 | 45 | 53 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 13 | M | 32 | Total | C | N | O | S | 0 | 0 |
| | | | 250 | 173 | 35 | 41 | 1 | | |
| 13 | m | 32 | Total | C | N | O | S | 0 | 0 |
| | | | 250 | 173 | 35 | 41 | 1 | | |
| 13 | A1 | 32 | Total | C | N | O | S | 0 | 0 |
| | | | 250 | 173 | 35 | 41 | 1 | | |
| 13 | BP | 32 | Total | C | N | O | S | 0 | 0 |
| | | | 250 | 173 | 35 | 41 | 1 | | |

- Molecule 14 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14 | S | 216 | Total | C | N | O | S | 0 | 0 |
| | | | 1670 | 1091 | 272 | 303 | 4 | | |
| 14 | s | 216 | Total | C | N | O | S | 0 | 0 |
| | | | 1670 | 1091 | 272 | 303 | 4 | | |
| 14 | A6 | 216 | Total | C | N | O | S | 0 | 0 |
| | | | 1670 | 1091 | 272 | 303 | 4 | | |
| 14 | BV | 216 | Total | C | N | O | S | 0 | 0 |
| | | | 1670 | 1091 | 272 | 303 | 4 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 15 | T | 29 | Total | C | N | O | S | 0 | 0 |
| | | | 239 | 168 | 33 | 37 | 1 | | |
| 15 | t | 29 | Total | C | N | O | S | 0 | 0 |
| | | | 239 | 168 | 33 | 37 | 1 | | |
| 15 | A7 | 29 | Total | C | N | O | S | 0 | 0 |
| | | | 239 | 168 | 33 | 37 | 1 | | |
| 15 | BW | 29 | Total | C | N | O | S | 0 | 0 |
| | | | 239 | 168 | 33 | 37 | 1 | | |

- Molecule 16 is a protein called Photosystem II 5 kDa protein, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 16 | U | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 195 | 122 | 36 | 34 | 3 | | |
| 16 | u | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 195 | 122 | 36 | 34 | 3 | | |
| 16 | A8 | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 195 | 122 | 36 | 34 | 3 | | |
| 16 | BX | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 195 | 122 | 36 | 34 | 3 | | |

- Molecule 17 is a protein called Photosystem II reaction center W protein, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 17 | W | 54 | Total | C | N | O | S | 0 | 0 |
| | | | 428 | 282 | 61 | 84 | 1 | | |
| 17 | w | 54 | Total | C | N | O | S | 0 | 0 |
| | | | 428 | 282 | 61 | 84 | 1 | | |
| 17 | A0 | 54 | Total | C | N | O | S | 0 | 0 |
| | | | 428 | 282 | 61 | 84 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 17 | BY | 54 | Total | C | N | O | S | 0 | 0 |
| | | | 428 | 282 | 61 | 84 | 1 | | |

- Molecule 18 is a protein called (thale cress) hypothetical protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 18 | X | 36 | Total | C | N | O | | 0 | 0 |
| | | | 248 | 162 | 39 | 47 | | | |
| 18 | x | 36 | Total | C | N | O | | 0 | 0 |
| | | | 248 | 162 | 39 | 47 | | | |
| 18 | BA | 36 | Total | C | N | O | | 0 | 0 |
| | | | 248 | 162 | 39 | 47 | | | |
| 18 | BZ | 36 | Total | C | N | O | | 0 | 0 |
| | | | 248 | 162 | 39 | 47 | | | |

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 19 | Z | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 465 | 313 | 69 | 82 | 1 | | |
| 19 | z | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 465 | 313 | 69 | 82 | 1 | | |
| 19 | BC | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 465 | 313 | 69 | 82 | 1 | | |
| 19 | Bb | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 465 | 313 | 69 | 82 | 1 | | |

- Molecule 20 is a protein called Photosystem II protein D1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20 | A | 323 | Total | C | N | O | S | 0 | 0 |
| | | | 2525 | 1652 | 415 | 445 | 13 | | |
| 20 | a | 323 | Total | C | N | O | S | 0 | 0 |
| | | | 2525 | 1652 | 415 | 445 | 13 | | |
| 20 | R | 323 | Total | C | N | O | S | 0 | 0 |
| | | | 2525 | 1652 | 415 | 445 | 13 | | |
| 20 | BD | 323 | Total | C | N | O | S | 0 | 0 |
| | | | 2525 | 1652 | 415 | 445 | 13 | | |

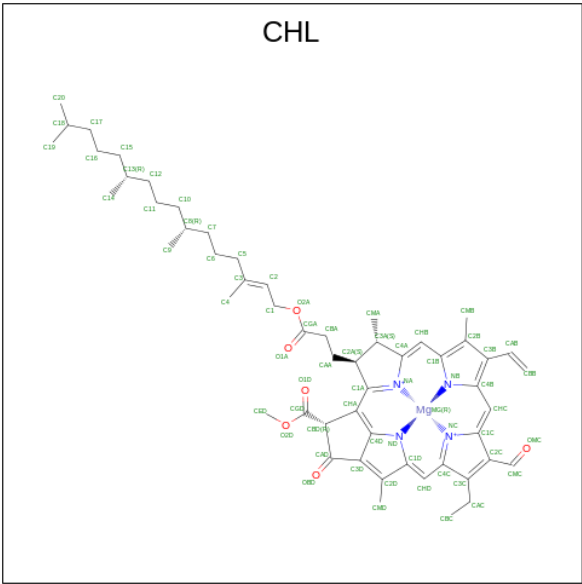
- Molecule 21 is a protein called Photosystem II CP43 reaction center protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 21 | C | 433 | Total | C | N | O | S | 0 | 0 |
| | | | 3373 | 2221 | 563 | 578 | 11 | | |
| 21 | c | 432 | Total | C | N | O | S | 0 | 0 |
| | | | 3365 | 2217 | 561 | 576 | 11 | | |
| 21 | 1 | 433 | Total | C | N | O | S | 0 | 0 |
| | | | 3373 | 2221 | 563 | 578 | 11 | | |
| 21 | BF | 432 | Total | C | N | O | S | 0 | 0 |
| | | | 3365 | 2217 | 561 | 576 | 11 | | |

- Molecule 22 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 22 | r | 197 | Total | C | N | O | S | 0 | 0 |
| | | | 1539 | 1004 | 251 | 281 | 3 | | |
| 22 | BU | 197 | Total | C | N | O | S | 0 | 0 |
| | | | 1539 | 1004 | 251 | 281 | 3 | | |

- Molecule 23 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 23 | 5 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 5 | 1 | Total 61 | C 50 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 6 | 1 | Total 63 | C 52 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 6 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 6 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 6 | 1 | Total 53 | C 42 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 6 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 6 | 1 | Total 60 | C 49 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 7 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 7 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 7 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 7 | 1 | Total 60 | C 49 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 7 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 7 | 1 | Total 60 | C 49 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 8 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 8 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 8 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 8 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | G | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | G | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | G | 1 | Total 50 | C 39 | Mg 1 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 23 | G | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | G | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | G | 1 | Total 58 | C 48 | Mg 1 | N 4 | O 5 | 0 |
| 23 | N | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | N | 1 | Total 48 | C 37 | Mg 1 | N 4 | O 6 | 0 |
| 23 | N | 1 | Total 50 | C 39 | Mg 1 | N 4 | O 6 | 0 |
| 23 | N | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | N | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | N | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | S | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | S | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | S | 1 | Total 57 | C 46 | Mg 1 | N 4 | O 6 | 0 |
| 23 | S | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | Y | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | Y | 1 | Total 48 | C 37 | Mg 1 | N 4 | O 6 | 0 |
| 23 | Y | 1 | Total 50 | C 39 | Mg 1 | N 4 | O 6 | 0 |
| 23 | Y | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | Y | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | Y | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | e | 1 | Total 45 | C 34 | Mg 1 | N 4 | O 6 | 0 |
| 23 | g | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 23 | g | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | g | 1 | Total 50 | C 39 | Mg 1 | N 4 | O 6 | 0 |
| 23 | g | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | g | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | g | 1 | Total 60 | C 49 | Mg 1 | N 4 | O 6 | 0 |
| 23 | n | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | n | 1 | Total 48 | C 37 | Mg 1 | N 4 | O 6 | 0 |
| 23 | n | 1 | Total 50 | C 39 | Mg 1 | N 4 | O 6 | 0 |
| 23 | n | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | n | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | n | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | s | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | s | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | s | 1 | Total 57 | C 46 | Mg 1 | N 4 | O 6 | 0 |
| 23 | s | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | y | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | y | 1 | Total 48 | C 37 | Mg 1 | N 4 | O 6 | 0 |
| 23 | y | 1 | Total 50 | C 39 | Mg 1 | N 4 | O 6 | 0 |
| 23 | y | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | y | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | y | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 23 | r | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | r | 1 | Total 55 | C 44 | Mg 1 | N 4 | O 6 | 0 |
| 23 | r | 1 | Total 60 | C 49 | Mg 1 | N 4 | O 6 | 0 |
| 23 | r | 1 | Total 42 | C 33 | Mg 1 | N 4 | O 4 | 0 |
| 23 | 9 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 9 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 9 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 9 | 1 | Total 62 | C 51 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 9 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 9 | 1 | Total 61 | C 50 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 0 | 1 | Total 63 | C 52 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 0 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 0 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 0 | 1 | Total 53 | C 42 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 0 | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | 0 | 1 | Total 60 | C 49 | Mg 1 | N 4 | O 6 | 0 |
| 23 | AA | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | AA | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | AA | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | AA | 1 | Total 60 | C 49 | Mg 1 | N 4 | O 6 | 0 |
| 23 | AA | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 23 | AA | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | |
| 23 | AB | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 23 | AB | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 23 | AB | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 23 | AB | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 23 | Au | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 23 | Au | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 23 | Au | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 39 | 1 | 4 | 6 | |
| 23 | Au | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 23 | Au | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 23 | Au | 1 | Total | C | Mg | N | O | 0 |
| | | | 58 | 48 | 1 | 4 | 5 | |
| 23 | A2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 23 | A2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 48 | 37 | 1 | 4 | 6 | |
| 23 | A2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 39 | 1 | 4 | 6 | |
| 23 | A2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 23 | A2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 23 | A2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 23 | A6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 23 | A6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 23 | A6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 57 | 46 | 1 | 4 | 6 | |
| 23 | A6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |

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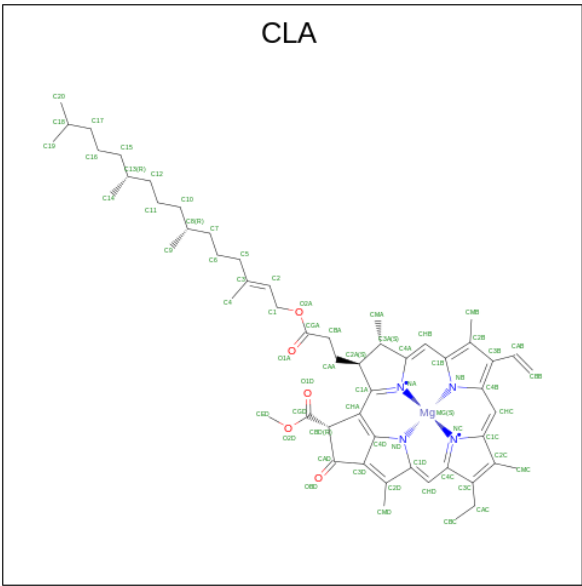
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 23 | BB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BB | 1 | Total 48 | C 37 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BB | 1 | Total 50 | C 39 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BB | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BH | 1 | Total 45 | C 34 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BJ | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BJ | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BJ | 1 | Total 50 | C 39 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BJ | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BJ | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BJ | 1 | Total 60 | C 49 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BQ | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BQ | 1 | Total 48 | C 37 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BQ | 1 | Total 50 | C 39 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BQ | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BQ | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BQ | 1 | Total 65 | C 54 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BV | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |
| 23 | BV | 1 | Total 46 | C 35 | Mg 1 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 23 | BV | 1 | Total | C | Mg | N | O | 0 |
| | | | 57 | 46 | 1 | 4 | 6 | |
| 23 | BV | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 23 | Ba | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 23 | Ba | 1 | Total | C | Mg | N | O | 0 |
| | | | 48 | 37 | 1 | 4 | 6 | |
| 23 | Ba | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 39 | 1 | 4 | 6 | |
| 23 | Ba | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 23 | Ba | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 23 | Ba | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 23 | BU | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 23 | BU | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 44 | 1 | 4 | 6 | |
| 23 | BU | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | |
| 23 | BU | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 33 | 1 | 4 | 4 | |

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 24 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 61 | 51 | 1 | 4 | 5 | |
| 24 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 24 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 24 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | |
| 24 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 24 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 24 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 24 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 24 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 24 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 24 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 24 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 24 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 24 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 24 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 58 | 48 | 1 | 4 | 5 | |
| 24 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 48 | 38 | 1 | 4 | 5 | |
| 24 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 61 | 51 | 1 | 4 | 5 | |
| 24 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 24 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 24 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 48 | 39 | 1 | 4 | 4 | |
| 24 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 24 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 24 | 7 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 7 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 8 | 1 | Total 41 | C 33 | Mg 1 | N 4 | O 3 | 0 |
| 24 | 8 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 8 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 8 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 8 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 8 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | D | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | D | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | G | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | G | 1 | Total 64 | C 54 | Mg 1 | N 4 | O 5 | 0 |
| 24 | G | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | G | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | G | 1 | Total 48 | C 38 | Mg 1 | N 4 | O 5 | 0 |
| 24 | I | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | N | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | N | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | N | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | N | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | N | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | N | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | N | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 24 | N | 1 | Total 48 | C 38 | Mg 1 | N 4 | O 5 | 0 |
| 24 | S | 1 | Total 61 | C 51 | Mg 1 | N 4 | O 5 | 0 |
| 24 | S | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | S | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | S | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | S | 1 | Total 53 | C 44 | Mg 1 | N 4 | O 4 | 0 |
| 24 | S | 1 | Total 56 | C 46 | Mg 1 | N 4 | O 5 | 0 |
| 24 | S | 1 | Total 49 | C 39 | Mg 1 | N 4 | O 5 | 0 |
| 24 | S | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 24 | S | 1 | Total 49 | C 39 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Y | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Y | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Y | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Y | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Y | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Y | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Y | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Y | 1 | Total 48 | C 38 | Mg 1 | N 4 | O 5 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | d | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | d | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | g | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | g | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | g | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | g | 1 | Total 64 | C 54 | Mg 1 | N 4 | O 5 | 0 |
| 24 | g | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | g | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 24 | g | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | g | 1 | Total 48 | C 38 | Mg 1 | N 4 | O 5 | 0 |
| 24 | n | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | n | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | n | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | n | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | n | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | n | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | n | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | n | 1 | Total 48 | C 38 | Mg 1 | N 4 | O 5 | 0 |
| 24 | s | 1 | Total 61 | C 51 | Mg 1 | N 4 | O 5 | 0 |
| 24 | s | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | s | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | s | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | s | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 24 | s | 1 | Total 56 | C 46 | Mg 1 | N 4 | O 5 | 0 |
| 24 | s | 1 | Total 49 | C 39 | Mg 1 | N 4 | O 5 | 0 |
| 24 | s | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 24 | s | 1 | Total 49 | C 39 | Mg 1 | N 4 | O 5 | 0 |
| 24 | y | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | y | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 24 | y | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | y | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | y | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | y | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | y | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | y | 1 | Total 48 | C 38 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 24 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | a | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | a | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | a | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | a | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | r | 1 | Total 49 | C 39 | Mg 1 | N 4 | O 5 | 0 |
| 24 | r | 1 | Total 58 | C 49 | Mg 1 | N 4 | O 4 | 0 |
| 24 | r | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 24 | r | 1 | Total 48 | C 38 | Mg 1 | N 4 | O 5 | 0 |
| 24 | r | 1 | Total 58 | C 48 | Mg 1 | N 4 | O 5 | 0 |
| 24 | r | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | r | 1 | Total 49 | C 39 | Mg 1 | N 4 | O 5 | 0 |
| 24 | r | 1 | Total 49 | C 39 | Mg 1 | N 4 | O 5 | 0 |
| 24 | r | 1 | Total 37 | C 31 | Mg 1 | N 4 | O 1 | 0 |
| 24 | r | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 9 | 1 | Total 61 | C 51 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 9 | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 9 | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 9 | 1 | Total 56 | C 46 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 9 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 9 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 9 | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 9 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 0 | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 0 | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 0 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 0 | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 0 | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 0 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 24 | 0 | 1 | Total 58 | C 48 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 0 | 1 | Total 48 | C 38 | Mg 1 | N 4 | O 5 | 0 |
| 24 | AA | 1 | Total 61 | C 51 | Mg 1 | N 4 | O 5 | 0 |
| 24 | AA | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 24 | AA | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | AA | 1 | Total 48 | C 39 | Mg 1 | N 4 | O 4 | 0 |
| 24 | AA | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | AA | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | AA | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | AA | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | AA | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | AB | 1 | Total 41 | C 33 | Mg 1 | N 4 | O 3 | 0 |
| 24 | AB | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | AB | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | AB | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | AB | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | AB | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | v | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | v | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | v | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | v | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | v | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 24 | v | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | v | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | v | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | v | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | v | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | v | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | v | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | v | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | v | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | v | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | v | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 2 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 2 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Au | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Au | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Au | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Au | 1 | Total 64 | C 54 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Au | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Au | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Au | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Au | 1 | Total 48 | C 38 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 24 | Aw | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A2 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A2 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A2 | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A2 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A2 | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A2 | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A2 | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A2 | 1 | Total 48 | C 38 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A6 | 1 | Total 61 | C 51 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A6 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A6 | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A6 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A6 | 1 | Total 53 | C 44 | Mg 1 | N 4 | O 4 | 0 |
| 24 | A6 | 1 | Total 56 | C 46 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A6 | 1 | Total 49 | C 39 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A6 | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 24 | A6 | 1 | Total 49 | C 39 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BB | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BB | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BB | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 24 | BB | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BB | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BB | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BB | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BB | 1 | Total 48 | C 38 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BE | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BE | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BE | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BE | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BE | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BE | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BE | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BE | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BE | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BE | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BE | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BE | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BE | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BE | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BE | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BE | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 24 | BG | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BG | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BJ | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BJ | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BJ | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BJ | 1 | Total 64 | C 54 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BJ | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BJ | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BJ | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BJ | 1 | Total 48 | C 38 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BQ | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BQ | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BQ | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BQ | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BQ | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BQ | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BQ | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BQ | 1 | Total 48 | C 38 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BV | 1 | Total 61 | C 51 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BV | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BV | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 24 | BV | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BV | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BV | 1 | Total 56 | C 46 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BV | 1 | Total 49 | C 39 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BV | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BV | 1 | Total 49 | C 39 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Ba | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Ba | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Ba | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Ba | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Ba | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Ba | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Ba | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | Ba | 1 | Total 48 | C 38 | Mg 1 | N 4 | O 5 | 0 |
| 24 | R | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | R | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | R | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | R | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 1 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 1 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 1 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |

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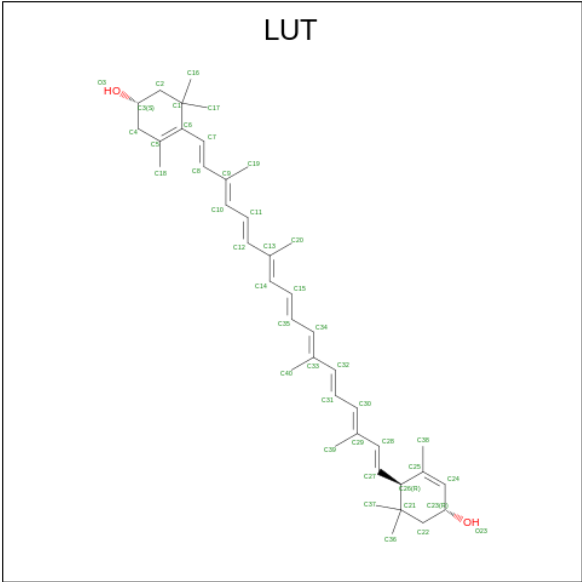
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 24 | 1 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 1 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 1 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 1 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 1 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 1 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 1 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 1 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | 1 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BD | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BD | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BD | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BD | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BF | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BF | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BF | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BF | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BF | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BF | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BF | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BF | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 24 | BF | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BF | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BF | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BF | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BF | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BU | 1 | Total 49 | C 39 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BU | 1 | Total 58 | C 49 | Mg 1 | N 4 | O 4 | 0 |
| 24 | BU | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BU | 1 | Total 48 | C 38 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BU | 1 | Total 58 | C 48 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BU | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BU | 1 | Total 49 | C 39 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BU | 1 | Total 49 | C 39 | Mg 1 | N 4 | O 5 | 0 |
| 24 | BU | 1 | Total 37 | C 31 | Mg 1 | N 4 | O 1 | 0 |
| 24 | BU | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |

- Molecule 25 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 25 | 5 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | 5 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | 6 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | 6 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | 7 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | 7 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | 8 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | G | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | G | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | N | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | N | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | S | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | S | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | Y | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |

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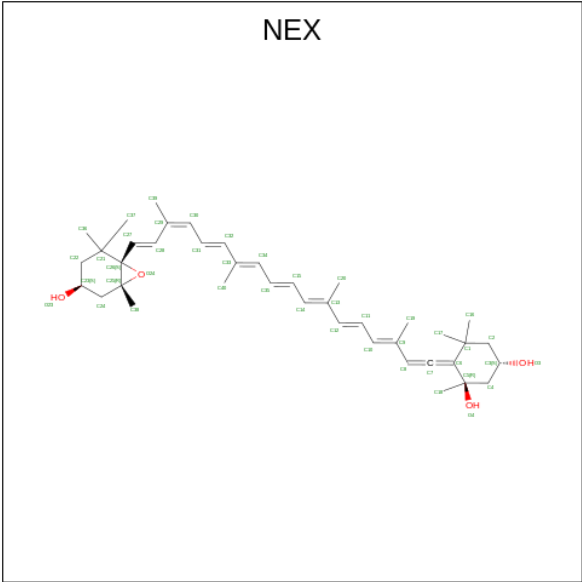
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 25 | Y | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | g | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | g | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | n | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | n | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | s | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | s | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | y | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | y | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | r | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | 9 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | 9 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | 0 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | 0 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | AA | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | AA | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | AB | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | Au | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | Au | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | A2 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | A2 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |

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| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 25 | A6 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | A6 | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | BB | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | BB | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | BJ | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | BJ | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | BQ | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | BQ | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | BV | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | BV | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | Ba | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | Ba | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |
| 25 | BU | 1 | Total | C | O | 0 |
| | | | 42 | 40 | 2 | |

- Molecule 26 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



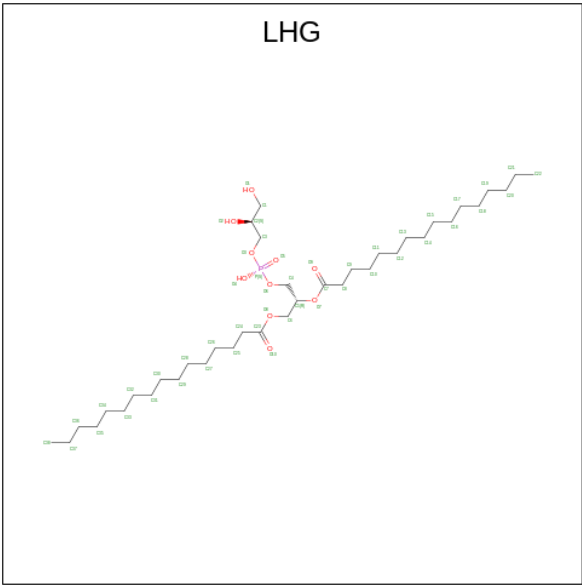
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 26 | 5 | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | 7 | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | G | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | N | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | S | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | Y | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | g | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | n | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | s | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | y | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | r | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | 9 | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | AA | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | Au | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |

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| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 26 | A2 | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | A6 | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | BB | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | BB | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | BJ | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | BQ | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | BV | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 26 | Ba | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 27 | 5 | 1 | Total | C | O | P | 0 |
| | | | 41 | 30 | 10 | 1 | |
| 27 | 6 | 1 | Total | C | O | P | 0 |
| | | | 47 | 36 | 10 | 1 | |
| 27 | B | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|
| 27 | B | 1 | Total 46 | C 35 | O 10 | P 1 | 0 |
| 27 | D | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | G | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | L | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | N | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | W | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | Y | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | b | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | b | 1 | Total 46 | C 35 | O 10 | P 1 | 0 |
| 27 | b | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | d | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | g | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | n | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | w | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | y | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | C | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | C | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | c | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | c | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | r | 1 | Total 42 | C 31 | O 10 | P 1 | 0 |
| 27 | 9 | 1 | Total 41 | C 30 | O 10 | P 1 | 0 |

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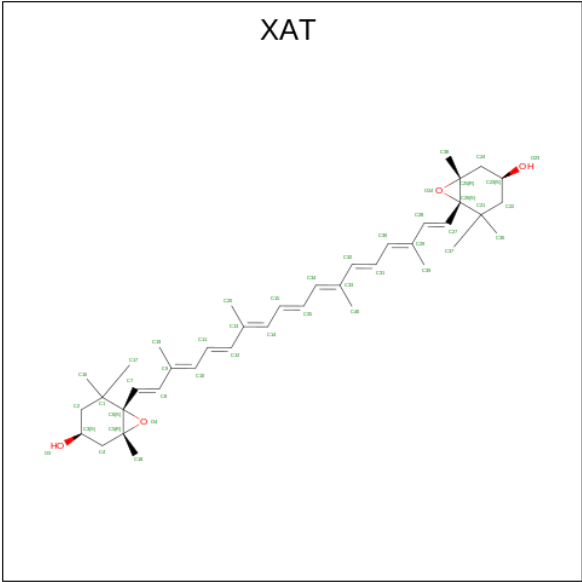
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|
| 27 | 0 | 1 | Total 47 | C 36 | O 10 | P 1 | 0 |
| 27 | v | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | 2 | 1 | Total 46 | C 35 | O 10 | P 1 | 0 |
| 27 | 2 | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | Au | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | Az | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | A2 | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | A0 | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | BB | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | BE | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | BE | 1 | Total 46 | C 35 | O 10 | P 1 | 0 |
| 27 | BE | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | BG | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | BJ | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | BQ | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | BY | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | Ba | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | 1 | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | 1 | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | BF | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |
| 27 | BF | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 27 | BU | 1 | Total | C | O | P | 0 |
| | | | 42 | 31 | 10 | 1 | |

- Molecule 28 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: C₄₀H₅₆O₄).



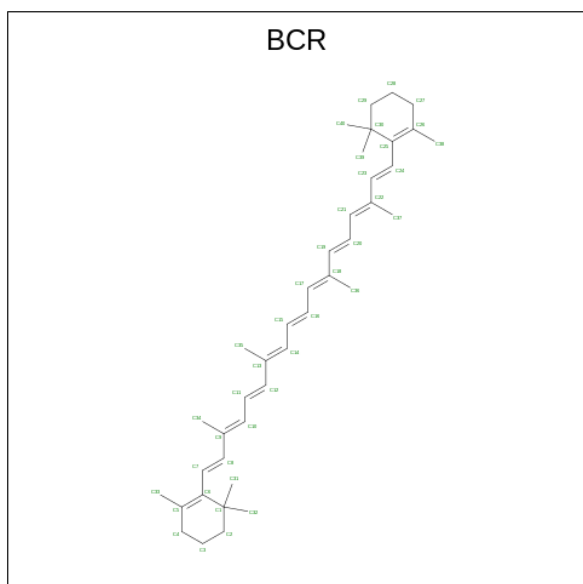
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 28 | 5 | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | 7 | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | 7 | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | 8 | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | G | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | N | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | Y | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | g | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | n | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | y | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |

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| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 28 | r | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | 9 | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | AA | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | AA | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | AB | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | Au | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | A2 | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | BB | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | BJ | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | BQ | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | Ba | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |
| 28 | BU | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------------|---------|
| 29 | 8 | 1 | Total C 40 40 | 0 |
| 29 | B | 1 | Total C 40 40 | 0 |
| 29 | B | 1 | Total C 40 40 | 0 |
| 29 | B | 1 | Total C 40 40 | 0 |
| 29 | B | 1 | Total C 40 40 | 0 |
| 29 | F | 1 | Total C 40 40 | 0 |
| 29 | H | 1 | Total C 40 40 | 0 |
| 29 | K | 1 | Total C 40 40 | 0 |
| 29 | K | 1 | Total C 40 40 | 0 |
| 29 | b | 1 | Total C 40 40 | 0 |
| 29 | b | 1 | Total C 40 40 | 0 |
| 29 | b | 1 | Total C 40 40 | 0 |
| 29 | b | 1 | Total C 40 40 | 0 |
| 29 | f | 1 | Total C 40 40 | 0 |
| 29 | h | 1 | Total C 40 40 | 0 |
| 29 | k | 1 | Total C 40 40 | 0 |
| 29 | z | 1 | Total C 40 40 | 0 |
| 29 | z | 1 | Total C 40 40 | 0 |
| 29 | A | 1 | Total C 40 40 | 0 |
| 29 | C | 1 | Total C 40 40 | 0 |
| 29 | C | 1 | Total C 40 40 | 0 |
| 29 | a | 1 | Total C 40 40 | 0 |

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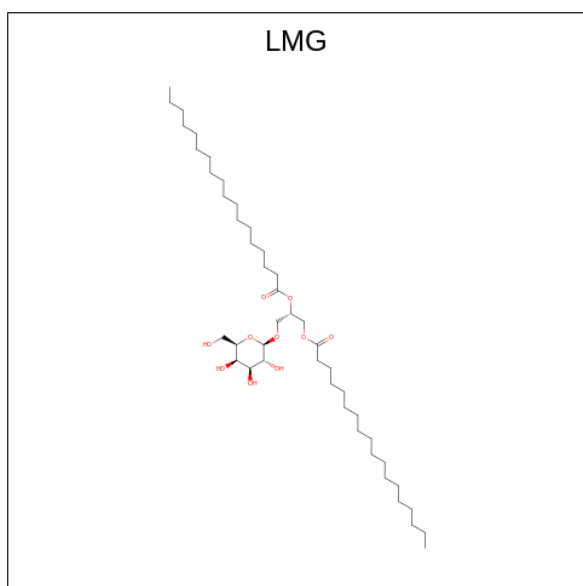
| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------------|---------|
| 29 | c | 1 | Total C 40 40 | 0 |
| 29 | AB | 1 | Total C 40 40 | 0 |
| 29 | v | 1 | Total C 40 40 | 0 |
| 29 | v | 1 | Total C 40 40 | 0 |
| 29 | v | 1 | Total C 40 40 | 0 |
| 29 | v | 1 | Total C 40 40 | 0 |
| 29 | 4 | 1 | Total C 40 40 | 0 |
| 29 | Av | 1 | Total C 40 40 | 0 |
| 29 | Ay | 1 | Total C 40 40 | 0 |
| 29 | Ay | 1 | Total C 40 40 | 0 |
| 29 | BE | 1 | Total C 40 40 | 0 |
| 29 | BE | 1 | Total C 40 40 | 0 |
| 29 | BE | 1 | Total C 40 40 | 0 |
| 29 | BE | 1 | Total C 40 40 | 0 |
| 29 | BI | 1 | Total C 40 40 | 0 |
| 29 | BK | 1 | Total C 40 40 | 0 |
| 29 | BN | 1 | Total C 40 40 | 0 |
| 29 | Bb | 1 | Total C 40 40 | 0 |
| 29 | R | 1 | Total C 40 40 | 0 |
| 29 | 1 | 1 | Total C 40 40 | 0 |
| 29 | 1 | 1 | Total C 40 40 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 29 | BD | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 29 | BF | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 29 | BF | 1 | Total | C | 0 |
| | | | 40 | 40 | |

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



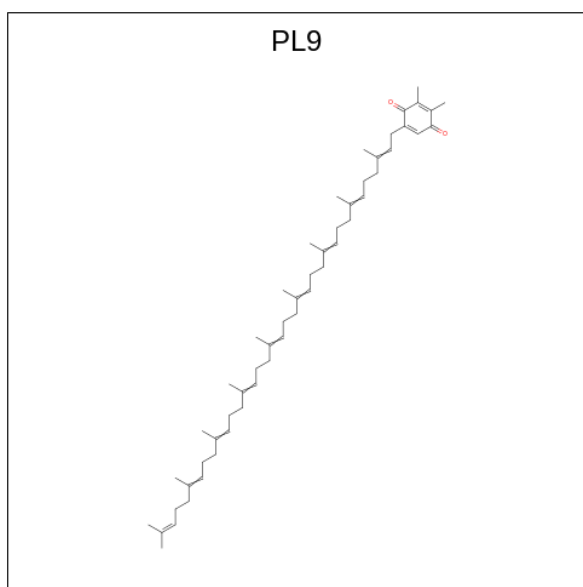
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 30 | B | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 30 | B | 1 | Total | C | O | 0 |
| | | | 40 | 30 | 10 | |
| 30 | D | 1 | Total | C | O | 0 |
| | | | 46 | 36 | 10 | |
| 30 | I | 1 | Total | C | O | 0 |
| | | | 40 | 30 | 10 | |
| 30 | b | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 30 | d | 1 | Total | C | O | 0 |
| | | | 46 | 36 | 10 | |
| 30 | i | 1 | Total | C | O | 0 |
| | | | 48 | 38 | 10 | |
| 30 | A | 1 | Total | C | O | 0 |
| | | | 48 | 38 | 10 | |

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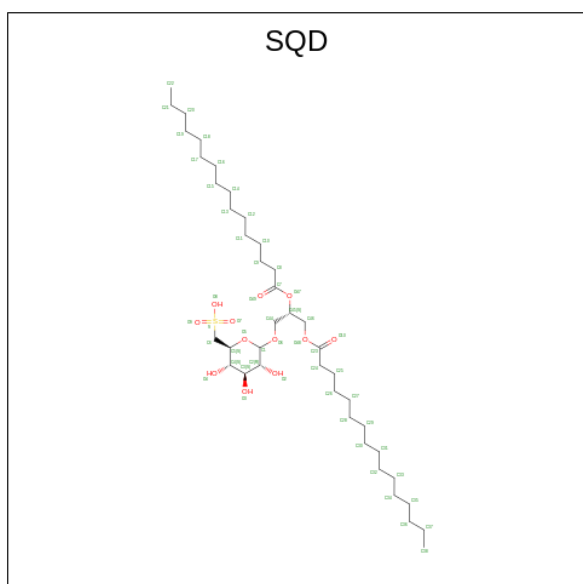
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 30 | C | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 30 | C | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 30 | c | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 30 | c | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 30 | v | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 30 | v | 1 | Total | C | O | 0 |
| | | | 40 | 30 | 10 | |
| 30 | 2 | 1 | Total | C | O | 0 |
| | | | 46 | 36 | 10 | |
| 30 | Aw | 1 | Total | C | O | 0 |
| | | | 40 | 30 | 10 | |
| 30 | A0 | 1 | Total | C | O | 0 |
| | | | 48 | 38 | 10 | |
| 30 | BE | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 30 | BG | 1 | Total | C | O | 0 |
| | | | 46 | 36 | 10 | |
| 30 | BL | 1 | Total | C | O | 0 |
| | | | 48 | 38 | 10 | |
| 30 | 1 | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 30 | 1 | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 30 | BF | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 30 | BF | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |

- Molecule 31 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: C₅₃H₈₀O₂).



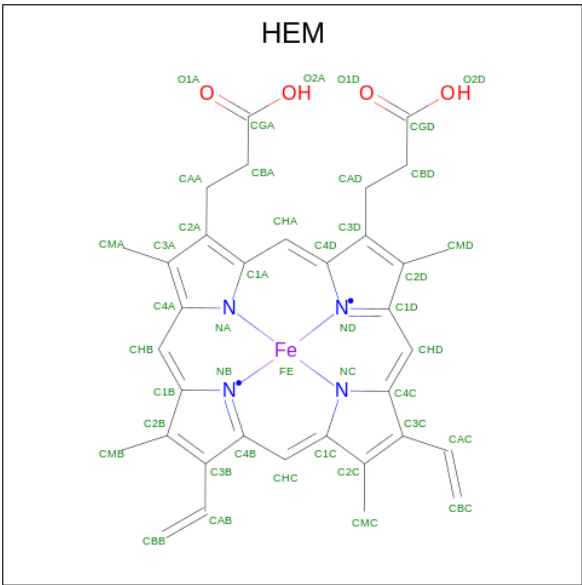
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 31 | D | 1 | Total | C | O | 0 |
| | | | 55 | 53 | 2 | |
| 31 | d | 1 | Total | C | O | 0 |
| | | | 55 | 53 | 2 | |
| 31 | 2 | 1 | Total | C | O | 0 |
| | | | 55 | 53 | 2 | |
| 31 | BG | 1 | Total | C | O | 0 |
| | | | 55 | 53 | 2 | |

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



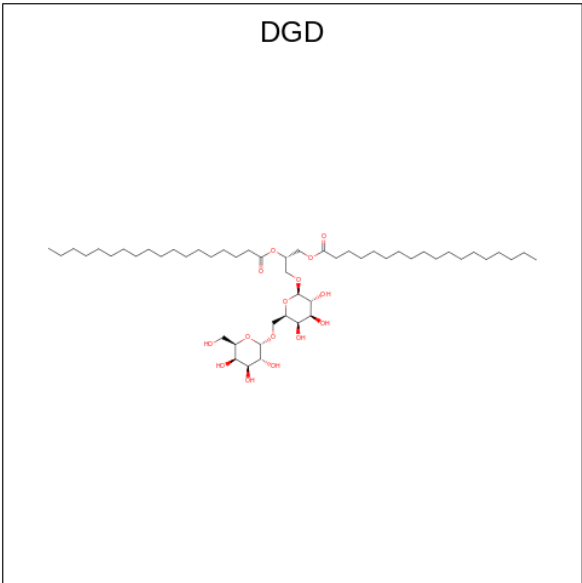
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 32 | D | 1 | Total | C | O | S | 0 |
| | | | 50 | 37 | 12 | 1 | |
| 32 | L | 1 | Total | C | O | S | 0 |
| | | | 42 | 29 | 12 | 1 | |
| 32 | L | 1 | Total | C | O | S | 0 |
| | | | 54 | 41 | 12 | 1 | |
| 32 | d | 1 | Total | C | O | S | 0 |
| | | | 50 | 37 | 12 | 1 | |
| 32 | l | 1 | Total | C | O | S | 0 |
| | | | 54 | 41 | 12 | 1 | |
| 32 | l | 1 | Total | C | O | S | 0 |
| | | | 42 | 29 | 12 | 1 | |
| 32 | A | 1 | Total | C | O | S | 0 |
| | | | 54 | 41 | 12 | 1 | |
| 32 | a | 1 | Total | C | O | S | 0 |
| | | | 54 | 41 | 12 | 1 | |
| 32 | 2 | 1 | Total | C | O | S | 0 |
| | | | 50 | 37 | 12 | 1 | |
| 32 | Az | 1 | Total | C | O | S | 0 |
| | | | 42 | 29 | 12 | 1 | |
| 32 | A1 | 1 | Total | C | O | S | 0 |
| | | | 54 | 41 | 12 | 1 | |
| 32 | BG | 1 | Total | C | O | S | 0 |
| | | | 50 | 37 | 12 | 1 | |
| 32 | BO | 1 | Total | C | O | S | 0 |
| | | | 54 | 41 | 12 | 1 | |
| 32 | BO | 1 | Total | C | O | S | 0 |
| | | | 42 | 29 | 12 | 1 | |
| 32 | R | 1 | Total | C | O | S | 0 |
| | | | 54 | 41 | 12 | 1 | |
| 32 | BD | 1 | Total | C | O | S | 0 |
| | | | 54 | 41 | 12 | 1 | |

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



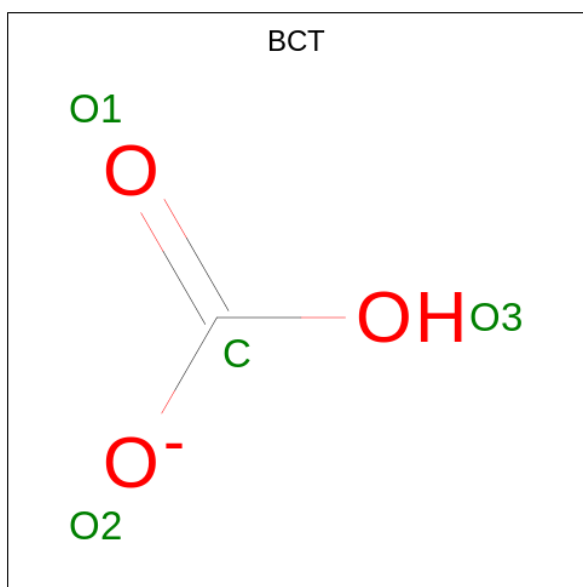
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 33 | F | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 |
| 33 | f | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 |
| 33 | 4 | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 |
| 33 | BI | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 |

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



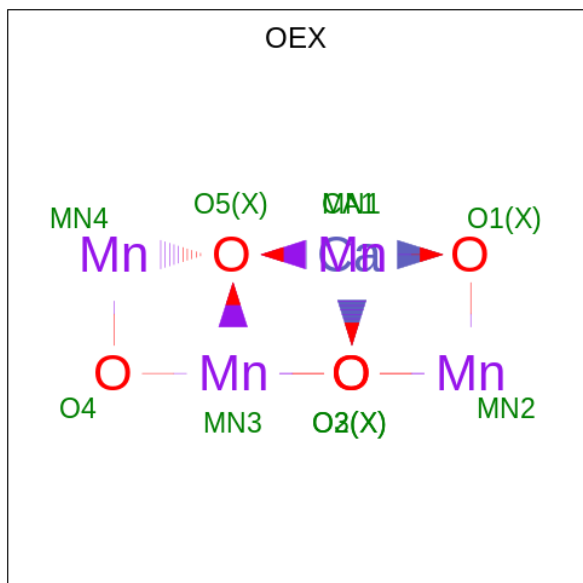
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 34 | H | 1 | Total | C | O | 0 |
| | | | 62 | 47 | 15 | |
| 34 | h | 1 | Total | C | O | 0 |
| | | | 62 | 47 | 15 | |
| 34 | A | 1 | Total | C | O | 0 |
| | | | 59 | 44 | 15 | |
| 34 | C | 1 | Total | C | O | 0 |
| | | | 55 | 40 | 15 | |
| 34 | C | 1 | Total | C | O | 0 |
| | | | 62 | 47 | 15 | |
| 34 | C | 1 | Total | C | O | 0 |
| | | | 60 | 45 | 15 | |
| 34 | a | 1 | Total | C | O | 0 |
| | | | 59 | 44 | 15 | |
| 34 | a | 1 | Total | C | O | 0 |
| | | | 60 | 45 | 15 | |
| 34 | c | 1 | Total | C | O | 0 |
| | | | 55 | 40 | 15 | |
| 34 | c | 1 | Total | C | O | 0 |
| | | | 62 | 47 | 15 | |
| 34 | Av | 1 | Total | C | O | 0 |
| | | | 62 | 47 | 15 | |
| 34 | BK | 1 | Total | C | O | 0 |
| | | | 62 | 47 | 15 | |
| 34 | R | 1 | Total | C | O | 0 |
| | | | 59 | 44 | 15 | |
| 34 | 1 | 1 | Total | C | O | 0 |
| | | | 55 | 40 | 15 | |
| 34 | 1 | 1 | Total | C | O | 0 |
| | | | 62 | 47 | 15 | |
| 34 | 1 | 1 | Total | C | O | 0 |
| | | | 60 | 45 | 15 | |
| 34 | BD | 1 | Total | C | O | 0 |
| | | | 59 | 44 | 15 | |
| 34 | BD | 1 | Total | C | O | 0 |
| | | | 60 | 45 | 15 | |
| 34 | BF | 1 | Total | C | O | 0 |
| | | | 55 | 40 | 15 | |
| 34 | BF | 1 | Total | C | O | 0 |
| | | | 62 | 47 | 15 | |

- Molecule 35 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 35 | A | 1 | Total | C | O | 0 |
| | | | 4 | 1 | 3 | |
| 35 | a | 1 | Total | C | O | 0 |
| | | | 4 | 1 | 3 | |
| 35 | 2 | 1 | Total | C | O | 0 |
| | | | 4 | 1 | 3 | |
| 35 | BD | 1 | Total | C | O | 0 |
| | | | 4 | 1 | 3 | |

- Molecule 36 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).

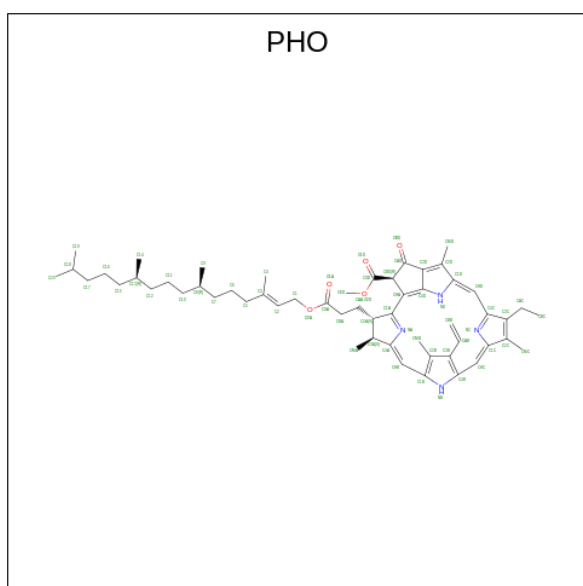


| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 36 | A | 1 | Total | Ca | Mn | O | 0 |
| | | | 10 | 1 | 4 | 5 | |
| 36 | a | 1 | Total | Ca | Mn | O | 0 |
| | | | 10 | 1 | 4 | 5 | |
| 36 | R | 1 | Total | Ca | Mn | O | 0 |
| | | | 10 | 1 | 4 | 5 | |
| 36 | BD | 1 | Total | Ca | Mn | O | 0 |
| | | | 10 | 1 | 4 | 5 | |

- Molecule 37 is FE (II) ION (CCD ID: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 37 | A | 1 | Total | Fe | 0 |
| | | | 1 | 1 | |
| 37 | a | 1 | Total | Fe | 0 |
| | | | 1 | 1 | |
| 37 | R | 1 | Total | Fe | 0 |
| | | | 1 | 1 | |
| 37 | BD | 1 | Total | Fe | 0 |
| | | | 1 | 1 | |

- Molecule 38 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 38 | A | 1 | Total | C | N | O | 0 |
| | | | 64 | 55 | 4 | 5 | |
| 38 | A | 1 | Total | C | N | O | 0 |
| | | | 64 | 55 | 4 | 5 | |

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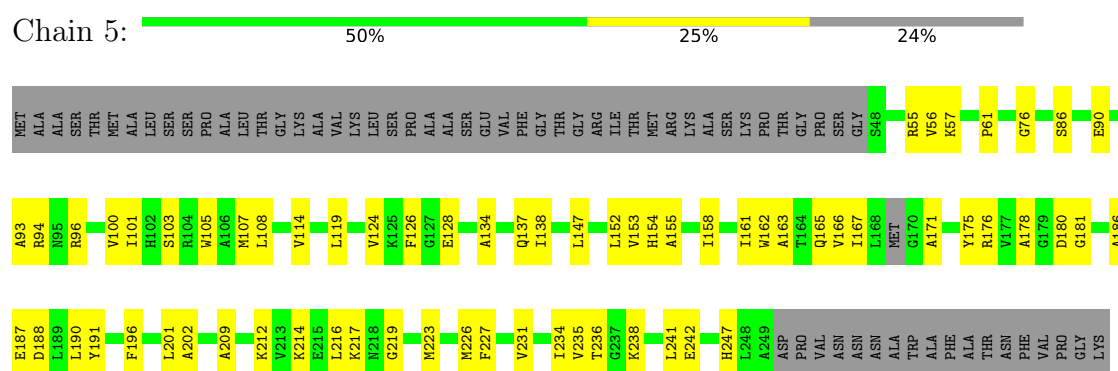
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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|
| 38 | a | 1 | Total 64 | C 55 | N 4 | O 5 | 0 |
| 38 | a | 1 | Total 64 | C 55 | N 4 | O 5 | 0 |
| 38 | R | 1 | Total 64 | C 55 | N 4 | O 5 | 0 |
| 38 | R | 1 | Total 64 | C 55 | N 4 | O 5 | 0 |
| 38 | BD | 1 | Total 64 | C 55 | N 4 | O 5 | 0 |
| 38 | BD | 1 | Total 64 | C 55 | N 4 | O 5 | 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.

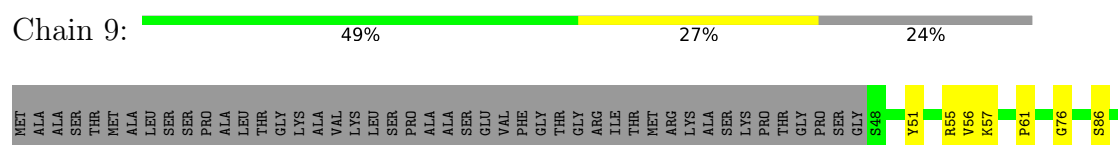
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

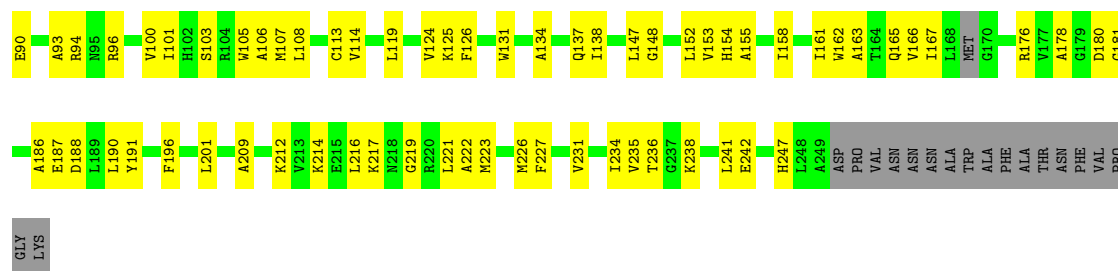


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



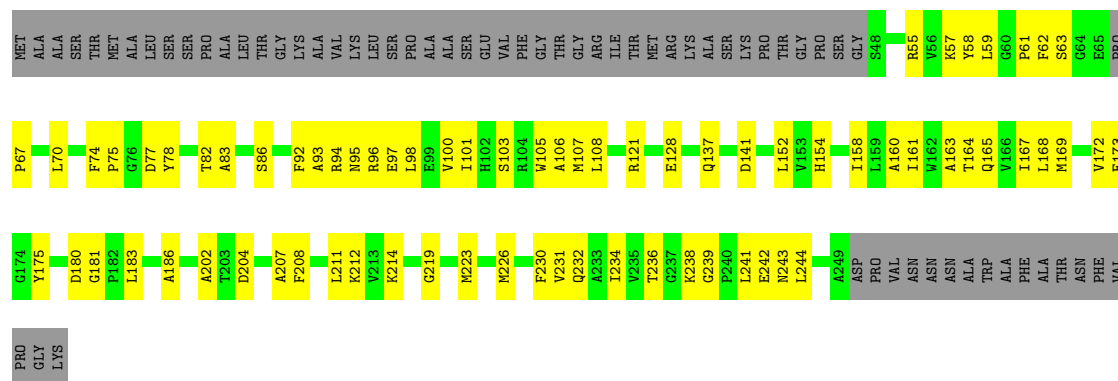
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic





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

Chain AA: 48% 27% 24%



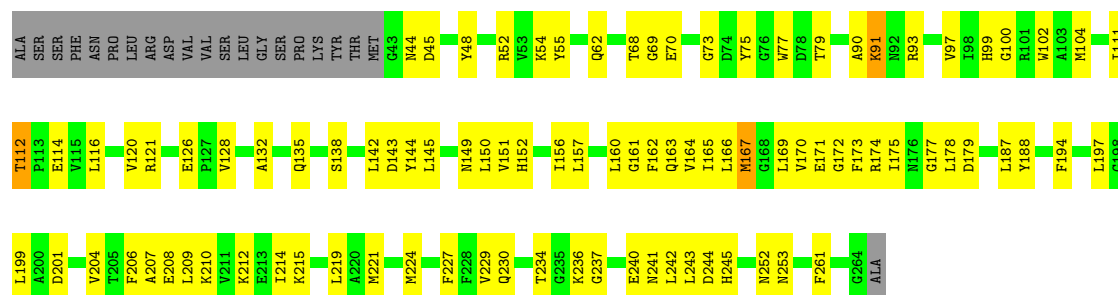
- Molecule 2: Chlorophyll a-b binding protein 3, chloroplastic

Chain 6: 53% 37% 9%

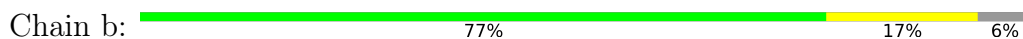
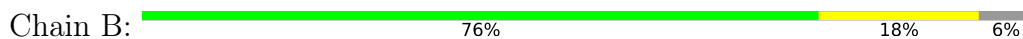


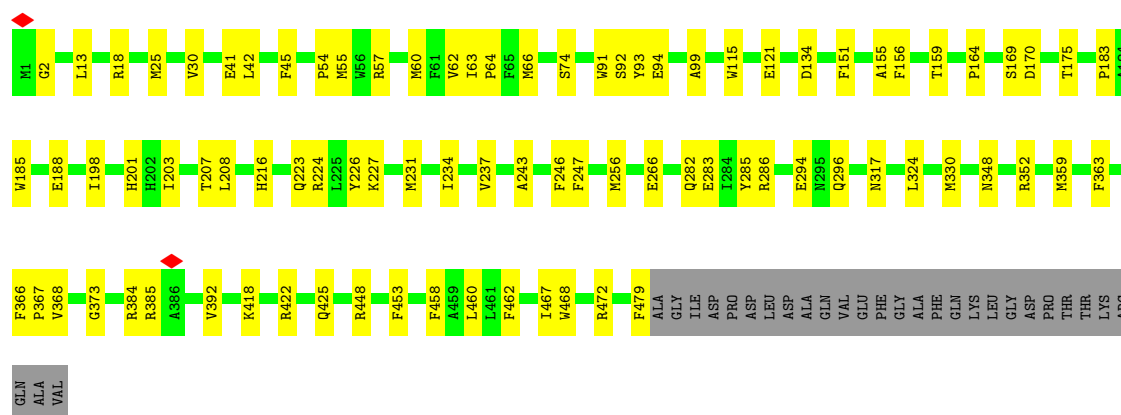
- Molecule 2: Chlorophyll a-b binding protein 3, chloroplastic

Chain 0: 53% 37% 9%



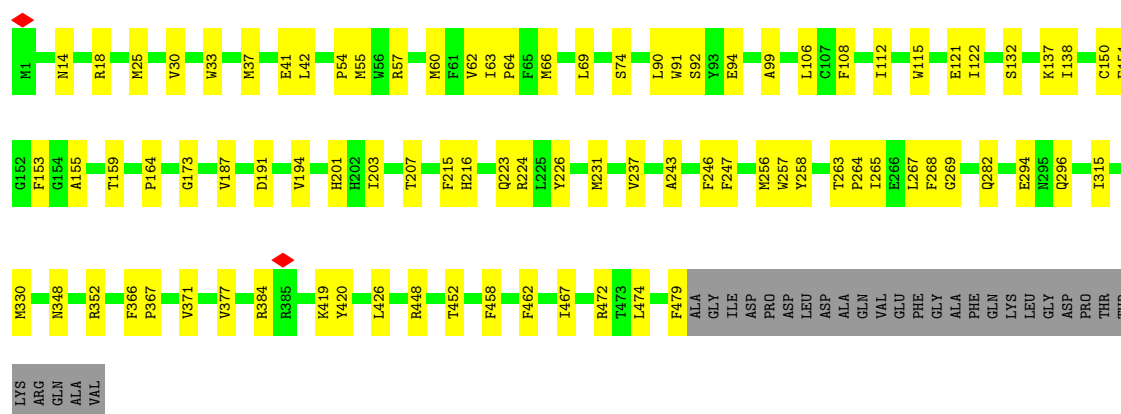
- Chain 8: 54% 36% 9%





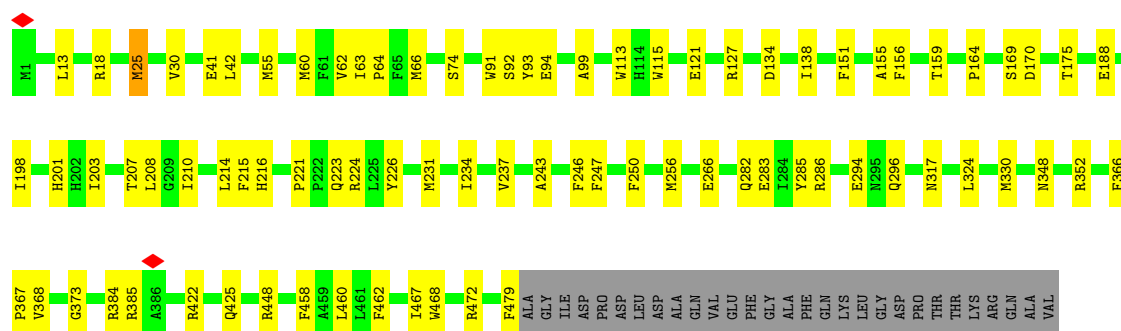
• Molecule 4: Photosystem II CP47 reaction center protein

Chain v: 77% 17% 6%



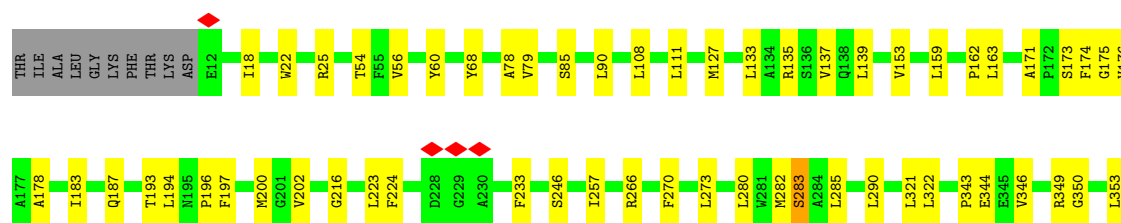
• Molecule 4: Photosystem II CP47 reaction center protein

Chain BE: 78% 16% 6%



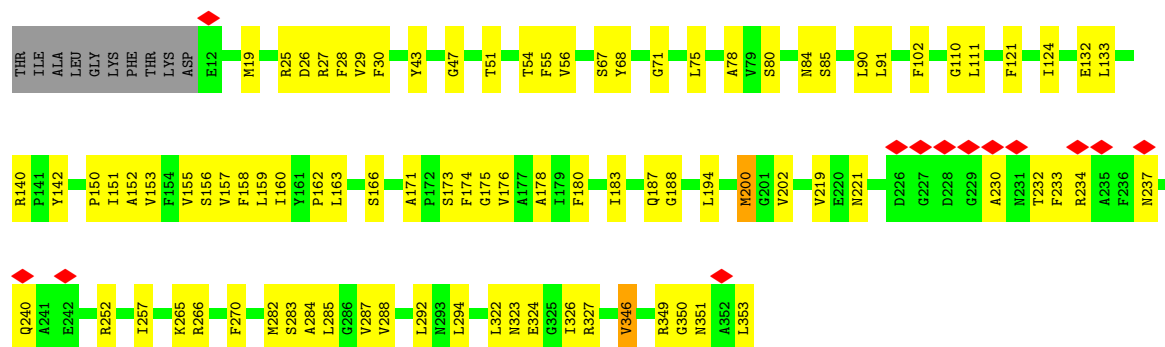
• Molecule 5: Photosystem II D2 protein

Chain D: 81% 16% 3%



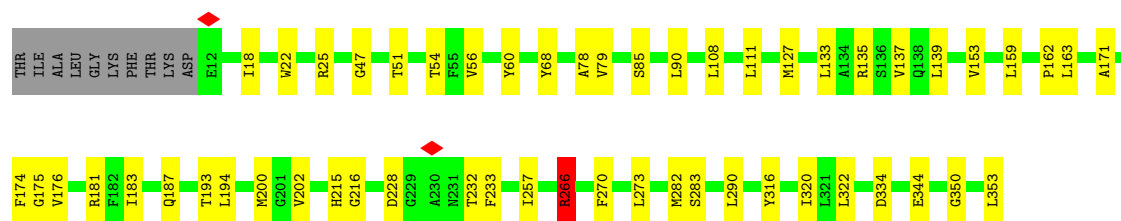
• Molecule 5: Photosystem II D2 protein

Chain d: 72% 25%



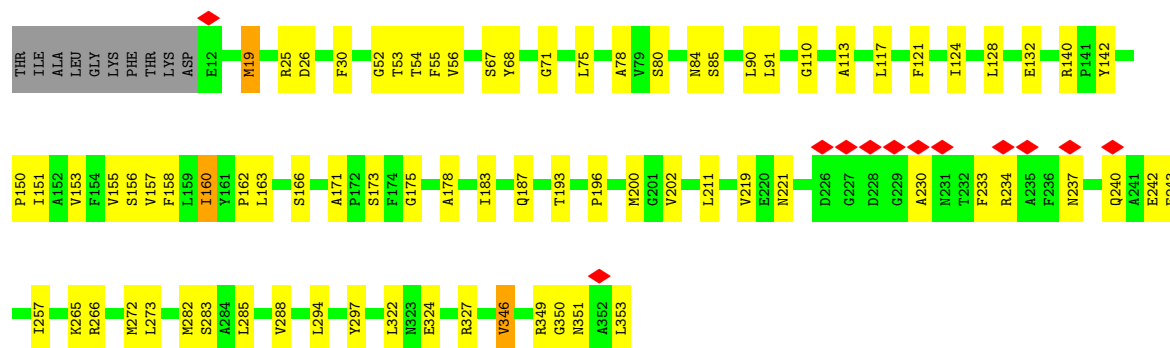
• Molecule 5: Photosystem II D2 protein

Chain 2: 82% 15%



• Molecule 5: Photosystem II D2 protein

Chain BG: 75% 21%



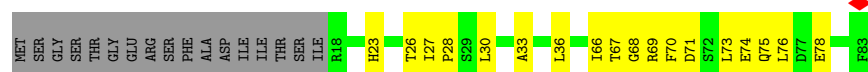
• Molecule 6: Cytochrome b559 subunit alpha



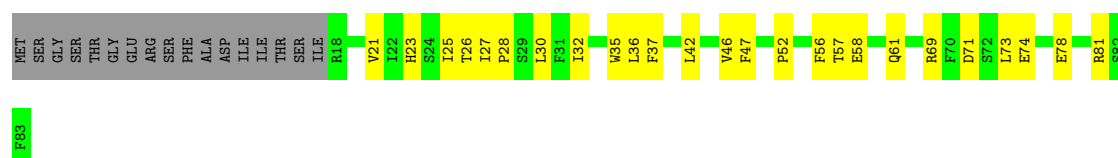
- Molecule 6: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit alpha



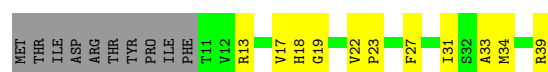
- Molecule 6: Cytochrome b559 subunit alpha



- Molecule 7: Cytochrome b559 subunit beta



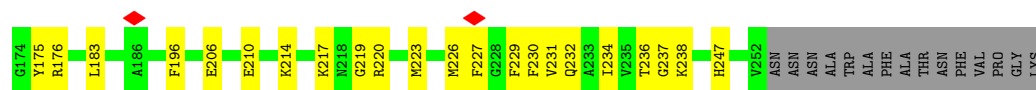
- Molecule 7: Cytochrome b559 subunit beta



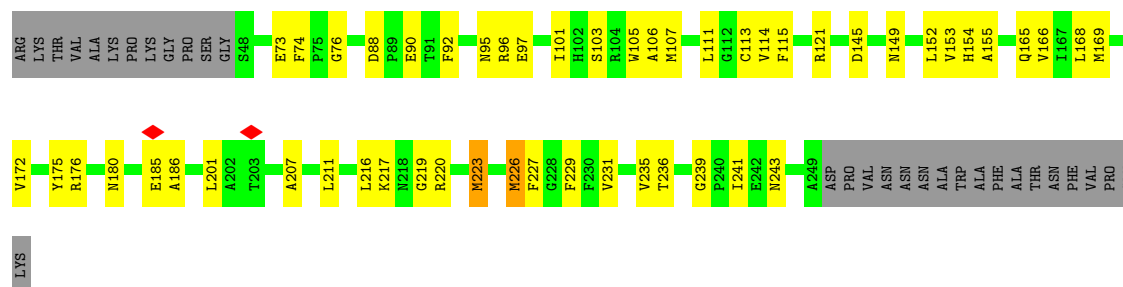
- Molecule 7: Cytochrome b559 subunit beta



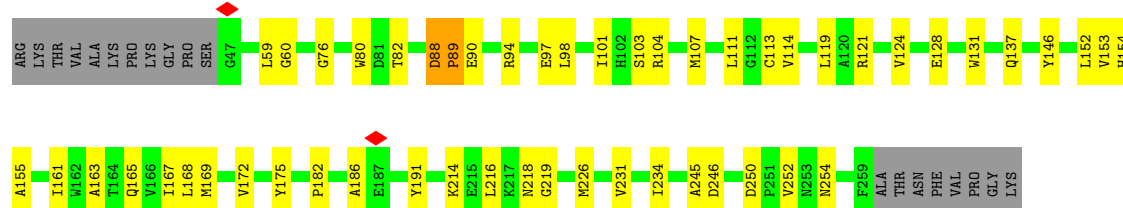




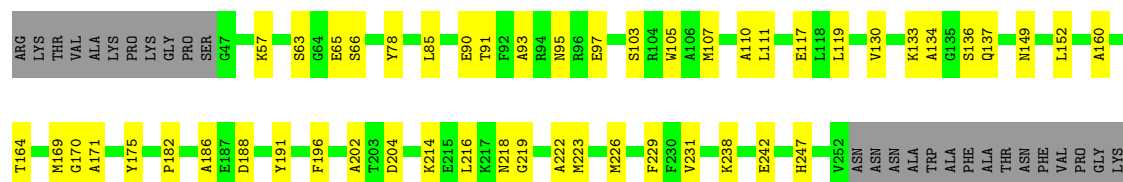
- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic



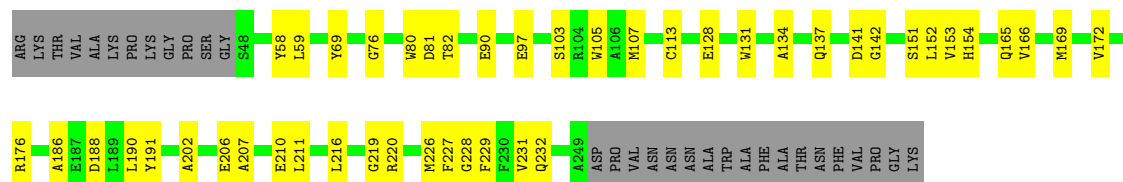
- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic




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

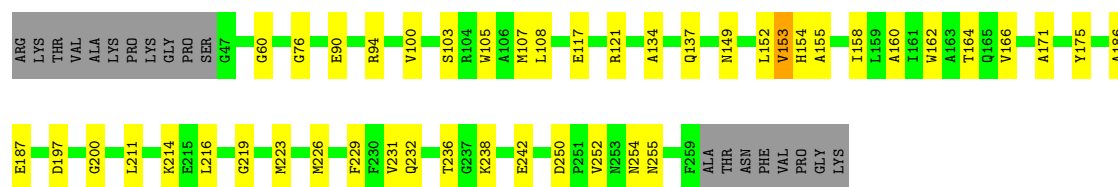


- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic



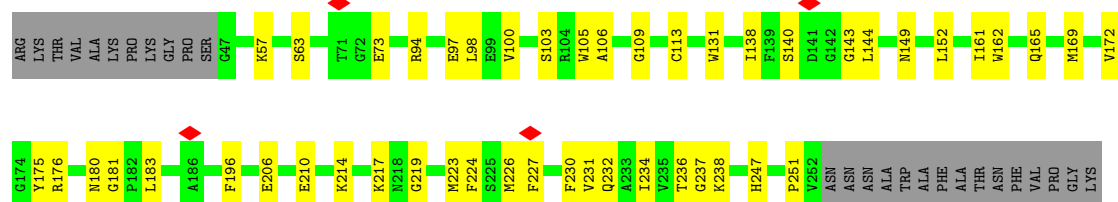
- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain BB: 



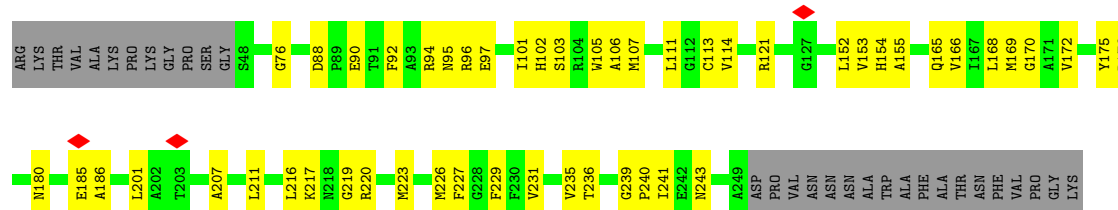
- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain BJ: 



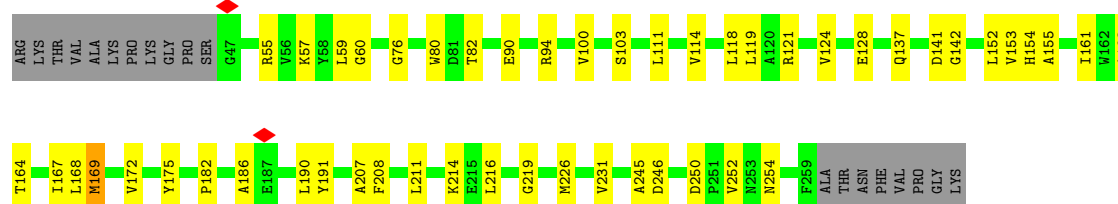
- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain BQ: 



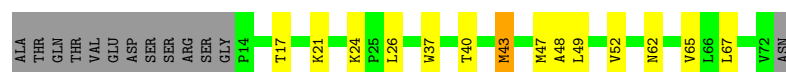
- Molecule 8: Chlorophyll a-b binding protein 1, chloroplastic

Chain Ba: 

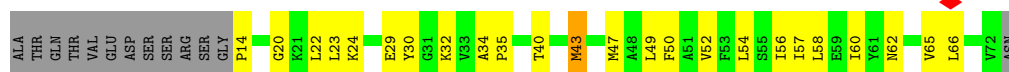


- Molecule 9: Photosystem II reaction center protein H

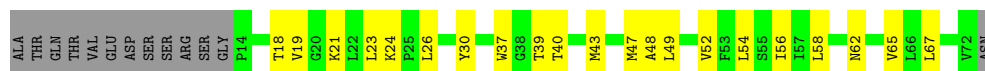
Chain H: 



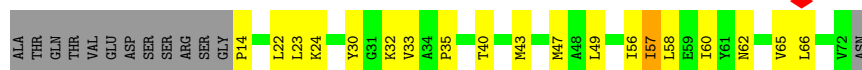
- Molecule 9: Photosystem II reaction center protein H



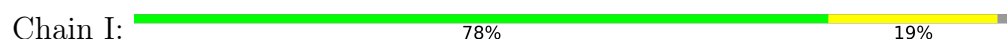
- Molecule 9: Photosystem II reaction center protein H



- Molecule 9: Photosystem II reaction center protein H



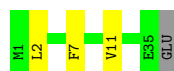
- Molecule 10: Photosystem II reaction center protein I



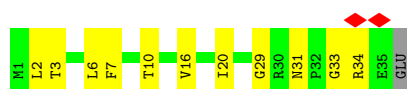
- Molecule 10: Photosystem II reaction center protein I



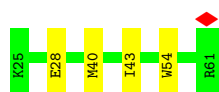
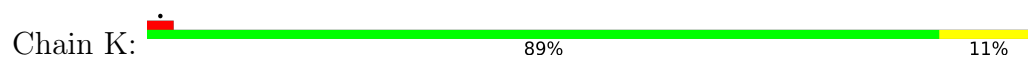
- Molecule 10: Photosystem II reaction center protein I



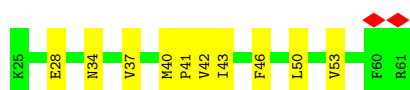
- Molecule 10: Photosystem II reaction center protein I



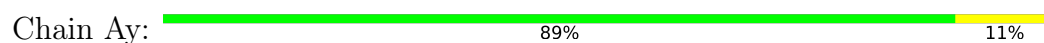
- Molecule 11: Photosystem II reaction center protein K



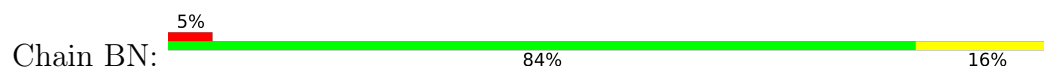
- Molecule 11: Photosystem II reaction center protein K



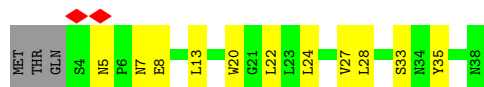
- Molecule 11: Photosystem II reaction center protein K



- 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 12: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein L

Chain BO:  63% 29% 8%



- Molecule 13: Photosystem II reaction center protein M

Chain M:  56% 32% 6% 6%



- Molecule 13: Photosystem II reaction center protein M

Chain m:  50% 41% 6% 6%



- Molecule 13: Photosystem II reaction center protein M

Chain A1:  50% 44% 6%



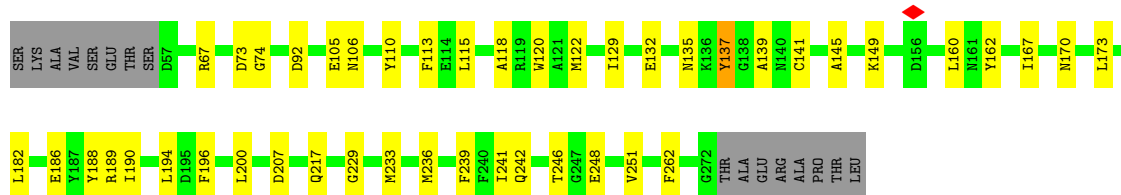
- Molecule 13: Photosystem II reaction center protein M

Chain BP:  56% 35% 6% 6%



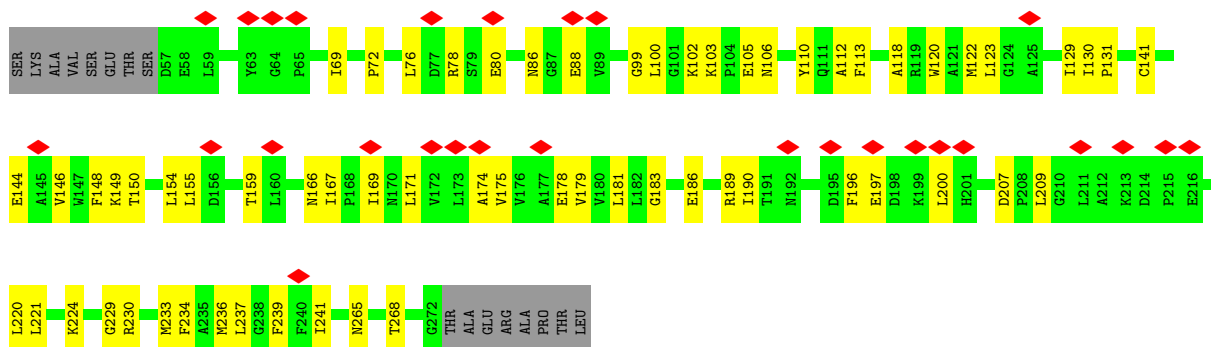
- Molecule 14: Chlorophyll a-b binding protein CP26, chloroplastic

Chain S:  74% 19% 7%

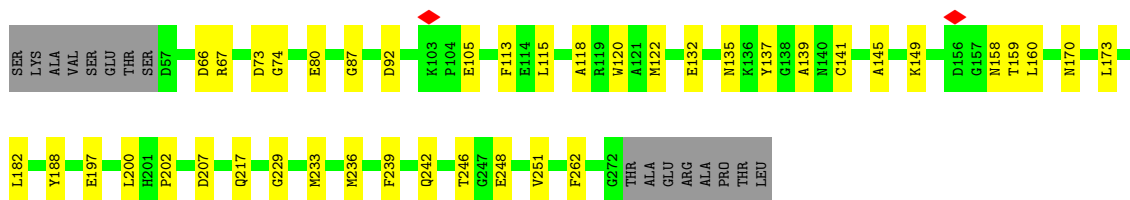
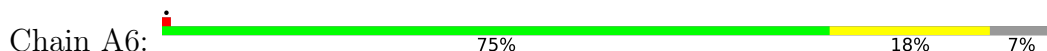


- Molecule 14: Chlorophyll a-b binding protein CP26, chloroplastic

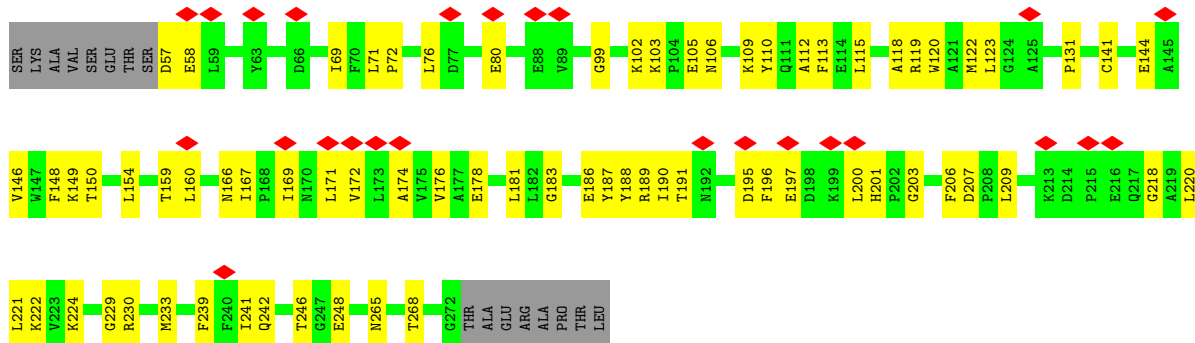
Chain s:  12% 66% 27% 7%



- Molecule 14: Chlorophyll a-b binding protein CP26, chloroplastic



- Molecule 14: Chlorophyll a-b binding protein CP26, chloroplastic



- Molecule 15: Photosystem II reaction center protein T

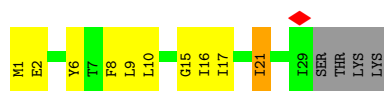


- Molecule 15: Photosystem II reaction center protein T





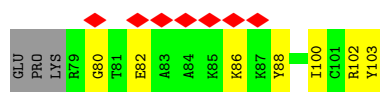
- Molecule 15: Photosystem II reaction center protein T



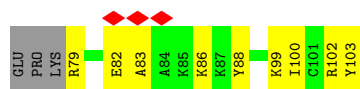
- Molecule 15: Photosystem II reaction center protein T



- Molecule 16: Photosystem II 5 kDa protein, chloroplastic



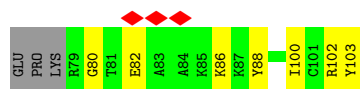
- Molecule 16: Photosystem II 5 kDa protein, chloroplastic



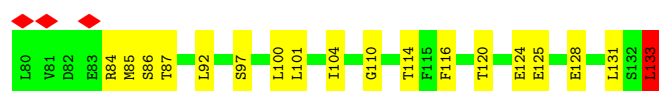
- Molecule 16: Photosystem II 5 kDa protein, chloroplastic



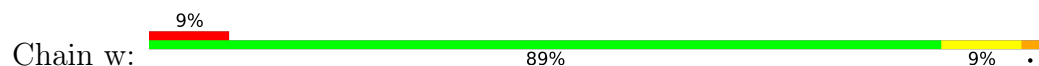
- Molecule 16: Photosystem II 5 kDa protein, chloroplastic



- Molecule 17: Photosystem II reaction center W protein, chloroplastic



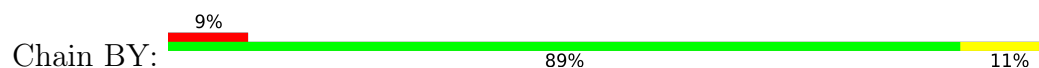
- Molecule 17: Photosystem II reaction center W protein, chloroplastic



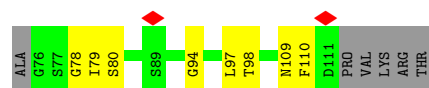
- Molecule 17: Photosystem II reaction center W protein, chloroplastic



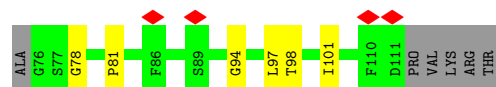
- Molecule 17: Photosystem II reaction center W protein, chloroplastic



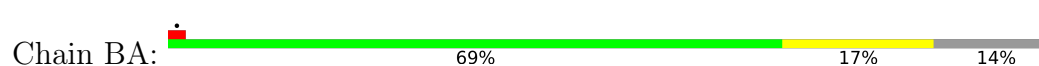
- Molecule 18: (thale cress) hypothetical protein



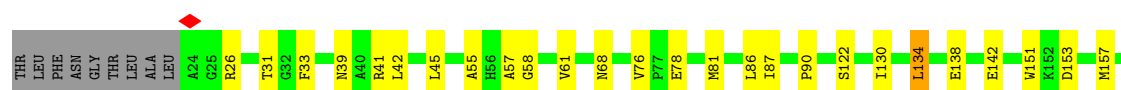
- Molecule 18: (thale cress) hypothetical protein

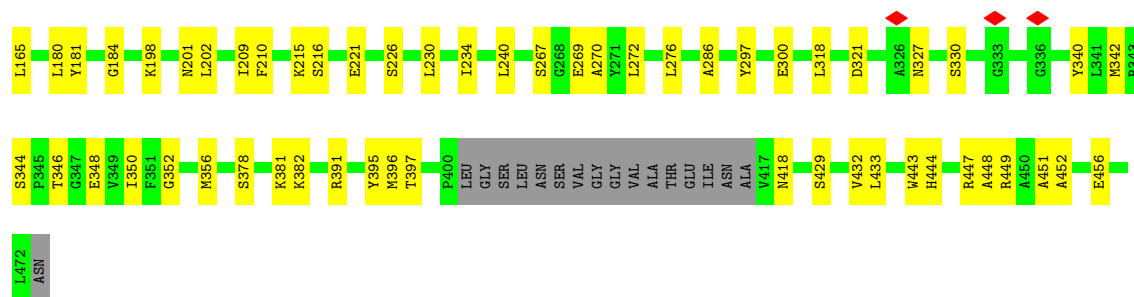


- Molecule 18: (thale cress) hypothetical protein

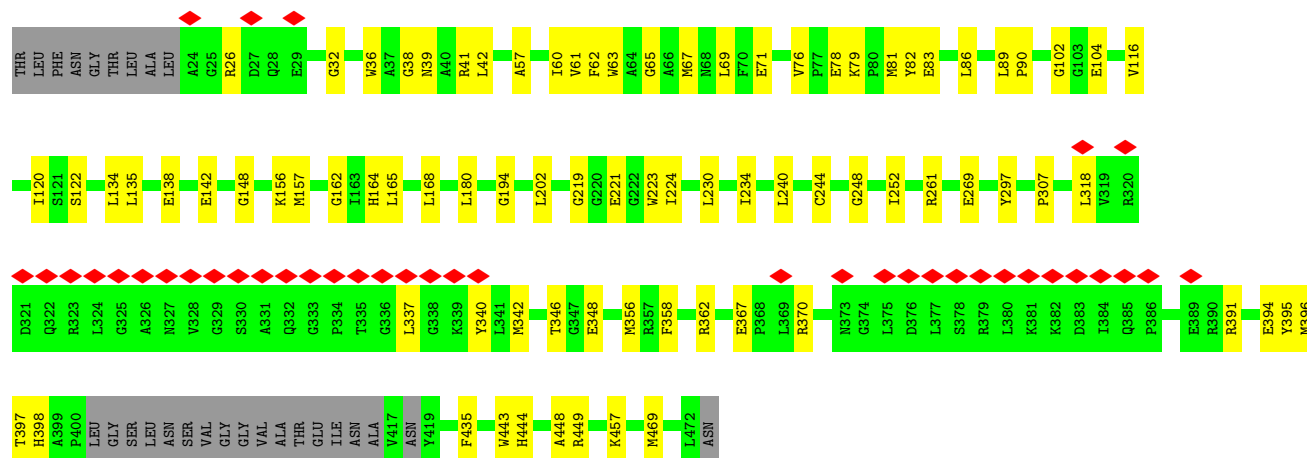
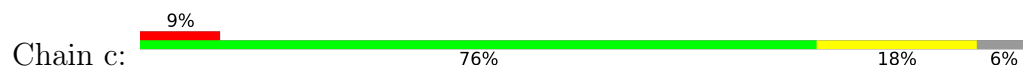


- 

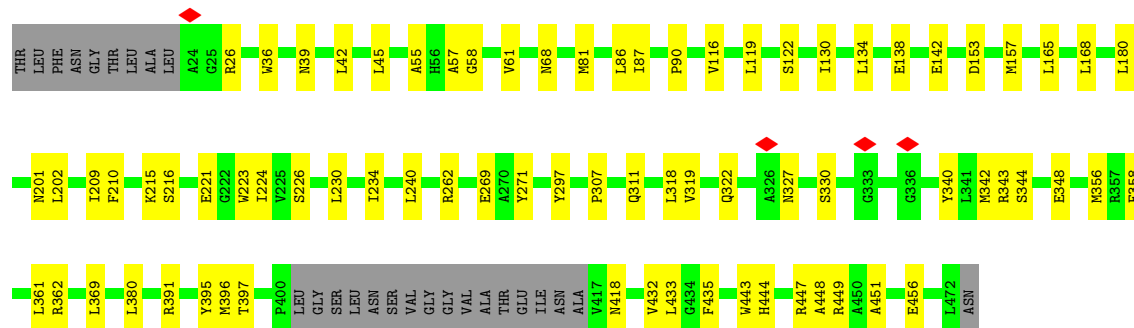
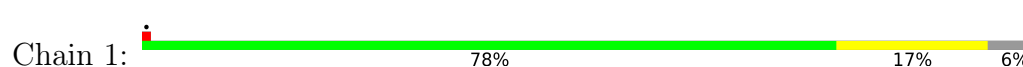




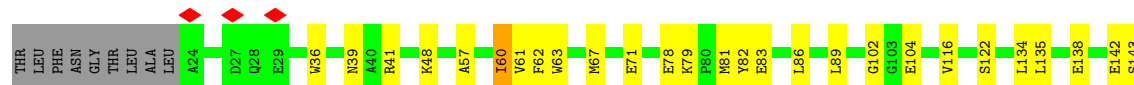
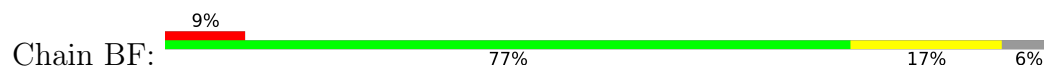
• Molecule 21: Photosystem II CP43 reaction center protein

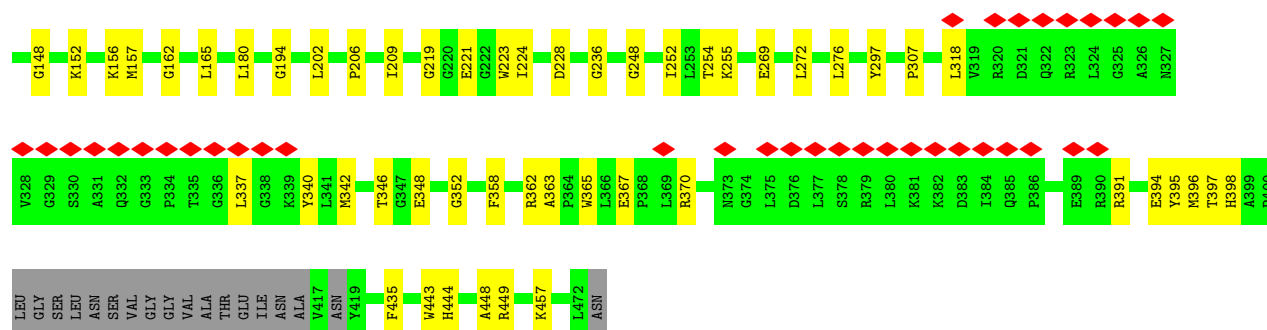


• Molecule 21: Photosystem II CP43 reaction center protein



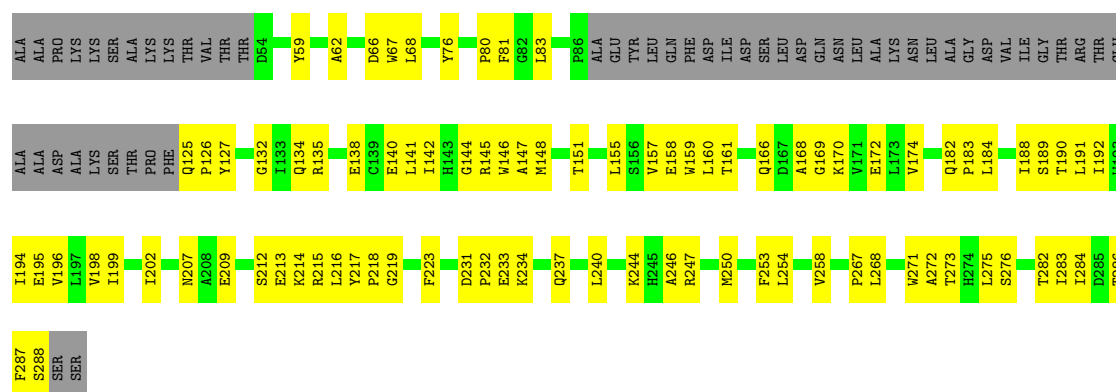
• Molecule 21: Photosystem II CP43 reaction center protein





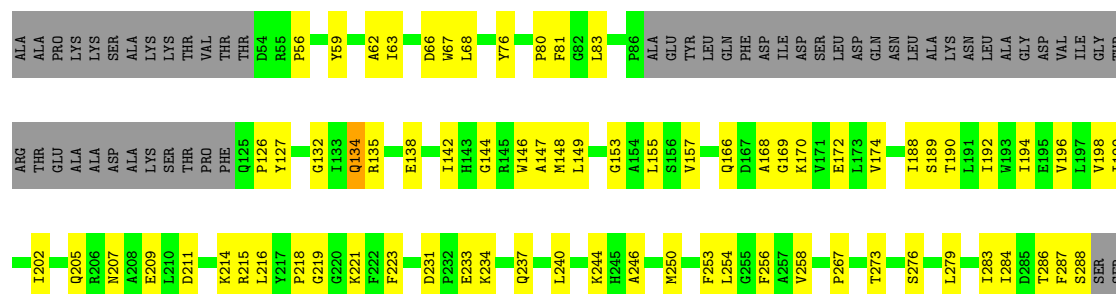
• Molecule 22: Chlorophyll a-b binding protein CP29.1, chloroplastic

Chain r:



• Molecule 22: Chlorophyll a-b binding protein CP29.1, chloroplastic

Chain BU:



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 48981 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TALOS ARCTICA | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 50.5 | Depositor |
| Minimum defocus (nm) | 1200 | Depositor |
| Maximum defocus (nm) | 2200 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 45.874 | Depositor |
| Minimum map value | -18.604 | Depositor |
| Average map value | 0.011 | Depositor |
| Map value standard deviation | 1.000 | Depositor |
| Recommended contour level | 4.5 | Depositor |
| Map size (Å) | 770.4, 770.4, 770.4 | wwPDB |
| Map dimensions | 720, 720, 720 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.07, 1.07, 1.07 | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 | 5 | 0.26 | 0/1573 | 0.44 | 0/2137 |
| 1 | 7 | 0.28 | 0/1573 | 0.45 | 0/2134 |
| 1 | 9 | 0.25 | 0/1573 | 0.38 | 0/2137 |
| 1 | AA | 0.31 | 0/1573 | 0.45 | 0/2134 |
| 2 | 0 | 0.34 | 0/1768 | 0.55 | 2/2405 (0.1%) |
| 2 | 6 | 0.36 | 0/1768 | 0.58 | 3/2405 (0.1%) |
| 3 | 8 | 0.27 | 0/1564 | 0.54 | 0/2123 |
| 3 | AB | 0.29 | 0/1564 | 0.55 | 0/2123 |
| 4 | B | 0.23 | 0/3886 | 0.34 | 1/5293 (0.0%) |
| 4 | BE | 0.24 | 0/3886 | 0.36 | 1/5293 (0.0%) |
| 4 | b | 0.22 | 0/3886 | 0.35 | 0/5293 |
| 4 | v | 0.23 | 0/3886 | 0.32 | 0/5293 |
| 5 | 2 | 0.35 | 0/2816 | 0.40 | 1/3837 (0.0%) |
| 5 | BG | 0.32 | 1/2816 (0.0%) | 0.41 | 0/3837 |
| 5 | D | 0.25 | 0/2816 | 0.35 | 0/3837 |
| 5 | d | 0.31 | 1/2816 (0.0%) | 0.41 | 1/3837 (0.0%) |
| 6 | 3 | 0.15 | 0/562 | 0.34 | 0/763 |
| 6 | BH | 0.17 | 0/562 | 0.33 | 0/763 |
| 6 | E | 0.15 | 0/562 | 0.34 | 0/763 |
| 6 | e | 0.15 | 0/562 | 0.30 | 0/763 |
| 7 | 4 | 0.17 | 0/230 | 0.34 | 0/311 |
| 7 | BI | 0.15 | 0/230 | 0.31 | 0/311 |
| 7 | F | 0.15 | 0/230 | 0.31 | 0/311 |
| 7 | f | 0.17 | 0/230 | 0.33 | 0/311 |
| 8 | A2 | 0.29 | 0/1580 | 0.40 | 0/2146 |
| 8 | Au | 0.23 | 0/1607 | 0.33 | 0/2184 |
| 8 | BB | 0.31 | 0/1669 | 0.37 | 0/2270 |
| 8 | BJ | 0.15 | 0/1607 | 0.38 | 0/2184 |
| 8 | BQ | 0.19 | 0/1580 | 0.40 | 0/2146 |
| 8 | Ba | 0.19 | 0/1669 | 0.37 | 1/2270 (0.0%) |
| 8 | G | 0.25 | 0/1607 | 0.38 | 1/2184 (0.0%) |
| 8 | N | 0.28 | 0/1580 | 0.40 | 0/2146 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 8 | Y | 0.31 | 0/1669 | 0.39 | 1/2270 (0.0%) |
| 8 | g | 0.15 | 0/1607 | 0.38 | 0/2184 |
| 8 | n | 0.26 | 0/1580 | 0.48 | 2/2146 (0.1%) |
| 8 | y | 0.25 | 0/1669 | 0.46 | 1/2270 (0.0%) |
| 9 | Av | 0.29 | 0/447 | 0.52 | 0/608 |
| 9 | BK | 0.27 | 0/447 | 0.48 | 0/608 |
| 9 | H | 0.28 | 0/447 | 0.48 | 1/608 (0.2%) |
| 9 | h | 0.28 | 0/447 | 0.52 | 1/608 (0.2%) |
| 10 | Aw | 0.28 | 0/294 | 0.41 | 0/397 |
| 10 | BL | 0.27 | 0/294 | 0.39 | 0/397 |
| 10 | I | 0.27 | 0/294 | 0.40 | 0/397 |
| 10 | i | 0.27 | 0/294 | 0.50 | 0/397 |
| 11 | Ay | 0.22 | 0/313 | 0.44 | 0/428 |
| 11 | BN | 0.22 | 0/313 | 0.45 | 0/428 |
| 11 | K | 0.20 | 0/313 | 0.40 | 0/428 |
| 11 | k | 0.21 | 0/313 | 0.45 | 0/428 |
| 12 | Az | 0.28 | 0/301 | 0.33 | 0/409 |
| 12 | BO | 0.25 | 0/301 | 0.30 | 0/409 |
| 12 | L | 0.25 | 0/301 | 0.39 | 0/409 |
| 12 | l | 0.26 | 0/301 | 0.33 | 0/409 |
| 13 | A1 | 0.26 | 0/254 | 0.50 | 0/347 |
| 13 | BP | 0.27 | 0/254 | 0.53 | 0/347 |
| 13 | M | 0.31 | 0/254 | 0.53 | 0/347 |
| 13 | m | 0.26 | 0/254 | 0.53 | 0/347 |
| 14 | A6 | 0.22 | 0/1715 | 0.37 | 0/2328 |
| 14 | BV | 0.17 | 0/1715 | 0.36 | 0/2328 |
| 14 | S | 0.19 | 0/1715 | 0.35 | 0/2328 |
| 14 | s | 0.16 | 0/1715 | 0.34 | 0/2328 |
| 15 | A7 | 0.26 | 0/246 | 0.34 | 0/333 |
| 15 | BW | 0.29 | 0/246 | 0.36 | 0/333 |
| 15 | T | 0.33 | 0/246 | 0.43 | 0/333 |
| 15 | t | 0.21 | 0/246 | 0.33 | 0/333 |
| 16 | A8 | 0.17 | 0/197 | 0.26 | 0/261 |
| 16 | BX | 0.15 | 0/197 | 0.36 | 0/261 |
| 16 | U | 0.16 | 0/197 | 0.28 | 0/261 |
| 16 | u | 0.16 | 0/197 | 0.34 | 0/261 |
| 17 | A0 | 0.26 | 0/439 | 0.41 | 0/594 |
| 17 | BY | 0.21 | 0/439 | 0.33 | 0/594 |
| 17 | W | 0.26 | 0/439 | 0.43 | 1/594 (0.2%) |
| 17 | w | 0.26 | 0/439 | 0.44 | 0/594 |
| 18 | BA | 0.15 | 0/250 | 0.42 | 0/339 |
| 18 | BZ | 0.16 | 0/250 | 0.39 | 0/339 |
| 18 | X | 0.15 | 0/250 | 0.42 | 0/339 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 18 | x | 0.16 | 0/250 | 0.44 | 0/339 |
| 19 | BC | 0.20 | 0/475 | 0.43 | 0/649 |
| 19 | Bb | 0.19 | 0/475 | 0.39 | 0/649 |
| 19 | Z | 0.23 | 0/475 | 0.49 | 0/649 |
| 19 | z | 0.19 | 0/475 | 0.37 | 0/649 |
| 20 | A | 0.27 | 0/2602 | 0.37 | 0/3546 |
| 20 | BD | 0.26 | 0/2602 | 0.37 | 0/3546 |
| 20 | R | 0.32 | 0/2602 | 0.42 | 1/3546 (0.0%) |
| 20 | a | 0.25 | 0/2602 | 0.38 | 1/3546 (0.0%) |
| 21 | 1 | 0.28 | 0/3487 | 0.37 | 0/4750 |
| 21 | BF | 0.27 | 0/3478 | 0.35 | 0/4736 |
| 21 | C | 0.24 | 0/3487 | 0.36 | 0/4750 |
| 21 | c | 0.26 | 0/3478 | 0.38 | 0/4736 |
| 22 | BU | 0.35 | 0/1585 | 0.48 | 0/2161 |
| 22 | r | 0.31 | 0/1585 | 0.52 | 0/2161 |
| All | All | 0.26 | 2/109588 (0.0%) | 0.40 | 20/149064 (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 |
|-----|-------|---------------------|---------------------|
| 2 | 6 | 0 | 1 |
| 3 | 8 | 0 | 1 |
| 5 | 2 | 0 | 1 |
| 17 | w | 0 | 1 |
| All | All | 0 | 4 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5 | d | 346 | VAL | CB-CG1 | -5.66 | 1.33 | 1.52 |
| 5 | BG | 346 | VAL | CB-CG1 | -5.54 | 1.34 | 1.52 |

The worst 5 of 20 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 0 | 167 | MET | CG-SD-CE | -9.25 | 80.54 | 100.90 |
| 8 | y | 89 | PRO | CA-N-CD | -8.75 | 99.75 | 112.00 |
| 20 | a | 328 | MET | CG-SD-CE | -7.01 | 85.48 | 100.90 |
| 8 | n | 226 | MET | CG-SD-CE | -6.92 | 85.69 | 100.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 6 | 167 | MET | CG-SD-CE | -6.76 | 86.02 | 100.90 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 5 | 2 | 266 | ARG | Sidechain |
| 2 | 6 | 93 | ARG | Sidechain |
| 3 | 8 | 223 | ARG | Sidechain |
| 17 | w | 84 | ARG | Sidechain |

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 | 5 | 1529 | 0 | 1470 | 72 | 0 |
| 1 | 7 | 1530 | 0 | 1473 | 68 | 0 |
| 1 | 9 | 1529 | 0 | 1470 | 68 | 0 |
| 1 | AA | 1530 | 0 | 1473 | 82 | 0 |
| 2 | 0 | 1716 | 0 | 1658 | 115 | 0 |
| 2 | 6 | 1716 | 0 | 1658 | 113 | 0 |
| 3 | 8 | 1512 | 0 | 1444 | 81 | 0 |
| 3 | AB | 1512 | 0 | 1444 | 95 | 0 |
| 4 | B | 3757 | 0 | 3641 | 84 | 0 |
| 4 | BE | 3757 | 0 | 3641 | 88 | 0 |
| 4 | b | 3757 | 0 | 3641 | 93 | 0 |
| 4 | v | 3757 | 0 | 3641 | 83 | 0 |
| 5 | 2 | 2723 | 0 | 2615 | 68 | 0 |
| 5 | BG | 2723 | 0 | 2615 | 85 | 0 |
| 5 | D | 2723 | 0 | 2615 | 65 | 0 |
| 5 | d | 2723 | 0 | 2615 | 99 | 0 |
| 6 | 3 | 544 | 0 | 519 | 17 | 0 |
| 6 | BH | 544 | 0 | 519 | 20 | 0 |
| 6 | E | 544 | 0 | 519 | 18 | 0 |
| 6 | e | 544 | 0 | 519 | 21 | 0 |
| 7 | 4 | 225 | 0 | 233 | 10 | 0 |
| 7 | BI | 225 | 0 | 233 | 13 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7 | F | 225 | 0 | 233 | 9 | 0 |
| 7 | f | 225 | 0 | 233 | 13 | 0 |
| 8 | A2 | 1536 | 0 | 1480 | 44 | 0 |
| 8 | Au | 1562 | 0 | 1503 | 43 | 0 |
| 8 | BB | 1621 | 0 | 1550 | 36 | 0 |
| 8 | BJ | 1562 | 0 | 1503 | 47 | 0 |
| 8 | BQ | 1536 | 0 | 1480 | 49 | 0 |
| 8 | Ba | 1621 | 0 | 1550 | 35 | 0 |
| 8 | G | 1562 | 0 | 1503 | 52 | 0 |
| 8 | N | 1536 | 0 | 1480 | 42 | 0 |
| 8 | Y | 1621 | 0 | 1550 | 43 | 0 |
| 8 | g | 1562 | 0 | 1503 | 47 | 0 |
| 8 | n | 1536 | 0 | 1480 | 51 | 0 |
| 8 | y | 1621 | 0 | 1550 | 42 | 0 |
| 9 | Av | 438 | 0 | 465 | 27 | 0 |
| 9 | BK | 438 | 0 | 465 | 23 | 0 |
| 9 | H | 438 | 0 | 465 | 19 | 0 |
| 9 | h | 438 | 0 | 465 | 29 | 0 |
| 10 | Aw | 286 | 0 | 295 | 2 | 0 |
| 10 | BL | 286 | 0 | 295 | 7 | 0 |
| 10 | I | 286 | 0 | 295 | 7 | 0 |
| 10 | i | 286 | 0 | 295 | 10 | 0 |
| 11 | Ay | 302 | 0 | 313 | 5 | 0 |
| 11 | BN | 302 | 0 | 313 | 4 | 0 |
| 11 | K | 302 | 0 | 313 | 5 | 0 |
| 11 | k | 302 | 0 | 313 | 9 | 0 |
| 12 | Az | 293 | 0 | 283 | 11 | 0 |
| 12 | BO | 293 | 0 | 283 | 12 | 0 |
| 12 | L | 293 | 0 | 283 | 13 | 0 |
| 12 | l | 293 | 0 | 283 | 16 | 0 |
| 13 | A1 | 250 | 0 | 279 | 16 | 0 |
| 13 | BP | 250 | 0 | 279 | 15 | 0 |
| 13 | M | 250 | 0 | 279 | 15 | 0 |
| 13 | m | 250 | 0 | 279 | 15 | 0 |
| 14 | A6 | 1670 | 0 | 1649 | 36 | 0 |
| 14 | BV | 1670 | 0 | 1649 | 74 | 0 |
| 14 | S | 1670 | 0 | 1649 | 42 | 0 |
| 14 | s | 1670 | 0 | 1649 | 67 | 0 |
| 15 | A7 | 239 | 0 | 255 | 9 | 0 |
| 15 | BW | 239 | 0 | 255 | 5 | 0 |
| 15 | T | 239 | 0 | 255 | 12 | 0 |
| 15 | t | 239 | 0 | 255 | 8 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16 | A8 | 195 | 0 | 206 | 14 | 0 |
| 16 | BX | 195 | 0 | 206 | 8 | 0 |
| 16 | U | 195 | 0 | 206 | 16 | 0 |
| 16 | u | 195 | 0 | 206 | 11 | 0 |
| 17 | A0 | 428 | 0 | 405 | 13 | 0 |
| 17 | BY | 428 | 0 | 405 | 4 | 0 |
| 17 | W | 428 | 0 | 405 | 17 | 0 |
| 17 | w | 428 | 0 | 405 | 8 | 0 |
| 18 | BA | 248 | 0 | 266 | 7 | 0 |
| 18 | BZ | 248 | 0 | 266 | 8 | 0 |
| 18 | X | 248 | 0 | 266 | 8 | 0 |
| 18 | x | 248 | 0 | 266 | 7 | 0 |
| 19 | BC | 465 | 0 | 495 | 16 | 0 |
| 19 | Bb | 465 | 0 | 495 | 15 | 0 |
| 19 | Z | 465 | 0 | 495 | 16 | 0 |
| 19 | z | 465 | 0 | 495 | 17 | 0 |
| 20 | A | 2525 | 0 | 2443 | 50 | 0 |
| 20 | BD | 2525 | 0 | 2443 | 68 | 0 |
| 20 | R | 2525 | 0 | 2443 | 58 | 0 |
| 20 | a | 2525 | 0 | 2443 | 65 | 0 |
| 21 | 1 | 3373 | 0 | 3302 | 58 | 0 |
| 21 | BF | 3365 | 0 | 3295 | 62 | 0 |
| 21 | C | 3373 | 0 | 3302 | 60 | 0 |
| 21 | c | 3365 | 0 | 3295 | 81 | 0 |
| 22 | BU | 1539 | 0 | 1502 | 75 | 0 |
| 22 | r | 1539 | 0 | 1502 | 93 | 0 |
| 23 | 0 | 314 | 0 | 238 | 35 | 0 |
| 23 | 5 | 307 | 0 | 228 | 43 | 0 |
| 23 | 6 | 314 | 0 | 238 | 42 | 0 |
| 23 | 7 | 304 | 0 | 222 | 32 | 0 |
| 23 | 8 | 184 | 0 | 124 | 10 | 0 |
| 23 | 9 | 307 | 0 | 228 | 40 | 0 |
| 23 | A2 | 358 | 0 | 318 | 47 | 0 |
| 23 | A6 | 195 | 0 | 136 | 15 | 0 |
| 23 | AA | 304 | 0 | 222 | 34 | 0 |
| 23 | AB | 184 | 0 | 124 | 15 | 0 |
| 23 | Au | 349 | 0 | 300 | 39 | 0 |
| 23 | BB | 358 | 0 | 318 | 48 | 0 |
| 23 | BH | 45 | 0 | 28 | 0 | 0 |
| 23 | BJ | 351 | 0 | 303 | 54 | 0 |
| 23 | BQ | 358 | 0 | 318 | 51 | 0 |
| 23 | BU | 222 | 0 | 179 | 36 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 23 | BV | 195 | 0 | 136 | 20 | 0 |
| 23 | Ba | 358 | 0 | 318 | 45 | 0 |
| 23 | G | 349 | 0 | 300 | 50 | 0 |
| 23 | N | 358 | 0 | 318 | 45 | 0 |
| 23 | S | 195 | 0 | 136 | 15 | 0 |
| 23 | Y | 358 | 0 | 318 | 47 | 0 |
| 23 | e | 45 | 0 | 28 | 0 | 0 |
| 23 | g | 351 | 0 | 303 | 52 | 0 |
| 23 | n | 358 | 0 | 318 | 54 | 0 |
| 23 | r | 222 | 0 | 179 | 35 | 0 |
| 23 | s | 195 | 0 | 136 | 20 | 0 |
| 23 | y | 358 | 0 | 318 | 45 | 0 |
| 24 | 0 | 426 | 0 | 373 | 37 | 0 |
| 24 | 1 | 780 | 0 | 864 | 34 | 0 |
| 24 | 2 | 130 | 0 | 144 | 8 | 0 |
| 24 | 5 | 412 | 0 | 348 | 41 | 0 |
| 24 | 6 | 426 | 0 | 373 | 43 | 0 |
| 24 | 7 | 389 | 0 | 311 | 28 | 0 |
| 24 | 8 | 266 | 0 | 194 | 20 | 0 |
| 24 | 9 | 412 | 0 | 348 | 37 | 0 |
| 24 | A | 240 | 0 | 242 | 14 | 0 |
| 24 | A2 | 473 | 0 | 468 | 23 | 0 |
| 24 | A6 | 463 | 0 | 390 | 14 | 0 |
| 24 | AA | 389 | 0 | 311 | 28 | 0 |
| 24 | AB | 266 | 0 | 194 | 25 | 0 |
| 24 | Au | 477 | 0 | 477 | 20 | 0 |
| 24 | Aw | 65 | 0 | 72 | 3 | 0 |
| 24 | B | 1040 | 0 | 1152 | 73 | 0 |
| 24 | BB | 473 | 0 | 468 | 18 | 0 |
| 24 | BD | 240 | 0 | 242 | 18 | 0 |
| 24 | BE | 1040 | 0 | 1152 | 69 | 0 |
| 24 | BF | 845 | 0 | 936 | 39 | 0 |
| 24 | BG | 130 | 0 | 144 | 8 | 0 |
| 24 | BJ | 477 | 0 | 477 | 25 | 0 |
| 24 | BQ | 473 | 0 | 468 | 27 | 0 |
| 24 | BU | 518 | 0 | 452 | 36 | 0 |
| 24 | BV | 465 | 0 | 393 | 29 | 0 |
| 24 | Ba | 473 | 0 | 468 | 21 | 0 |
| 24 | C | 780 | 0 | 864 | 36 | 0 |
| 24 | D | 130 | 0 | 144 | 7 | 0 |
| 24 | G | 477 | 0 | 477 | 21 | 0 |
| 24 | I | 65 | 0 | 72 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24 | N | 473 | 0 | 468 | 23 | 0 |
| 24 | R | 240 | 0 | 242 | 12 | 0 |
| 24 | S | 463 | 0 | 390 | 20 | 0 |
| 24 | Y | 473 | 0 | 468 | 22 | 0 |
| 24 | a | 240 | 0 | 242 | 17 | 0 |
| 24 | b | 1040 | 0 | 1152 | 74 | 0 |
| 24 | c | 845 | 0 | 936 | 47 | 0 |
| 24 | d | 130 | 0 | 144 | 7 | 0 |
| 24 | g | 477 | 0 | 477 | 21 | 0 |
| 24 | n | 473 | 0 | 468 | 25 | 0 |
| 24 | r | 518 | 0 | 452 | 37 | 0 |
| 24 | s | 465 | 0 | 393 | 29 | 0 |
| 24 | v | 1040 | 0 | 1152 | 79 | 0 |
| 24 | y | 473 | 0 | 468 | 19 | 0 |
| 25 | 0 | 84 | 0 | 112 | 19 | 0 |
| 25 | 5 | 84 | 0 | 112 | 15 | 0 |
| 25 | 6 | 84 | 0 | 112 | 17 | 0 |
| 25 | 7 | 84 | 0 | 112 | 13 | 0 |
| 25 | 8 | 42 | 0 | 56 | 6 | 0 |
| 25 | 9 | 84 | 0 | 112 | 18 | 0 |
| 25 | A2 | 84 | 0 | 112 | 12 | 0 |
| 25 | A6 | 84 | 0 | 112 | 10 | 0 |
| 25 | AA | 84 | 0 | 112 | 14 | 0 |
| 25 | AB | 42 | 0 | 56 | 9 | 0 |
| 25 | Au | 84 | 0 | 112 | 12 | 0 |
| 25 | BB | 84 | 0 | 112 | 11 | 0 |
| 25 | BJ | 84 | 0 | 112 | 17 | 0 |
| 25 | BQ | 84 | 0 | 112 | 11 | 0 |
| 25 | BU | 42 | 0 | 56 | 10 | 0 |
| 25 | BV | 84 | 0 | 112 | 10 | 0 |
| 25 | Ba | 84 | 0 | 112 | 7 | 0 |
| 25 | G | 84 | 0 | 112 | 11 | 0 |
| 25 | N | 84 | 0 | 112 | 10 | 0 |
| 25 | S | 84 | 0 | 112 | 11 | 0 |
| 25 | Y | 84 | 0 | 112 | 9 | 0 |
| 25 | g | 84 | 0 | 112 | 16 | 0 |
| 25 | n | 84 | 0 | 112 | 11 | 0 |
| 25 | r | 42 | 0 | 56 | 9 | 0 |
| 25 | s | 84 | 0 | 112 | 16 | 0 |
| 25 | y | 84 | 0 | 112 | 9 | 0 |
| 26 | 5 | 44 | 0 | 56 | 1 | 0 |
| 26 | 7 | 44 | 0 | 56 | 5 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 26 | 9 | 44 | 0 | 56 | 1 | 0 |
| 26 | A2 | 44 | 0 | 56 | 3 | 0 |
| 26 | A6 | 44 | 0 | 56 | 2 | 0 |
| 26 | AA | 44 | 0 | 56 | 4 | 0 |
| 26 | Au | 44 | 0 | 56 | 1 | 0 |
| 26 | BB | 88 | 0 | 112 | 8 | 0 |
| 26 | BJ | 44 | 0 | 56 | 1 | 0 |
| 26 | BQ | 44 | 0 | 56 | 3 | 0 |
| 26 | BV | 44 | 0 | 56 | 5 | 0 |
| 26 | Ba | 44 | 0 | 56 | 2 | 0 |
| 26 | G | 44 | 0 | 56 | 1 | 0 |
| 26 | N | 44 | 0 | 56 | 3 | 0 |
| 26 | S | 44 | 0 | 56 | 3 | 0 |
| 26 | Y | 44 | 0 | 56 | 1 | 0 |
| 26 | g | 44 | 0 | 56 | 1 | 0 |
| 26 | n | 44 | 0 | 56 | 3 | 0 |
| 26 | r | 44 | 0 | 56 | 5 | 0 |
| 26 | s | 44 | 0 | 56 | 5 | 0 |
| 26 | y | 44 | 0 | 56 | 3 | 0 |
| 27 | 0 | 47 | 0 | 67 | 8 | 0 |
| 27 | 1 | 98 | 0 | 148 | 4 | 0 |
| 27 | 2 | 95 | 0 | 139 | 1 | 0 |
| 27 | 5 | 41 | 0 | 55 | 3 | 0 |
| 27 | 6 | 47 | 0 | 67 | 5 | 0 |
| 27 | 9 | 41 | 0 | 55 | 3 | 0 |
| 27 | A0 | 49 | 0 | 74 | 1 | 0 |
| 27 | A2 | 49 | 0 | 74 | 3 | 0 |
| 27 | Au | 49 | 0 | 74 | 4 | 0 |
| 27 | Az | 49 | 0 | 74 | 3 | 0 |
| 27 | B | 95 | 0 | 139 | 2 | 0 |
| 27 | BB | 49 | 0 | 74 | 7 | 0 |
| 27 | BE | 144 | 0 | 213 | 3 | 0 |
| 27 | BF | 98 | 0 | 148 | 3 | 0 |
| 27 | BG | 49 | 0 | 74 | 1 | 0 |
| 27 | BJ | 49 | 0 | 74 | 4 | 0 |
| 27 | BQ | 49 | 0 | 74 | 6 | 0 |
| 27 | BU | 42 | 0 | 57 | 5 | 0 |
| 27 | BY | 49 | 0 | 74 | 1 | 0 |
| 27 | Ba | 49 | 0 | 74 | 4 | 0 |
| 27 | C | 98 | 0 | 148 | 5 | 0 |
| 27 | D | 49 | 0 | 74 | 3 | 0 |
| 27 | G | 49 | 0 | 74 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 27 | L | 49 | 0 | 74 | 3 | 0 |
| 27 | N | 49 | 0 | 74 | 5 | 0 |
| 27 | W | 49 | 0 | 74 | 1 | 0 |
| 27 | Y | 49 | 0 | 74 | 6 | 0 |
| 27 | b | 144 | 0 | 213 | 6 | 0 |
| 27 | c | 98 | 0 | 148 | 3 | 0 |
| 27 | d | 49 | 0 | 74 | 1 | 0 |
| 27 | g | 49 | 0 | 74 | 4 | 0 |
| 27 | n | 49 | 0 | 74 | 5 | 0 |
| 27 | r | 42 | 0 | 57 | 6 | 0 |
| 27 | v | 49 | 0 | 74 | 2 | 0 |
| 27 | w | 49 | 0 | 74 | 1 | 0 |
| 27 | y | 49 | 0 | 74 | 5 | 0 |
| 28 | 5 | 44 | 0 | 56 | 11 | 0 |
| 28 | 7 | 88 | 0 | 112 | 4 | 0 |
| 28 | 8 | 44 | 0 | 56 | 6 | 0 |
| 28 | 9 | 44 | 0 | 56 | 11 | 0 |
| 28 | A2 | 44 | 0 | 56 | 6 | 0 |
| 28 | AA | 88 | 0 | 112 | 6 | 0 |
| 28 | AB | 44 | 0 | 56 | 6 | 0 |
| 28 | Au | 44 | 0 | 56 | 4 | 0 |
| 28 | BB | 44 | 0 | 56 | 6 | 0 |
| 28 | BJ | 44 | 0 | 56 | 1 | 0 |
| 28 | BQ | 44 | 0 | 56 | 5 | 0 |
| 28 | BU | 44 | 0 | 56 | 4 | 0 |
| 28 | Ba | 44 | 0 | 56 | 2 | 0 |
| 28 | G | 44 | 0 | 56 | 4 | 0 |
| 28 | N | 44 | 0 | 56 | 5 | 0 |
| 28 | Y | 44 | 0 | 56 | 5 | 0 |
| 28 | g | 44 | 0 | 56 | 1 | 0 |
| 28 | n | 44 | 0 | 56 | 2 | 0 |
| 28 | r | 44 | 0 | 56 | 5 | 0 |
| 28 | y | 44 | 0 | 56 | 3 | 0 |
| 29 | 1 | 80 | 0 | 112 | 7 | 0 |
| 29 | 4 | 40 | 0 | 56 | 3 | 0 |
| 29 | 8 | 40 | 0 | 56 | 6 | 0 |
| 29 | A | 40 | 0 | 56 | 3 | 0 |
| 29 | AB | 40 | 0 | 56 | 5 | 0 |
| 29 | Av | 40 | 0 | 56 | 4 | 0 |
| 29 | Ay | 80 | 0 | 112 | 8 | 0 |
| 29 | B | 160 | 0 | 224 | 20 | 0 |
| 29 | BD | 40 | 0 | 56 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29 | BE | 160 | 0 | 224 | 15 | 0 |
| 29 | BF | 80 | 0 | 112 | 6 | 0 |
| 29 | BI | 40 | 0 | 56 | 2 | 0 |
| 29 | BK | 40 | 0 | 56 | 8 | 0 |
| 29 | BN | 40 | 0 | 56 | 2 | 0 |
| 29 | Bb | 40 | 0 | 56 | 3 | 0 |
| 29 | C | 80 | 0 | 112 | 5 | 0 |
| 29 | F | 40 | 0 | 56 | 1 | 0 |
| 29 | H | 40 | 0 | 56 | 5 | 0 |
| 29 | K | 80 | 0 | 112 | 5 | 0 |
| 29 | R | 40 | 0 | 56 | 1 | 0 |
| 29 | a | 40 | 0 | 56 | 3 | 0 |
| 29 | b | 160 | 0 | 224 | 16 | 0 |
| 29 | c | 40 | 0 | 56 | 3 | 0 |
| 29 | f | 40 | 0 | 56 | 2 | 0 |
| 29 | h | 40 | 0 | 56 | 7 | 0 |
| 29 | k | 40 | 0 | 56 | 1 | 0 |
| 29 | v | 160 | 0 | 224 | 16 | 0 |
| 29 | z | 80 | 0 | 112 | 8 | 0 |
| 30 | 1 | 102 | 0 | 144 | 5 | 0 |
| 30 | 2 | 46 | 0 | 62 | 0 | 0 |
| 30 | A | 48 | 0 | 66 | 1 | 0 |
| 30 | A0 | 48 | 0 | 66 | 1 | 0 |
| 30 | Aw | 40 | 0 | 50 | 1 | 0 |
| 30 | B | 91 | 0 | 122 | 0 | 0 |
| 30 | BE | 51 | 0 | 72 | 1 | 0 |
| 30 | BF | 102 | 0 | 144 | 5 | 0 |
| 30 | BG | 46 | 0 | 62 | 0 | 0 |
| 30 | BL | 48 | 0 | 66 | 2 | 0 |
| 30 | C | 102 | 0 | 144 | 5 | 0 |
| 30 | D | 46 | 0 | 62 | 0 | 0 |
| 30 | I | 40 | 0 | 50 | 3 | 0 |
| 30 | b | 51 | 0 | 72 | 1 | 0 |
| 30 | c | 102 | 0 | 144 | 7 | 0 |
| 30 | d | 46 | 0 | 62 | 0 | 0 |
| 30 | i | 48 | 0 | 66 | 2 | 0 |
| 30 | v | 91 | 0 | 122 | 0 | 0 |
| 31 | 2 | 55 | 0 | 80 | 1 | 0 |
| 31 | BG | 55 | 0 | 80 | 2 | 0 |
| 31 | D | 55 | 0 | 80 | 1 | 0 |
| 31 | d | 55 | 0 | 80 | 3 | 0 |
| 32 | 2 | 50 | 0 | 67 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 32 | A | 54 | 0 | 78 | 8 | 0 |
| 32 | A1 | 54 | 0 | 78 | 2 | 0 |
| 32 | Az | 42 | 0 | 48 | 3 | 0 |
| 32 | BD | 54 | 0 | 78 | 6 | 0 |
| 32 | BG | 50 | 0 | 67 | 4 | 0 |
| 32 | BO | 96 | 0 | 126 | 6 | 0 |
| 32 | D | 50 | 0 | 67 | 1 | 0 |
| 32 | L | 96 | 0 | 126 | 5 | 0 |
| 32 | R | 54 | 0 | 78 | 9 | 0 |
| 32 | a | 54 | 0 | 78 | 6 | 0 |
| 32 | d | 50 | 0 | 67 | 3 | 0 |
| 32 | l | 96 | 0 | 126 | 7 | 0 |
| 33 | 4 | 43 | 0 | 30 | 3 | 0 |
| 33 | BI | 43 | 0 | 30 | 2 | 0 |
| 33 | F | 43 | 0 | 30 | 1 | 0 |
| 33 | f | 43 | 0 | 30 | 2 | 0 |
| 34 | 1 | 177 | 0 | 228 | 7 | 0 |
| 34 | A | 59 | 0 | 76 | 2 | 0 |
| 34 | Av | 62 | 0 | 82 | 6 | 0 |
| 34 | BD | 119 | 0 | 154 | 2 | 0 |
| 34 | BF | 117 | 0 | 150 | 4 | 0 |
| 34 | BK | 62 | 0 | 82 | 6 | 0 |
| 34 | C | 177 | 0 | 228 | 5 | 0 |
| 34 | H | 62 | 0 | 82 | 6 | 0 |
| 34 | R | 59 | 0 | 76 | 2 | 0 |
| 34 | a | 119 | 0 | 154 | 3 | 0 |
| 34 | c | 117 | 0 | 150 | 4 | 0 |
| 34 | h | 62 | 0 | 82 | 4 | 0 |
| 35 | 2 | 4 | 0 | 1 | 0 | 0 |
| 35 | A | 4 | 0 | 1 | 0 | 0 |
| 35 | BD | 4 | 0 | 1 | 0 | 0 |
| 35 | a | 4 | 0 | 1 | 0 | 0 |
| 36 | A | 10 | 0 | 0 | 0 | 0 |
| 36 | BD | 10 | 0 | 0 | 1 | 0 |
| 36 | R | 10 | 0 | 0 | 0 | 0 |
| 36 | a | 10 | 0 | 0 | 1 | 0 |
| 37 | A | 1 | 0 | 0 | 0 | 0 |
| 37 | BD | 1 | 0 | 0 | 0 | 0 |
| 37 | R | 1 | 0 | 0 | 0 | 0 |
| 37 | a | 1 | 0 | 0 | 0 | 0 |
| 38 | A | 128 | 0 | 148 | 8 | 0 |
| 38 | BD | 128 | 0 | 148 | 6 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 38 | R | 128 | 0 | 148 | 7 | 0 |
| 38 | a | 128 | 0 | 148 | 4 | 0 |
| All | All | 146846 | 0 | 146920 | 4896 | 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 17.

The worst 5 of 4896 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:n:103:SER:HA | 8:n:223:MET:HE1 | 1.25 | 1.18 |
| 8:BJ:226:MET:HE1 | 25:BJ:616:LUT:H12 | 1.27 | 1.14 |
| 4:BE:223:GLN:HE22 | 9:BK:35:PRO:HA | 0.97 | 1.11 |
| 5:d:326:ILE:HG12 | 20:a:328:MET:HE1 | 1.39 | 1.05 |
| 2:0:172:GLY:HA3 | 1:AA:62:PHE:CE1 | 1.96 | 1.01 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1 | 5 | 197/266 (74%) | 196 (100%) | 0 | 1 (0%) | 25 | 58 |
| 1 | 7 | 197/266 (74%) | 193 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 9 | 197/266 (74%) | 196 (100%) | 0 | 1 (0%) | 25 | 58 |
| 1 | AA | 197/266 (74%) | 194 (98%) | 3 (2%) | 0 | 100 | 100 |
| 2 | 0 | 220/243 (90%) | 211 (96%) | 8 (4%) | 1 (0%) | 25 | 58 |
| 2 | 6 | 220/243 (90%) | 212 (96%) | 7 (3%) | 1 (0%) | 25 | 58 |
| 3 | 8 | 190/212 (90%) | 184 (97%) | 6 (3%) | 0 | 100 | 100 |
| 3 | AB | 190/212 (90%) | 182 (96%) | 8 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 4 | B | 477/508 (94%) | 468 (98%) | 9 (2%) | 0 | 100 | 100 |
| 4 | BE | 477/508 (94%) | 473 (99%) | 4 (1%) | 0 | 100 | 100 |
| 4 | b | 477/508 (94%) | 473 (99%) | 4 (1%) | 0 | 100 | 100 |
| 4 | v | 477/508 (94%) | 467 (98%) | 10 (2%) | 0 | 100 | 100 |
| 5 | 2 | 340/352 (97%) | 336 (99%) | 4 (1%) | 0 | 100 | 100 |
| 5 | BG | 340/352 (97%) | 336 (99%) | 4 (1%) | 0 | 100 | 100 |
| 5 | D | 340/352 (97%) | 334 (98%) | 6 (2%) | 0 | 100 | 100 |
| 5 | d | 340/352 (97%) | 335 (98%) | 5 (2%) | 0 | 100 | 100 |
| 6 | 3 | 64/83 (77%) | 63 (98%) | 1 (2%) | 0 | 100 | 100 |
| 6 | BH | 64/83 (77%) | 61 (95%) | 3 (5%) | 0 | 100 | 100 |
| 6 | E | 64/83 (77%) | 63 (98%) | 1 (2%) | 0 | 100 | 100 |
| 6 | e | 64/83 (77%) | 61 (95%) | 3 (5%) | 0 | 100 | 100 |
| 7 | 4 | 27/39 (69%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 7 | BI | 27/39 (69%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 7 | F | 27/39 (69%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 7 | f | 27/39 (69%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 8 | A2 | 200/232 (86%) | 198 (99%) | 1 (0%) | 1 (0%) | 25 | 58 |
| 8 | Au | 204/232 (88%) | 202 (99%) | 2 (1%) | 0 | 100 | 100 |
| 8 | BB | 211/232 (91%) | 209 (99%) | 1 (0%) | 1 (0%) | 25 | 58 |
| 8 | BJ | 204/232 (88%) | 201 (98%) | 3 (2%) | 0 | 100 | 100 |
| 8 | BQ | 200/232 (86%) | 199 (100%) | 0 | 1 (0%) | 25 | 58 |
| 8 | Ba | 211/232 (91%) | 209 (99%) | 1 (0%) | 1 (0%) | 25 | 58 |
| 8 | G | 204/232 (88%) | 201 (98%) | 3 (2%) | 0 | 100 | 100 |
| 8 | N | 200/232 (86%) | 199 (100%) | 0 | 1 (0%) | 25 | 58 |
| 8 | Y | 211/232 (91%) | 209 (99%) | 1 (0%) | 1 (0%) | 25 | 58 |
| 8 | g | 204/232 (88%) | 202 (99%) | 2 (1%) | 0 | 100 | 100 |
| 8 | n | 200/232 (86%) | 199 (100%) | 0 | 1 (0%) | 25 | 58 |
| 8 | y | 211/232 (91%) | 209 (99%) | 1 (0%) | 1 (0%) | 25 | 58 |
| 9 | Av | 57/72 (79%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 9 | BK | 57/72 (79%) | 52 (91%) | 5 (9%) | 0 | 100 | 100 |
| 9 | H | 57/72 (79%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 9 | h | 57/72 (79%) | 52 (91%) | 5 (9%) | 0 | 100 | 100 |
| 10 | Aw | 33/36 (92%) | 33 (100%) | 0 | 0 | 100 | 100 |
| 10 | BL | 33/36 (92%) | 33 (100%) | 0 | 0 | 100 | 100 |
| 10 | I | 33/36 (92%) | 33 (100%) | 0 | 0 | 100 | 100 |
| 10 | i | 33/36 (92%) | 33 (100%) | 0 | 0 | 100 | 100 |
| 11 | Ay | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 11 | BN | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 11 | K | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 11 | k | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 12 | Az | 33/38 (87%) | 32 (97%) | 1 (3%) | 0 | 100 | 100 |
| 12 | BO | 33/38 (87%) | 33 (100%) | 0 | 0 | 100 | 100 |
| 12 | L | 33/38 (87%) | 32 (97%) | 1 (3%) | 0 | 100 | 100 |
| 12 | l | 33/38 (87%) | 33 (100%) | 0 | 0 | 100 | 100 |
| 13 | A1 | 30/34 (88%) | 28 (93%) | 1 (3%) | 1 (3%) | 3 | 24 |
| 13 | BP | 30/34 (88%) | 29 (97%) | 0 | 1 (3%) | 3 | 24 |
| 13 | M | 30/34 (88%) | 28 (93%) | 1 (3%) | 1 (3%) | 3 | 24 |
| 13 | m | 30/34 (88%) | 29 (97%) | 0 | 1 (3%) | 3 | 24 |
| 14 | A6 | 214/232 (92%) | 211 (99%) | 3 (1%) | 0 | 100 | 100 |
| 14 | BV | 214/232 (92%) | 210 (98%) | 4 (2%) | 0 | 100 | 100 |
| 14 | S | 214/232 (92%) | 212 (99%) | 2 (1%) | 0 | 100 | 100 |
| 14 | s | 214/232 (92%) | 211 (99%) | 3 (1%) | 0 | 100 | 100 |
| 15 | A7 | 27/33 (82%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 15 | BW | 27/33 (82%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 15 | T | 27/33 (82%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 15 | t | 27/33 (82%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 16 | A8 | 23/28 (82%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 16 | BX | 23/28 (82%) | 22 (96%) | 1 (4%) | 0 | 100 | 100 |
| 16 | U | 23/28 (82%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 16 | u | 23/28 (82%) | 22 (96%) | 1 (4%) | 0 | 100 | 100 |
| 17 | A0 | 52/54 (96%) | 51 (98%) | 1 (2%) | 0 | 100 | 100 |
| 17 | BY | 52/54 (96%) | 51 (98%) | 1 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 17 | W | 52/54 (96%) | 51 (98%) | 1 (2%) | 0 | 100 | 100 |
| 17 | w | 52/54 (96%) | 50 (96%) | 2 (4%) | 0 | 100 | 100 |
| 18 | BA | 34/42 (81%) | 33 (97%) | 0 | 1 (3%) | 3 | 26 |
| 18 | BZ | 34/42 (81%) | 33 (97%) | 1 (3%) | 0 | 100 | 100 |
| 18 | X | 34/42 (81%) | 33 (97%) | 0 | 1 (3%) | 3 | 26 |
| 18 | x | 34/42 (81%) | 33 (97%) | 1 (3%) | 0 | 100 | 100 |
| 19 | BC | 60/62 (97%) | 59 (98%) | 1 (2%) | 0 | 100 | 100 |
| 19 | Bb | 60/62 (97%) | 60 (100%) | 0 | 0 | 100 | 100 |
| 19 | Z | 60/62 (97%) | 60 (100%) | 0 | 0 | 100 | 100 |
| 19 | z | 60/62 (97%) | 60 (100%) | 0 | 0 | 100 | 100 |
| 20 | A | 319/352 (91%) | 308 (97%) | 11 (3%) | 0 | 100 | 100 |
| 20 | BD | 319/352 (91%) | 310 (97%) | 9 (3%) | 0 | 100 | 100 |
| 20 | R | 319/352 (91%) | 309 (97%) | 10 (3%) | 0 | 100 | 100 |
| 20 | a | 319/352 (91%) | 310 (97%) | 9 (3%) | 0 | 100 | 100 |
| 21 | 1 | 429/459 (94%) | 428 (100%) | 1 (0%) | 0 | 100 | 100 |
| 21 | BF | 427/459 (93%) | 425 (100%) | 2 (0%) | 0 | 100 | 100 |
| 21 | C | 429/459 (94%) | 427 (100%) | 2 (0%) | 0 | 100 | 100 |
| 21 | c | 427/459 (93%) | 425 (100%) | 2 (0%) | 0 | 100 | 100 |
| 22 | BU | 193/250 (77%) | 189 (98%) | 4 (2%) | 0 | 100 | 100 |
| 22 | r | 193/250 (77%) | 185 (96%) | 8 (4%) | 0 | 100 | 100 |
| All | All | 13466/15102 (89%) | 13241 (98%) | 207 (2%) | 18 (0%) | 50 | 79 |

5 of 18 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | m | 3 | VAL |
| 13 | A1 | 3 | VAL |
| 13 | BP | 3 | VAL |
| 13 | M | 3 | VAL |
| 18 | BA | 79 | ILE |

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 | 5 | 153/201 (76%) | 153 (100%) | 0 | 100 | 100 |
| 1 | 7 | 153/201 (76%) | 152 (99%) | 1 (1%) | 81 | 86 |
| 1 | 9 | 153/201 (76%) | 153 (100%) | 0 | 100 | 100 |
| 1 | AA | 153/201 (76%) | 153 (100%) | 0 | 100 | 100 |
| 2 | 0 | 174/192 (91%) | 173 (99%) | 1 (1%) | 84 | 88 |
| 2 | 6 | 174/192 (91%) | 171 (98%) | 3 (2%) | 56 | 72 |
| 3 | 8 | 148/159 (93%) | 147 (99%) | 1 (1%) | 81 | 86 |
| 3 | AB | 148/159 (93%) | 146 (99%) | 2 (1%) | 62 | 75 |
| 4 | B | 379/402 (94%) | 379 (100%) | 0 | 100 | 100 |
| 4 | BE | 379/402 (94%) | 379 (100%) | 0 | 100 | 100 |
| 4 | b | 379/402 (94%) | 379 (100%) | 0 | 100 | 100 |
| 4 | v | 379/402 (94%) | 379 (100%) | 0 | 100 | 100 |
| 5 | 2 | 274/282 (97%) | 274 (100%) | 0 | 100 | 100 |
| 5 | BG | 274/282 (97%) | 272 (99%) | 2 (1%) | 81 | 86 |
| 5 | D | 274/282 (97%) | 273 (100%) | 1 (0%) | 89 | 91 |
| 5 | d | 274/282 (97%) | 273 (100%) | 1 (0%) | 89 | 91 |
| 6 | 3 | 59/73 (81%) | 59 (100%) | 0 | 100 | 100 |
| 6 | BH | 59/73 (81%) | 59 (100%) | 0 | 100 | 100 |
| 6 | E | 59/73 (81%) | 59 (100%) | 0 | 100 | 100 |
| 6 | e | 59/73 (81%) | 59 (100%) | 0 | 100 | 100 |
| 7 | 4 | 24/34 (71%) | 24 (100%) | 0 | 100 | 100 |
| 7 | BI | 24/34 (71%) | 24 (100%) | 0 | 100 | 100 |
| 7 | F | 24/34 (71%) | 23 (96%) | 1 (4%) | 25 | 49 |
| 7 | f | 24/34 (71%) | 24 (100%) | 0 | 100 | 100 |
| 8 | A2 | 154/177 (87%) | 154 (100%) | 0 | 100 | 100 |
| 8 | Au | 157/177 (89%) | 156 (99%) | 1 (1%) | 84 | 88 |
| 8 | BB | 162/177 (92%) | 161 (99%) | 1 (1%) | 84 | 88 |
| 8 | BJ | 157/177 (89%) | 157 (100%) | 0 | 100 | 100 |
| 8 | BQ | 154/177 (87%) | 154 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 8 | Ba | 162/177 (92%) | 162 (100%) | 0 | 100 | 100 |
| 8 | G | 157/177 (89%) | 157 (100%) | 0 | 100 | 100 |
| 8 | N | 154/177 (87%) | 154 (100%) | 0 | 100 | 100 |
| 8 | Y | 162/177 (92%) | 160 (99%) | 2 (1%) | 67 | 77 |
| 8 | g | 157/177 (89%) | 157 (100%) | 0 | 100 | 100 |
| 8 | n | 154/177 (87%) | 154 (100%) | 0 | 100 | 100 |
| 8 | y | 162/177 (92%) | 161 (99%) | 1 (1%) | 84 | 88 |
| 9 | Av | 49/60 (82%) | 49 (100%) | 0 | 100 | 100 |
| 9 | BK | 49/60 (82%) | 48 (98%) | 1 (2%) | 50 | 68 |
| 9 | H | 49/60 (82%) | 49 (100%) | 0 | 100 | 100 |
| 9 | h | 49/60 (82%) | 49 (100%) | 0 | 100 | 100 |
| 10 | Aw | 32/33 (97%) | 32 (100%) | 0 | 100 | 100 |
| 10 | BL | 32/33 (97%) | 32 (100%) | 0 | 100 | 100 |
| 10 | I | 32/33 (97%) | 32 (100%) | 0 | 100 | 100 |
| 10 | i | 32/33 (97%) | 32 (100%) | 0 | 100 | 100 |
| 11 | Ay | 32/32 (100%) | 32 (100%) | 0 | 100 | 100 |
| 11 | BN | 32/32 (100%) | 32 (100%) | 0 | 100 | 100 |
| 11 | K | 32/32 (100%) | 32 (100%) | 0 | 100 | 100 |
| 11 | k | 32/32 (100%) | 32 (100%) | 0 | 100 | 100 |
| 12 | Az | 33/36 (92%) | 33 (100%) | 0 | 100 | 100 |
| 12 | BO | 33/36 (92%) | 33 (100%) | 0 | 100 | 100 |
| 12 | L | 33/36 (92%) | 32 (97%) | 1 (3%) | 36 | 58 |
| 12 | l | 33/36 (92%) | 33 (100%) | 0 | 100 | 100 |
| 13 | A1 | 28/30 (93%) | 28 (100%) | 0 | 100 | 100 |
| 13 | BP | 28/30 (93%) | 28 (100%) | 0 | 100 | 100 |
| 13 | M | 28/30 (93%) | 27 (96%) | 1 (4%) | 30 | 54 |
| 13 | m | 28/30 (93%) | 28 (100%) | 0 | 100 | 100 |
| 14 | A6 | 167/180 (93%) | 166 (99%) | 1 (1%) | 84 | 88 |
| 14 | BV | 167/180 (93%) | 167 (100%) | 0 | 100 | 100 |
| 14 | S | 167/180 (93%) | 166 (99%) | 1 (1%) | 84 | 88 |
| 14 | s | 167/180 (93%) | 166 (99%) | 1 (1%) | 84 | 88 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 15 | A7 | 26/30 (87%) | 25 (96%) | 1 (4%) | 28 | 52 |
| 15 | BW | 26/30 (87%) | 26 (100%) | 0 | 100 | 100 |
| 15 | T | 26/30 (87%) | 26 (100%) | 0 | 100 | 100 |
| 15 | t | 26/30 (87%) | 26 (100%) | 0 | 100 | 100 |
| 16 | A8 | 20/23 (87%) | 20 (100%) | 0 | 100 | 100 |
| 16 | BX | 20/23 (87%) | 20 (100%) | 0 | 100 | 100 |
| 16 | U | 20/23 (87%) | 20 (100%) | 0 | 100 | 100 |
| 16 | u | 20/23 (87%) | 20 (100%) | 0 | 100 | 100 |
| 17 | A0 | 47/47 (100%) | 46 (98%) | 1 (2%) | 48 | 66 |
| 17 | BY | 47/47 (100%) | 47 (100%) | 0 | 100 | 100 |
| 17 | W | 47/47 (100%) | 46 (98%) | 1 (2%) | 48 | 66 |
| 17 | w | 47/47 (100%) | 47 (100%) | 0 | 100 | 100 |
| 18 | BA | 29/34 (85%) | 29 (100%) | 0 | 100 | 100 |
| 18 | BZ | 29/34 (85%) | 29 (100%) | 0 | 100 | 100 |
| 18 | X | 29/34 (85%) | 29 (100%) | 0 | 100 | 100 |
| 18 | x | 29/34 (85%) | 29 (100%) | 0 | 100 | 100 |
| 19 | BC | 54/54 (100%) | 54 (100%) | 0 | 100 | 100 |
| 19 | Bb | 54/54 (100%) | 54 (100%) | 0 | 100 | 100 |
| 19 | Z | 54/54 (100%) | 54 (100%) | 0 | 100 | 100 |
| 19 | z | 54/54 (100%) | 54 (100%) | 0 | 100 | 100 |
| 20 | A | 260/284 (92%) | 260 (100%) | 0 | 100 | 100 |
| 20 | BD | 260/284 (92%) | 260 (100%) | 0 | 100 | 100 |
| 20 | R | 260/284 (92%) | 259 (100%) | 1 (0%) | 89 | 91 |
| 20 | a | 260/284 (92%) | 260 (100%) | 0 | 100 | 100 |
| 21 | 1 | 340/359 (95%) | 340 (100%) | 0 | 100 | 100 |
| 21 | BF | 339/359 (94%) | 338 (100%) | 1 (0%) | 91 | 92 |
| 21 | C | 340/359 (95%) | 338 (99%) | 2 (1%) | 84 | 88 |
| 21 | c | 339/359 (94%) | 339 (100%) | 0 | 100 | 100 |
| 22 | BU | 159/201 (79%) | 156 (98%) | 3 (2%) | 52 | 69 |
| 22 | r | 159/201 (79%) | 159 (100%) | 0 | 100 | 100 |
| All | All | 10876/12004 (91%) | 10842 (100%) | 34 (0%) | 90 | 92 |

5 of 34 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | BK | 57 | ILE |
| 20 | R | 290 | ILE |
| 22 | BU | 134 | GLN |
| 8 | Y | 226 | MET |
| 8 | Y | 158 | ILE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | A6 | 228 | ASN |
| 14 | BV | 242 | GLN |
| 4 | BE | 26 | HIS |
| 8 | BJ | 232 | GLN |
| 20 | R | 181 | 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 766 ligands modelled in this entry, 4 are monoatomic - leaving 762 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 |
| 24 | CLA | BU | 609 | 22 | 65,73,73 | 1.43 | 10 (15%) | 76,113,113 | 1.43 | 6 (7%) |
| 24 | CLA | BD | 407 | - | 50,58,73 | 1.64 | 7 (14%) | 58,95,113 | 1.61 | 9 (15%) |
| 24 | CLA | 5 | 614 | 1 | 45,53,73 | 1.75 | 5 (11%) | 52,89,113 | 1.68 | 6 (11%) |
| 23 | CHL | 6 | 606 | - | 46,54,74 | 2.21 | 14 (30%) | 49,90,114 | 2.83 | 18 (36%) |
| 26 | NEX | s | 616 | - | 38,46,46 | 1.61 | 7 (18%) | 50,70,70 | 1.62 | 9 (18%) |
| 23 | CHL | A2 | 605 | 8 | 48,56,74 | 2.15 | 14 (29%) | 51,92,114 | 2.75 | 18 (35%) |
| 23 | CHL | 5 | 601 | 1 | 46,54,74 | 2.28 | 15 (32%) | 49,90,114 | 2.88 | 19 (38%) |
| 23 | CHL | AA | 310 | - | 58,66,74 | 2.13 | 16 (27%) | 61,103,114 | 2.68 | 24 (39%) |
| 24 | CLA | v | 608 | 4 | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.44 | 6 (7%) |
| 24 | CLA | 1 | 506 | 21 | 65,73,73 | 1.48 | 10 (15%) | 76,113,113 | 1.35 | 8 (10%) |
| 24 | CLA | Au | 611 | 27 | 60,68,73 | 1.50 | 7 (11%) | 70,107,113 | 1.38 | 7 (10%) |
| 24 | CLA | C | 510 | 21 | 65,73,73 | 1.44 | 8 (12%) | 76,113,113 | 1.39 | 6 (7%) |
| 23 | CHL | BU | 605 | 22 | 63,71,74 | 1.82 | 14 (22%) | 68,109,114 | 2.47 | 24 (35%) |
| 24 | CLA | b | 608 | - | 65,73,73 | 1.45 | 7 (10%) | 76,113,113 | 1.40 | 7 (9%) |
| 24 | CLA | BU | 608 | 22 | 58,66,73 | 1.55 | 10 (17%) | 67,104,113 | 1.49 | 7 (10%) |
| 23 | CHL | BB | 306 | 8 | 48,56,74 | 2.22 | 15 (31%) | 51,92,114 | 2.65 | 20 (39%) |
| 24 | CLA | C | 502 | 21 | 65,73,73 | 1.46 | 8 (12%) | 76,113,113 | 1.35 | 6 (7%) |
| 28 | XAT | 7 | 318 | - | 39,47,47 | 6.13 | 21 (53%) | 54,74,74 | 7.80 | 34 (62%) |
| 23 | CHL | 9 | 609 | - | 59,67,74 | 2.21 | 19 (32%) | 63,104,114 | 2.77 | 24 (38%) |
| 24 | CLA | AB | 303 | - | 45,53,73 | 1.71 | 8 (17%) | 52,89,113 | 1.62 | 6 (11%) |
| 24 | CLA | 6 | 613 | - | 58,66,73 | 1.57 | 10 (17%) | 67,104,113 | 1.55 | 9 (13%) |
| 30 | LMG | b | 621 | - | 51,51,55 | 0.72 | 0 | 59,59,63 | 1.39 | 7 (11%) |
| 24 | CLA | Au | 602 | 8 | 65,73,73 | 1.44 | 7 (10%) | 76,113,113 | 1.46 | 8 (10%) |
| 24 | CLA | s | 608 | - | 45,53,73 | 1.80 | 6 (13%) | 52,89,113 | 1.49 | 6 (11%) |
| 30 | LMG | C | 519 | - | 51,51,55 | 0.72 | 1 (1%) | 59,59,63 | 1.32 | 5 (8%) |
| 34 | DGD | BD | 413 | - | 61,61,67 | 0.90 | 2 (3%) | 75,75,81 | 1.41 | 8 (10%) |
| 24 | CLA | 0 | 602 | 2 | 60,68,73 | 1.45 | 10 (16%) | 70,107,113 | 1.43 | 8 (11%) |
| 23 | CHL | r | 606 | - | 53,61,74 | 2.14 | 15 (28%) | 57,98,114 | 2.65 | 23 (40%) |
| 34 | DGD | C | 517 | - | 63,63,67 | 0.88 | 2 (3%) | 77,77,81 | 1.44 | 8 (10%) |
| 23 | CHL | y | 306 | 8 | 48,56,74 | 2.26 | 16 (33%) | 51,92,114 | 2.69 | 19 (37%) |
| 24 | CLA | s | 609 | 14 | 55,63,73 | 1.58 | 7 (12%) | 64,101,113 | 1.55 | 8 (12%) |
| 23 | CHL | Ba | 308 | - | 63,71,74 | 1.94 | 14 (22%) | 68,109,114 | 2.48 | 22 (32%) |
| 24 | CLA | B | 615 | - | 65,73,73 | 1.46 | 8 (12%) | 76,113,113 | 1.38 | 7 (9%) |
| 29 | BCR | BI | 101 | - | 41,41,41 | 1.18 | 3 (7%) | 56,56,56 | 1.21 | 5 (8%) |
| 24 | CLA | b | 615 | - | 65,73,73 | 1.44 | 7 (10%) | 76,113,113 | 1.44 | 8 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 23 | CHL | Y | 306 | 8 | 48,56,74 | 2.22 | 15 (31%) | 51,92,114 | 2.66 | 20 (39%) |
| 23 | CHL | G | 601 | 8 | 63,71,74 | 1.91 | 15 (23%) | 68,109,114 | 2.53 | 24 (35%) |
| 24 | CLA | 2 | 402 | 5 | 65,73,73 | 1.43 | 8 (12%) | 76,113,113 | 1.43 | 10 (13%) |
| 24 | CLA | C | 503 | 21 | 65,73,73 | 1.45 | 8 (12%) | 76,113,113 | 1.41 | 7 (9%) |
| 23 | CHL | s | 605 | 14 | 46,54,74 | 2.30 | 16 (34%) | 49,90,114 | 2.78 | 21 (42%) |
| 24 | CLA | B | 604 | 4 | 65,73,73 | 1.43 | 8 (12%) | 76,113,113 | 1.42 | 8 (10%) |
| 24 | CLA | R | 405 | - | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.46 | 10 (13%) |
| 24 | CLA | v | 609 | 4 | 65,73,73 | 1.42 | 8 (12%) | 76,113,113 | 1.40 | 7 (9%) |
| 24 | CLA | BE | 603 | 4 | 65,73,73 | 1.47 | 7 (10%) | 76,113,113 | 1.40 | 6 (7%) |
| 23 | CHL | 7 | 307 | 1 | 46,54,74 | 2.28 | 16 (34%) | 49,90,114 | 2.73 | 19 (38%) |
| 28 | XAT | AA | 301 | - | 39,47,47 | 6.20 | 22 (56%) | 54,74,74 | 7.72 | 34 (62%) |
| 24 | CLA | BV | 608 | - | 45,53,73 | 1.80 | 6 (13%) | 52,89,113 | 1.50 | 6 (11%) |
| 24 | CLA | 1 | 507 | - | 65,73,73 | 1.44 | 10 (15%) | 76,113,113 | 1.38 | 6 (7%) |
| 25 | LUT | 6 | 615 | - | 42,43,43 | 1.59 | 9 (21%) | 51,60,60 | 1.39 | 10 (19%) |
| 24 | CLA | BE | 613 | - | 65,73,73 | 1.43 | 10 (15%) | 76,113,113 | 1.38 | 8 (10%) |
| 24 | CLA | n | 604 | - | 50,58,73 | 1.68 | 6 (12%) | 58,95,113 | 1.52 | 7 (12%) |
| 23 | CHL | BV | 605 | 14 | 46,54,74 | 2.29 | 16 (34%) | 49,90,114 | 2.77 | 21 (42%) |
| 24 | CLA | y | 313 | - | 60,68,73 | 1.53 | 7 (11%) | 70,107,113 | 1.44 | 8 (11%) |
| 24 | CLA | BD | 406 | - | 65,73,73 | 1.44 | 8 (12%) | 76,113,113 | 1.46 | 8 (10%) |
| 25 | LUT | 0 | 616 | - | 42,43,43 | 1.70 | 8 (19%) | 51,60,60 | 1.63 | 10 (19%) |
| 24 | CLA | BQ | 610 | 8 | 65,73,73 | 1.47 | 6 (9%) | 76,113,113 | 1.56 | 10 (13%) |
| 27 | LHG | Ba | 319 | 24 | 48,48,48 | 0.61 | 1 (2%) | 51,54,54 | 1.28 | 6 (11%) |
| 23 | CHL | g | 609 | - | 58,66,74 | 2.19 | 16 (27%) | 61,103,114 | 2.65 | 21 (34%) |
| 23 | CHL | n | 605 | 8 | 48,56,74 | 2.21 | 14 (29%) | 51,92,114 | 2.76 | 18 (35%) |
| 24 | CLA | 1 | 504 | 21 | 65,73,73 | 1.43 | 8 (12%) | 76,113,113 | 1.42 | 7 (9%) |
| 34 | DGD | 1 | 516 | - | 56,56,67 | 0.99 | 4 (7%) | 70,70,81 | 1.50 | 11 (15%) |
| 24 | CLA | BJ | 602 | 8 | 65,73,73 | 1.46 | 6 (9%) | 76,113,113 | 1.39 | 8 (10%) |
| 29 | BCR | z | 101 | - | 41,41,41 | 1.29 | 4 (9%) | 56,56,56 | 1.27 | 5 (8%) |
| 24 | CLA | BF | 504 | 21 | 65,73,73 | 1.44 | 10 (15%) | 76,113,113 | 1.43 | 8 (10%) |
| 29 | BCR | h | 101 | - | 41,41,41 | 1.17 | 2 (4%) | 56,56,56 | 1.34 | 8 (14%) |
| 24 | CLA | 9 | 603 | - | 55,63,73 | 1.58 | 9 (16%) | 64,101,113 | 1.40 | 9 (14%) |
| 24 | CLA | c | 507 | 21 | 65,73,73 | 1.47 | 10 (15%) | 76,113,113 | 1.39 | 8 (10%) |
| 23 | CHL | BB | 310 | - | 63,71,74 | 1.92 | 14 (22%) | 68,109,114 | 2.46 | 20 (29%) |
| 24 | CLA | r | 602 | 22 | 58,66,73 | 1.49 | 10 (17%) | 65,104,113 | 1.52 | 7 (10%) |
| 27 | LHG | BE | 623 | - | 45,45,48 | 0.68 | 1 (2%) | 48,51,54 | 1.25 | 4 (8%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 23 | CHL | Ba | 302 | 8 | 63,71,74 | 1.98 | 16 (25%) | 68,109,114 | 2.51 | 24 (35%) |
| 24 | CLA | c | 511 | 21 | 65,73,73 | 1.42 | 9 (13%) | 76,113,113 | 1.43 | 7 (9%) |
| 29 | BCR | v | 617 | - | 41,41,41 | 1.23 | 2 (4%) | 56,56,56 | 1.34 | 8 (14%) |
| 24 | CLA | g | 602 | 8 | 65,73,73 | 1.47 | 6 (9%) | 76,113,113 | 1.39 | 8 (10%) |
| 24 | CLA | B | 601 | - | 65,73,73 | 1.49 | 6 (9%) | 76,113,113 | 1.36 | 8 (10%) |
| 23 | CHL | N | 607 | - | 63,71,74 | 1.90 | 15 (23%) | 68,109,114 | 2.54 | 24 (35%) |
| 38 | PHO | a | 408 | - | 51,69,69 | 1.09 | 6 (11%) | 47,99,99 | 1.15 | 5 (10%) |
| 24 | CLA | 0 | 611 | 27 | 55,63,73 | 1.56 | 10 (18%) | 64,101,113 | 1.58 | 10 (15%) |
| 23 | CHL | g | 606 | - | 50,58,74 | 2.21 | 15 (30%) | 52,94,114 | 2.73 | 20 (38%) |
| 31 | PL9 | 2 | 404 | - | 55,55,55 | 1.68 | 10 (18%) | 68,69,69 | 1.52 | 13 (19%) |
| 30 | LMG | A | 412 | - | 48,48,55 | 0.75 | 0 | 56,56,63 | 1.32 | 5 (8%) |
| 23 | CHL | A6 | 605 | 14 | 46,54,74 | 2.21 | 16 (34%) | 49,90,114 | 2.90 | 18 (36%) |
| 25 | LUT | AA | 317 | - | 42,43,43 | 1.61 | 8 (19%) | 51,60,60 | 1.51 | 10 (19%) |
| 24 | CLA | 5 | 602 | 1 | 61,69,73 | 1.47 | 7 (11%) | 71,108,113 | 1.41 | 6 (8%) |
| 24 | CLA | r | 601 | 22 | 49,57,73 | 1.64 | 9 (18%) | 55,93,113 | 1.64 | 7 (12%) |
| 27 | LHG | 2 | 405 | - | 45,45,48 | 0.68 | 1 (2%) | 48,51,54 | 1.23 | 4 (8%) |
| 23 | CHL | BJ | 607 | - | 63,71,74 | 1.95 | 13 (20%) | 68,109,114 | 2.48 | 22 (32%) |
| 23 | CHL | Au | 606 | - | 50,58,74 | 2.16 | 15 (30%) | 52,94,114 | 2.73 | 21 (40%) |
| 34 | DGD | A | 402 | - | 60,60,67 | 0.93 | 2 (3%) | 74,74,81 | 1.38 | 8 (10%) |
| 24 | CLA | BQ | 612 | - | 60,68,73 | 1.52 | 6 (10%) | 70,107,113 | 1.48 | 8 (11%) |
| 26 | NEX | n | 617 | - | 38,46,46 | 1.62 | 7 (18%) | 50,70,70 | 1.60 | 9 (18%) |
| 24 | CLA | B | 612 | 4 | 65,73,73 | 1.44 | 10 (15%) | 76,113,113 | 1.41 | 8 (10%) |
| 24 | CLA | c | 513 | - | 65,73,73 | 1.43 | 10 (15%) | 76,113,113 | 1.41 | 8 (10%) |
| 28 | XAT | 5 | 619 | - | 39,47,47 | 6.02 | 19 (48%) | 54,74,74 | 7.65 | 35 (64%) |
| 24 | CLA | B | 605 | 4 | 65,73,73 | 1.46 | 9 (13%) | 76,113,113 | 1.37 | 8 (10%) |
| 23 | CHL | 6 | 608 | 2 | 46,54,74 | 2.27 | 15 (32%) | 49,90,114 | 2.81 | 20 (40%) |
| 23 | CHL | 8 | 305 | - | 46,54,74 | 2.28 | 15 (32%) | 49,90,114 | 2.74 | 17 (34%) |
| 24 | CLA | AB | 308 | - | 45,53,73 | 1.70 | 8 (17%) | 52,89,113 | 1.89 | 12 (23%) |
| 24 | CLA | R | 404 | 20 | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.40 | 8 (10%) |
| 28 | XAT | N | 619 | - | 39,47,47 | 6.10 | 20 (51%) | 54,74,74 | 7.74 | 35 (64%) |
| 24 | CLA | BV | 609 | 14 | 55,63,73 | 1.57 | 6 (10%) | 64,101,113 | 1.56 | 7 (10%) |
| 24 | CLA | 5 | 611 | 27 | 45,53,73 | 1.76 | 6 (13%) | 52,89,113 | 1.56 | 7 (13%) |
| 24 | CLA | v | 612 | 4 | 65,73,73 | 1.44 | 10 (15%) | 76,113,113 | 1.42 | 9 (11%) |
| 24 | CLA | 8 | 310 | - | 45,53,73 | 1.78 | 6 (13%) | 52,89,113 | 1.68 | 8 (15%) |
| 29 | BCR | v | 618 | - | 41,41,41 | 1.22 | 2 (4%) | 56,56,56 | 1.23 | 5 (8%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 35 | BCT | a | 402 | - | 2,3,3 | 1.31 | 0 | 2,3,3 | 4.15 | 1 (50%) |
| 23 | CHL | G | 607 | - | 63,71,74 | 1.91 | 15 (23%) | 68,109,114 | 2.49 | 22 (32%) |
| 24 | CLA | R | 406 | - | 50,58,73 | 1.64 | 9 (18%) | 58,95,113 | 1.61 | 9 (15%) |
| 25 | LUT | BB | 317 | - | 42,43,43 | 1.67 | 8 (19%) | 51,60,60 | 1.54 | 9 (17%) |
| 23 | CHL | 6 | 607 | - | 53,61,74 | 2.10 | 14 (26%) | 57,98,114 | 2.65 | 22 (38%) |
| 24 | CLA | Ba | 312 | 27 | 60,68,73 | 1.52 | 7 (11%) | 70,107,113 | 1.42 | 9 (12%) |
| 24 | CLA | AA | 313 | - | 45,53,73 | 1.75 | 6 (13%) | 52,89,113 | 1.64 | 7 (13%) |
| 34 | DGD | h | 102 | - | 63,63,67 | 0.89 | 2 (3%) | 77,77,81 | 1.40 | 9 (11%) |
| 27 | LHG | L | 102 | - | 48,48,48 | 0.66 | 1 (2%) | 51,54,54 | 1.28 | 7 (13%) |
| 25 | LUT | A6 | 615 | - | 42,43,43 | 1.62 | 8 (19%) | 51,60,60 | 1.75 | 14 (27%) |
| 24 | CLA | a | 407 | - | 50,58,73 | 1.64 | 7 (14%) | 58,95,113 | 1.61 | 8 (13%) |
| 24 | CLA | v | 616 | 4 | 65,73,73 | 1.46 | 7 (10%) | 76,113,113 | 1.43 | 8 (10%) |
| 24 | CLA | b | 613 | 4 | 65,73,73 | 1.43 | 8 (12%) | 76,113,113 | 1.38 | 8 (10%) |
| 24 | CLA | Ba | 311 | 8 | 60,68,73 | 1.54 | 7 (11%) | 70,107,113 | 1.45 | 10 (14%) |
| 36 | OEX | BD | 403 | 20 | 0,15,15 | - | - | - | - | - |
| 28 | XAT | r | 616 | - | 39,47,47 | 6.05 | 20 (51%) | 54,74,74 | 7.70 | 38 (70%) |
| 23 | CHL | Au | 609 | 8 | 56,64,74 | 1.92 | 14 (25%) | 56,100,114 | 2.61 | 21 (37%) |
| 30 | LMG | c | 518 | - | 51,51,55 | 0.72 | 1 (1%) | 59,59,63 | 1.33 | 5 (8%) |
| 38 | PHO | BD | 408 | - | 51,69,69 | 1.10 | 6 (11%) | 47,99,99 | 1.16 | 5 (10%) |
| 27 | LHG | g | 618 | 24 | 48,48,48 | 0.63 | 1 (2%) | 51,54,54 | 1.27 | 6 (11%) |
| 24 | CLA | 9 | 611 | 27 | 45,53,73 | 1.76 | 6 (13%) | 52,89,113 | 1.57 | 7 (13%) |
| 29 | BCR | BF | 515 | - | 41,41,41 | 1.31 | 4 (9%) | 56,56,56 | 1.26 | 5 (8%) |
| 27 | LHG | 0 | 617 | 24 | 46,46,48 | 0.68 | 1 (2%) | 49,52,54 | 1.33 | 6 (12%) |
| 24 | CLA | y | 311 | 8 | 60,68,73 | 1.53 | 7 (11%) | 70,107,113 | 1.50 | 10 (14%) |
| 28 | XAT | g | 619 | - | 39,47,47 | 6.17 | 22 (56%) | 54,74,74 | 7.66 | 34 (62%) |
| 26 | NEX | A2 | 617 | - | 38,46,46 | 1.85 | 9 (23%) | 50,70,70 | 1.70 | 10 (20%) |
| 27 | LHG | N | 618 | 24 | 48,48,48 | 0.61 | 1 (2%) | 51,54,54 | 1.27 | 6 (11%) |
| 24 | CLA | c | 502 | 21 | 65,73,73 | 1.47 | 8 (12%) | 76,113,113 | 1.36 | 7 (9%) |
| 25 | LUT | A2 | 616 | - | 42,43,43 | 1.64 | 8 (19%) | 51,60,60 | 1.57 | 10 (19%) |
| 27 | LHG | b | 622 | - | 48,48,48 | 0.62 | 1 (2%) | 51,54,54 | 1.27 | 6 (11%) |
| 24 | CLA | G | 610 | 8 | 64,72,73 | 1.43 | 8 (12%) | 74,111,113 | 1.43 | 8 (10%) |
| 24 | CLA | Au | 610 | 8 | 64,72,73 | 1.43 | 8 (12%) | 74,111,113 | 1.45 | 8 (10%) |
| 24 | CLA | A2 | 602 | 8 | 65,73,73 | 1.47 | 9 (13%) | 76,113,113 | 1.41 | 7 (9%) |
| 23 | CHL | e | 601 | - | 44,53,74 | 2.27 | 15 (34%) | 46,89,114 | 2.78 | 18 (39%) |
| 24 | CLA | BE | 606 | 4 | 65,73,73 | 1.48 | 7 (10%) | 76,113,113 | 1.36 | 8 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 29 | BCR | F | 101 | - | 41,41,41 | 1.20 | 3 (7%) | 56,56,56 | 1.21 | 5 (8%) |
| 23 | CHL | y | 308 | - | 63,71,74 | 1.94 | 14 (22%) | 68,109,114 | 2.48 | 21 (30%) |
| 23 | CHL | G | 608 | - | 63,71,74 | 1.94 | 16 (25%) | 68,109,114 | 2.45 | 22 (32%) |
| 24 | CLA | G | 612 | - | 60,68,73 | 1.52 | 7 (11%) | 70,107,113 | 1.39 | 7 (10%) |
| 29 | BCR | K | 102 | - | 41,41,41 | 1.25 | 3 (7%) | 56,56,56 | 1.30 | 8 (14%) |
| 23 | CHL | Y | 308 | - | 63,71,74 | 1.87 | 14 (22%) | 68,109,114 | 2.54 | 23 (33%) |
| 24 | CLA | 7 | 303 | 1 | 61,69,73 | 1.45 | 8 (13%) | 71,108,113 | 1.52 | 7 (9%) |
| 24 | CLA | b | 604 | 4 | 65,73,73 | 1.44 | 6 (9%) | 76,113,113 | 1.39 | 6 (7%) |
| 31 | PL9 | D | 403 | - | 55,55,55 | 1.80 | 9 (16%) | 68,69,69 | 1.49 | 11 (16%) |
| 25 | LUT | 9 | 616 | - | 42,43,43 | 1.66 | 8 (19%) | 51,60,60 | 1.65 | 11 (21%) |
| 24 | CLA | C | 512 | - | 65,73,73 | 1.43 | 8 (12%) | 76,113,113 | 1.42 | 8 (10%) |
| 28 | XAT | G | 619 | - | 39,47,47 | 6.18 | 22 (56%) | 54,74,74 | 7.66 | 34 (62%) |
| 24 | CLA | B | 606 | - | 65,73,73 | 1.49 | 8 (12%) | 76,113,113 | 1.39 | 7 (9%) |
| 24 | CLA | r | 609 | 22 | 65,73,73 | 1.43 | 10 (15%) | 76,113,113 | 1.42 | 6 (7%) |
| 24 | CLA | Y | 304 | 8 | 65,73,73 | 1.48 | 9 (13%) | 76,113,113 | 1.38 | 7 (9%) |
| 24 | CLA | 1 | 505 | - | 65,73,73 | 1.43 | 7 (10%) | 76,113,113 | 1.38 | 7 (9%) |
| 25 | LUT | Au | 615 | - | 42,43,43 | 1.65 | 8 (19%) | 51,60,60 | 1.65 | 11 (21%) |
| 24 | CLA | d | 401 | 5 | 65,73,73 | 1.41 | 8 (12%) | 76,113,113 | 1.43 | 9 (11%) |
| 23 | CHL | AA | 308 | - | 58,66,74 | 1.99 | 15 (25%) | 61,103,114 | 2.66 | 23 (37%) |
| 24 | CLA | B | 607 | - | 65,73,73 | 1.43 | 7 (10%) | 76,113,113 | 1.44 | 6 (7%) |
| 25 | LUT | G | 615 | - | 42,43,43 | 1.65 | 8 (19%) | 51,60,60 | 1.64 | 11 (21%) |
| 29 | BCR | B | 623 | - | 41,41,41 | 1.16 | 2 (4%) | 56,56,56 | 1.22 | 5 (8%) |
| 25 | LUT | 8 | 311 | - | 42,43,43 | 1.59 | 8 (19%) | 51,60,60 | 1.41 | 9 (17%) |
| 23 | CHL | N | 606 | 8 | 50,58,74 | 2.16 | 15 (30%) | 52,94,114 | 2.72 | 20 (38%) |
| 23 | CHL | g | 605 | 8 | 46,54,74 | 2.29 | 15 (32%) | 49,90,114 | 2.84 | 20 (40%) |
| 24 | CLA | 9 | 602 | 1 | 61,69,73 | 1.48 | 9 (14%) | 71,108,113 | 1.40 | 7 (9%) |
| 23 | CHL | BQ | 606 | 8 | 50,58,74 | 2.22 | 16 (32%) | 52,94,114 | 2.71 | 21 (40%) |
| 24 | CLA | 7 | 312 | - | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.61 | 7 (13%) |
| 29 | BCR | BE | 620 | - | 41,41,41 | 1.18 | 2 (4%) | 56,56,56 | 1.22 | 4 (7%) |
| 30 | LMG | c | 501 | - | 51,51,55 | 0.73 | 0 | 59,59,63 | 1.34 | 6 (10%) |
| 24 | CLA | BE | 617 | 4 | 65,73,73 | 1.45 | 7 (10%) | 76,113,113 | 1.40 | 7 (9%) |
| 23 | CHL | A2 | 607 | - | 63,71,74 | 1.90 | 15 (23%) | 68,109,114 | 2.56 | 25 (36%) |
| 24 | CLA | S | 613 | 14 | 49,57,73 | 1.67 | 7 (14%) | 55,93,113 | 1.58 | 9 (16%) |
| 27 | LHG | 1 | 521 | - | 48,48,48 | 0.61 | 0 | 51,54,54 | 1.27 | 6 (11%) |
| 25 | LUT | BQ | 616 | - | 42,43,43 | 1.66 | 8 (19%) | 51,60,60 | 1.52 | 11 (21%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 27 | LHG | Az | 102 | - | 48,48,48 | 0.67 | 1 (2%) | 51,54,54 | 1.29 | 7 (13%) |
| 24 | CLA | BU | 614 | - | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.64 | 8 (15%) |
| 23 | CHL | BJ | 606 | - | 50,58,74 | 2.20 | 15 (30%) | 52,94,114 | 2.72 | 22 (42%) |
| 23 | CHL | BQ | 609 | - | 63,71,74 | 1.99 | 16 (25%) | 68,109,114 | 2.42 | 23 (33%) |
| 23 | CHL | 5 | 609 | - | 59,67,74 | 2.17 | 17 (28%) | 63,104,114 | 2.73 | 24 (38%) |
| 24 | CLA | Ba | 314 | 8 | 65,73,73 | 1.49 | 7 (10%) | 76,113,113 | 1.37 | 7 (9%) |
| 29 | BCR | 1 | 515 | - | 41,41,41 | 1.35 | 4 (9%) | 56,56,56 | 1.28 | 6 (10%) |
| 23 | CHL | S | 606 | - | 55,63,74 | 2.06 | 16 (29%) | 57,99,114 | 2.78 | 22 (38%) |
| 33 | HEM | f | 102 | 7,6 | 41,50,50 | 1.46 | 4 (9%) | 45,82,82 | 1.24 | 3 (6%) |
| 23 | CHL | 0 | 608 | 2 | 46,54,74 | 2.26 | 15 (32%) | 49,90,114 | 2.82 | 19 (38%) |
| 23 | CHL | BH | 601 | - | 44,53,74 | 2.27 | 15 (34%) | 46,89,114 | 2.79 | 18 (39%) |
| 24 | CLA | 0 | 612 | - | 45,53,73 | 1.71 | 8 (17%) | 52,89,113 | 1.61 | 7 (13%) |
| 25 | LUT | r | 615 | - | 42,43,43 | 1.60 | 8 (19%) | 51,60,60 | 1.55 | 11 (21%) |
| 34 | DGD | a | 413 | - | 61,61,67 | 0.90 | 2 (3%) | 75,75,81 | 1.41 | 9 (12%) |
| 24 | CLA | 8 | 308 | - | 45,53,73 | 1.68 | 9 (20%) | 52,89,113 | 1.95 | 14 (26%) |
| 29 | BCR | BE | 618 | - | 41,41,41 | 1.16 | 2 (4%) | 56,56,56 | 1.41 | 10 (17%) |
| 32 | SQD | A1 | 101 | - | 53,54,54 | 1.52 | 7 (13%) | 62,65,65 | 1.37 | 6 (9%) |
| 30 | LMG | BL | 101 | - | 48,48,55 | 0.74 | 1 (2%) | 56,56,63 | 1.32 | 6 (10%) |
| 24 | CLA | BF | 508 | - | 65,73,73 | 1.44 | 11 (16%) | 76,113,113 | 1.36 | 7 (9%) |
| 24 | CLA | b | 614 | - | 65,73,73 | 1.44 | 9 (13%) | 76,113,113 | 1.40 | 6 (7%) |
| 25 | LUT | g | 615 | - | 42,43,43 | 1.61 | 8 (19%) | 51,60,60 | 1.52 | 9 (17%) |
| 33 | HEM | F | 102 | 7 | 41,50,50 | 1.46 | 5 (12%) | 45,82,82 | 1.29 | 4 (8%) |
| 27 | LHG | r | 618 | 24 | 41,41,48 | 0.72 | 1 (2%) | 44,47,54 | 1.34 | 7 (15%) |
| 32 | SQD | l | 102 | - | 41,42,54 | 1.63 | 7 (17%) | 50,53,65 | 1.45 | 7 (14%) |
| 29 | BCR | Ay | 101 | - | 41,41,41 | 1.17 | 2 (4%) | 56,56,56 | 1.29 | 7 (12%) |
| 24 | CLA | c | 504 | 21 | 65,73,73 | 1.46 | 10 (15%) | 76,113,113 | 1.41 | 8 (10%) |
| 23 | CHL | 5 | 606 | 1 | 46,54,74 | 2.23 | 14 (30%) | 49,90,114 | 2.91 | 20 (40%) |
| 23 | CHL | s | 601 | - | 46,54,74 | 2.31 | 16 (34%) | 49,90,114 | 2.75 | 18 (36%) |
| 24 | CLA | G | 603 | 8 | 65,73,73 | 1.44 | 8 (12%) | 76,113,113 | 1.40 | 9 (11%) |
| 24 | CLA | Au | 603 | 8 | 65,73,73 | 1.44 | 8 (12%) | 76,113,113 | 1.37 | 6 (7%) |
| 27 | LHG | 9 | 618 | 24 | 40,40,48 | 0.63 | 0 | 43,46,54 | 1.30 | 6 (13%) |
| 32 | SQD | a | 412 | - | 53,54,54 | 1.53 | 7 (13%) | 62,65,65 | 1.34 | 6 (9%) |
| 23 | CHL | n | 601 | 8 | 63,71,74 | 2.00 | 15 (23%) | 68,109,114 | 2.43 | 21 (30%) |
| 24 | CLA | C | 507 | - | 65,73,73 | 1.44 | 10 (15%) | 76,113,113 | 1.37 | 6 (7%) |
| 24 | CLA | N | 612 | - | 60,68,73 | 1.49 | 7 (11%) | 70,107,113 | 1.48 | 6 (8%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | CLA | BQ | 613 | - | 60,68,73 | 1.55 | 7 (11%) | 70,107,113 | 1.41 | 8 (11%) |
| 24 | CLA | G | 614 | - | 48,56,73 | 1.68 | 6 (12%) | 55,92,113 | 1.58 | 8 (14%) |
| 25 | LUT | 7 | 316 | - | 42,43,43 | 1.68 | 8 (19%) | 51,60,60 | 1.59 | 7 (13%) |
| 23 | CHL | BJ | 605 | 8 | 46,54,74 | 2.29 | 15 (32%) | 49,90,114 | 2.84 | 20 (40%) |
| 26 | NEX | A6 | 616 | - | 38,46,46 | 1.63 | 7 (18%) | 50,70,70 | 1.64 | 9 (18%) |
| 24 | CLA | s | 604 | - | 50,58,73 | 1.74 | 9 (18%) | 58,95,113 | 1.50 | 6 (10%) |
| 24 | CLA | D | 401 | 5 | 65,73,73 | 1.43 | 8 (12%) | 76,113,113 | 1.42 | 9 (11%) |
| 27 | LHG | y | 319 | 24 | 48,48,48 | 0.61 | 1 (2%) | 51,54,54 | 1.28 | 6 (11%) |
| 24 | CLA | v | 603 | 4 | 65,73,73 | 1.43 | 8 (12%) | 76,113,113 | 1.38 | 7 (9%) |
| 24 | CLA | Aw | 102 | - | 65,73,73 | 1.43 | 10 (15%) | 76,113,113 | 1.48 | 9 (11%) |
| 27 | LHG | W | 201 | - | 48,48,48 | 0.60 | 0 | 51,54,54 | 1.26 | 6 (11%) |
| 25 | LUT | 7 | 317 | - | 42,43,43 | 1.64 | 8 (19%) | 51,60,60 | 1.50 | 9 (17%) |
| 38 | PHO | R | 408 | - | 51,69,69 | 1.06 | 6 (11%) | 47,99,99 | 1.15 | 4 (8%) |
| 24 | CLA | b | 611 | - | 65,73,73 | 1.48 | 9 (13%) | 76,113,113 | 1.71 | 12 (15%) |
| 24 | CLA | v | 614 | - | 65,73,73 | 1.44 | 7 (10%) | 76,113,113 | 1.46 | 8 (10%) |
| 24 | CLA | AA | 303 | 1 | 61,69,73 | 1.44 | 8 (13%) | 71,108,113 | 1.53 | 9 (12%) |
| 24 | CLA | A6 | 609 | 14 | 53,61,73 | 1.62 | 9 (16%) | 59,98,113 | 1.47 | 7 (11%) |
| 23 | CHL | N | 609 | 8 | 63,71,74 | 1.92 | 14 (22%) | 68,109,114 | 2.44 | 19 (27%) |
| 23 | CHL | n | 607 | - | 63,71,74 | 1.96 | 14 (22%) | 68,109,114 | 2.49 | 22 (32%) |
| 23 | CHL | Au | 608 | - | 63,71,74 | 1.93 | 16 (25%) | 68,109,114 | 2.47 | 22 (32%) |
| 24 | CLA | Au | 612 | - | 60,68,73 | 1.51 | 7 (11%) | 70,107,113 | 1.42 | 7 (10%) |
| 24 | CLA | I | 102 | - | 65,73,73 | 1.42 | 10 (15%) | 76,113,113 | 1.47 | 8 (10%) |
| 27 | LHG | c | 519 | - | 48,48,48 | 0.55 | 0 | 51,54,54 | 1.26 | 6 (11%) |
| 29 | BCR | z | 102 | - | 41,41,41 | 1.27 | 3 (7%) | 56,56,56 | 1.32 | 8 (14%) |
| 25 | LUT | 0 | 615 | - | 42,43,43 | 1.69 | 8 (19%) | 51,60,60 | 1.48 | 10 (19%) |
| 24 | CLA | BU | 611 | 22 | 49,57,73 | 1.65 | 9 (18%) | 55,93,113 | 1.54 | 6 (10%) |
| 36 | OEX | a | 403 | 20 | 0,15,15 | - | - | - | - | - |
| 24 | CLA | BJ | 610 | 8 | 64,72,73 | 1.49 | 5 (7%) | 74,111,113 | 1.38 | 9 (12%) |
| 23 | CHL | S | 605 | 14 | 46,54,74 | 2.22 | 15 (32%) | 49,90,114 | 2.91 | 18 (36%) |
| 29 | BCR | 1 | 514 | - | 41,41,41 | 1.28 | 4 (9%) | 56,56,56 | 1.22 | 6 (10%) |
| 24 | CLA | 1 | 508 | 21 | 65,73,73 | 1.42 | 10 (15%) | 76,113,113 | 1.43 | 6 (7%) |
| 23 | CHL | G | 609 | - | 56,64,74 | 2.08 | 16 (28%) | 56,100,114 | 2.56 | 21 (37%) |
| 24 | CLA | C | 511 | 21 | 65,73,73 | 1.46 | 9 (13%) | 76,113,113 | 1.41 | 12 (15%) |
| 23 | CHL | s | 607 | - | 46,54,74 | 2.38 | 15 (32%) | 49,90,114 | 2.74 | 20 (40%) |
| 30 | LMG | 1 | 501 | - | 51,51,55 | 0.74 | 0 | 59,59,63 | 1.35 | 6 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | CLA | B | 608 | 4 | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.42 | 6 (7%) |
| 24 | CLA | Y | 315 | - | 48,56,73 | 1.68 | 8 (16%) | 55,92,113 | 1.63 | 7 (12%) |
| 25 | LUT | 5 | 615 | - | 42,43,43 | 1.70 | 8 (19%) | 51,60,60 | 1.68 | 12 (23%) |
| 24 | CLA | S | 604 | - | 50,58,73 | 1.66 | 7 (14%) | 58,95,113 | 1.56 | 7 (12%) |
| 23 | CHL | Ba | 309 | - | 63,71,74 | 2.01 | 16 (25%) | 68,109,114 | 2.47 | 22 (32%) |
| 24 | CLA | Au | 613 | - | 65,73,73 | 1.44 | 7 (10%) | 76,113,113 | 1.42 | 6 (7%) |
| 23 | CHL | A2 | 606 | 8 | 50,58,74 | 2.15 | 14 (28%) | 52,94,114 | 2.74 | 20 (38%) |
| 23 | CHL | A6 | 607 | 14 | 46,54,74 | 2.38 | 16 (34%) | 49,90,114 | 3.07 | 16 (32%) |
| 24 | CLA | 0 | 613 | - | 58,66,73 | 1.55 | 10 (17%) | 67,104,113 | 1.57 | 9 (13%) |
| 30 | LMG | Aw | 101 | - | 40,40,55 | 0.81 | 0 | 48,48,63 | 1.34 | 7 (14%) |
| 25 | LUT | A2 | 615 | - | 42,43,43 | 1.67 | 8 (19%) | 51,60,60 | 1.53 | 10 (19%) |
| 24 | CLA | BB | 311 | 8 | 60,68,73 | 1.48 | 9 (15%) | 70,107,113 | 1.47 | 7 (10%) |
| 24 | CLA | v | 611 | 4 | 65,73,73 | 1.45 | 7 (10%) | 76,113,113 | 1.51 | 8 (10%) |
| 24 | CLA | BU | 610 | 27 | 49,57,73 | 1.61 | 8 (16%) | 55,93,113 | 1.57 | 7 (12%) |
| 24 | CLA | BV | 603 | 14 | 45,53,73 | 1.78 | 6 (13%) | 52,89,113 | 1.57 | 7 (13%) |
| 25 | LUT | AB | 311 | - | 42,43,43 | 1.64 | 8 (19%) | 51,60,60 | 1.61 | 10 (19%) |
| 29 | BCR | f | 101 | - | 41,41,41 | 1.17 | 3 (7%) | 56,56,56 | 1.22 | 5 (8%) |
| 23 | CHL | BQ | 607 | - | 63,71,74 | 1.95 | 14 (22%) | 68,109,114 | 2.49 | 22 (32%) |
| 26 | NEX | BV | 616 | - | 38,46,46 | 1.61 | 7 (18%) | 50,70,70 | 1.61 | 9 (18%) |
| 24 | CLA | G | 611 | 27 | 60,68,73 | 1.52 | 7 (11%) | 70,107,113 | 1.47 | 10 (14%) |
| 25 | LUT | 9 | 615 | - | 42,43,43 | 1.66 | 8 (19%) | 51,60,60 | 1.69 | 9 (17%) |
| 38 | PHO | R | 407 | - | 51,69,69 | 1.12 | 6 (11%) | 47,99,99 | 1.14 | 5 (10%) |
| 25 | LUT | G | 616 | - | 42,43,43 | 1.63 | 8 (19%) | 51,60,60 | 1.53 | 10 (19%) |
| 23 | CHL | BV | 607 | - | 46,54,74 | 2.38 | 15 (32%) | 49,90,114 | 2.74 | 20 (40%) |
| 24 | CLA | BE | 609 | 4 | 65,73,73 | 1.45 | 7 (10%) | 76,113,113 | 1.56 | 8 (10%) |
| 24 | CLA | 6 | 604 | - | 45,53,73 | 1.72 | 8 (17%) | 52,89,113 | 1.80 | 12 (23%) |
| 24 | CLA | N | 614 | - | 48,56,73 | 1.75 | 6 (12%) | 55,92,113 | 1.61 | 7 (12%) |
| 23 | CHL | 9 | 606 | 1 | 46,54,74 | 2.24 | 14 (30%) | 49,90,114 | 2.88 | 21 (42%) |
| 27 | LHG | BG | 404 | - | 48,48,48 | 0.67 | 1 (2%) | 51,54,54 | 1.26 | 6 (11%) |
| 24 | CLA | AB | 309 | - | 45,53,73 | 1.77 | 5 (11%) | 52,89,113 | 1.56 | 7 (13%) |
| 24 | CLA | r | 603 | 22 | 60,68,73 | 1.50 | 9 (15%) | 70,107,113 | 1.39 | 6 (8%) |
| 24 | CLA | 0 | 603 | - | 55,63,73 | 1.58 | 8 (14%) | 64,101,113 | 1.47 | 7 (10%) |
| 24 | CLA | c | 510 | 21 | 65,73,73 | 1.45 | 10 (15%) | 76,113,113 | 1.41 | 7 (9%) |
| 34 | DGD | BD | 401 | - | 60,60,67 | 0.94 | 2 (3%) | 74,74,81 | 1.38 | 6 (8%) |
| 24 | CLA | BJ | 614 | 8 | 48,56,73 | 1.71 | 5 (10%) | 55,92,113 | 1.59 | 6 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | CLA | B | 609 | - | 65,73,73 | 1.41 | 9 (13%) | 76,113,113 | 1.40 | 7 (9%) |
| 28 | XAT | 7 | 301 | - | 39,47,47 | 6.21 | 21 (53%) | 54,74,74 | 7.69 | 34 (62%) |
| 29 | BCR | R | 410 | - | 41,41,41 | 1.29 | 3 (7%) | 56,56,56 | 1.25 | 5 (8%) |
| 24 | CLA | v | 615 | - | 65,73,73 | 1.45 | 8 (12%) | 76,113,113 | 1.38 | 7 (9%) |
| 30 | LMG | BG | 405 | - | 46,46,55 | 0.78 | 1 (2%) | 54,54,63 | 1.34 | 5 (9%) |
| 34 | DGD | C | 518 | - | 61,61,67 | 0.90 | 2 (3%) | 75,75,81 | 1.40 | 10 (13%) |
| 23 | CHL | y | 310 | - | 63,71,74 | 2.09 | 16 (25%) | 68,109,114 | 2.48 | 23 (33%) |
| 24 | CLA | A2 | 610 | - | 65,73,73 | 1.44 | 7 (10%) | 76,113,113 | 1.48 | 9 (11%) |
| 23 | CHL | 7 | 302 | 1 | 46,54,74 | 2.37 | 16 (34%) | 49,90,114 | 2.84 | 19 (38%) |
| 24 | CLA | G | 602 | 8 | 65,73,73 | 1.42 | 7 (10%) | 76,113,113 | 1.46 | 8 (10%) |
| 24 | CLA | c | 509 | 21 | 65,73,73 | 1.43 | 9 (13%) | 76,113,113 | 1.42 | 7 (9%) |
| 24 | CLA | BU | 612 | 22 | 36,44,73 | 1.83 | 11 (30%) | 40,76,113 | 1.66 | 6 (15%) |
| 24 | CLA | S | 602 | 14 | 61,69,73 | 1.49 | 6 (9%) | 71,108,113 | 1.46 | 7 (9%) |
| 25 | LUT | g | 616 | - | 42,43,43 | 1.65 | 7 (16%) | 51,60,60 | 1.59 | 10 (19%) |
| 28 | XAT | y | 301 | - | 39,47,47 | 6.11 | 22 (56%) | 54,74,74 | 7.77 | 34 (62%) |
| 24 | CLA | 1 | 511 | 21 | 65,73,73 | 1.46 | 9 (13%) | 76,113,113 | 1.41 | 7 (9%) |
| 34 | DGD | 1 | 518 | - | 61,61,67 | 0.90 | 2 (3%) | 75,75,81 | 1.40 | 10 (13%) |
| 26 | NEX | Y | 318 | - | 38,46,46 | 1.63 | 7 (18%) | 50,70,70 | 1.62 | 9 (18%) |
| 24 | CLA | BE | 614 | - | 65,73,73 | 1.44 | 10 (15%) | 76,113,113 | 1.41 | 6 (7%) |
| 23 | CHL | BJ | 601 | 8 | 63,71,74 | 1.94 | 14 (22%) | 68,109,114 | 2.55 | 23 (33%) |
| 24 | CLA | 6 | 603 | - | 55,63,73 | 1.57 | 8 (14%) | 64,101,113 | 1.48 | 7 (10%) |
| 24 | CLA | BF | 510 | 21 | 65,73,73 | 1.47 | 10 (15%) | 76,113,113 | 1.40 | 7 (9%) |
| 24 | CLA | A2 | 603 | 8 | 65,73,73 | 1.44 | 9 (13%) | 76,113,113 | 1.40 | 7 (9%) |
| 23 | CHL | 7 | 309 | - | 46,54,74 | 2.29 | 16 (34%) | 49,90,114 | 2.82 | 18 (36%) |
| 24 | CLA | BV | 610 | - | 56,64,73 | 1.58 | 7 (12%) | 65,102,113 | 1.58 | 9 (13%) |
| 24 | CLA | G | 613 | - | 65,73,73 | 1.44 | 7 (10%) | 76,113,113 | 1.42 | 6 (7%) |
| 26 | NEX | y | 318 | - | 38,46,46 | 1.65 | 7 (18%) | 50,70,70 | 1.62 | 9 (18%) |
| 27 | LHG | 6 | 617 | 24 | 46,46,48 | 0.66 | 1 (2%) | 49,52,54 | 1.32 | 6 (12%) |
| 29 | BCR | B | 619 | - | 41,41,41 | 1.17 | 2 (4%) | 56,56,56 | 1.17 | 5 (8%) |
| 24 | CLA | N | 611 | 27 | 60,68,73 | 1.51 | 7 (11%) | 70,107,113 | 1.44 | 8 (11%) |
| 24 | CLA | n | 610 | 8 | 65,73,73 | 1.41 | 5 (7%) | 76,113,113 | 1.56 | 10 (13%) |
| 24 | CLA | BQ | 611 | 27 | 60,68,73 | 1.55 | 5 (8%) | 70,107,113 | 1.45 | 7 (10%) |
| 24 | CLA | b | 610 | - | 65,73,73 | 1.45 | 7 (10%) | 76,113,113 | 1.43 | 7 (9%) |
| 32 | SQD | D | 406 | - | 49,50,54 | 1.57 | 7 (14%) | 58,61,65 | 1.45 | 7 (12%) |
| 30 | LMG | v | 623 | - | 40,40,55 | 0.85 | 1 (2%) | 48,48,63 | 1.30 | 5 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 35 | BCT | A | 401 | - | 2,3,3 | 1.30 | 0 | 2,3,3 | 4.03 | 1 (50%) |
| 29 | BCR | Ay | 102 | - | 41,41,41 | 1.25 | 4 (9%) | 56,56,56 | 1.30 | 8 (14%) |
| 30 | LMG | d | 405 | - | 46,46,55 | 0.77 | 1 (2%) | 54,54,63 | 1.34 | 5 (9%) |
| 24 | CLA | BJ | 611 | 27 | 60,68,73 | 1.54 | 5 (8%) | 70,107,113 | 1.44 | 8 (11%) |
| 23 | CHL | g | 608 | - | 63,71,74 | 1.94 | 15 (23%) | 68,109,114 | 2.55 | 24 (35%) |
| 23 | CHL | r | 607 | 22 | 58,66,74 | 1.98 | 14 (24%) | 61,103,114 | 2.62 | 22 (36%) |
| 29 | BCR | v | 619 | - | 41,41,41 | 1.18 | 2 (4%) | 56,56,56 | 1.23 | 6 (10%) |
| 32 | SQD | BO | 101 | - | 53,54,54 | 1.53 | 8 (15%) | 62,65,65 | 1.36 | 6 (9%) |
| 24 | CLA | b | 603 | 4 | 65,73,73 | 1.47 | 7 (10%) | 76,113,113 | 1.39 | 7 (9%) |
| 24 | CLA | a | 406 | - | 65,73,73 | 1.43 | 7 (10%) | 76,113,113 | 1.46 | 8 (10%) |
| 24 | CLA | s | 610 | - | 56,64,73 | 1.57 | 7 (12%) | 65,102,113 | 1.57 | 9 (13%) |
| 24 | CLA | C | 508 | 21 | 65,73,73 | 1.42 | 9 (13%) | 76,113,113 | 1.43 | 6 (7%) |
| 27 | LHG | C | 521 | - | 48,48,48 | 0.61 | 1 (2%) | 51,54,54 | 1.27 | 6 (11%) |
| 27 | LHG | B | 621 | - | 48,48,48 | 0.61 | 1 (2%) | 51,54,54 | 1.26 | 6 (11%) |
| 23 | CHL | A2 | 601 | 8 | 63,71,74 | 1.92 | 15 (23%) | 68,109,114 | 2.48 | 23 (33%) |
| 23 | CHL | AA | 307 | 1 | 46,54,74 | 2.28 | 16 (34%) | 49,90,114 | 2.72 | 19 (38%) |
| 24 | CLA | BF | 512 | 21 | 65,73,73 | 1.48 | 10 (15%) | 76,113,113 | 1.43 | 9 (11%) |
| 29 | BCR | 4 | 101 | - | 41,41,41 | 1.22 | 3 (7%) | 56,56,56 | 1.21 | 5 (8%) |
| 24 | CLA | N | 604 | - | 50,58,73 | 1.62 | 7 (14%) | 58,95,113 | 1.62 | 8 (13%) |
| 27 | LHG | b | 624 | - | 48,48,48 | 0.67 | 1 (2%) | 51,54,54 | 1.28 | 7 (13%) |
| 23 | CHL | AB | 307 | 3 | 46,54,74 | 2.33 | 16 (34%) | 49,90,114 | 2.78 | 19 (38%) |
| 24 | CLA | b | 607 | - | 65,73,73 | 1.49 | 8 (12%) | 76,113,113 | 1.35 | 7 (9%) |
| 23 | CHL | AB | 306 | - | 46,54,74 | 2.33 | 16 (34%) | 49,90,114 | 2.74 | 20 (40%) |
| 23 | CHL | Y | 302 | 8 | 63,71,74 | 1.91 | 15 (23%) | 68,109,114 | 2.54 | 24 (35%) |
| 23 | CHL | 0 | 607 | - | 53,61,74 | 2.11 | 14 (26%) | 57,98,114 | 2.64 | 23 (40%) |
| 24 | CLA | s | 603 | 14 | 45,53,73 | 1.79 | 6 (13%) | 52,89,113 | 1.58 | 7 (13%) |
| 24 | CLA | BF | 514 | - | 65,73,73 | 1.41 | 8 (12%) | 76,113,113 | 1.44 | 6 (7%) |
| 24 | CLA | A6 | 610 | - | 56,64,73 | 1.58 | 8 (14%) | 65,102,113 | 1.46 | 6 (9%) |
| 24 | CLA | BE | 611 | - | 65,73,73 | 1.47 | 9 (13%) | 76,113,113 | 1.42 | 9 (11%) |
| 23 | CHL | BV | 601 | - | 46,54,74 | 2.31 | 16 (34%) | 49,90,114 | 2.74 | 17 (34%) |
| 24 | CLA | n | 614 | - | 48,56,73 | 1.76 | 5 (10%) | 55,92,113 | 1.62 | 9 (16%) |
| 25 | LUT | BJ | 616 | - | 42,43,43 | 1.65 | 7 (16%) | 51,60,60 | 1.65 | 9 (17%) |
| 28 | XAT | BQ | 619 | - | 39,47,47 | 6.12 | 21 (53%) | 54,74,74 | 7.75 | 34 (62%) |
| 27 | LHG | b | 623 | - | 45,45,48 | 0.66 | 1 (2%) | 48,51,54 | 1.25 | 4 (8%) |
| 24 | CLA | Ba | 304 | - | 65,73,73 | 1.50 | 6 (9%) | 76,113,113 | 1.34 | 7 (9%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | CLA | 6 | 614 | 2 | 48,56,73 | 1.66 | 8 (16%) | 55,92,113 | 1.50 | 7 (12%) |
| 24 | CLA | b | 612 | 4 | 65,73,73 | 1.44 | 7 (10%) | 76,113,113 | 1.43 | 9 (11%) |
| 27 | LHG | BF | 520 | - | 48,48,48 | 0.55 | 0 | 51,54,54 | 1.27 | 6 (11%) |
| 25 | LUT | n | 616 | - | 42,43,43 | 1.62 | 8 (19%) | 51,60,60 | 1.53 | 11 (21%) |
| 25 | LUT | BU | 615 | - | 42,43,43 | 1.60 | 8 (19%) | 51,60,60 | 1.55 | 11 (21%) |
| 23 | CHL | 9 | 605 | 1 | 46,54,74 | 2.33 | 16 (34%) | 49,90,114 | 2.75 | 18 (36%) |
| 24 | CLA | 1 | 510 | 21 | 65,73,73 | 1.46 | 10 (15%) | 76,113,113 | 1.42 | 6 (7%) |
| 30 | LMG | BF | 519 | - | 51,51,55 | 0.71 | 1 (1%) | 59,59,63 | 1.33 | 4 (6%) |
| 24 | CLA | BV | 604 | - | 50,58,73 | 1.76 | 10 (20%) | 58,95,113 | 1.52 | 6 (10%) |
| 24 | CLA | BD | 410 | - | 60,68,73 | 1.48 | 7 (11%) | 70,107,113 | 1.50 | 8 (11%) |
| 25 | LUT | Y | 316 | - | 42,43,43 | 1.65 | 8 (19%) | 51,60,60 | 1.52 | 11 (21%) |
| 27 | LHG | 5 | 618 | 24 | 40,40,48 | 0.64 | 1 (2%) | 43,46,54 | 1.30 | 6 (13%) |
| 24 | CLA | s | 612 | 14 | 55,63,73 | 1.61 | 6 (10%) | 64,101,113 | 1.46 | 7 (10%) |
| 23 | CHL | BB | 307 | - | 50,58,74 | 2.06 | 13 (26%) | 52,94,114 | 2.87 | 20 (38%) |
| 35 | BCT | 2 | 401 | - | 2,3,3 | 1.31 | 0 | 2,3,3 | 3.99 | 1 (50%) |
| 27 | LHG | 2 | 406 | - | 48,48,48 | 0.65 | 1 (2%) | 51,54,54 | 1.27 | 5 (9%) |
| 36 | OEX | A | 403 | 20 | 0,15,15 | - | - | - | - | - |
| 26 | NEX | BB | 318 | - | 38,46,46 | 1.61 | 7 (18%) | 50,70,70 | 1.66 | 9 (18%) |
| 29 | BCR | b | 620 | - | 41,41,41 | 1.17 | 2 (4%) | 56,56,56 | 1.22 | 4 (7%) |
| 24 | CLA | BE | 608 | - | 65,73,73 | 1.45 | 7 (10%) | 76,113,113 | 1.41 | 7 (9%) |
| 23 | CHL | AB | 304 | 3 | 46,54,74 | 2.29 | 16 (34%) | 49,90,114 | 2.70 | 19 (38%) |
| 23 | CHL | A6 | 601 | 14 | 46,54,74 | 2.26 | 16 (34%) | 49,90,114 | 2.75 | 20 (40%) |
| 24 | CLA | AB | 301 | 3 | 42,49,73 | 1.77 | 7 (16%) | 48,83,113 | 1.67 | 8 (16%) |
| 34 | DGD | H | 102 | - | 63,63,67 | 0.90 | 2 (3%) | 77,77,81 | 1.38 | 7 (9%) |
| 23 | CHL | 7 | 306 | 1 | 46,54,74 | 2.41 | 15 (32%) | 49,90,114 | 2.72 | 18 (36%) |
| 24 | CLA | c | 512 | 21 | 65,73,73 | 1.48 | 9 (13%) | 76,113,113 | 1.47 | 8 (10%) |
| 23 | CHL | g | 607 | - | 63,71,74 | 1.96 | 13 (20%) | 68,109,114 | 2.47 | 22 (32%) |
| 23 | CHL | BU | 606 | - | 53,61,74 | 2.14 | 15 (28%) | 57,98,114 | 2.65 | 22 (38%) |
| 28 | XAT | BJ | 619 | - | 39,47,47 | 6.17 | 22 (56%) | 54,74,74 | 7.65 | 34 (62%) |
| 29 | BCR | a | 411 | - | 41,41,41 | 1.23 | 2 (4%) | 56,56,56 | 1.19 | 5 (8%) |
| 24 | CLA | G | 604 | - | 50,58,73 | 1.64 | 6 (12%) | 58,95,113 | 1.59 | 7 (12%) |
| 24 | CLA | A2 | 612 | - | 60,68,73 | 1.49 | 7 (11%) | 70,107,113 | 1.49 | 6 (8%) |
| 30 | LMG | BE | 621 | - | 51,51,55 | 0.72 | 1 (1%) | 59,59,63 | 1.40 | 8 (13%) |
| 24 | CLA | Y | 305 | - | 50,58,73 | 1.66 | 9 (18%) | 58,95,113 | 1.56 | 8 (13%) |
| 24 | CLA | n | 613 | - | 60,68,73 | 1.56 | 7 (11%) | 70,107,113 | 1.42 | 8 (11%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | CLA | BF | 507 | 21 | 65,73,73 | 1.48 | 10 (15%) | 76,113,113 | 1.39 | 8 (10%) |
| 29 | BCR | k | 101 | - | 41,41,41 | 1.19 | 2 (4%) | 56,56,56 | 1.24 | 6 (10%) |
| 29 | BCR | H | 101 | - | 41,41,41 | 1.18 | 2 (4%) | 56,56,56 | 1.29 | 9 (16%) |
| 23 | CHL | r | 605 | 22 | 63,71,74 | 1.82 | 13 (20%) | 68,109,114 | 2.48 | 23 (33%) |
| 24 | CLA | AB | 310 | - | 45,53,73 | 1.75 | 6 (13%) | 52,89,113 | 1.70 | 8 (15%) |
| 24 | CLA | B | 602 | 4 | 65,73,73 | 1.44 | 7 (10%) | 76,113,113 | 1.45 | 7 (9%) |
| 24 | CLA | C | 505 | - | 65,73,73 | 1.43 | 7 (10%) | 76,113,113 | 1.38 | 7 (9%) |
| 23 | CHL | AA | 302 | 1 | 46,54,74 | 2.38 | 15 (32%) | 49,90,114 | 2.85 | 19 (38%) |
| 23 | CHL | s | 606 | - | 55,63,74 | 2.07 | 15 (27%) | 57,99,114 | 2.80 | 22 (38%) |
| 23 | CHL | y | 302 | 8 | 63,71,74 | 1.99 | 16 (25%) | 68,109,114 | 2.53 | 23 (33%) |
| 24 | CLA | BV | 612 | 14 | 55,63,73 | 1.61 | 6 (10%) | 64,101,113 | 1.46 | 7 (10%) |
| 27 | LHG | c | 520 | - | 48,48,48 | 0.61 | 0 | 51,54,54 | 1.26 | 6 (11%) |
| 27 | LHG | l | 520 | - | 48,48,48 | 0.57 | 0 | 51,54,54 | 1.26 | 6 (11%) |
| 24 | CLA | A6 | 603 | - | 45,53,73 | 1.74 | 7 (15%) | 52,89,113 | 1.66 | 6 (11%) |
| 24 | CLA | AA | 315 | 1 | 45,53,73 | 1.77 | 6 (13%) | 52,89,113 | 1.60 | 6 (11%) |
| 23 | CHL | Ba | 307 | - | 50,58,74 | 2.20 | 16 (32%) | 52,94,114 | 2.73 | 20 (38%) |
| 25 | LUT | BQ | 615 | - | 42,43,43 | 1.68 | 8 (19%) | 51,60,60 | 1.51 | 9 (17%) |
| 27 | LHG | BF | 521 | - | 48,48,48 | 0.61 | 1 (2%) | 51,54,54 | 1.26 | 6 (11%) |
| 24 | CLA | b | 605 | 4 | 65,73,73 | 1.44 | 8 (12%) | 76,113,113 | 1.43 | 9 (11%) |
| 23 | CHL | n | 609 | - | 63,71,74 | 1.98 | 15 (23%) | 68,109,114 | 2.44 | 23 (33%) |
| 23 | CHL | G | 606 | - | 50,58,74 | 2.17 | 15 (30%) | 52,94,114 | 2.73 | 20 (38%) |
| 24 | CLA | A2 | 613 | 8 | 60,68,73 | 1.53 | 8 (13%) | 70,107,113 | 1.47 | 8 (11%) |
| 24 | CLA | 7 | 304 | - | 55,63,73 | 1.60 | 8 (14%) | 64,101,113 | 1.38 | 8 (12%) |
| 29 | BCR | c | 515 | - | 41,41,41 | 1.30 | 4 (9%) | 56,56,56 | 1.28 | 6 (10%) |
| 24 | CLA | y | 304 | - | 65,73,73 | 1.49 | 6 (9%) | 76,113,113 | 1.34 | 7 (9%) |
| 24 | CLA | r | 610 | 27 | 49,57,73 | 1.62 | 8 (16%) | 55,93,113 | 1.56 | 7 (12%) |
| 24 | CLA | Y | 312 | - | 60,68,73 | 1.52 | 9 (15%) | 70,107,113 | 1.46 | 10 (14%) |
| 24 | CLA | BU | 603 | 22 | 60,68,73 | 1.51 | 9 (15%) | 70,107,113 | 1.40 | 6 (8%) |
| 38 | PHO | a | 409 | - | 51,69,69 | 1.07 | 6 (11%) | 47,99,99 | 1.13 | 6 (12%) |
| 23 | CHL | BV | 606 | - | 55,63,74 | 2.07 | 14 (25%) | 57,99,114 | 2.80 | 22 (38%) |
| 24 | CLA | g | 610 | 8 | 64,72,73 | 1.49 | 6 (9%) | 74,111,113 | 1.38 | 9 (12%) |
| 24 | CLA | BV | 613 | 14 | 49,57,73 | 1.67 | 8 (16%) | 55,93,113 | 1.57 | 7 (12%) |
| 24 | CLA | Au | 604 | - | 50,58,73 | 1.64 | 6 (12%) | 58,95,113 | 1.58 | 7 (12%) |
| 24 | CLA | b | 606 | 4 | 65,73,73 | 1.47 | 7 (10%) | 76,113,113 | 1.36 | 8 (10%) |
| 28 | XAT | Ba | 301 | - | 39,47,47 | 6.12 | 22 (56%) | 54,74,74 | 7.78 | 34 (62%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 29 | BCR | C | 514 | - | 41,41,41 | 1.27 | 2 (4%) | 56,56,56 | 1.22 | 5 (8%) |
| 23 | CHL | r | 613 | 22 | 42,50,74 | 2.34 | 16 (38%) | 44,85,114 | 3.00 | 22 (50%) |
| 24 | CLA | S | 603 | - | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.65 | 6 (11%) |
| 24 | CLA | c | 505 | - | 65,73,73 | 1.46 | 7 (10%) | 76,113,113 | 1.38 | 7 (9%) |
| 23 | CHL | BB | 302 | 8 | 63,71,74 | 1.89 | 14 (22%) | 68,109,114 | 2.56 | 25 (36%) |
| 29 | BCR | b | 619 | - | 41,41,41 | 1.16 | 2 (4%) | 56,56,56 | 1.21 | 5 (8%) |
| 30 | LMG | v | 620 | - | 51,51,55 | 0.72 | 0 | 59,59,63 | 1.38 | 7 (11%) |
| 29 | BCR | BD | 411 | - | 41,41,41 | 1.25 | 2 (4%) | 56,56,56 | 1.20 | 5 (8%) |
| 24 | CLA | D | 402 | - | 65,73,73 | 1.46 | 6 (9%) | 76,113,113 | 1.38 | 7 (9%) |
| 24 | CLA | BG | 402 | - | 65,73,73 | 1.44 | 6 (9%) | 76,113,113 | 1.37 | 7 (9%) |
| 28 | XAT | 9 | 619 | - | 39,47,47 | 6.07 | 20 (51%) | 54,74,74 | 7.51 | 33 (61%) |
| 23 | CHL | 5 | 608 | - | 46,54,74 | 2.27 | 15 (32%) | 49,90,114 | 2.74 | 17 (34%) |
| 24 | CLA | s | 613 | 14 | 49,57,73 | 1.66 | 9 (18%) | 55,93,113 | 1.56 | 7 (12%) |
| 24 | CLA | Ba | 305 | - | 50,58,73 | 1.67 | 7 (14%) | 58,95,113 | 1.53 | 7 (12%) |
| 23 | CHL | N | 608 | - | 63,71,74 | 1.93 | 16 (25%) | 68,109,114 | 2.48 | 23 (33%) |
| 27 | LHG | A2 | 618 | 24 | 48,48,48 | 0.63 | 1 (2%) | 51,54,54 | 1.27 | 6 (11%) |
| 24 | CLA | BB | 312 | - | 60,68,73 | 1.52 | 9 (15%) | 70,107,113 | 1.47 | 10 (14%) |
| 24 | CLA | Y | 311 | 8 | 60,68,73 | 1.47 | 9 (15%) | 70,107,113 | 1.50 | 8 (11%) |
| 26 | NEX | 9 | 617 | - | 38,46,46 | 1.66 | 7 (18%) | 50,70,70 | 1.68 | 9 (18%) |
| 27 | LHG | BJ | 618 | 24 | 48,48,48 | 0.62 | 1 (2%) | 51,54,54 | 1.27 | 6 (11%) |
| 23 | CHL | Au | 607 | - | 63,71,74 | 1.90 | 15 (23%) | 68,109,114 | 2.51 | 23 (33%) |
| 24 | CLA | BQ | 602 | 8 | 65,73,73 | 1.48 | 6 (9%) | 76,113,113 | 1.34 | 6 (7%) |
| 24 | CLA | N | 602 | 8 | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.40 | 8 (10%) |
| 24 | CLA | b | 609 | 4 | 65,73,73 | 1.43 | 7 (10%) | 76,113,113 | 1.51 | 8 (10%) |
| 24 | CLA | r | 604 | - | 48,56,73 | 1.62 | 9 (18%) | 55,92,113 | 1.65 | 7 (12%) |
| 23 | CHL | Ba | 306 | 8 | 48,56,74 | 2.26 | 16 (33%) | 51,92,114 | 2.68 | 18 (35%) |
| 32 | SQD | R | 411 | - | 53,54,54 | 1.51 | 7 (13%) | 62,65,65 | 1.34 | 6 (9%) |
| 28 | XAT | A2 | 619 | - | 39,47,47 | 6.09 | 20 (51%) | 54,74,74 | 7.74 | 35 (64%) |
| 27 | LHG | n | 618 | 24 | 48,48,48 | 0.62 | 1 (2%) | 51,54,54 | 1.28 | 6 (11%) |
| 23 | CHL | g | 601 | 8 | 63,71,74 | 1.94 | 14 (22%) | 68,109,114 | 2.55 | 23 (33%) |
| 24 | CLA | Y | 313 | - | 60,68,73 | 1.51 | 9 (15%) | 70,107,113 | 1.43 | 7 (10%) |
| 30 | LMG | A0 | 201 | - | 48,48,55 | 0.75 | 0 | 56,56,63 | 1.32 | 6 (10%) |
| 24 | CLA | 8 | 303 | - | 45,53,73 | 1.71 | 8 (17%) | 52,89,113 | 1.63 | 6 (11%) |
| 34 | DGD | C | 516 | - | 56,56,67 | 0.96 | 2 (3%) | 70,70,81 | 1.49 | 10 (14%) |
| 24 | CLA | A | 407 | - | 50,58,73 | 1.64 | 8 (16%) | 58,95,113 | 1.61 | 10 (17%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | CLA | C | 509 | 21 | 65,73,73 | 1.45 | 10 (15%) | 76,113,113 | 1.42 | 8 (10%) |
| 25 | LUT | N | 615 | - | 42,43,43 | 1.68 | 8 (19%) | 51,60,60 | 1.53 | 9 (17%) |
| 23 | CHL | Y | 309 | - | 63,71,74 | 1.91 | 15 (23%) | 68,109,114 | 2.48 | 21 (30%) |
| 24 | CLA | BF | 503 | 21 | 65,73,73 | 1.46 | 9 (13%) | 76,113,113 | 1.41 | 7 (9%) |
| 27 | LHG | B | 622 | - | 45,45,48 | 0.66 | 1 (2%) | 48,51,54 | 1.23 | 4 (8%) |
| 25 | LUT | y | 316 | - | 42,43,43 | 1.62 | 8 (19%) | 51,60,60 | 1.47 | 10 (19%) |
| 23 | CHL | 8 | 304 | - | 46,54,74 | 2.30 | 16 (34%) | 49,90,114 | 2.69 | 19 (38%) |
| 27 | LHG | A0 | 202 | - | 48,48,48 | 0.59 | 0 | 51,54,54 | 1.27 | 6 (11%) |
| 24 | CLA | BG | 401 | 5 | 65,73,73 | 1.41 | 8 (12%) | 76,113,113 | 1.46 | 9 (11%) |
| 23 | CHL | 8 | 306 | - | 46,54,74 | 2.34 | 16 (34%) | 49,90,114 | 2.75 | 21 (42%) |
| 24 | CLA | g | 604 | - | 50,58,73 | 1.70 | 6 (12%) | 58,95,113 | 1.57 | 7 (12%) |
| 24 | CLA | BV | 602 | 14 | 61,69,73 | 1.53 | 6 (9%) | 71,108,113 | 1.41 | 7 (9%) |
| 25 | LUT | BJ | 615 | - | 42,43,43 | 1.61 | 8 (19%) | 51,60,60 | 1.52 | 9 (17%) |
| 26 | NEX | 7 | 319 | - | 38,46,46 | 1.65 | 7 (18%) | 50,70,70 | 1.70 | 10 (20%) |
| 26 | NEX | N | 617 | - | 38,46,46 | 1.57 | 7 (18%) | 50,70,70 | 1.59 | 9 (18%) |
| 24 | CLA | A | 406 | - | 65,73,73 | 1.46 | 9 (13%) | 76,113,113 | 1.47 | 10 (13%) |
| 29 | BCR | AB | 313 | - | 41,41,41 | 1.29 | 3 (7%) | 56,56,56 | 1.30 | 7 (12%) |
| 24 | CLA | BE | 612 | 4 | 65,73,73 | 1.45 | 8 (12%) | 76,113,113 | 1.45 | 8 (10%) |
| 23 | CHL | S | 607 | - | 46,54,74 | 2.25 | 15 (32%) | 49,90,114 | 3.06 | 19 (38%) |
| 29 | BCR | BE | 601 | - | 41,41,41 | 1.18 | 2 (4%) | 56,56,56 | 1.30 | 6 (10%) |
| 24 | CLA | 5 | 604 | - | 50,58,73 | 1.70 | 9 (18%) | 58,95,113 | 1.49 | 9 (15%) |
| 25 | LUT | n | 615 | - | 42,43,43 | 1.68 | 8 (19%) | 51,60,60 | 1.51 | 9 (17%) |
| 24 | CLA | BB | 315 | - | 48,56,73 | 1.68 | 8 (16%) | 55,92,113 | 1.63 | 7 (12%) |
| 24 | CLA | BD | 405 | 20 | 65,73,73 | 1.46 | 10 (15%) | 76,113,113 | 1.40 | 8 (10%) |
| 34 | DGD | Av | 102 | - | 63,63,67 | 0.91 | 2 (3%) | 77,77,81 | 1.38 | 9 (11%) |
| 25 | LUT | s | 614 | - | 42,43,43 | 1.64 | 8 (19%) | 51,60,60 | 1.46 | 11 (21%) |
| 26 | NEX | BB | 320 | - | 38,46,46 | 1.65 | 7 (18%) | 50,70,70 | 1.63 | 10 (20%) |
| 24 | CLA | AA | 311 | 1 | 48,56,73 | 1.74 | 10 (20%) | 53,92,113 | 1.53 | 8 (15%) |
| 24 | CLA | A2 | 614 | - | 48,56,73 | 1.75 | 6 (12%) | 55,92,113 | 1.60 | 7 (12%) |
| 24 | CLA | BB | 304 | 8 | 65,73,73 | 1.47 | 9 (13%) | 76,113,113 | 1.39 | 7 (9%) |
| 24 | CLA | Ba | 315 | - | 48,56,73 | 1.69 | 6 (12%) | 55,92,113 | 1.57 | 6 (10%) |
| 29 | BCR | B | 618 | - | 41,41,41 | 1.21 | 2 (4%) | 56,56,56 | 1.23 | 5 (8%) |
| 24 | CLA | BF | 502 | 21 | 65,73,73 | 1.48 | 9 (13%) | 76,113,113 | 1.36 | 7 (9%) |
| 23 | CHL | 6 | 605 | 2 | 46,54,74 | 2.34 | 16 (34%) | 49,90,114 | 2.77 | 19 (38%) |
| 23 | CHL | y | 307 | - | 50,58,74 | 2.21 | 16 (32%) | 52,94,114 | 2.73 | 20 (38%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | CLA | r | 614 | - | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.66 | 8 (15%) |
| 27 | LHG | BB | 319 | - | 48,48,48 | 0.67 | 1 (2%) | 51,54,54 | 1.27 | 6 (11%) |
| 26 | NEX | g | 617 | - | 38,46,46 | 1.65 | 6 (15%) | 50,70,70 | 1.68 | 9 (18%) |
| 24 | CLA | BF | 509 | 21 | 65,73,73 | 1.43 | 9 (13%) | 76,113,113 | 1.43 | 7 (9%) |
| 29 | BCR | Bb | 101 | - | 41,41,41 | 1.29 | 4 (9%) | 56,56,56 | 1.33 | 9 (16%) |
| 24 | CLA | r | 612 | 22 | 36,44,73 | 1.85 | 10 (27%) | 40,76,113 | 1.65 | 7 (17%) |
| 28 | XAT | AB | 312 | - | 39,47,47 | 6.08 | 19 (48%) | 54,74,74 | 7.74 | 36 (66%) |
| 24 | CLA | g | 614 | 8 | 48,56,73 | 1.71 | 5 (10%) | 55,92,113 | 1.59 | 6 (10%) |
| 24 | CLA | BJ | 613 | - | 65,73,73 | 1.50 | 5 (7%) | 76,113,113 | 1.40 | 8 (10%) |
| 26 | NEX | 5 | 617 | - | 38,46,46 | 1.66 | 7 (18%) | 50,70,70 | 1.67 | 9 (18%) |
| 24 | CLA | AA | 314 | 1 | 45,53,73 | 1.72 | 7 (15%) | 52,89,113 | 1.61 | 6 (11%) |
| 27 | LHG | Au | 618 | 24 | 48,48,48 | 0.60 | 0 | 51,54,54 | 1.27 | 6 (11%) |
| 32 | SQD | BD | 412 | - | 53,54,54 | 1.52 | 7 (13%) | 62,65,65 | 1.35 | 6 (9%) |
| 25 | LUT | BV | 614 | - | 42,43,43 | 1.66 | 8 (19%) | 51,60,60 | 1.47 | 10 (19%) |
| 23 | CHL | 5 | 607 | - | 60,68,74 | 1.97 | 15 (25%) | 64,105,114 | 2.49 | 23 (35%) |
| 24 | CLA | Y | 314 | 8 | 65,73,73 | 1.44 | 10 (15%) | 76,113,113 | 1.42 | 6 (7%) |
| 24 | CLA | BE | 615 | - | 65,73,73 | 1.44 | 7 (10%) | 76,113,113 | 1.45 | 8 (10%) |
| 24 | CLA | 7 | 305 | - | 45,53,73 | 1.75 | 6 (13%) | 52,89,113 | 1.56 | 7 (13%) |
| 24 | CLA | R | 409 | - | 60,68,73 | 1.47 | 8 (13%) | 70,107,113 | 1.50 | 7 (10%) |
| 23 | CHL | 0 | 601 | 2 | 61,69,74 | 2.01 | 16 (26%) | 65,106,114 | 2.52 | 23 (35%) |
| 26 | NEX | Ba | 318 | - | 38,46,46 | 1.64 | 7 (18%) | 50,70,70 | 1.59 | 9 (18%) |
| 24 | CLA | v | 602 | 4 | 65,73,73 | 1.43 | 7 (10%) | 76,113,113 | 1.43 | 7 (9%) |
| 24 | CLA | A6 | 608 | - | 45,53,73 | 1.74 | 6 (13%) | 52,89,113 | 1.54 | 7 (13%) |
| 24 | CLA | BU | 602 | 22 | 58,66,73 | 1.50 | 10 (17%) | 65,104,113 | 1.51 | 7 (10%) |
| 27 | LHG | Y | 319 | - | 48,48,48 | 0.63 | 1 (2%) | 51,54,54 | 1.27 | 6 (11%) |
| 24 | CLA | S | 610 | - | 56,64,73 | 1.58 | 8 (14%) | 65,102,113 | 1.45 | 6 (9%) |
| 24 | CLA | S | 611 | - | 49,57,73 | 1.65 | 8 (16%) | 55,93,113 | 1.54 | 7 (12%) |
| 24 | CLA | BU | 604 | - | 48,56,73 | 1.61 | 9 (18%) | 55,92,113 | 1.70 | 9 (16%) |
| 38 | PHO | A | 409 | - | 51,69,69 | 1.05 | 5 (9%) | 47,99,99 | 1.14 | 4 (8%) |
| 23 | CHL | BJ | 609 | - | 58,66,74 | 2.19 | 17 (29%) | 61,103,114 | 2.65 | 21 (34%) |
| 24 | CLA | n | 612 | - | 60,68,73 | 1.52 | 6 (10%) | 70,107,113 | 1.49 | 8 (11%) |
| 24 | CLA | v | 606 | - | 65,73,73 | 1.49 | 8 (12%) | 76,113,113 | 1.41 | 8 (10%) |
| 24 | CLA | B | 610 | - | 65,73,73 | 1.46 | 7 (10%) | 76,113,113 | 1.42 | 8 (10%) |
| 25 | LUT | AA | 316 | - | 42,43,43 | 1.64 | 8 (19%) | 51,60,60 | 1.55 | 11 (21%) |
| 23 | CHL | 9 | 608 | - | 46,54,74 | 2.26 | 15 (32%) | 49,90,114 | 2.75 | 17 (34%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | CLA | A2 | 611 | 27 | 60,68,73 | 1.51 | 8 (13%) | 70,107,113 | 1.43 | 8 (11%) |
| 24 | CLA | C | 513 | 21 | 65,73,73 | 1.43 | 6 (9%) | 76,113,113 | 1.45 | 7 (9%) |
| 29 | BCR | b | 601 | - | 41,41,41 | 1.16 | 2 (4%) | 56,56,56 | 1.31 | 8 (14%) |
| 24 | CLA | BB | 303 | 8 | 65,73,73 | 1.41 | 9 (13%) | 76,113,113 | 1.47 | 7 (9%) |
| 27 | LHG | w | 201 | - | 48,48,48 | 0.62 | 1 (2%) | 51,54,54 | 1.25 | 6 (11%) |
| 23 | CHL | y | 309 | - | 63,71,74 | 2.08 | 16 (25%) | 68,109,114 | 2.47 | 23 (33%) |
| 24 | CLA | BJ | 603 | 8 | 65,73,73 | 1.48 | 6 (9%) | 76,113,113 | 1.37 | 6 (7%) |
| 27 | LHG | C | 520 | - | 48,48,48 | 0.58 | 0 | 51,54,54 | 1.25 | 6 (11%) |
| 26 | NEX | r | 617 | - | 38,46,46 | 1.61 | 7 (18%) | 50,70,70 | 1.62 | 9 (18%) |
| 24 | CLA | s | 602 | 14 | 61,69,73 | 1.53 | 6 (9%) | 71,108,113 | 1.43 | 7 (9%) |
| 25 | LUT | Y | 317 | - | 42,43,43 | 1.66 | 8 (19%) | 51,60,60 | 1.54 | 10 (19%) |
| 27 | LHG | BU | 617 | 24 | 41,41,48 | 0.74 | 1 (2%) | 44,47,54 | 1.35 | 7 (15%) |
| 23 | CHL | 6 | 609 | - | 58,66,74 | 2.17 | 19 (32%) | 61,103,114 | 2.79 | 21 (34%) |
| 24 | CLA | c | 506 | - | 65,73,73 | 1.45 | 8 (12%) | 76,113,113 | 1.47 | 8 (10%) |
| 23 | CHL | n | 608 | - | 63,71,74 | 1.99 | 16 (25%) | 68,109,114 | 2.44 | 23 (33%) |
| 24 | CLA | 9 | 613 | 1 | 55,63,73 | 1.54 | 7 (12%) | 64,101,113 | 1.53 | 7 (10%) |
| 34 | DGD | c | 516 | - | 56,56,67 | 0.97 | 2 (3%) | 70,70,81 | 1.50 | 12 (17%) |
| 28 | XAT | BU | 616 | - | 39,47,47 | 6.03 | 19 (48%) | 54,74,74 | 7.69 | 38 (70%) |
| 24 | CLA | 2 | 403 | - | 65,73,73 | 1.45 | 6 (9%) | 76,113,113 | 1.39 | 7 (9%) |
| 29 | BCR | A | 411 | - | 41,41,41 | 1.27 | 3 (7%) | 56,56,56 | 1.25 | 6 (10%) |
| 24 | CLA | Ba | 313 | - | 60,68,73 | 1.54 | 7 (11%) | 70,107,113 | 1.44 | 9 (12%) |
| 24 | CLA | BF | 506 | - | 65,73,73 | 1.45 | 8 (12%) | 76,113,113 | 1.49 | 8 (10%) |
| 28 | XAT | n | 619 | - | 39,47,47 | 6.12 | 21 (53%) | 54,74,74 | 7.74 | 34 (62%) |
| 24 | CLA | 8 | 302 | - | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.57 | 6 (11%) |
| 24 | CLA | 9 | 614 | 1 | 45,53,73 | 1.76 | 5 (11%) | 52,89,113 | 1.70 | 6 (11%) |
| 24 | CLA | 0 | 614 | 2 | 48,56,73 | 1.67 | 9 (18%) | 55,92,113 | 1.51 | 8 (14%) |
| 23 | CHL | A2 | 609 | 8 | 63,71,74 | 1.92 | 14 (22%) | 68,109,114 | 2.45 | 19 (27%) |
| 24 | CLA | S | 609 | 14 | 53,61,73 | 1.62 | 9 (16%) | 59,98,113 | 1.47 | 6 (10%) |
| 29 | BCR | BK | 101 | - | 41,41,41 | 1.18 | 2 (4%) | 56,56,56 | 1.32 | 9 (16%) |
| 24 | CLA | 7 | 313 | - | 45,53,73 | 1.74 | 6 (13%) | 52,89,113 | 1.61 | 6 (11%) |
| 24 | CLA | a | 405 | 20 | 65,73,73 | 1.46 | 9 (13%) | 76,113,113 | 1.37 | 7 (9%) |
| 30 | LMG | D | 405 | - | 46,46,55 | 0.77 | 1 (2%) | 54,54,63 | 1.35 | 5 (9%) |
| 24 | CLA | 5 | 603 | 1 | 55,63,73 | 1.59 | 9 (16%) | 64,101,113 | 1.40 | 9 (14%) |
| 24 | CLA | A6 | 612 | 14 | 55,63,73 | 1.57 | 8 (14%) | 64,101,113 | 1.52 | 7 (10%) |
| 24 | CLA | BU | 601 | 22 | 49,57,73 | 1.64 | 9 (18%) | 55,93,113 | 1.66 | 8 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 29 | BCR | BF | 516 | - | 41,41,41 | 1.37 | 3 (7%) | 56,56,56 | 1.31 | 8 (14%) |
| 24 | CLA | S | 608 | - | 45,53,73 | 1.73 | 6 (13%) | 52,89,113 | 1.53 | 6 (11%) |
| 24 | CLA | BF | 513 | - | 65,73,73 | 1.43 | 10 (15%) | 76,113,113 | 1.43 | 8 (10%) |
| 23 | CHL | N | 605 | 8 | 48,56,74 | 2.16 | 16 (33%) | 51,92,114 | 2.75 | 18 (35%) |
| 29 | BCR | v | 622 | - | 41,41,41 | 1.17 | 2 (4%) | 56,56,56 | 1.23 | 5 (8%) |
| 24 | CLA | s | 611 | - | 49,57,73 | 1.69 | 7 (14%) | 55,93,113 | 1.59 | 7 (12%) |
| 24 | CLA | v | 604 | 4 | 65,73,73 | 1.44 | 8 (12%) | 76,113,113 | 1.41 | 8 (10%) |
| 29 | BCR | Av | 101 | - | 41,41,41 | 1.19 | 2 (4%) | 56,56,56 | 1.30 | 9 (16%) |
| 24 | CLA | 9 | 604 | - | 50,58,73 | 1.71 | 10 (20%) | 58,95,113 | 1.49 | 8 (13%) |
| 24 | CLA | v | 610 | - | 65,73,73 | 1.45 | 8 (12%) | 76,113,113 | 1.40 | 8 (10%) |
| 30 | LMG | B | 624 | - | 40,40,55 | 0.84 | 1 (2%) | 48,48,63 | 1.31 | 5 (10%) |
| 23 | CHL | 9 | 601 | 1 | 46,54,74 | 2.27 | 15 (32%) | 49,90,114 | 2.88 | 18 (36%) |
| 24 | CLA | Y | 303 | 8 | 65,73,73 | 1.41 | 9 (13%) | 76,113,113 | 1.44 | 6 (7%) |
| 27 | LHG | BE | 624 | - | 48,48,48 | 0.66 | 1 (2%) | 51,54,54 | 1.28 | 7 (13%) |
| 30 | LMG | B | 620 | - | 51,51,55 | 0.72 | 0 | 59,59,63 | 1.37 | 7 (11%) |
| 34 | DGD | 1 | 517 | - | 63,63,67 | 0.90 | 2 (3%) | 77,77,81 | 1.44 | 8 (10%) |
| 29 | BCR | K | 101 | - | 41,41,41 | 1.20 | 3 (7%) | 56,56,56 | 1.34 | 5 (8%) |
| 27 | LHG | d | 404 | - | 48,48,48 | 0.65 | 1 (2%) | 51,54,54 | 1.26 | 6 (11%) |
| 26 | NEX | S | 616 | - | 38,46,46 | 1.65 | 7 (18%) | 50,70,70 | 1.63 | 9 (18%) |
| 24 | CLA | BB | 314 | 8 | 65,73,73 | 1.44 | 10 (15%) | 76,113,113 | 1.43 | 8 (10%) |
| 24 | CLA | N | 610 | - | 65,73,73 | 1.44 | 7 (10%) | 76,113,113 | 1.55 | 9 (11%) |
| 28 | XAT | BB | 301 | - | 39,47,47 | 6.17 | 20 (51%) | 54,74,74 | 7.80 | 34 (62%) |
| 24 | CLA | BJ | 612 | - | 60,68,73 | 1.58 | 5 (8%) | 70,107,113 | 1.36 | 6 (8%) |
| 24 | CLA | BV | 611 | - | 49,57,73 | 1.68 | 7 (14%) | 55,93,113 | 1.58 | 7 (12%) |
| 24 | CLA | c | 508 | - | 65,73,73 | 1.43 | 10 (15%) | 76,113,113 | 1.35 | 6 (7%) |
| 23 | CHL | 5 | 605 | 1 | 46,54,74 | 2.33 | 16 (34%) | 49,90,114 | 2.74 | 18 (36%) |
| 24 | CLA | BB | 305 | - | 50,58,73 | 1.66 | 10 (20%) | 58,95,113 | 1.57 | 8 (13%) |
| 29 | BCR | C | 515 | - | 41,41,41 | 1.32 | 3 (7%) | 56,56,56 | 1.28 | 6 (10%) |
| 23 | CHL | AA | 309 | - | 46,54,74 | 2.29 | 16 (34%) | 49,90,114 | 2.82 | 18 (36%) |
| 28 | XAT | AA | 318 | - | 39,47,47 | 6.12 | 21 (53%) | 54,74,74 | 7.81 | 34 (62%) |
| 24 | CLA | n | 603 | 8 | 65,73,73 | 1.48 | 6 (9%) | 76,113,113 | 1.35 | 8 (10%) |
| 24 | CLA | C | 504 | 21 | 65,73,73 | 1.43 | 6 (9%) | 76,113,113 | 1.41 | 8 (10%) |
| 23 | CHL | 9 | 607 | - | 60,68,74 | 1.94 | 14 (23%) | 64,105,114 | 2.55 | 23 (35%) |
| 35 | BCT | BD | 402 | - | 2,3,3 | 1.33 | 0 | 2,3,3 | 4.13 | 1 (50%) |
| 24 | CLA | a | 410 | - | 60,68,73 | 1.49 | 7 (11%) | 70,107,113 | 1.50 | 8 (11%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 38 | PHO | A | 408 | - | 51,69,69 | 1.11 | 6 (11%) | 47,99,99 | 1.13 | 5 (10%) |
| 27 | LHG | BQ | 618 | 24 | 48,48,48 | 0.62 | 1 (2%) | 51,54,54 | 1.28 | 6 (11%) |
| 30 | LMG | i | 101 | - | 48,48,55 | 0.74 | 1 (2%) | 56,56,63 | 1.32 | 6 (10%) |
| 23 | CHL | 6 | 601 | 2 | 61,69,74 | 2.01 | 16 (26%) | 65,106,114 | 2.52 | 24 (36%) |
| 24 | CLA | v | 601 | - | 65,73,73 | 1.49 | 6 (9%) | 76,113,113 | 1.36 | 8 (10%) |
| 24 | CLA | A2 | 604 | - | 50,58,73 | 1.62 | 7 (14%) | 58,95,113 | 1.62 | 8 (13%) |
| 24 | CLA | A | 410 | - | 60,68,73 | 1.47 | 6 (10%) | 70,107,113 | 1.47 | 7 (10%) |
| 25 | LUT | BB | 316 | - | 42,43,43 | 1.66 | 8 (19%) | 51,60,60 | 1.53 | 11 (21%) |
| 23 | CHL | AA | 306 | 1 | 46,54,74 | 2.41 | 16 (34%) | 49,90,114 | 2.72 | 18 (36%) |
| 34 | DGD | BK | 102 | - | 63,63,67 | 0.95 | 3 (4%) | 77,77,81 | 1.47 | 10 (12%) |
| 27 | LHG | G | 618 | 24 | 48,48,48 | 0.60 | 0 | 51,54,54 | 1.27 | 6 (11%) |
| 24 | CLA | 5 | 610 | 1 | 56,64,73 | 1.56 | 10 (17%) | 65,102,113 | 1.50 | 10 (15%) |
| 25 | LUT | Ba | 316 | - | 42,43,43 | 1.62 | 8 (19%) | 51,60,60 | 1.46 | 9 (17%) |
| 28 | XAT | Y | 301 | - | 39,47,47 | 6.16 | 21 (53%) | 54,74,74 | 7.77 | 34 (62%) |
| 23 | CHL | Au | 605 | 8 | 46,54,74 | 2.31 | 15 (32%) | 49,90,114 | 2.82 | 19 (38%) |
| 24 | CLA | y | 314 | 8 | 65,73,73 | 1.48 | 6 (9%) | 76,113,113 | 1.37 | 7 (9%) |
| 24 | CLA | BF | 511 | 21 | 65,73,73 | 1.42 | 10 (15%) | 76,113,113 | 1.44 | 7 (9%) |
| 27 | LHG | BE | 622 | - | 48,48,48 | 0.62 | 1 (2%) | 51,54,54 | 1.27 | 6 (11%) |
| 24 | CLA | AB | 302 | - | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.57 | 6 (11%) |
| 24 | CLA | y | 315 | - | 48,56,73 | 1.68 | 6 (12%) | 55,92,113 | 1.57 | 6 (10%) |
| 34 | DGD | BF | 518 | - | 63,63,67 | 0.87 | 2 (3%) | 77,77,81 | 1.41 | 7 (9%) |
| 24 | CLA | 1 | 502 | 21 | 65,73,73 | 1.46 | 8 (12%) | 76,113,113 | 1.35 | 7 (9%) |
| 34 | DGD | BF | 517 | - | 56,56,67 | 0.96 | 2 (3%) | 70,70,81 | 1.50 | 11 (15%) |
| 24 | CLA | B | 616 | 4 | 65,73,73 | 1.46 | 7 (10%) | 76,113,113 | 1.42 | 8 (10%) |
| 24 | CLA | BE | 607 | - | 65,73,73 | 1.48 | 7 (10%) | 76,113,113 | 1.36 | 7 (9%) |
| 24 | CLA | b | 616 | - | 65,73,73 | 1.46 | 8 (12%) | 76,113,113 | 1.39 | 7 (9%) |
| 24 | CLA | A6 | 611 | - | 49,57,73 | 1.65 | 9 (18%) | 55,93,113 | 1.53 | 7 (12%) |
| 33 | HEM | 4 | 102 | 7 | 41,50,50 | 1.45 | 4 (9%) | 45,82,82 | 1.29 | 4 (8%) |
| 36 | OEX | R | 402 | 20 | 0,15,15 | - | - | - | - | - |
| 24 | CLA | A6 | 613 | 14 | 49,57,73 | 1.66 | 8 (16%) | 55,93,113 | 1.60 | 9 (16%) |
| 38 | PHO | BD | 409 | - | 51,69,69 | 1.08 | 6 (11%) | 47,99,99 | 1.14 | 6 (12%) |
| 24 | CLA | AA | 305 | - | 45,53,73 | 1.74 | 7 (15%) | 52,89,113 | 1.56 | 7 (13%) |
| 27 | LHG | D | 404 | - | 48,48,48 | 0.63 | 1 (2%) | 51,54,54 | 1.27 | 5 (9%) |
| 32 | SQD | Az | 101 | - | 41,42,54 | 1.59 | 8 (19%) | 50,53,65 | 1.83 | 9 (18%) |
| 24 | CLA | 7 | 311 | 1 | 48,56,73 | 1.70 | 10 (20%) | 53,92,113 | 1.54 | 8 (15%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | CLA | y | 312 | 27 | 60,68,73 | 1.53 | 7 (11%) | 70,107,113 | 1.42 | 9 (12%) |
| 24 | CLA | g | 612 | - | 60,68,73 | 1.58 | 5 (8%) | 70,107,113 | 1.36 | 6 (8%) |
| 25 | LUT | 6 | 616 | - | 42,43,43 | 1.71 | 7 (16%) | 51,60,60 | 1.65 | 10 (19%) |
| 24 | CLA | B | 614 | - | 65,73,73 | 1.44 | 7 (10%) | 76,113,113 | 1.47 | 8 (10%) |
| 23 | CHL | BQ | 605 | 8 | 48,56,74 | 2.21 | 13 (27%) | 51,92,114 | 2.75 | 17 (33%) |
| 24 | CLA | c | 514 | 21 | 65,73,73 | 1.41 | 7 (10%) | 76,113,113 | 1.45 | 6 (7%) |
| 23 | CHL | Ba | 310 | - | 63,71,74 | 2.11 | 16 (25%) | 68,109,114 | 2.48 | 24 (35%) |
| 24 | CLA | 5 | 612 | - | 45,53,73 | 1.75 | 8 (17%) | 52,89,113 | 1.61 | 6 (11%) |
| 29 | BCR | 8 | 313 | - | 41,41,41 | 1.26 | 3 (7%) | 56,56,56 | 1.29 | 7 (12%) |
| 24 | CLA | v | 607 | - | 65,73,73 | 1.43 | 7 (10%) | 76,113,113 | 1.46 | 6 (7%) |
| 32 | SQD | BG | 406 | - | 49,50,54 | 1.58 | 7 (14%) | 58,61,65 | 1.44 | 7 (12%) |
| 23 | CHL | G | 605 | 8 | 46,54,74 | 2.31 | 15 (32%) | 49,90,114 | 2.82 | 18 (36%) |
| 23 | CHL | n | 606 | 8 | 50,58,74 | 2.19 | 17 (34%) | 52,94,114 | 2.73 | 21 (40%) |
| 34 | DGD | c | 517 | - | 63,63,67 | 0.87 | 2 (3%) | 77,77,81 | 1.41 | 8 (10%) |
| 24 | CLA | 7 | 315 | 1 | 45,53,73 | 1.77 | 6 (13%) | 52,89,113 | 1.61 | 6 (11%) |
| 24 | CLA | Ba | 303 | 8 | 65,73,73 | 1.47 | 6 (9%) | 76,113,113 | 1.37 | 7 (9%) |
| 24 | CLA | 6 | 612 | - | 45,53,73 | 1.73 | 8 (17%) | 52,89,113 | 1.64 | 7 (13%) |
| 24 | CLA | 6 | 602 | 2 | 60,68,73 | 1.47 | 9 (15%) | 70,107,113 | 1.38 | 7 (10%) |
| 23 | CHL | S | 601 | 14 | 46,54,74 | 2.27 | 15 (32%) | 49,90,114 | 2.77 | 19 (38%) |
| 30 | LMG | C | 501 | - | 51,51,55 | 0.74 | 0 | 59,59,63 | 1.35 | 6 (10%) |
| 25 | LUT | A6 | 614 | - | 42,43,43 | 1.67 | 8 (19%) | 51,60,60 | 1.50 | 10 (19%) |
| 24 | CLA | S | 612 | 14 | 55,63,73 | 1.59 | 8 (14%) | 64,101,113 | 1.50 | 8 (12%) |
| 23 | CHL | BB | 309 | - | 63,71,74 | 1.91 | 15 (23%) | 68,109,114 | 2.49 | 21 (30%) |
| 27 | LHG | v | 621 | - | 48,48,48 | 0.62 | 1 (2%) | 51,54,54 | 1.26 | 6 (11%) |
| 24 | CLA | BE | 602 | - | 65,73,73 | 1.47 | 7 (10%) | 76,113,113 | 1.35 | 7 (9%) |
| 30 | LMG | 2 | 407 | - | 46,46,55 | 0.78 | 1 (2%) | 54,54,63 | 1.35 | 5 (9%) |
| 31 | PL9 | BG | 403 | - | 55,55,55 | 1.50 | 6 (10%) | 68,69,69 | 1.54 | 14 (20%) |
| 34 | DGD | R | 401 | - | 60,60,67 | 0.92 | 2 (3%) | 74,74,81 | 1.38 | 8 (10%) |
| 23 | CHL | A2 | 608 | - | 63,71,74 | 1.93 | 15 (23%) | 68,109,114 | 2.47 | 23 (33%) |
| 24 | CLA | BE | 610 | - | 65,73,73 | 1.45 | 7 (10%) | 76,113,113 | 1.41 | 7 (9%) |
| 24 | CLA | y | 303 | 8 | 65,73,73 | 1.47 | 6 (9%) | 76,113,113 | 1.38 | 7 (9%) |
| 24 | CLA | 6 | 611 | 27 | 55,63,73 | 1.56 | 10 (18%) | 64,101,113 | 1.59 | 10 (15%) |
| 23 | CHL | 7 | 310 | - | 58,66,74 | 2.12 | 16 (27%) | 61,103,114 | 2.68 | 24 (39%) |
| 24 | CLA | B | 603 | 4 | 65,73,73 | 1.45 | 8 (12%) | 76,113,113 | 1.37 | 6 (7%) |
| 23 | CHL | BQ | 608 | - | 63,71,74 | 1.99 | 16 (25%) | 68,109,114 | 2.45 | 23 (33%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 32 | SQD | L | 103 | - | 53,54,54 | 1.52 | 8 (15%) | 62,65,65 | 1.37 | 6 (9%) |
| 24 | CLA | 1 | 513 | 21 | 65,73,73 | 1.43 | 7 (10%) | 76,113,113 | 1.46 | 8 (10%) |
| 24 | CLA | 8 | 309 | - | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.55 | 6 (11%) |
| 24 | CLA | b | 602 | - | 65,73,73 | 1.47 | 6 (9%) | 76,113,113 | 1.35 | 7 (9%) |
| 25 | LUT | S | 615 | - | 42,43,43 | 1.62 | 8 (19%) | 51,60,60 | 1.75 | 15 (29%) |
| 24 | CLA | B | 611 | 4 | 65,73,73 | 1.43 | 7 (10%) | 76,113,113 | 1.51 | 8 (10%) |
| 24 | CLA | c | 503 | 21 | 65,73,73 | 1.46 | 9 (13%) | 76,113,113 | 1.41 | 7 (9%) |
| 32 | SQD | BO | 102 | - | 41,42,54 | 1.63 | 7 (17%) | 50,53,65 | 1.46 | 7 (14%) |
| 24 | CLA | d | 402 | - | 65,73,73 | 1.45 | 6 (9%) | 76,113,113 | 1.37 | 7 (9%) |
| 24 | CLA | 0 | 604 | - | 45,53,73 | 1.71 | 9 (20%) | 52,89,113 | 1.55 | 8 (15%) |
| 23 | CHL | Au | 601 | 8 | 63,71,74 | 1.90 | 16 (25%) | 68,109,114 | 2.53 | 22 (32%) |
| 24 | CLA | 9 | 610 | 1 | 56,64,73 | 1.57 | 10 (17%) | 65,102,113 | 1.46 | 8 (12%) |
| 23 | CHL | BB | 308 | - | 63,71,74 | 1.86 | 14 (22%) | 68,109,114 | 2.55 | 23 (33%) |
| 24 | CLA | 8 | 301 | 3 | 42,49,73 | 1.77 | 7 (16%) | 48,83,113 | 1.68 | 8 (16%) |
| 24 | CLA | B | 613 | 4 | 65,73,73 | 1.43 | 9 (13%) | 76,113,113 | 1.42 | 6 (7%) |
| 32 | SQD | 2 | 408 | - | 49,50,54 | 1.57 | 9 (18%) | 58,61,65 | 1.52 | 8 (13%) |
| 29 | BCR | b | 618 | - | 41,41,41 | 1.18 | 2 (4%) | 56,56,56 | 1.28 | 8 (14%) |
| 24 | CLA | BE | 605 | 4 | 65,73,73 | 1.44 | 9 (13%) | 76,113,113 | 1.43 | 9 (11%) |
| 24 | CLA | r | 611 | 22 | 49,57,73 | 1.65 | 9 (18%) | 55,93,113 | 1.54 | 6 (10%) |
| 24 | CLA | BB | 313 | - | 60,68,73 | 1.51 | 9 (15%) | 70,107,113 | 1.44 | 7 (10%) |
| 25 | LUT | BV | 615 | - | 42,43,43 | 1.64 | 8 (19%) | 51,60,60 | 1.52 | 11 (21%) |
| 32 | SQD | l | 101 | - | 53,54,54 | 1.53 | 8 (15%) | 62,65,65 | 1.36 | 6 (9%) |
| 29 | BCR | B | 617 | - | 41,41,41 | 1.22 | 2 (4%) | 56,56,56 | 1.34 | 8 (14%) |
| 24 | CLA | g | 611 | 27 | 60,68,73 | 1.55 | 5 (8%) | 70,107,113 | 1.44 | 8 (11%) |
| 32 | SQD | A | 413 | - | 53,54,54 | 1.51 | 7 (13%) | 62,65,65 | 1.33 | 6 (9%) |
| 26 | NEX | AA | 319 | - | 38,46,46 | 1.66 | 6 (15%) | 50,70,70 | 1.69 | 10 (20%) |
| 25 | LUT | N | 616 | - | 42,43,43 | 1.64 | 8 (19%) | 51,60,60 | 1.55 | 9 (17%) |
| 24 | CLA | v | 613 | 4 | 65,73,73 | 1.44 | 9 (13%) | 76,113,113 | 1.43 | 6 (7%) |
| 24 | CLA | n | 611 | 27 | 60,68,73 | 1.55 | 5 (8%) | 70,107,113 | 1.45 | 7 (10%) |
| 24 | CLA | A | 405 | 20 | 65,73,73 | 1.45 | 10 (15%) | 76,113,113 | 1.39 | 8 (10%) |
| 24 | CLA | n | 602 | 8 | 65,73,73 | 1.47 | 6 (9%) | 76,113,113 | 1.35 | 8 (10%) |
| 24 | CLA | 1 | 503 | 21 | 65,73,73 | 1.46 | 10 (15%) | 76,113,113 | 1.43 | 7 (9%) |
| 26 | NEX | BJ | 617 | - | 38,46,46 | 1.66 | 6 (15%) | 50,70,70 | 1.69 | 9 (18%) |
| 23 | CHL | BU | 607 | 22 | 58,66,74 | 1.98 | 14 (24%) | 61,103,114 | 2.64 | 22 (36%) |
| 28 | XAT | 8 | 312 | - | 39,47,47 | 6.10 | 19 (48%) | 54,74,74 | 7.74 | 36 (66%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | CLA | AA | 312 | - | 45,53,73 | 1.74 | 7 (15%) | 52,89,113 | 1.60 | 7 (13%) |
| 24 | CLA | C | 506 | 21 | 65,73,73 | 1.47 | 10 (15%) | 76,113,113 | 1.36 | 8 (10%) |
| 24 | CLA | BQ | 604 | - | 50,58,73 | 1.68 | 6 (12%) | 58,95,113 | 1.52 | 7 (12%) |
| 23 | CHL | 7 | 308 | - | 58,66,74 | 1.98 | 15 (25%) | 61,103,114 | 2.62 | 22 (36%) |
| 24 | CLA | Au | 614 | - | 48,56,73 | 1.67 | 6 (12%) | 55,92,113 | 1.59 | 8 (14%) |
| 23 | CHL | Y | 310 | 8 | 63,71,74 | 1.94 | 15 (23%) | 68,109,114 | 2.46 | 20 (29%) |
| 29 | BCR | BE | 619 | - | 41,41,41 | 1.16 | 2 (4%) | 56,56,56 | 1.20 | 5 (8%) |
| 25 | LUT | s | 615 | - | 42,43,43 | 1.64 | 8 (19%) | 51,60,60 | 1.52 | 11 (21%) |
| 24 | CLA | v | 605 | 4 | 65,73,73 | 1.46 | 9 (13%) | 76,113,113 | 1.36 | 8 (10%) |
| 24 | CLA | BJ | 604 | - | 50,58,73 | 1.69 | 5 (10%) | 58,95,113 | 1.57 | 7 (12%) |
| 25 | LUT | S | 614 | - | 42,43,43 | 1.67 | 8 (19%) | 51,60,60 | 1.50 | 10 (19%) |
| 24 | CLA | 9 | 612 | - | 45,53,73 | 1.73 | 8 (17%) | 52,89,113 | 1.62 | 6 (11%) |
| 23 | CHL | A6 | 606 | - | 55,63,74 | 2.05 | 15 (27%) | 57,99,114 | 2.78 | 22 (38%) |
| 27 | LHG | BY | 201 | - | 48,48,48 | 0.62 | 1 (2%) | 51,54,54 | 1.25 | 6 (11%) |
| 24 | CLA | BQ | 603 | 8 | 65,73,73 | 1.48 | 7 (10%) | 76,113,113 | 1.36 | 8 (10%) |
| 25 | LUT | 5 | 616 | - | 42,43,43 | 1.69 | 8 (19%) | 51,60,60 | 1.68 | 12 (23%) |
| 24 | CLA | N | 603 | 8 | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.39 | 8 (10%) |
| 23 | CHL | AB | 305 | - | 46,54,74 | 2.28 | 15 (32%) | 49,90,114 | 2.72 | 17 (34%) |
| 24 | CLA | r | 608 | 22 | 58,66,73 | 1.55 | 10 (17%) | 67,104,113 | 1.49 | 6 (8%) |
| 23 | CHL | 0 | 609 | - | 58,66,74 | 2.18 | 19 (32%) | 61,103,114 | 2.79 | 22 (36%) |
| 23 | CHL | 0 | 605 | 2 | 46,54,74 | 2.34 | 16 (34%) | 49,90,114 | 2.76 | 21 (42%) |
| 24 | CLA | 1 | 509 | 21 | 65,73,73 | 1.45 | 10 (15%) | 76,113,113 | 1.43 | 9 (11%) |
| 25 | LUT | Ba | 317 | - | 42,43,43 | 1.61 | 8 (19%) | 51,60,60 | 1.52 | 10 (19%) |
| 24 | CLA | b | 617 | 4 | 65,73,73 | 1.44 | 7 (10%) | 76,113,113 | 1.41 | 7 (9%) |
| 26 | NEX | BQ | 617 | - | 38,46,46 | 1.68 | 7 (18%) | 50,70,70 | 1.66 | 9 (18%) |
| 32 | SQD | d | 406 | - | 49,50,54 | 1.57 | 7 (14%) | 58,61,65 | 1.44 | 7 (12%) |
| 24 | CLA | AA | 304 | - | 55,63,73 | 1.60 | 8 (14%) | 64,101,113 | 1.37 | 8 (12%) |
| 24 | CLA | BQ | 614 | - | 48,56,73 | 1.75 | 5 (10%) | 55,92,113 | 1.62 | 9 (16%) |
| 32 | SQD | L | 101 | - | 41,42,54 | 1.62 | 7 (17%) | 50,53,65 | 1.57 | 9 (18%) |
| 23 | CHL | BQ | 601 | 8 | 63,71,74 | 2.00 | 15 (23%) | 68,109,114 | 2.43 | 21 (30%) |
| 24 | CLA | N | 613 | 8 | 60,68,73 | 1.52 | 8 (13%) | 70,107,113 | 1.47 | 8 (11%) |
| 26 | NEX | G | 617 | - | 38,46,46 | 1.64 | 7 (18%) | 50,70,70 | 1.69 | 9 (18%) |
| 24 | CLA | BE | 604 | 4 | 65,73,73 | 1.43 | 6 (9%) | 76,113,113 | 1.40 | 6 (7%) |
| 26 | NEX | Au | 617 | - | 38,46,46 | 1.64 | 6 (15%) | 50,70,70 | 1.69 | 9 (18%) |
| 30 | LMG | BF | 501 | - | 51,51,55 | 0.74 | 0 | 59,59,63 | 1.34 | 7 (11%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 25 | LUT | y | 317 | - | 42,43,43 | 1.61 | 8 (19%) | 51,60,60 | 1.52 | 10 (19%) |
| 23 | CHL | 0 | 606 | - | 46,54,74 | 2.19 | 14 (30%) | 49,90,114 | 2.83 | 18 (36%) |
| 24 | CLA | 7 | 314 | 1 | 45,53,73 | 1.73 | 8 (17%) | 52,89,113 | 1.61 | 6 (11%) |
| 24 | CLA | BE | 616 | - | 65,73,73 | 1.45 | 8 (12%) | 76,113,113 | 1.39 | 8 (10%) |
| 30 | LMG | 1 | 519 | - | 51,51,55 | 0.73 | 1 (1%) | 59,59,63 | 1.32 | 4 (6%) |
| 25 | LUT | Au | 616 | - | 42,43,43 | 1.64 | 8 (19%) | 51,60,60 | 1.54 | 9 (17%) |
| 31 | PL9 | d | 403 | - | 55,55,55 | 1.65 | 9 (16%) | 68,69,69 | 1.66 | 14 (20%) |
| 29 | BCR | BN | 101 | - | 41,41,41 | 1.24 | 3 (7%) | 56,56,56 | 1.32 | 6 (10%) |
| 24 | CLA | 0 | 610 | 2 | 60,68,73 | 1.50 | 9 (15%) | 70,107,113 | 1.56 | 13 (18%) |
| 23 | CHL | N | 601 | 8 | 63,71,74 | 1.92 | 15 (23%) | 68,109,114 | 2.48 | 22 (32%) |
| 33 | HEM | BI | 102 | 7,6 | 41,50,50 | 1.45 | 4 (9%) | 45,82,82 | 1.23 | 3 (6%) |
| 23 | CHL | BJ | 608 | - | 63,71,74 | 1.94 | 15 (23%) | 68,109,114 | 2.55 | 24 (35%) |
| 24 | CLA | A6 | 602 | 14 | 61,69,73 | 1.46 | 6 (9%) | 71,108,113 | 1.46 | 7 (9%) |
| 24 | CLA | g | 613 | - | 65,73,73 | 1.50 | 6 (9%) | 76,113,113 | 1.42 | 8 (10%) |
| 24 | CLA | g | 603 | 8 | 65,73,73 | 1.48 | 6 (9%) | 76,113,113 | 1.38 | 7 (9%) |
| 24 | CLA | A6 | 604 | - | 50,58,73 | 1.65 | 7 (14%) | 58,95,113 | 1.56 | 7 (12%) |
| 23 | CHL | Y | 307 | - | 50,58,74 | 2.07 | 13 (26%) | 52,94,114 | 2.88 | 20 (38%) |
| 24 | CLA | 1 | 512 | - | 65,73,73 | 1.42 | 7 (10%) | 76,113,113 | 1.43 | 9 (11%) |
| 23 | CHL | BU | 613 | 22 | 42,50,74 | 2.33 | 16 (38%) | 44,85,114 | 3.01 | 22 (50%) |
| 24 | CLA | y | 305 | - | 50,58,73 | 1.67 | 7 (14%) | 58,95,113 | 1.54 | 7 (12%) |
| 30 | LMG | I | 101 | - | 40,40,55 | 0.81 | 0 | 48,48,63 | 1.31 | 6 (12%) |
| 24 | CLA | BF | 505 | - | 65,73,73 | 1.45 | 7 (10%) | 76,113,113 | 1.35 | 6 (7%) |
| 24 | CLA | 6 | 610 | 2 | 60,68,73 | 1.50 | 10 (16%) | 70,107,113 | 1.65 | 13 (18%) |
| 28 | XAT | Au | 619 | - | 39,47,47 | 6.18 | 21 (53%) | 54,74,74 | 7.66 | 34 (62%) |
| 24 | CLA | 5 | 613 | 1 | 55,63,73 | 1.55 | 7 (12%) | 64,101,113 | 1.54 | 7 (10%) |
| 34 | DGD | a | 401 | - | 60,60,67 | 0.94 | 2 (3%) | 74,74,81 | 1.38 | 7 (9%) |
| 23 | CHL | 8 | 307 | 3 | 46,54,74 | 2.29 | 15 (32%) | 49,90,114 | 2.80 | 22 (44%) |

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 |
|-----|------|-------|-----|------|-----------|---------------|-------|
| 24 | CLA | BU | 609 | 22 | 1/1/15/20 | 12/37/115/115 | - |
| 24 | CLA | BD | 407 | - | 1/1/12/20 | 6/19/97/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24 | CLA | 5 | 614 | 1 | 1/1/11/20 | 6/13/91/115 | - |
| 23 | CHL | 6 | 606 | - | 3/3/16/26 | 7/15/113/137 | - |
| 26 | NEX | s | 616 | - | - | 15/27/83/83 | 0/3/3/3 |
| 23 | CHL | A2 | 605 | 8 | 3/3/16/26 | 9/18/116/137 | - |
| 23 | CHL | 5 | 601 | 1 | 3/3/16/26 | 9/15/113/137 | - |
| 23 | CHL | AA | 310 | - | 3/3/18/26 | 12/27/125/137 | - |
| 24 | CLA | v | 608 | 4 | 1/1/15/20 | 13/37/115/115 | - |
| 24 | CLA | 1 | 506 | 21 | 1/1/15/20 | 15/37/115/115 | - |
| 24 | CLA | Au | 611 | 27 | 1/1/14/20 | 9/31/109/115 | - |
| 24 | CLA | C | 510 | 21 | 1/1/15/20 | 16/37/115/115 | - |
| 23 | CHL | BU | 605 | 22 | 3/3/19/26 | 22/33/131/137 | - |
| 24 | CLA | b | 608 | - | 1/1/15/20 | 19/37/115/115 | - |
| 24 | CLA | BU | 608 | 22 | 1/1/13/20 | 11/29/107/115 | - |
| 23 | CHL | BB | 306 | 8 | 3/3/16/26 | 7/18/116/137 | - |
| 24 | CLA | C | 502 | 21 | 1/1/15/20 | 16/37/115/115 | - |
| 28 | XAT | 7 | 318 | - | - | 12/31/93/93 | 0/4/4/4 |
| 23 | CHL | 9 | 609 | - | 3/3/18/26 | 13/29/127/137 | - |
| 24 | CLA | AB | 303 | - | 1/1/11/20 | 5/13/91/115 | - |
| 24 | CLA | 6 | 613 | - | 1/1/13/20 | 13/29/107/115 | - |
| 30 | LMG | b | 621 | - | - | 25/46/66/70 | 0/1/1/1 |
| 24 | CLA | Au | 602 | 8 | 1/1/15/20 | 13/37/115/115 | - |
| 24 | CLA | s | 608 | - | 1/1/11/20 | 5/13/91/115 | - |
| 30 | LMG | C | 519 | - | - | 22/46/66/70 | 0/1/1/1 |
| 34 | DGD | BD | 413 | - | - | 26/49/89/95 | 0/2/2/2 |
| 24 | CLA | 0 | 602 | 2 | 1/1/14/20 | 16/31/109/115 | - |
| 23 | CHL | r | 606 | - | 3/3/17/26 | 6/24/122/137 | - |
| 34 | DGD | C | 517 | - | - | 20/51/91/95 | 0/2/2/2 |
| 23 | CHL | y | 306 | 8 | 3/3/16/26 | 7/18/116/137 | - |
| 24 | CLA | s | 609 | 14 | 1/1/13/20 | 8/25/103/115 | - |
| 23 | CHL | Ba | 308 | - | 3/3/19/26 | 18/33/131/137 | - |
| 24 | CLA | B | 615 | - | 1/1/15/20 | 17/37/115/115 | - |
| 29 | BCR | BI | 101 | - | - | 11/29/63/63 | 0/2/2/2 |
| 24 | CLA | b | 615 | - | 1/1/15/20 | 18/37/115/115 | - |
| 23 | CHL | Y | 306 | 8 | 3/3/16/26 | 7/18/116/137 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 23 | CHL | G | 601 | 8 | 3/3/19/26 | 16/33/131/137 | - |
| 24 | CLA | 2 | 402 | 5 | 1/1/15/20 | 17/37/115/115 | - |
| 24 | CLA | C | 503 | 21 | 1/1/15/20 | 16/37/115/115 | - |
| 23 | CHL | s | 605 | 14 | 3/3/16/26 | 11/15/113/137 | - |
| 24 | CLA | B | 604 | 4 | 1/1/15/20 | 14/37/115/115 | - |
| 24 | CLA | R | 405 | - | 1/1/15/20 | 6/37/115/115 | - |
| 24 | CLA | v | 609 | 4 | 1/1/15/20 | 13/37/115/115 | - |
| 24 | CLA | BE | 603 | 4 | 1/1/15/20 | 16/37/115/115 | - |
| 23 | CHL | 7 | 307 | 1 | 3/3/16/26 | 6/15/113/137 | - |
| 28 | XAT | AA | 301 | - | - | 11/31/93/93 | 0/4/4/4 |
| 24 | CLA | BV | 608 | - | 1/1/11/20 | 5/13/91/115 | - |
| 24 | CLA | 1 | 507 | - | 1/1/15/20 | 16/37/115/115 | - |
| 25 | LUT | 6 | 615 | - | - | 2/29/67/67 | 0/2/2/2 |
| 24 | CLA | BE | 613 | - | 1/1/15/20 | 15/37/115/115 | - |
| 24 | CLA | n | 604 | - | 1/1/12/20 | 9/19/97/115 | - |
| 23 | CHL | BV | 605 | 14 | 3/3/16/26 | 10/15/113/137 | - |
| 24 | CLA | y | 313 | - | 1/1/14/20 | 12/31/109/115 | - |
| 24 | CLA | BD | 406 | - | 1/1/15/20 | 7/37/115/115 | - |
| 25 | LUT | 0 | 616 | - | - | 1/29/67/67 | 0/2/2/2 |
| 24 | CLA | BQ | 610 | 8 | 1/1/15/20 | 14/37/115/115 | - |
| 27 | LHG | Ba | 319 | 24 | - | 20/53/53/53 | - |
| 23 | CHL | g | 609 | - | 3/3/18/26 | 10/27/125/137 | - |
| 23 | CHL | n | 605 | 8 | 3/3/16/26 | 6/18/116/137 | - |
| 24 | CLA | 1 | 504 | 21 | 1/1/15/20 | 14/37/115/115 | - |
| 34 | DGD | 1 | 516 | - | - | 12/44/84/95 | 0/2/2/2 |
| 24 | CLA | BJ | 602 | 8 | 1/1/15/20 | 15/37/115/115 | - |
| 29 | BCR | z | 101 | - | - | 3/29/63/63 | 0/2/2/2 |
| 24 | CLA | BF | 504 | 21 | 1/1/15/20 | 17/37/115/115 | - |
| 29 | BCR | h | 101 | - | - | 5/29/63/63 | 0/2/2/2 |
| 24 | CLA | 9 | 603 | - | 1/1/13/20 | 9/25/103/115 | - |
| 24 | CLA | c | 507 | 21 | 1/1/15/20 | 17/37/115/115 | - |
| 23 | CHL | BB | 310 | - | 3/3/19/26 | 17/33/131/137 | - |
| 24 | CLA | r | 602 | 22 | 1/1/13/20 | 8/25/105/115 | - |
| 27 | LHG | BE | 623 | - | - | 15/50/50/53 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 23 | CHL | Ba | 302 | 8 | 3/3/19/26 | 14/33/131/137 | - |
| 24 | CLA | c | 511 | 21 | 1/1/15/20 | 15/37/115/115 | - |
| 29 | BCR | v | 617 | - | - | 5/29/63/63 | 0/2/2/2 |
| 24 | CLA | g | 602 | 8 | 1/1/15/20 | 15/37/115/115 | - |
| 24 | CLA | B | 601 | - | 1/1/15/20 | 15/37/115/115 | - |
| 23 | CHL | N | 607 | - | 3/3/19/26 | 14/33/131/137 | - |
| 38 | PHO | a | 408 | - | - | 6/37/103/103 | 0/5/6/6 |
| 24 | CLA | 0 | 611 | 27 | 1/1/13/20 | 12/25/103/115 | - |
| 23 | CHL | g | 606 | - | 3/3/16/26 | 4/20/118/137 | - |
| 31 | PL9 | 2 | 404 | - | - | 5/53/73/73 | 0/1/1/1 |
| 30 | LMG | A | 412 | - | - | 16/43/63/70 | 0/1/1/1 |
| 23 | CHL | A6 | 605 | 14 | 3/3/16/26 | 9/15/113/137 | - |
| 25 | LUT | AA | 317 | - | - | 1/29/67/67 | 0/2/2/2 |
| 24 | CLA | 5 | 602 | 1 | 1/1/14/20 | 15/33/111/115 | - |
| 24 | CLA | r | 601 | 22 | 1/1/11/20 | 8/18/96/115 | - |
| 27 | LHG | 2 | 405 | - | - | 15/50/50/53 | - |
| 23 | CHL | BJ | 607 | - | 3/3/19/26 | 18/33/131/137 | - |
| 23 | CHL | Au | 606 | - | 3/3/16/26 | 7/20/118/137 | - |
| 34 | DGD | A | 402 | - | - | 24/48/88/95 | 0/2/2/2 |
| 24 | CLA | BQ | 612 | - | 1/1/14/20 | 6/31/109/115 | - |
| 26 | NEX | n | 617 | - | - | 15/27/83/83 | 0/3/3/3 |
| 24 | CLA | B | 612 | 4 | 1/1/15/20 | 13/37/115/115 | - |
| 24 | CLA | c | 513 | - | 1/1/15/20 | 12/37/115/115 | - |
| 28 | XAT | 5 | 619 | - | - | 15/31/93/93 | 0/4/4/4 |
| 24 | CLA | B | 605 | 4 | 1/1/15/20 | 20/37/115/115 | - |
| 23 | CHL | 6 | 608 | 2 | 3/3/16/26 | 7/15/113/137 | - |
| 23 | CHL | 8 | 305 | - | 3/3/16/26 | 7/15/113/137 | - |
| 24 | CLA | AB | 308 | - | 1/1/11/20 | 6/13/91/115 | - |
| 24 | CLA | R | 404 | 20 | 1/1/15/20 | 8/37/115/115 | - |
| 28 | XAT | N | 619 | - | - | 17/31/93/93 | 0/4/4/4 |
| 24 | CLA | BV | 609 | 14 | 1/1/13/20 | 9/25/103/115 | - |
| 24 | CLA | 5 | 611 | 27 | 1/1/11/20 | 6/13/91/115 | - |
| 24 | CLA | v | 612 | 4 | 1/1/15/20 | 13/37/115/115 | - |
| 24 | CLA | 8 | 310 | - | 1/1/11/20 | 4/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 29 | BCR | v | 618 | - | - | 7/29/63/63 | 0/2/2/2 |
| 23 | CHL | G | 607 | - | 3/3/19/26 | 15/33/131/137 | - |
| 24 | CLA | R | 406 | - | 1/1/12/20 | 5/19/97/115 | - |
| 25 | LUT | BB | 317 | - | - | 1/29/67/67 | 0/2/2/2 |
| 23 | CHL | 6 | 607 | - | 3/3/17/26 | 12/24/122/137 | - |
| 24 | CLA | Ba | 312 | 27 | 1/1/14/20 | 12/31/109/115 | - |
| 24 | CLA | AA | 313 | - | 1/1/11/20 | 4/13/91/115 | - |
| 34 | DGD | h | 102 | - | - | 15/51/91/95 | 0/2/2/2 |
| 27 | LHG | L | 102 | - | - | 19/53/53/53 | - |
| 25 | LUT | A6 | 615 | - | - | 1/29/67/67 | 0/2/2/2 |
| 24 | CLA | a | 407 | - | 1/1/12/20 | 6/19/97/115 | - |
| 24 | CLA | v | 616 | 4 | 1/1/15/20 | 17/37/115/115 | - |
| 24 | CLA | b | 613 | 4 | 1/1/15/20 | 14/37/115/115 | - |
| 24 | CLA | Ba | 311 | 8 | 1/1/14/20 | 10/31/109/115 | - |
| 28 | XAT | r | 616 | - | - | 17/31/93/93 | 0/4/4/4 |
| 23 | CHL | Au | 609 | 8 | 3/3/17/26 | 8/21/121/137 | - |
| 30 | LMG | c | 518 | - | - | 23/46/66/70 | 0/1/1/1 |
| 38 | PHO | BD | 408 | - | - | 7/37/103/103 | 0/5/6/6 |
| 27 | LHG | g | 618 | 24 | - | 18/53/53/53 | - |
| 24 | CLA | 9 | 611 | 27 | 1/1/11/20 | 6/13/91/115 | - |
| 29 | BCR | BF | 515 | - | - | 3/29/63/63 | 0/2/2/2 |
| 27 | LHG | 0 | 617 | 24 | - | 12/51/51/53 | - |
| 24 | CLA | y | 311 | 8 | 1/1/14/20 | 10/31/109/115 | - |
| 28 | XAT | g | 619 | - | - | 12/31/93/93 | 0/4/4/4 |
| 26 | NEX | A2 | 617 | - | - | 15/27/83/83 | 0/3/3/3 |
| 27 | LHG | N | 618 | 24 | - | 16/53/53/53 | - |
| 24 | CLA | c | 502 | 21 | 1/1/15/20 | 14/37/115/115 | - |
| 25 | LUT | A2 | 616 | - | - | 1/29/67/67 | 0/2/2/2 |
| 27 | LHG | b | 622 | - | - | 24/53/53/53 | - |
| 24 | CLA | G | 610 | 8 | 1/1/14/20 | 19/36/114/115 | - |
| 24 | CLA | Au | 610 | 8 | 1/1/14/20 | 19/36/114/115 | - |
| 24 | CLA | A2 | 602 | 8 | 1/1/15/20 | 13/37/115/115 | - |
| 23 | CHL | e | 601 | - | 3/3/16/26 | 2/13/111/137 | - |
| 24 | CLA | BE | 606 | 4 | 1/1/15/20 | 17/37/115/115 | - |
| 29 | BCR | F | 101 | - | - | 8/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 23 | CHL | y | 308 | - | 3/3/19/26 | 18/33/131/137 | - |
| 23 | CHL | G | 608 | - | 3/3/19/26 | 23/33/131/137 | - |
| 24 | CLA | G | 612 | - | 1/1/14/20 | 9/31/109/115 | - |
| 29 | BCR | K | 102 | - | - | 6/29/63/63 | 0/2/2/2 |
| 23 | CHL | Y | 308 | - | 3/3/19/26 | 15/33/131/137 | - |
| 24 | CLA | 7 | 303 | 1 | 1/1/14/20 | 8/33/111/115 | - |
| 24 | CLA | b | 604 | 4 | 1/1/15/20 | 13/37/115/115 | - |
| 31 | PL9 | D | 403 | - | - | 5/53/73/73 | 0/1/1/1 |
| 25 | LUT | 9 | 616 | - | - | 1/29/67/67 | 0/2/2/2 |
| 24 | CLA | C | 512 | - | 1/1/15/20 | 11/37/115/115 | - |
| 28 | XAT | G | 619 | - | - | 14/31/93/93 | 0/4/4/4 |
| 24 | CLA | B | 606 | - | 1/1/15/20 | 17/37/115/115 | - |
| 24 | CLA | r | 609 | 22 | 1/1/15/20 | 12/37/115/115 | - |
| 24 | CLA | Y | 304 | 8 | 1/1/15/20 | 9/37/115/115 | - |
| 24 | CLA | 1 | 505 | - | 1/1/15/20 | 8/37/115/115 | - |
| 25 | LUT | Au | 615 | - | - | 1/29/67/67 | 0/2/2/2 |
| 24 | CLA | d | 401 | 5 | 1/1/15/20 | 16/37/115/115 | - |
| 23 | CHL | AA | 308 | - | 3/3/18/26 | 15/27/125/137 | - |
| 24 | CLA | B | 607 | - | 1/1/15/20 | 20/37/115/115 | - |
| 25 | LUT | G | 615 | - | - | 1/29/67/67 | 0/2/2/2 |
| 29 | BCR | B | 623 | - | - | 13/29/63/63 | 0/2/2/2 |
| 25 | LUT | 8 | 311 | - | - | 1/29/67/67 | 0/2/2/2 |
| 23 | CHL | N | 606 | 8 | 3/3/16/26 | 8/20/118/137 | - |
| 23 | CHL | g | 605 | 8 | 3/3/16/26 | 7/15/113/137 | - |
| 24 | CLA | 9 | 602 | 1 | 1/1/14/20 | 14/33/111/115 | - |
| 23 | CHL | BQ | 606 | 8 | 3/3/16/26 | 9/20/118/137 | - |
| 24 | CLA | 7 | 312 | - | 1/1/11/20 | 9/13/91/115 | - |
| 29 | BCR | BE | 620 | - | - | 5/29/63/63 | 0/2/2/2 |
| 30 | LMG | c | 501 | - | - | 23/46/66/70 | 0/1/1/1 |
| 24 | CLA | BE | 617 | 4 | 1/1/15/20 | 17/37/115/115 | - |
| 23 | CHL | A2 | 607 | - | 3/3/19/26 | 16/33/131/137 | - |
| 24 | CLA | S | 613 | 14 | 1/1/11/20 | 7/18/96/115 | - |
| 27 | LHG | 1 | 521 | - | - | 23/53/53/53 | - |
| 25 | LUT | BQ | 616 | - | - | 1/29/67/67 | 0/2/2/2 |
| 27 | LHG | Az | 102 | - | - | 19/53/53/53 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24 | CLA | BU | 614 | - | 1/1/11/20 | 7/13/91/115 | - |
| 23 | CHL | BJ | 606 | - | 3/3/16/26 | 4/20/118/137 | - |
| 23 | CHL | BQ | 609 | - | 3/3/19/26 | 15/33/131/137 | - |
| 23 | CHL | 5 | 609 | - | 3/3/18/26 | 12/29/127/137 | - |
| 24 | CLA | Ba | 314 | 8 | 1/1/15/20 | 15/37/115/115 | - |
| 29 | BCR | 1 | 515 | - | - | 5/29/63/63 | 0/2/2/2 |
| 23 | CHL | S | 606 | - | 3/3/17/26 | 8/24/122/137 | - |
| 33 | HEM | f | 102 | 7,6 | - | 3/12/54/54 | - |
| 23 | CHL | 0 | 608 | 2 | 3/3/16/26 | 7/15/113/137 | - |
| 23 | CHL | BH | 601 | - | 3/3/16/26 | 2/13/111/137 | - |
| 24 | CLA | 0 | 612 | - | 1/1/11/20 | 6/13/91/115 | - |
| 25 | LUT | r | 615 | - | - | 3/29/67/67 | 0/2/2/2 |
| 34 | DGD | a | 413 | - | - | 26/49/89/95 | 0/2/2/2 |
| 24 | CLA | 8 | 308 | - | 1/1/11/20 | 5/13/91/115 | - |
| 29 | BCR | BE | 618 | - | - | 4/29/63/63 | 0/2/2/2 |
| 32 | SQD | A1 | 101 | - | - | 19/49/69/69 | 0/1/1/1 |
| 30 | LMG | BL | 101 | - | - | 17/43/63/70 | 0/1/1/1 |
| 24 | CLA | BF | 508 | - | 1/1/15/20 | 13/37/115/115 | - |
| 24 | CLA | b | 614 | - | 1/1/15/20 | 12/37/115/115 | - |
| 25 | LUT | g | 615 | - | - | 2/29/67/67 | 0/2/2/2 |
| 33 | HEM | F | 102 | 7 | - | 4/12/54/54 | - |
| 27 | LHG | r | 618 | 24 | - | 12/46/46/53 | - |
| 32 | SQD | l | 102 | - | - | 21/37/57/69 | 0/1/1/1 |
| 29 | BCR | Ay | 101 | - | - | 11/29/63/63 | 0/2/2/2 |
| 24 | CLA | c | 504 | 21 | 1/1/15/20 | 20/37/115/115 | - |
| 23 | CHL | 5 | 606 | 1 | 3/3/16/26 | 4/15/113/137 | - |
| 23 | CHL | s | 601 | - | 3/3/16/26 | 6/15/113/137 | - |
| 24 | CLA | G | 603 | 8 | 1/1/15/20 | 12/37/115/115 | - |
| 24 | CLA | Au | 603 | 8 | 1/1/15/20 | 12/37/115/115 | - |
| 27 | LHG | 9 | 618 | 24 | - | 18/45/45/53 | - |
| 32 | SQD | a | 412 | - | - | 28/49/69/69 | 0/1/1/1 |
| 23 | CHL | n | 601 | 8 | 3/3/19/26 | 19/33/131/137 | - |
| 24 | CLA | C | 507 | - | 1/1/15/20 | 14/37/115/115 | - |
| 24 | CLA | N | 612 | - | 1/1/14/20 | 6/31/109/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24 | CLA | BQ | 613 | - | 1/1/14/20 | 9/31/109/115 | - |
| 24 | CLA | G | 614 | - | 1/1/11/20 | 5/17/95/115 | - |
| 25 | LUT | 7 | 316 | - | - | 3/29/67/67 | 0/2/2/2 |
| 23 | CHL | BJ | 605 | 8 | 3/3/16/26 | 7/15/113/137 | - |
| 26 | NEX | A6 | 616 | - | - | 13/27/83/83 | 0/3/3/3 |
| 24 | CLA | s | 604 | - | 1/1/12/20 | 7/19/97/115 | - |
| 24 | CLA | D | 401 | 5 | 1/1/15/20 | 18/37/115/115 | - |
| 27 | LHG | y | 319 | 24 | - | 20/53/53/53 | - |
| 24 | CLA | v | 603 | 4 | 1/1/15/20 | 13/37/115/115 | - |
| 24 | CLA | Aw | 102 | - | 1/1/15/20 | 14/37/115/115 | - |
| 27 | LHG | W | 201 | - | - | 15/53/53/53 | - |
| 25 | LUT | 7 | 317 | - | - | 1/29/67/67 | 0/2/2/2 |
| 38 | PHO | R | 408 | - | - | 15/37/103/103 | 0/5/6/6 |
| 24 | CLA | b | 611 | - | 1/1/15/20 | 13/37/115/115 | - |
| 24 | CLA | v | 614 | - | 1/1/15/20 | 20/37/115/115 | - |
| 24 | CLA | AA | 303 | 1 | 1/1/14/20 | 6/33/111/115 | - |
| 24 | CLA | A6 | 609 | 14 | 1/1/12/20 | 2/19/99/115 | - |
| 23 | CHL | N | 609 | 8 | 3/3/19/26 | 12/33/131/137 | - |
| 23 | CHL | n | 607 | - | 3/3/19/26 | 16/33/131/137 | - |
| 23 | CHL | Au | 608 | - | 3/3/19/26 | 22/33/131/137 | - |
| 24 | CLA | Au | 612 | - | 1/1/14/20 | 8/31/109/115 | - |
| 24 | CLA | I | 102 | - | 1/1/15/20 | 14/37/115/115 | - |
| 27 | LHG | c | 519 | - | - | 26/53/53/53 | - |
| 29 | BCR | z | 102 | - | - | 7/29/63/63 | 0/2/2/2 |
| 25 | LUT | 0 | 615 | - | - | 2/29/67/67 | 0/2/2/2 |
| 24 | CLA | BU | 611 | 22 | 1/1/11/20 | 6/18/96/115 | - |
| 24 | CLA | BJ | 610 | 8 | 1/1/14/20 | 19/36/114/115 | - |
| 23 | CHL | S | 605 | 14 | 3/3/16/26 | 9/15/113/137 | - |
| 29 | BCR | 1 | 514 | - | - | 3/29/63/63 | 0/2/2/2 |
| 24 | CLA | 1 | 508 | 21 | 1/1/15/20 | 16/37/115/115 | - |
| 23 | CHL | G | 609 | - | 3/3/17/26 | 8/21/121/137 | - |
| 24 | CLA | C | 511 | 21 | 1/1/15/20 | 11/37/115/115 | - |
| 23 | CHL | s | 607 | - | 3/3/16/26 | 9/15/113/137 | - |
| 30 | LMG | 1 | 501 | - | - | 18/46/66/70 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24 | CLA | B | 608 | 4 | 1/1/15/20 | 13/37/115/115 | - |
| 24 | CLA | Y | 315 | - | 1/1/11/20 | 6/17/95/115 | - |
| 25 | LUT | 5 | 615 | - | - | 3/29/67/67 | 0/2/2/2 |
| 24 | CLA | S | 604 | - | 1/1/12/20 | 7/19/97/115 | - |
| 23 | CHL | Ba | 309 | - | 3/3/19/26 | 15/33/131/137 | - |
| 24 | CLA | Au | 613 | - | 1/1/15/20 | 12/37/115/115 | - |
| 23 | CHL | A2 | 606 | 8 | 3/3/16/26 | 8/20/118/137 | - |
| 23 | CHL | A6 | 607 | 14 | 3/3/16/26 | 12/15/113/137 | - |
| 24 | CLA | 0 | 613 | - | 1/1/13/20 | 11/29/107/115 | - |
| 30 | LMG | Aw | 101 | - | - | 12/35/55/70 | 0/1/1/1 |
| 25 | LUT | A2 | 615 | - | - | 1/29/67/67 | 0/2/2/2 |
| 24 | CLA | BB | 311 | 8 | 1/1/14/20 | 11/31/109/115 | - |
| 24 | CLA | v | 611 | 4 | 1/1/15/20 | 11/37/115/115 | - |
| 24 | CLA | BU | 610 | 27 | 1/1/11/20 | 8/18/96/115 | - |
| 24 | CLA | BV | 603 | 14 | 1/1/11/20 | 4/13/91/115 | - |
| 25 | LUT | AB | 311 | - | - | 1/29/67/67 | 0/2/2/2 |
| 29 | BCR | f | 101 | - | - | 11/29/63/63 | 0/2/2/2 |
| 23 | CHL | BQ | 607 | - | 3/3/19/26 | 16/33/131/137 | - |
| 26 | NEX | BV | 616 | - | - | 15/27/83/83 | 0/3/3/3 |
| 24 | CLA | G | 611 | 27 | 1/1/14/20 | 9/31/109/115 | - |
| 25 | LUT | 9 | 615 | - | - | 3/29/67/67 | 0/2/2/2 |
| 38 | PHO | R | 407 | - | - | 7/37/103/103 | 0/5/6/6 |
| 25 | LUT | G | 616 | - | - | 2/29/67/67 | 0/2/2/2 |
| 23 | CHL | BV | 607 | - | 3/3/16/26 | 10/15/113/137 | - |
| 24 | CLA | BE | 609 | 4 | 1/1/15/20 | 13/37/115/115 | - |
| 24 | CLA | 6 | 604 | - | 1/1/11/20 | 10/13/91/115 | - |
| 24 | CLA | N | 614 | - | 1/1/11/20 | 8/17/95/115 | - |
| 23 | CHL | 9 | 606 | 1 | 3/3/16/26 | 3/15/113/137 | - |
| 27 | LHG | BG | 404 | - | - | 18/53/53/53 | - |
| 24 | CLA | AB | 309 | - | 1/1/11/20 | 3/13/91/115 | - |
| 24 | CLA | r | 603 | 22 | 1/1/14/20 | 7/31/109/115 | - |
| 24 | CLA | 0 | 603 | - | 1/1/13/20 | 8/25/103/115 | - |
| 24 | CLA | c | 510 | 21 | 1/1/15/20 | 8/37/115/115 | - |
| 34 | DGD | BD | 401 | - | - | 21/48/88/95 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24 | CLA | BJ | 614 | 8 | 1/1/11/20 | 5/17/95/115 | - |
| 24 | CLA | B | 609 | - | 1/1/15/20 | 13/37/115/115 | - |
| 28 | XAT | 7 | 301 | - | - | 11/31/93/93 | 0/4/4/4 |
| 29 | BCR | R | 410 | - | - | 5/29/63/63 | 0/2/2/2 |
| 24 | CLA | v | 615 | - | 1/1/15/20 | 17/37/115/115 | - |
| 30 | LMG | BG | 405 | - | - | 14/41/61/70 | 0/1/1/1 |
| 34 | DGD | C | 518 | - | - | 20/49/89/95 | 0/2/2/2 |
| 23 | CHL | y | 310 | - | 3/3/19/26 | 20/33/131/137 | - |
| 24 | CLA | A2 | 610 | - | 1/1/15/20 | 15/37/115/115 | - |
| 23 | CHL | 7 | 302 | 1 | 3/3/16/26 | 6/15/113/137 | - |
| 24 | CLA | G | 602 | 8 | 1/1/15/20 | 13/37/115/115 | - |
| 24 | CLA | c | 509 | 21 | 1/1/15/20 | 16/37/115/115 | - |
| 24 | CLA | BU | 612 | 22 | 1/1/7/20 | 0/2/72/115 | - |
| 24 | CLA | S | 602 | 14 | 1/1/14/20 | 13/33/111/115 | - |
| 25 | LUT | g | 616 | - | - | 1/29/67/67 | 0/2/2/2 |
| 28 | XAT | y | 301 | - | - | 15/31/93/93 | 0/4/4/4 |
| 24 | CLA | 1 | 511 | 21 | 1/1/15/20 | 12/37/115/115 | - |
| 34 | DGD | 1 | 518 | - | - | 20/49/89/95 | 0/2/2/2 |
| 26 | NEX | Y | 318 | - | - | 12/27/83/83 | 0/3/3/3 |
| 24 | CLA | BE | 614 | - | 1/1/15/20 | 12/37/115/115 | - |
| 23 | CHL | BJ | 601 | 8 | 3/3/19/26 | 17/33/131/137 | - |
| 24 | CLA | 6 | 603 | - | 1/1/13/20 | 9/25/103/115 | - |
| 24 | CLA | BF | 510 | 21 | 1/1/15/20 | 8/37/115/115 | - |
| 24 | CLA | A2 | 603 | 8 | 1/1/15/20 | 11/37/115/115 | - |
| 23 | CHL | 7 | 309 | - | 3/3/16/26 | 8/15/113/137 | - |
| 24 | CLA | BV | 610 | - | 1/1/13/20 | 10/27/105/115 | - |
| 24 | CLA | G | 613 | - | 1/1/15/20 | 12/37/115/115 | - |
| 26 | NEX | y | 318 | - | - | 13/27/83/83 | 0/3/3/3 |
| 27 | LHG | 6 | 617 | 24 | - | 13/51/51/53 | - |
| 29 | BCR | B | 619 | - | - | 6/29/63/63 | 0/2/2/2 |
| 24 | CLA | N | 611 | 27 | 1/1/14/20 | 13/31/109/115 | - |
| 24 | CLA | n | 610 | 8 | 1/1/15/20 | 14/37/115/115 | - |
| 24 | CLA | BQ | 611 | 27 | 1/1/14/20 | 12/31/109/115 | - |
| 24 | CLA | b | 610 | - | 1/1/15/20 | 12/37/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 32 | SQD | D | 406 | - | - | 21/45/65/69 | 0/1/1/1 |
| 30 | LMG | v | 623 | - | - | 16/35/55/70 | 0/1/1/1 |
| 29 | BCR | Ay | 102 | - | - | 6/29/63/63 | 0/2/2/2 |
| 30 | LMG | d | 405 | - | - | 14/41/61/70 | 0/1/1/1 |
| 24 | CLA | BJ | 611 | 27 | 1/1/14/20 | 9/31/109/115 | - |
| 23 | CHL | g | 608 | - | 3/3/19/26 | 21/33/131/137 | - |
| 23 | CHL | r | 607 | 22 | 3/3/18/26 | 19/27/125/137 | - |
| 29 | BCR | v | 619 | - | - | 7/29/63/63 | 0/2/2/2 |
| 32 | SQD | BO | 101 | - | - | 21/49/69/69 | 0/1/1/1 |
| 24 | CLA | b | 603 | 4 | 1/1/15/20 | 14/37/115/115 | - |
| 24 | CLA | a | 406 | - | 1/1/15/20 | 7/37/115/115 | - |
| 24 | CLA | s | 610 | - | 1/1/13/20 | 10/27/105/115 | - |
| 24 | CLA | C | 508 | 21 | 1/1/15/20 | 15/37/115/115 | - |
| 27 | LHG | C | 521 | - | - | 23/53/53/53 | - |
| 27 | LHG | B | 621 | - | - | 23/53/53/53 | - |
| 23 | CHL | A2 | 601 | 8 | 3/3/19/26 | 17/33/131/137 | - |
| 23 | CHL | AA | 307 | 1 | 3/3/16/26 | 6/15/113/137 | - |
| 24 | CLA | BF | 512 | 21 | 1/1/15/20 | 11/37/115/115 | - |
| 29 | BCR | 4 | 101 | - | - | 8/29/63/63 | 0/2/2/2 |
| 24 | CLA | N | 604 | - | 1/1/12/20 | 9/19/97/115 | - |
| 27 | LHG | b | 624 | - | - | 19/53/53/53 | - |
| 23 | CHL | AB | 307 | 3 | 3/3/16/26 | 8/15/113/137 | - |
| 24 | CLA | b | 607 | - | 1/1/15/20 | 14/37/115/115 | - |
| 23 | CHL | AB | 306 | - | 3/3/16/26 | 5/15/113/137 | - |
| 23 | CHL | Y | 302 | 8 | 3/3/19/26 | 15/33/131/137 | - |
| 23 | CHL | 0 | 607 | - | 3/3/17/26 | 12/24/122/137 | - |
| 24 | CLA | s | 603 | 14 | 1/1/11/20 | 4/13/91/115 | - |
| 24 | CLA | BF | 514 | - | 1/1/15/20 | 13/37/115/115 | - |
| 24 | CLA | A6 | 610 | - | 1/1/13/20 | 10/27/105/115 | - |
| 24 | CLA | BE | 611 | - | 1/1/15/20 | 14/37/115/115 | - |
| 23 | CHL | BV | 601 | - | 3/3/16/26 | 6/15/113/137 | - |
| 24 | CLA | n | 614 | - | 1/1/11/20 | 7/17/95/115 | - |
| 25 | LUT | BJ | 616 | - | - | 1/29/67/67 | 0/2/2/2 |
| 28 | XAT | BQ | 619 | - | - | 19/31/93/93 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 27 | LHG | b | 623 | - | - | 15/50/50/53 | - |
| 24 | CLA | Ba | 304 | - | 1/1/15/20 | 9/37/115/115 | - |
| 24 | CLA | 6 | 614 | 2 | 1/1/11/20 | 10/17/95/115 | - |
| 24 | CLA | b | 612 | 4 | 1/1/15/20 | 12/37/115/115 | - |
| 27 | LHG | BF | 520 | - | - | 27/53/53/53 | - |
| 25 | LUT | n | 616 | - | - | 1/29/67/67 | 0/2/2/2 |
| 25 | LUT | BU | 615 | - | - | 3/29/67/67 | 0/2/2/2 |
| 23 | CHL | 9 | 605 | 1 | 3/3/16/26 | 5/15/113/137 | - |
| 24 | CLA | 1 | 510 | 21 | 1/1/15/20 | 16/37/115/115 | - |
| 30 | LMG | BF | 519 | - | - | 22/46/66/70 | 0/1/1/1 |
| 24 | CLA | BV | 604 | - | 1/1/12/20 | 6/19/97/115 | - |
| 24 | CLA | BD | 410 | - | 1/1/14/20 | 9/31/109/115 | - |
| 25 | LUT | Y | 316 | - | - | 3/29/67/67 | 0/2/2/2 |
| 27 | LHG | 5 | 618 | 24 | - | 18/45/45/53 | - |
| 24 | CLA | s | 612 | 14 | 1/1/13/20 | 10/25/103/115 | - |
| 23 | CHL | BB | 307 | - | 3/3/16/26 | 8/20/118/137 | - |
| 27 | LHG | 2 | 406 | - | - | 18/53/53/53 | - |
| 26 | NEX | BB | 318 | - | - | 10/27/83/83 | 0/3/3/3 |
| 29 | BCR | b | 620 | - | - | 4/29/63/63 | 0/2/2/2 |
| 24 | CLA | BE | 608 | - | 1/1/15/20 | 19/37/115/115 | - |
| 23 | CHL | AB | 304 | 3 | 3/3/16/26 | 10/15/113/137 | - |
| 23 | CHL | A6 | 601 | 14 | 3/3/16/26 | 5/15/113/137 | - |
| 24 | CLA | AB | 301 | 3 | 1/1/9/20 | 5/7/81/115 | - |
| 34 | DGD | H | 102 | - | - | 14/51/91/95 | 0/2/2/2 |
| 23 | CHL | 7 | 306 | 1 | 3/3/16/26 | 5/15/113/137 | - |
| 24 | CLA | c | 512 | 21 | 1/1/15/20 | 10/37/115/115 | - |
| 23 | CHL | g | 607 | - | 3/3/19/26 | 18/33/131/137 | - |
| 23 | CHL | BU | 606 | - | 3/3/17/26 | 6/24/122/137 | - |
| 28 | XAT | BJ | 619 | - | - | 12/31/93/93 | 0/4/4/4 |
| 29 | BCR | a | 411 | - | - | 5/29/63/63 | 0/2/2/2 |
| 24 | CLA | G | 604 | - | 1/1/12/20 | 6/19/97/115 | - |
| 24 | CLA | A2 | 612 | - | 1/1/14/20 | 6/31/109/115 | - |
| 30 | LMG | BE | 621 | - | - | 23/46/66/70 | 0/1/1/1 |
| 24 | CLA | Y | 305 | - | 1/1/12/20 | 11/19/97/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24 | CLA | n | 613 | - | 1/1/14/20 | 9/31/109/115 | - |
| 24 | CLA | BF | 507 | 21 | 1/1/15/20 | 17/37/115/115 | - |
| 29 | BCR | k | 101 | - | - | 11/29/63/63 | 0/2/2/2 |
| 29 | BCR | H | 101 | - | - | 5/29/63/63 | 0/2/2/2 |
| 23 | CHL | r | 605 | 22 | 3/3/19/26 | 22/33/131/137 | - |
| 24 | CLA | AB | 310 | - | 1/1/11/20 | 5/13/91/115 | - |
| 24 | CLA | B | 602 | 4 | 1/1/15/20 | 15/37/115/115 | - |
| 24 | CLA | C | 505 | - | 1/1/15/20 | 8/37/115/115 | - |
| 23 | CHL | AA | 302 | 1 | 3/3/16/26 | 6/15/113/137 | - |
| 23 | CHL | s | 606 | - | 3/3/17/26 | 8/24/122/137 | - |
| 23 | CHL | y | 302 | 8 | 3/3/19/26 | 14/33/131/137 | - |
| 24 | CLA | BV | 612 | 14 | 1/1/13/20 | 10/25/103/115 | - |
| 27 | LHG | c | 520 | - | - | 22/53/53/53 | - |
| 27 | LHG | l | 520 | - | - | 25/53/53/53 | - |
| 24 | CLA | A6 | 603 | - | 1/1/11/20 | 5/13/91/115 | - |
| 24 | CLA | AA | 315 | 1 | 1/1/11/20 | 3/13/91/115 | - |
| 23 | CHL | Ba | 307 | - | 3/3/16/26 | 7/20/118/137 | - |
| 25 | LUT | BQ | 615 | - | - | 1/29/67/67 | 0/2/2/2 |
| 27 | LHG | BF | 521 | - | - | 22/53/53/53 | - |
| 24 | CLA | b | 605 | 4 | 1/1/15/20 | 19/37/115/115 | - |
| 23 | CHL | n | 609 | - | 3/3/19/26 | 15/33/131/137 | - |
| 23 | CHL | G | 606 | - | 3/3/16/26 | 7/20/118/137 | - |
| 24 | CLA | A2 | 613 | 8 | 1/1/14/20 | 11/31/109/115 | - |
| 24 | CLA | 7 | 304 | - | 1/1/13/20 | 10/25/103/115 | - |
| 29 | BCR | c | 515 | - | - | 6/29/63/63 | 0/2/2/2 |
| 24 | CLA | y | 304 | - | 1/1/15/20 | 9/37/115/115 | - |
| 24 | CLA | r | 610 | 27 | 1/1/11/20 | 9/18/96/115 | - |
| 24 | CLA | Y | 312 | - | 1/1/14/20 | 11/31/109/115 | - |
| 24 | CLA | BU | 603 | 22 | 1/1/14/20 | 8/31/109/115 | - |
| 38 | PHO | a | 409 | - | - | 15/37/103/103 | 0/5/6/6 |
| 23 | CHL | BV | 606 | - | 3/3/17/26 | 8/24/122/137 | - |
| 24 | CLA | g | 610 | 8 | 1/1/14/20 | 19/36/114/115 | - |
| 24 | CLA | BV | 613 | 14 | 1/1/11/20 | 6/18/96/115 | - |
| 24 | CLA | Au | 604 | - | 1/1/12/20 | 6/19/97/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24 | CLA | b | 606 | 4 | 1/1/15/20 | 16/37/115/115 | - |
| 28 | XAT | Ba | 301 | - | - | 15/31/93/93 | 0/4/4/4 |
| 29 | BCR | C | 514 | - | - | 3/29/63/63 | 0/2/2/2 |
| 23 | CHL | r | 613 | 22 | 3/3/15/26 | 2/10/108/137 | - |
| 24 | CLA | S | 603 | - | 1/1/11/20 | 5/13/91/115 | - |
| 24 | CLA | c | 505 | - | 1/1/15/20 | 10/37/115/115 | - |
| 23 | CHL | BB | 302 | 8 | 3/3/19/26 | 16/33/131/137 | - |
| 29 | BCR | b | 619 | - | - | 7/29/63/63 | 0/2/2/2 |
| 30 | LMG | v | 620 | - | - | 18/46/66/70 | 0/1/1/1 |
| 29 | BCR | BD | 411 | - | - | 5/29/63/63 | 0/2/2/2 |
| 24 | CLA | D | 402 | - | 1/1/15/20 | 11/37/115/115 | - |
| 24 | CLA | BG | 402 | - | 1/1/15/20 | 10/37/115/115 | - |
| 28 | XAT | 9 | 619 | - | - | 16/31/93/93 | 0/4/4/4 |
| 23 | CHL | 5 | 608 | - | 3/3/16/26 | 7/15/113/137 | - |
| 24 | CLA | s | 613 | 14 | 1/1/11/20 | 7/18/96/115 | - |
| 24 | CLA | Ba | 305 | - | 1/1/12/20 | 9/19/97/115 | - |
| 23 | CHL | N | 608 | - | 3/3/19/26 | 14/33/131/137 | - |
| 27 | LHG | A2 | 618 | 24 | - | 17/53/53/53 | - |
| 24 | CLA | BB | 312 | - | 1/1/14/20 | 11/31/109/115 | - |
| 24 | CLA | Y | 311 | 8 | 1/1/14/20 | 11/31/109/115 | - |
| 26 | NEX | 9 | 617 | - | - | 17/27/83/83 | 0/3/3/3 |
| 27 | LHG | BJ | 618 | 24 | - | 18/53/53/53 | - |
| 23 | CHL | Au | 607 | - | 3/3/19/26 | 15/33/131/137 | - |
| 24 | CLA | BQ | 602 | 8 | 1/1/15/20 | 16/37/115/115 | - |
| 24 | CLA | N | 602 | 8 | 1/1/15/20 | 13/37/115/115 | - |
| 24 | CLA | b | 609 | 4 | 1/1/15/20 | 13/37/115/115 | - |
| 24 | CLA | r | 604 | - | 1/1/11/20 | 9/17/95/115 | - |
| 23 | CHL | Ba | 306 | 8 | 3/3/16/26 | 7/18/116/137 | - |
| 32 | SQD | R | 411 | - | - | 26/49/69/69 | 0/1/1/1 |
| 28 | XAT | A2 | 619 | - | - | 17/31/93/93 | 0/4/4/4 |
| 27 | LHG | n | 618 | 24 | - | 20/53/53/53 | - |
| 23 | CHL | g | 601 | 8 | 3/3/19/26 | 16/33/131/137 | - |
| 24 | CLA | Y | 313 | - | 1/1/14/20 | 9/31/109/115 | - |
| 30 | LMG | A0 | 201 | - | - | 16/43/63/70 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24 | CLA | 8 | 303 | - | 1/1/11/20 | 5/13/91/115 | - |
| 34 | DGD | C | 516 | - | - | 13/44/84/95 | 0/2/2/2 |
| 24 | CLA | A | 407 | - | 1/1/12/20 | 5/19/97/115 | - |
| 24 | CLA | C | 509 | 21 | 1/1/15/20 | 8/37/115/115 | - |
| 25 | LUT | N | 615 | - | - | 1/29/67/67 | 0/2/2/2 |
| 23 | CHL | Y | 309 | - | 3/3/19/26 | 14/33/131/137 | - |
| 24 | CLA | BF | 503 | 21 | 1/1/15/20 | 15/37/115/115 | - |
| 27 | LHG | B | 622 | - | - | 16/50/50/53 | - |
| 25 | LUT | y | 316 | - | - | 2/29/67/67 | 0/2/2/2 |
| 23 | CHL | 8 | 304 | - | 3/3/16/26 | 9/15/113/137 | - |
| 27 | LHG | A0 | 202 | - | - | 14/53/53/53 | - |
| 24 | CLA | BG | 401 | 5 | 1/1/15/20 | 16/37/115/115 | - |
| 23 | CHL | 8 | 306 | - | 3/3/16/26 | 6/15/113/137 | - |
| 24 | CLA | g | 604 | - | 1/1/12/20 | 9/19/97/115 | - |
| 24 | CLA | BV | 602 | 14 | 1/1/14/20 | 9/33/111/115 | - |
| 25 | LUT | BJ | 615 | - | - | 2/29/67/67 | 0/2/2/2 |
| 26 | NEX | 7 | 319 | - | - | 22/27/83/83 | 0/3/3/3 |
| 26 | NEX | N | 617 | - | - | 15/27/83/83 | 0/3/3/3 |
| 24 | CLA | A | 406 | - | 1/1/15/20 | 6/37/115/115 | - |
| 29 | BCR | AB | 313 | - | - | 16/29/63/63 | 0/2/2/2 |
| 24 | CLA | BE | 612 | 4 | 1/1/15/20 | 11/37/115/115 | - |
| 23 | CHL | S | 607 | - | 3/3/16/26 | 9/15/113/137 | - |
| 29 | BCR | BE | 601 | - | - | 15/29/63/63 | 0/2/2/2 |
| 24 | CLA | 5 | 604 | - | 1/1/12/20 | 10/19/97/115 | - |
| 25 | LUT | n | 615 | - | - | 1/29/67/67 | 0/2/2/2 |
| 24 | CLA | BB | 315 | - | 1/1/11/20 | 6/17/95/115 | - |
| 24 | CLA | BD | 405 | 20 | 1/1/15/20 | 7/37/115/115 | - |
| 34 | DGD | Av | 102 | - | - | 14/51/91/95 | 0/2/2/2 |
| 25 | LUT | s | 614 | - | - | 2/29/67/67 | 0/2/2/2 |
| 26 | NEX | BB | 320 | - | - | 17/27/83/83 | 0/3/3/3 |
| 24 | CLA | AA | 311 | 1 | 1/1/11/20 | 4/13/93/115 | - |
| 24 | CLA | A2 | 614 | - | 1/1/11/20 | 8/17/95/115 | - |
| 24 | CLA | BB | 304 | 8 | 1/1/15/20 | 9/37/115/115 | - |
| 24 | CLA | Ba | 315 | - | 1/1/11/20 | 6/17/95/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 29 | BCR | B | 618 | - | - | 7/29/63/63 | 0/2/2/2 |
| 24 | CLA | BF | 502 | 21 | 1/1/15/20 | 14/37/115/115 | - |
| 23 | CHL | 6 | 605 | 2 | 3/3/16/26 | 5/15/113/137 | - |
| 23 | CHL | y | 307 | - | 3/3/16/26 | 7/20/118/137 | - |
| 24 | CLA | r | 614 | - | 1/1/11/20 | 7/13/91/115 | - |
| 27 | LHG | BB | 319 | - | - | 18/53/53/53 | - |
| 26 | NEX | g | 617 | - | - | 17/27/83/83 | 0/3/3/3 |
| 24 | CLA | BF | 509 | 21 | 1/1/15/20 | 16/37/115/115 | - |
| 29 | BCR | Bb | 101 | - | - | 7/29/63/63 | 0/2/2/2 |
| 24 | CLA | r | 612 | 22 | 1/1/7/20 | 0/2/72/115 | - |
| 28 | XAT | AB | 312 | - | - | 16/31/93/93 | 0/4/4/4 |
| 24 | CLA | g | 614 | 8 | 1/1/11/20 | 5/17/95/115 | - |
| 24 | CLA | BJ | 613 | - | 1/1/15/20 | 13/37/115/115 | - |
| 26 | NEX | 5 | 617 | - | - | 17/27/83/83 | 0/3/3/3 |
| 24 | CLA | AA | 314 | 1 | 1/1/11/20 | 7/13/91/115 | - |
| 27 | LHG | Au | 618 | 24 | - | 17/53/53/53 | - |
| 32 | SQD | BD | 412 | - | - | 28/49/69/69 | 0/1/1/1 |
| 25 | LUT | BV | 614 | - | - | 2/29/67/67 | 0/2/2/2 |
| 23 | CHL | 5 | 607 | - | 3/3/18/26 | 19/30/128/137 | - |
| 24 | CLA | Y | 314 | 8 | 1/1/15/20 | 14/37/115/115 | - |
| 24 | CLA | BE | 615 | - | 1/1/15/20 | 18/37/115/115 | - |
| 24 | CLA | 7 | 305 | - | 1/1/11/20 | 7/13/91/115 | - |
| 24 | CLA | R | 409 | - | 1/1/14/20 | 11/31/109/115 | - |
| 23 | CHL | 0 | 601 | 2 | 3/3/18/26 | 15/31/129/137 | - |
| 26 | NEX | Ba | 318 | - | - | 13/27/83/83 | 0/3/3/3 |
| 24 | CLA | v | 602 | 4 | 1/1/15/20 | 15/37/115/115 | - |
| 24 | CLA | A6 | 608 | - | 1/1/11/20 | 4/13/91/115 | - |
| 24 | CLA | BU | 602 | 22 | 1/1/13/20 | 8/25/105/115 | - |
| 27 | LHG | Y | 319 | - | - | 20/53/53/53 | - |
| 24 | CLA | S | 610 | - | 1/1/13/20 | 10/27/105/115 | - |
| 24 | CLA | S | 611 | - | 1/1/11/20 | 4/18/96/115 | - |
| 24 | CLA | BU | 604 | - | 1/1/11/20 | 10/17/95/115 | - |
| 38 | PHO | A | 409 | - | - | 16/37/103/103 | 0/5/6/6 |
| 23 | CHL | BJ | 609 | - | 3/3/18/26 | 10/27/125/137 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24 | CLA | n | 612 | - | 1/1/14/20 | 6/31/109/115 | - |
| 24 | CLA | v | 606 | - | 1/1/15/20 | 17/37/115/115 | - |
| 24 | CLA | B | 610 | - | 1/1/15/20 | 14/37/115/115 | - |
| 25 | LUT | AA | 316 | - | - | 3/29/67/67 | 0/2/2/2 |
| 23 | CHL | 9 | 608 | - | 3/3/16/26 | 7/15/113/137 | - |
| 24 | CLA | A2 | 611 | 27 | 1/1/14/20 | 13/31/109/115 | - |
| 24 | CLA | C | 513 | 21 | 1/1/15/20 | 14/37/115/115 | - |
| 29 | BCR | b | 601 | - | - | 15/29/63/63 | 0/2/2/2 |
| 24 | CLA | BB | 303 | 8 | 1/1/15/20 | 23/37/115/115 | - |
| 27 | LHG | w | 201 | - | - | 16/53/53/53 | - |
| 23 | CHL | y | 309 | - | 3/3/19/26 | 14/33/131/137 | - |
| 24 | CLA | BJ | 603 | 8 | 1/1/15/20 | 11/37/115/115 | - |
| 27 | LHG | C | 520 | - | - | 25/53/53/53 | - |
| 26 | NEX | r | 617 | - | - | 17/27/83/83 | 0/3/3/3 |
| 24 | CLA | s | 602 | 14 | 1/1/14/20 | 12/33/111/115 | - |
| 25 | LUT | Y | 317 | - | - | 1/29/67/67 | 0/2/2/2 |
| 27 | LHG | BU | 617 | 24 | - | 12/46/46/53 | - |
| 23 | CHL | 6 | 609 | - | 3/3/18/26 | 10/27/125/137 | - |
| 24 | CLA | c | 506 | - | 1/1/15/20 | 13/37/115/115 | - |
| 23 | CHL | n | 608 | - | 3/3/19/26 | 13/33/131/137 | - |
| 24 | CLA | 9 | 613 | 1 | 1/1/13/20 | 9/25/103/115 | - |
| 34 | DGD | c | 516 | - | - | 14/44/84/95 | 0/2/2/2 |
| 28 | XAT | BU | 616 | - | - | 17/31/93/93 | 0/4/4/4 |
| 24 | CLA | 2 | 403 | - | 1/1/15/20 | 11/37/115/115 | - |
| 29 | BCR | A | 411 | - | - | 5/29/63/63 | 0/2/2/2 |
| 24 | CLA | Ba | 313 | - | 1/1/14/20 | 12/31/109/115 | - |
| 24 | CLA | BF | 506 | - | 1/1/15/20 | 14/37/115/115 | - |
| 28 | XAT | n | 619 | - | - | 19/31/93/93 | 0/4/4/4 |
| 24 | CLA | 8 | 302 | - | 1/1/11/20 | 4/13/91/115 | - |
| 24 | CLA | 9 | 614 | 1 | 1/1/11/20 | 6/13/91/115 | - |
| 24 | CLA | 0 | 614 | 2 | 1/1/11/20 | 9/17/95/115 | - |
| 23 | CHL | A2 | 609 | 8 | 3/3/19/26 | 11/33/131/137 | - |
| 24 | CLA | S | 609 | 14 | 1/1/12/20 | 2/19/99/115 | - |
| 29 | BCR | BK | 101 | - | - | 6/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24 | CLA | 7 | 313 | - | 1/1/11/20 | 5/13/91/115 | - |
| 24 | CLA | a | 405 | 20 | 1/1/15/20 | 7/37/115/115 | - |
| 30 | LMG | D | 405 | - | - | 13/41/61/70 | 0/1/1/1 |
| 24 | CLA | 5 | 603 | 1 | 1/1/13/20 | 10/25/103/115 | - |
| 24 | CLA | A6 | 612 | 14 | 1/1/13/20 | 11/25/103/115 | - |
| 24 | CLA | BU | 601 | 22 | 1/1/11/20 | 9/18/96/115 | - |
| 29 | BCR | BF | 516 | - | - | 6/29/63/63 | 0/2/2/2 |
| 24 | CLA | S | 608 | - | 1/1/11/20 | 4/13/91/115 | - |
| 24 | CLA | BF | 513 | - | 1/1/15/20 | 13/37/115/115 | - |
| 23 | CHL | N | 605 | 8 | 3/3/16/26 | 9/18/116/137 | - |
| 29 | BCR | v | 622 | - | - | 13/29/63/63 | 0/2/2/2 |
| 24 | CLA | s | 611 | - | 1/1/11/20 | 4/18/96/115 | - |
| 24 | CLA | v | 604 | 4 | 1/1/15/20 | 14/37/115/115 | - |
| 29 | BCR | Av | 101 | - | - | 4/29/63/63 | 0/2/2/2 |
| 24 | CLA | 9 | 604 | - | 1/1/12/20 | 10/19/97/115 | - |
| 24 | CLA | v | 610 | - | 1/1/15/20 | 15/37/115/115 | - |
| 30 | LMG | B | 624 | - | - | 17/35/55/70 | 0/1/1/1 |
| 23 | CHL | 9 | 601 | 1 | 3/3/16/26 | 9/15/113/137 | - |
| 24 | CLA | Y | 303 | 8 | 1/1/15/20 | 22/37/115/115 | - |
| 27 | LHG | BE | 624 | - | - | 19/53/53/53 | - |
| 30 | LMG | B | 620 | - | - | 18/46/66/70 | 0/1/1/1 |
| 34 | DGD | 1 | 517 | - | - | 21/51/91/95 | 0/2/2/2 |
| 29 | BCR | K | 101 | - | - | 11/29/63/63 | 0/2/2/2 |
| 27 | LHG | d | 404 | - | - | 16/53/53/53 | - |
| 26 | NEX | S | 616 | - | - | 15/27/83/83 | 0/3/3/3 |
| 24 | CLA | BB | 314 | 8 | 1/1/15/20 | 13/37/115/115 | - |
| 24 | CLA | N | 610 | - | 1/1/15/20 | 16/37/115/115 | - |
| 28 | XAT | BB | 301 | - | - | 17/31/93/93 | 0/4/4/4 |
| 24 | CLA | BJ | 612 | - | 1/1/14/20 | 6/31/109/115 | - |
| 24 | CLA | BV | 611 | - | 1/1/11/20 | 5/18/96/115 | - |
| 24 | CLA | c | 508 | - | 1/1/15/20 | 12/37/115/115 | - |
| 23 | CHL | 5 | 605 | 1 | 3/3/16/26 | 5/15/113/137 | - |
| 24 | CLA | BB | 305 | - | 1/1/12/20 | 11/19/97/115 | - |
| 29 | BCR | C | 515 | - | - | 5/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 23 | CHL | AA | 309 | - | 3/3/16/26 | 8/15/113/137 | - |
| 28 | XAT | AA | 318 | - | - | 12/31/93/93 | 0/4/4/4 |
| 24 | CLA | n | 603 | 8 | 1/1/15/20 | 14/37/115/115 | - |
| 24 | CLA | C | 504 | 21 | 1/1/15/20 | 14/37/115/115 | - |
| 23 | CHL | 9 | 607 | - | 3/3/18/26 | 18/30/128/137 | - |
| 24 | CLA | a | 410 | - | 1/1/14/20 | 9/31/109/115 | - |
| 38 | PHO | A | 408 | - | - | 7/37/103/103 | 0/5/6/6 |
| 27 | LHG | BQ | 618 | 24 | - | 20/53/53/53 | - |
| 30 | LMG | i | 101 | - | - | 17/43/63/70 | 0/1/1/1 |
| 23 | CHL | 6 | 601 | 2 | 3/3/18/26 | 16/31/129/137 | - |
| 24 | CLA | v | 601 | - | 1/1/15/20 | 15/37/115/115 | - |
| 24 | CLA | A2 | 604 | - | 1/1/12/20 | 9/19/97/115 | - |
| 24 | CLA | A | 410 | - | 1/1/14/20 | 10/31/109/115 | - |
| 25 | LUT | BB | 316 | - | - | 3/29/67/67 | 0/2/2/2 |
| 23 | CHL | AA | 306 | 1 | 3/3/16/26 | 5/15/113/137 | - |
| 34 | DGD | BK | 102 | - | - | 18/51/91/95 | 0/2/2/2 |
| 27 | LHG | G | 618 | 24 | - | 17/53/53/53 | - |
| 24 | CLA | 5 | 610 | 1 | 1/1/13/20 | 6/27/105/115 | - |
| 25 | LUT | Ba | 316 | - | - | 2/29/67/67 | 0/2/2/2 |
| 28 | XAT | Y | 301 | - | - | 18/31/93/93 | 0/4/4/4 |
| 23 | CHL | Au | 605 | 8 | 3/3/16/26 | 7/15/113/137 | - |
| 24 | CLA | y | 314 | 8 | 1/1/15/20 | 15/37/115/115 | - |
| 24 | CLA | BF | 511 | 21 | 1/1/15/20 | 15/37/115/115 | - |
| 27 | LHG | BE | 622 | - | - | 24/53/53/53 | - |
| 24 | CLA | AB | 302 | - | 1/1/11/20 | 4/13/91/115 | - |
| 24 | CLA | y | 315 | - | 1/1/11/20 | 6/17/95/115 | - |
| 34 | DGD | BF | 518 | - | - | 21/51/91/95 | 0/2/2/2 |
| 24 | CLA | 1 | 502 | 21 | 1/1/15/20 | 15/37/115/115 | - |
| 34 | DGD | BF | 517 | - | - | 14/44/84/95 | 0/2/2/2 |
| 24 | CLA | B | 616 | 4 | 1/1/15/20 | 17/37/115/115 | - |
| 24 | CLA | BE | 607 | - | 1/1/15/20 | 14/37/115/115 | - |
| 24 | CLA | b | 616 | - | 1/1/15/20 | 10/37/115/115 | - |
| 24 | CLA | A6 | 611 | - | 1/1/11/20 | 4/18/96/115 | - |
| 33 | HEM | 4 | 102 | 7 | - | 5/12/54/54 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24 | CLA | A6 | 613 | 14 | 1/1/11/20 | 7/18/96/115 | - |
| 38 | PHO | BD | 409 | - | - | 15/37/103/103 | 0/5/6/6 |
| 24 | CLA | AA | 305 | - | 1/1/11/20 | 7/13/91/115 | - |
| 27 | LHG | D | 404 | - | - | 16/53/53/53 | - |
| 32 | SQD | Az | 101 | - | - | 18/37/57/69 | 0/1/1/1 |
| 24 | CLA | 7 | 311 | 1 | 1/1/11/20 | 4/13/93/115 | - |
| 24 | CLA | y | 312 | 27 | 1/1/14/20 | 11/31/109/115 | - |
| 24 | CLA | g | 612 | - | 1/1/14/20 | 6/31/109/115 | - |
| 25 | LUT | 6 | 616 | - | - | 1/29/67/67 | 0/2/2/2 |
| 24 | CLA | B | 614 | - | 1/1/15/20 | 19/37/115/115 | - |
| 23 | CHL | BQ | 605 | 8 | 3/3/16/26 | 7/18/116/137 | - |
| 24 | CLA | c | 514 | 21 | 1/1/15/20 | 14/37/115/115 | - |
| 23 | CHL | Ba | 310 | - | 3/3/19/26 | 19/33/131/137 | - |
| 24 | CLA | 5 | 612 | - | 1/1/11/20 | 6/13/91/115 | - |
| 29 | BCR | 8 | 313 | - | - | 16/29/63/63 | 0/2/2/2 |
| 24 | CLA | v | 607 | - | 1/1/15/20 | 20/37/115/115 | - |
| 32 | SQD | BG | 406 | - | - | 23/45/65/69 | 0/1/1/1 |
| 23 | CHL | G | 605 | 8 | 3/3/16/26 | 7/15/113/137 | - |
| 23 | CHL | n | 606 | 8 | 3/3/16/26 | 9/20/118/137 | - |
| 34 | DGD | c | 517 | - | - | 21/51/91/95 | 0/2/2/2 |
| 24 | CLA | 7 | 315 | 1 | 1/1/11/20 | 3/13/91/115 | - |
| 24 | CLA | Ba | 303 | 8 | 1/1/15/20 | 15/37/115/115 | - |
| 24 | CLA | 6 | 612 | - | 1/1/11/20 | 6/13/91/115 | - |
| 24 | CLA | 6 | 602 | 2 | 1/1/14/20 | 16/31/109/115 | - |
| 23 | CHL | S | 601 | 14 | 3/3/16/26 | 5/15/113/137 | - |
| 30 | LMG | C | 501 | - | - | 18/46/66/70 | 0/1/1/1 |
| 25 | LUT | A6 | 614 | - | - | 2/29/67/67 | 0/2/2/2 |
| 24 | CLA | S | 612 | 14 | 1/1/13/20 | 10/25/103/115 | - |
| 23 | CHL | BB | 309 | - | 3/3/19/26 | 14/33/131/137 | - |
| 27 | LHG | v | 621 | - | - | 23/53/53/53 | - |
| 24 | CLA | BE | 602 | - | 1/1/15/20 | 15/37/115/115 | - |
| 30 | LMG | 2 | 407 | - | - | 13/41/61/70 | 0/1/1/1 |
| 31 | PL9 | BG | 403 | - | - | 8/53/73/73 | 0/1/1/1 |
| 34 | DGD | R | 401 | - | - | 24/48/88/95 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 23 | CHL | A2 | 608 | - | 3/3/19/26 | 14/33/131/137 | - |
| 24 | CLA | BE | 610 | - | 1/1/15/20 | 14/37/115/115 | - |
| 24 | CLA | y | 303 | 8 | 1/1/15/20 | 16/37/115/115 | - |
| 24 | CLA | 6 | 611 | 27 | 1/1/13/20 | 12/25/103/115 | - |
| 23 | CHL | 7 | 310 | - | 3/3/18/26 | 14/27/125/137 | - |
| 24 | CLA | B | 603 | 4 | 1/1/15/20 | 12/37/115/115 | - |
| 23 | CHL | BQ | 608 | - | 3/3/19/26 | 13/33/131/137 | - |
| 32 | SQD | L | 103 | - | - | 18/49/69/69 | 0/1/1/1 |
| 24 | CLA | 1 | 513 | 21 | 1/1/15/20 | 14/37/115/115 | - |
| 24 | CLA | 8 | 309 | - | 1/1/11/20 | 3/13/91/115 | - |
| 24 | CLA | b | 602 | - | 1/1/15/20 | 16/37/115/115 | - |
| 25 | LUT | S | 615 | - | - | 0/29/67/67 | 0/2/2/2 |
| 24 | CLA | B | 611 | 4 | 1/1/15/20 | 11/37/115/115 | - |
| 24 | CLA | c | 503 | 21 | 1/1/15/20 | 15/37/115/115 | - |
| 32 | SQD | BO | 102 | - | - | 21/37/57/69 | 0/1/1/1 |
| 24 | CLA | d | 402 | - | 1/1/15/20 | 11/37/115/115 | - |
| 24 | CLA | 0 | 604 | - | 1/1/11/20 | 8/13/91/115 | - |
| 23 | CHL | Au | 601 | 8 | 3/3/19/26 | 17/33/131/137 | - |
| 24 | CLA | 9 | 610 | 1 | 1/1/13/20 | 6/27/105/115 | - |
| 23 | CHL | BB | 308 | - | 3/3/19/26 | 15/33/131/137 | - |
| 24 | CLA | 8 | 301 | 3 | 1/1/9/20 | 5/7/81/115 | - |
| 24 | CLA | B | 613 | 4 | 1/1/15/20 | 13/37/115/115 | - |
| 32 | SQD | 2 | 408 | - | - | 24/45/65/69 | 0/1/1/1 |
| 29 | BCR | b | 618 | - | - | 3/29/63/63 | 0/2/2/2 |
| 24 | CLA | BE | 605 | 4 | 1/1/15/20 | 19/37/115/115 | - |
| 24 | CLA | r | 611 | 22 | 1/1/11/20 | 6/18/96/115 | - |
| 24 | CLA | BB | 313 | - | 1/1/14/20 | 9/31/109/115 | - |
| 25 | LUT | BV | 615 | - | - | 1/29/67/67 | 0/2/2/2 |
| 32 | SQD | l | 101 | - | - | 21/49/69/69 | 0/1/1/1 |
| 29 | BCR | B | 617 | - | - | 5/29/63/63 | 0/2/2/2 |
| 24 | CLA | g | 611 | 27 | 1/1/14/20 | 9/31/109/115 | - |
| 32 | SQD | A | 413 | - | - | 26/49/69/69 | 0/1/1/1 |
| 26 | NEX | AA | 319 | - | - | 22/27/83/83 | 0/3/3/3 |
| 25 | LUT | N | 616 | - | - | 1/29/67/67 | 0/2/2/2 |
| 24 | CLA | v | 613 | 4 | 1/1/15/20 | 14/37/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24 | CLA | n | 611 | 27 | 1/1/14/20 | 12/31/109/115 | - |
| 24 | CLA | A | 405 | 20 | 1/1/15/20 | 8/37/115/115 | - |
| 24 | CLA | n | 602 | 8 | 1/1/15/20 | 16/37/115/115 | - |
| 24 | CLA | 1 | 503 | 21 | 1/1/15/20 | 13/37/115/115 | - |
| 26 | NEX | BJ | 617 | - | - | 17/27/83/83 | 0/3/3/3 |
| 23 | CHL | BU | 607 | 22 | 3/3/18/26 | 18/27/125/137 | - |
| 28 | XAT | 8 | 312 | - | - | 16/31/93/93 | 0/4/4/4 |
| 24 | CLA | AA | 312 | - | 1/1/11/20 | 9/13/91/115 | - |
| 24 | CLA | C | 506 | 21 | 1/1/15/20 | 15/37/115/115 | - |
| 24 | CLA | BQ | 604 | - | 1/1/12/20 | 9/19/97/115 | - |
| 23 | CHL | 7 | 308 | - | 3/3/18/26 | 13/27/125/137 | - |
| 24 | CLA | Au | 614 | - | 1/1/11/20 | 5/17/95/115 | - |
| 23 | CHL | Y | 310 | 8 | 3/3/19/26 | 17/33/131/137 | - |
| 29 | BCR | BE | 619 | - | - | 7/29/63/63 | 0/2/2/2 |
| 25 | LUT | s | 615 | - | - | 1/29/67/67 | 0/2/2/2 |
| 24 | CLA | v | 605 | 4 | 1/1/15/20 | 21/37/115/115 | - |
| 24 | CLA | BJ | 604 | - | 1/1/12/20 | 9/19/97/115 | - |
| 25 | LUT | S | 614 | - | - | 2/29/67/67 | 0/2/2/2 |
| 24 | CLA | 9 | 612 | - | 1/1/11/20 | 6/13/91/115 | - |
| 23 | CHL | A6 | 606 | - | 3/3/17/26 | 7/24/122/137 | - |
| 27 | LHG | BY | 201 | - | - | 16/53/53/53 | - |
| 24 | CLA | BQ | 603 | 8 | 1/1/15/20 | 12/37/115/115 | - |
| 25 | LUT | 5 | 616 | - | - | 2/29/67/67 | 0/2/2/2 |
| 24 | CLA | N | 603 | 8 | 1/1/15/20 | 11/37/115/115 | - |
| 23 | CHL | AB | 305 | - | 3/3/16/26 | 7/15/113/137 | - |
| 24 | CLA | r | 608 | 22 | 1/1/13/20 | 11/29/107/115 | - |
| 23 | CHL | 0 | 609 | - | 3/3/18/26 | 9/27/125/137 | - |
| 23 | CHL | 0 | 605 | 2 | 3/3/16/26 | 5/15/113/137 | - |
| 24 | CLA | 1 | 509 | 21 | 1/1/15/20 | 8/37/115/115 | - |
| 25 | LUT | Ba | 317 | - | - | 1/29/67/67 | 0/2/2/2 |
| 24 | CLA | b | 617 | 4 | 1/1/15/20 | 17/37/115/115 | - |
| 26 | NEX | BQ | 617 | - | - | 16/27/83/83 | 0/3/3/3 |
| 32 | SQD | d | 406 | - | - | 21/45/65/69 | 0/1/1/1 |
| 24 | CLA | AA | 304 | - | 1/1/13/20 | 10/25/103/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24 | CLA | BQ | 614 | - | 1/1/11/20 | 7/17/95/115 | - |
| 32 | SQD | L | 101 | - | - | 19/37/57/69 | 0/1/1/1 |
| 23 | CHL | BQ | 601 | 8 | 3/3/19/26 | 18/33/131/137 | - |
| 24 | CLA | N | 613 | 8 | 1/1/14/20 | 9/31/109/115 | - |
| 26 | NEX | G | 617 | - | - | 19/27/83/83 | 0/3/3/3 |
| 24 | CLA | BE | 604 | 4 | 1/1/15/20 | 13/37/115/115 | - |
| 26 | NEX | Au | 617 | - | - | 19/27/83/83 | 0/3/3/3 |
| 30 | LMG | BF | 501 | - | - | 22/46/66/70 | 0/1/1/1 |
| 25 | LUT | y | 317 | - | - | 1/29/67/67 | 0/2/2/2 |
| 23 | CHL | 0 | 606 | - | 3/3/16/26 | 7/15/113/137 | - |
| 24 | CLA | 7 | 314 | 1 | 1/1/11/20 | 7/13/91/115 | - |
| 24 | CLA | BE | 616 | - | 1/1/15/20 | 10/37/115/115 | - |
| 30 | LMG | 1 | 519 | - | - | 22/46/66/70 | 0/1/1/1 |
| 25 | LUT | Au | 616 | - | - | 2/29/67/67 | 0/2/2/2 |
| 31 | PL9 | d | 403 | - | - | 10/53/73/73 | 0/1/1/1 |
| 29 | BCR | BN | 101 | - | - | 11/29/63/63 | 0/2/2/2 |
| 24 | CLA | 0 | 610 | 2 | 1/1/14/20 | 9/31/109/115 | - |
| 23 | CHL | N | 601 | 8 | 3/3/19/26 | 17/33/131/137 | - |
| 33 | HEM | BI | 102 | 7,6 | - | 3/12/54/54 | - |
| 23 | CHL | BJ | 608 | - | 3/3/19/26 | 21/33/131/137 | - |
| 24 | CLA | A6 | 602 | 14 | 1/1/14/20 | 13/33/111/115 | - |
| 24 | CLA | g | 613 | - | 1/1/15/20 | 13/37/115/115 | - |
| 24 | CLA | g | 603 | 8 | 1/1/15/20 | 11/37/115/115 | - |
| 24 | CLA | A6 | 604 | - | 1/1/12/20 | 7/19/97/115 | - |
| 23 | CHL | Y | 307 | - | 3/3/16/26 | 9/20/118/137 | - |
| 24 | CLA | 1 | 512 | - | 1/1/15/20 | 11/37/115/115 | - |
| 23 | CHL | BU | 613 | 22 | 3/3/15/26 | 4/10/108/137 | - |
| 24 | CLA | y | 305 | - | 1/1/12/20 | 10/19/97/115 | - |
| 30 | LMG | I | 101 | - | - | 12/35/55/70 | 0/1/1/1 |
| 24 | CLA | BF | 505 | - | 1/1/15/20 | 8/37/115/115 | - |
| 24 | CLA | 6 | 610 | 2 | 1/1/14/20 | 8/31/109/115 | - |
| 28 | XAT | Au | 619 | - | - | 14/31/93/93 | 0/4/4/4 |
| 24 | CLA | 5 | 613 | 1 | 1/1/13/20 | 8/25/103/115 | - |
| 34 | DGD | a | 401 | - | - | 21/48/88/95 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|--------------|-------|
| 23 | CHL | 8 | 307 | 3 | 3/3/16/26 | 8/15/113/137 | - |

The worst 5 of 6294 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 28 | 7 | 301 | XAT | C10-C9 | 15.13 | 1.55 | 1.35 |
| 28 | AA | 301 | XAT | C10-C9 | 15.11 | 1.55 | 1.35 |
| 28 | Au | 619 | XAT | C10-C9 | 15.10 | 1.55 | 1.35 |
| 28 | G | 619 | XAT | C10-C9 | 15.07 | 1.55 | 1.35 |
| 28 | AA | 318 | XAT | C10-C9 | 15.04 | 1.55 | 1.35 |

The worst 5 of 8154 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28 | BB | 301 | XAT | O24-C25-C24 | 33.02 | 138.19 | 113.38 |
| 28 | AA | 301 | XAT | O24-C25-C24 | 32.93 | 138.12 | 113.38 |
| 28 | N | 619 | XAT | O24-C25-C24 | 32.85 | 138.06 | 113.38 |
| 28 | 5 | 619 | XAT | O4-C5-C4 | 32.85 | 138.06 | 113.38 |
| 28 | A2 | 619 | XAT | O24-C25-C24 | 32.82 | 138.04 | 113.38 |

5 of 778 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 23 | 5 | 601 | CHL | ND |
| 23 | 5 | 601 | CHL | NC |
| 23 | 5 | 601 | CHL | NA |
| 23 | 5 | 605 | CHL | ND |
| 23 | 5 | 605 | CHL | NC |

5 of 8592 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 23 | 5 | 601 | CHL | C1A-C2A-CAA-CBA |
| 23 | 5 | 601 | CHL | C3A-C2A-CAA-CBA |
| 23 | 5 | 601 | CHL | CBD-CGD-O2D-CED |
| 23 | 5 | 605 | CHL | C1A-C2A-CAA-CBA |
| 23 | 5 | 607 | CHL | C3A-C2A-CAA-CBA |

There are no ring outliers.

699 monomers are involved in 2718 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24 | BU | 609 | CLA | 5 | 0 |
| 24 | BD | 407 | CLA | 3 | 0 |
| 24 | 5 | 614 | CLA | 1 | 0 |
| 23 | 6 | 606 | CHL | 7 | 0 |
| 26 | s | 616 | NEX | 5 | 0 |
| 23 | A2 | 605 | CHL | 2 | 0 |
| 23 | 5 | 601 | CHL | 5 | 0 |
| 23 | AA | 310 | CHL | 10 | 0 |
| 24 | v | 608 | CLA | 5 | 0 |
| 24 | 1 | 506 | CLA | 5 | 0 |
| 24 | Au | 611 | CLA | 3 | 0 |
| 24 | C | 510 | CLA | 1 | 0 |
| 23 | BU | 605 | CHL | 17 | 0 |
| 24 | b | 608 | CLA | 3 | 0 |
| 24 | BU | 608 | CLA | 3 | 0 |
| 23 | BB | 306 | CHL | 5 | 0 |
| 24 | C | 502 | CLA | 3 | 0 |
| 28 | 7 | 318 | XAT | 1 | 0 |
| 23 | 9 | 609 | CHL | 15 | 0 |
| 24 | AB | 303 | CLA | 3 | 0 |
| 24 | 6 | 613 | CLA | 11 | 0 |
| 30 | b | 621 | LMG | 1 | 0 |
| 24 | Au | 602 | CLA | 6 | 0 |
| 24 | s | 608 | CLA | 6 | 0 |
| 30 | C | 519 | LMG | 3 | 0 |
| 24 | 0 | 602 | CLA | 5 | 0 |
| 23 | r | 606 | CHL | 13 | 0 |
| 34 | C | 517 | DGD | 4 | 0 |
| 23 | y | 306 | CHL | 3 | 0 |
| 24 | s | 609 | CLA | 4 | 0 |
| 23 | Ba | 308 | CHL | 8 | 0 |
| 24 | B | 615 | CLA | 4 | 0 |
| 29 | BI | 101 | BCR | 2 | 0 |
| 24 | b | 615 | CLA | 4 | 0 |
| 23 | Y | 306 | CHL | 6 | 0 |
| 23 | G | 601 | CHL | 13 | 0 |
| 24 | 2 | 402 | CLA | 7 | 0 |
| 24 | C | 503 | CLA | 1 | 0 |
| 23 | s | 605 | CHL | 5 | 0 |
| 24 | B | 604 | CLA | 6 | 0 |
| 24 | R | 405 | CLA | 6 | 0 |
| 24 | v | 609 | CLA | 12 | 0 |
| 24 | BE | 603 | CLA | 13 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23 | 7 | 307 | CHL | 2 | 0 |
| 28 | AA | 301 | XAT | 3 | 0 |
| 24 | BV | 608 | CLA | 6 | 0 |
| 24 | 1 | 507 | CLA | 4 | 0 |
| 25 | 6 | 615 | LUT | 8 | 0 |
| 24 | BE | 613 | CLA | 4 | 0 |
| 23 | BV | 605 | CHL | 5 | 0 |
| 24 | y | 313 | CLA | 3 | 0 |
| 24 | BD | 406 | CLA | 8 | 0 |
| 25 | 0 | 616 | LUT | 9 | 0 |
| 24 | BQ | 610 | CLA | 12 | 0 |
| 27 | Ba | 319 | LHG | 4 | 0 |
| 23 | g | 609 | CHL | 16 | 0 |
| 23 | n | 605 | CHL | 2 | 0 |
| 24 | 1 | 504 | CLA | 2 | 0 |
| 34 | 1 | 516 | DGD | 1 | 0 |
| 24 | BJ | 602 | CLA | 6 | 0 |
| 29 | z | 101 | BCR | 5 | 0 |
| 24 | BF | 504 | CLA | 2 | 0 |
| 29 | h | 101 | BCR | 7 | 0 |
| 24 | 9 | 603 | CLA | 4 | 0 |
| 24 | c | 507 | CLA | 4 | 0 |
| 23 | BB | 310 | CHL | 10 | 0 |
| 24 | r | 602 | CLA | 10 | 0 |
| 27 | BE | 623 | LHG | 1 | 0 |
| 23 | Ba | 302 | CHL | 10 | 0 |
| 24 | c | 511 | CLA | 3 | 0 |
| 29 | v | 617 | BCR | 5 | 0 |
| 24 | g | 602 | CLA | 5 | 0 |
| 24 | B | 601 | CLA | 4 | 0 |
| 23 | N | 607 | CHL | 8 | 0 |
| 38 | a | 408 | PHO | 4 | 0 |
| 24 | 0 | 611 | CLA | 6 | 0 |
| 23 | g | 606 | CHL | 7 | 0 |
| 31 | 2 | 404 | PL9 | 1 | 0 |
| 30 | A | 412 | LMG | 1 | 0 |
| 23 | A6 | 605 | CHL | 1 | 0 |
| 25 | AA | 317 | LUT | 7 | 0 |
| 24 | 5 | 602 | CLA | 8 | 0 |
| 24 | r | 601 | CLA | 4 | 0 |
| 27 | 2 | 405 | LHG | 1 | 0 |
| 23 | BJ | 607 | CHL | 10 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23 | Au | 606 | CHL | 2 | 0 |
| 34 | A | 402 | DGD | 2 | 0 |
| 24 | BQ | 612 | CLA | 4 | 0 |
| 26 | n | 617 | NEX | 3 | 0 |
| 24 | B | 612 | CLA | 3 | 0 |
| 24 | c | 513 | CLA | 3 | 0 |
| 28 | 5 | 619 | XAT | 11 | 0 |
| 24 | B | 605 | CLA | 10 | 0 |
| 23 | 6 | 608 | CHL | 2 | 0 |
| 23 | 8 | 305 | CHL | 2 | 0 |
| 24 | AB | 308 | CLA | 11 | 0 |
| 24 | R | 404 | CLA | 5 | 0 |
| 28 | N | 619 | XAT | 5 | 0 |
| 24 | BV | 609 | CLA | 7 | 0 |
| 24 | 5 | 611 | CLA | 2 | 0 |
| 24 | v | 612 | CLA | 4 | 0 |
| 24 | 8 | 310 | CLA | 2 | 0 |
| 23 | G | 607 | CHL | 11 | 0 |
| 24 | R | 406 | CLA | 2 | 0 |
| 25 | BB | 317 | LUT | 6 | 0 |
| 23 | 6 | 607 | CHL | 7 | 0 |
| 24 | Ba | 312 | CLA | 1 | 0 |
| 24 | AA | 313 | CLA | 2 | 0 |
| 34 | h | 102 | DGD | 4 | 0 |
| 27 | L | 102 | LHG | 3 | 0 |
| 25 | A6 | 615 | LUT | 8 | 0 |
| 24 | a | 407 | CLA | 6 | 0 |
| 24 | v | 616 | CLA | 3 | 0 |
| 24 | b | 613 | CLA | 5 | 0 |
| 24 | Ba | 311 | CLA | 4 | 0 |
| 36 | BD | 403 | OEX | 1 | 0 |
| 28 | r | 616 | XAT | 5 | 0 |
| 23 | Au | 609 | CHL | 8 | 0 |
| 30 | c | 518 | LMG | 4 | 0 |
| 38 | BD | 408 | PHO | 5 | 0 |
| 27 | g | 618 | LHG | 4 | 0 |
| 24 | 9 | 611 | CLA | 2 | 0 |
| 29 | BF | 515 | BCR | 4 | 0 |
| 27 | 0 | 617 | LHG | 8 | 0 |
| 24 | y | 311 | CLA | 4 | 0 |
| 28 | g | 619 | XAT | 1 | 0 |
| 26 | A2 | 617 | NEX | 3 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 27 | N | 618 | LHG | 5 | 0 |
| 24 | c | 502 | CLA | 4 | 0 |
| 25 | A2 | 616 | LUT | 7 | 0 |
| 24 | G | 610 | CLA | 4 | 0 |
| 24 | Au | 610 | CLA | 3 | 0 |
| 24 | A2 | 602 | CLA | 2 | 0 |
| 24 | BE | 606 | CLA | 5 | 0 |
| 29 | F | 101 | BCR | 1 | 0 |
| 23 | y | 308 | CHL | 6 | 0 |
| 23 | G | 608 | CHL | 7 | 0 |
| 24 | G | 612 | CLA | 3 | 0 |
| 29 | K | 102 | BCR | 2 | 0 |
| 23 | Y | 308 | CHL | 9 | 0 |
| 24 | 7 | 303 | CLA | 8 | 0 |
| 24 | b | 604 | CLA | 1 | 0 |
| 31 | D | 403 | PL9 | 1 | 0 |
| 25 | 9 | 616 | LUT | 10 | 0 |
| 24 | C | 512 | CLA | 3 | 0 |
| 28 | G | 619 | XAT | 4 | 0 |
| 24 | B | 606 | CLA | 8 | 0 |
| 24 | r | 609 | CLA | 6 | 0 |
| 24 | Y | 304 | CLA | 2 | 0 |
| 24 | 1 | 505 | CLA | 2 | 0 |
| 25 | Au | 615 | LUT | 7 | 0 |
| 24 | d | 401 | CLA | 6 | 0 |
| 23 | AA | 308 | CHL | 7 | 0 |
| 24 | B | 607 | CLA | 2 | 0 |
| 25 | G | 615 | LUT | 6 | 0 |
| 29 | B | 623 | BCR | 8 | 0 |
| 25 | 8 | 311 | LUT | 6 | 0 |
| 23 | N | 606 | CHL | 5 | 0 |
| 23 | g | 605 | CHL | 3 | 0 |
| 24 | 9 | 602 | CLA | 7 | 0 |
| 23 | BQ | 606 | CHL | 7 | 0 |
| 24 | 7 | 312 | CLA | 2 | 0 |
| 29 | BE | 620 | BCR | 5 | 0 |
| 30 | c | 501 | LMG | 3 | 0 |
| 24 | BE | 617 | CLA | 3 | 0 |
| 23 | A2 | 607 | CHL | 11 | 0 |
| 27 | 1 | 521 | LHG | 3 | 0 |
| 25 | BQ | 616 | LUT | 6 | 0 |
| 27 | Az | 102 | LHG | 3 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24 | BU | 614 | CLA | 1 | 0 |
| 23 | BJ | 606 | CHL | 6 | 0 |
| 23 | BQ | 609 | CHL | 15 | 0 |
| 23 | 5 | 609 | CHL | 15 | 0 |
| 24 | Ba | 314 | CLA | 7 | 0 |
| 29 | 1 | 515 | BCR | 4 | 0 |
| 23 | S | 606 | CHL | 7 | 0 |
| 33 | f | 102 | HEM | 2 | 0 |
| 23 | 0 | 608 | CHL | 2 | 0 |
| 24 | 0 | 612 | CLA | 3 | 0 |
| 25 | r | 615 | LUT | 9 | 0 |
| 34 | a | 413 | DGD | 1 | 0 |
| 24 | 8 | 308 | CLA | 7 | 0 |
| 29 | BE | 618 | BCR | 4 | 0 |
| 32 | A1 | 101 | SQD | 2 | 0 |
| 30 | BL | 101 | LMG | 2 | 0 |
| 24 | BF | 508 | CLA | 2 | 0 |
| 24 | b | 614 | CLA | 2 | 0 |
| 25 | g | 615 | LUT | 7 | 0 |
| 33 | F | 102 | HEM | 1 | 0 |
| 27 | r | 618 | LHG | 6 | 0 |
| 32 | l | 102 | SQD | 2 | 0 |
| 29 | Ay | 101 | BCR | 3 | 0 |
| 24 | c | 504 | CLA | 4 | 0 |
| 23 | 5 | 606 | CHL | 7 | 0 |
| 23 | s | 601 | CHL | 3 | 0 |
| 24 | G | 603 | CLA | 1 | 0 |
| 27 | 9 | 618 | LHG | 3 | 0 |
| 32 | a | 412 | SQD | 6 | 0 |
| 23 | n | 601 | CHL | 12 | 0 |
| 24 | C | 507 | CLA | 2 | 0 |
| 24 | N | 612 | CLA | 1 | 0 |
| 24 | BQ | 613 | CLA | 4 | 0 |
| 25 | 7 | 316 | LUT | 6 | 0 |
| 23 | BJ | 605 | CHL | 3 | 0 |
| 26 | A6 | 616 | NEX | 2 | 0 |
| 24 | s | 604 | CLA | 6 | 0 |
| 24 | D | 401 | CLA | 7 | 0 |
| 27 | y | 319 | LHG | 5 | 0 |
| 24 | v | 603 | CLA | 3 | 0 |
| 24 | Aw | 102 | CLA | 3 | 0 |
| 27 | W | 201 | LHG | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25 | 7 | 317 | LUT | 7 | 0 |
| 24 | b | 611 | CLA | 6 | 0 |
| 24 | v | 614 | CLA | 8 | 0 |
| 24 | AA | 303 | CLA | 11 | 0 |
| 24 | A6 | 609 | CLA | 3 | 0 |
| 23 | N | 609 | CHL | 9 | 0 |
| 23 | n | 607 | CHL | 10 | 0 |
| 23 | Au | 608 | CHL | 6 | 0 |
| 24 | Au | 612 | CLA | 3 | 0 |
| 24 | I | 102 | CLA | 3 | 0 |
| 29 | z | 102 | BCR | 3 | 0 |
| 25 | 0 | 615 | LUT | 10 | 0 |
| 36 | a | 403 | OEX | 1 | 0 |
| 24 | BJ | 610 | CLA | 3 | 0 |
| 23 | S | 605 | CHL | 1 | 0 |
| 29 | 1 | 514 | BCR | 3 | 0 |
| 24 | 1 | 508 | CLA | 7 | 0 |
| 23 | G | 609 | CHL | 18 | 0 |
| 24 | C | 511 | CLA | 5 | 0 |
| 23 | s | 607 | CHL | 4 | 0 |
| 30 | 1 | 501 | LMG | 2 | 0 |
| 24 | B | 608 | CLA | 5 | 0 |
| 24 | Y | 315 | CLA | 1 | 0 |
| 25 | 5 | 615 | LUT | 6 | 0 |
| 24 | S | 604 | CLA | 3 | 0 |
| 23 | Ba | 309 | CHL | 8 | 0 |
| 24 | Au | 613 | CLA | 6 | 0 |
| 23 | A2 | 606 | CHL | 5 | 0 |
| 23 | A6 | 607 | CHL | 6 | 0 |
| 24 | 0 | 613 | CLA | 10 | 0 |
| 30 | Aw | 101 | LMG | 1 | 0 |
| 25 | A2 | 615 | LUT | 5 | 0 |
| 24 | BB | 311 | CLA | 3 | 0 |
| 24 | v | 611 | CLA | 5 | 0 |
| 24 | BU | 610 | CLA | 3 | 0 |
| 24 | BV | 603 | CLA | 1 | 0 |
| 25 | AB | 311 | LUT | 9 | 0 |
| 29 | f | 101 | BCR | 2 | 0 |
| 23 | BQ | 607 | CHL | 10 | 0 |
| 26 | BV | 616 | NEX | 5 | 0 |
| 24 | G | 611 | CLA | 4 | 0 |
| 25 | 9 | 615 | LUT | 8 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 38 | R | 407 | PHO | 7 | 0 |
| 25 | G | 616 | LUT | 5 | 0 |
| 23 | BV | 607 | CHL | 5 | 0 |
| 24 | BE | 609 | CLA | 4 | 0 |
| 24 | 6 | 604 | CLA | 6 | 0 |
| 24 | N | 614 | CLA | 3 | 0 |
| 23 | 9 | 606 | CHL | 5 | 0 |
| 27 | BG | 404 | LHG | 1 | 0 |
| 24 | AB | 309 | CLA | 1 | 0 |
| 24 | r | 603 | CLA | 1 | 0 |
| 24 | 0 | 603 | CLA | 1 | 0 |
| 24 | c | 510 | CLA | 2 | 0 |
| 34 | BD | 401 | DGD | 2 | 0 |
| 24 | B | 609 | CLA | 11 | 0 |
| 28 | 7 | 301 | XAT | 3 | 0 |
| 29 | R | 410 | BCR | 1 | 0 |
| 24 | v | 615 | CLA | 4 | 0 |
| 34 | C | 518 | DGD | 1 | 0 |
| 23 | y | 310 | CHL | 12 | 0 |
| 24 | A2 | 610 | CLA | 6 | 0 |
| 23 | 7 | 302 | CHL | 9 | 0 |
| 24 | G | 602 | CLA | 4 | 0 |
| 24 | c | 509 | CLA | 5 | 0 |
| 24 | BU | 612 | CLA | 4 | 0 |
| 24 | S | 602 | CLA | 8 | 0 |
| 25 | g | 616 | LUT | 9 | 0 |
| 28 | y | 301 | XAT | 3 | 0 |
| 24 | 1 | 511 | CLA | 3 | 0 |
| 34 | 1 | 518 | DGD | 2 | 0 |
| 26 | Y | 318 | NEX | 1 | 0 |
| 24 | BE | 614 | CLA | 2 | 0 |
| 23 | BJ | 601 | CHL | 15 | 0 |
| 24 | 6 | 603 | CLA | 1 | 0 |
| 24 | BF | 510 | CLA | 3 | 0 |
| 24 | A2 | 603 | CLA | 3 | 0 |
| 23 | 7 | 309 | CHL | 5 | 0 |
| 24 | BV | 610 | CLA | 2 | 0 |
| 24 | G | 613 | CLA | 6 | 0 |
| 26 | y | 318 | NEX | 3 | 0 |
| 27 | 6 | 617 | LHG | 5 | 0 |
| 29 | B | 619 | BCR | 6 | 0 |
| 24 | N | 611 | CLA | 3 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24 | n | 610 | CLA | 10 | 0 |
| 24 | BQ | 611 | CLA | 2 | 0 |
| 24 | b | 610 | CLA | 12 | 0 |
| 32 | D | 406 | SQD | 1 | 0 |
| 29 | Ay | 102 | BCR | 5 | 0 |
| 24 | BJ | 611 | CLA | 3 | 0 |
| 23 | g | 608 | CHL | 6 | 0 |
| 23 | r | 607 | CHL | 10 | 0 |
| 29 | v | 619 | BCR | 6 | 0 |
| 32 | BO | 101 | SQD | 5 | 0 |
| 24 | b | 603 | CLA | 10 | 0 |
| 24 | a | 406 | CLA | 7 | 0 |
| 24 | s | 610 | CLA | 3 | 0 |
| 24 | C | 508 | CLA | 5 | 0 |
| 27 | C | 521 | LHG | 3 | 0 |
| 27 | B | 621 | LHG | 2 | 0 |
| 23 | A2 | 601 | CHL | 9 | 0 |
| 23 | AA | 307 | CHL | 2 | 0 |
| 24 | BF | 512 | CLA | 3 | 0 |
| 29 | 4 | 101 | BCR | 3 | 0 |
| 27 | b | 624 | LHG | 4 | 0 |
| 23 | AB | 307 | CHL | 8 | 0 |
| 24 | b | 607 | CLA | 9 | 0 |
| 23 | AB | 306 | CHL | 3 | 0 |
| 23 | Y | 302 | CHL | 12 | 0 |
| 23 | 0 | 607 | CHL | 6 | 0 |
| 24 | s | 603 | CLA | 1 | 0 |
| 24 | BF | 514 | CLA | 7 | 0 |
| 24 | A6 | 610 | CLA | 1 | 0 |
| 24 | BE | 611 | CLA | 3 | 0 |
| 23 | BV | 601 | CHL | 3 | 0 |
| 24 | n | 614 | CLA | 2 | 0 |
| 25 | BJ | 616 | LUT | 10 | 0 |
| 28 | BQ | 619 | XAT | 5 | 0 |
| 27 | b | 623 | LHG | 2 | 0 |
| 24 | Ba | 304 | CLA | 3 | 0 |
| 24 | 6 | 614 | CLA | 4 | 0 |
| 24 | b | 612 | CLA | 3 | 0 |
| 25 | n | 616 | LUT | 6 | 0 |
| 25 | BU | 615 | LUT | 10 | 0 |
| 23 | 9 | 605 | CHL | 2 | 0 |
| 24 | 1 | 510 | CLA | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 30 | BF | 519 | LMG | 4 | 0 |
| 24 | BV | 604 | CLA | 6 | 0 |
| 24 | BD | 410 | CLA | 1 | 0 |
| 25 | Y | 316 | LUT | 4 | 0 |
| 27 | 5 | 618 | LHG | 3 | 0 |
| 24 | s | 612 | CLA | 1 | 0 |
| 23 | BB | 307 | CHL | 4 | 0 |
| 26 | BB | 318 | NEX | 3 | 0 |
| 29 | b | 620 | BCR | 3 | 0 |
| 24 | BE | 608 | CLA | 3 | 0 |
| 23 | AB | 304 | CHL | 3 | 0 |
| 23 | A6 | 601 | CHL | 2 | 0 |
| 24 | AB | 301 | CLA | 6 | 0 |
| 34 | H | 102 | DGD | 6 | 0 |
| 24 | c | 512 | CLA | 5 | 0 |
| 23 | g | 607 | CHL | 8 | 0 |
| 23 | BU | 606 | CHL | 12 | 0 |
| 28 | BJ | 619 | XAT | 1 | 0 |
| 29 | a | 411 | BCR | 3 | 0 |
| 24 | A2 | 612 | CLA | 1 | 0 |
| 30 | BE | 621 | LMG | 1 | 0 |
| 24 | n | 613 | CLA | 5 | 0 |
| 24 | BF | 507 | CLA | 4 | 0 |
| 29 | k | 101 | BCR | 1 | 0 |
| 29 | H | 101 | BCR | 5 | 0 |
| 23 | r | 605 | CHL | 17 | 0 |
| 24 | AB | 310 | CLA | 2 | 0 |
| 24 | B | 602 | CLA | 6 | 0 |
| 24 | C | 505 | CLA | 3 | 0 |
| 23 | AA | 302 | CHL | 11 | 0 |
| 23 | s | 606 | CHL | 11 | 0 |
| 23 | y | 302 | CHL | 11 | 0 |
| 24 | BV | 612 | CLA | 1 | 0 |
| 27 | c | 520 | LHG | 3 | 0 |
| 27 | 1 | 520 | LHG | 1 | 0 |
| 23 | Ba | 307 | CHL | 6 | 0 |
| 25 | BQ | 615 | LUT | 5 | 0 |
| 27 | BF | 521 | LHG | 3 | 0 |
| 24 | b | 605 | CLA | 6 | 0 |
| 23 | n | 609 | CHL | 15 | 0 |
| 23 | G | 606 | CHL | 3 | 0 |
| 24 | A2 | 613 | CLA | 5 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24 | 7 | 304 | CLA | 5 | 0 |
| 29 | c | 515 | BCR | 3 | 0 |
| 24 | y | 304 | CLA | 3 | 0 |
| 24 | r | 610 | CLA | 3 | 0 |
| 24 | Y | 312 | CLA | 6 | 0 |
| 24 | BU | 603 | CLA | 3 | 0 |
| 23 | BV | 606 | CHL | 10 | 0 |
| 24 | g | 610 | CLA | 2 | 0 |
| 24 | b | 606 | CLA | 5 | 0 |
| 28 | Ba | 301 | XAT | 2 | 0 |
| 29 | C | 514 | BCR | 2 | 0 |
| 23 | r | 613 | CHL | 3 | 0 |
| 24 | c | 505 | CLA | 5 | 0 |
| 23 | BB | 302 | CHL | 14 | 0 |
| 29 | b | 619 | BCR | 3 | 0 |
| 29 | BD | 411 | BCR | 2 | 0 |
| 24 | BG | 402 | CLA | 1 | 0 |
| 28 | 9 | 619 | XAT | 11 | 0 |
| 23 | 5 | 608 | CHL | 4 | 0 |
| 24 | Ba | 305 | CLA | 2 | 0 |
| 23 | N | 608 | CHL | 12 | 0 |
| 27 | A2 | 618 | LHG | 3 | 0 |
| 24 | BB | 312 | CLA | 3 | 0 |
| 24 | Y | 311 | CLA | 5 | 0 |
| 26 | 9 | 617 | NEX | 1 | 0 |
| 27 | BJ | 618 | LHG | 4 | 0 |
| 23 | Au | 607 | CHL | 10 | 0 |
| 24 | BQ | 602 | CLA | 6 | 0 |
| 24 | N | 602 | CLA | 2 | 0 |
| 24 | b | 609 | CLA | 5 | 0 |
| 24 | r | 604 | CLA | 3 | 0 |
| 23 | Ba | 306 | CHL | 3 | 0 |
| 32 | R | 411 | SQD | 9 | 0 |
| 28 | A2 | 619 | XAT | 6 | 0 |
| 27 | n | 618 | LHG | 5 | 0 |
| 23 | g | 601 | CHL | 14 | 0 |
| 24 | Y | 313 | CLA | 1 | 0 |
| 30 | A0 | 201 | LMG | 1 | 0 |
| 24 | 8 | 303 | CLA | 2 | 0 |
| 24 | A | 407 | CLA | 3 | 0 |
| 24 | C | 509 | CLA | 2 | 0 |
| 25 | N | 615 | LUT | 4 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23 | Y | 309 | CHL | 5 | 0 |
| 25 | y | 316 | LUT | 5 | 0 |
| 23 | 8 | 304 | CHL | 2 | 0 |
| 27 | A0 | 202 | LHG | 1 | 0 |
| 24 | BG | 401 | CLA | 7 | 0 |
| 23 | 8 | 306 | CHL | 3 | 0 |
| 24 | g | 604 | CLA | 2 | 0 |
| 24 | BV | 602 | CLA | 4 | 0 |
| 25 | BJ | 615 | LUT | 7 | 0 |
| 26 | 7 | 319 | NEX | 5 | 0 |
| 26 | N | 617 | NEX | 3 | 0 |
| 24 | A | 406 | CLA | 5 | 0 |
| 29 | AB | 313 | BCR | 5 | 0 |
| 24 | BE | 612 | CLA | 3 | 0 |
| 23 | S | 607 | CHL | 6 | 0 |
| 29 | BE | 601 | BCR | 6 | 0 |
| 24 | 5 | 604 | CLA | 6 | 0 |
| 25 | n | 615 | LUT | 5 | 0 |
| 24 | BB | 315 | CLA | 1 | 0 |
| 24 | BD | 405 | CLA | 8 | 0 |
| 34 | Av | 102 | DGD | 6 | 0 |
| 25 | s | 614 | LUT | 7 | 0 |
| 26 | BB | 320 | NEX | 5 | 0 |
| 24 | AA | 311 | CLA | 4 | 0 |
| 24 | A2 | 614 | CLA | 3 | 0 |
| 24 | BB | 304 | CLA | 1 | 0 |
| 29 | B | 618 | BCR | 1 | 0 |
| 24 | BF | 502 | CLA | 2 | 0 |
| 23 | y | 307 | CHL | 7 | 0 |
| 24 | r | 614 | CLA | 3 | 0 |
| 27 | BB | 319 | LHG | 7 | 0 |
| 26 | g | 617 | NEX | 1 | 0 |
| 24 | BF | 509 | CLA | 9 | 0 |
| 29 | Bb | 101 | BCR | 3 | 0 |
| 24 | r | 612 | CLA | 4 | 0 |
| 28 | AB | 312 | XAT | 6 | 0 |
| 24 | BJ | 613 | CLA | 6 | 0 |
| 26 | 5 | 617 | NEX | 1 | 0 |
| 24 | AA | 314 | CLA | 3 | 0 |
| 27 | Au | 618 | LHG | 4 | 0 |
| 32 | BD | 412 | SQD | 6 | 0 |
| 25 | BV | 614 | LUT | 6 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23 | 5 | 607 | CHL | 11 | 0 |
| 24 | Y | 314 | CLA | 5 | 0 |
| 24 | BE | 615 | CLA | 4 | 0 |
| 24 | 7 | 305 | CLA | 4 | 0 |
| 23 | 0 | 601 | CHL | 12 | 0 |
| 26 | Ba | 318 | NEX | 2 | 0 |
| 24 | v | 602 | CLA | 6 | 0 |
| 24 | A6 | 608 | CLA | 2 | 0 |
| 24 | BU | 602 | CLA | 12 | 0 |
| 27 | Y | 319 | LHG | 6 | 0 |
| 24 | S | 610 | CLA | 1 | 0 |
| 24 | BU | 604 | CLA | 3 | 0 |
| 38 | A | 409 | PHO | 2 | 0 |
| 23 | BJ | 609 | CHL | 15 | 0 |
| 24 | n | 612 | CLA | 3 | 0 |
| 24 | v | 606 | CLA | 9 | 0 |
| 24 | B | 610 | CLA | 2 | 0 |
| 25 | AA | 316 | LUT | 7 | 0 |
| 23 | 9 | 608 | CHL | 4 | 0 |
| 24 | A2 | 611 | CLA | 3 | 0 |
| 24 | C | 513 | CLA | 6 | 0 |
| 29 | b | 601 | BCR | 7 | 0 |
| 24 | BB | 303 | CLA | 3 | 0 |
| 27 | w | 201 | LHG | 1 | 0 |
| 23 | y | 309 | CHL | 8 | 0 |
| 24 | BJ | 603 | CLA | 3 | 0 |
| 27 | C | 520 | LHG | 2 | 0 |
| 26 | r | 617 | NEX | 5 | 0 |
| 24 | s | 602 | CLA | 6 | 0 |
| 25 | Y | 317 | LUT | 5 | 0 |
| 27 | BU | 617 | LHG | 5 | 0 |
| 23 | 6 | 609 | CHL | 13 | 0 |
| 24 | c | 506 | CLA | 3 | 0 |
| 23 | n | 608 | CHL | 10 | 0 |
| 24 | 9 | 613 | CLA | 7 | 0 |
| 28 | BU | 616 | XAT | 4 | 0 |
| 24 | 2 | 403 | CLA | 1 | 0 |
| 29 | A | 411 | BCR | 3 | 0 |
| 24 | Ba | 313 | CLA | 2 | 0 |
| 24 | BF | 506 | CLA | 3 | 0 |
| 28 | n | 619 | XAT | 2 | 0 |
| 24 | 8 | 302 | CLA | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24 | 9 | 614 | CLA | 1 | 0 |
| 24 | 0 | 614 | CLA | 4 | 0 |
| 23 | A2 | 609 | CHL | 10 | 0 |
| 24 | S | 609 | CLA | 4 | 0 |
| 29 | BK | 101 | BCR | 8 | 0 |
| 24 | 7 | 313 | CLA | 3 | 0 |
| 24 | a | 405 | CLA | 5 | 0 |
| 24 | 5 | 603 | CLA | 3 | 0 |
| 24 | BU | 601 | CLA | 3 | 0 |
| 29 | BF | 516 | BCR | 2 | 0 |
| 24 | S | 608 | CLA | 3 | 0 |
| 24 | BF | 513 | CLA | 3 | 0 |
| 23 | N | 605 | CHL | 2 | 0 |
| 29 | v | 622 | BCR | 5 | 0 |
| 24 | s | 611 | CLA | 2 | 0 |
| 24 | v | 604 | CLA | 6 | 0 |
| 29 | Av | 101 | BCR | 4 | 0 |
| 24 | 9 | 604 | CLA | 5 | 0 |
| 24 | v | 610 | CLA | 2 | 0 |
| 23 | 9 | 601 | CHL | 6 | 0 |
| 24 | Y | 303 | CLA | 3 | 0 |
| 27 | BE | 624 | LHG | 2 | 0 |
| 34 | 1 | 517 | DGD | 4 | 0 |
| 29 | K | 101 | BCR | 3 | 0 |
| 27 | d | 404 | LHG | 1 | 0 |
| 26 | S | 616 | NEX | 3 | 0 |
| 24 | BB | 314 | CLA | 5 | 0 |
| 24 | N | 610 | CLA | 9 | 0 |
| 28 | BB | 301 | XAT | 6 | 0 |
| 24 | BJ | 612 | CLA | 3 | 0 |
| 24 | BV | 611 | CLA | 2 | 0 |
| 24 | c | 508 | CLA | 5 | 0 |
| 23 | 5 | 605 | CHL | 2 | 0 |
| 24 | BB | 305 | CLA | 1 | 0 |
| 29 | C | 515 | BCR | 3 | 0 |
| 23 | AA | 309 | CHL | 4 | 0 |
| 28 | AA | 318 | XAT | 3 | 0 |
| 24 | n | 603 | CLA | 1 | 0 |
| 24 | C | 504 | CLA | 2 | 0 |
| 23 | 9 | 607 | CHL | 8 | 0 |
| 24 | a | 410 | CLA | 1 | 0 |
| 38 | A | 408 | PHO | 6 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 27 | BQ | 618 | LHG | 6 | 0 |
| 30 | i | 101 | LMG | 2 | 0 |
| 23 | 6 | 601 | CHL | 16 | 0 |
| 24 | v | 601 | CLA | 5 | 0 |
| 24 | A2 | 604 | CLA | 1 | 0 |
| 24 | A | 410 | CLA | 1 | 0 |
| 25 | BB | 316 | LUT | 5 | 0 |
| 34 | BK | 102 | DGD | 6 | 0 |
| 27 | G | 618 | LHG | 3 | 0 |
| 24 | 5 | 610 | CLA | 13 | 0 |
| 25 | Ba | 316 | LUT | 4 | 0 |
| 28 | Y | 301 | XAT | 5 | 0 |
| 24 | y | 314 | CLA | 3 | 0 |
| 24 | BF | 511 | CLA | 5 | 0 |
| 24 | AB | 302 | CLA | 2 | 0 |
| 34 | BF | 518 | DGD | 4 | 0 |
| 24 | 1 | 502 | CLA | 2 | 0 |
| 24 | B | 616 | CLA | 3 | 0 |
| 24 | BE | 607 | CLA | 8 | 0 |
| 24 | b | 616 | CLA | 4 | 0 |
| 33 | 4 | 102 | HEM | 3 | 0 |
| 38 | BD | 409 | PHO | 1 | 0 |
| 24 | AA | 305 | CLA | 4 | 0 |
| 27 | D | 404 | LHG | 3 | 0 |
| 32 | Az | 101 | SQD | 3 | 0 |
| 24 | 7 | 311 | CLA | 4 | 0 |
| 24 | y | 312 | CLA | 1 | 0 |
| 24 | g | 612 | CLA | 3 | 0 |
| 25 | 6 | 616 | LUT | 9 | 0 |
| 24 | B | 614 | CLA | 7 | 0 |
| 23 | BQ | 605 | CHL | 2 | 0 |
| 24 | c | 514 | CLA | 7 | 0 |
| 23 | Ba | 310 | CHL | 12 | 0 |
| 24 | 5 | 612 | CLA | 1 | 0 |
| 29 | 8 | 313 | BCR | 6 | 0 |
| 24 | v | 607 | CLA | 5 | 0 |
| 32 | BG | 406 | SQD | 4 | 0 |
| 23 | G | 605 | CHL | 1 | 0 |
| 23 | n | 606 | CHL | 8 | 0 |
| 34 | c | 517 | DGD | 4 | 0 |
| 24 | Ba | 303 | CLA | 2 | 0 |
| 24 | 6 | 612 | CLA | 3 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24 | 6 | 602 | CLA | 12 | 0 |
| 23 | S | 601 | CHL | 2 | 0 |
| 30 | C | 501 | LMG | 2 | 0 |
| 25 | A6 | 614 | LUT | 2 | 0 |
| 24 | S | 612 | CLA | 1 | 0 |
| 23 | BB | 309 | CHL | 7 | 0 |
| 27 | v | 621 | LHG | 2 | 0 |
| 24 | BE | 602 | CLA | 5 | 0 |
| 31 | BG | 403 | PL9 | 2 | 0 |
| 34 | R | 401 | DGD | 2 | 0 |
| 23 | A2 | 608 | CHL | 11 | 0 |
| 24 | BE | 610 | CLA | 11 | 0 |
| 24 | y | 303 | CLA | 3 | 0 |
| 24 | 6 | 611 | CLA | 5 | 0 |
| 23 | 7 | 310 | CHL | 11 | 0 |
| 24 | B | 603 | CLA | 4 | 0 |
| 23 | BQ | 608 | CHL | 9 | 0 |
| 32 | L | 103 | SQD | 2 | 0 |
| 24 | 1 | 513 | CLA | 7 | 0 |
| 24 | 8 | 309 | CLA | 1 | 0 |
| 24 | b | 602 | CLA | 4 | 0 |
| 25 | S | 615 | LUT | 7 | 0 |
| 24 | B | 611 | CLA | 5 | 0 |
| 24 | c | 503 | CLA | 1 | 0 |
| 32 | BO | 102 | SQD | 1 | 0 |
| 24 | d | 402 | CLA | 1 | 0 |
| 24 | 0 | 604 | CLA | 2 | 0 |
| 23 | Au | 601 | CHL | 14 | 0 |
| 24 | 9 | 610 | CLA | 9 | 0 |
| 23 | BB | 308 | CHL | 9 | 0 |
| 24 | 8 | 301 | CLA | 6 | 0 |
| 24 | B | 613 | CLA | 2 | 0 |
| 32 | 2 | 408 | SQD | 3 | 0 |
| 29 | b | 618 | BCR | 3 | 0 |
| 24 | BE | 605 | CLA | 5 | 0 |
| 24 | r | 611 | CLA | 1 | 0 |
| 24 | BB | 313 | CLA | 2 | 0 |
| 25 | BV | 615 | LUT | 4 | 0 |
| 32 | l | 101 | SQD | 5 | 0 |
| 29 | B | 617 | BCR | 6 | 0 |
| 24 | g | 611 | CLA | 3 | 0 |
| 32 | A | 413 | SQD | 8 | 0 |

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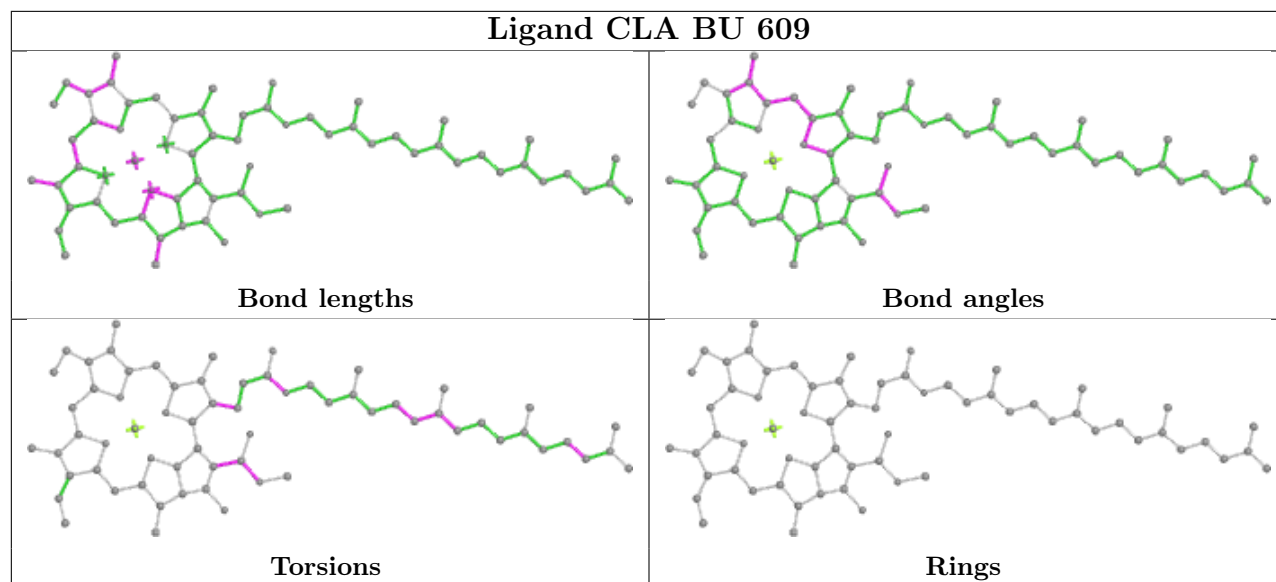
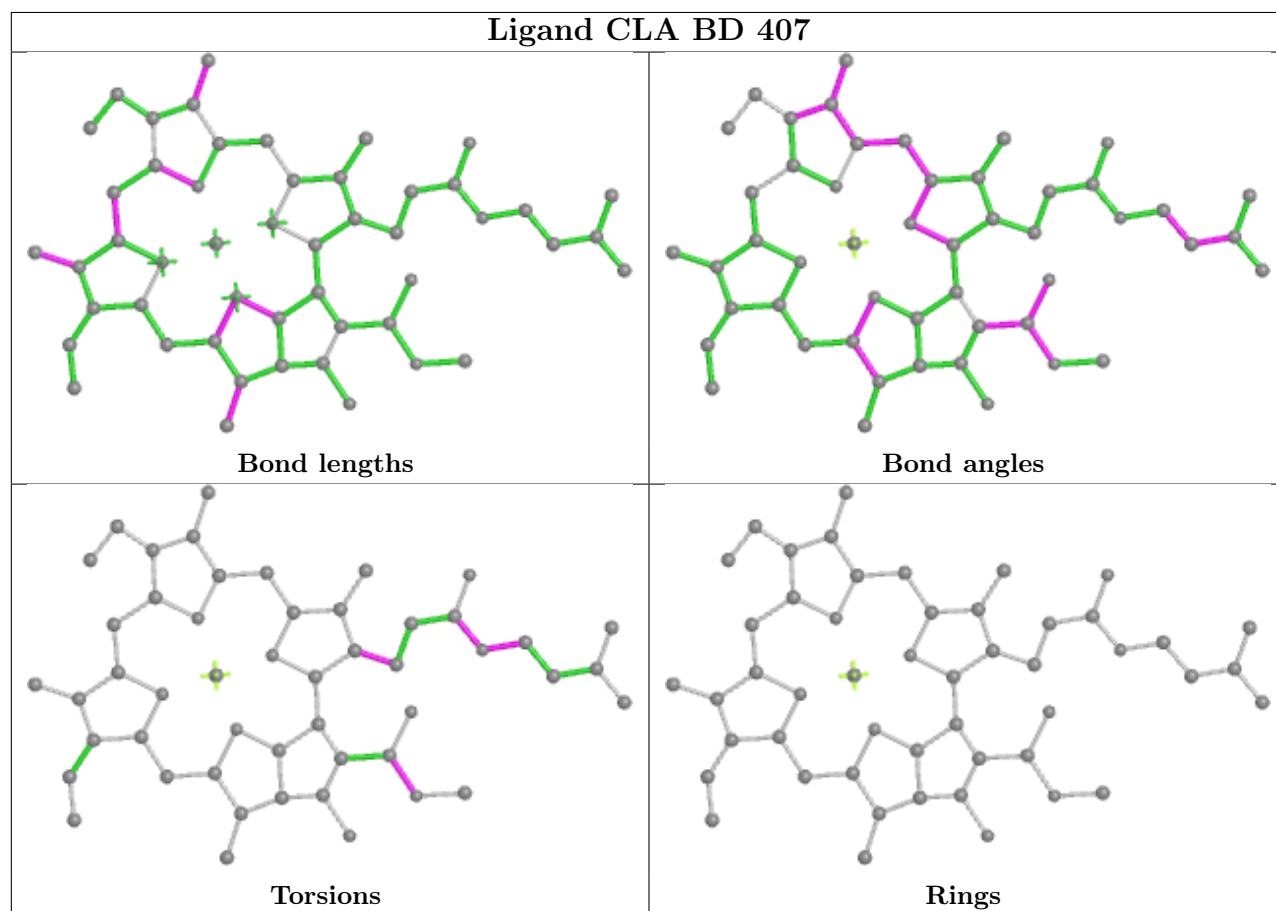
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
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| 25 | N | 616 | LUT | 6 | 0 |
| 24 | v | 613 | CLA | 2 | 0 |
| 24 | n | 611 | CLA | 2 | 0 |
| 24 | A | 405 | CLA | 6 | 0 |
| 24 | n | 602 | CLA | 5 | 0 |
| 24 | 1 | 503 | CLA | 1 | 0 |
| 26 | BJ | 617 | NEX | 1 | 0 |
| 23 | BU | 607 | CHL | 12 | 0 |
| 28 | 8 | 312 | XAT | 6 | 0 |
| 24 | AA | 312 | CLA | 1 | 0 |
| 24 | C | 506 | CLA | 5 | 0 |
| 23 | 7 | 308 | CHL | 6 | 0 |
| 23 | Y | 310 | CHL | 12 | 0 |
| 25 | s | 615 | LUT | 9 | 0 |
| 24 | v | 605 | CLA | 9 | 0 |
| 24 | BJ | 604 | CLA | 2 | 0 |
| 25 | S | 614 | LUT | 4 | 0 |
| 24 | 9 | 612 | CLA | 2 | 0 |
| 23 | A6 | 606 | CHL | 7 | 0 |
| 27 | BY | 201 | LHG | 1 | 0 |
| 24 | BQ | 603 | CLA | 1 | 0 |
| 25 | 5 | 616 | LUT | 9 | 0 |
| 24 | N | 603 | CLA | 1 | 0 |
| 23 | AB | 305 | CHL | 2 | 0 |
| 24 | r | 608 | CLA | 2 | 0 |
| 23 | 0 | 609 | CHL | 12 | 0 |
| 24 | 1 | 509 | CLA | 1 | 0 |
| 25 | Ba | 317 | LUT | 3 | 0 |
| 24 | b | 617 | CLA | 3 | 0 |
| 26 | BQ | 617 | NEX | 3 | 0 |
| 32 | d | 406 | SQD | 3 | 0 |
| 24 | AA | 304 | CLA | 4 | 0 |
| 24 | BQ | 614 | CLA | 2 | 0 |
| 32 | L | 101 | SQD | 3 | 0 |
| 23 | BQ | 601 | CHL | 11 | 0 |
| 24 | N | 613 | CLA | 5 | 0 |
| 26 | G | 617 | NEX | 1 | 0 |
| 24 | BE | 604 | CLA | 1 | 0 |
| 26 | Au | 617 | NEX | 1 | 0 |
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| 25 | y | 317 | LUT | 4 | 0 |

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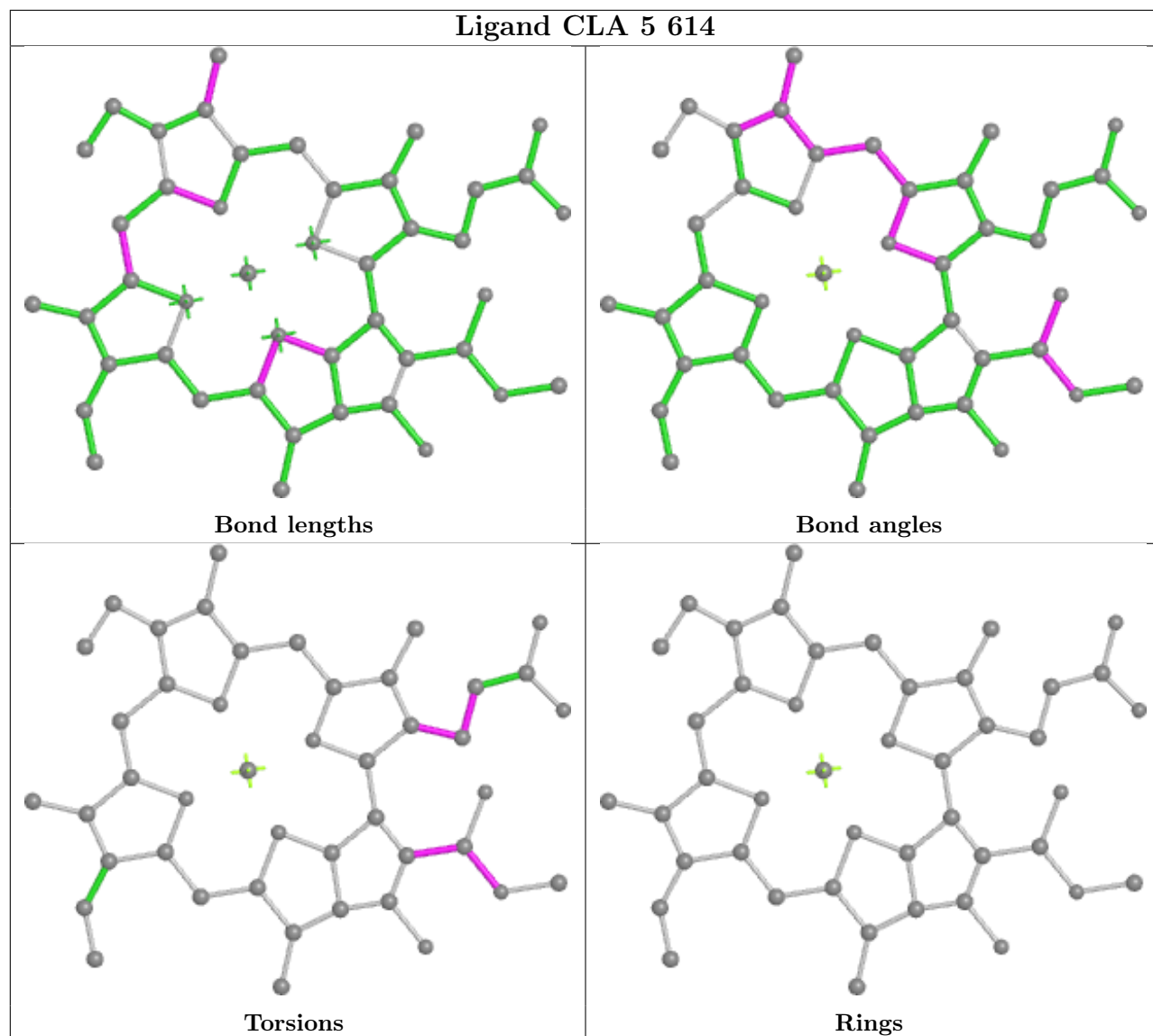
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
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| 24 | 7 | 314 | CLA | 3 | 0 |
| 24 | BE | 616 | CLA | 2 | 0 |
| 30 | 1 | 519 | LMG | 3 | 0 |
| 25 | Au | 616 | LUT | 5 | 0 |
| 31 | d | 403 | PL9 | 3 | 0 |
| 29 | BN | 101 | BCR | 2 | 0 |
| 24 | 0 | 610 | CLA | 10 | 0 |
| 23 | N | 601 | CHL | 10 | 0 |
| 33 | BI | 102 | HEM | 2 | 0 |
| 23 | BJ | 608 | CHL | 7 | 0 |
| 24 | A6 | 602 | CLA | 5 | 0 |
| 24 | g | 613 | CLA | 5 | 0 |
| 24 | g | 603 | CLA | 2 | 0 |
| 24 | A6 | 604 | CLA | 3 | 0 |
| 23 | Y | 307 | CHL | 5 | 0 |
| 24 | 1 | 512 | CLA | 2 | 0 |
| 23 | BU | 613 | CHL | 2 | 0 |
| 24 | y | 305 | CLA | 2 | 0 |
| 30 | I | 101 | LMG | 3 | 0 |
| 24 | BF | 505 | CLA | 2 | 0 |
| 24 | 6 | 610 | CLA | 5 | 0 |
| 28 | Au | 619 | XAT | 4 | 0 |
| 24 | 5 | 613 | CLA | 7 | 0 |
| 34 | a | 401 | DGD | 2 | 0 |
| 23 | 8 | 307 | CHL | 4 | 0 |

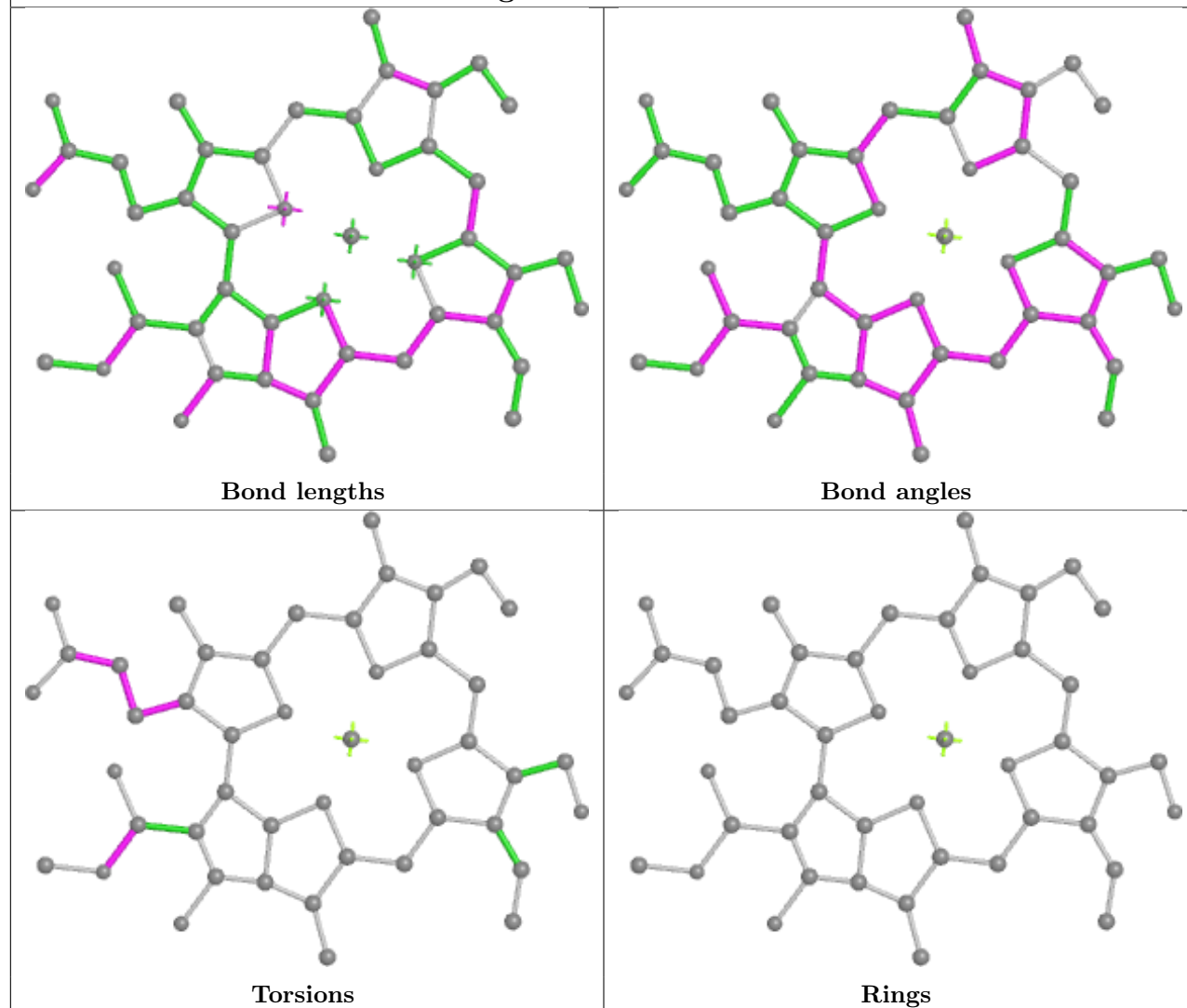
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 BU 609**Ligand CLA BD 407**

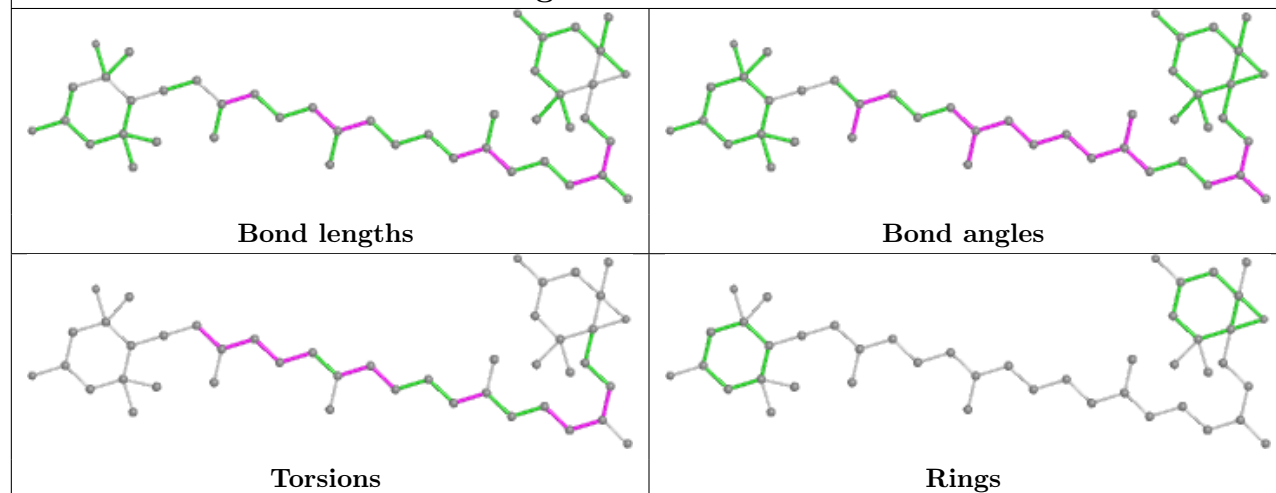
Ligand CLA 5 614

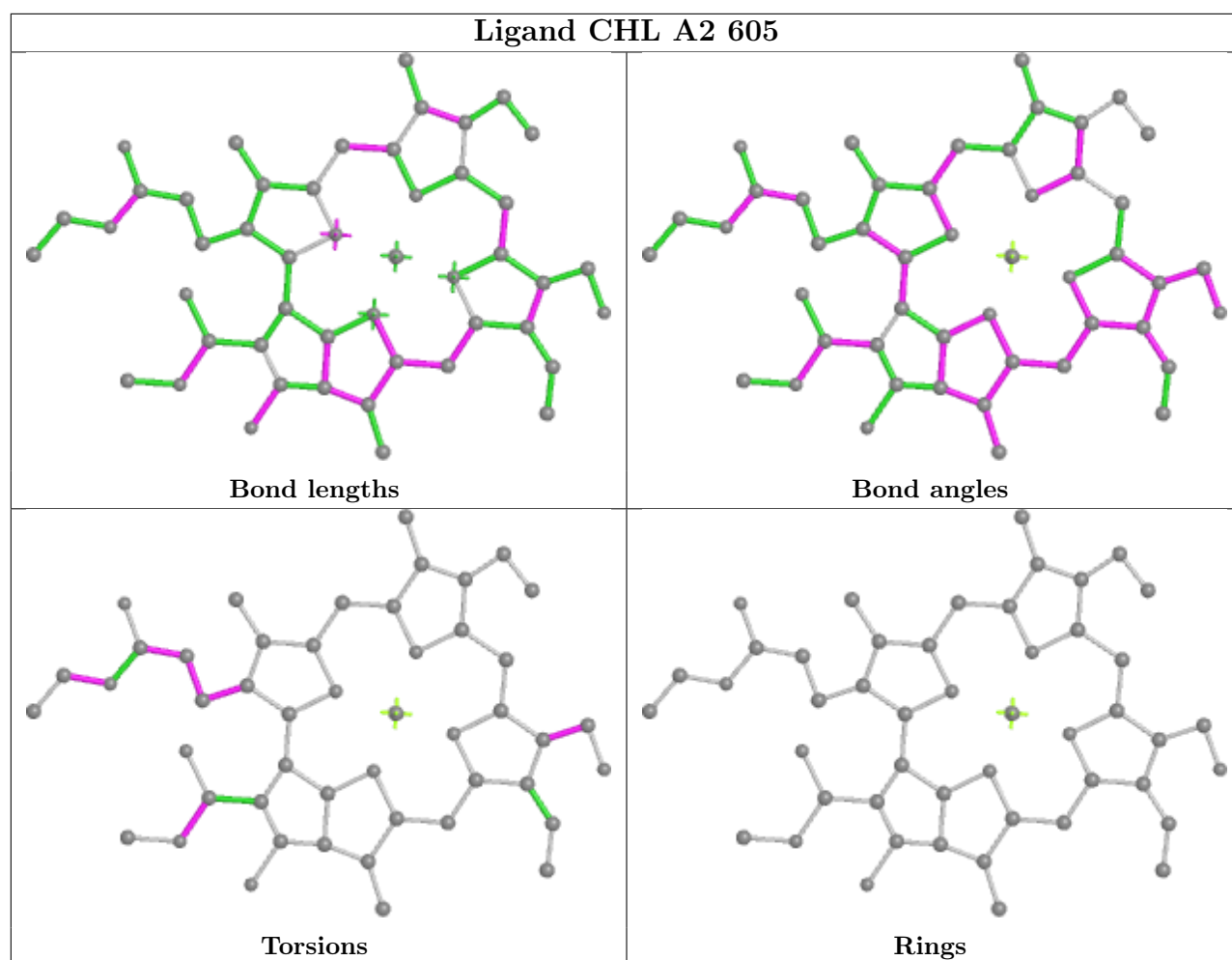


Ligand CHL 6 606

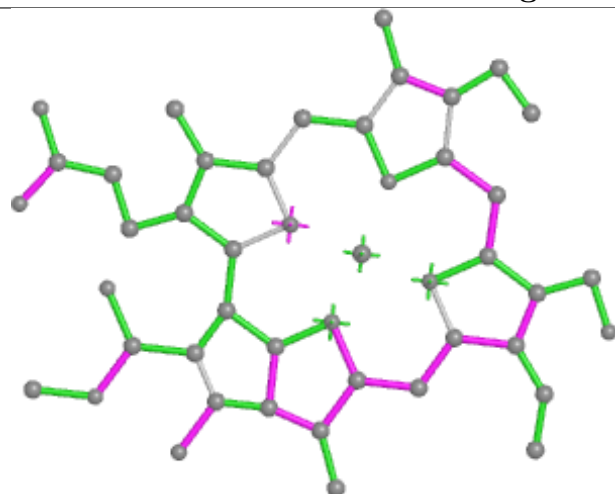


Ligand NEX s 616

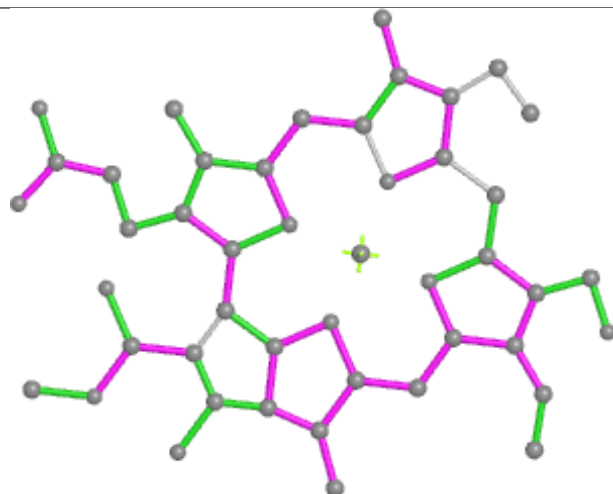




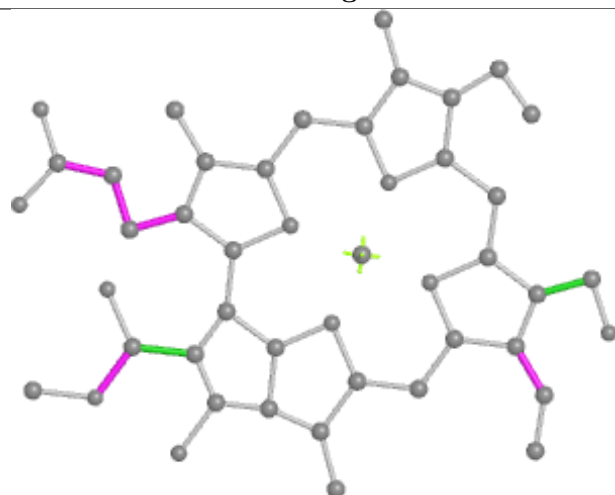
Ligand CHL 5 601



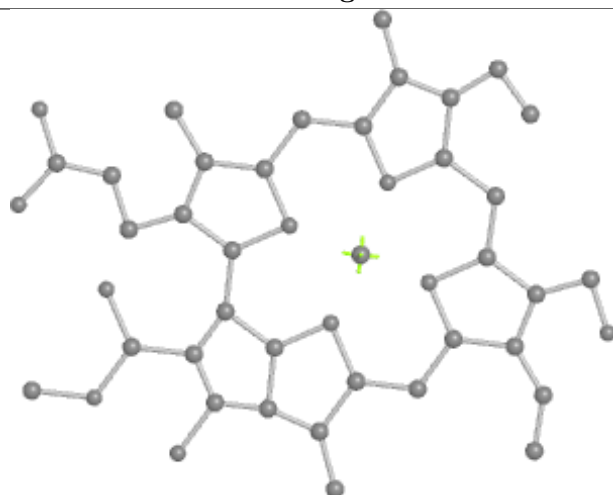
Bond lengths



Bond angles

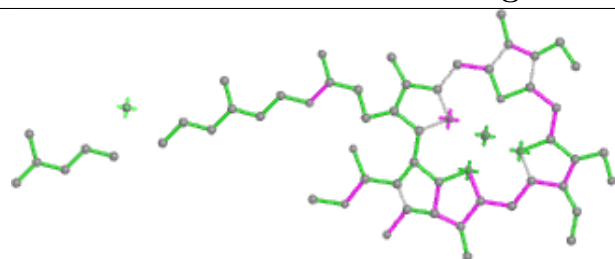


Torsions

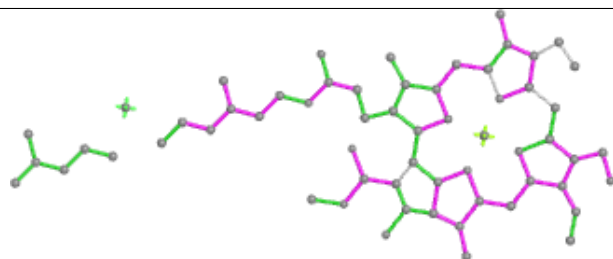


Rings

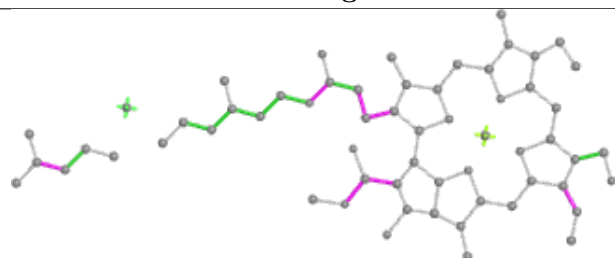
Ligand CHL AA 310



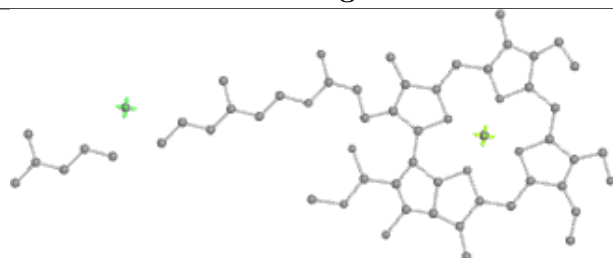
Bond lengths



Bond angles

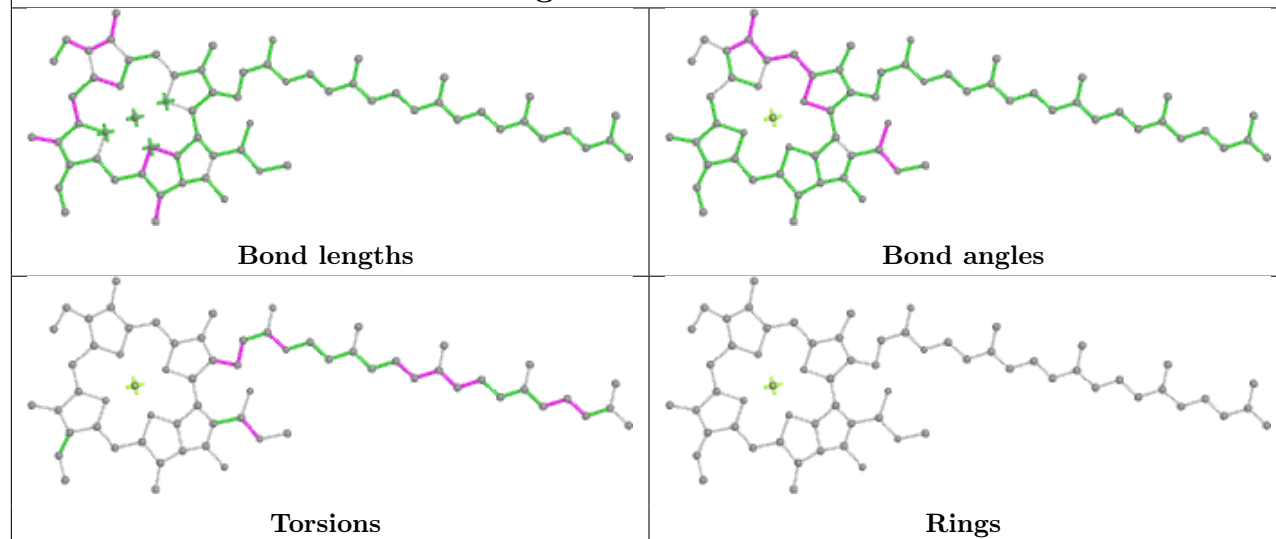


Torsions

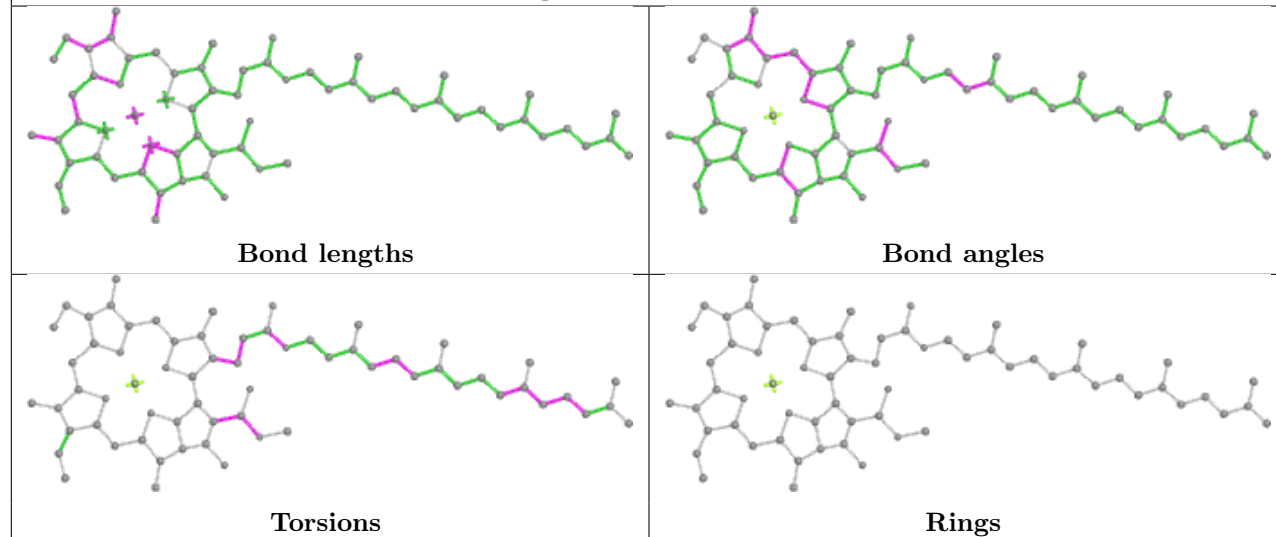


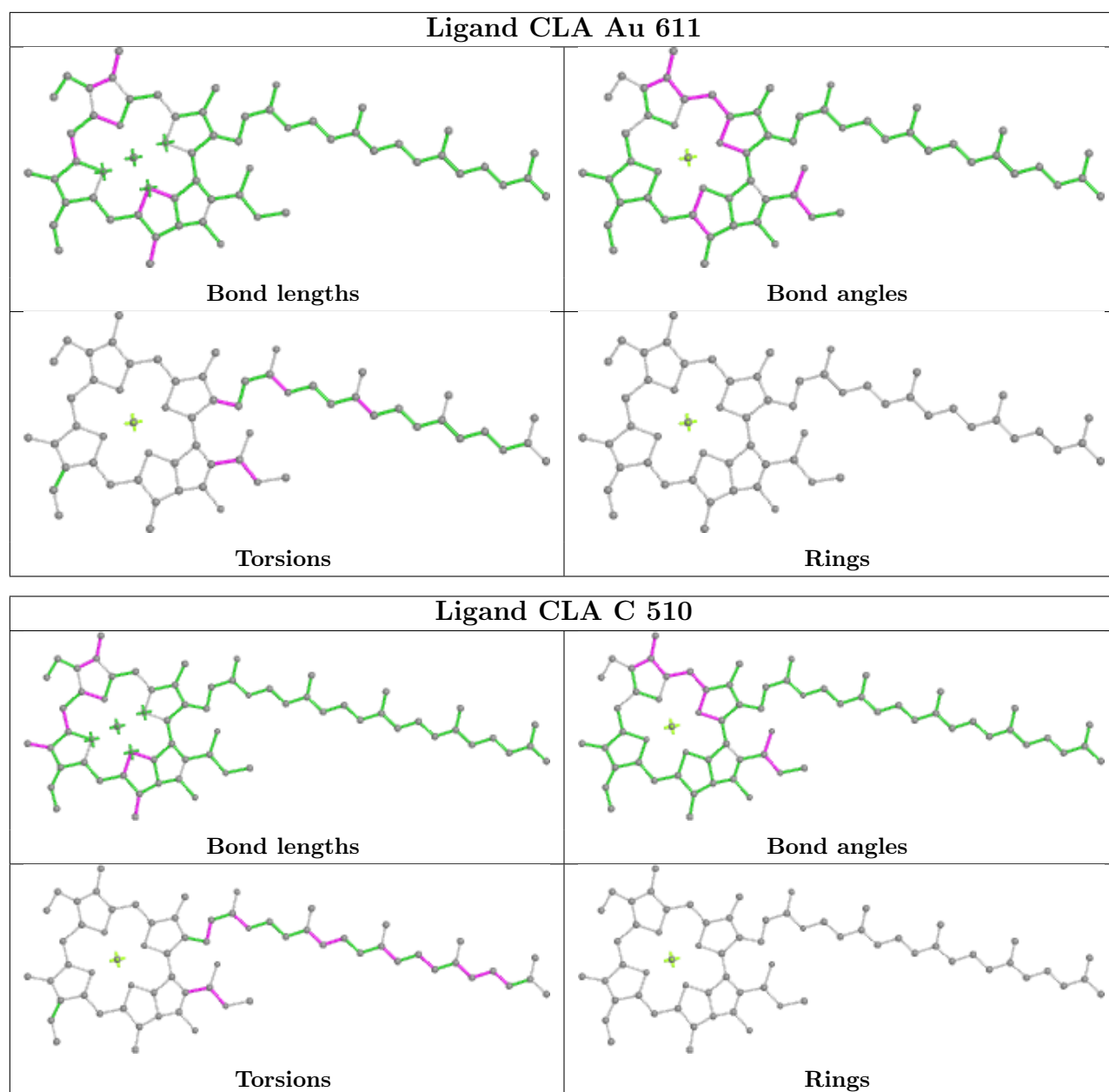
Rings

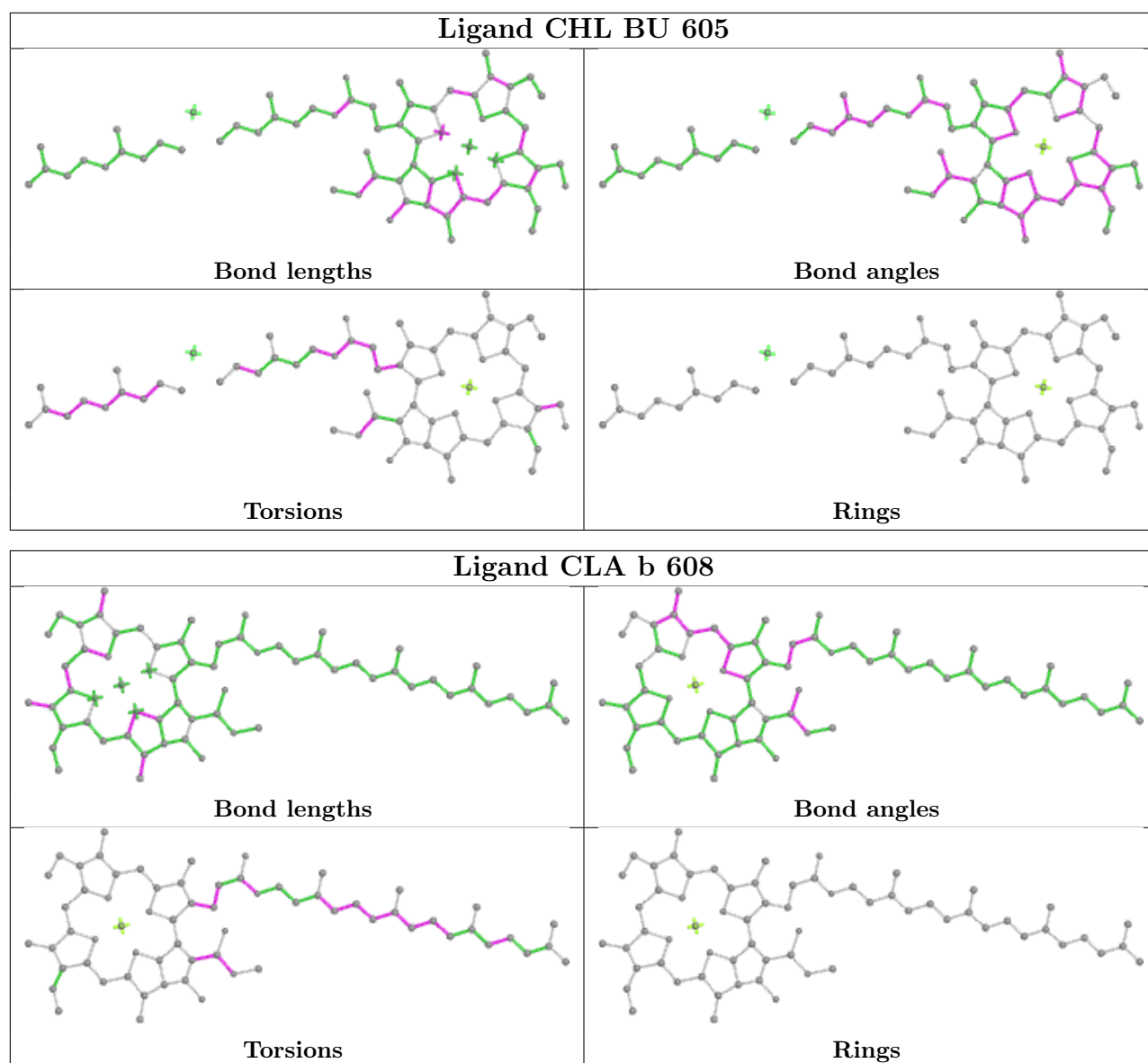
Ligand CLA v 608

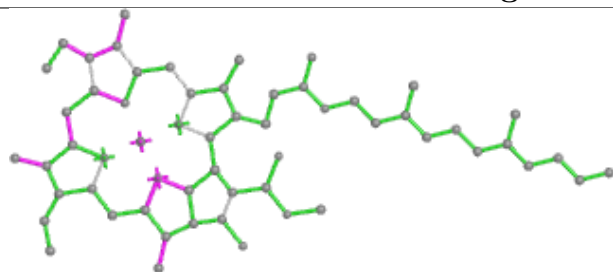


Ligand CLA 1 506

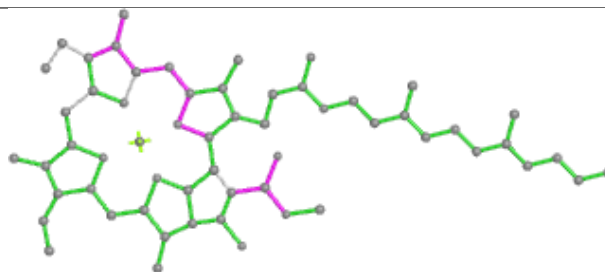




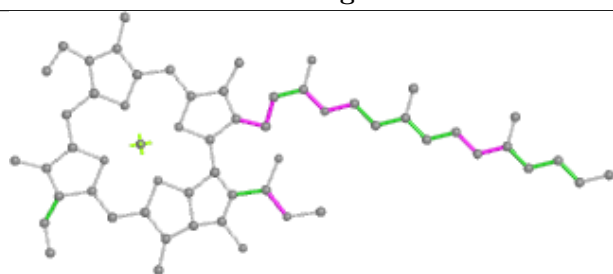


Ligand CLA BU 608

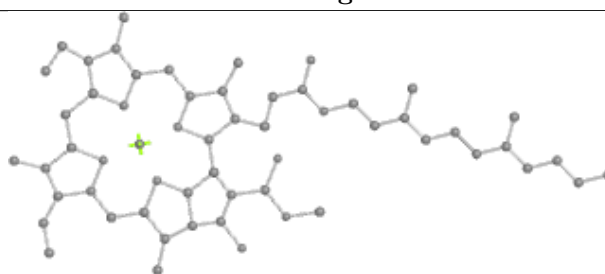
Bond lengths



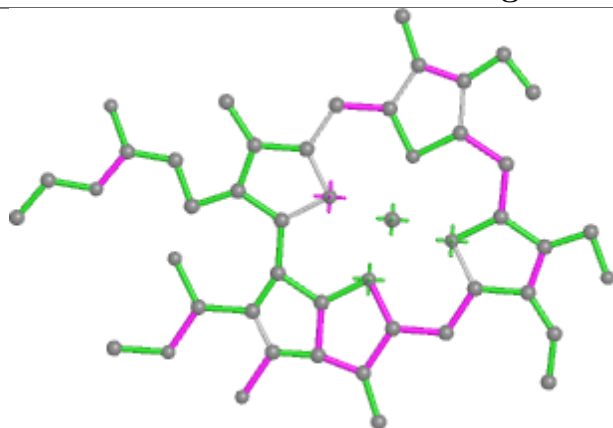
Bond angles



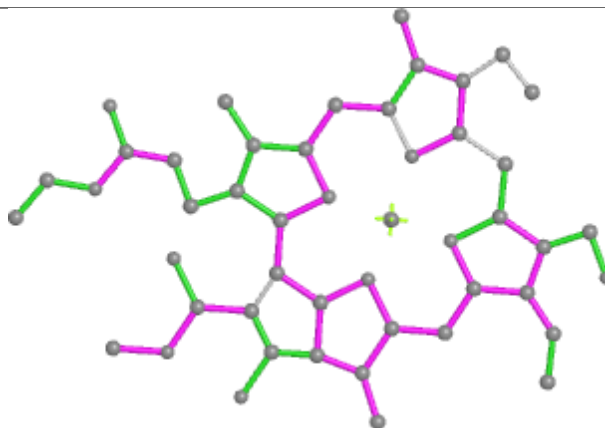
Torsions



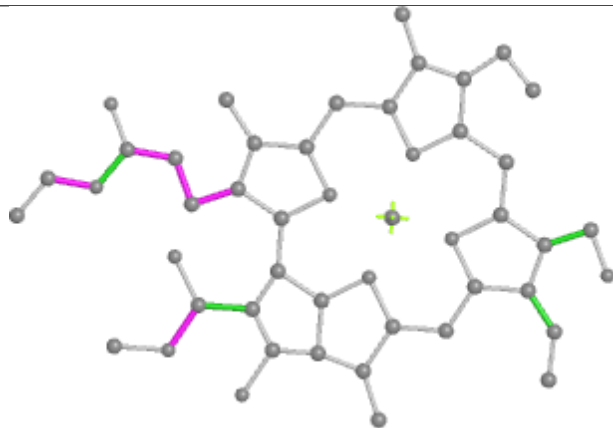
Rings

Ligand CHL BB 306

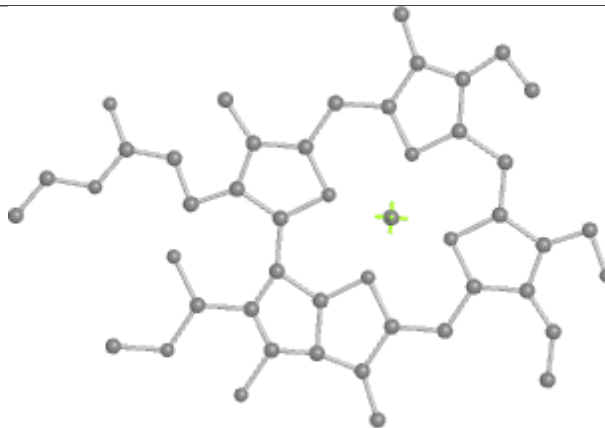
Bond lengths



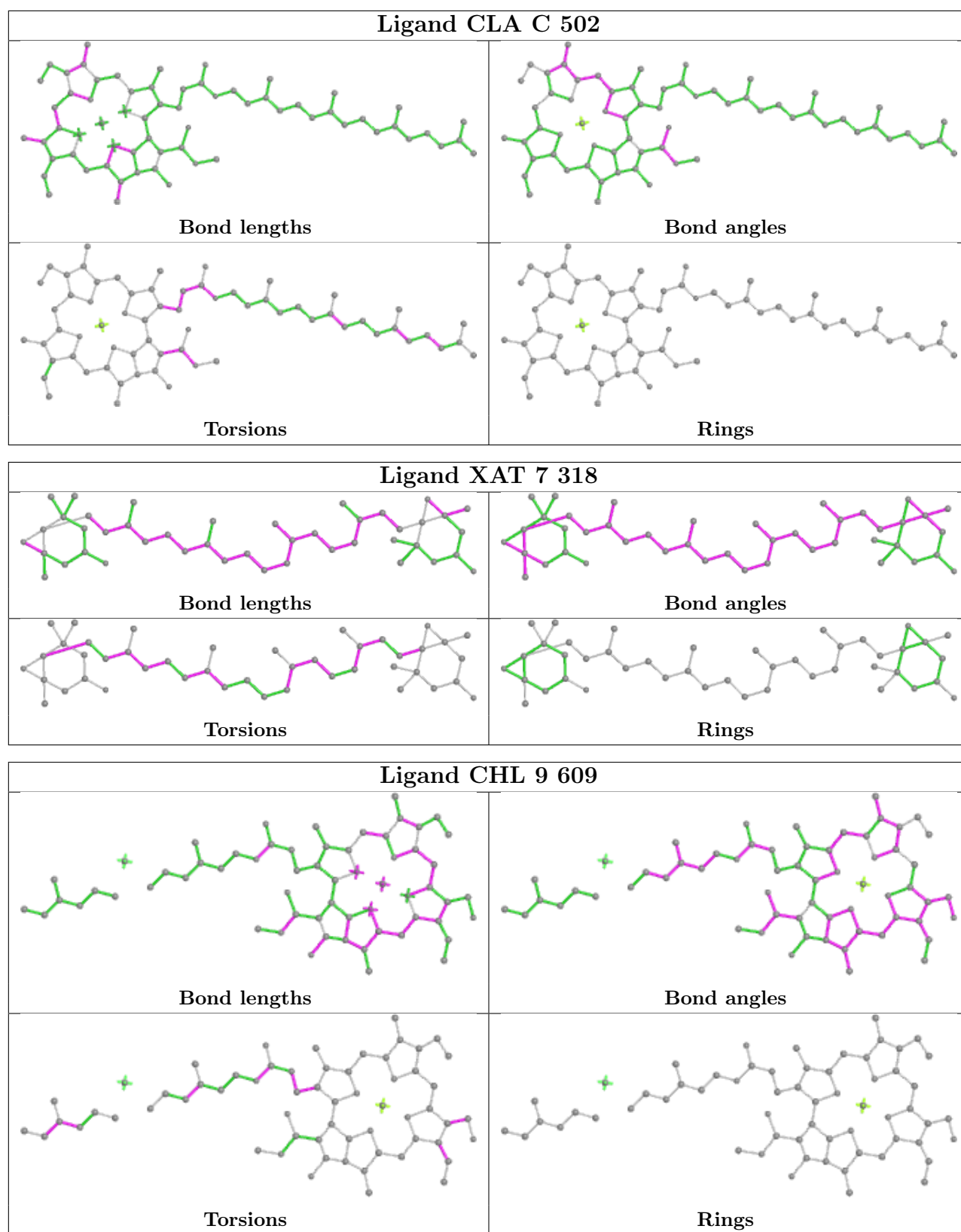
Bond angles



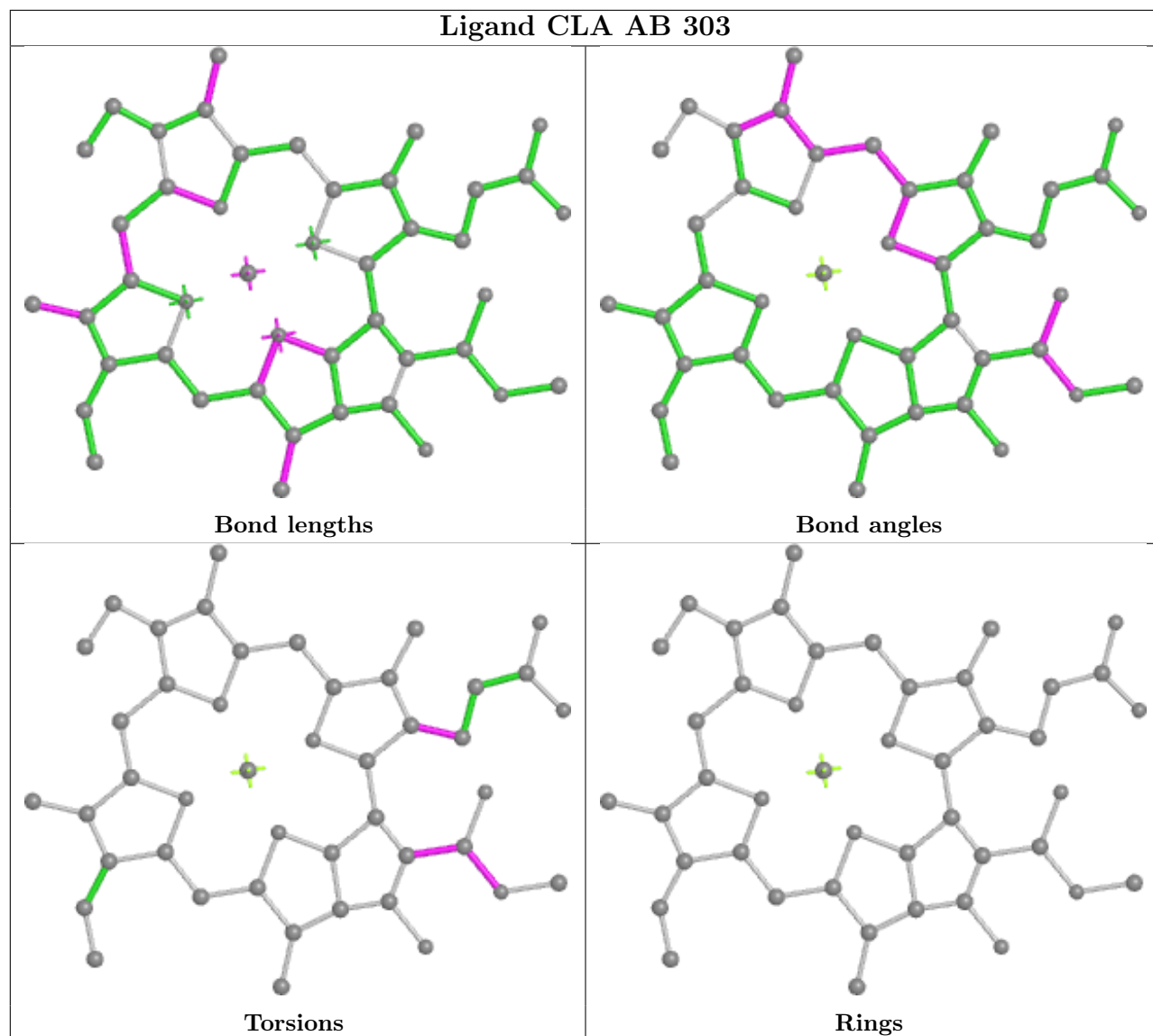
Torsions

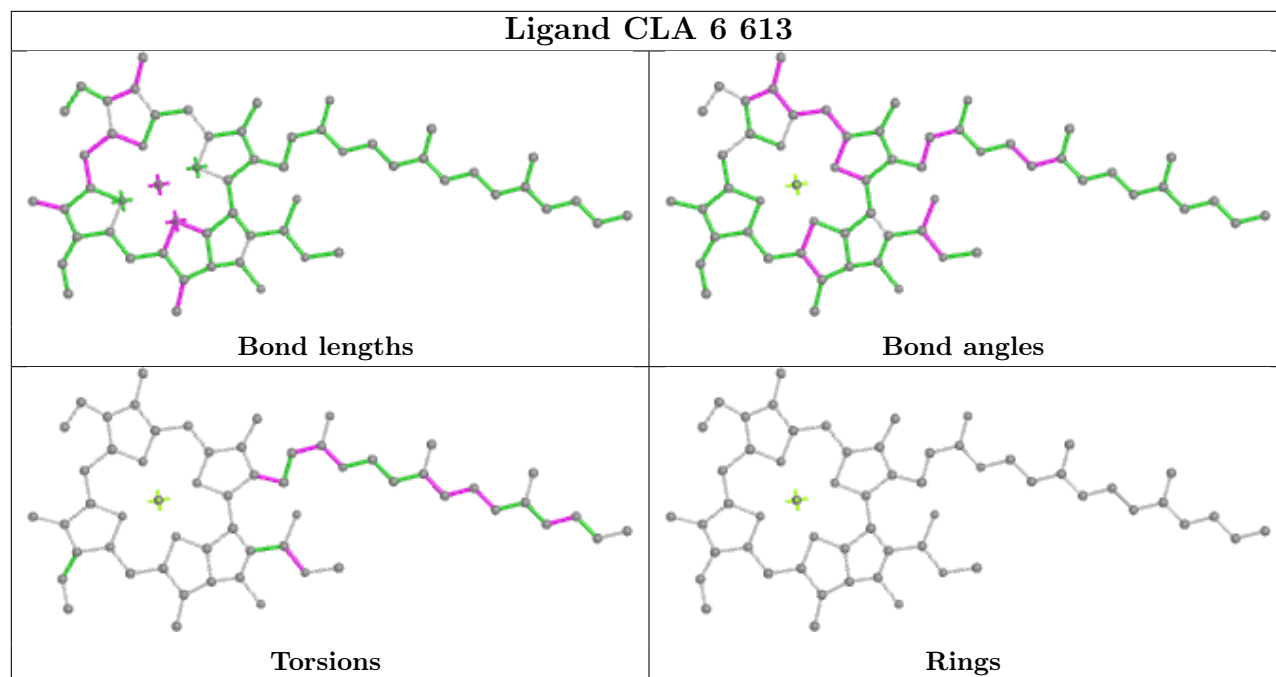
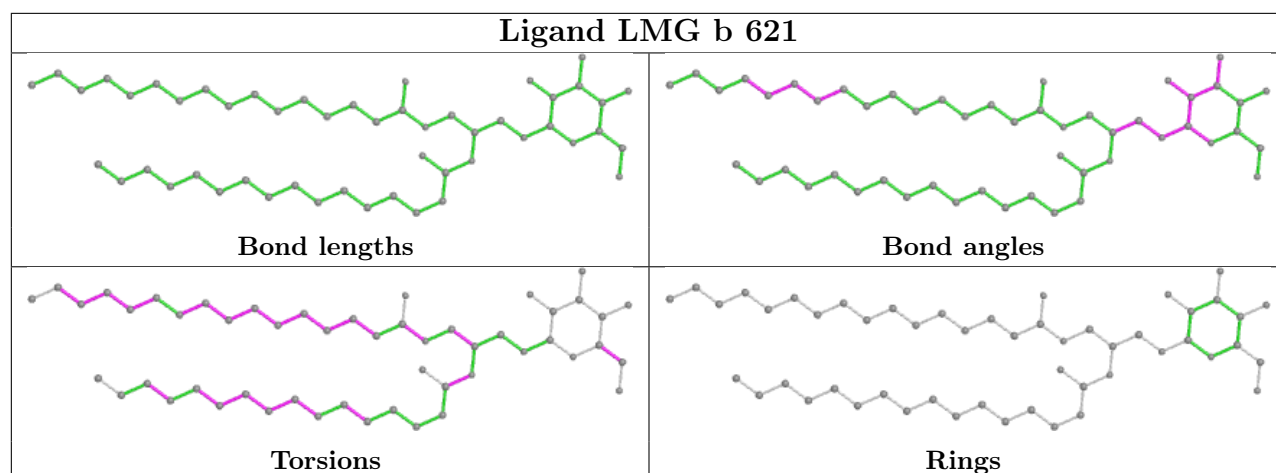
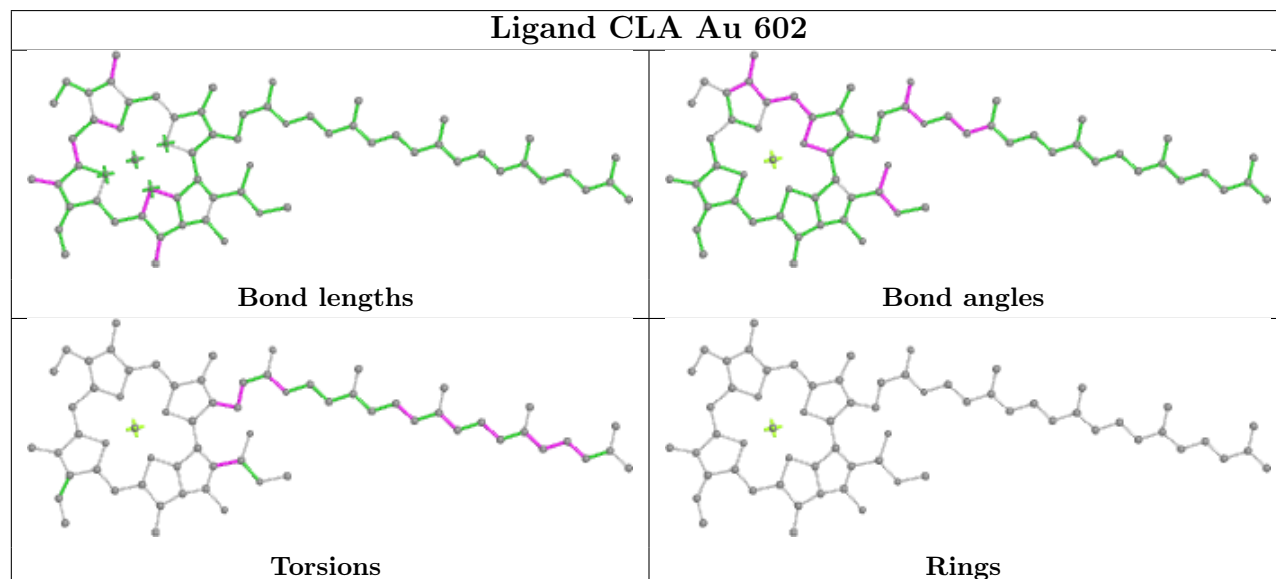


Rings

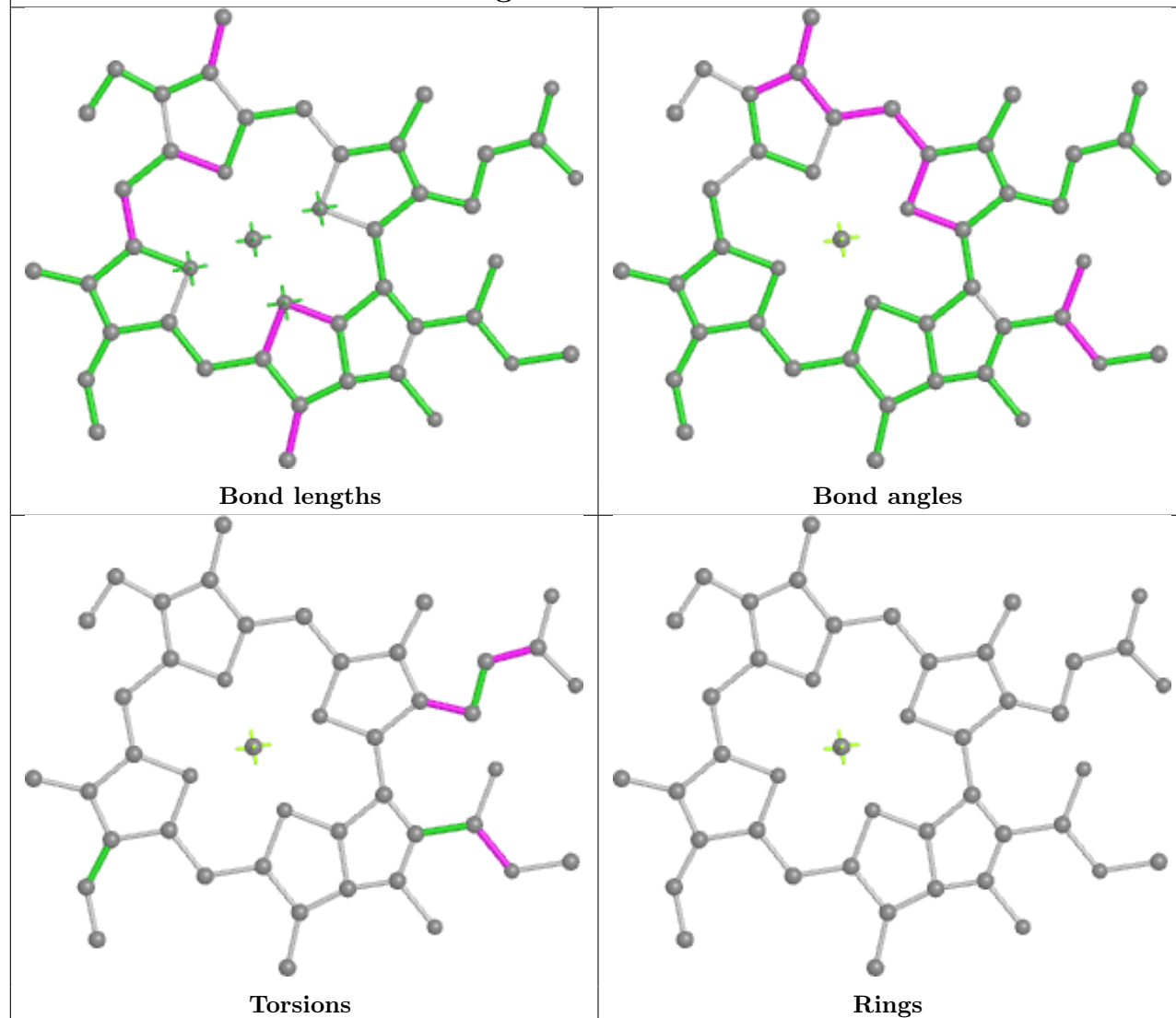


Ligand CLA AB 303

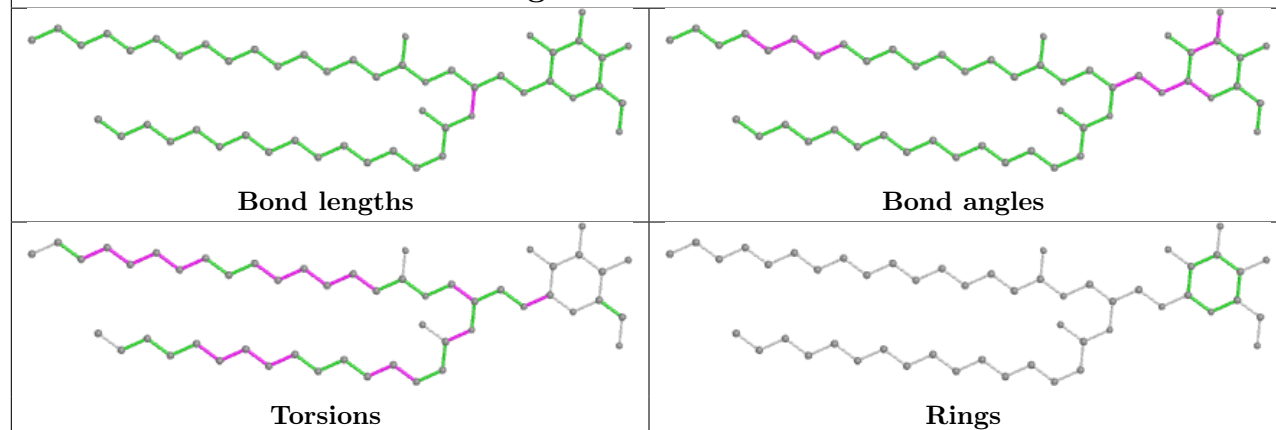


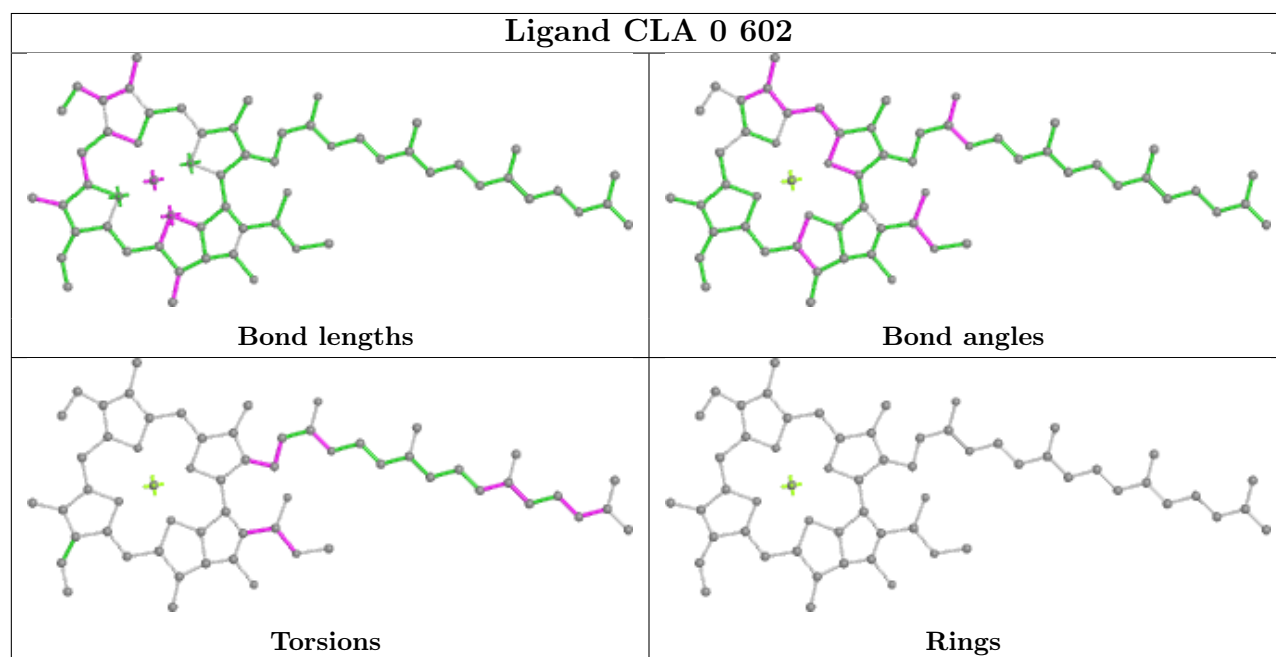
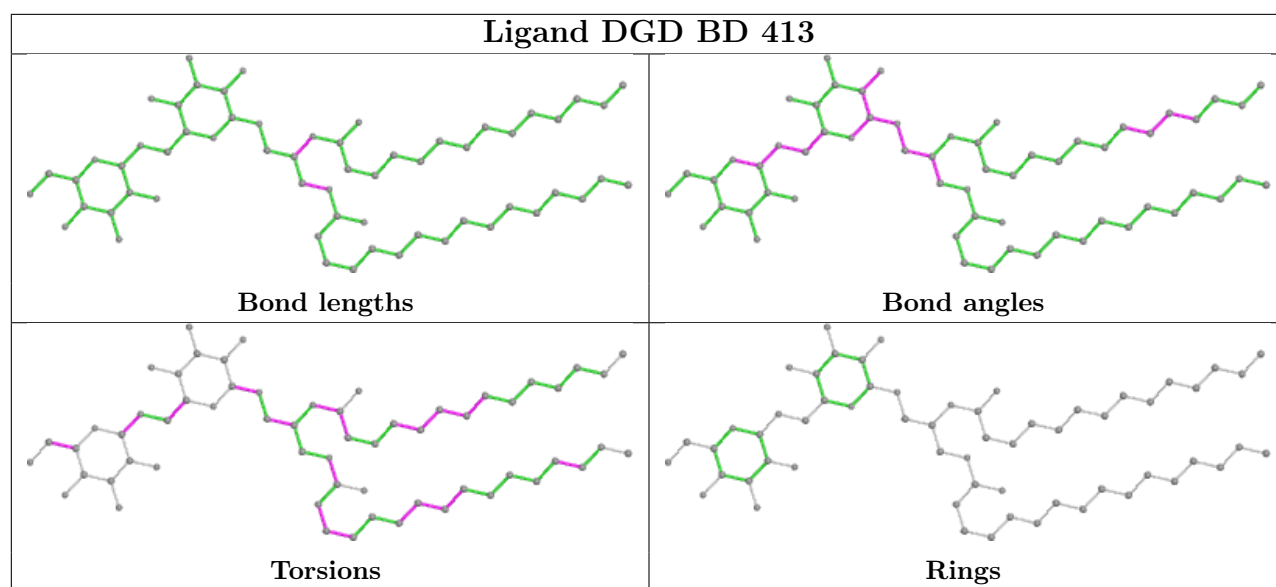
Ligand CLA 6 613**Ligand LMG b 621****Ligand CLA Au 602**

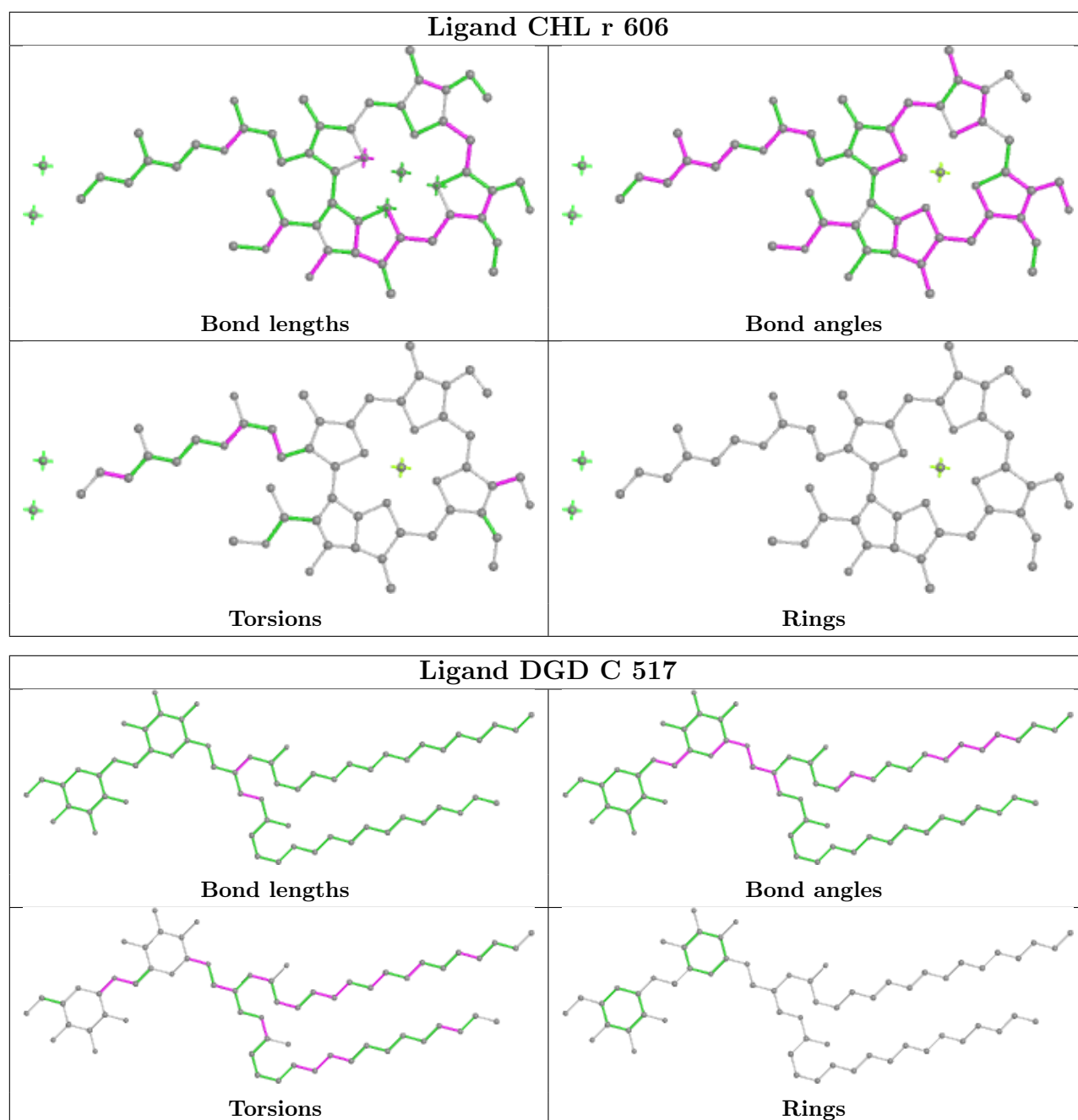
Ligand CLA s 608



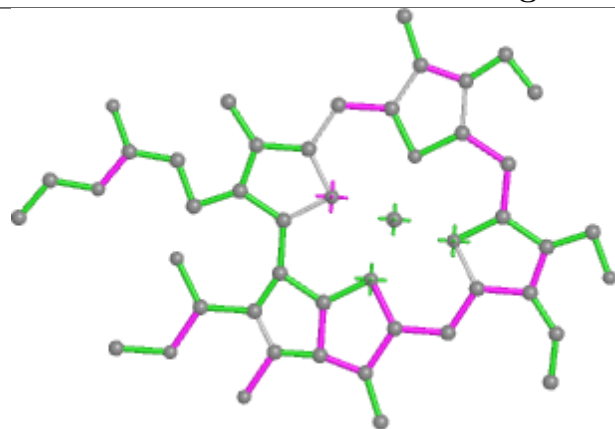
Ligand LMG C 519



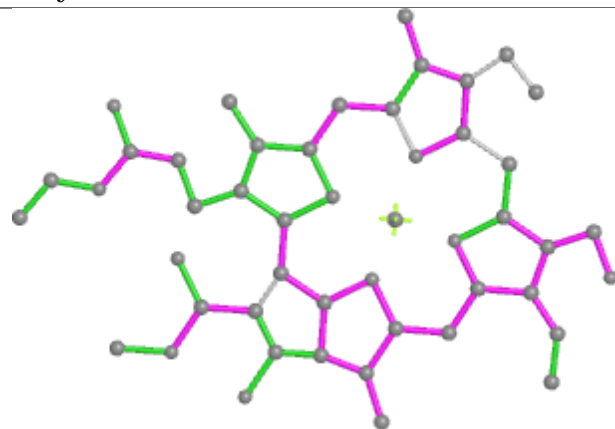




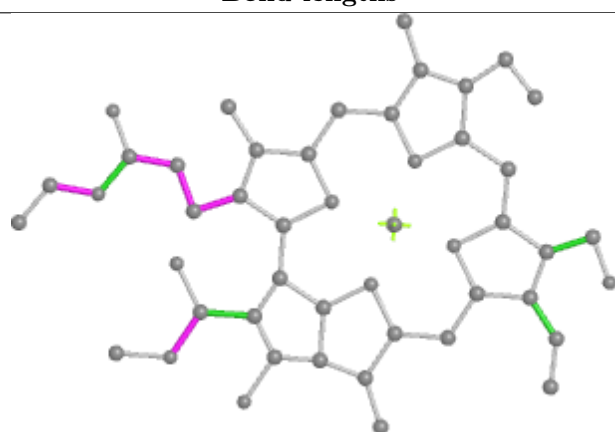
Ligand CHL y 306



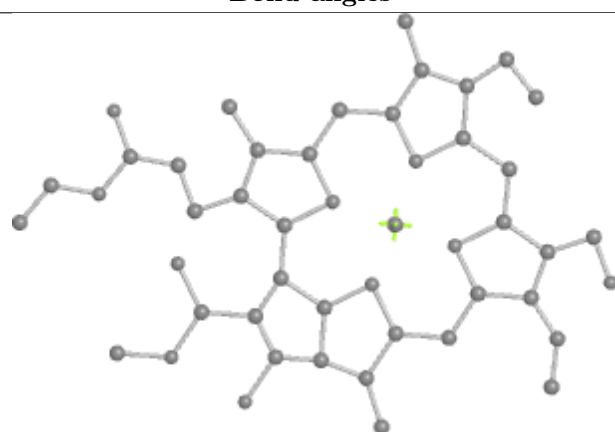
Bond lengths



Bond angles

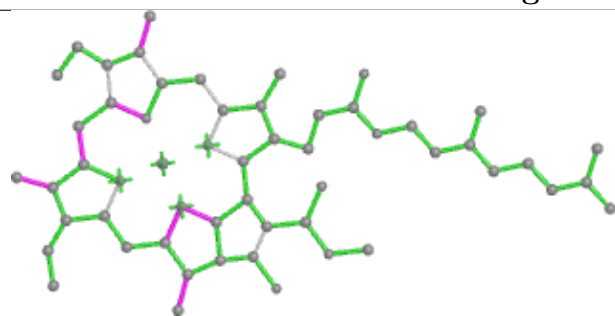


Torsions

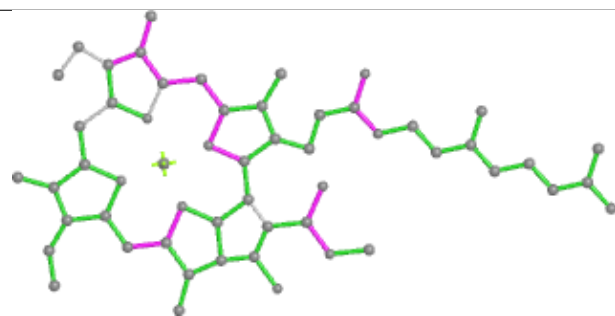


Rings

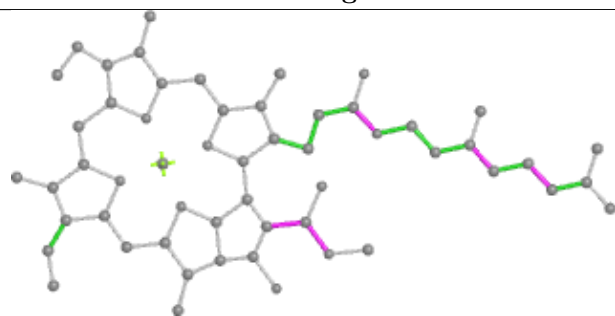
Ligand CLA s 609



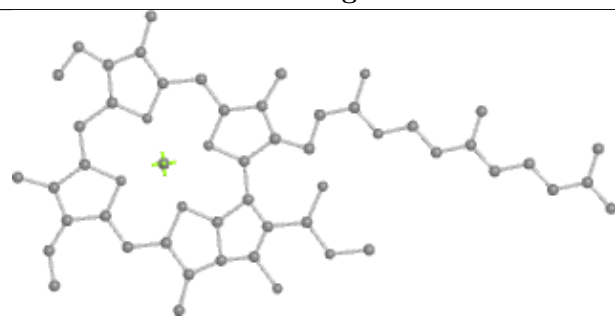
Bond lengths



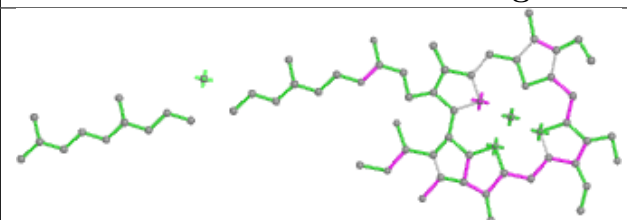
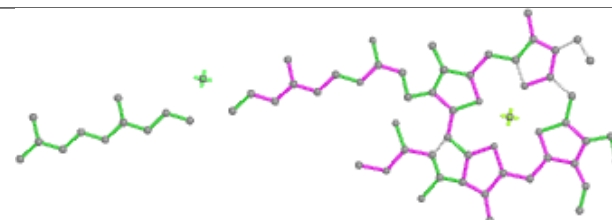
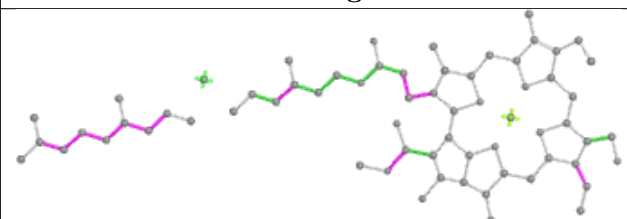
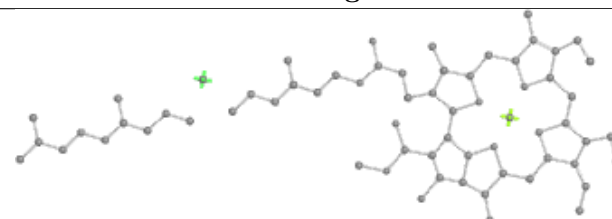
Bond angles

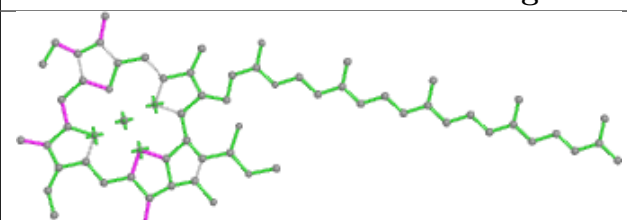
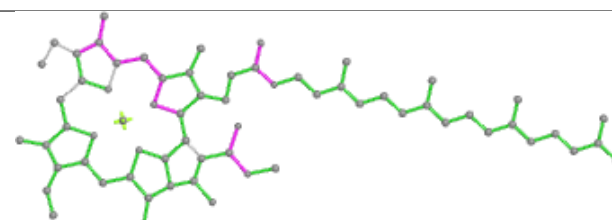
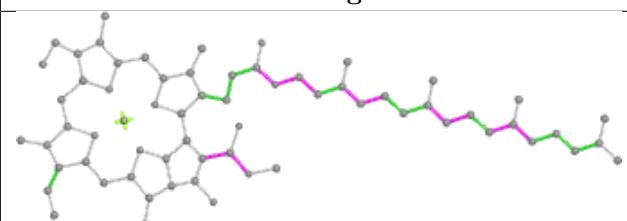
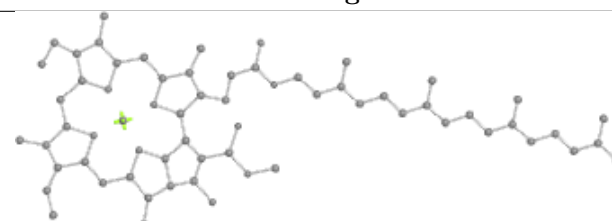


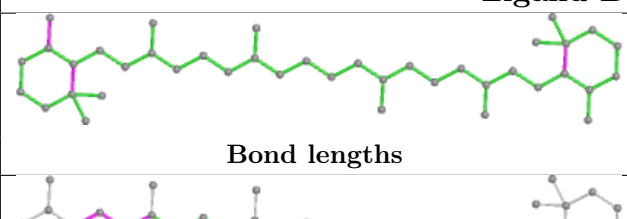
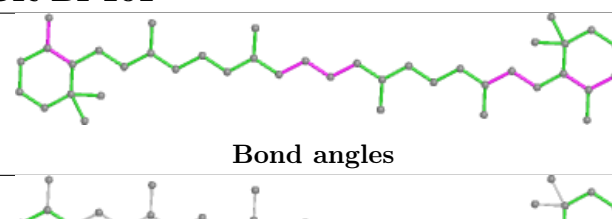


Torsions



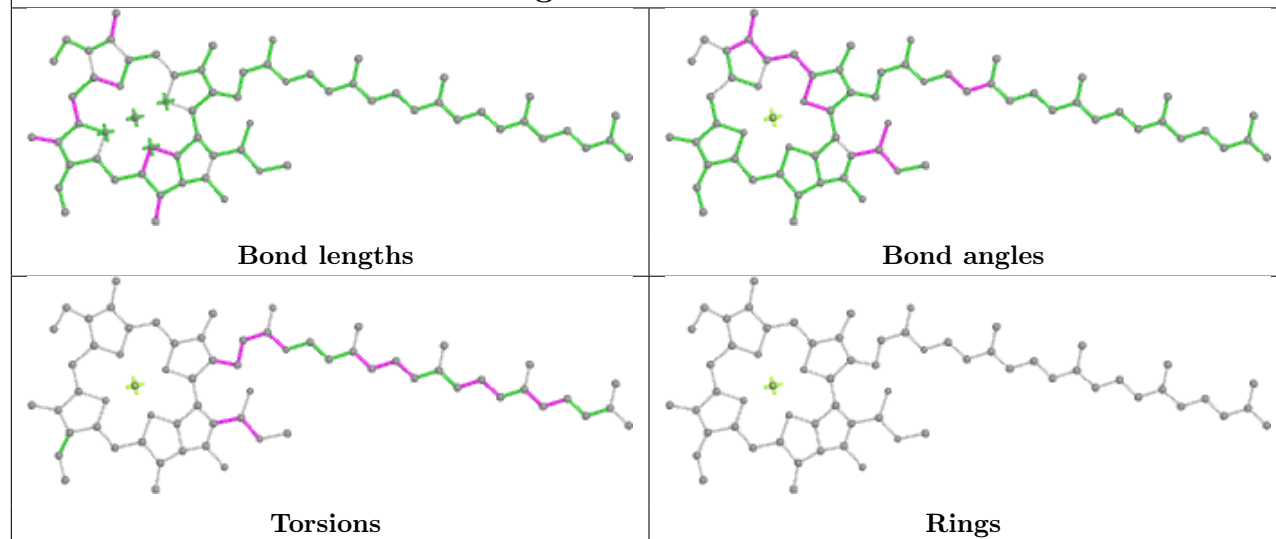
Rings

| Ligand CHL Ba 308 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

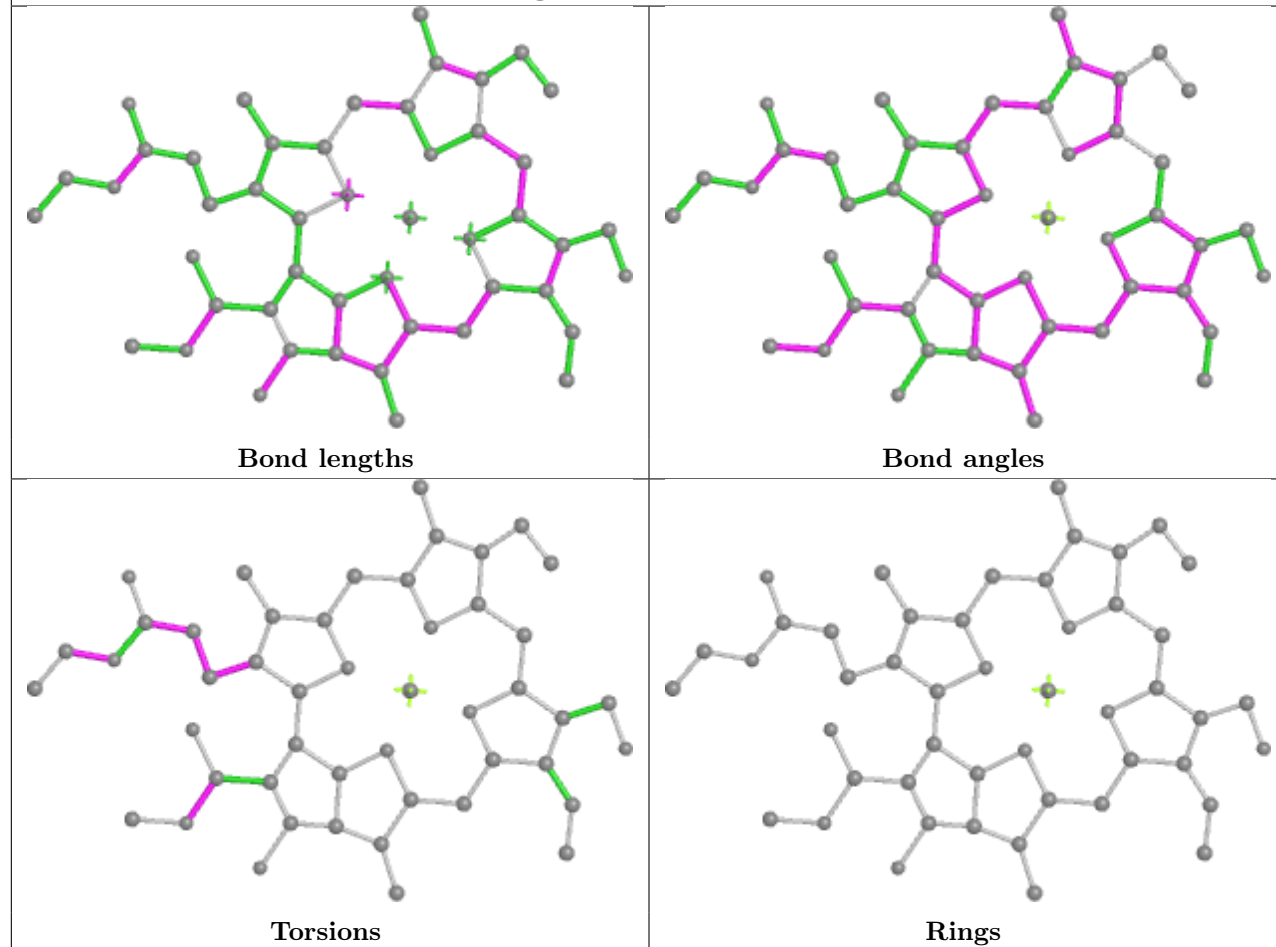
| Ligand CLA B 615 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

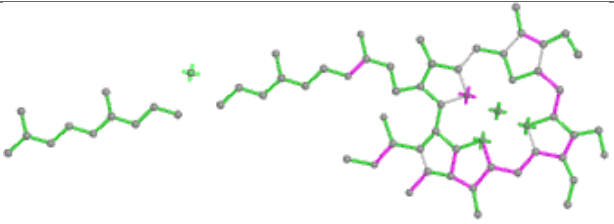
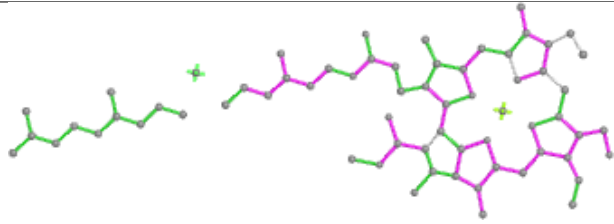
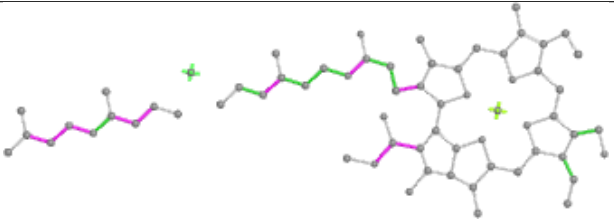
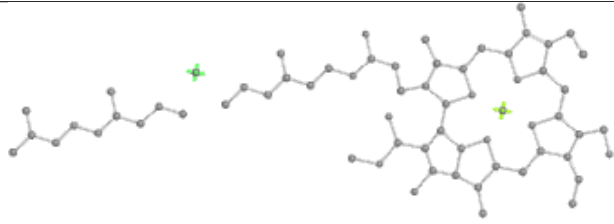
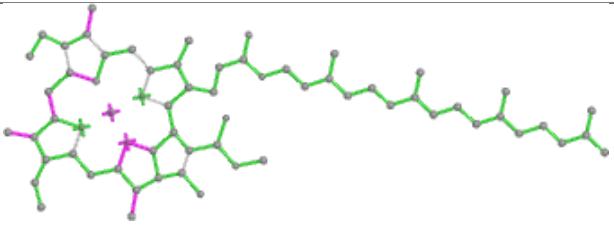
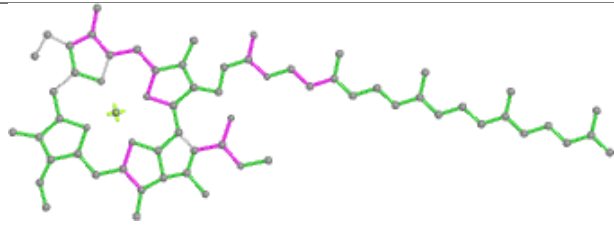
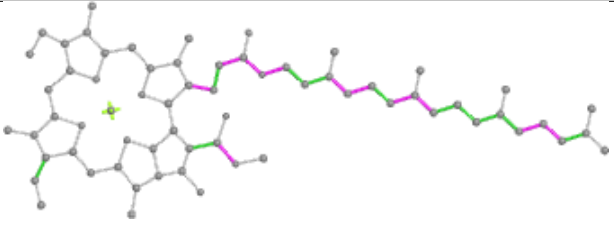
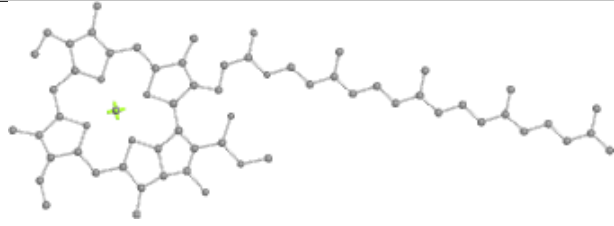
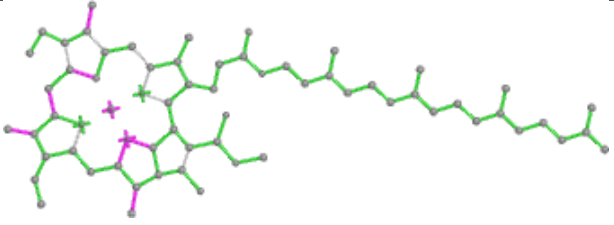
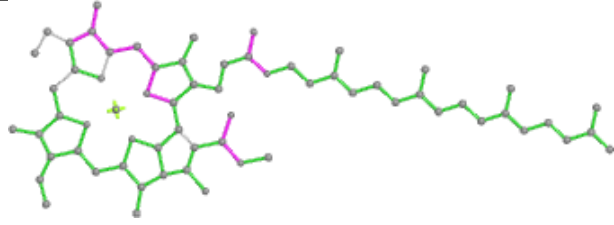
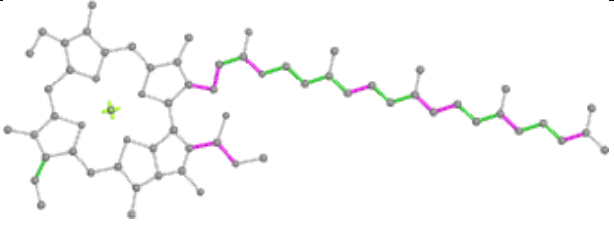
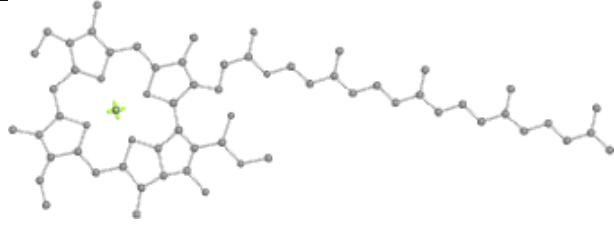
| Ligand BCR BI 101 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

Ligand CLA b 615

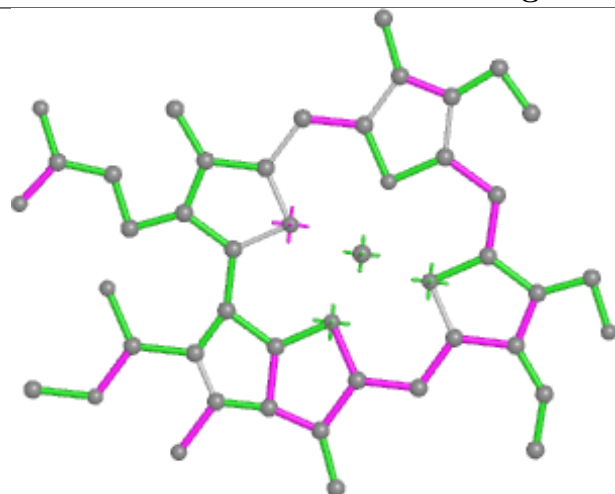


Ligand CHL Y 306

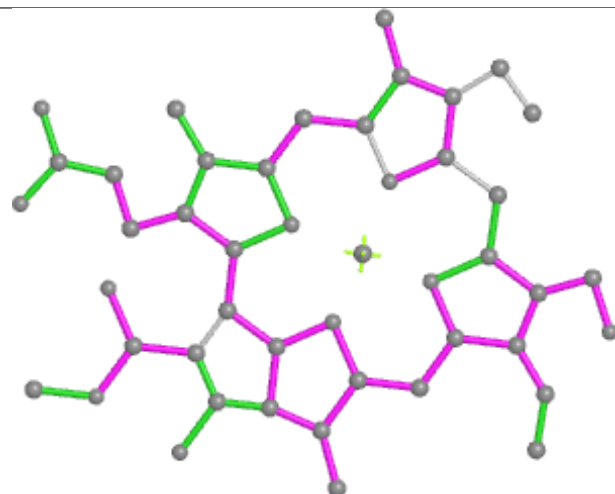


| Ligand CHL G 601 | |
|---|---|
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |
| Ligand CLA 2 402 | |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |
| Ligand CLA C 503 | |
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|  <p>Torsions</p> |  <p>Rings</p> |

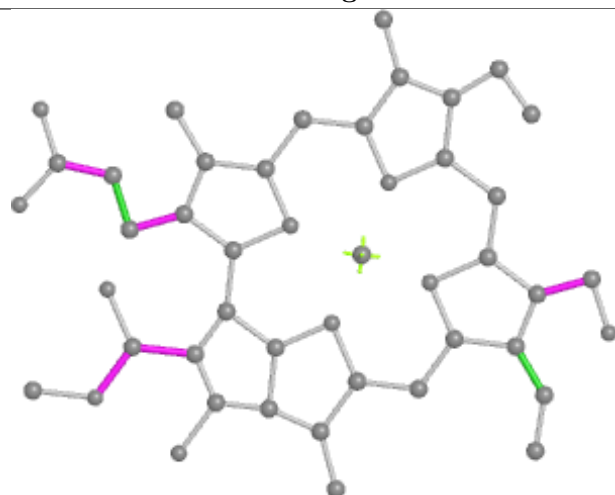
Ligand CHL s 605



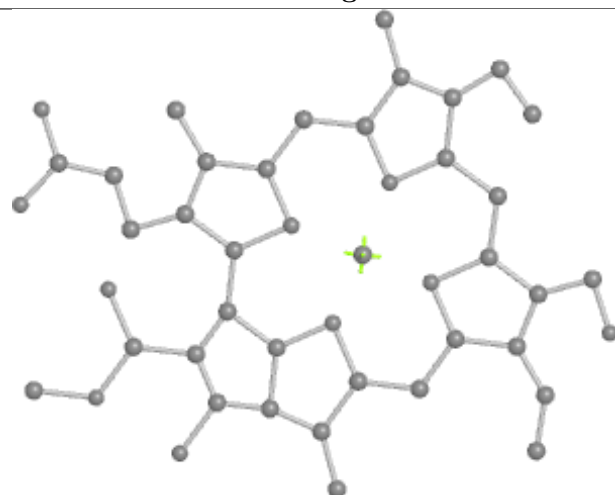
Bond lengths



Bond angles

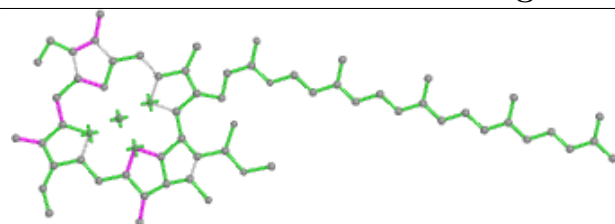


Torsions

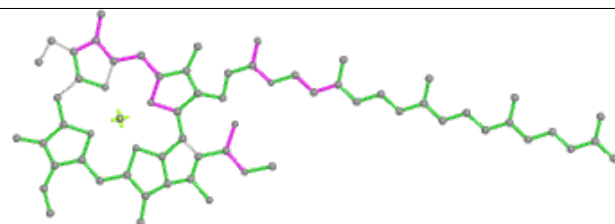


Rings

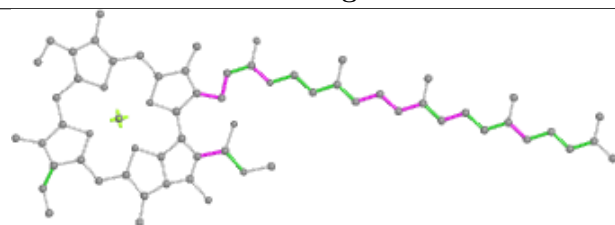
Ligand CLA B 604



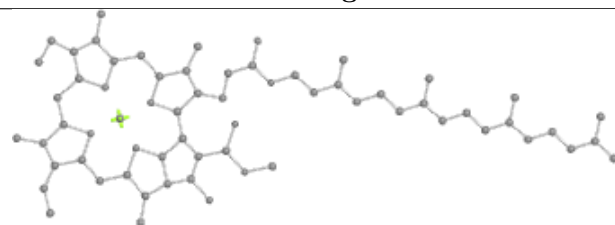
Bond lengths



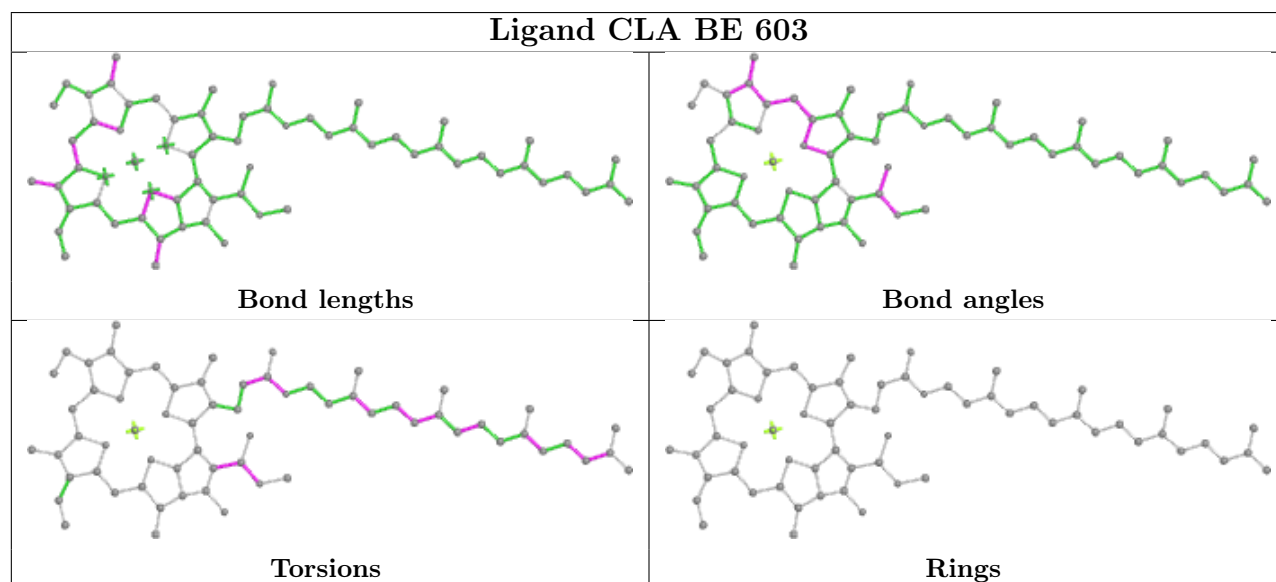
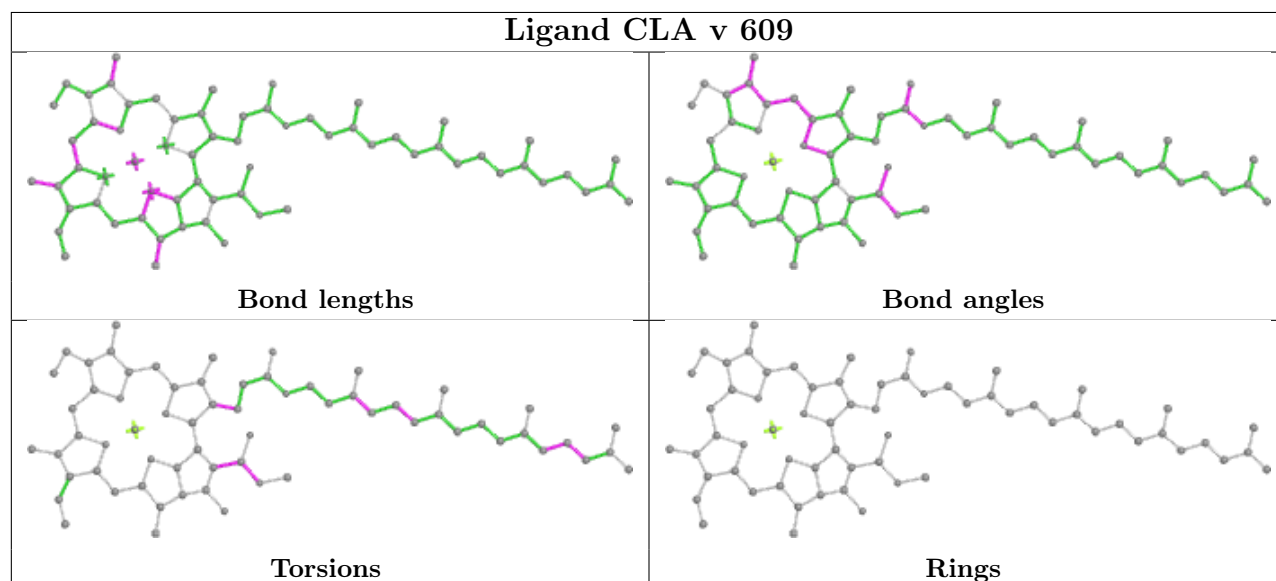
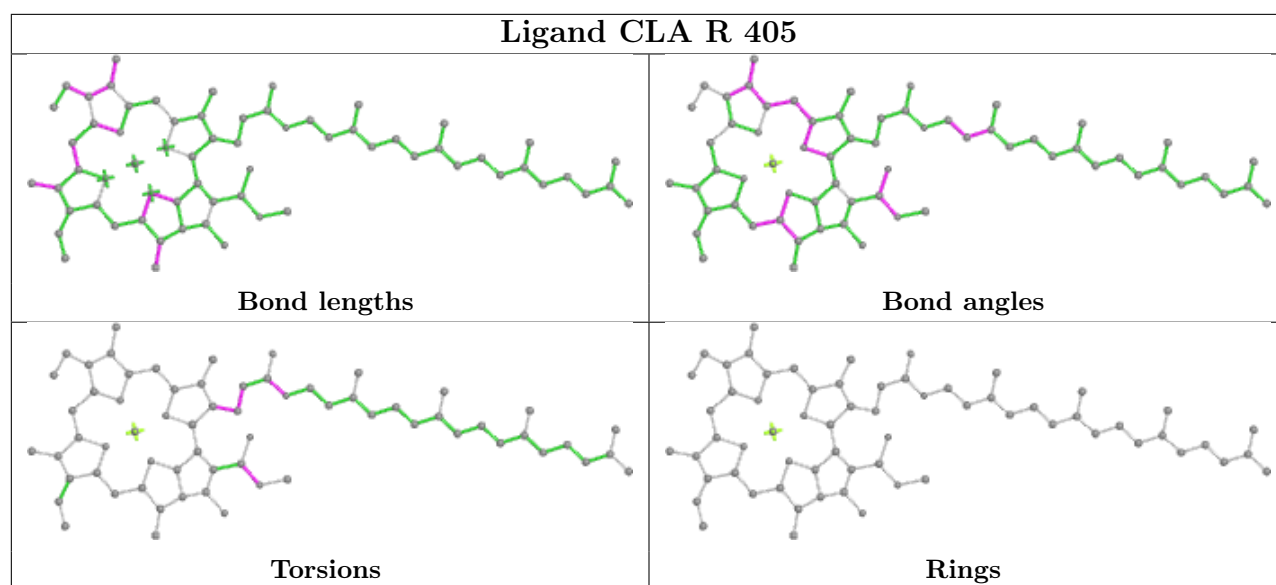
Bond angles



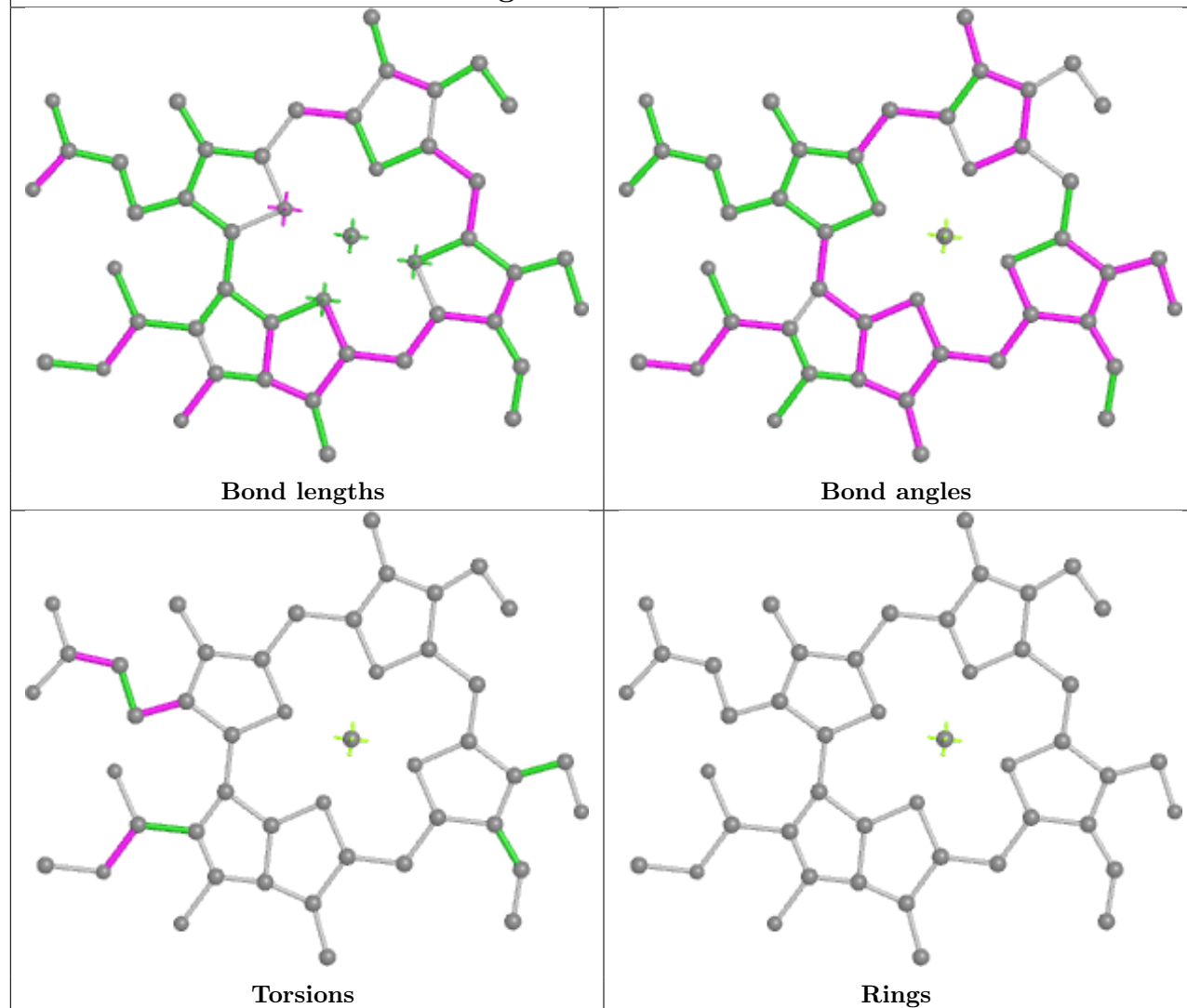
Torsions



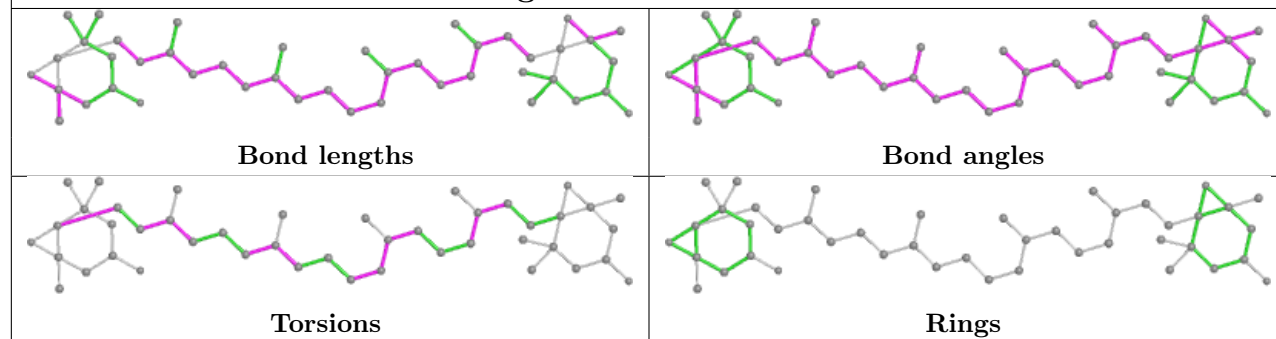
Rings



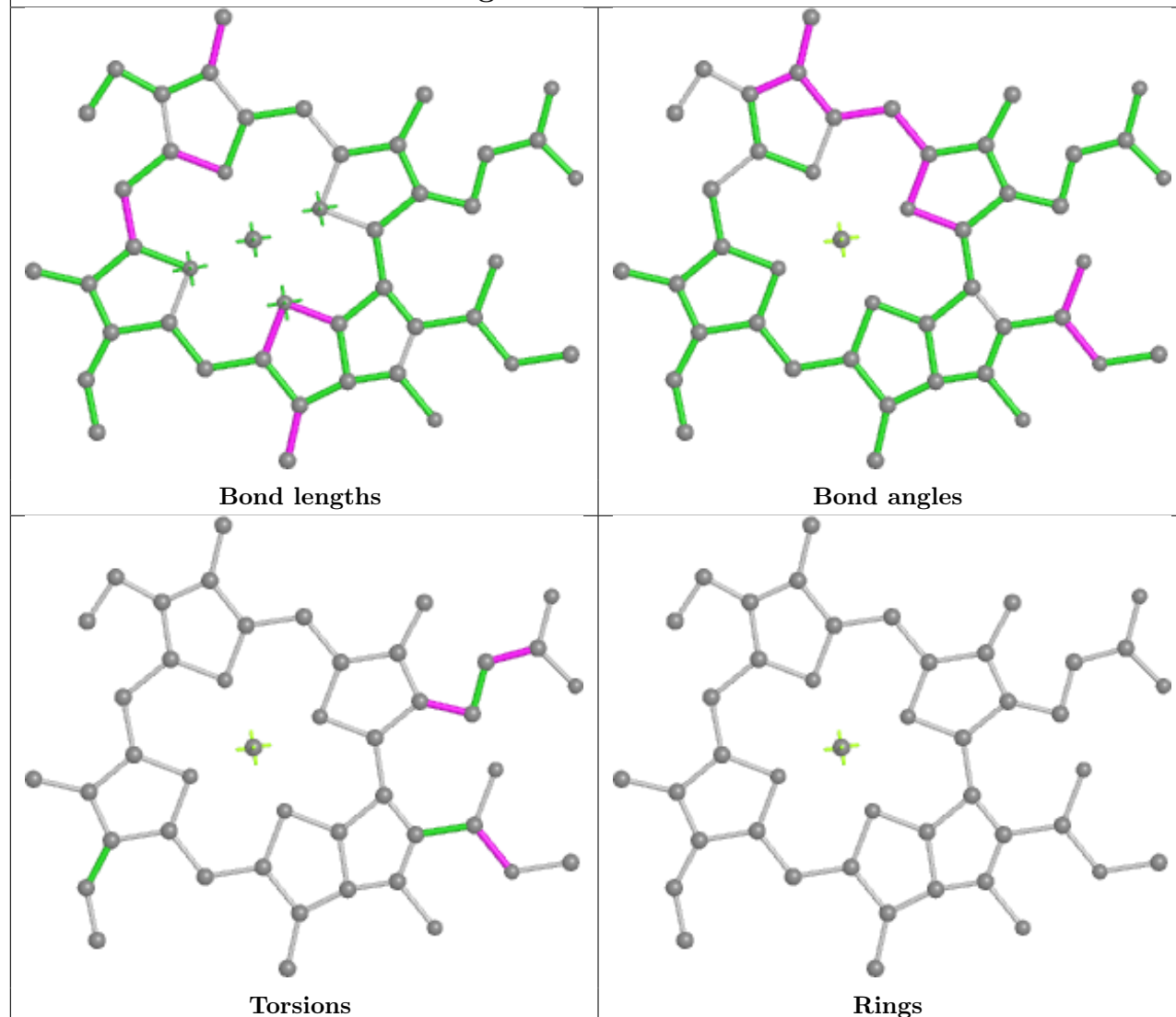
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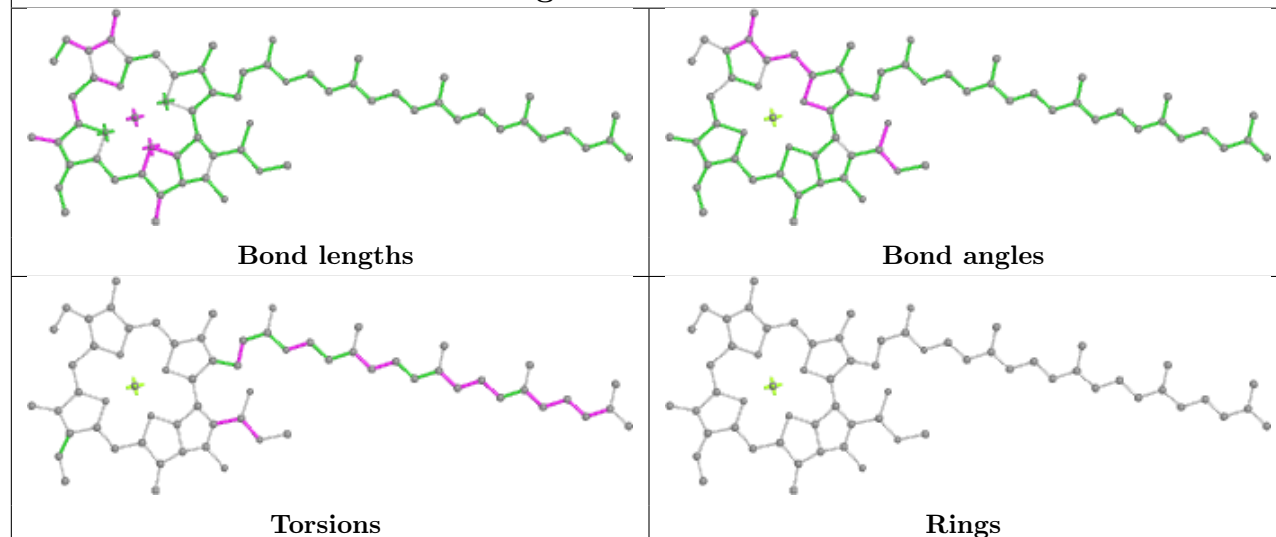
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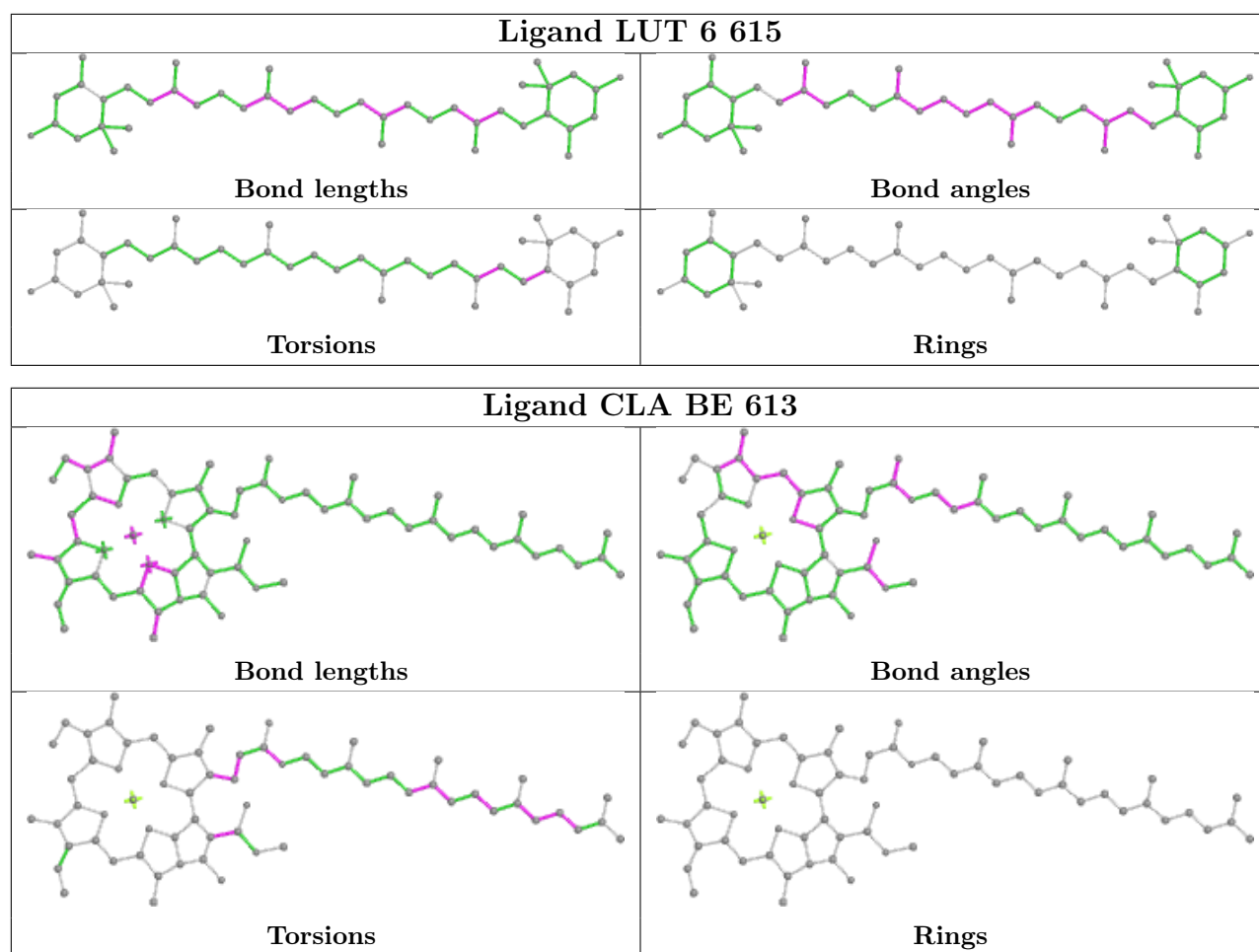


Ligand CLA BV 608

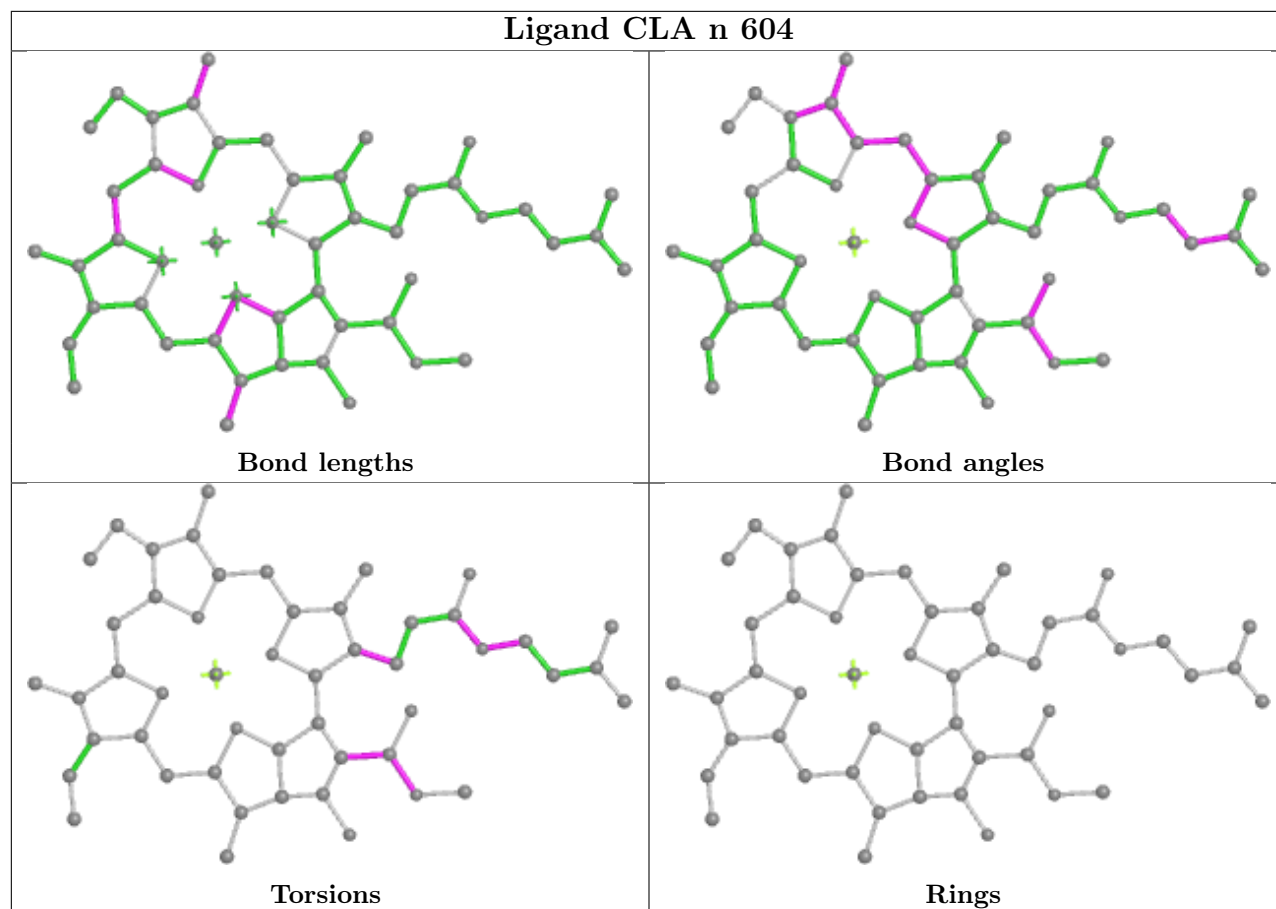


Ligand CLA 1 507

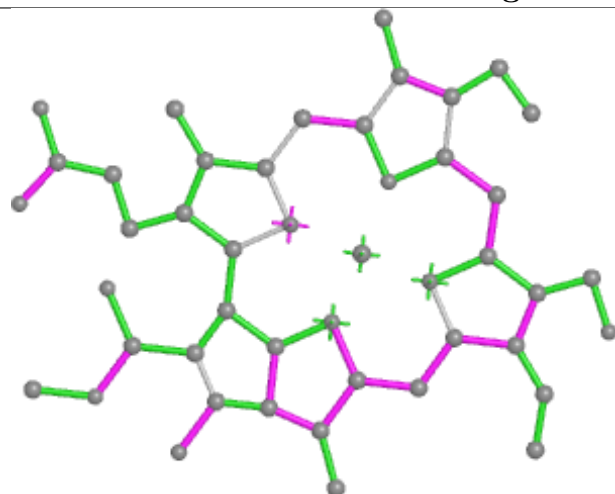




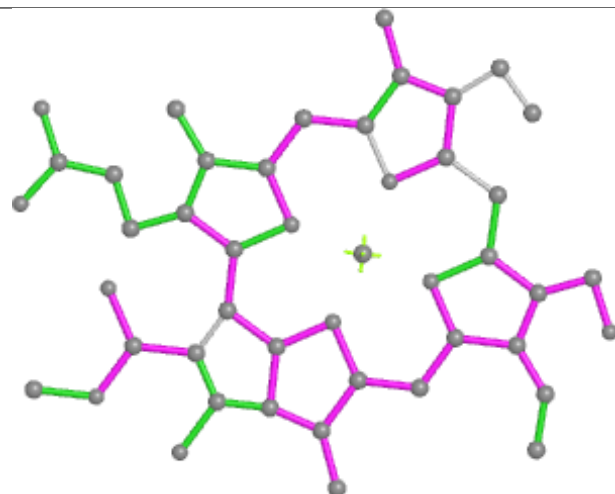
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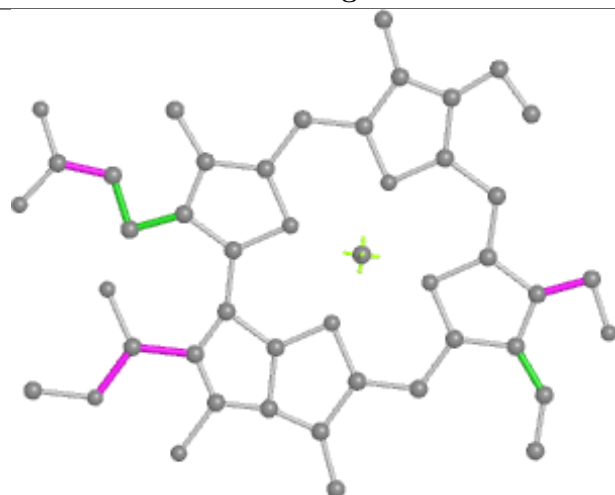
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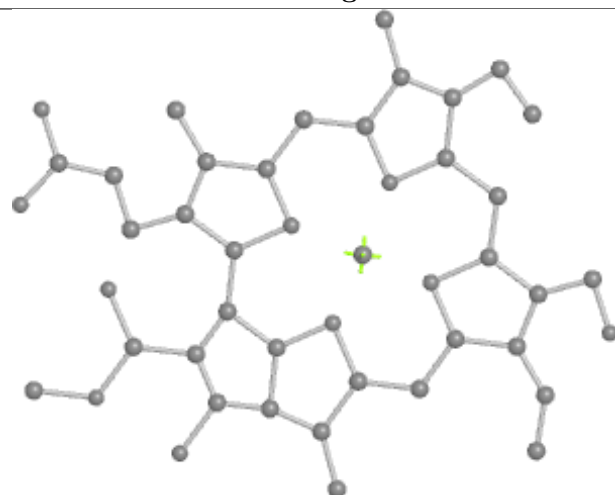
Bond lengths



Bond angles

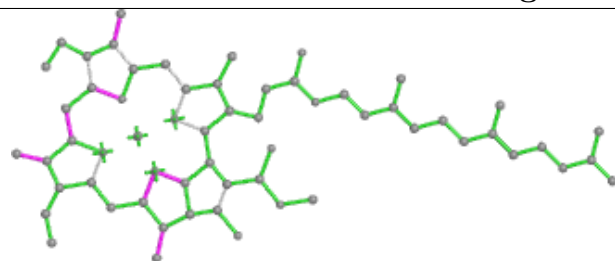


Torsions

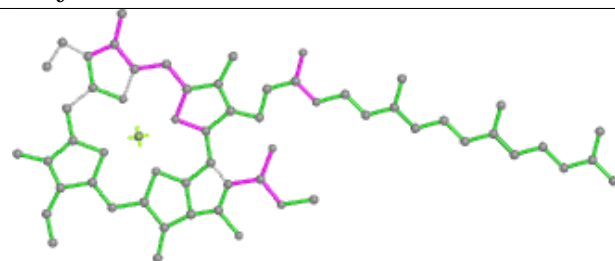


Rings

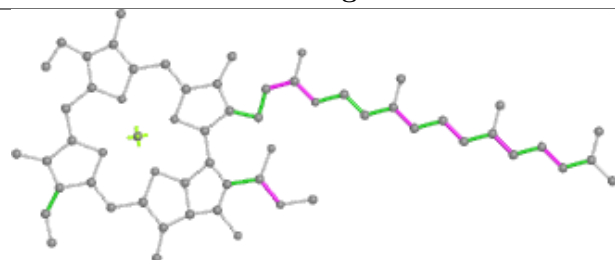
Ligand CLA y 313



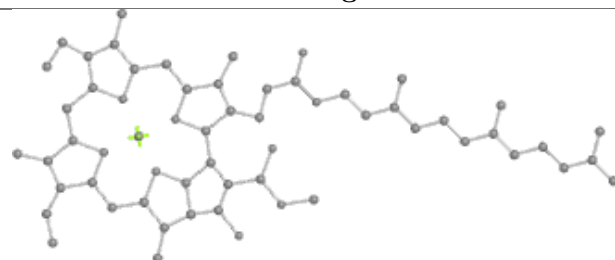
Bond lengths



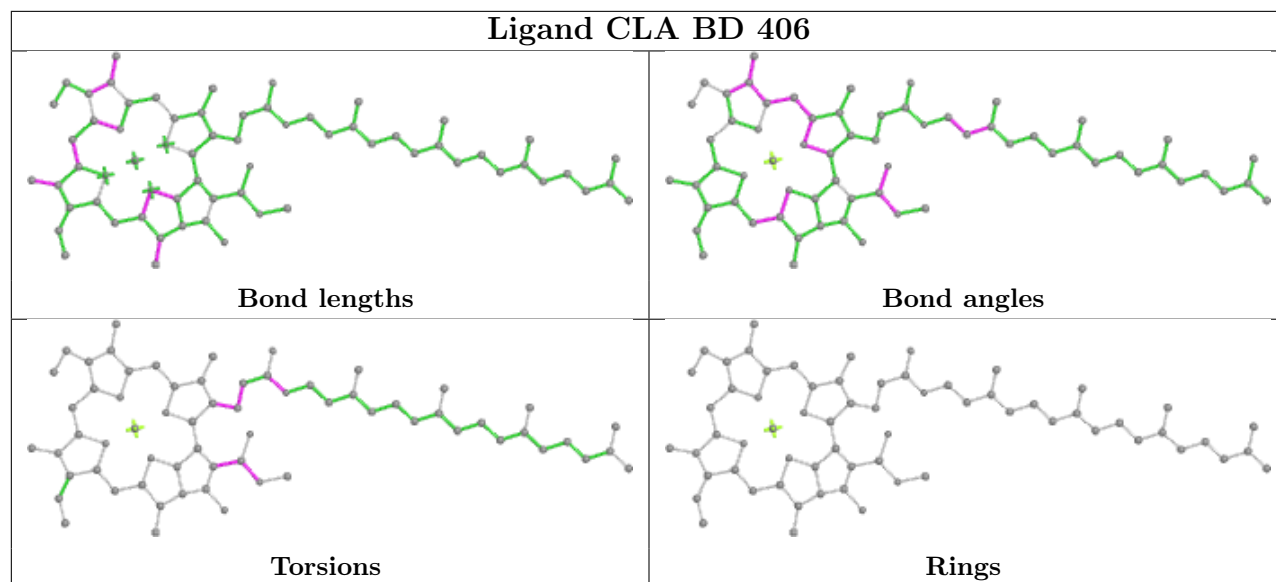
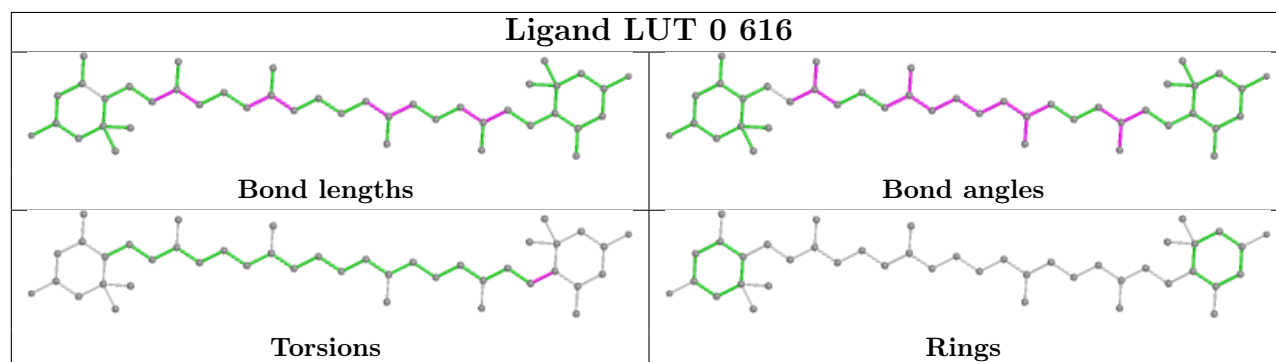
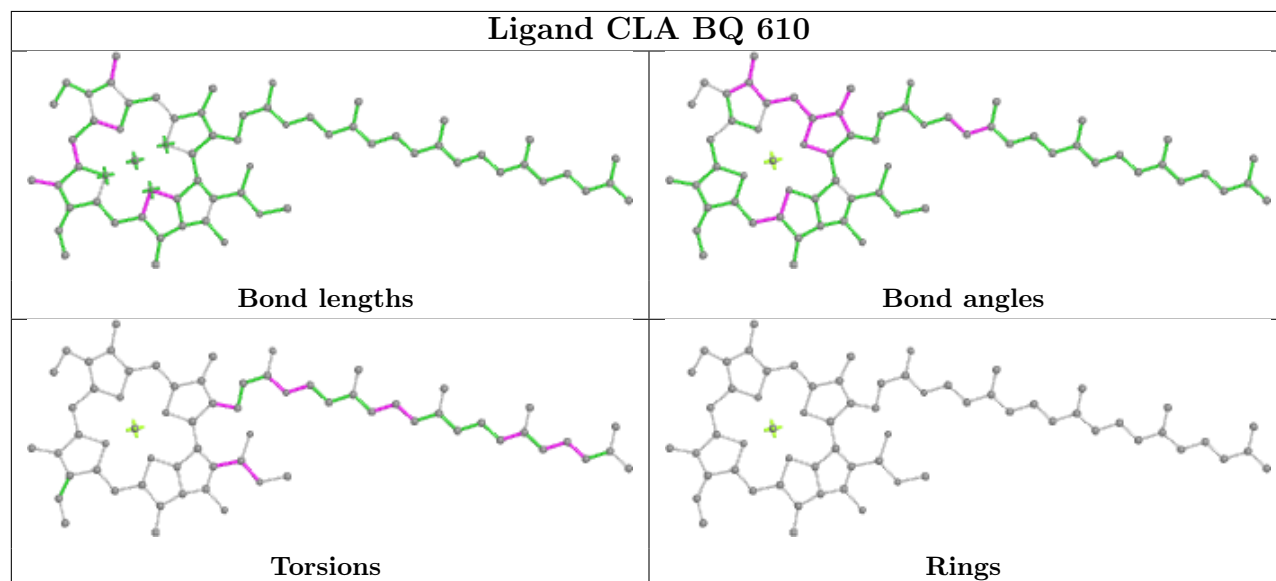
Bond angles

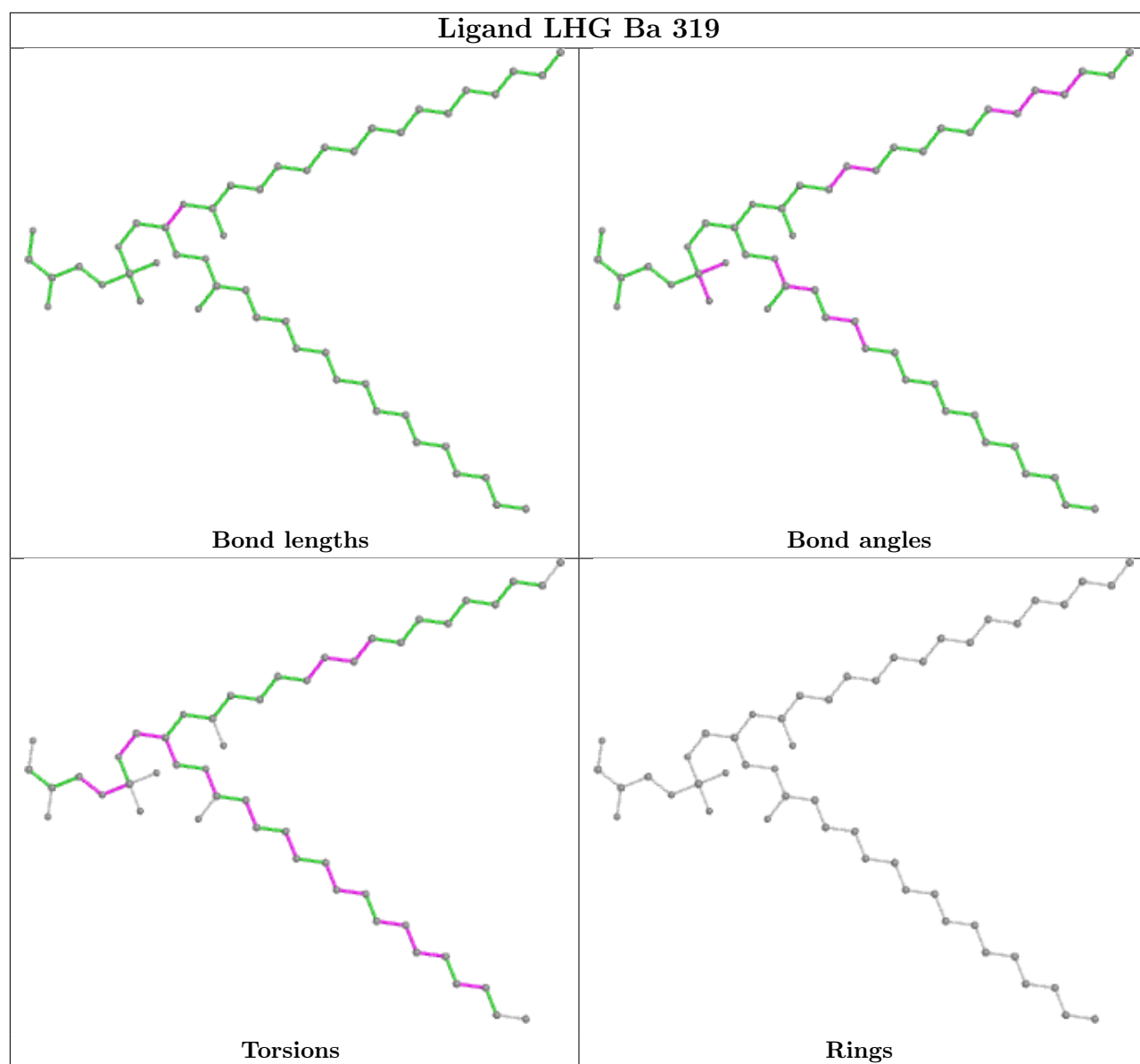


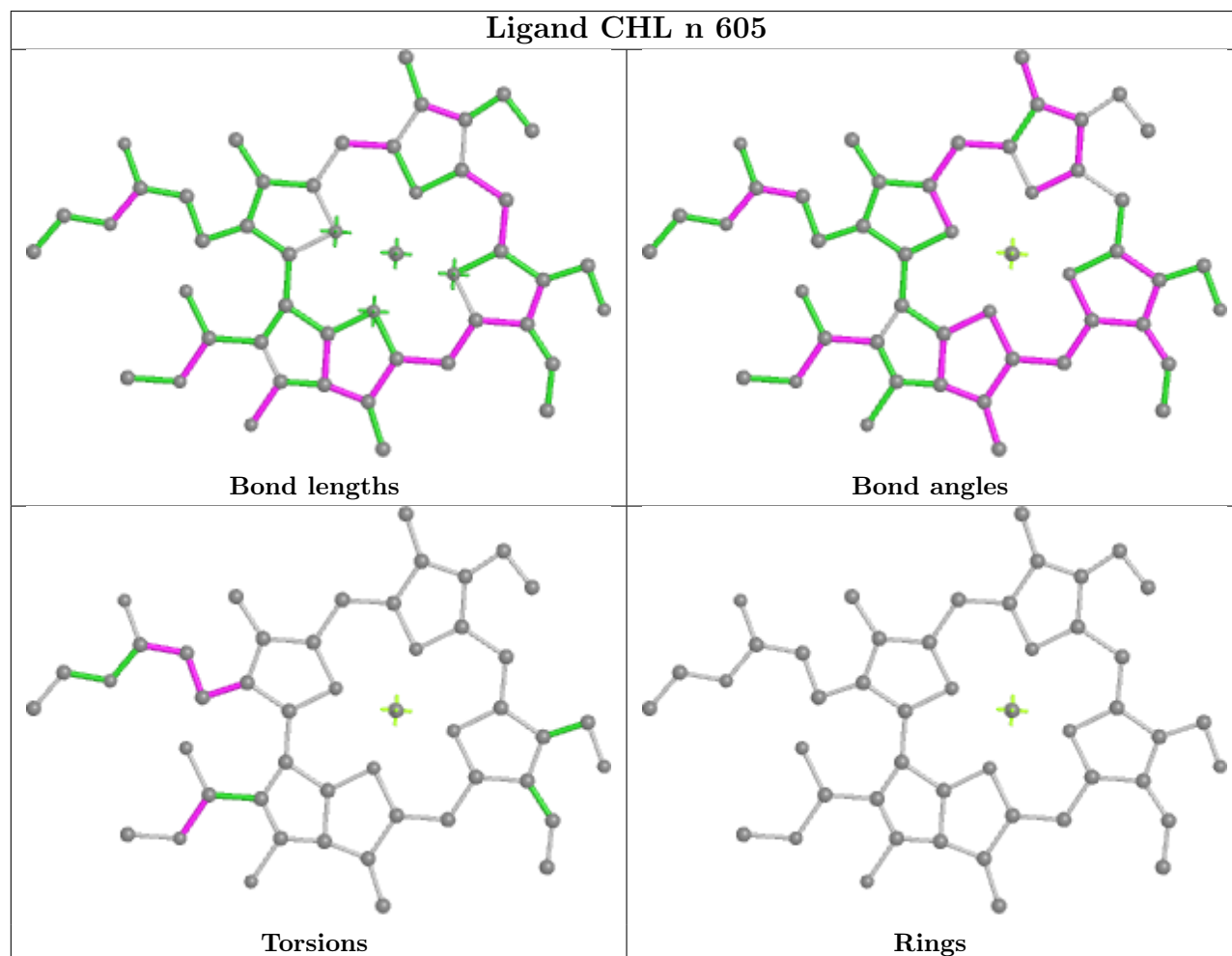
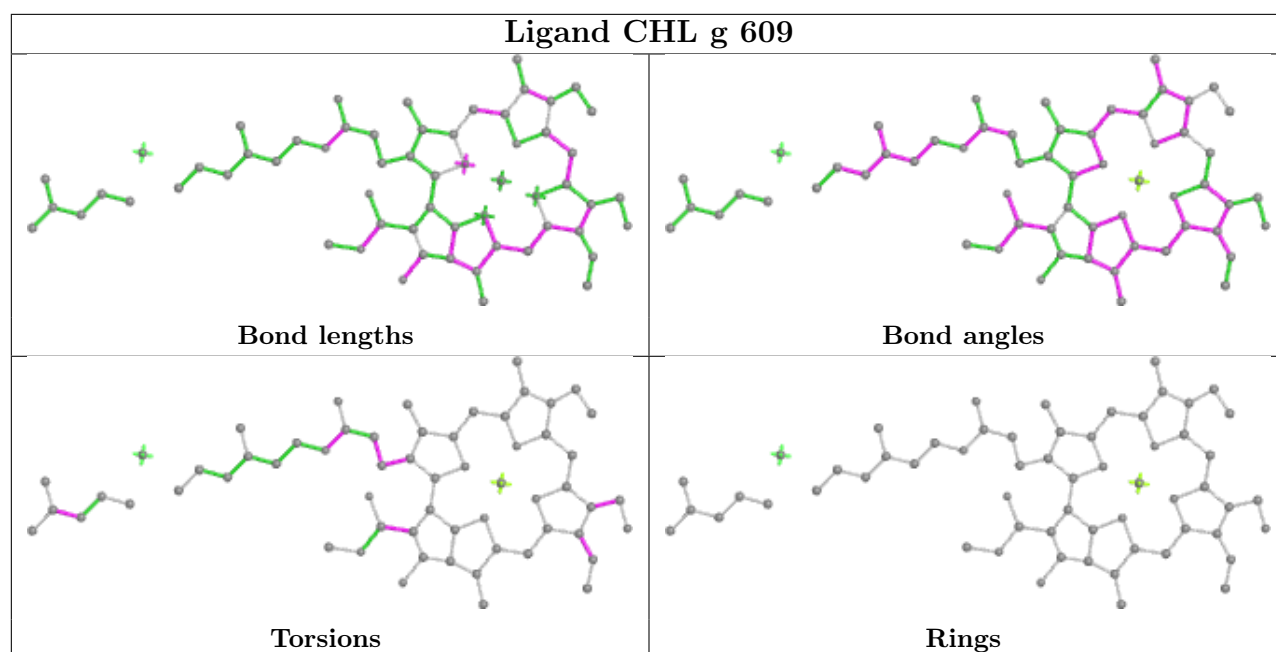
Torsions

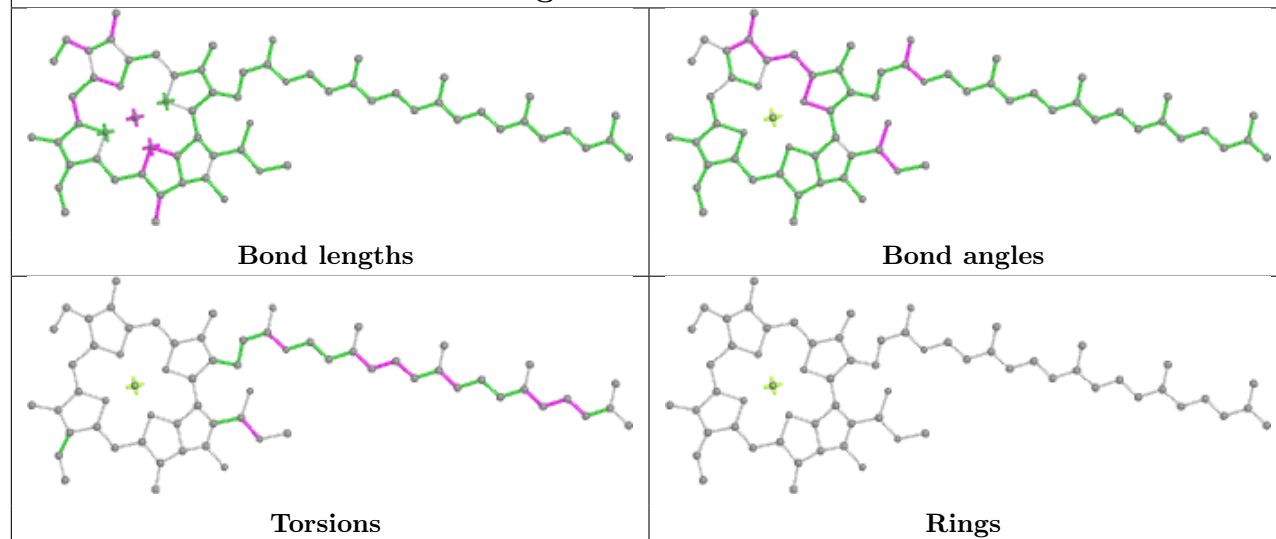
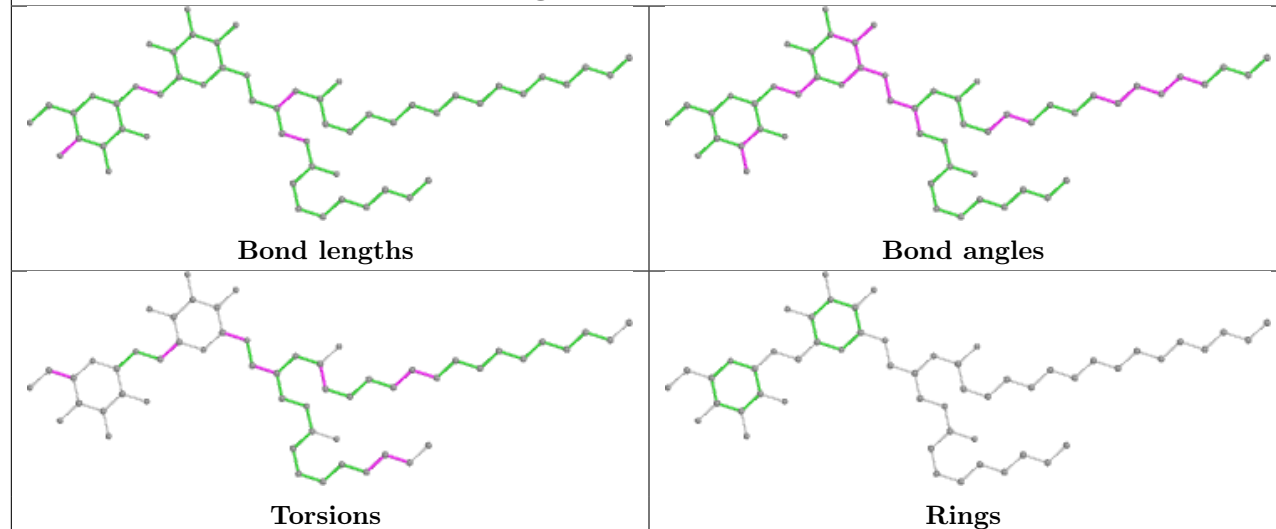
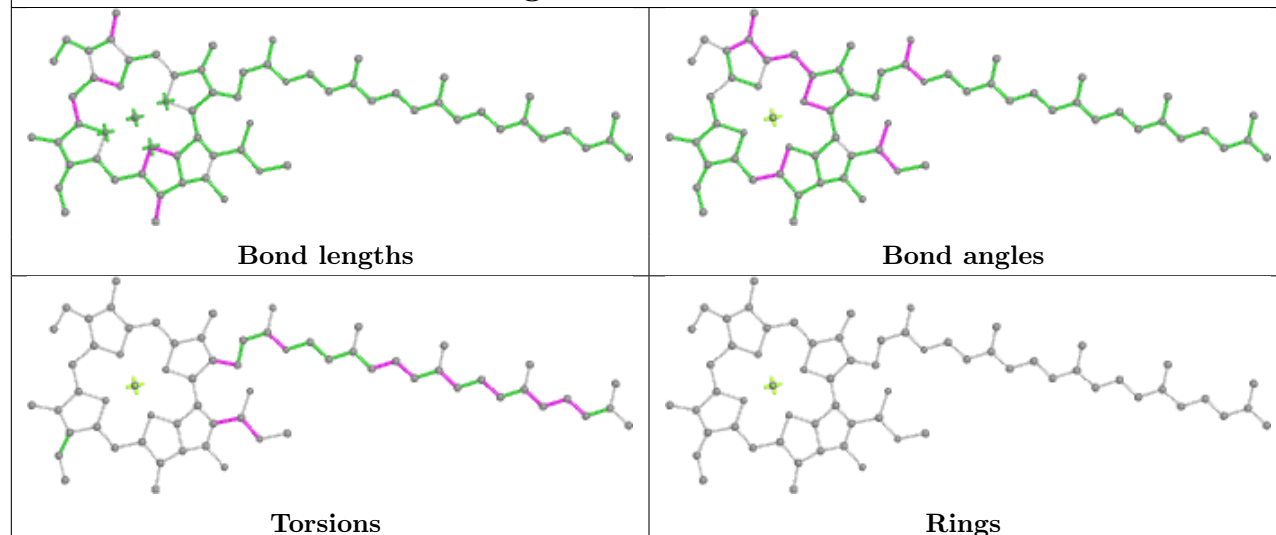


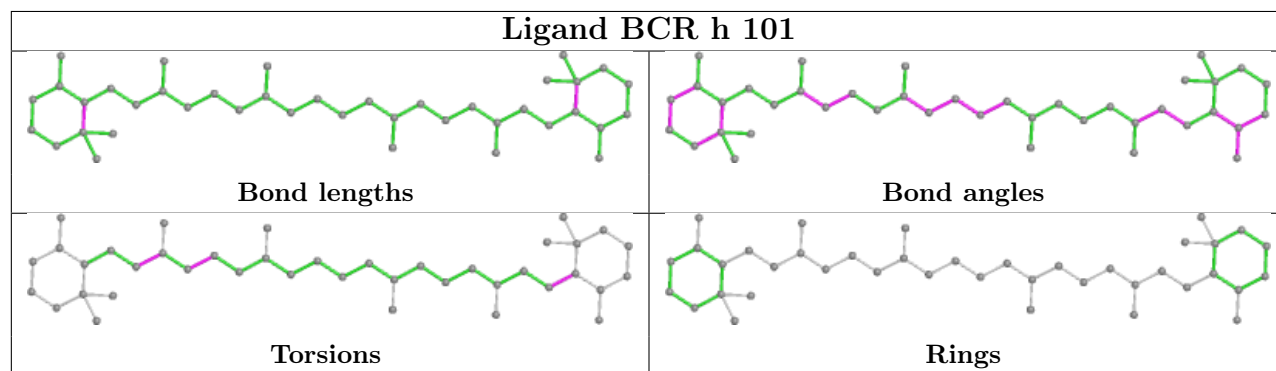
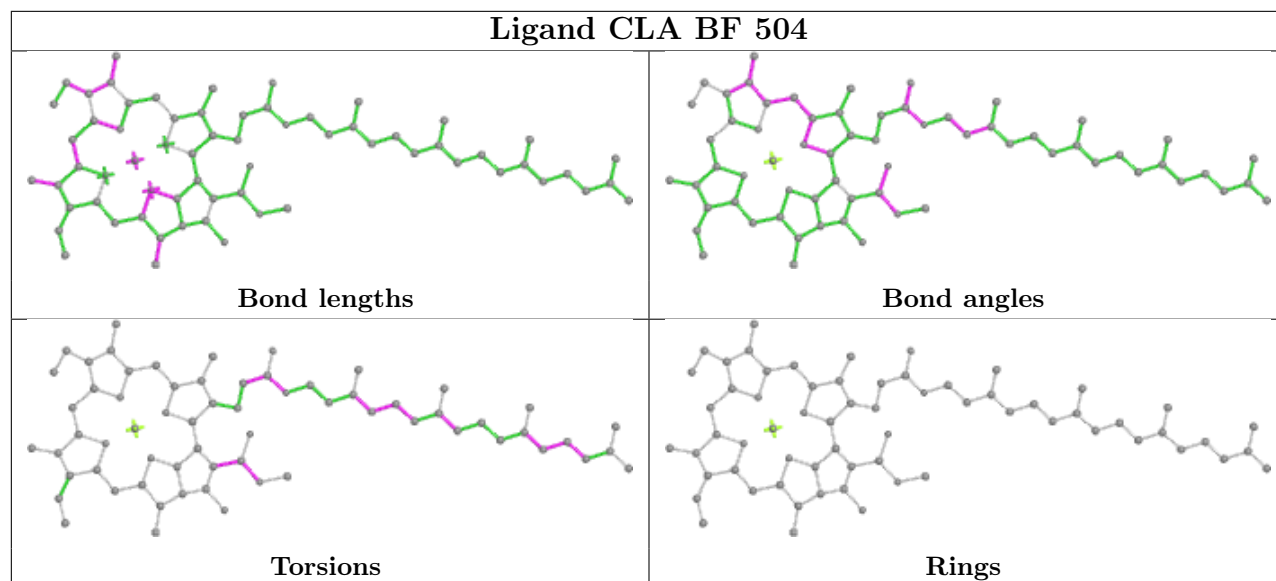
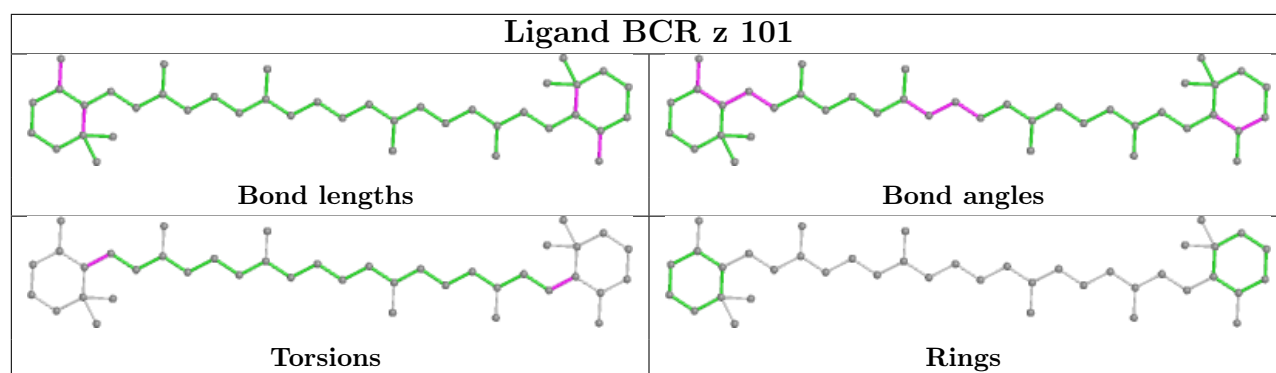
Rings

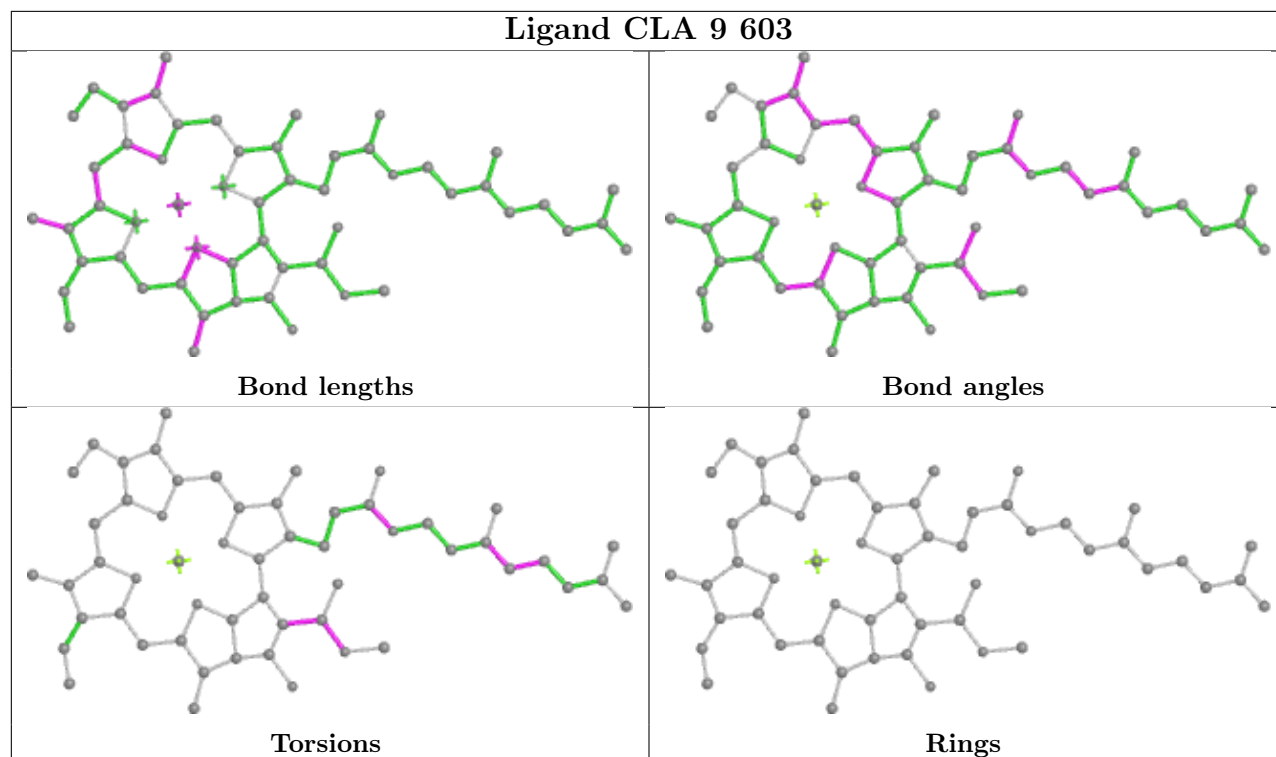
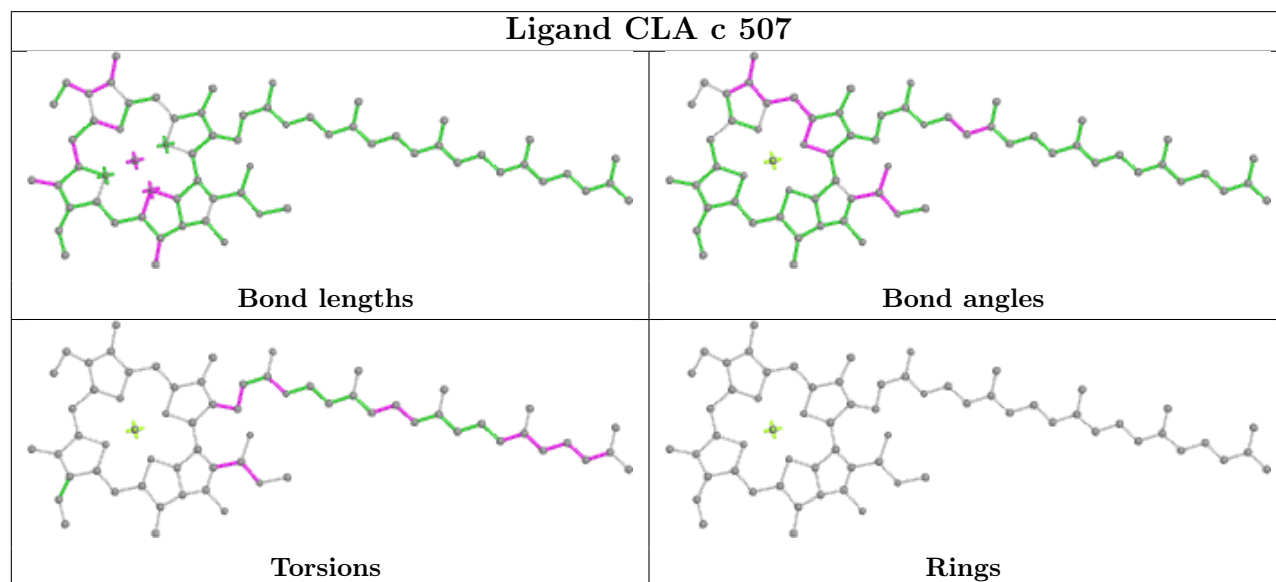
Ligand CLA BD 406**Ligand LUT 0 616****Ligand CLA BQ 610**

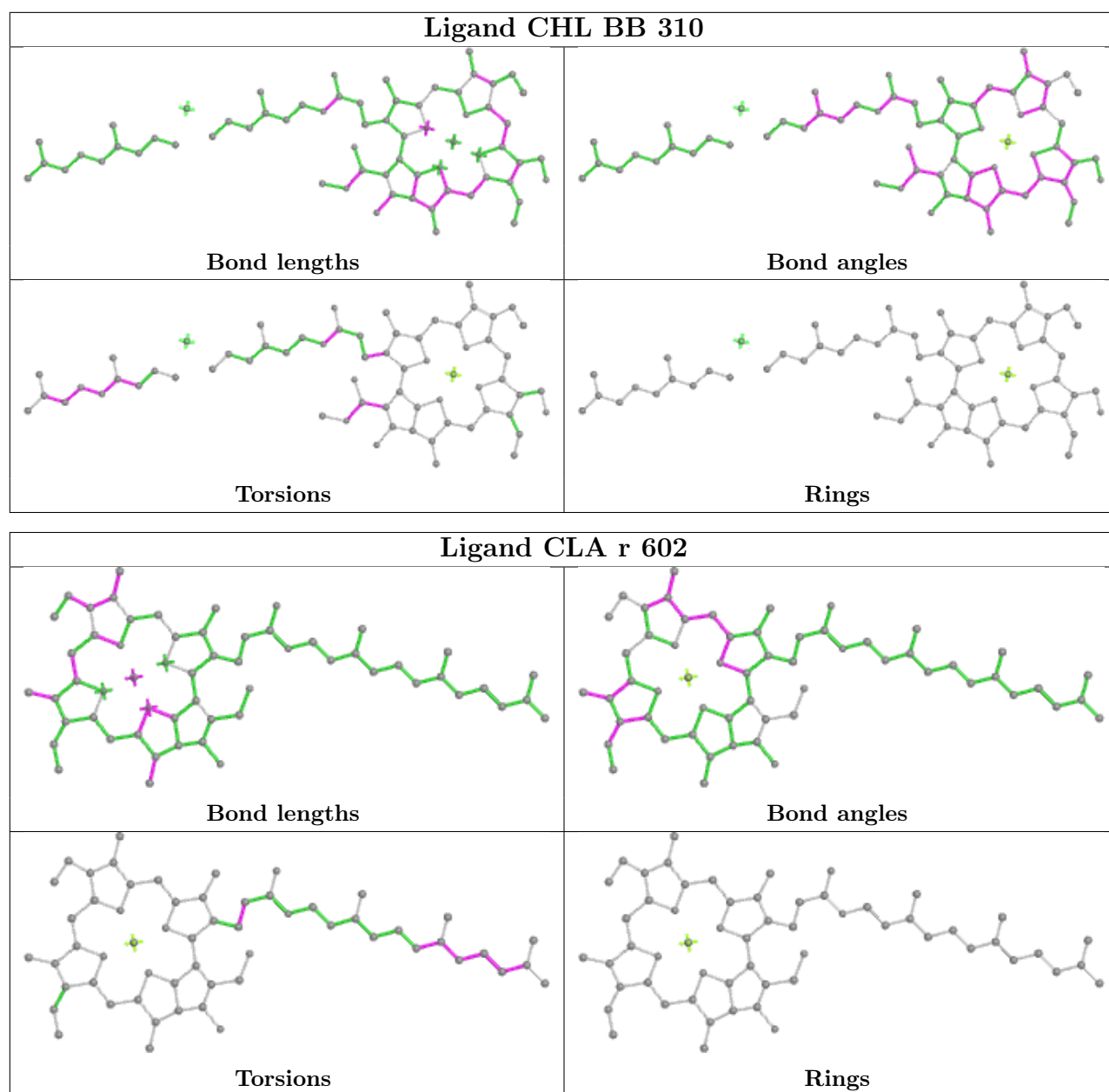


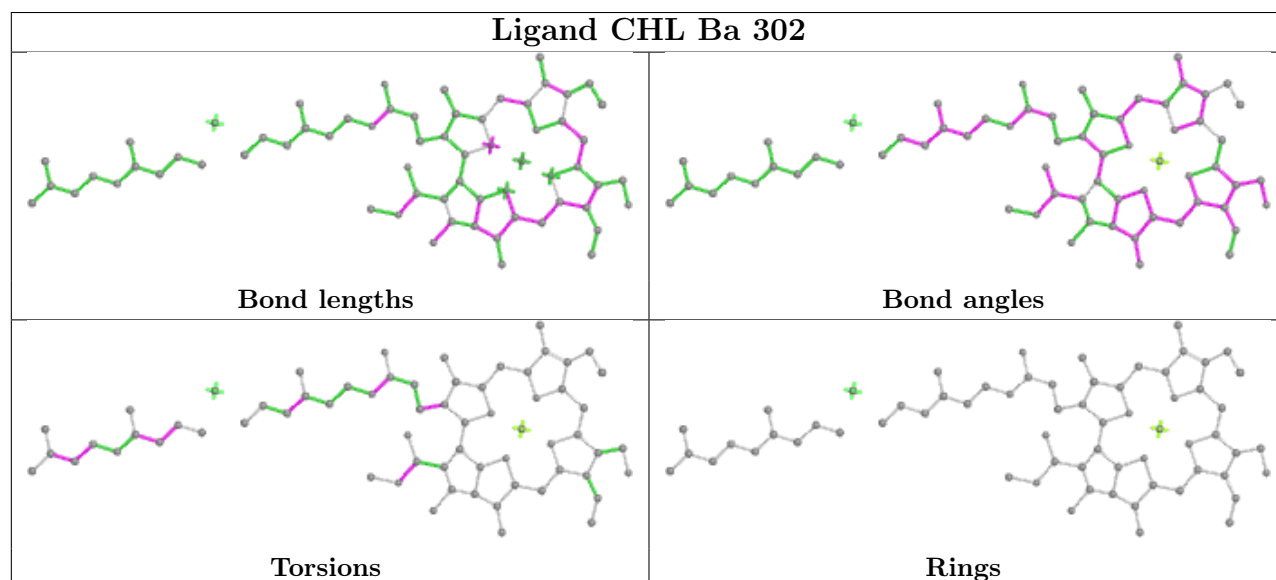
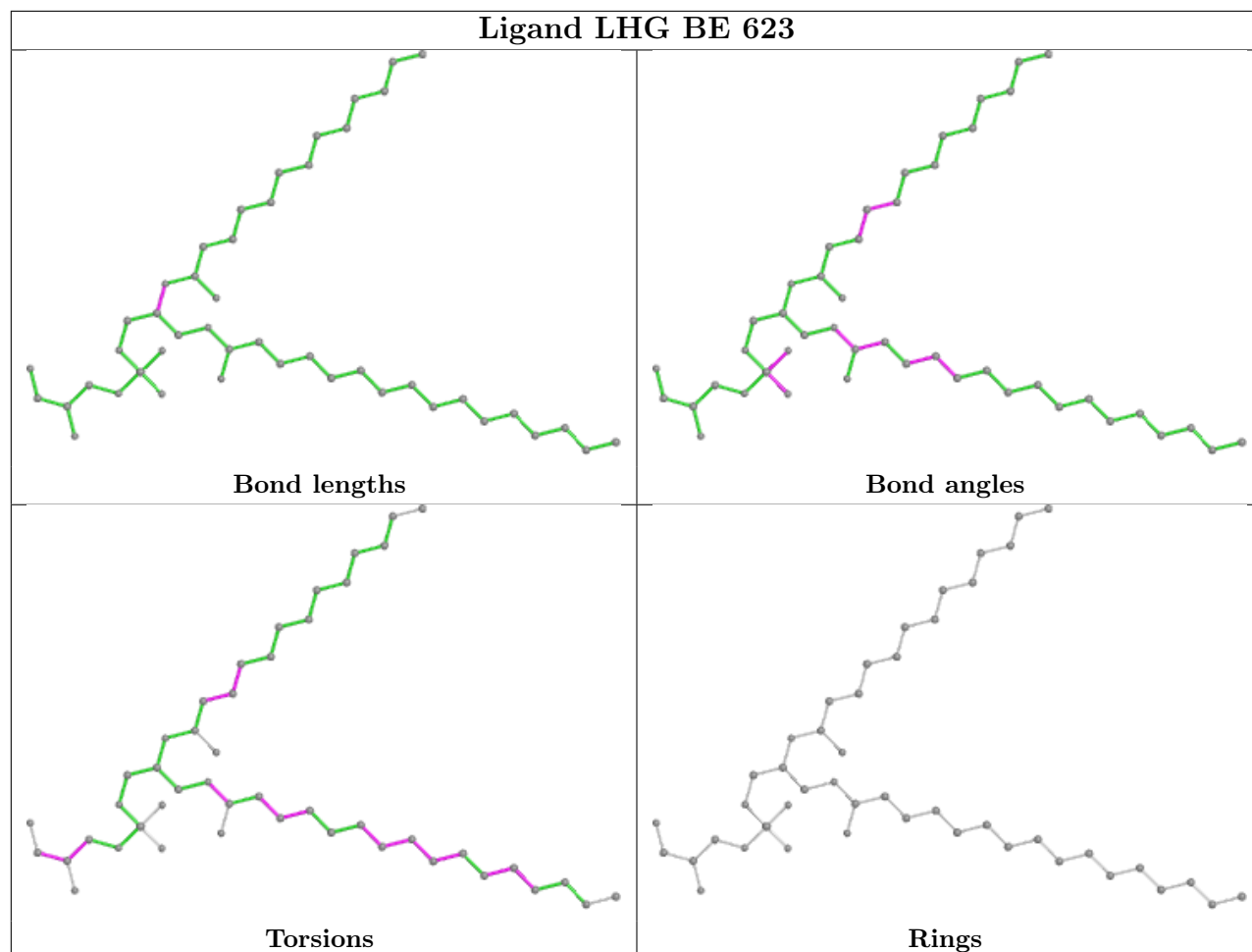


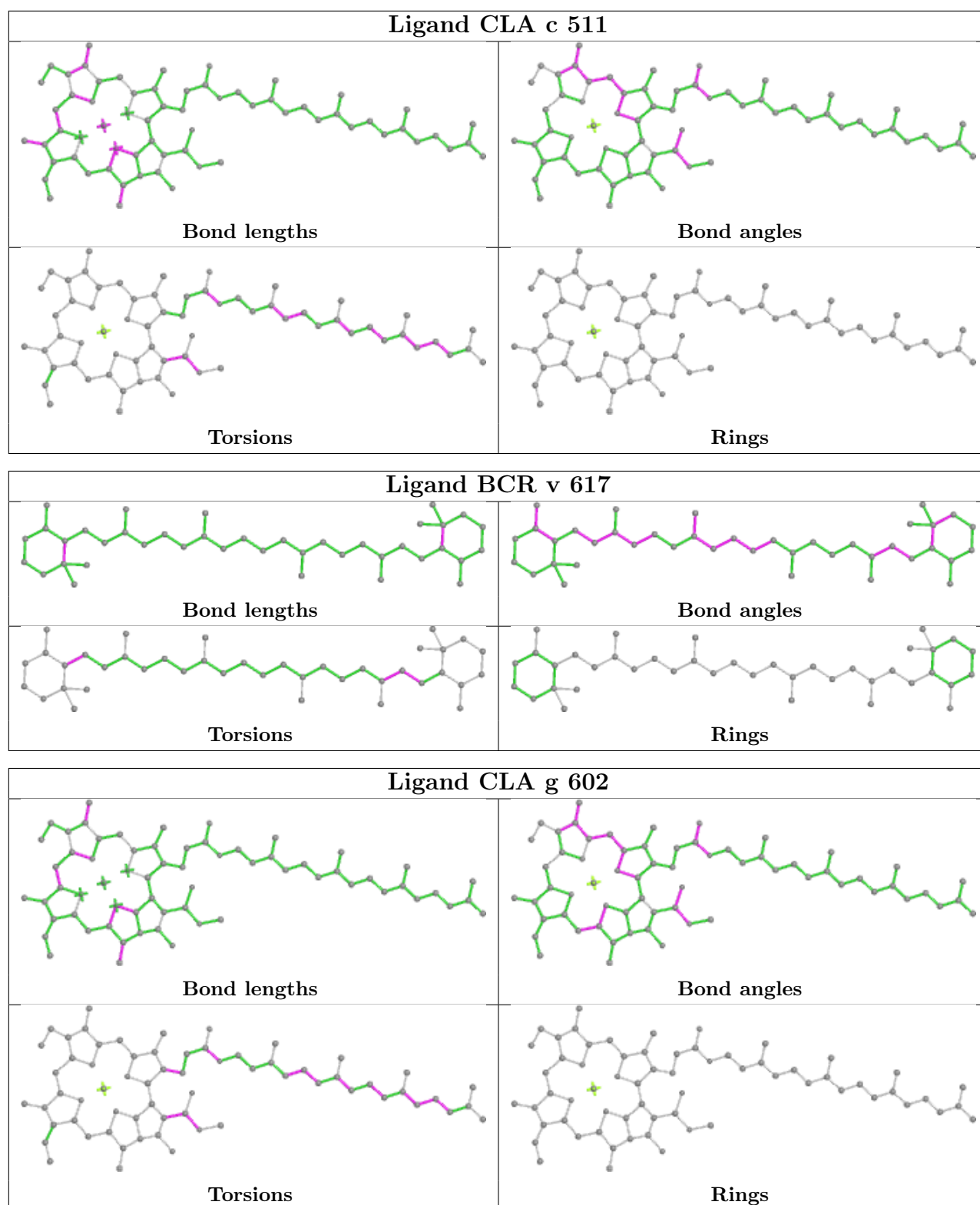
Ligand CLA 1 504**Ligand DGD 1 516****Ligand CLA BJ 602**

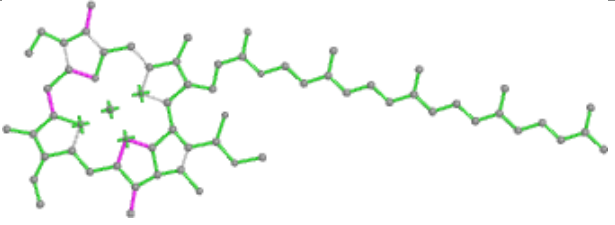
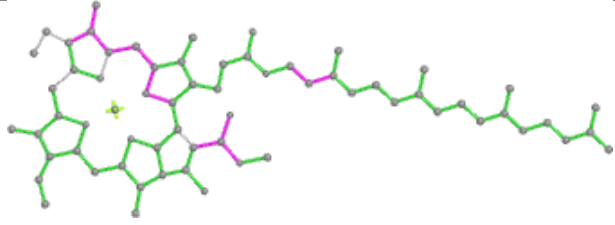
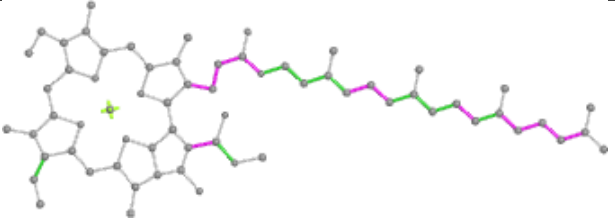
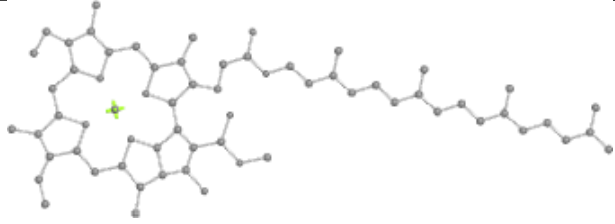
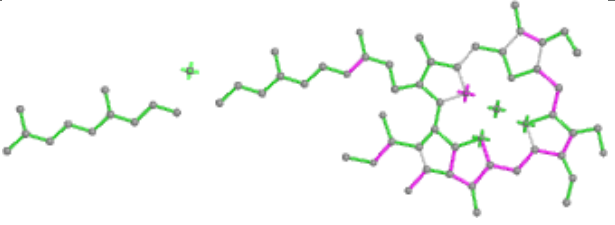
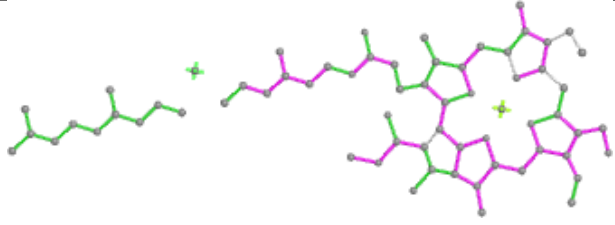
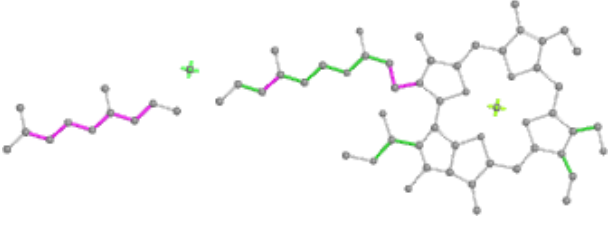
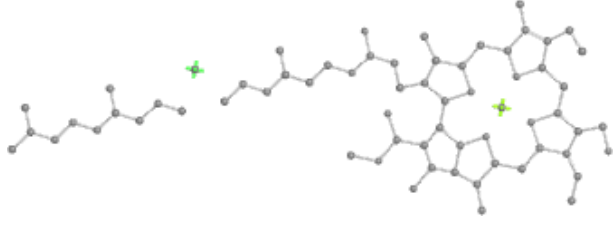
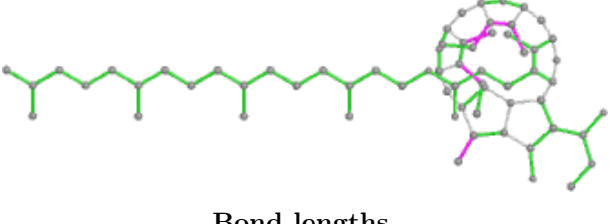
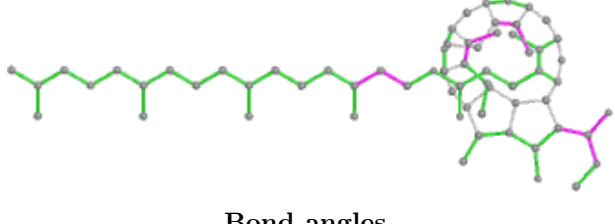
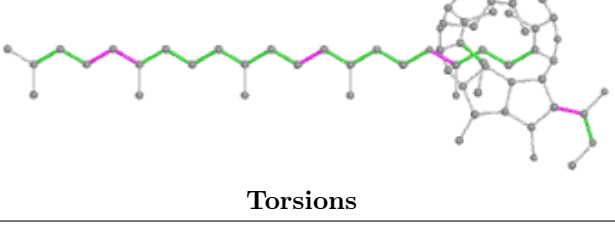
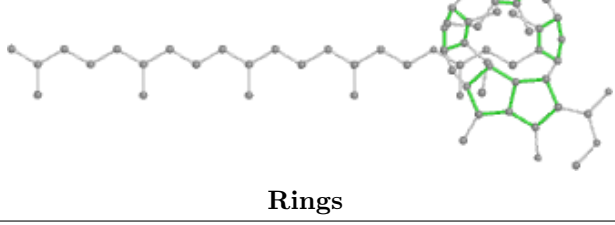


Ligand CLA 9 603**Ligand CLA c 507**

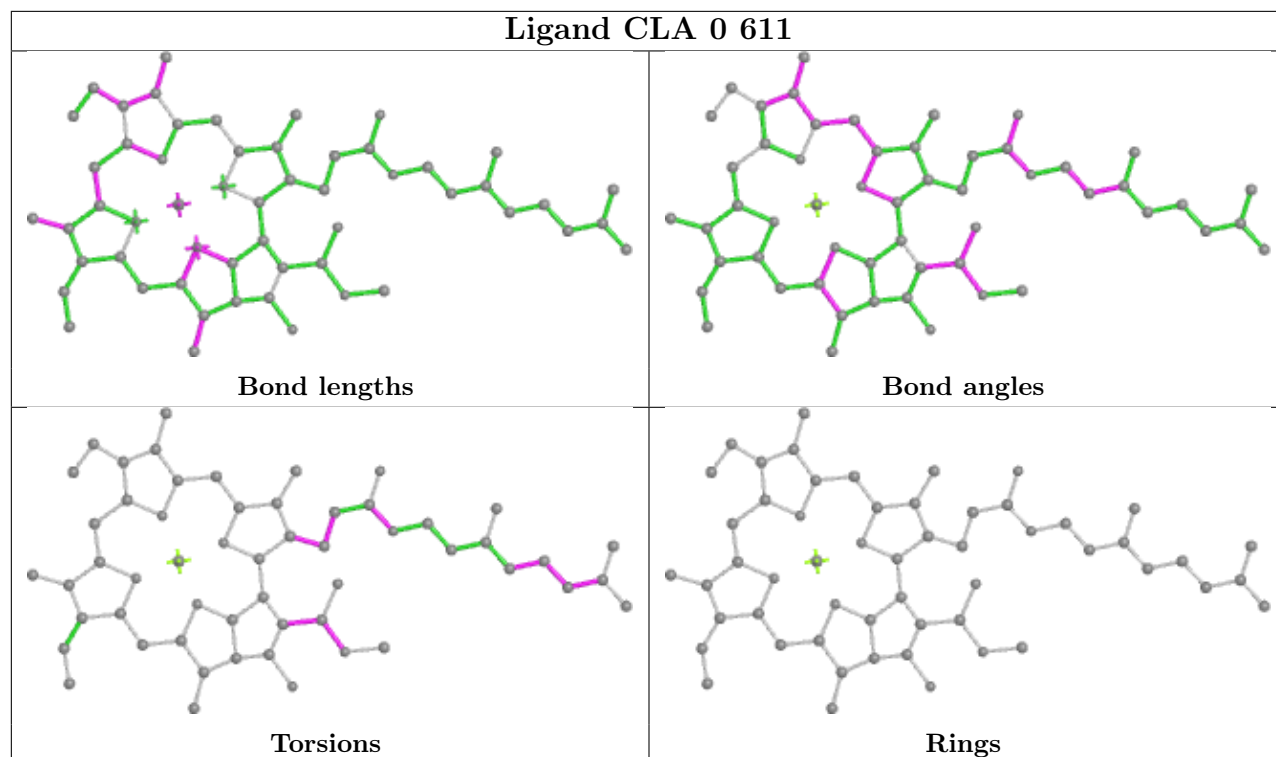




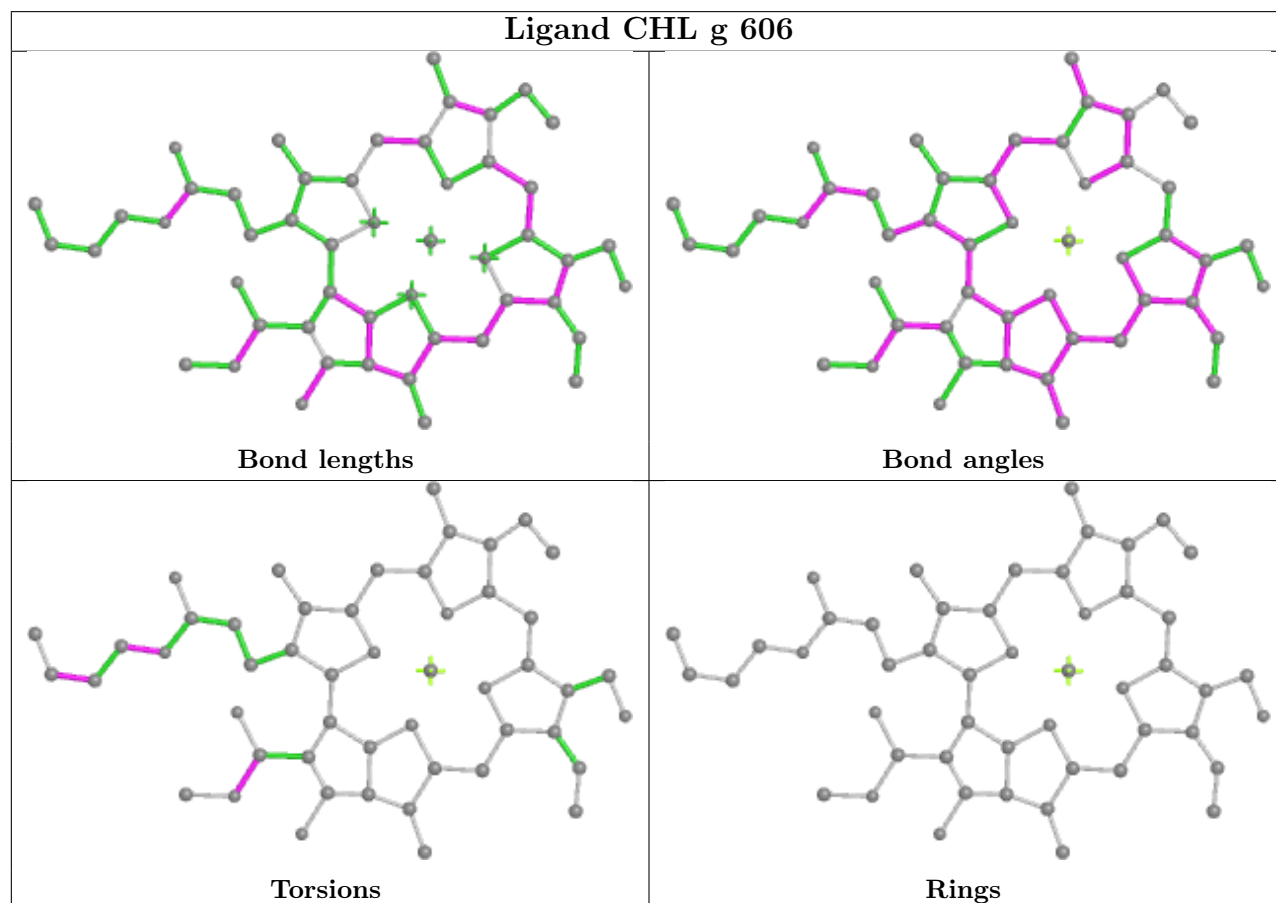


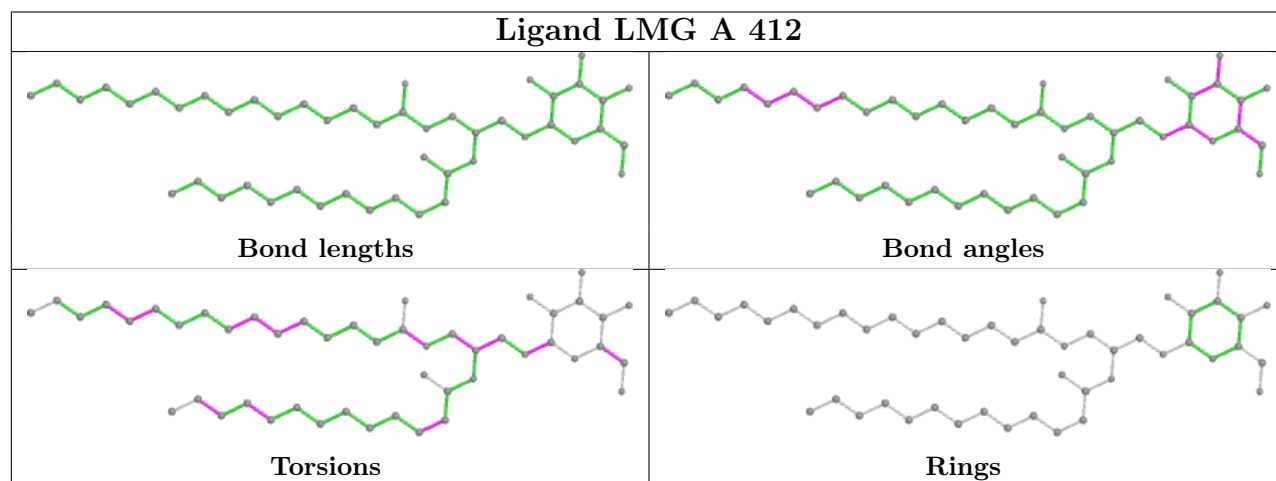
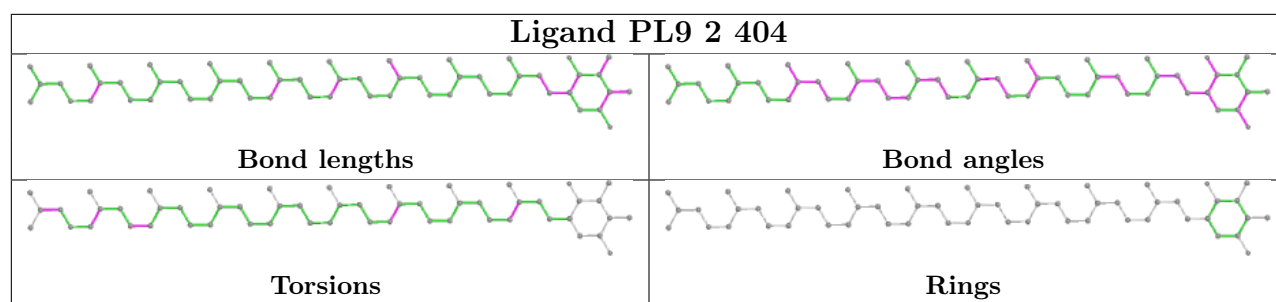
| Ligand CLA B 601 | |
|---|---|
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |
| Ligand CHL N 607 | |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |
| Ligand PHO a 408 | |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |

Ligand CLA 0 611

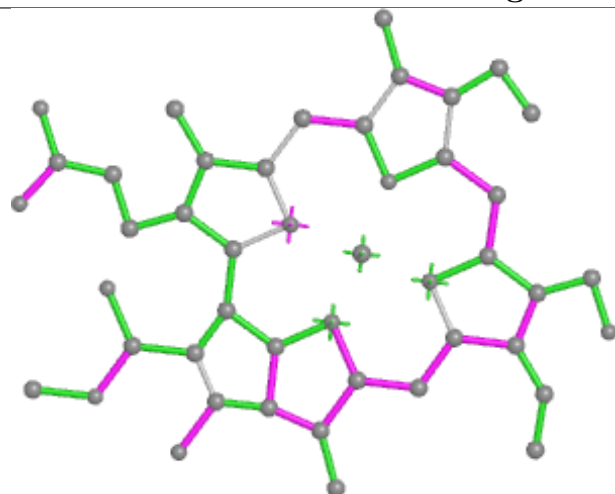


Ligand CHL g 606

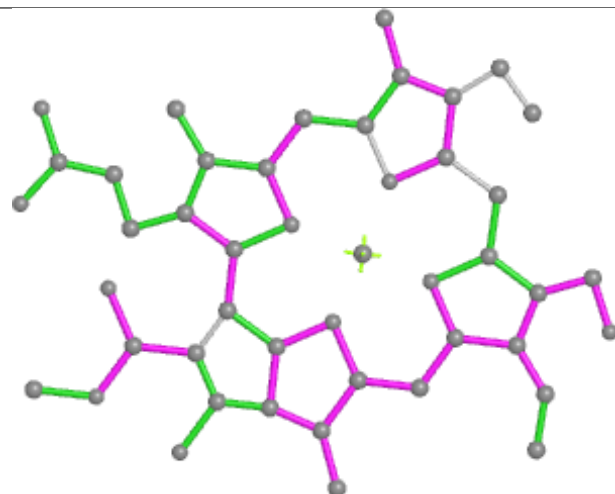




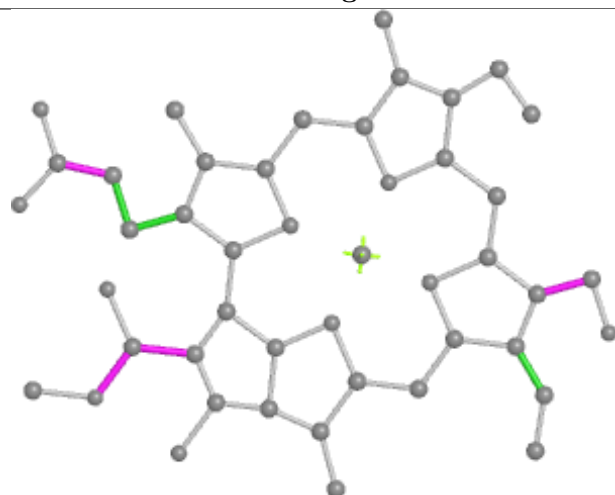
Ligand CHL A6 605



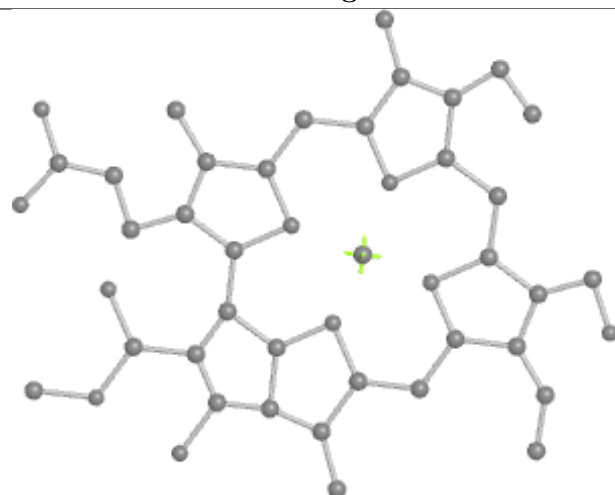
Bond lengths



Bond angles

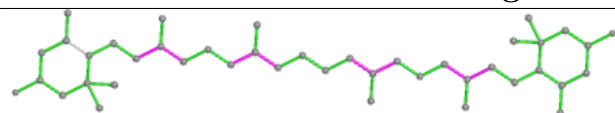


Torsions

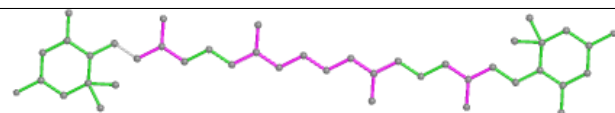


Rings

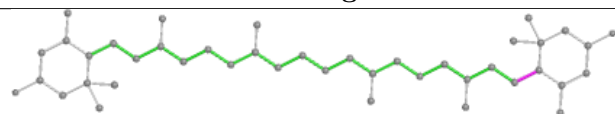
Ligand LUT AA 317



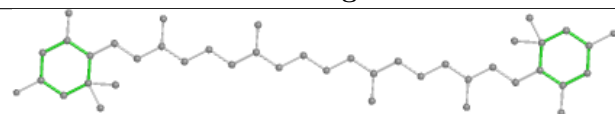
Bond lengths



Bond angles

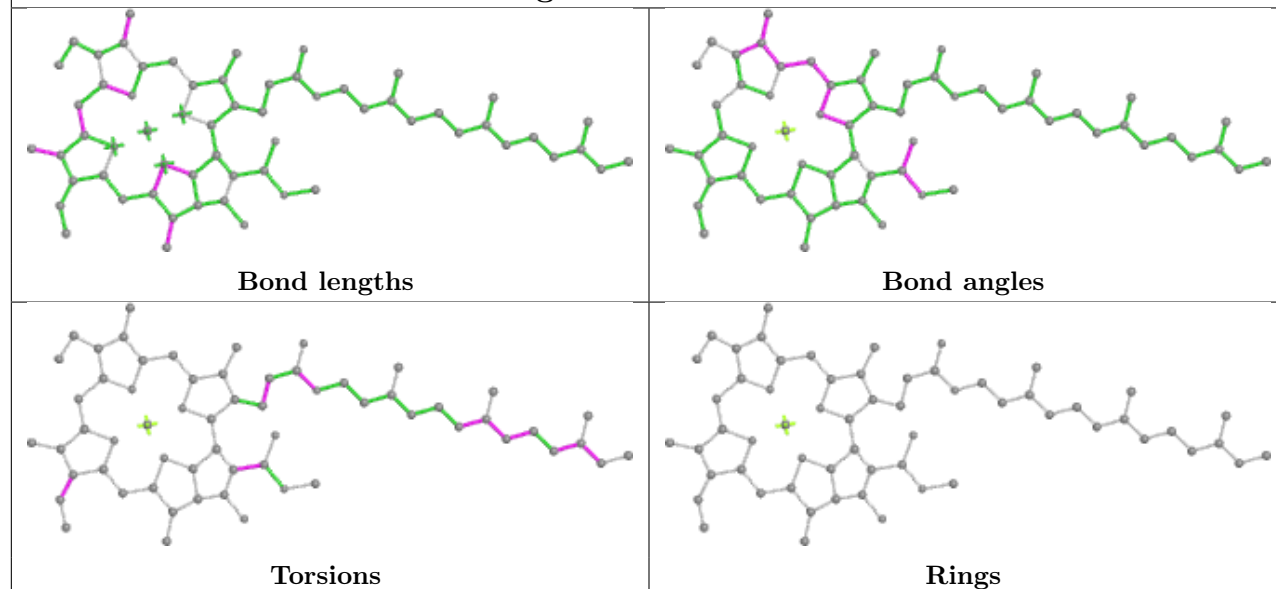


Torsions

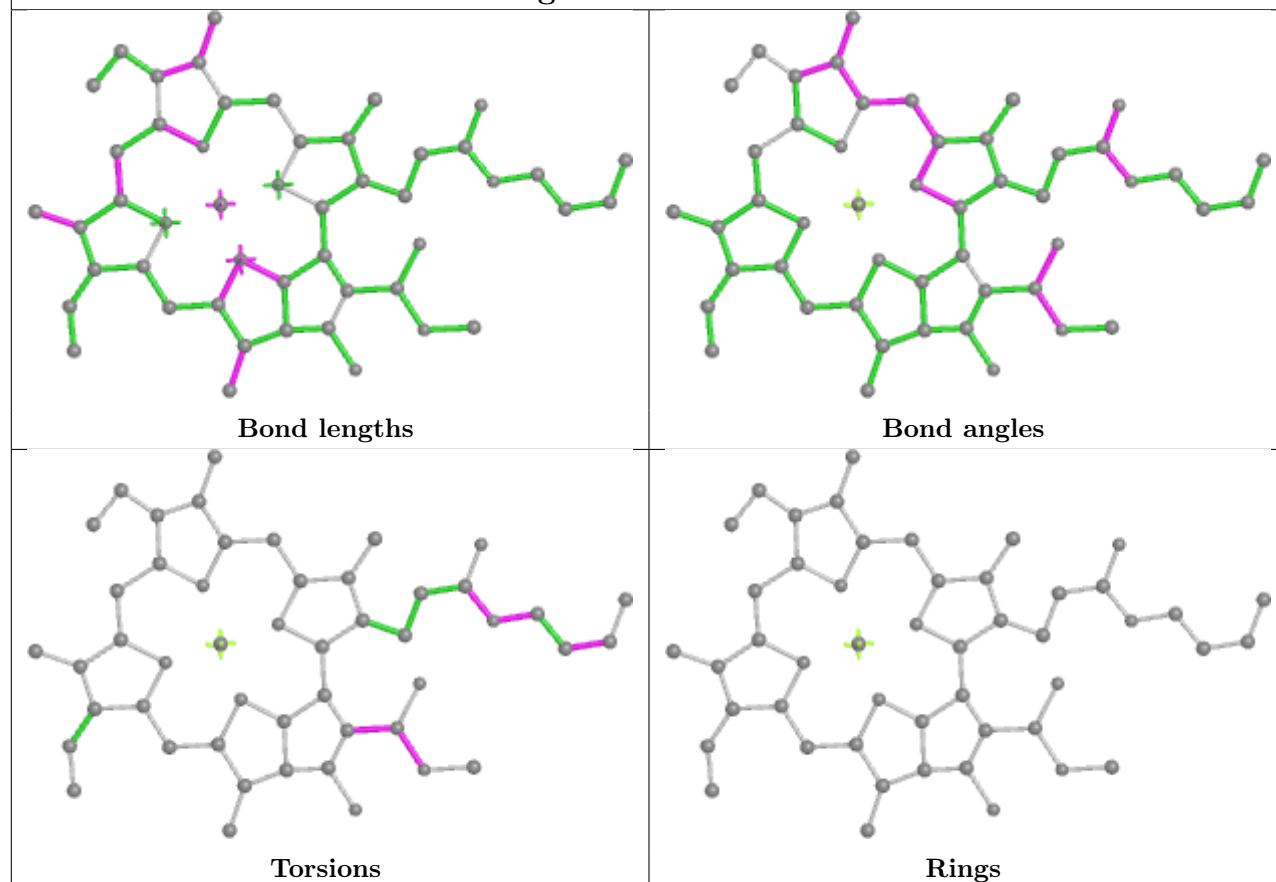


Rings

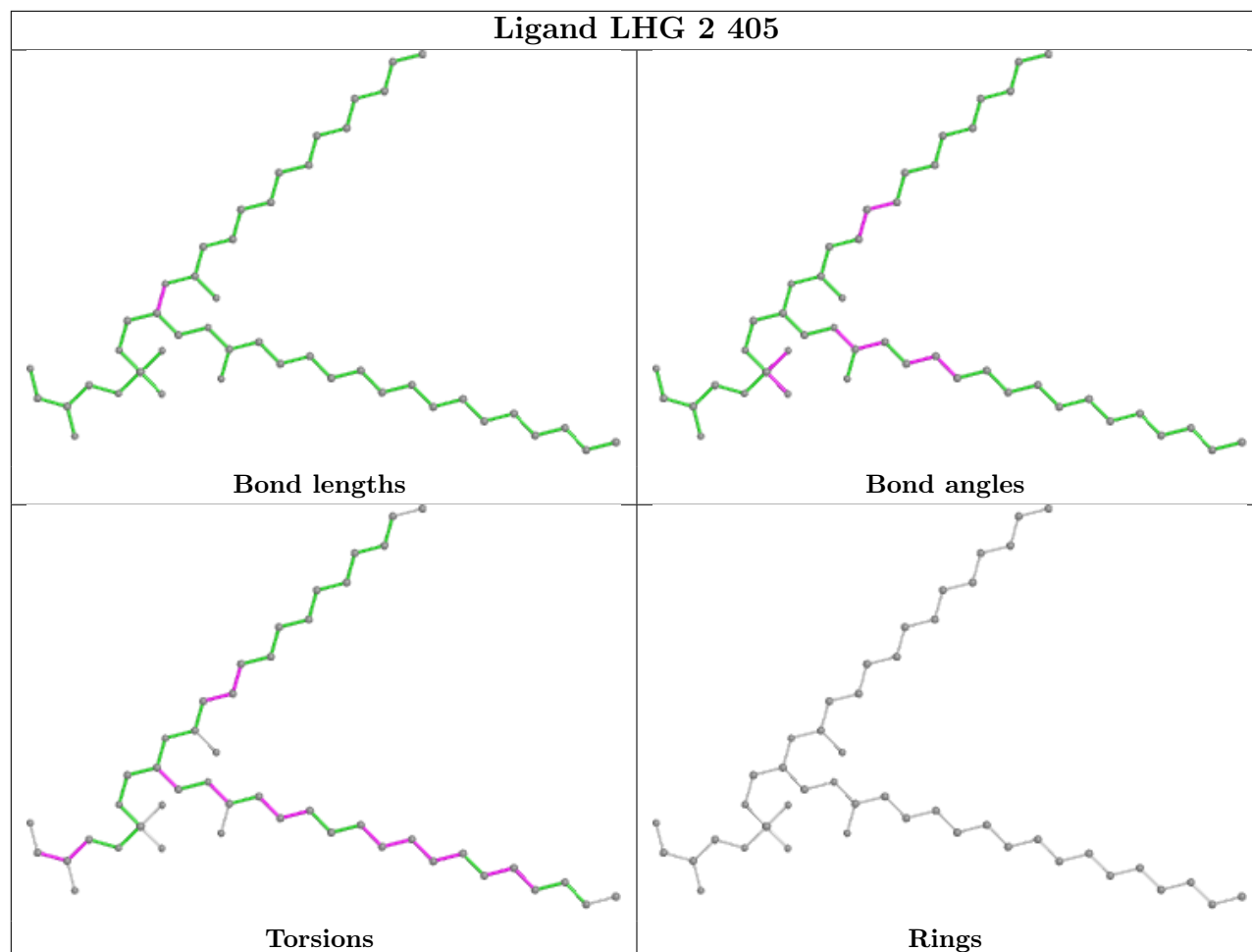
Ligand CLA 5 602



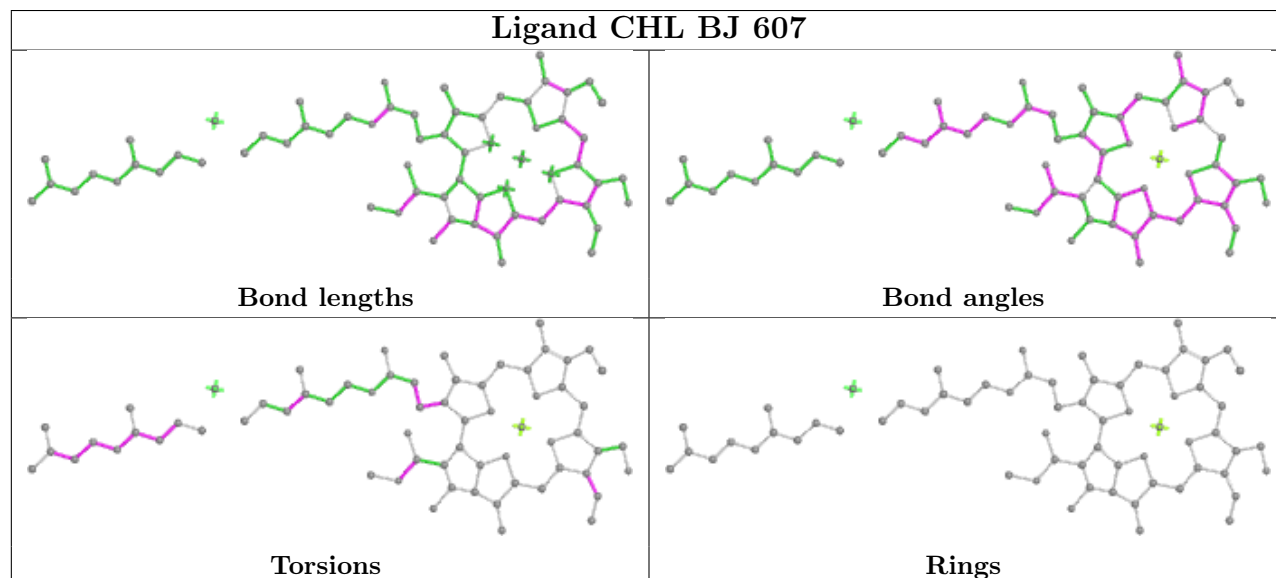
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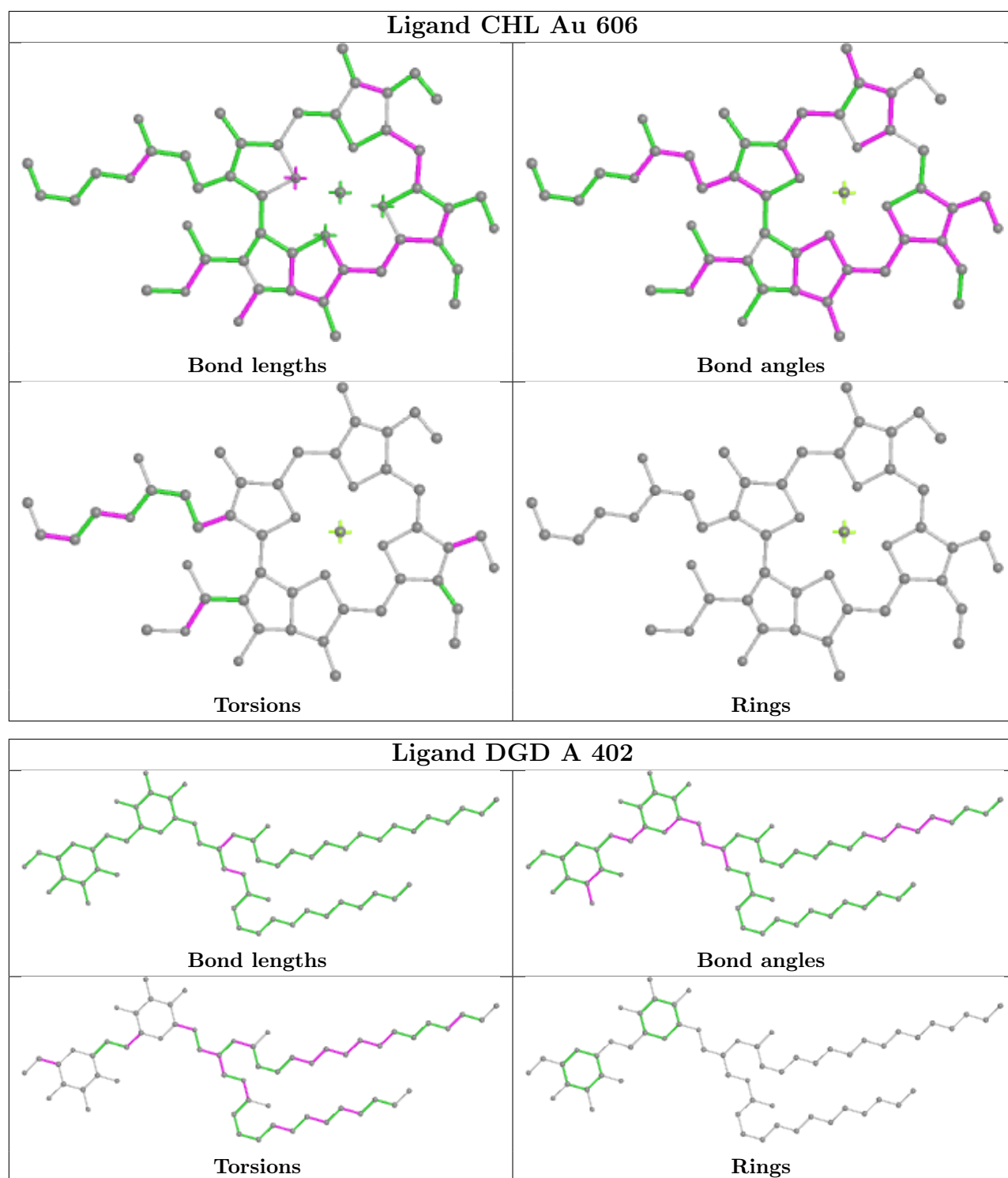


Ligand LHG 2 405

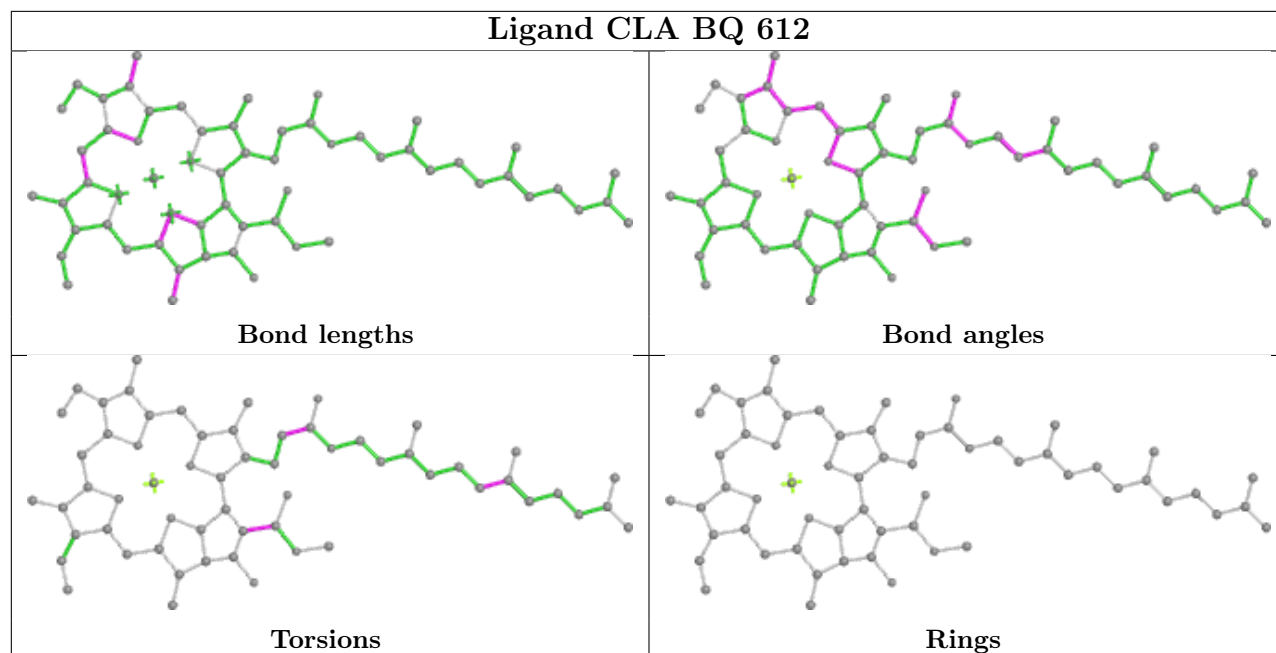


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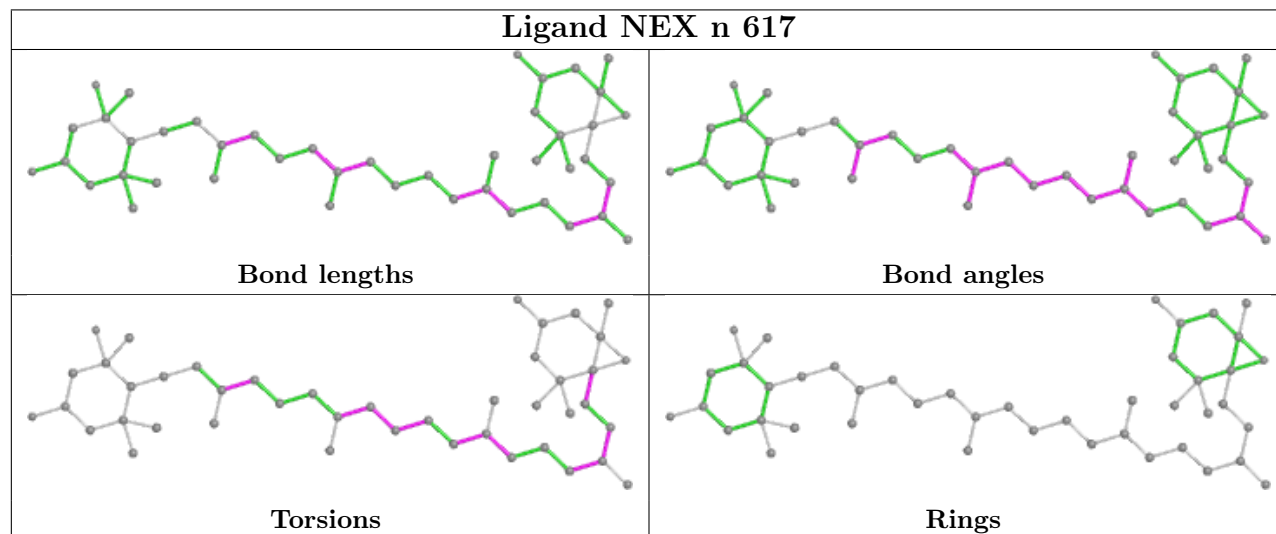




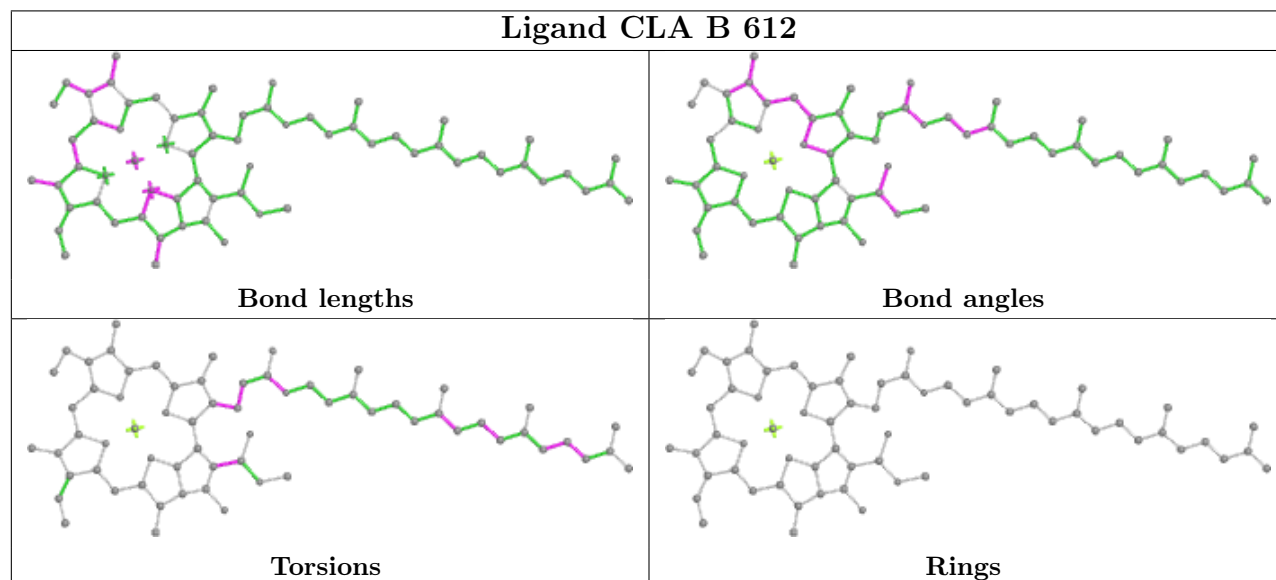
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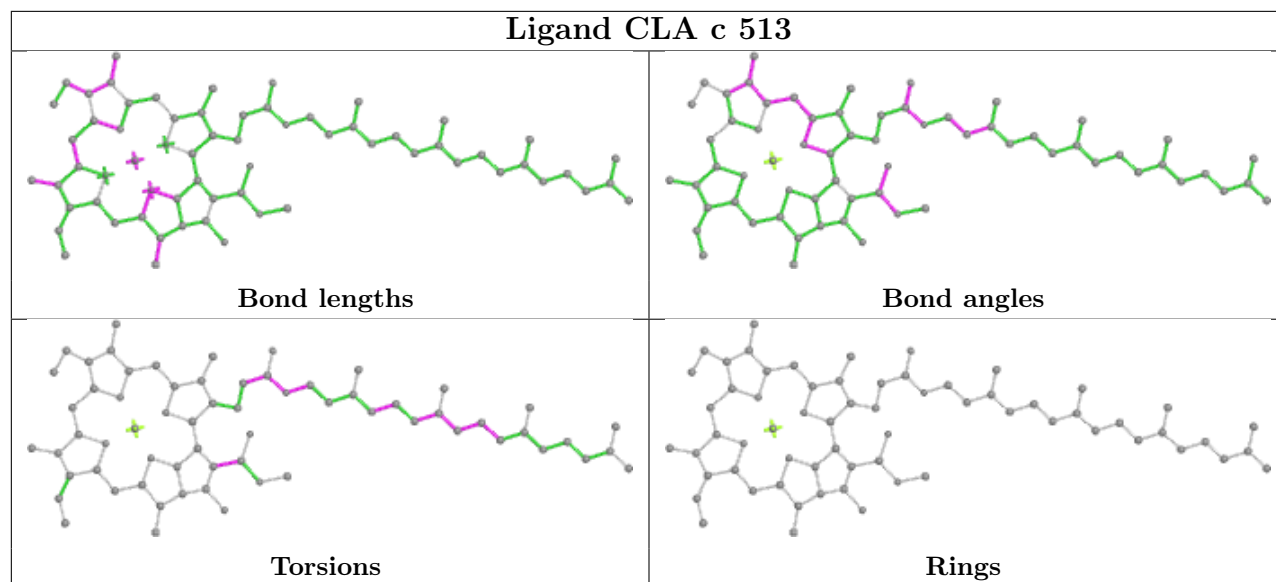
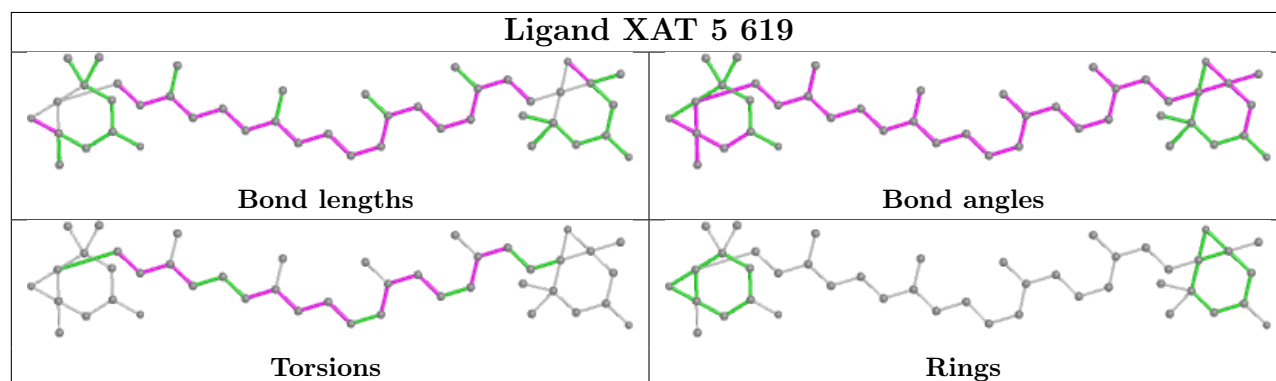
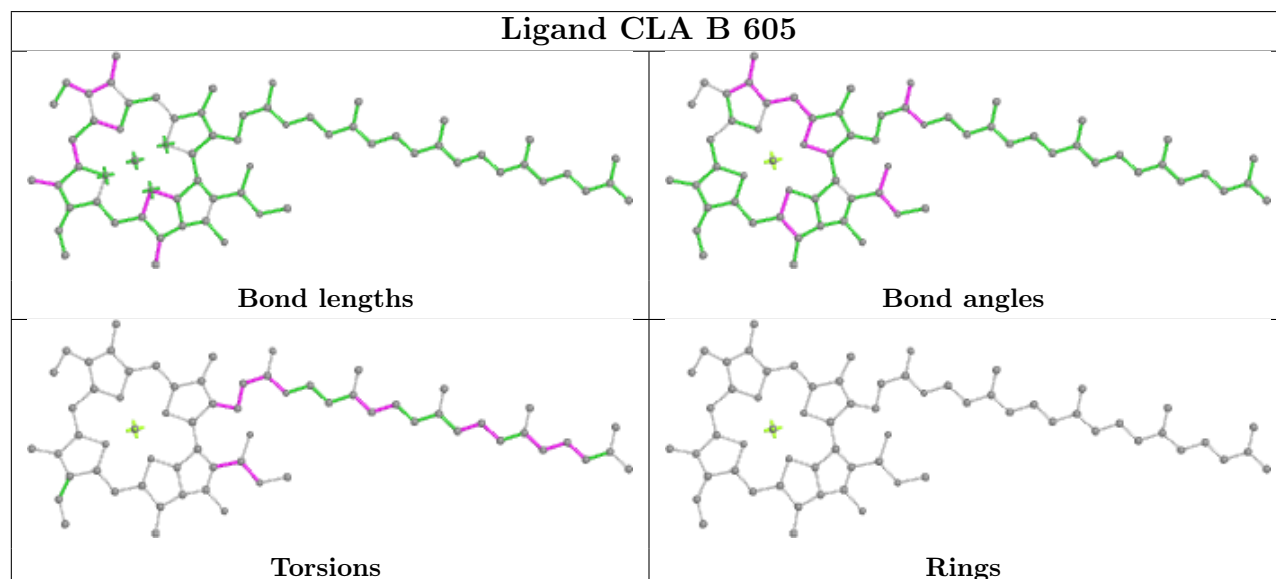


Ligand NEX n 617

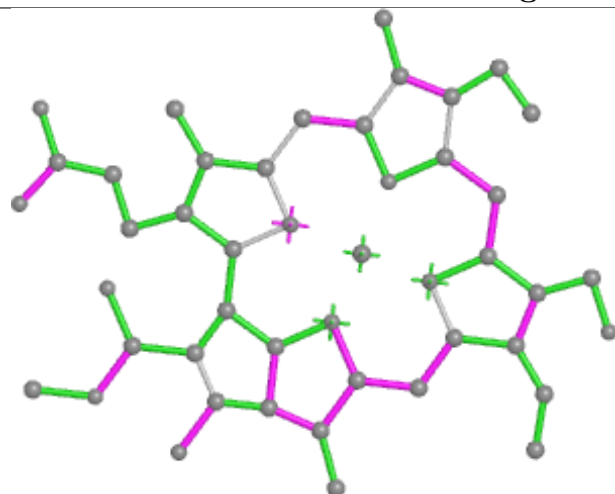


Ligand CLA B 612

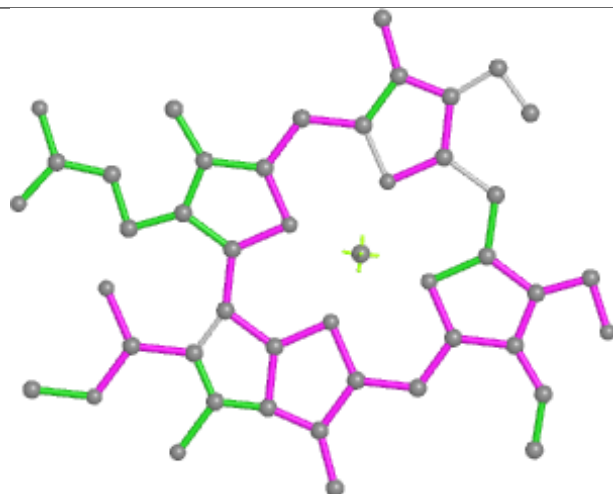


Ligand CLA c 513**Ligand XAT 5 619****Ligand CLA B 605**

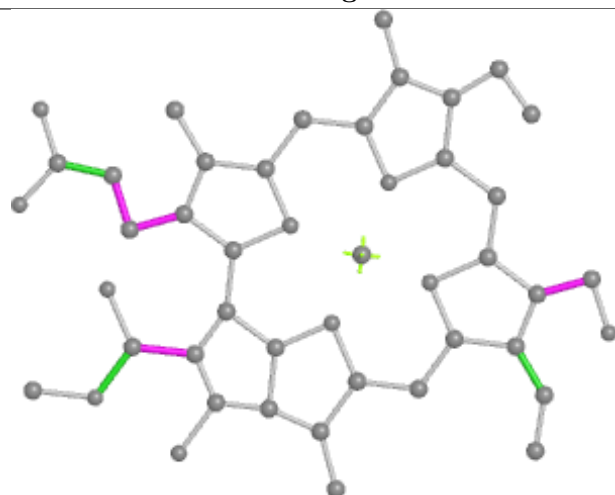
Ligand CHL 6 608



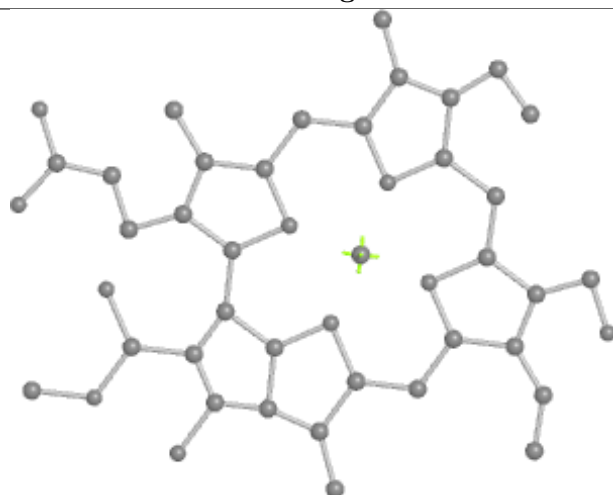
Bond lengths



Bond angles

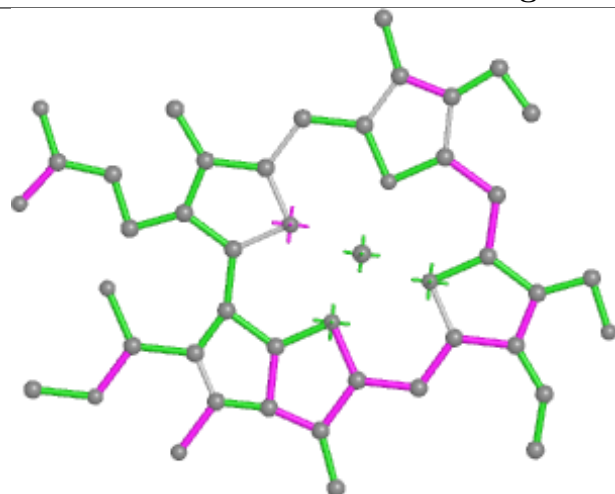


Torsions

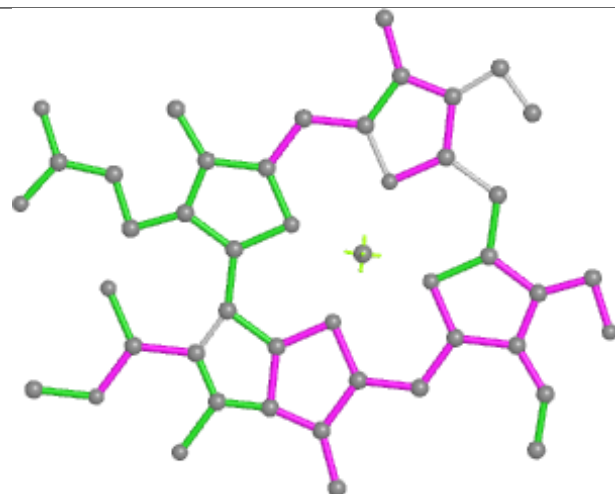


Rings

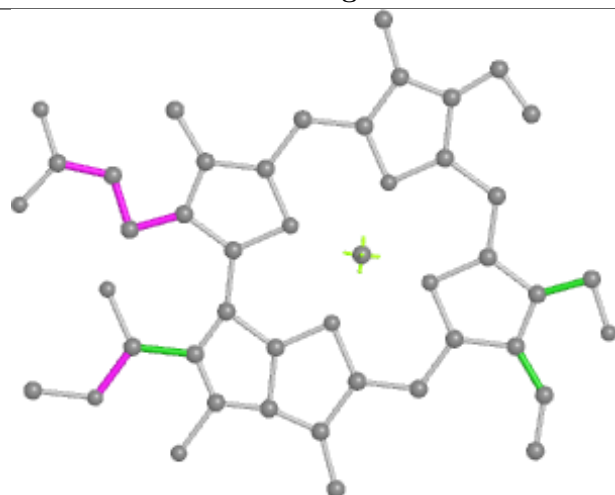
Ligand CHL 8 305



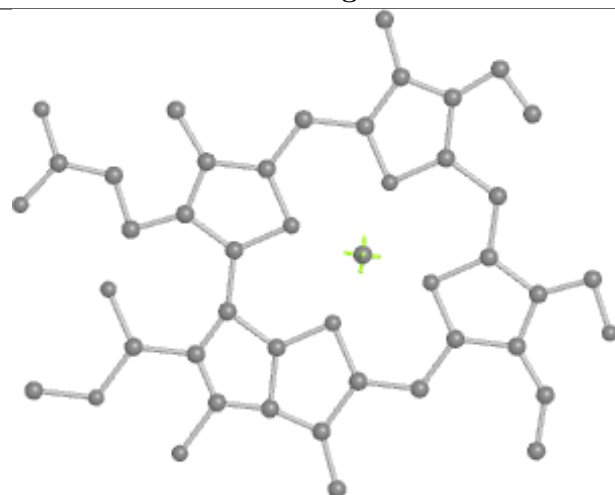
Bond lengths



Bond angles

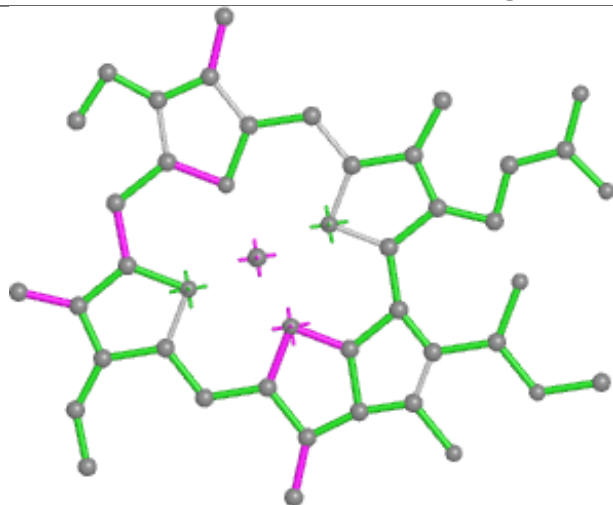


Torsions

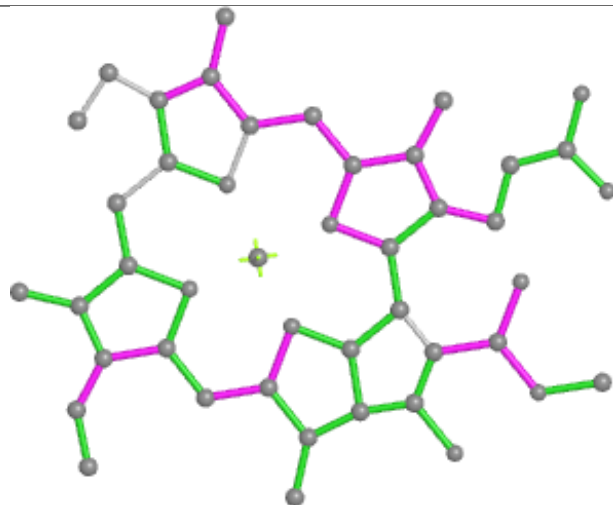


Rings

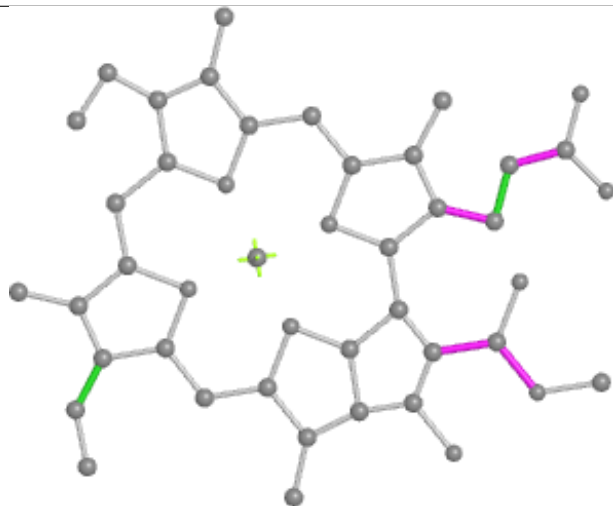
Ligand CLA AB 308



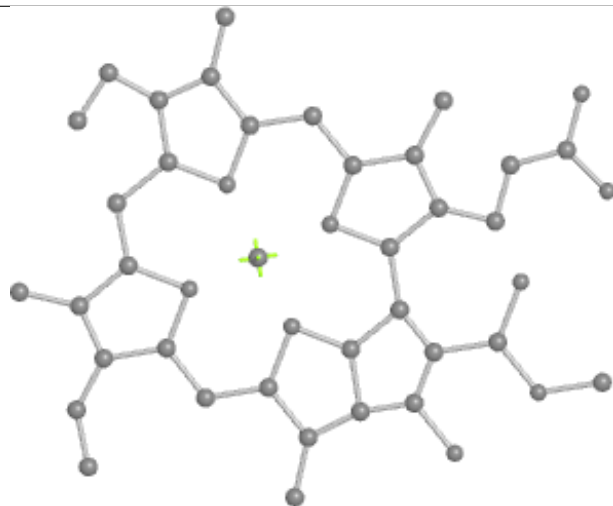
Bond lengths



Bond angles

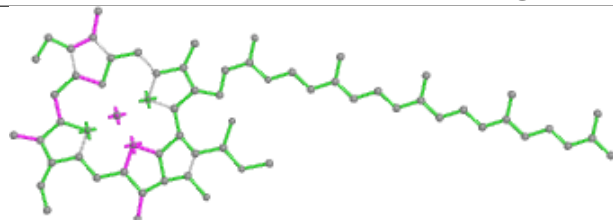


Torsions

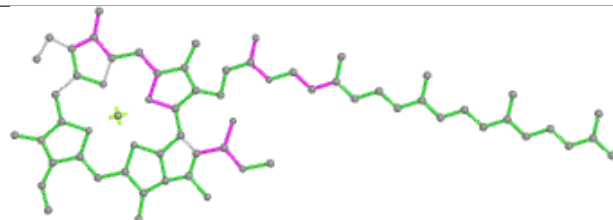


Rings

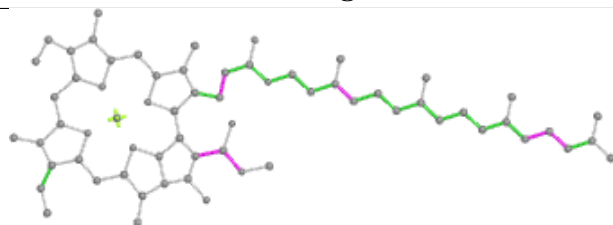
Ligand CLA R 404



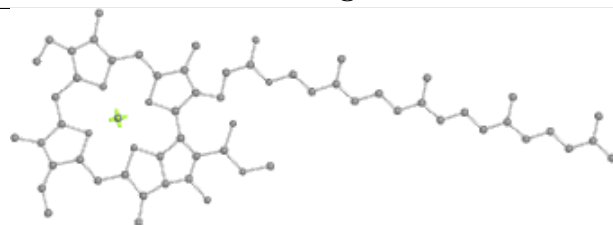
Bond lengths



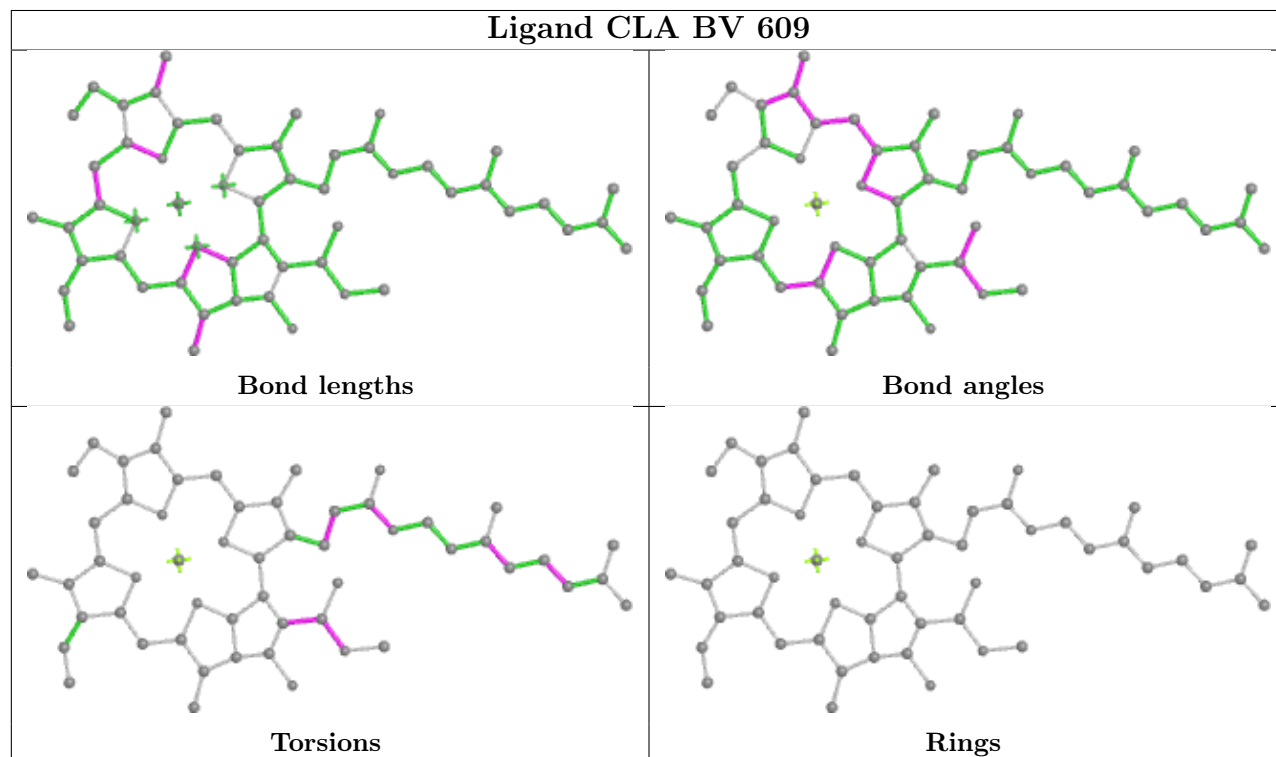
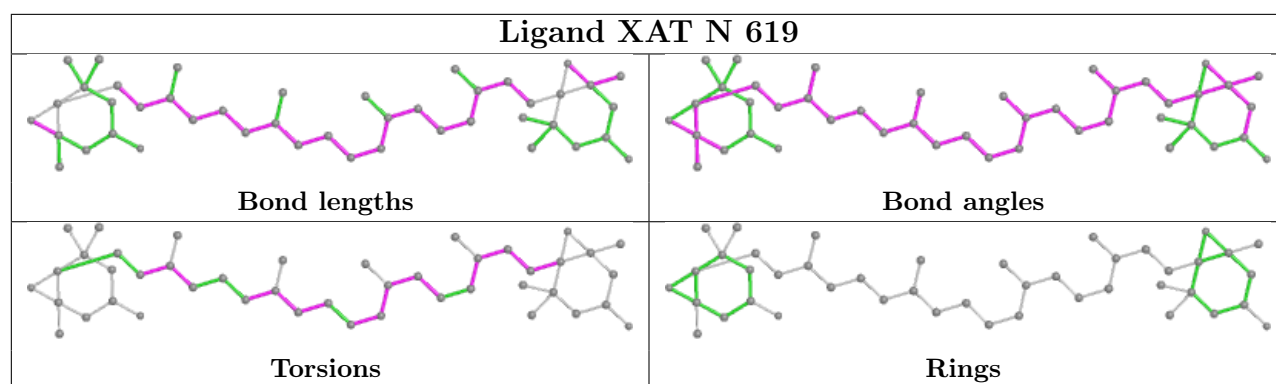
Bond angles



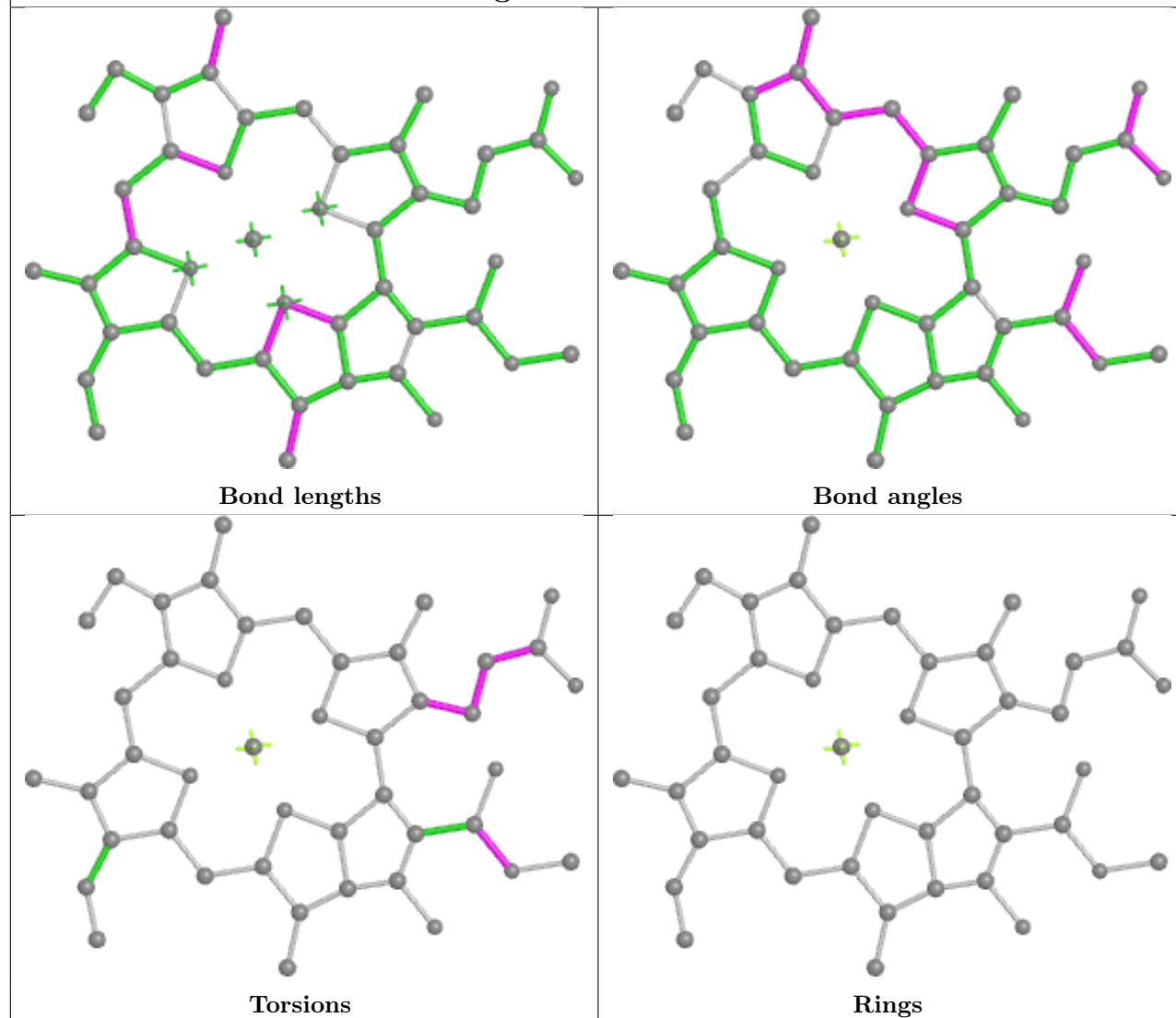
Torsions



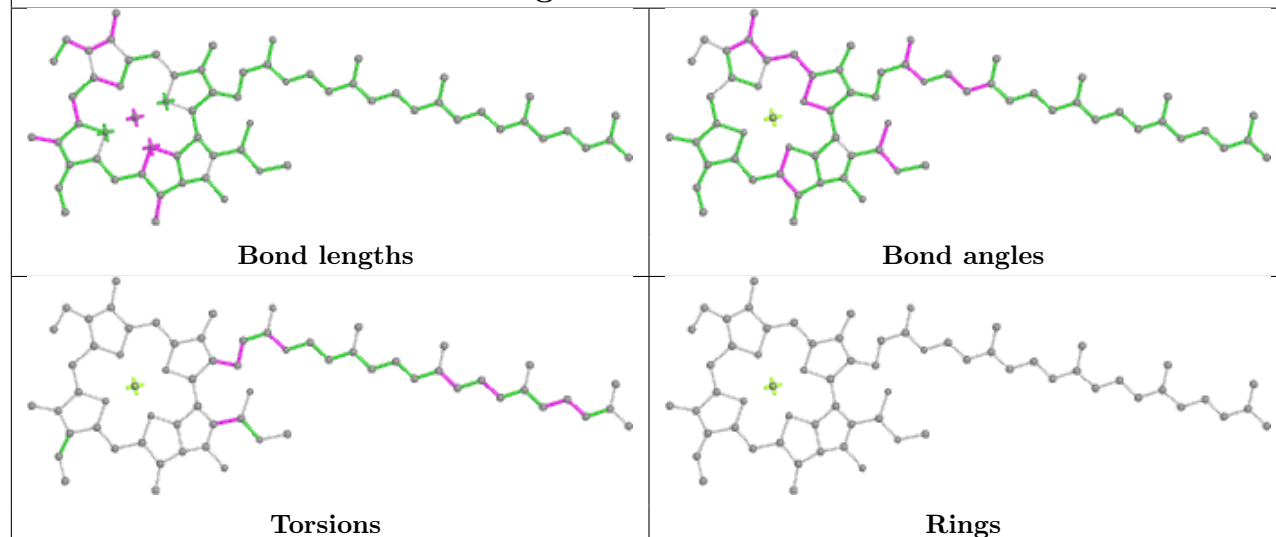
Rings



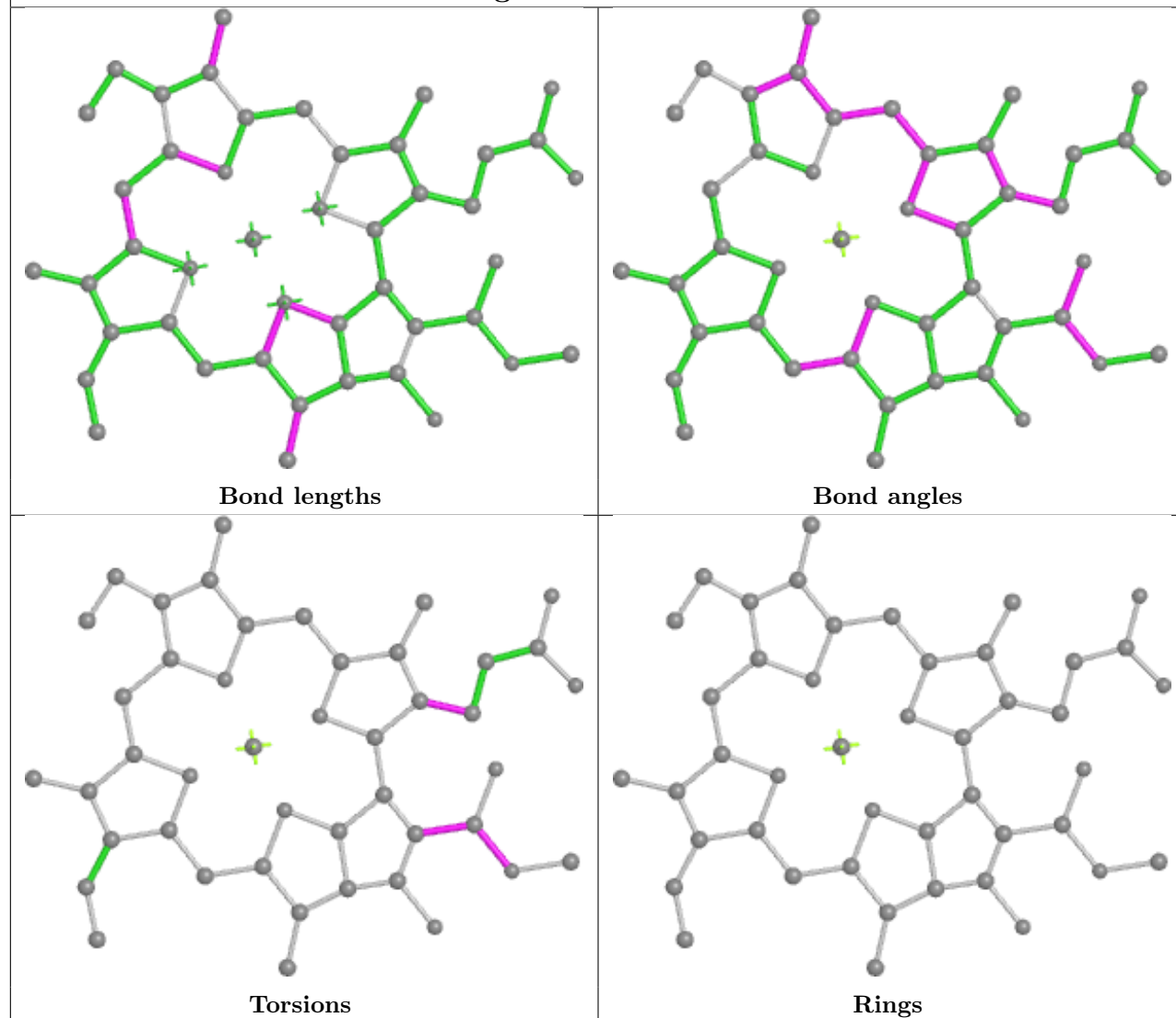
Ligand CLA 5 611



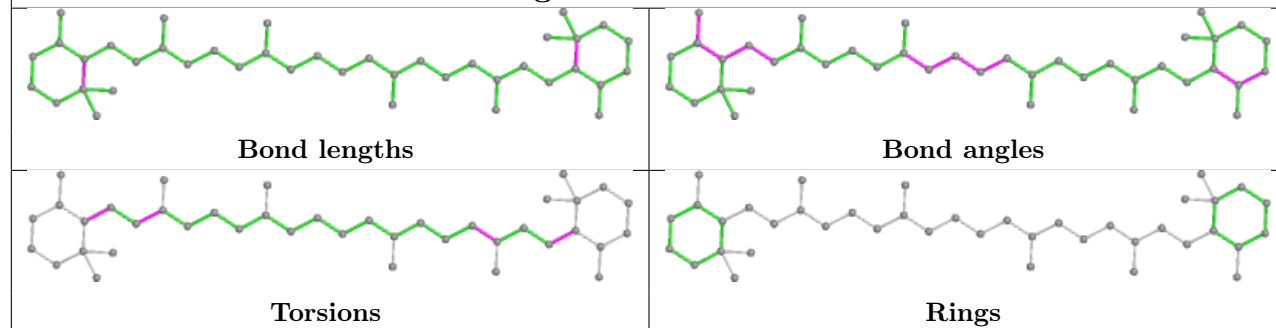
Ligand CLA v 612

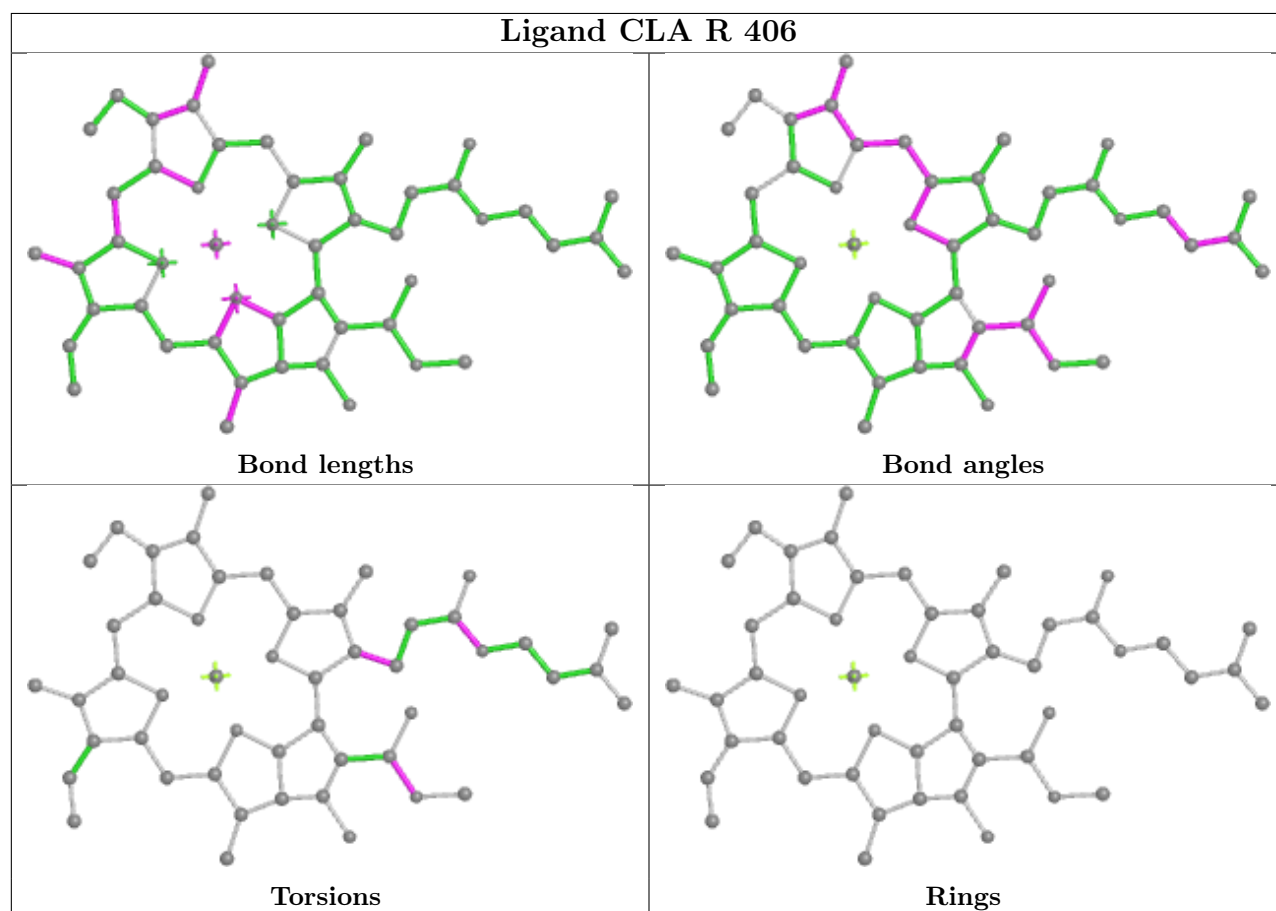
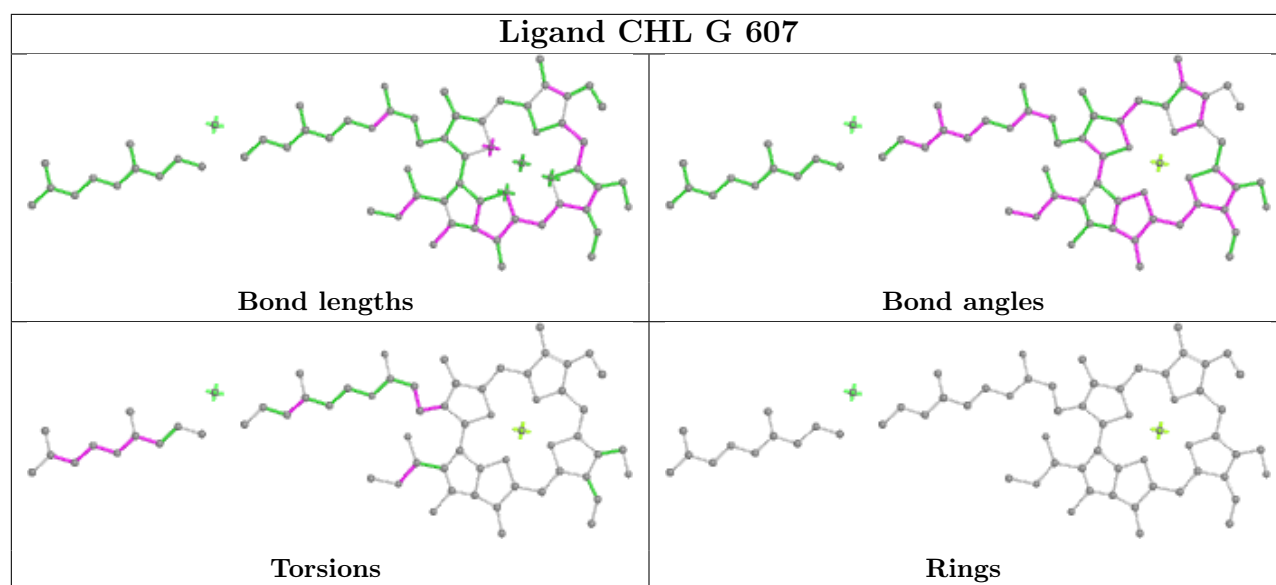


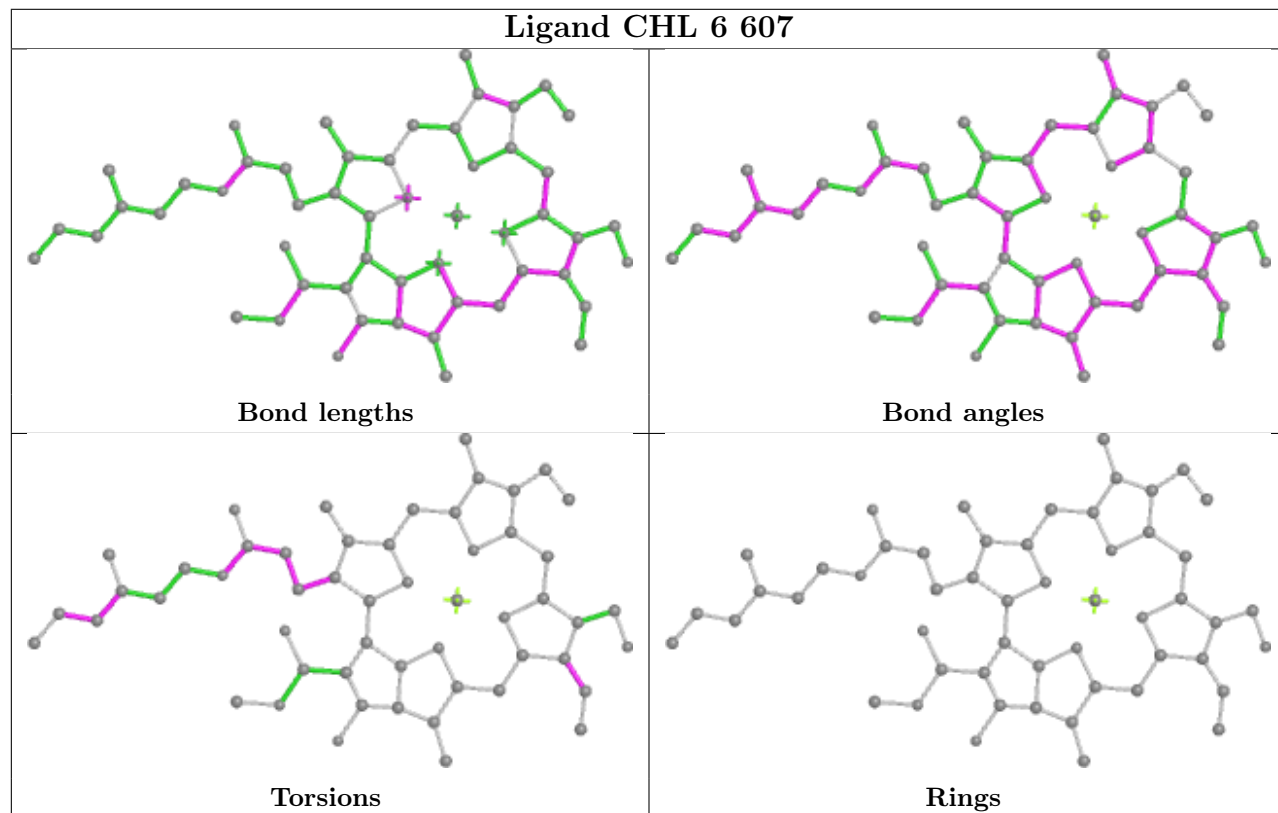
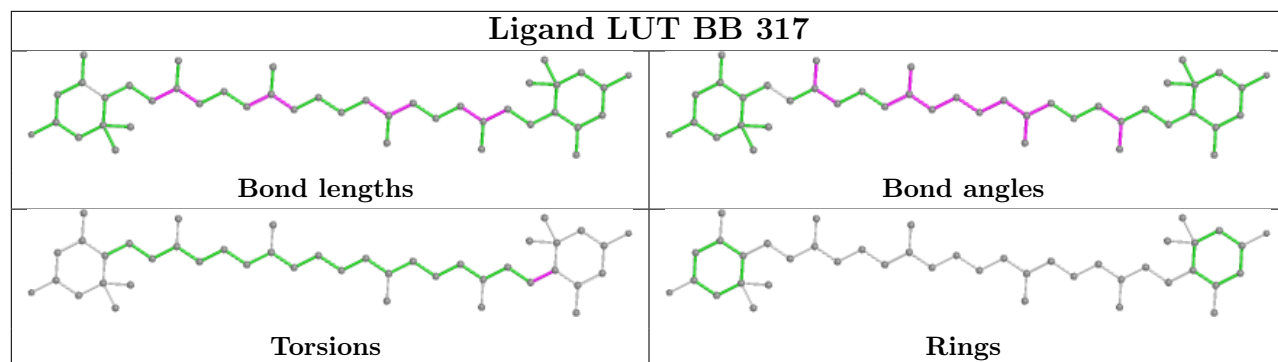
Ligand CLA 8 310



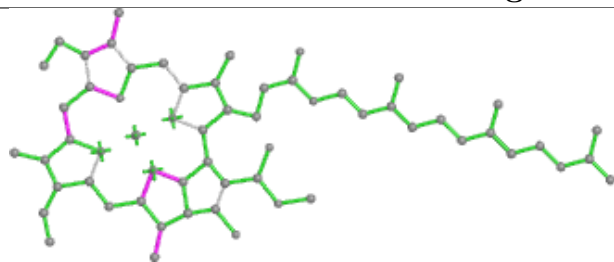
Ligand BCR v 618



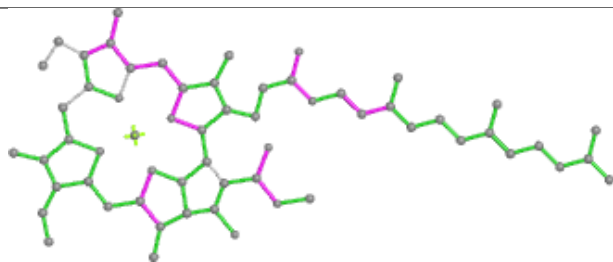




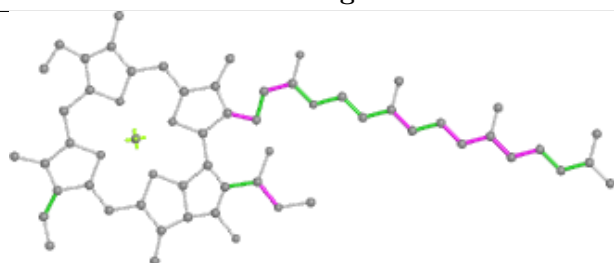
Ligand CLA Ba 312



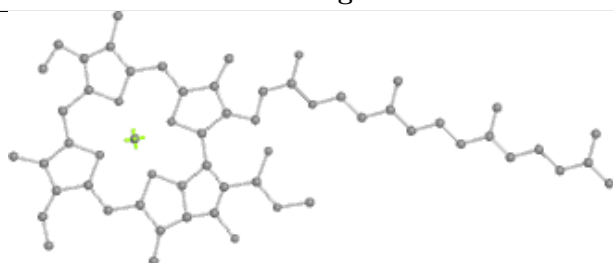
Bond lengths



Bond angles

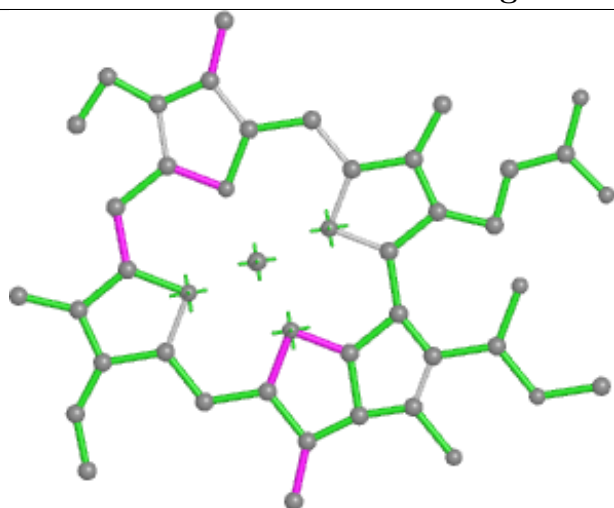


Torsions

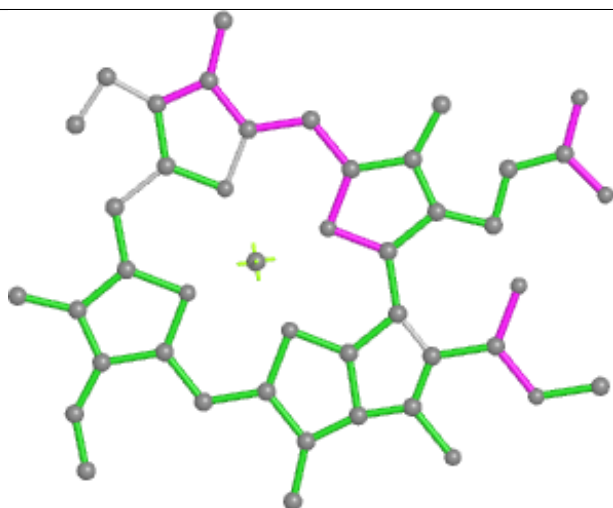


Rings

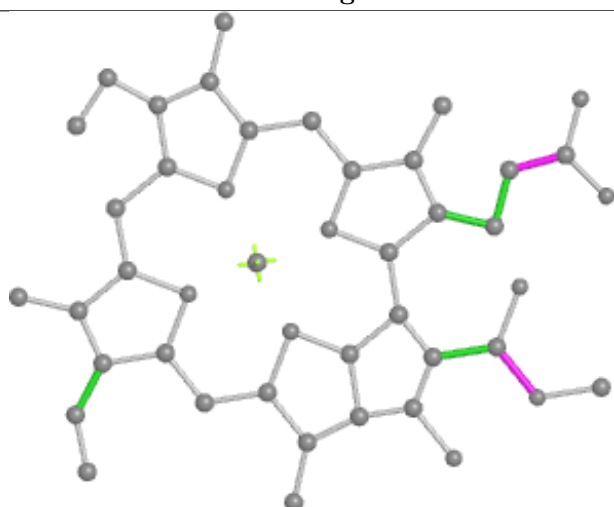
Ligand CLA AA 313



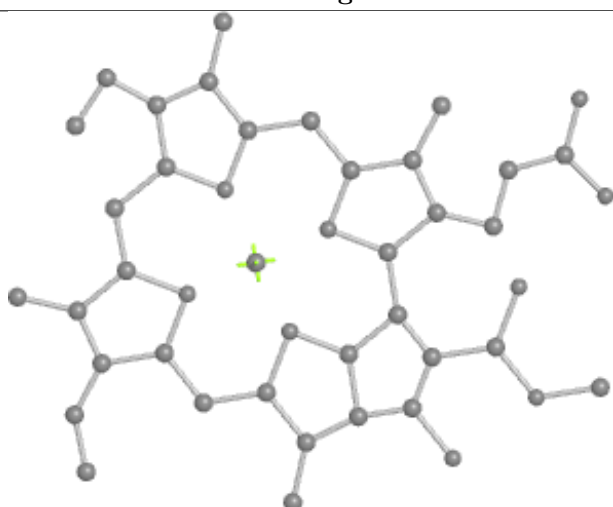
Bond lengths



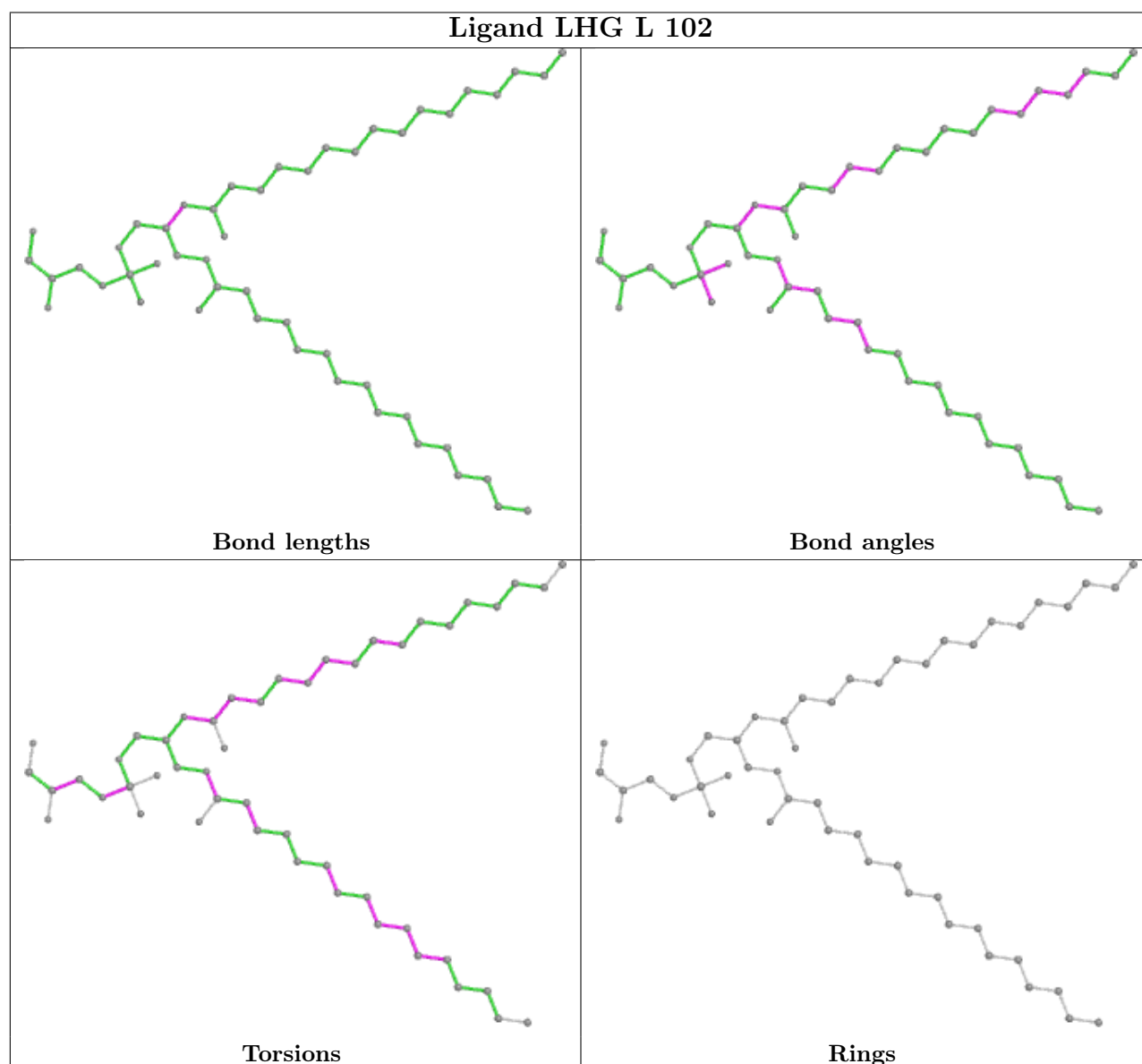
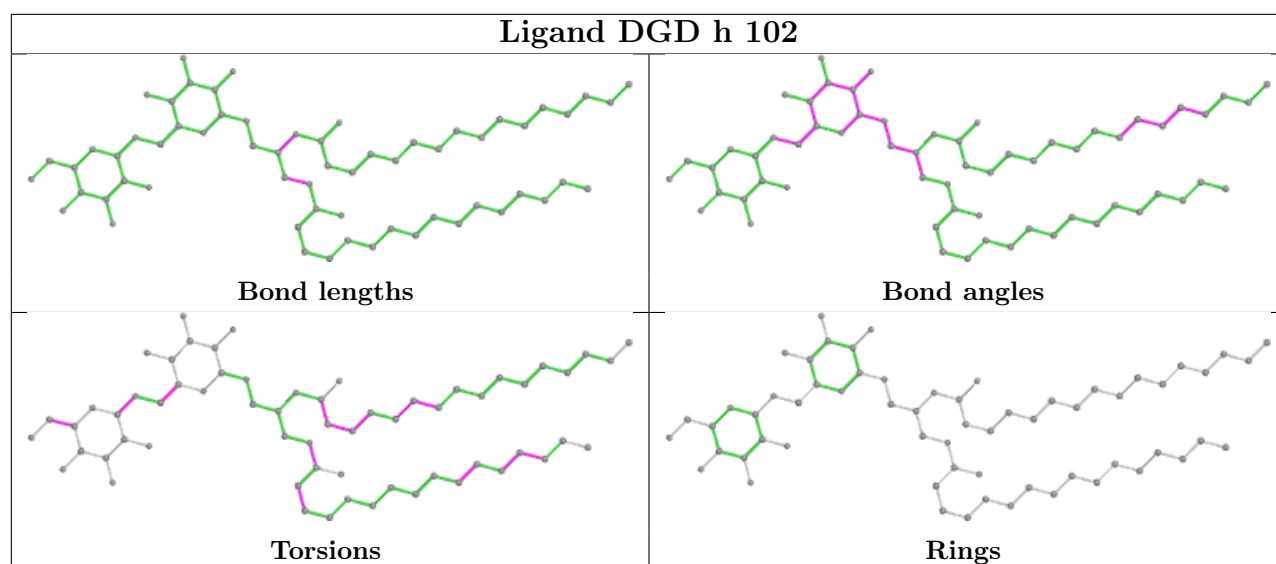
Bond angles

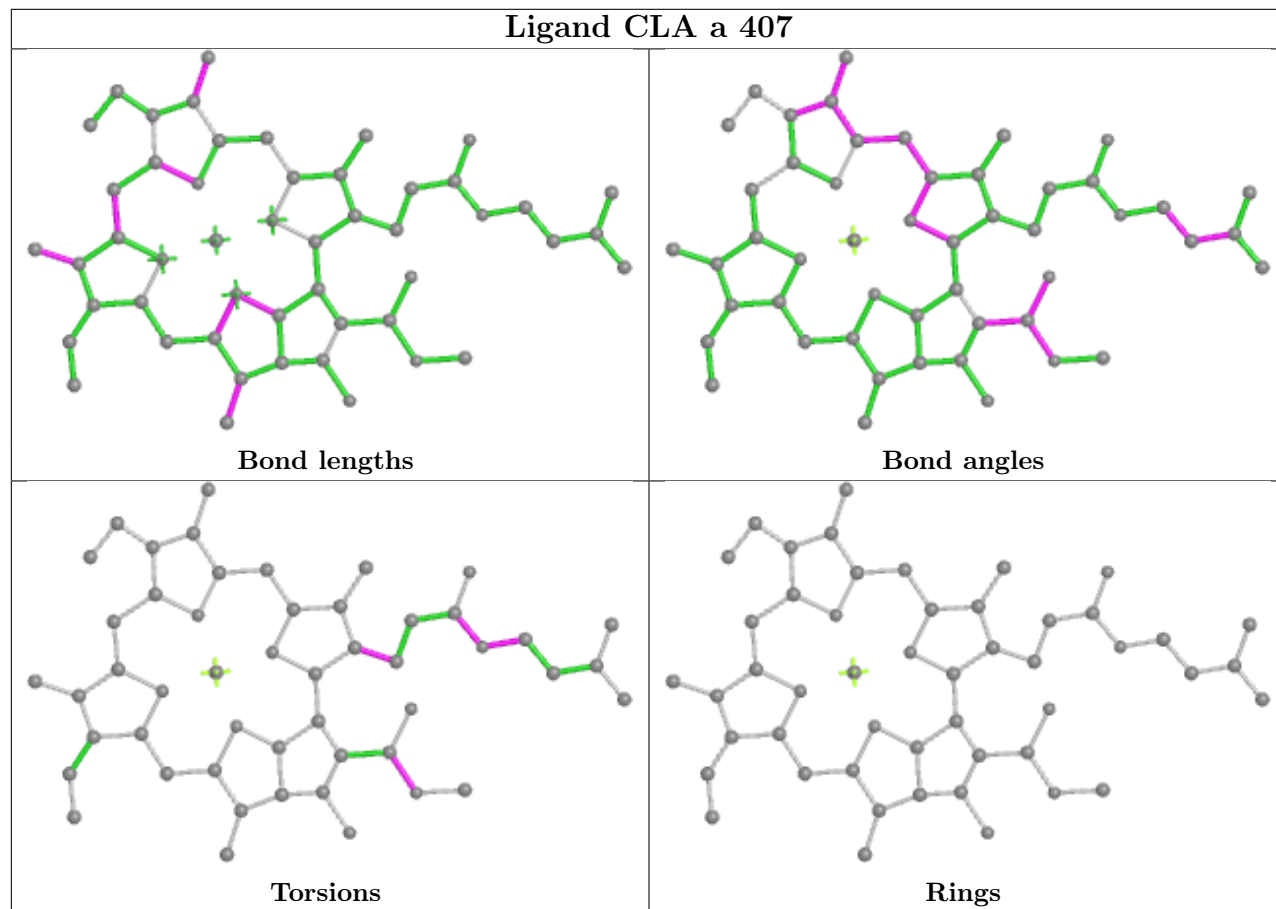
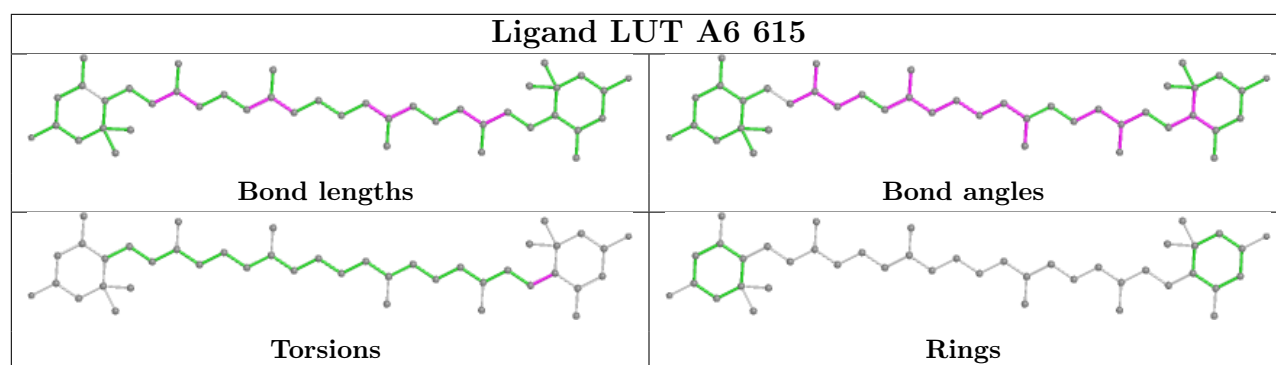


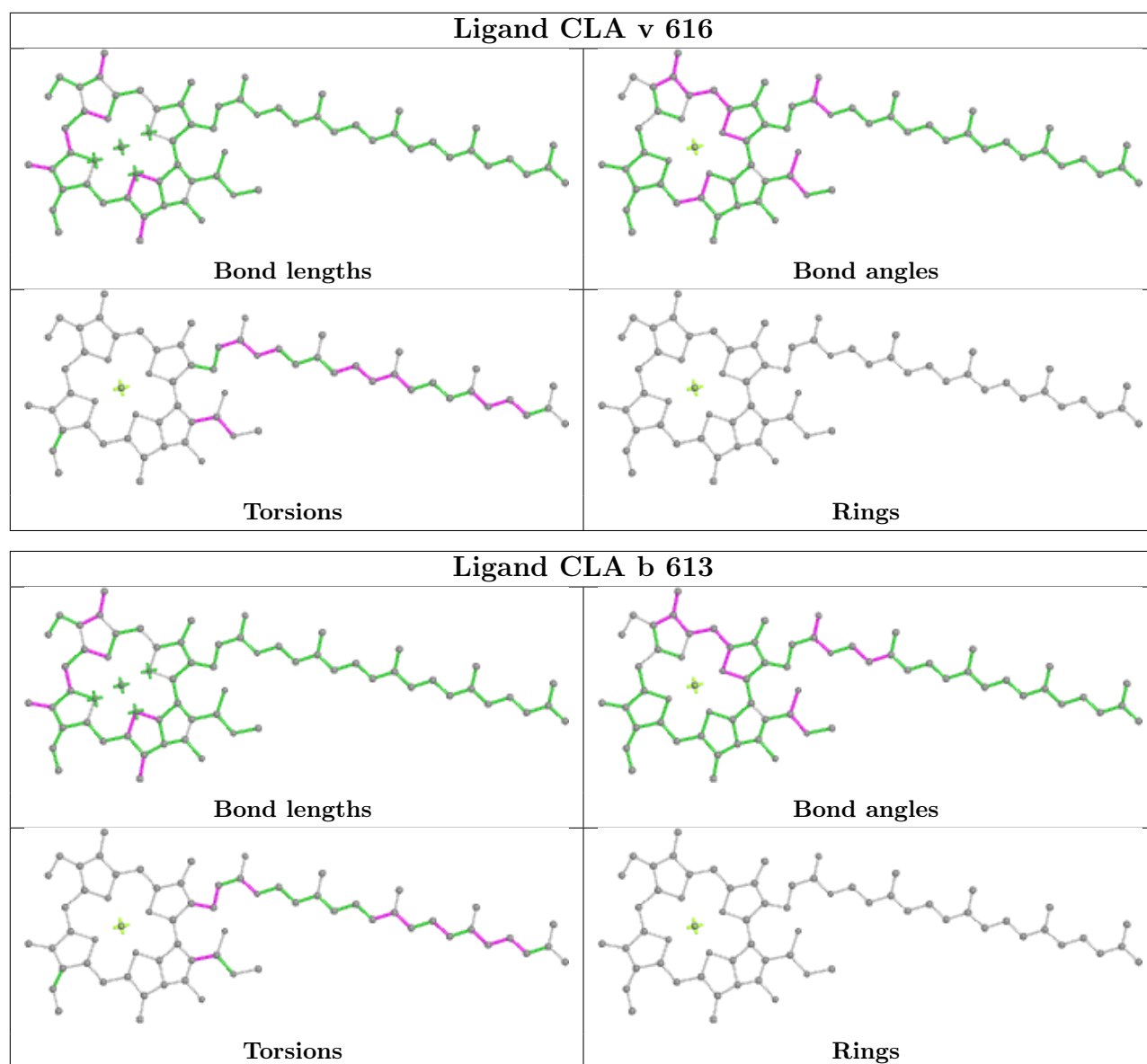
Torsions

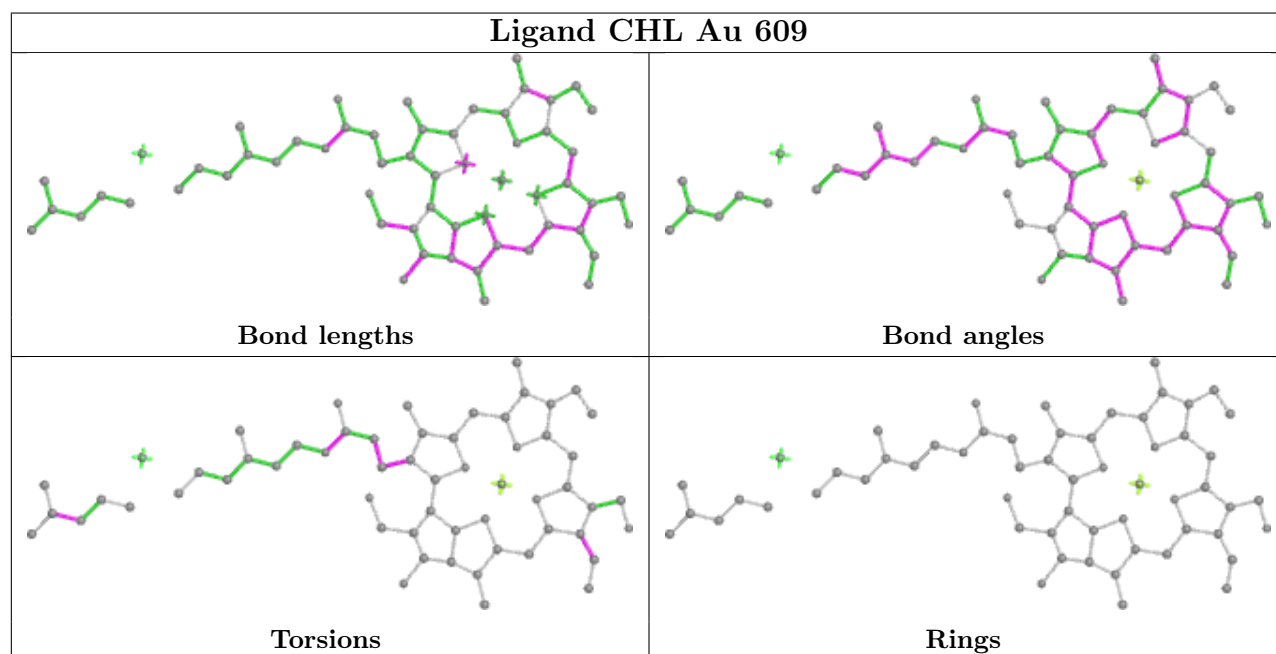
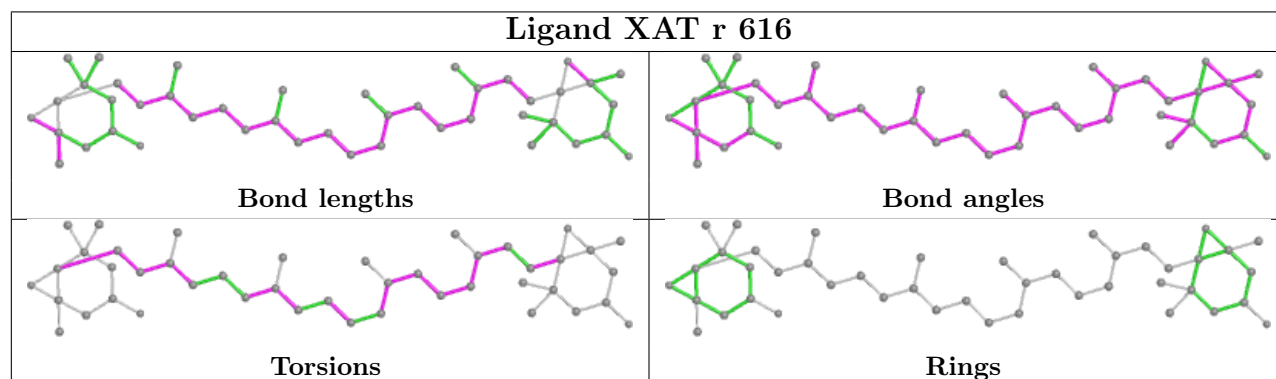
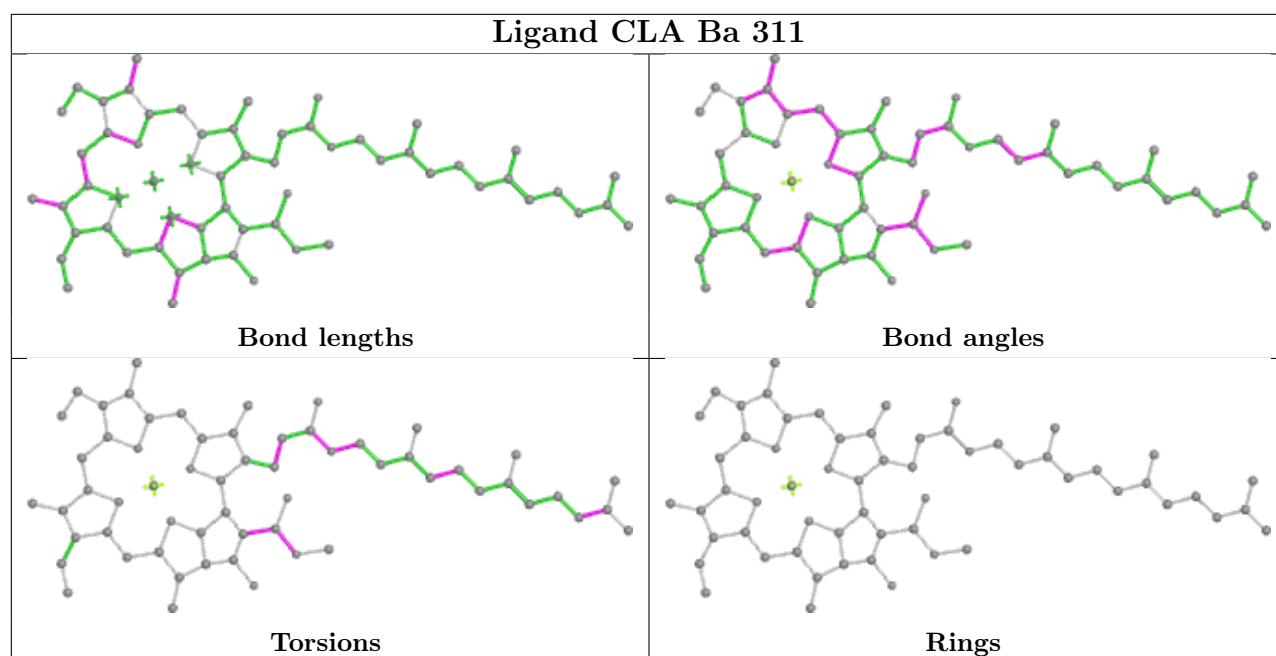


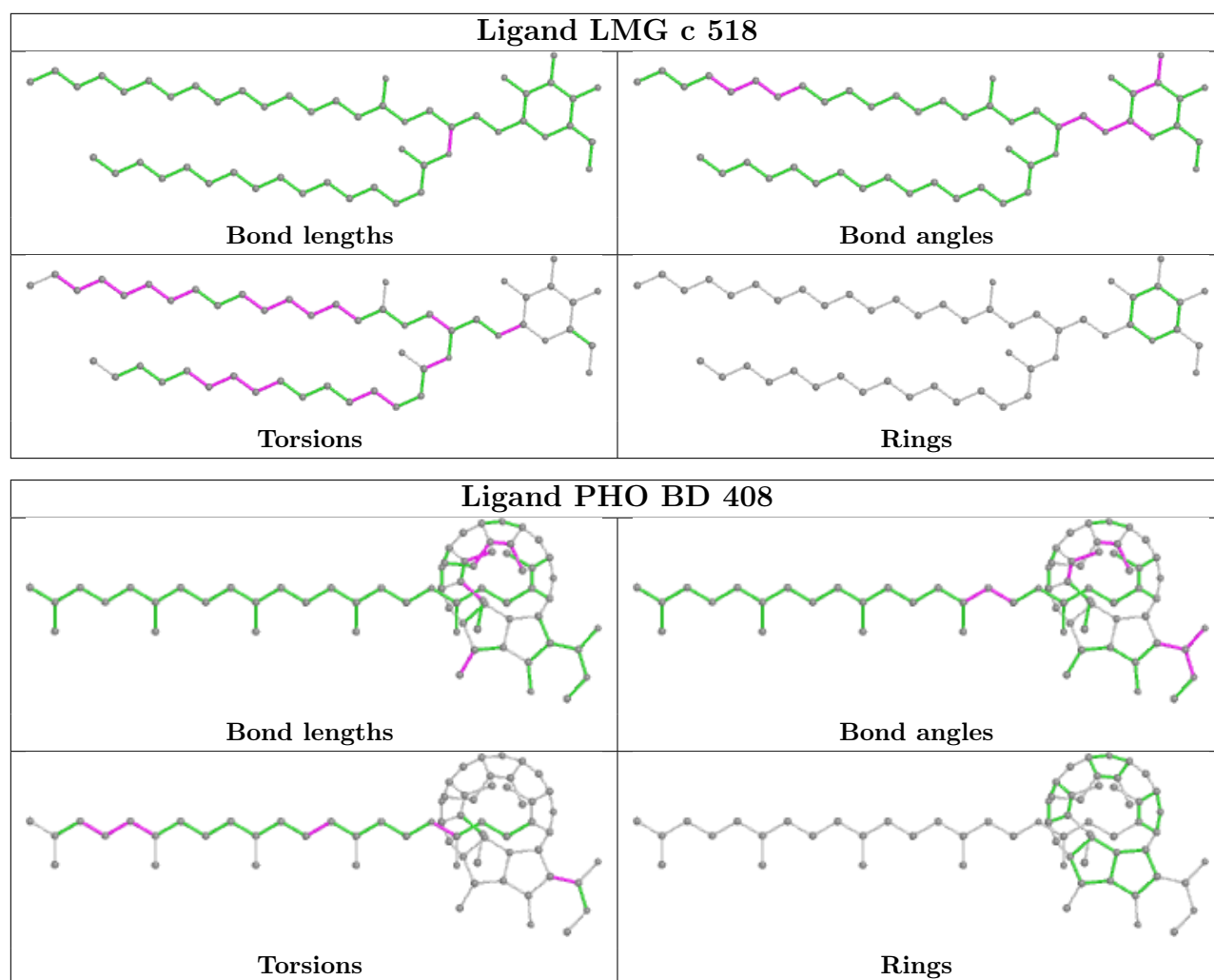
Rings

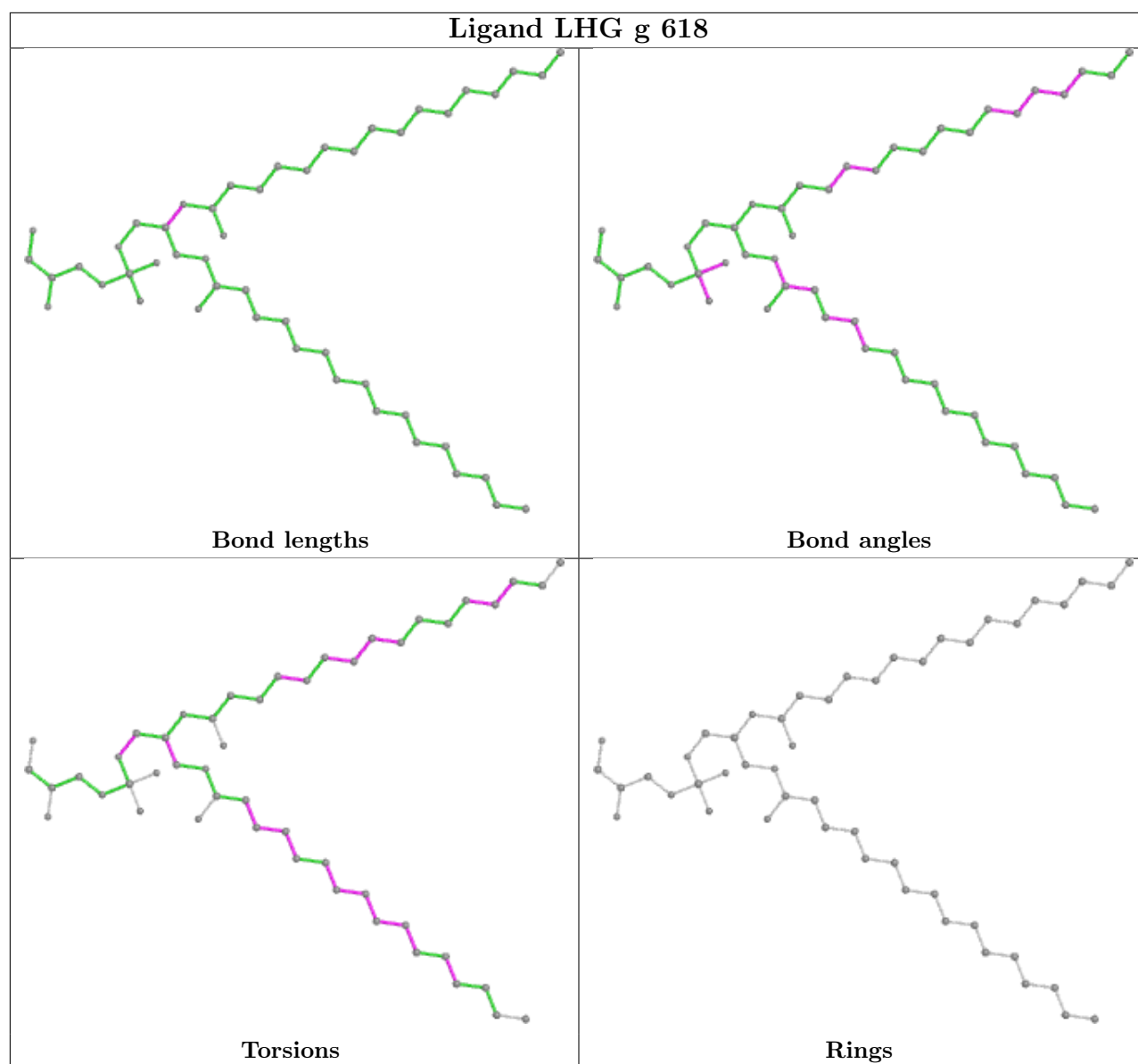




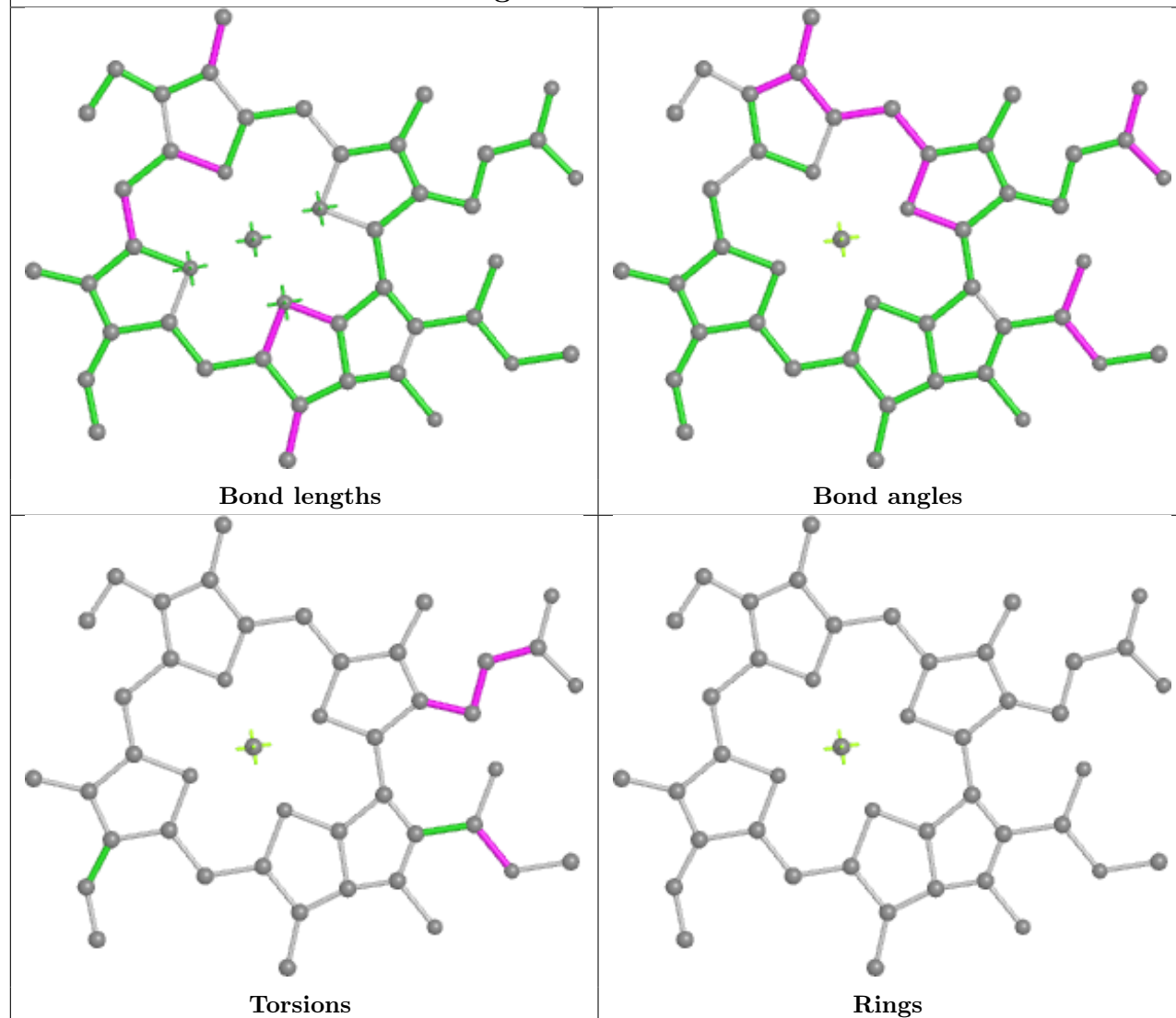




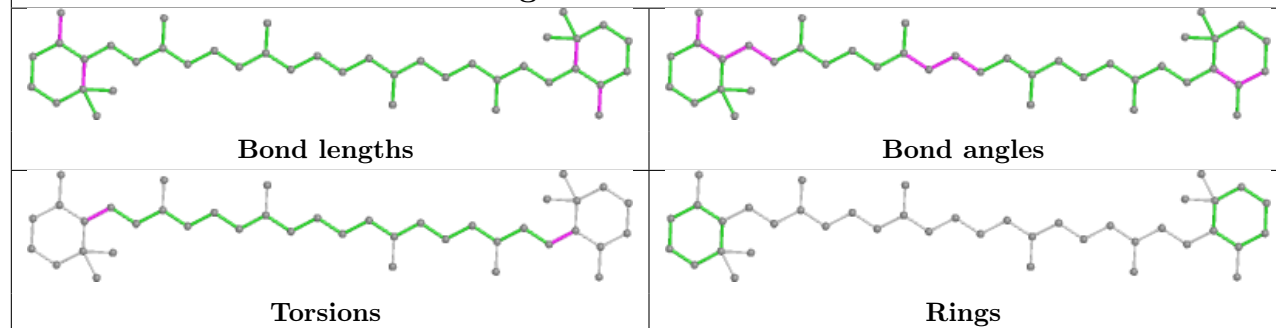




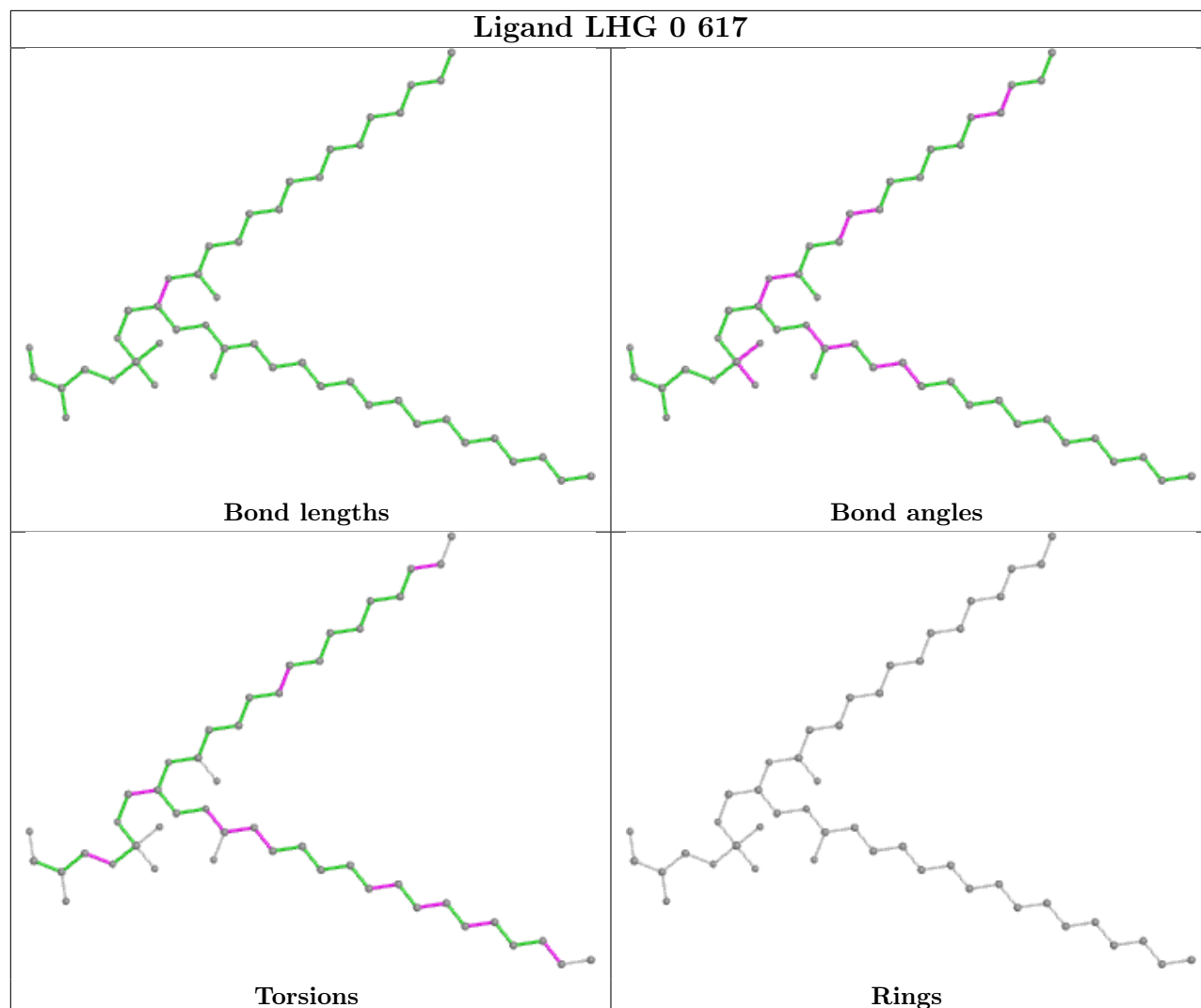
Ligand CLA 9 611



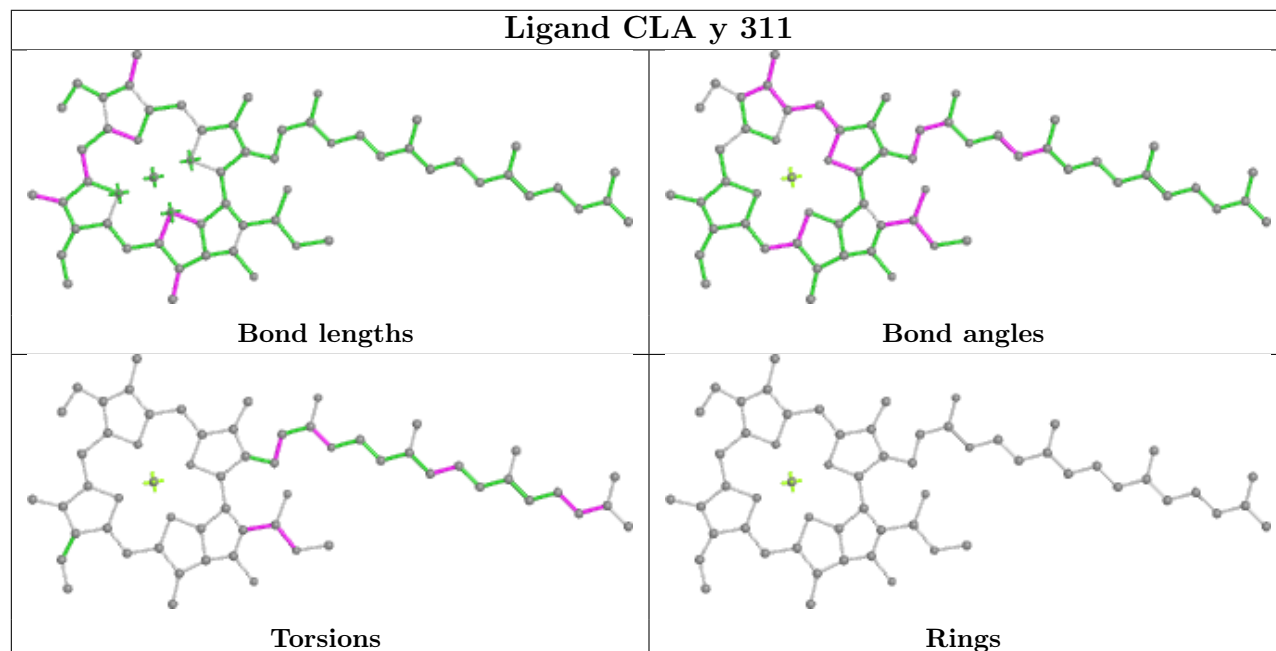
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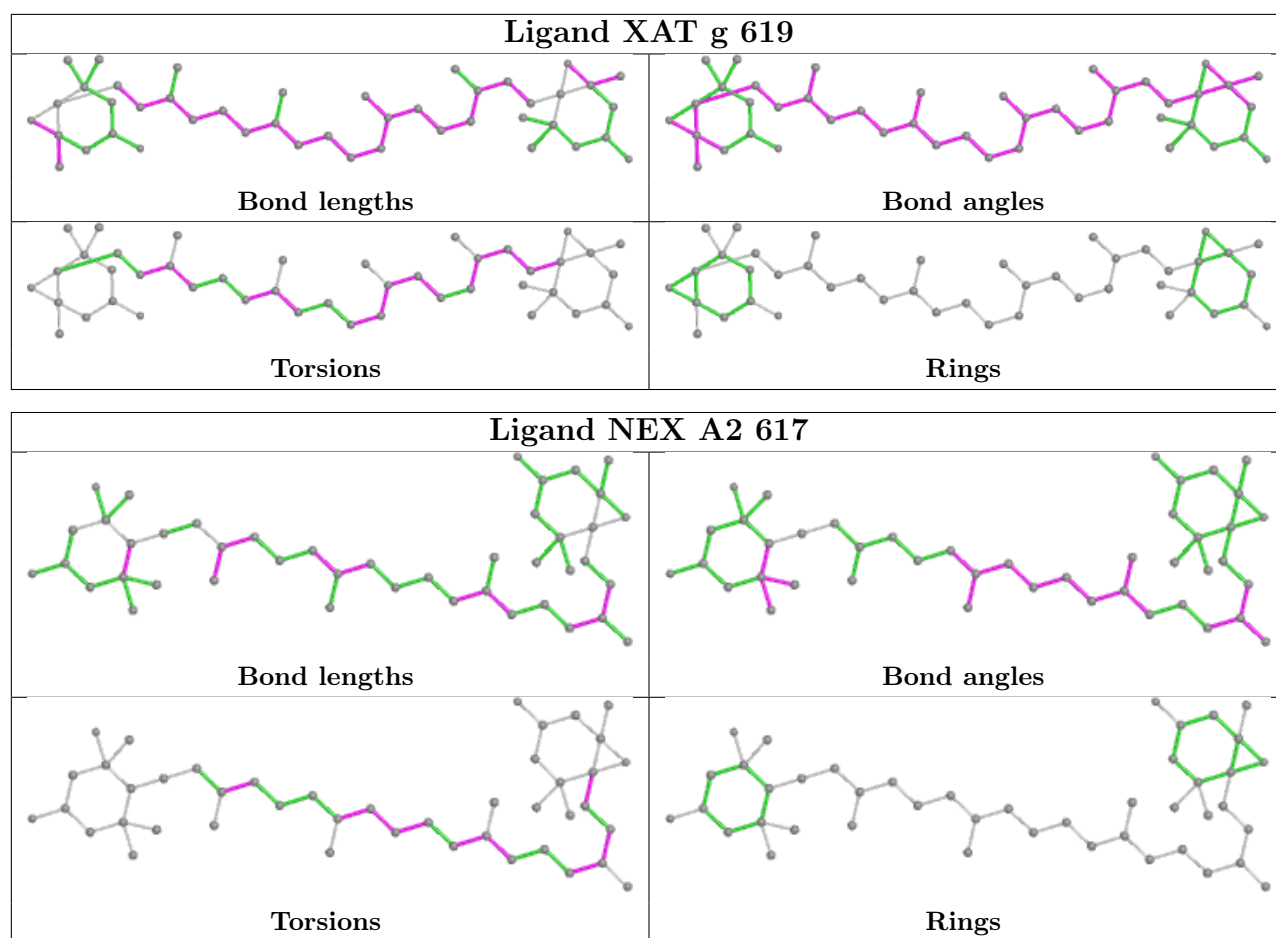


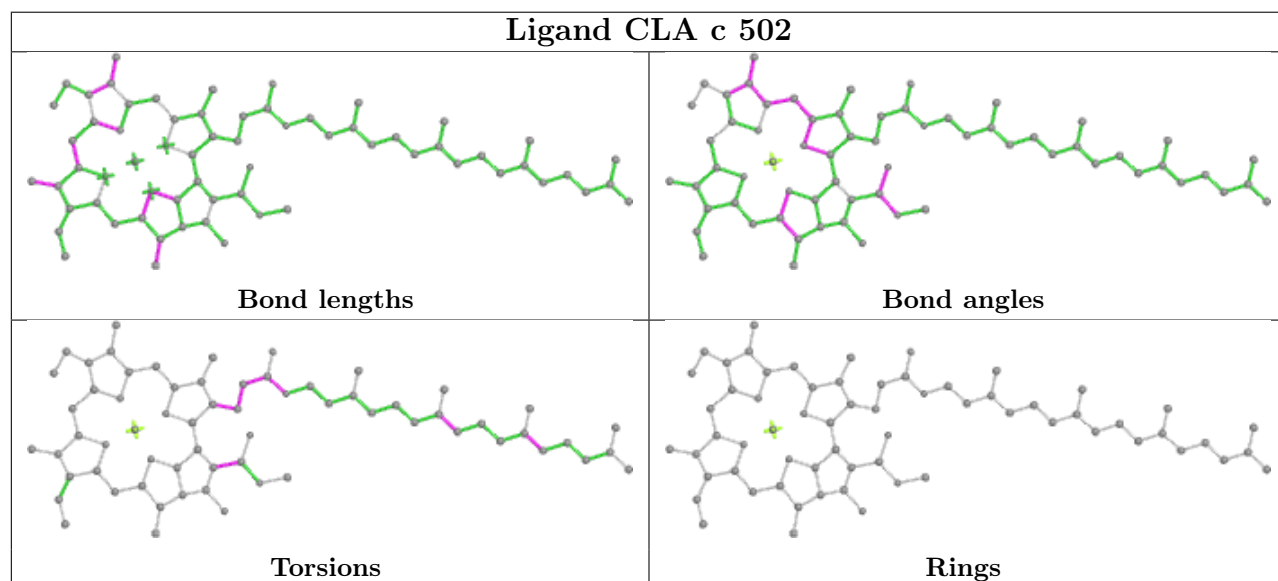
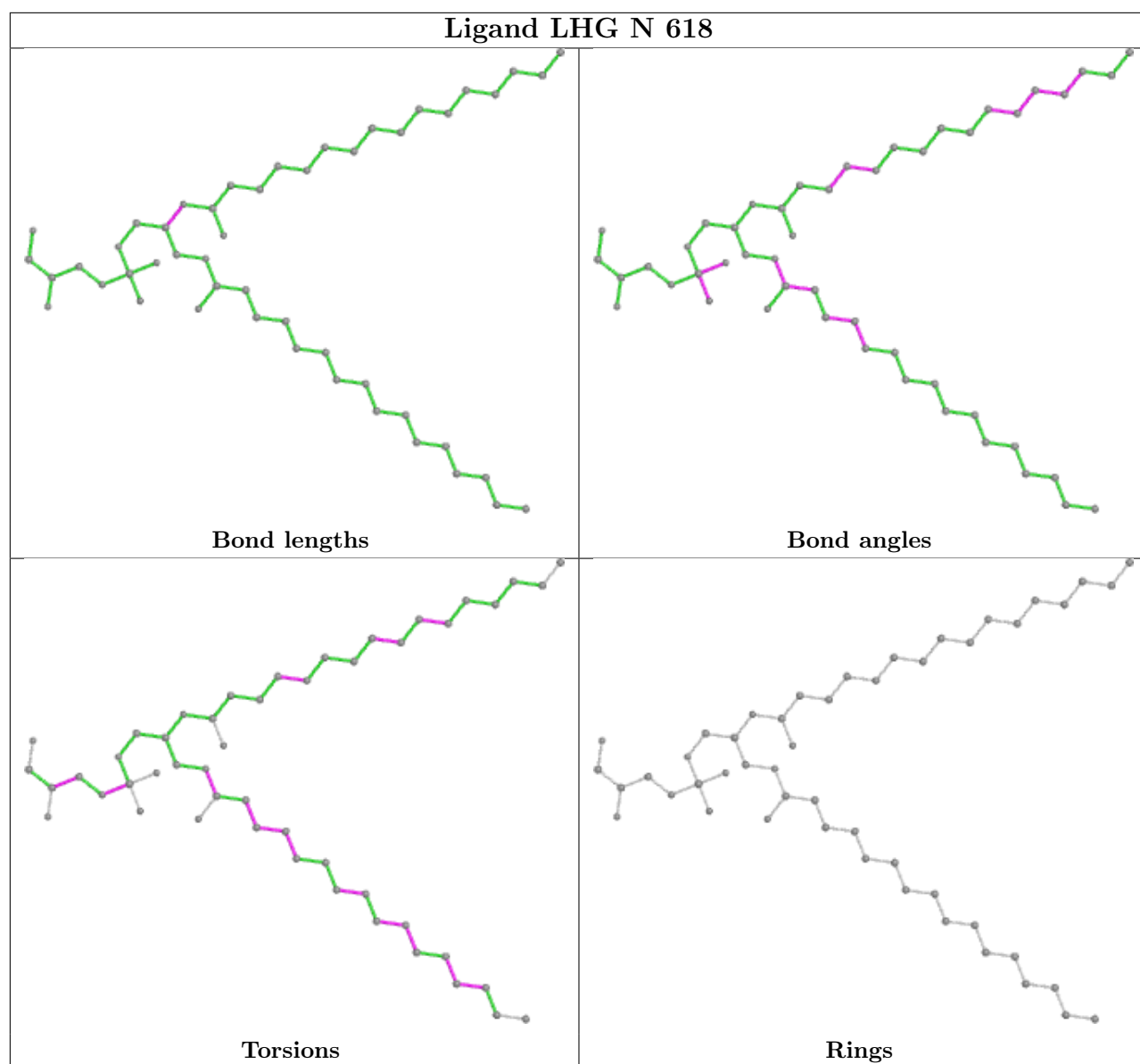
Ligand LHG 0 617

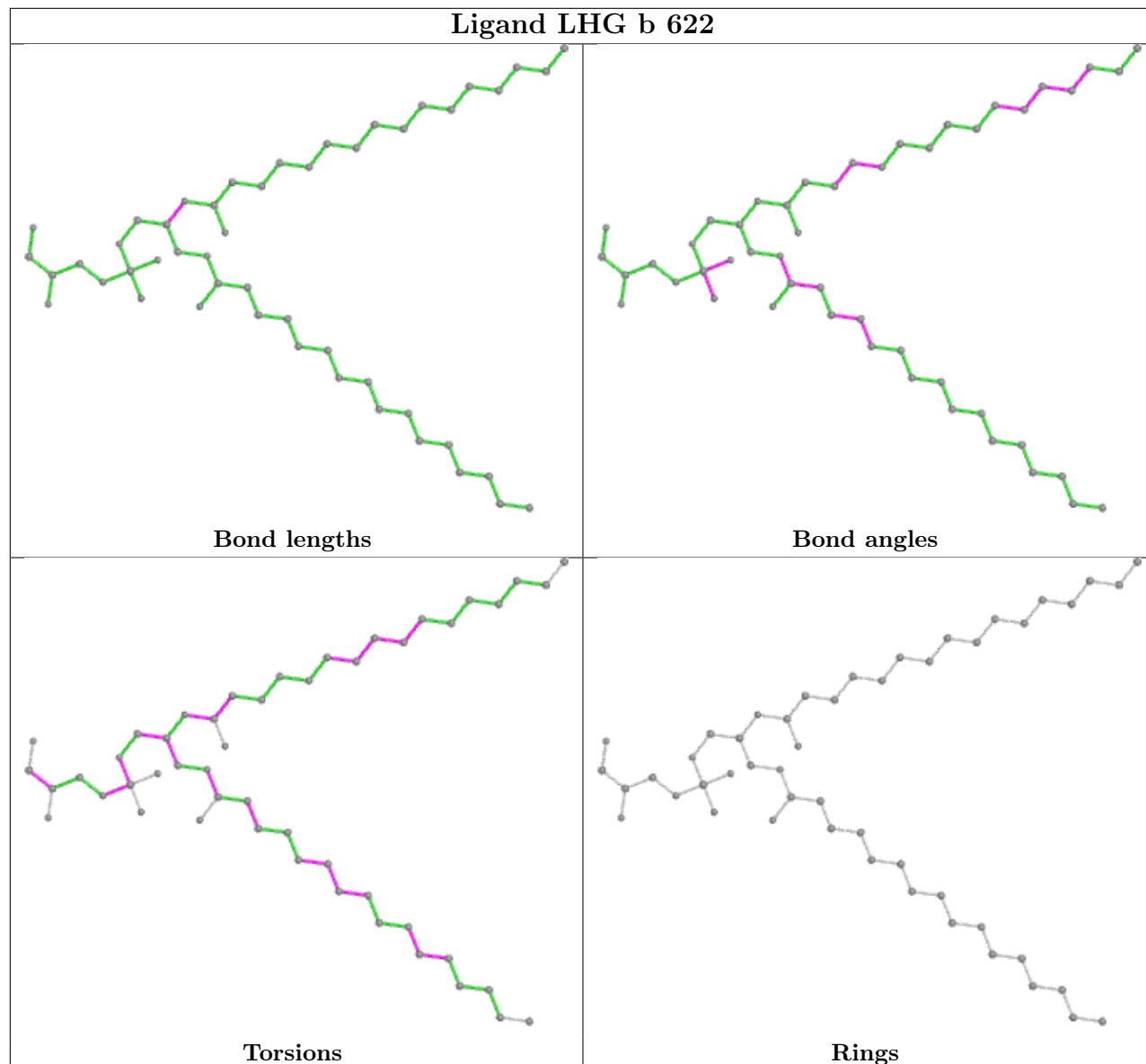
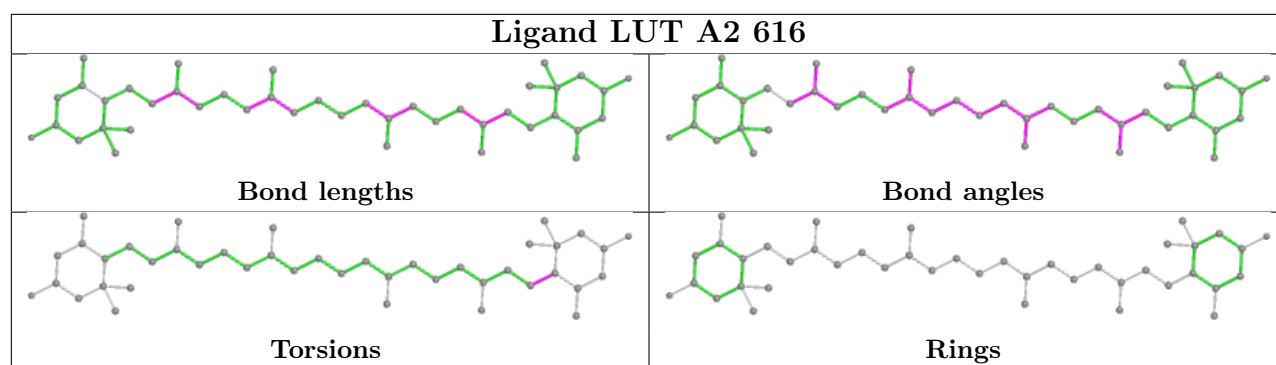


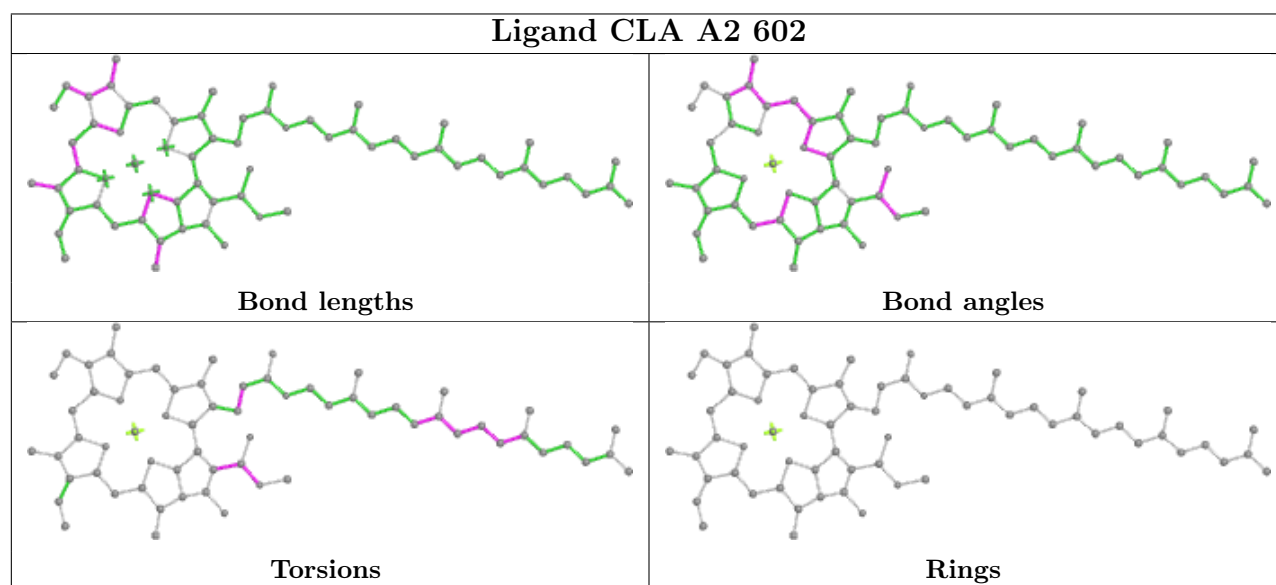
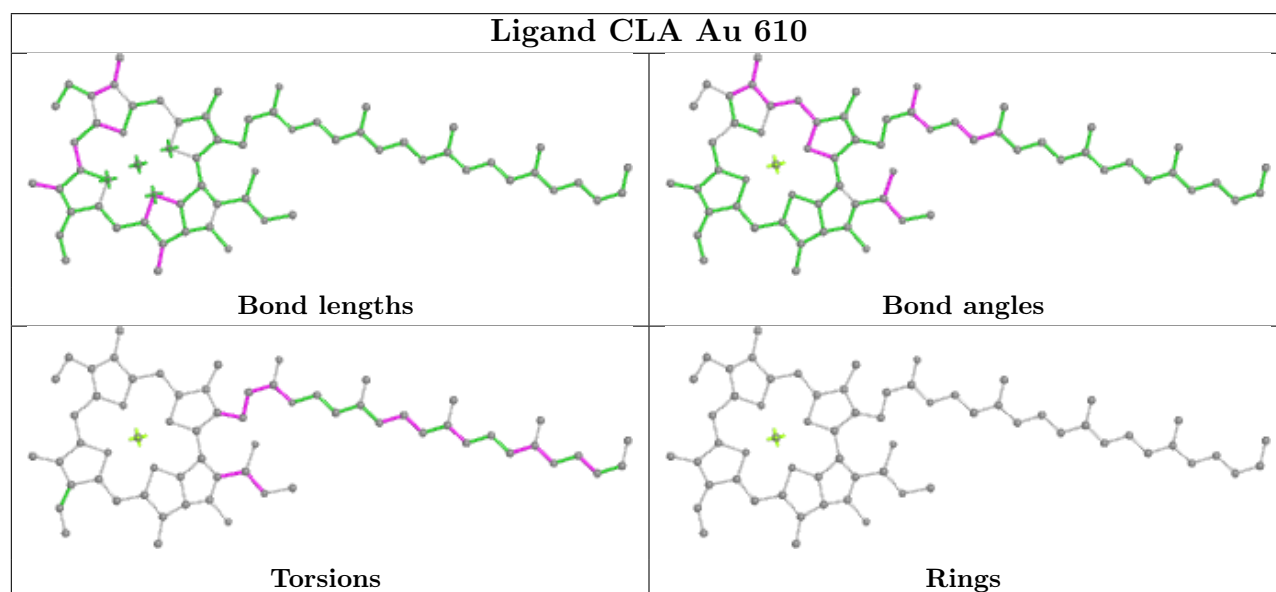
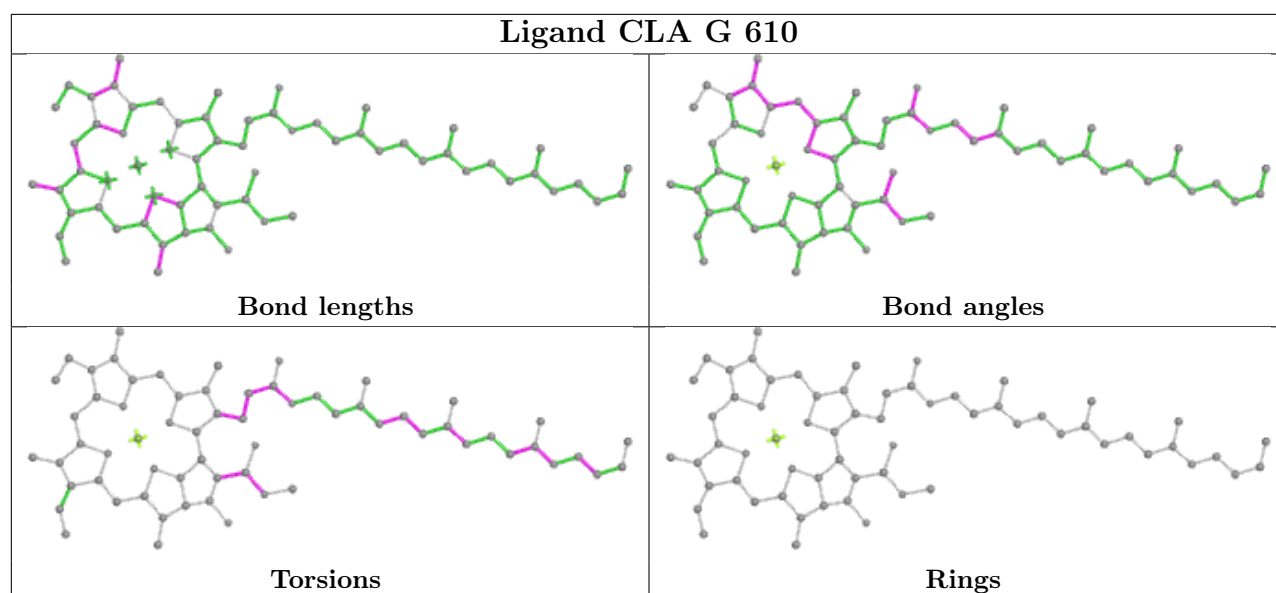
Ligand CLA y 311

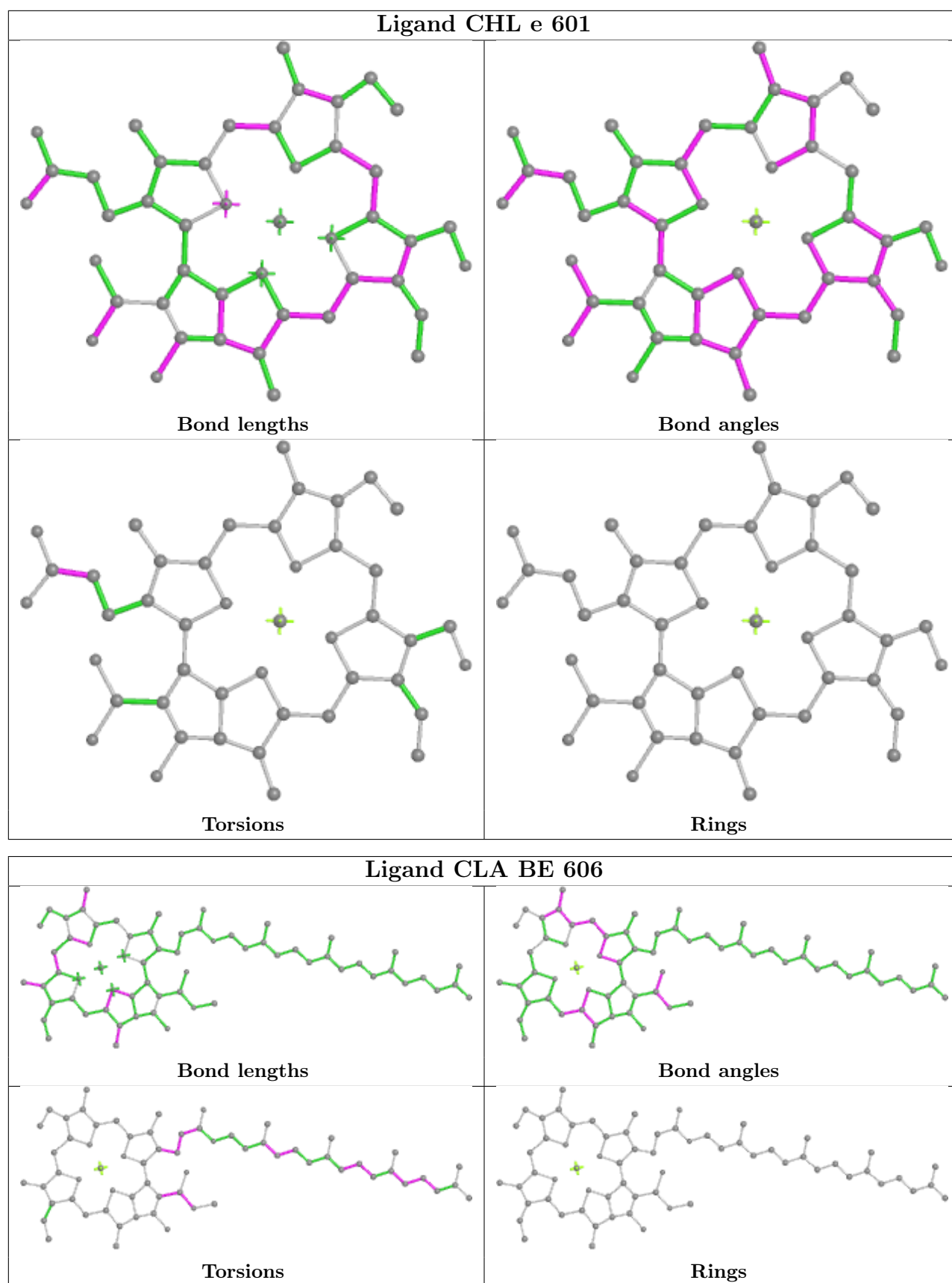


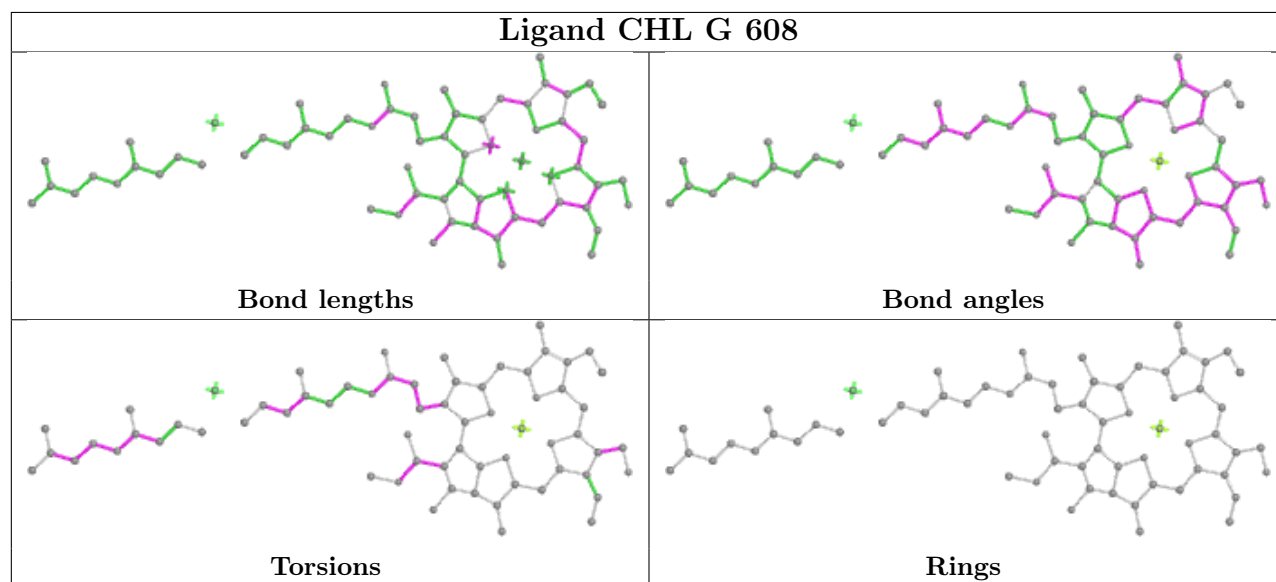
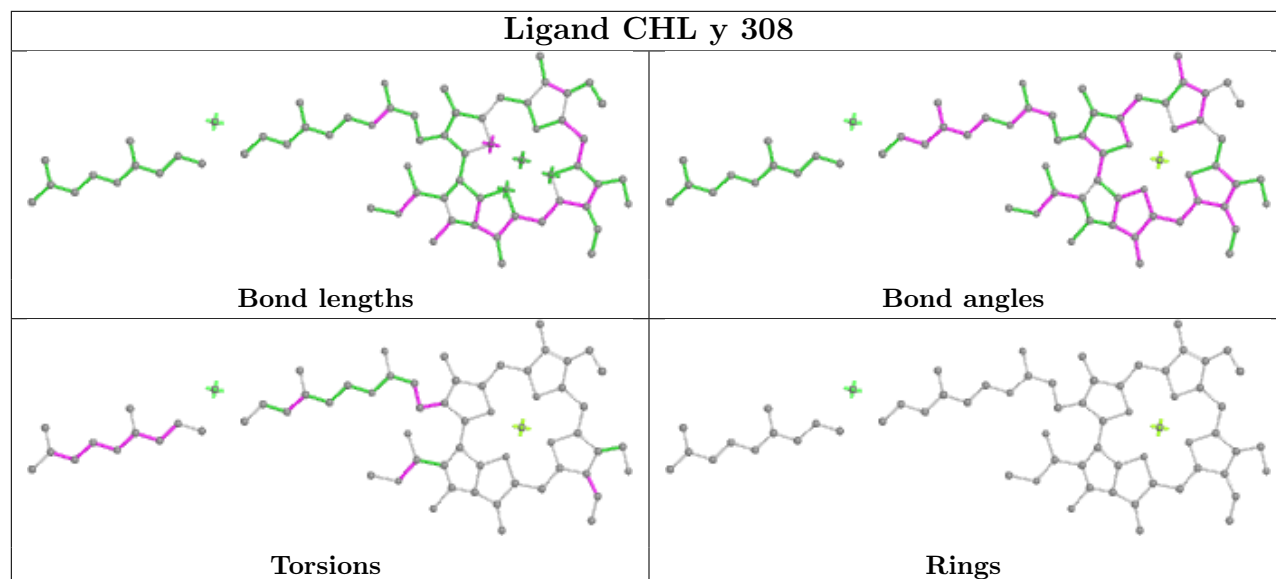
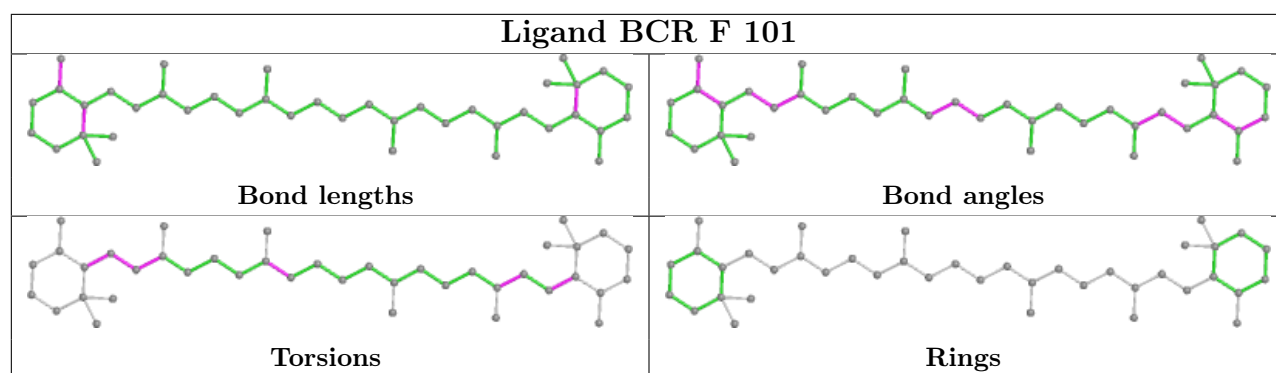


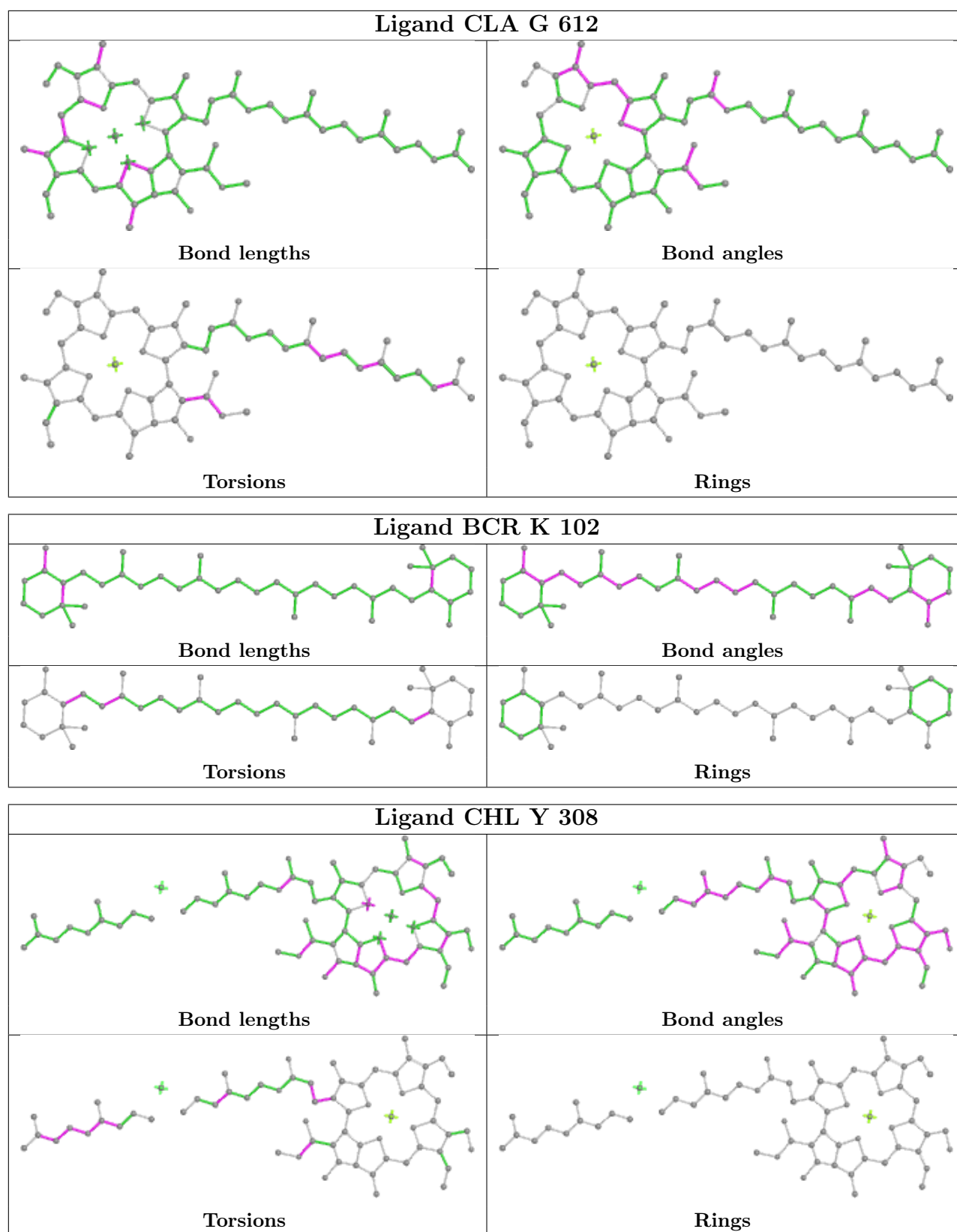


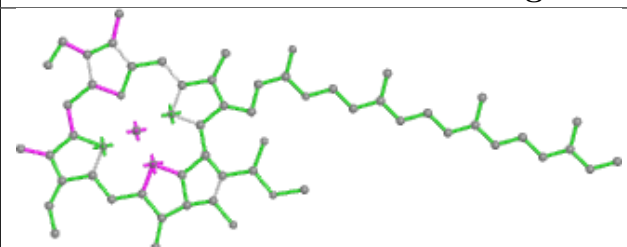
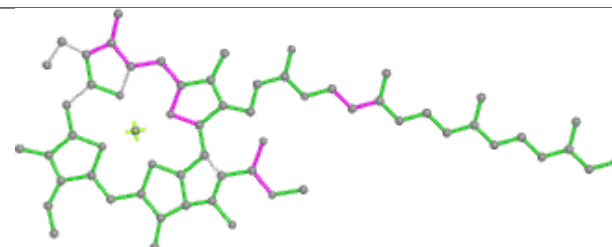
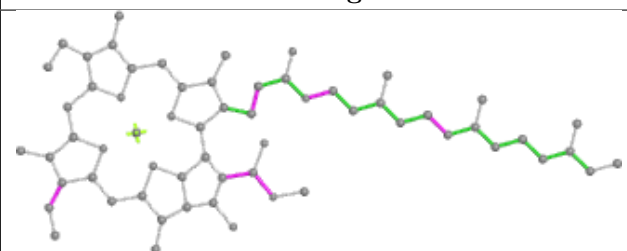
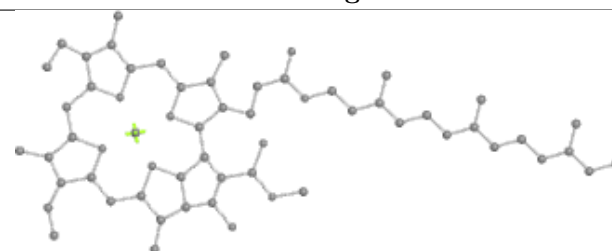


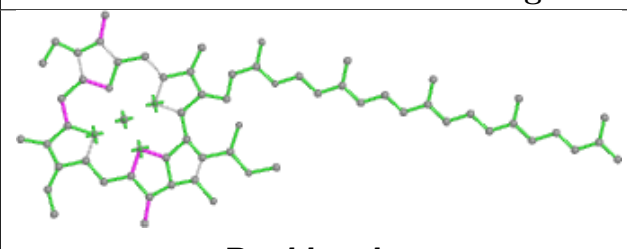
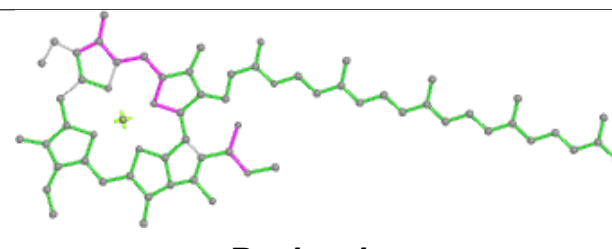
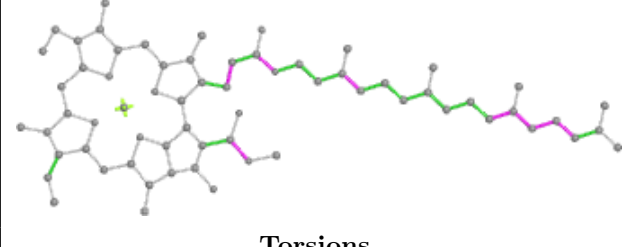
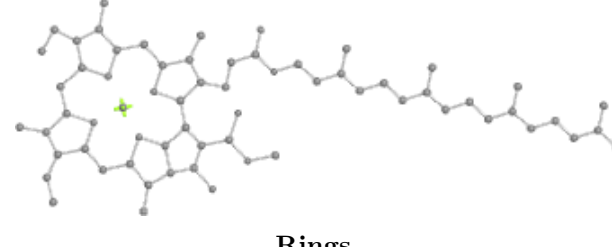


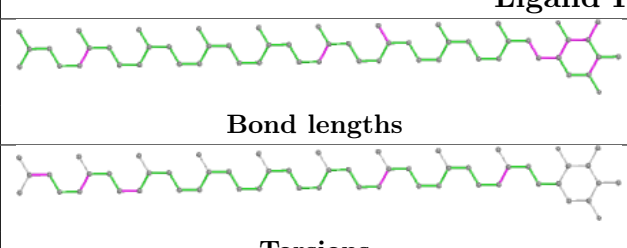
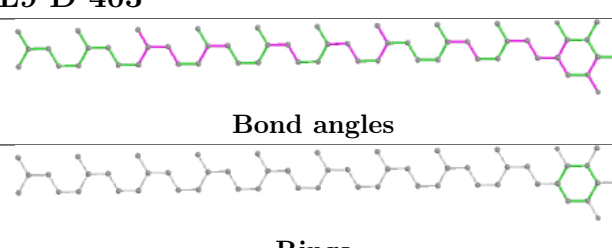
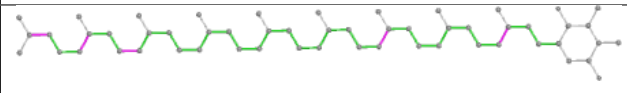
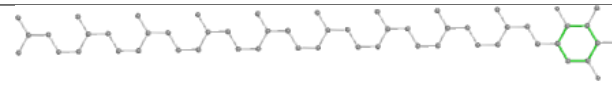


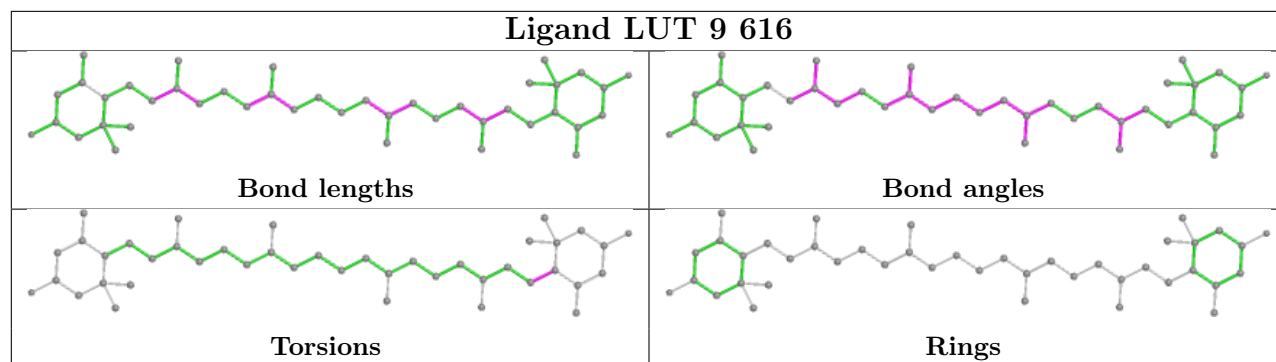
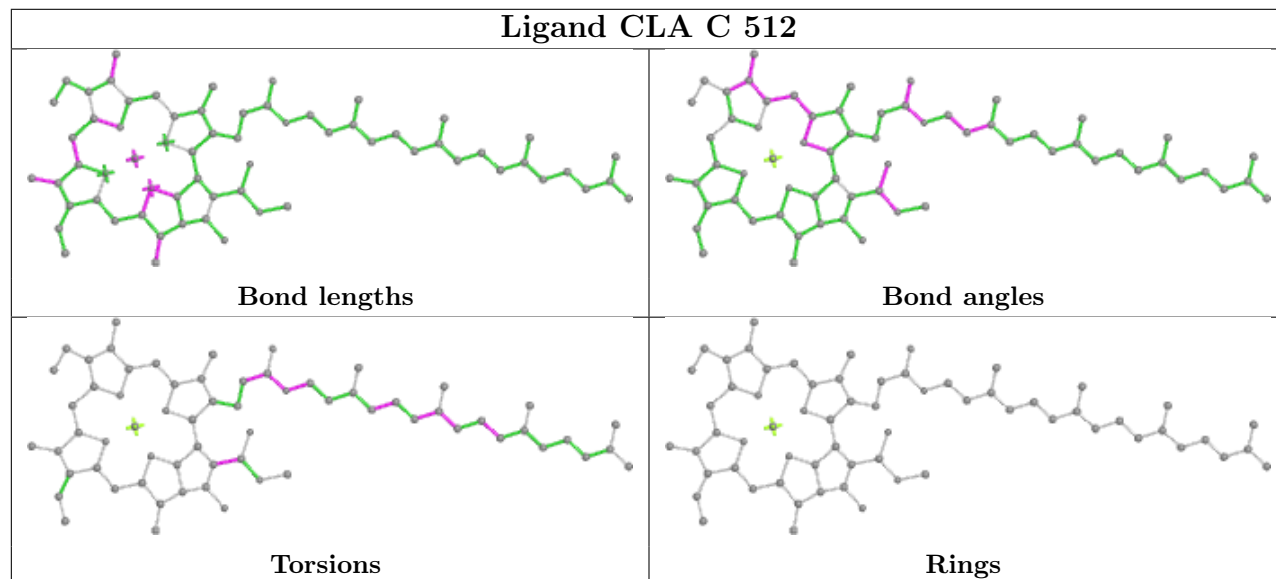
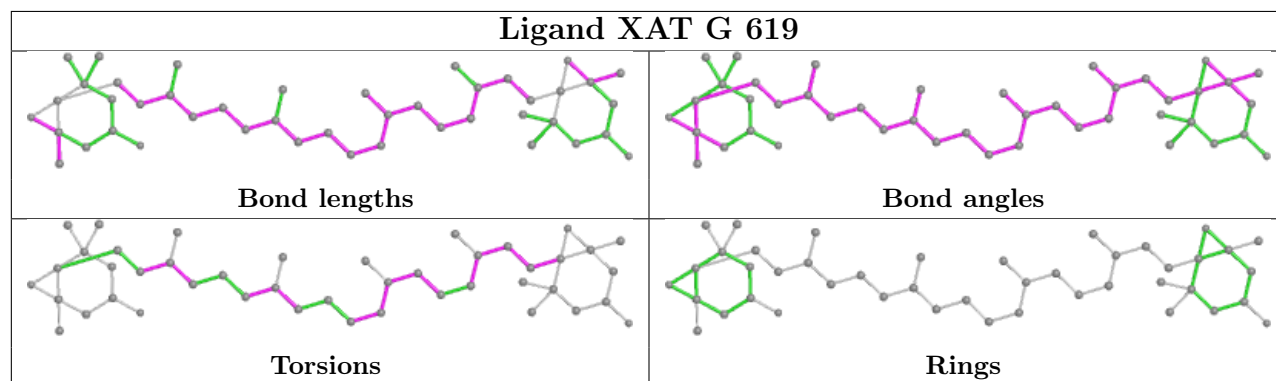


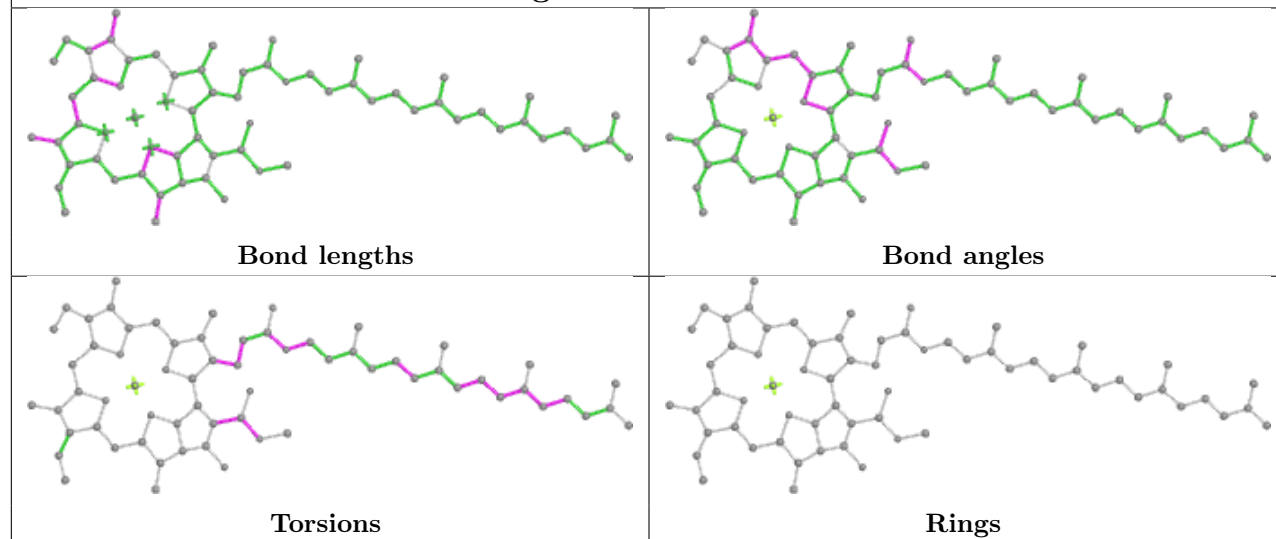
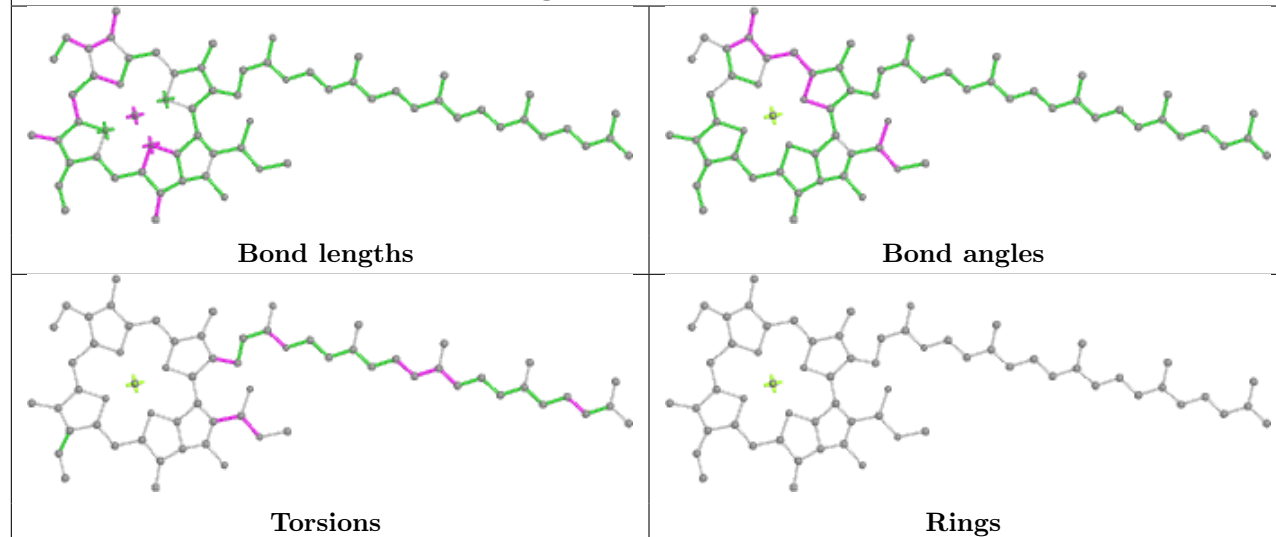
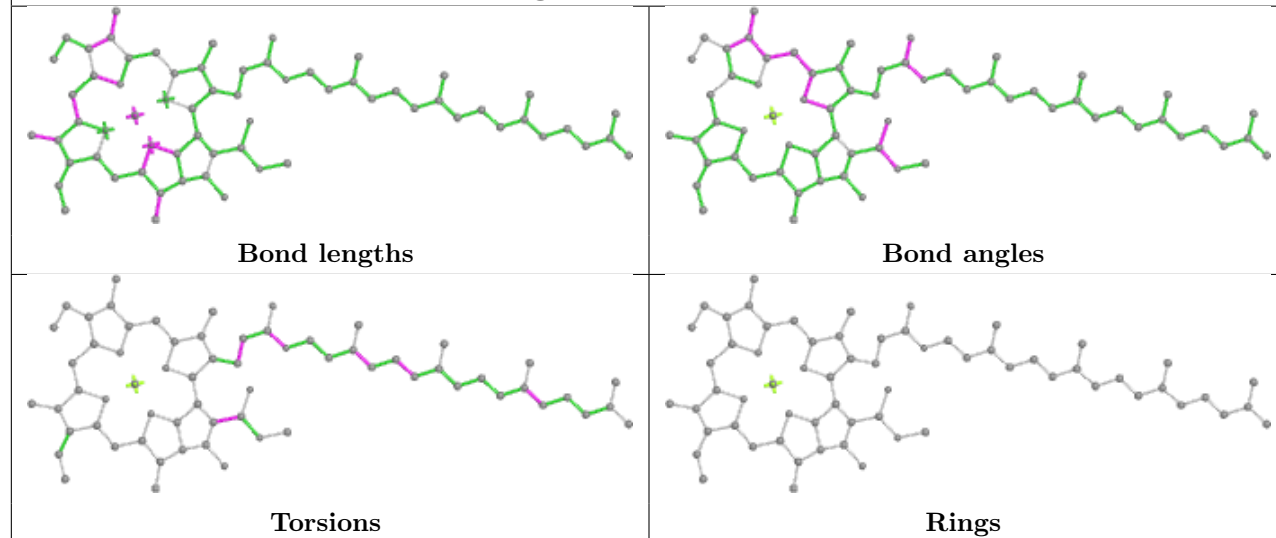


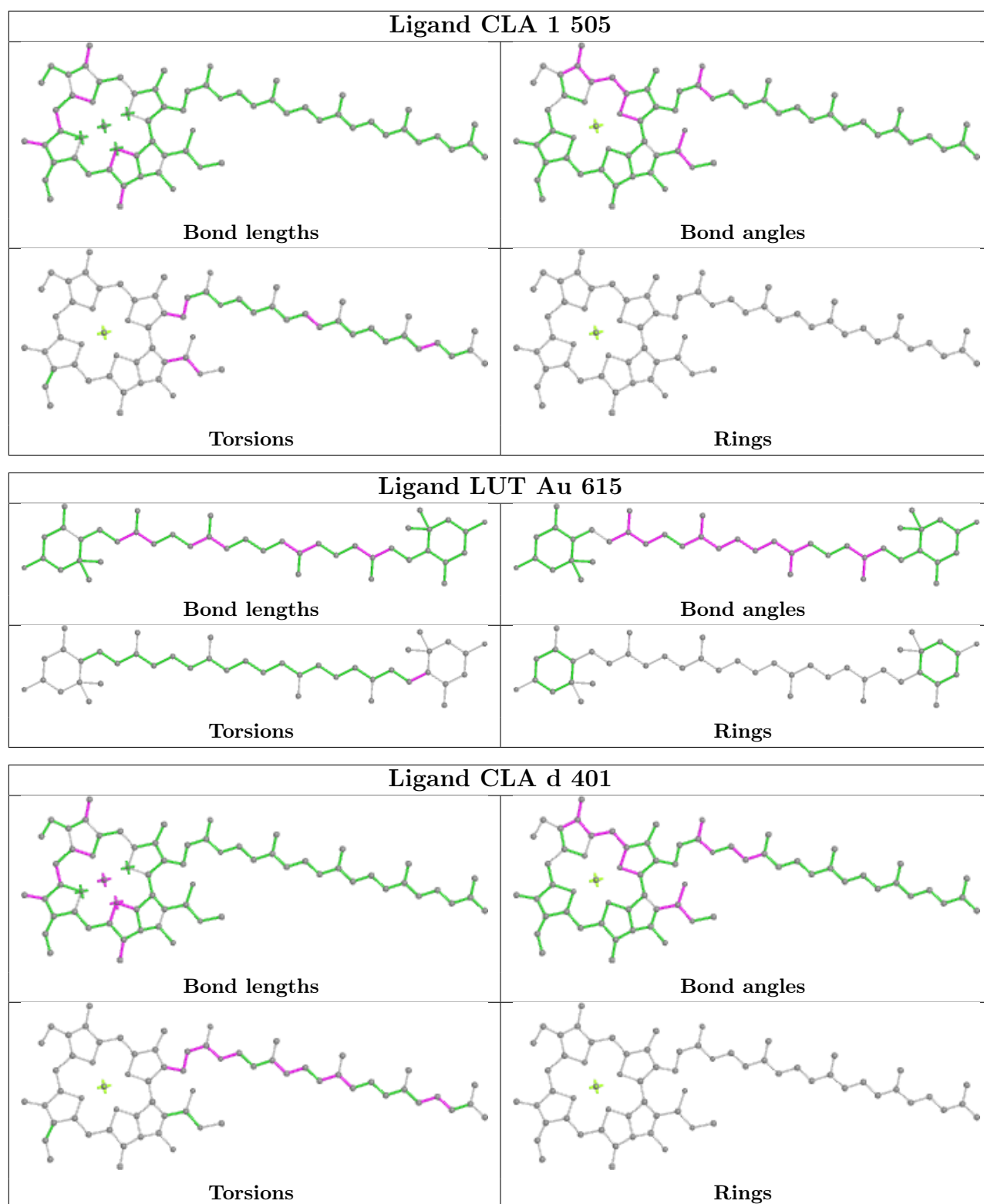
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|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

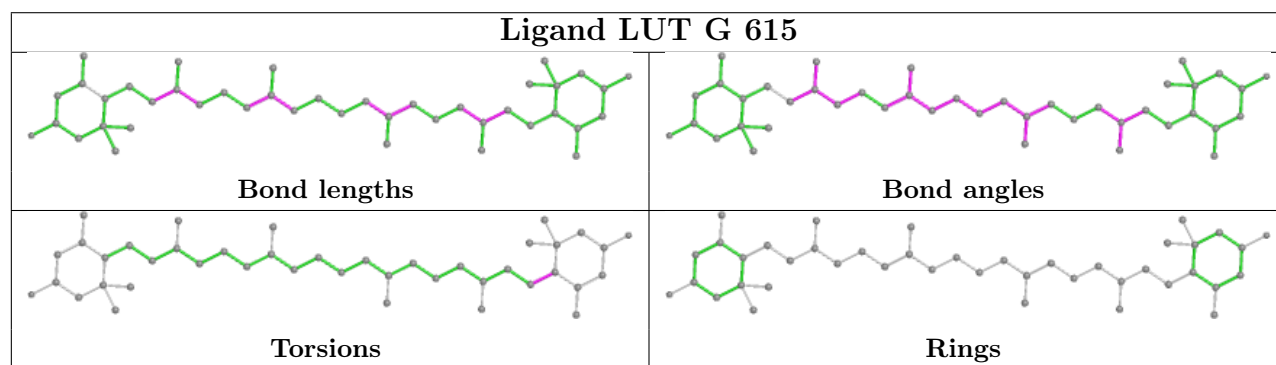
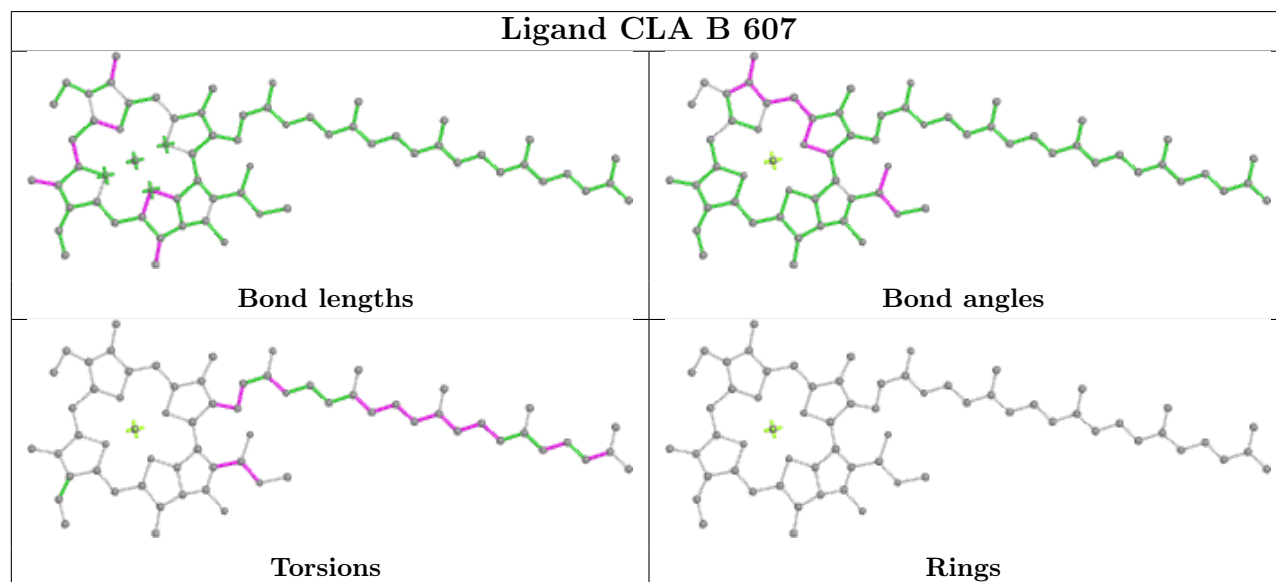
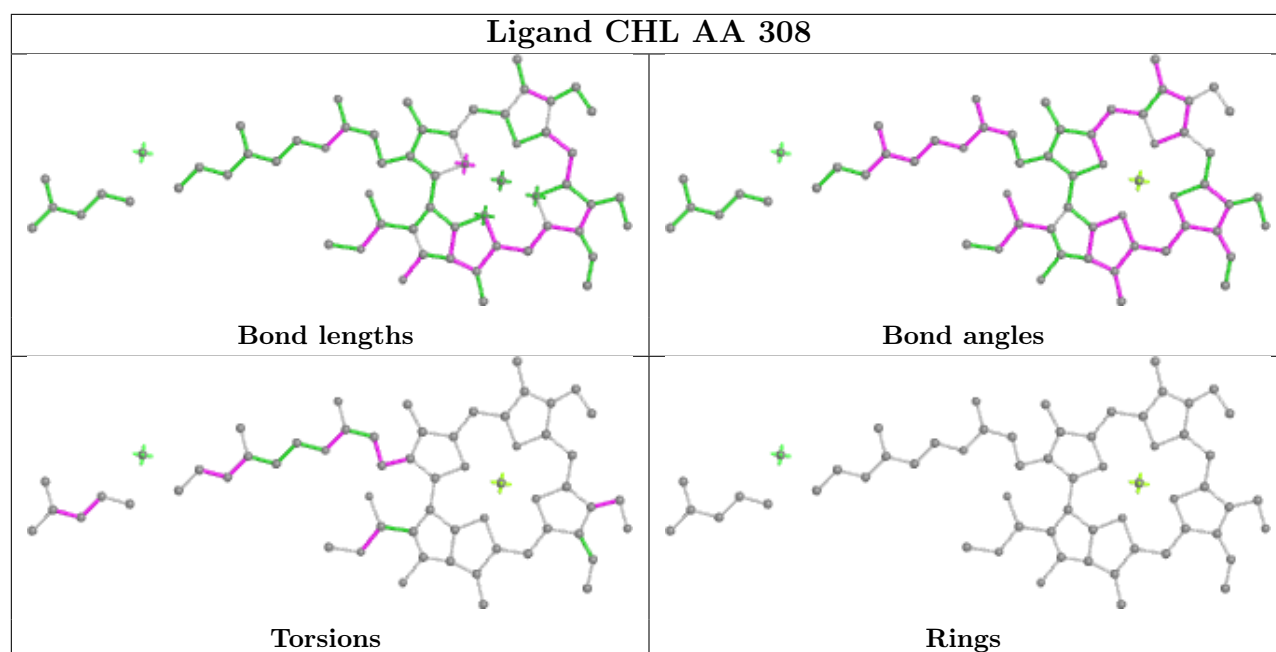
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| Bond lengths | Bond angles |
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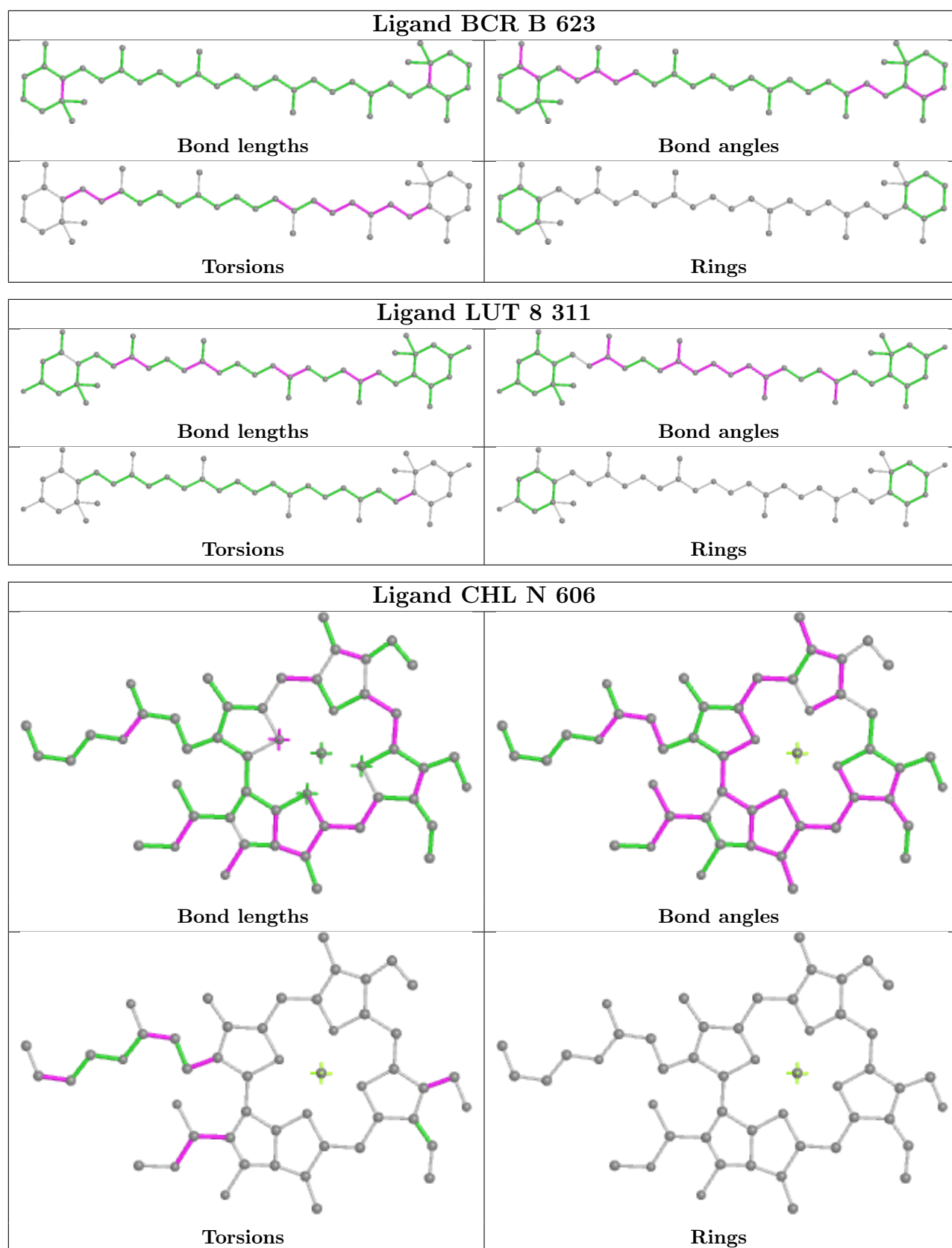
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| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

Ligand LUT 9 616**Ligand CLA C 512****Ligand XAT G 619**

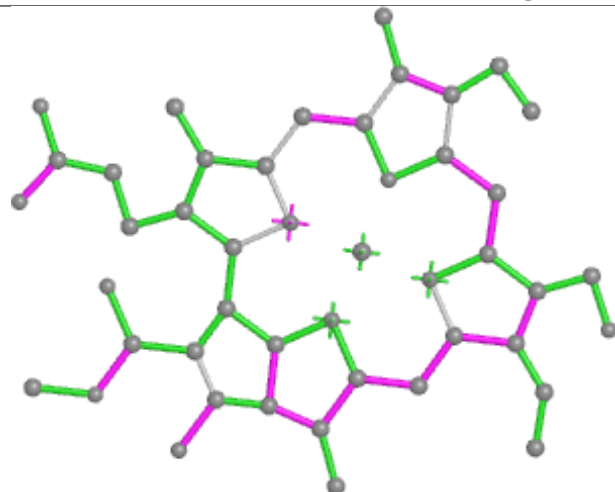
Ligand CLA B 606**Ligand CLA r 609****Ligand CLA Y 304**



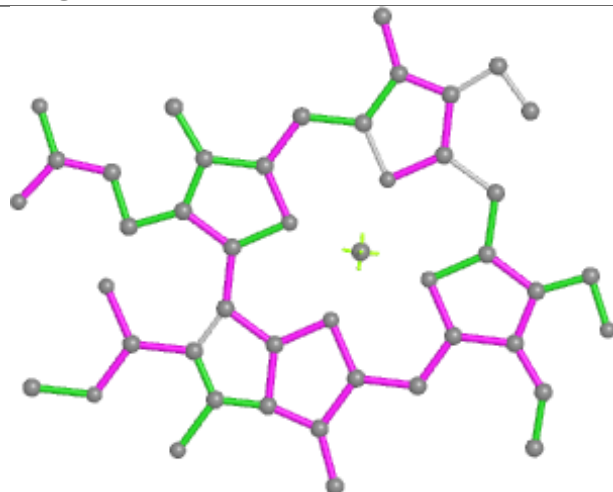




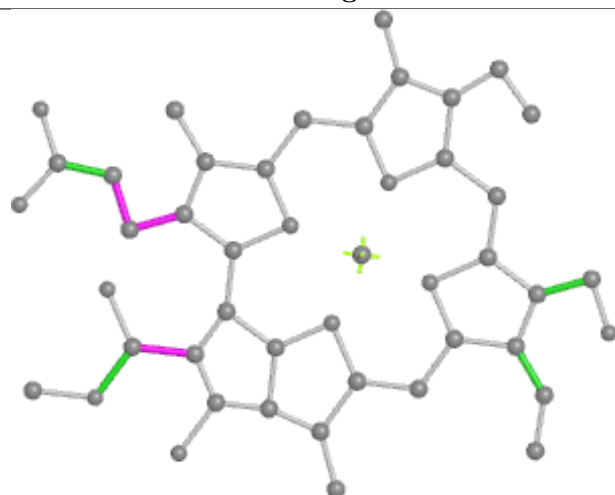
Ligand CHL g 605



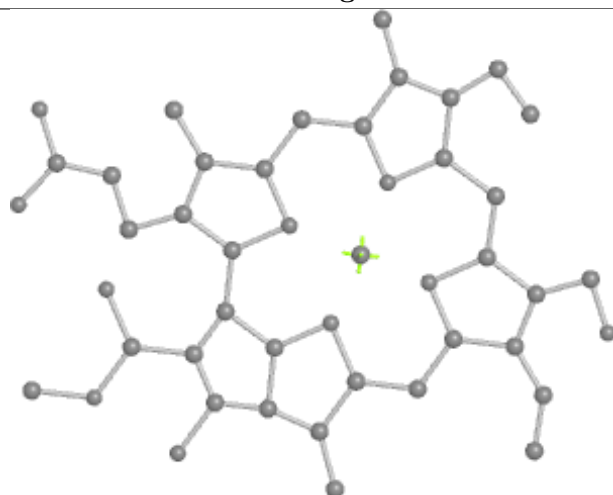
Bond lengths



Bond angles

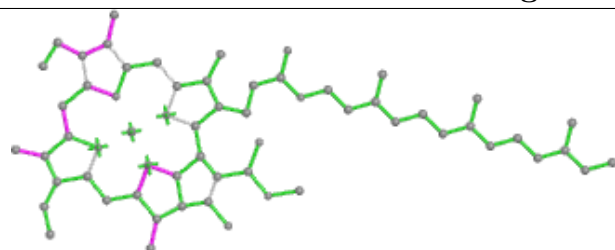


Torsions

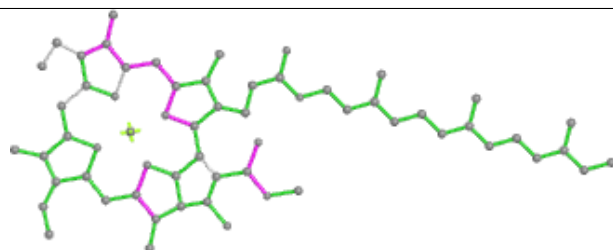


Rings

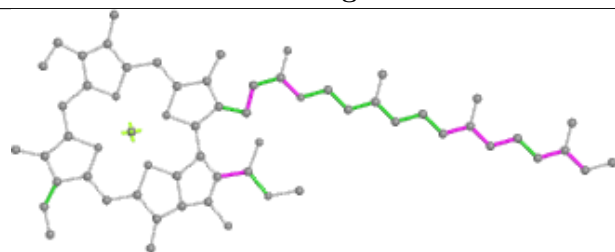
Ligand CLA 9 602



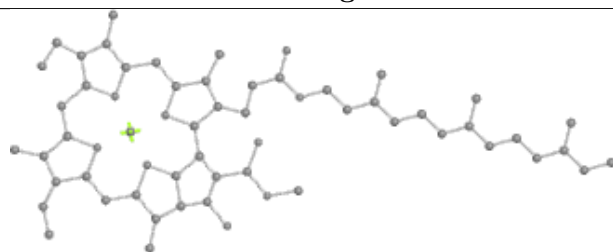
Bond lengths



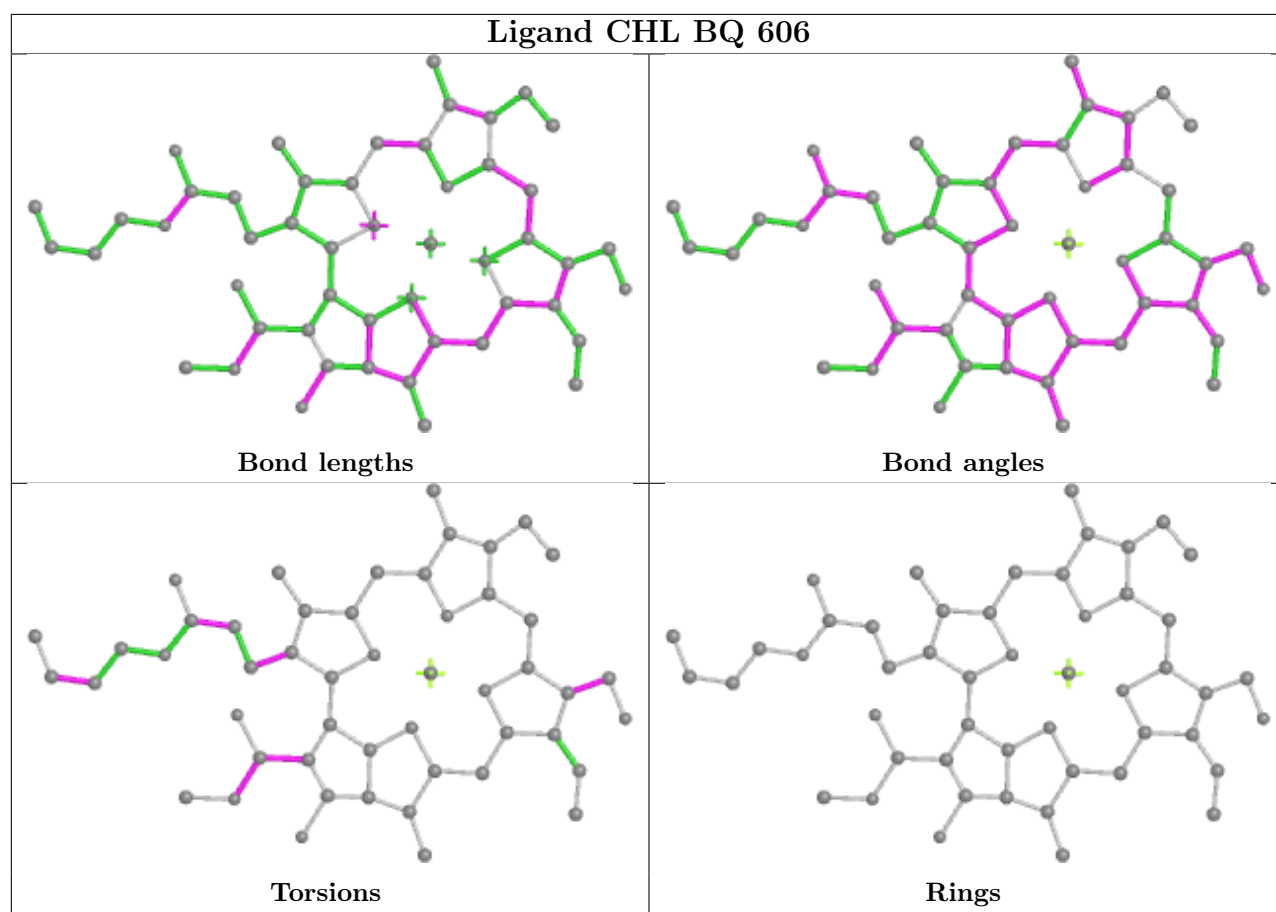
Bond angles



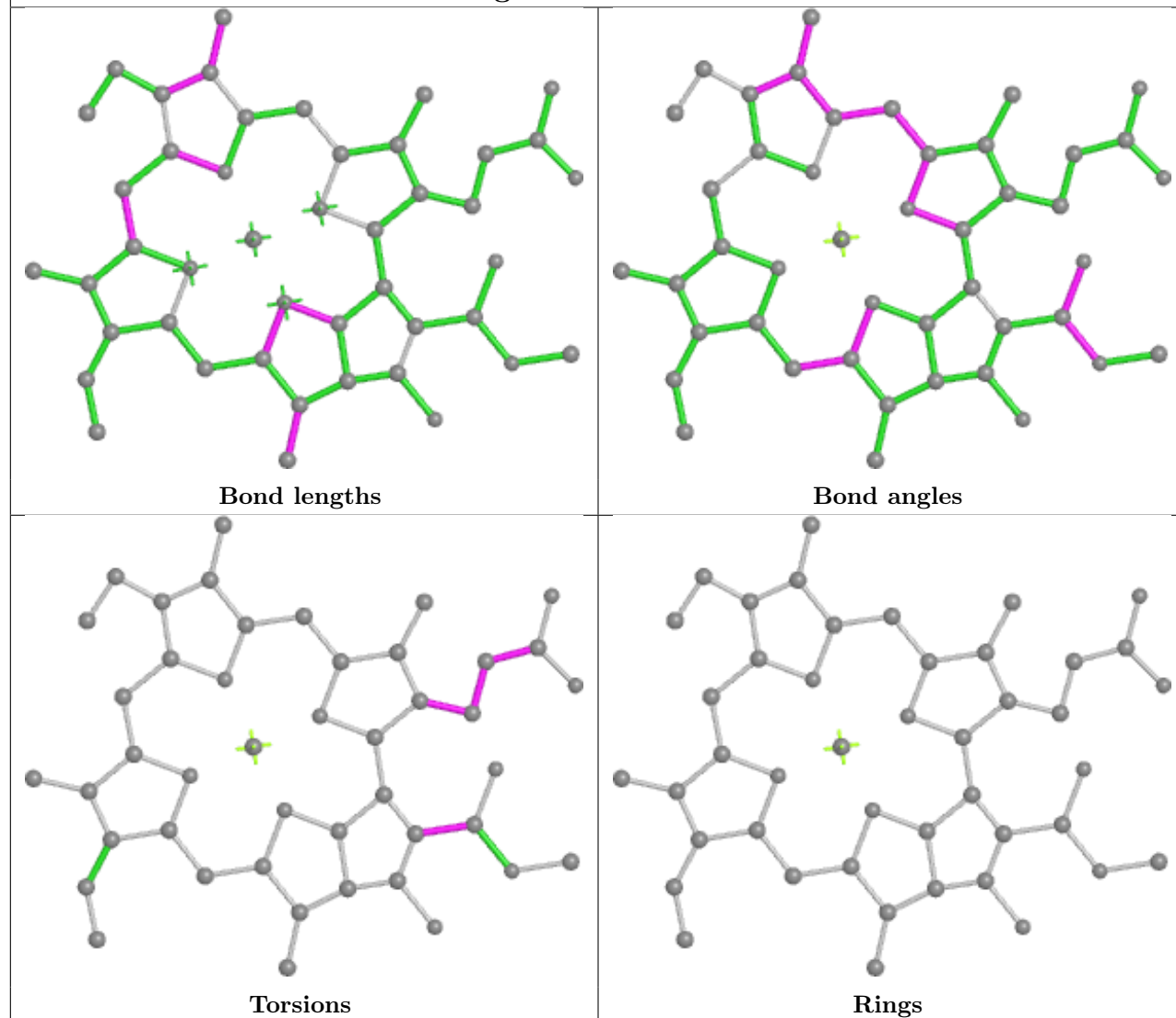
Torsions



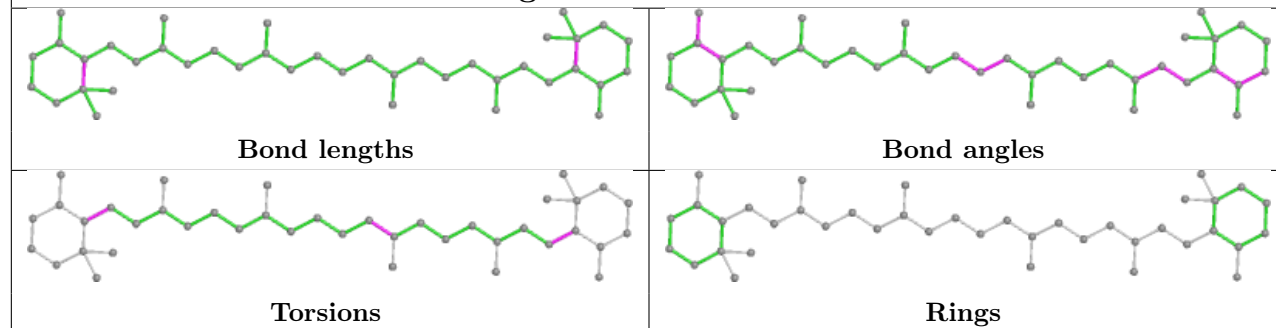
Rings

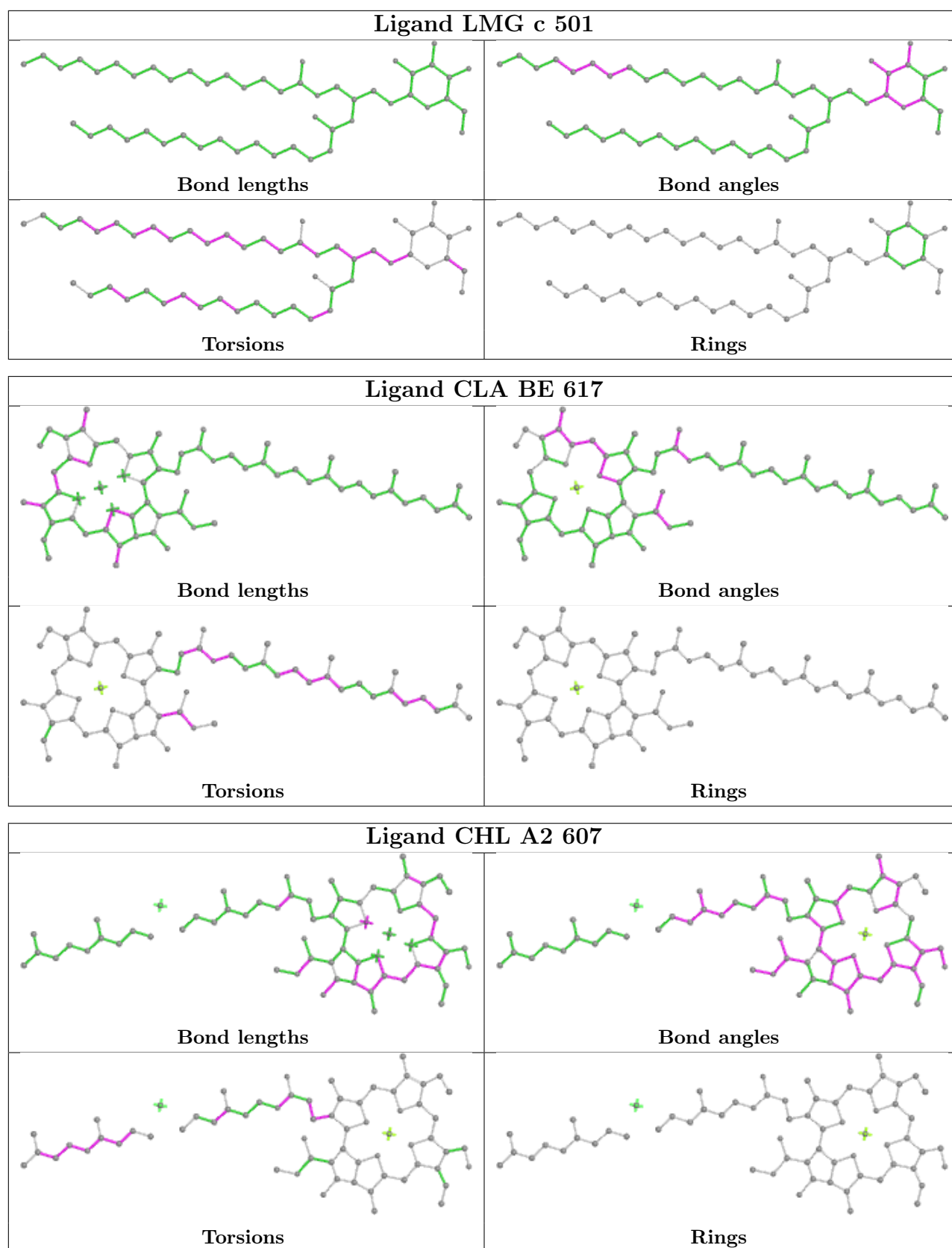


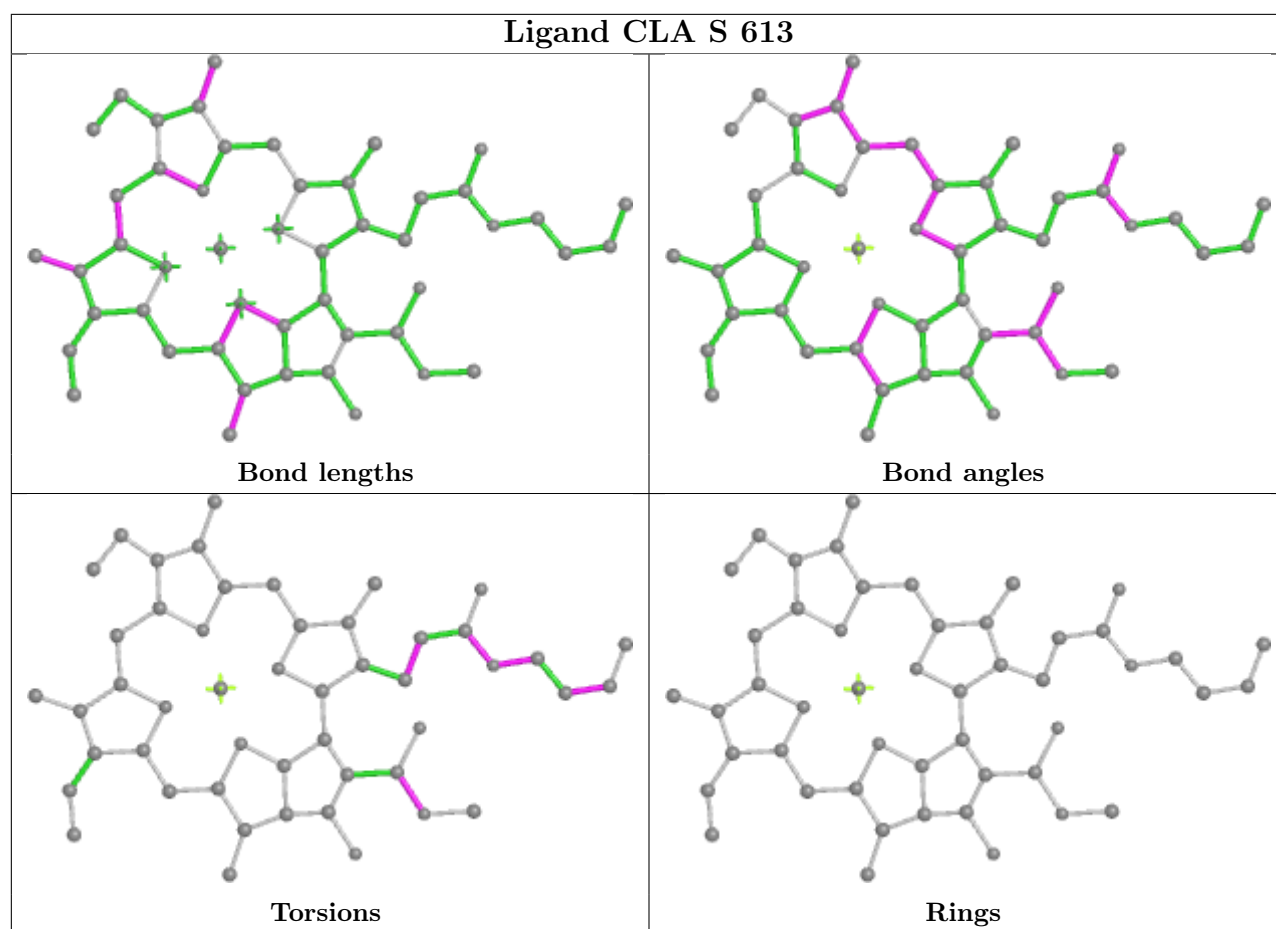
Ligand CLA 7 312



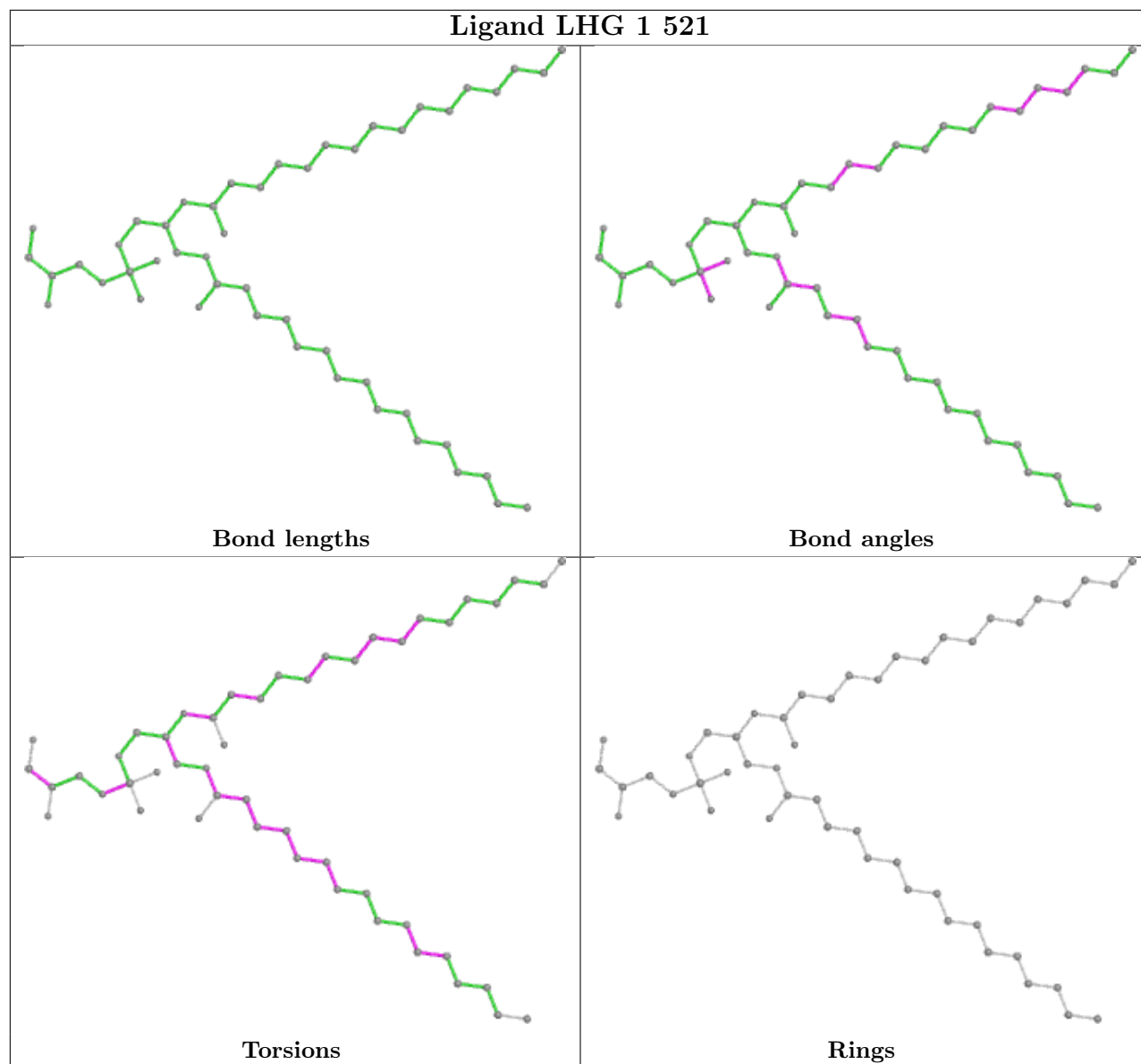
Ligand BCR BE 620



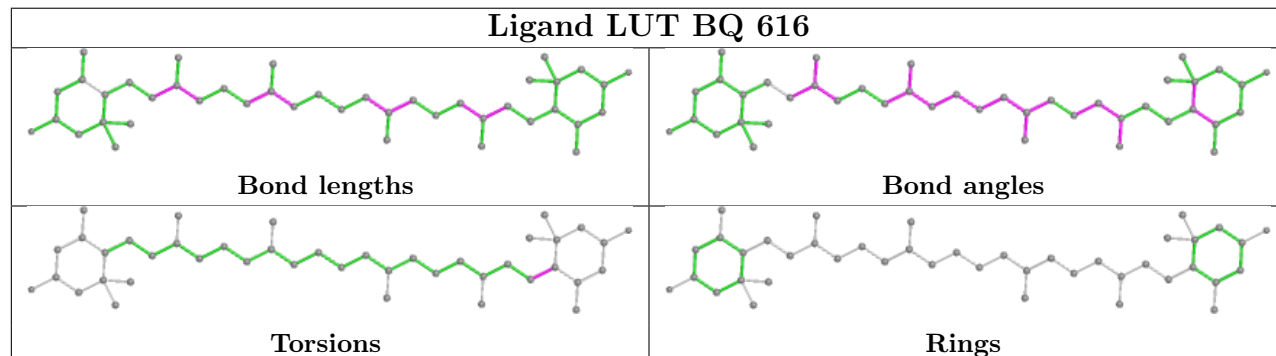


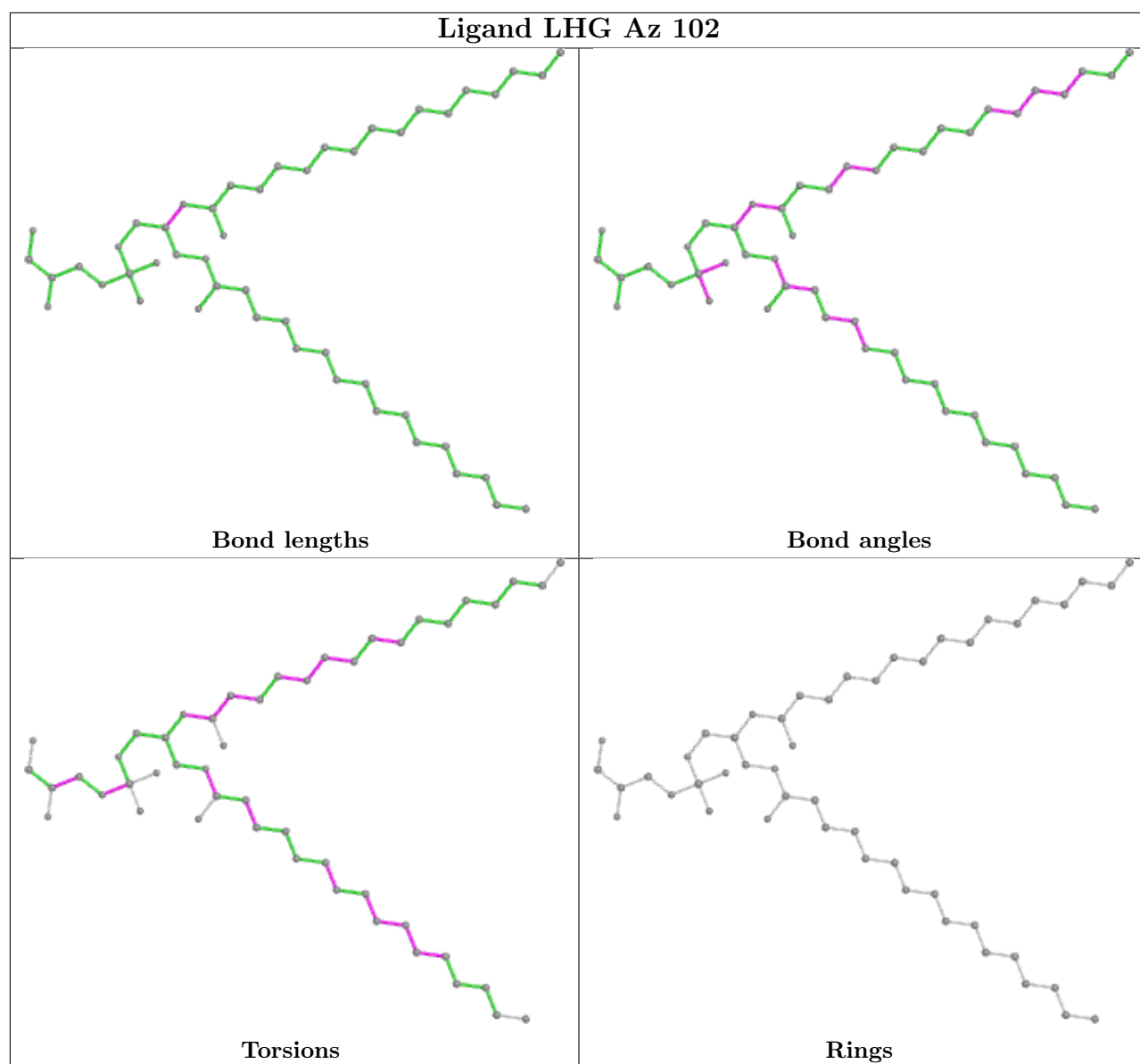


Ligand LHG 1 521

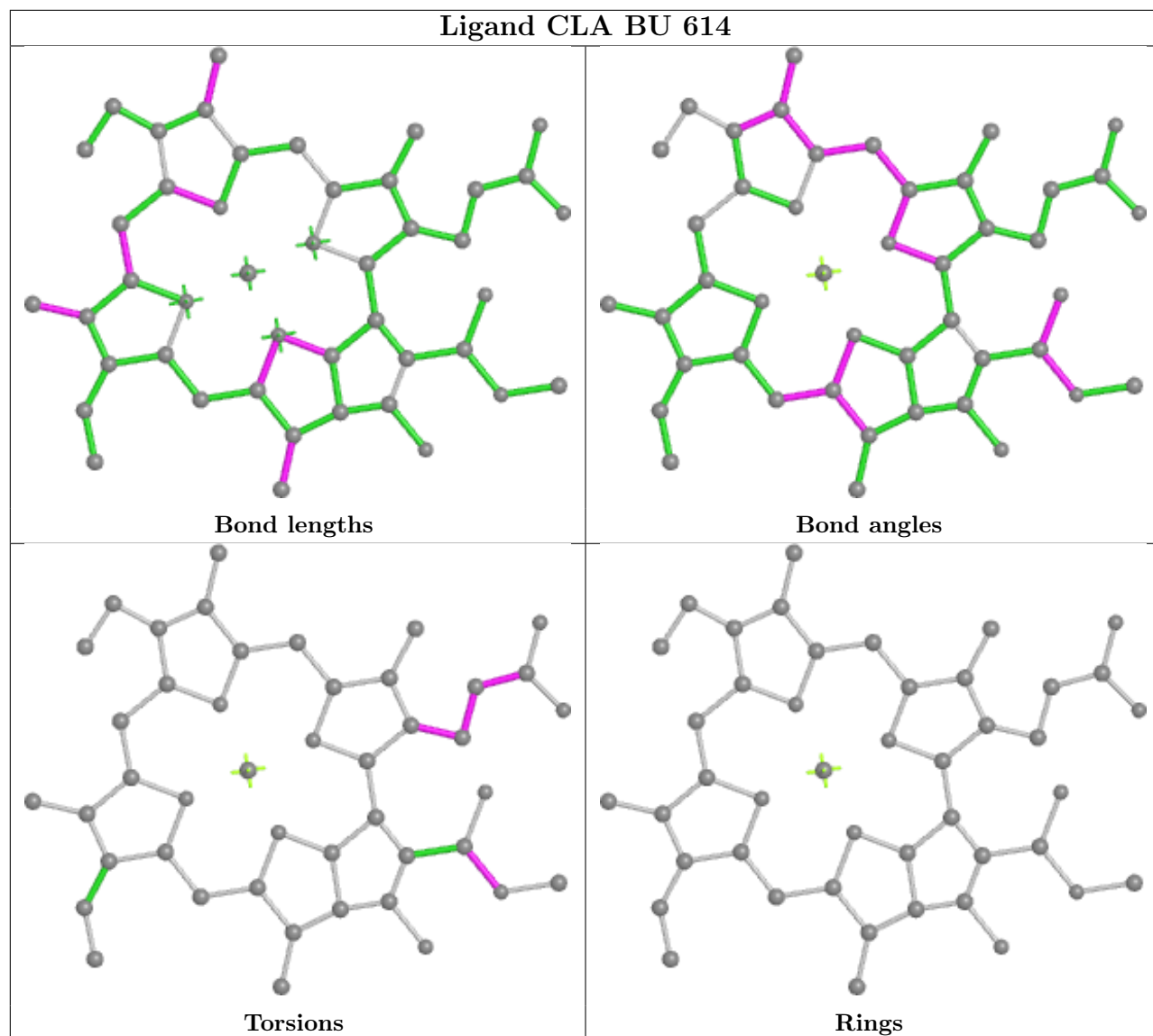


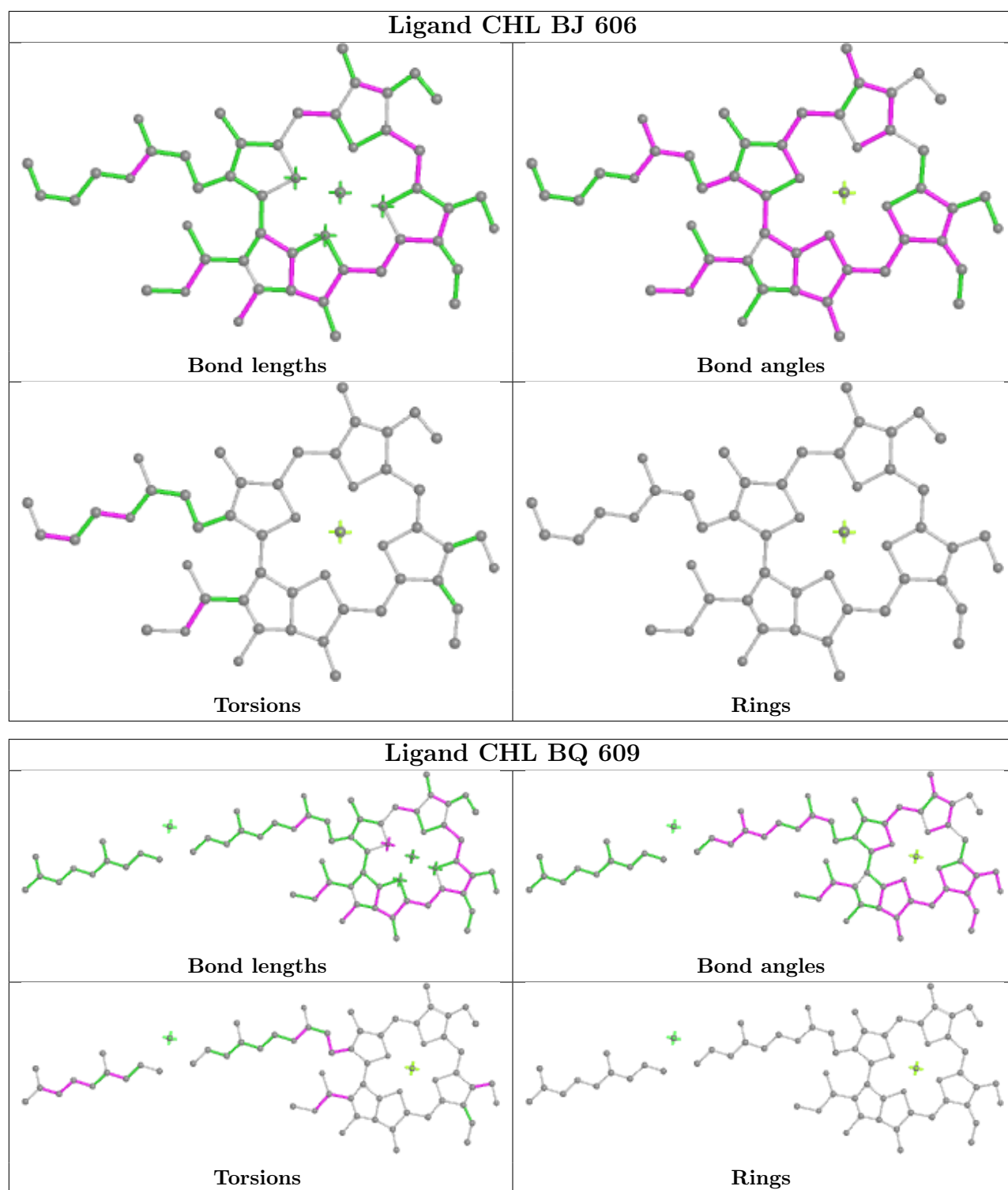
Ligand LUT BQ 616

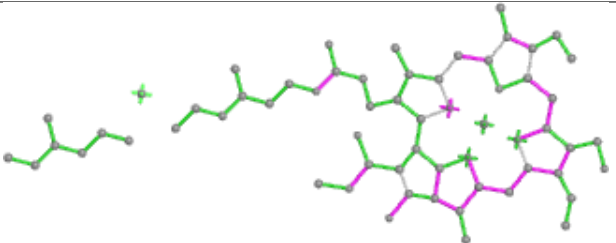
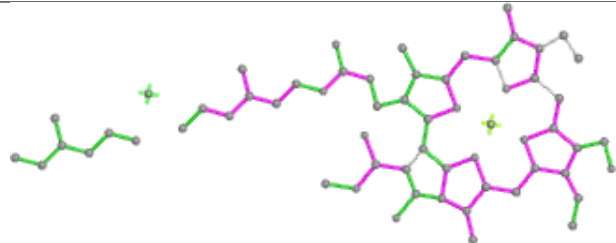
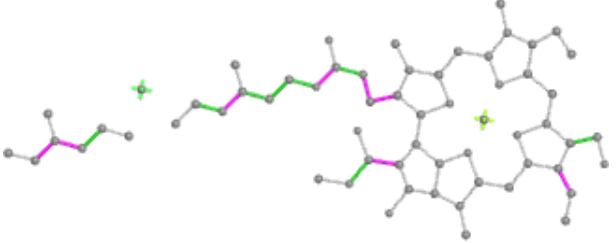
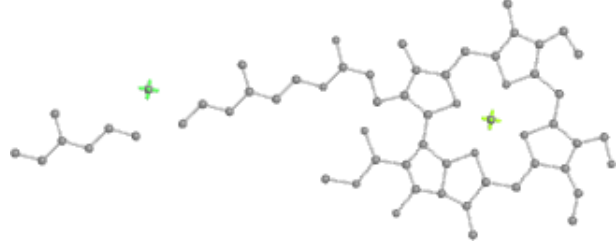


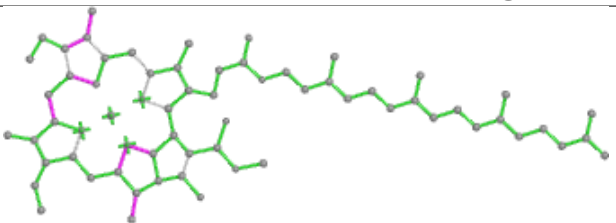
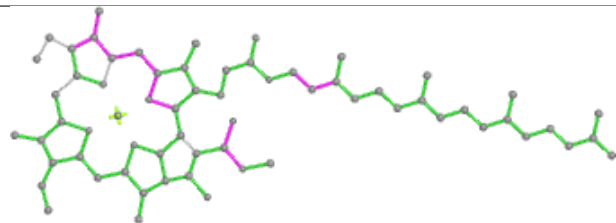
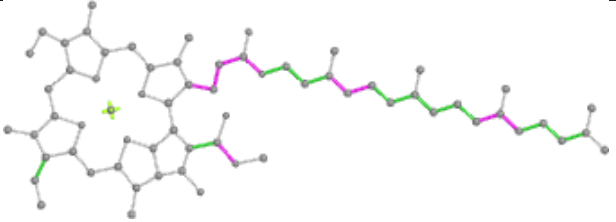
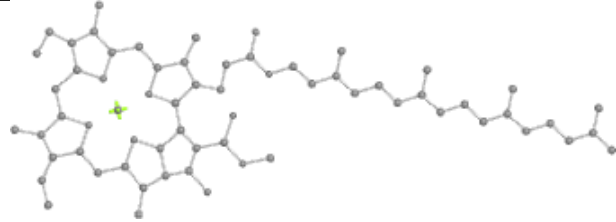


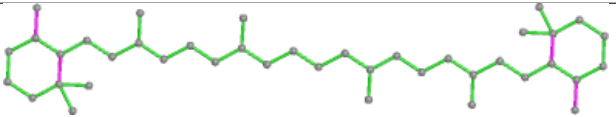
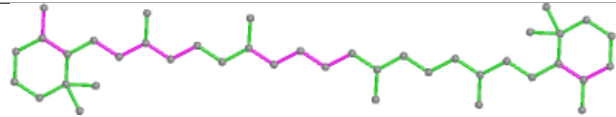
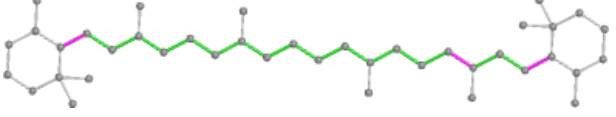
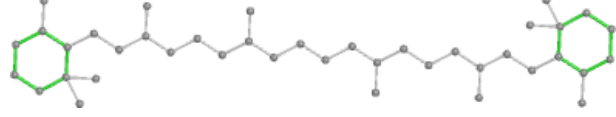
Ligand CLA BU 614



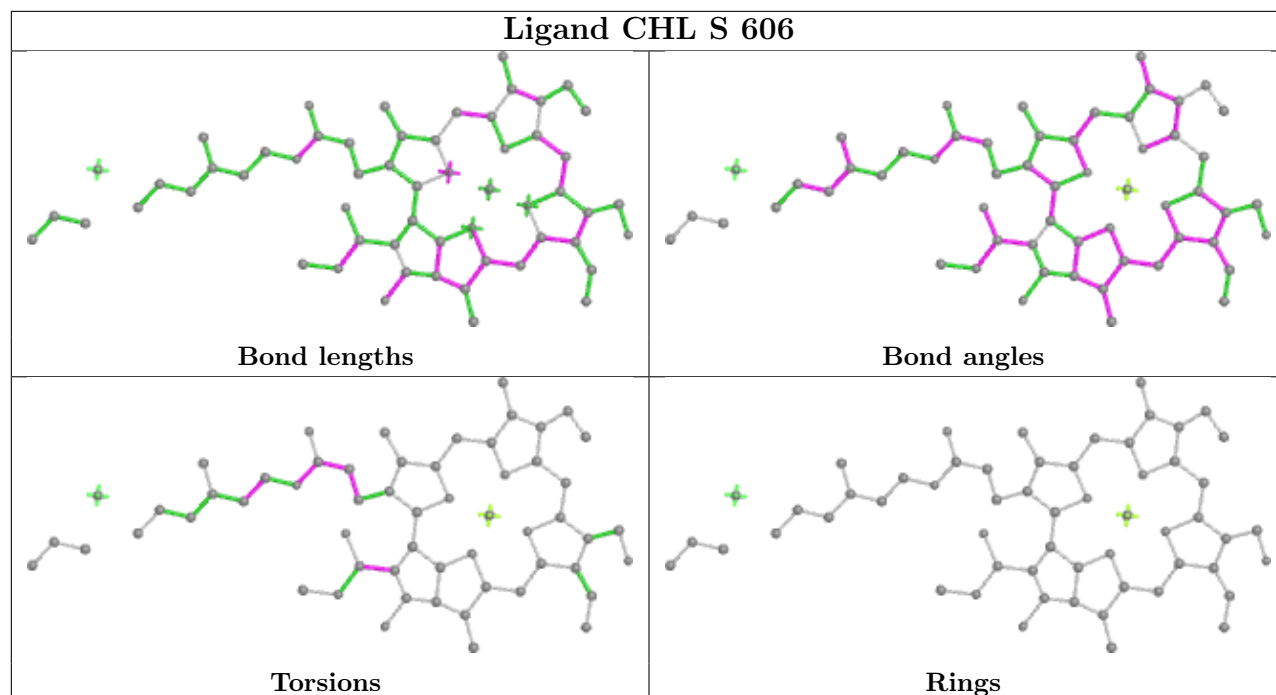


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|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

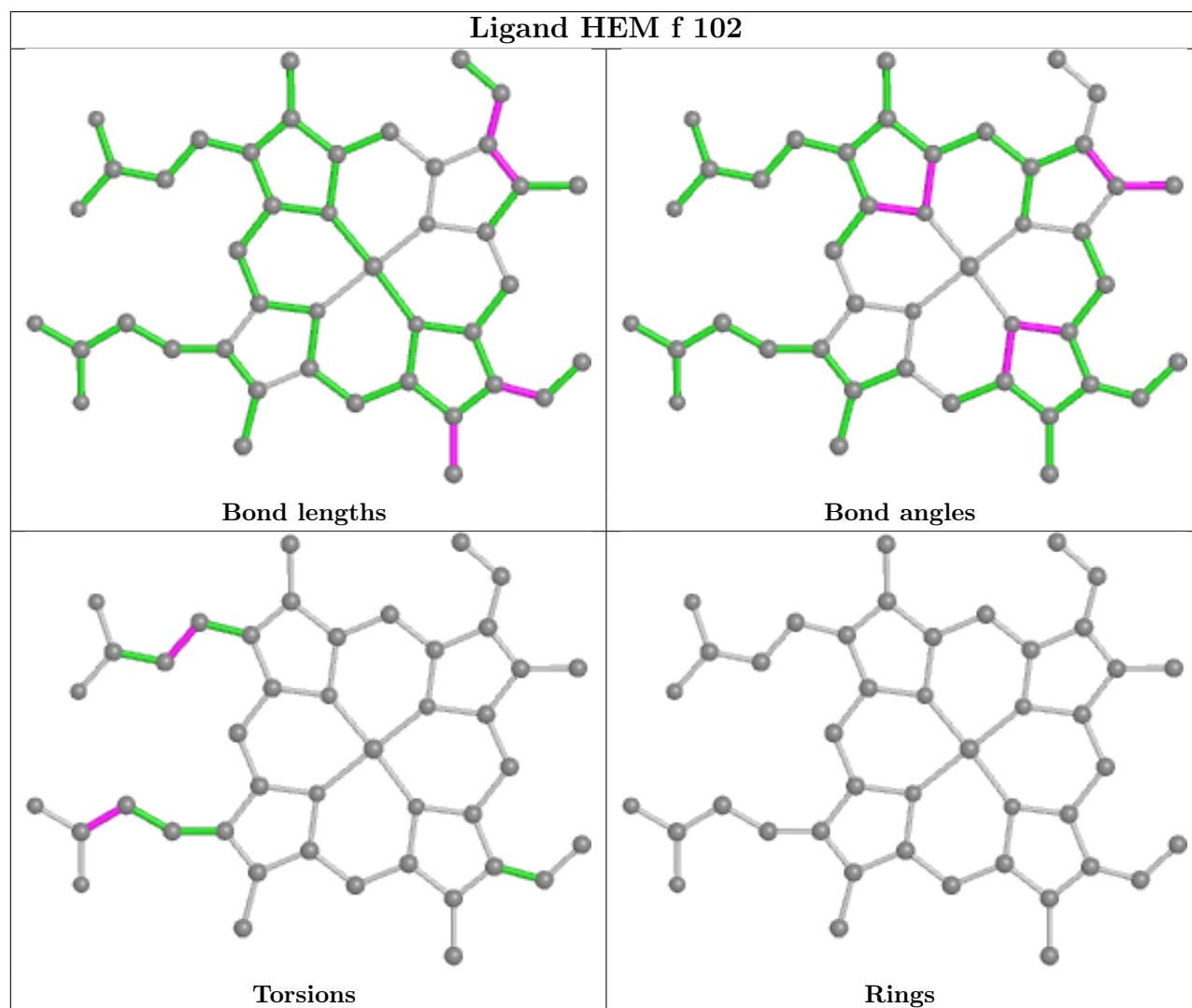
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| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand BCR 1 515 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

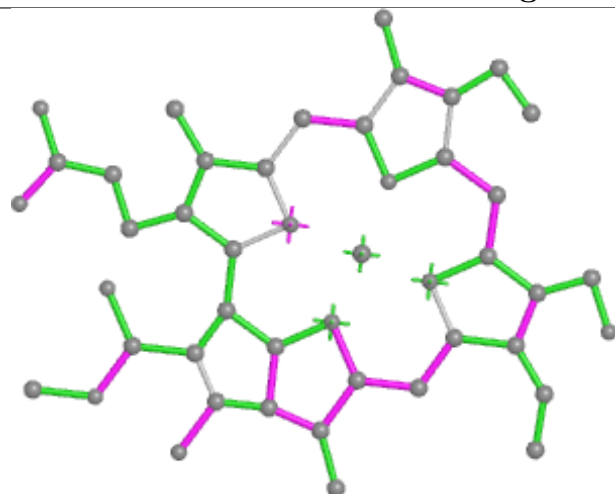
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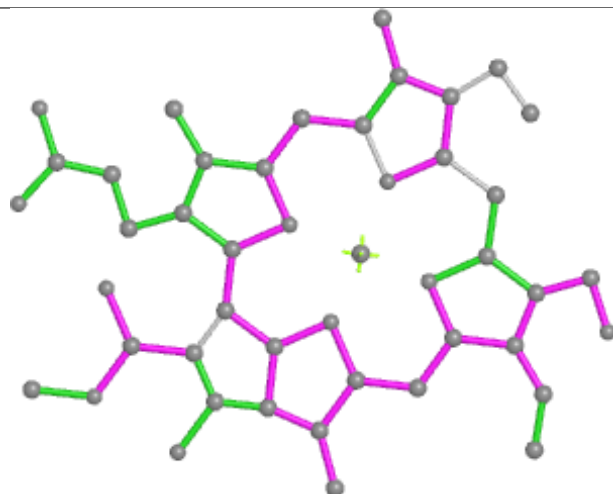
Ligand HEM f 102



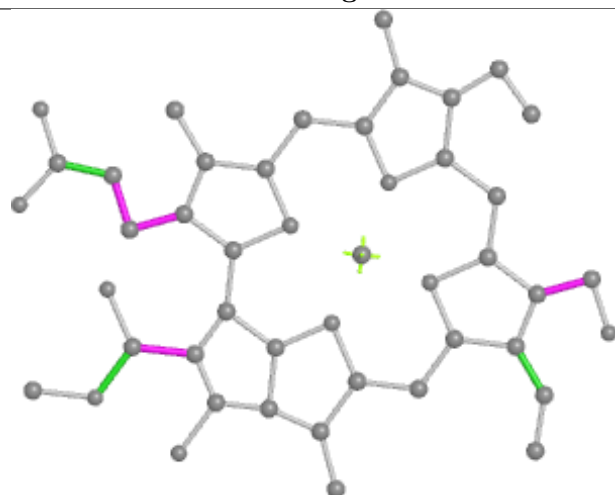
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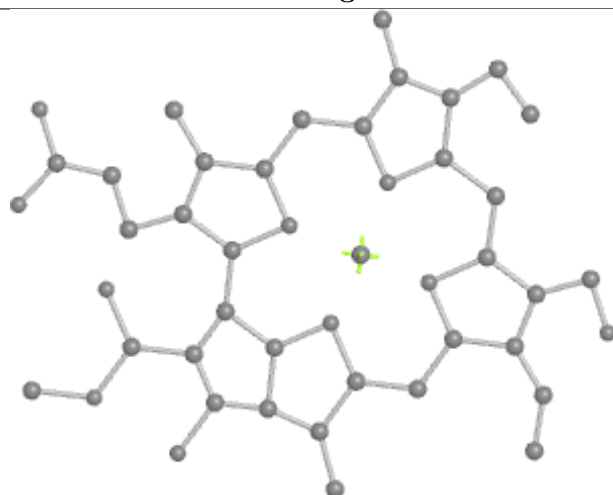
Bond lengths



Bond angles

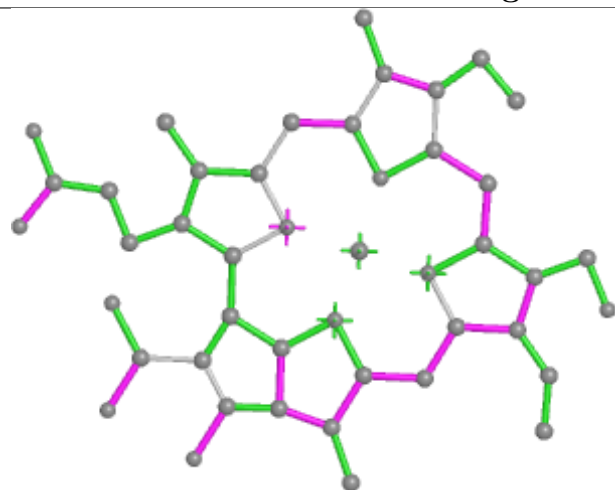


Torsions

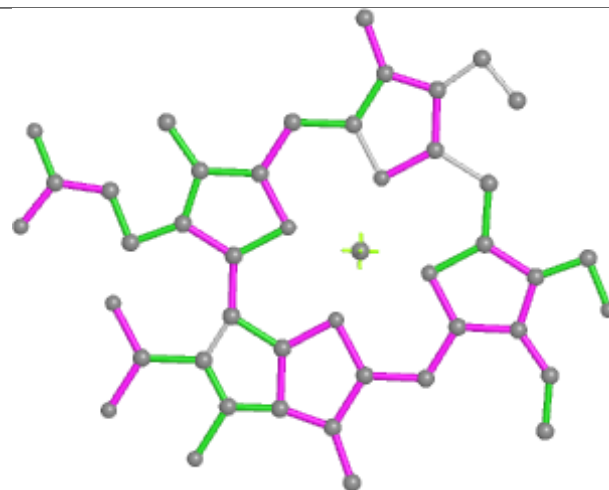


Rings

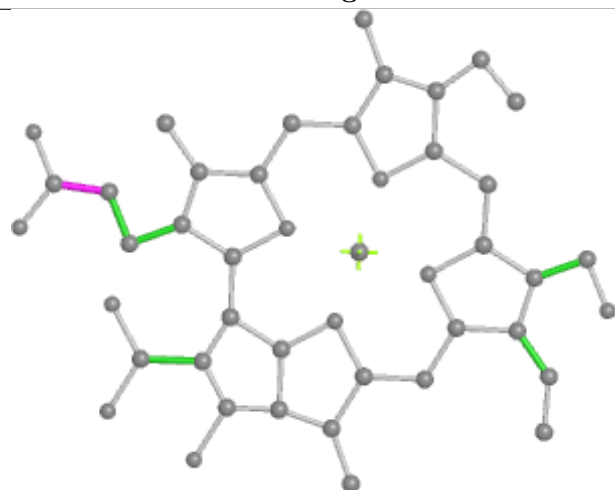
Ligand CHL BH 601



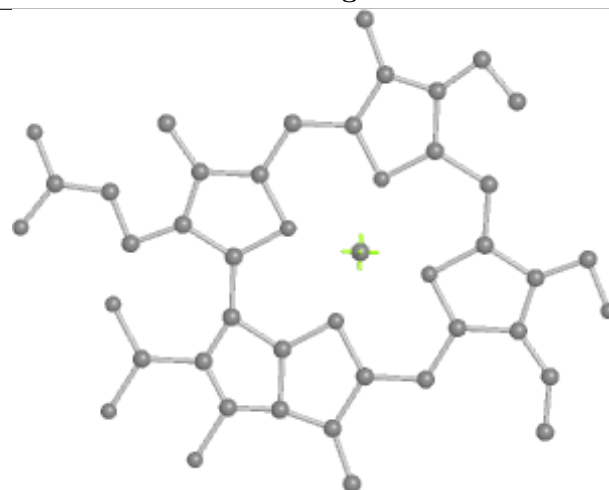
Bond lengths



Bond angles

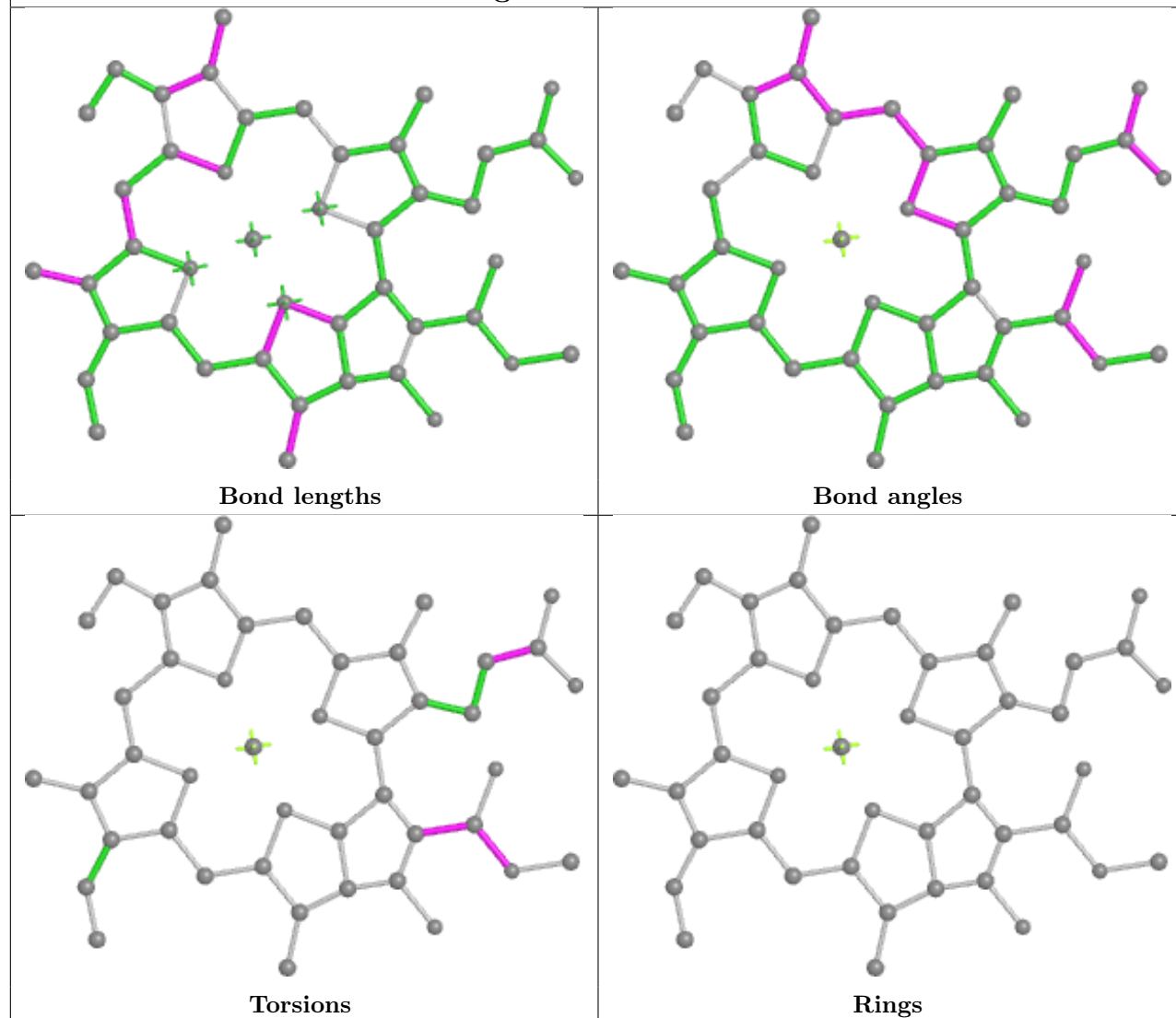


Torsions

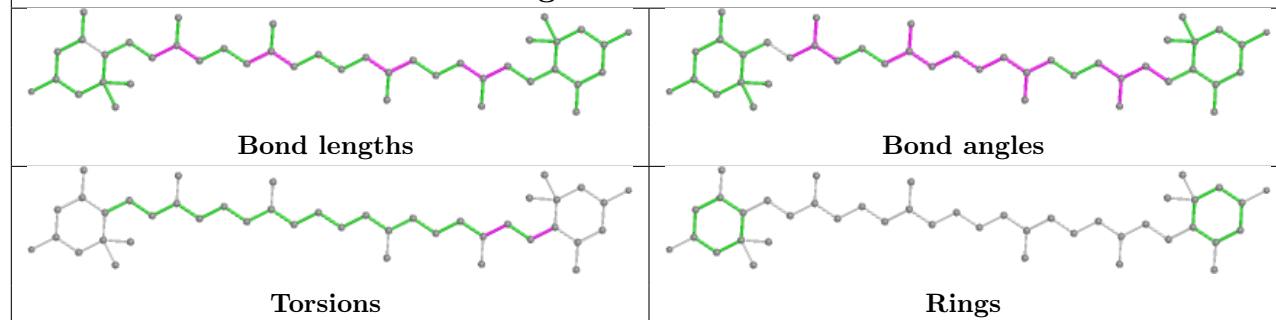


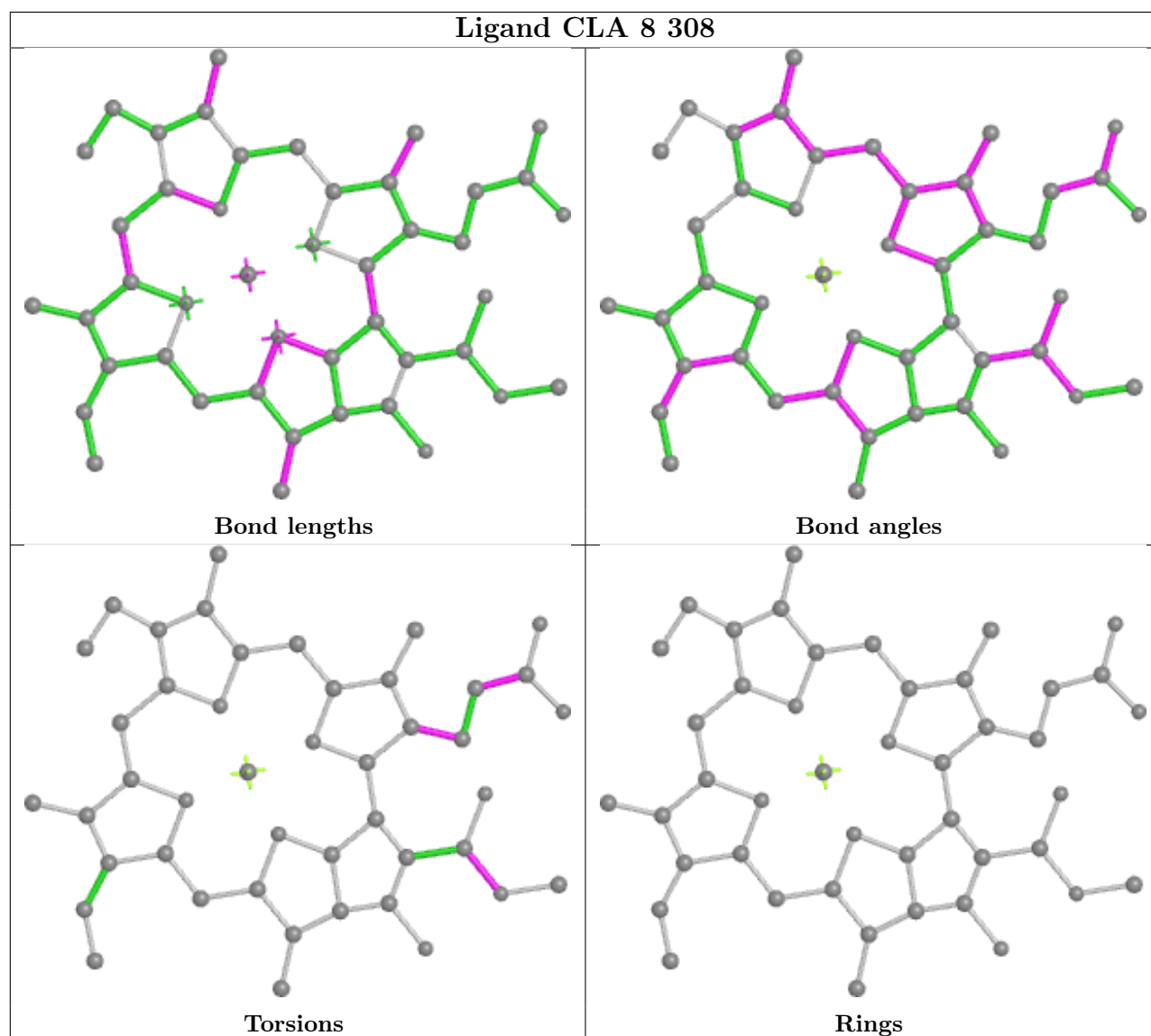
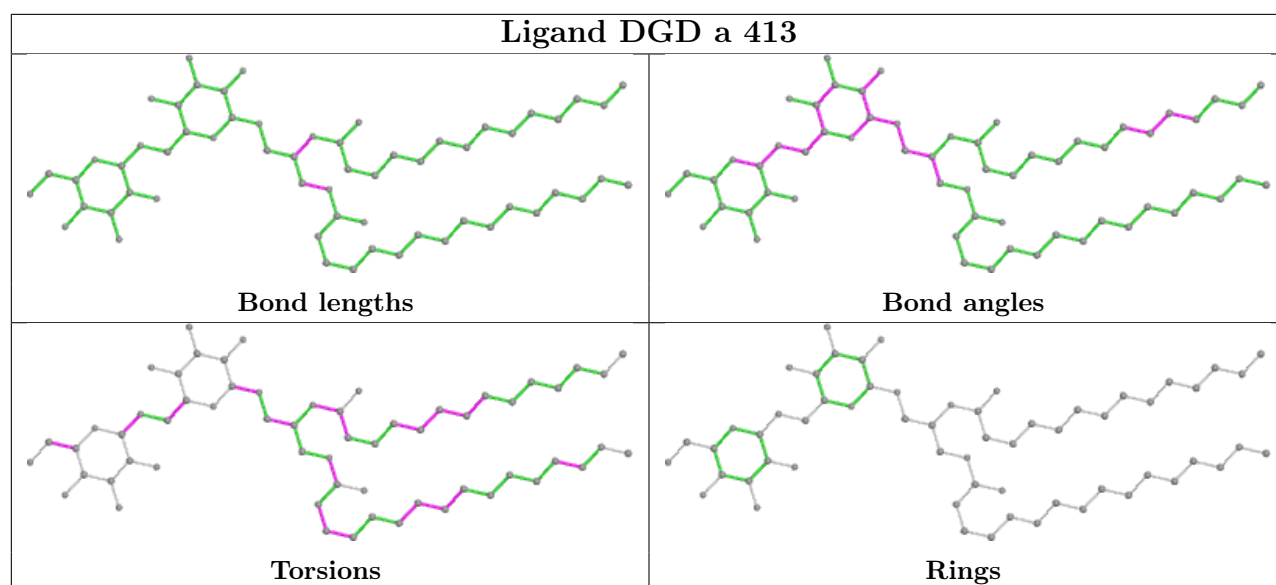
Rings

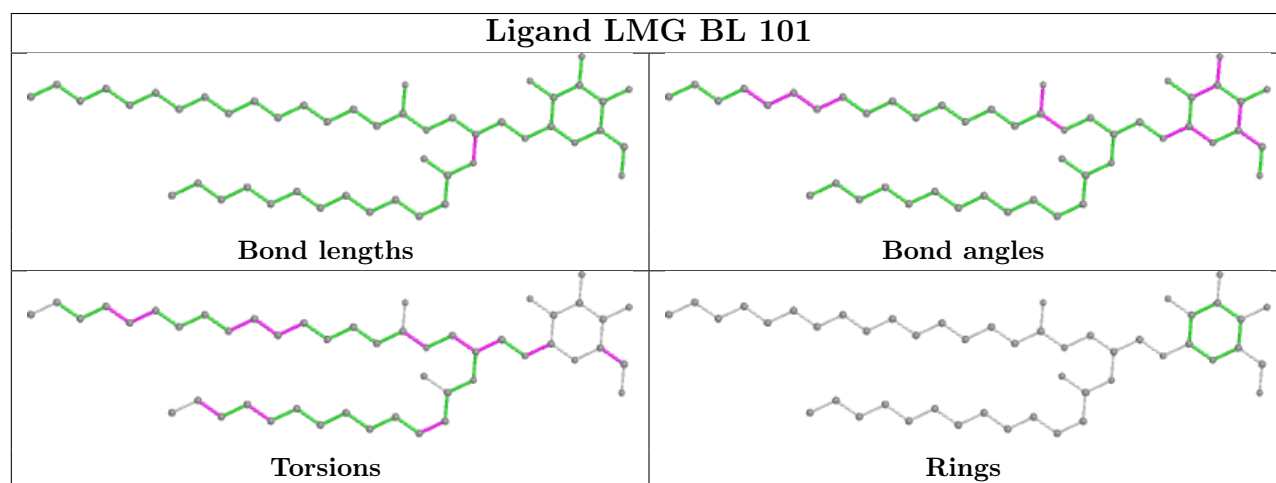
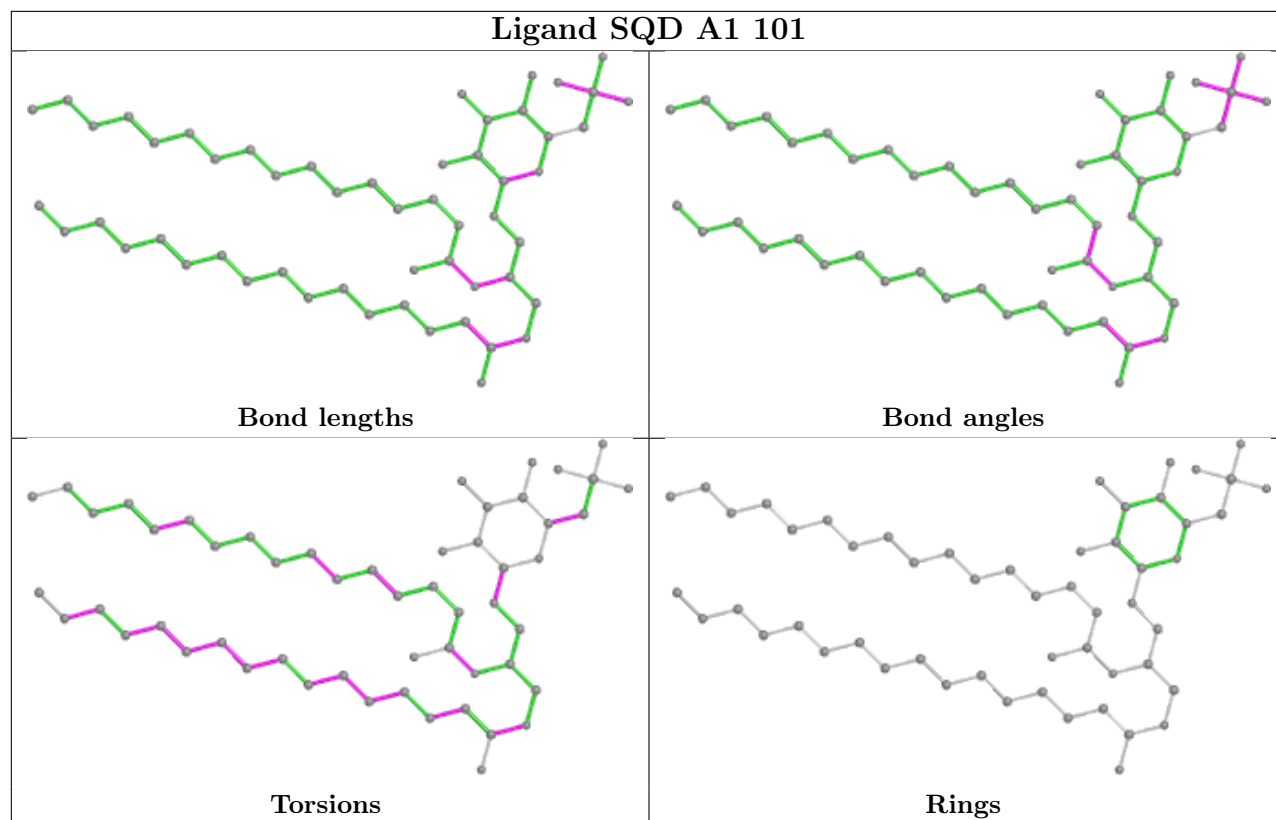
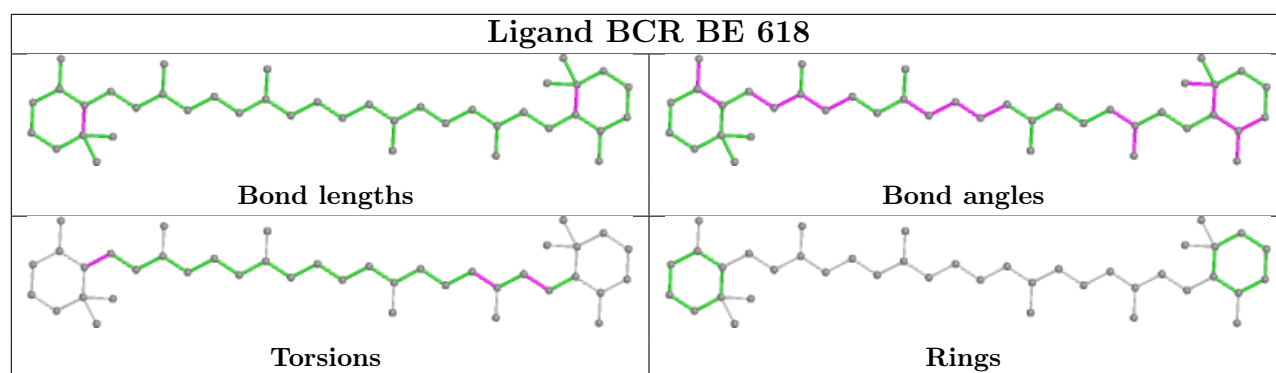
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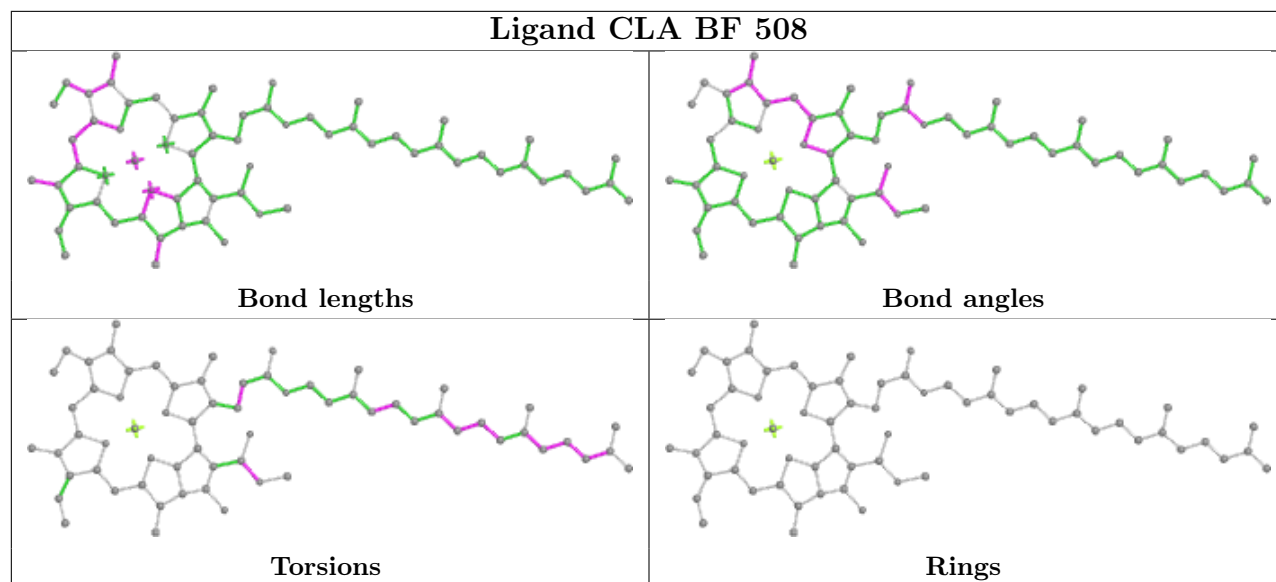
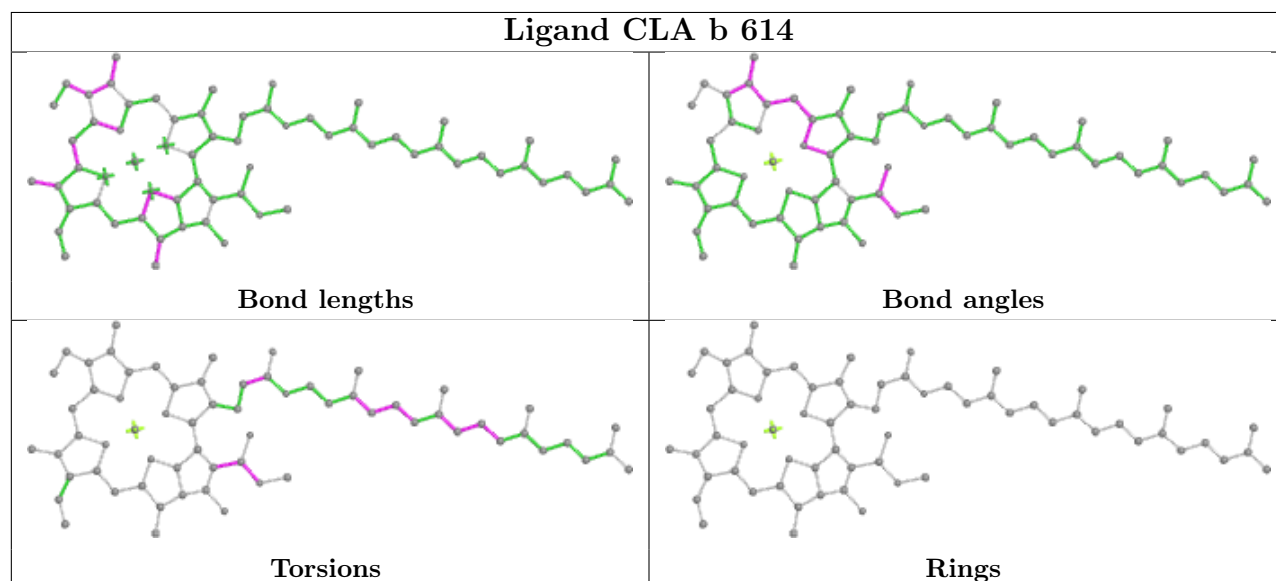
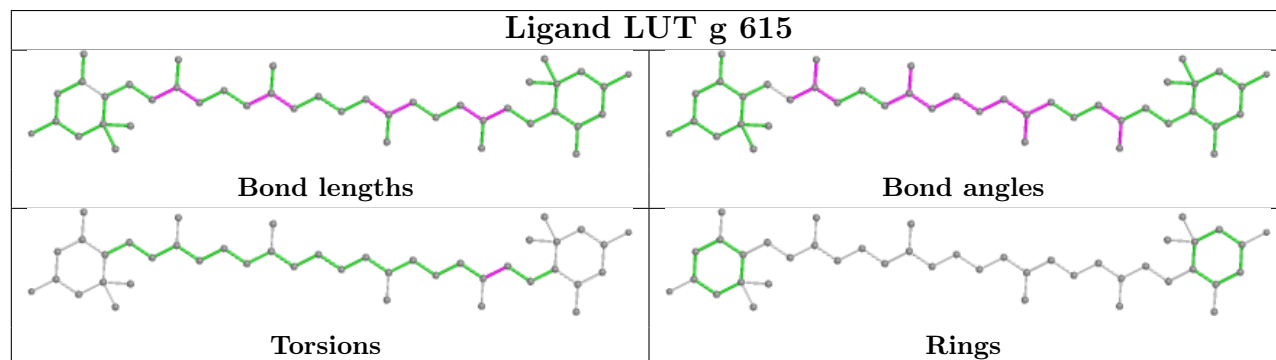


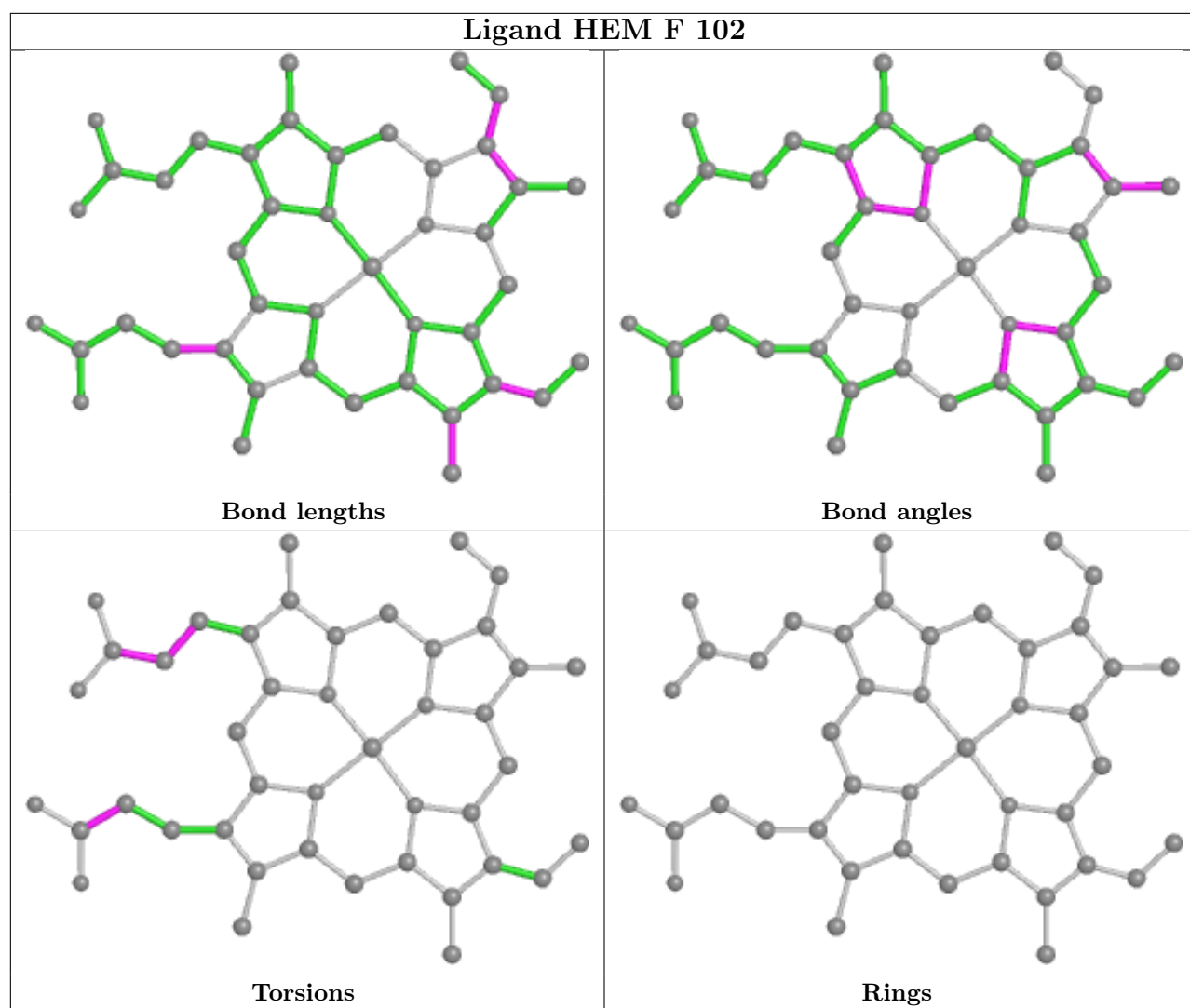
Ligand LUT r 615

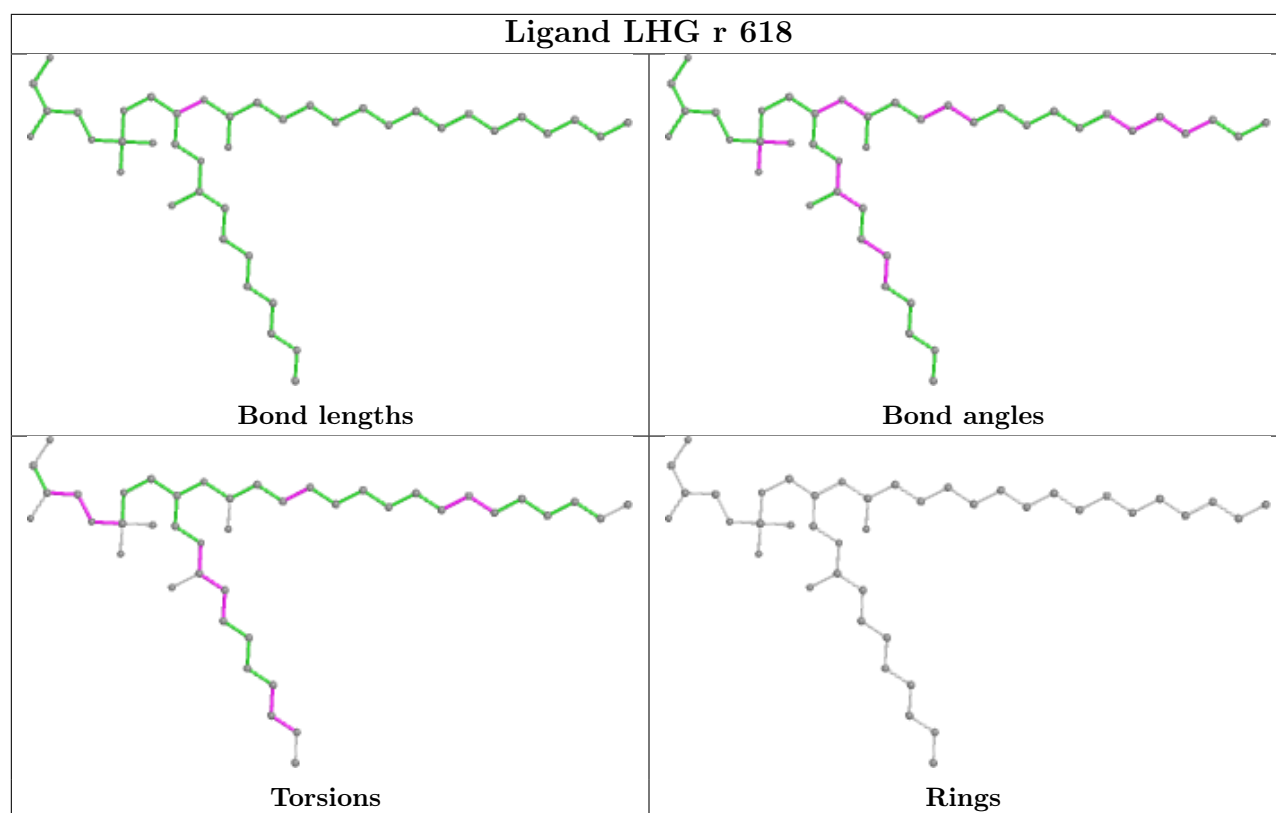




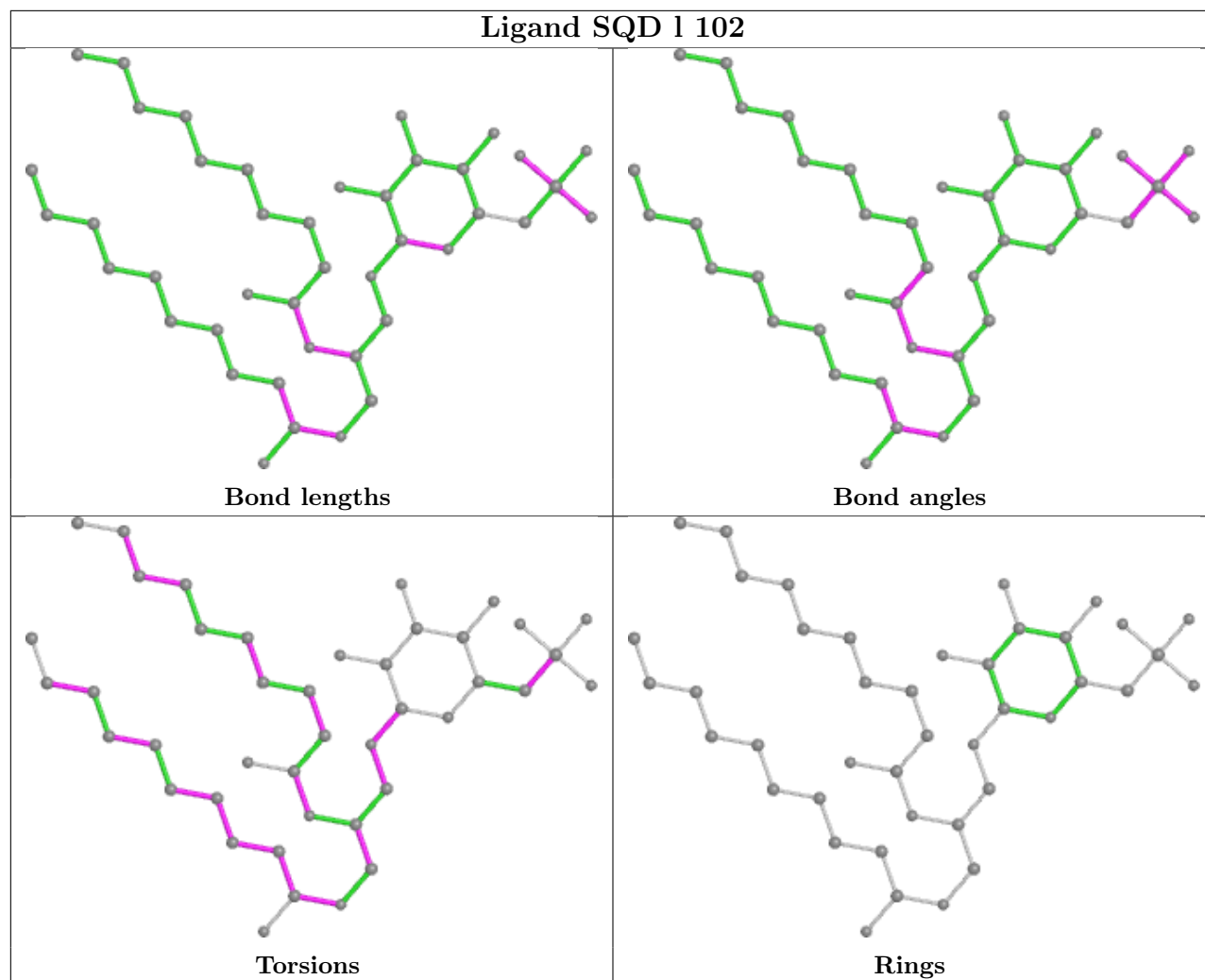


Ligand CLA BF 508**Ligand CLA b 614****Ligand LUT g 615**

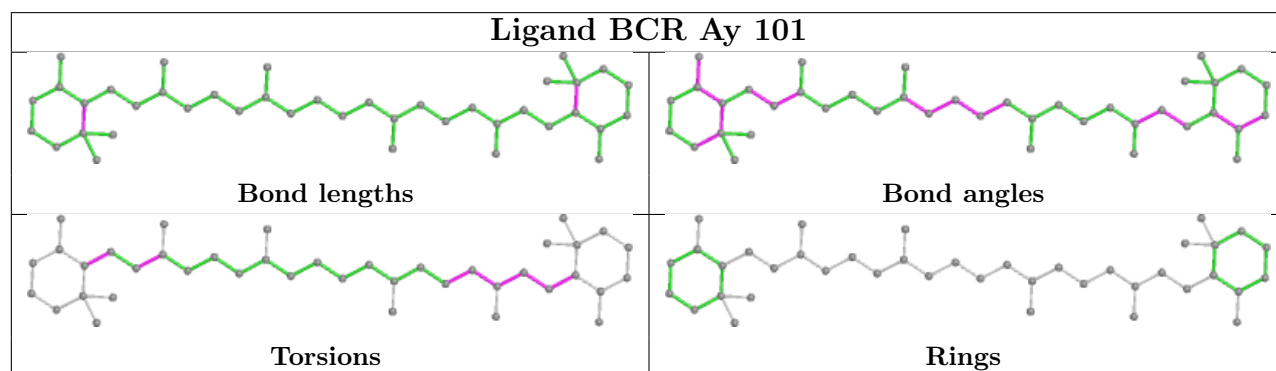




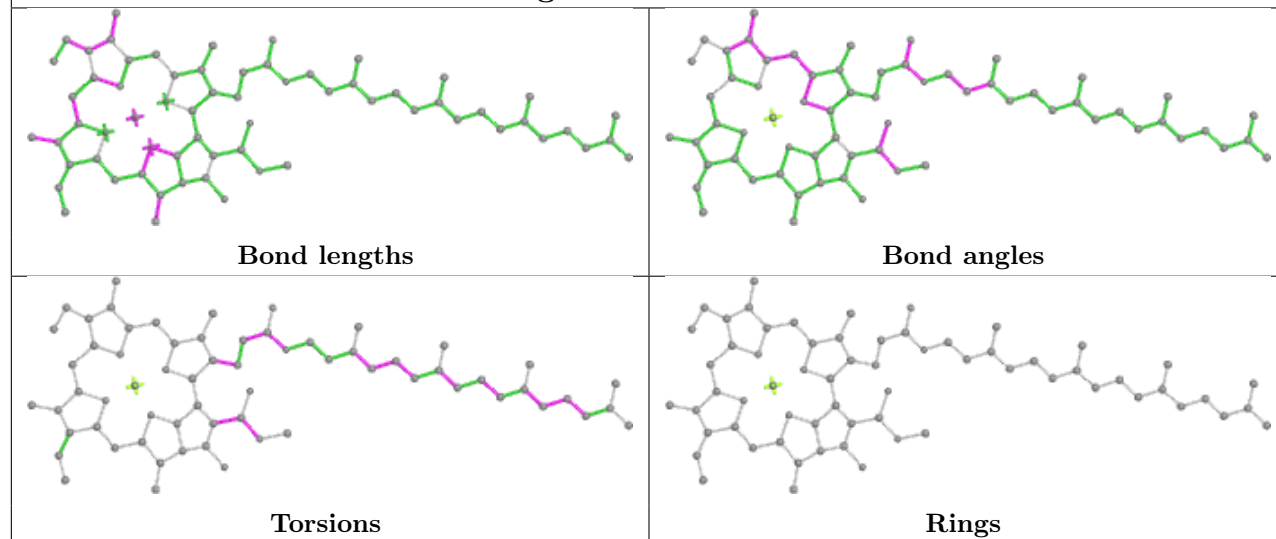
Ligand SQD I 102



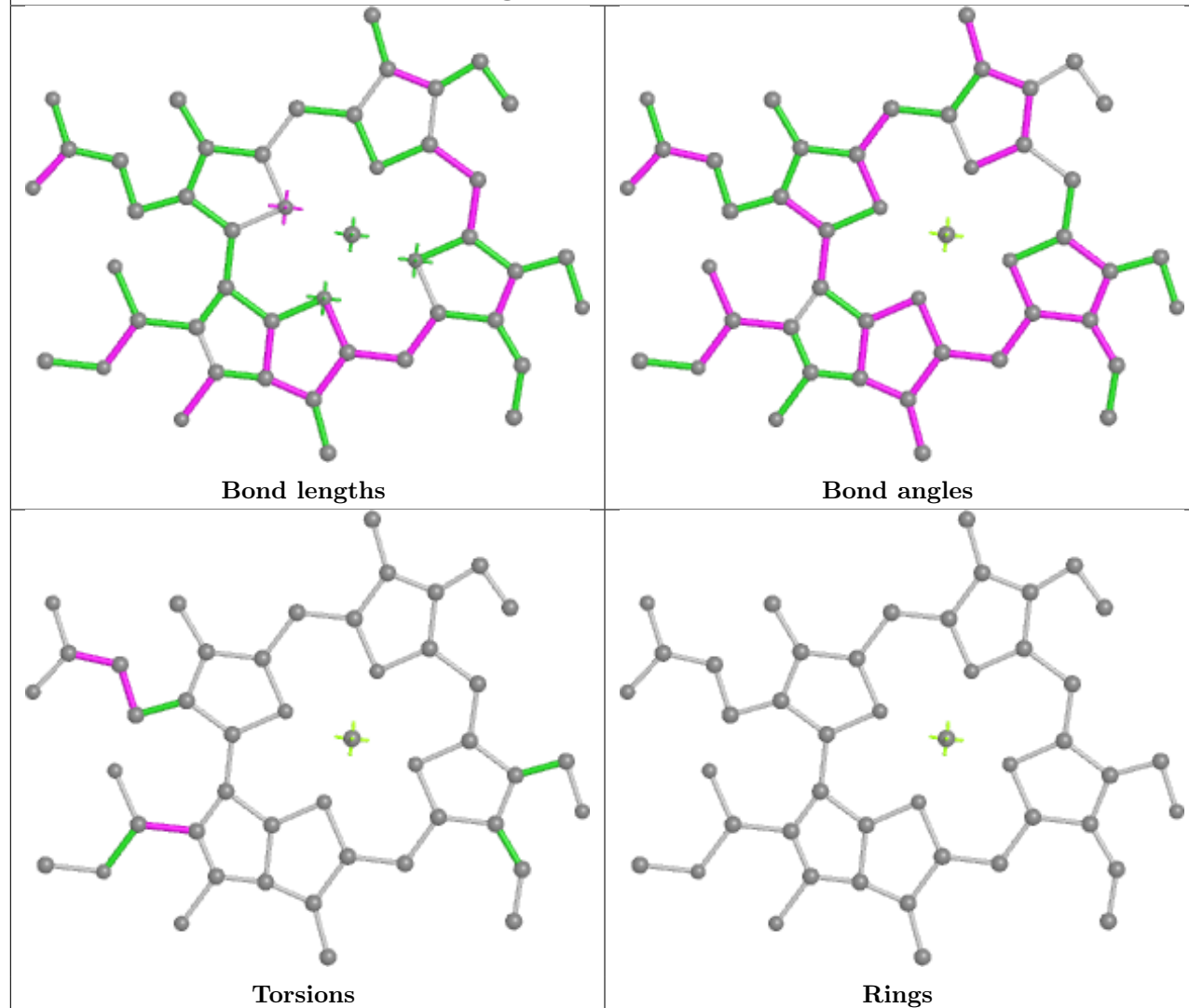
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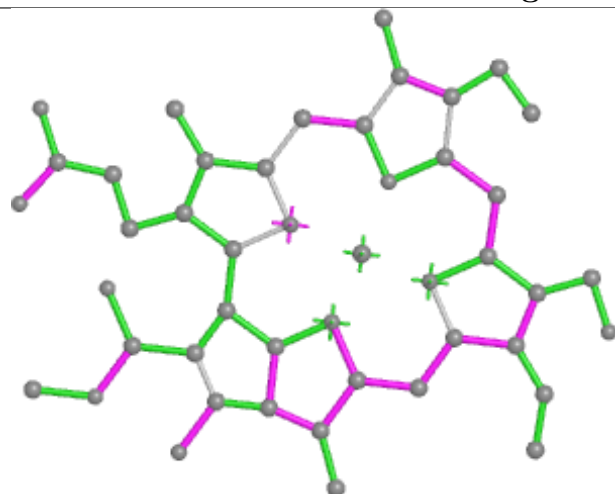
Ligand CLA c 504



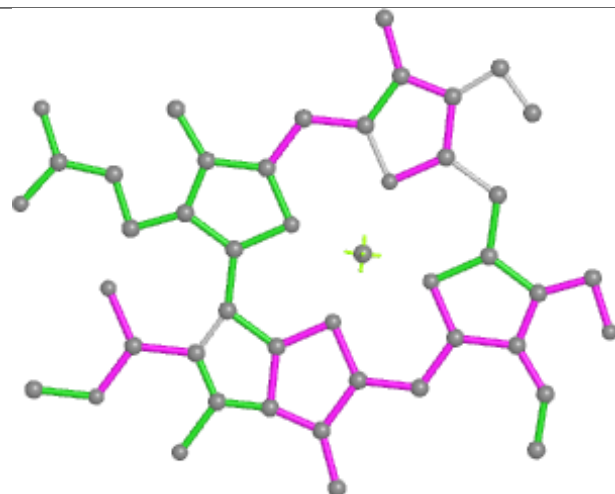
Ligand CHL 5 606



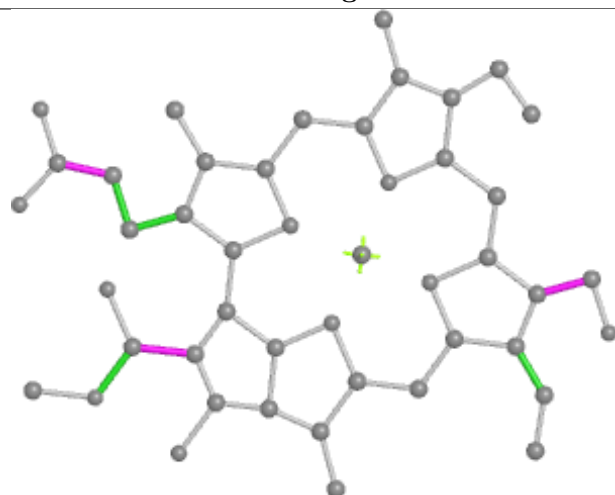
Ligand CHL s 601



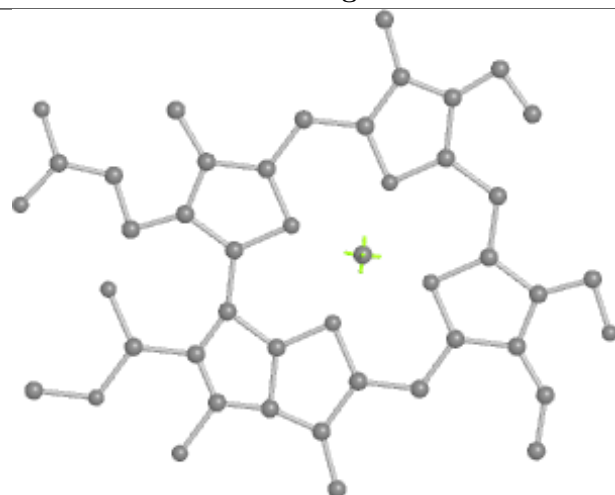
Bond lengths



Bond angles

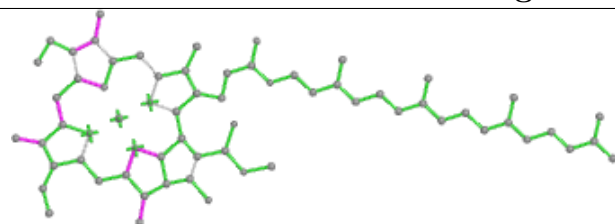


Torsions

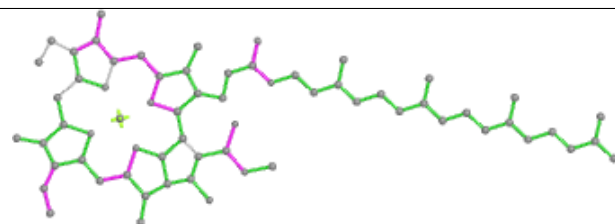


Rings

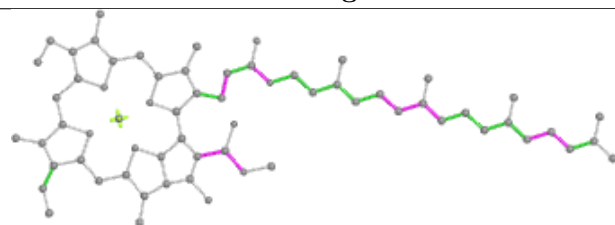
Ligand CLA G 603



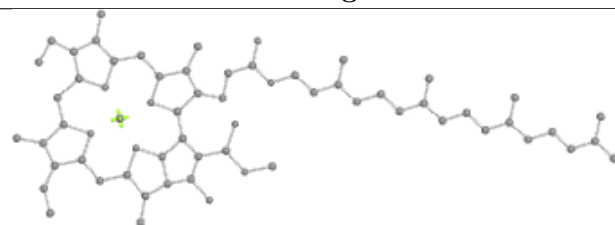
Bond lengths



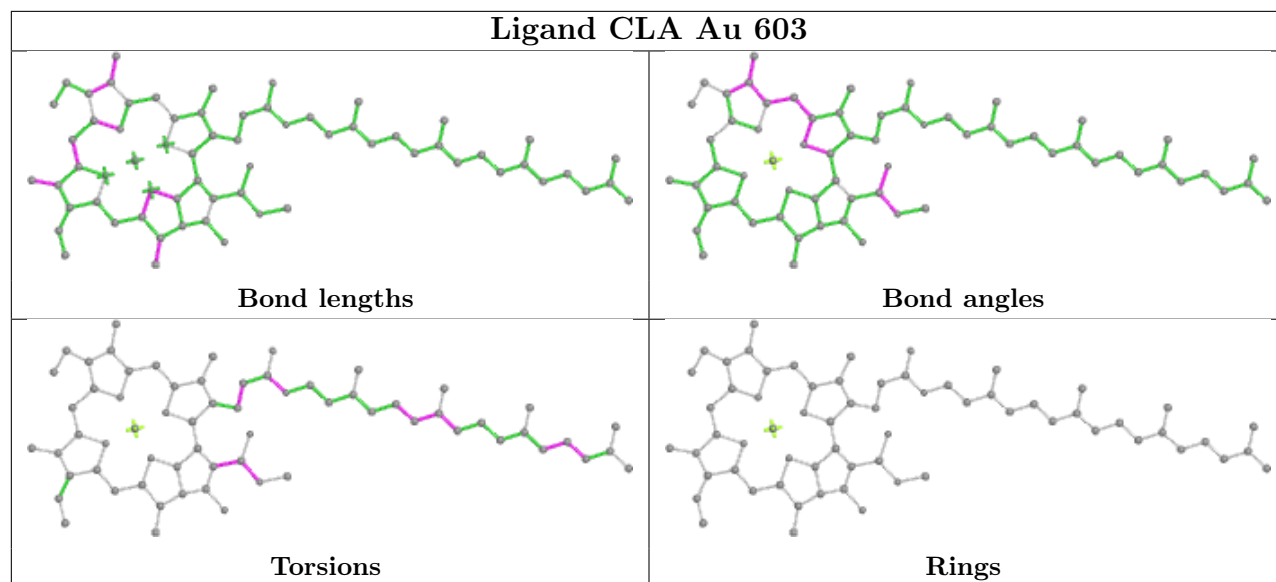
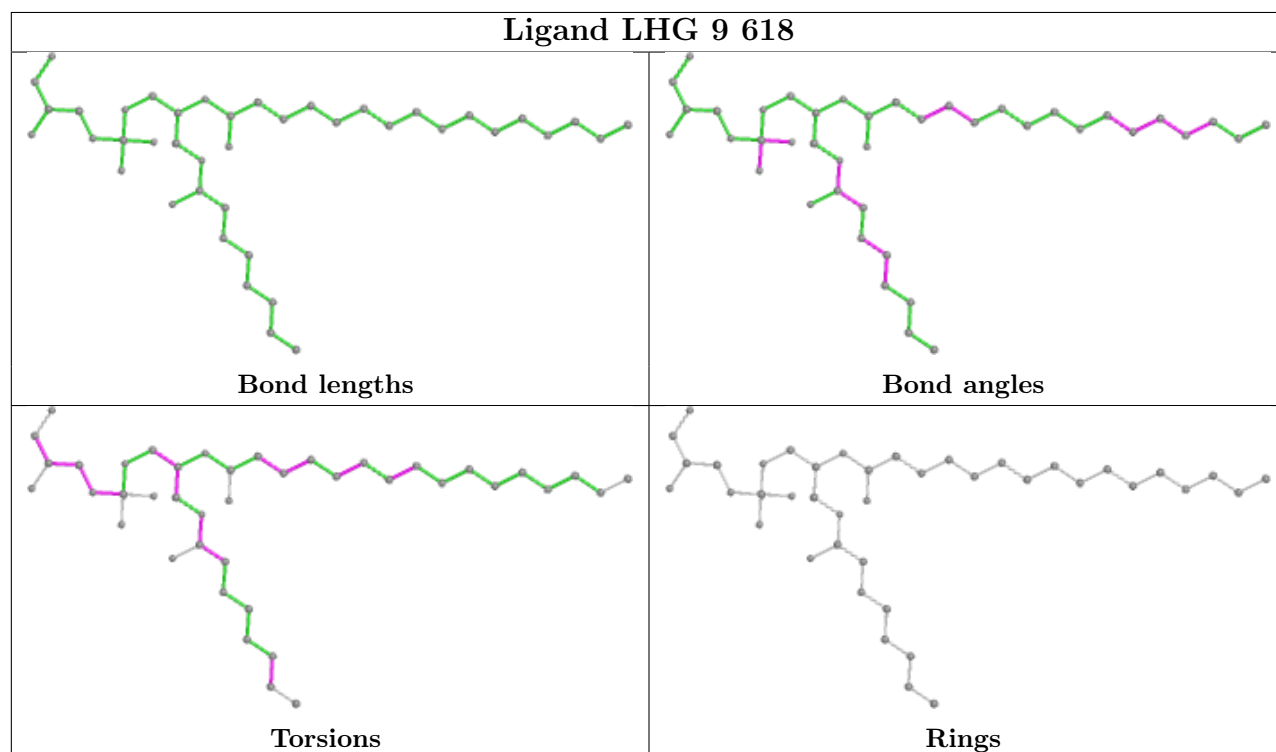
Bond angles

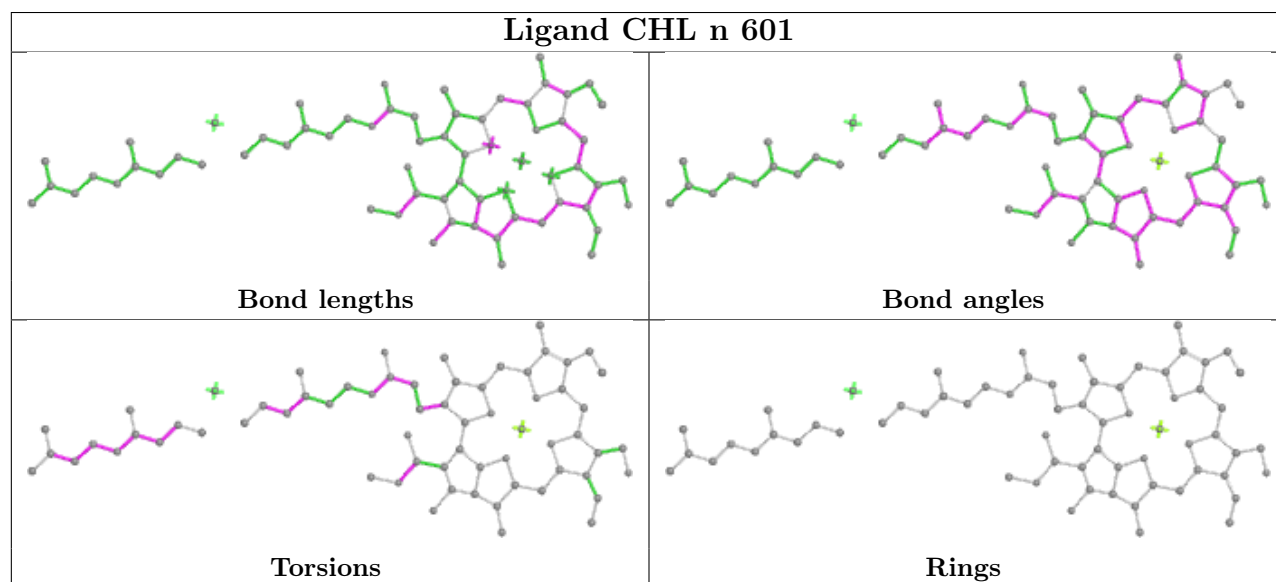
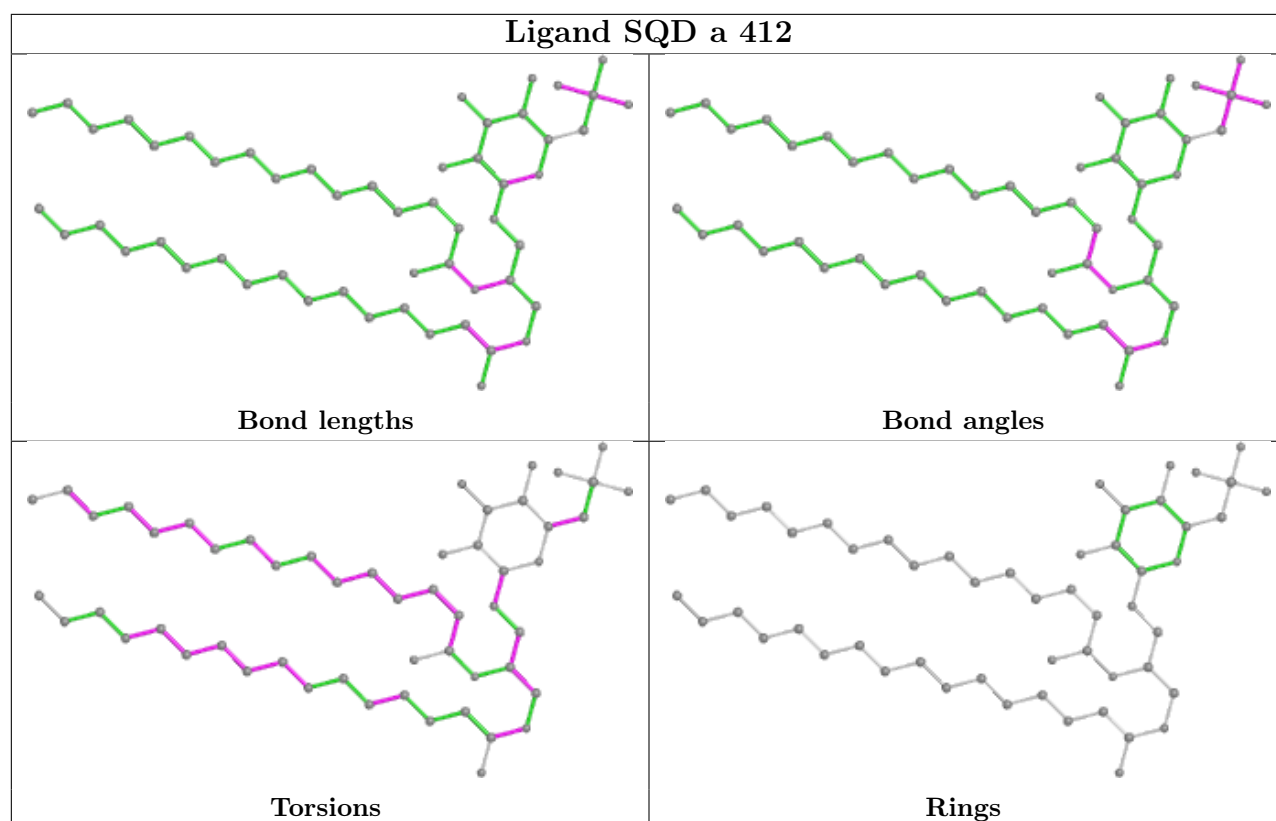


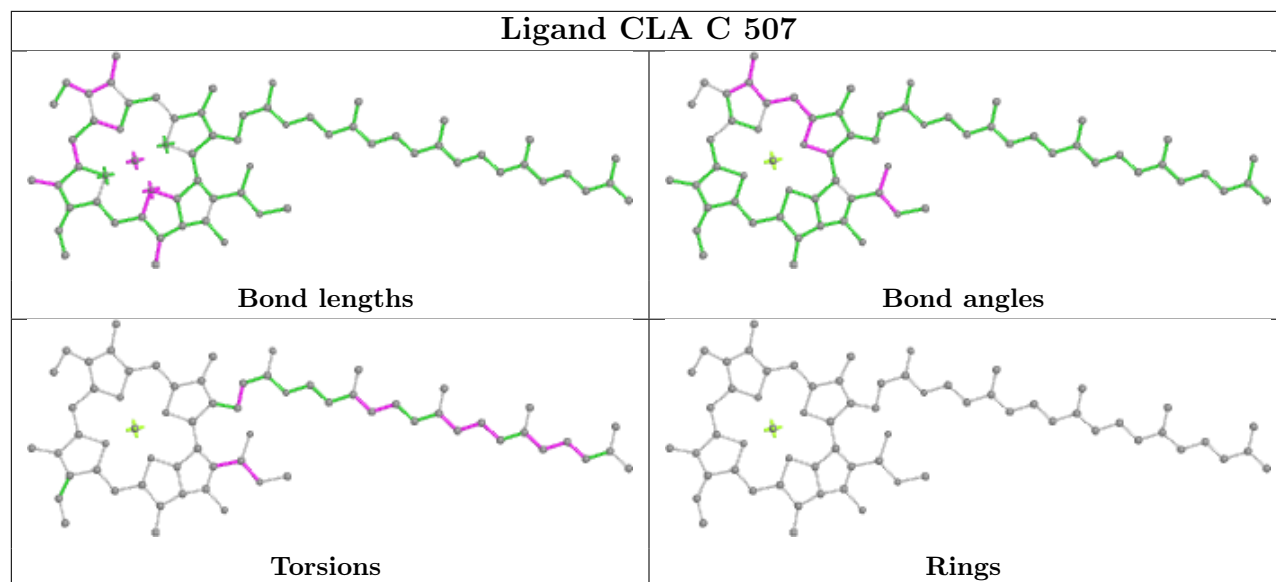
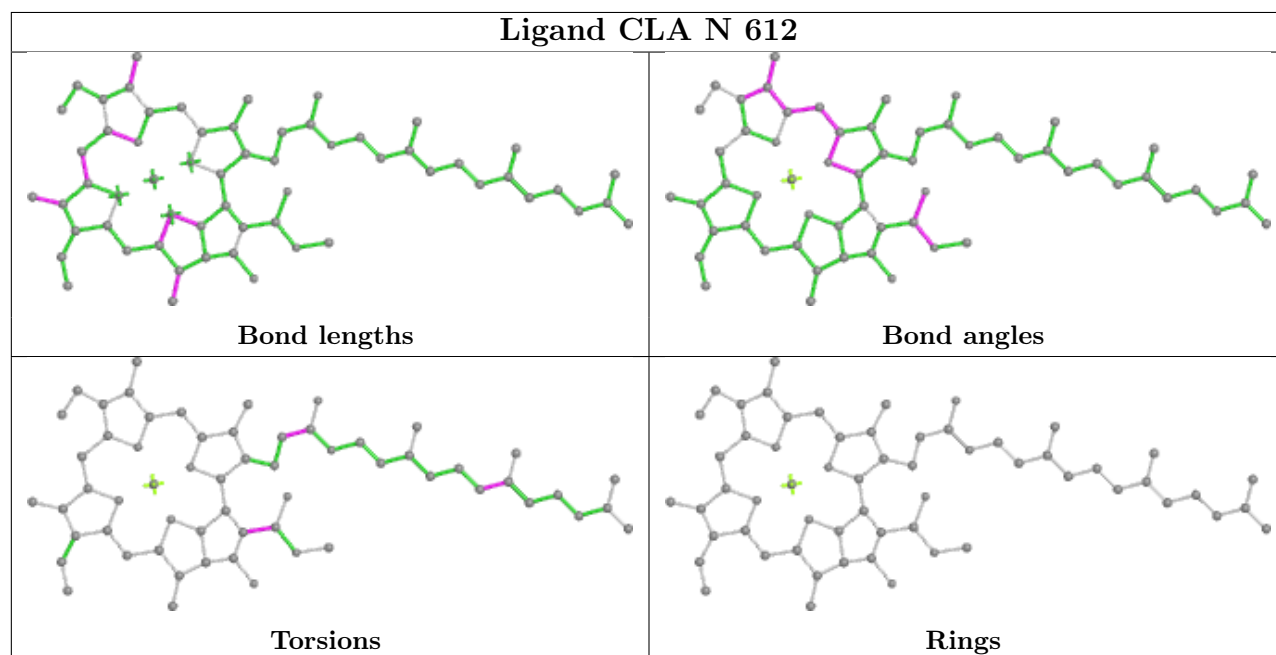
Torsions



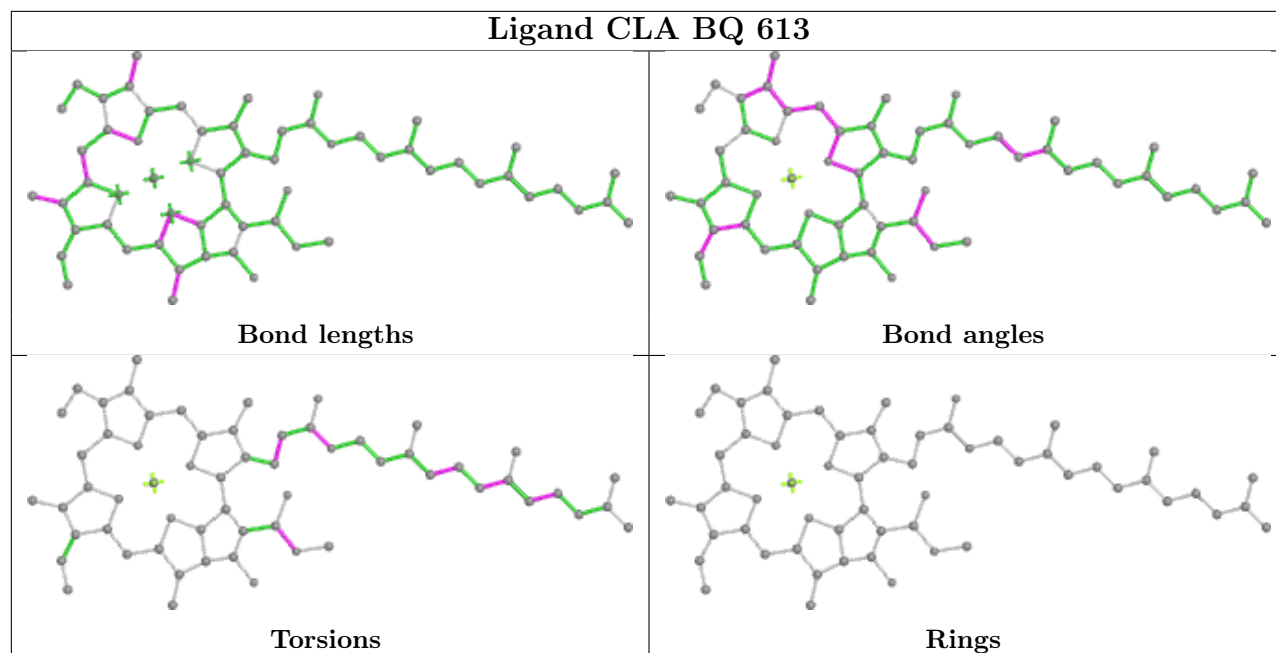
Rings

Ligand CLA Au 603**Ligand LHG 9 618**

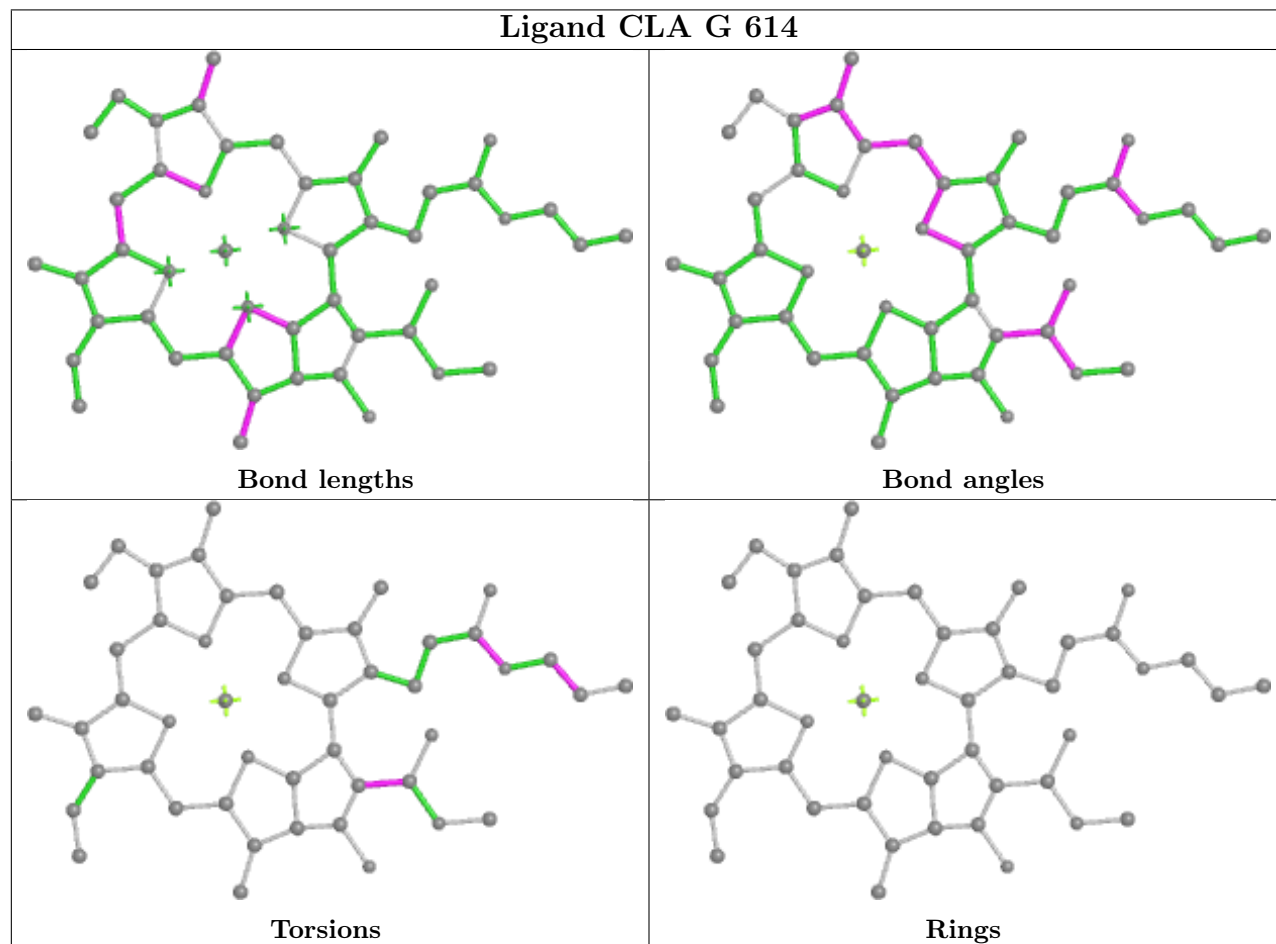


Ligand CLA C 507**Ligand CLA N 612**

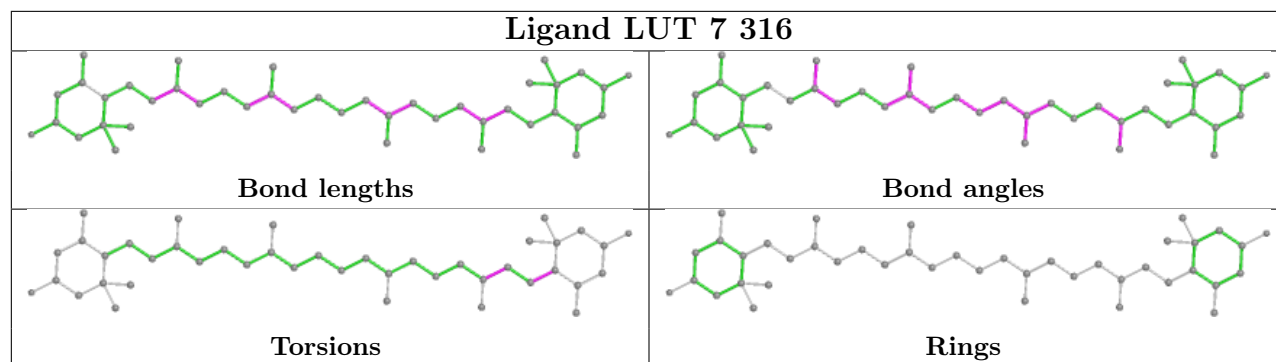
Ligand CLA BQ 613



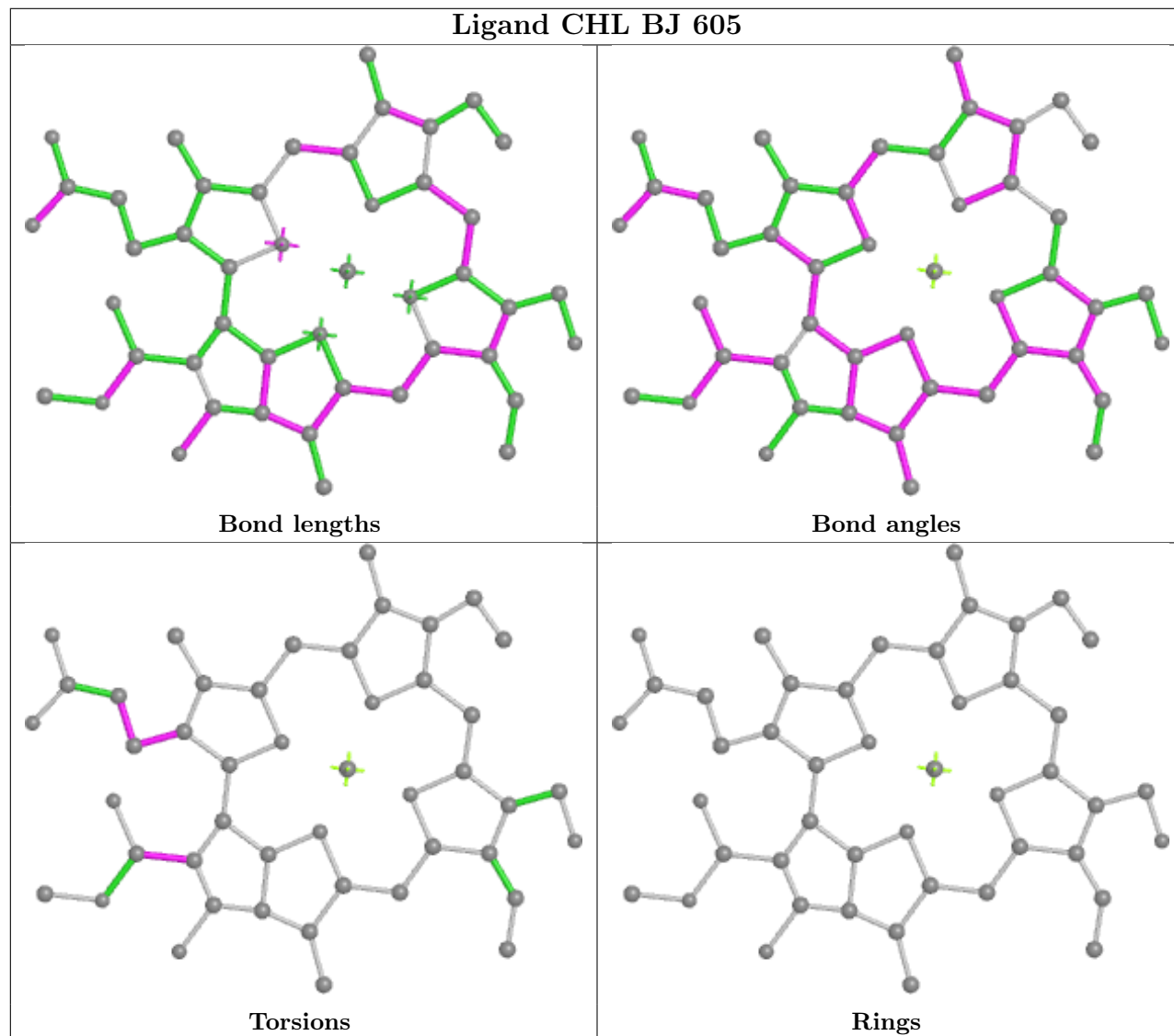
Ligand CLA G 614



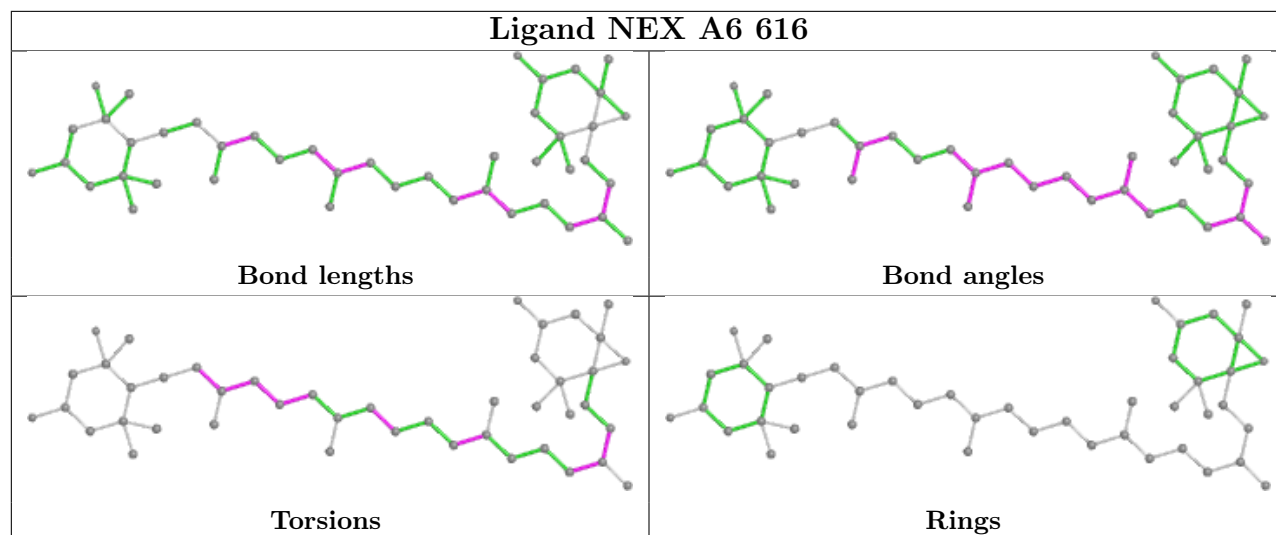
Ligand LUT 7 316



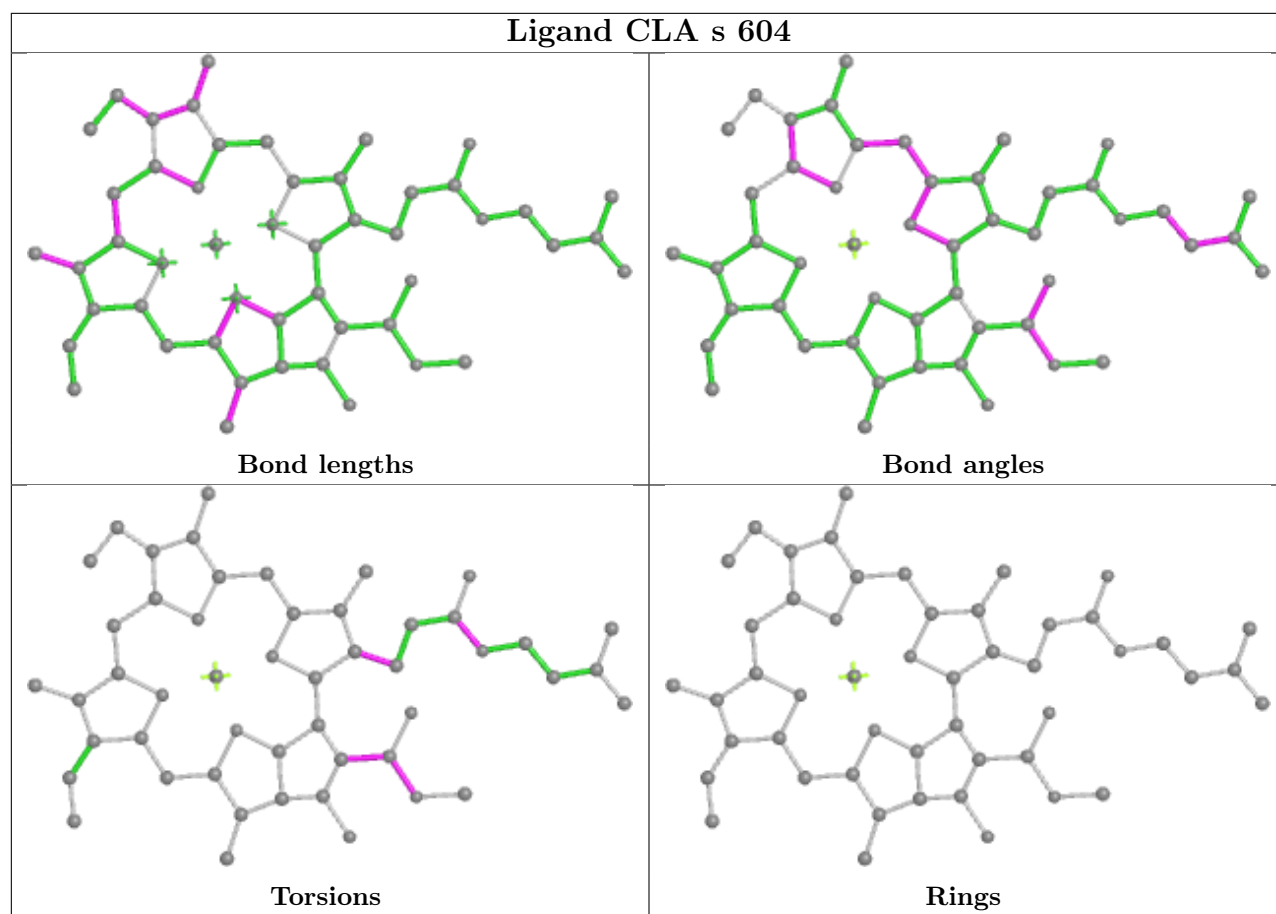
Ligand CHL BJ 605

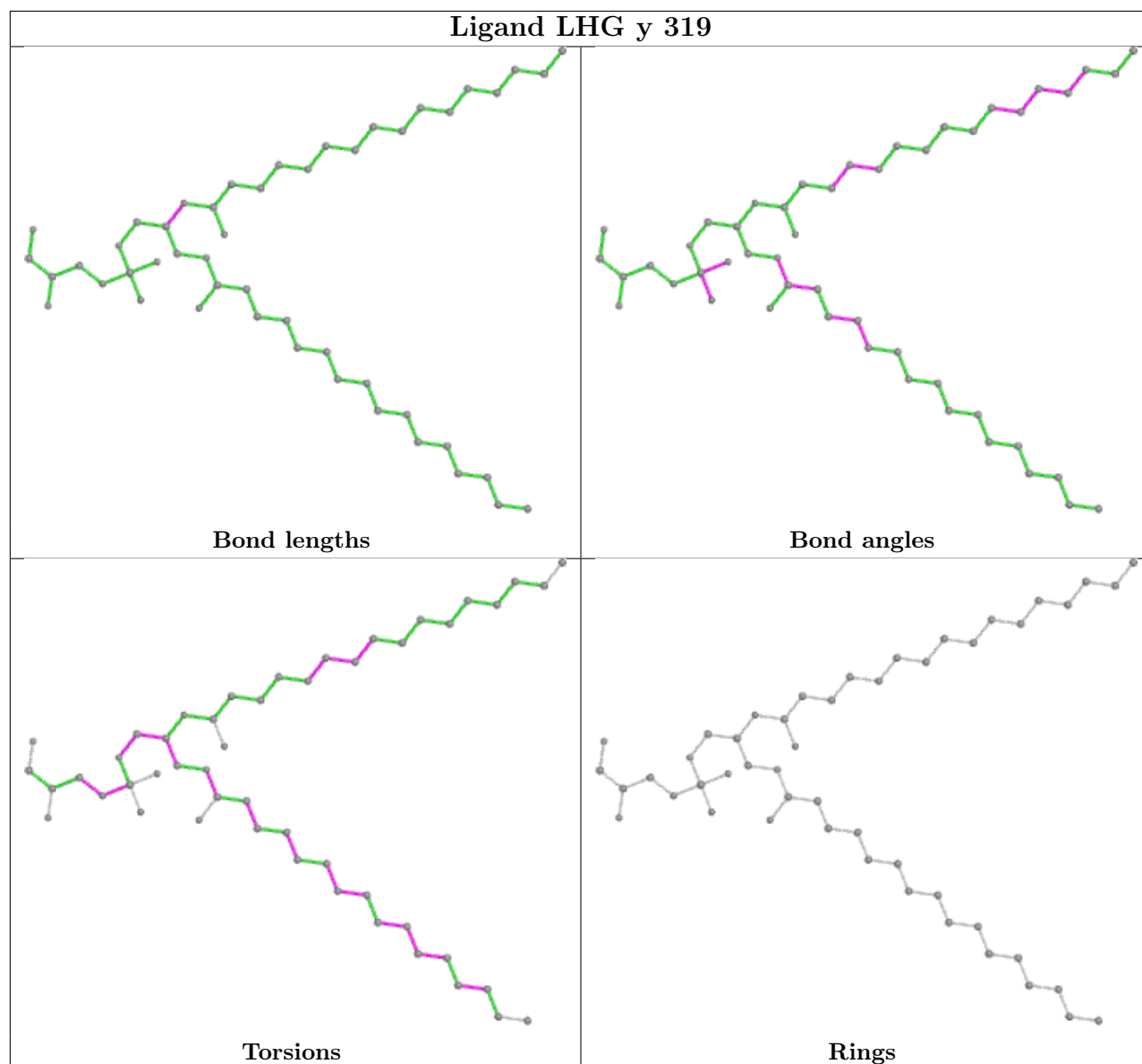
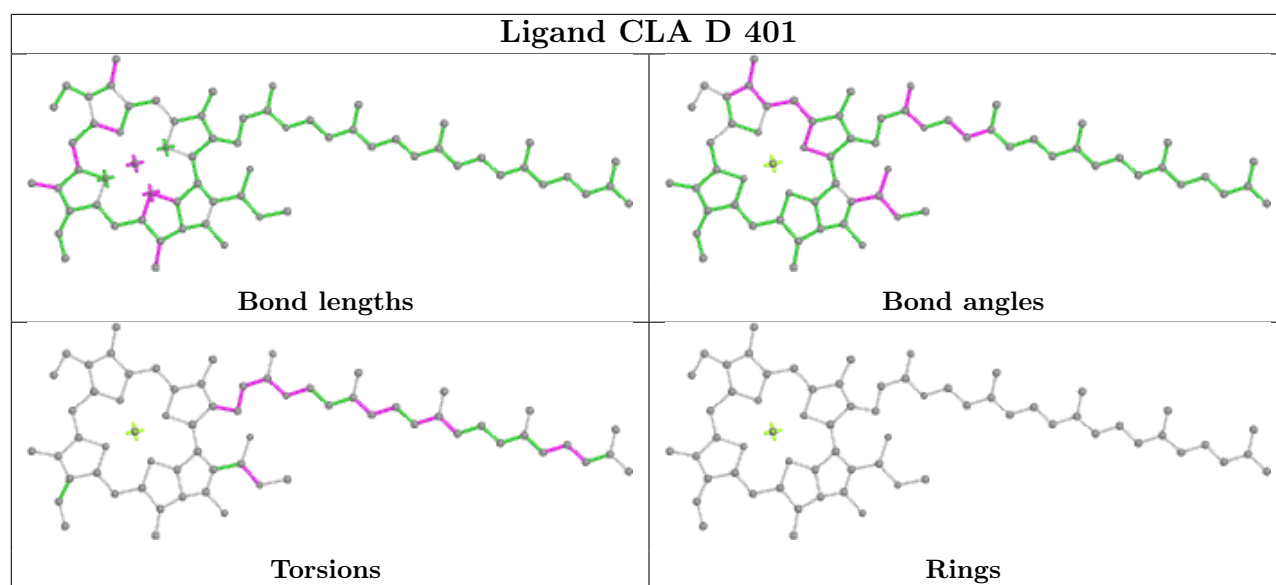


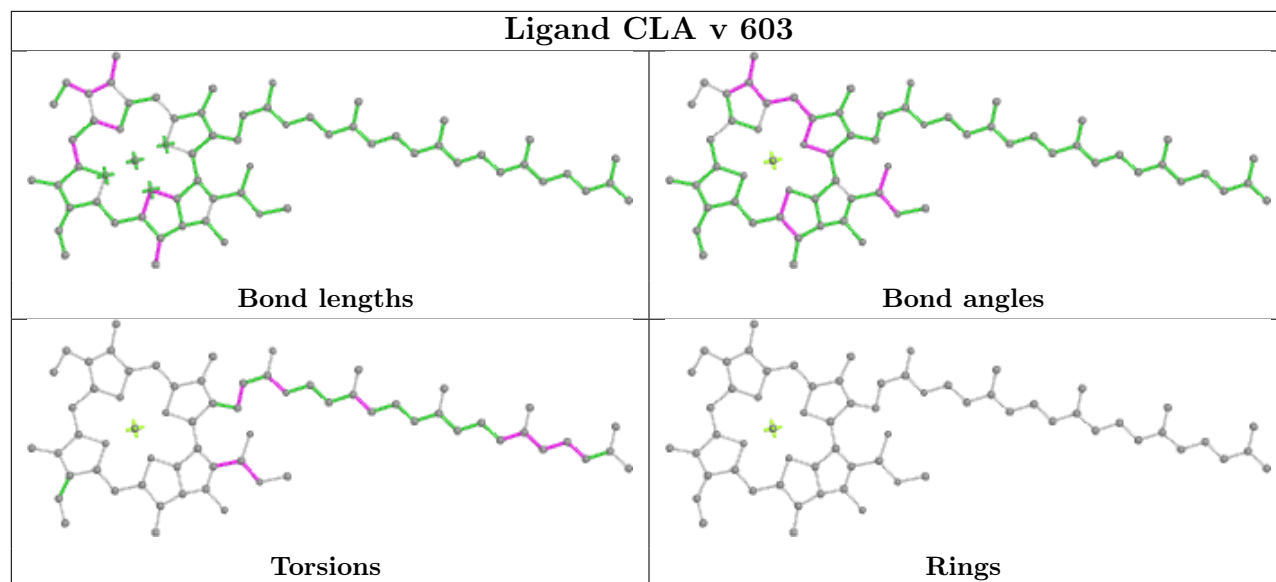
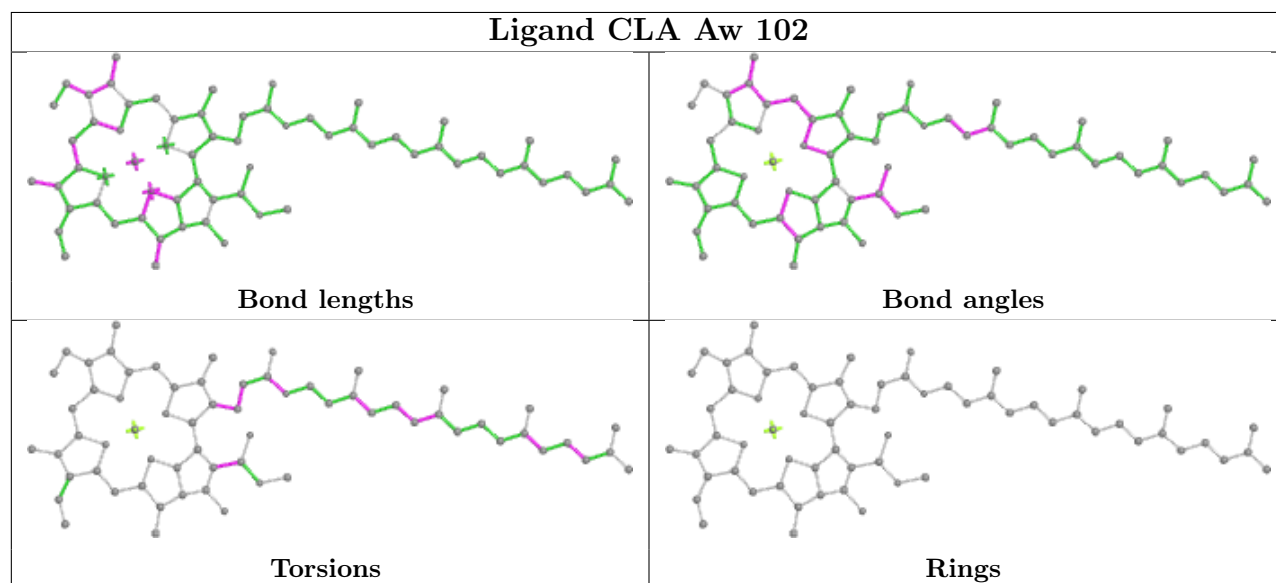
Ligand NEX A6 616

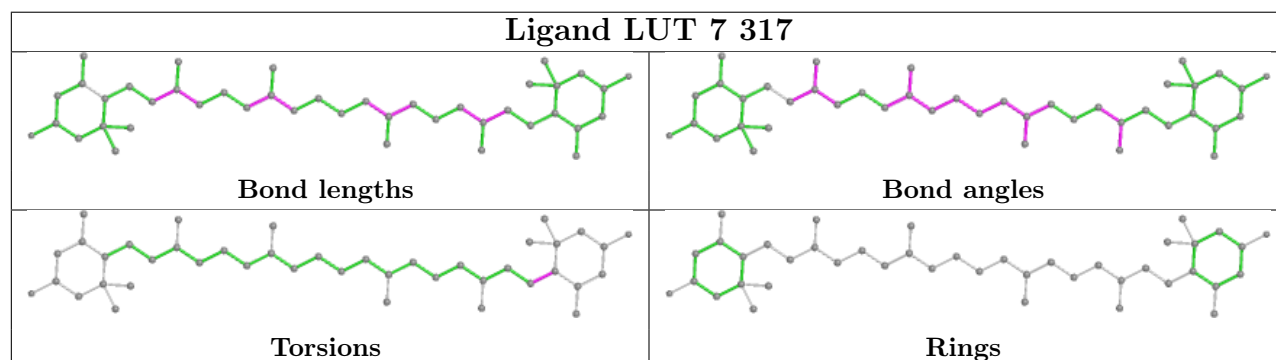
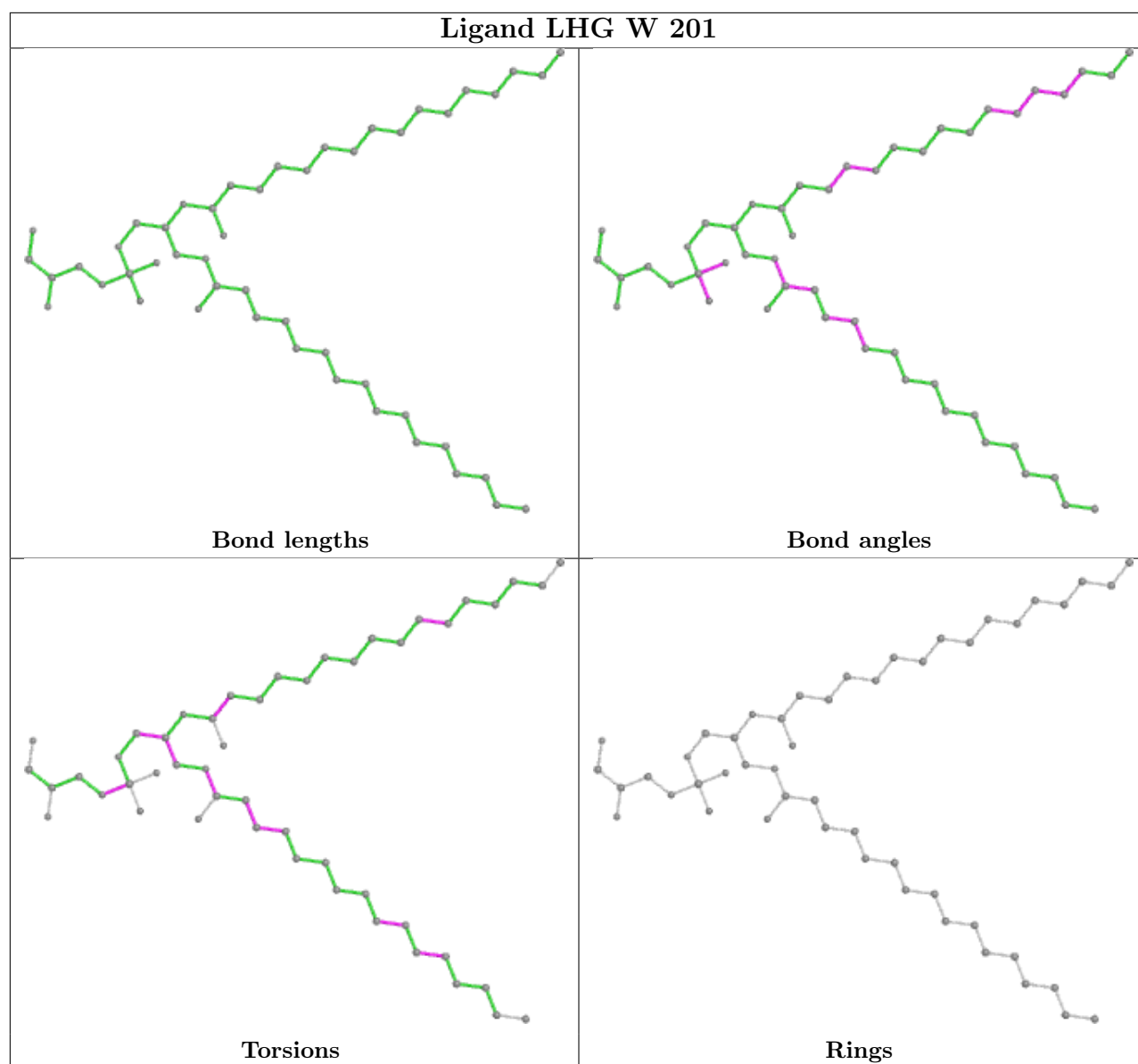


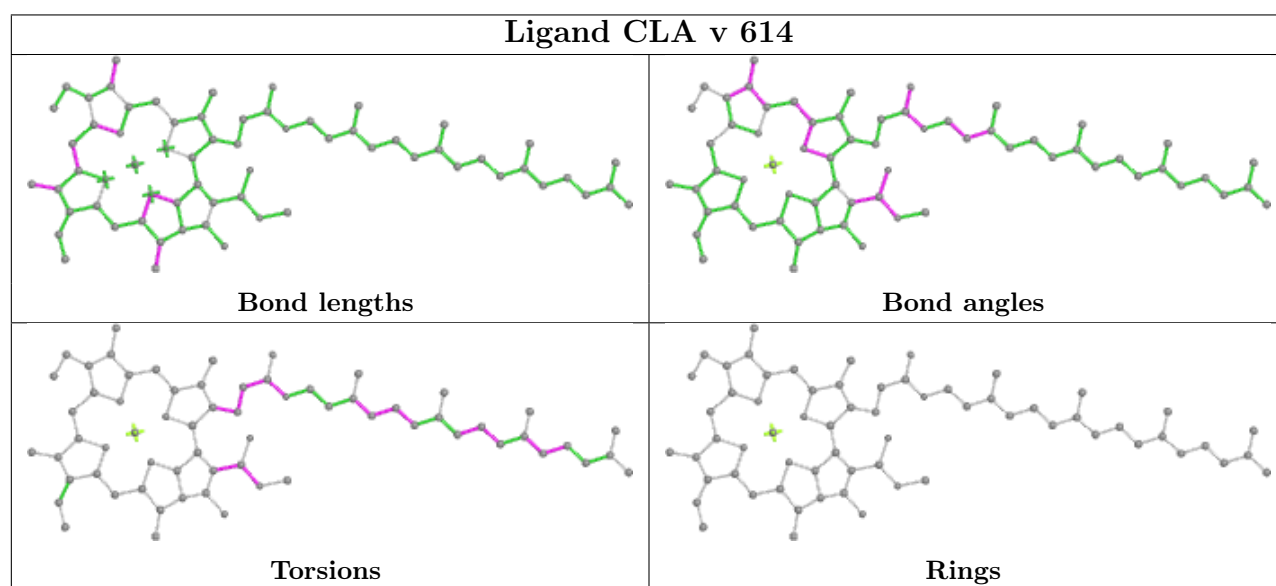
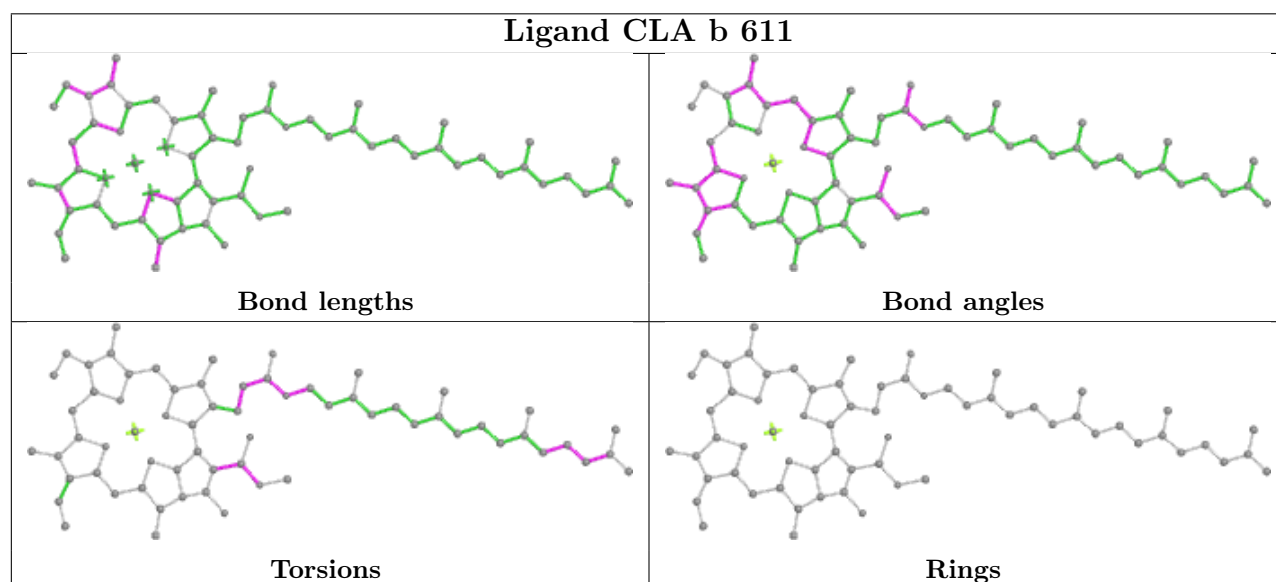
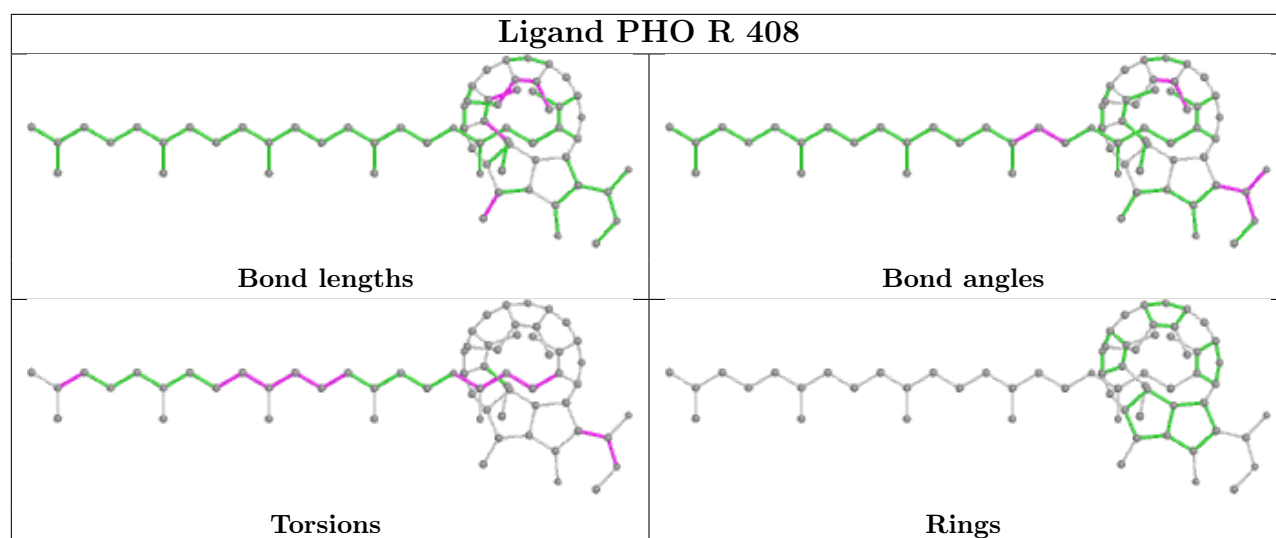
Ligand CLA s 604



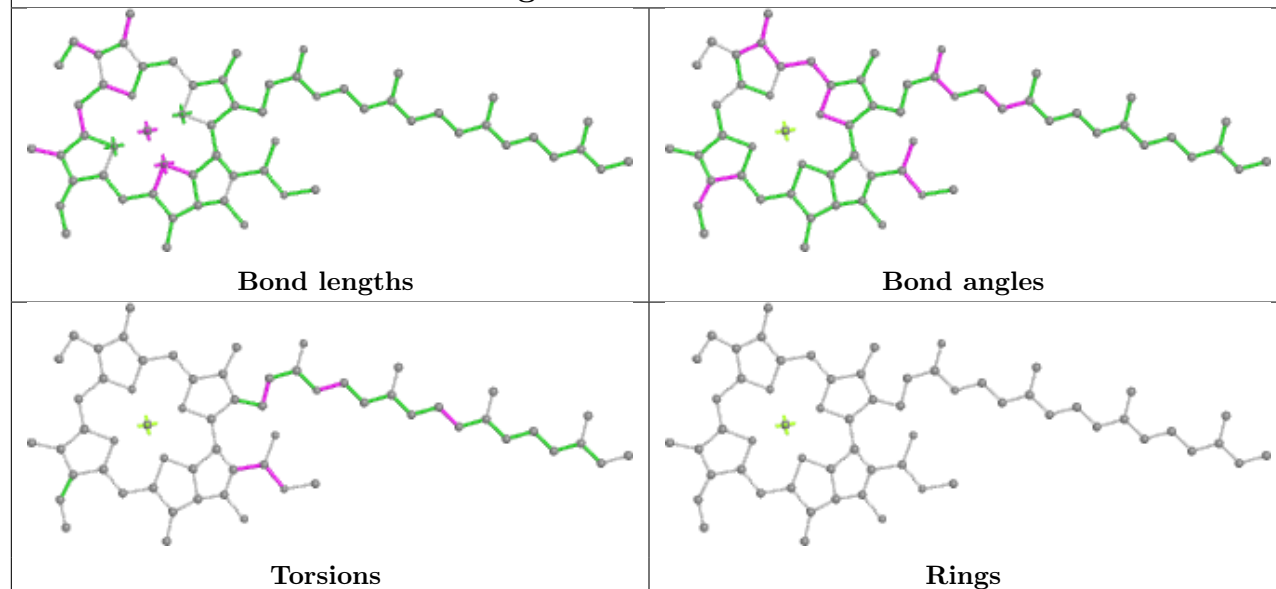


Ligand CLA v 603**Ligand CLA Aw 102**

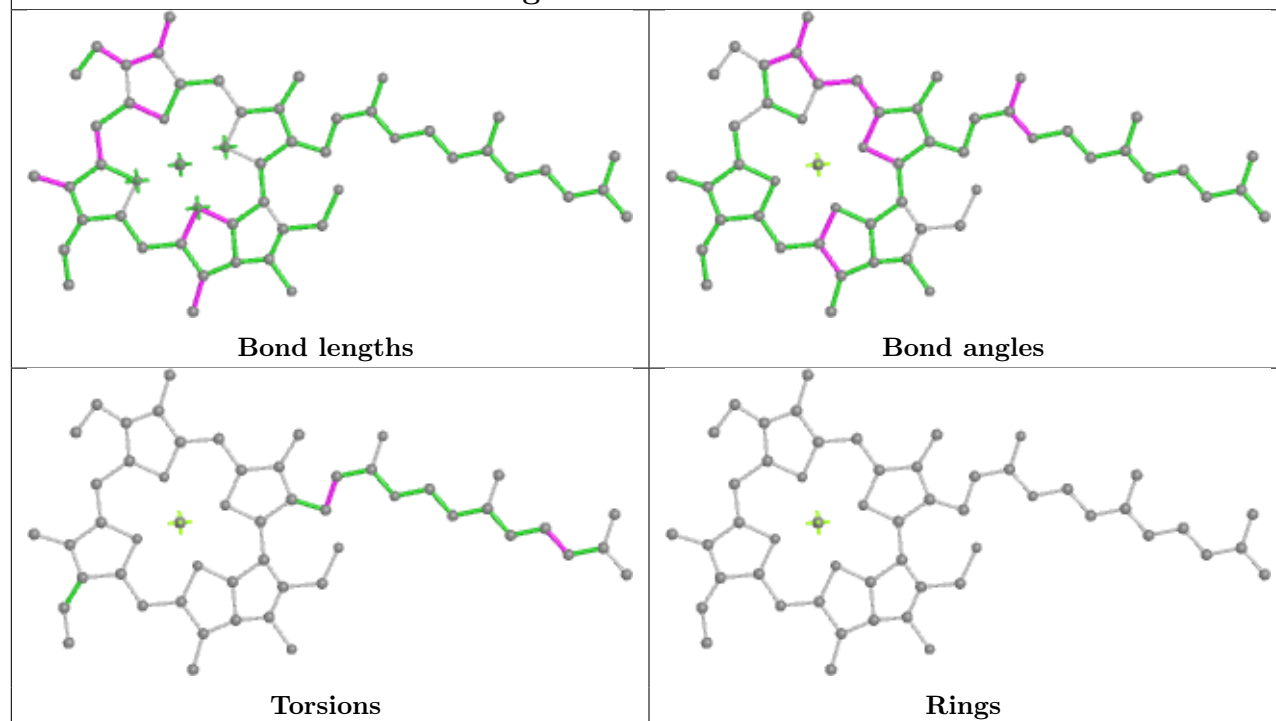


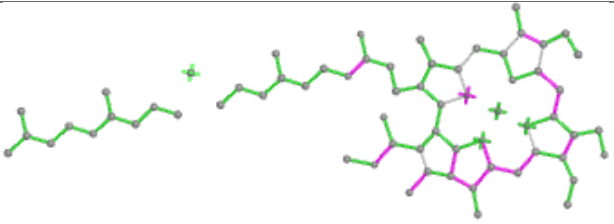
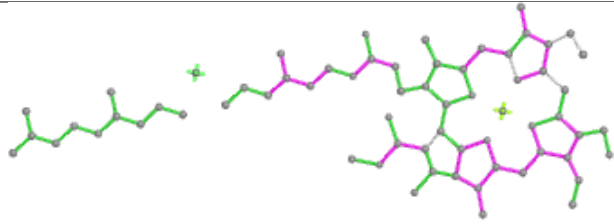
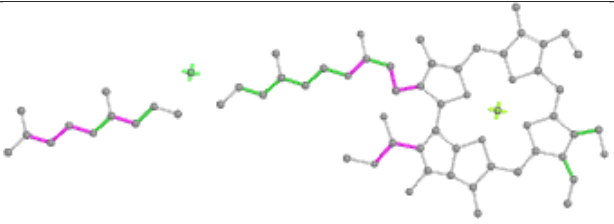
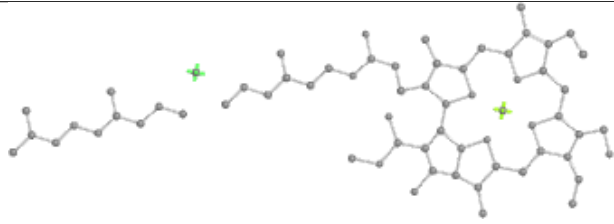
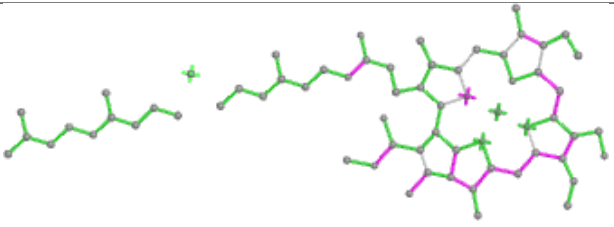
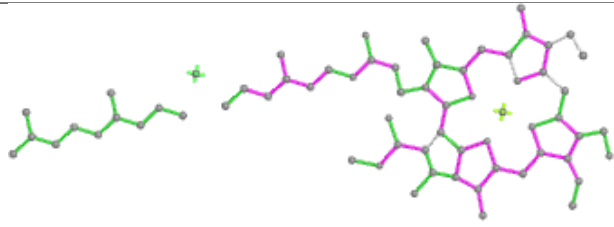
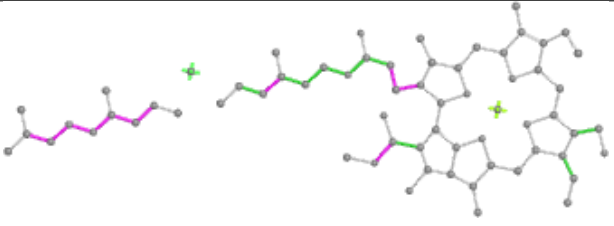
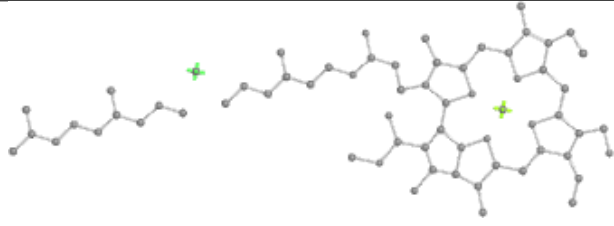
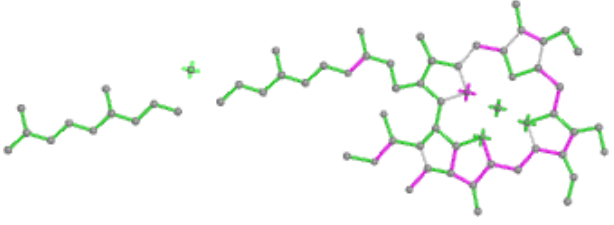
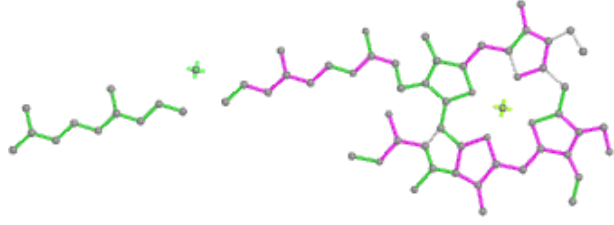
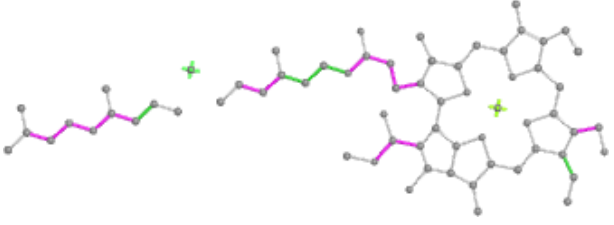
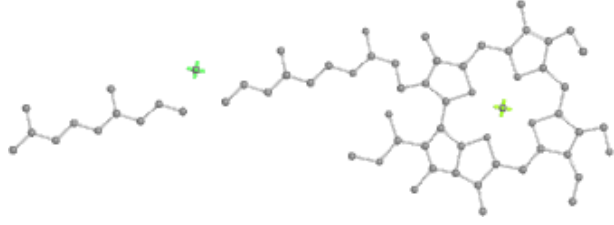


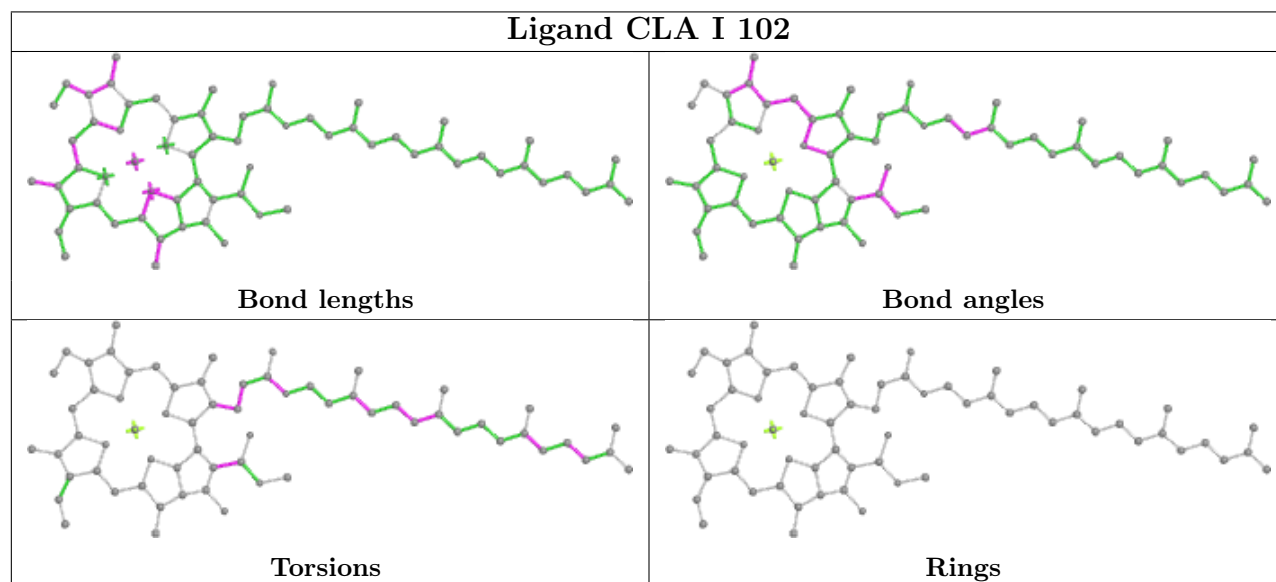
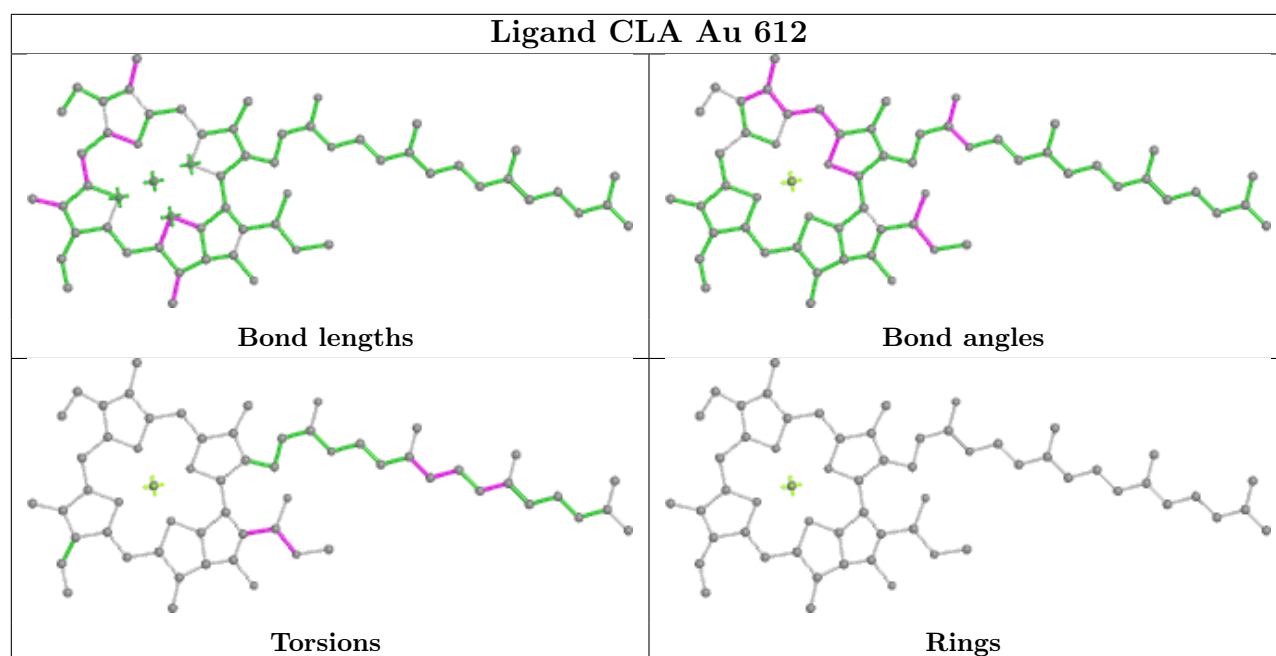
Ligand CLA AA 303

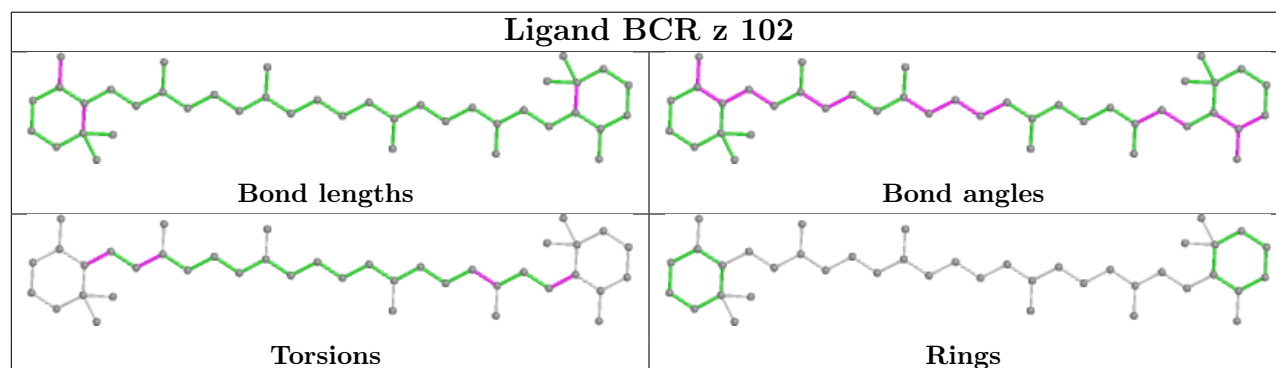
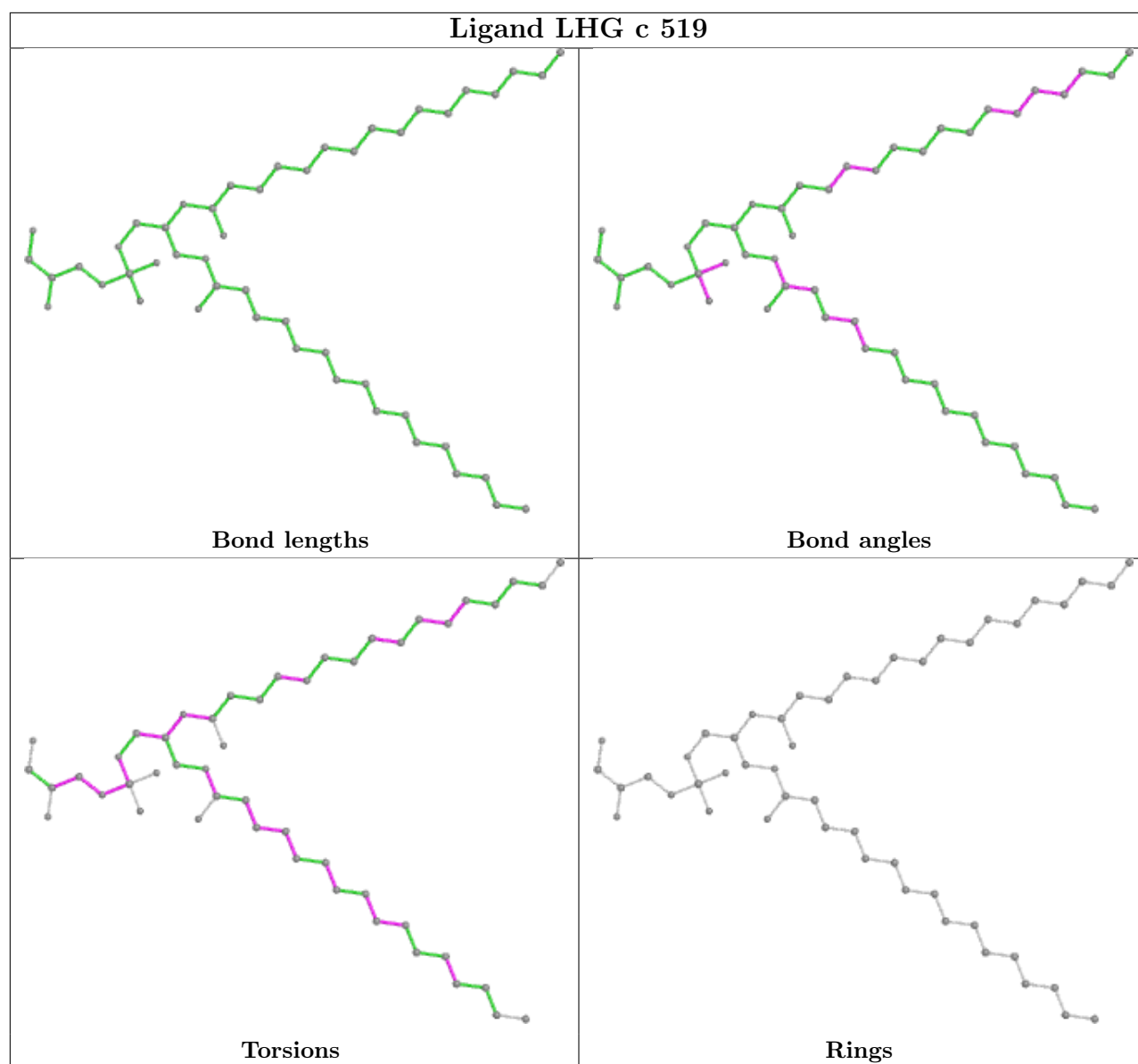


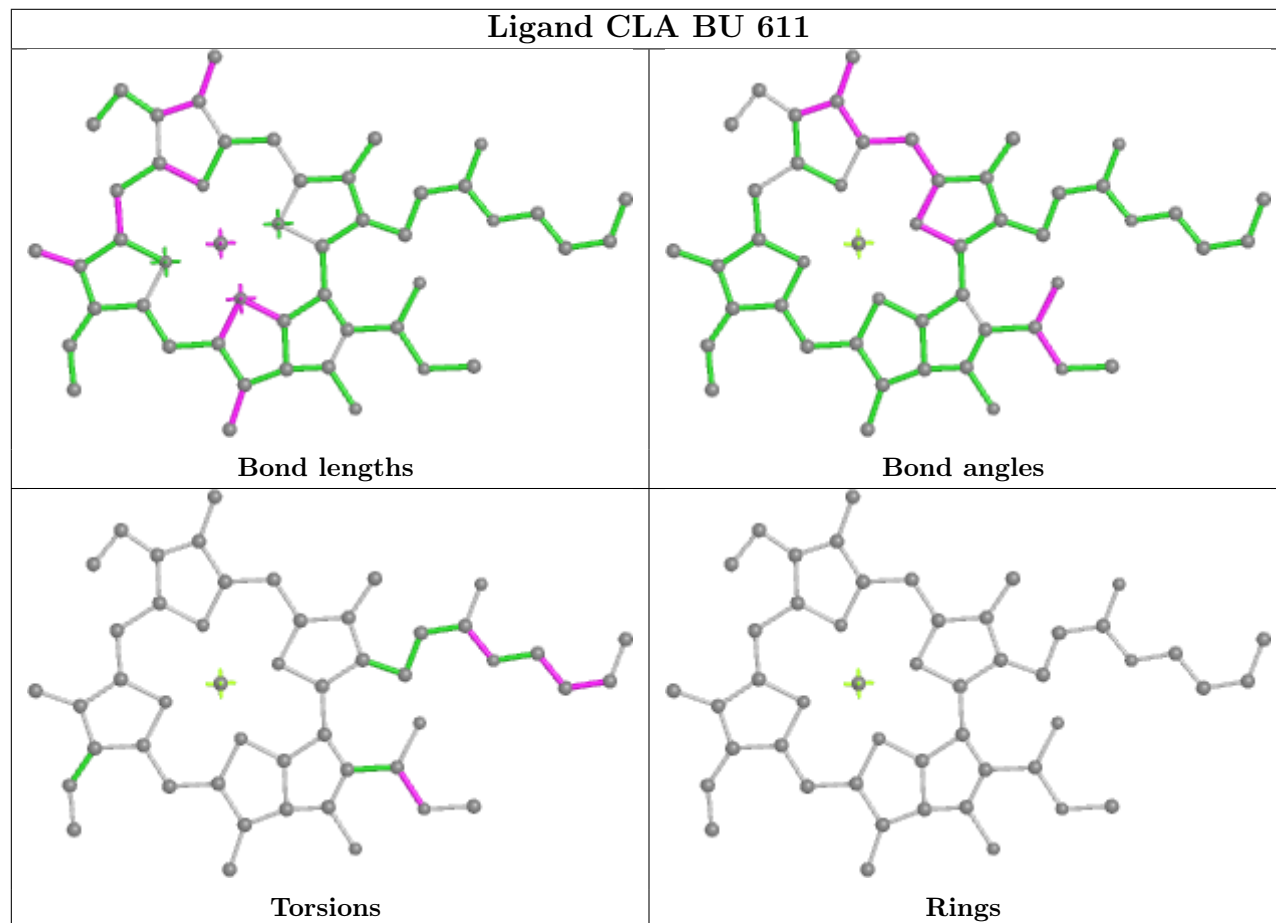
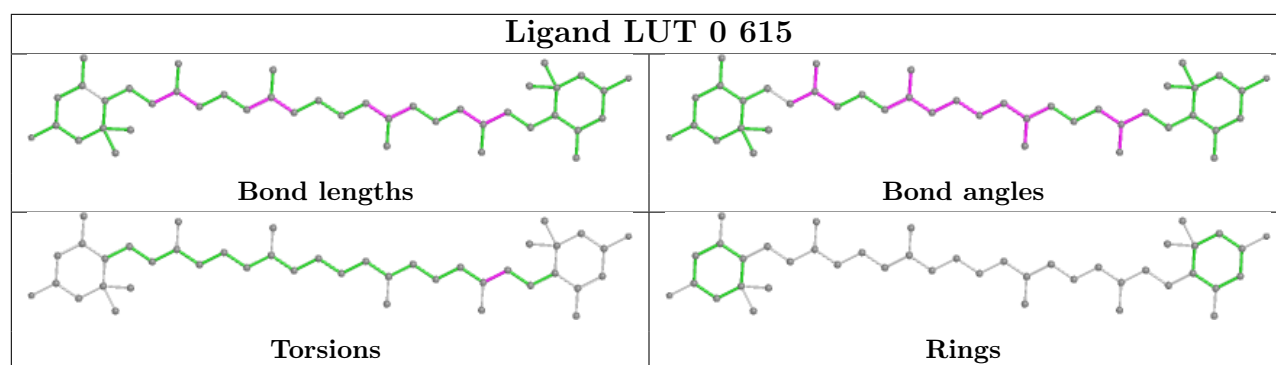
Ligand CLA A6 609

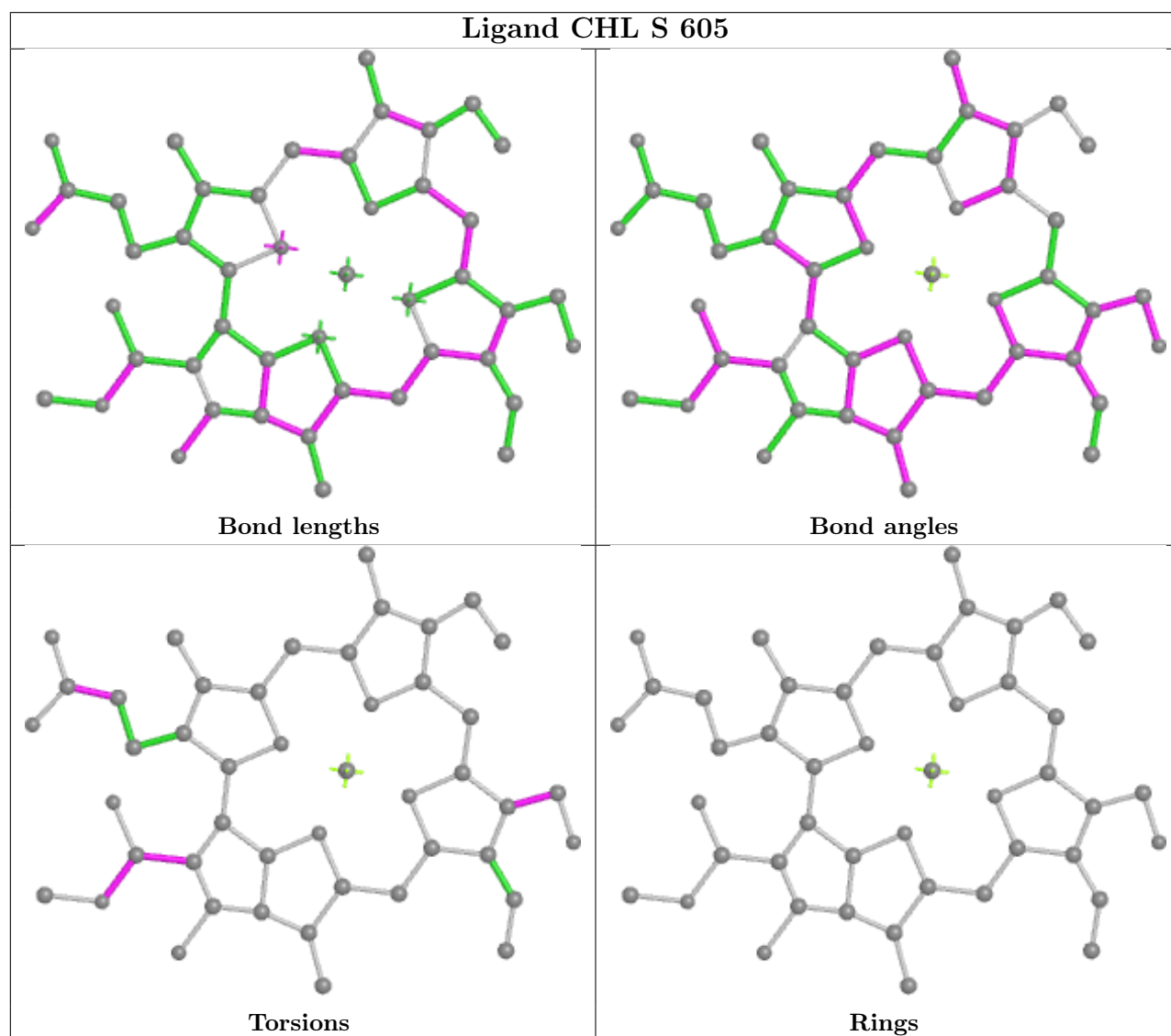
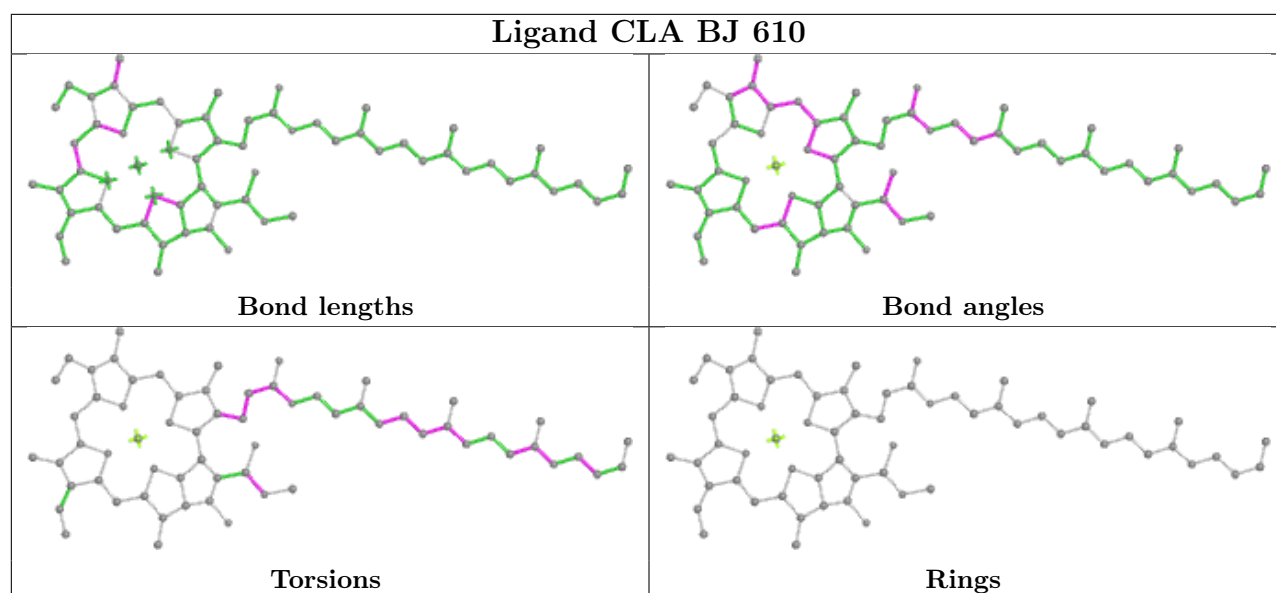


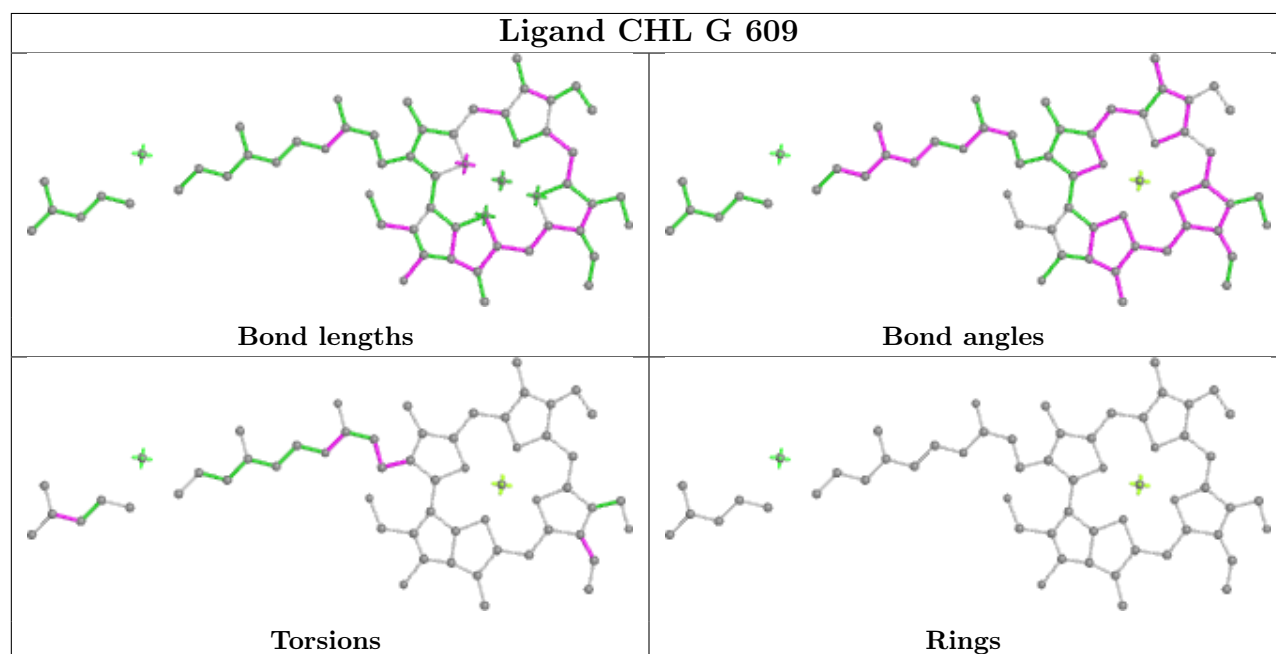
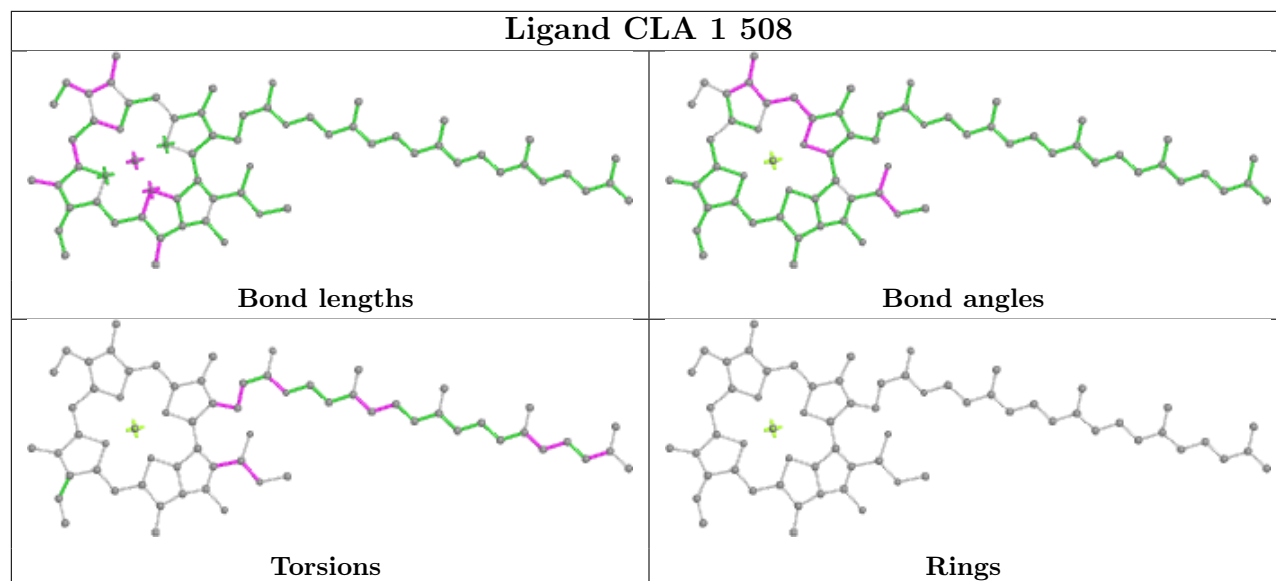
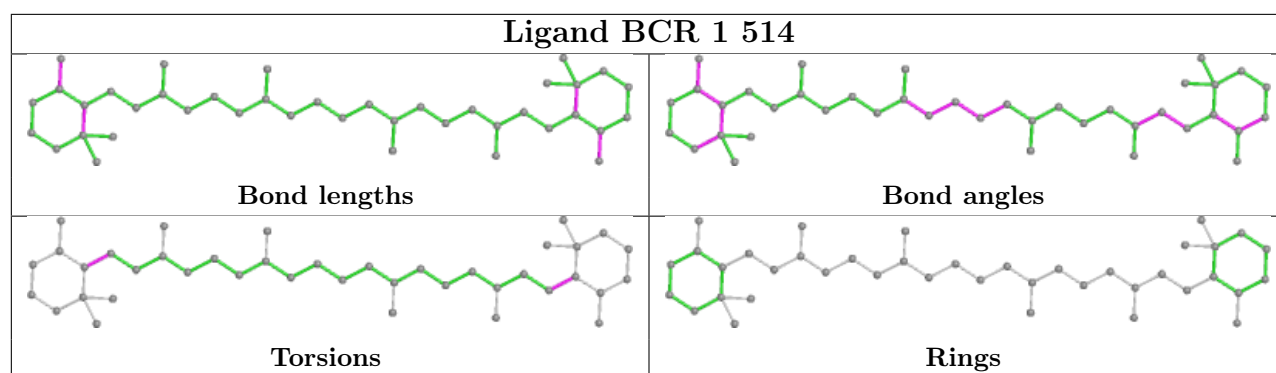
| Ligand CHL N 609 | |
|---|---|
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |
| Ligand CHL n 607 | |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |
| Ligand CHL Au 608 | |
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|  <p>Torsions</p> |  <p>Rings</p> |



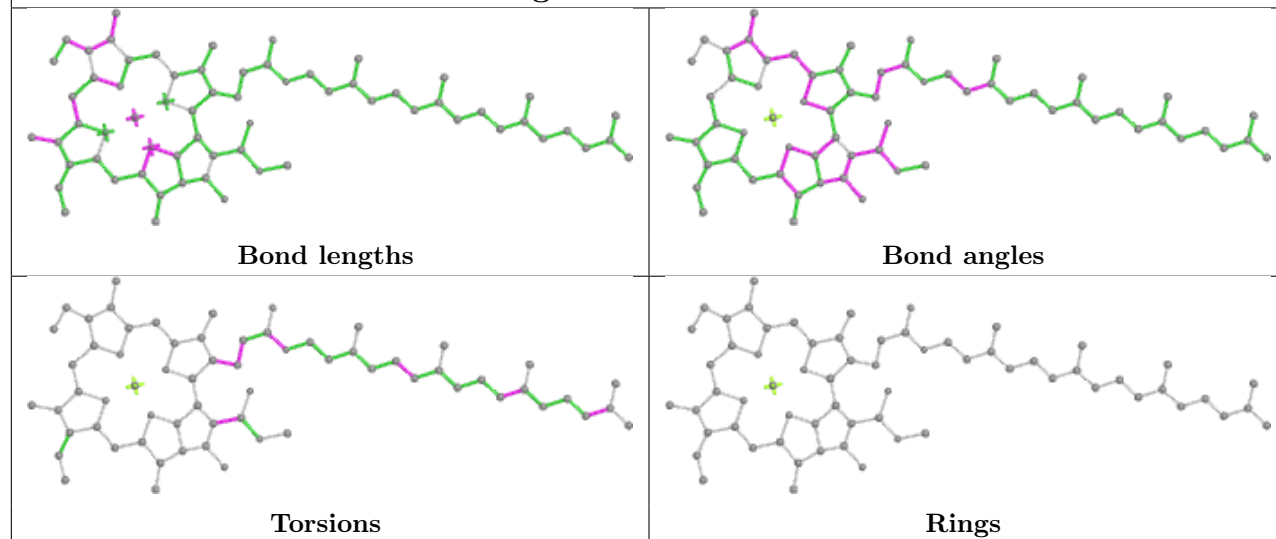




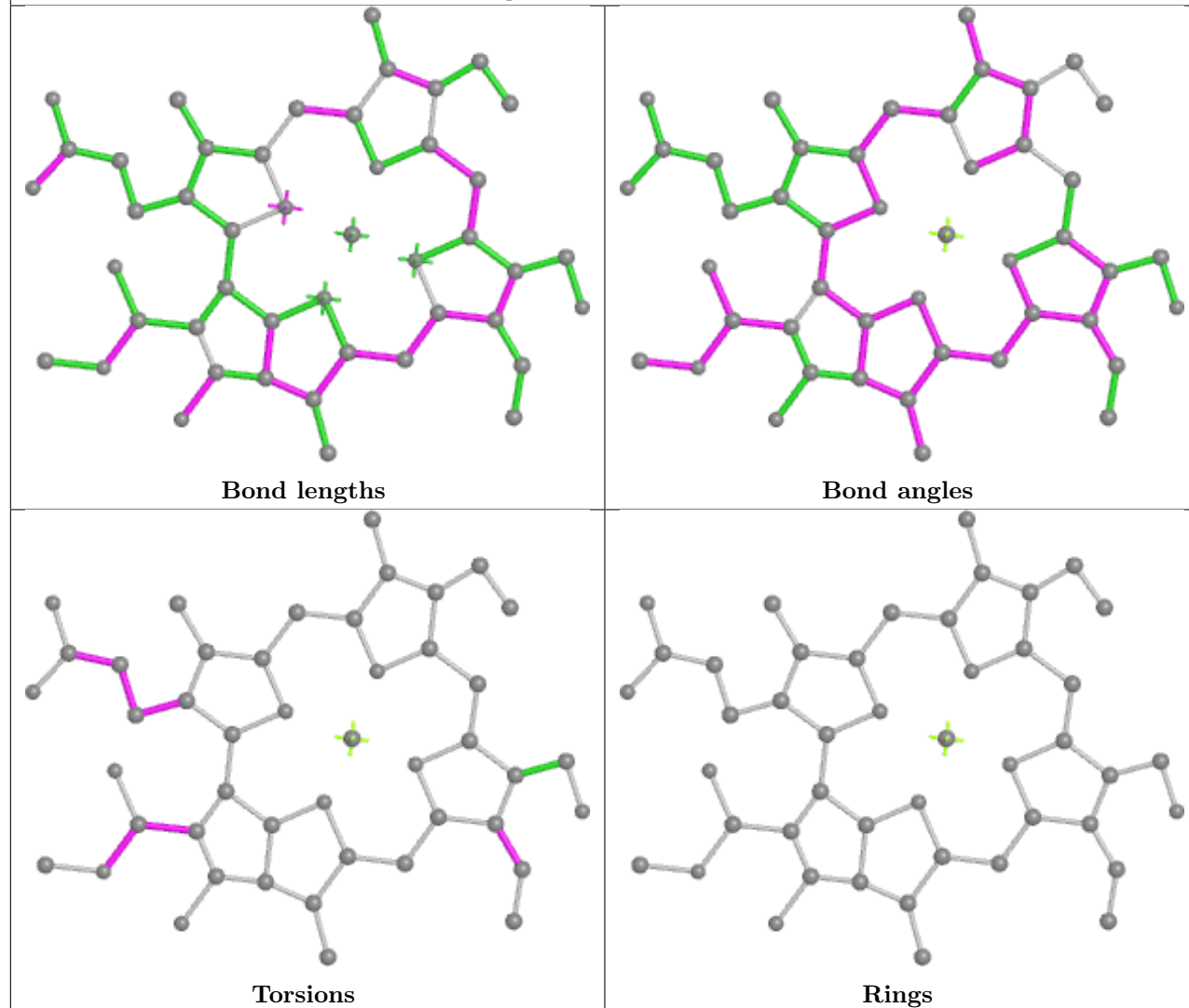


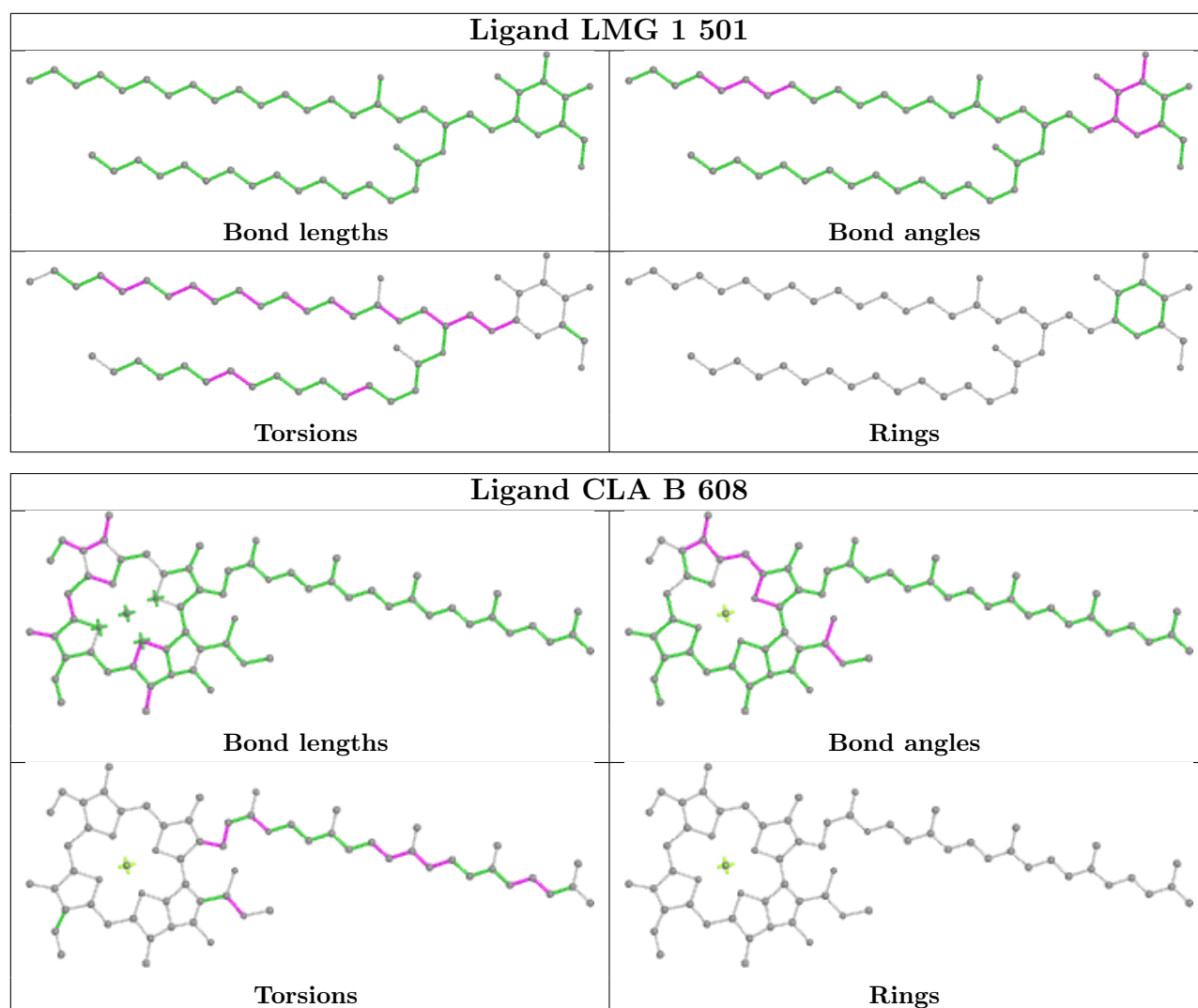


Ligand CLA C 511

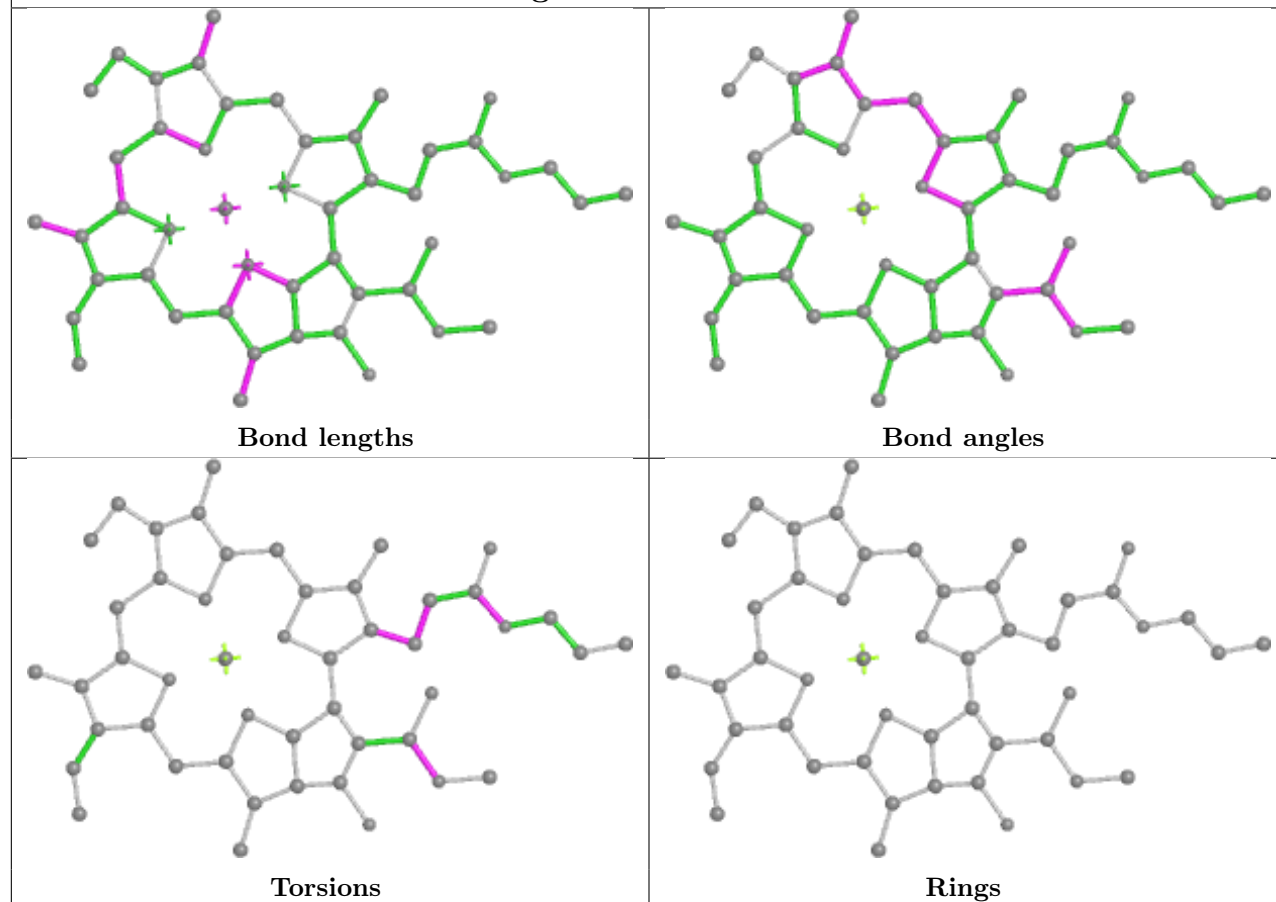


Ligand CHL s 607

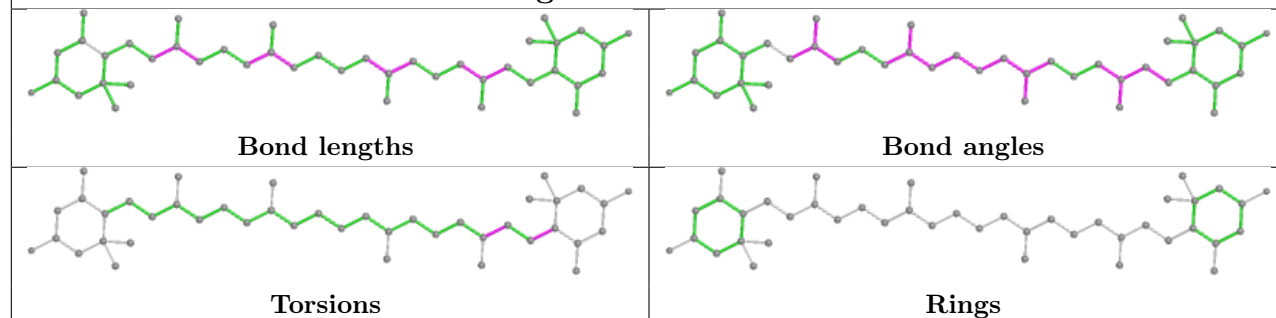




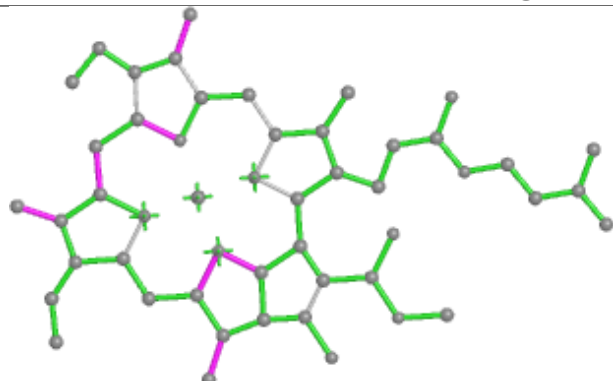
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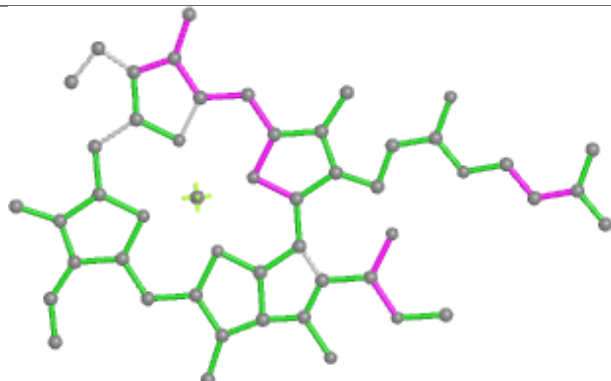
Ligand LUT 5 615



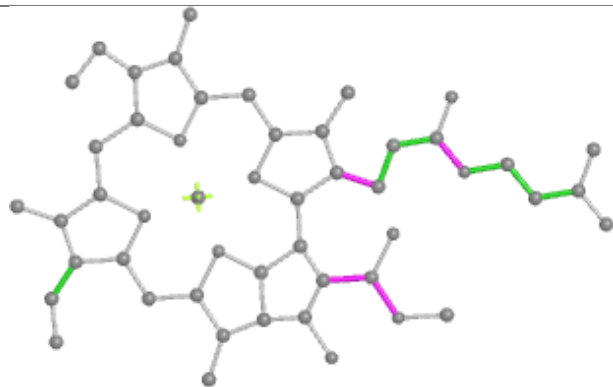
Ligand CLA S 604



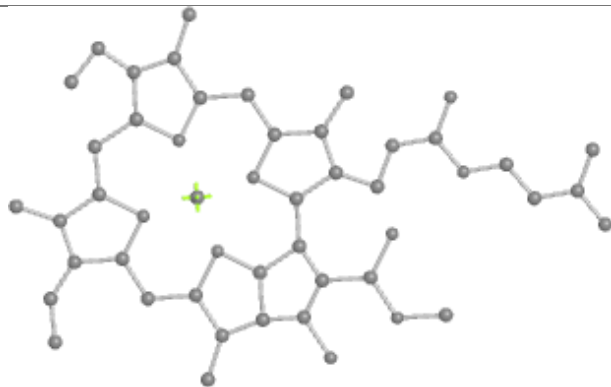
Bond lengths



Bond angles

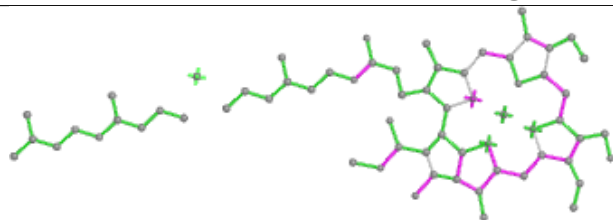


Torsions

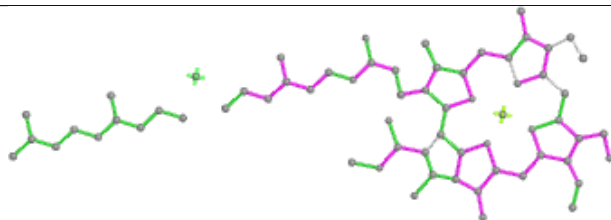


Rings

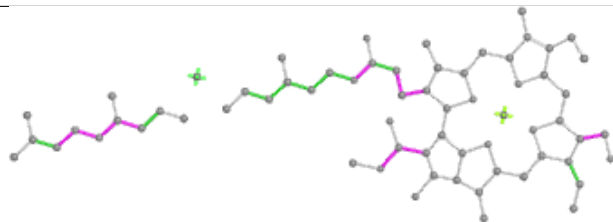
Ligand CHL Ba 309



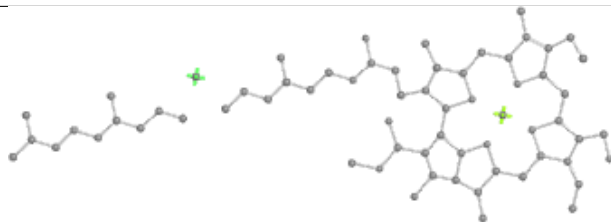
Bond lengths



Bond angles

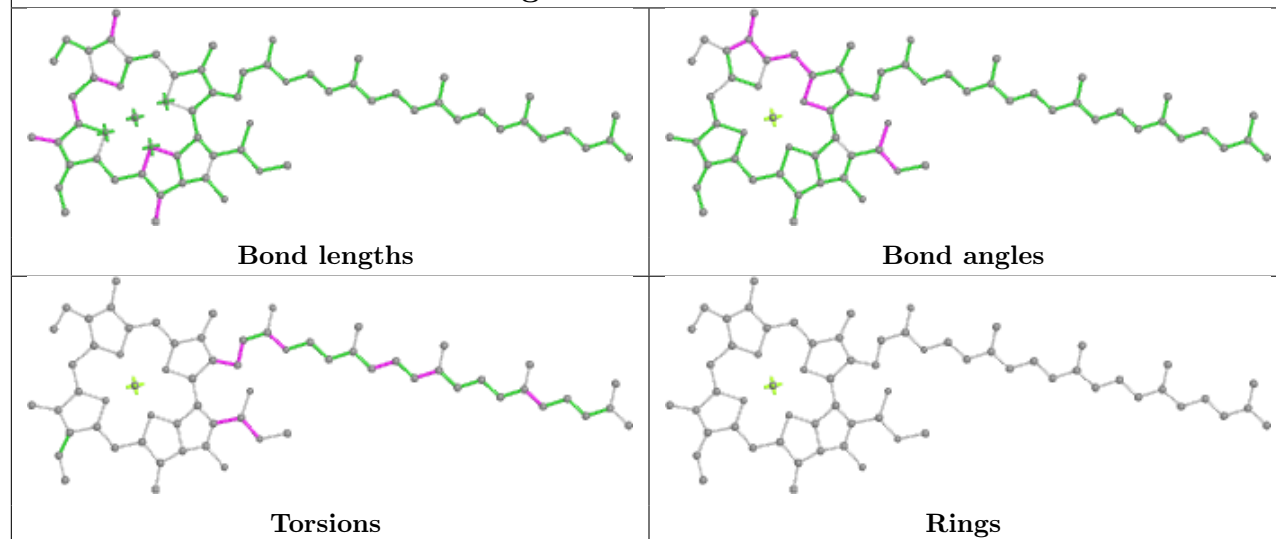


Torsions

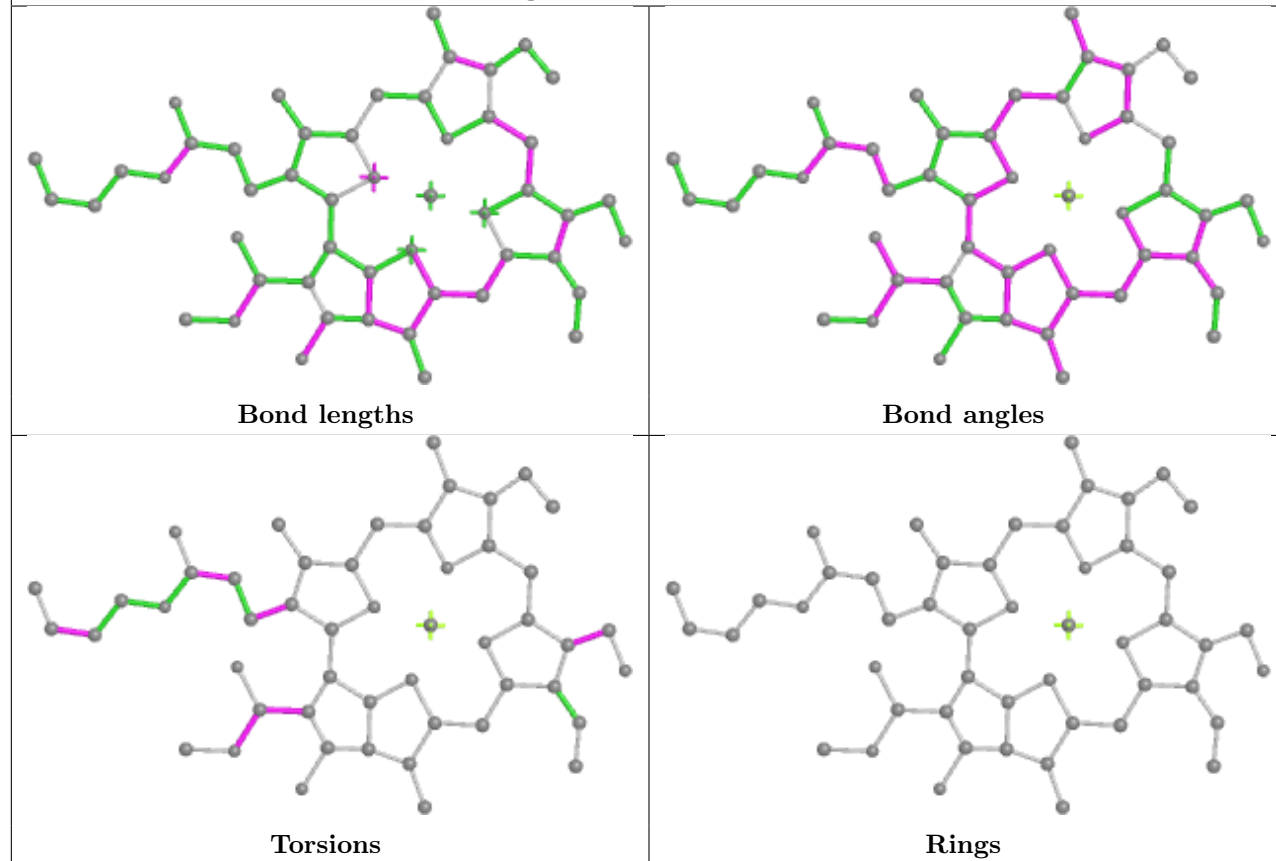


Rings

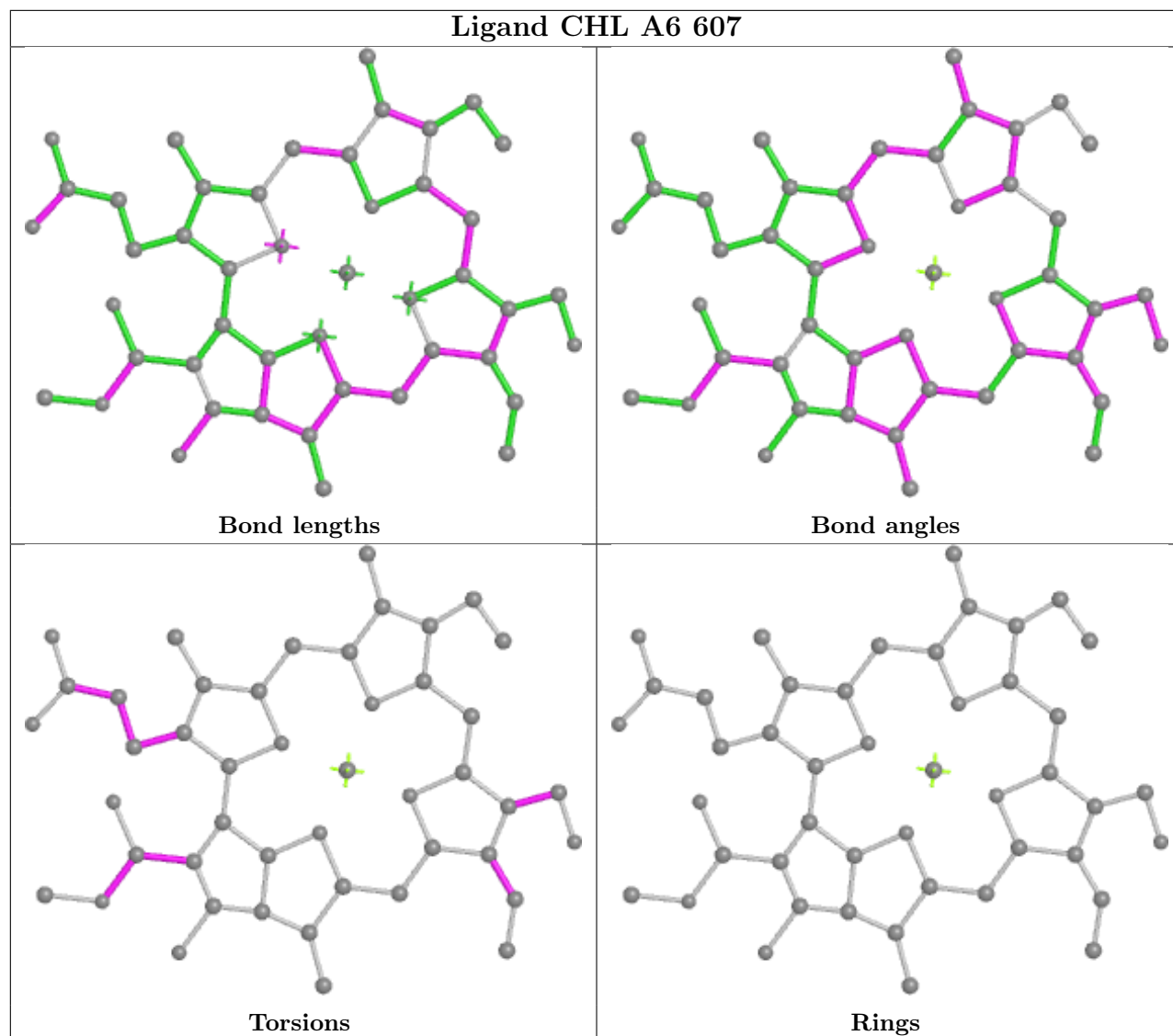
Ligand CLA Au 613

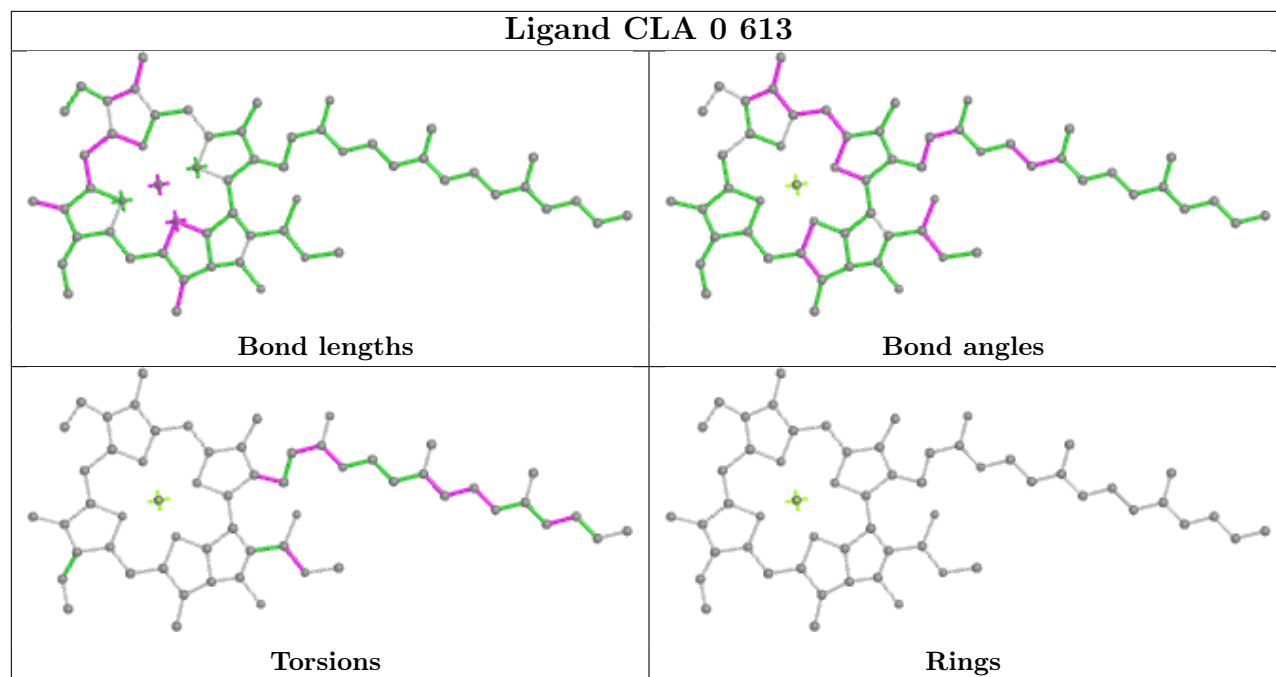
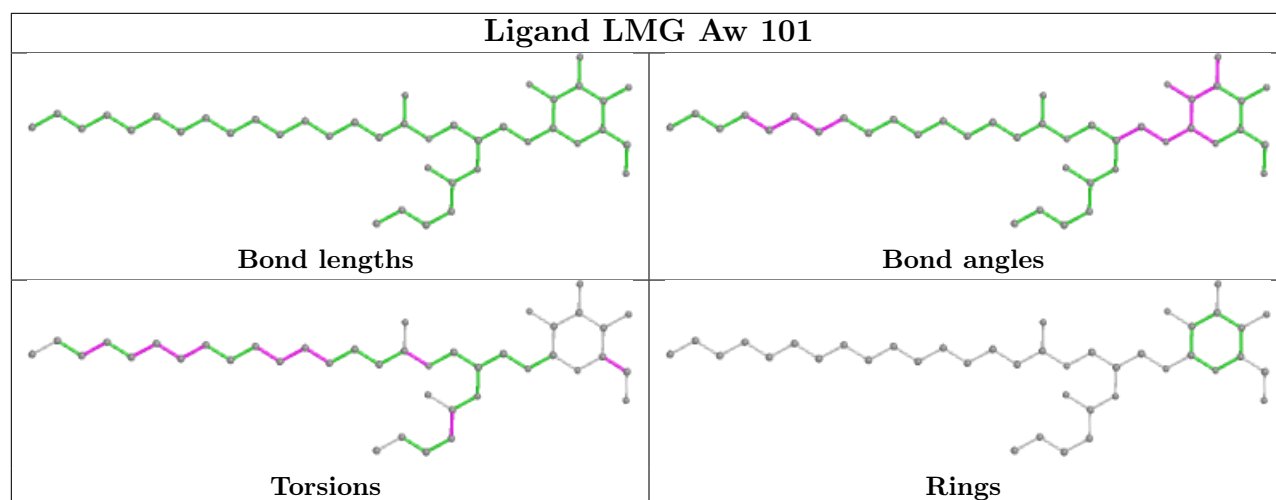
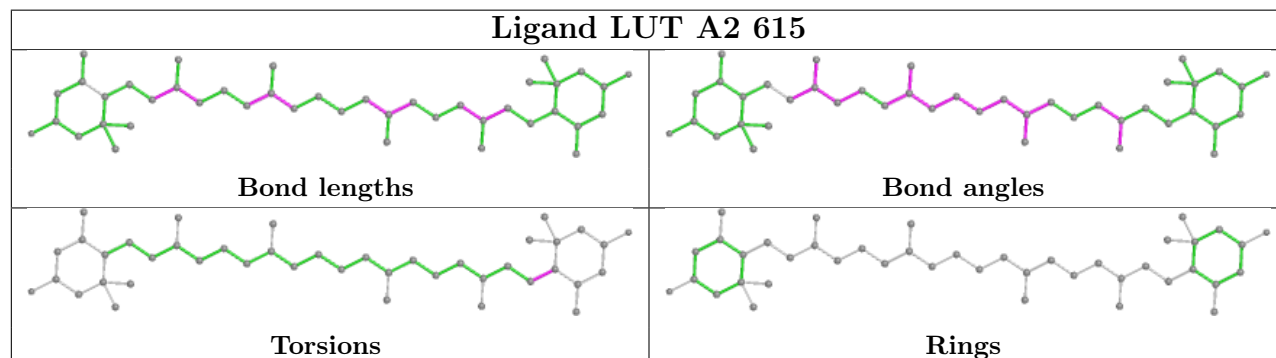


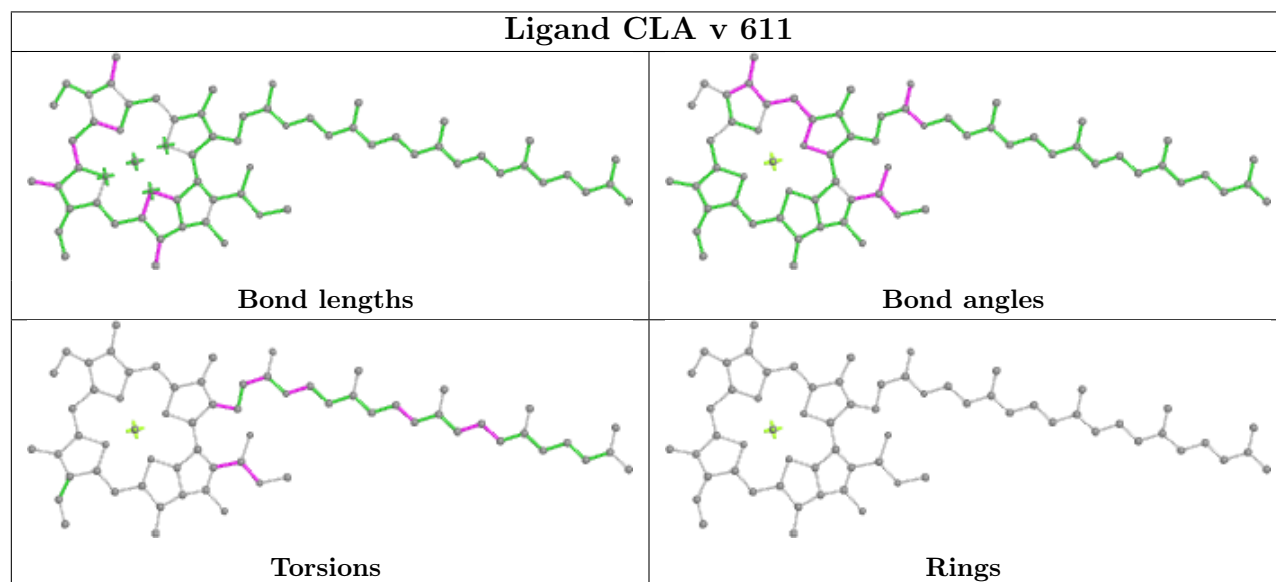
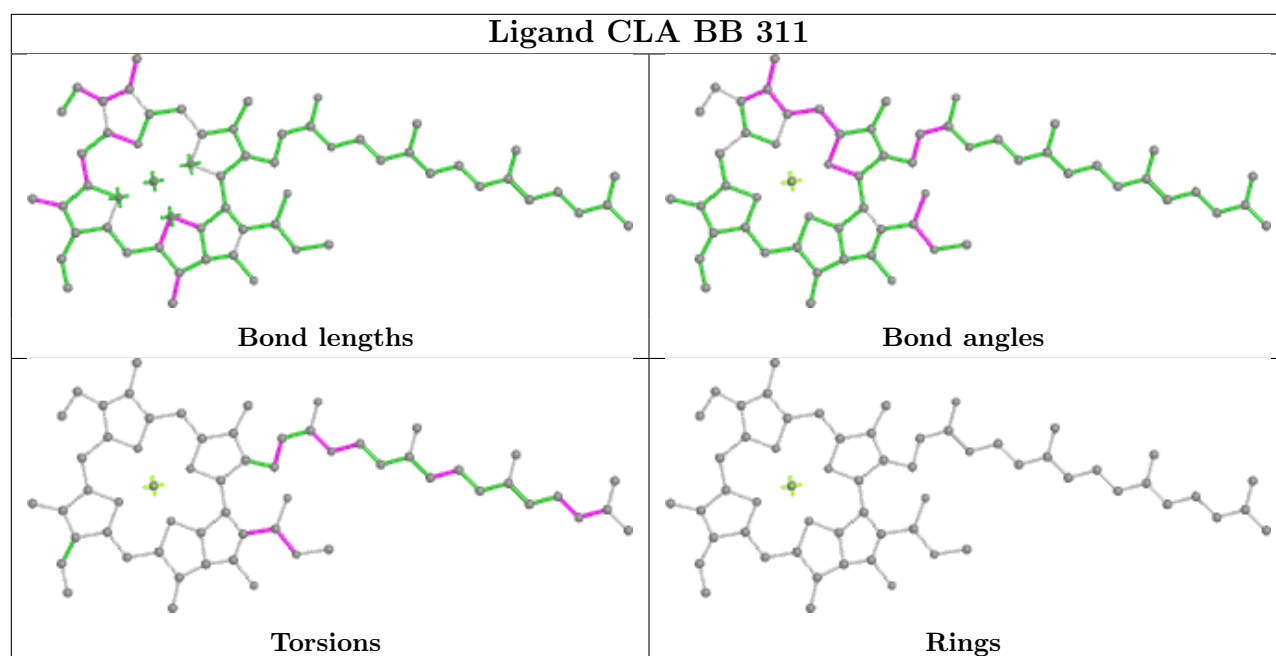
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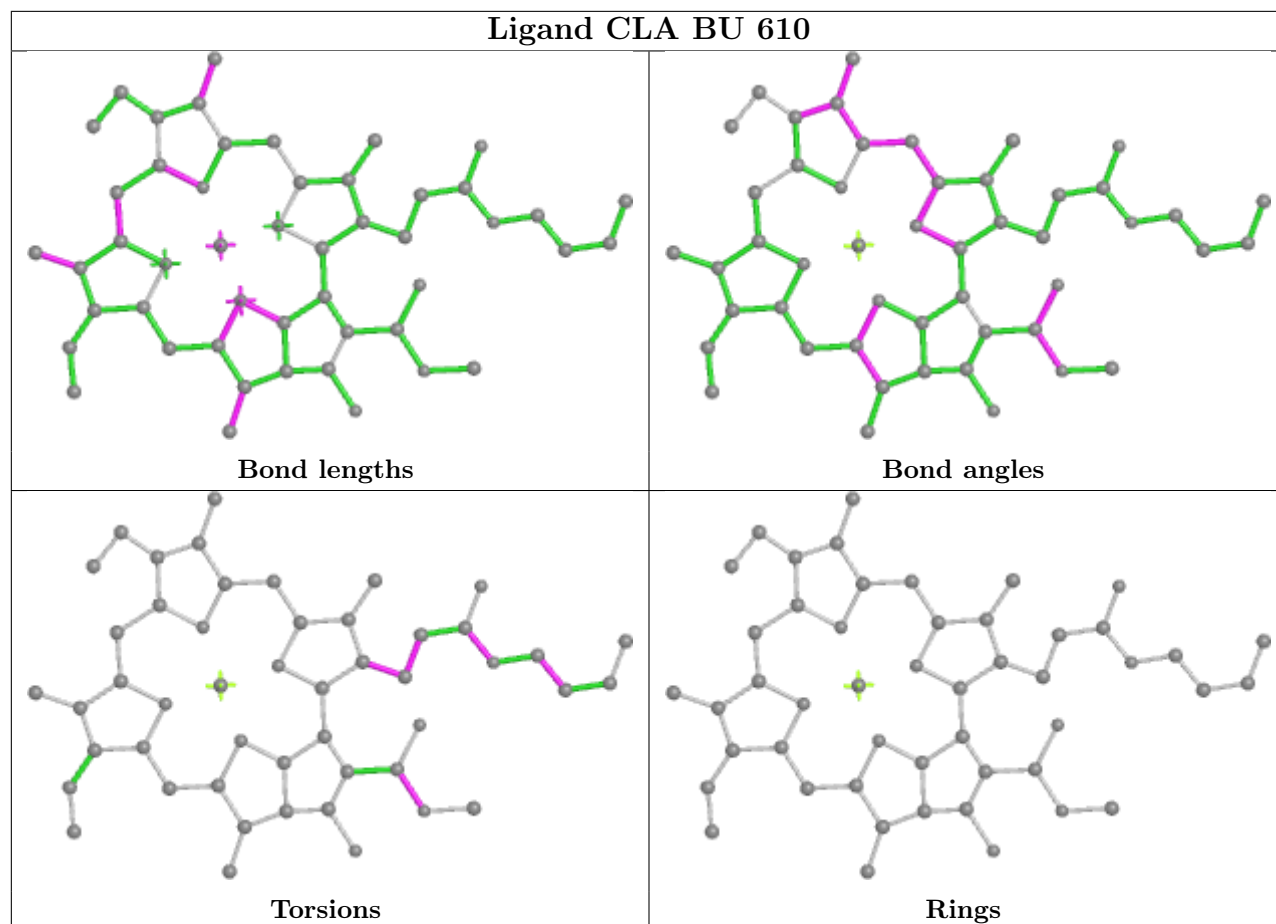
Ligand CHL A6 607



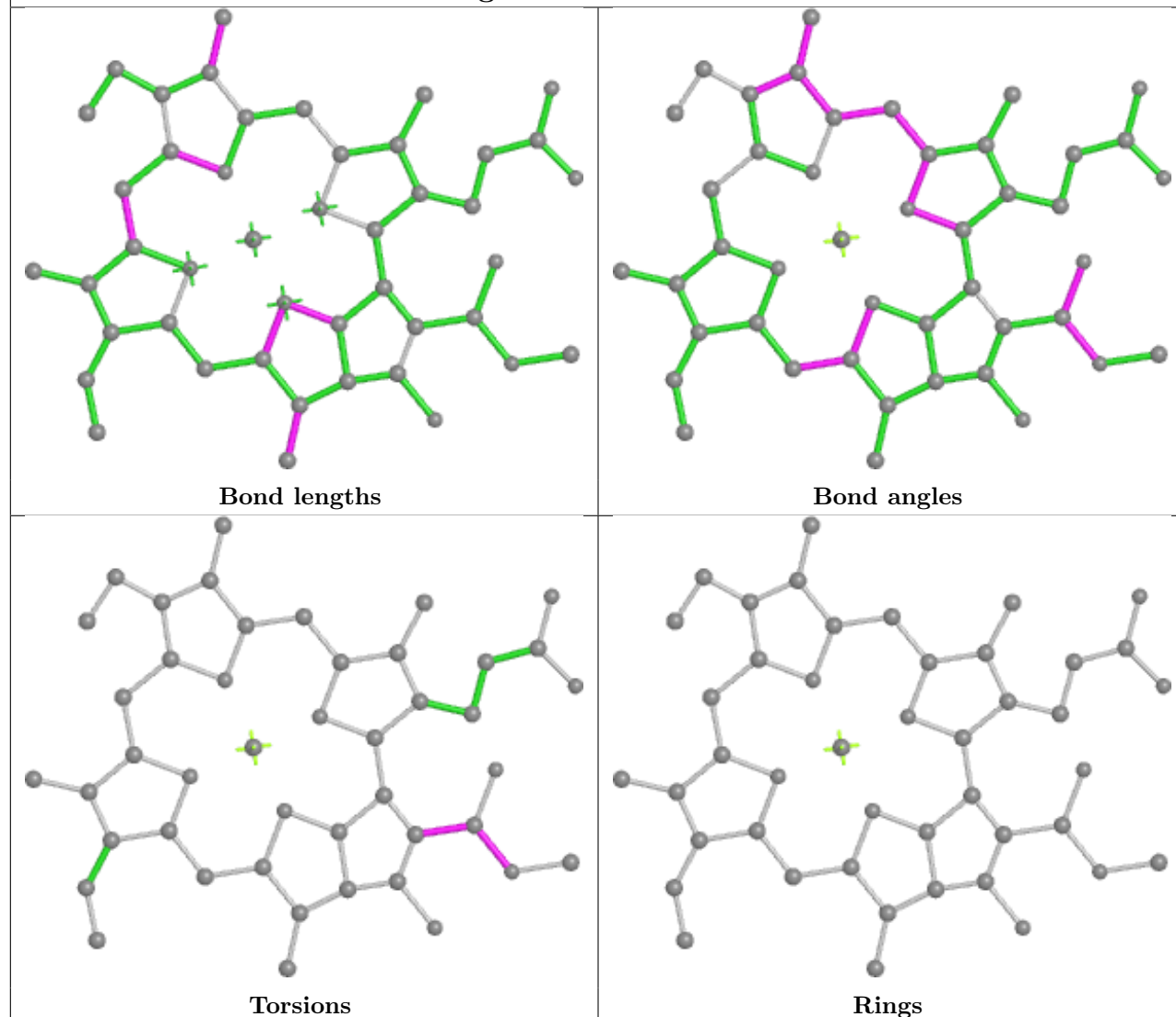
Ligand CLA 0 613**Ligand LMG Aw 101****Ligand LUT A2 615**



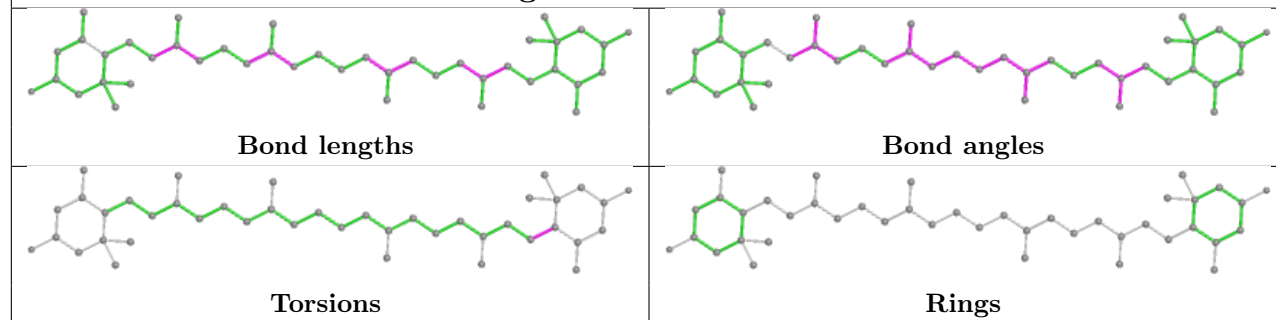
Ligand CLA BU 610

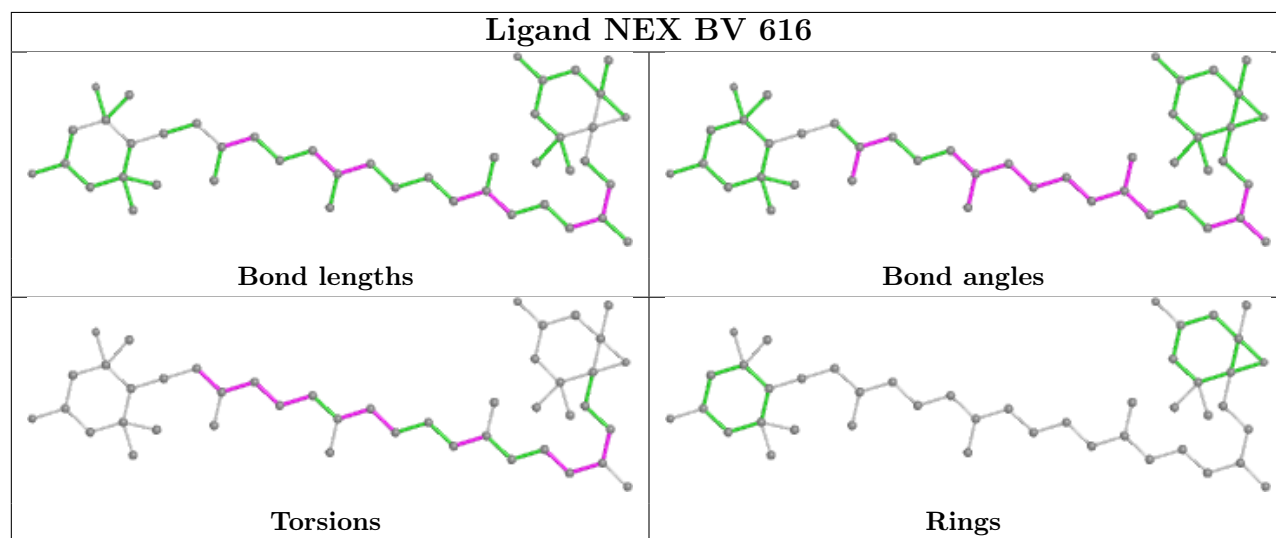
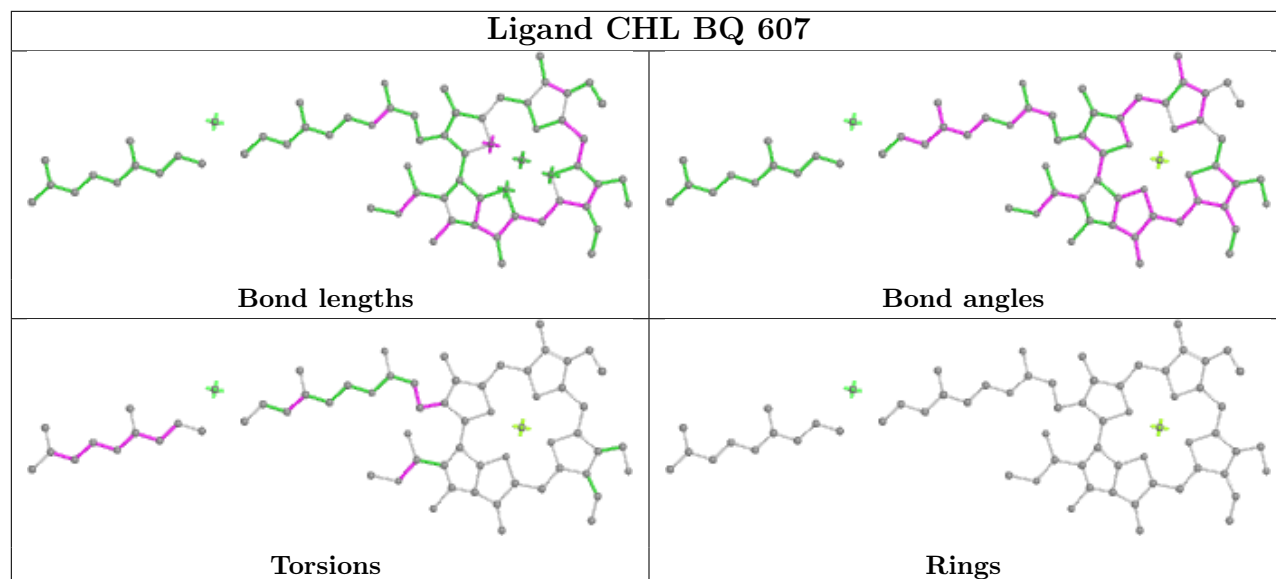
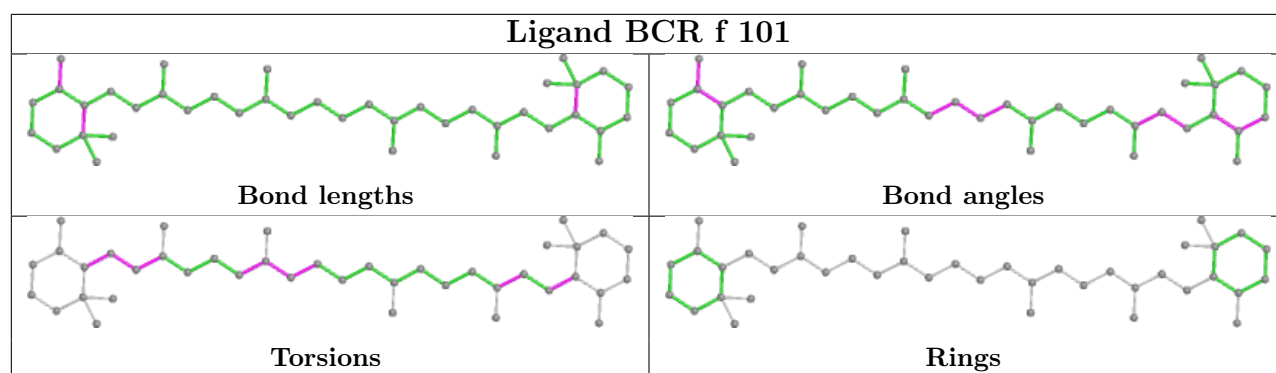


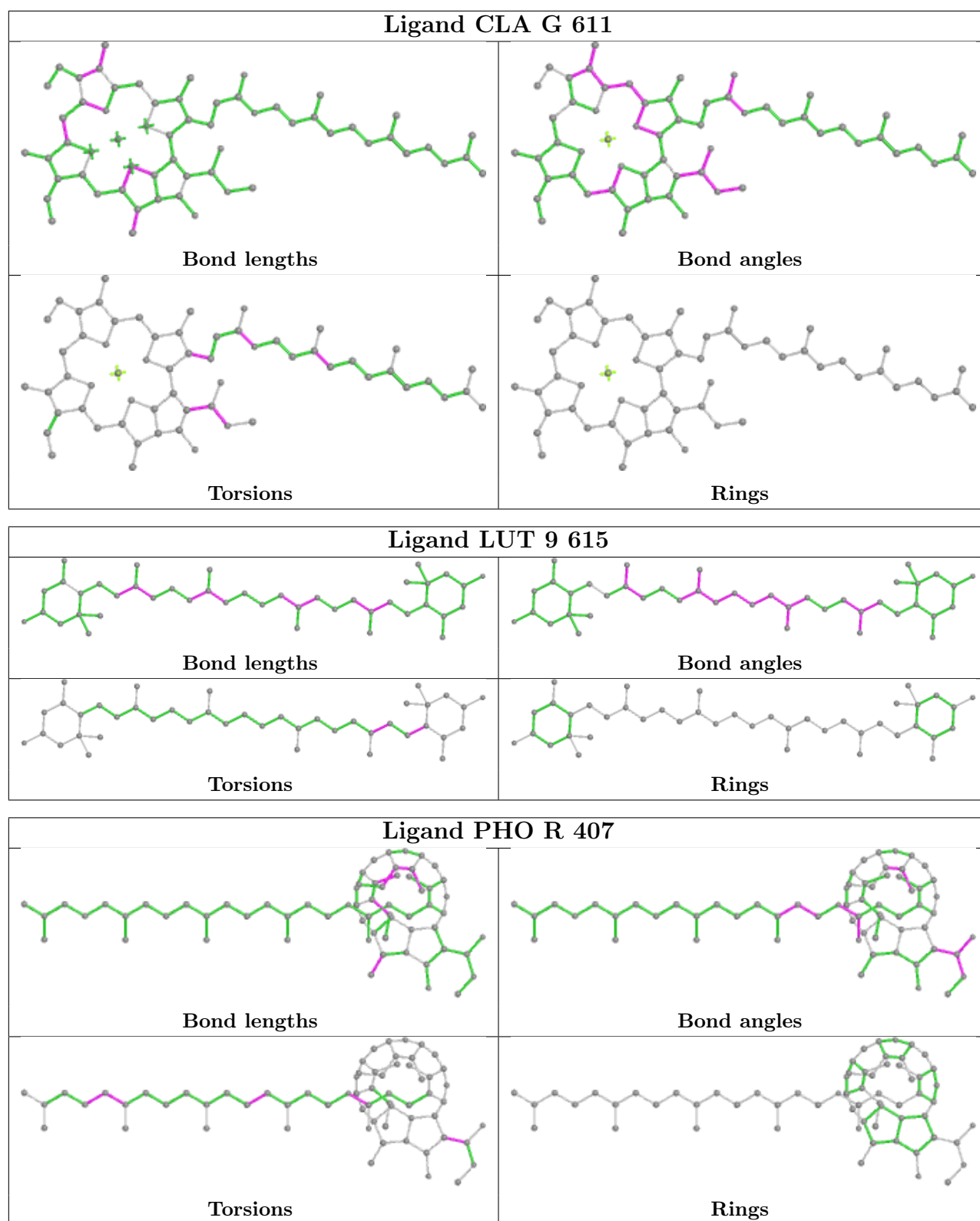
Ligand CLA BV 603

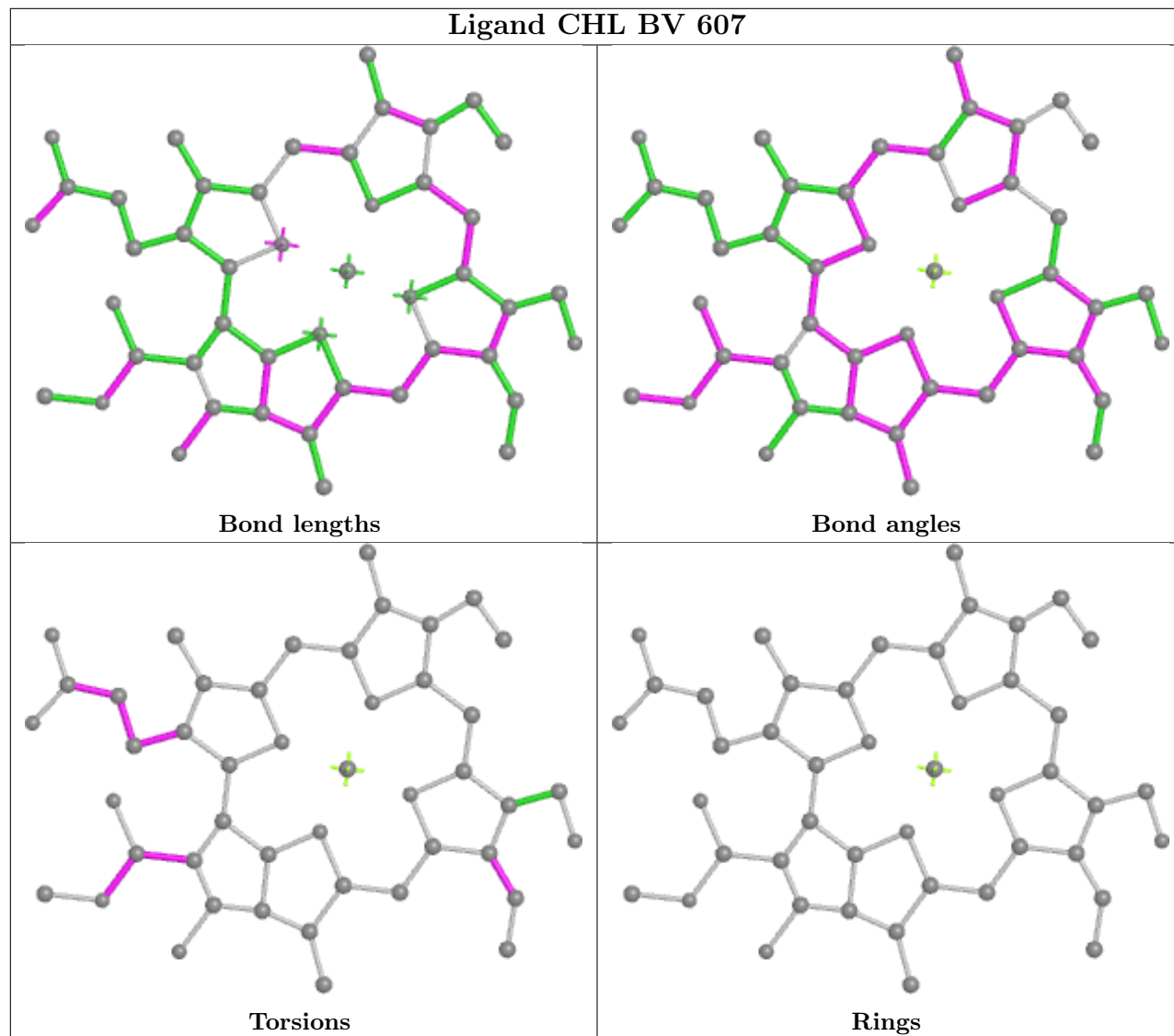
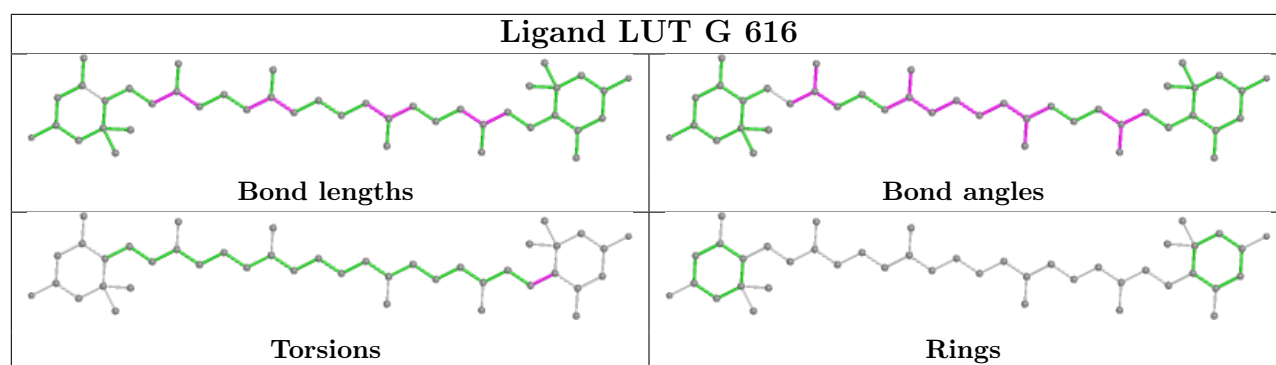


Ligand LUT AB 311

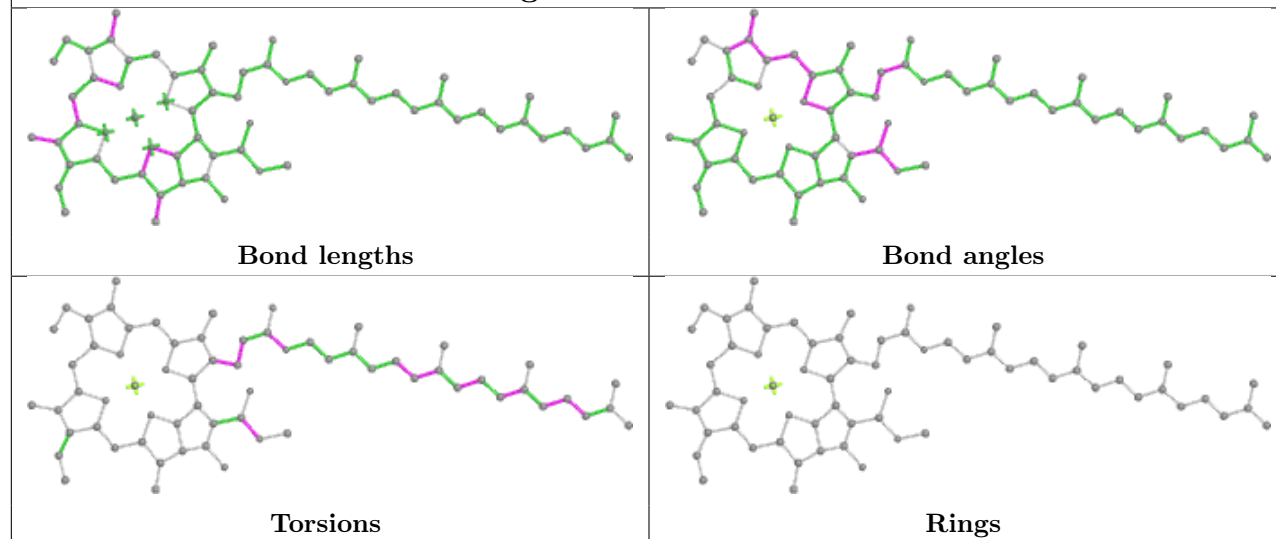




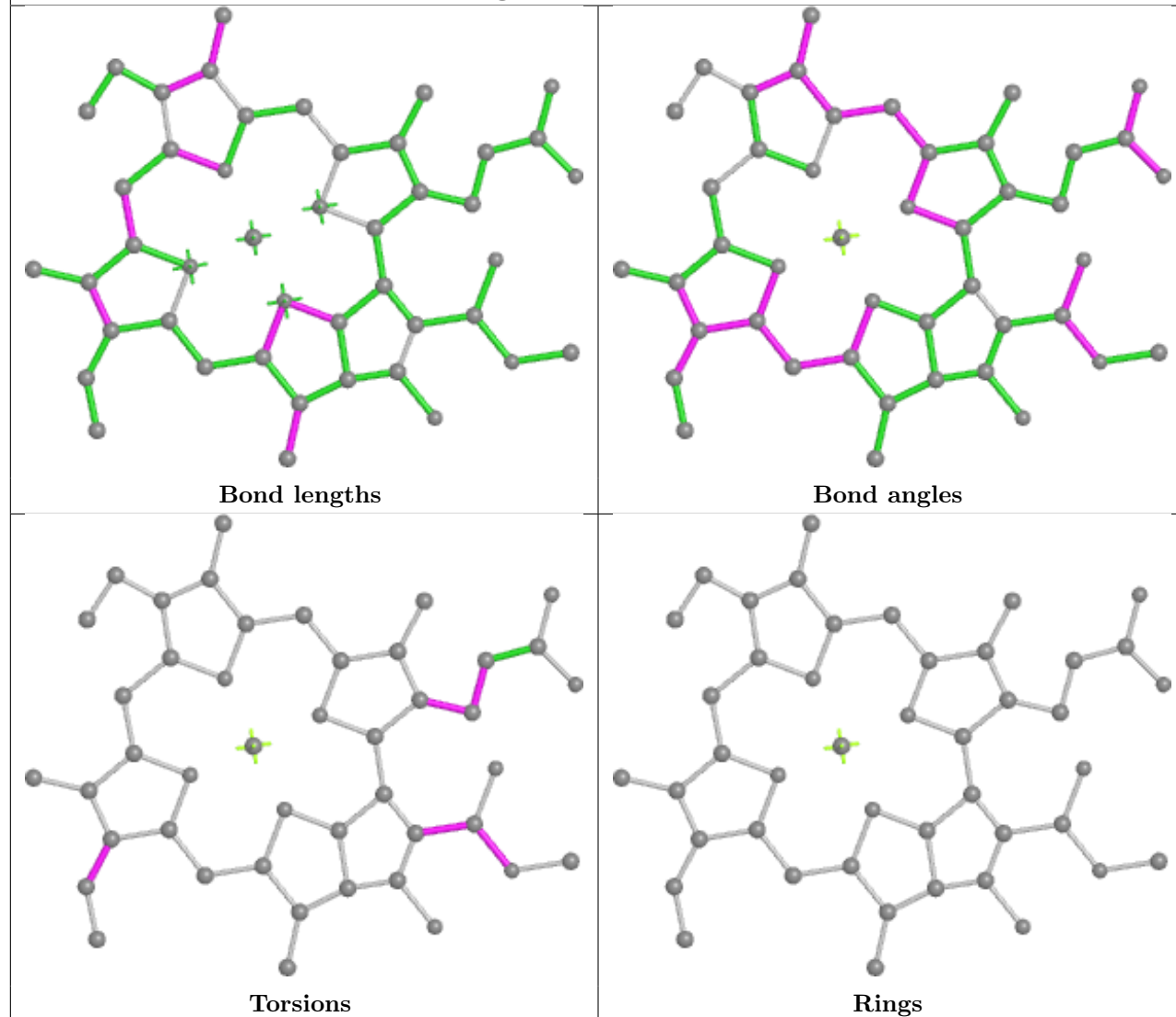


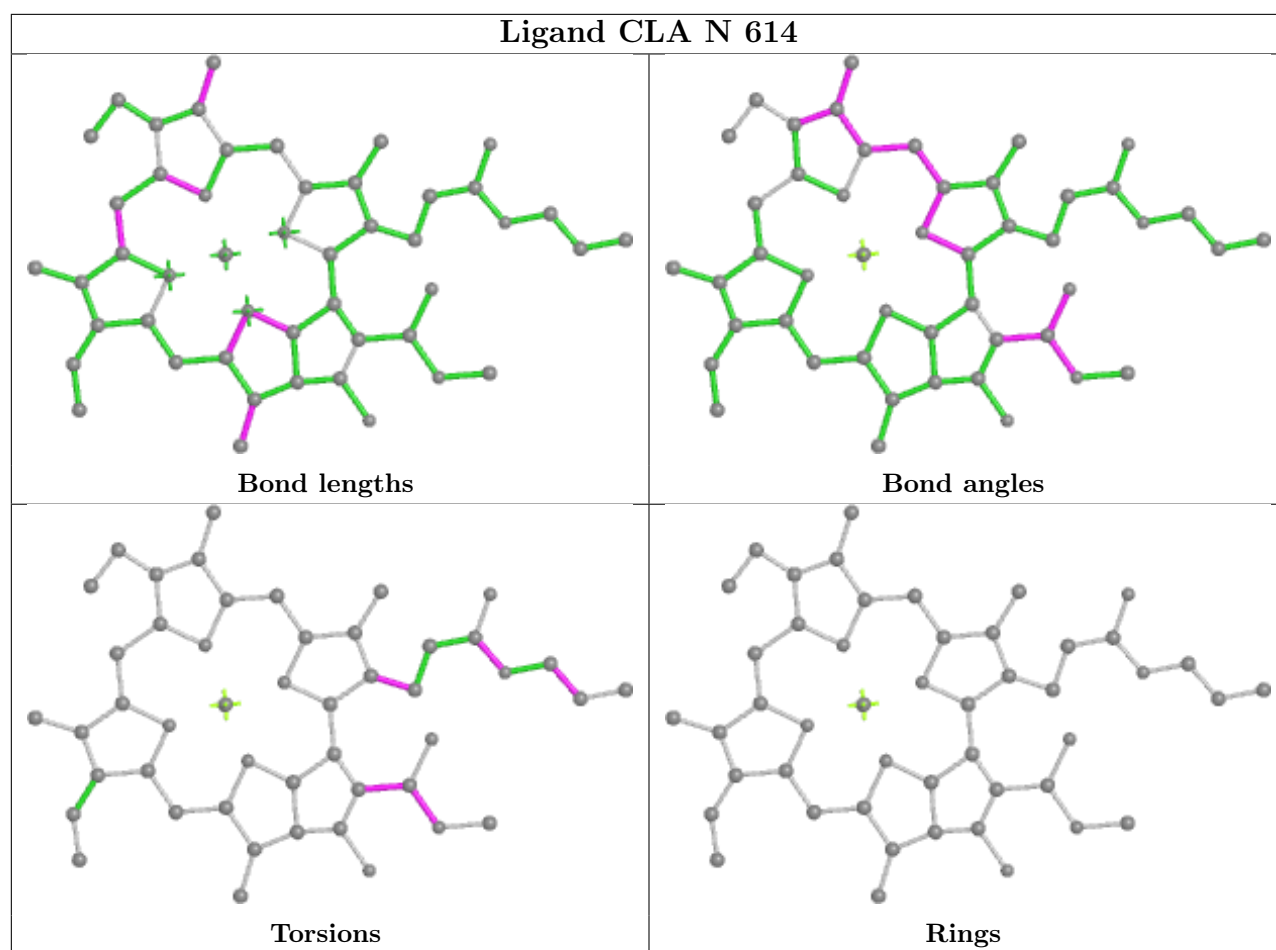


Ligand CLA BE 609

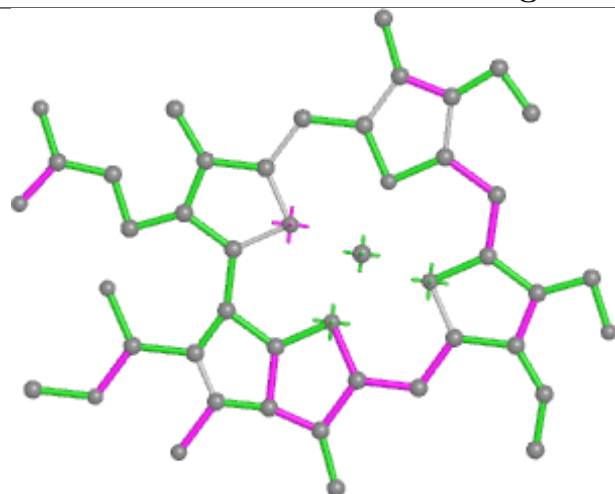


Ligand CLA 6 604

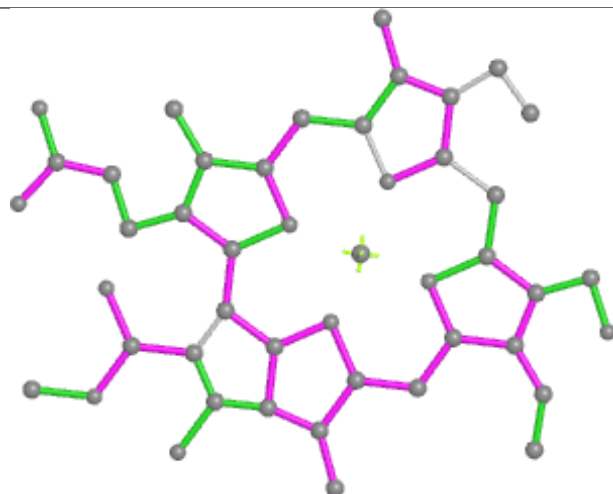




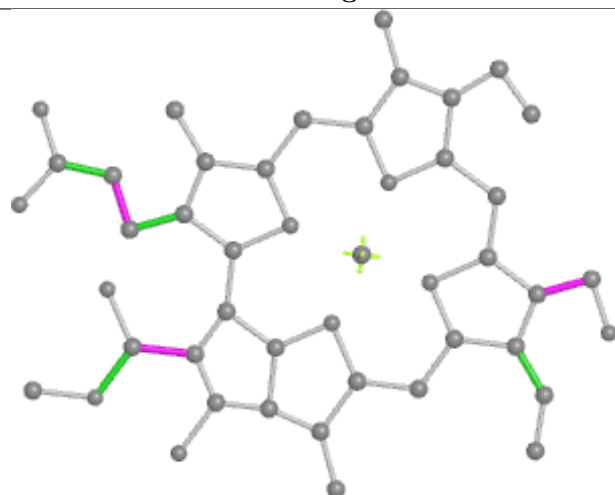
Ligand CHL 9 606



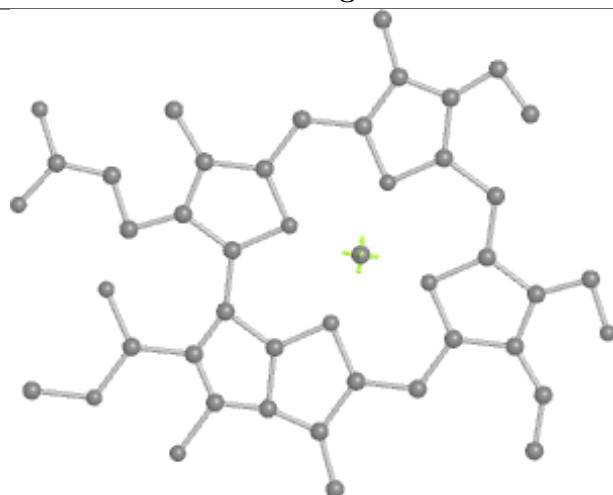
Bond lengths



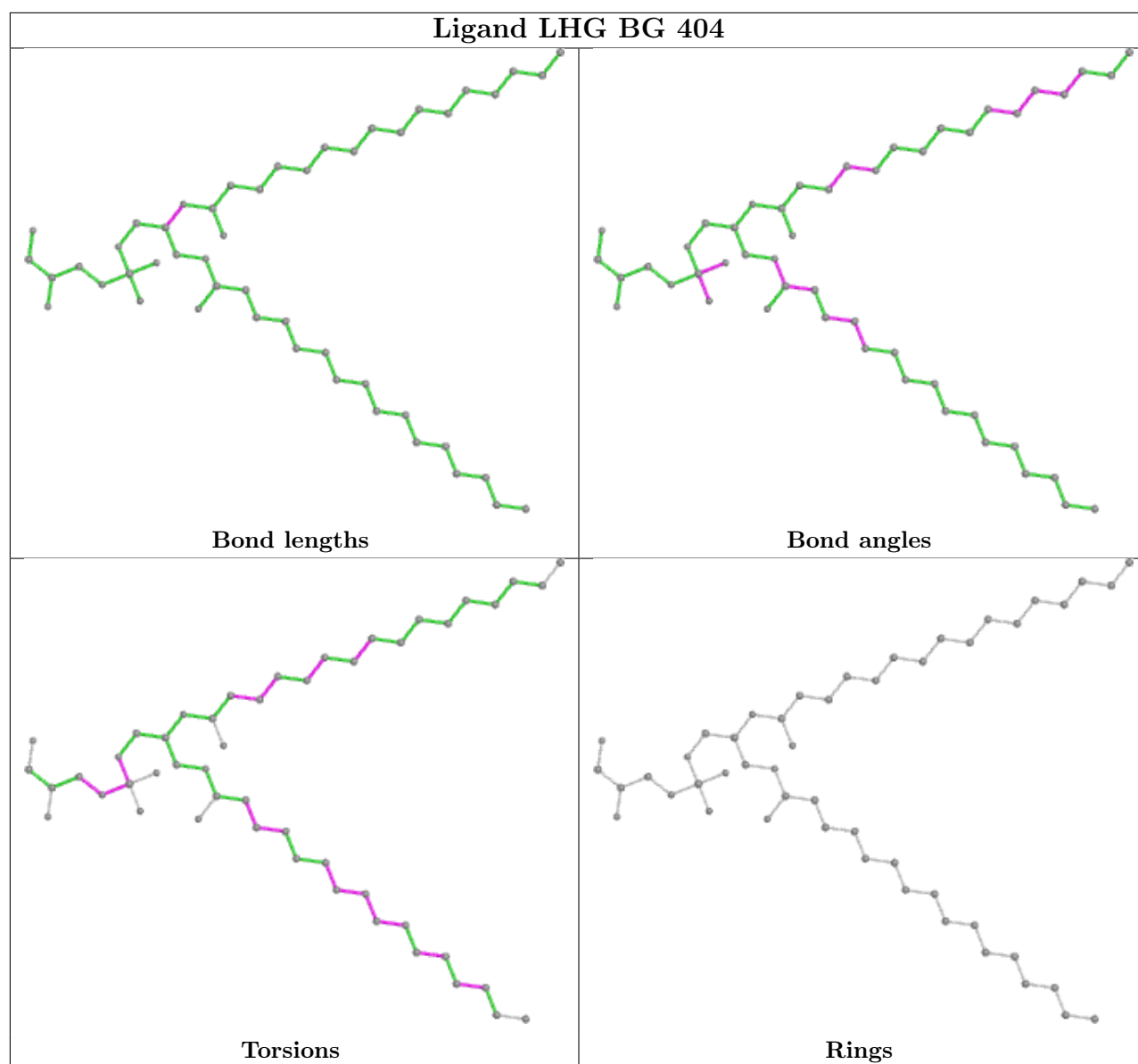
Bond angles



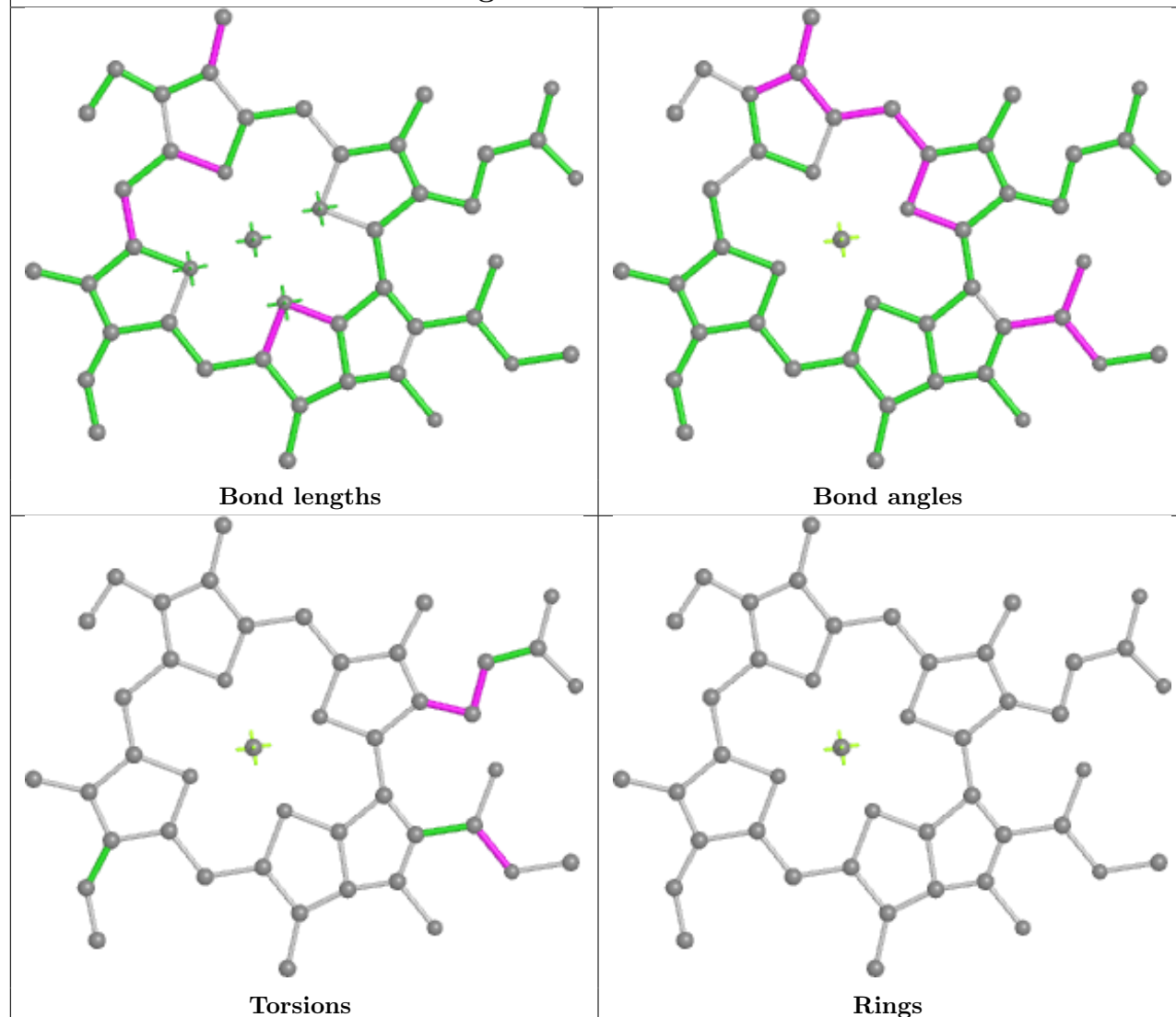
Torsions



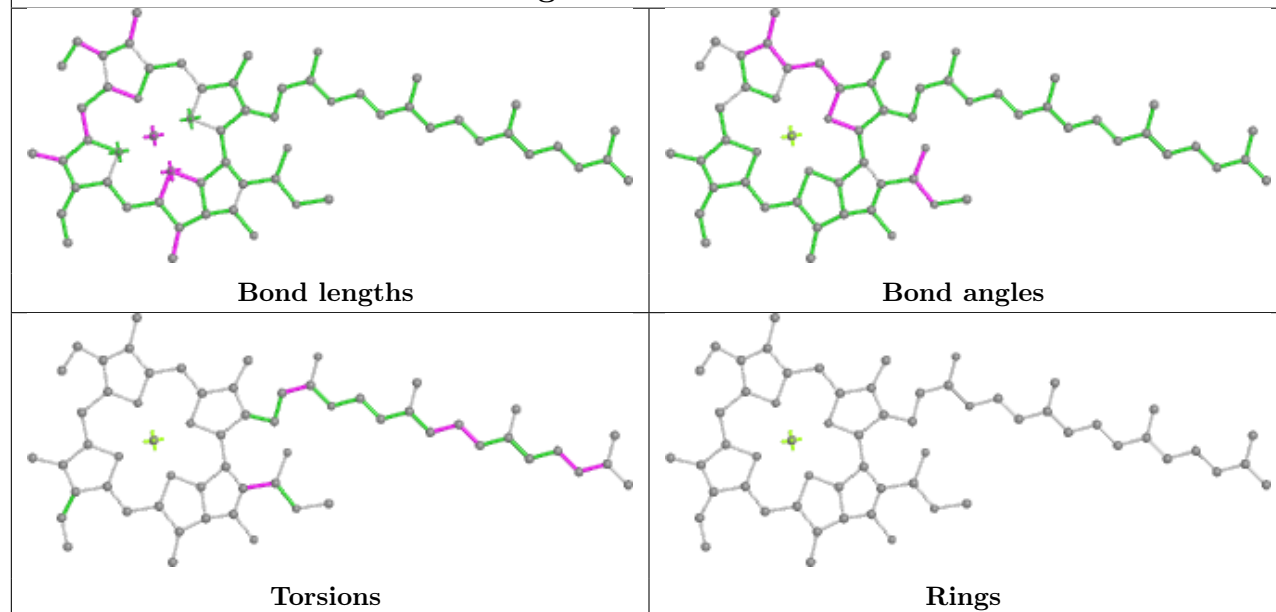
Rings

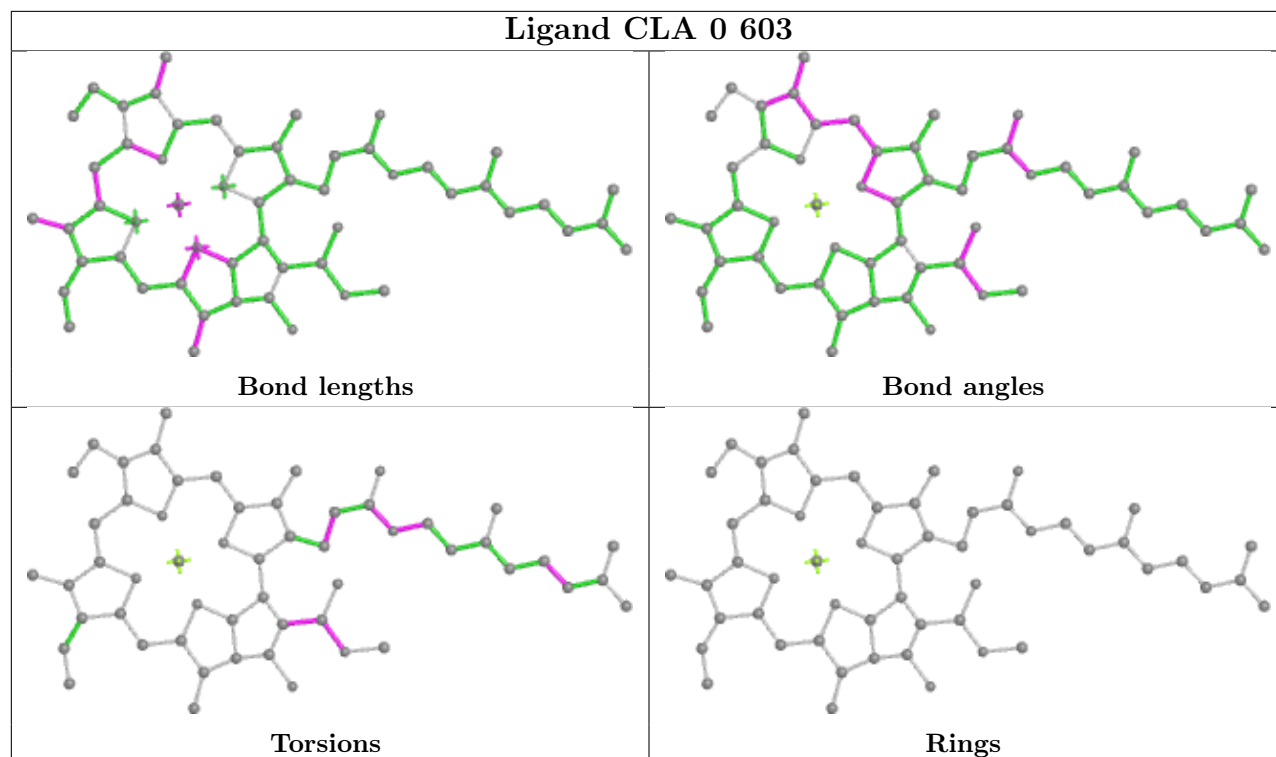
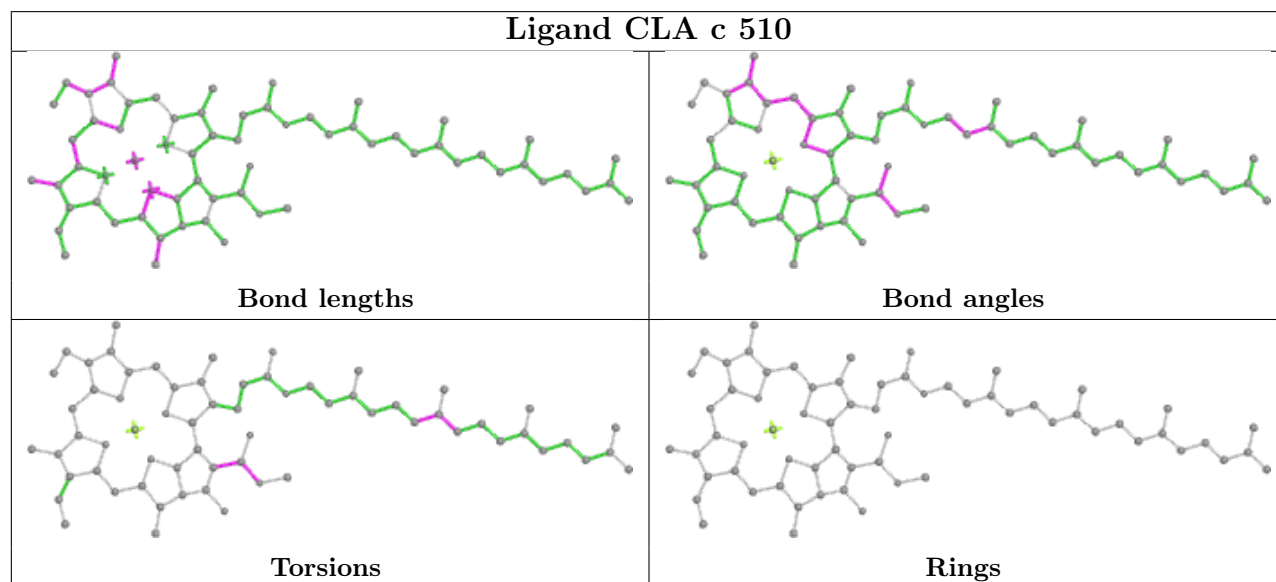


Ligand CLA AB 309

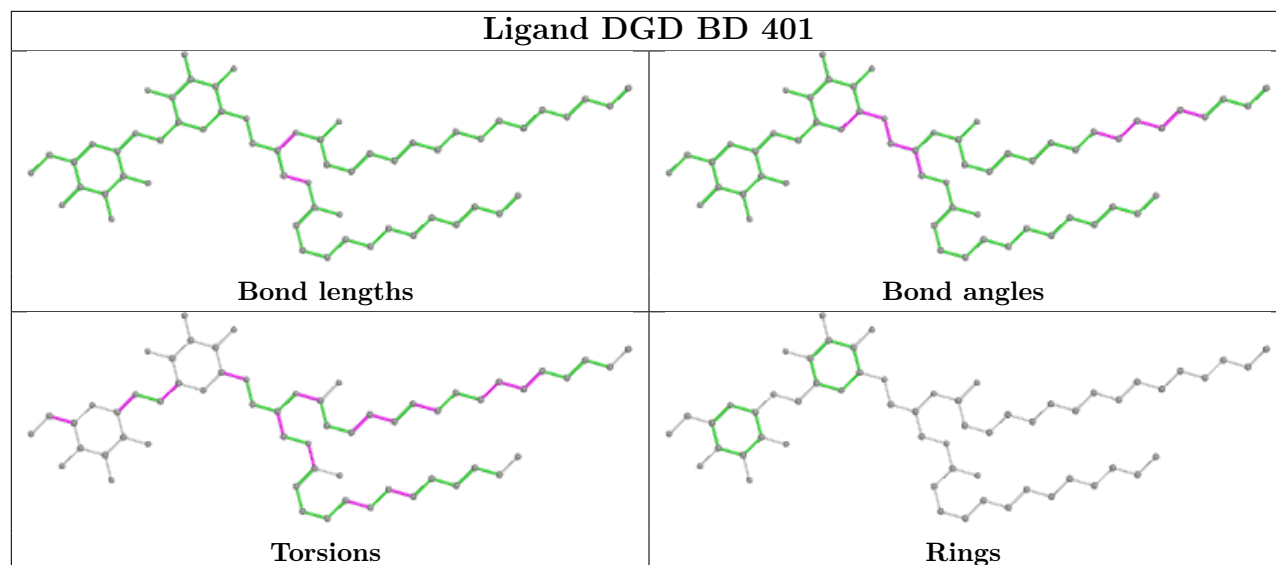


Ligand CLA r 603

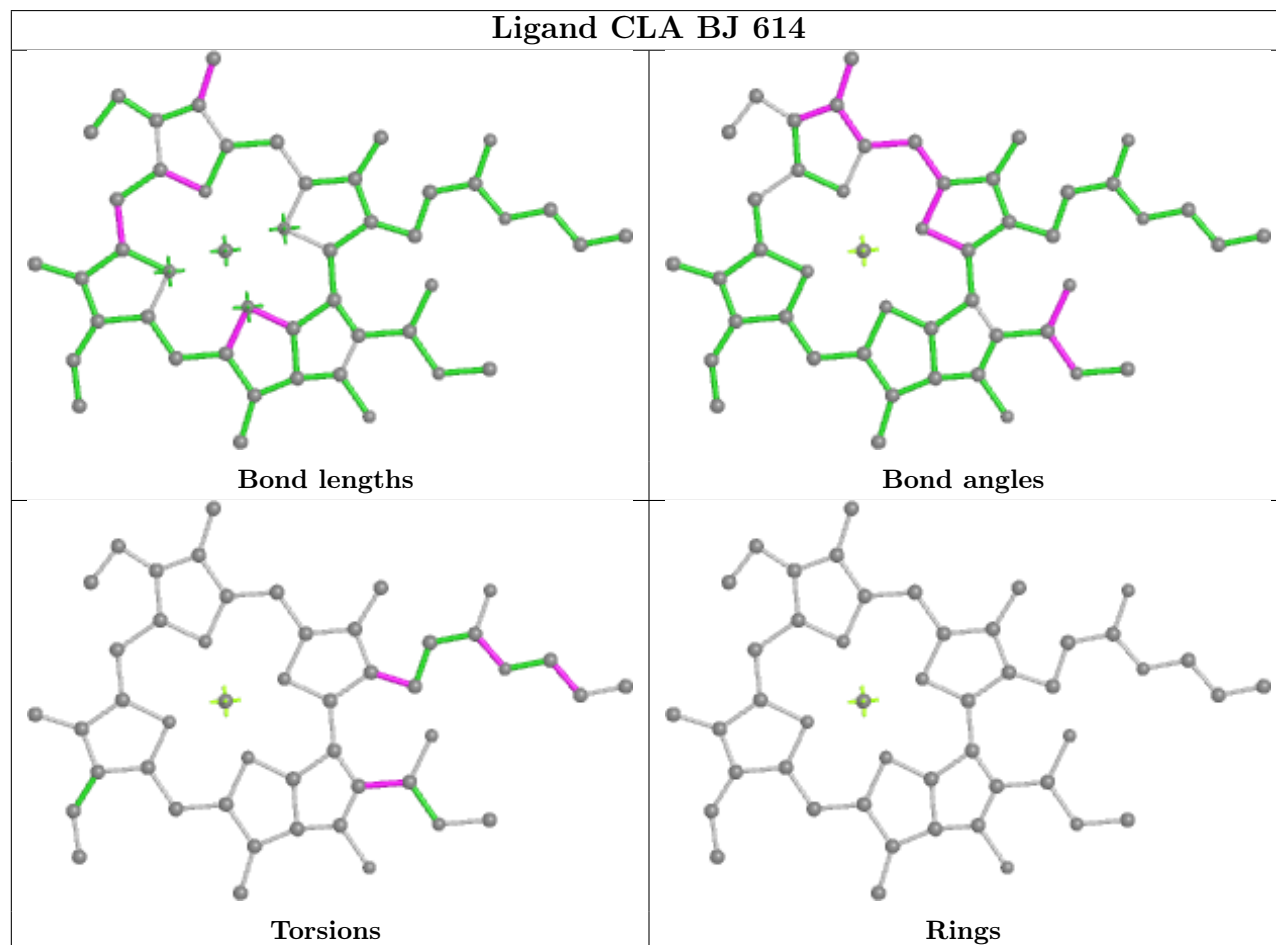


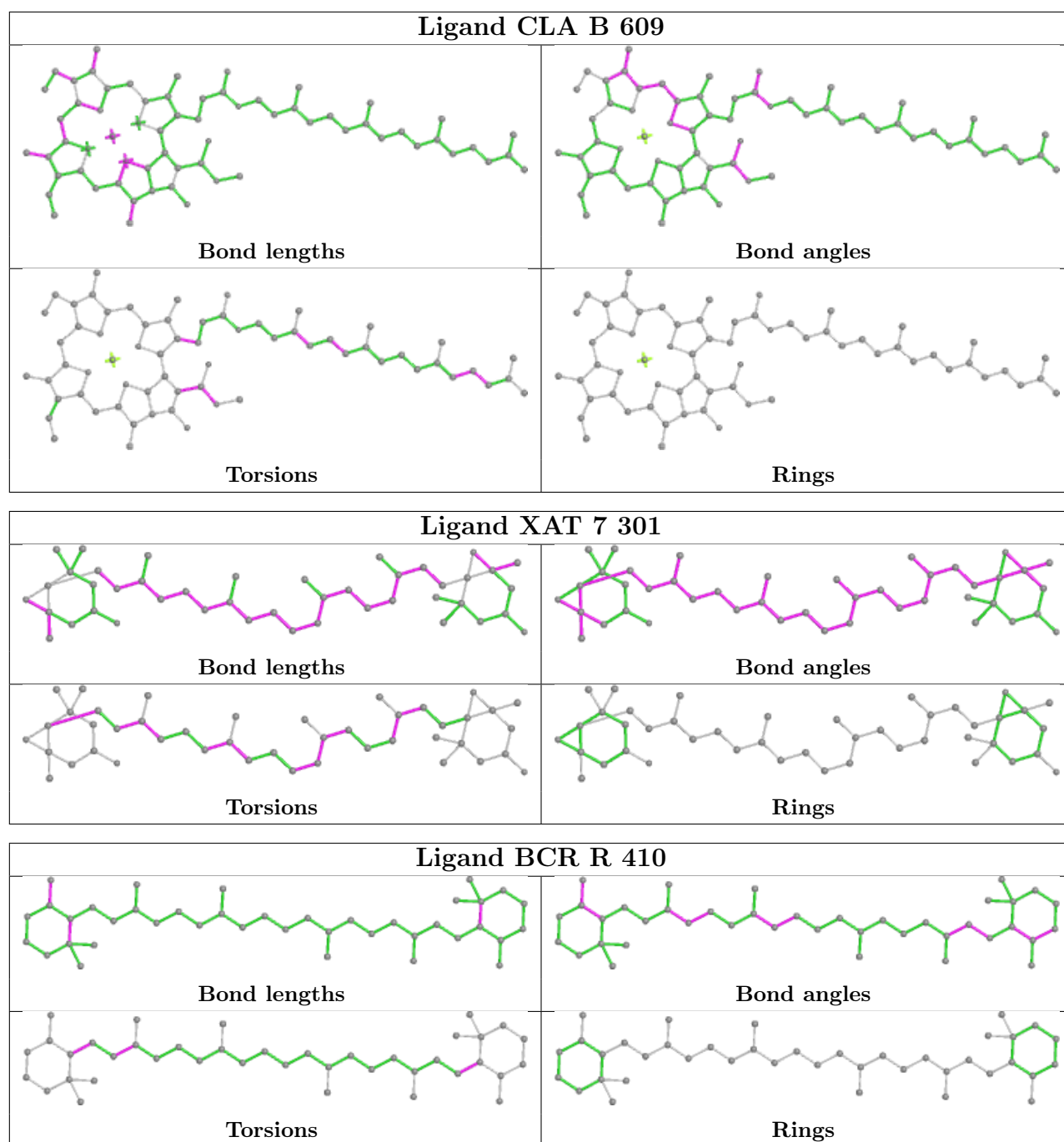
Ligand CLA 0 603**Ligand CLA c 510**

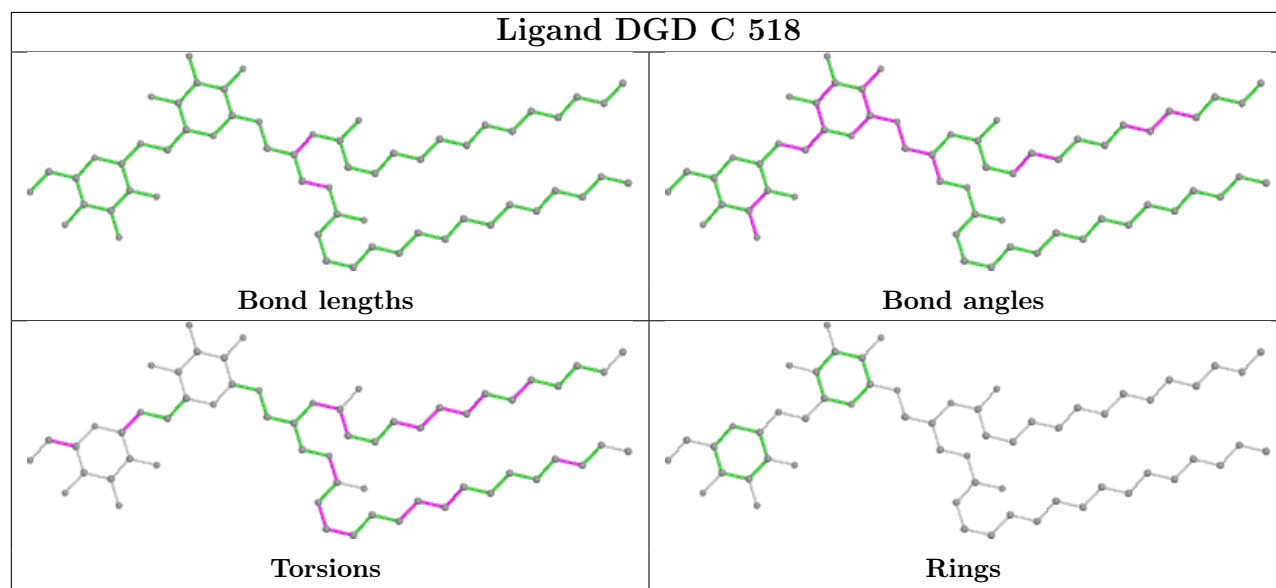
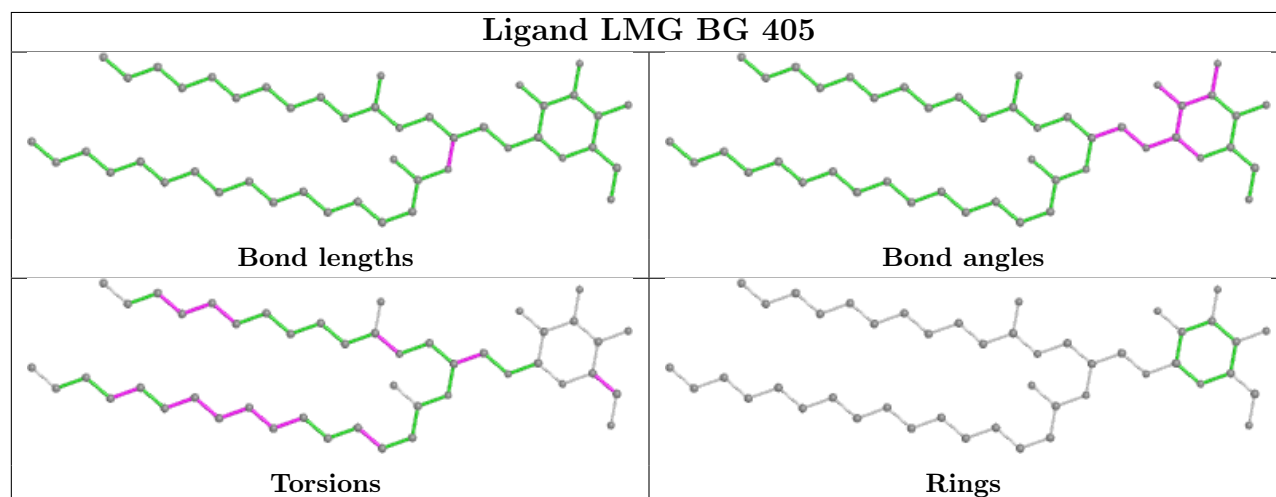
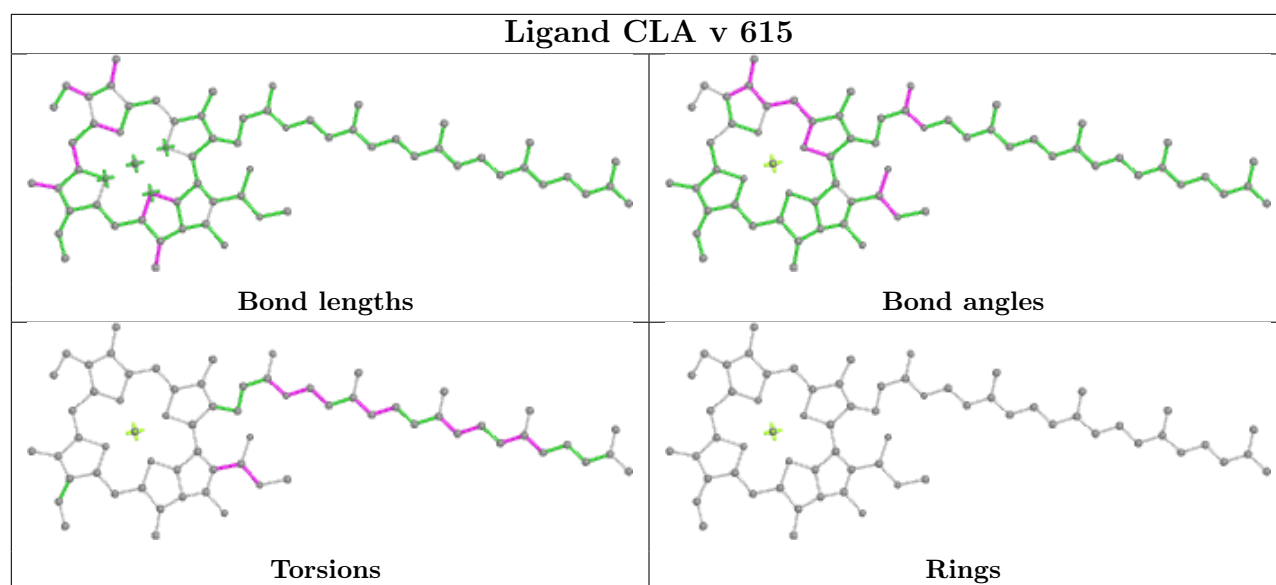
Ligand DGD BD 401

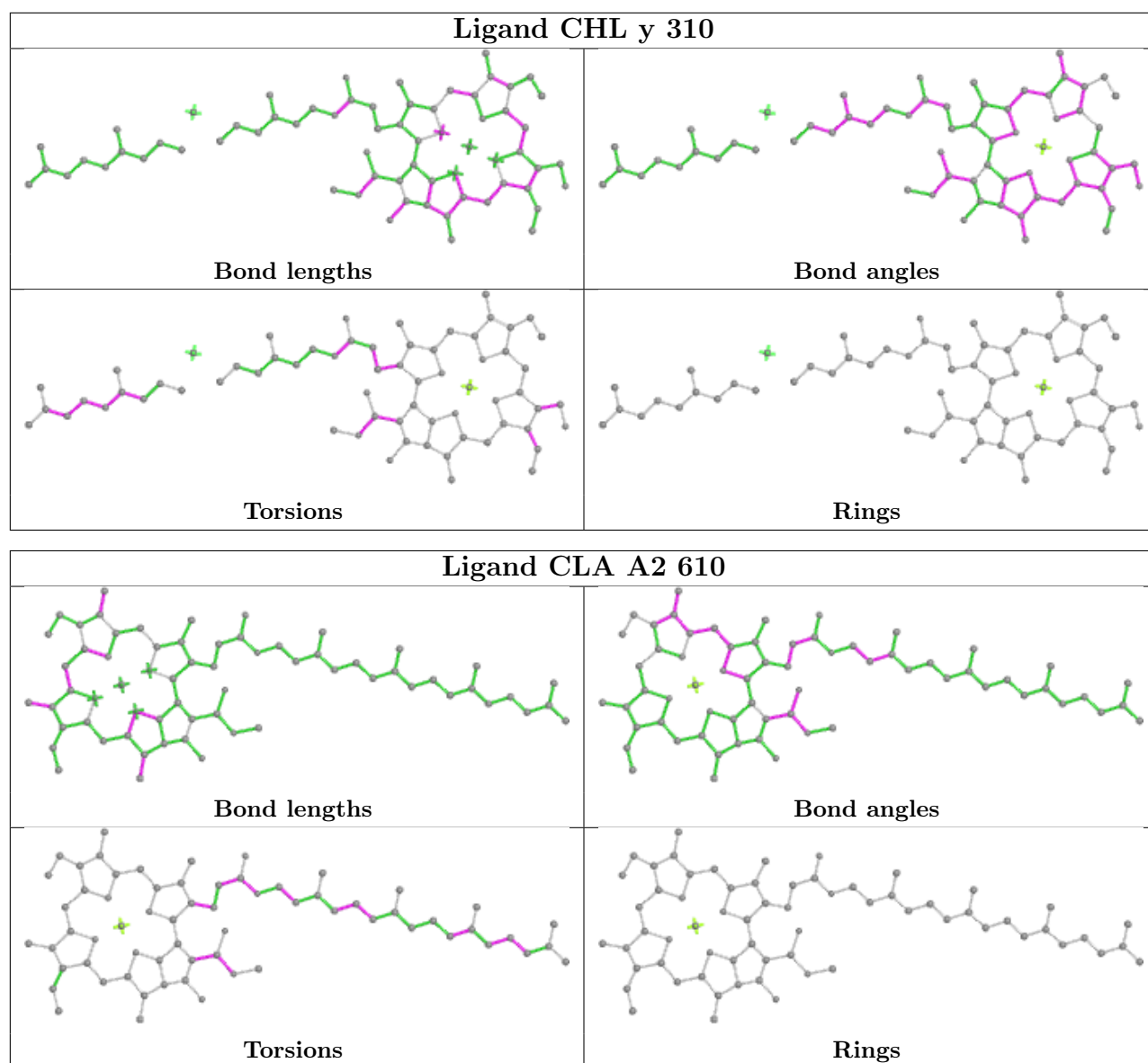


Ligand CLA BJ 614

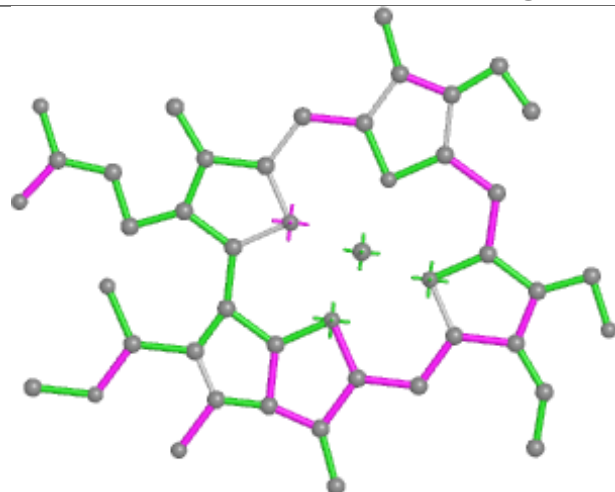




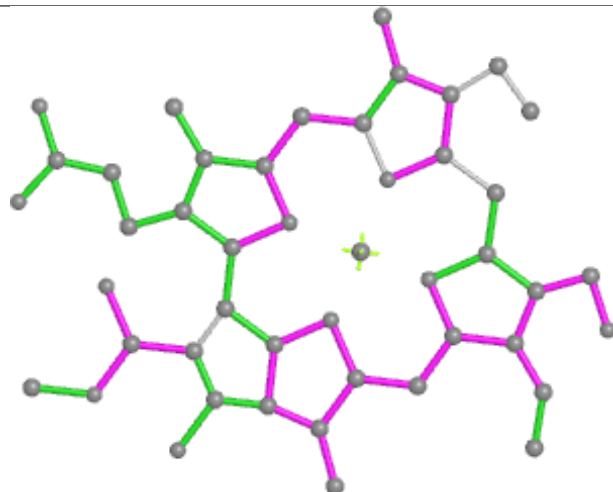




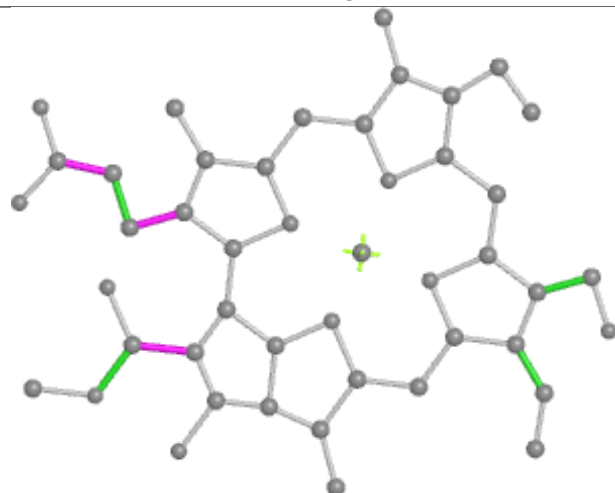
Ligand CHL 7 302



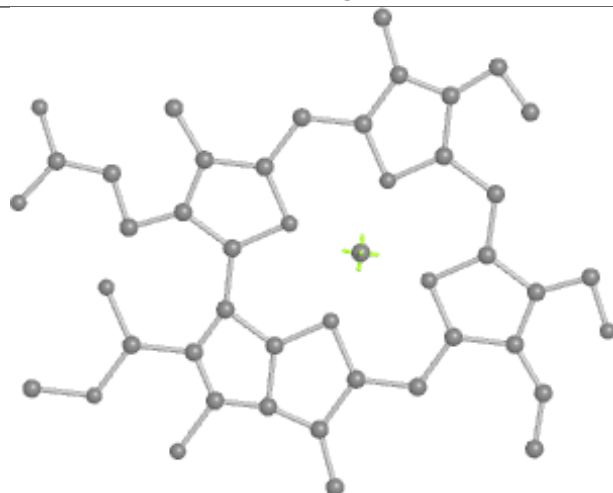
Bond lengths



Bond angles

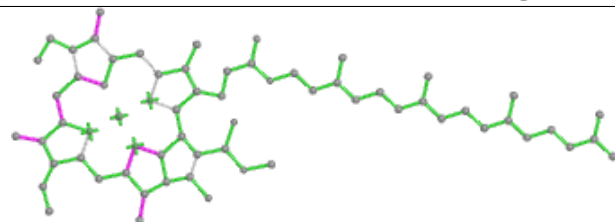


Torsions

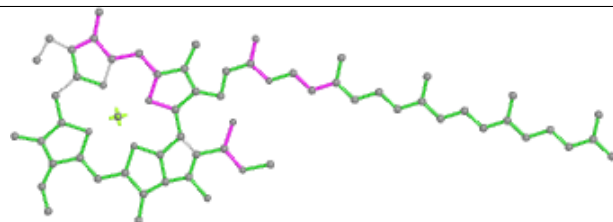


Rings

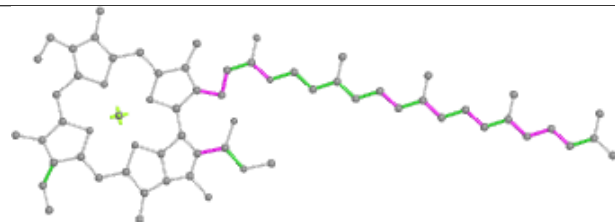
Ligand CLA G 602



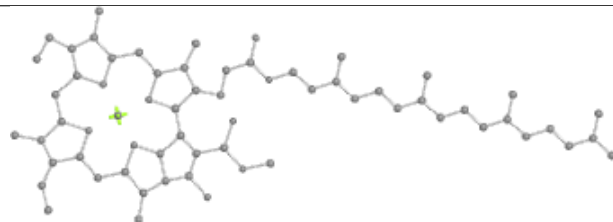
Bond lengths



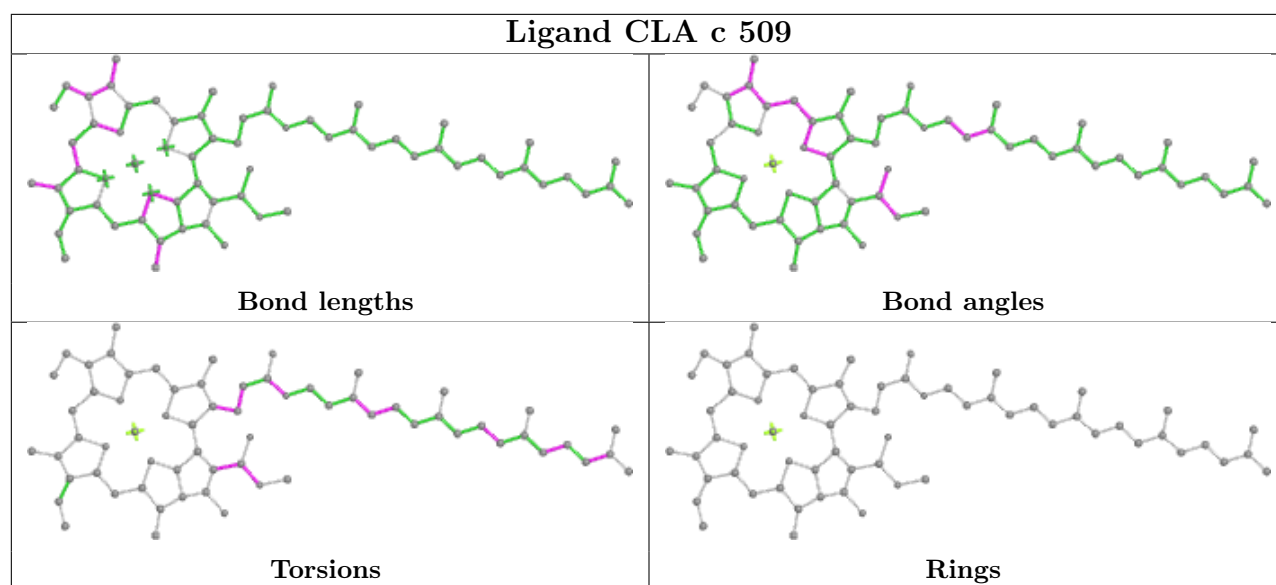
Bond angles



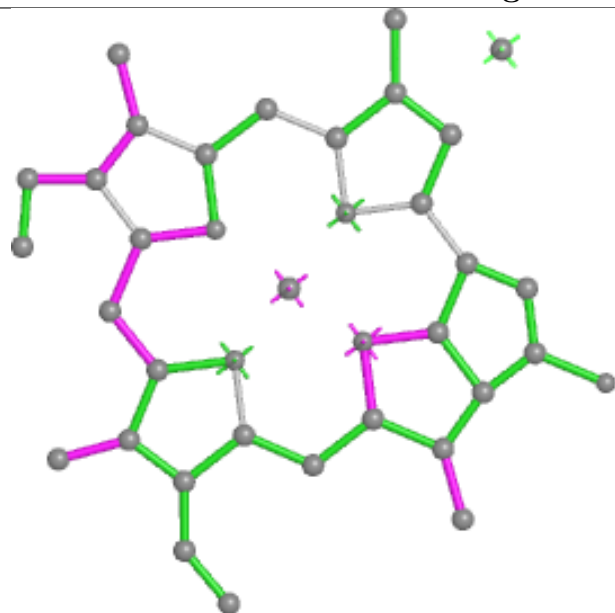
Torsions



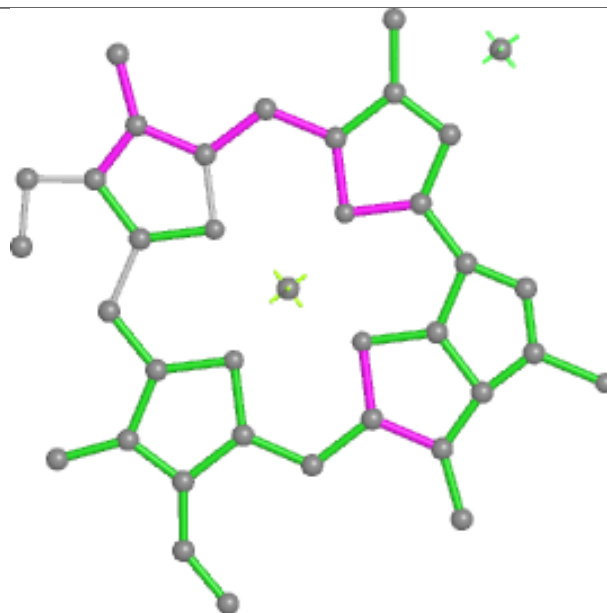
Rings



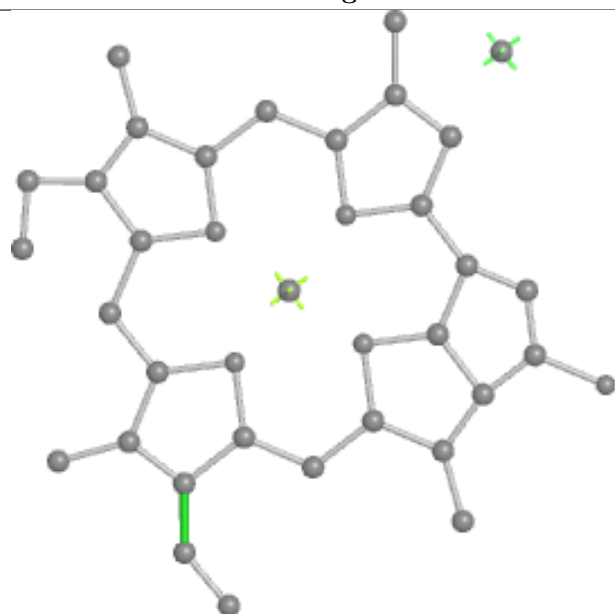
Ligand CLA BU 612



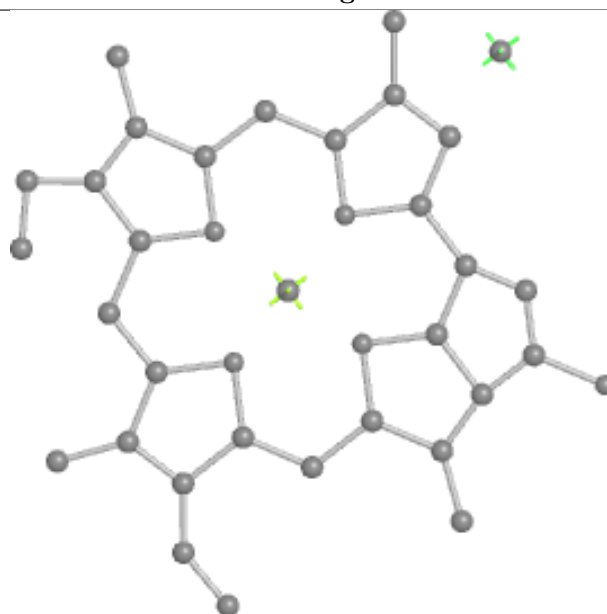
Bond lengths



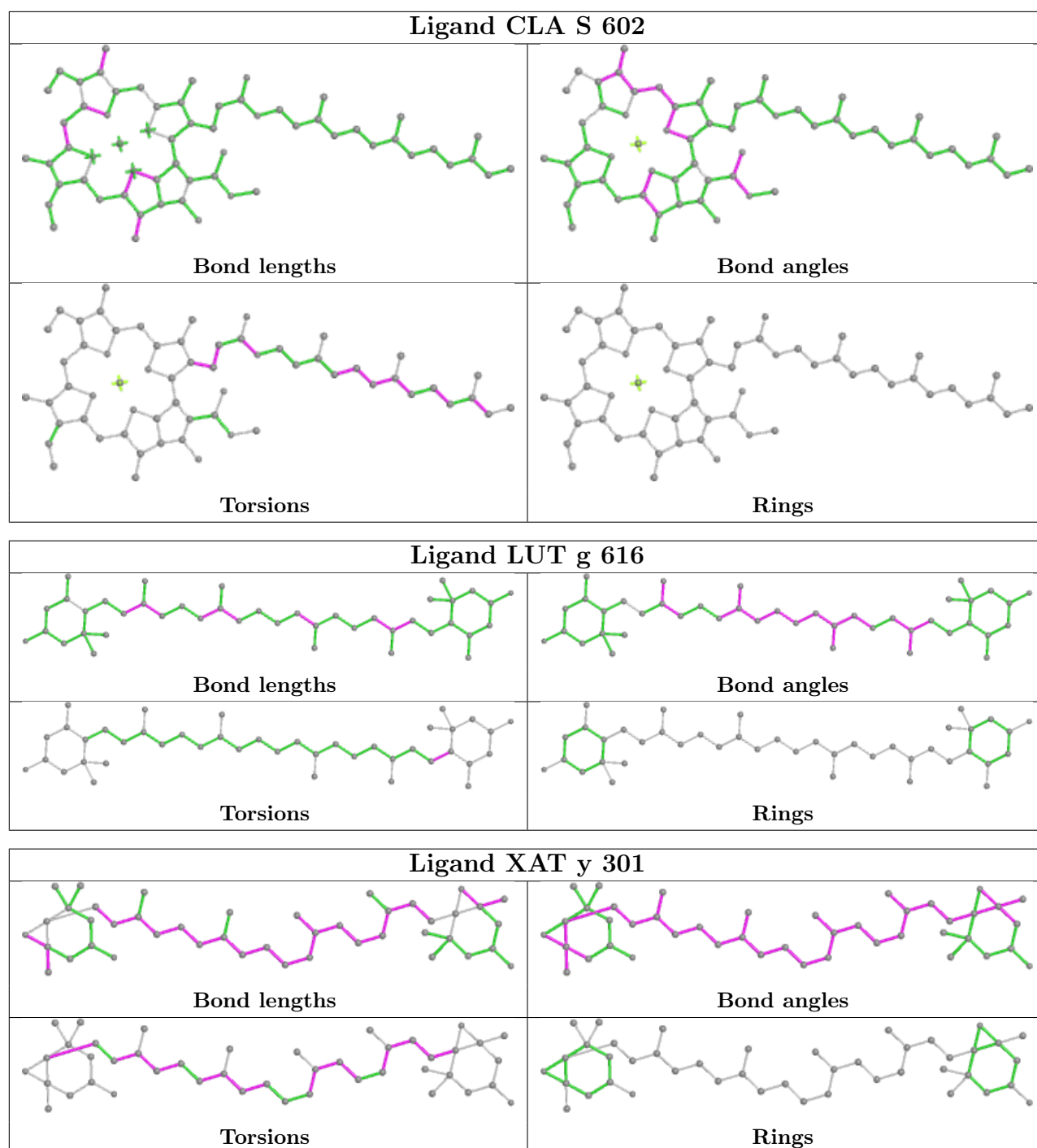
Bond angles



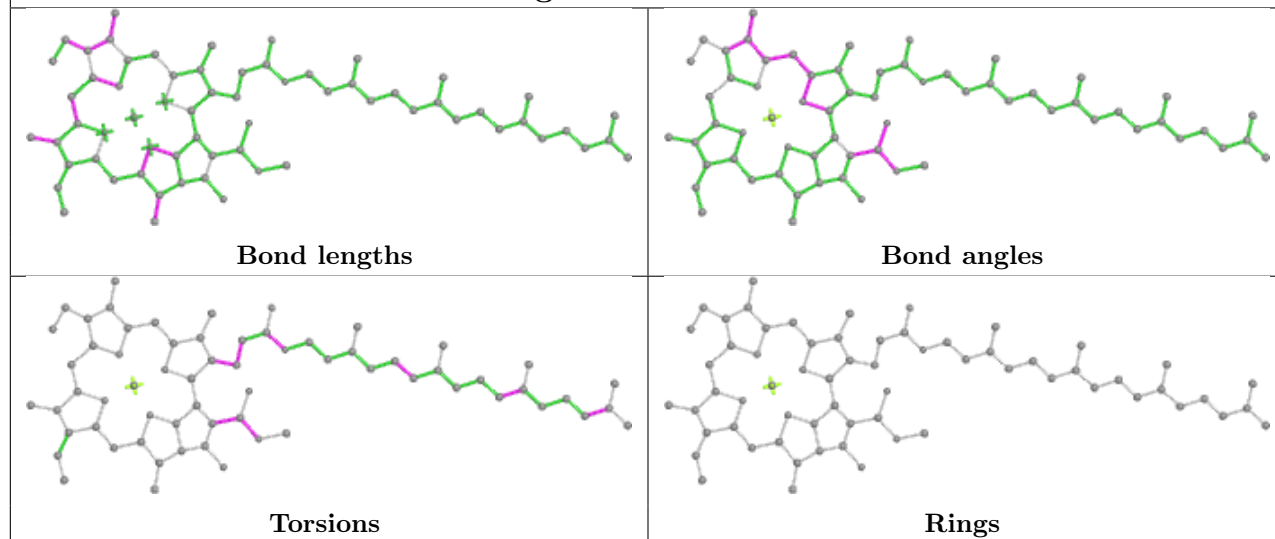
Torsions



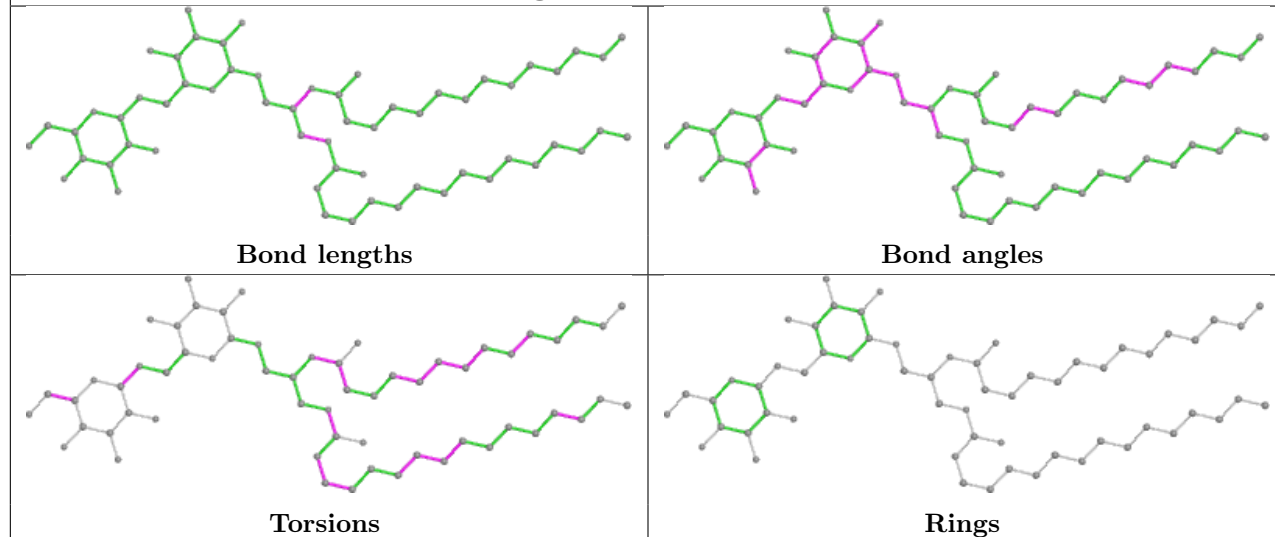
Rings



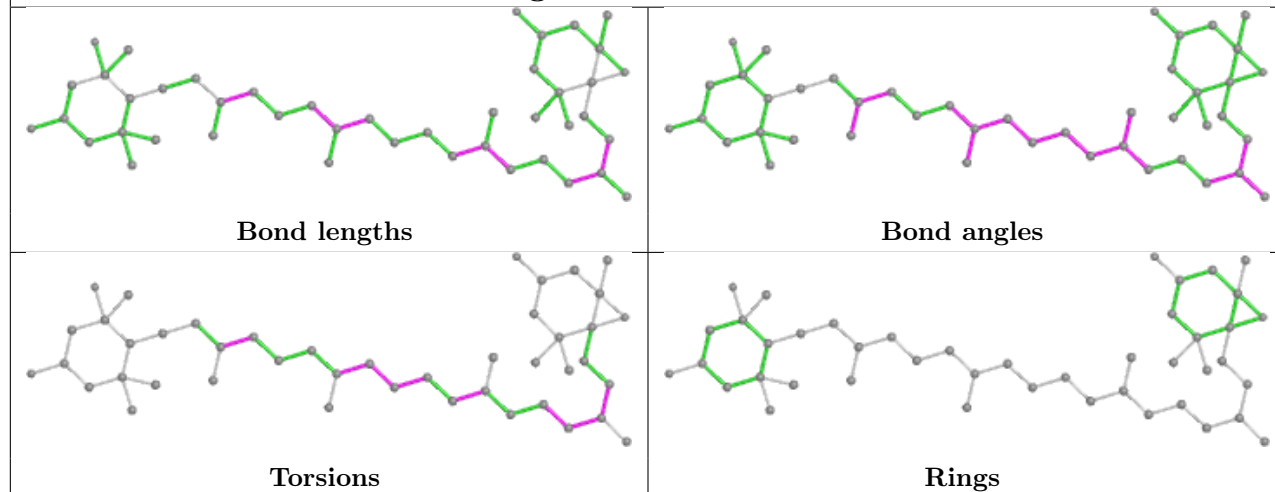
Ligand CLA 1 511

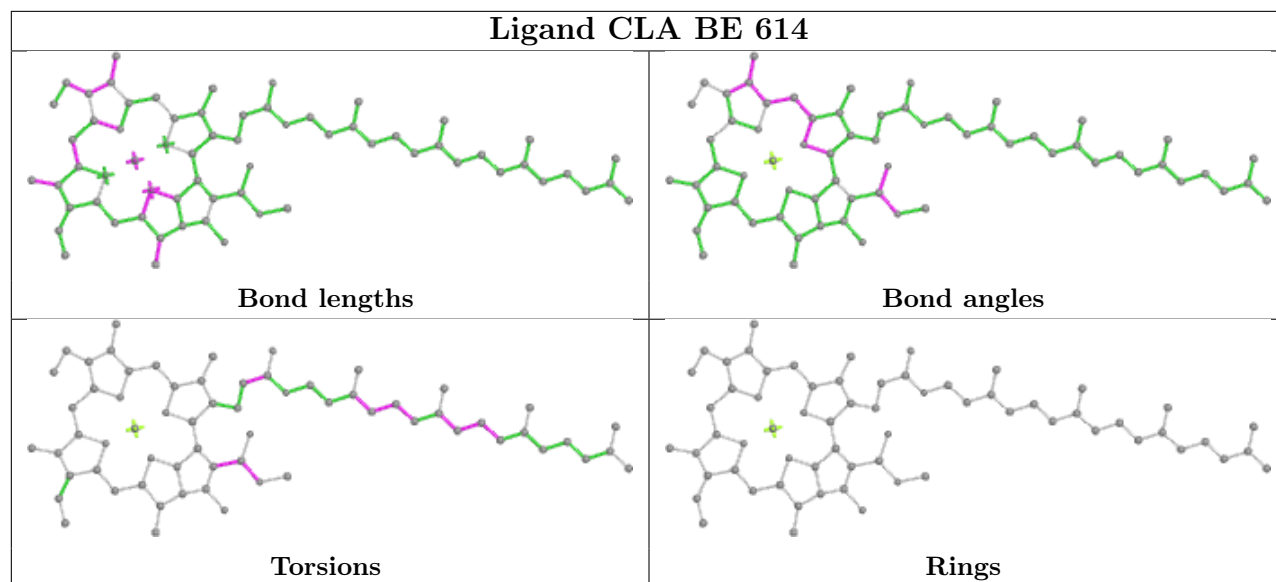
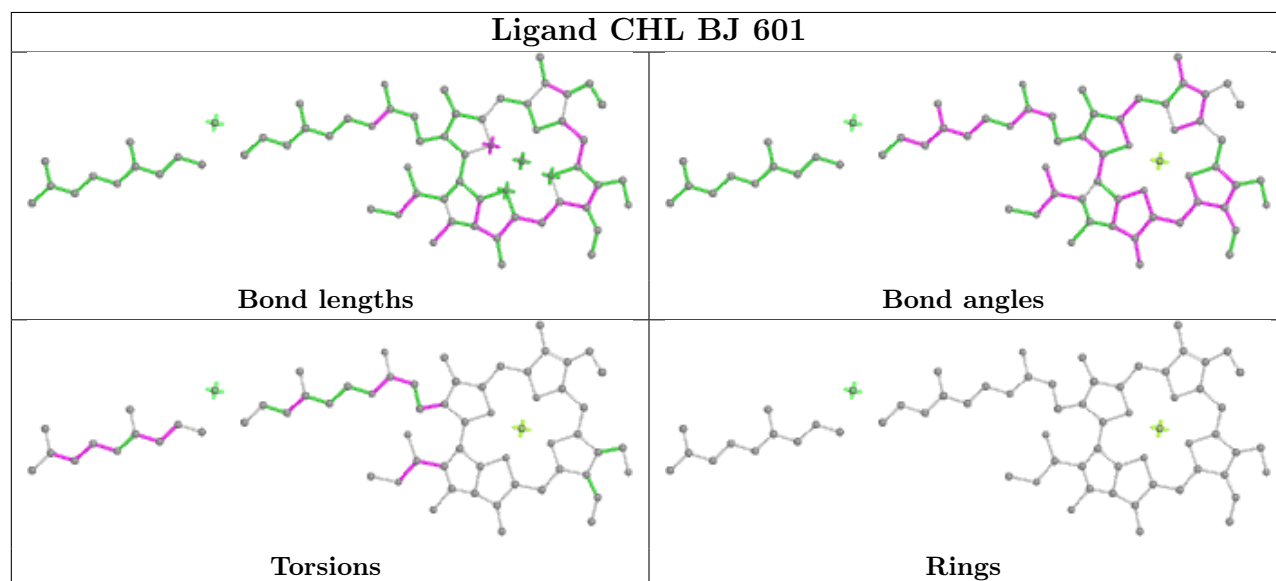


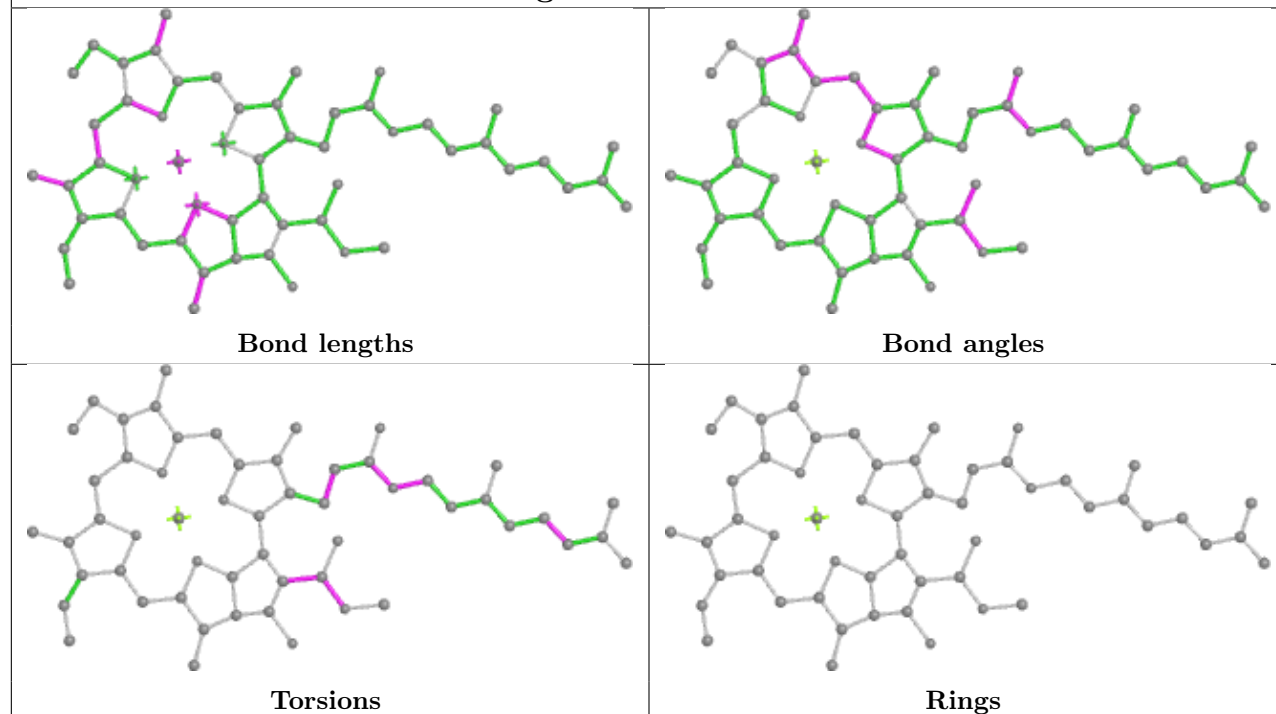
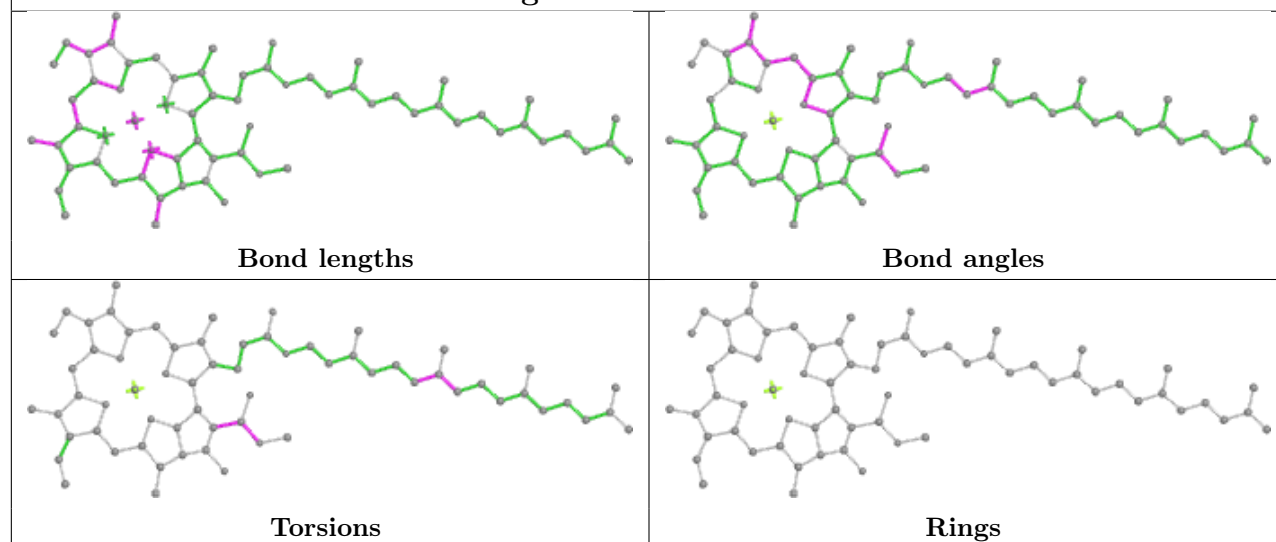
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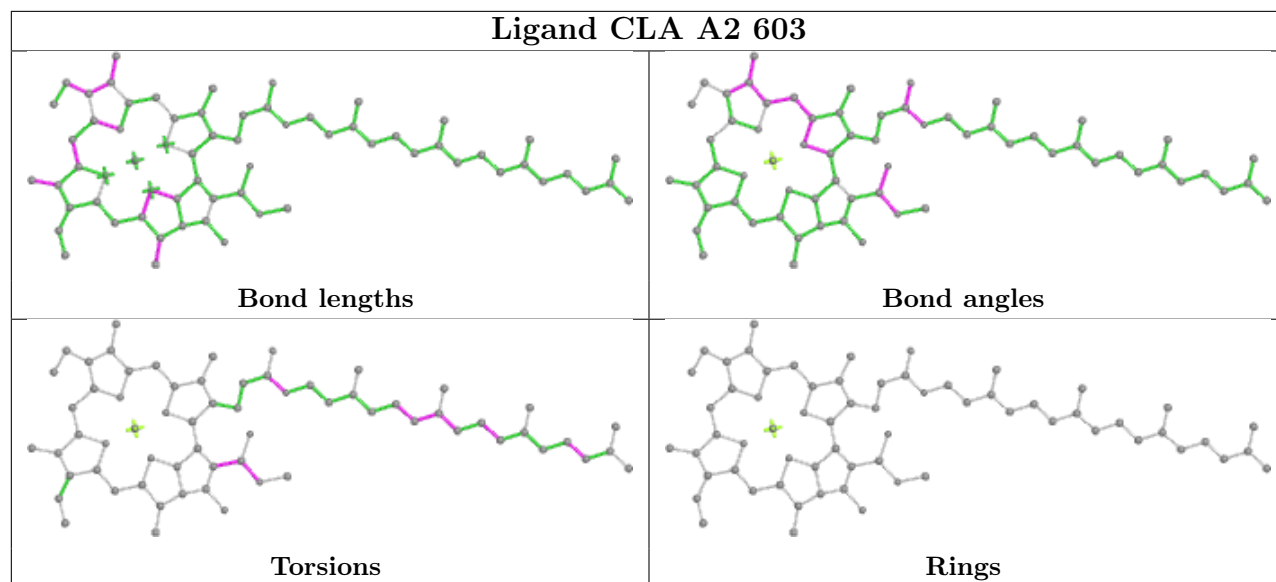
Ligand NEX Y 318



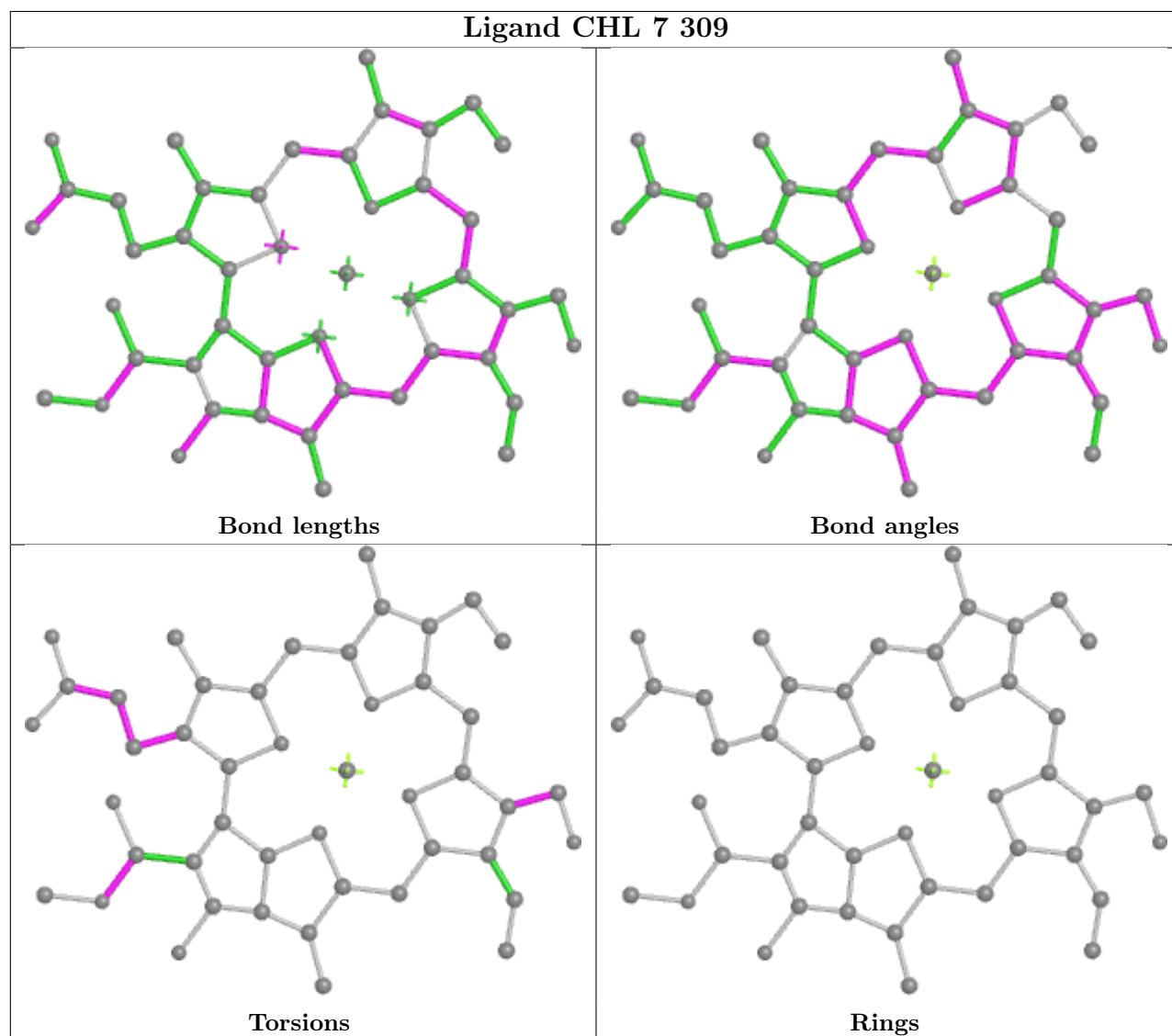
Ligand CLA BE 614**Ligand CHL BJ 601**

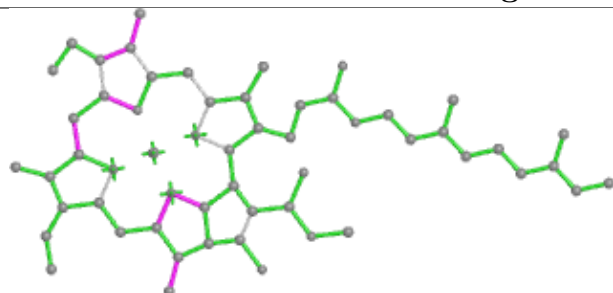
Ligand CLA 6 603**Ligand CLA BF 510**

Ligand CLA A2 603

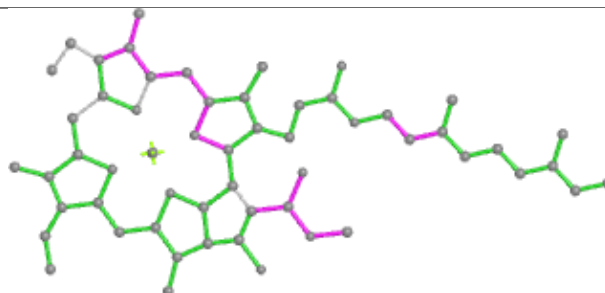


Ligand CHL 7 309

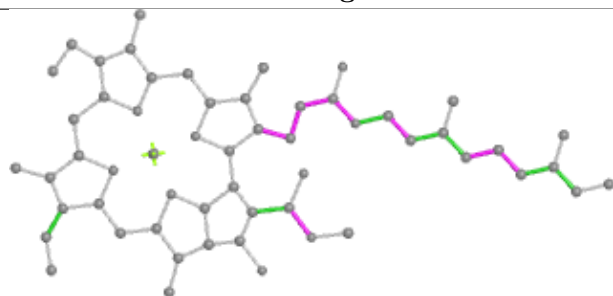


Ligand CLA BV 610

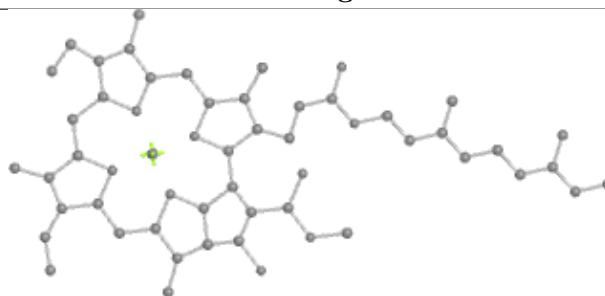
Bond lengths



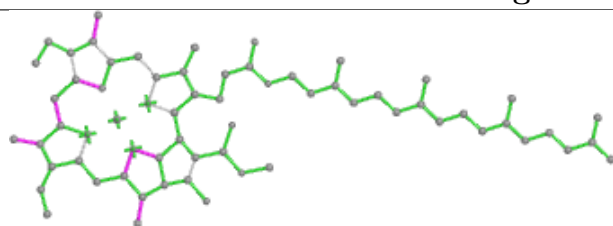
Bond angles



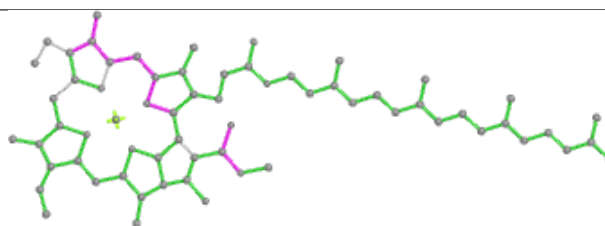
Torsions



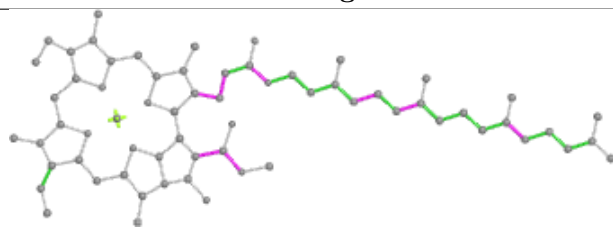
Rings

Ligand CLA G 613

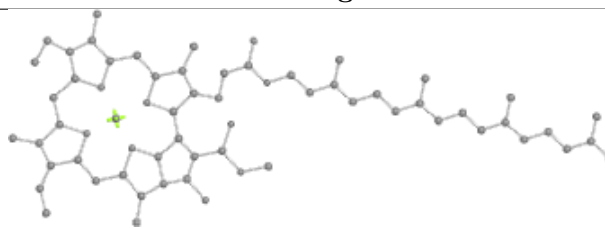
Bond lengths



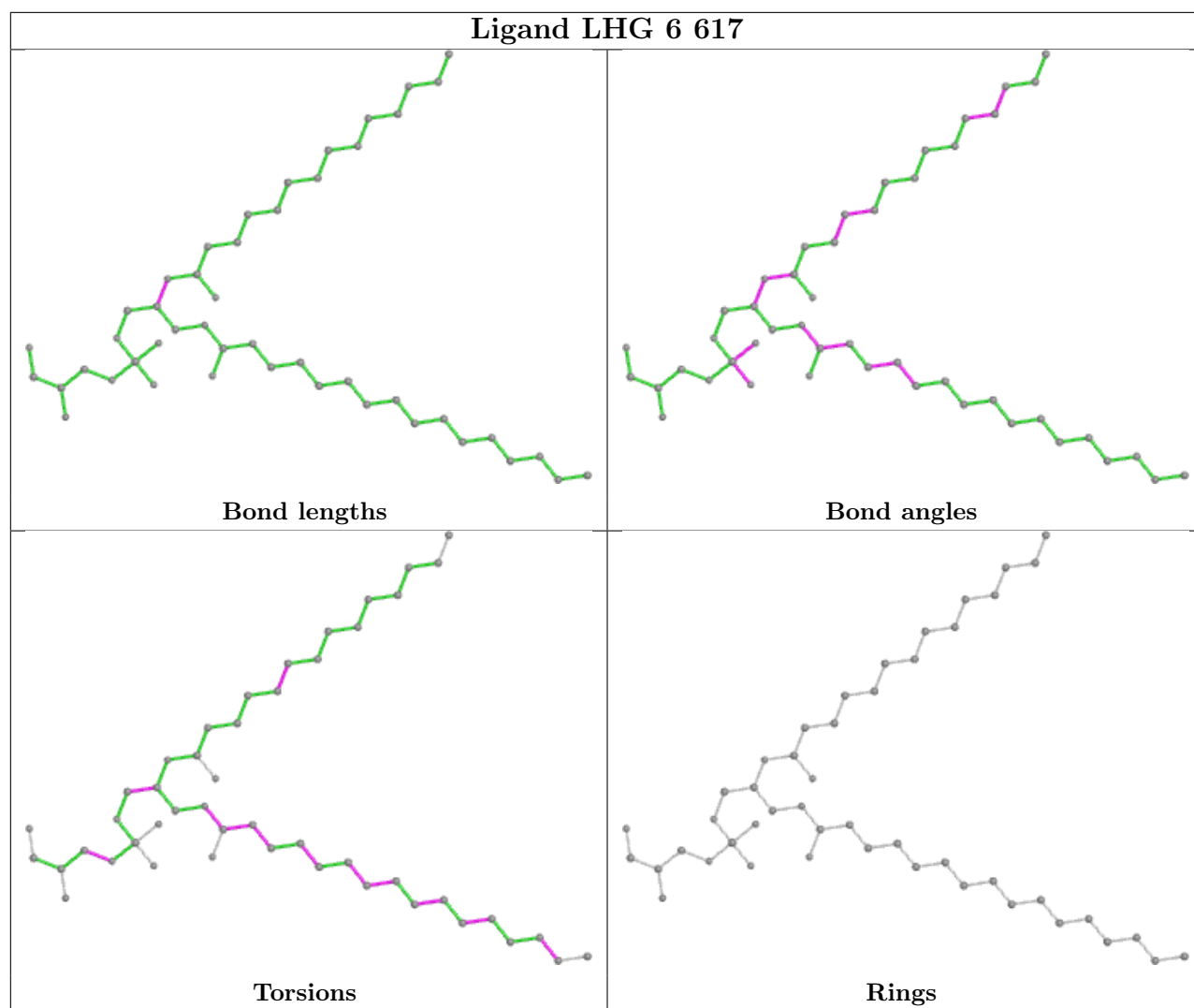
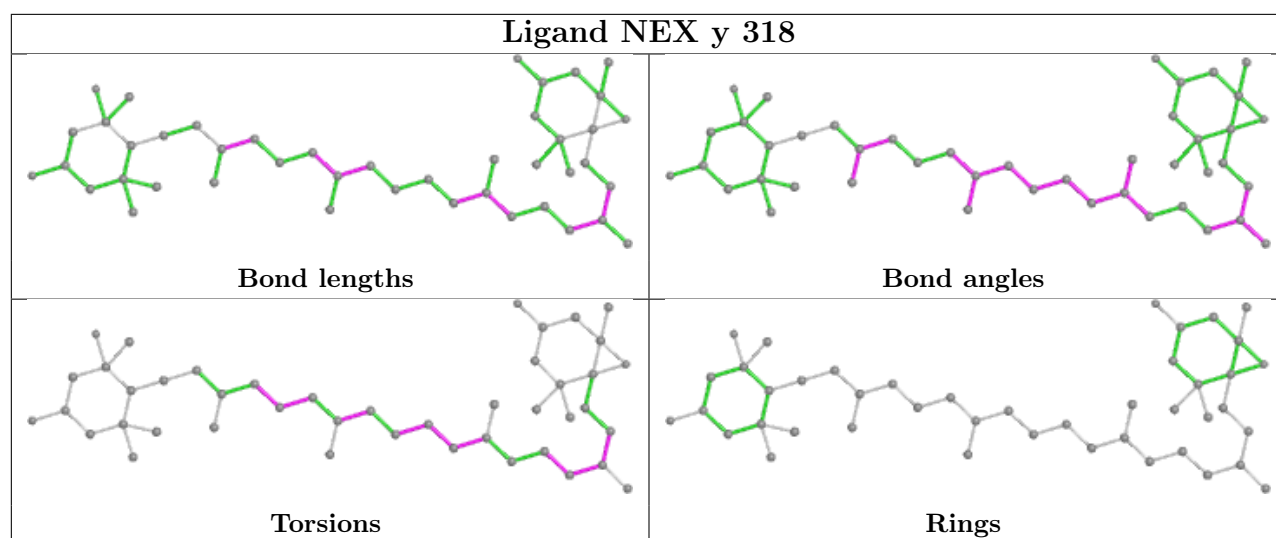
Bond angles

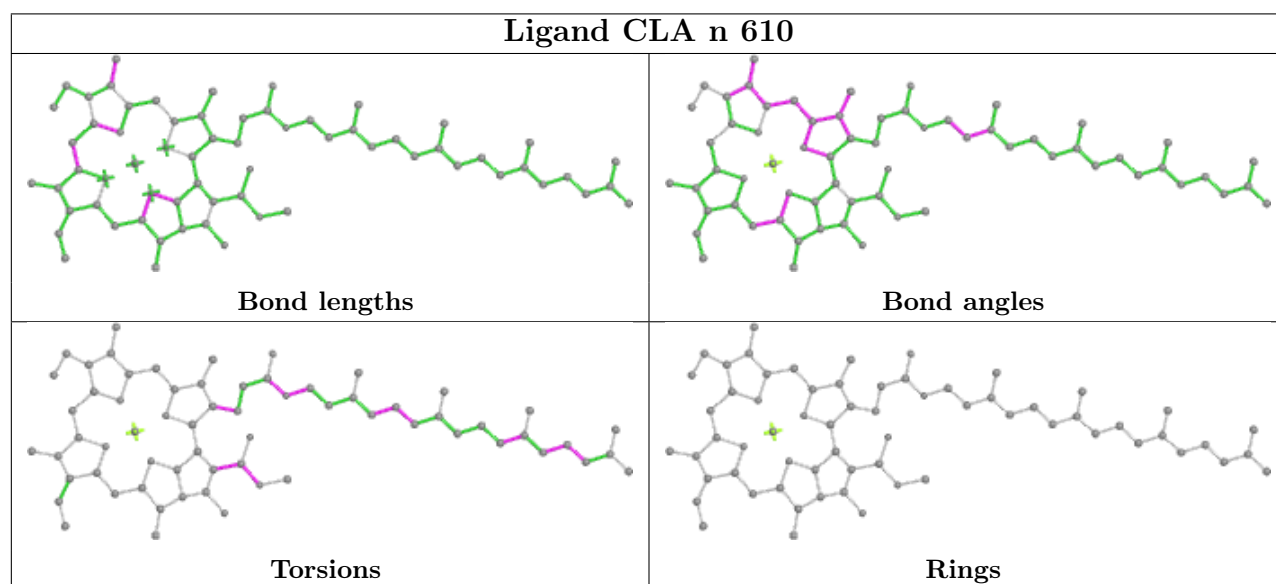
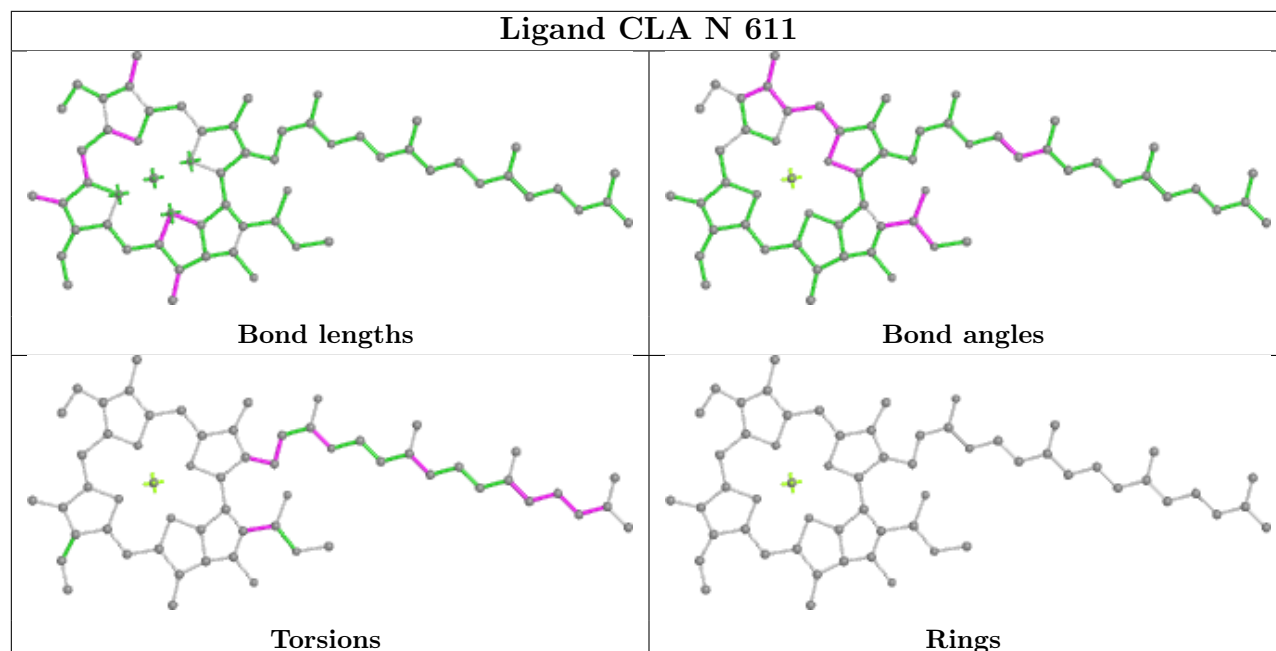
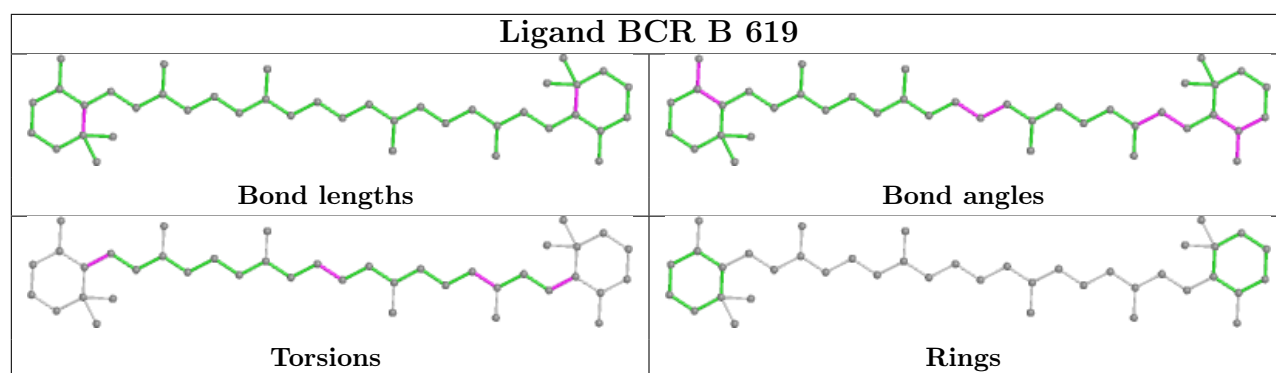


Torsions

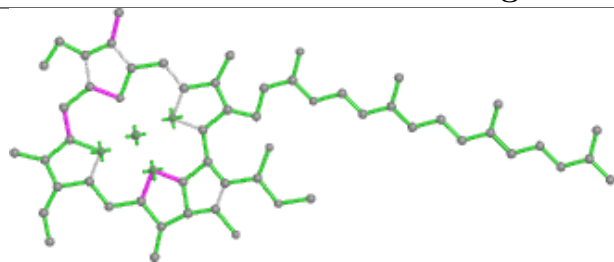


Rings

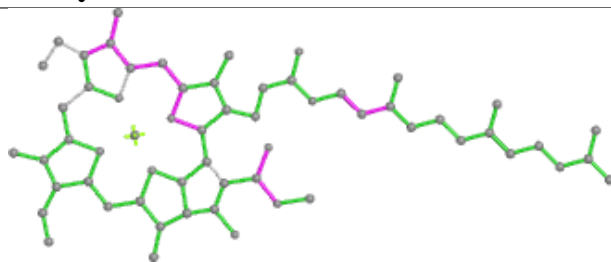




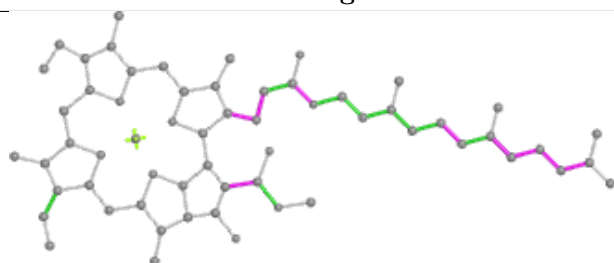
Ligand CLA BQ 611



Bond lengths



Bond angles

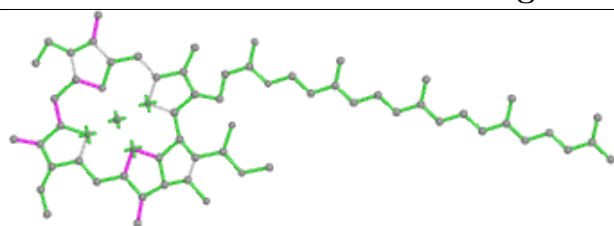


Torsions

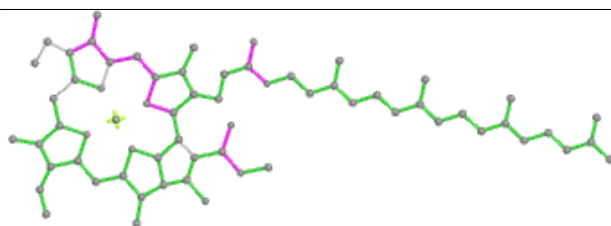


Rings

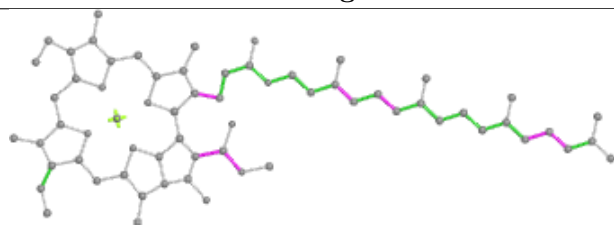
Ligand CLA b 610



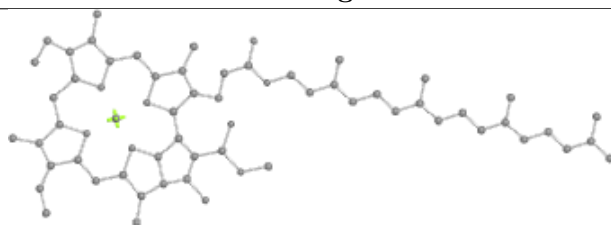
Bond lengths



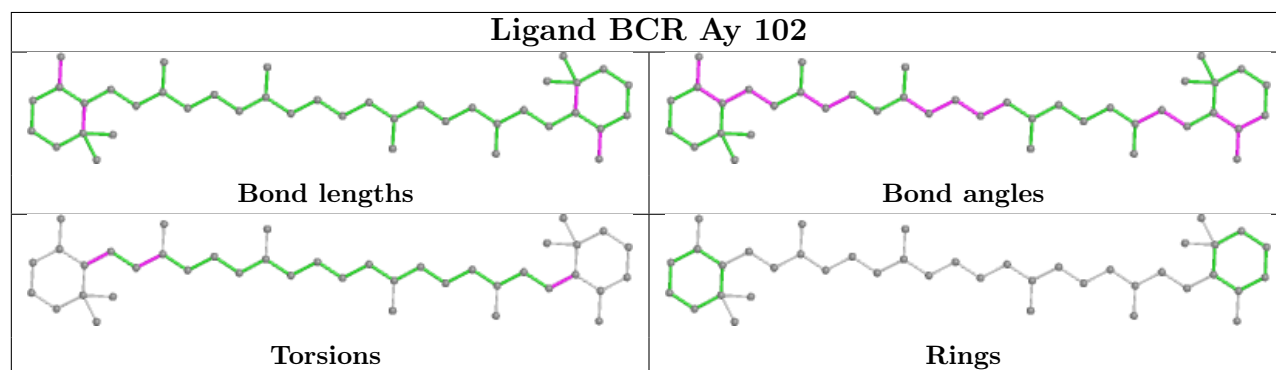
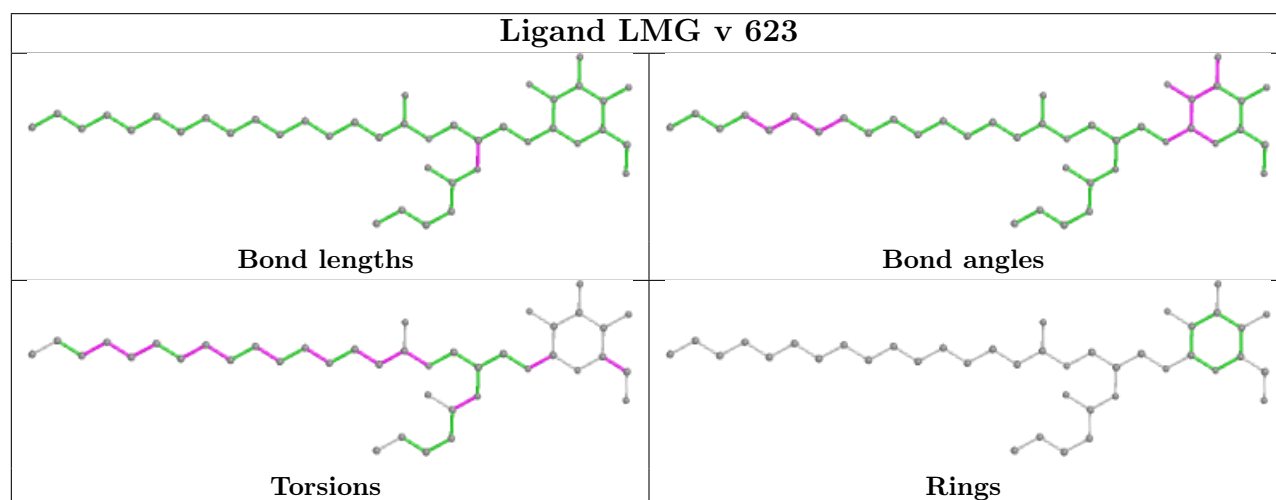
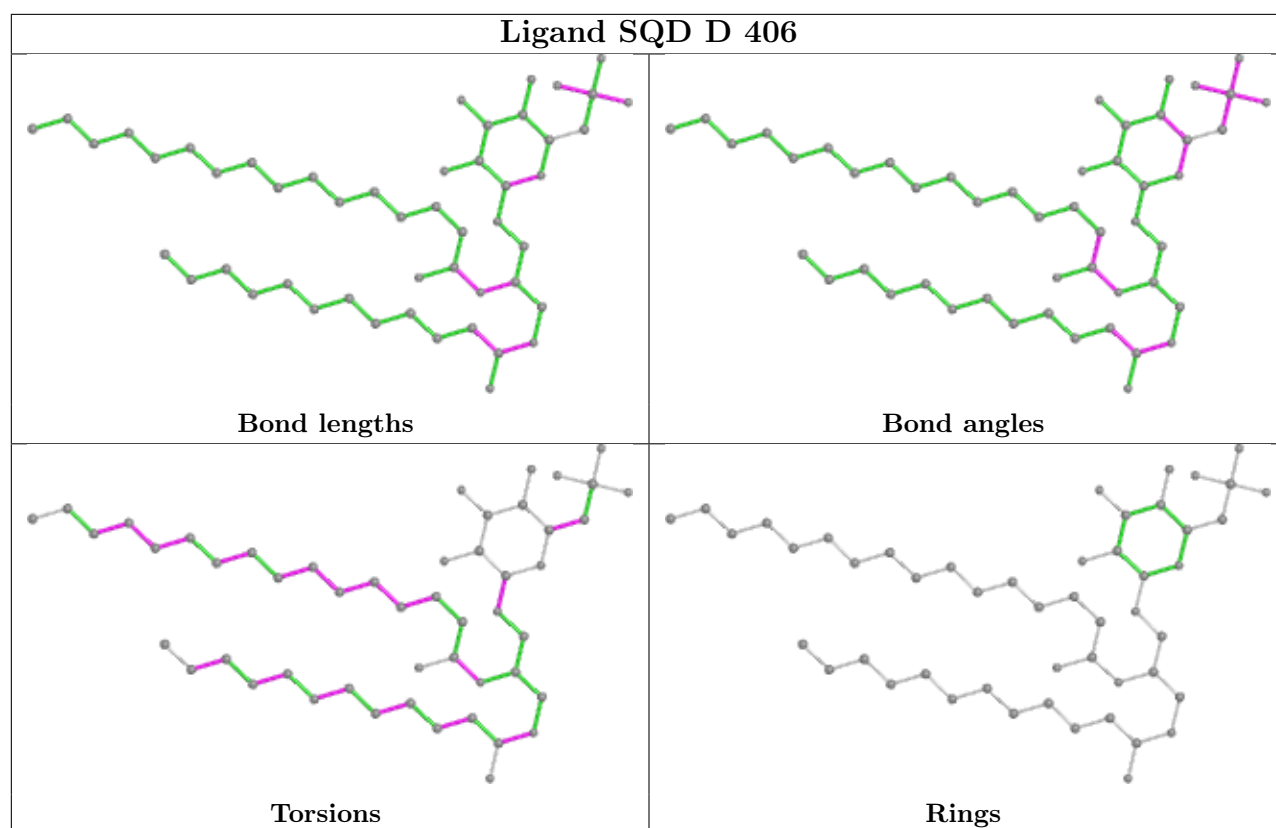
Bond angles

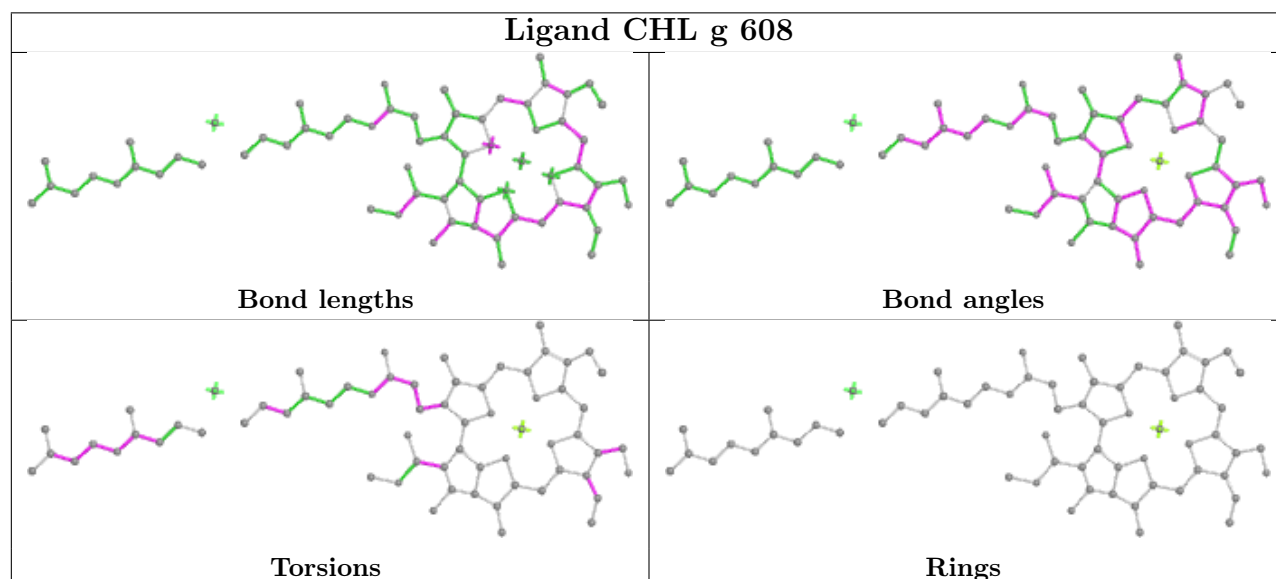
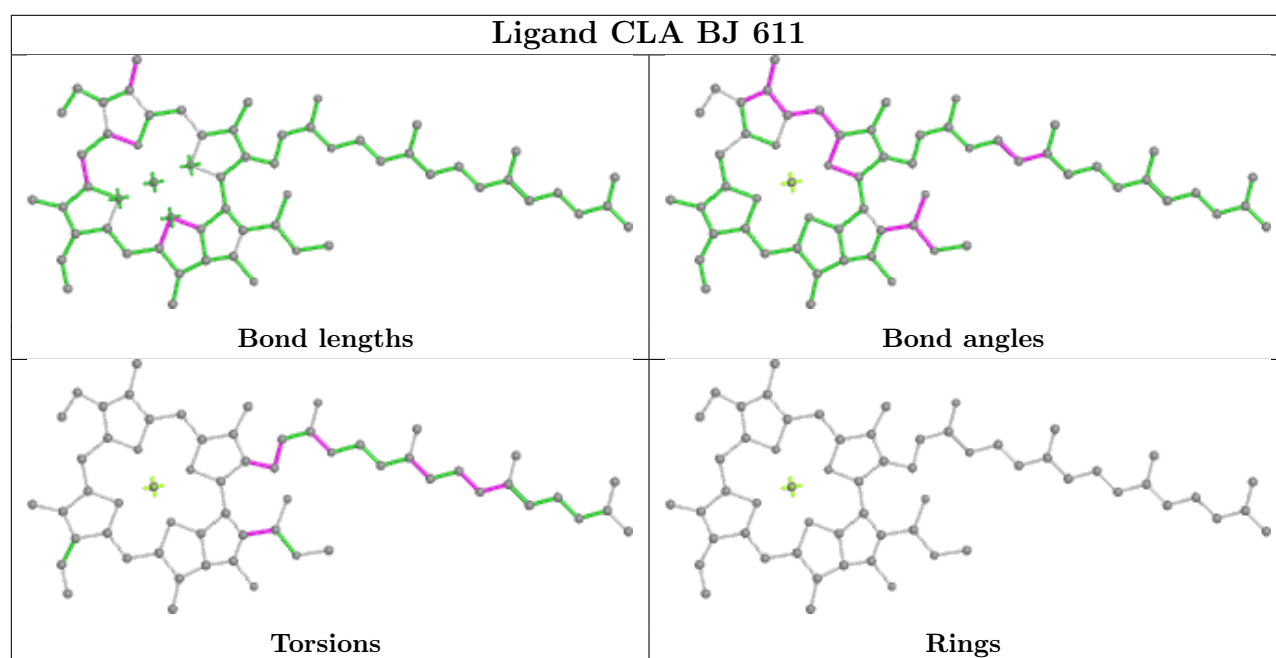
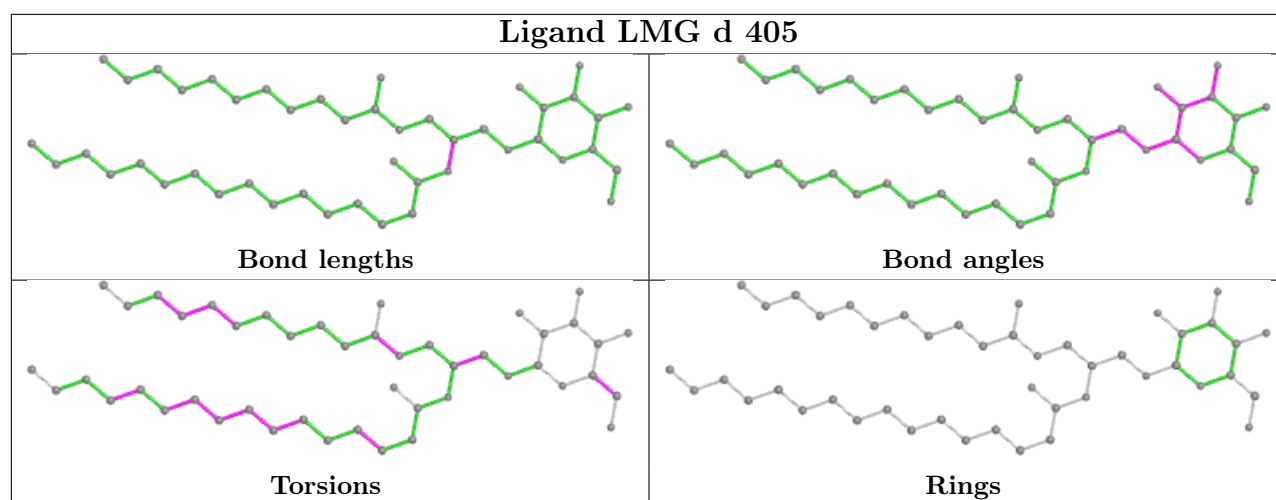


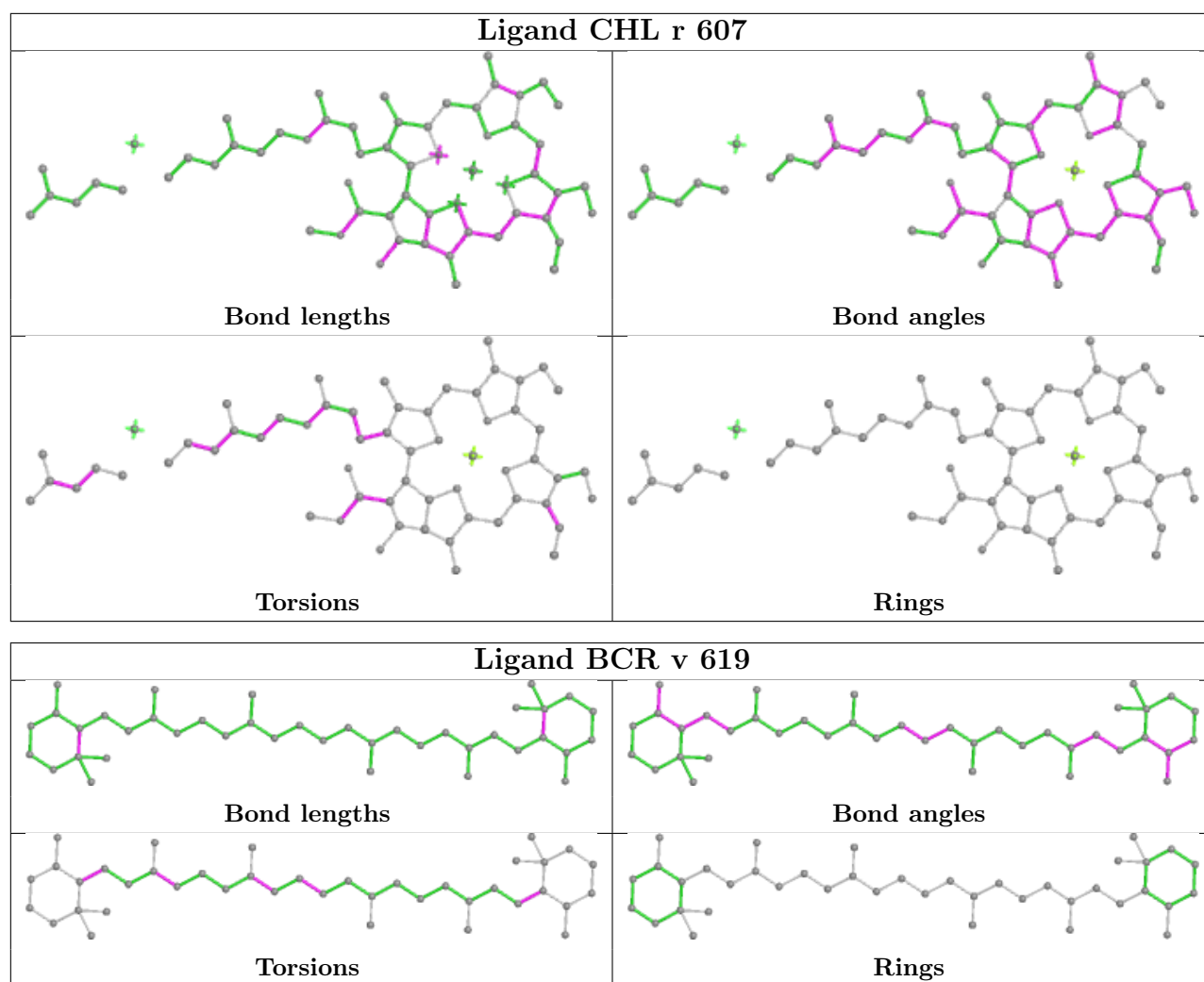
Torsions

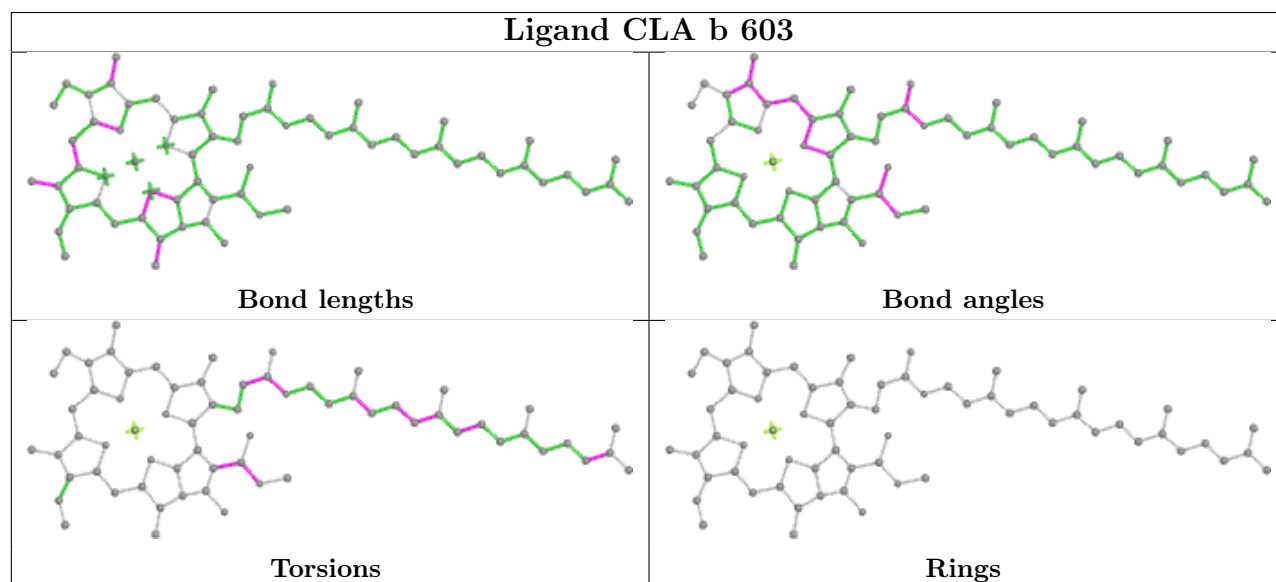
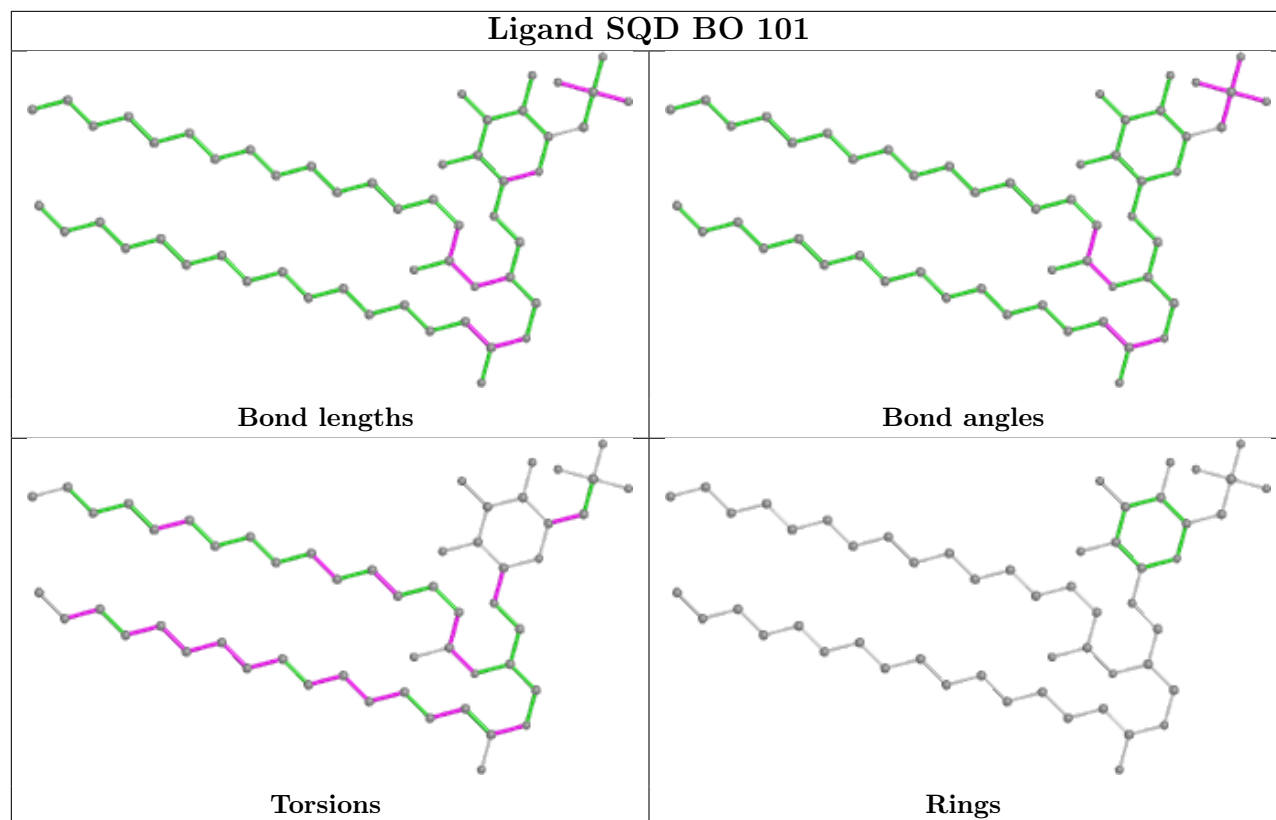


Rings

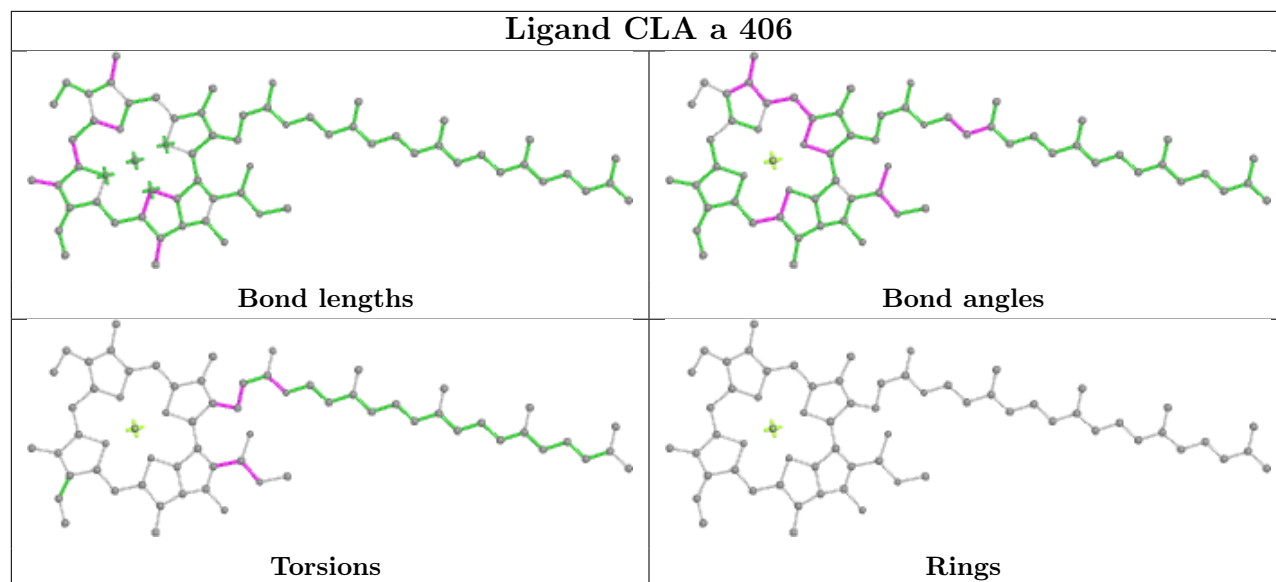




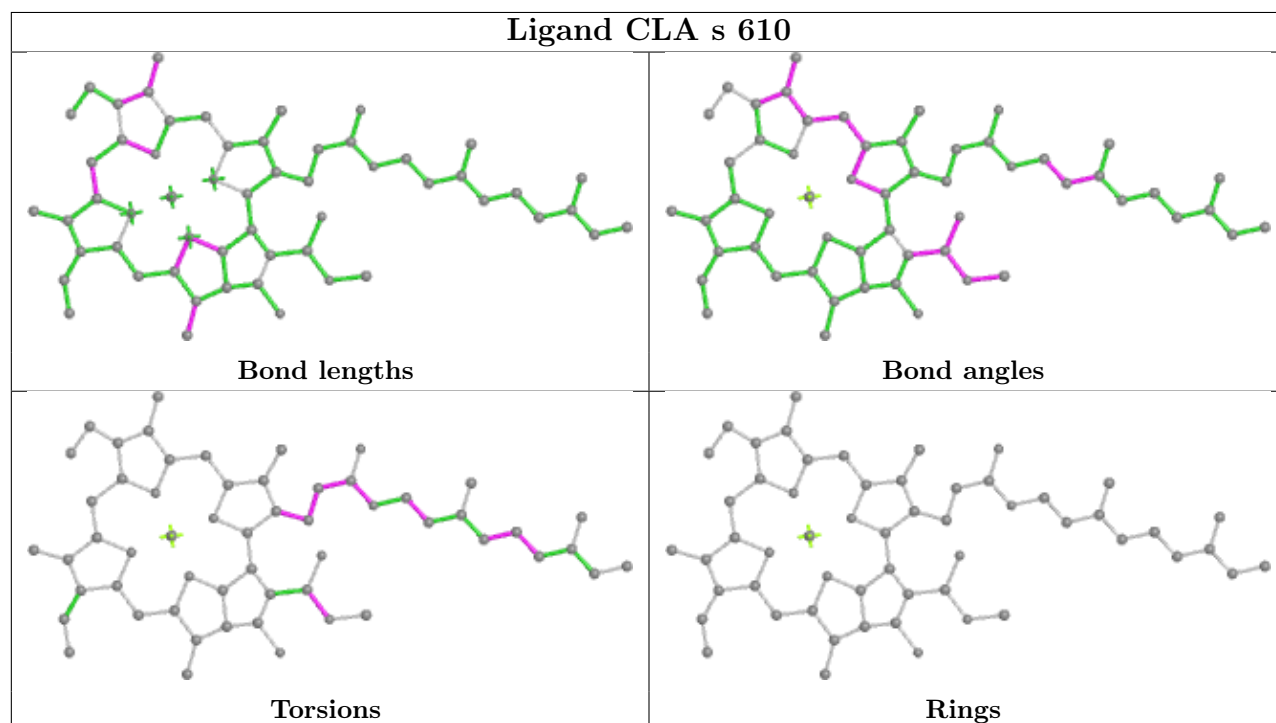


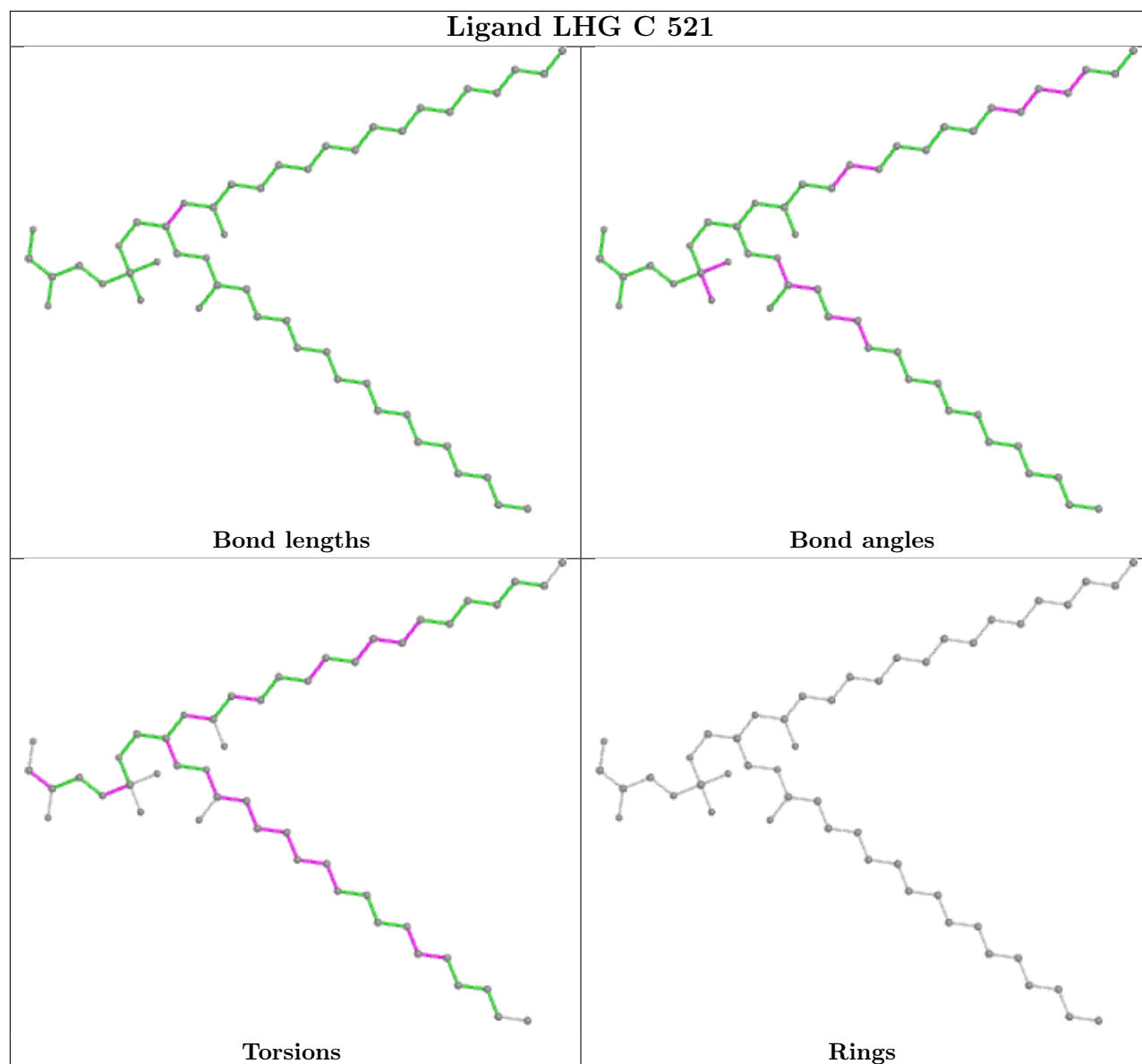
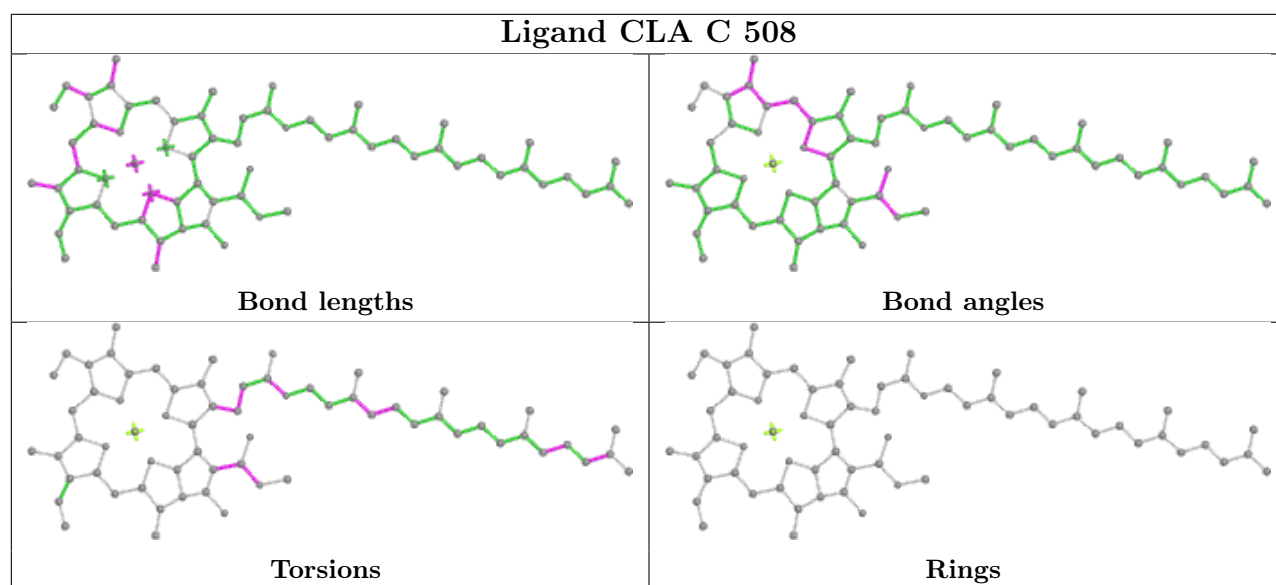


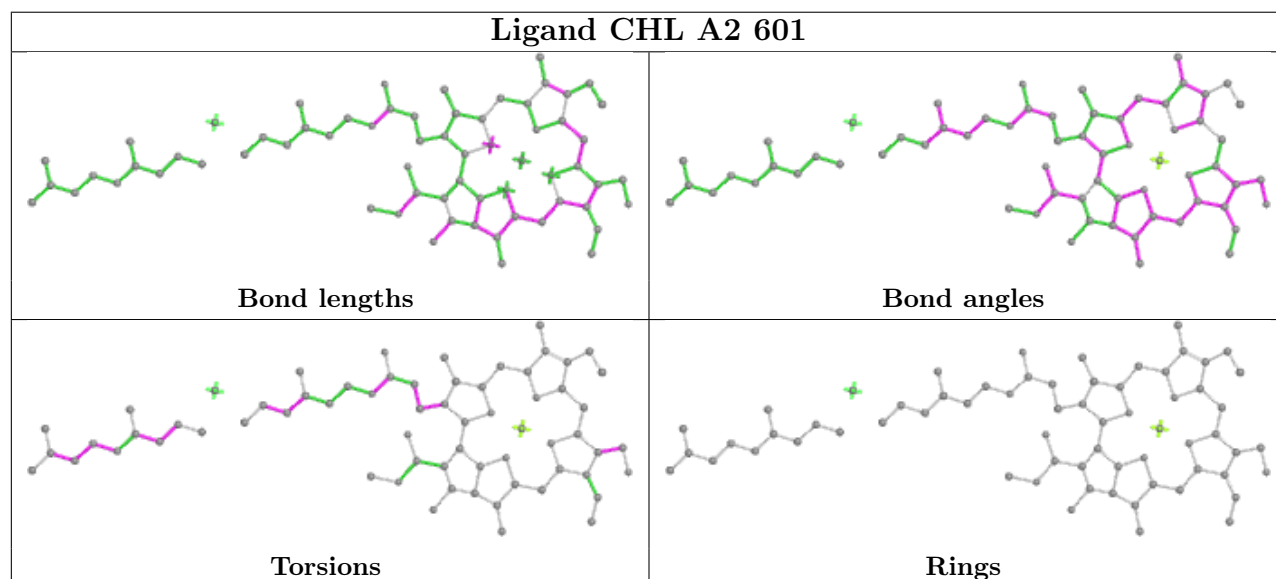
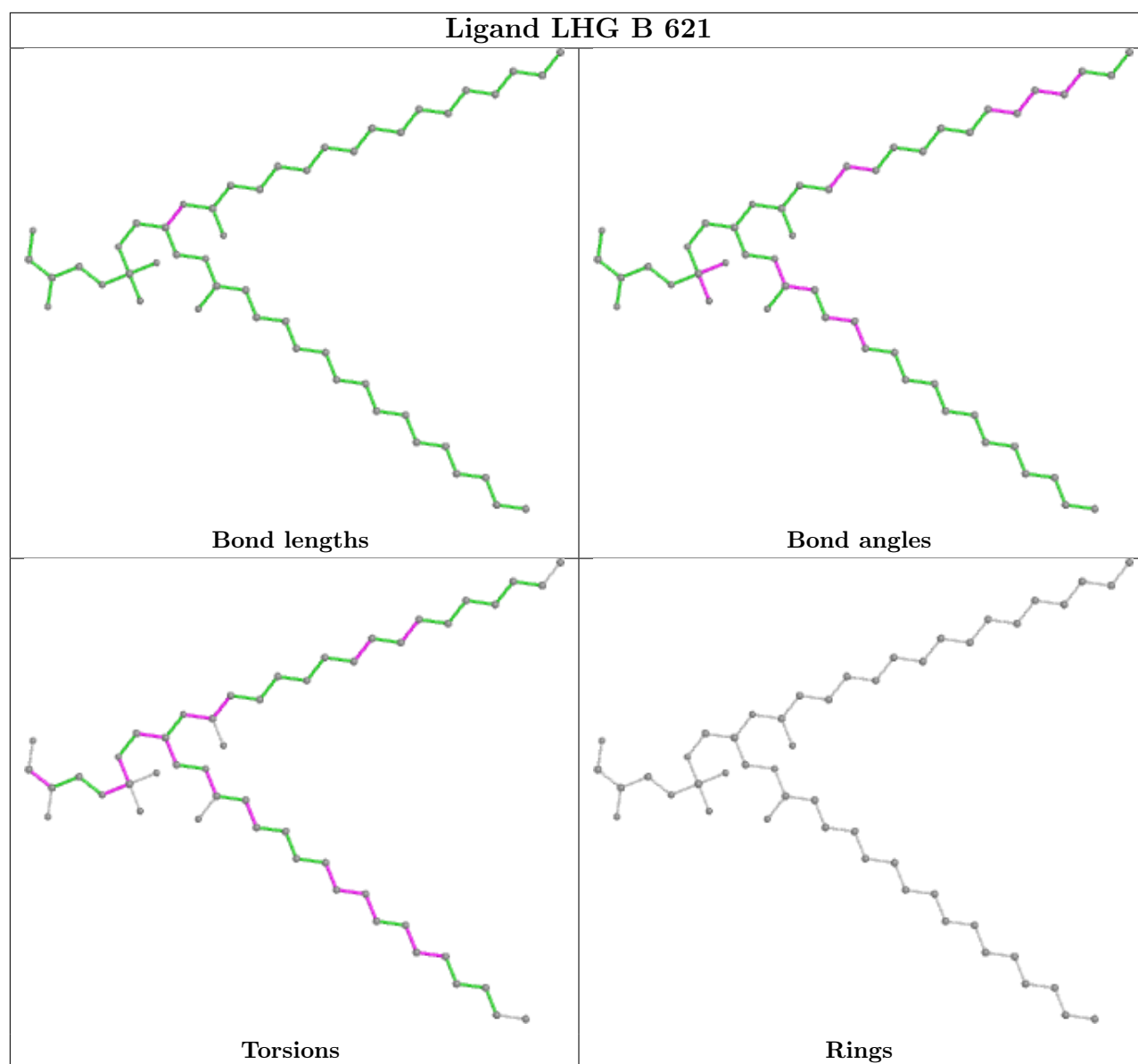
Ligand CLA a 406



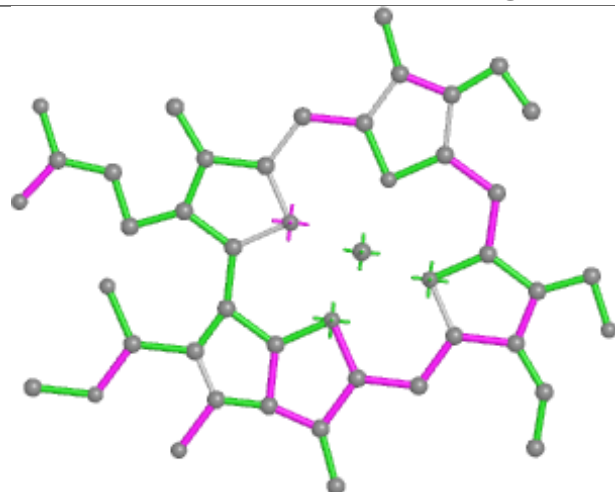
Ligand CLA s 610



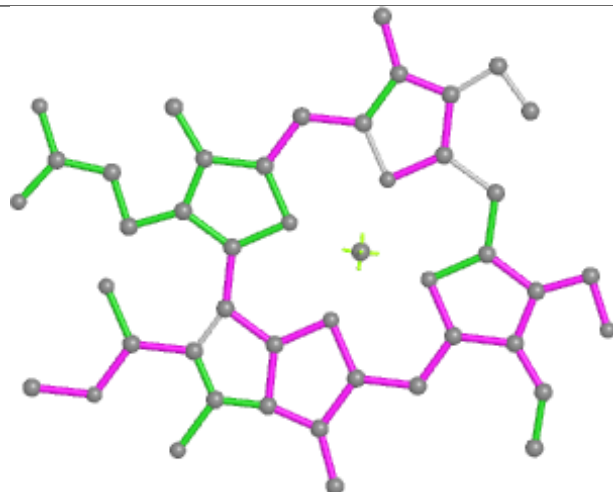




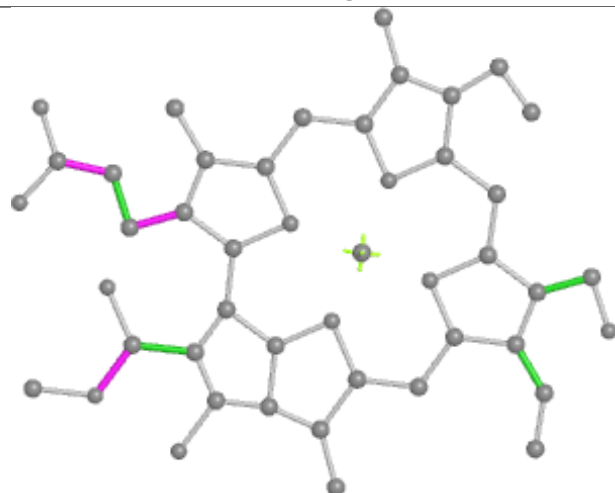
Ligand CHL AA 307



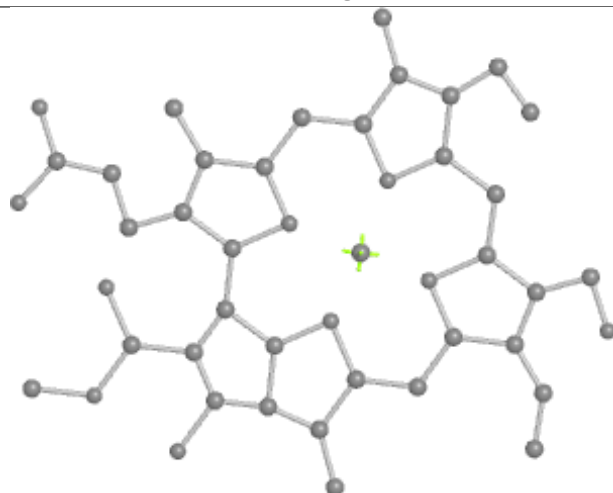
Bond lengths



Bond angles

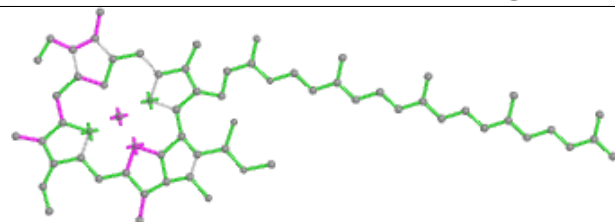


Torsions

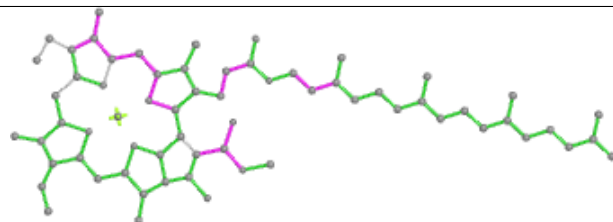


Rings

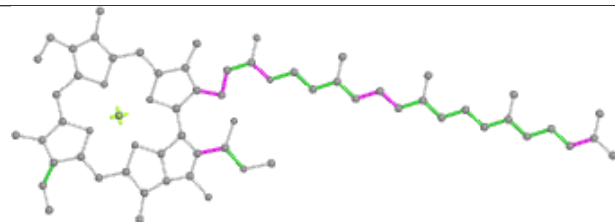
Ligand CLA BF 512



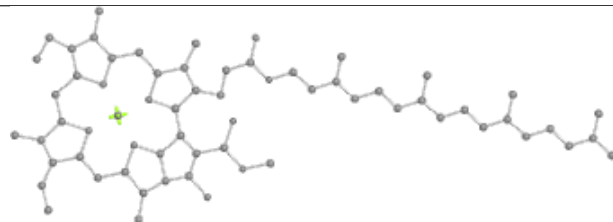
Bond lengths



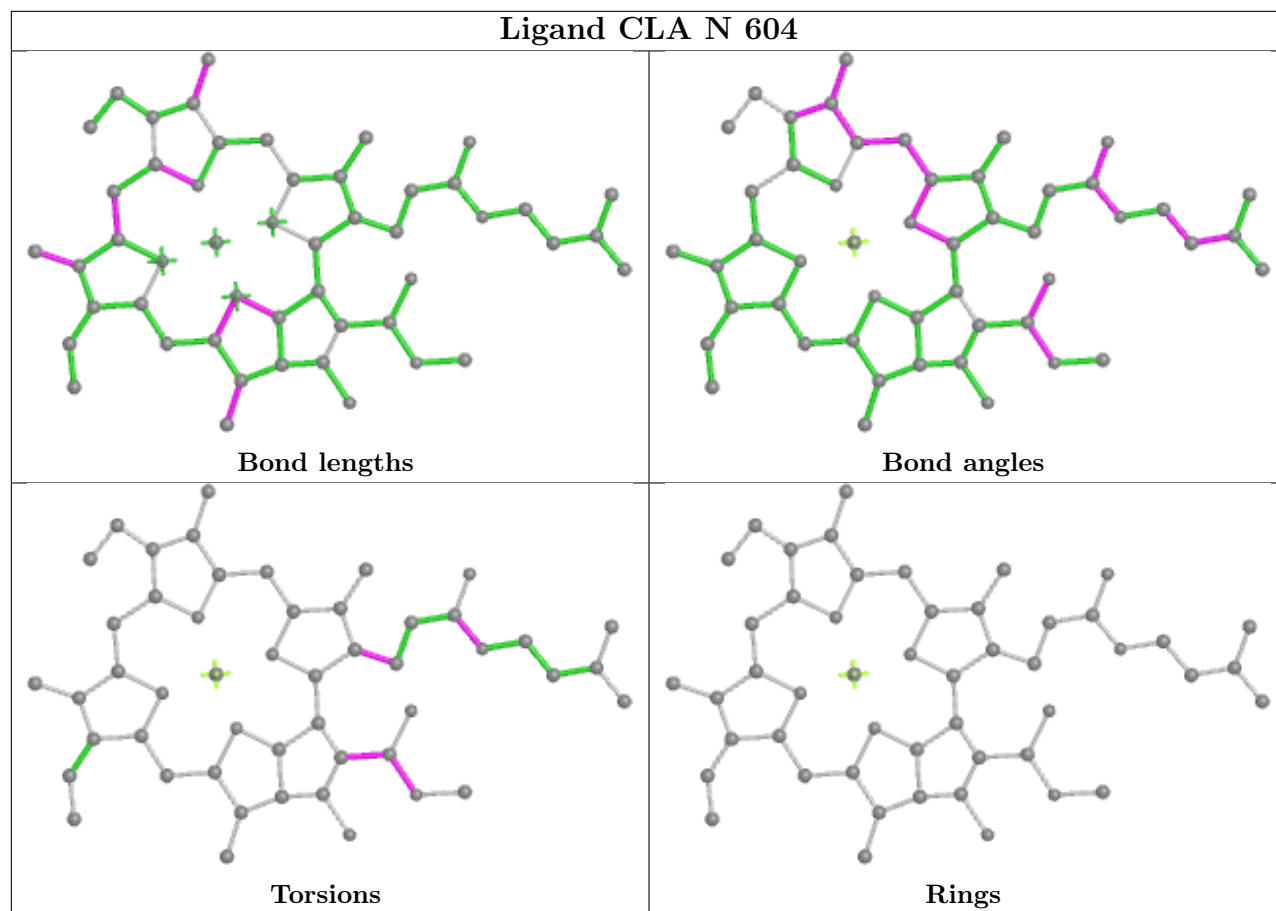
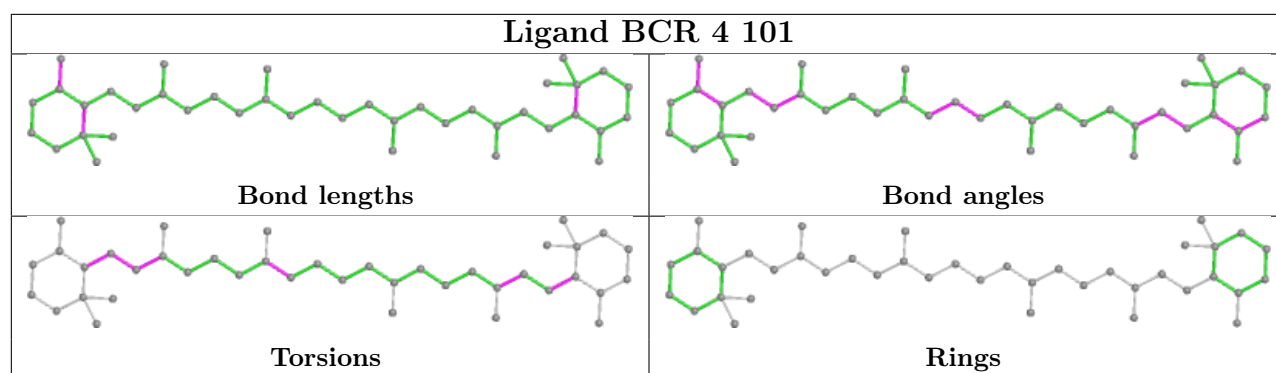
Bond angles

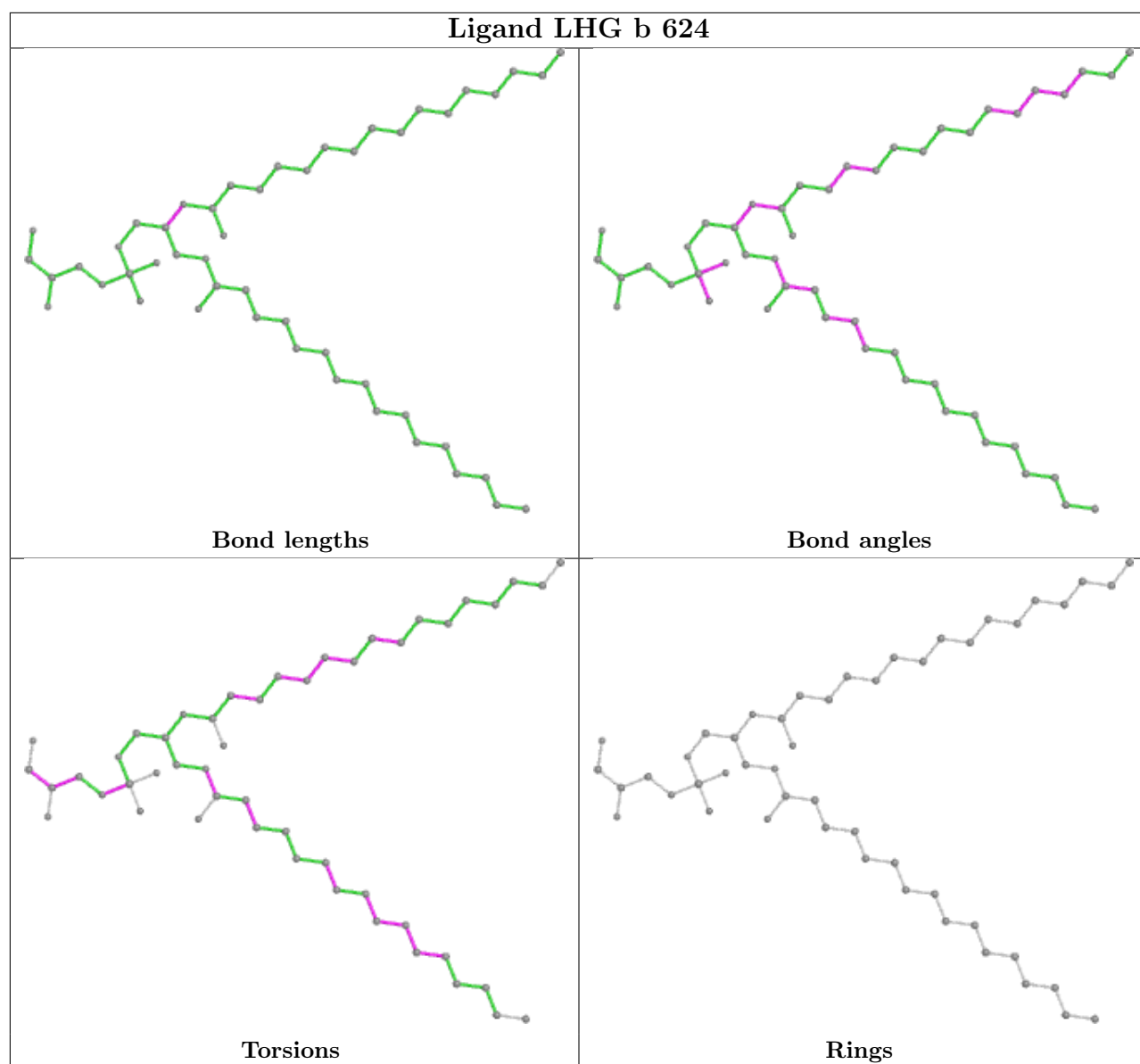


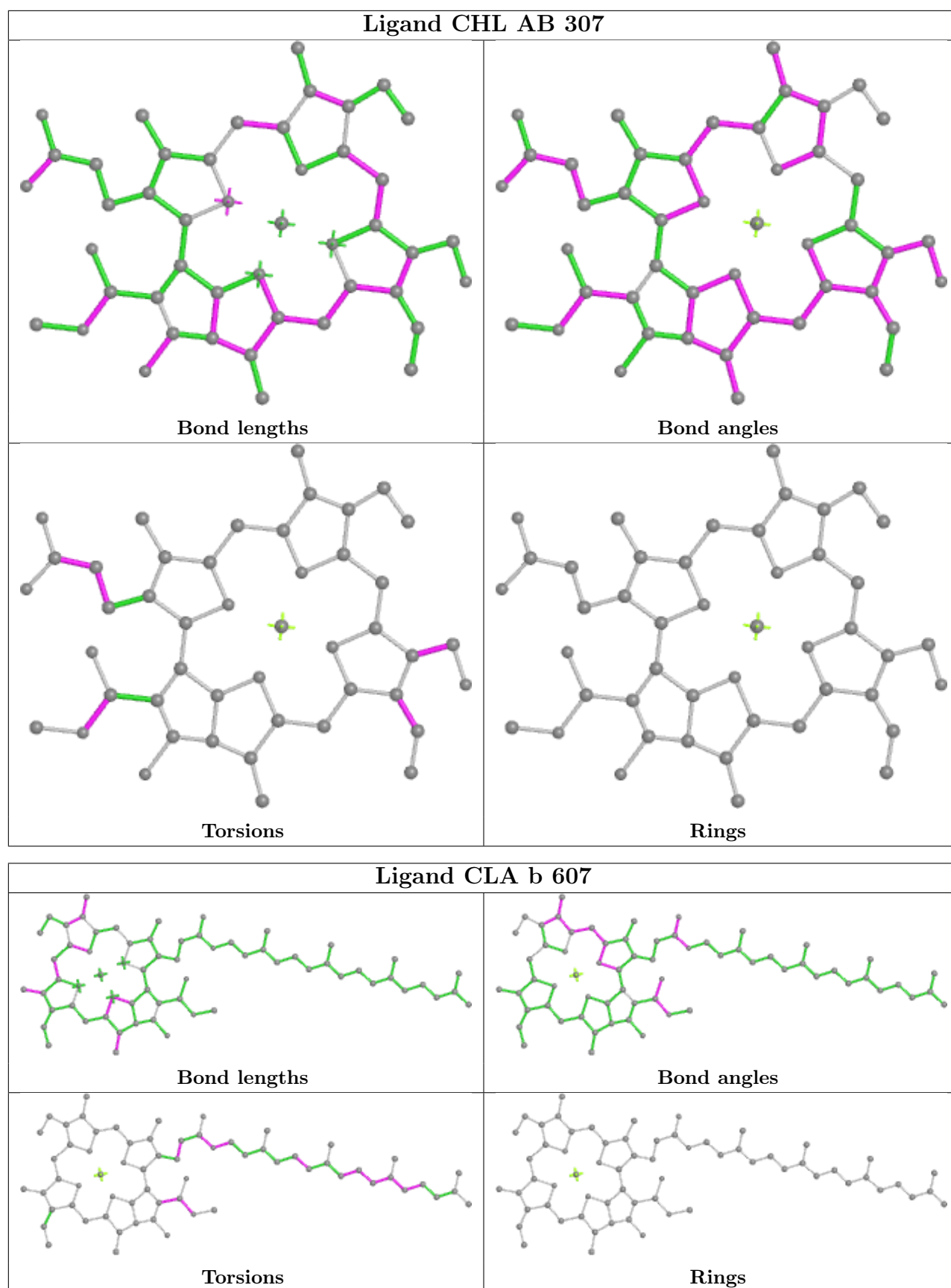
Torsions



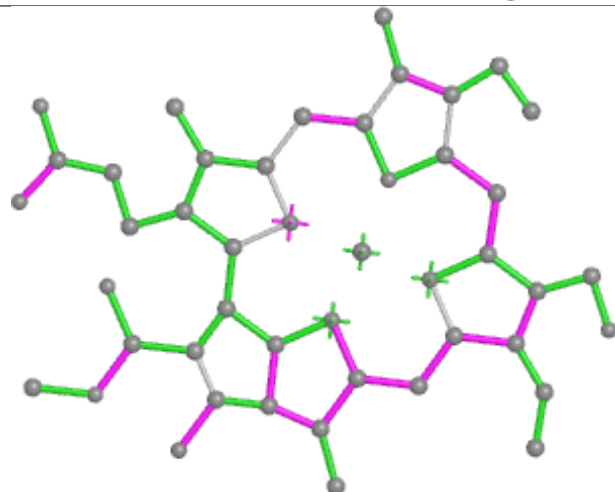
Rings



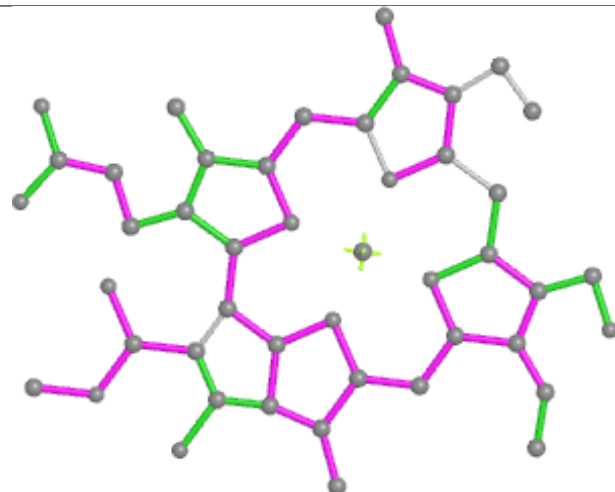




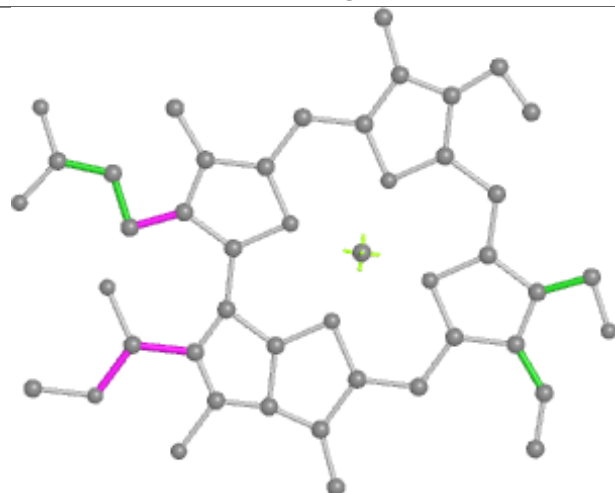
Ligand CHL AB 306



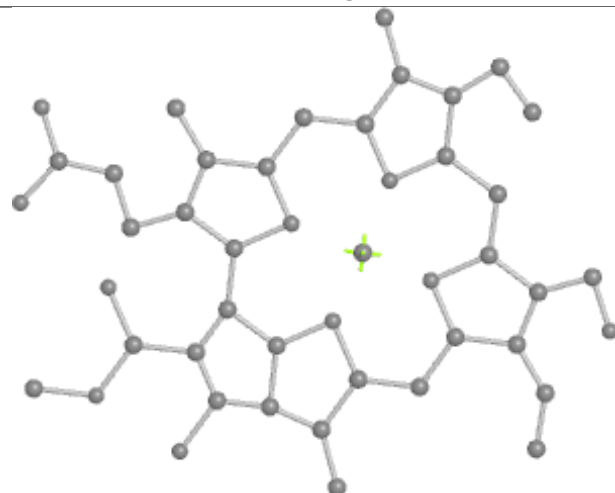
Bond lengths



Bond angles

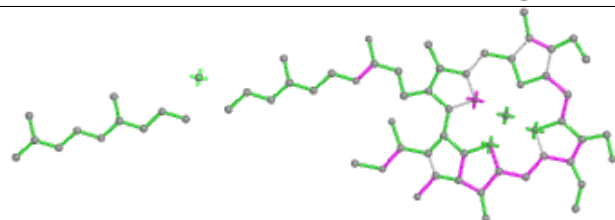


Torsions

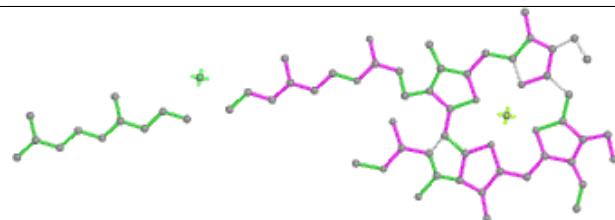


Rings

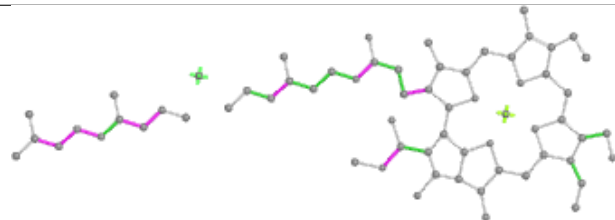
Ligand CHL Y 302



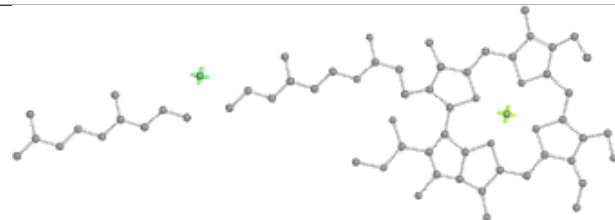
Bond lengths



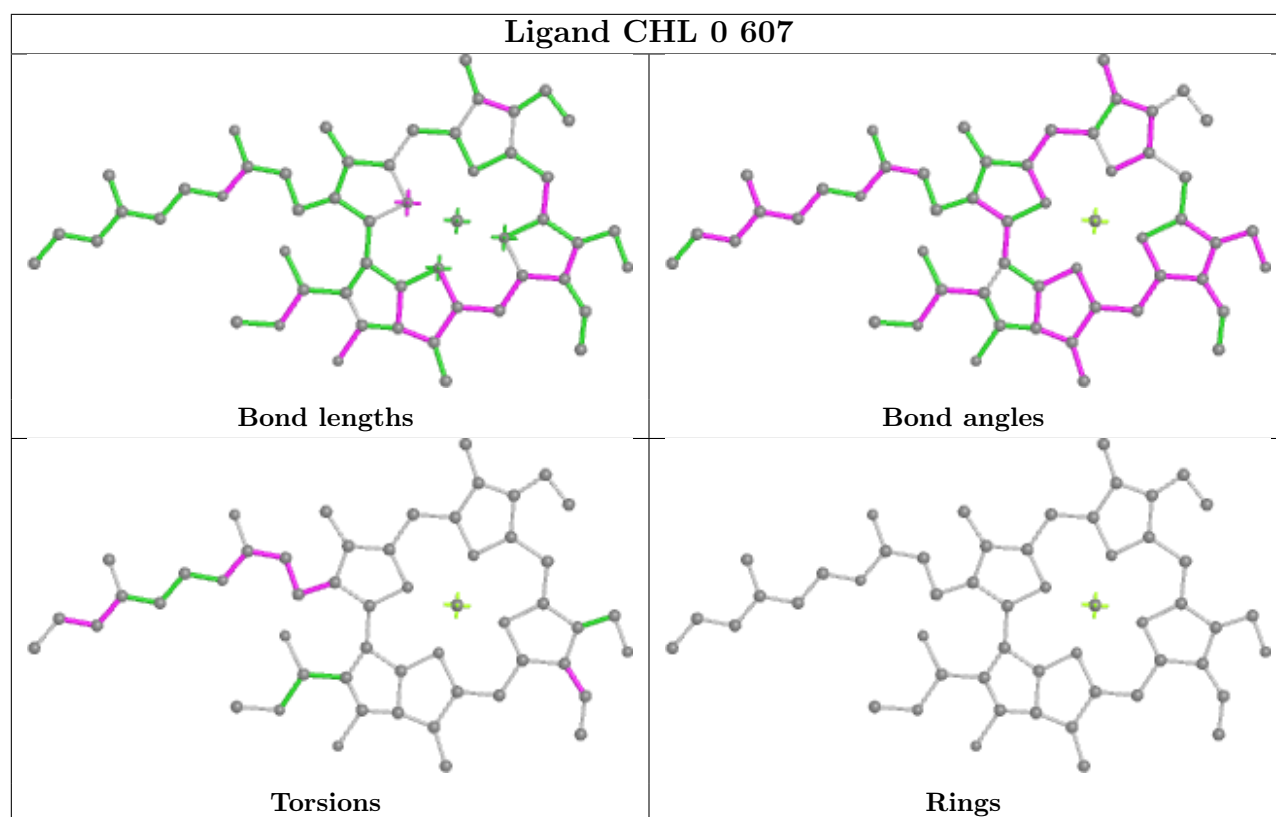
Bond angles



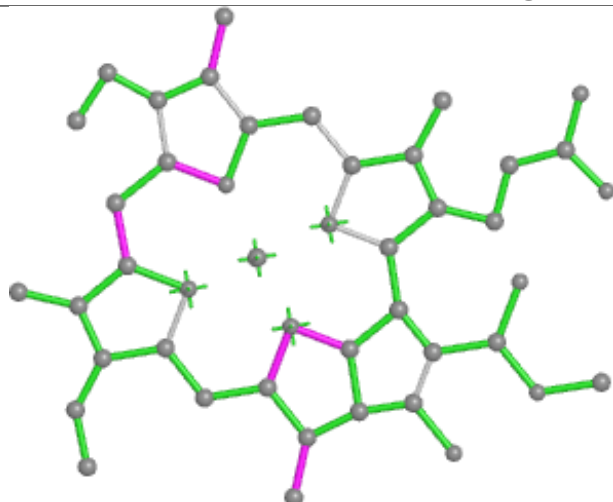
Torsions



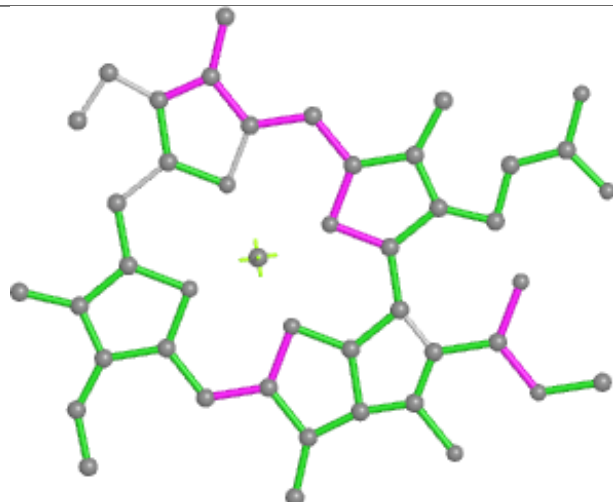
Rings



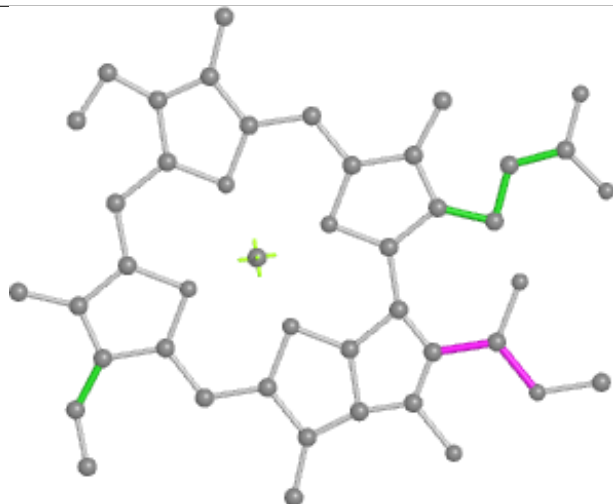
Ligand CLA s 603



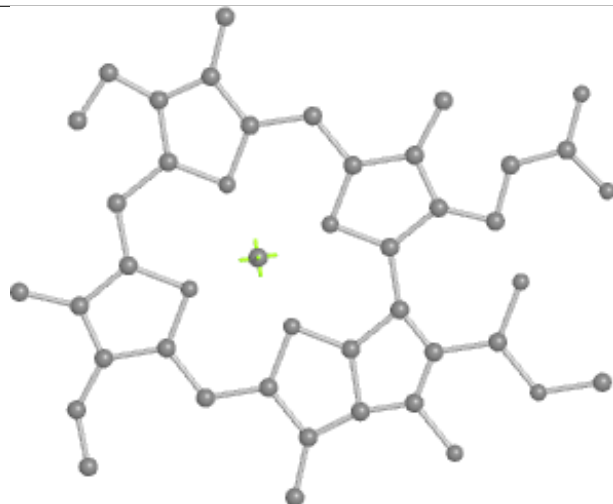
Bond lengths



Bond angles

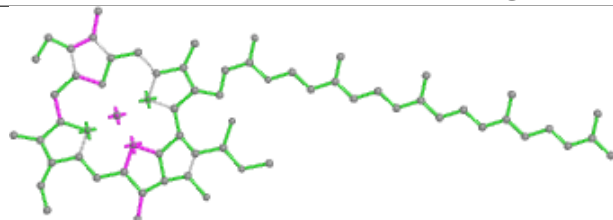


Torsions

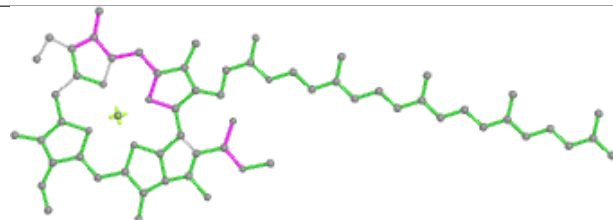


Rings

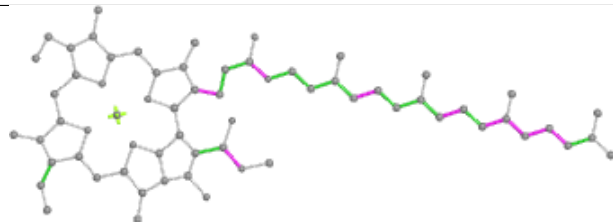
Ligand CLA BF 514



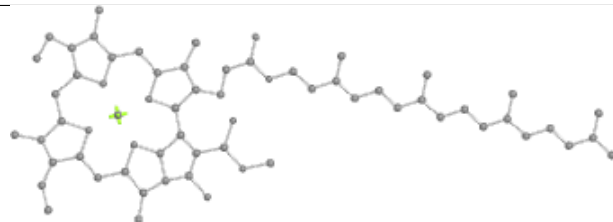
Bond lengths



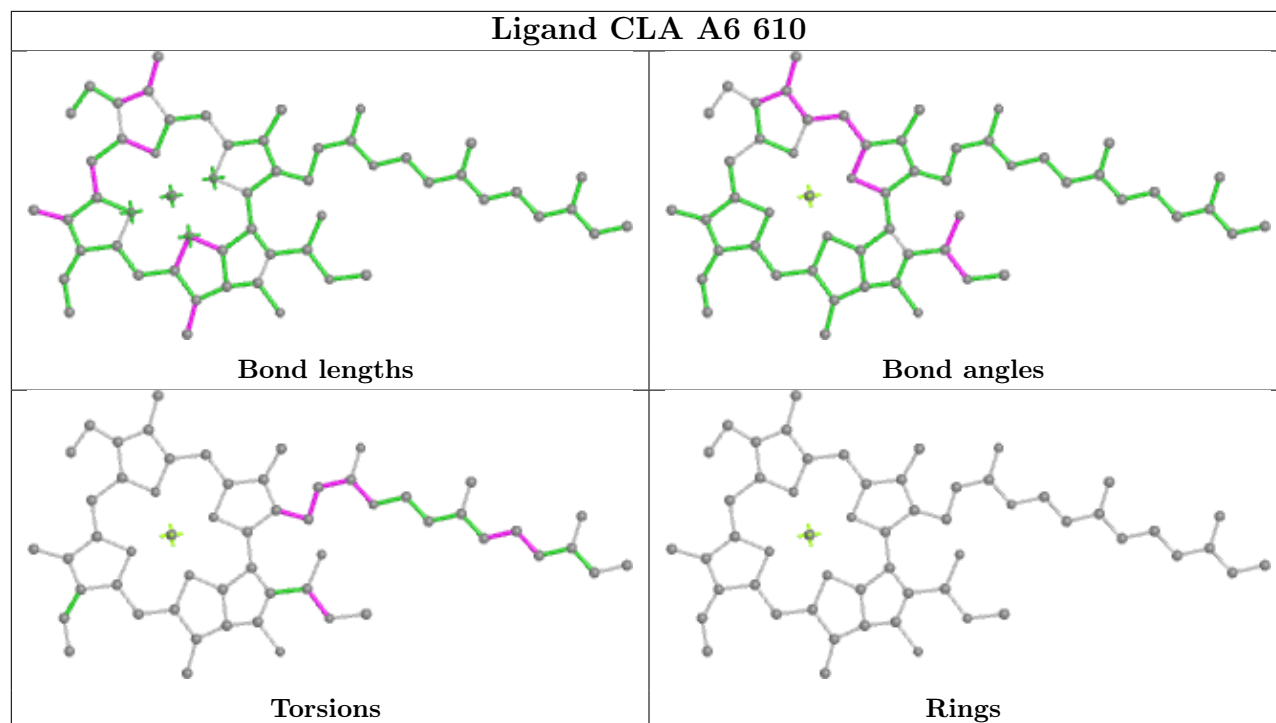
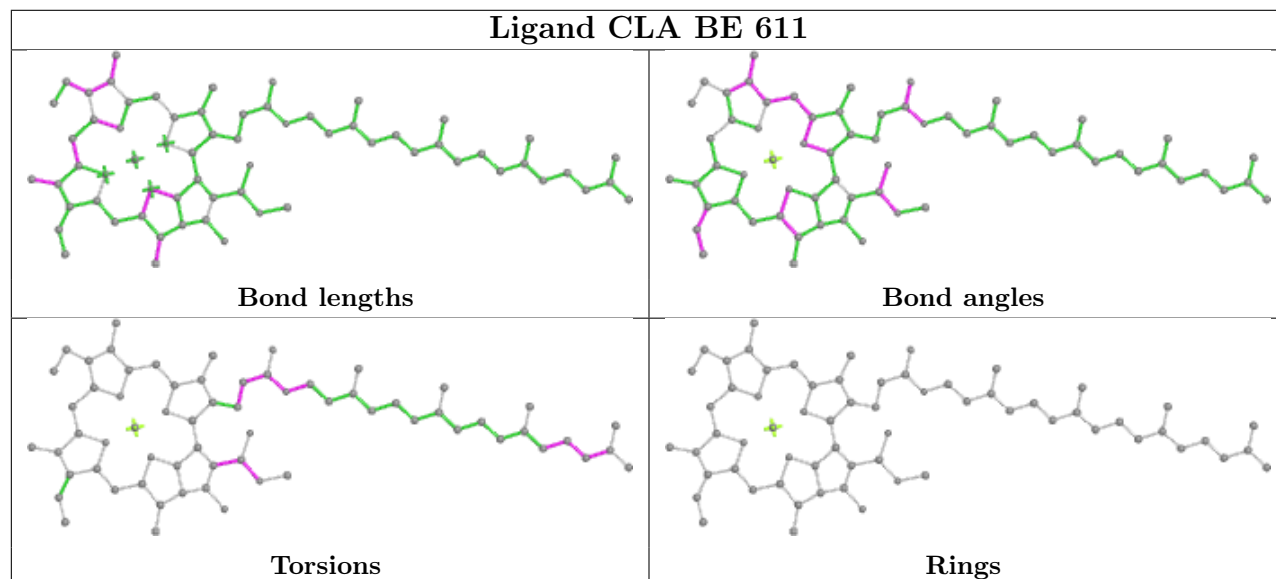
Bond angles



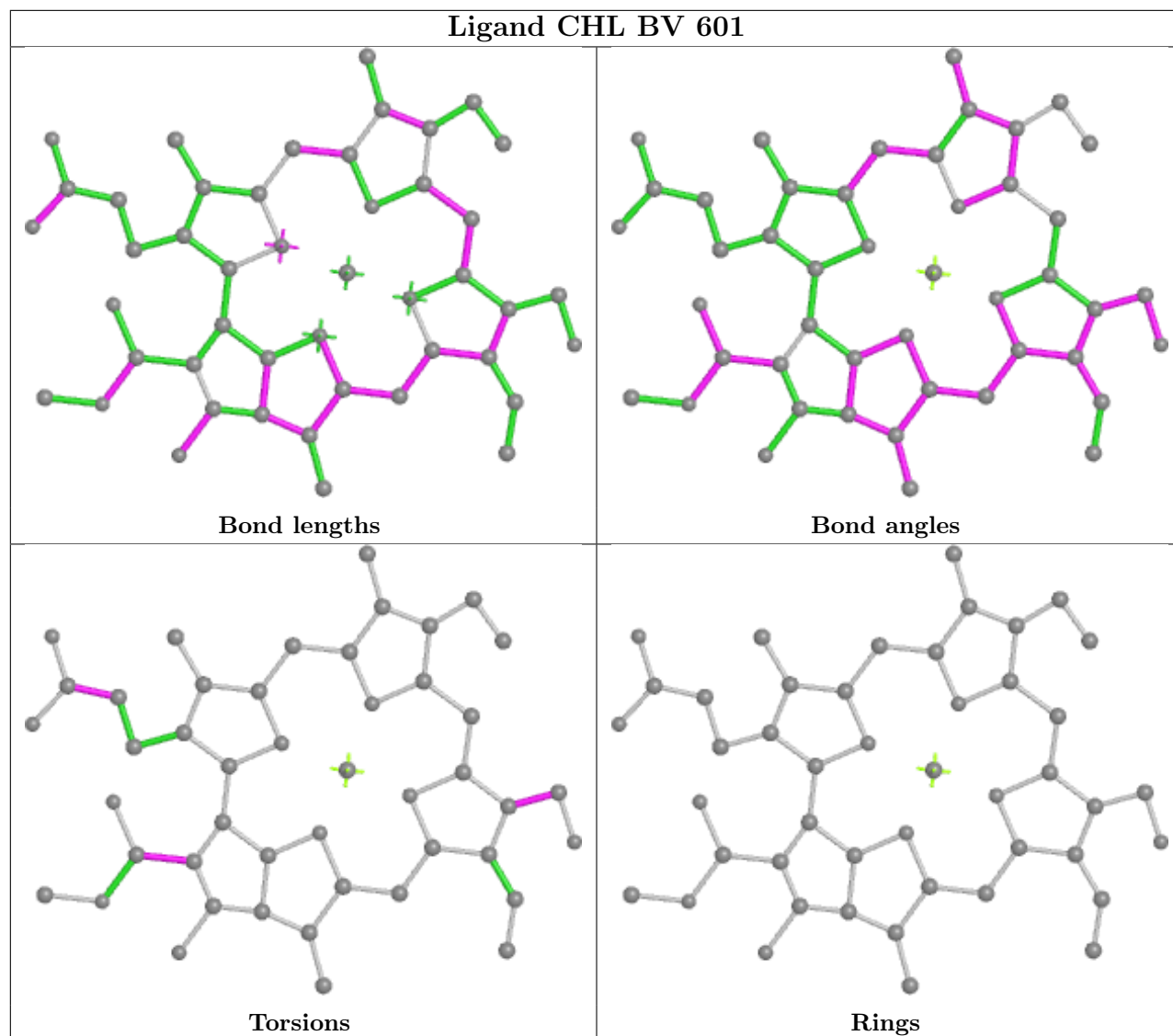
Torsions

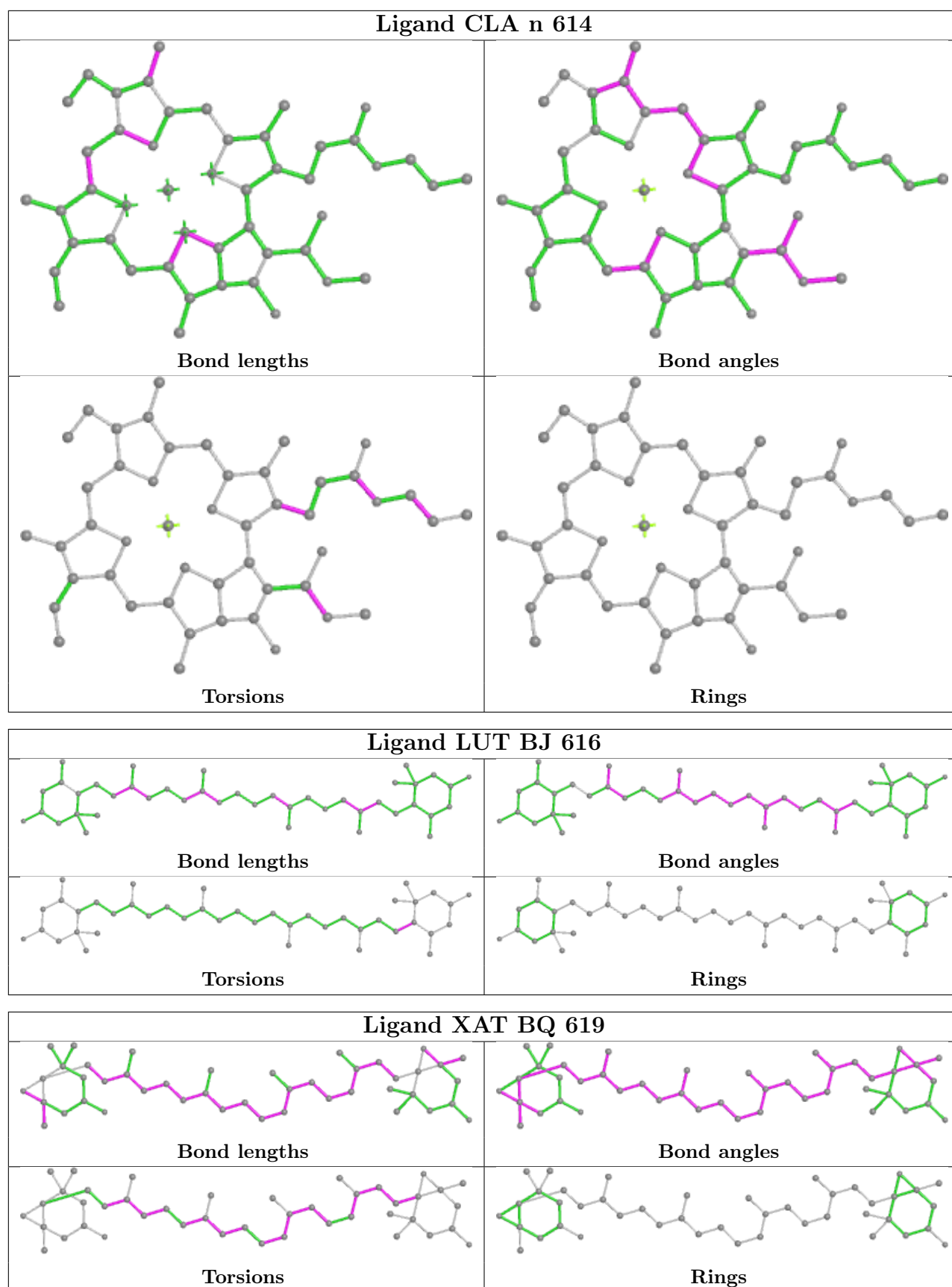


Rings

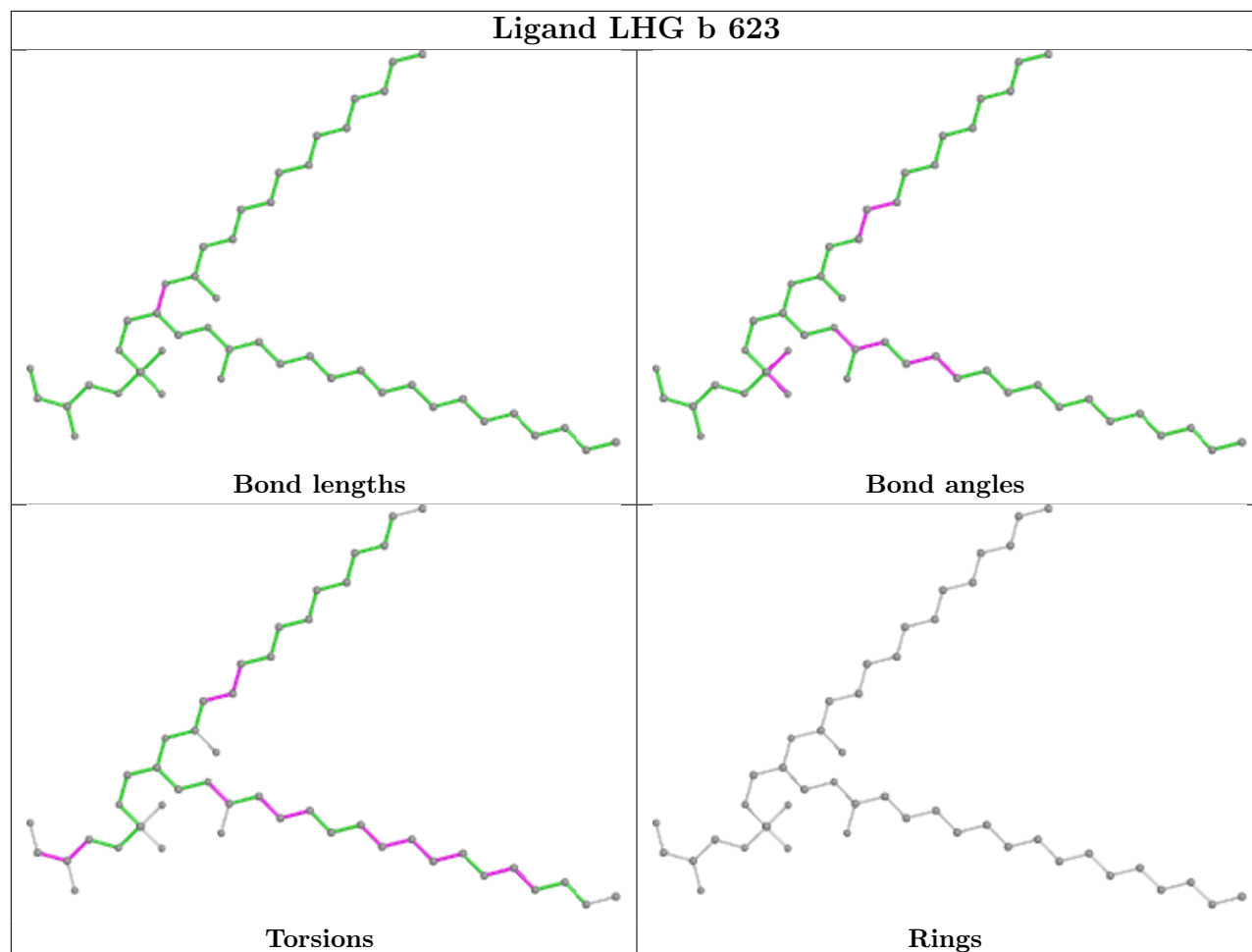
Ligand CLA A6 610**Ligand CLA BE 611**

Ligand CHL BV 601

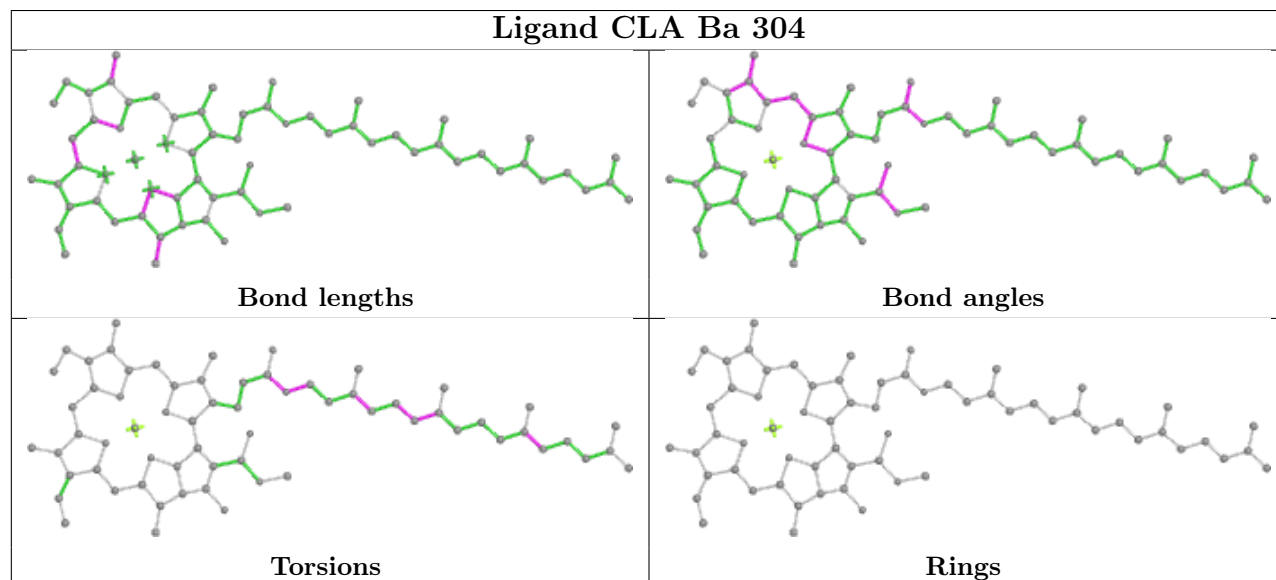




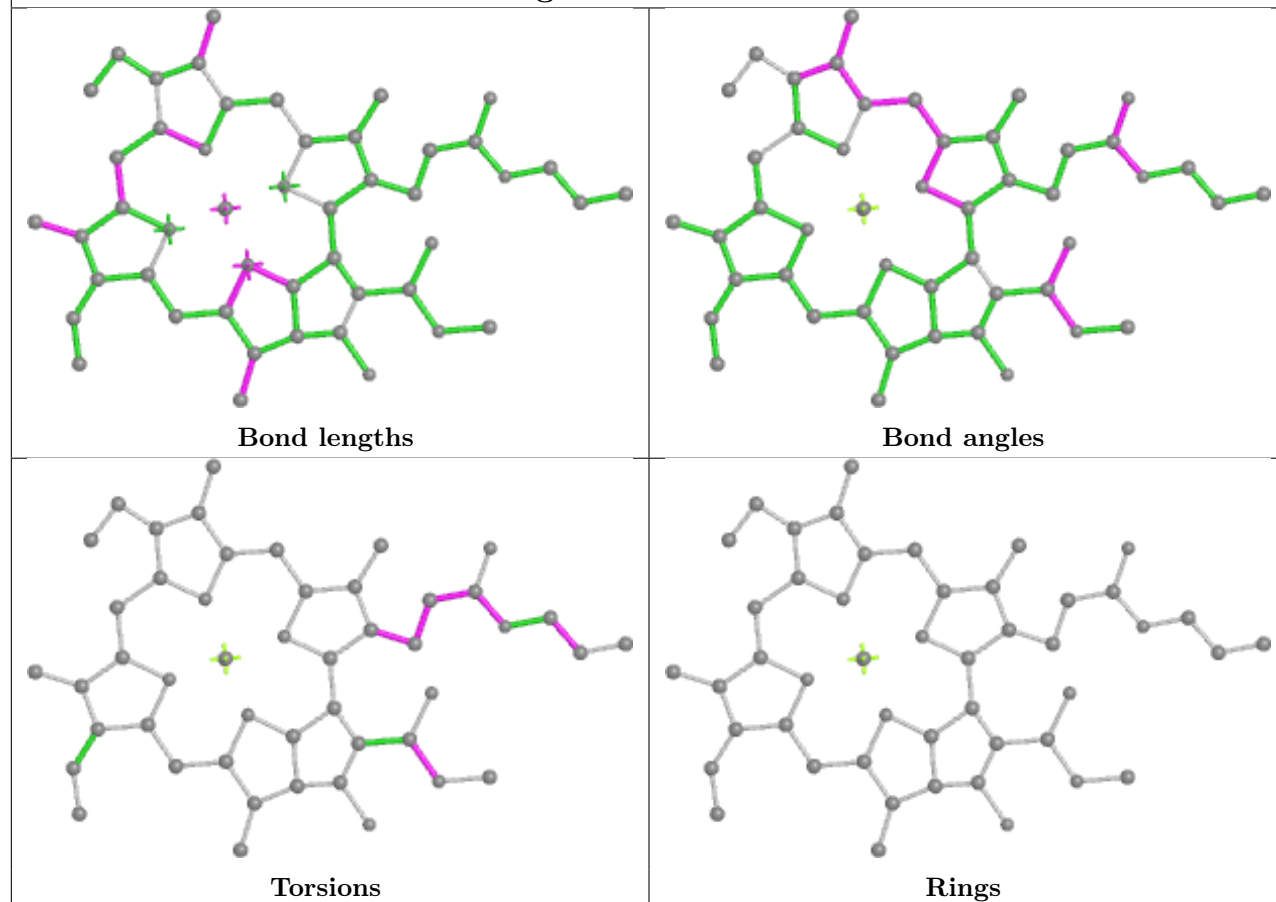
Ligand LHG b 623



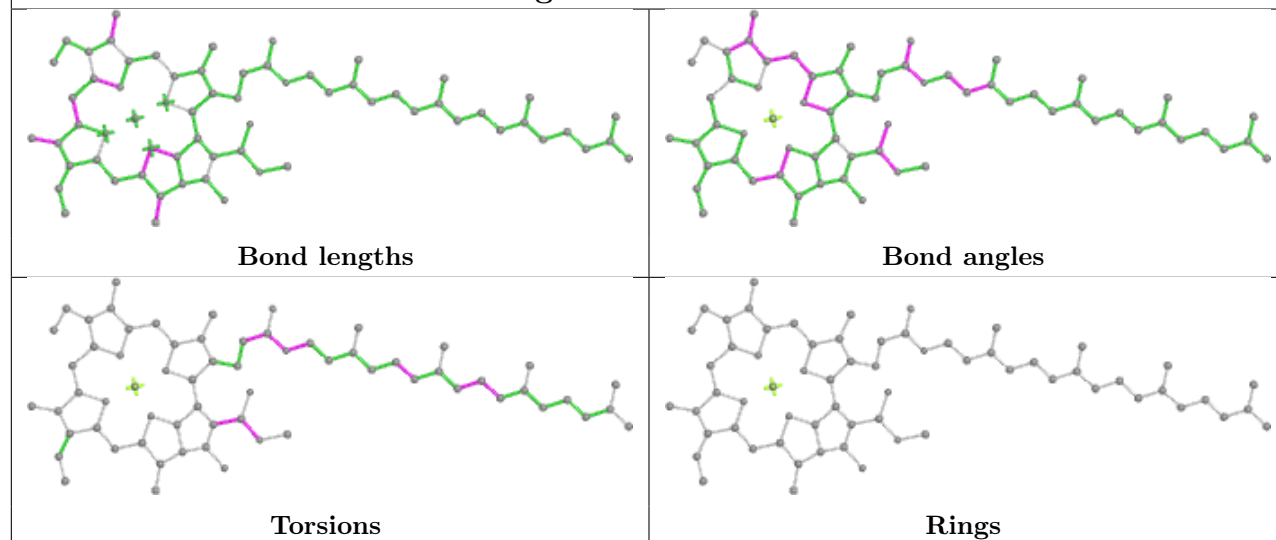
Ligand CLA Ba 304



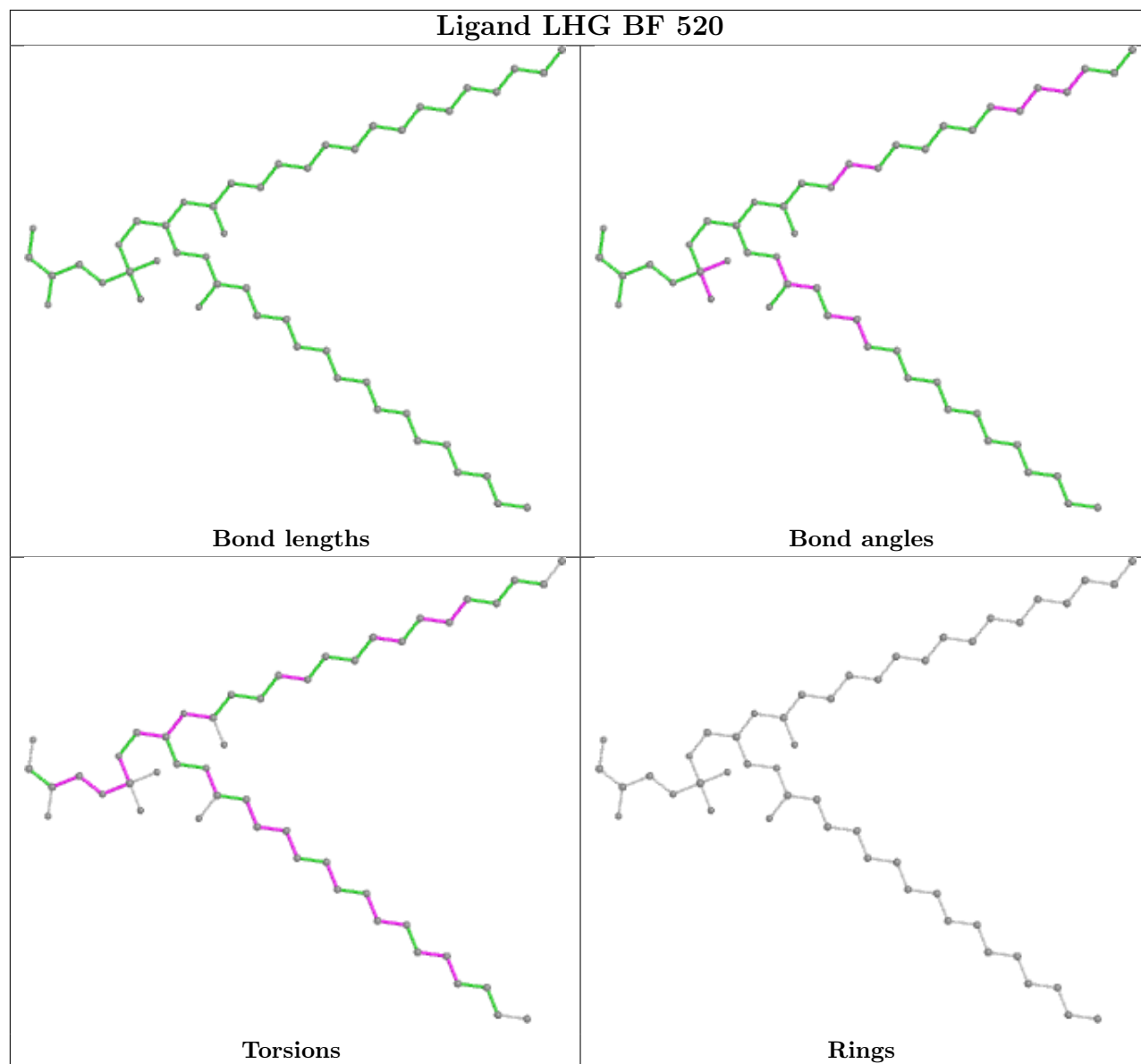
Ligand CLA 6 614



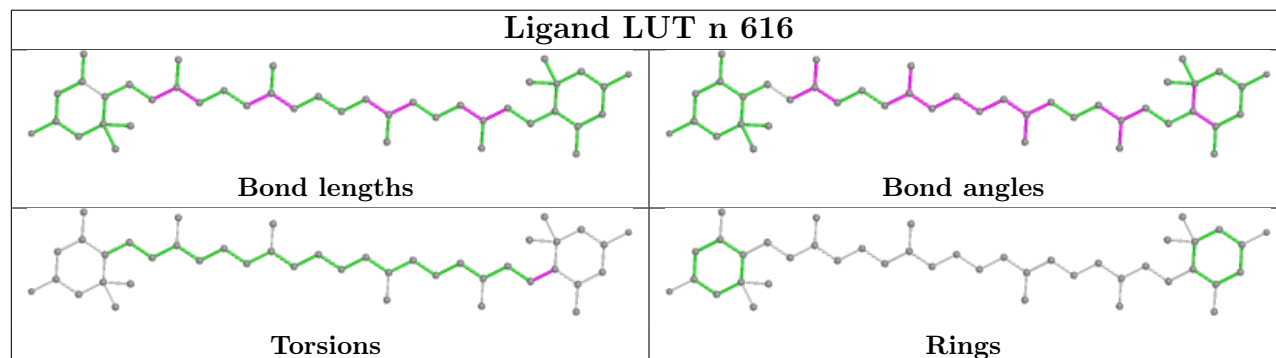
Ligand CLA b 612

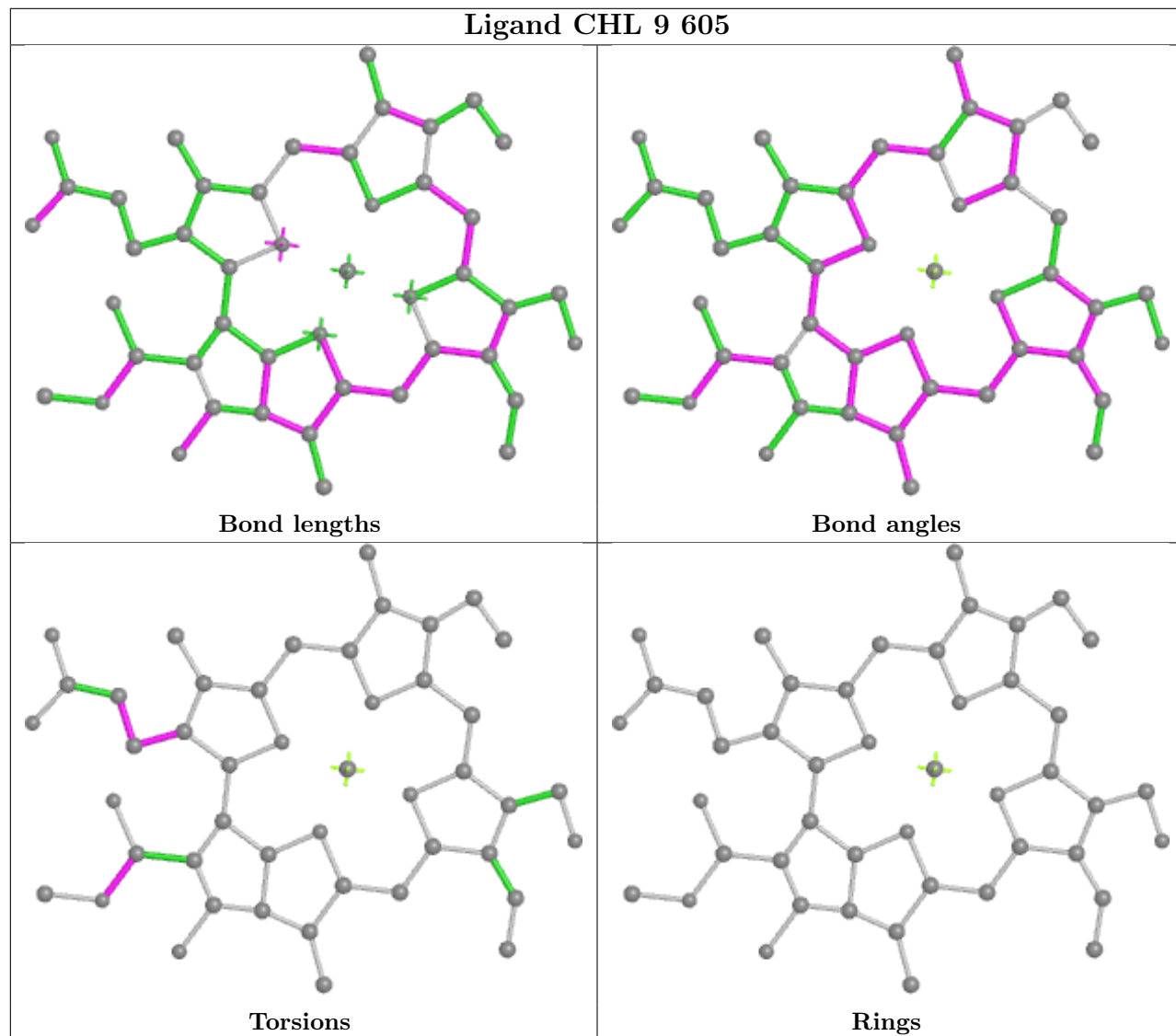
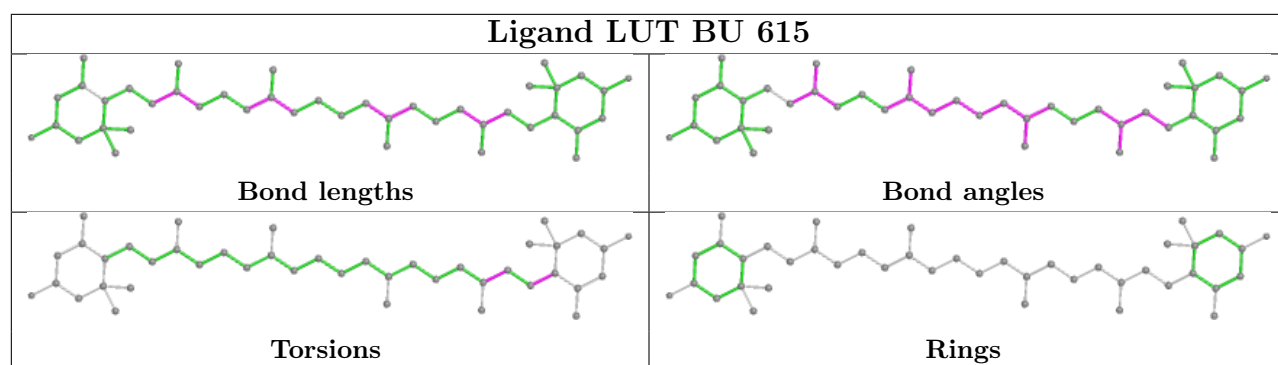


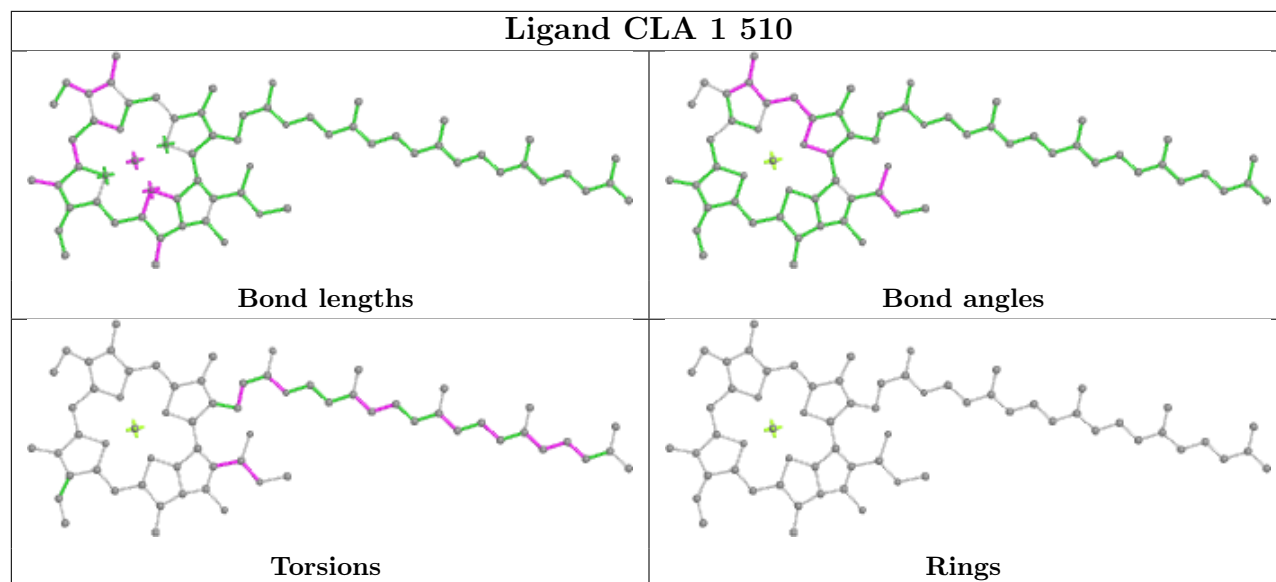
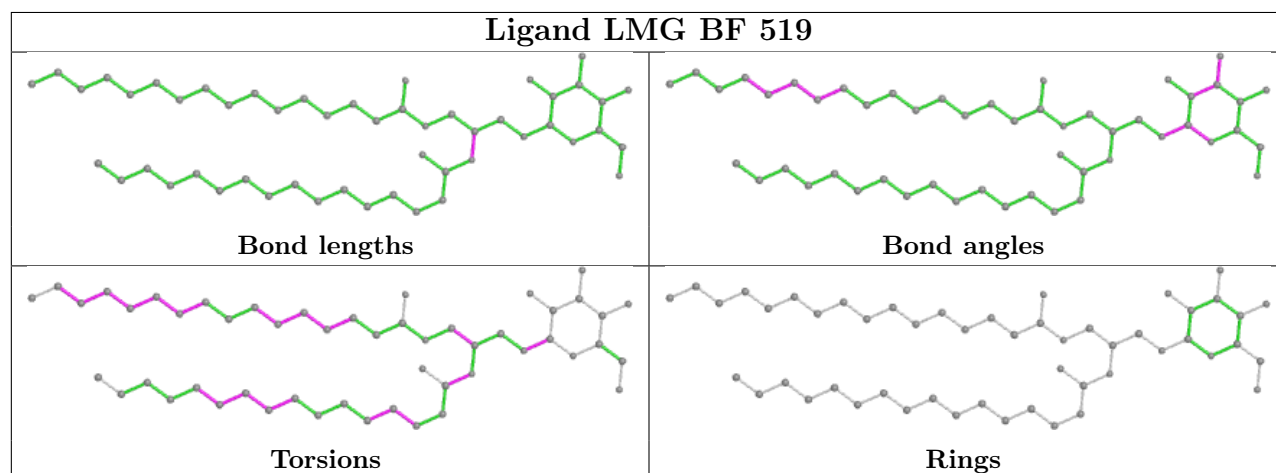
Ligand LHG BF 520



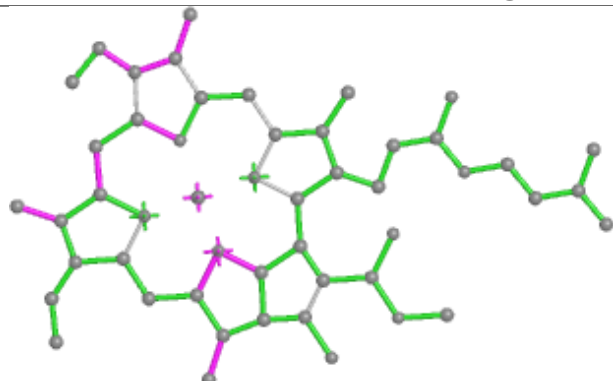
Ligand LUT n 616



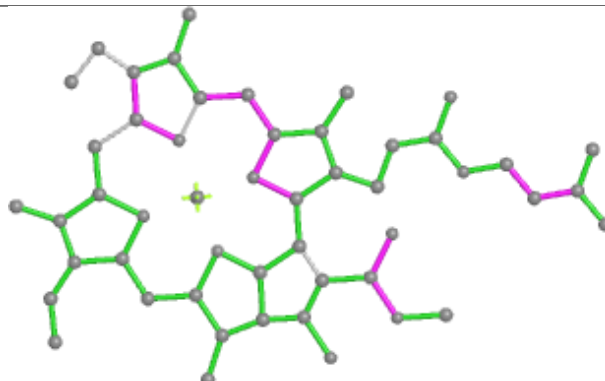


Ligand CLA 1 510**Ligand LMG BF 519**

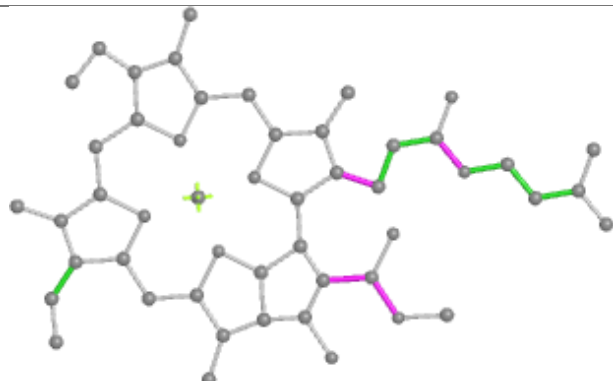
Ligand CLA BV 604



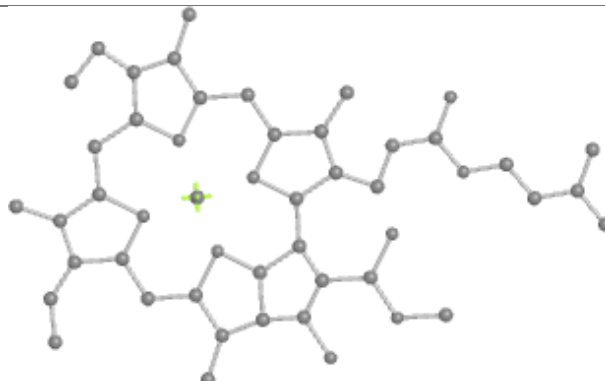
Bond lengths



Bond angles

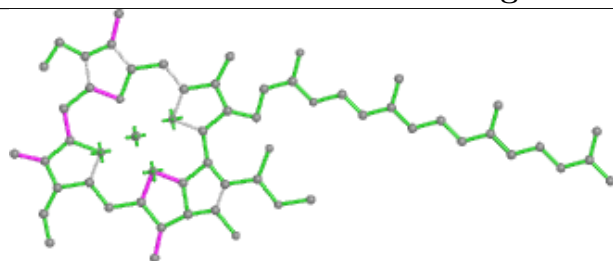


Torsions

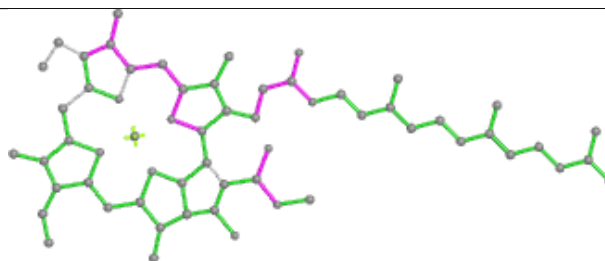


Rings

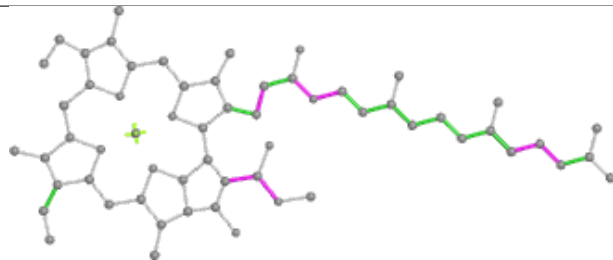
Ligand CLA BD 410



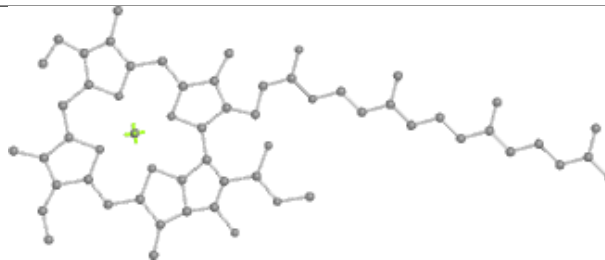
Bond lengths



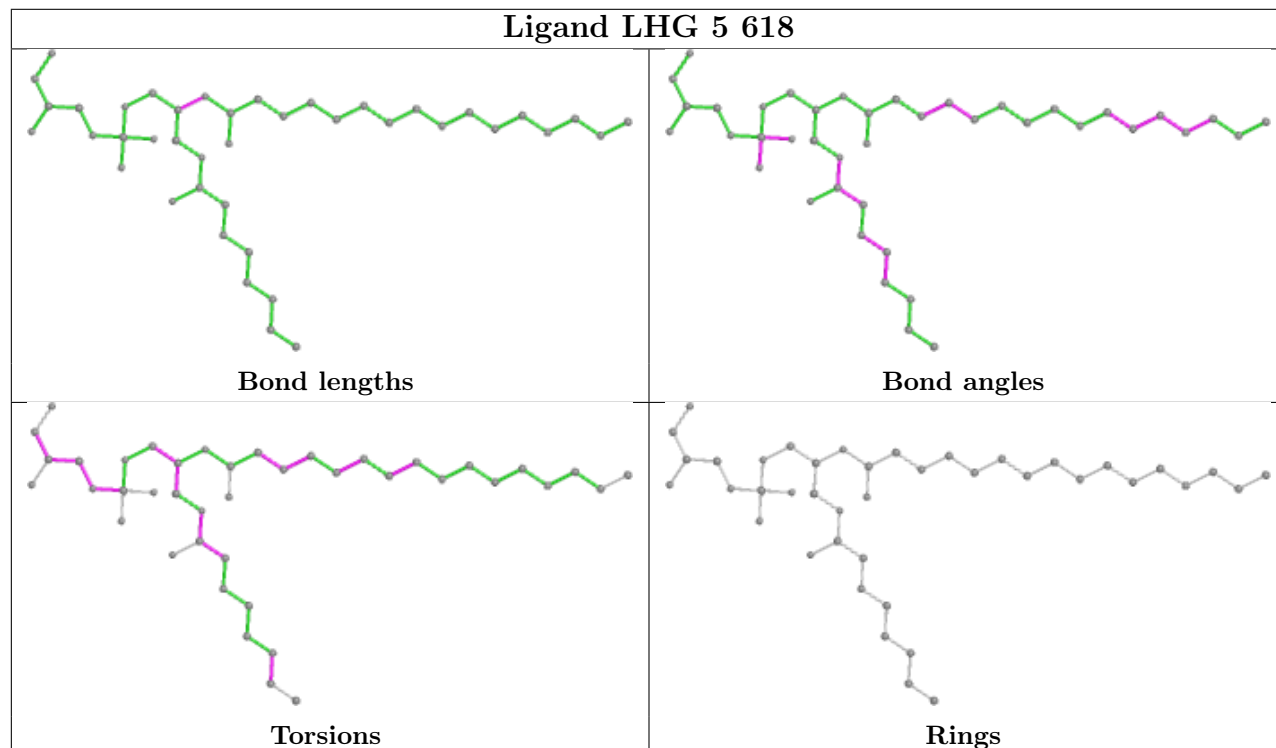
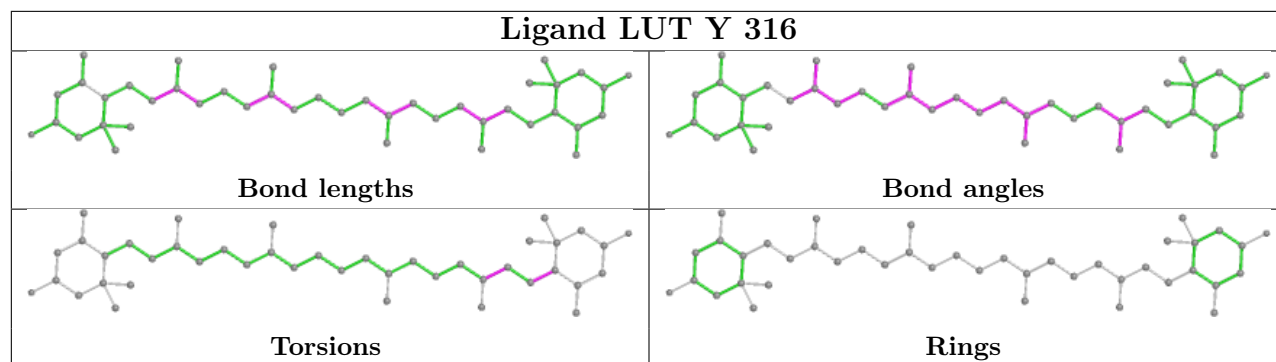
Bond angles



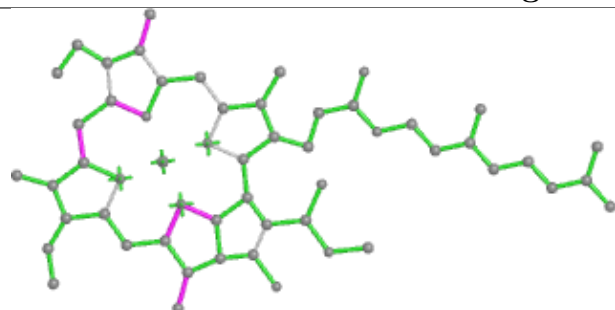
Torsions



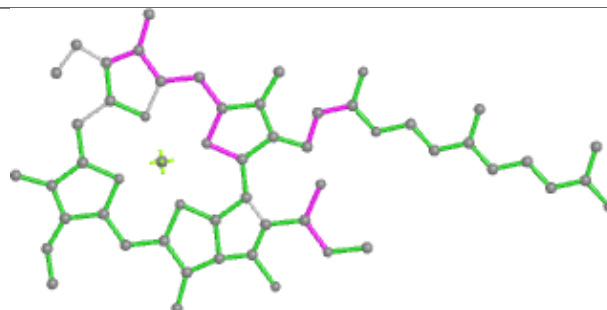
Rings



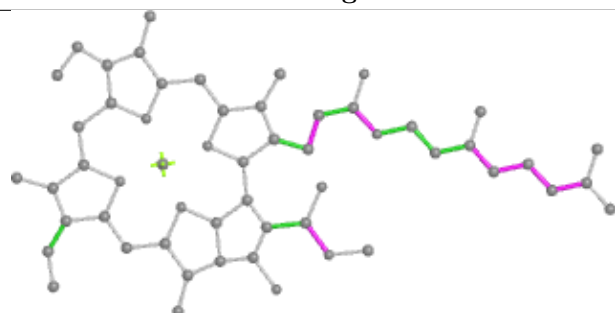
Ligand CLA s 612



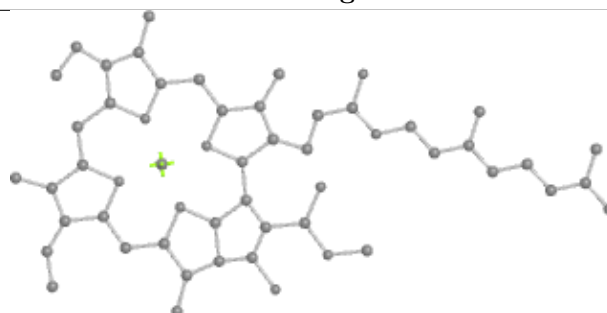
Bond lengths



Bond angles

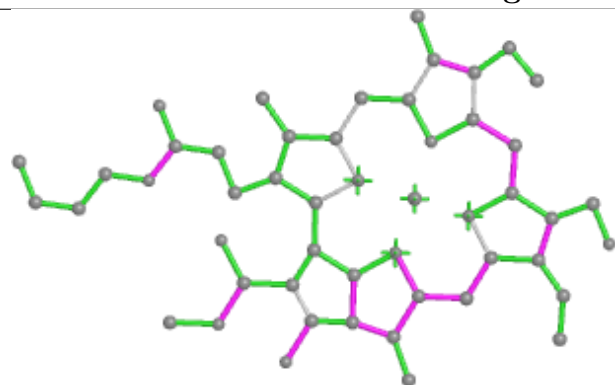


Torsions

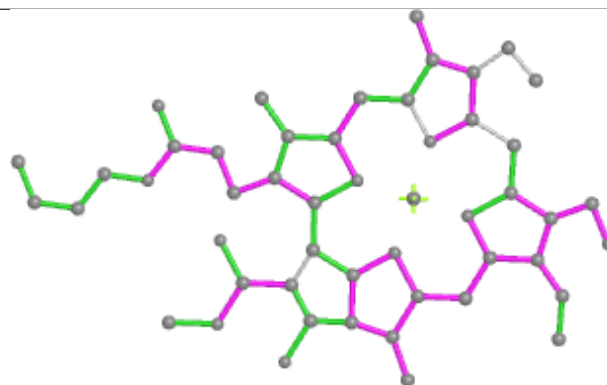


Rings

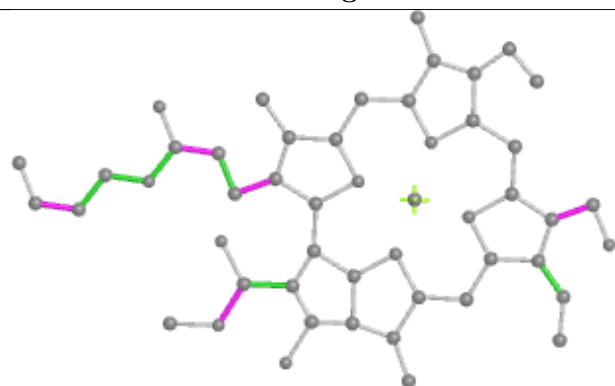
Ligand CHL BB 307



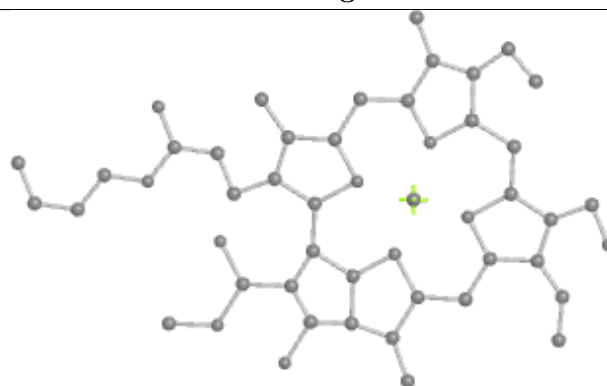
Bond lengths



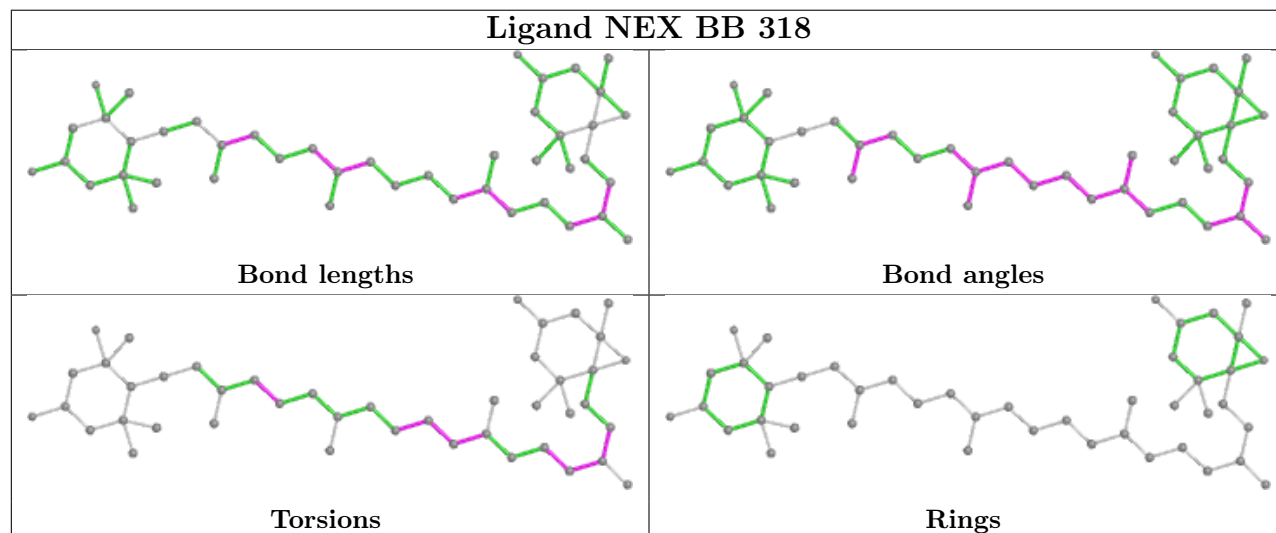
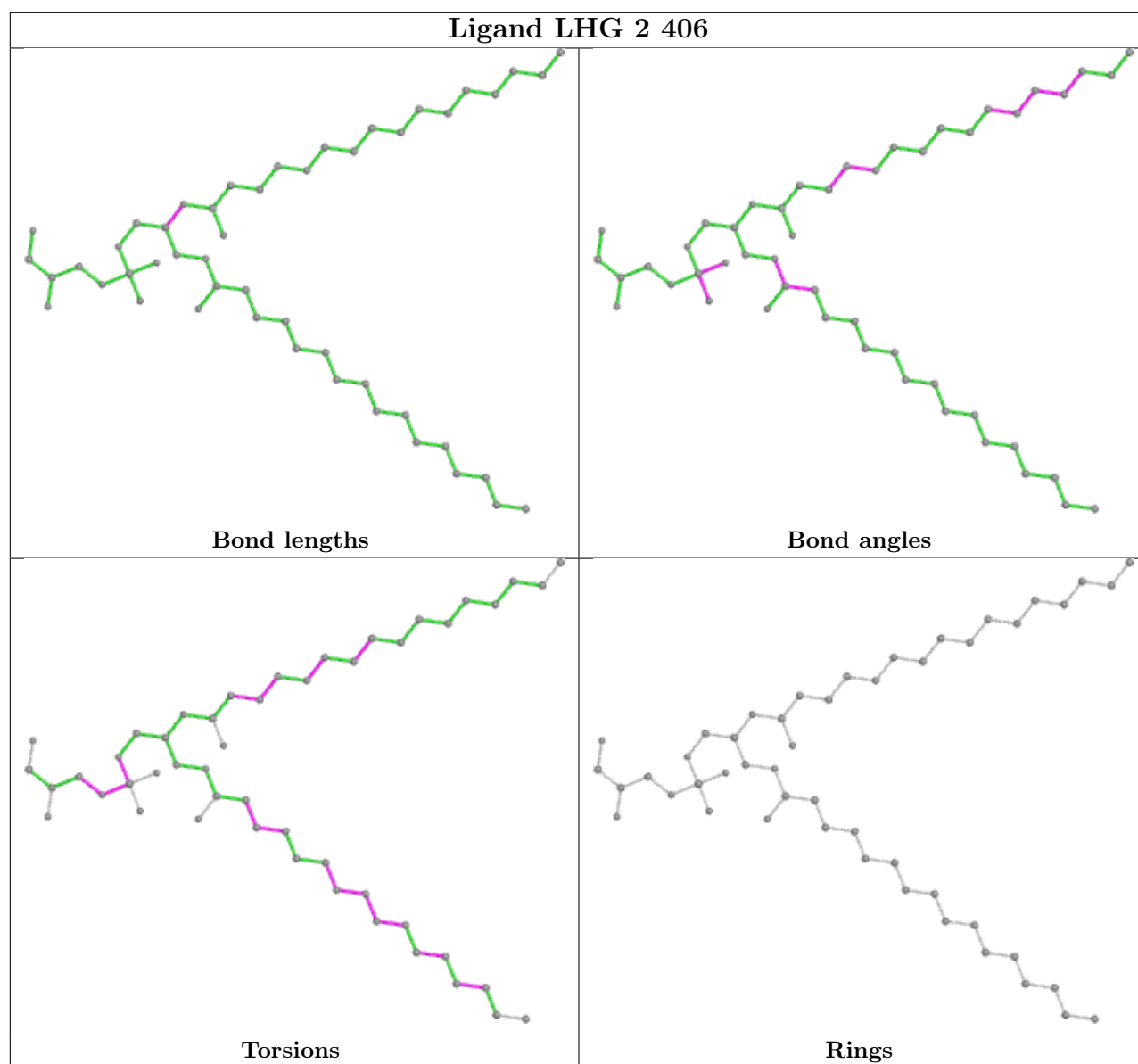
Bond angles

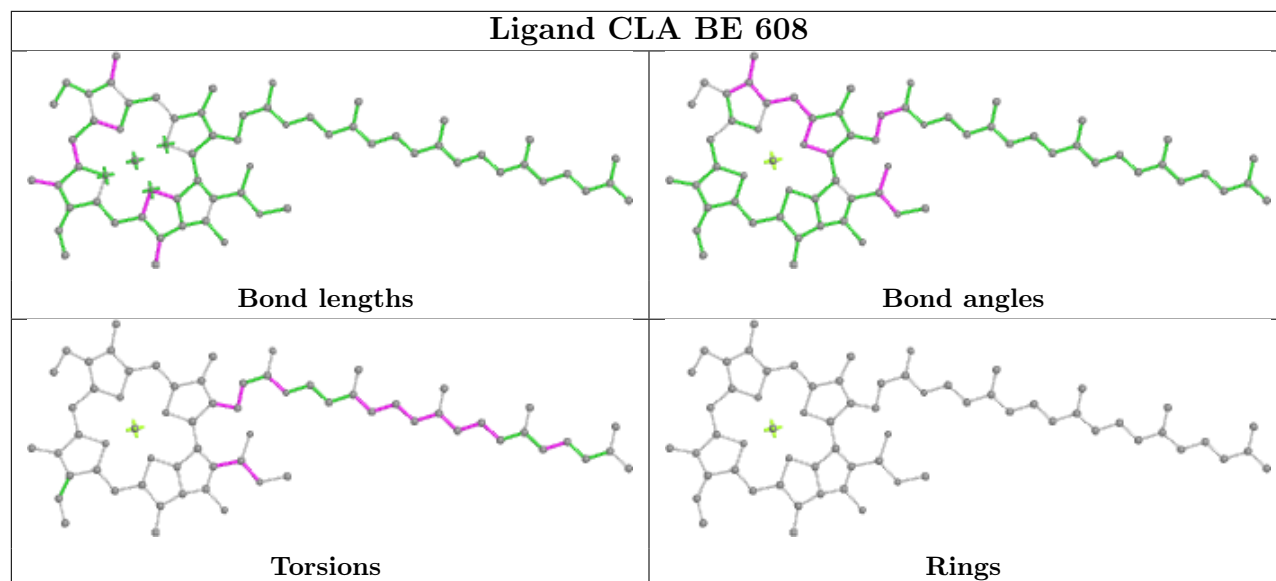
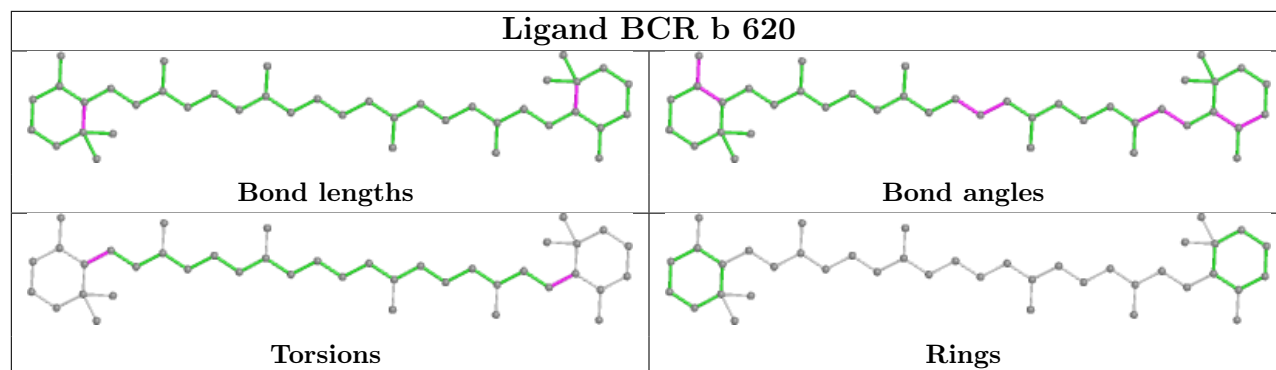


Torsions

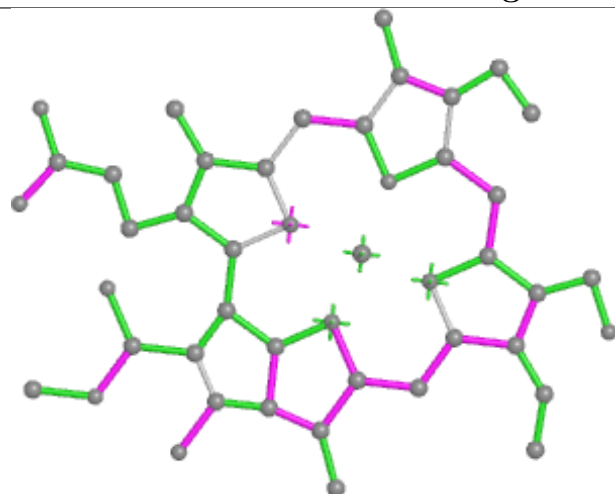


Rings

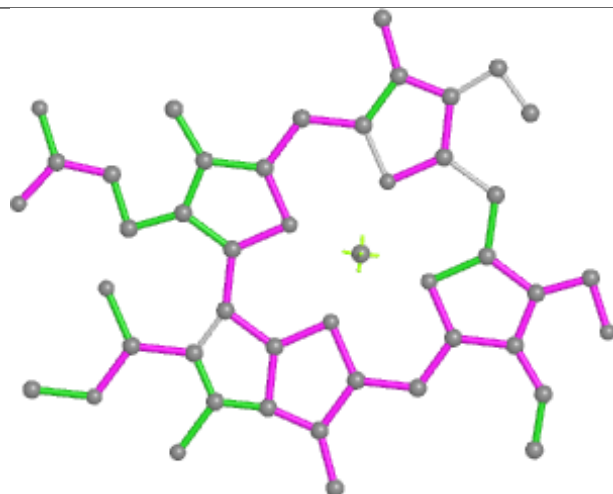




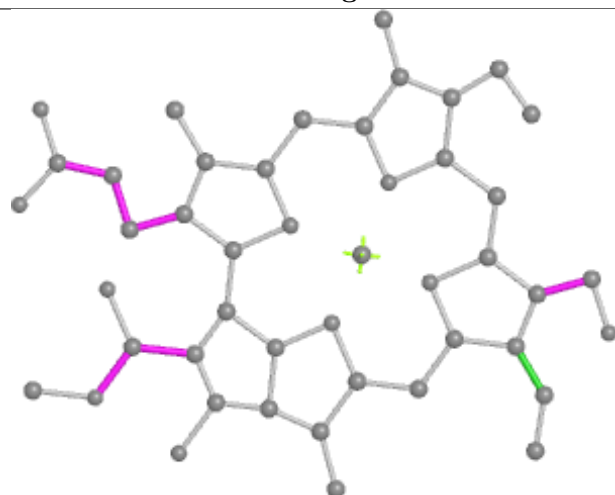
Ligand CHL AB 304



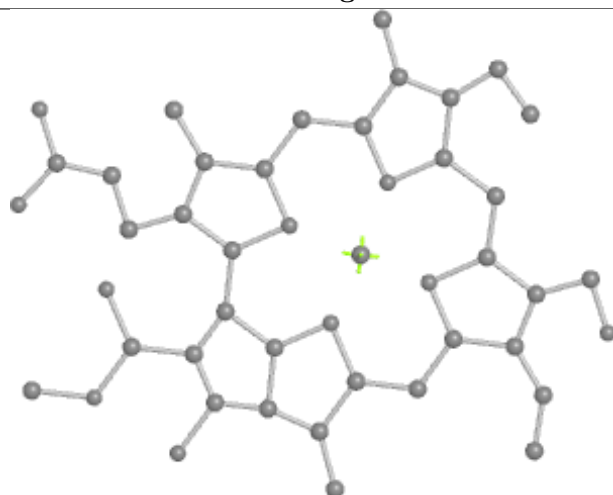
Bond lengths



Bond angles

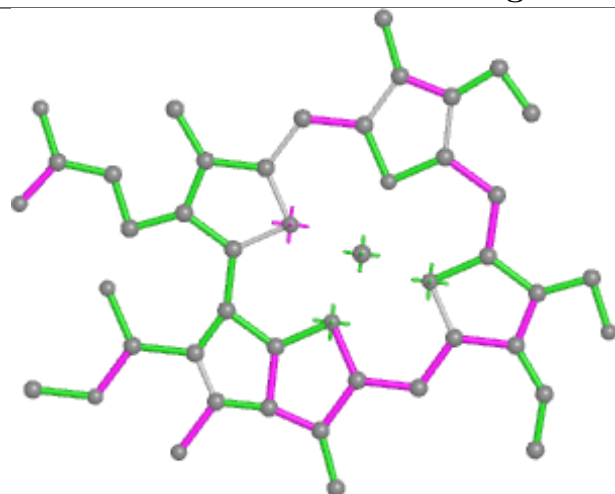


Torsions

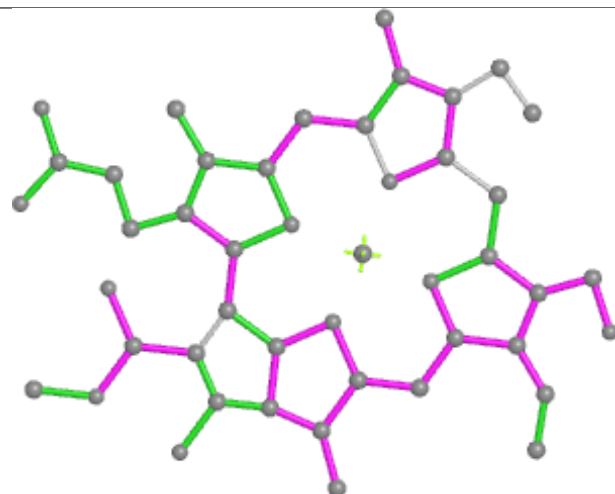


Rings

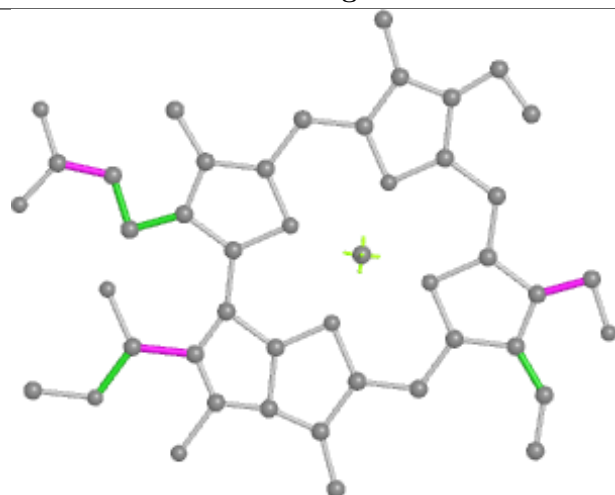
Ligand CHL A6 601



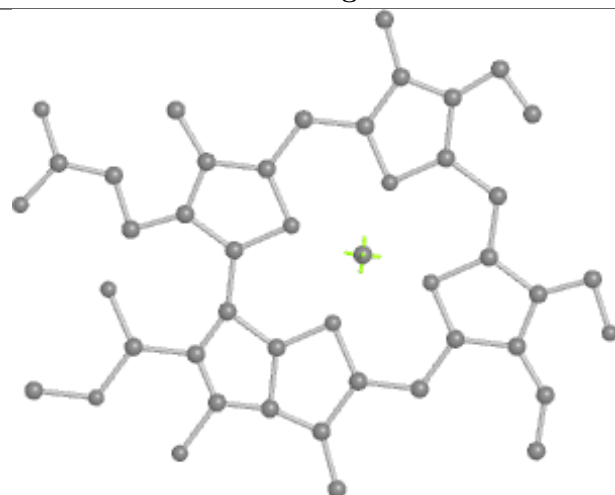
Bond lengths



Bond angles

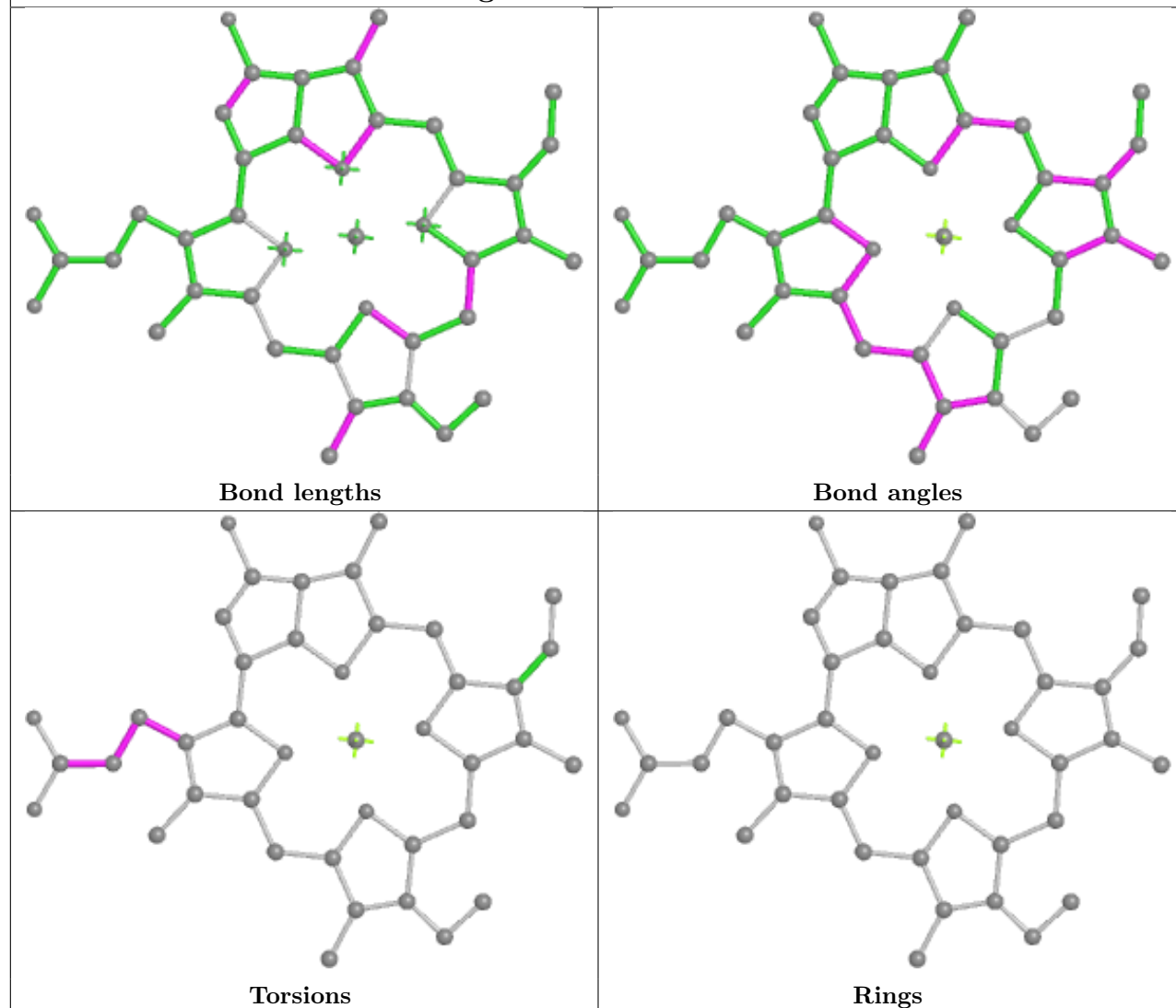


Torsions

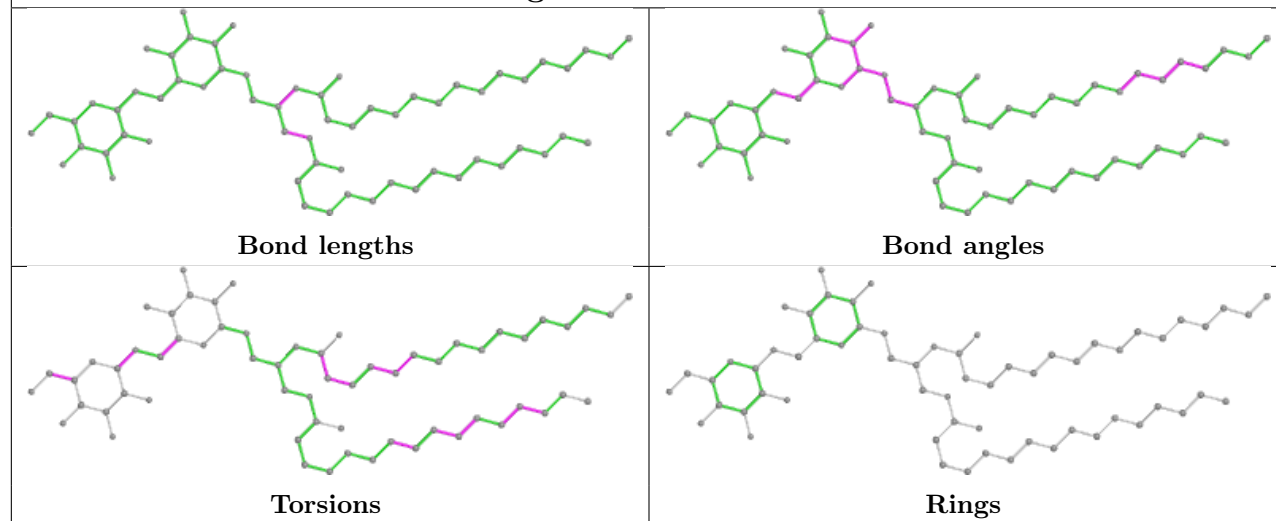


Rings

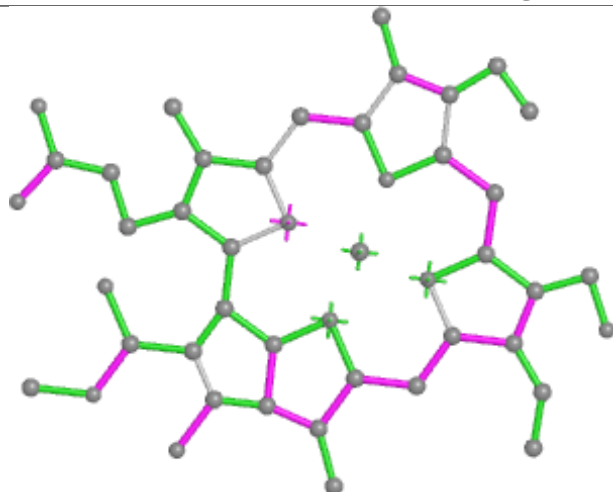
Ligand CLA AB 301



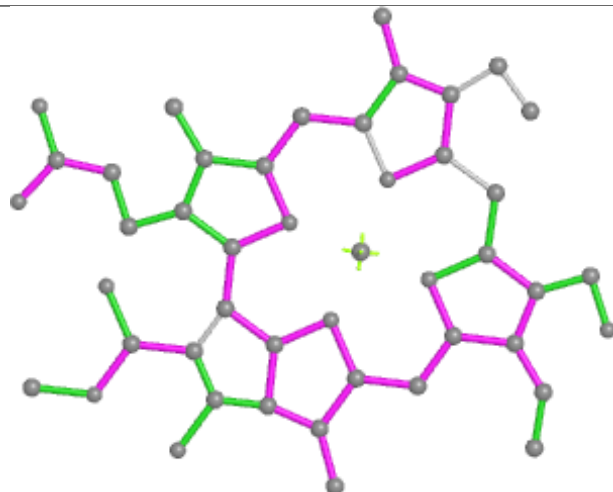
Ligand DGD H 102



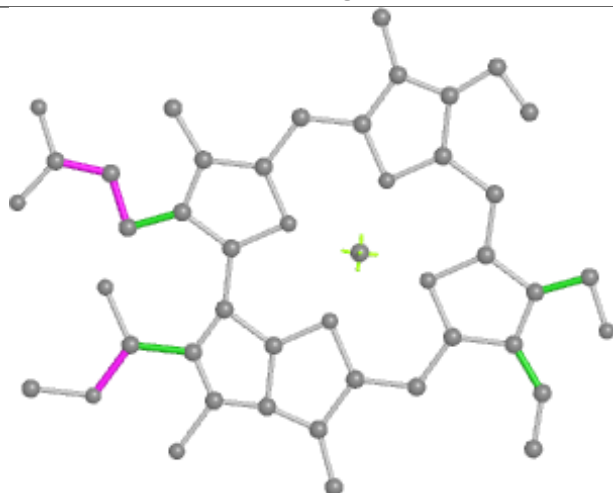
Ligand CHL 7 306



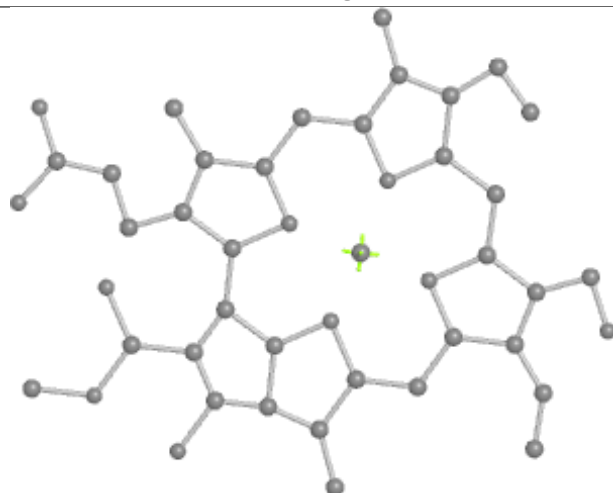
Bond lengths



Bond angles

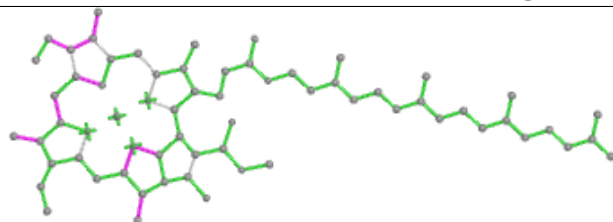


Torsions

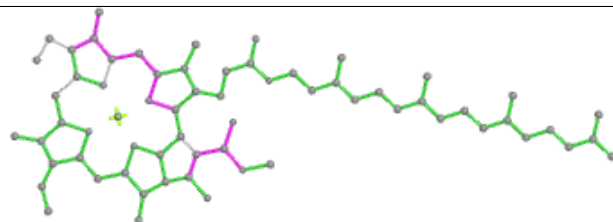


Rings

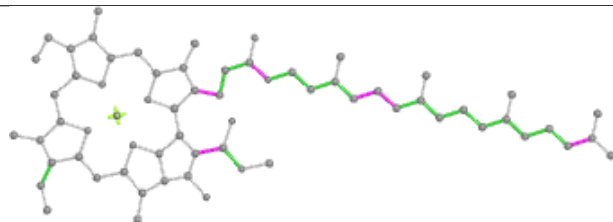
Ligand CLA c 512



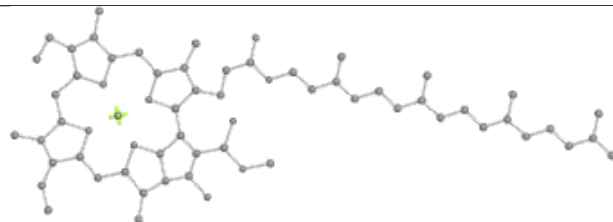
Bond lengths



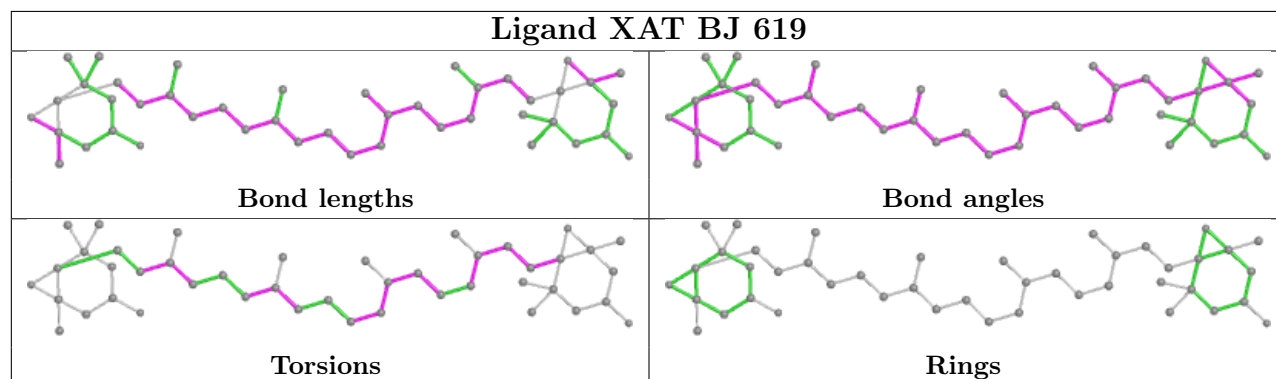
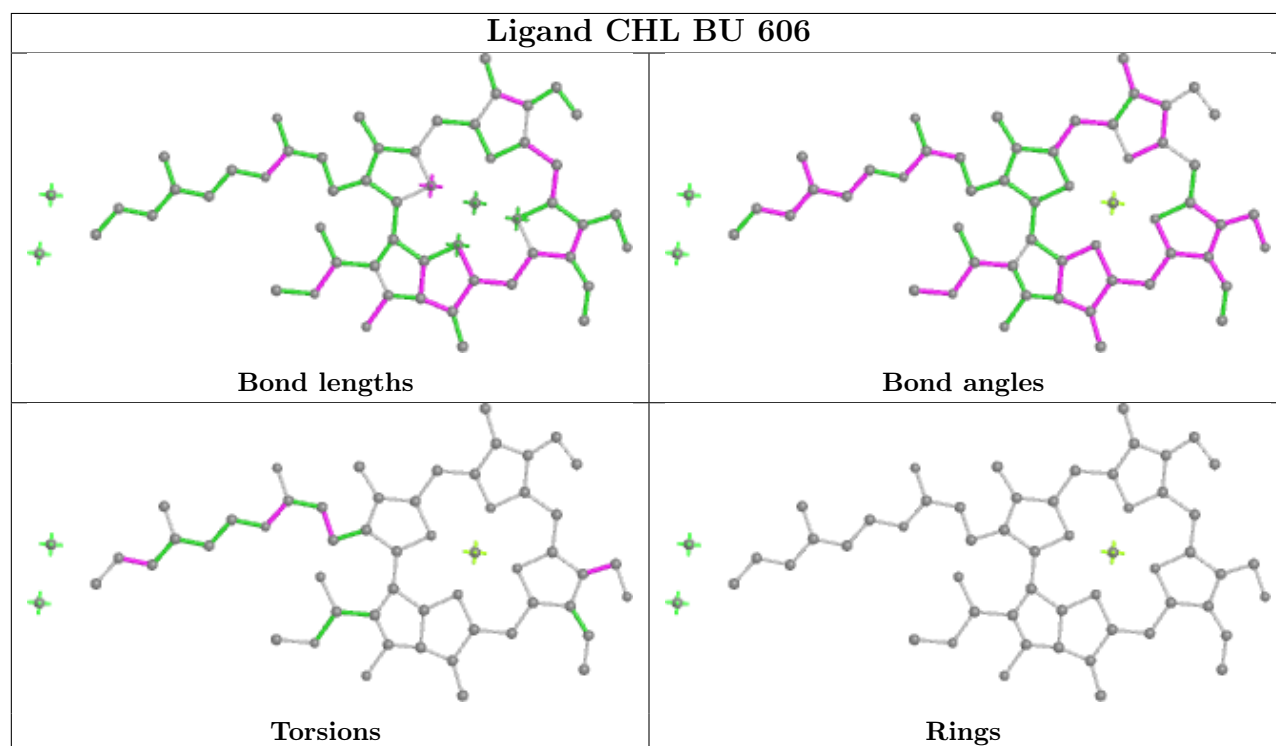
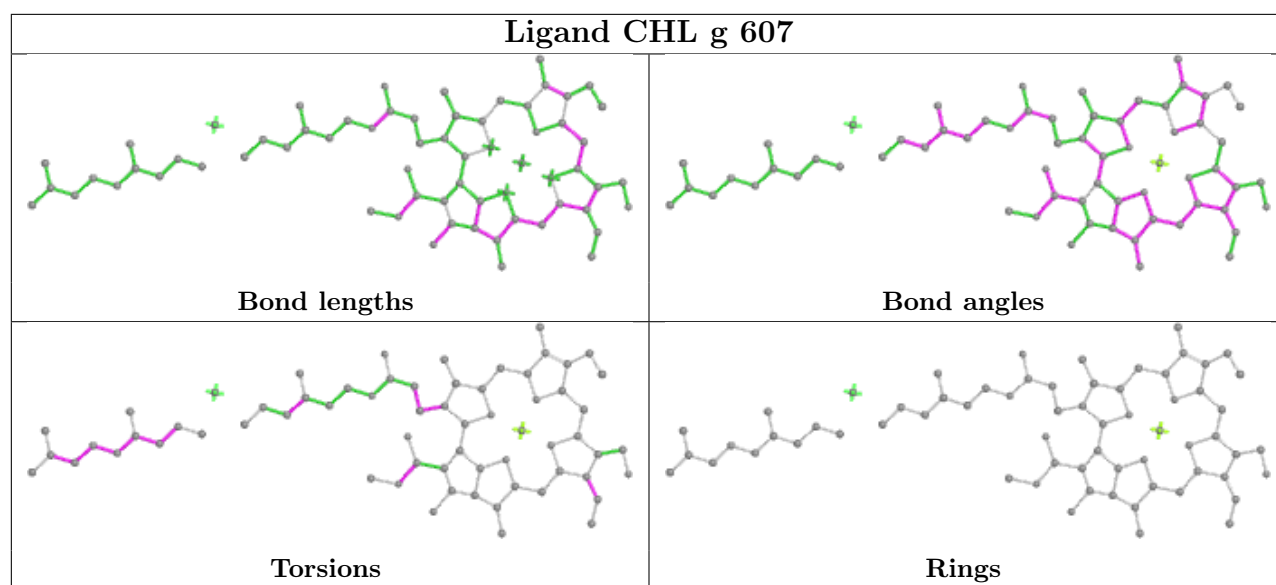
Bond angles

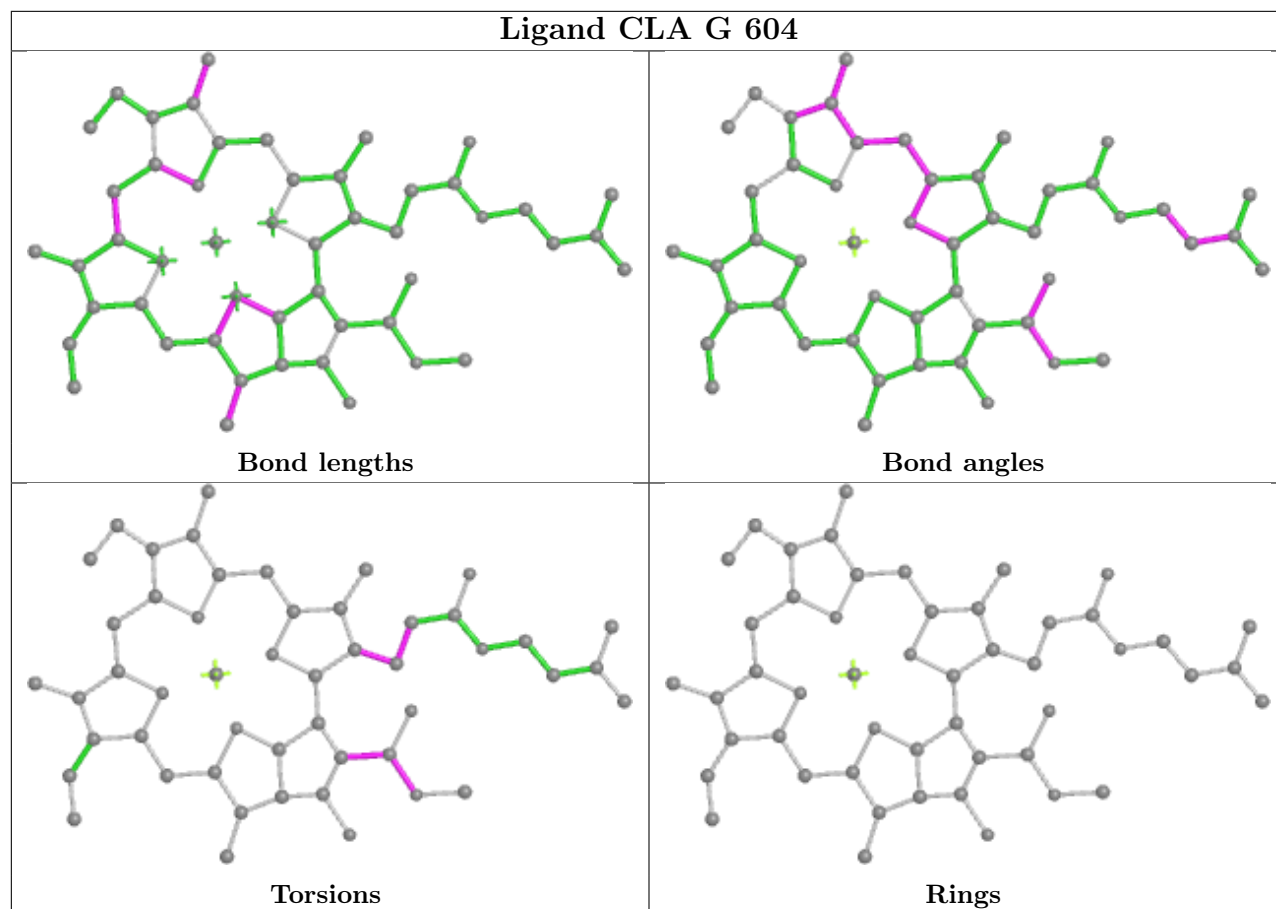
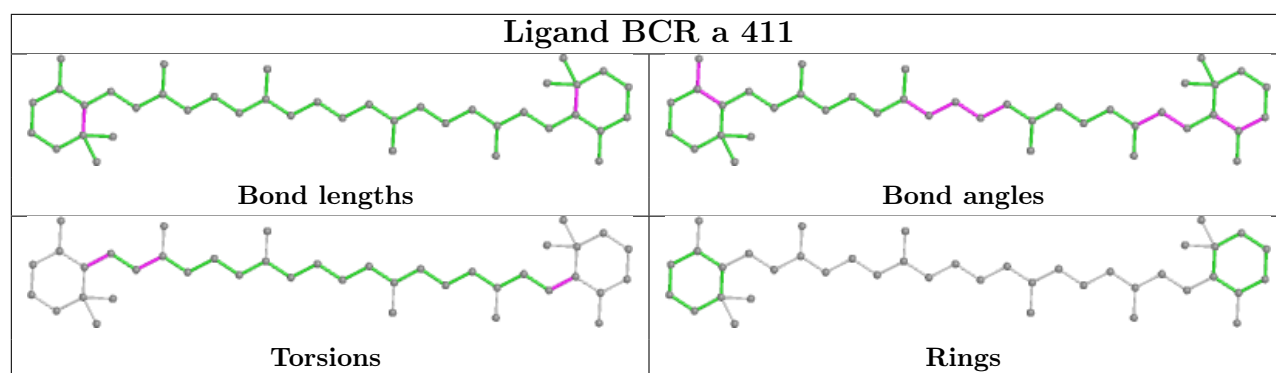


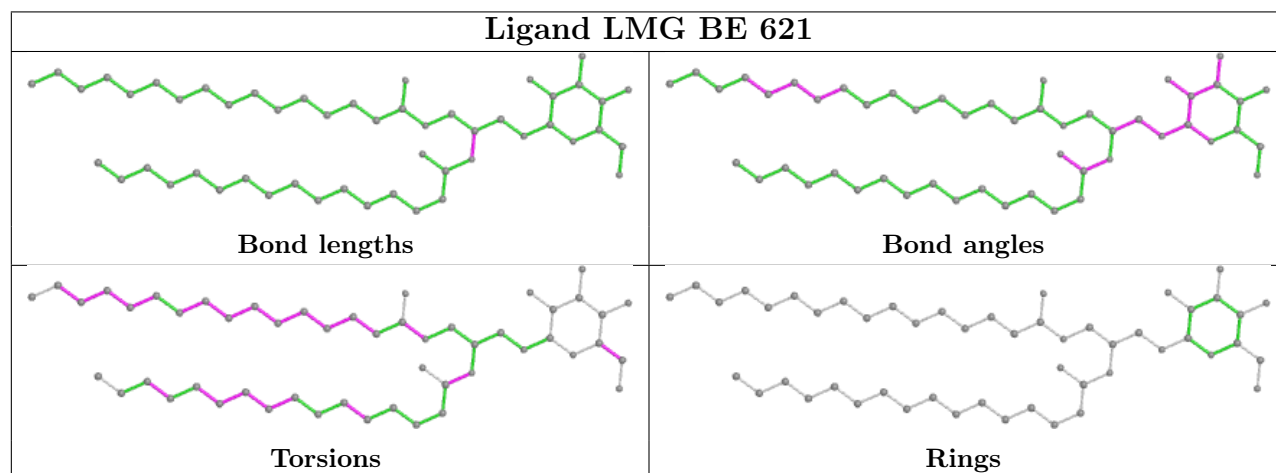
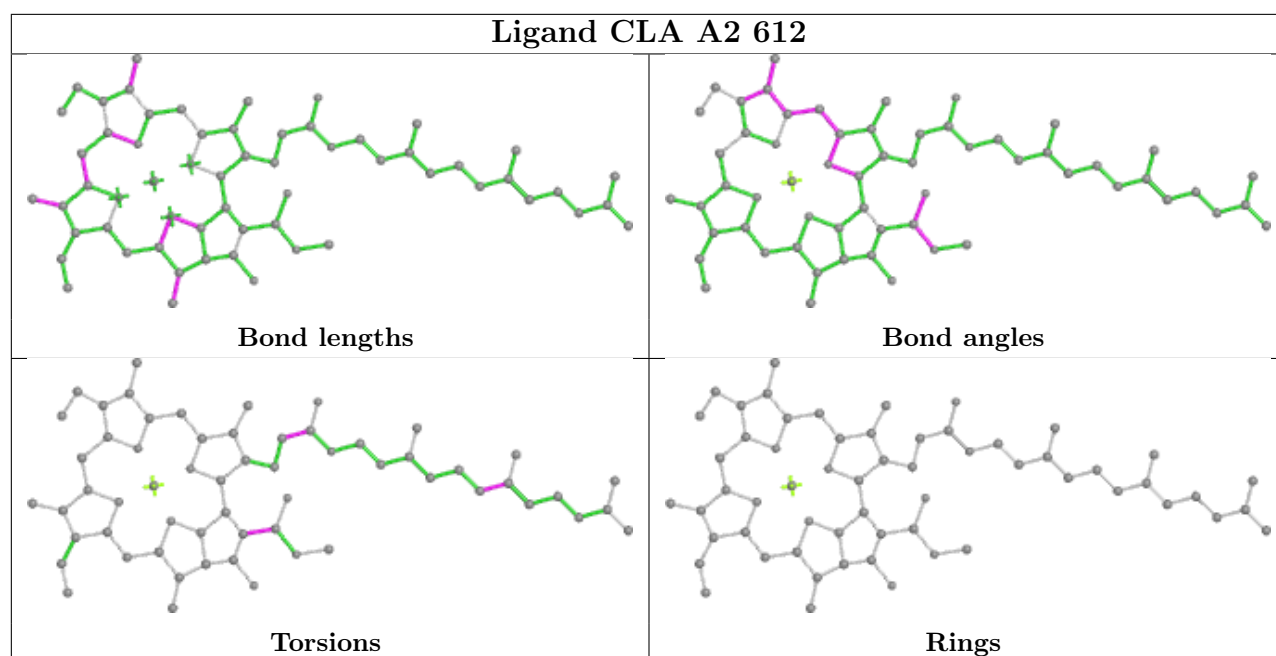
Torsions



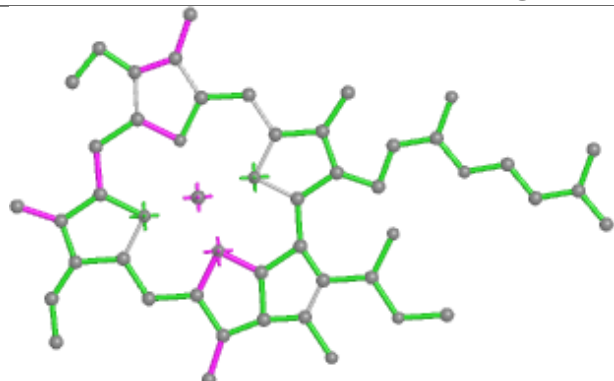
Rings



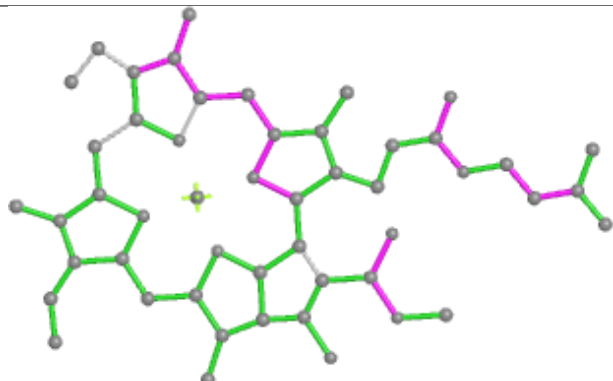




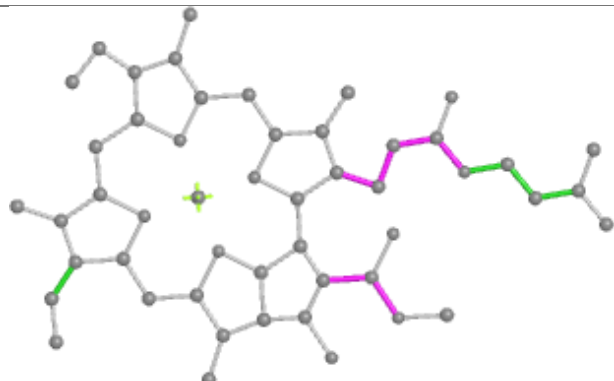
Ligand CLA Y 305



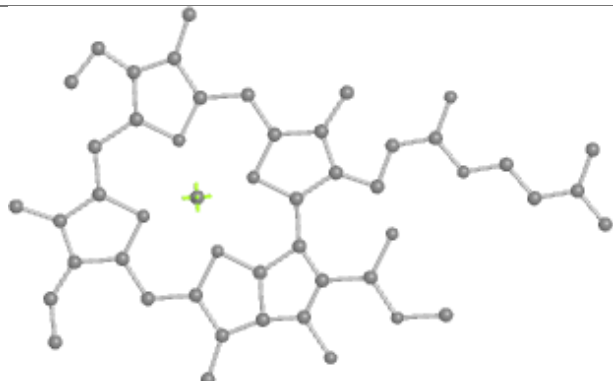
Bond lengths



Bond angles

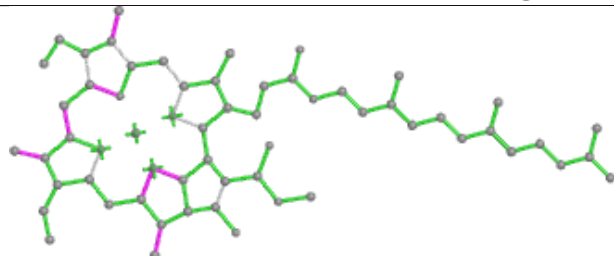


Torsions

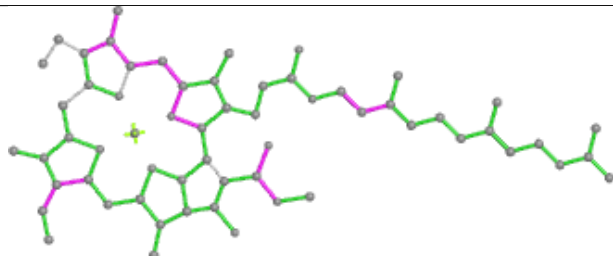


Rings

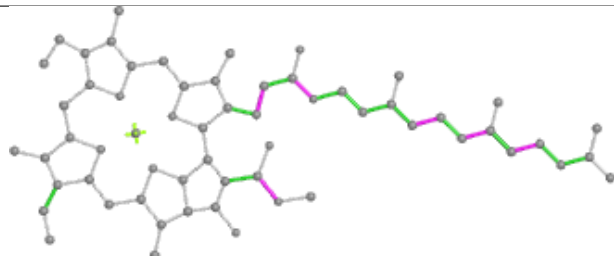
Ligand CLA n 613



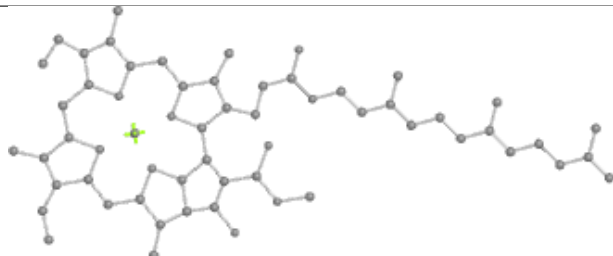
Bond lengths



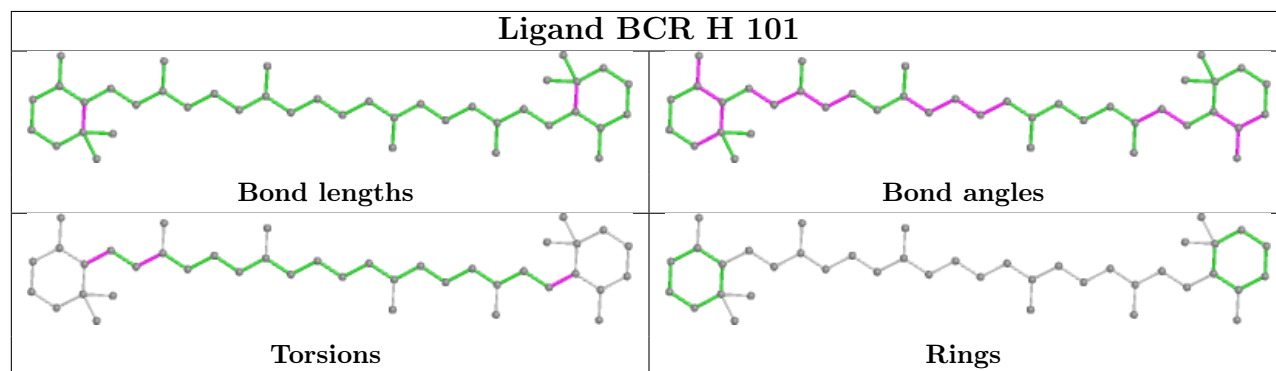
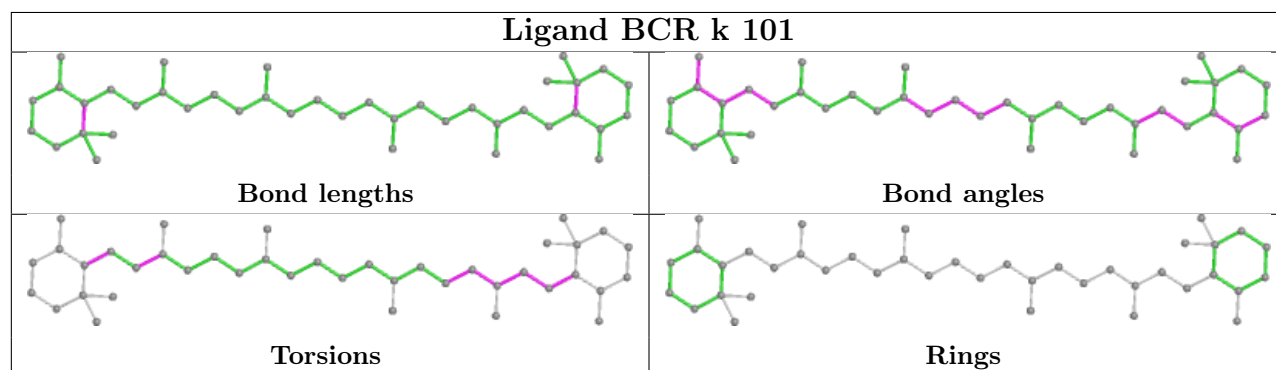
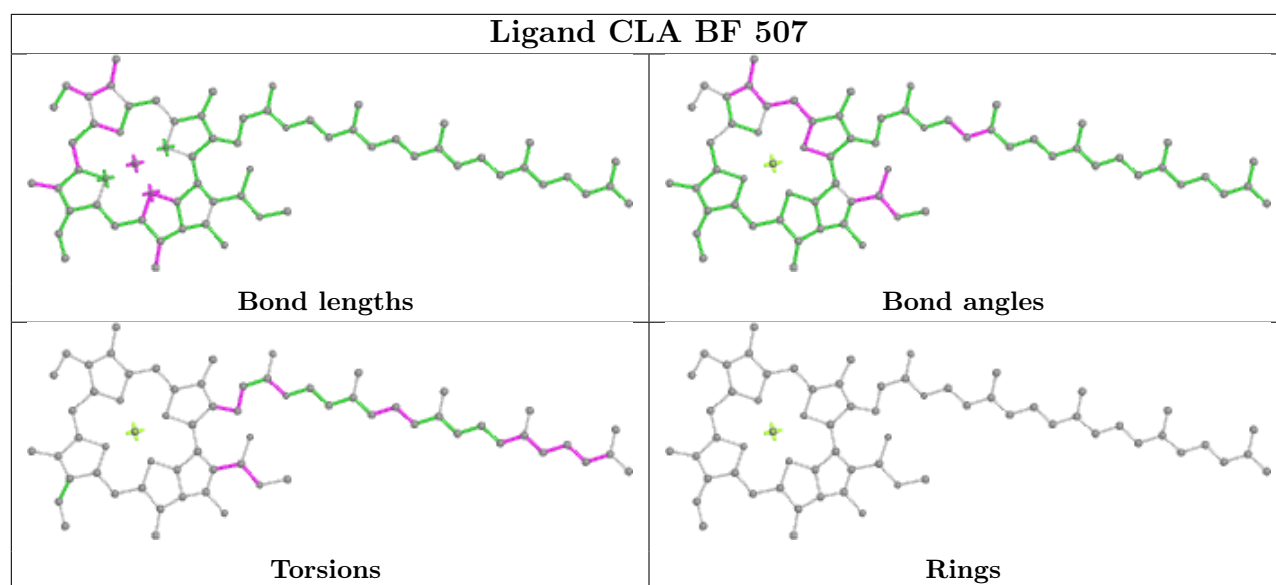
Bond angles

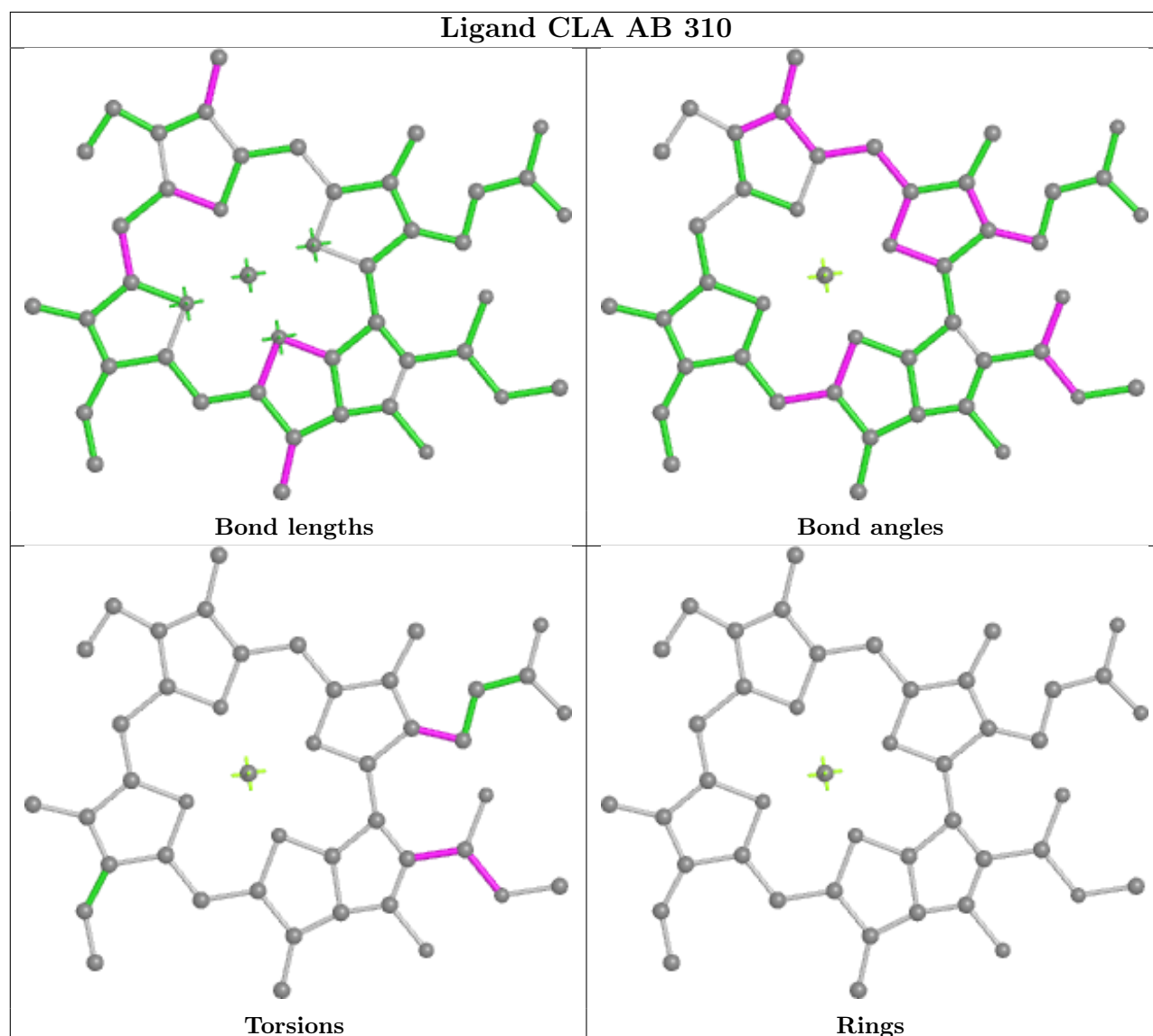
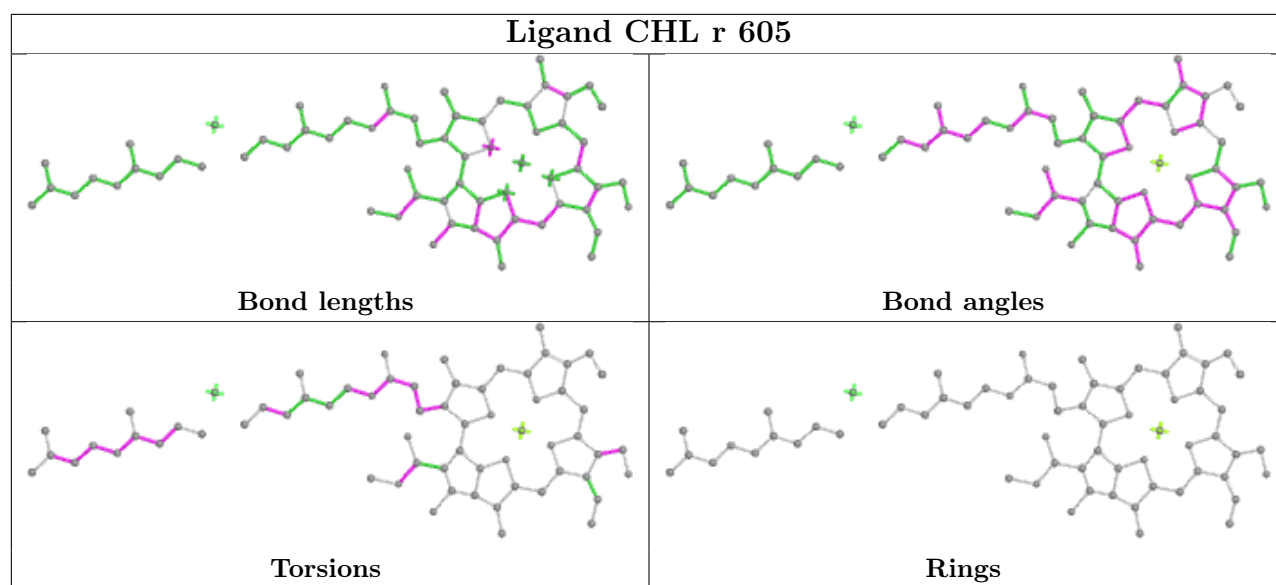


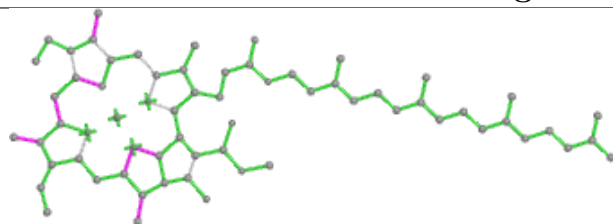
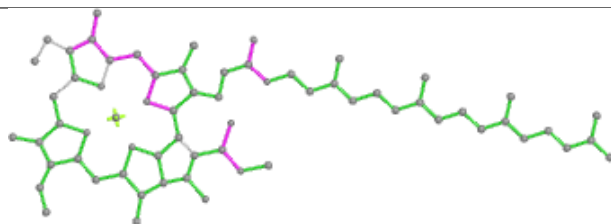
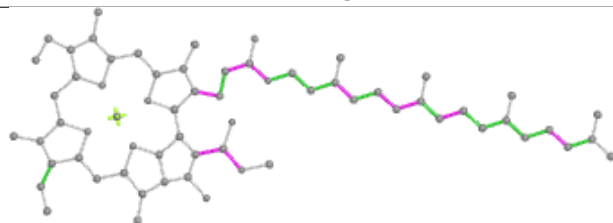
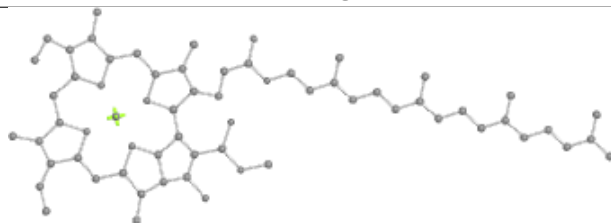
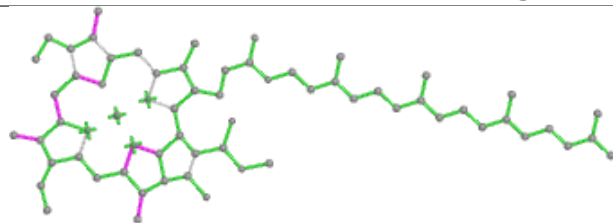
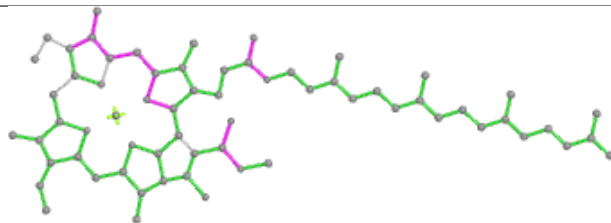
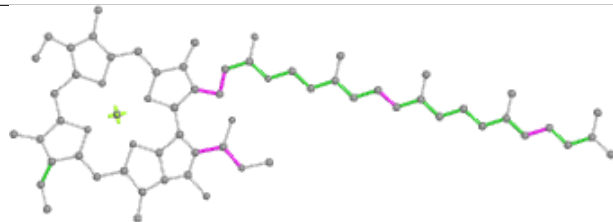
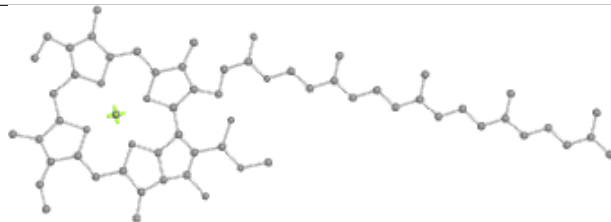
Torsions



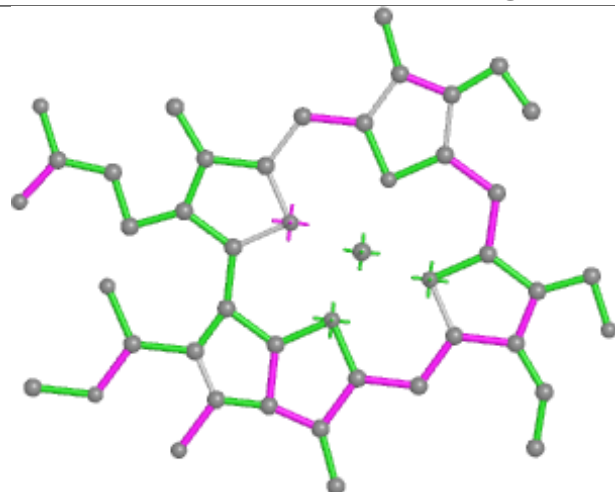
Rings



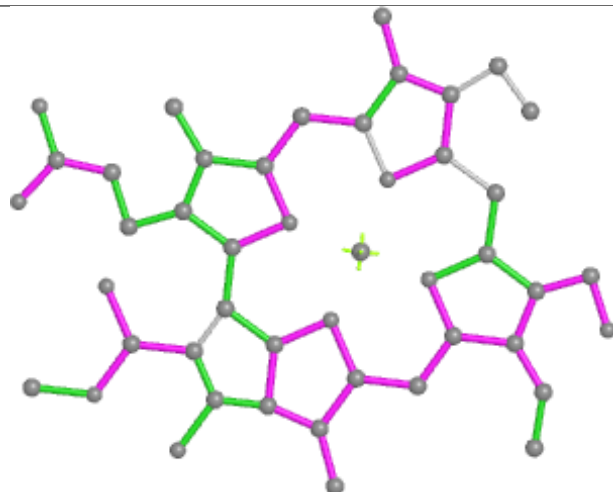


Ligand CLA B 602**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA C 505****Bond lengths****Bond angles****Torsions****Rings**

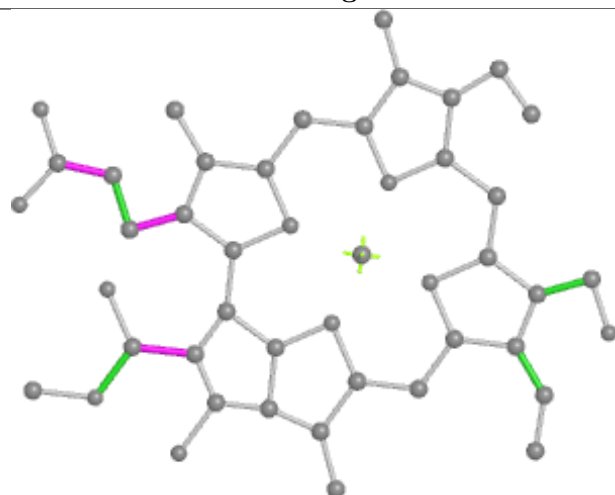
Ligand CHL AA 302



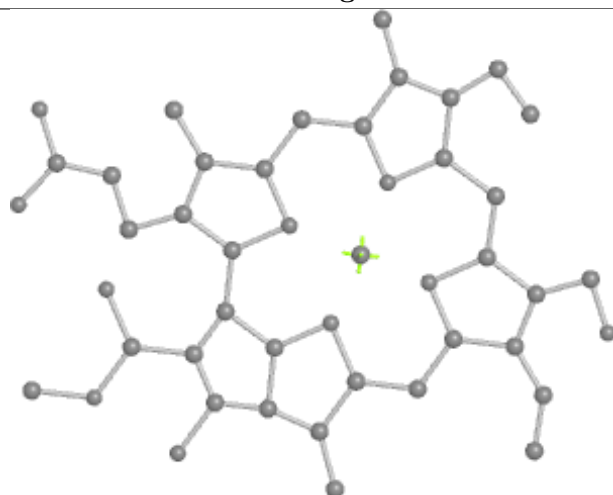
Bond lengths



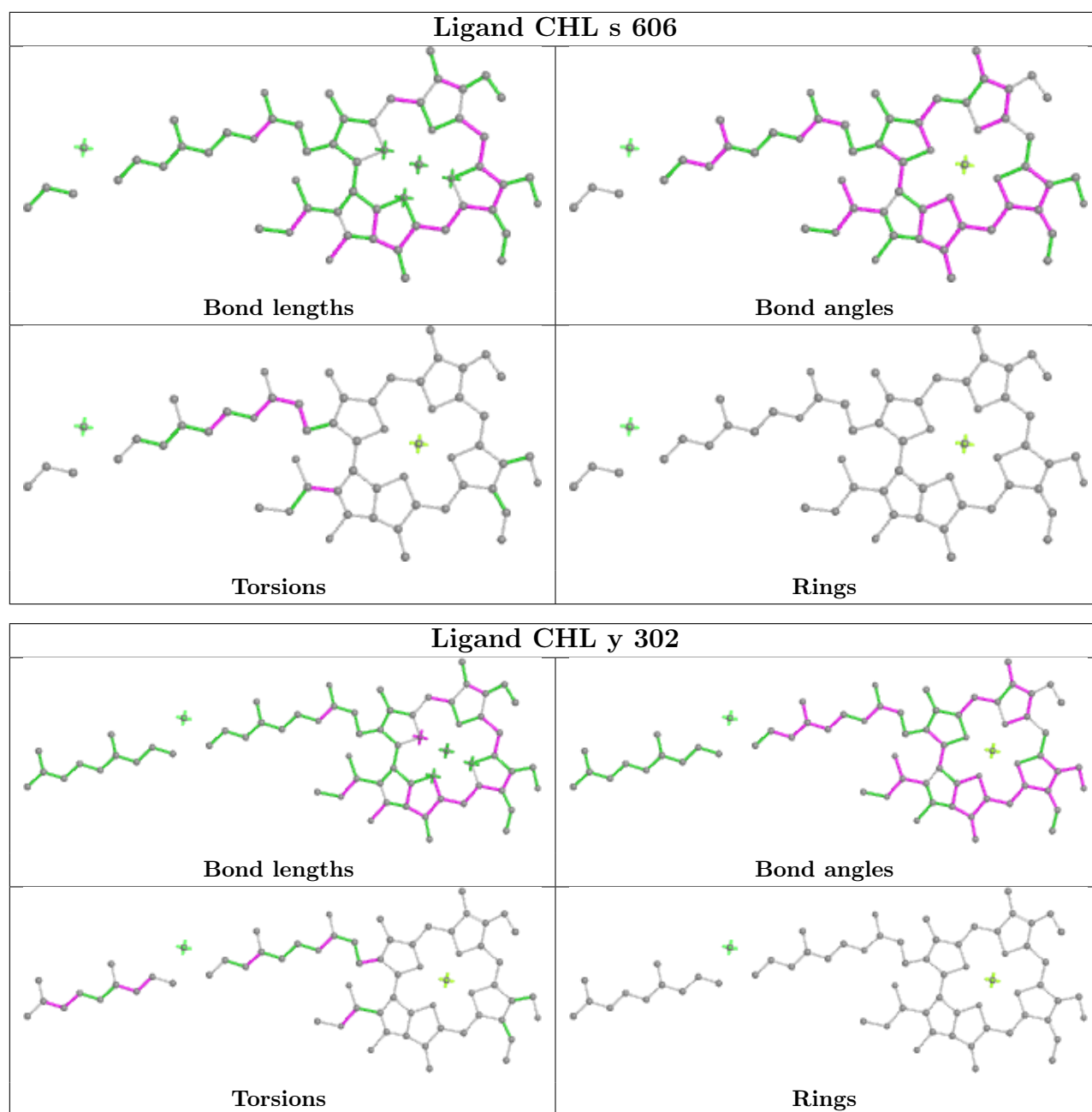
Bond angles

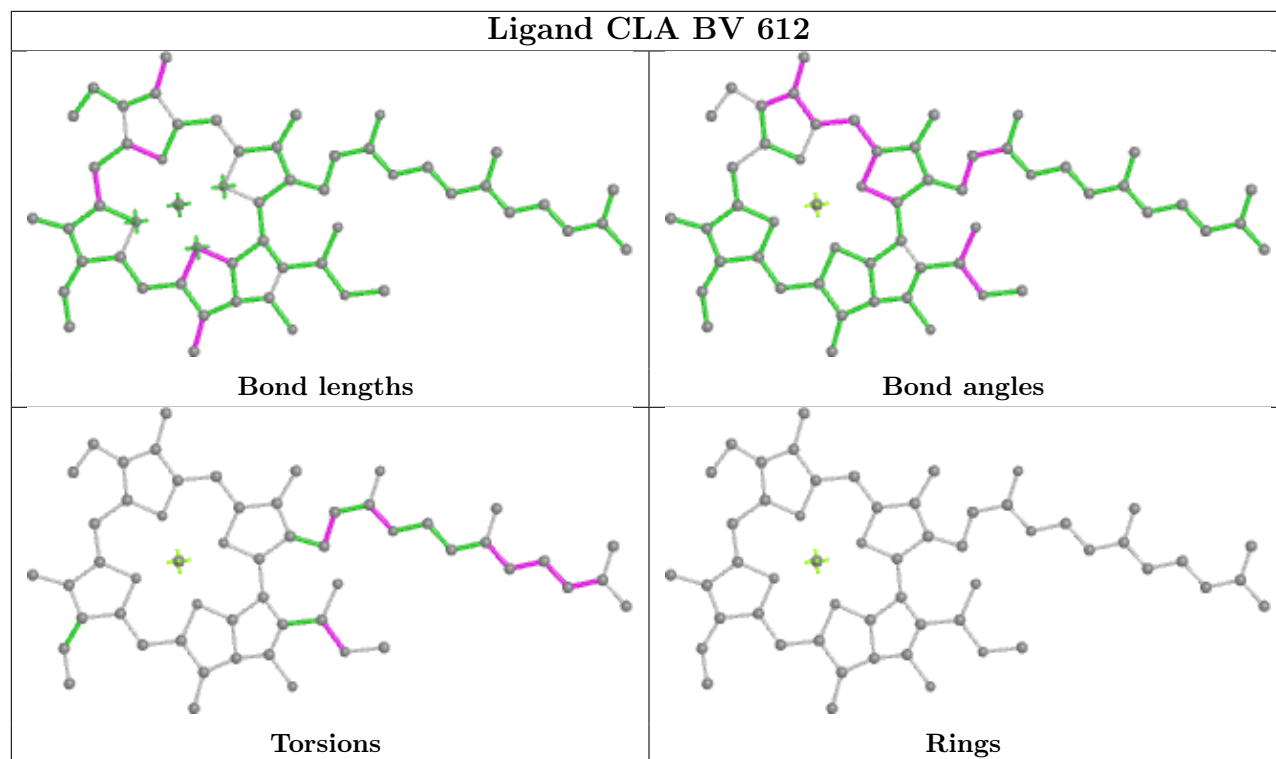


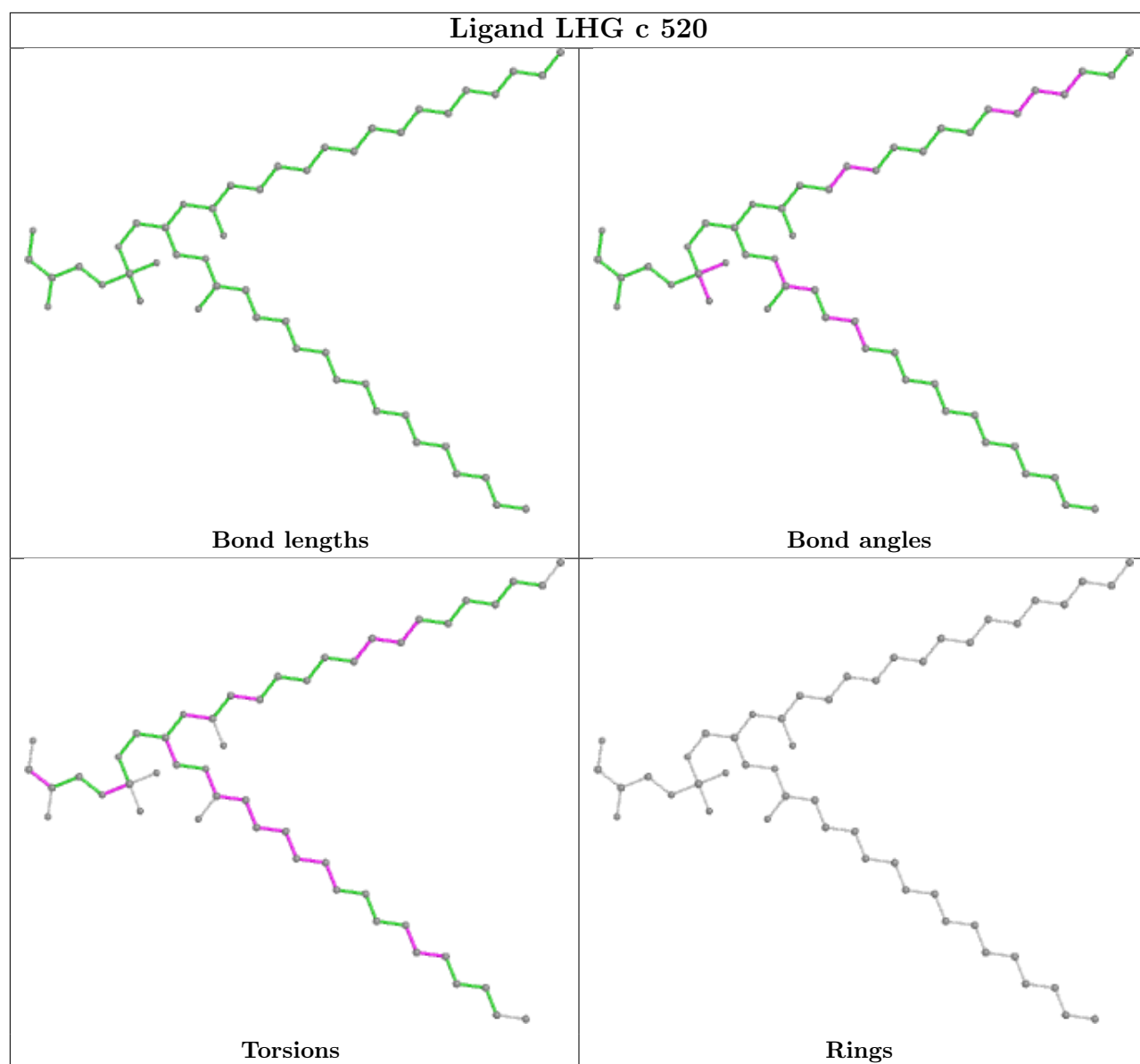
Torsions

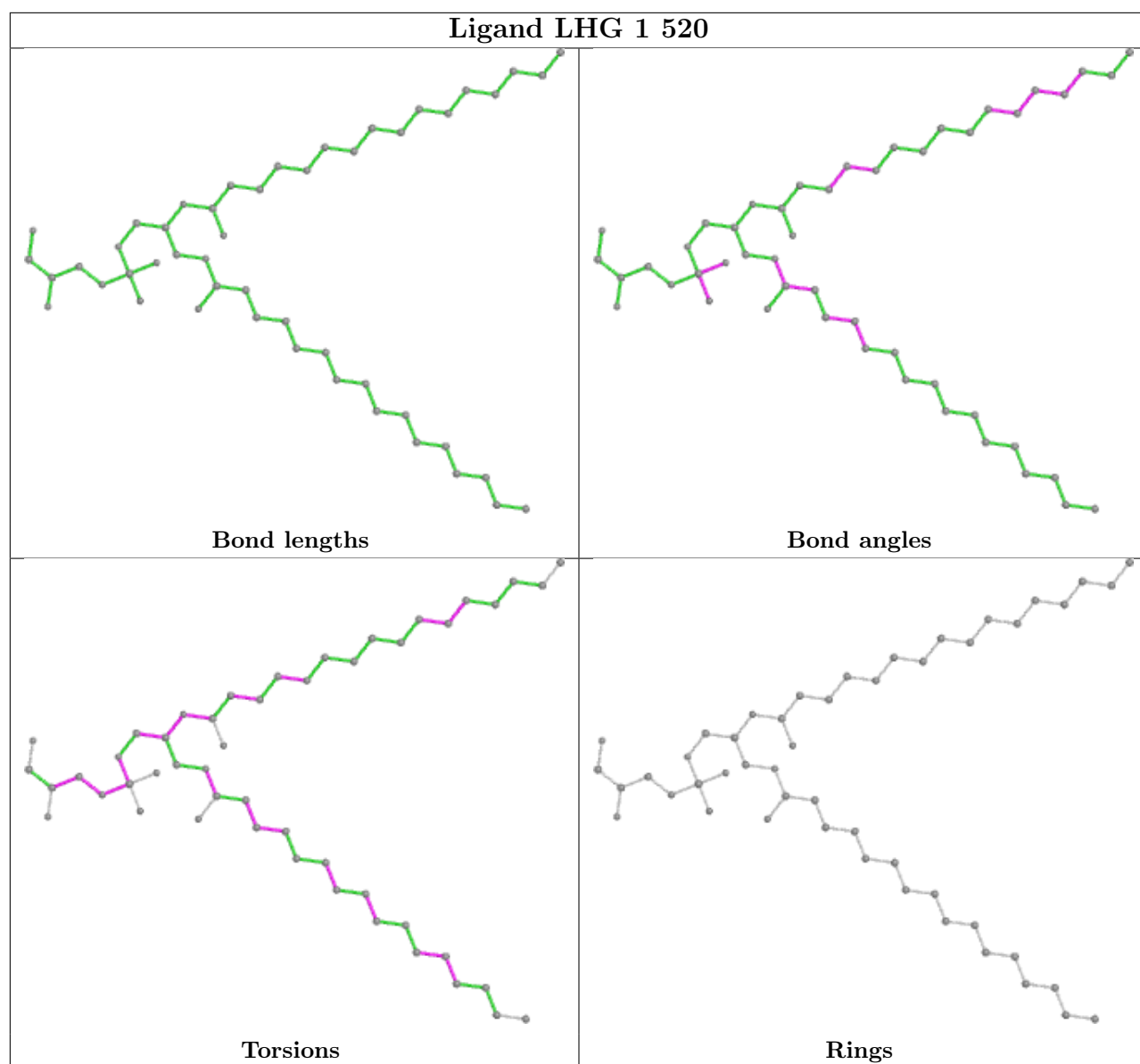


Rings

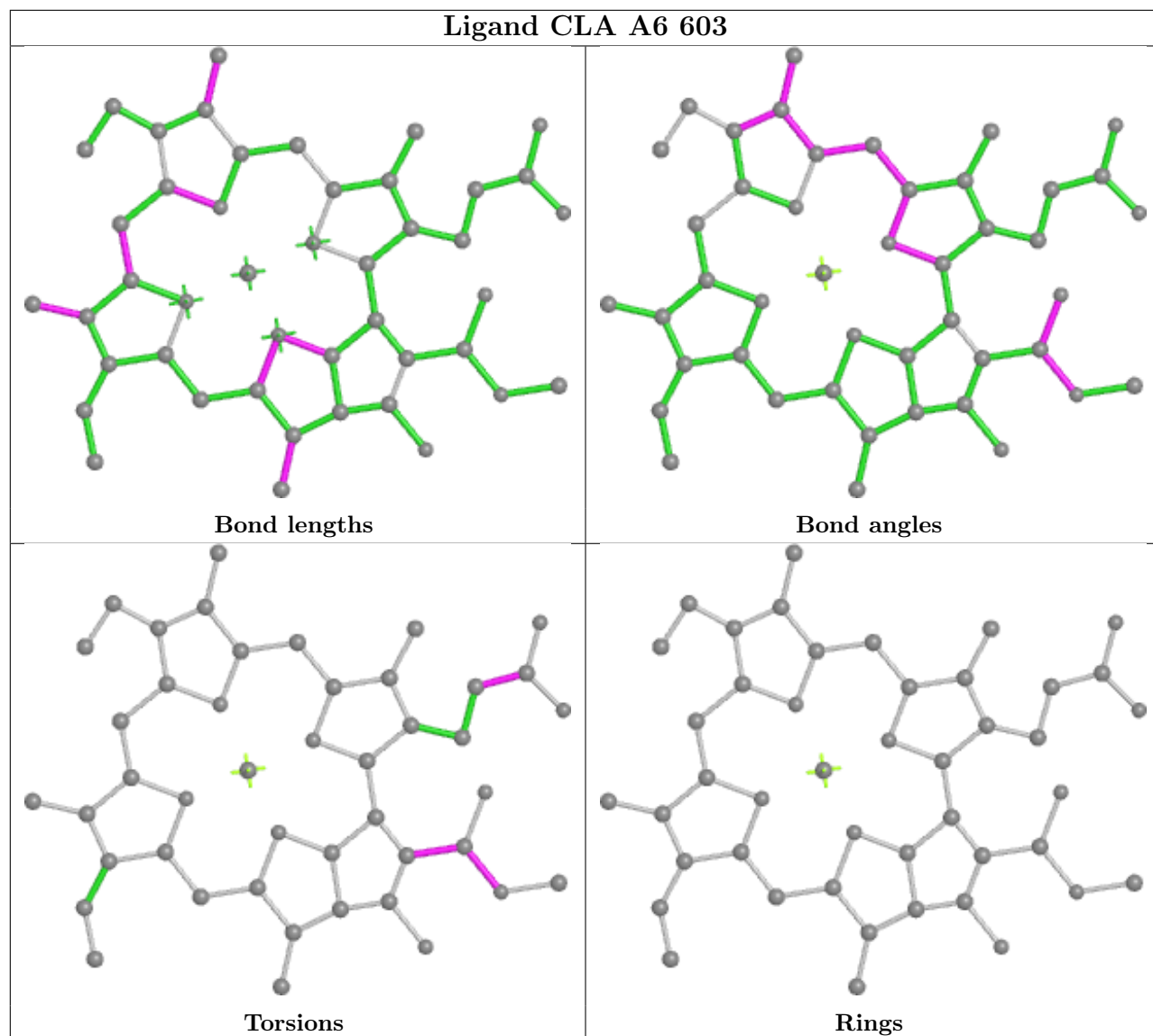




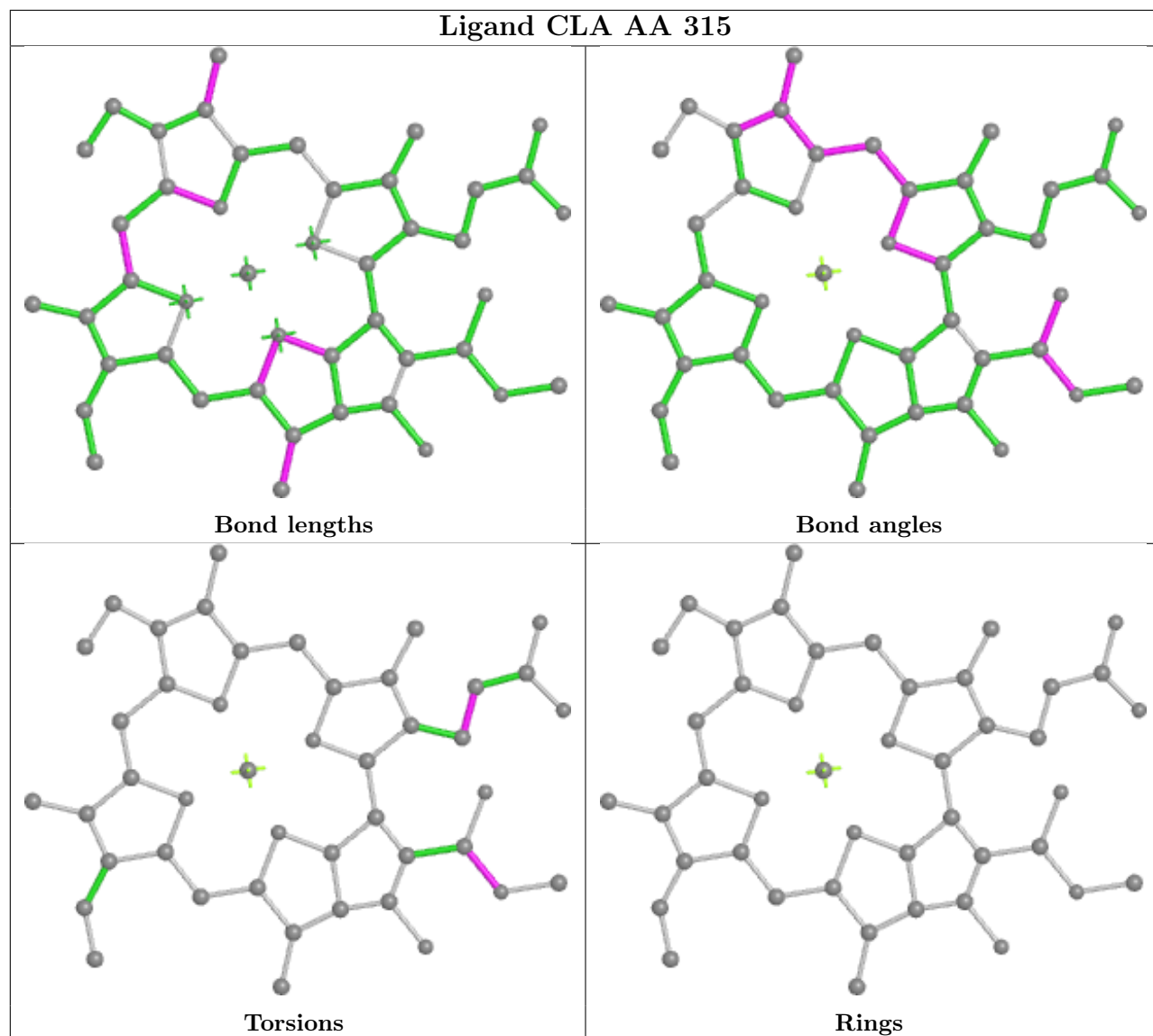


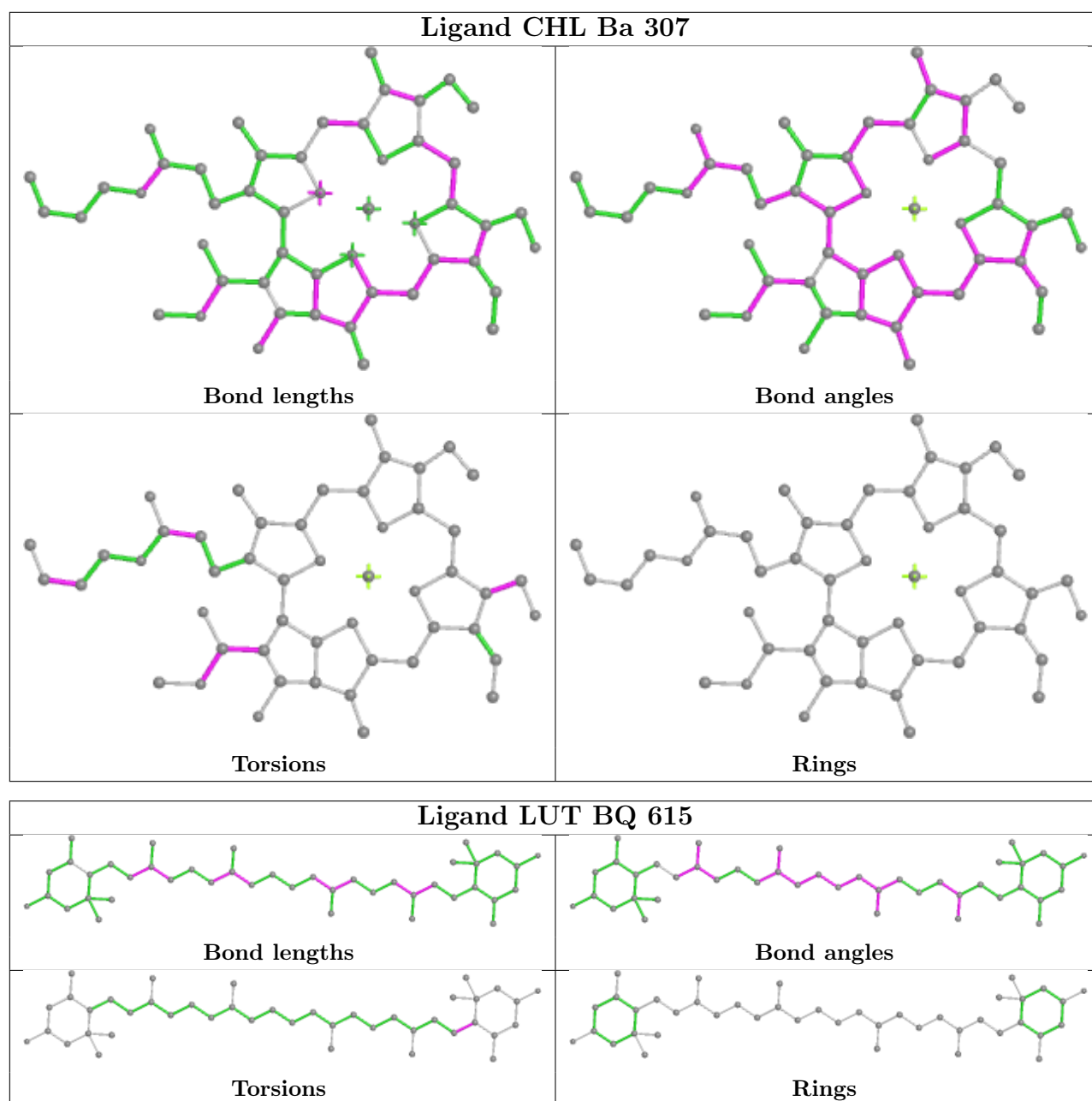


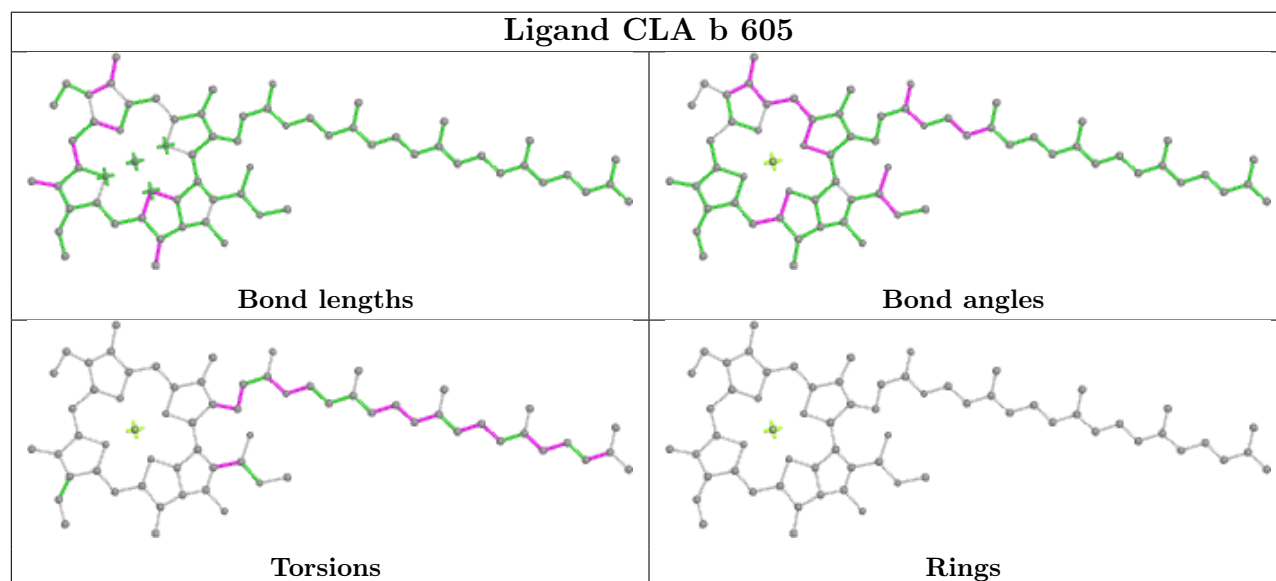
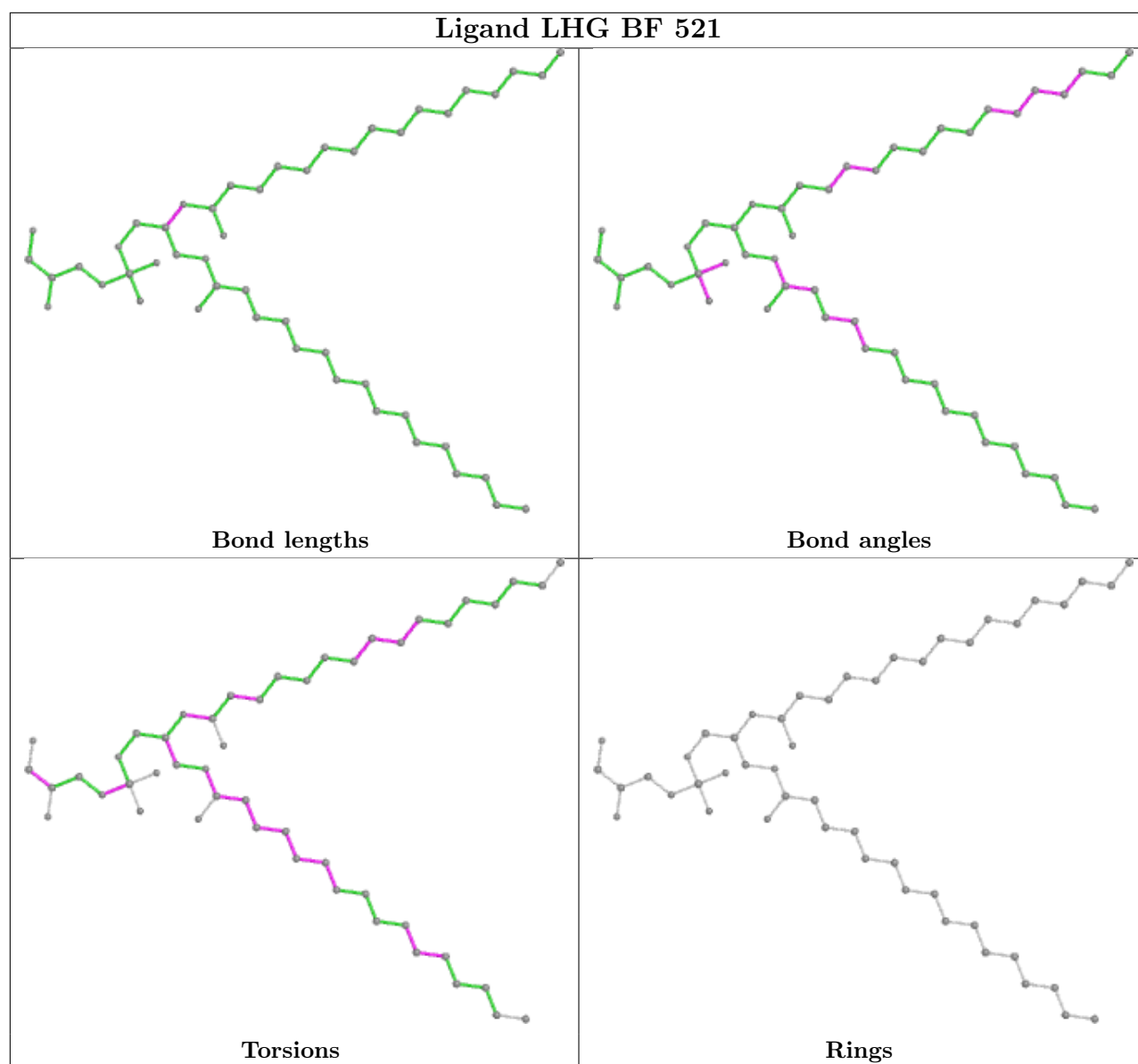
Ligand CLA A6 603

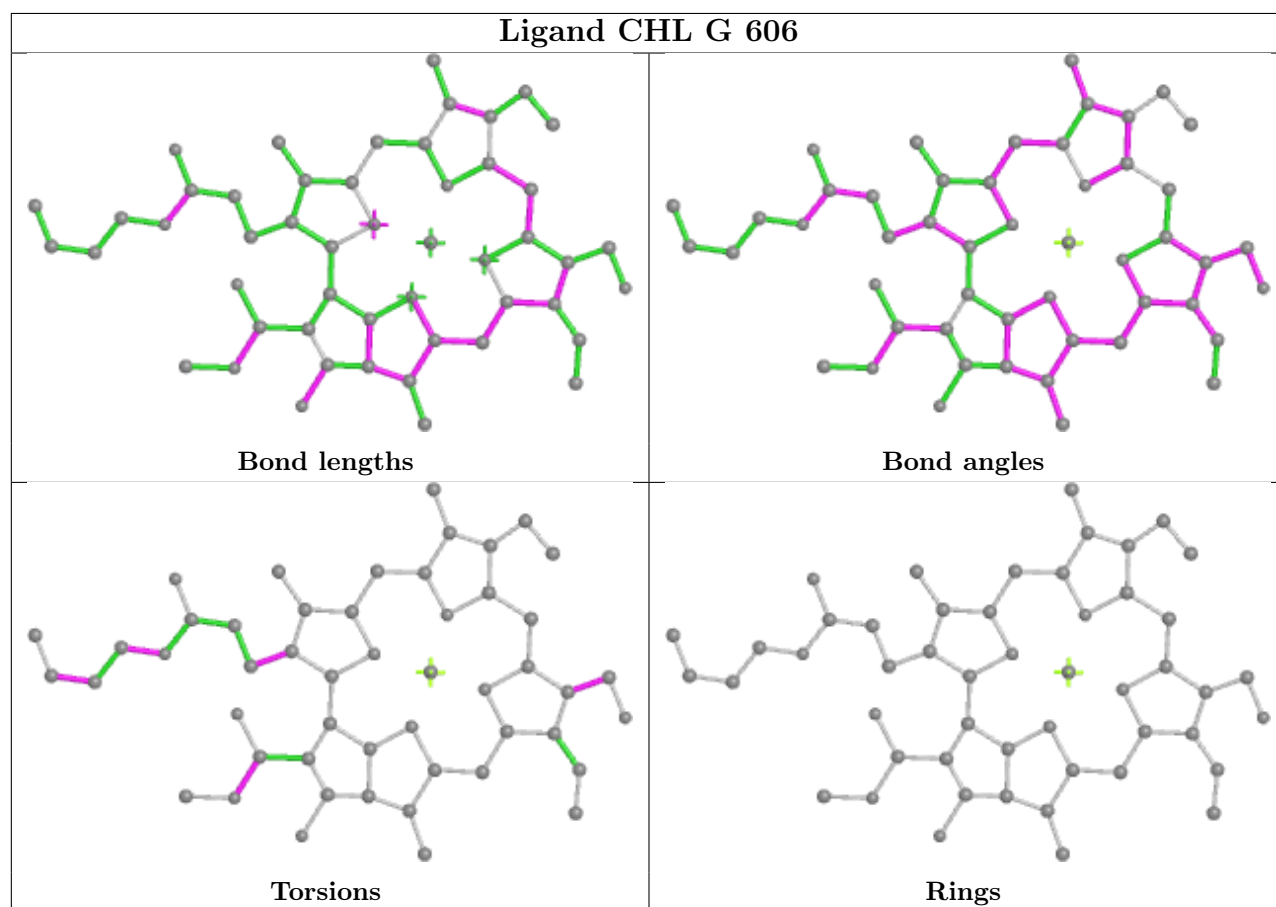
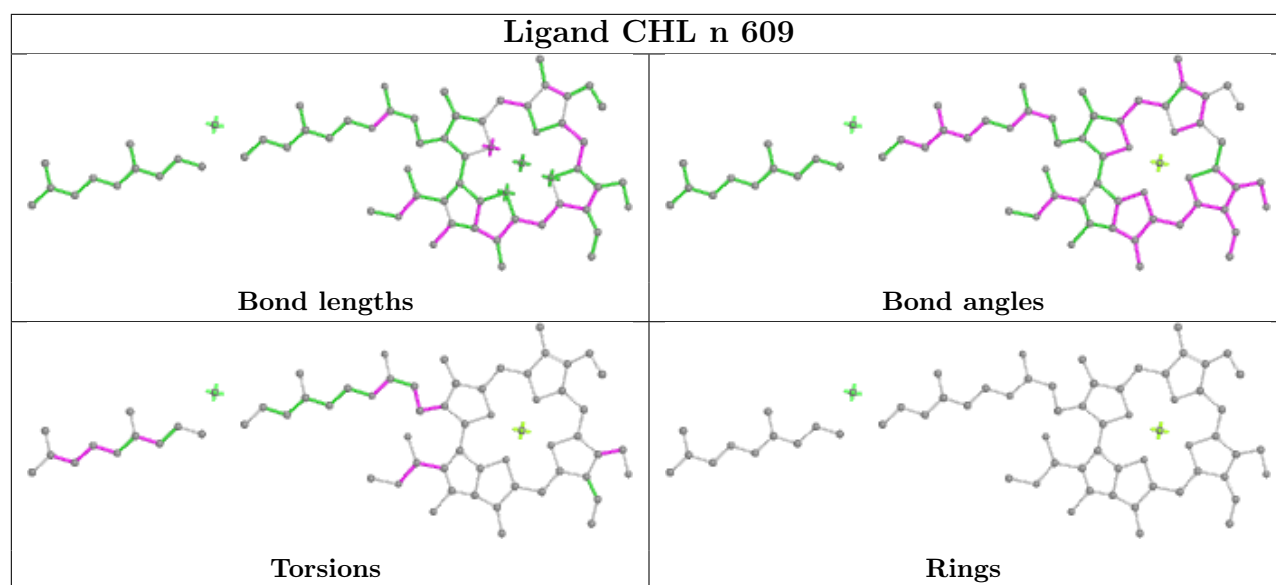


Ligand CLA AA 315

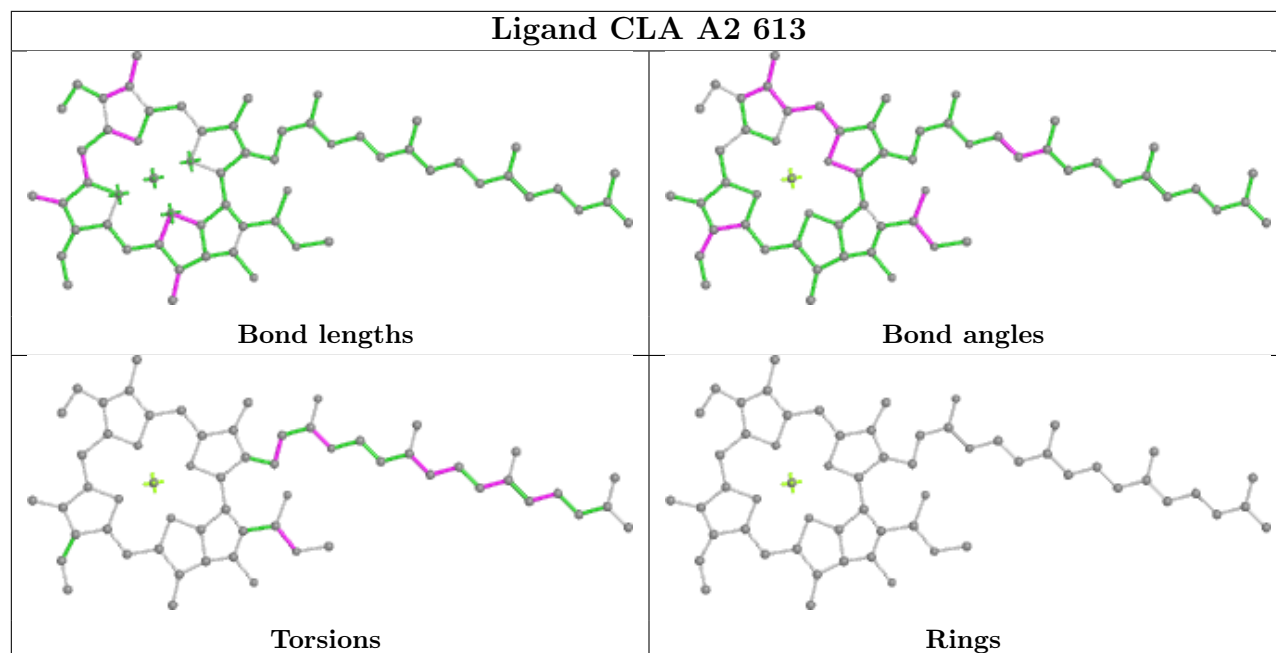




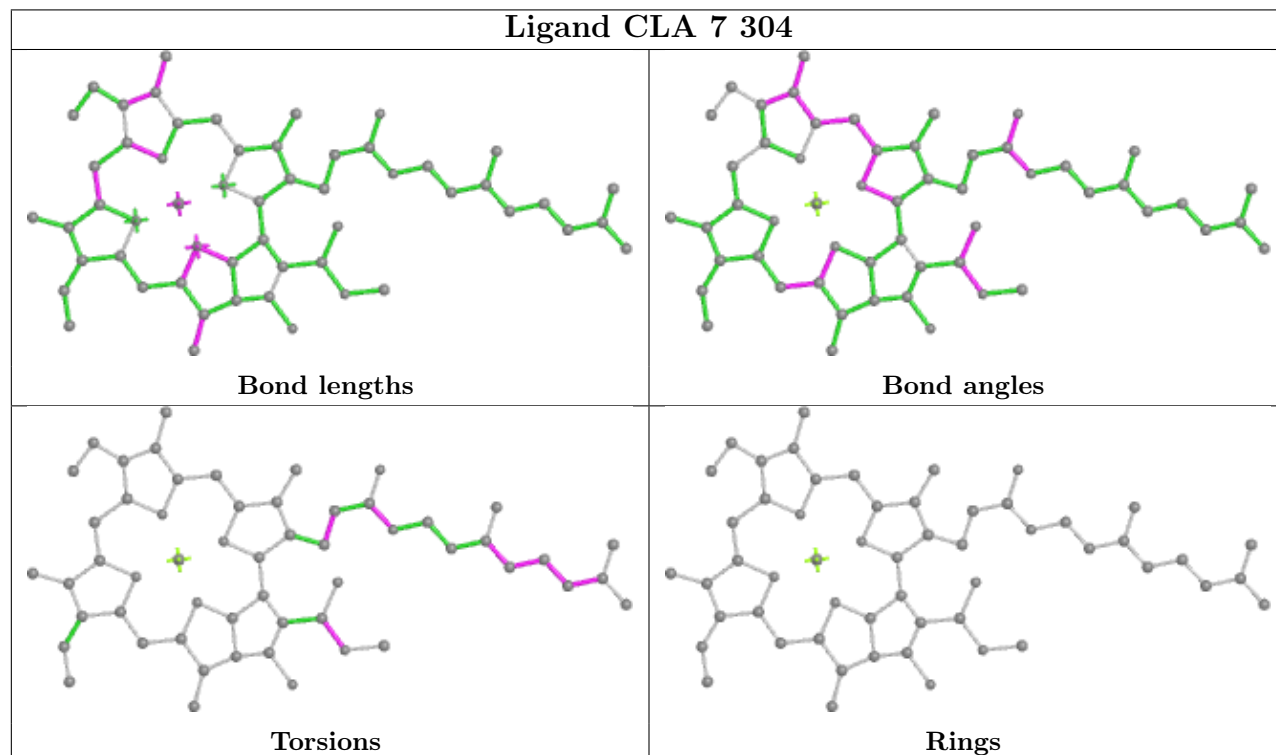




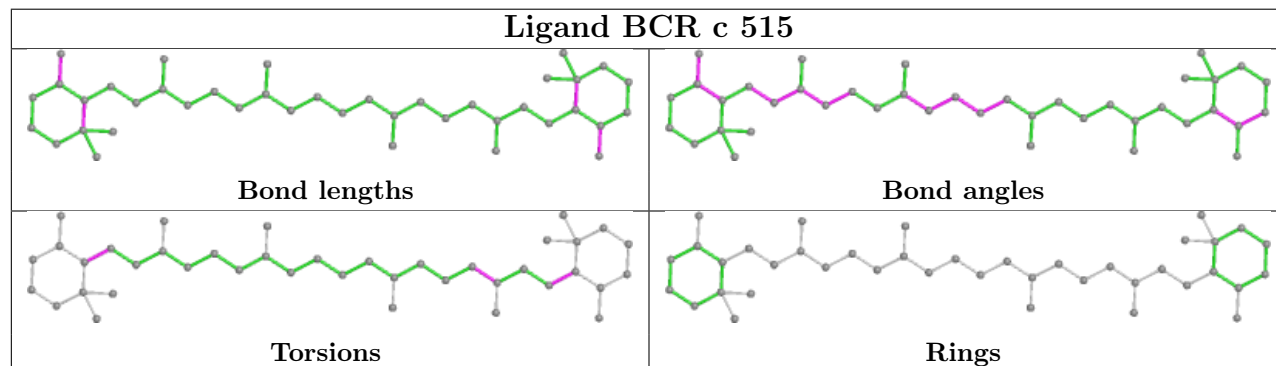
Ligand CLA A2 613



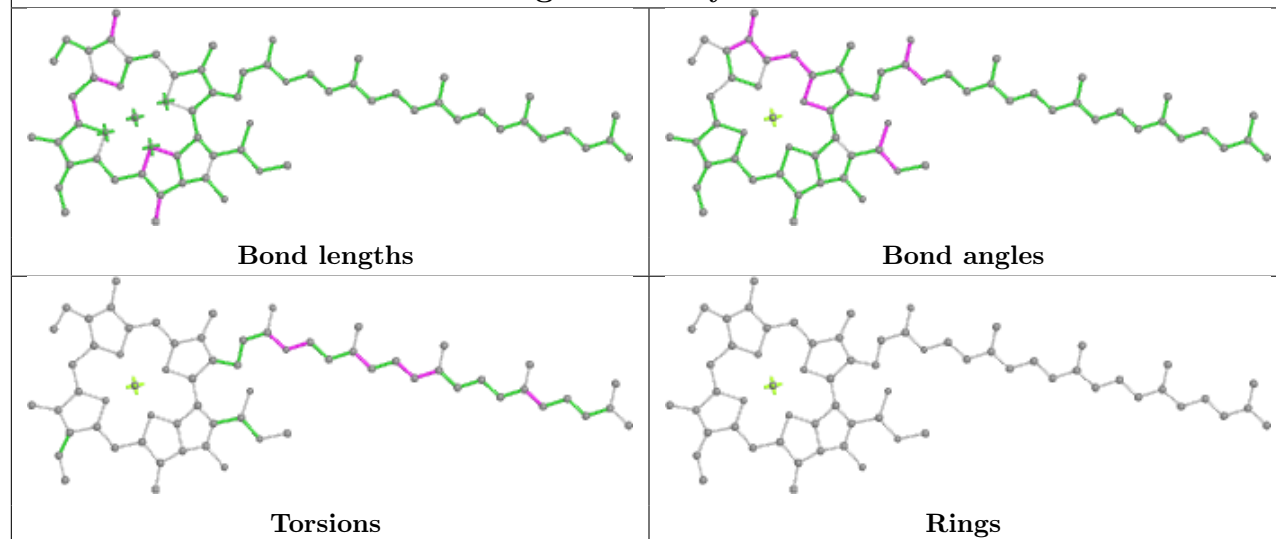
Ligand CLA 7 304



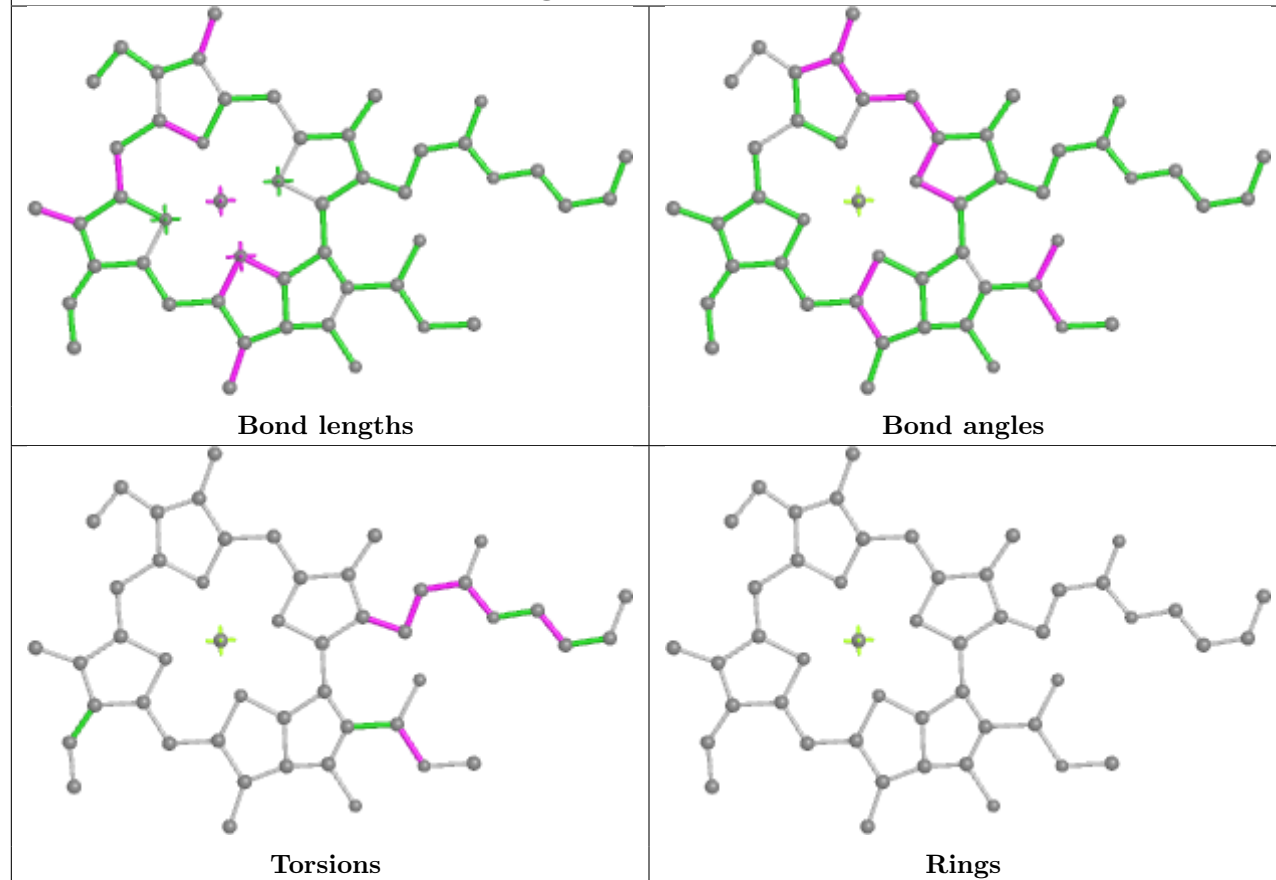
Ligand BCR c 515

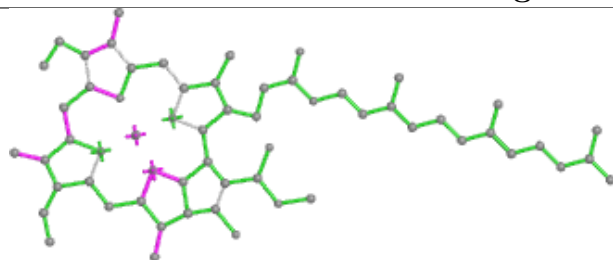


Ligand CLA y 304

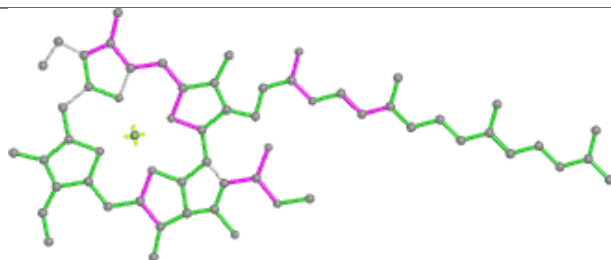


Ligand CLA r 610

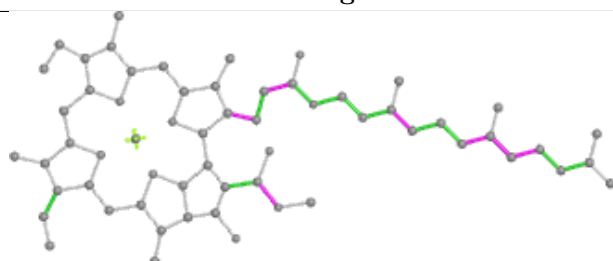


Ligand CLA Y 312

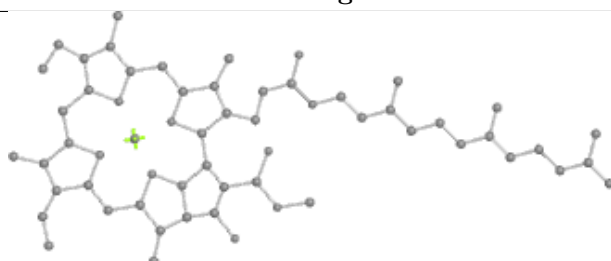
Bond lengths



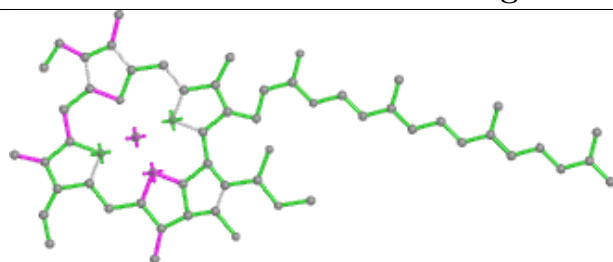
Bond angles



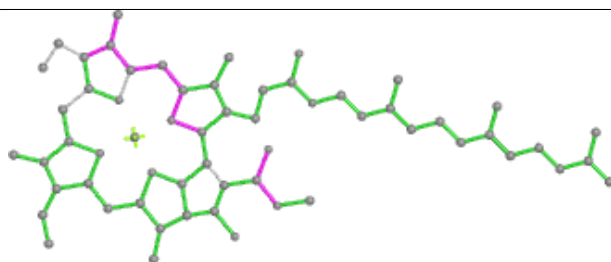
Torsions



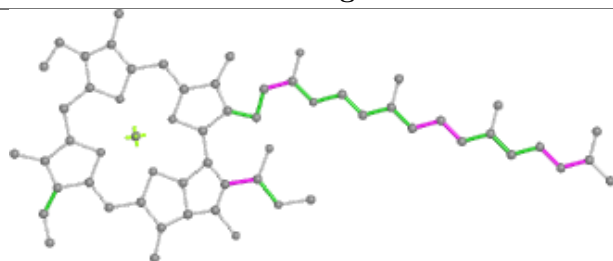
Rings

Ligand CLA BU 603

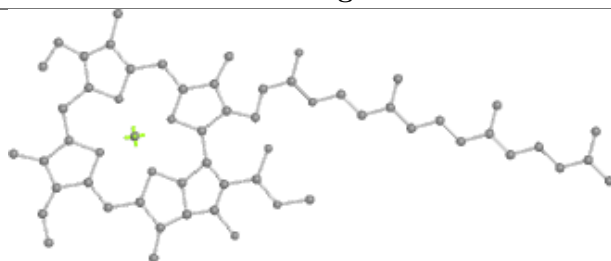
Bond lengths



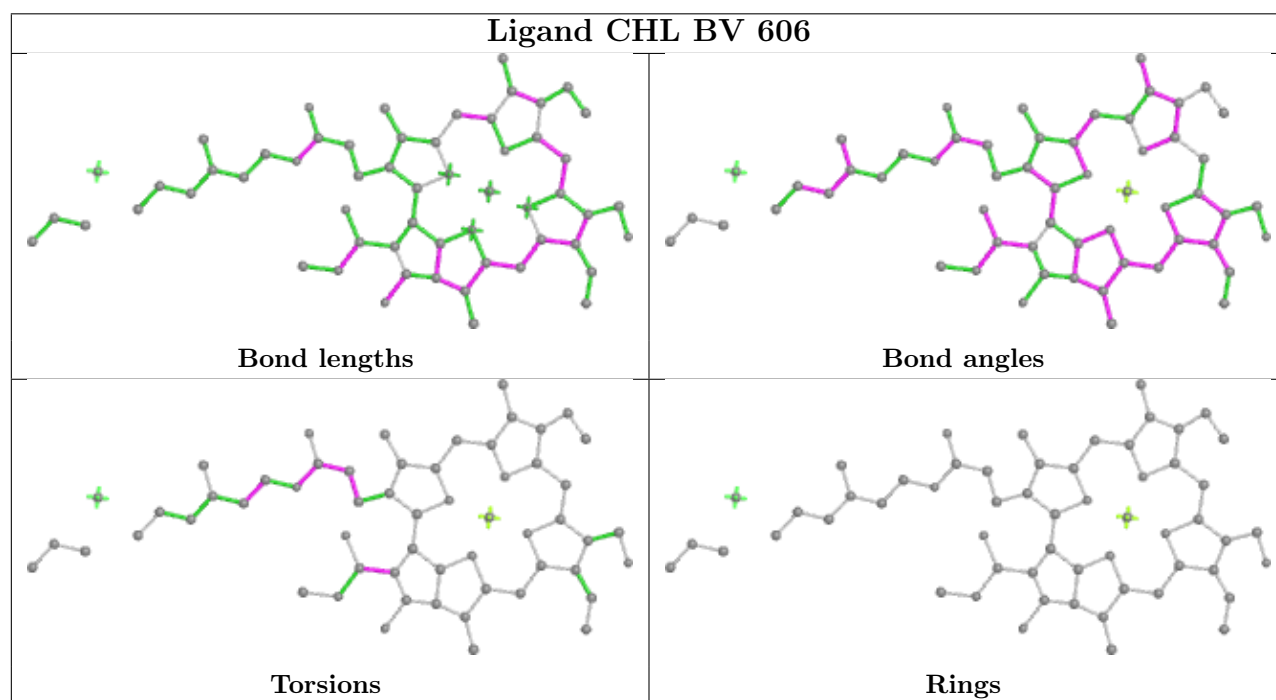
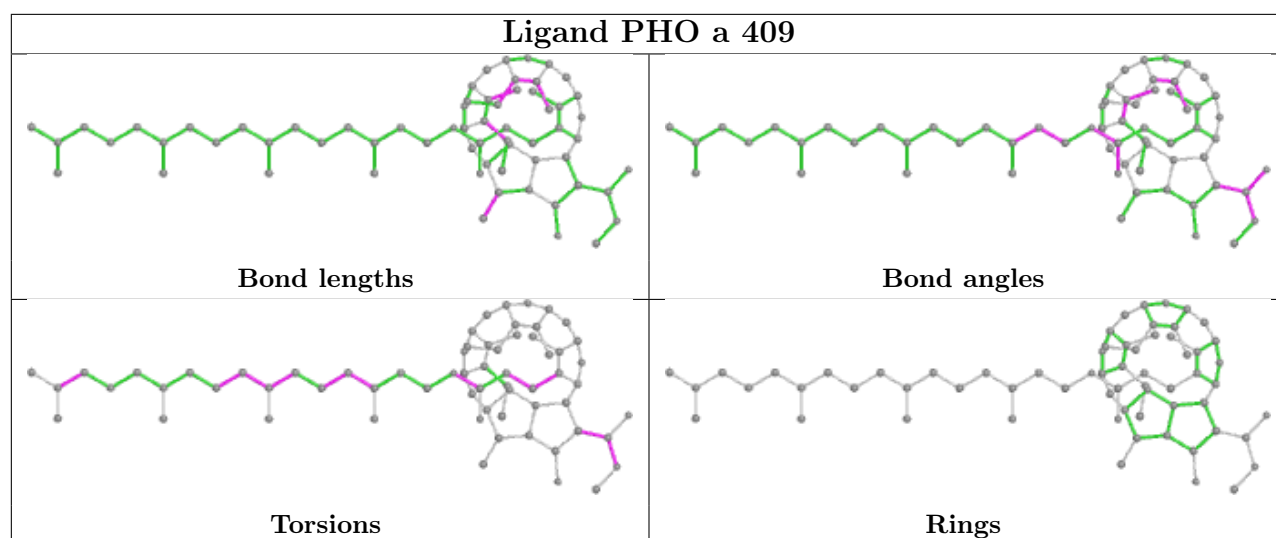
Bond angles



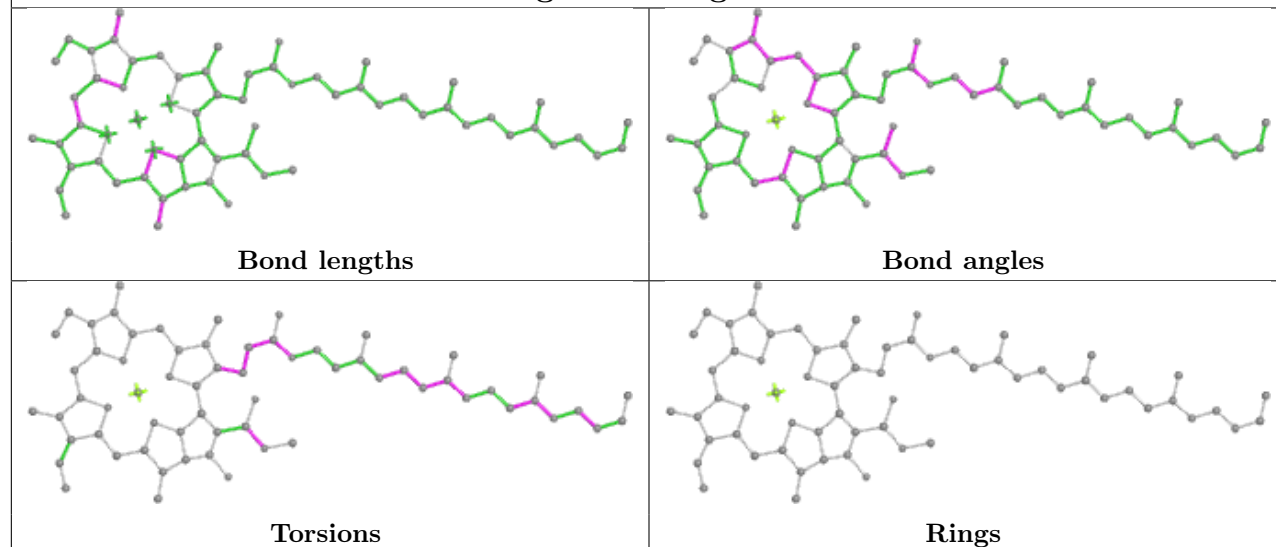
Torsions



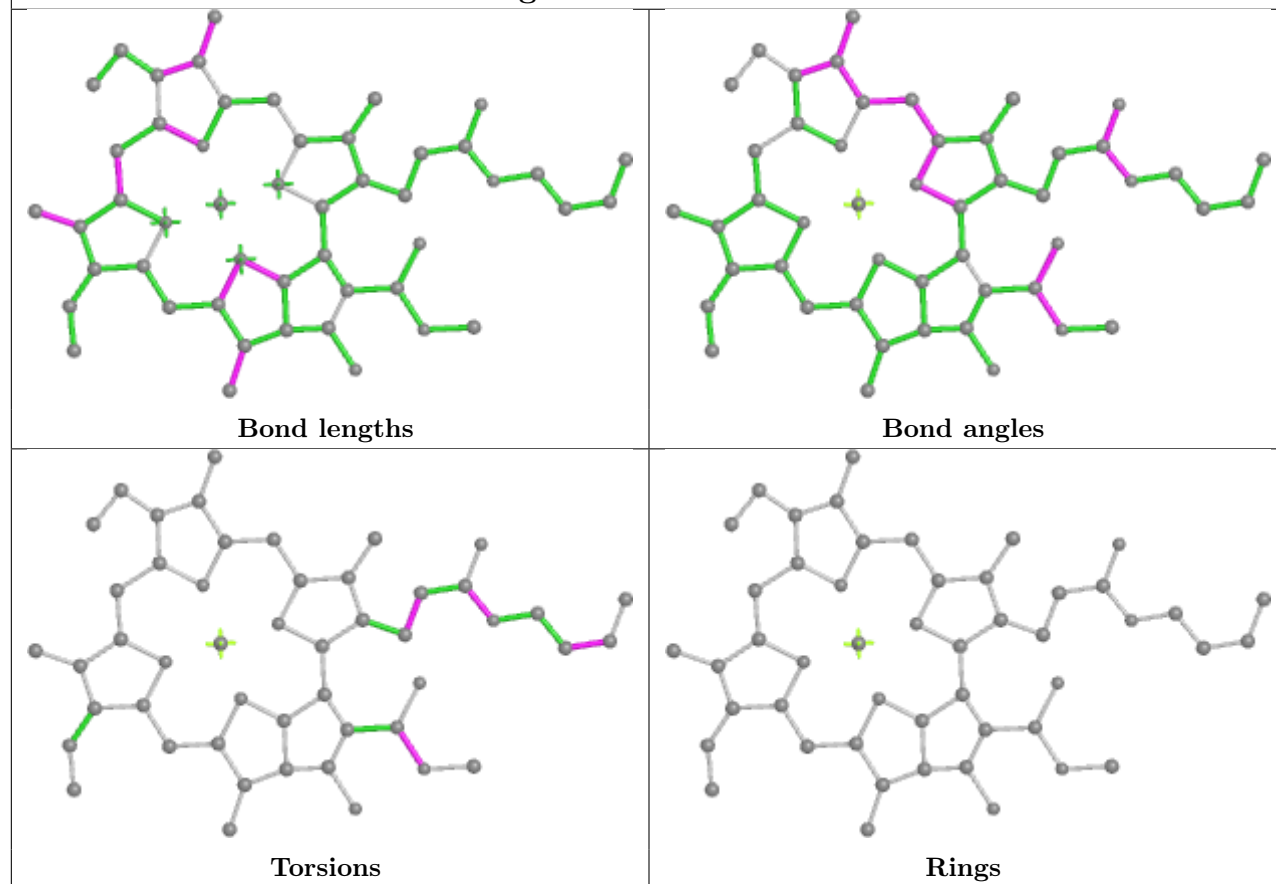
Rings



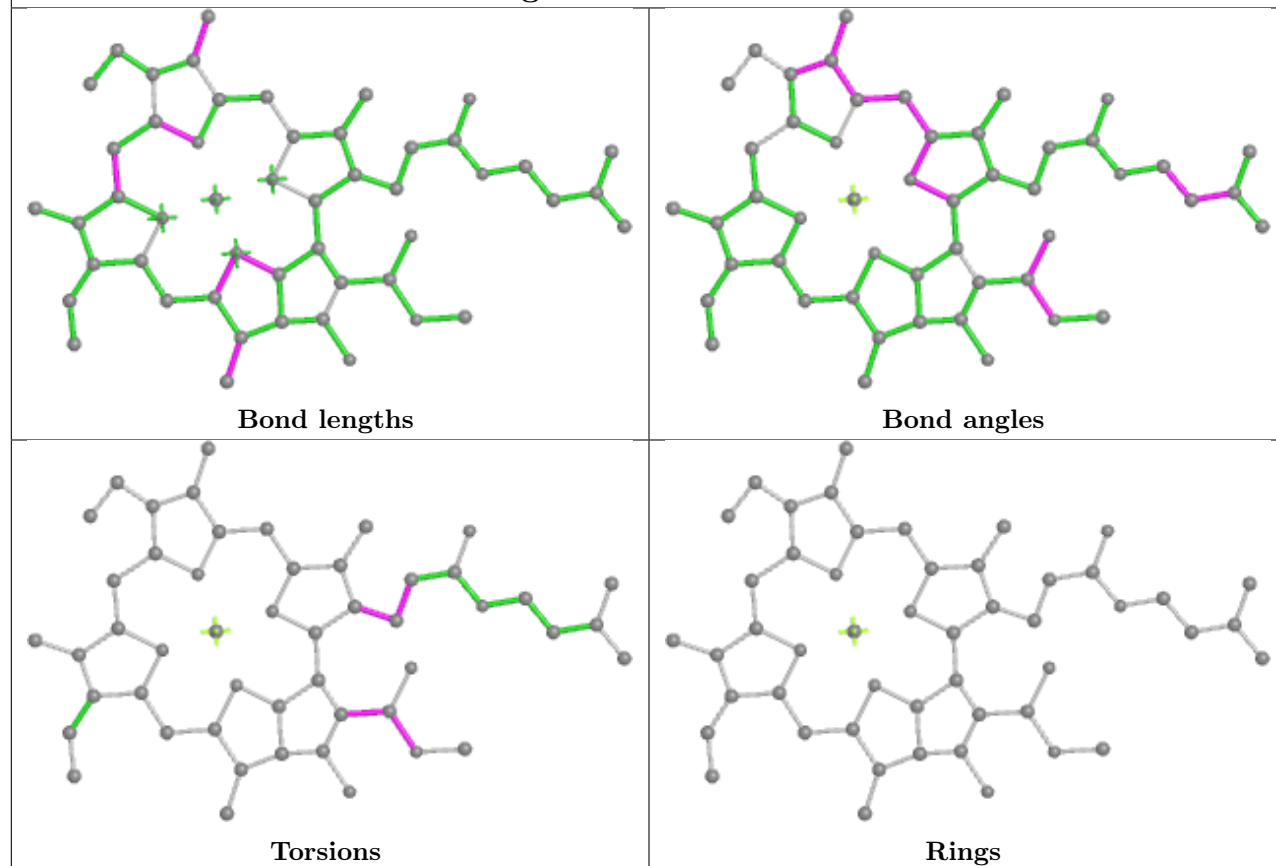
Ligand CLA g 610



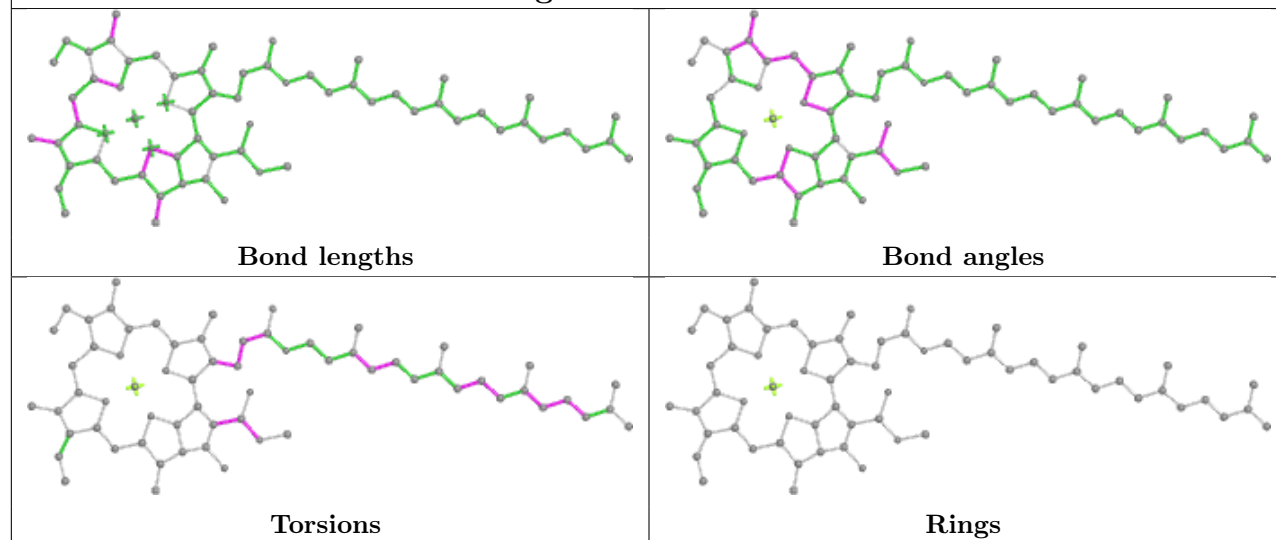
Ligand CLA BV 613

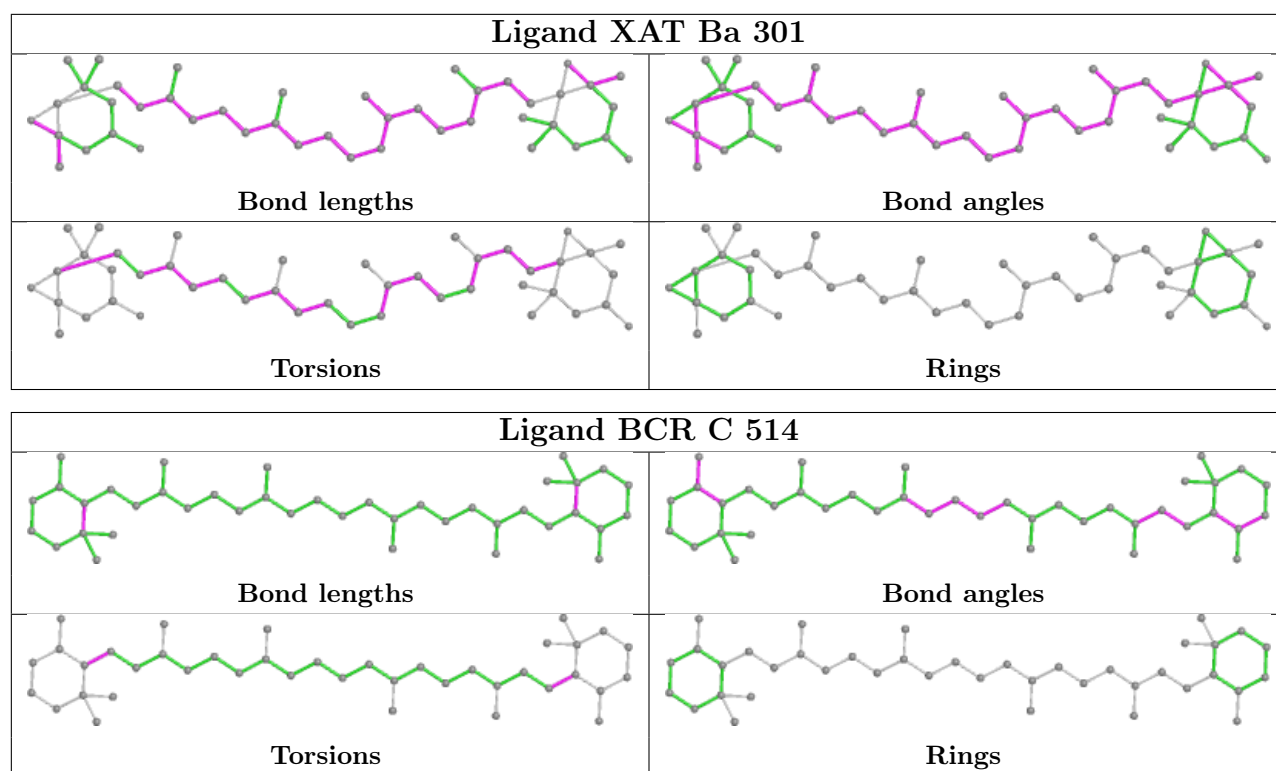


Ligand CLA Au 604

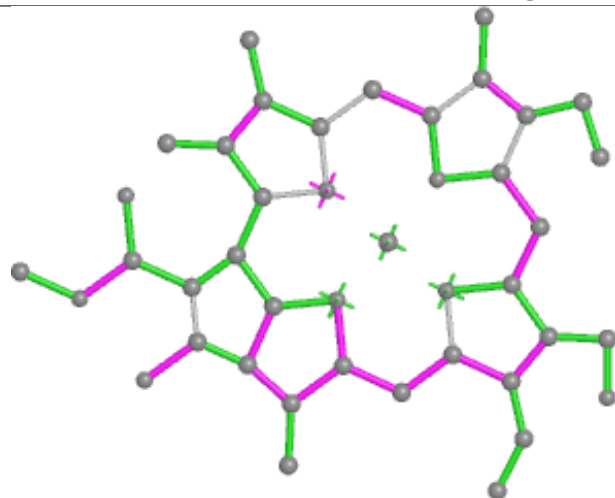


Ligand CLA b 606

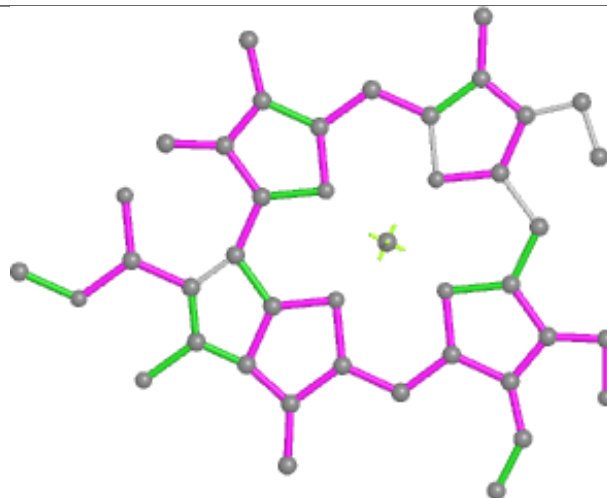




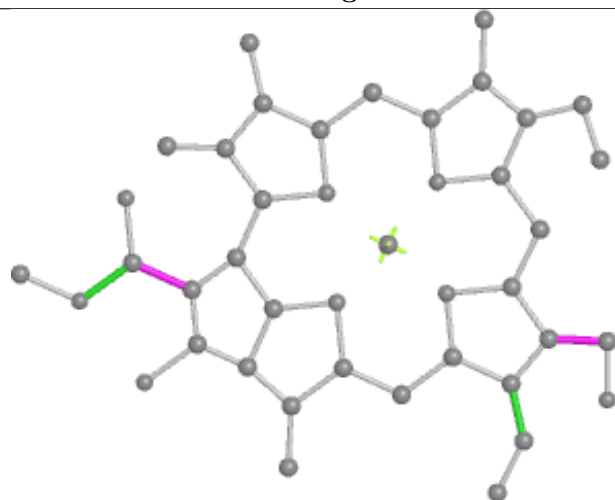
Ligand CHL r 613



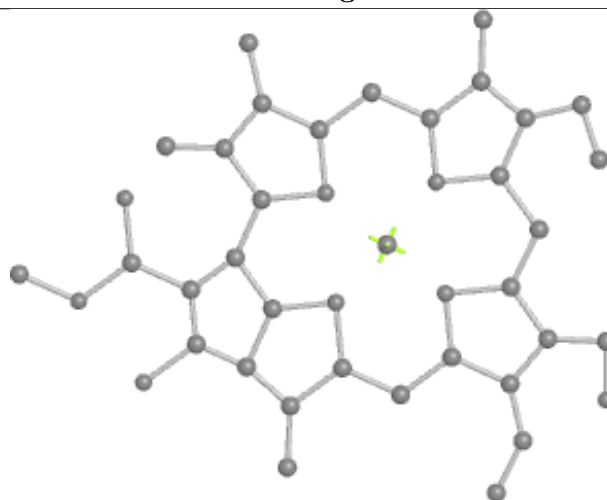
Bond lengths



Bond angles

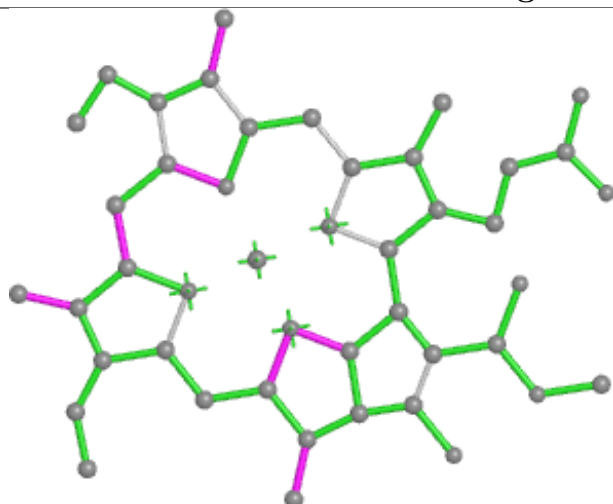


Torsions

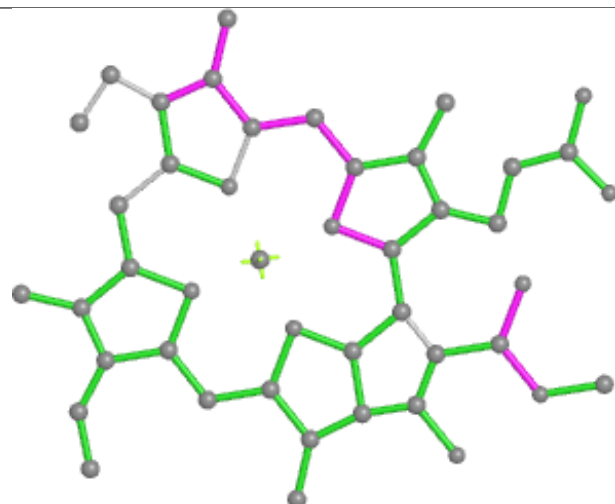


Rings

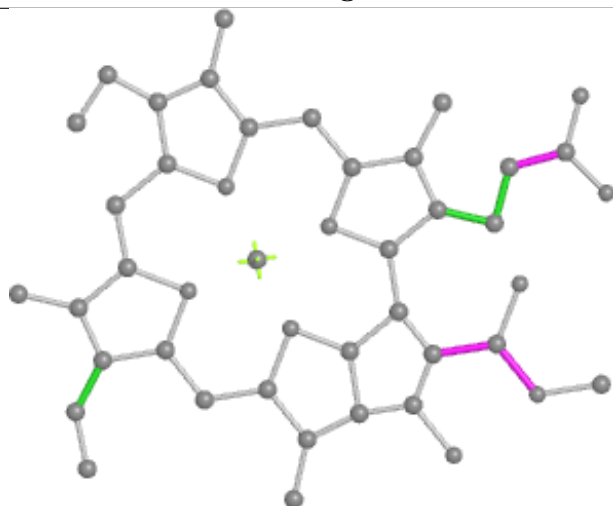
Ligand CLA S 603



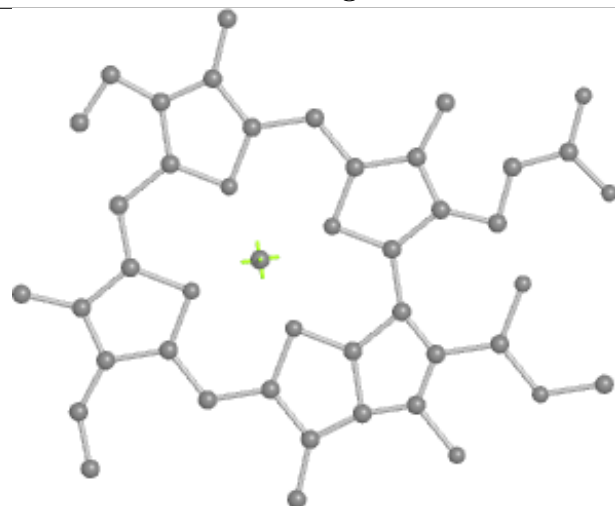
Bond lengths



Bond angles

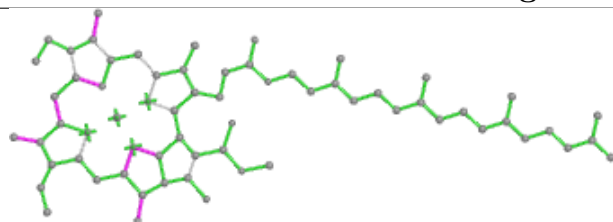


Torsions

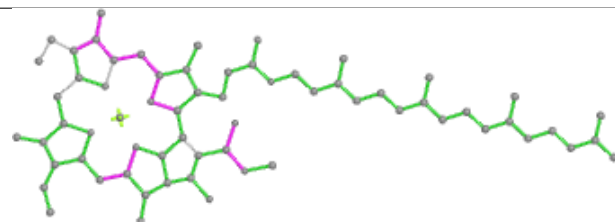


Rings

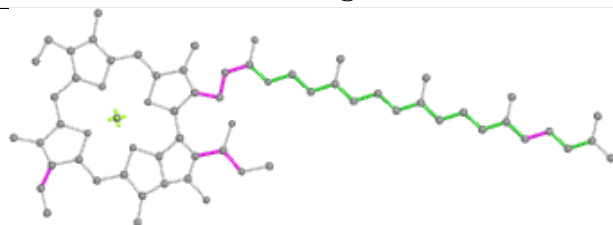
Ligand CLA c 505



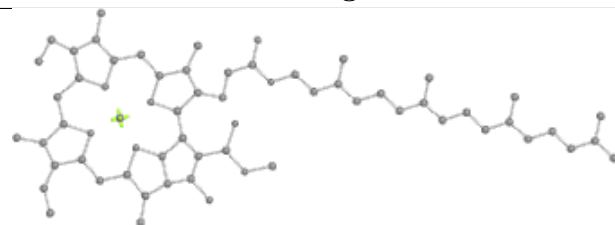
Bond lengths



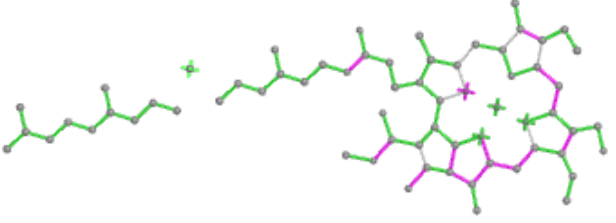
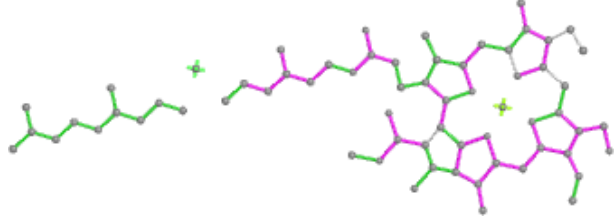
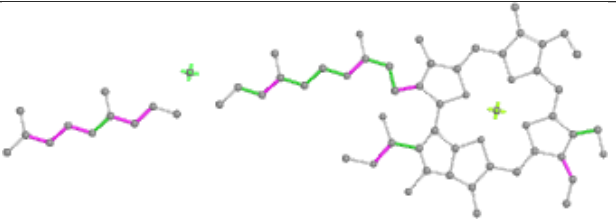
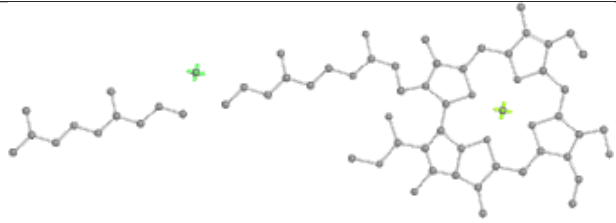
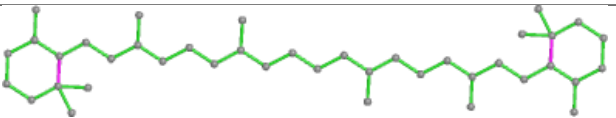
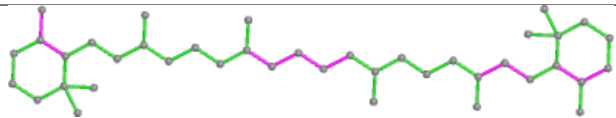
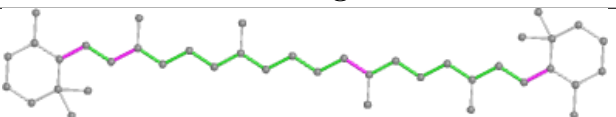
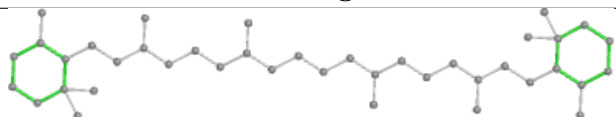
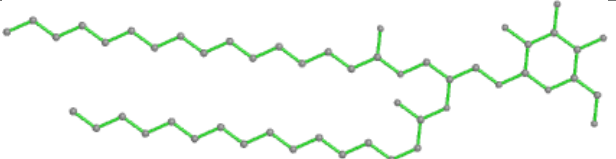
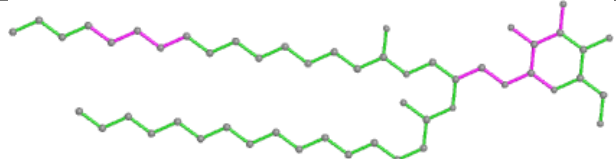
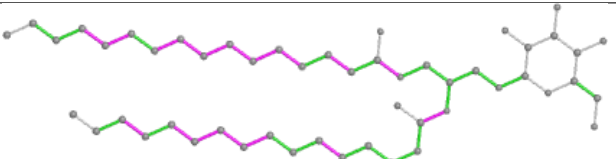
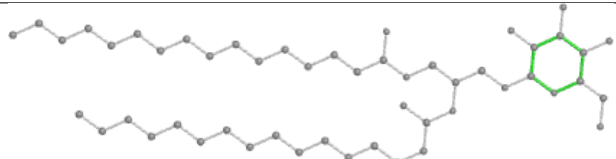
Bond angles

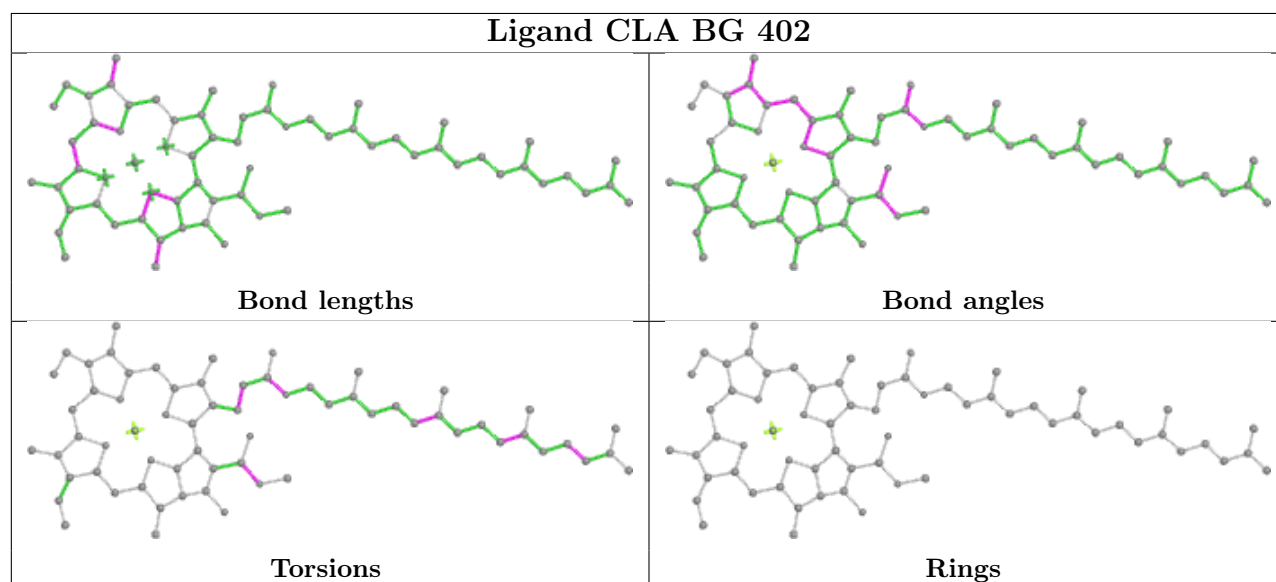
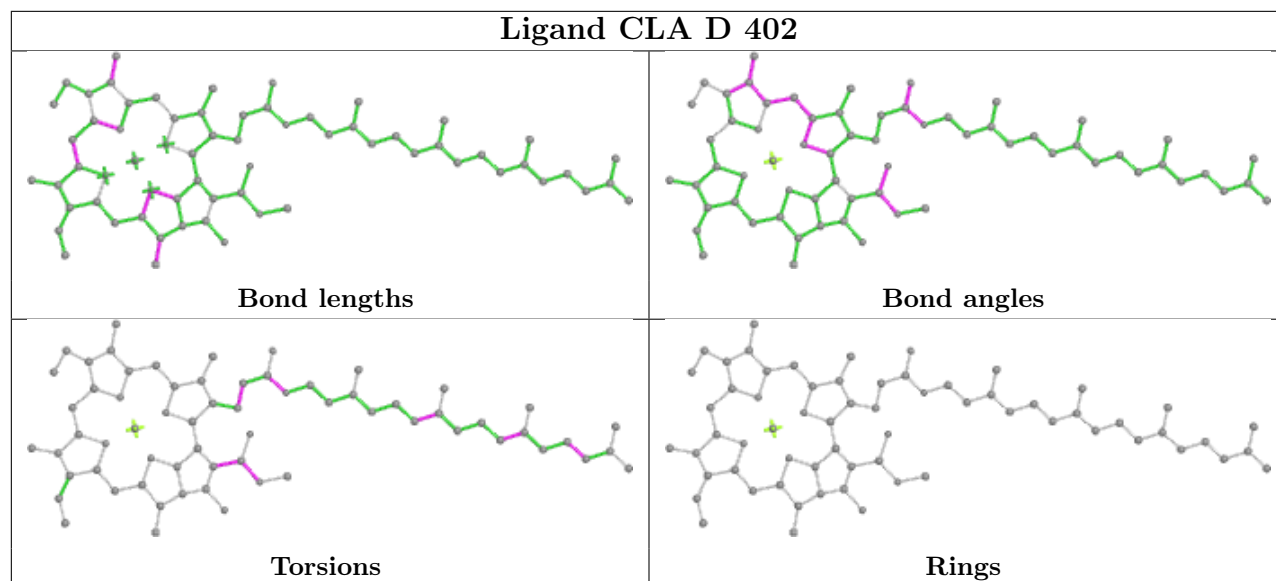
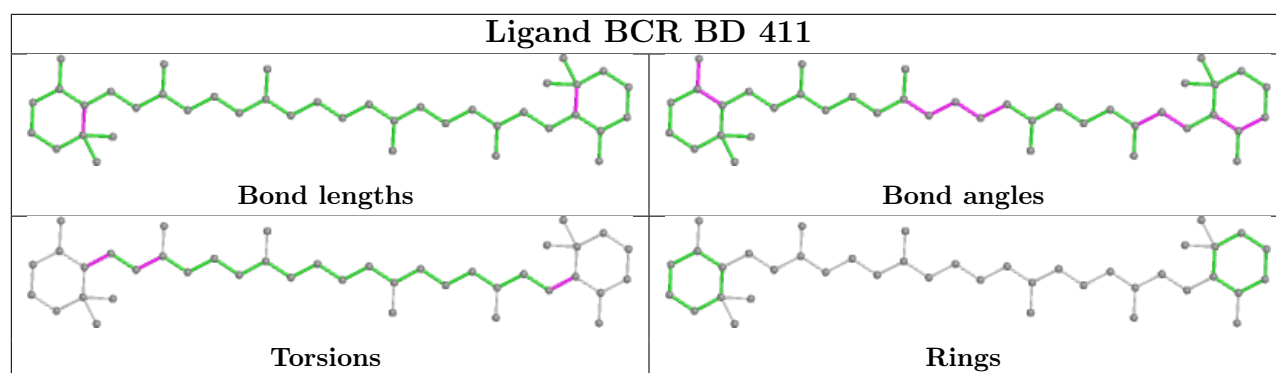


Torsions

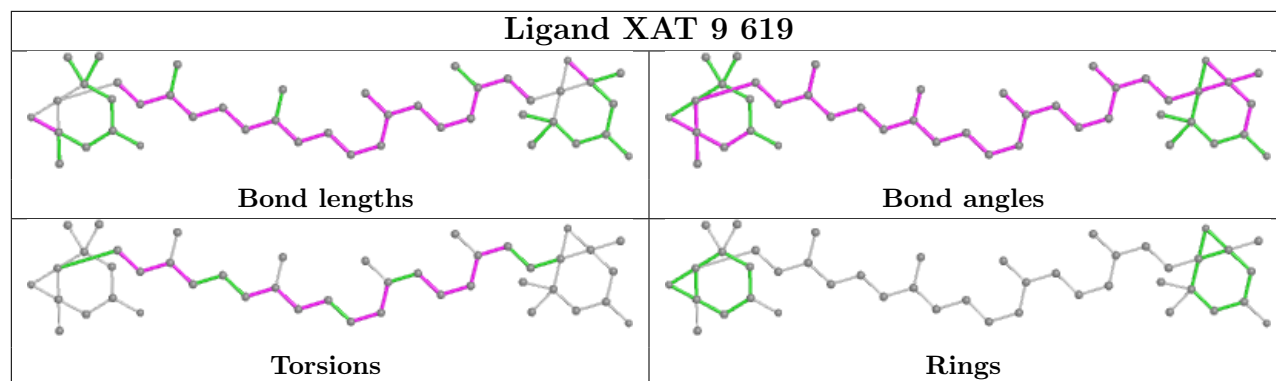


Rings

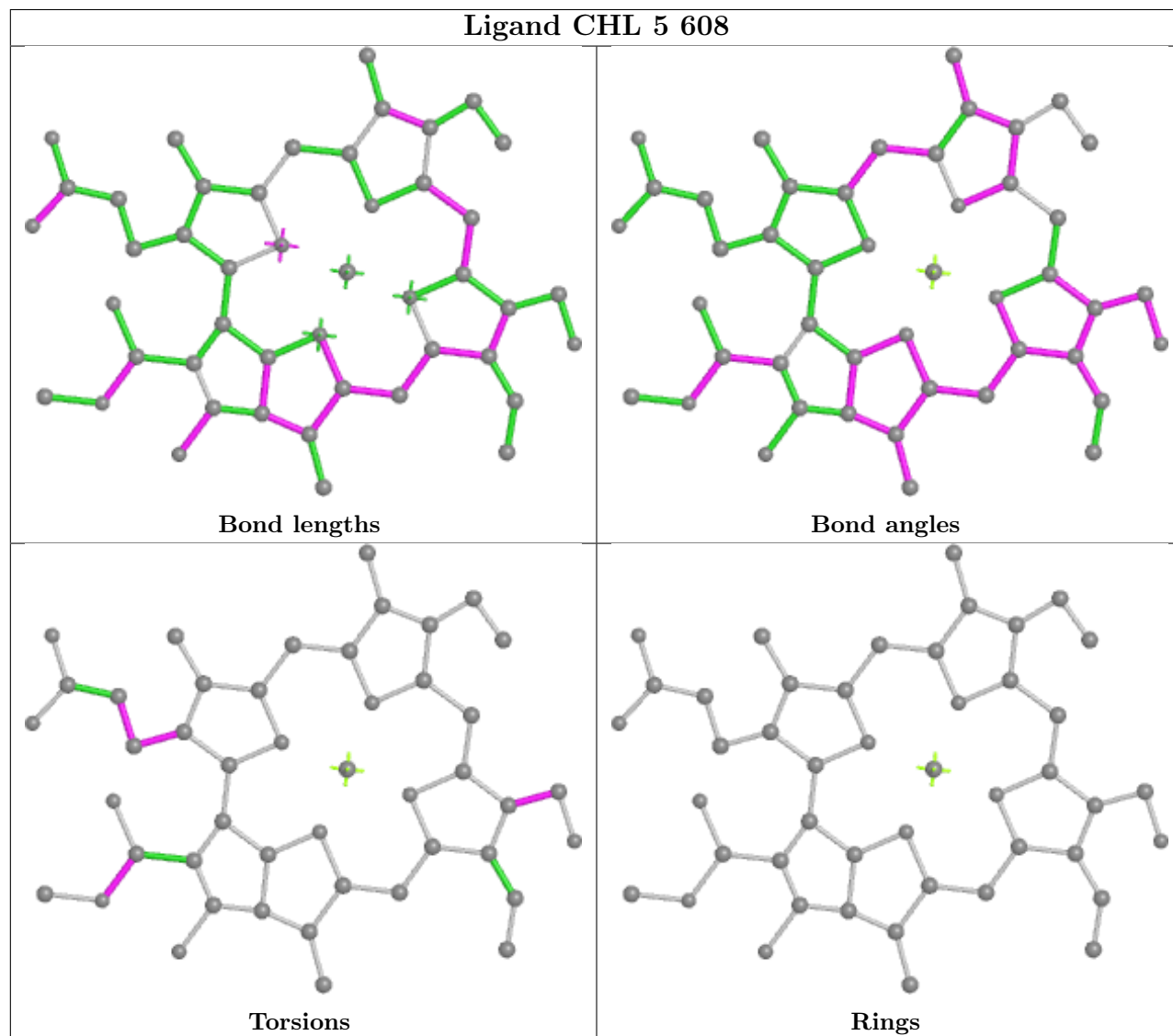
| Ligand CHL BB 302 | |
|---|---|
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |
| Ligand BCR b 619 | |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |
| Ligand LMG v 620 | |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |



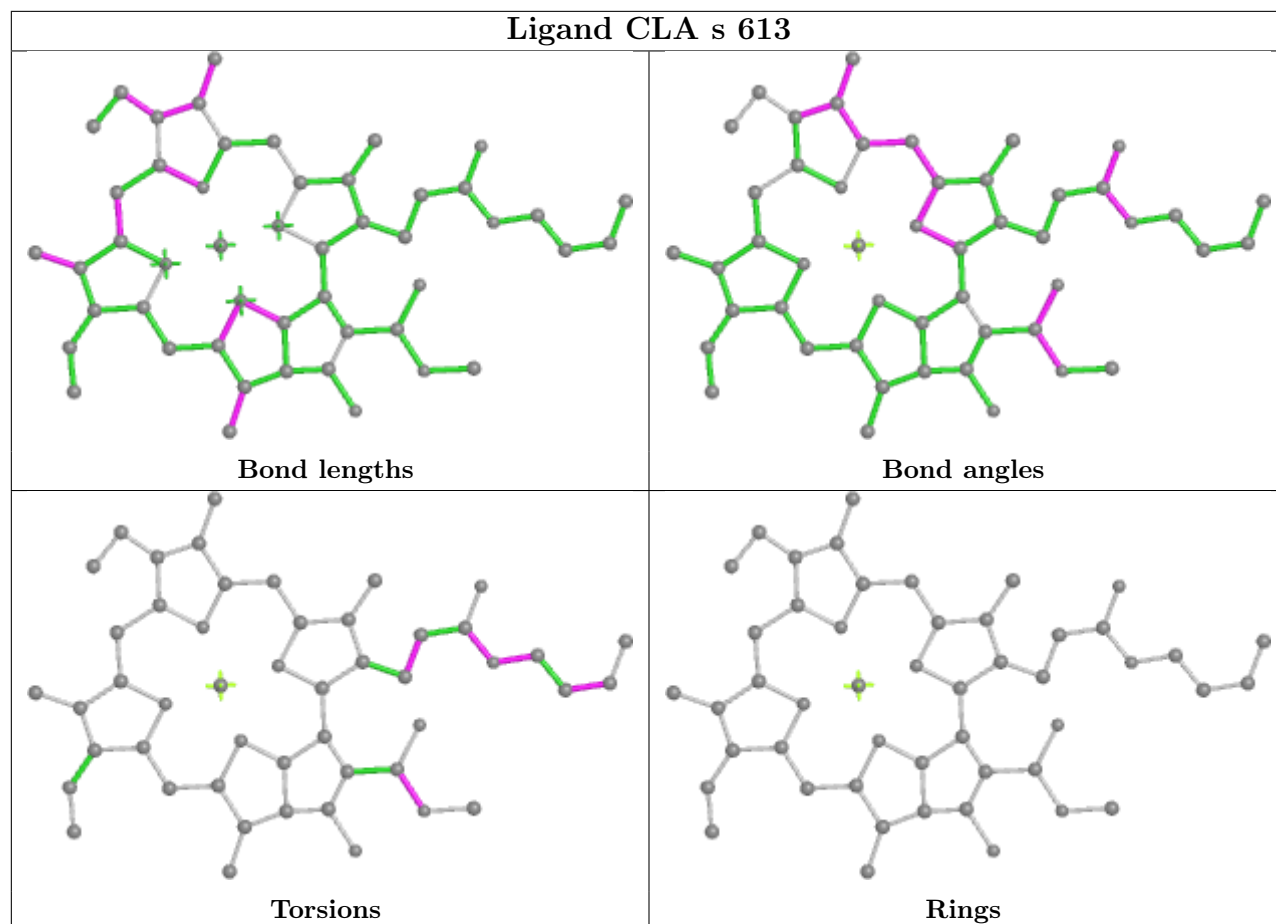
Ligand XAT 9 619



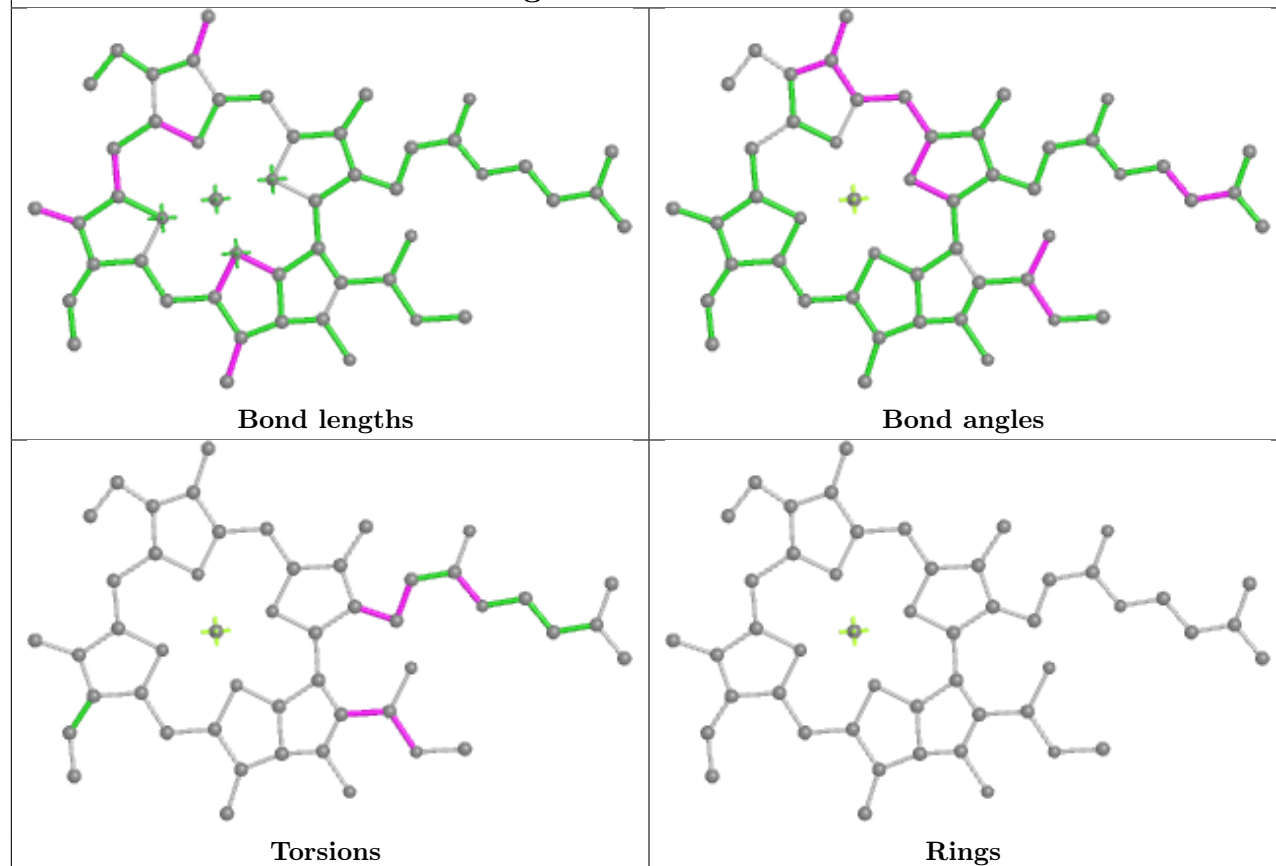
Ligand CHL 5 608



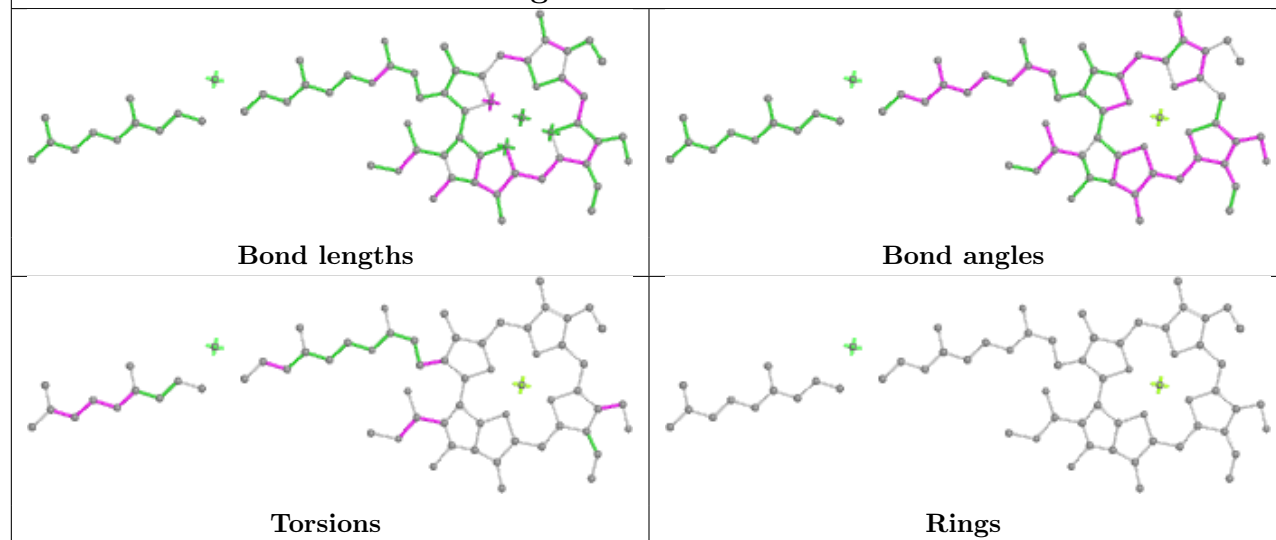
Ligand CLA s 613

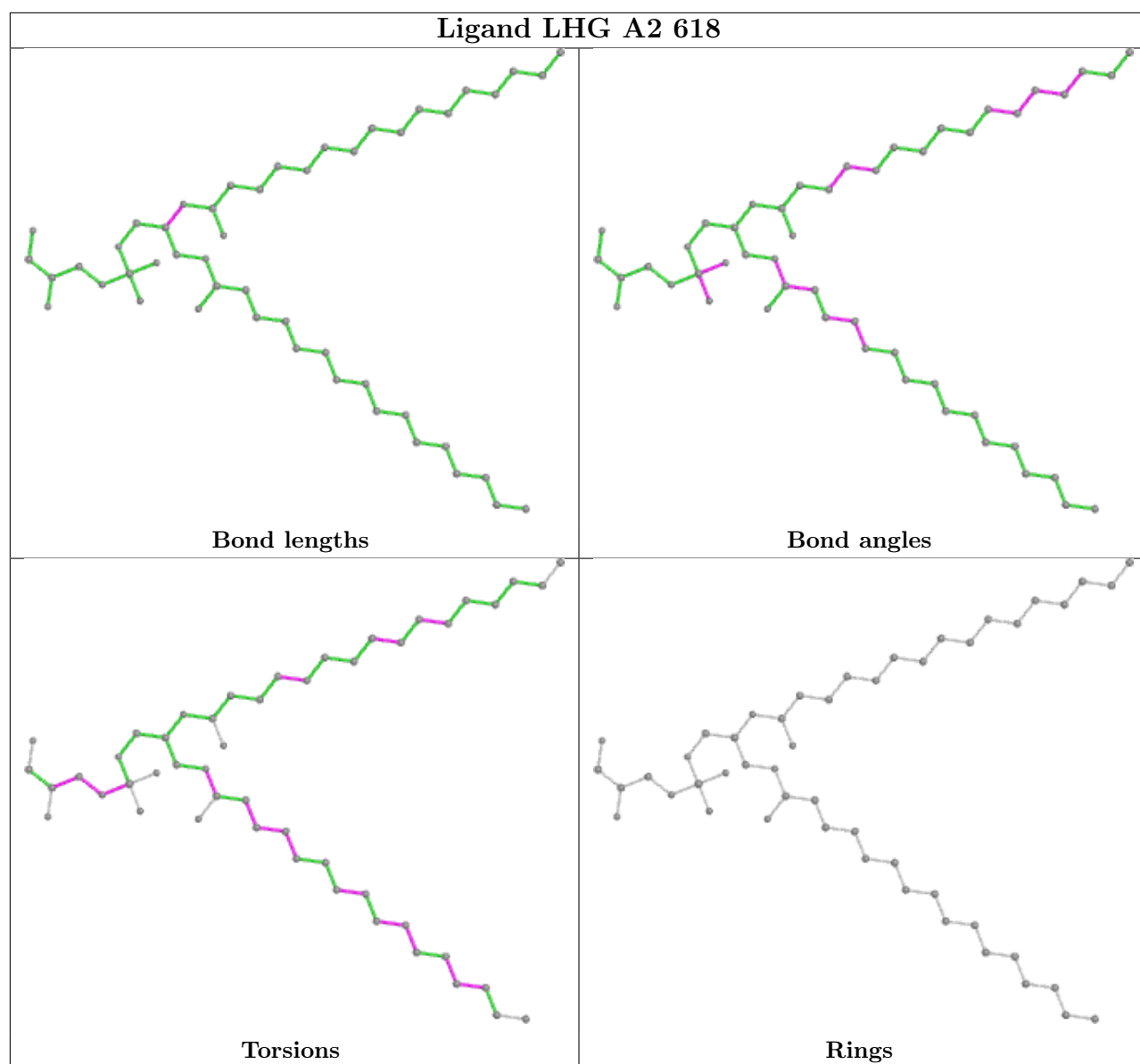


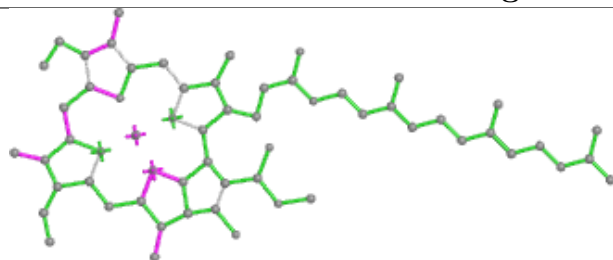
Ligand CLA Ba 305



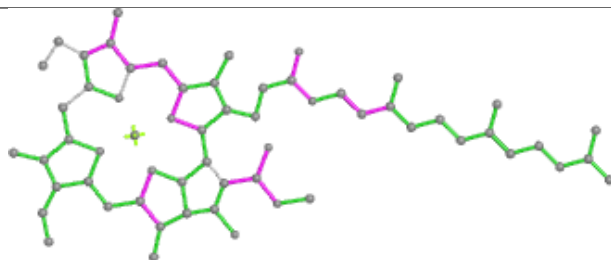
Ligand CHL N 608



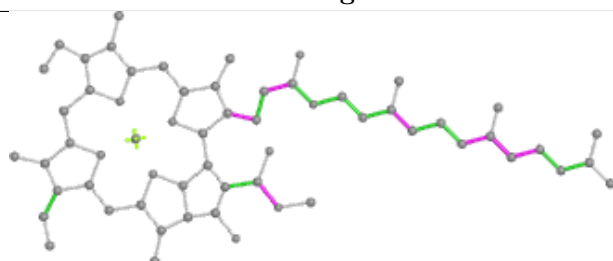


Ligand CLA BB 312

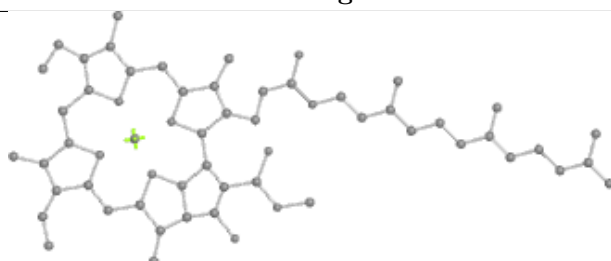
Bond lengths



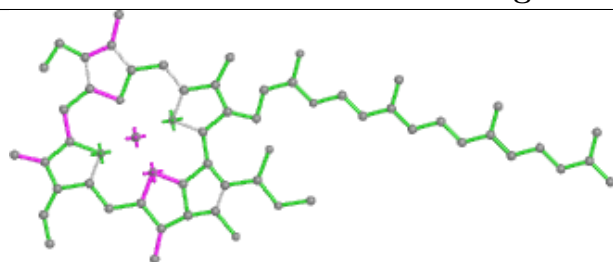
Bond angles



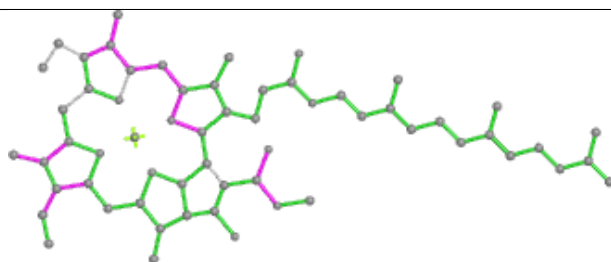
Torsions



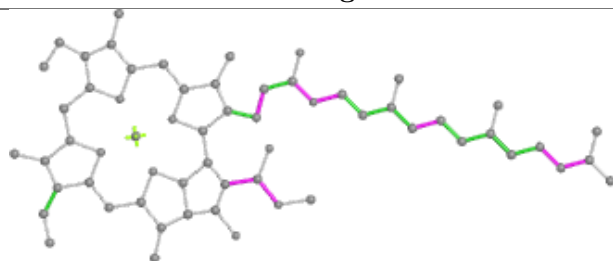
Rings

Ligand CLA Y 311

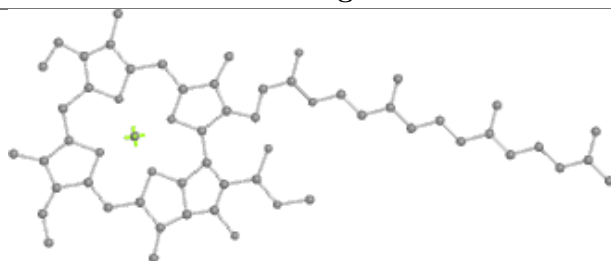
Bond lengths



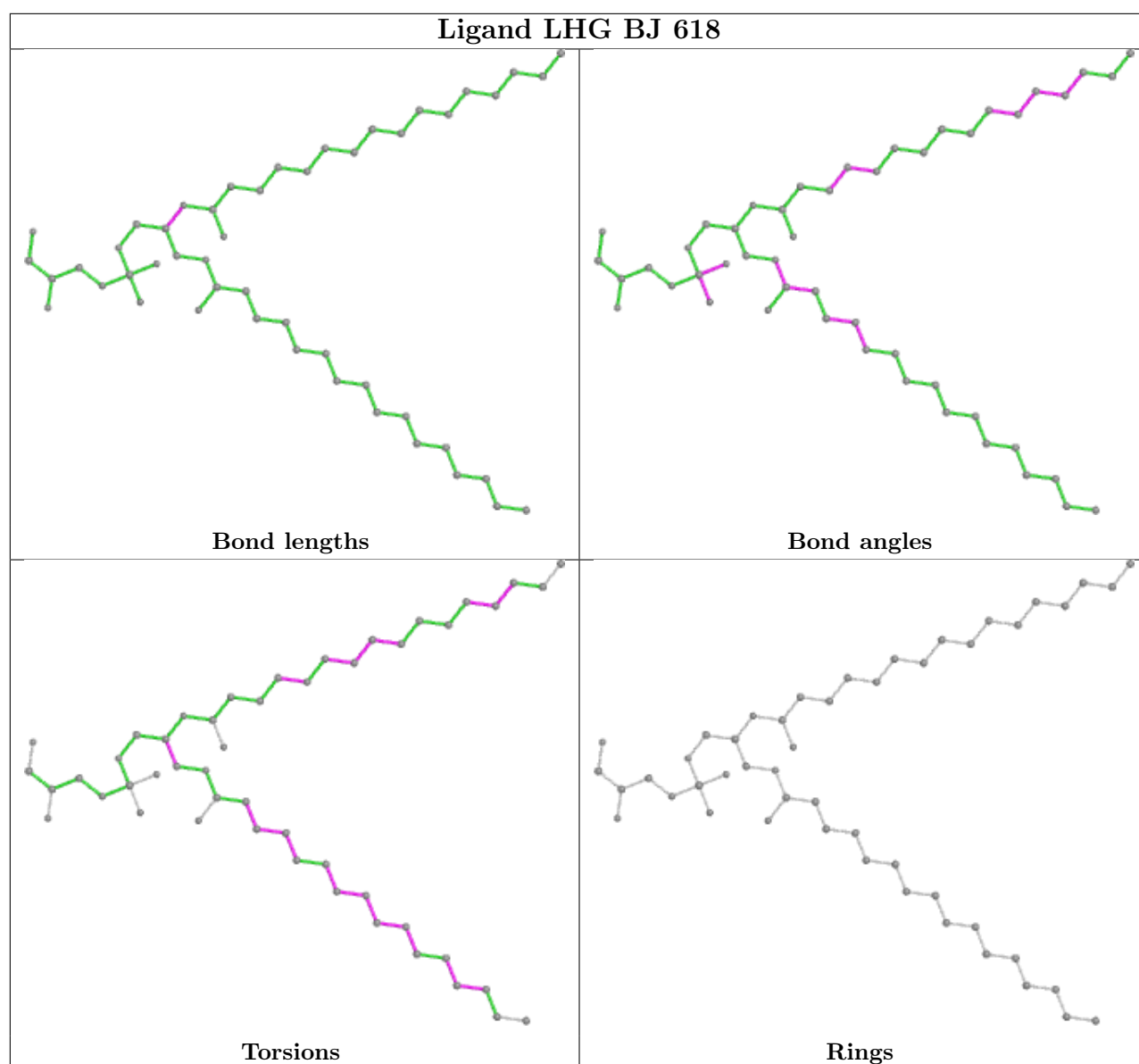
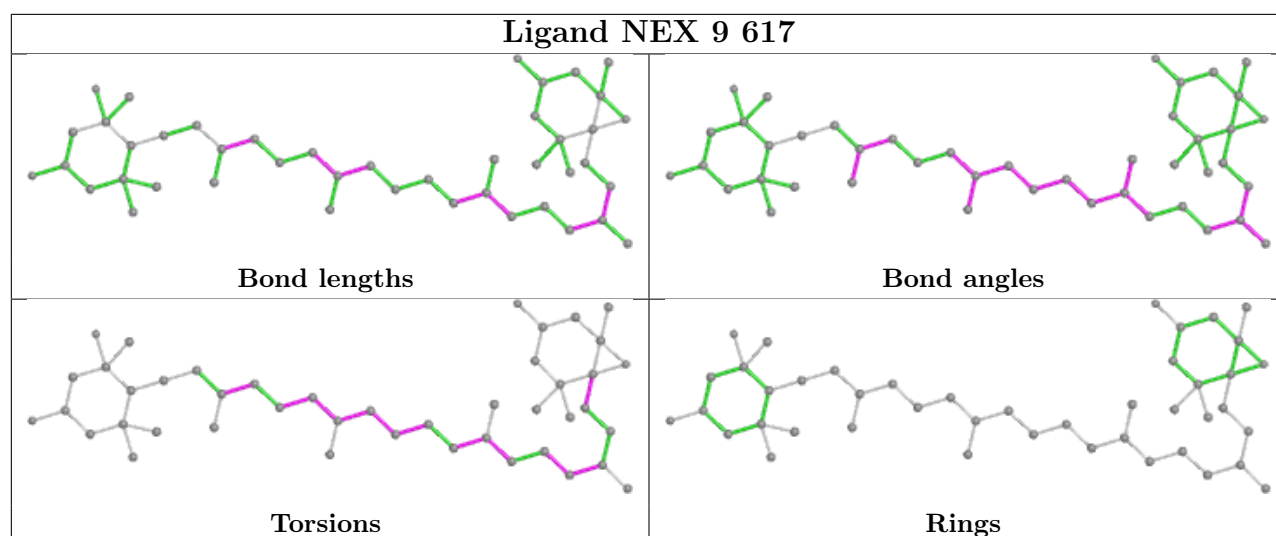
Bond angles

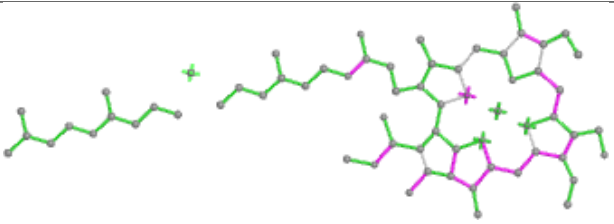
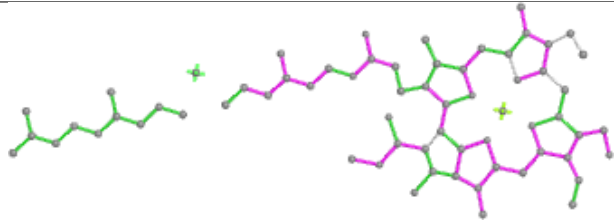
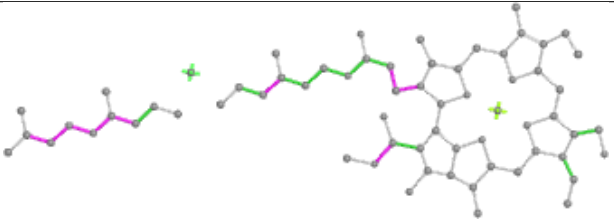
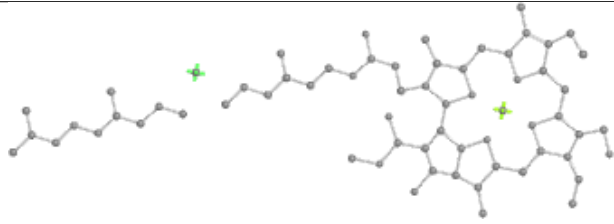
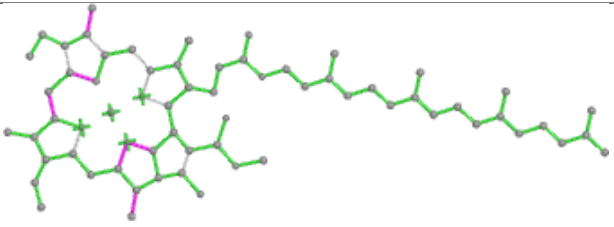
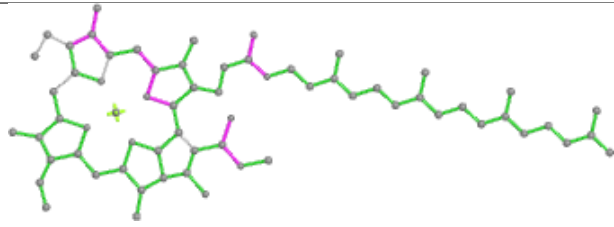
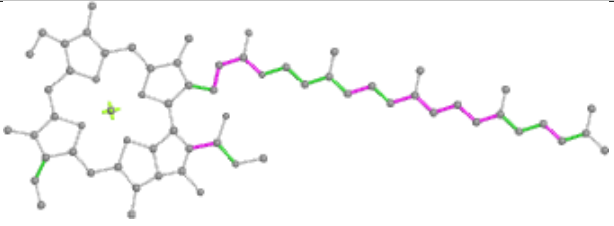
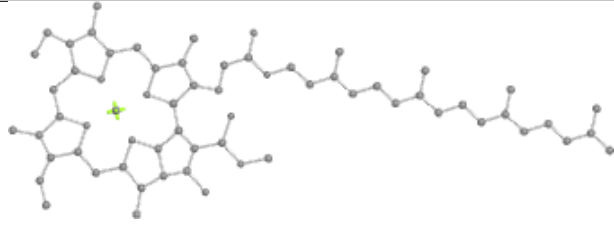
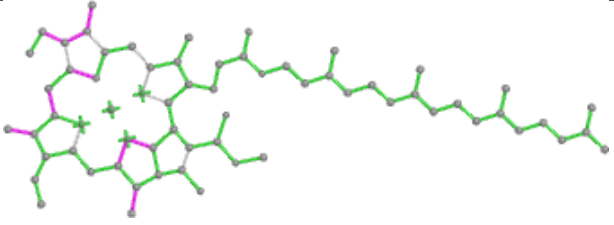
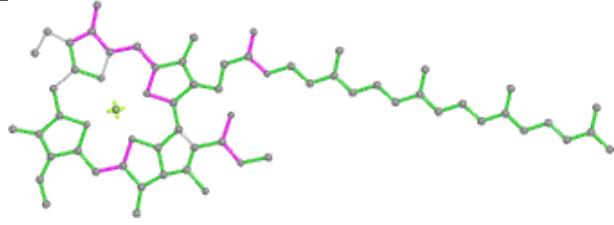
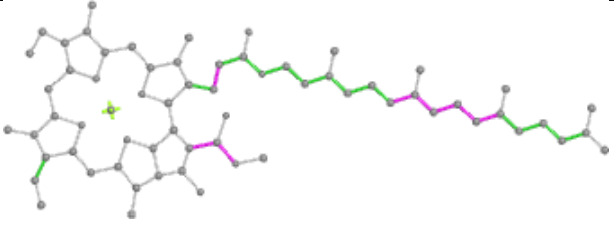
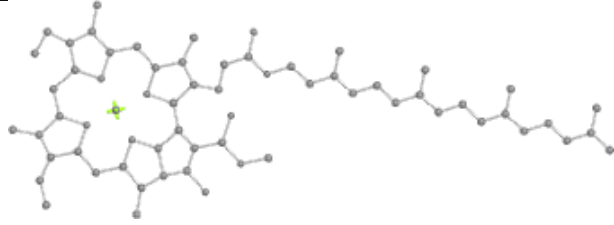


Torsions

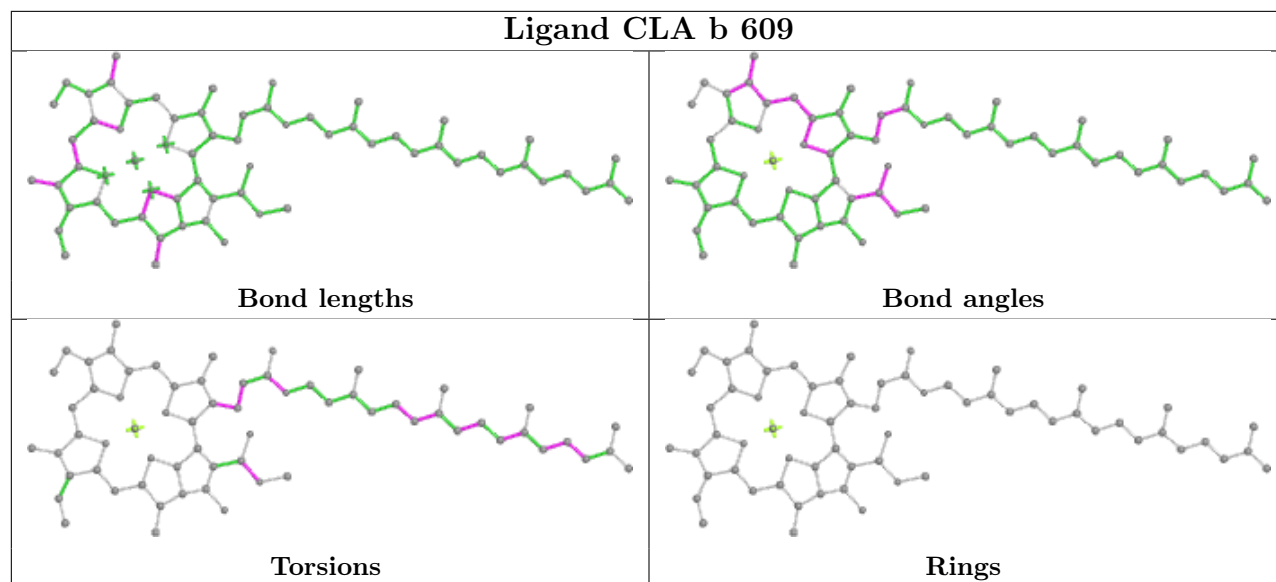


Rings

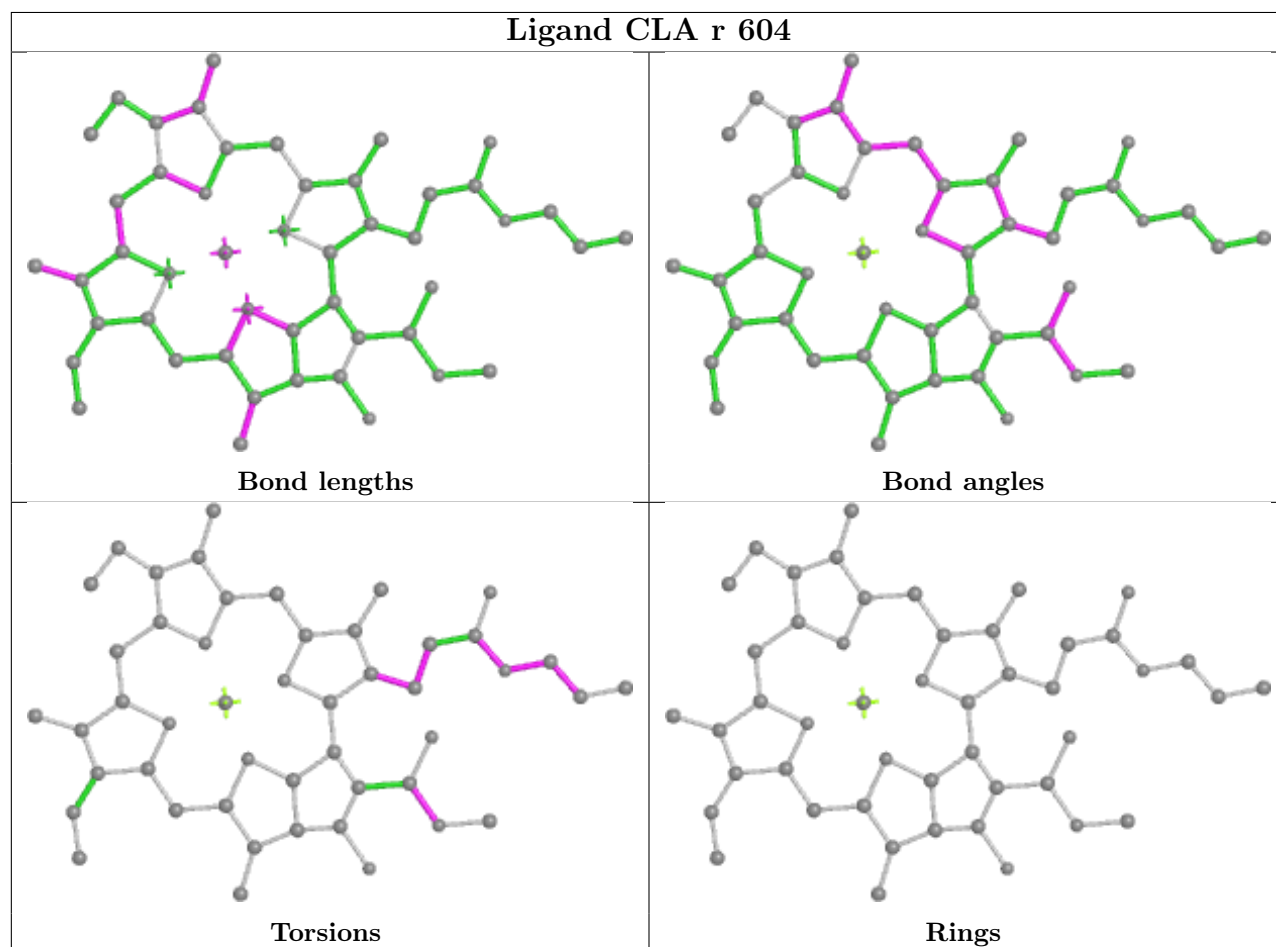


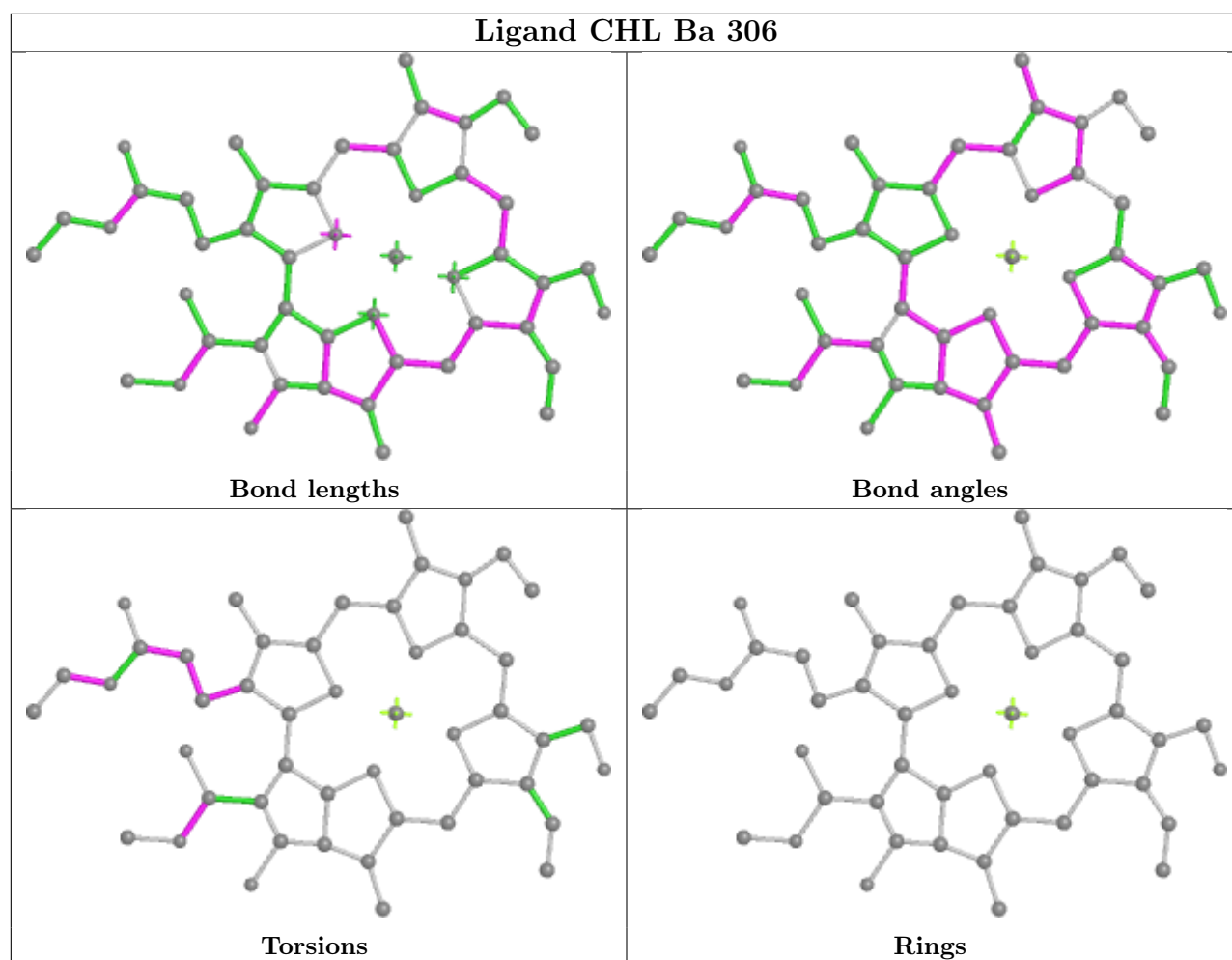
| Ligand CHL Au 607 | |
|---|---|
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |
| Ligand CLA BQ 602 | |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |
| Ligand CLA N 602 | |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p> |  <p>Rings</p> |

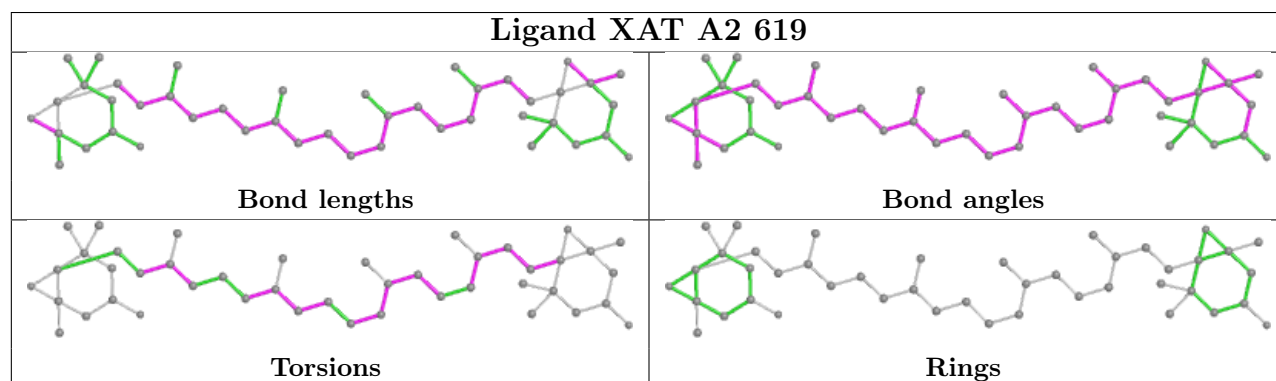
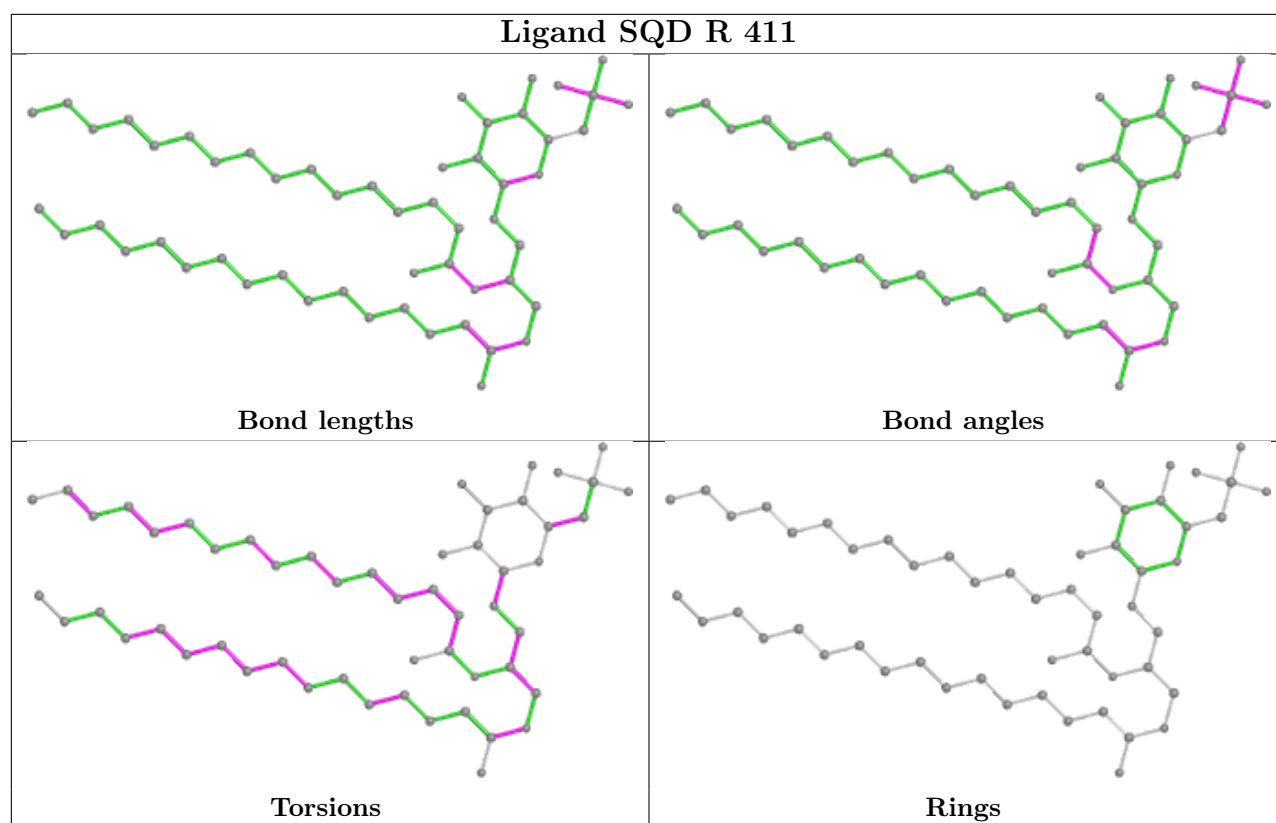
Ligand CLA b 609

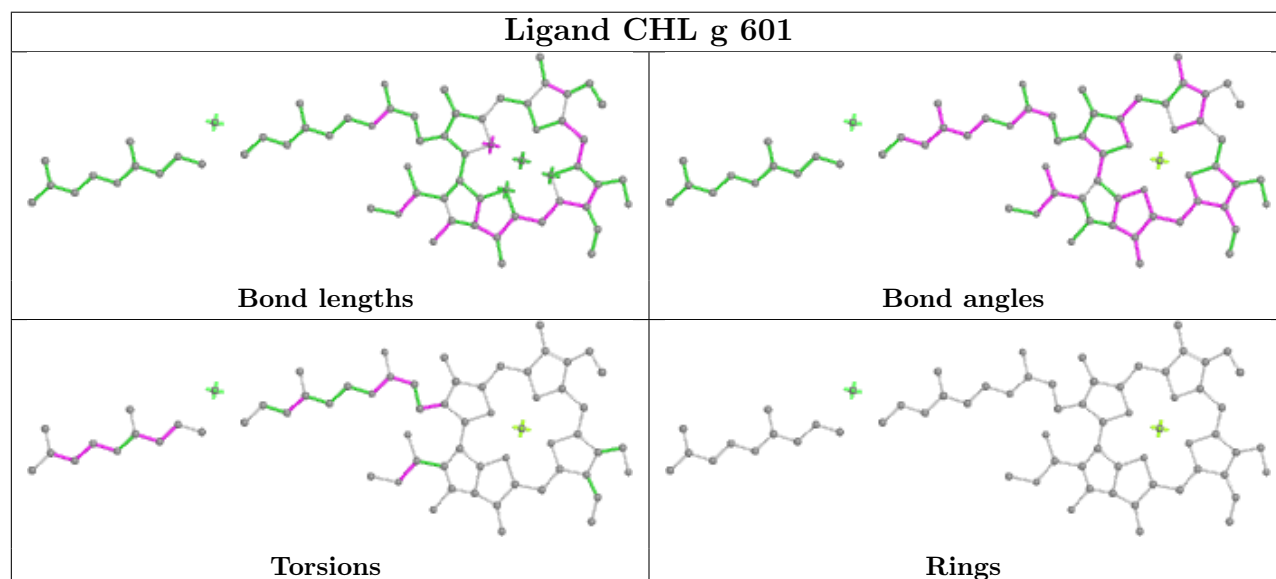
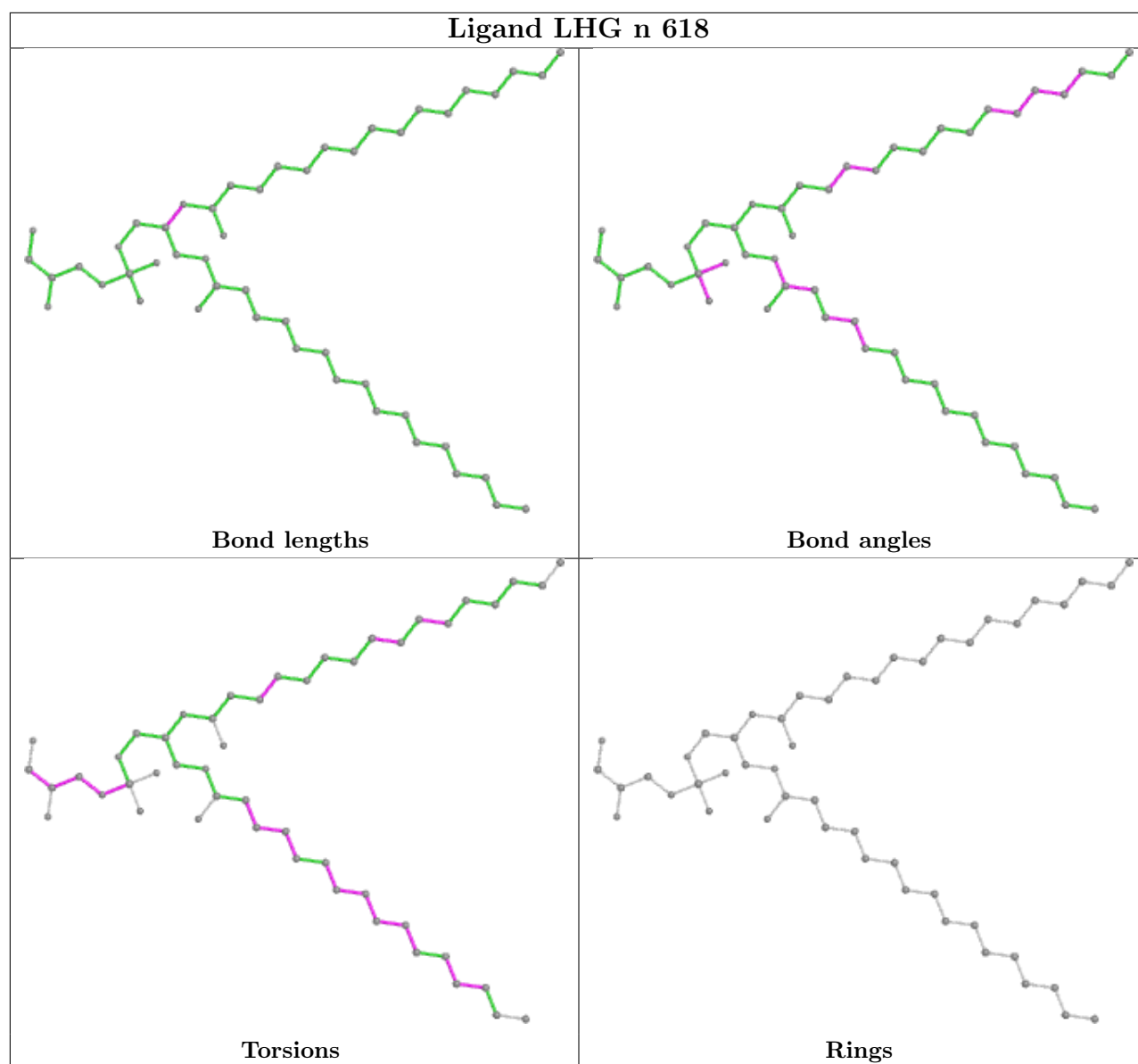


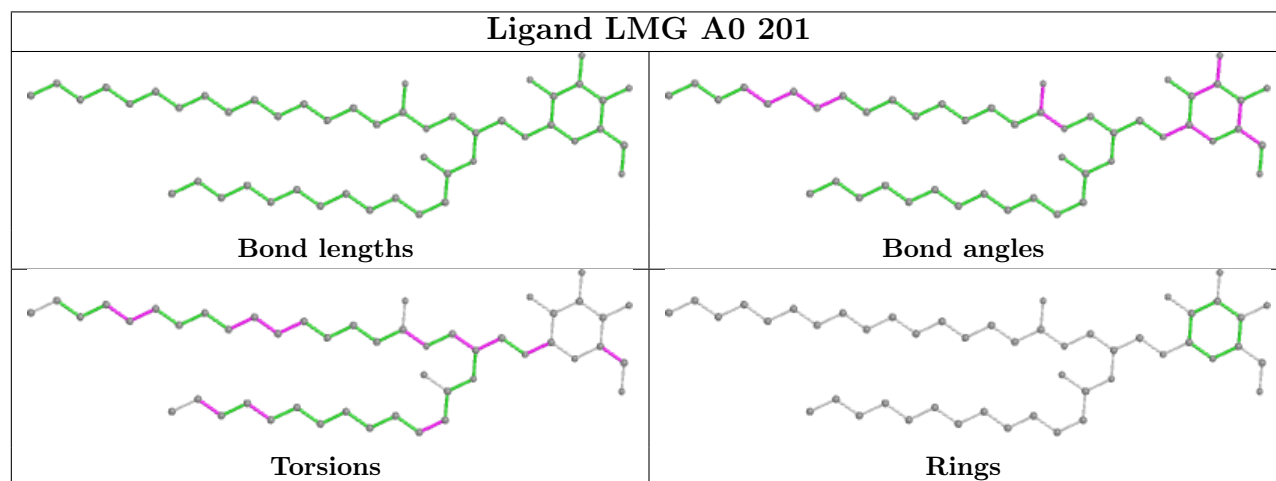
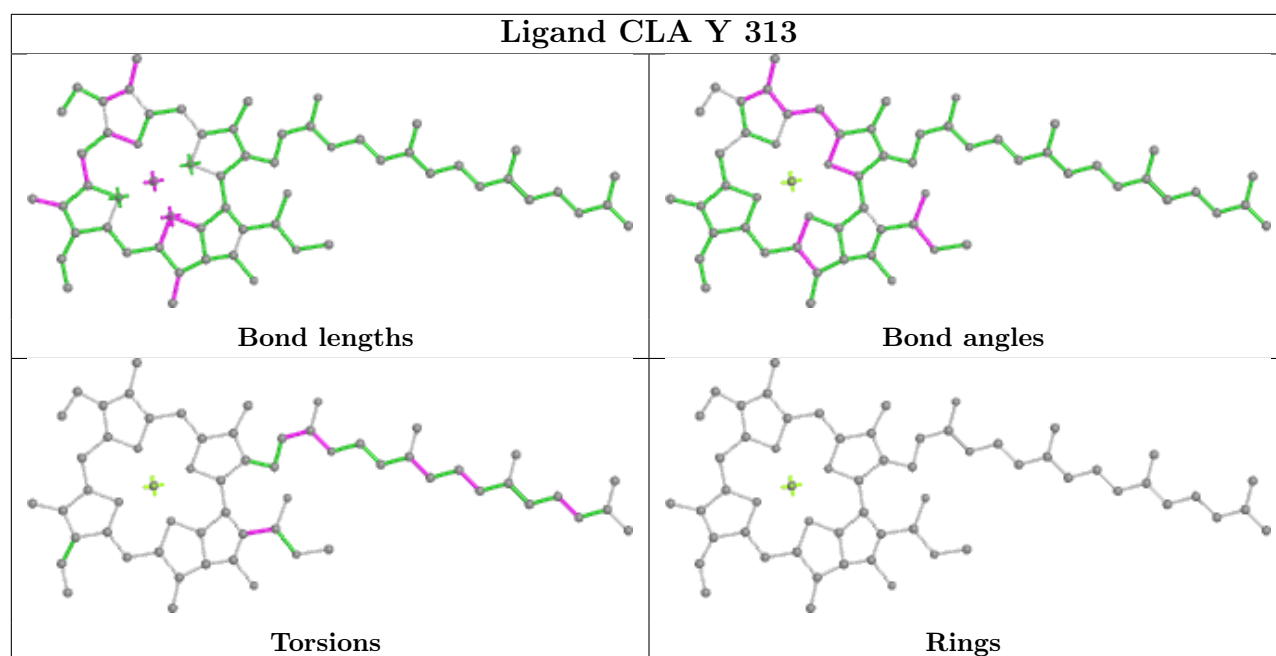
Ligand CLA r 604



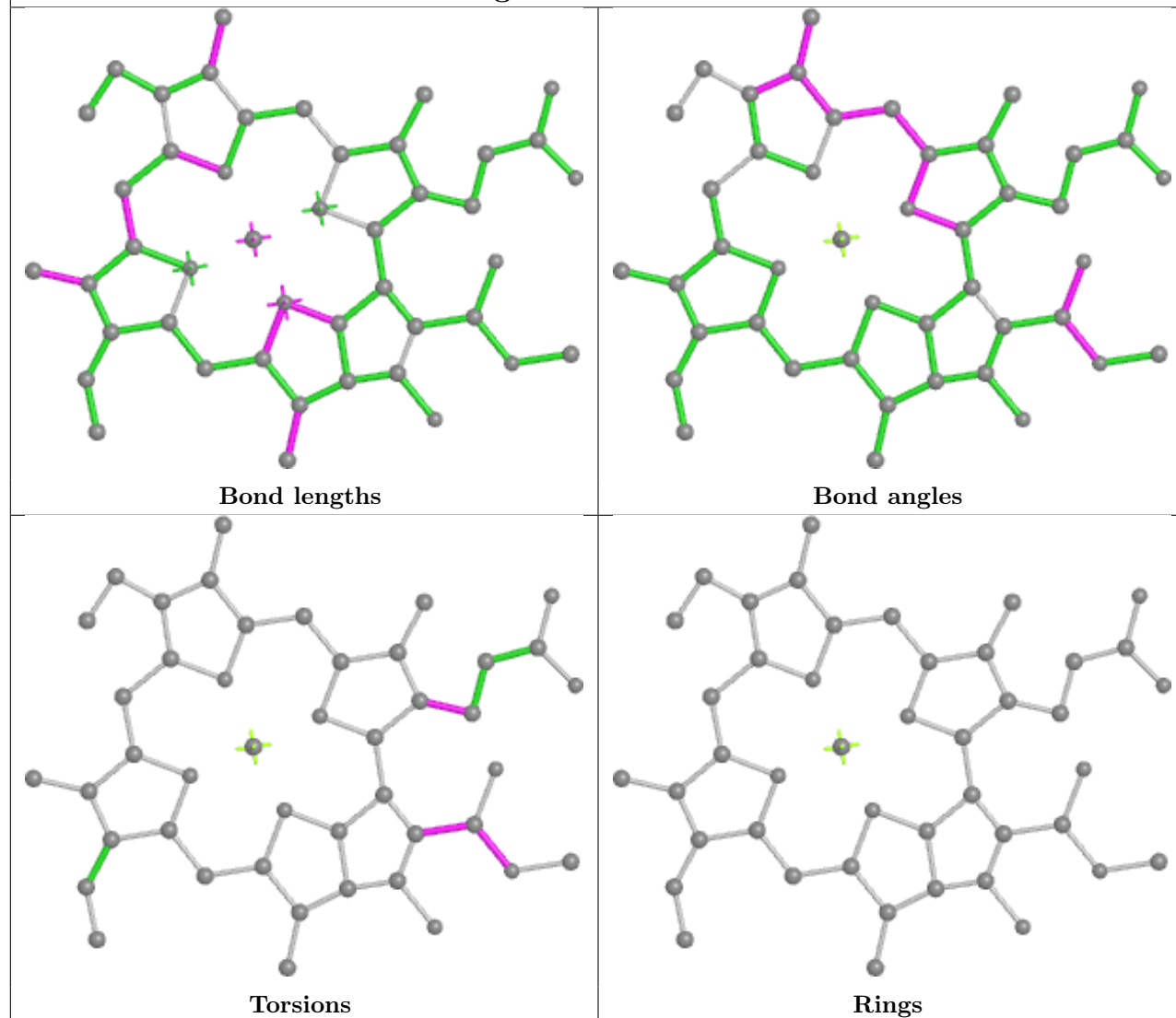




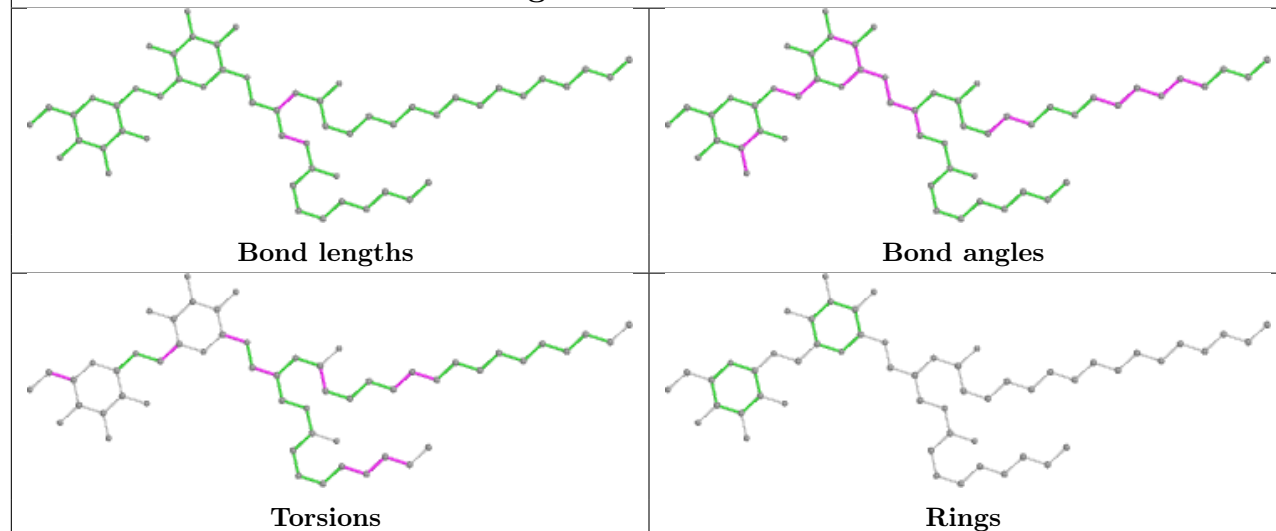




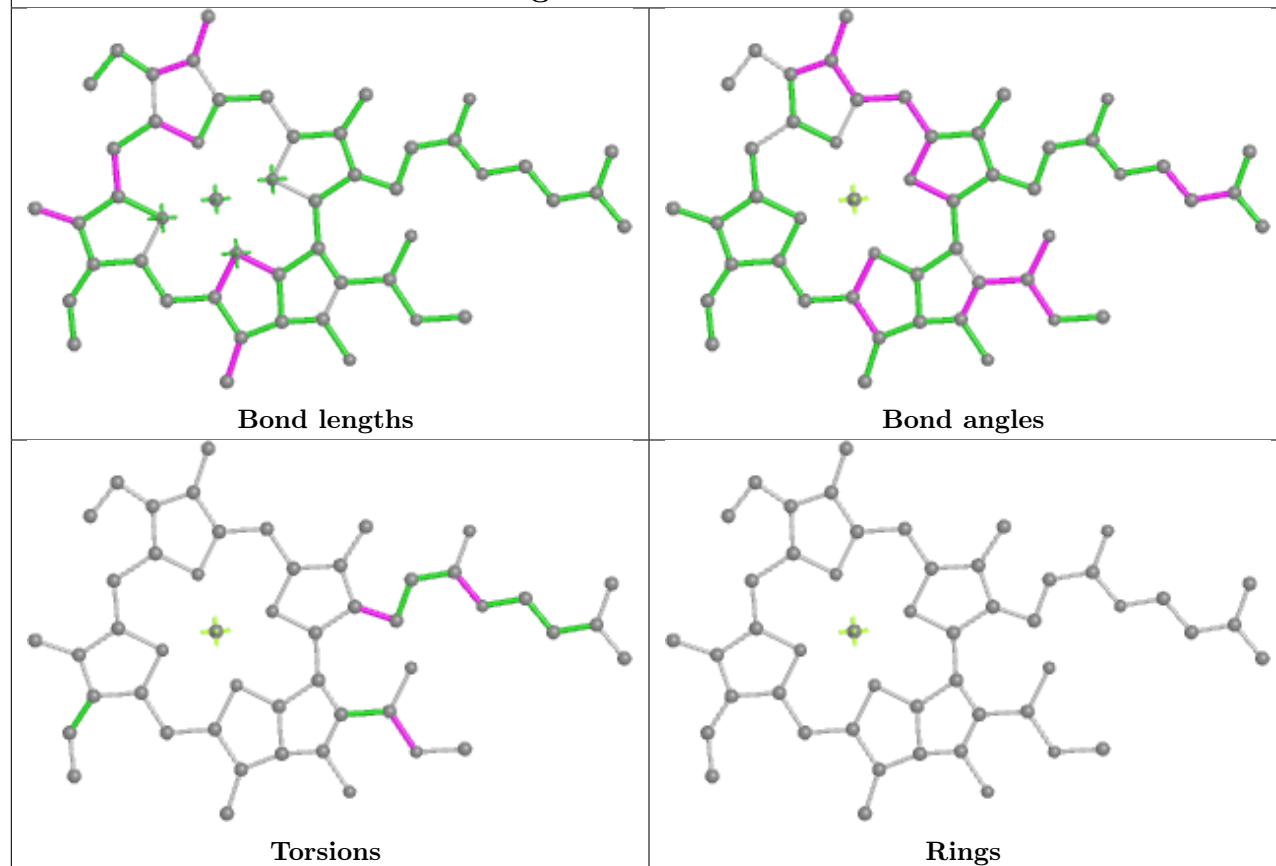
Ligand CLA 8 303



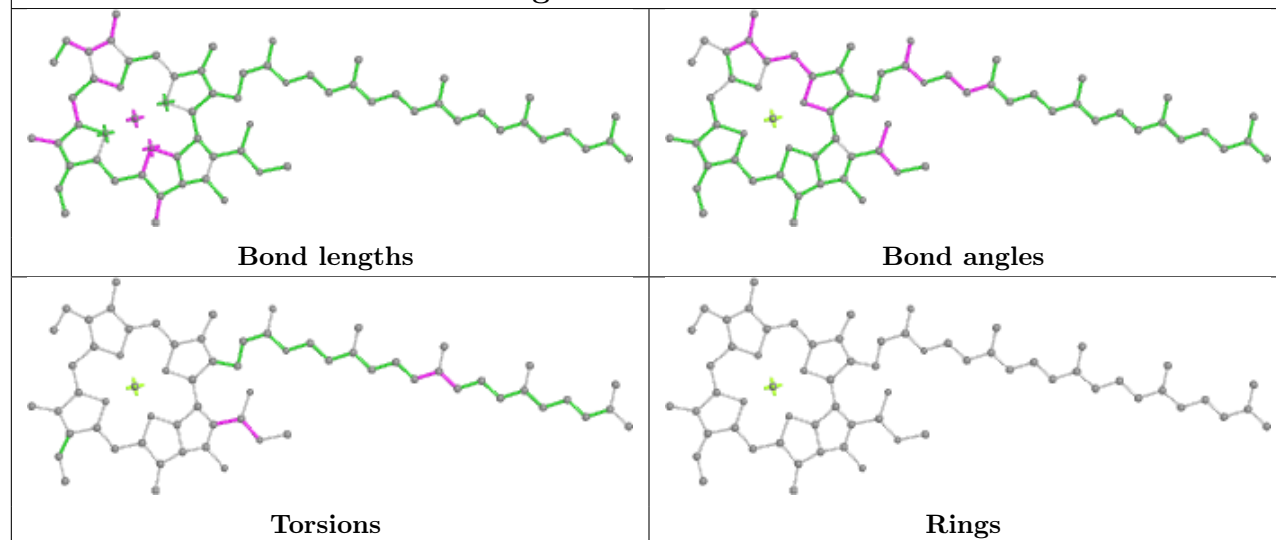
Ligand DGD C 516

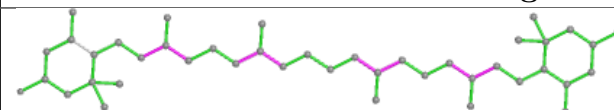
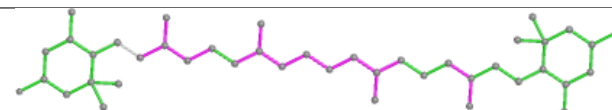
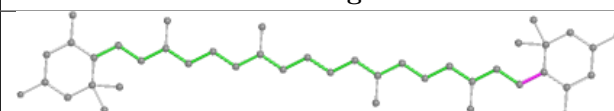
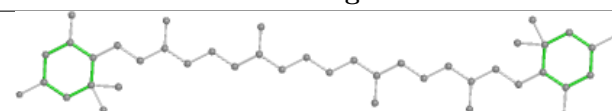


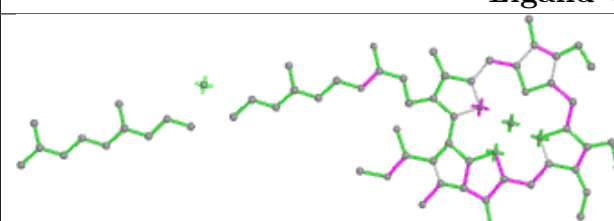
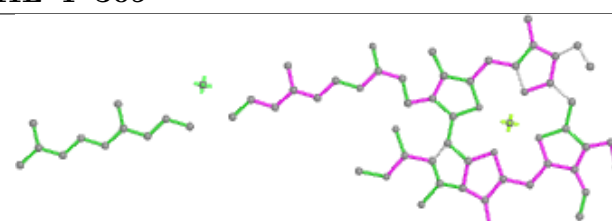
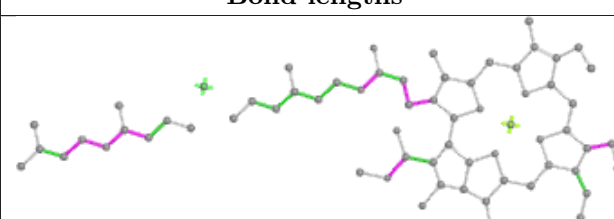
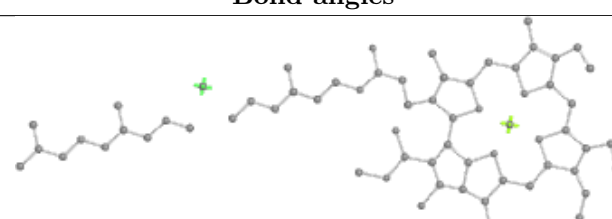
Ligand CLA A 407

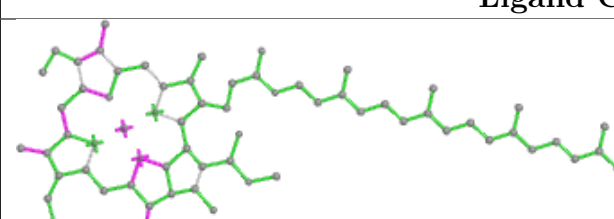
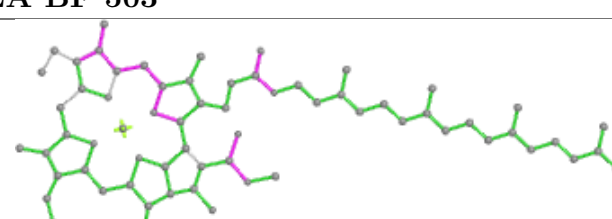
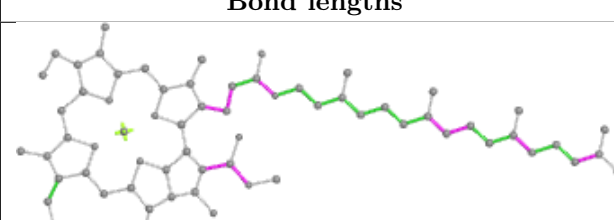
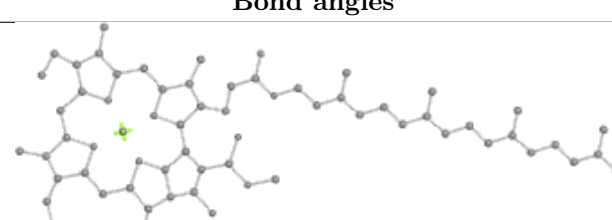


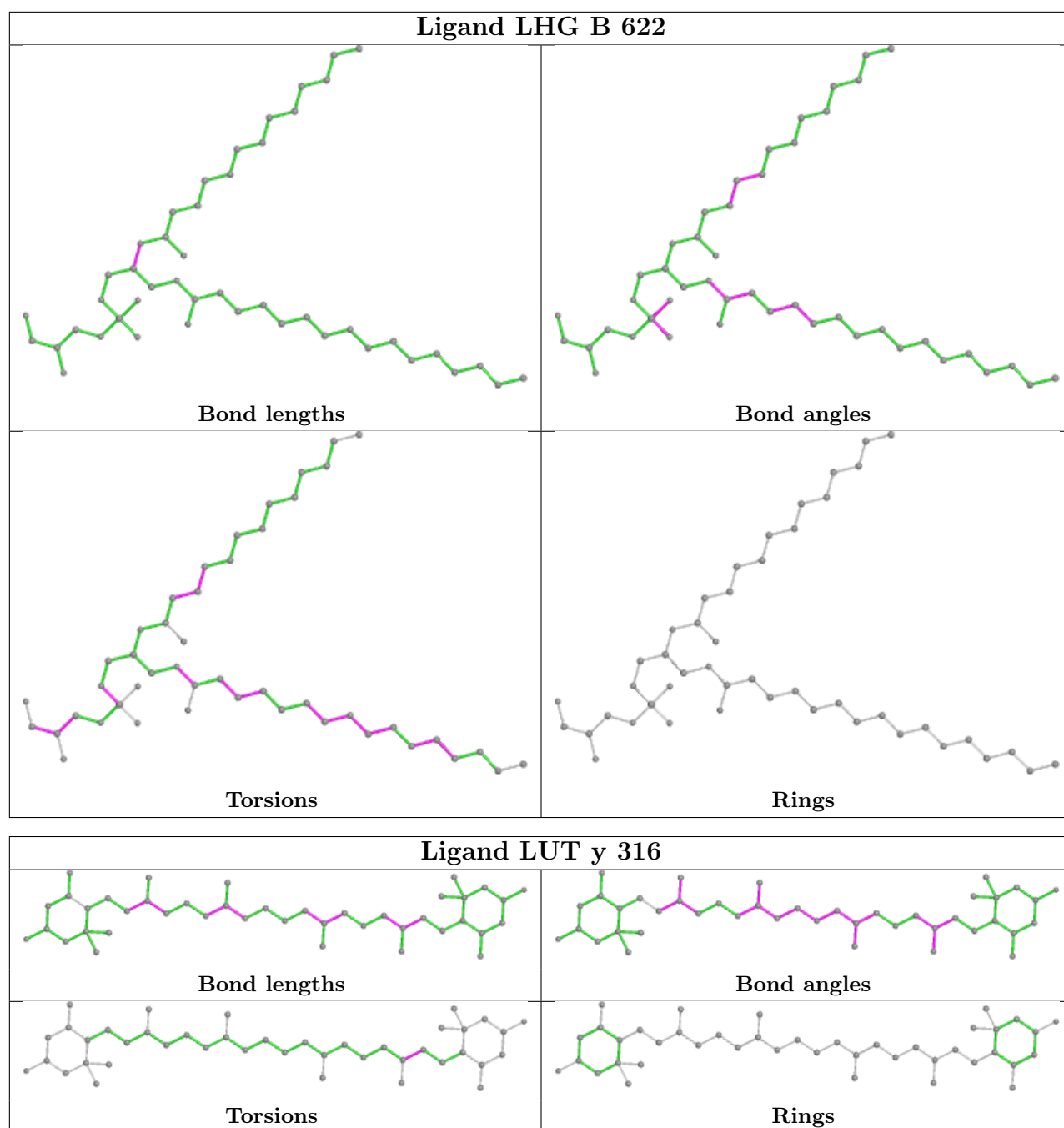
Ligand CLA C 509



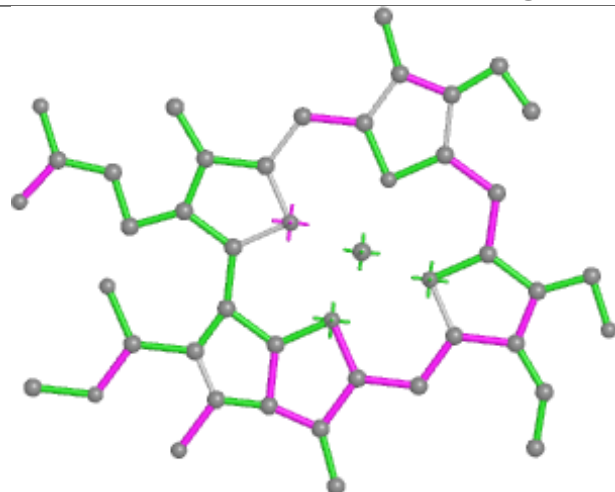
| Ligand LUT N 615 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CHL Y 309 | |
|--|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

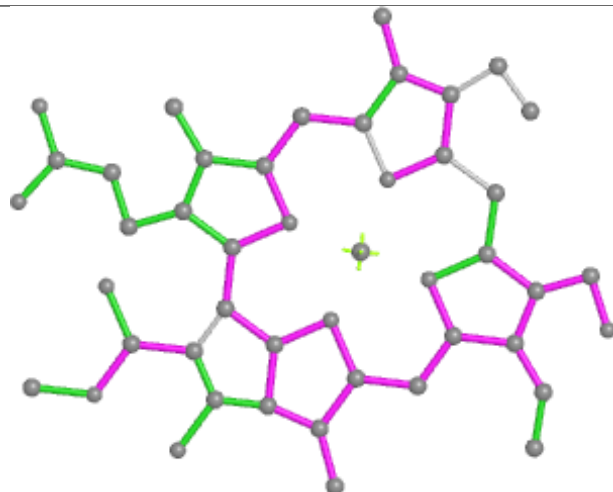
| Ligand CLA BF 503 | |
|---|--|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |



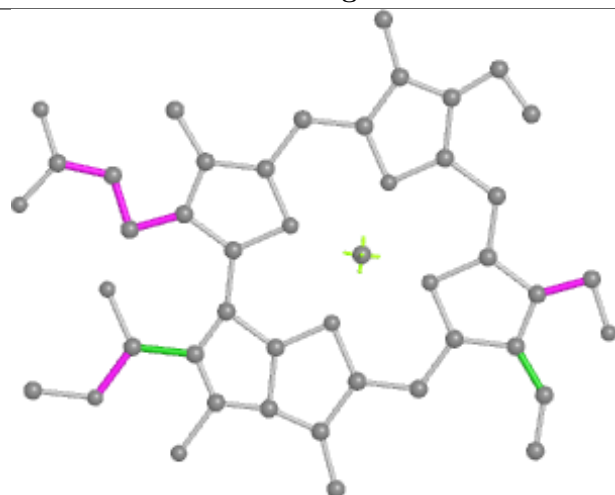
Ligand CHL 8 304



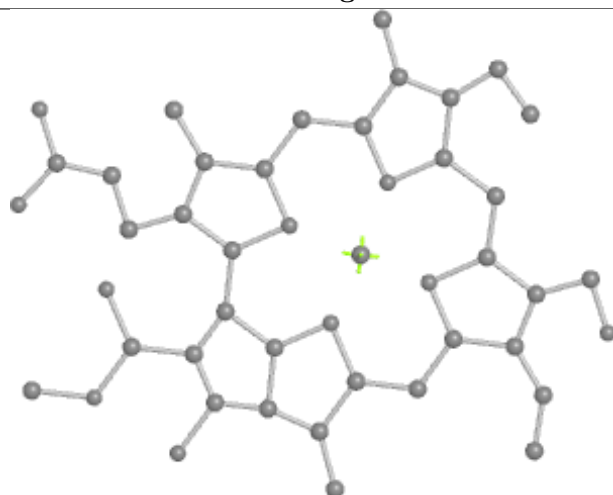
Bond lengths



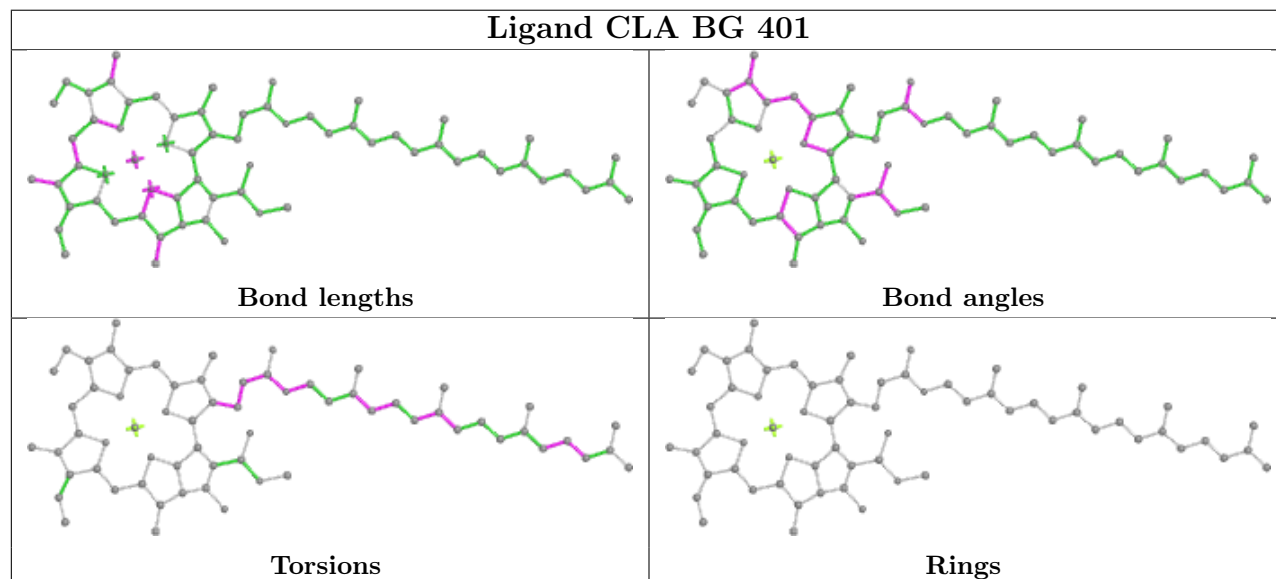
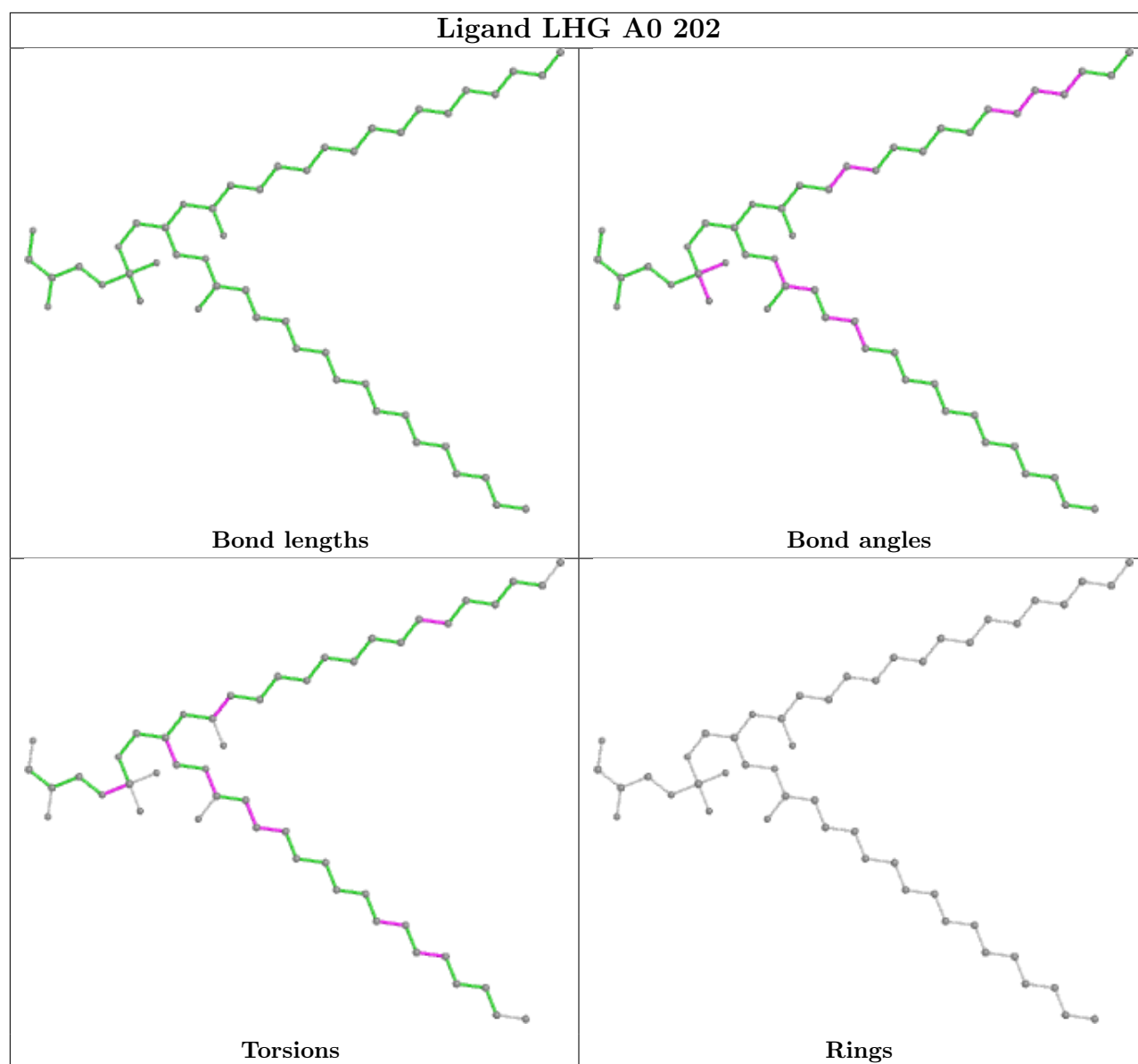
Bond angles



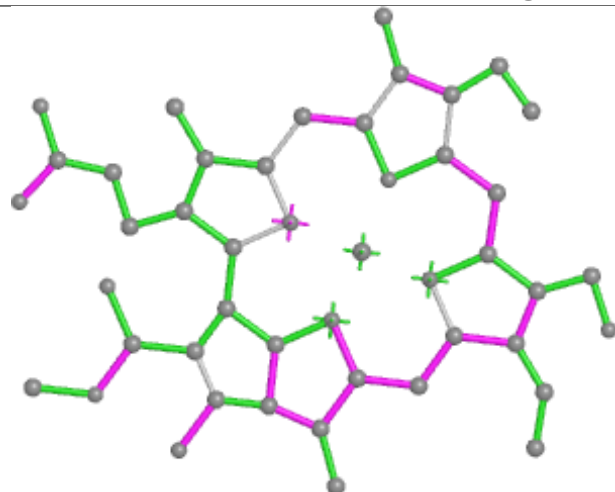
Torsions



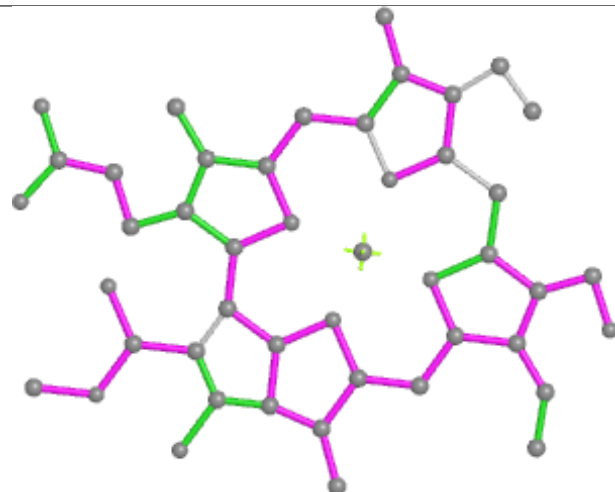
Rings



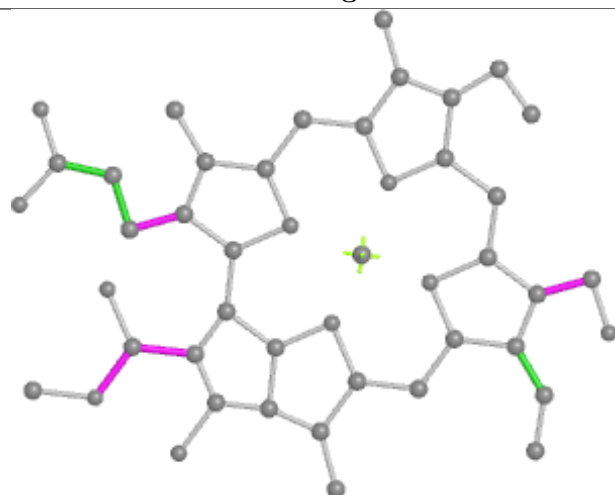
Ligand CHL 8 306



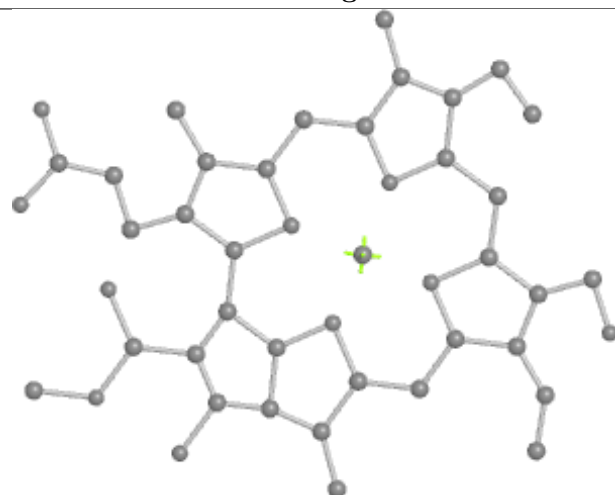
Bond lengths



Bond angles

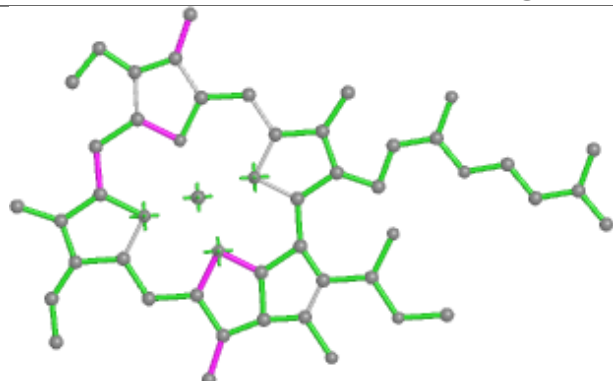


Torsions

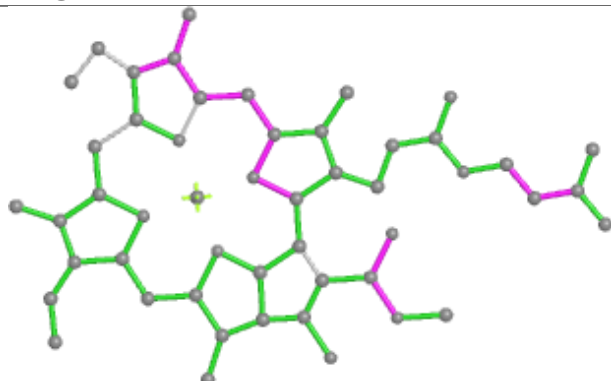


Rings

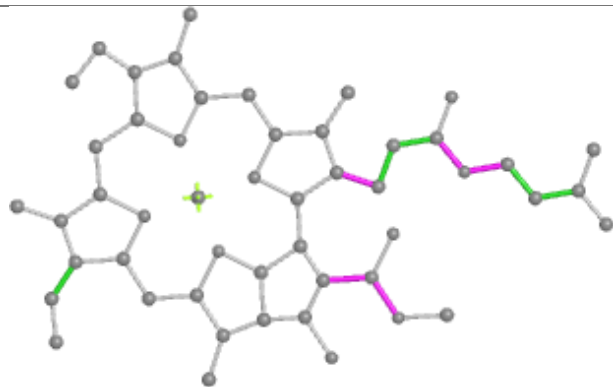
Ligand CLA g 604



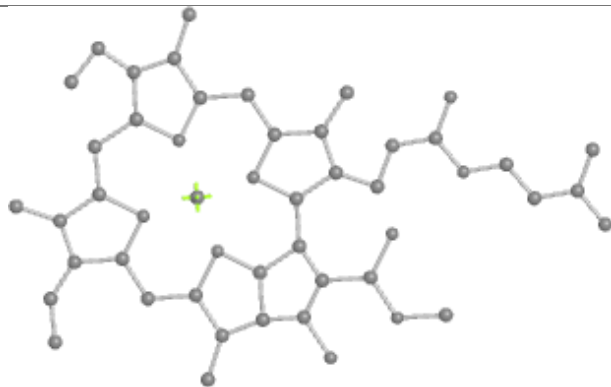
Bond lengths



Bond angles

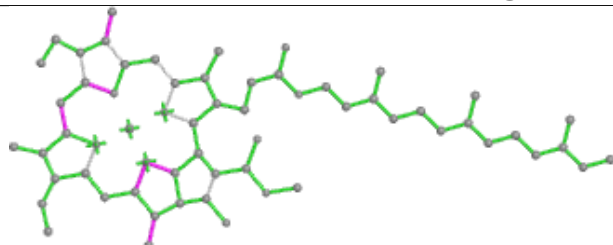


Torsions

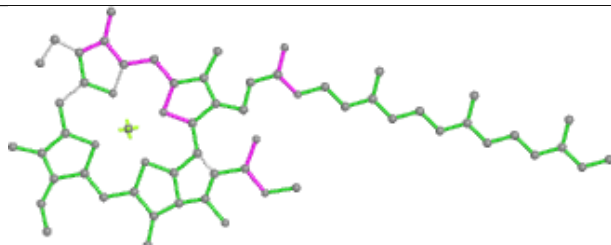


Rings

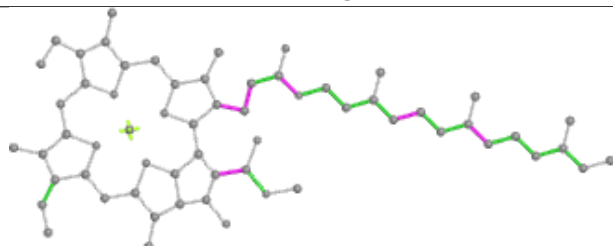
Ligand CLA BV 602



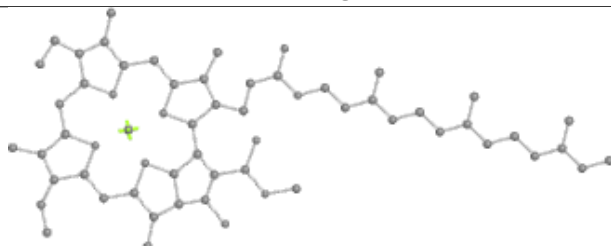
Bond lengths



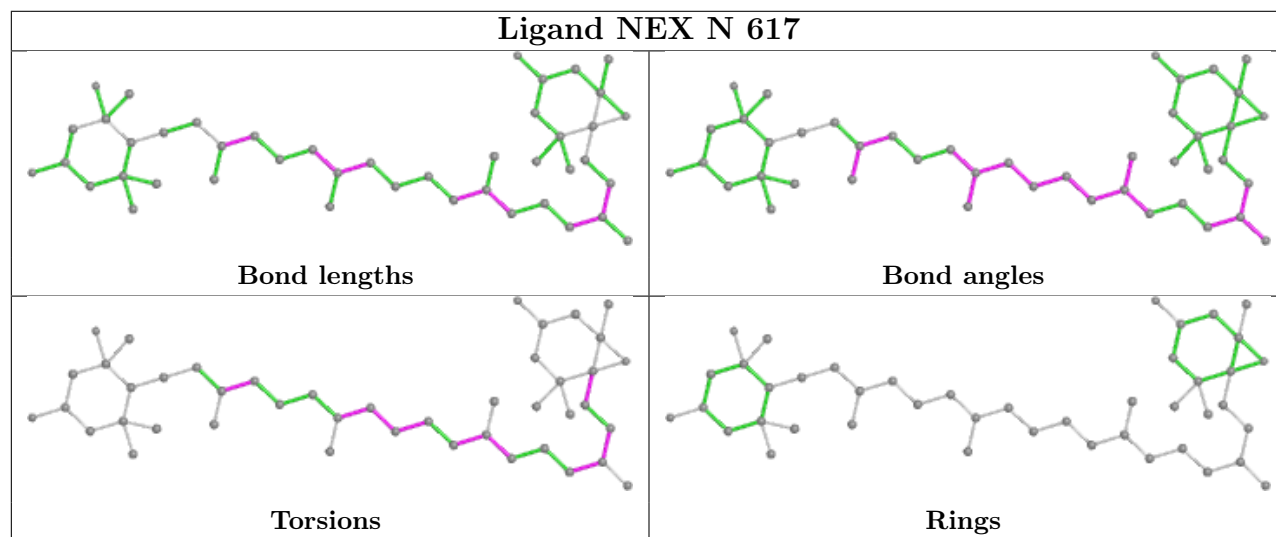
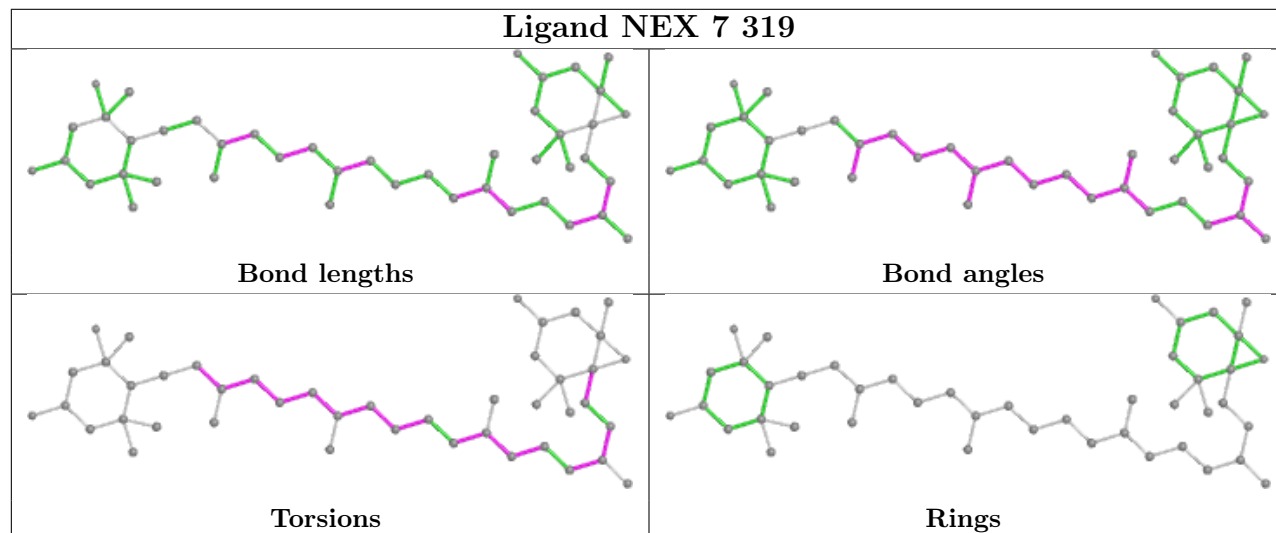
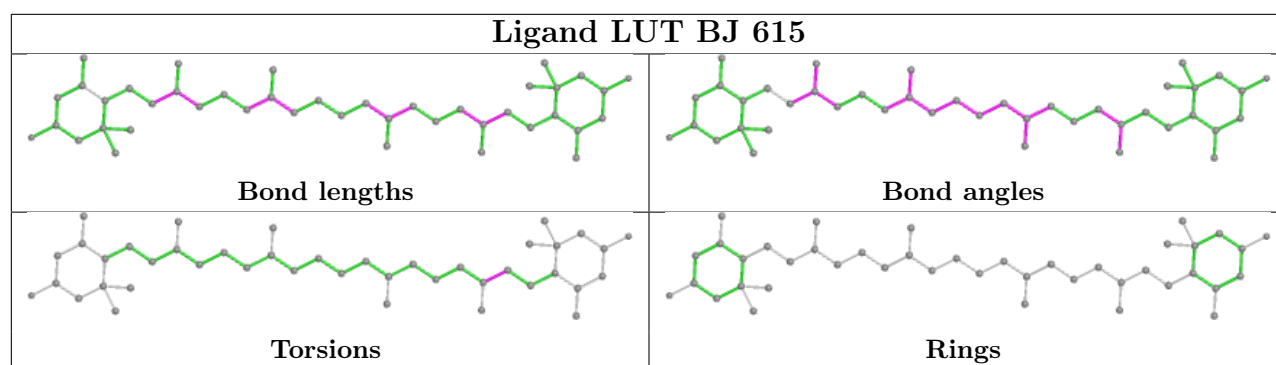
Bond angles

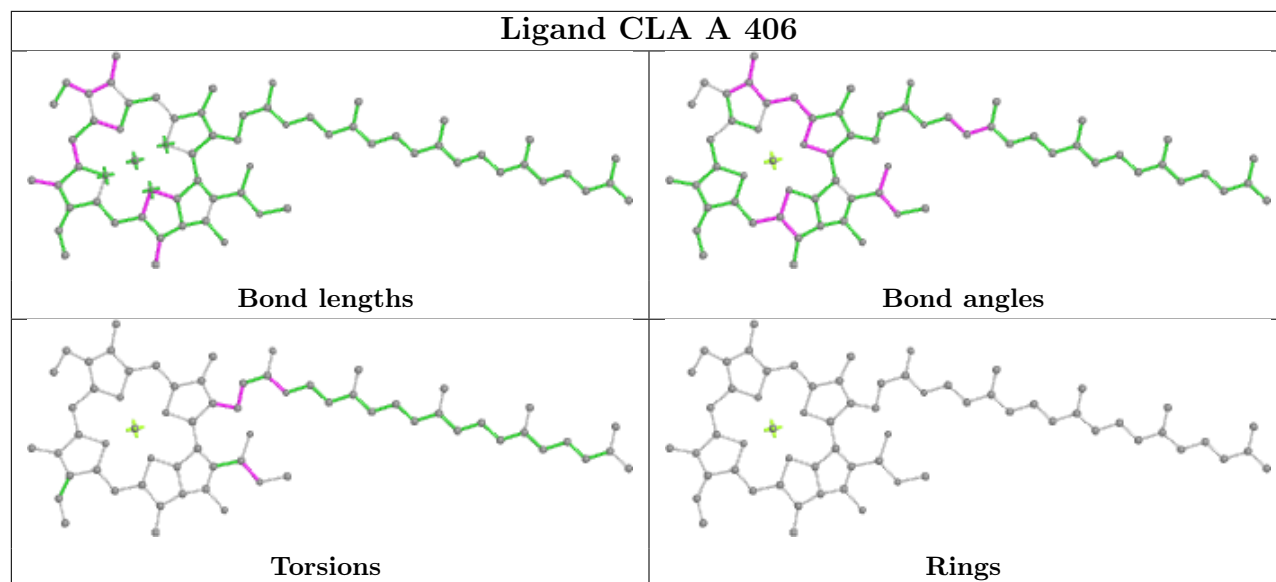
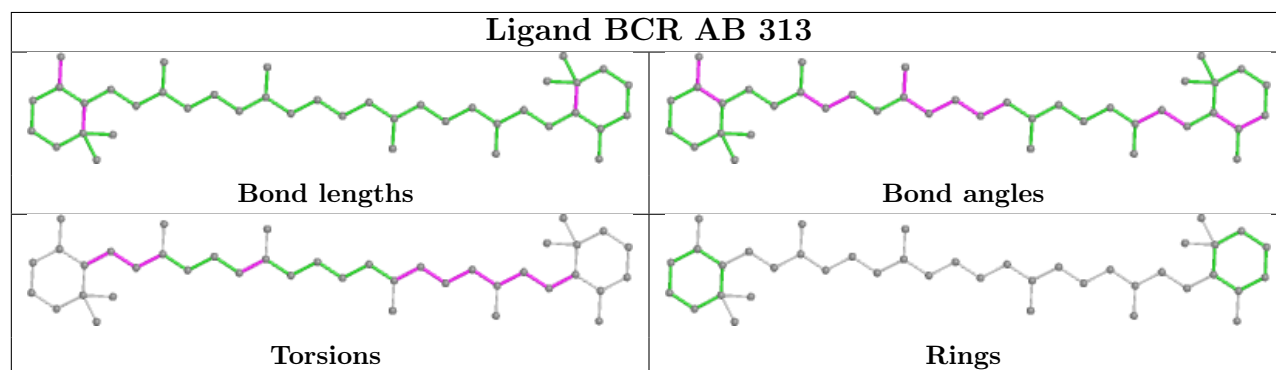
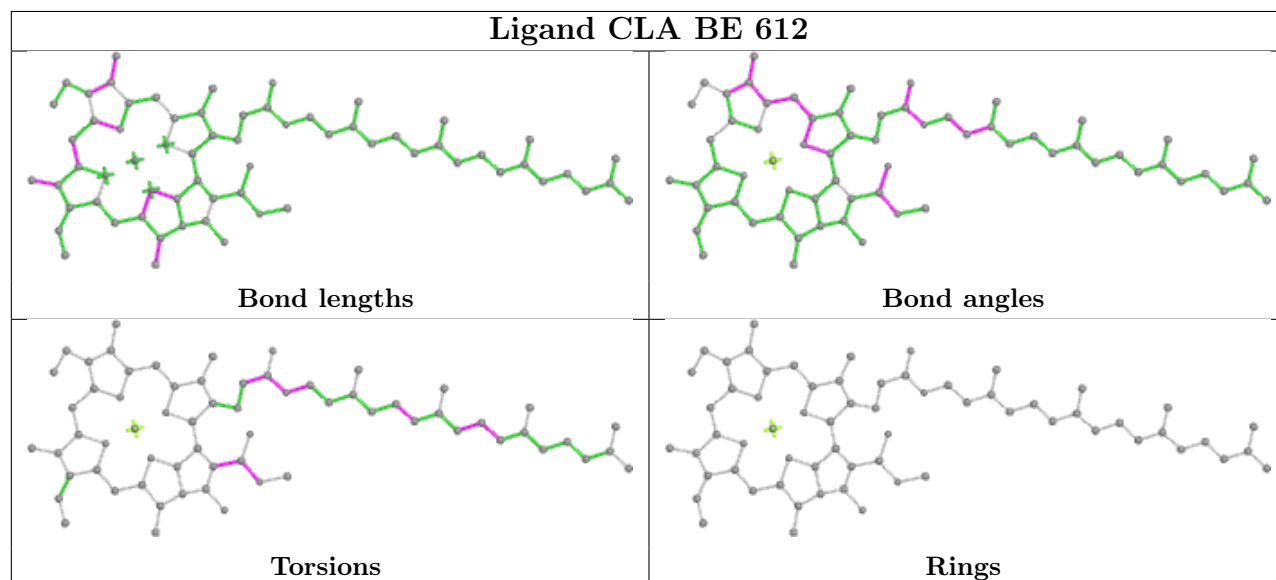


Torsions

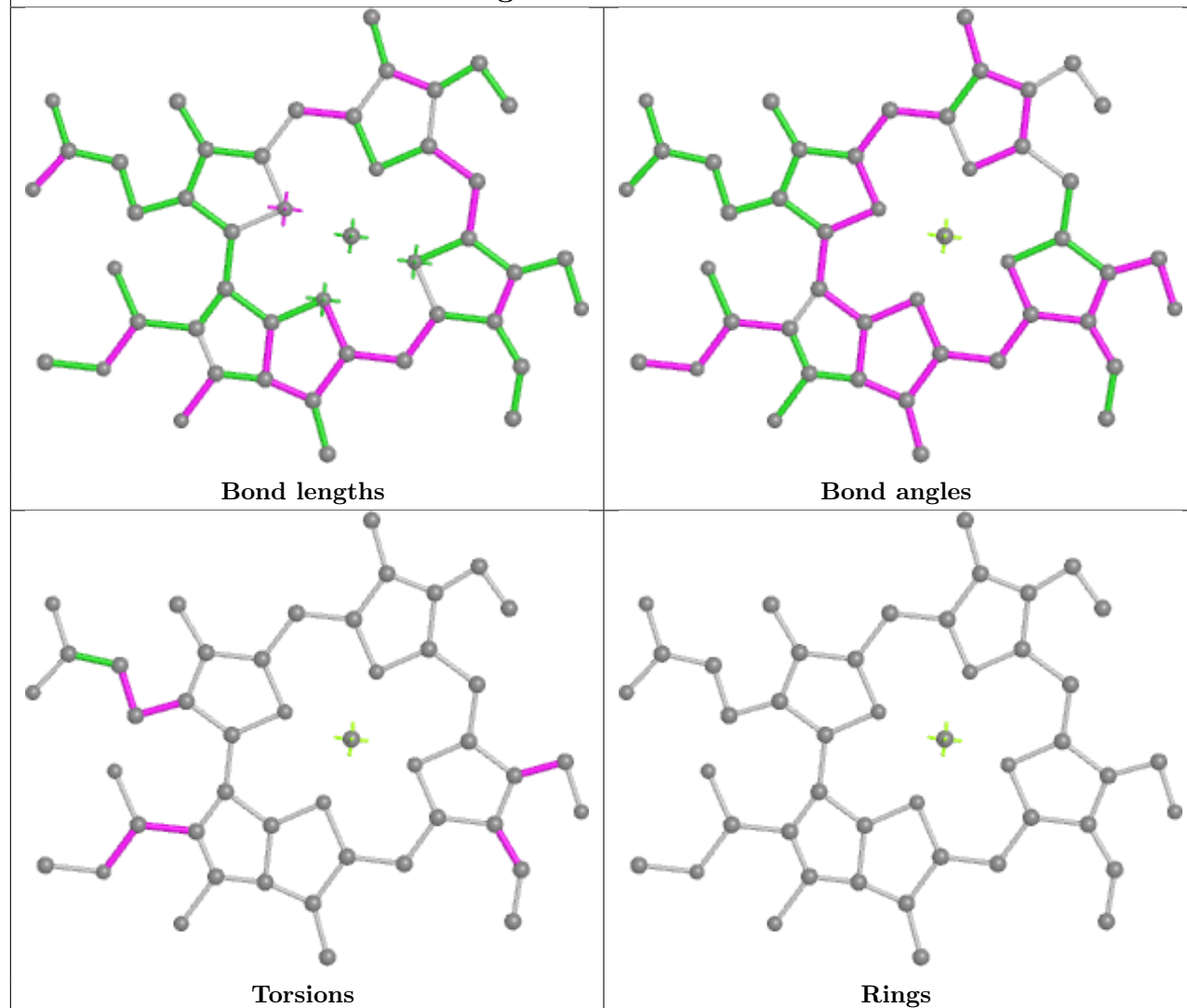


Rings

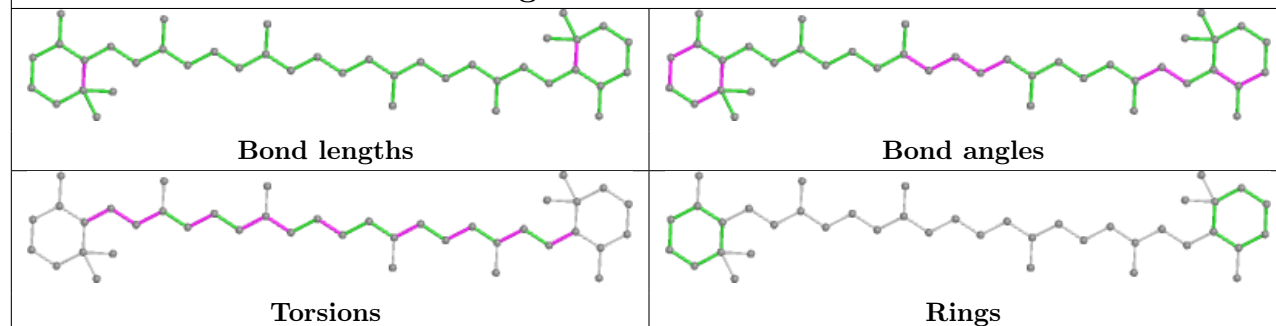


Ligand CLA A 406**Ligand BCR AB 313****Ligand CLA BE 612**

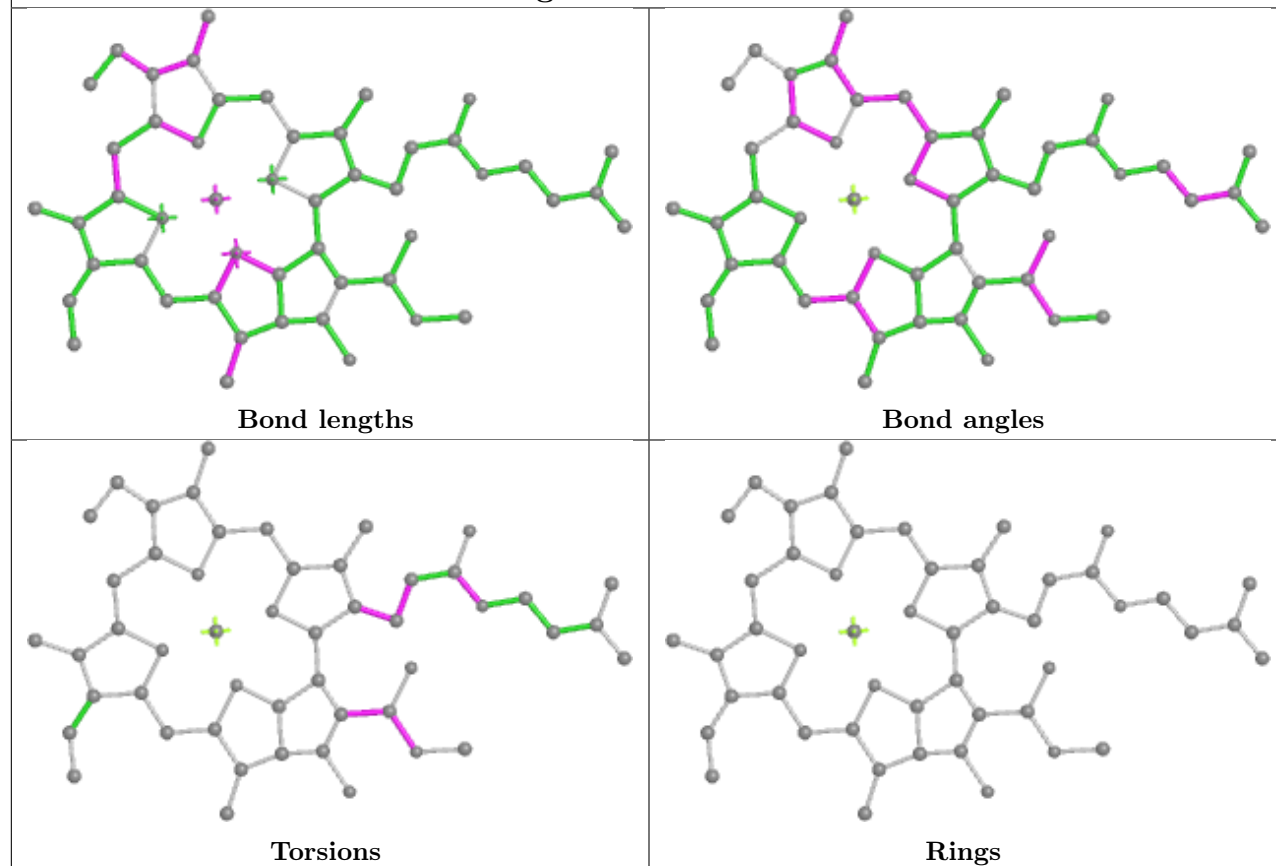
Ligand CHL S 607



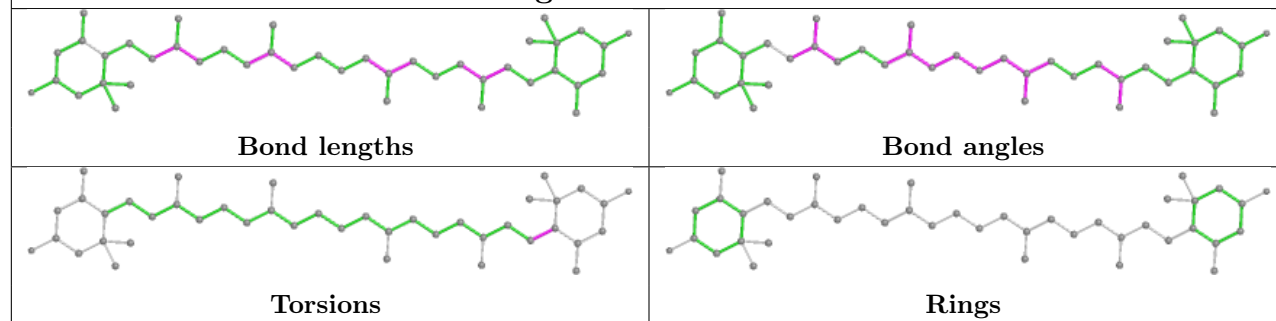
Ligand BCR BE 601



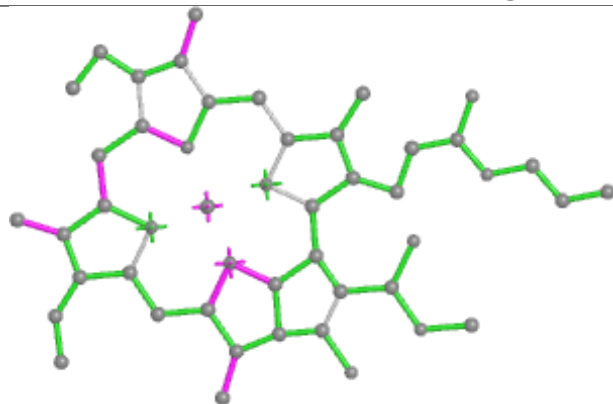
Ligand CLA 5 604



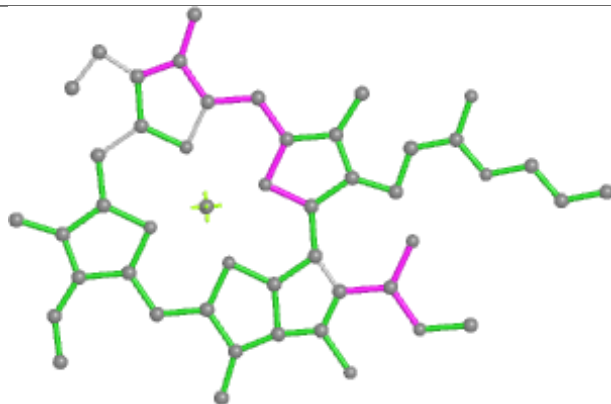
Ligand LUT n 615



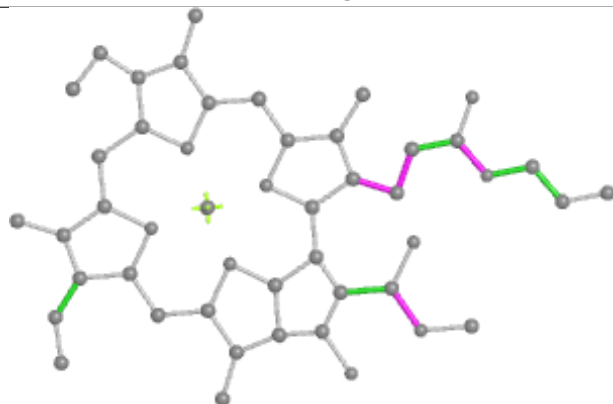
Ligand CLA BB 315



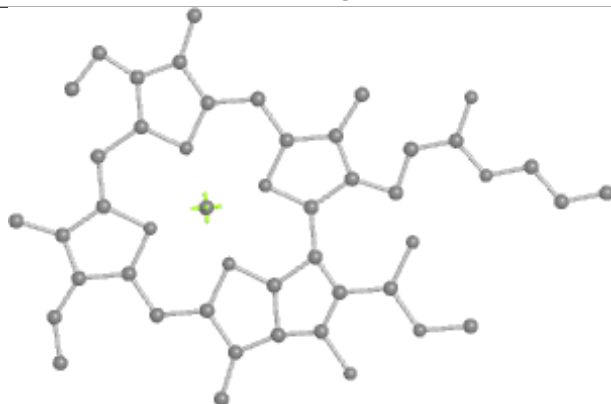
Bond lengths



Bond angles

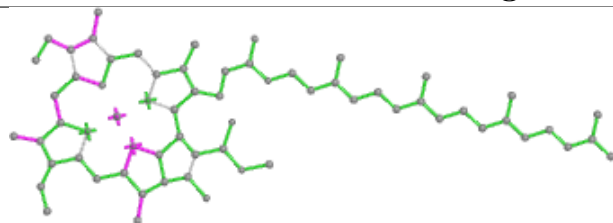


Torsions

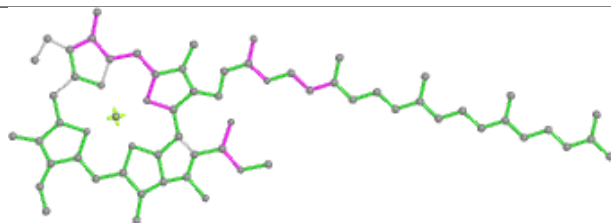


Rings

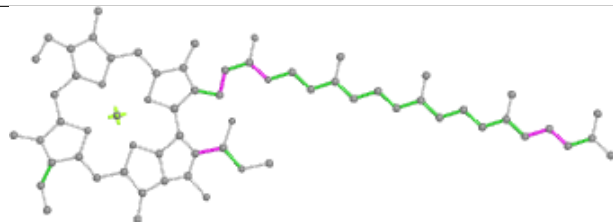
Ligand CLA BD 405



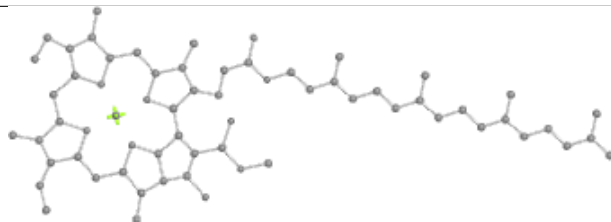
Bond lengths



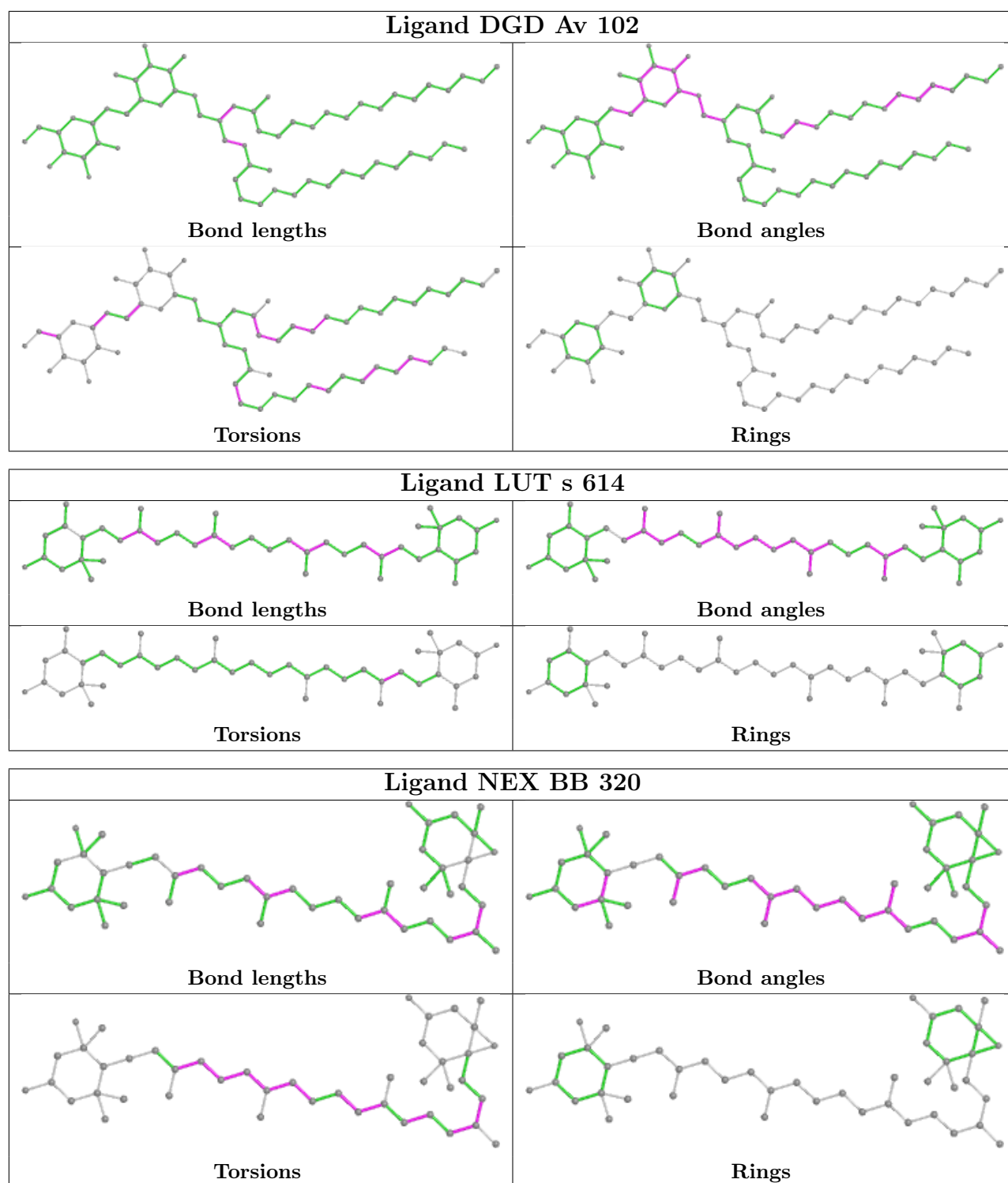
Bond angles



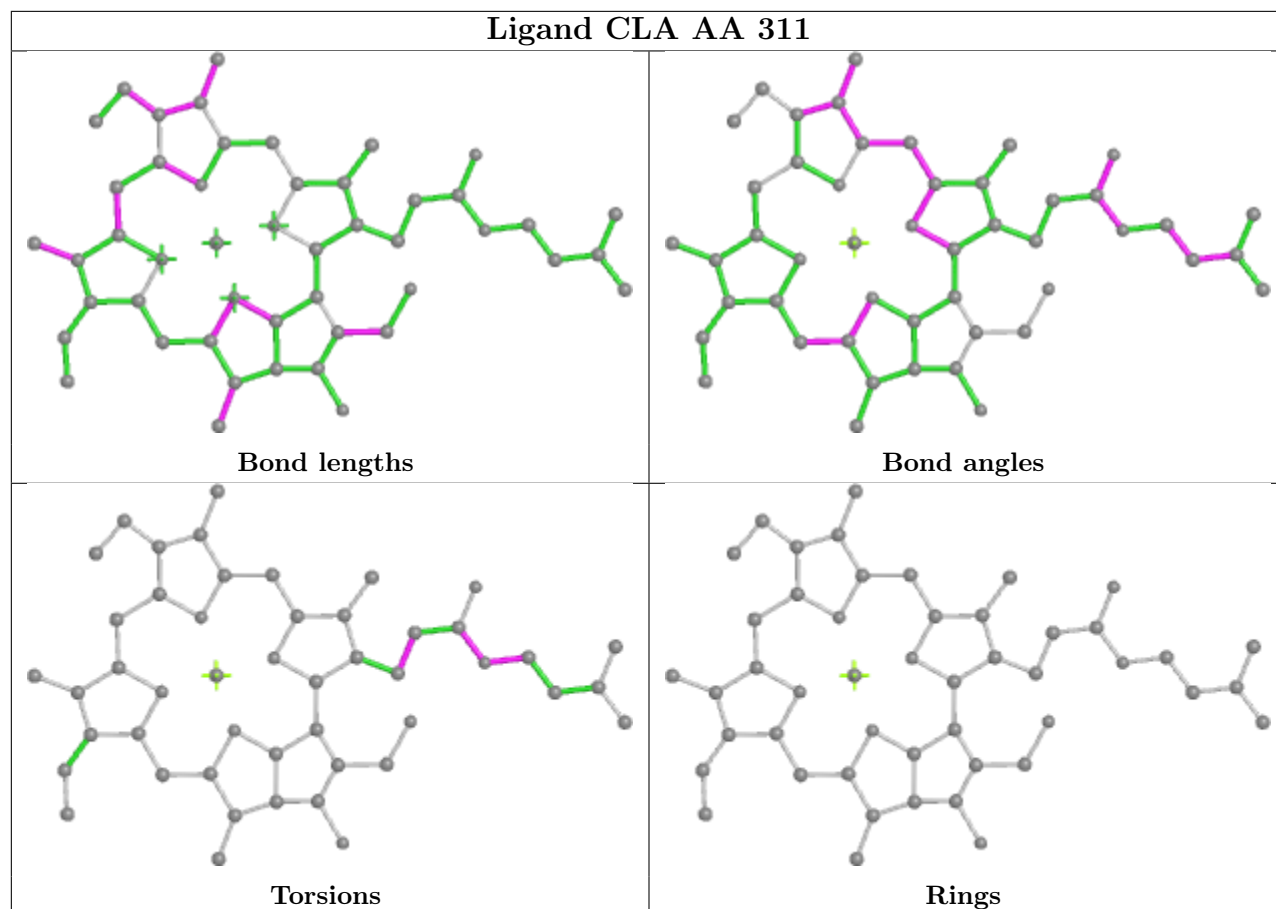
Torsions



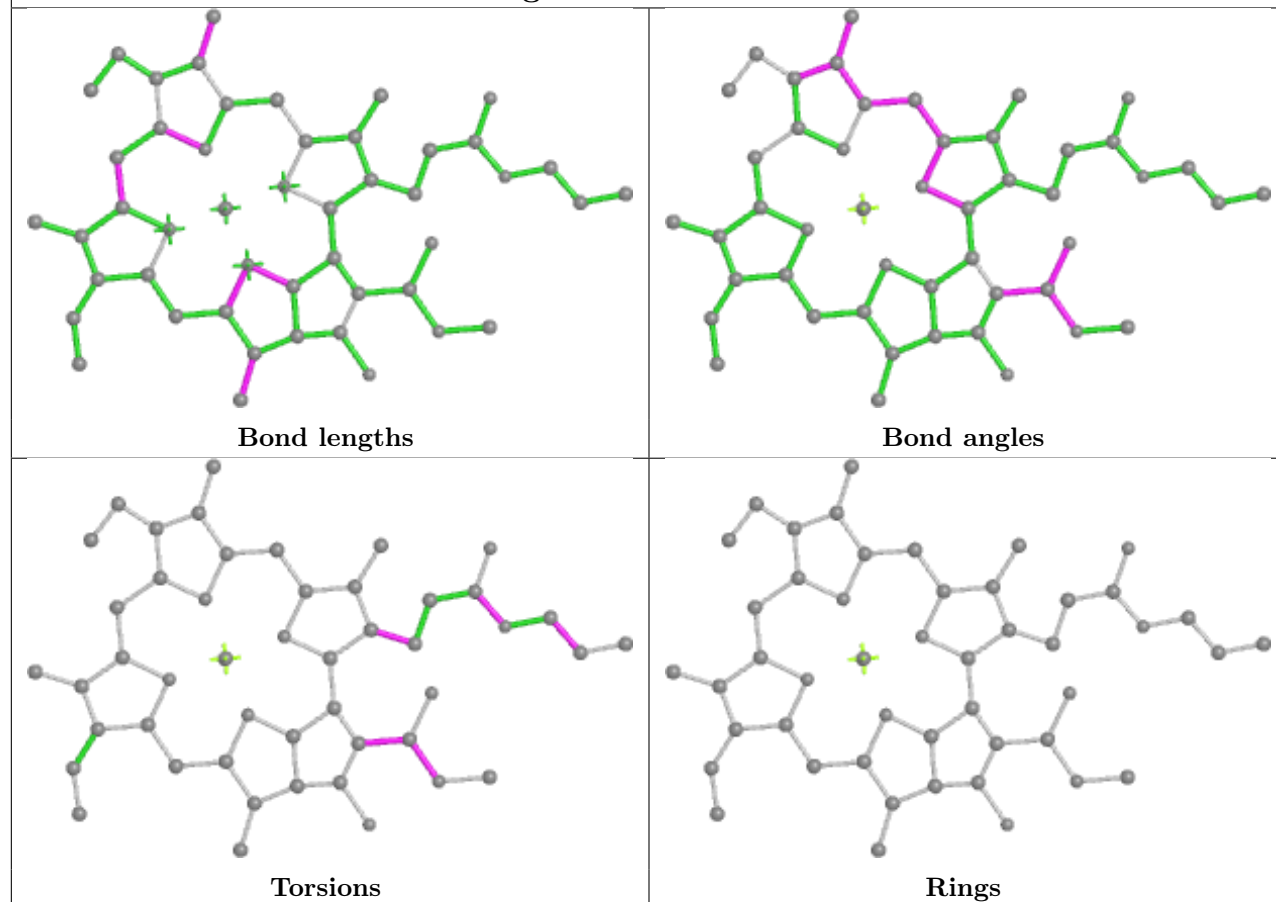
Rings



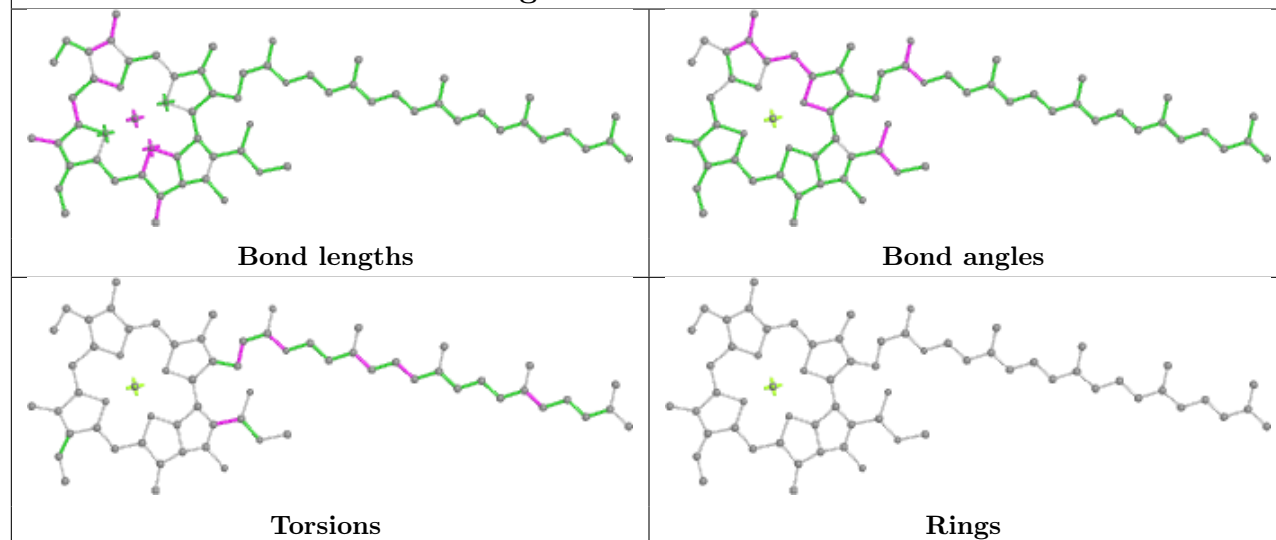
Ligand CLA AA 311

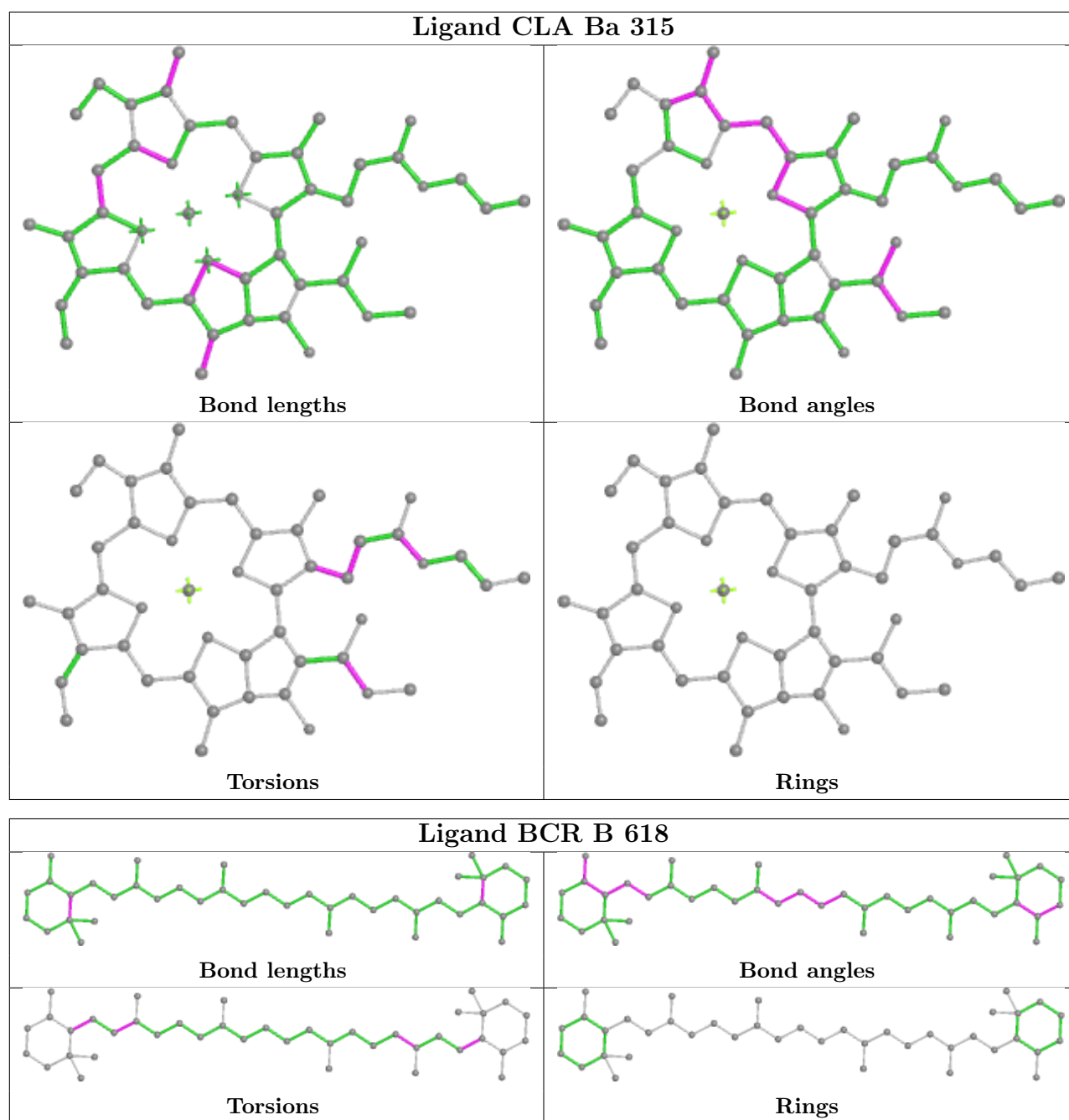


Ligand CLA A2 614

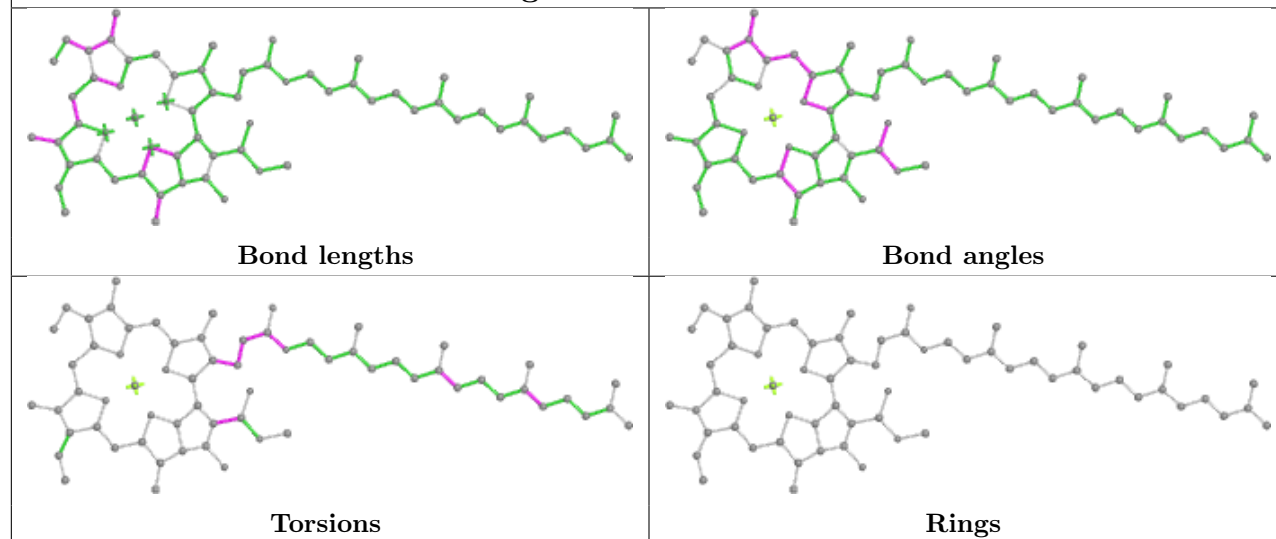


Ligand CLA BB 304

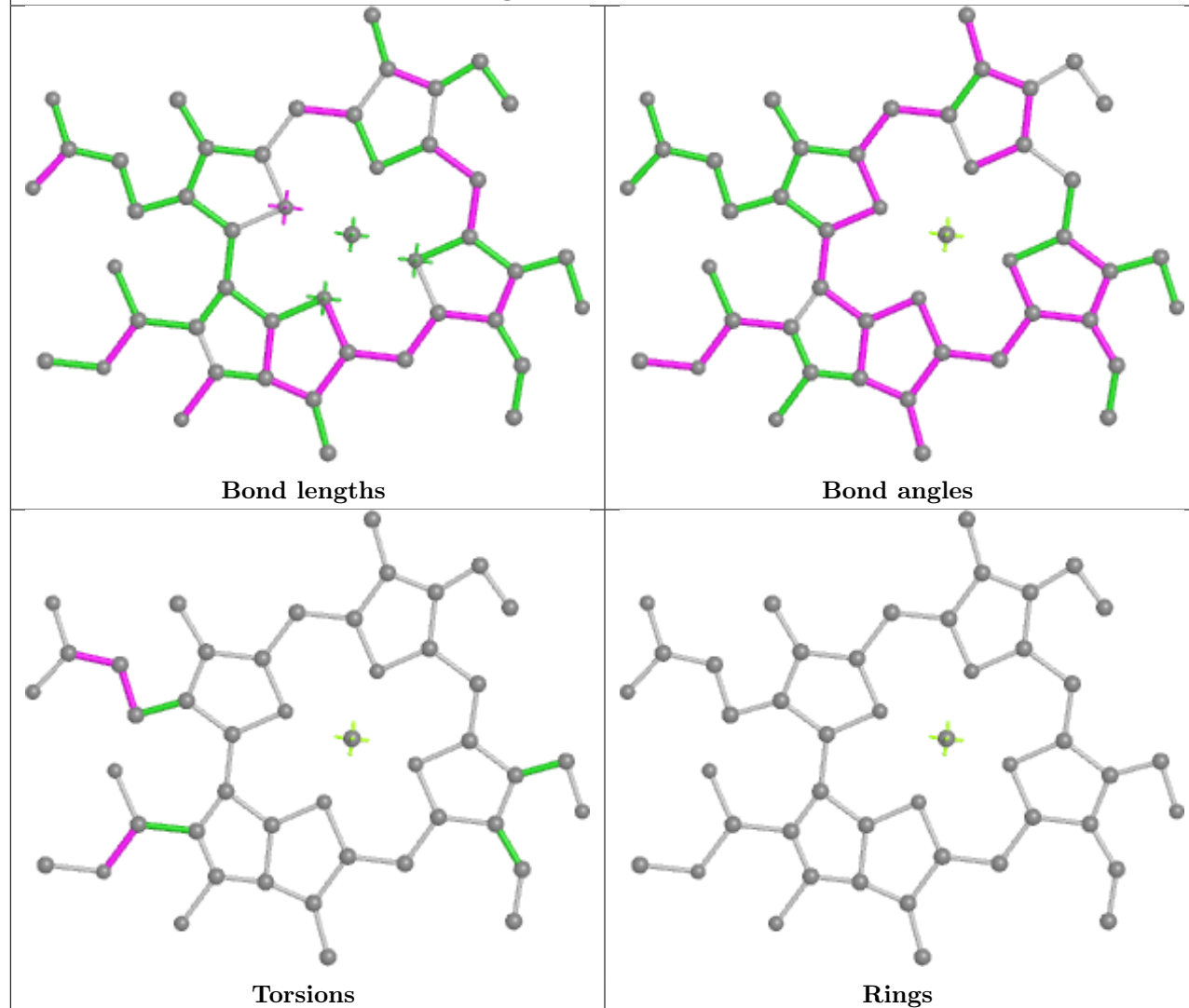




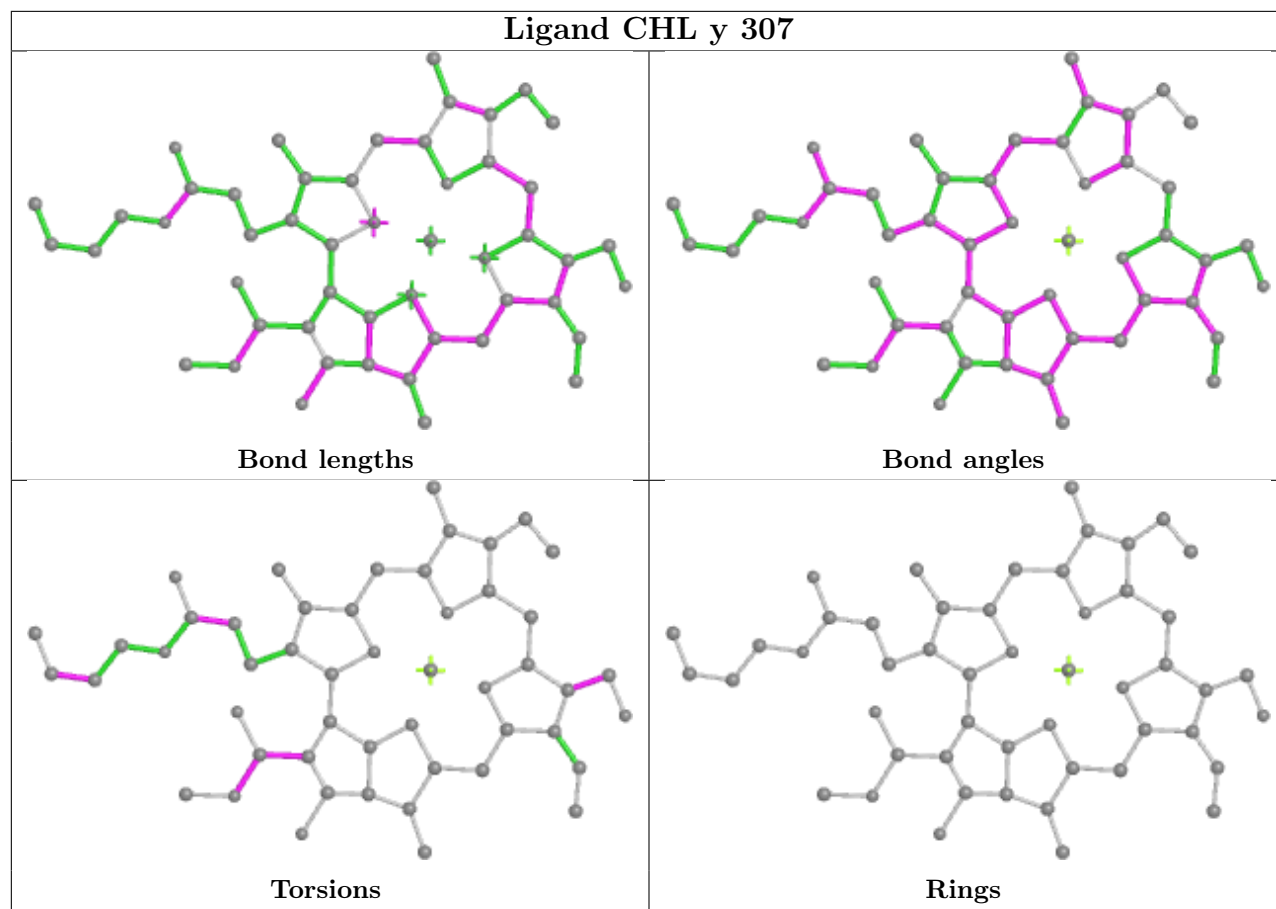
Ligand CLA BF 502



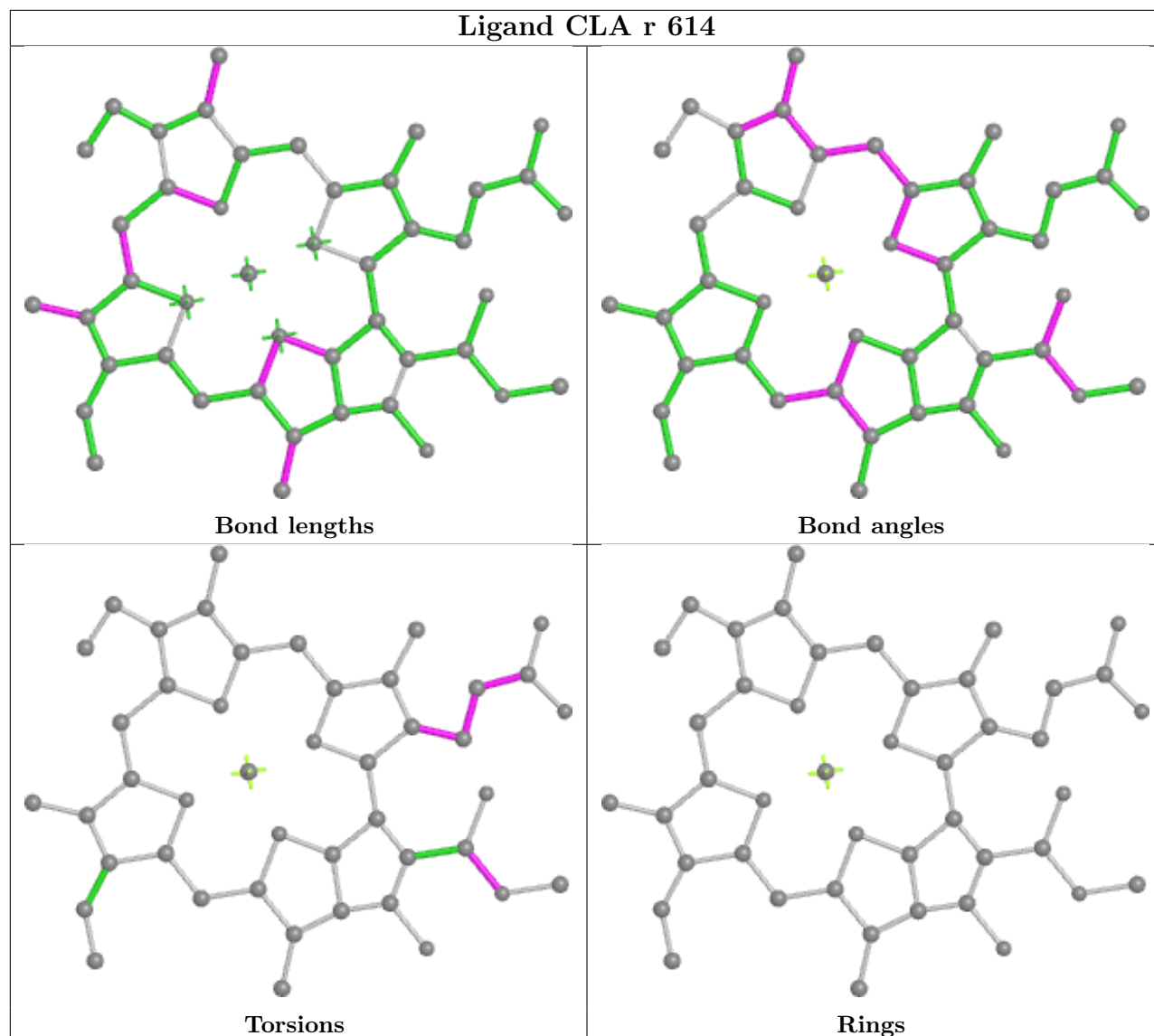
Ligand CHL 6 605

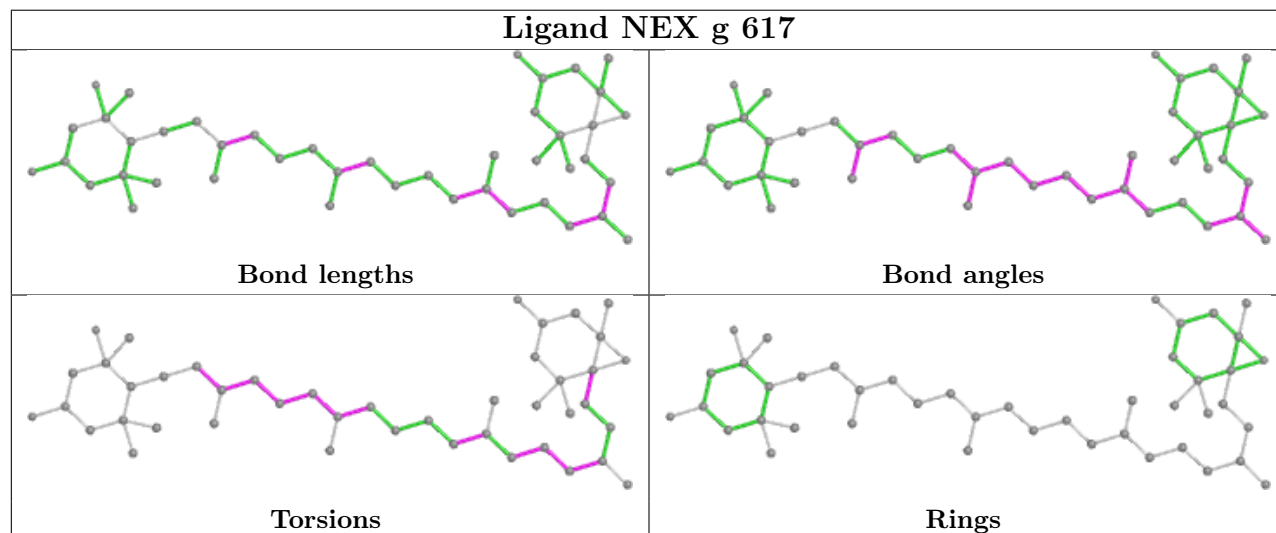
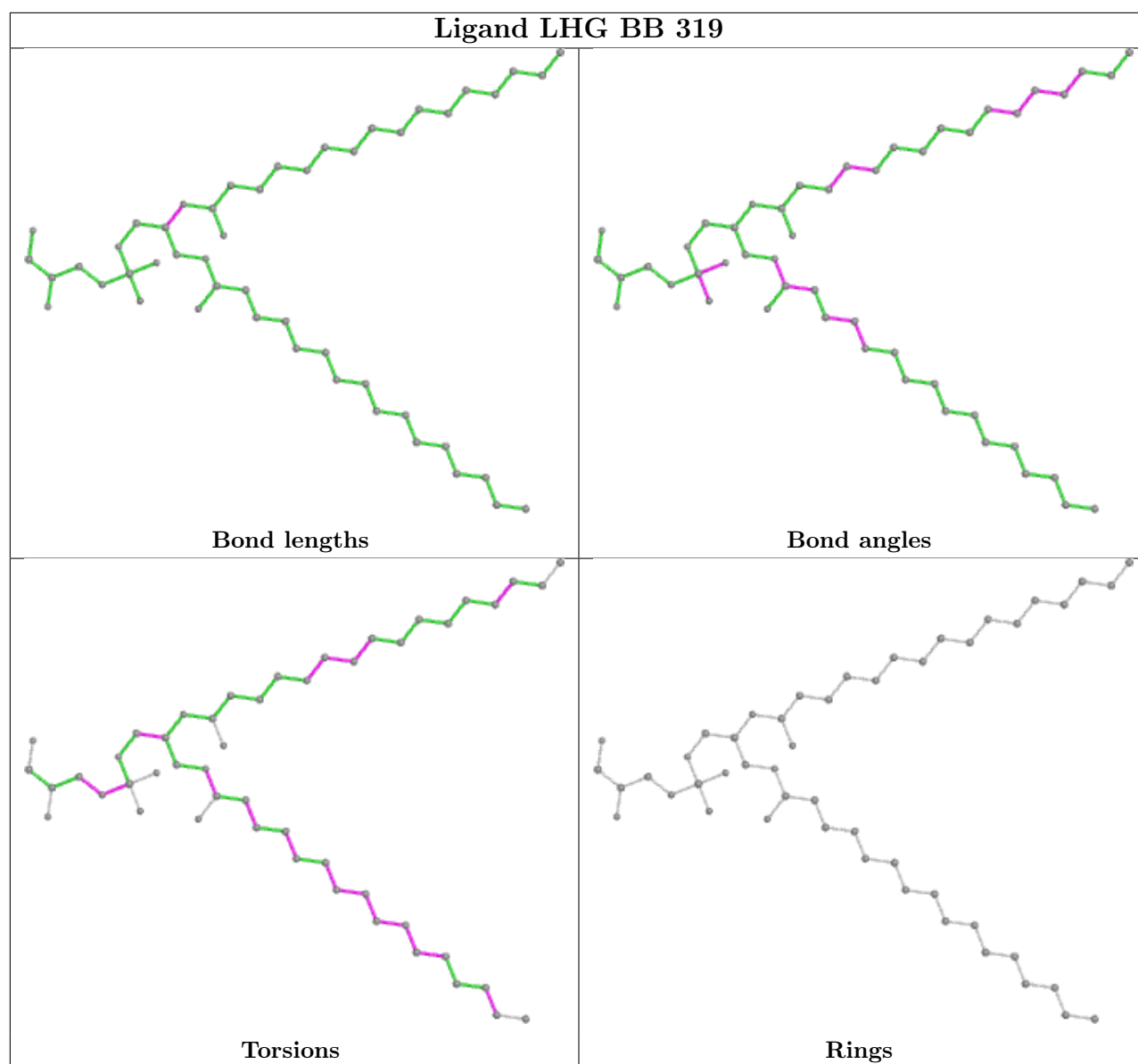


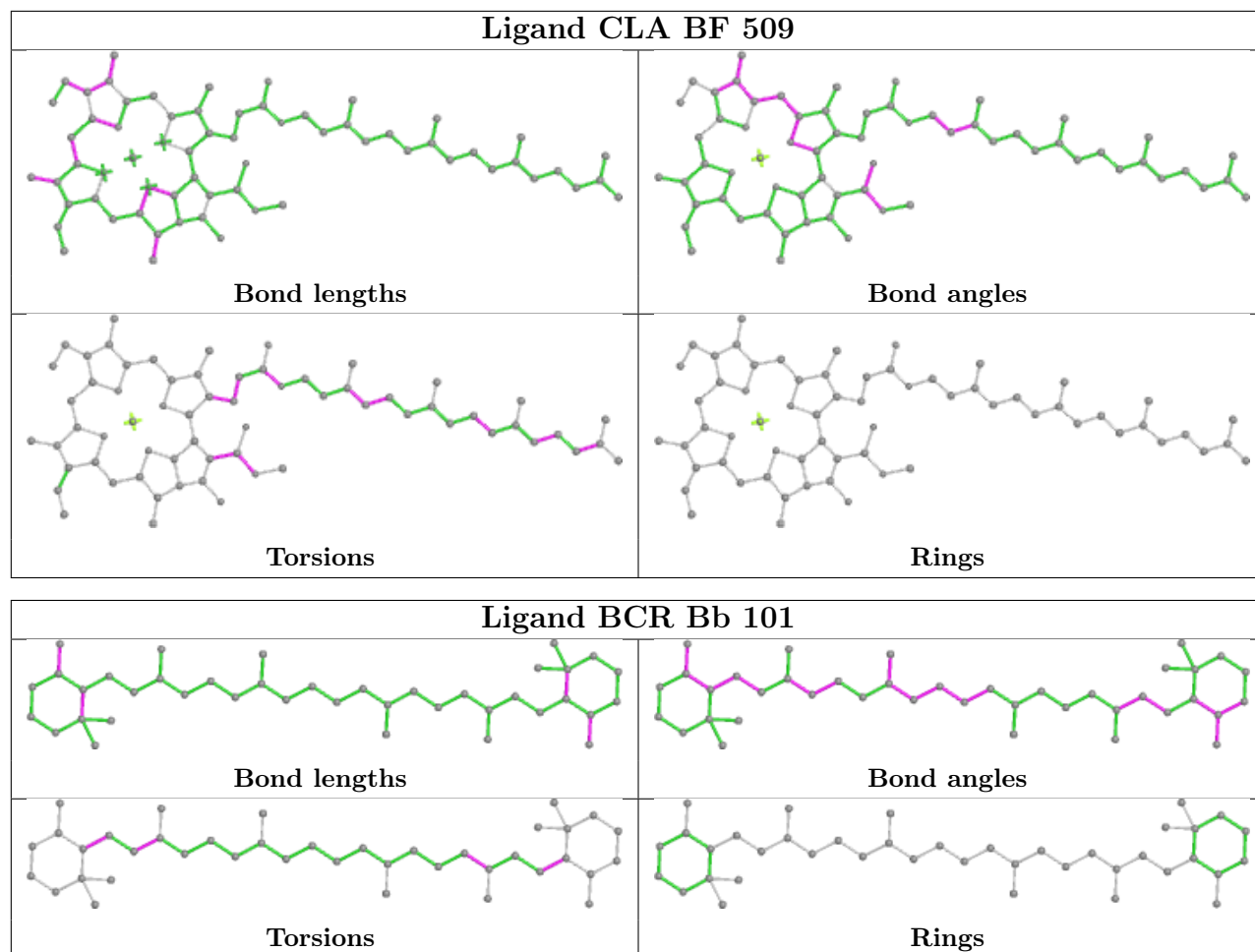
Ligand CHL y 307



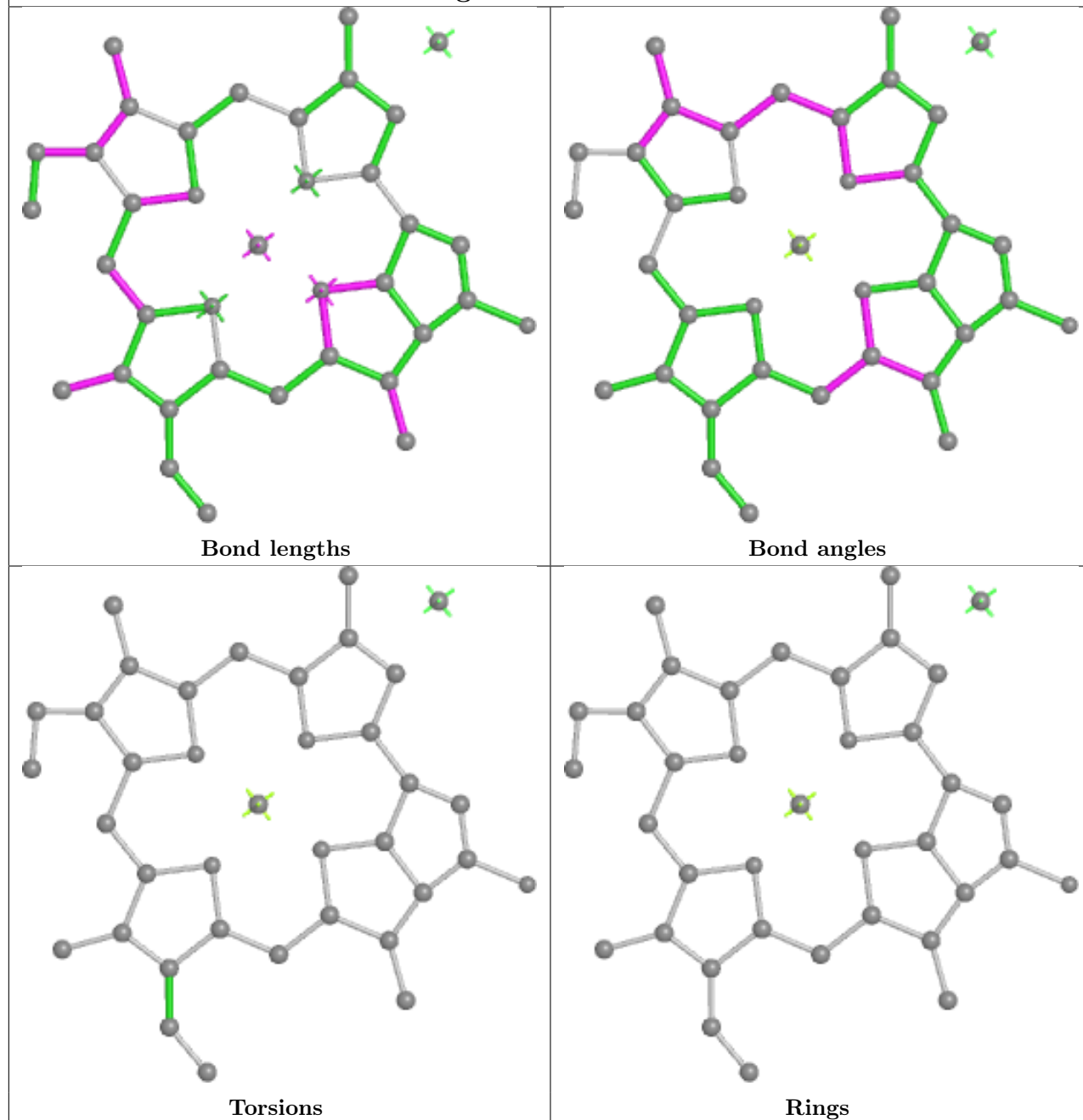
Ligand CLA r 614



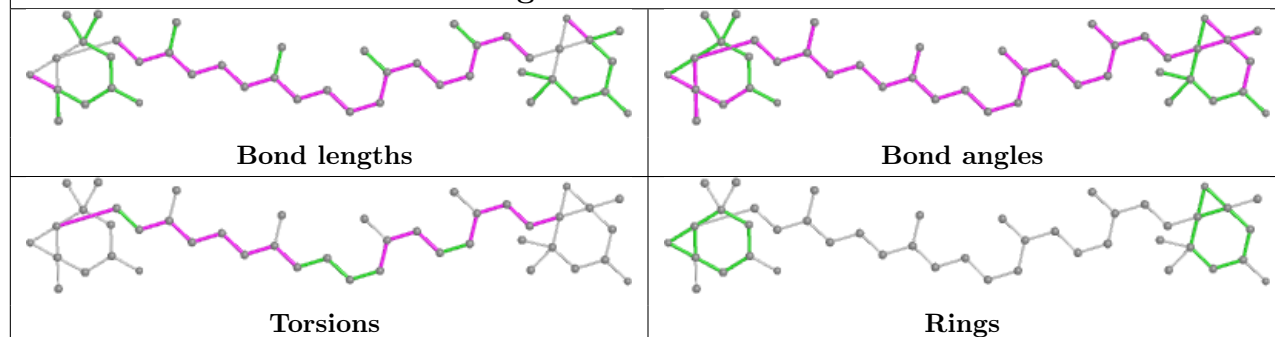




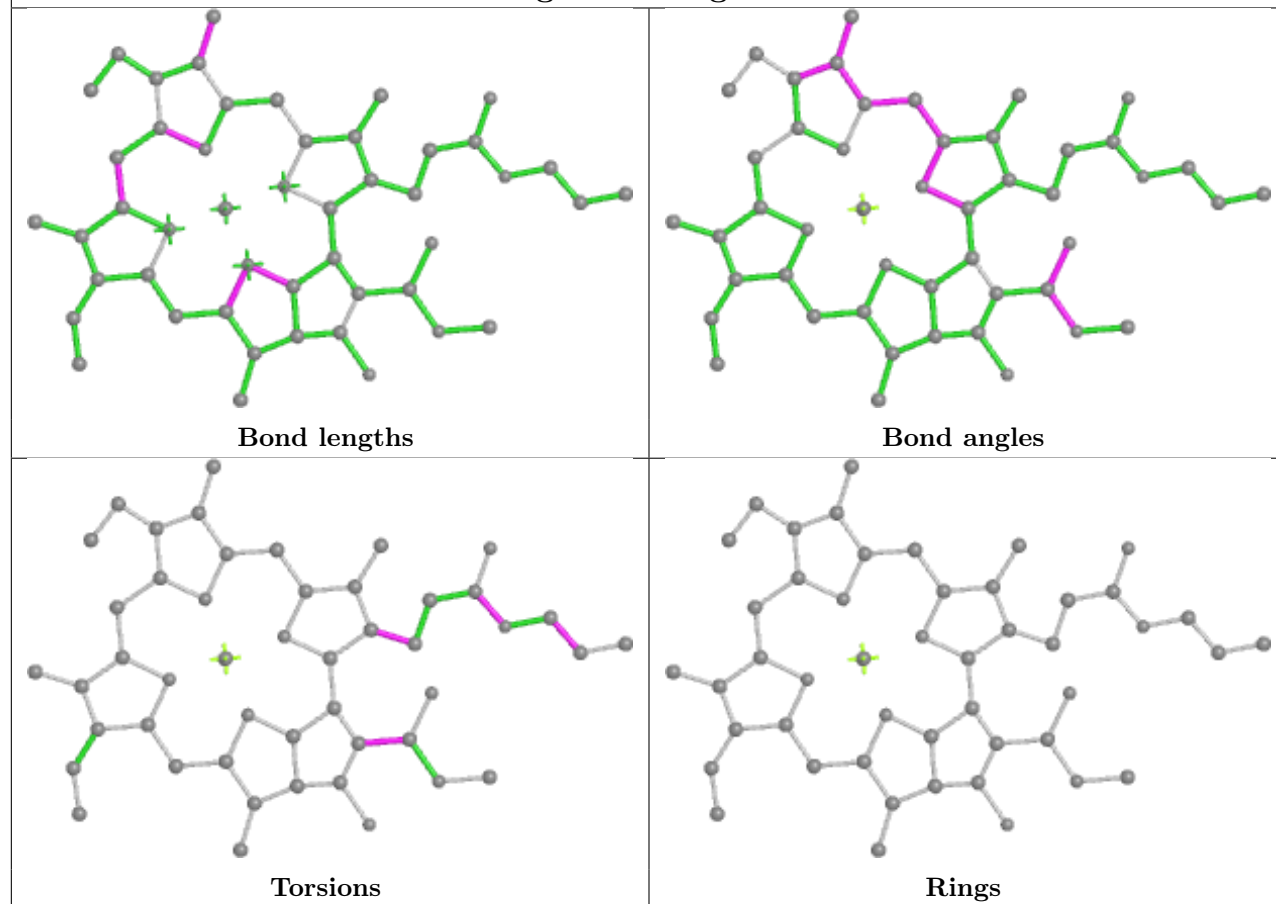
Ligand CLA r 612



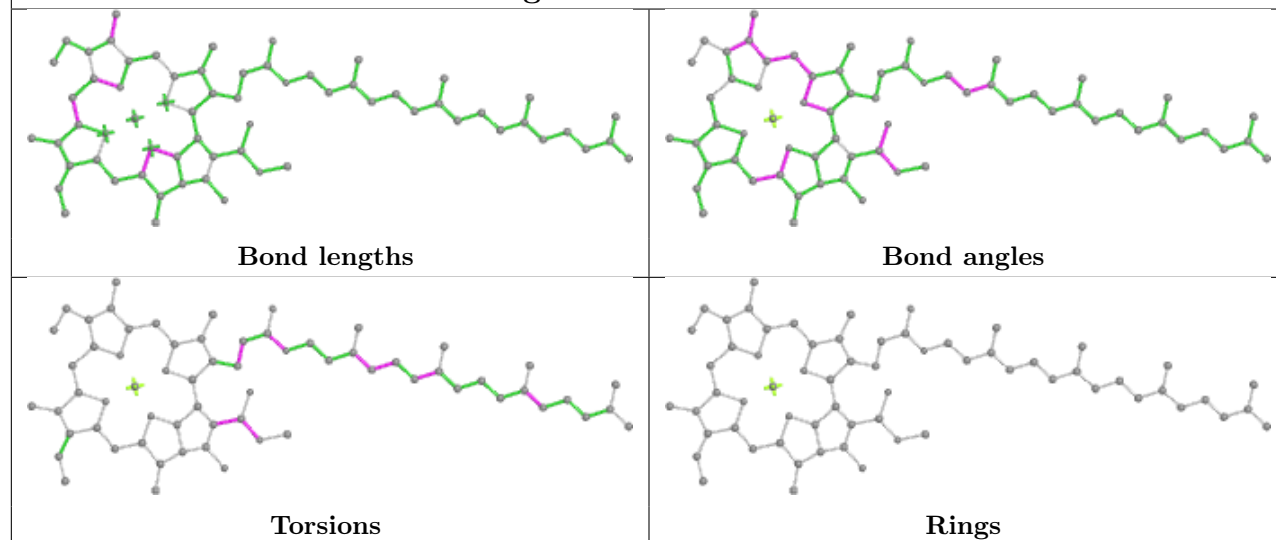
Ligand XAT AB 312

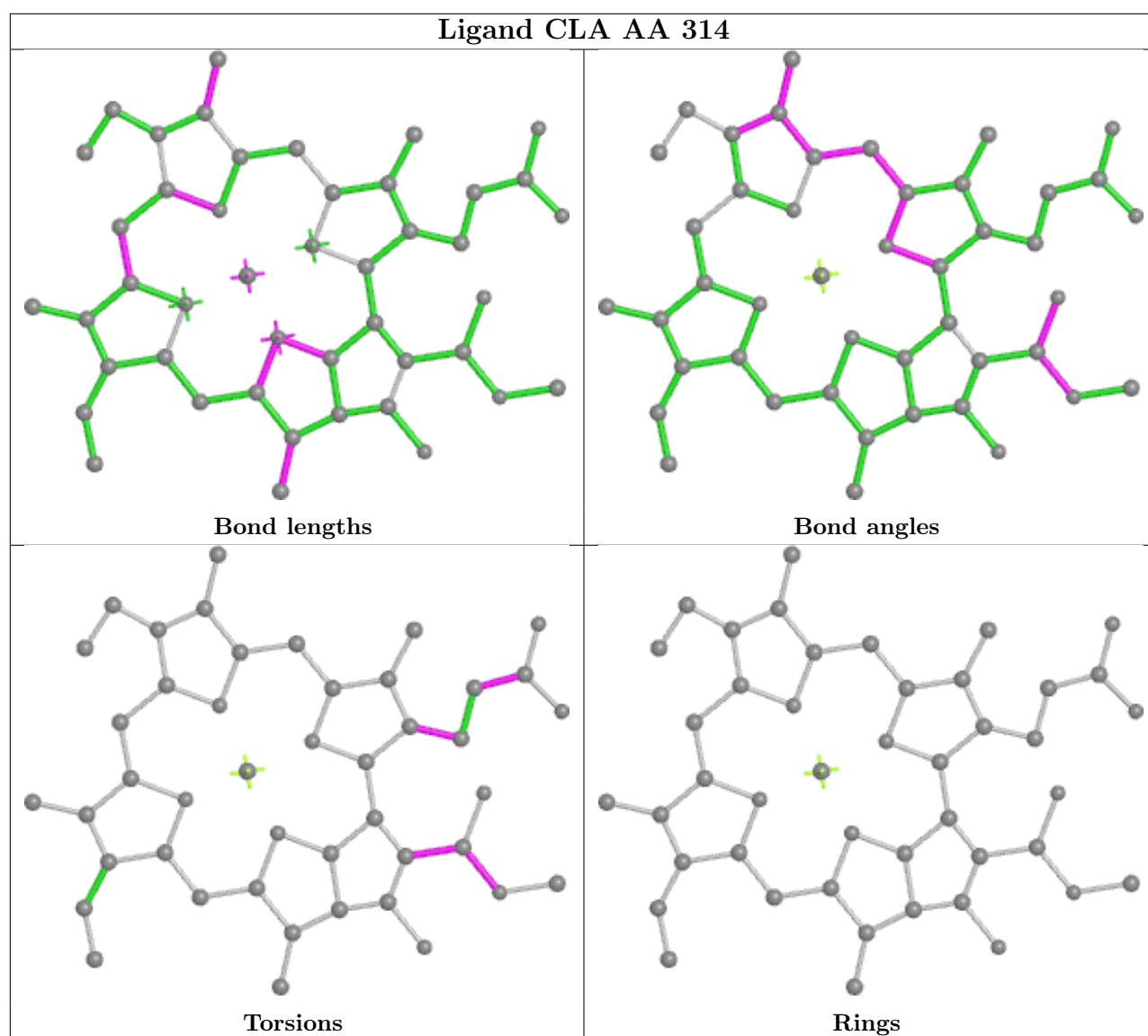
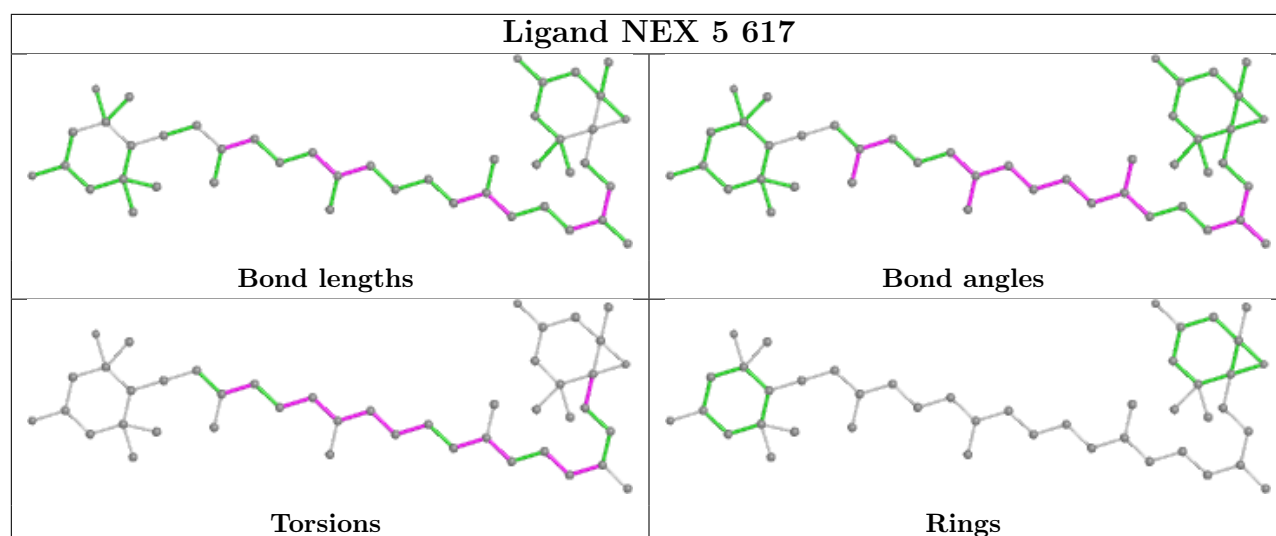


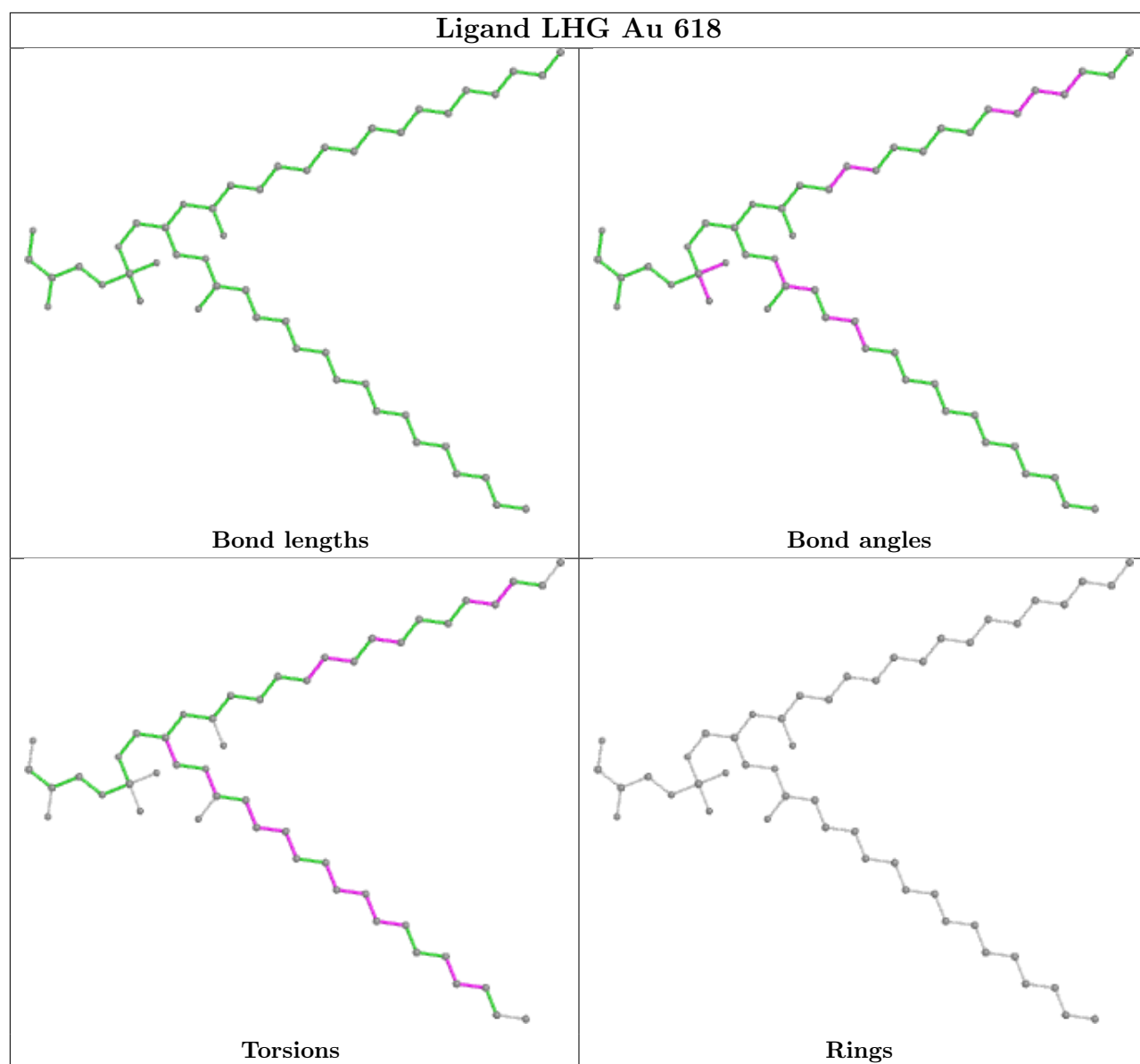
Ligand CLA g 614

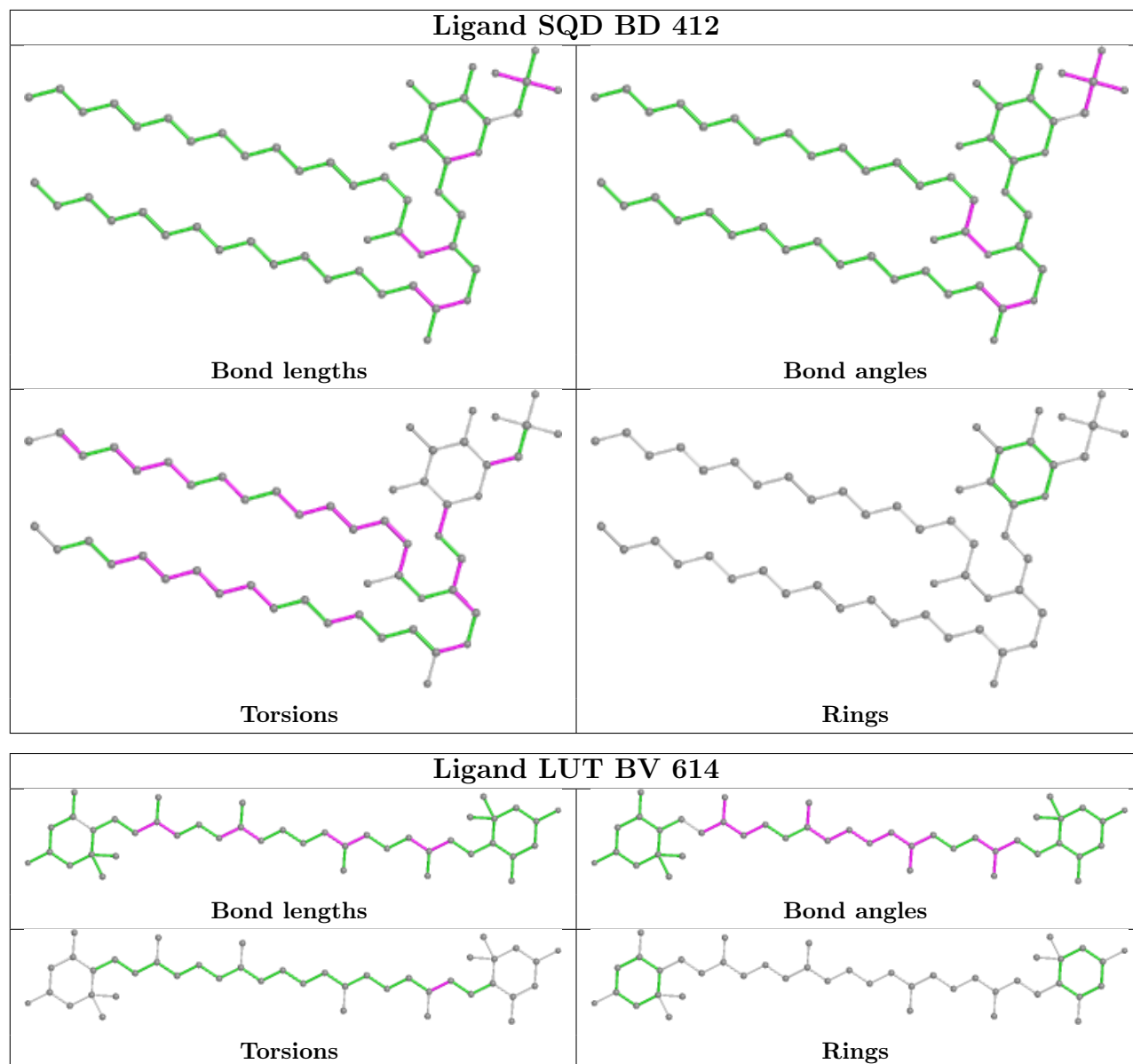


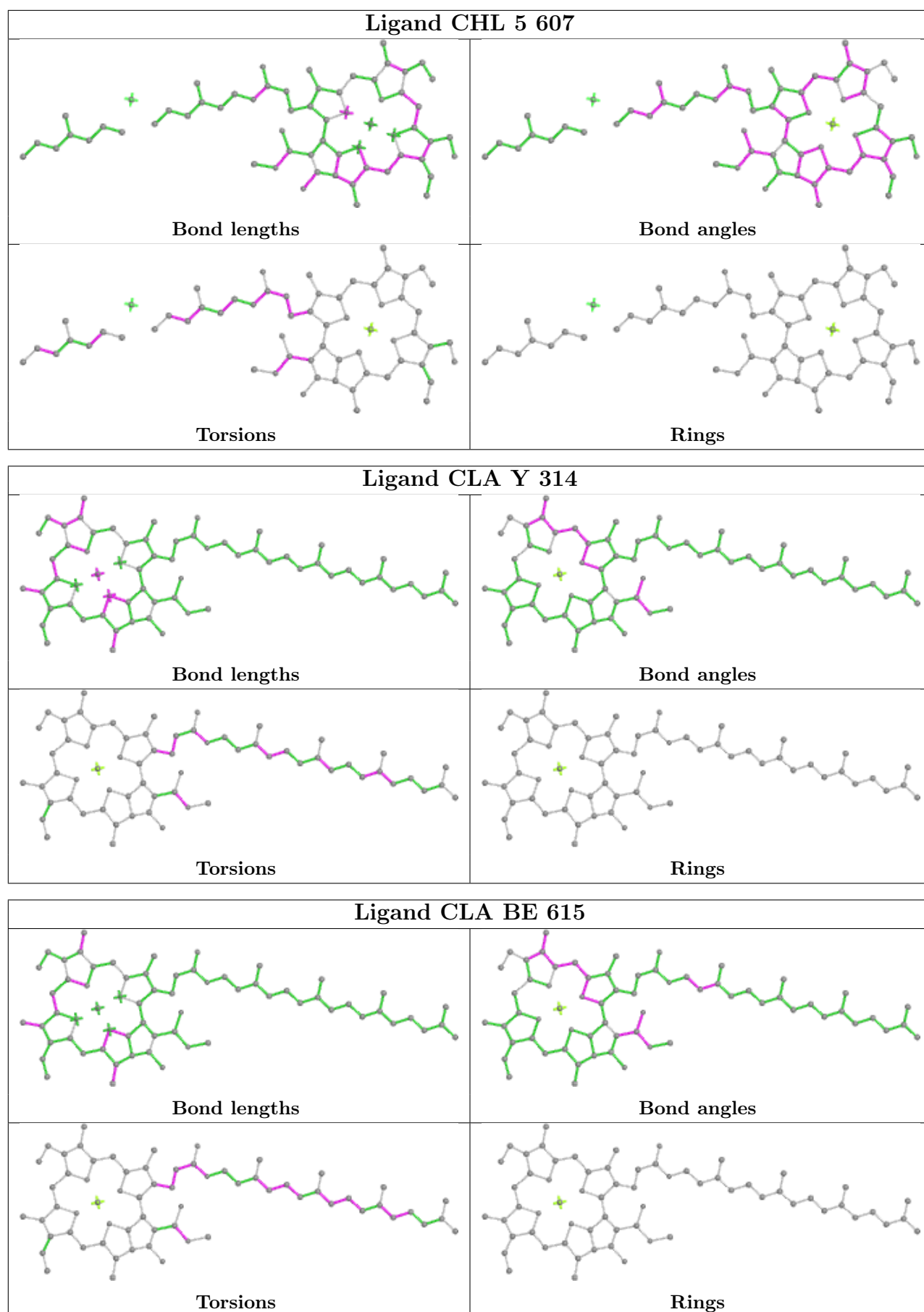
Ligand CLA BJ 613



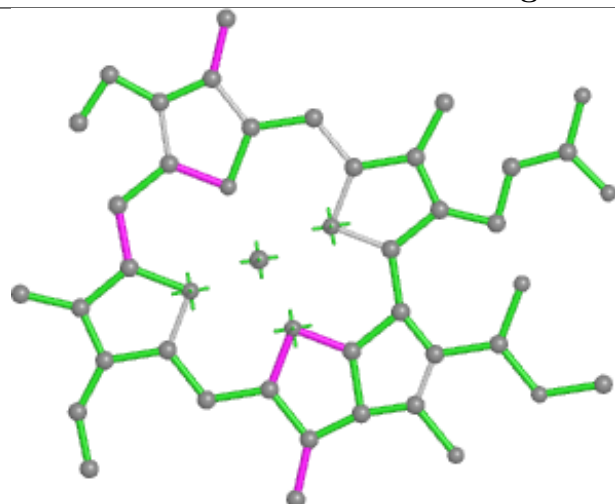




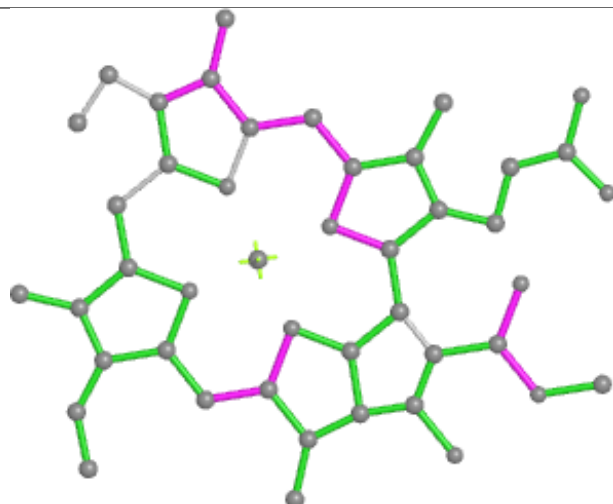




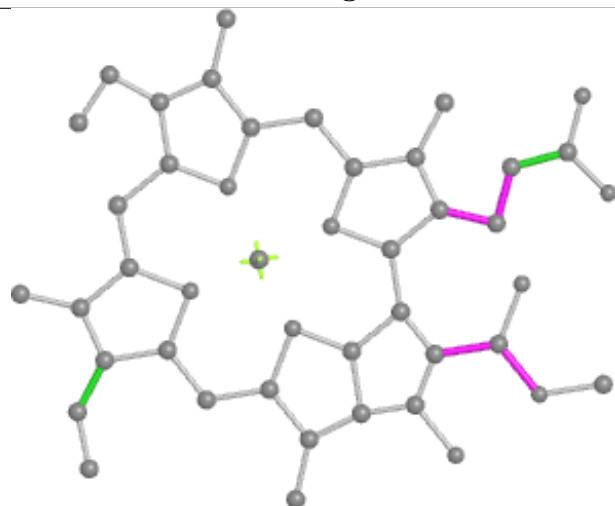
Ligand CLA 7 305



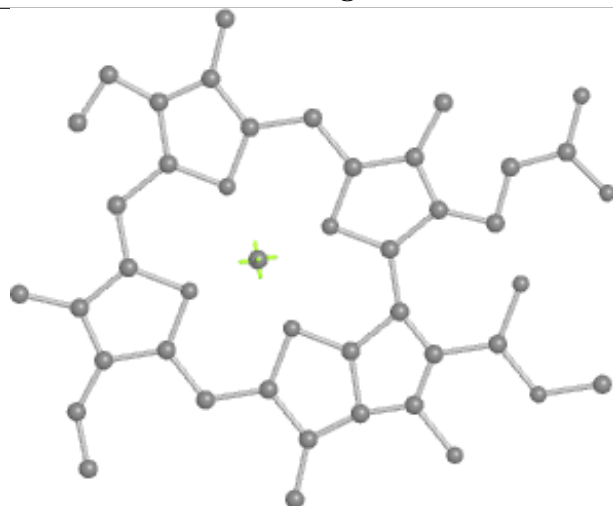
Bond lengths



Bond angles

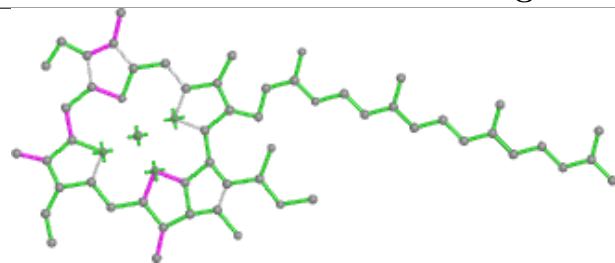


Torsions

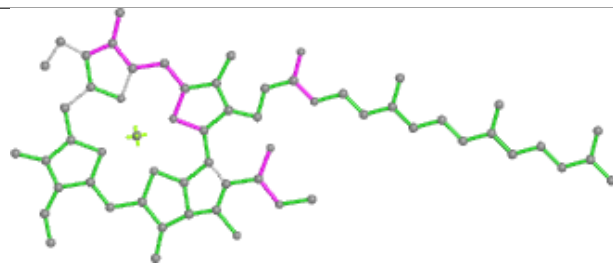


Rings

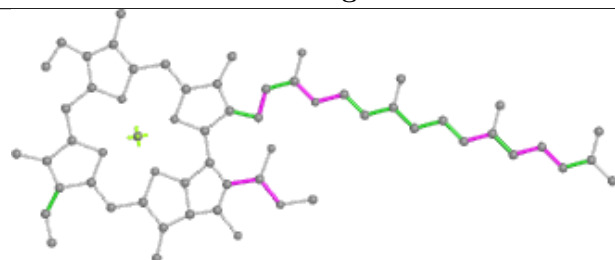
Ligand CLA R 409



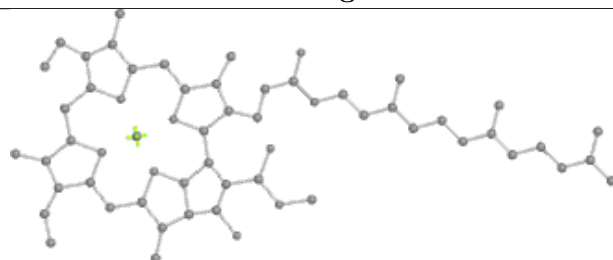
Bond lengths



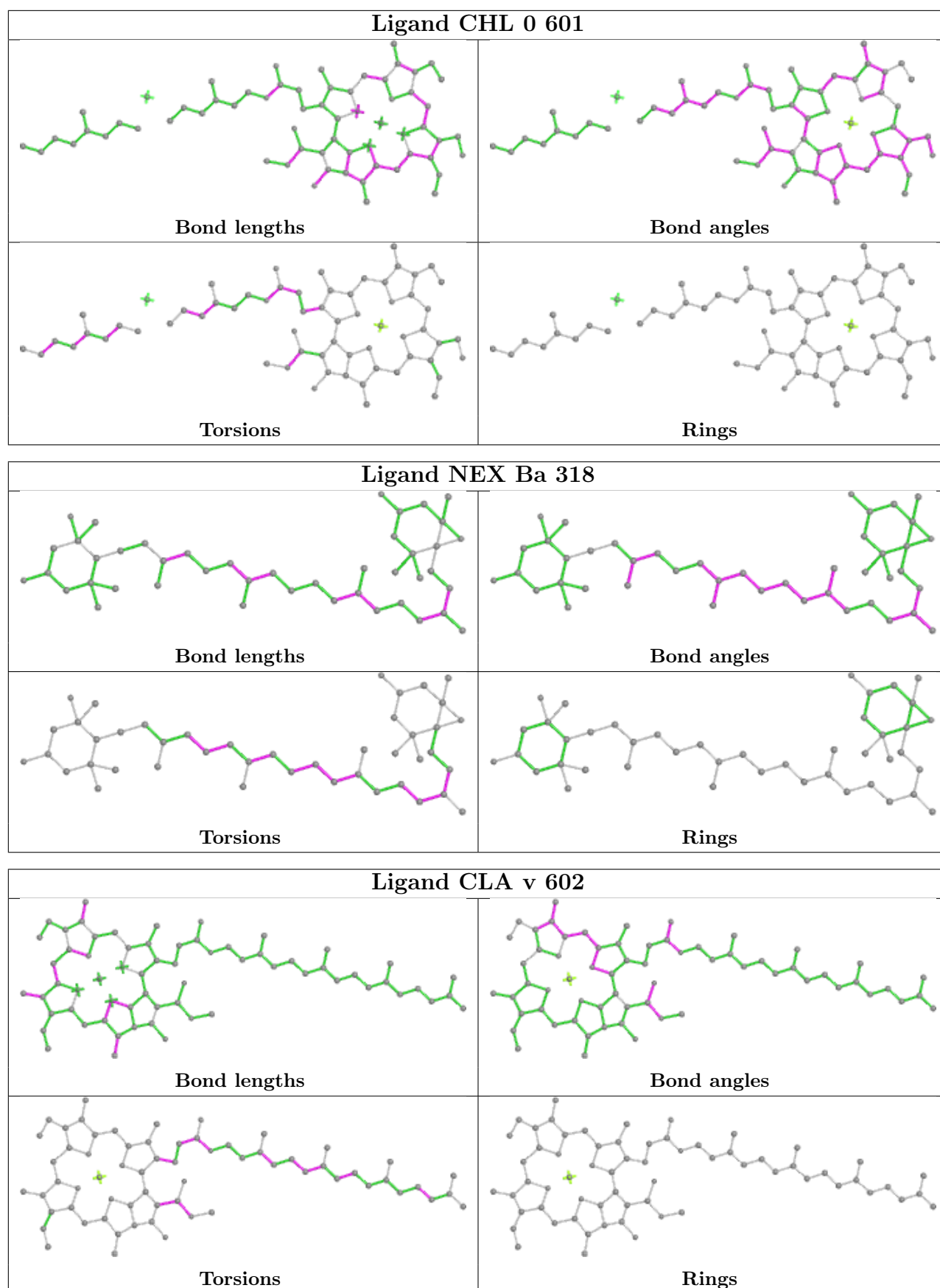
Bond angles



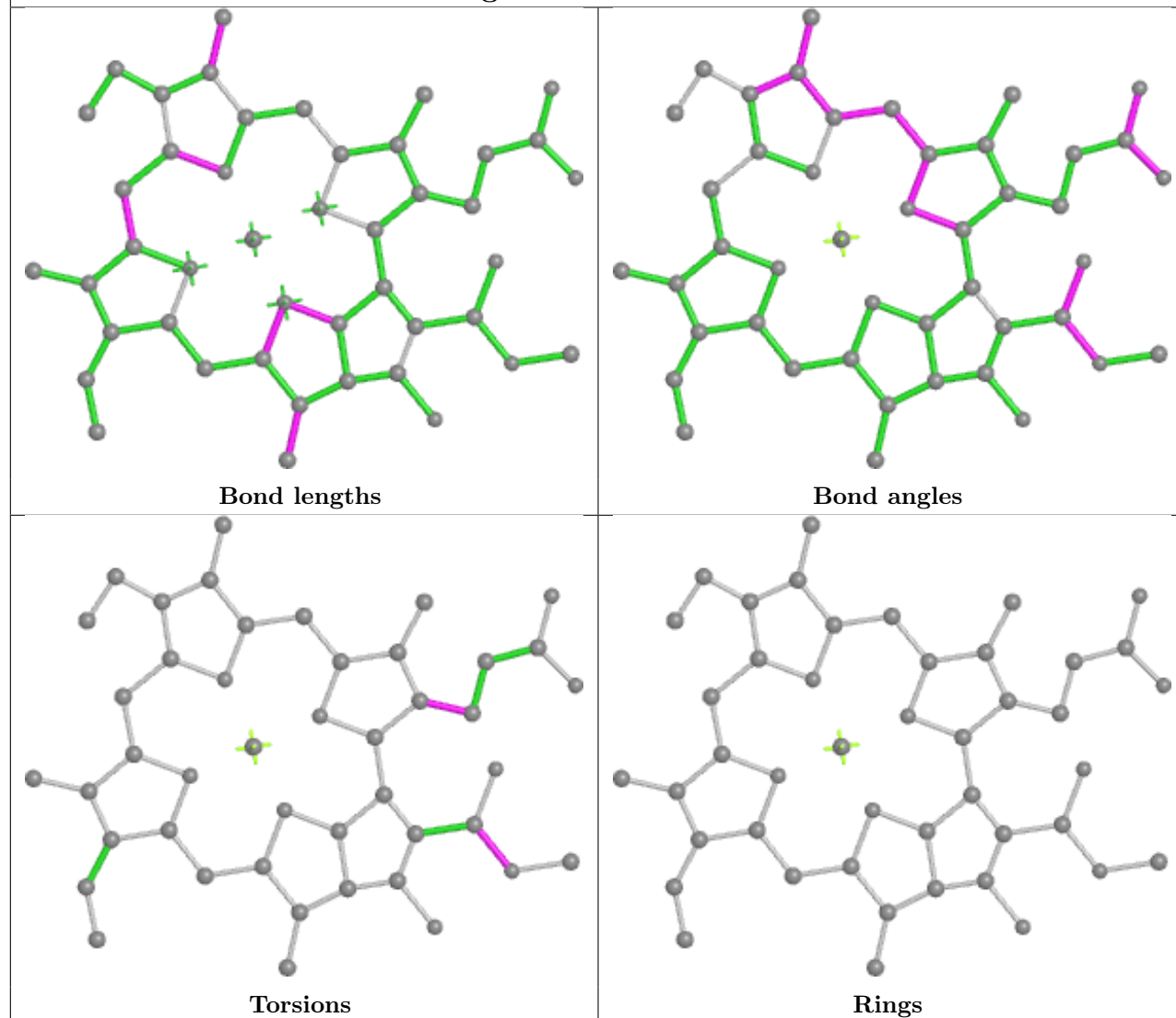
Torsions



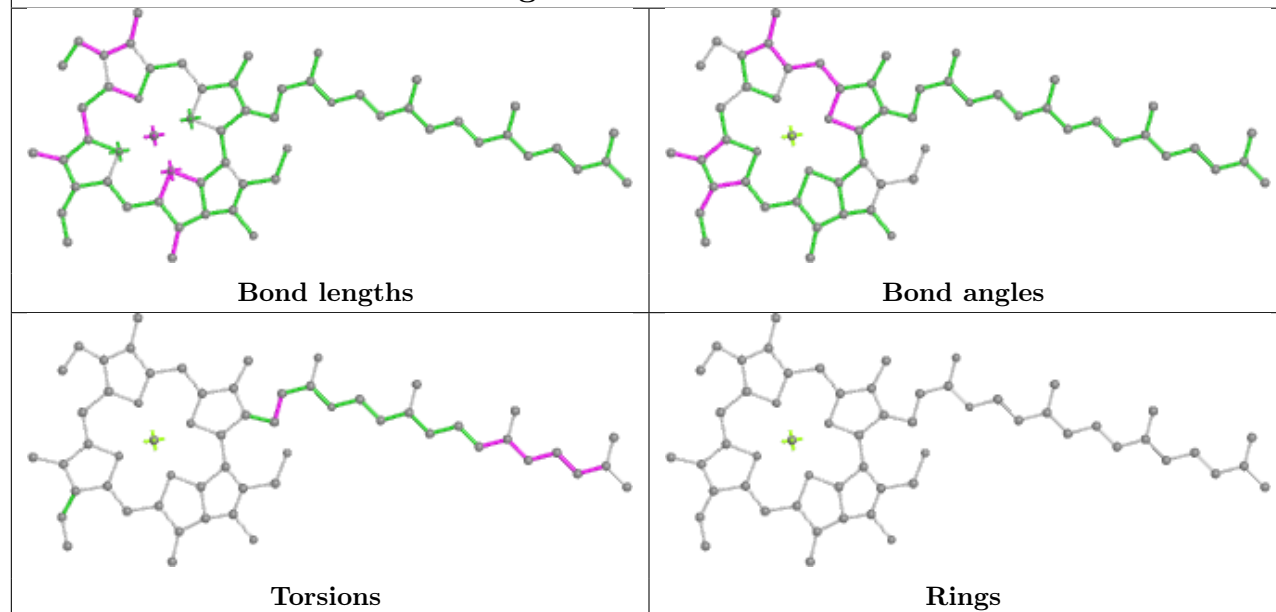
Rings

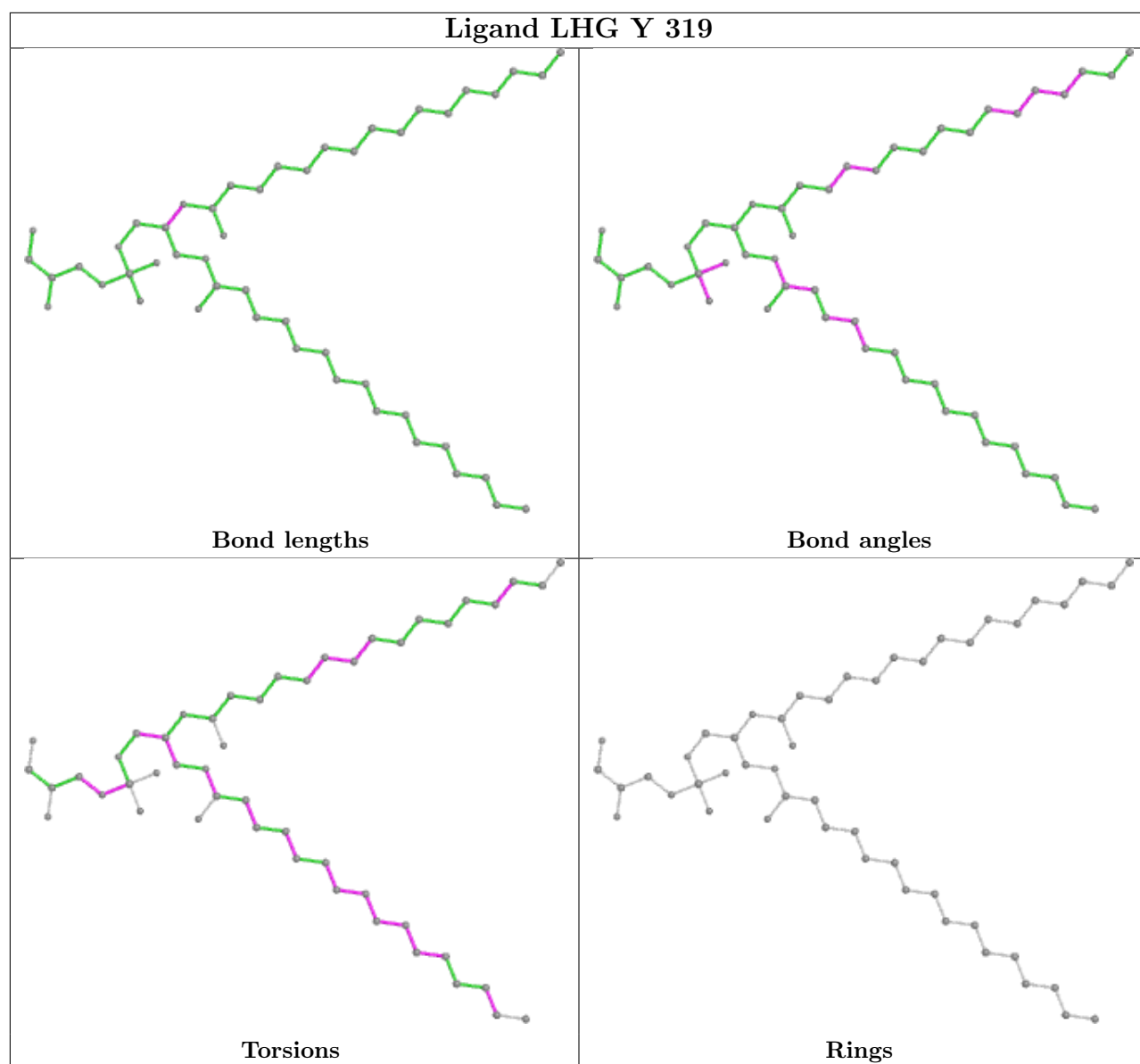


Ligand CLA A6 608

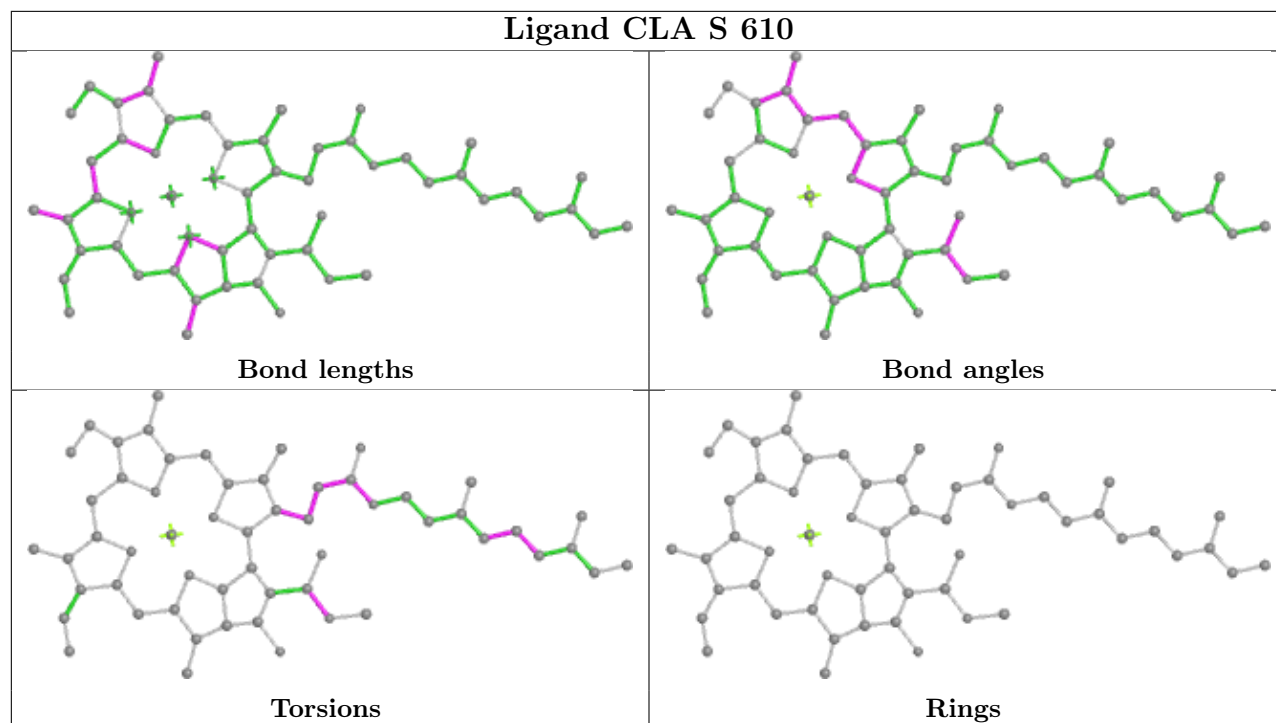


Ligand CLA BU 602

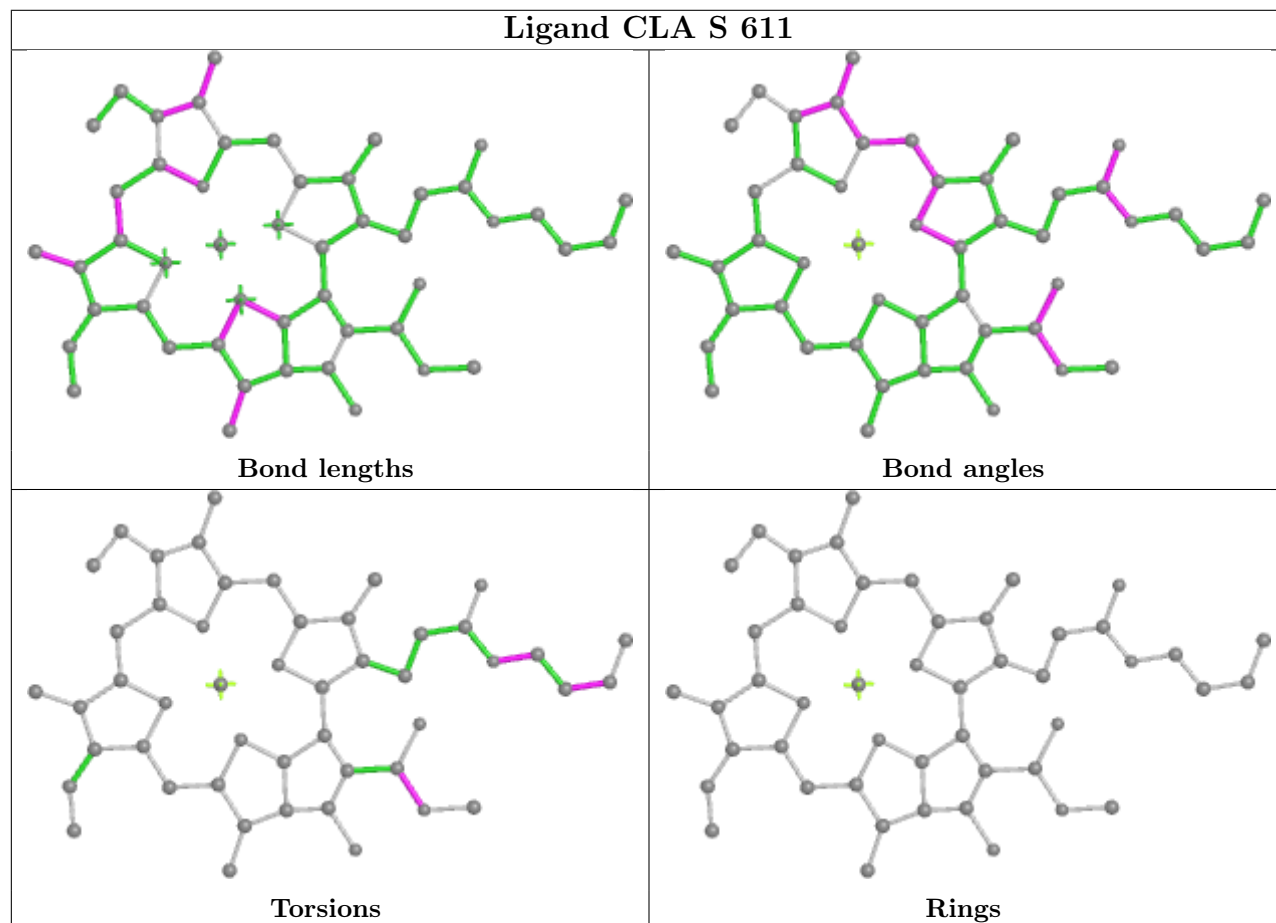




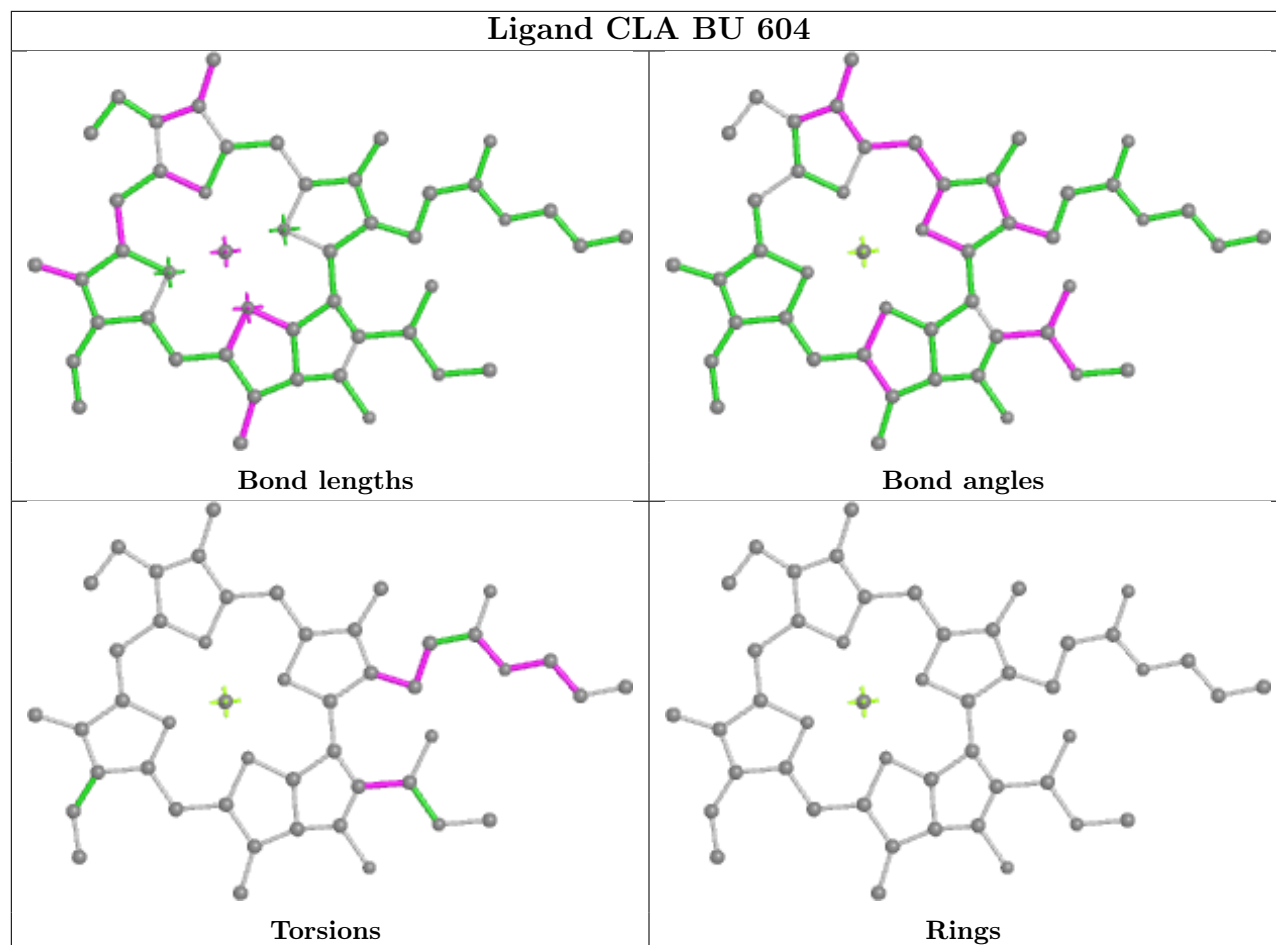
Ligand CLA S 610



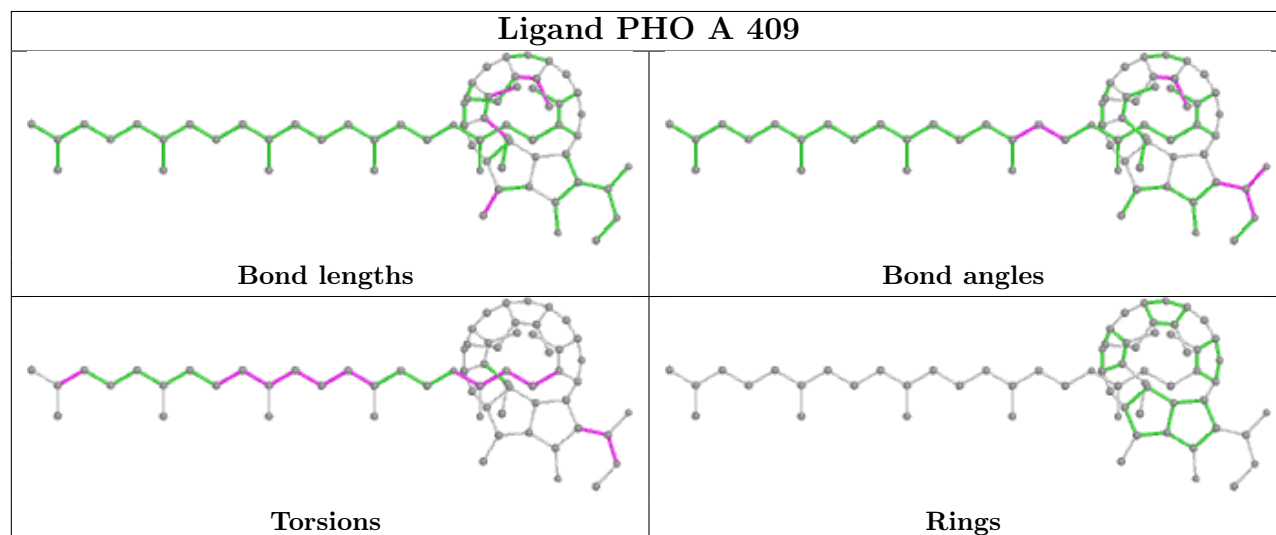
Ligand CLA S 611

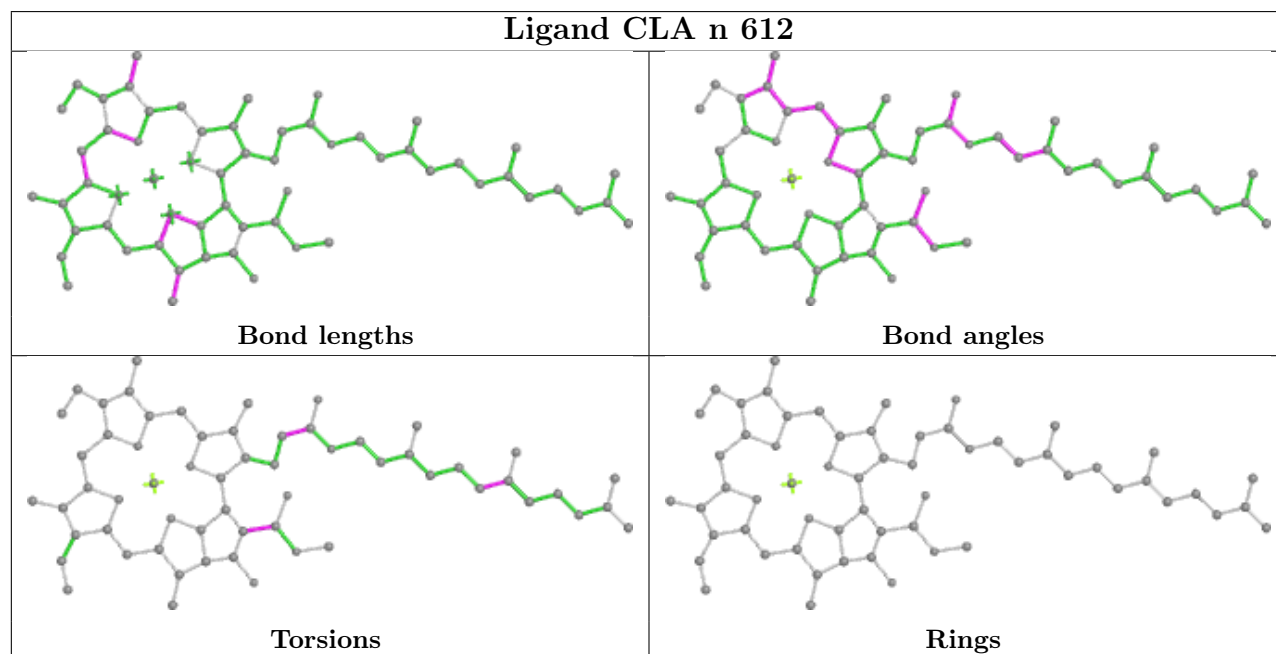
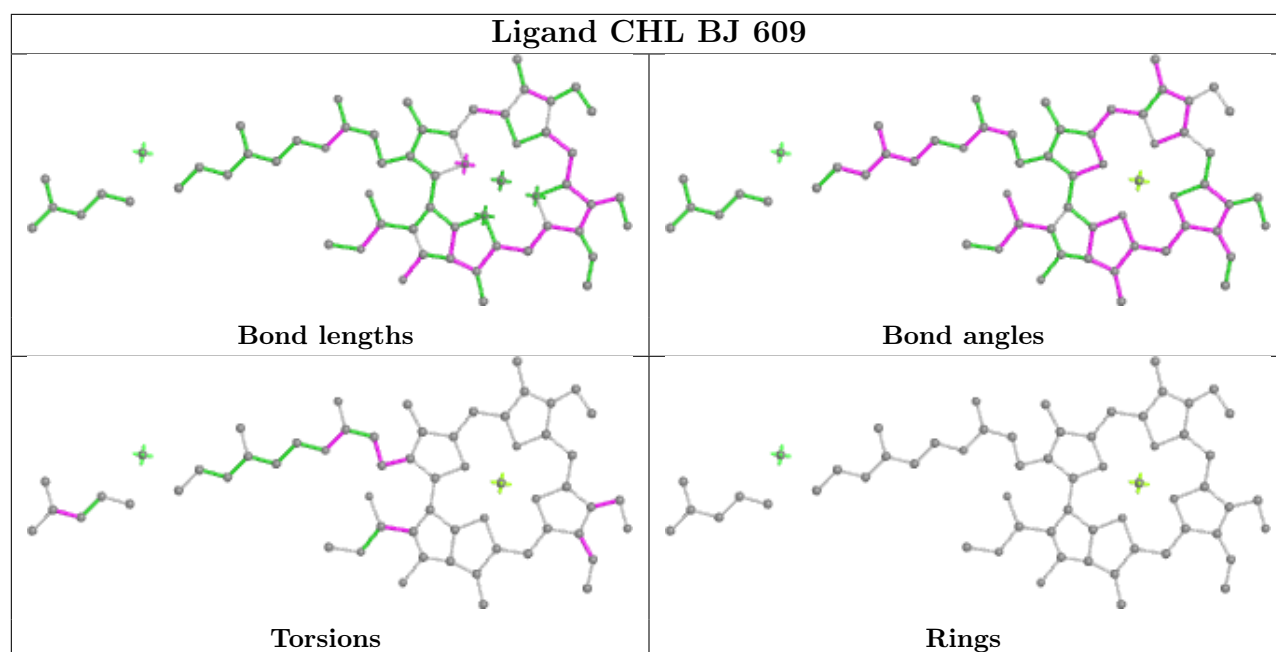


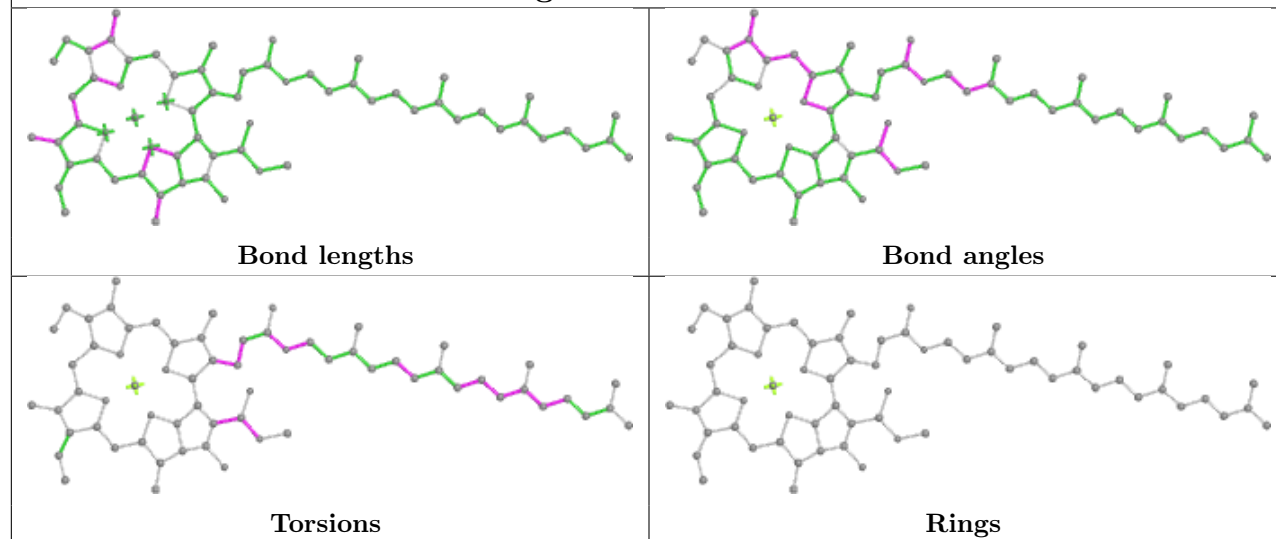
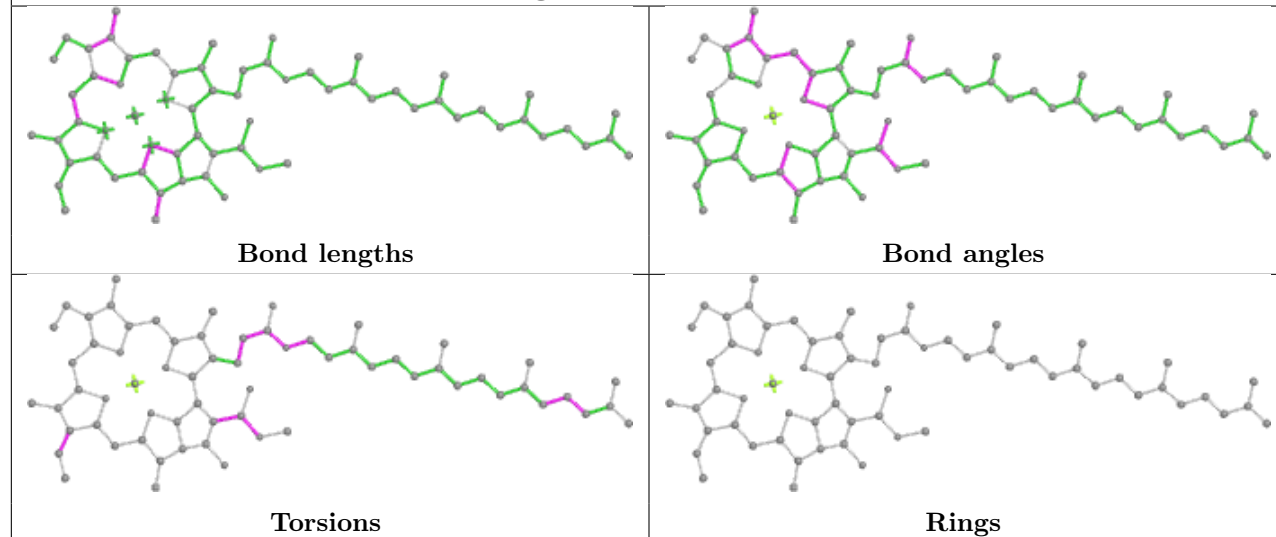
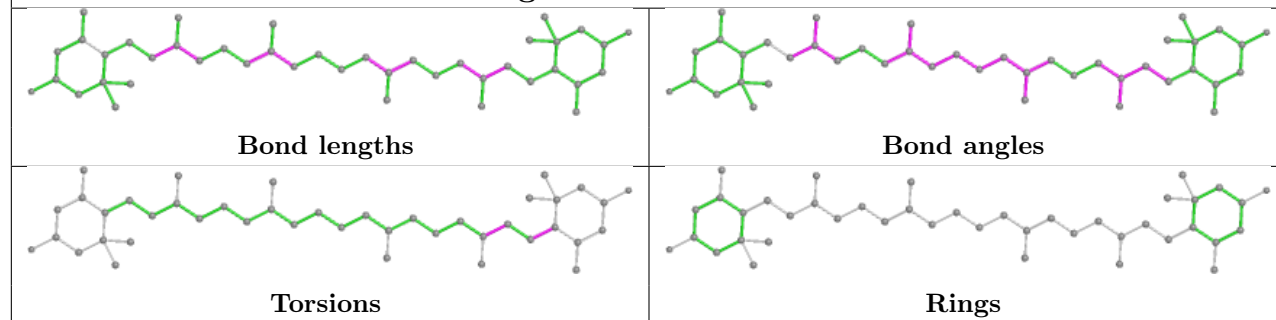
Ligand CLA BU 604



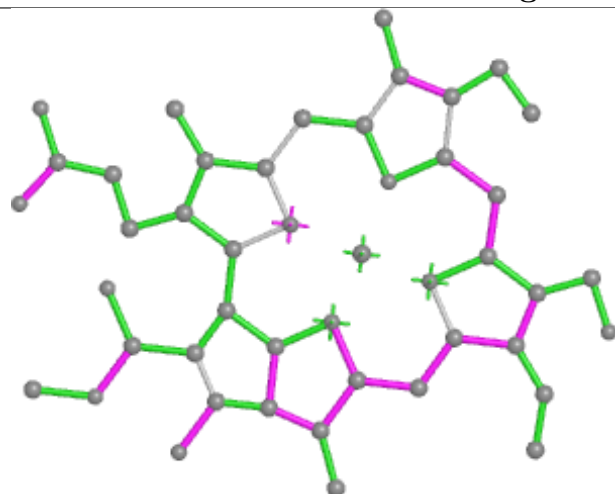
Ligand PHO A 409



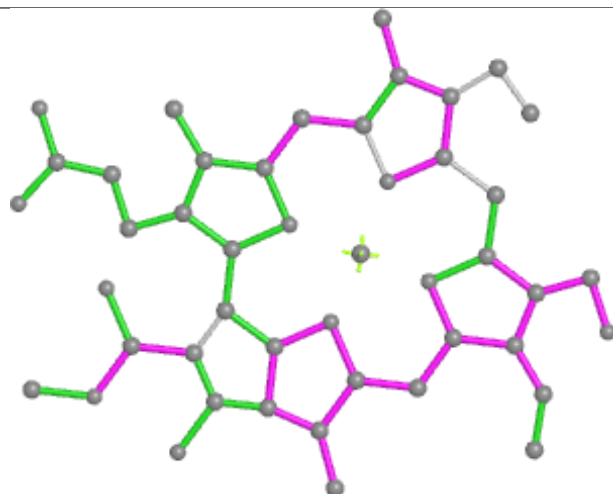


Ligand CLA v 606**Ligand CLA B 610****Ligand LUT AA 316**

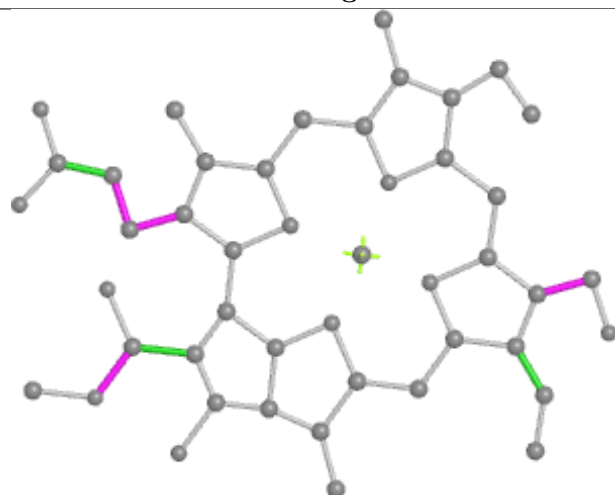
Ligand CHL 9 608



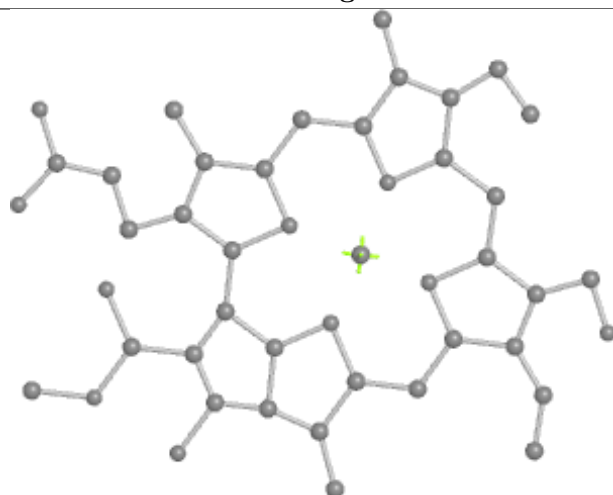
Bond lengths



Bond angles

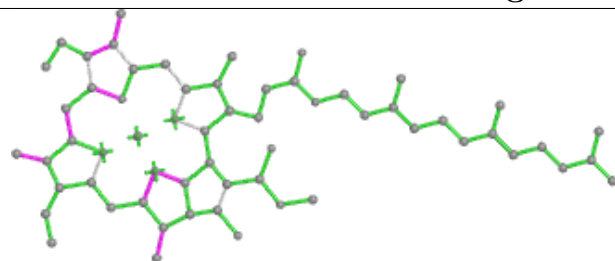


Torsions

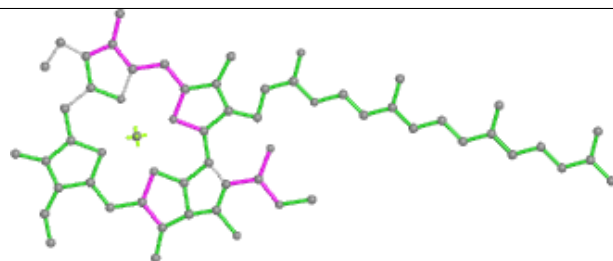


Rings

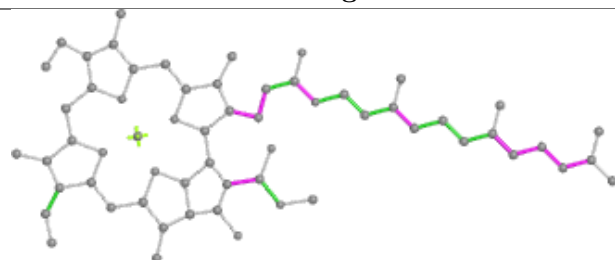
Ligand CLA A2 611



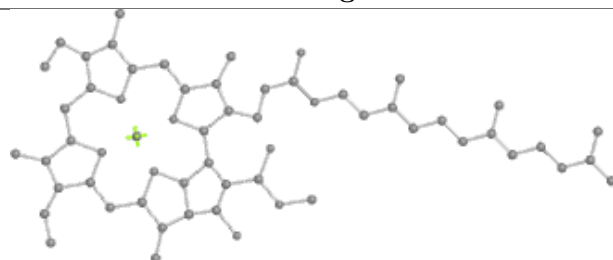
Bond lengths



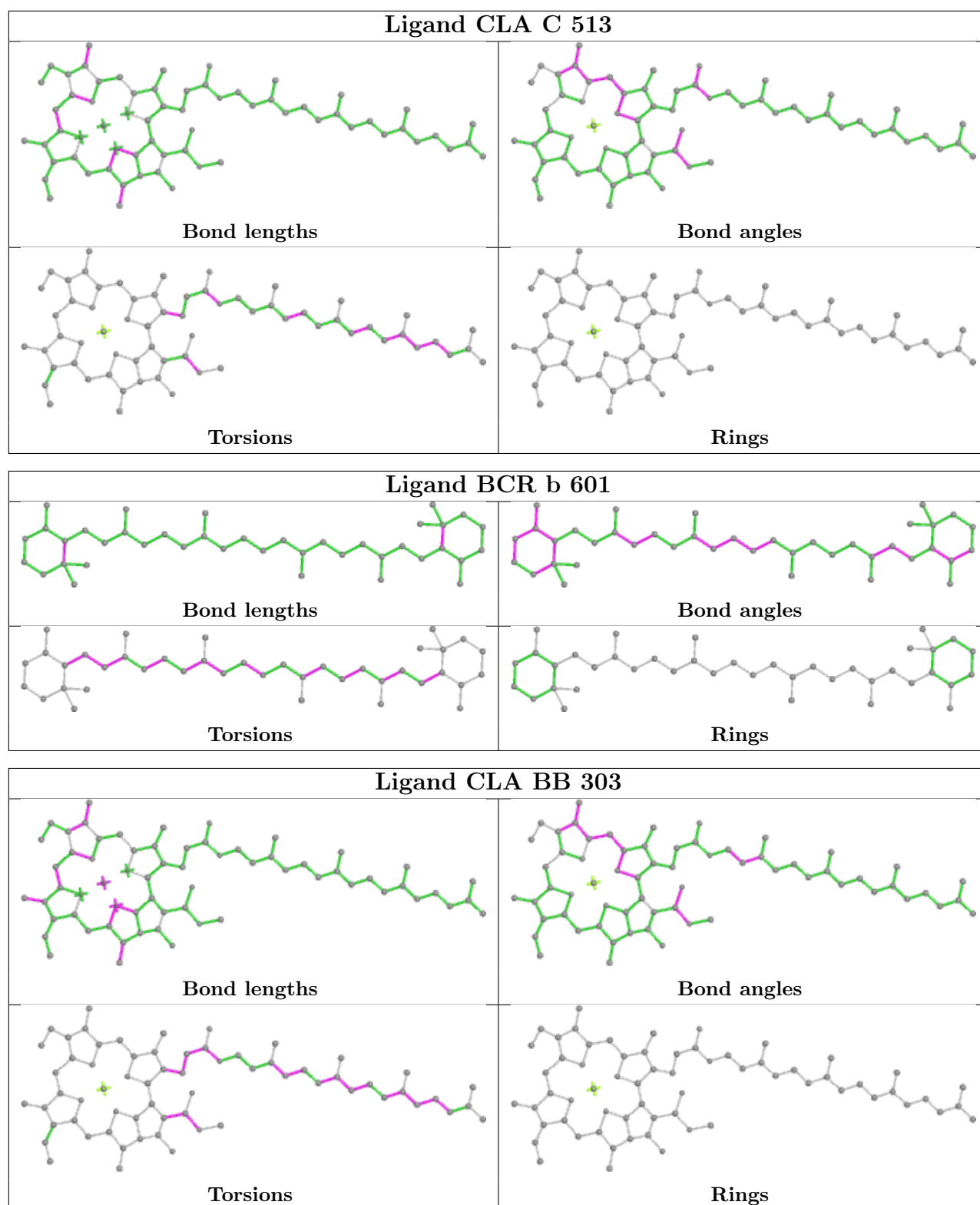
Bond angles

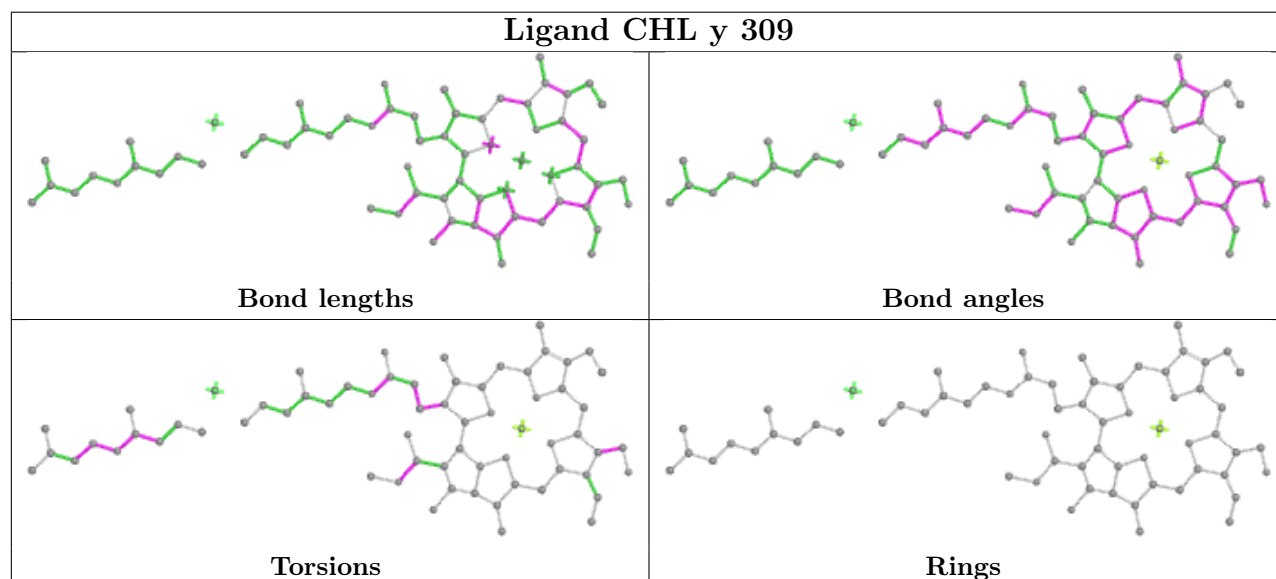
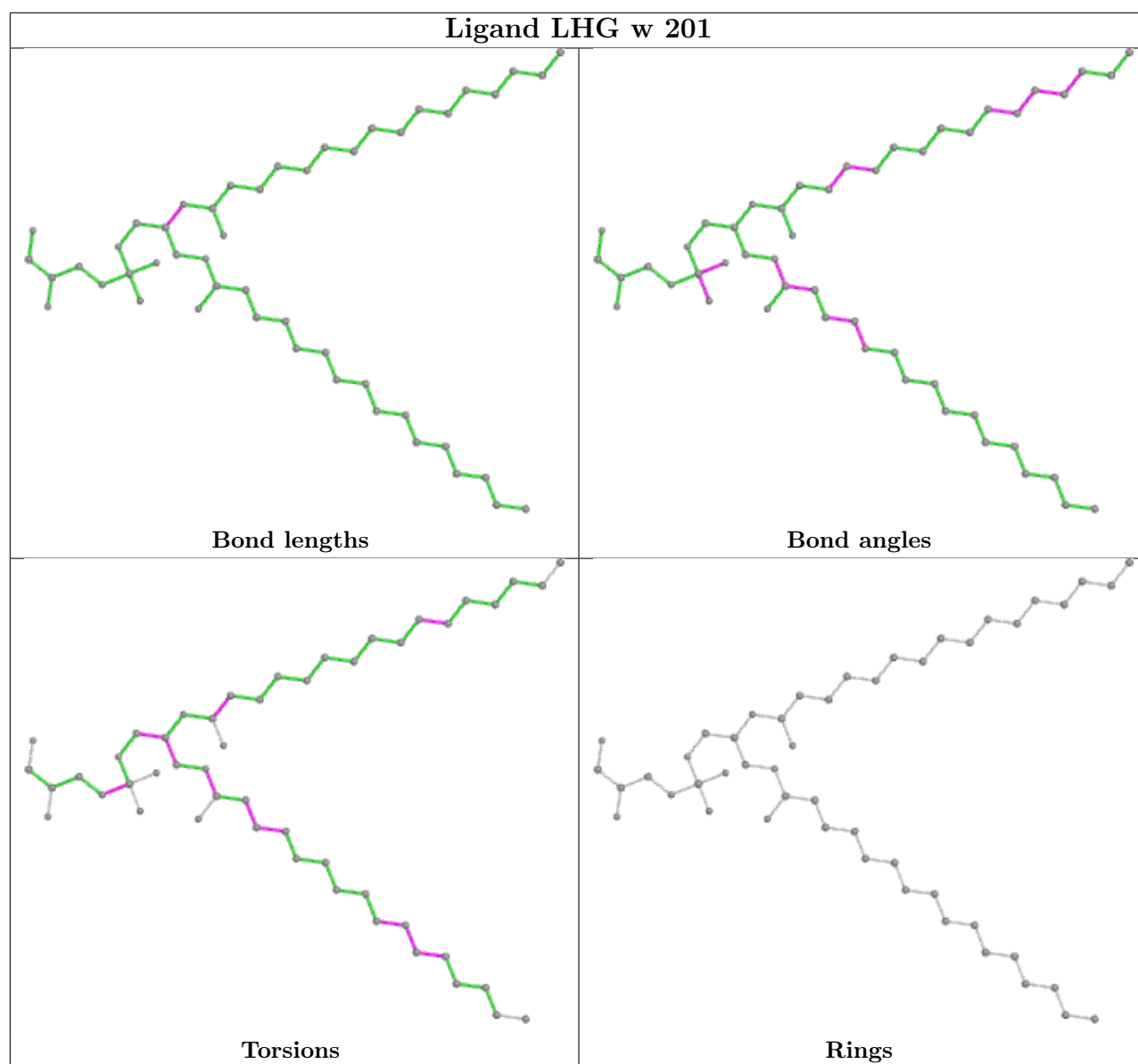


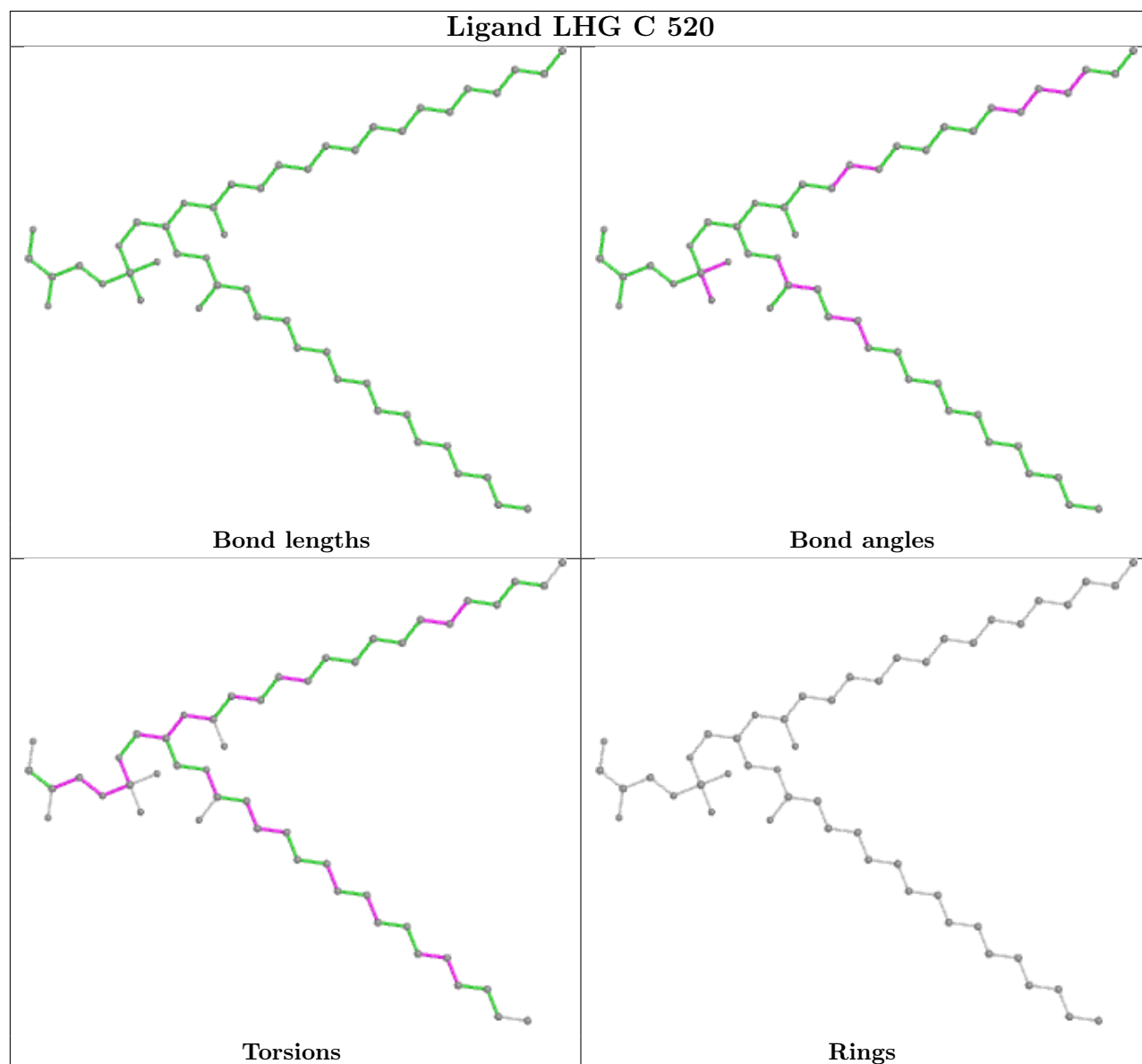
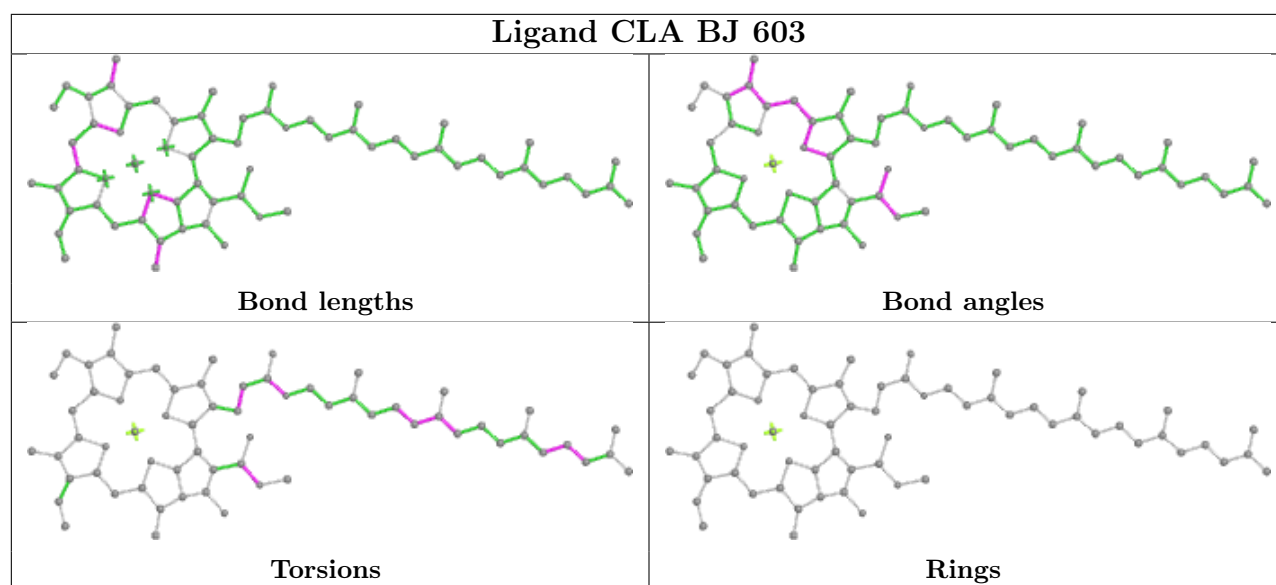
Torsions

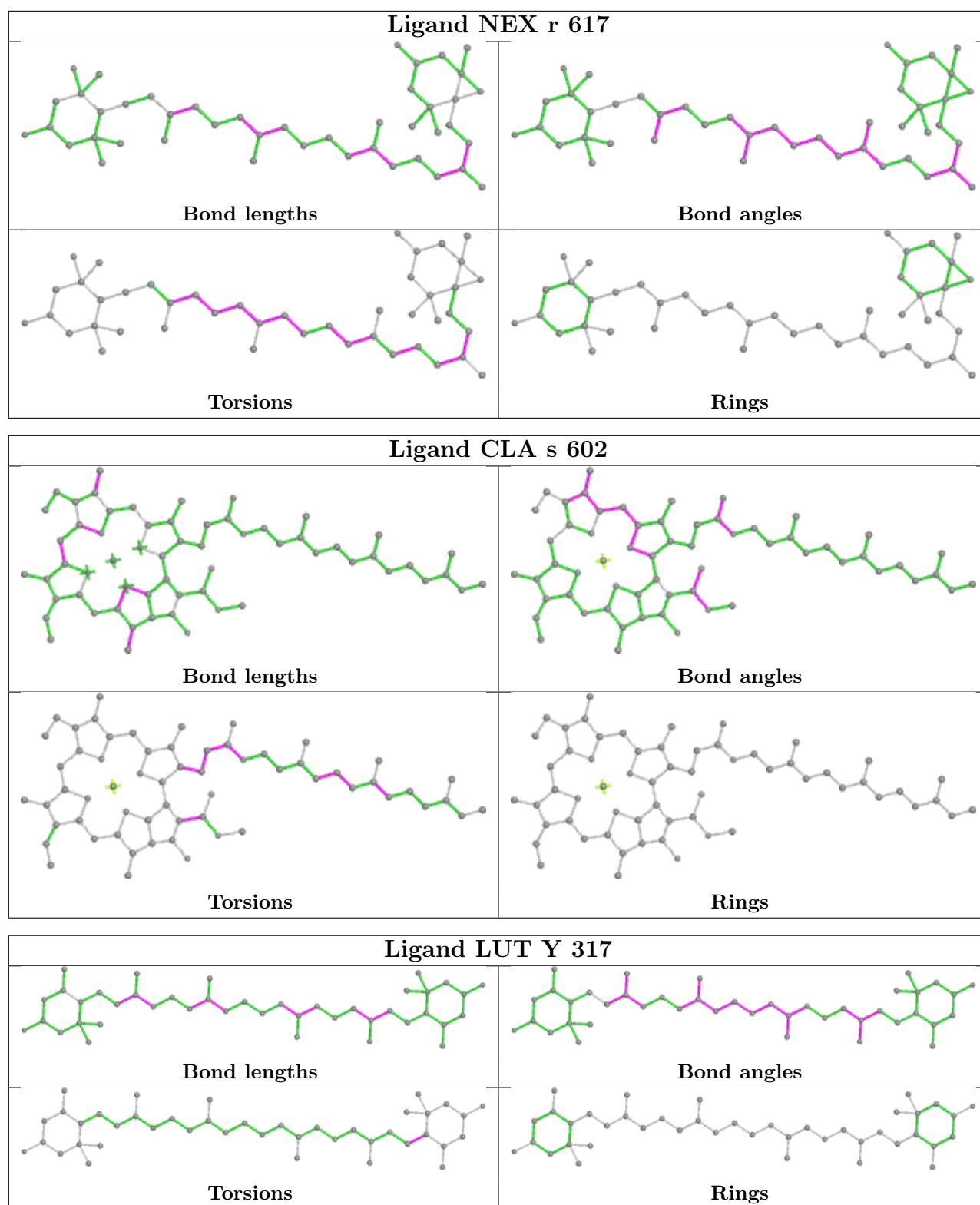


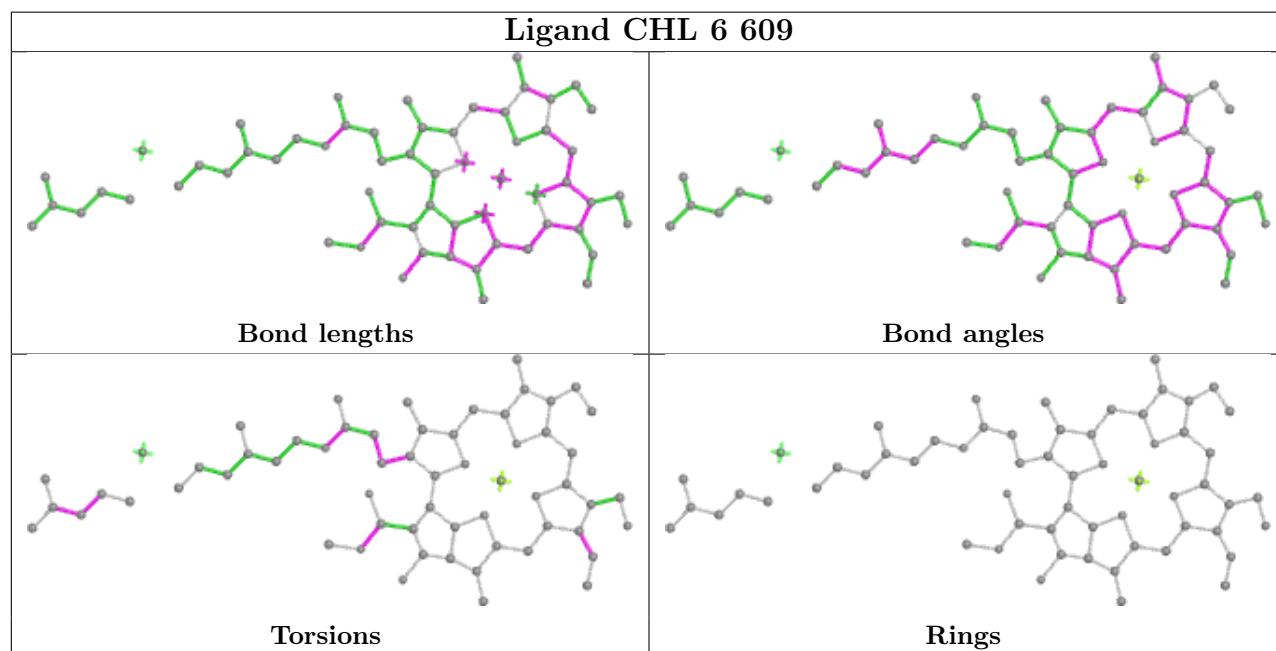
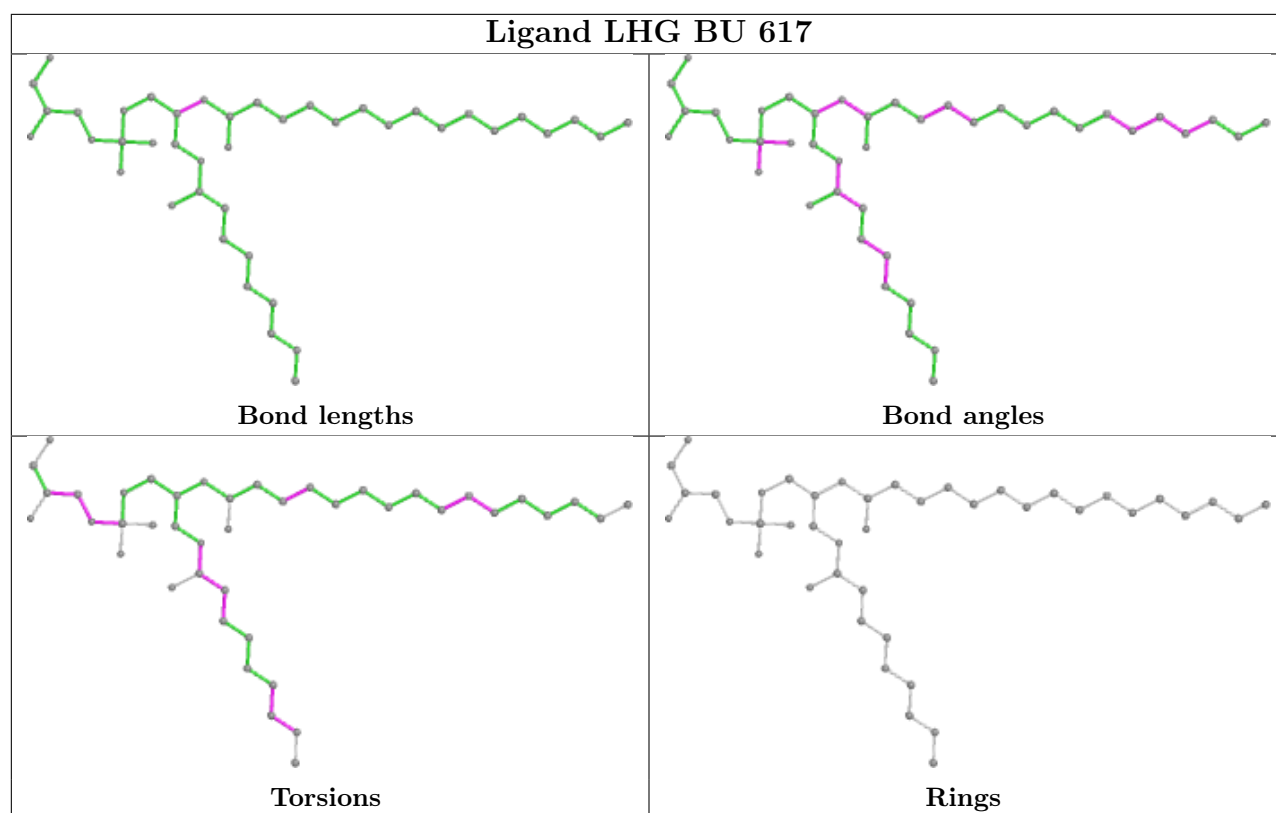
Rings

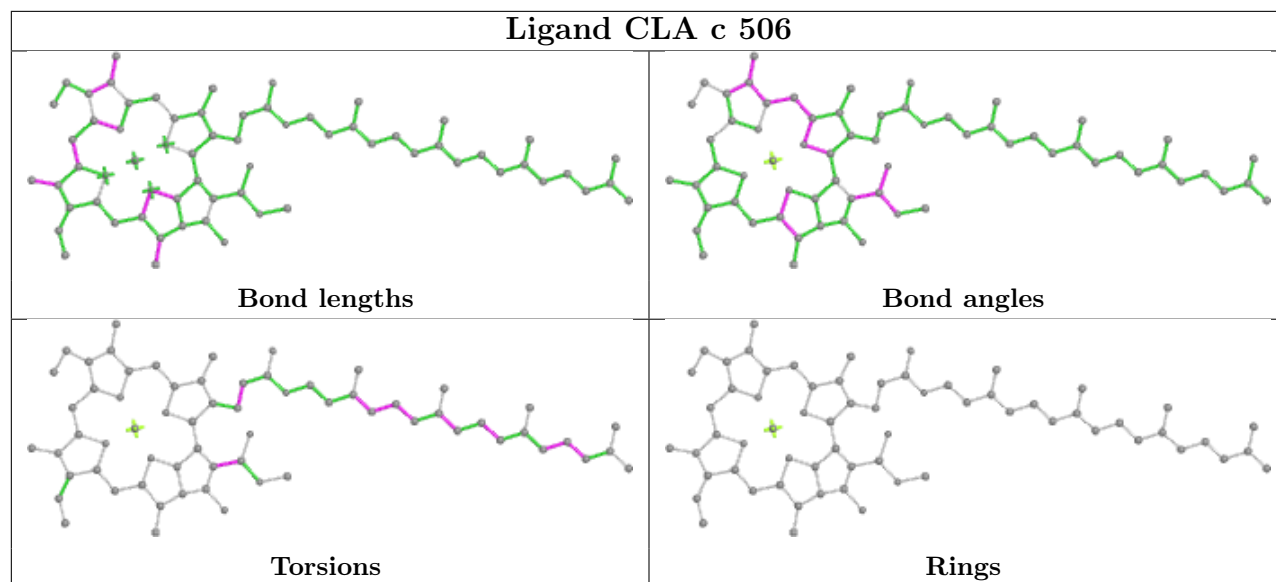
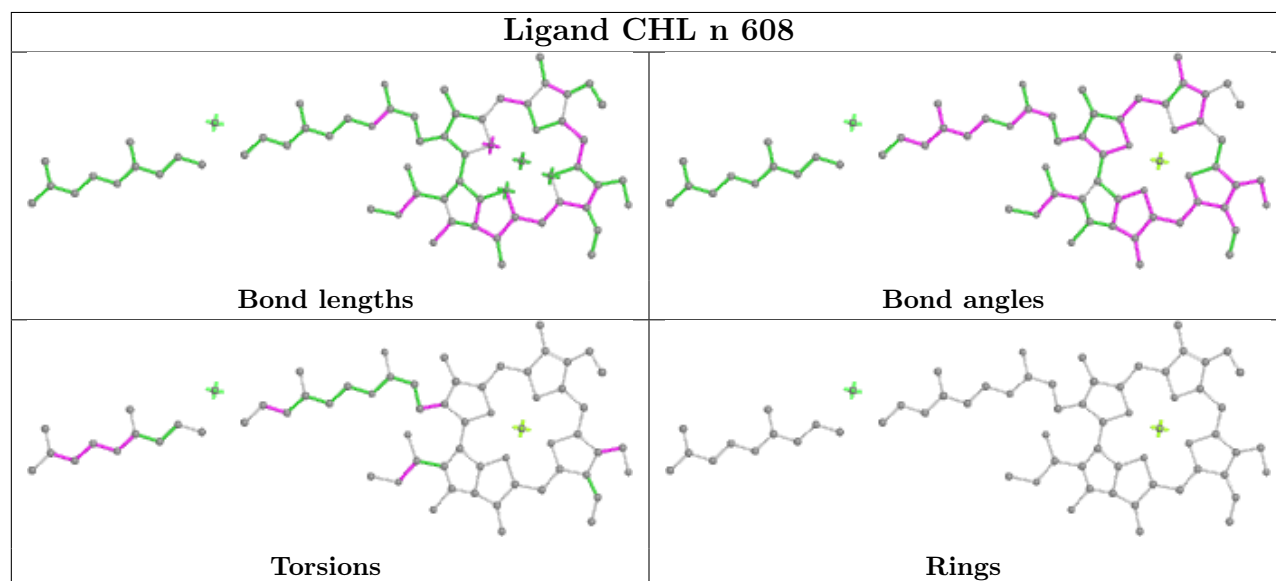


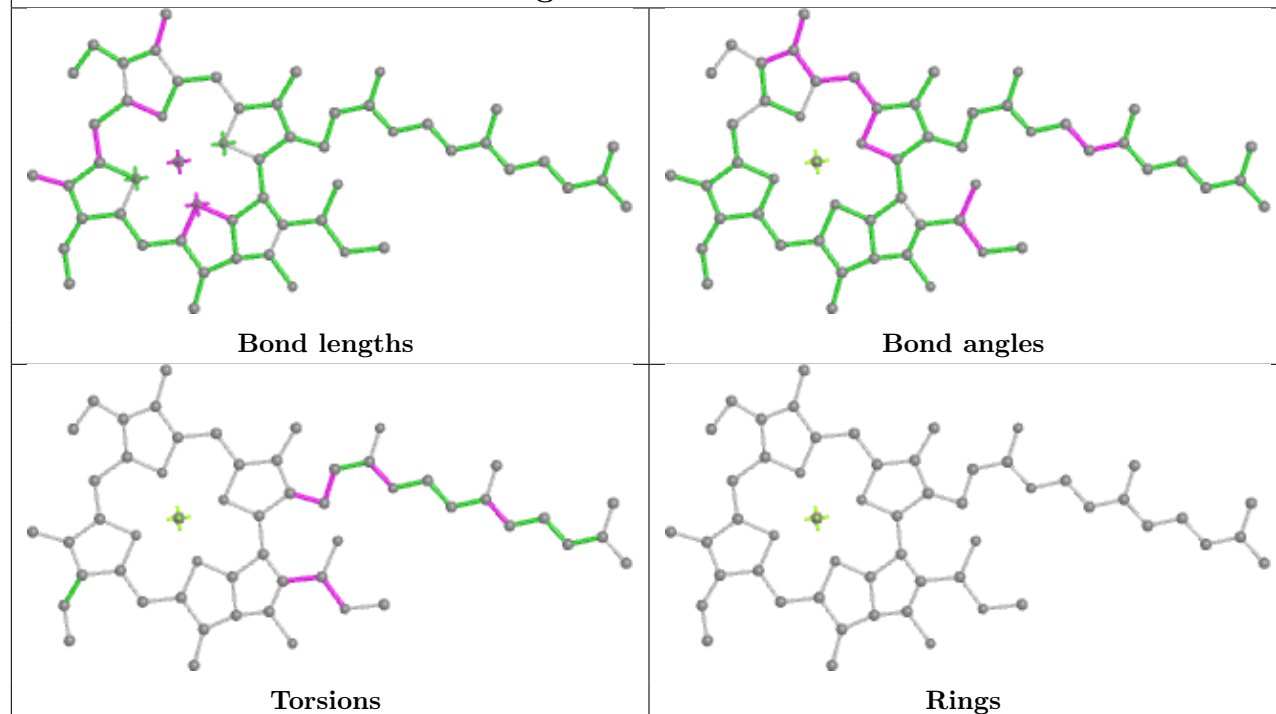
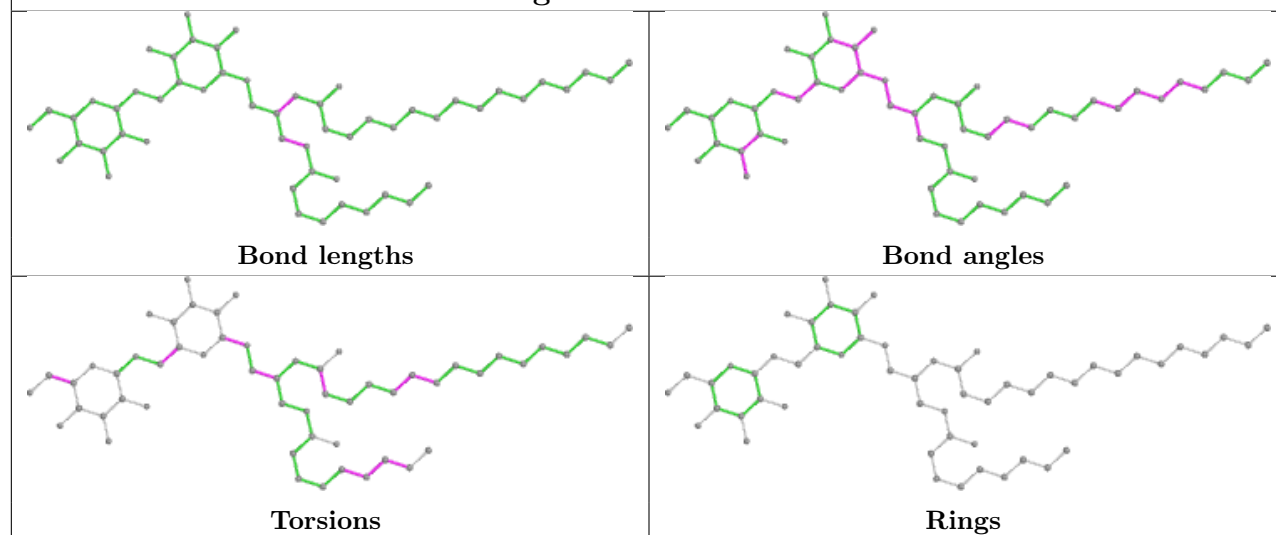
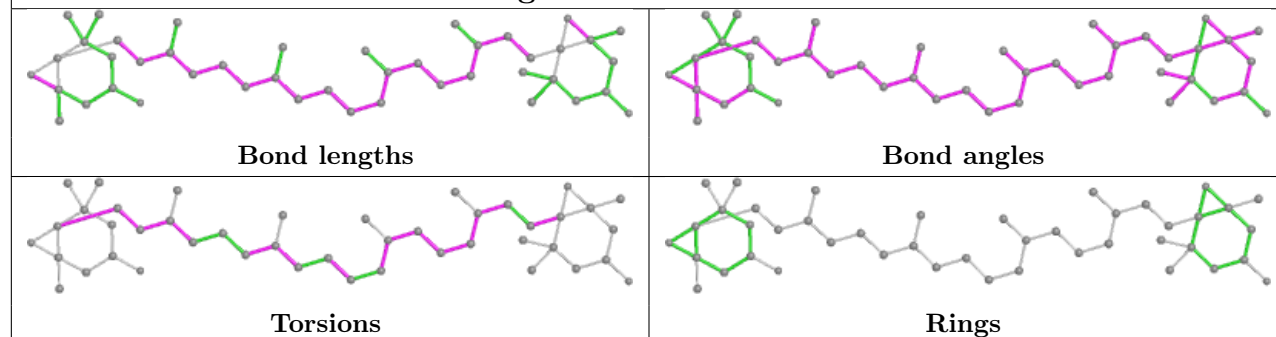


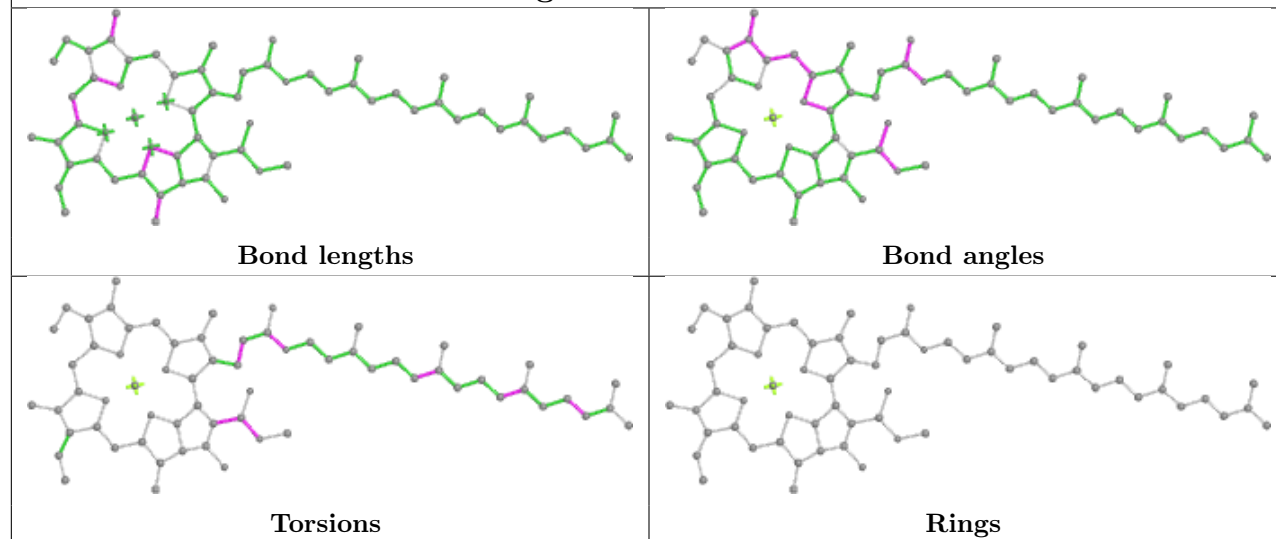
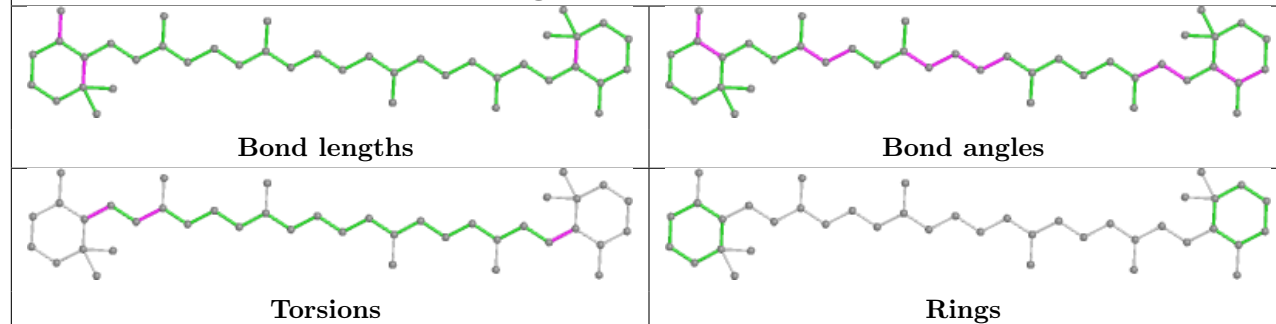
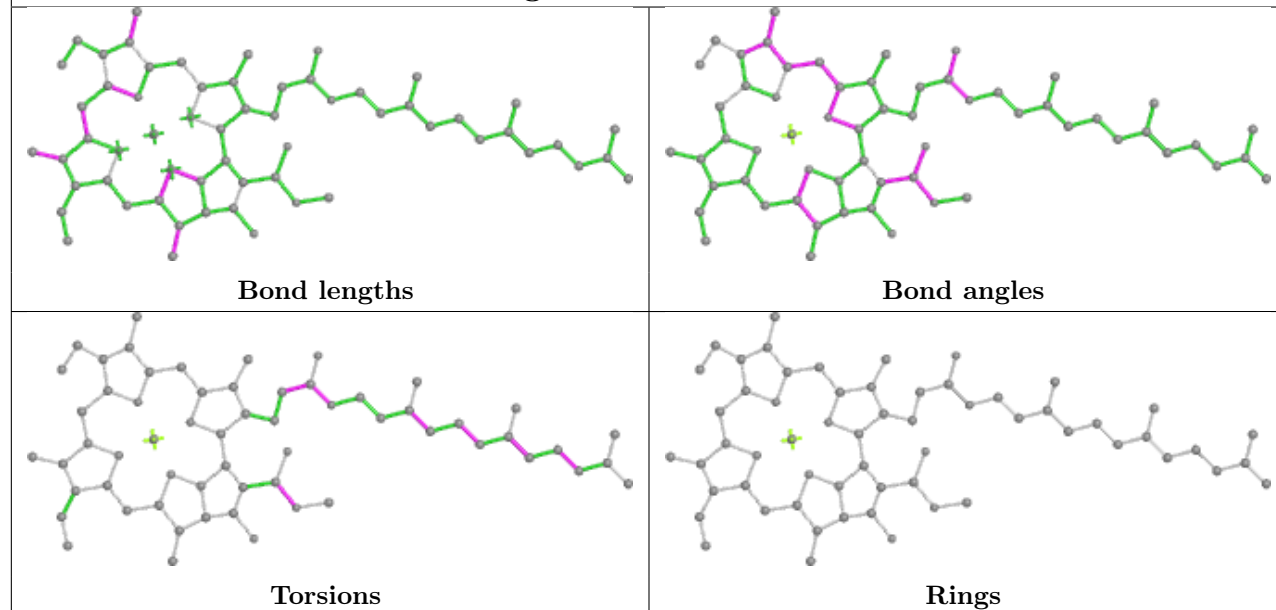


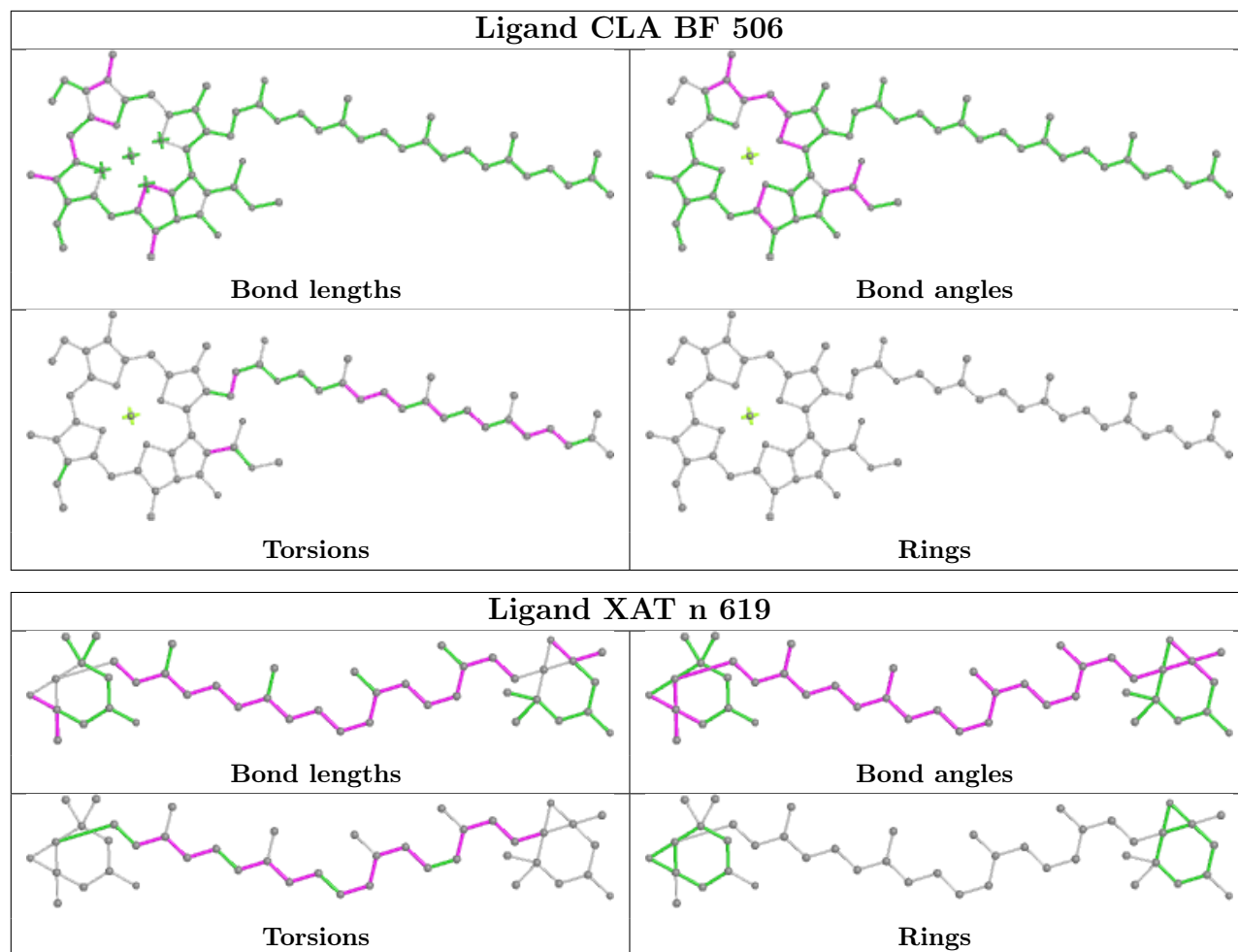




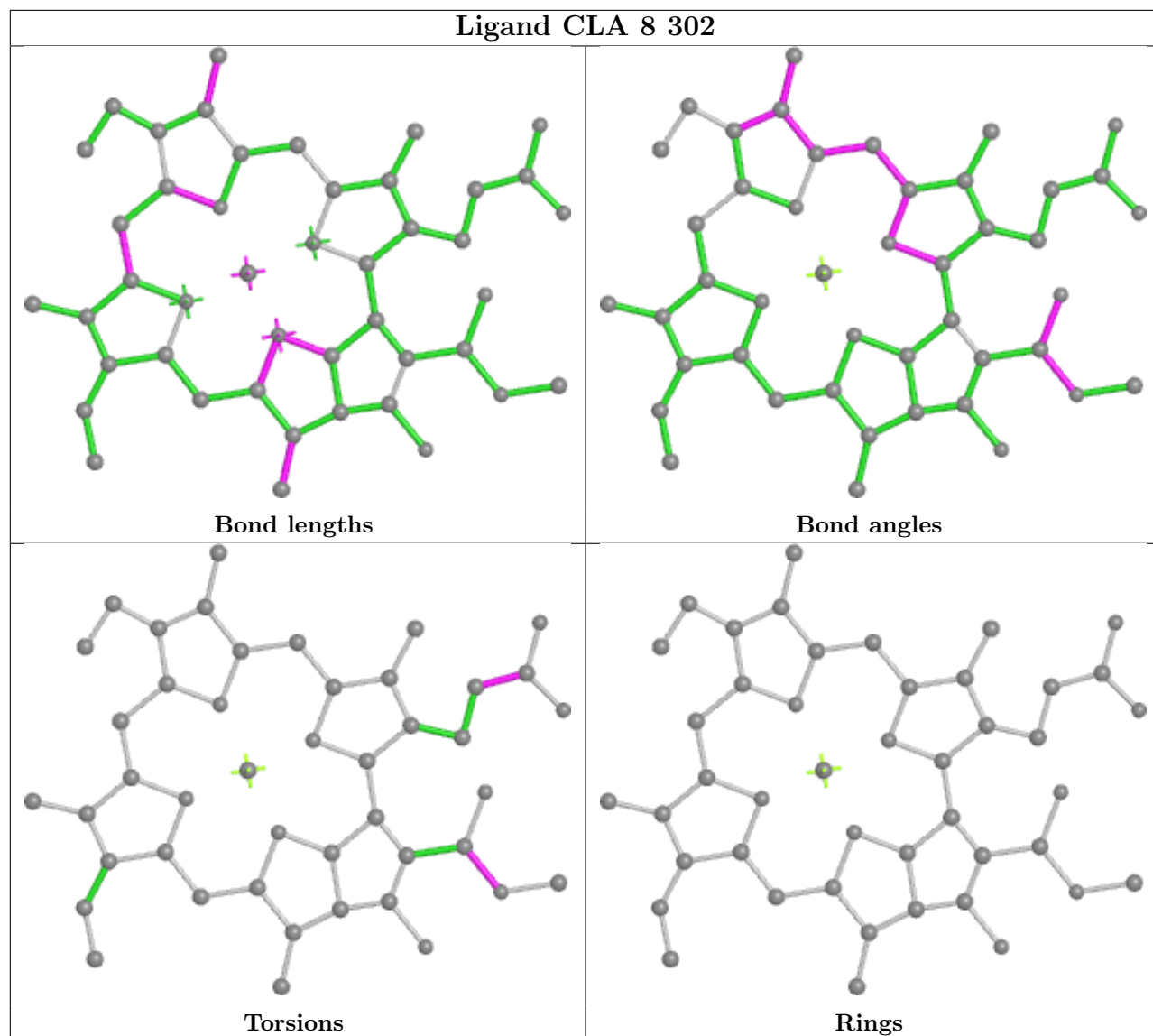
Ligand CLA c 506**Ligand CHL n 608**

Ligand CLA 9 613**Ligand DGD c 516****Ligand XAT BU 616**

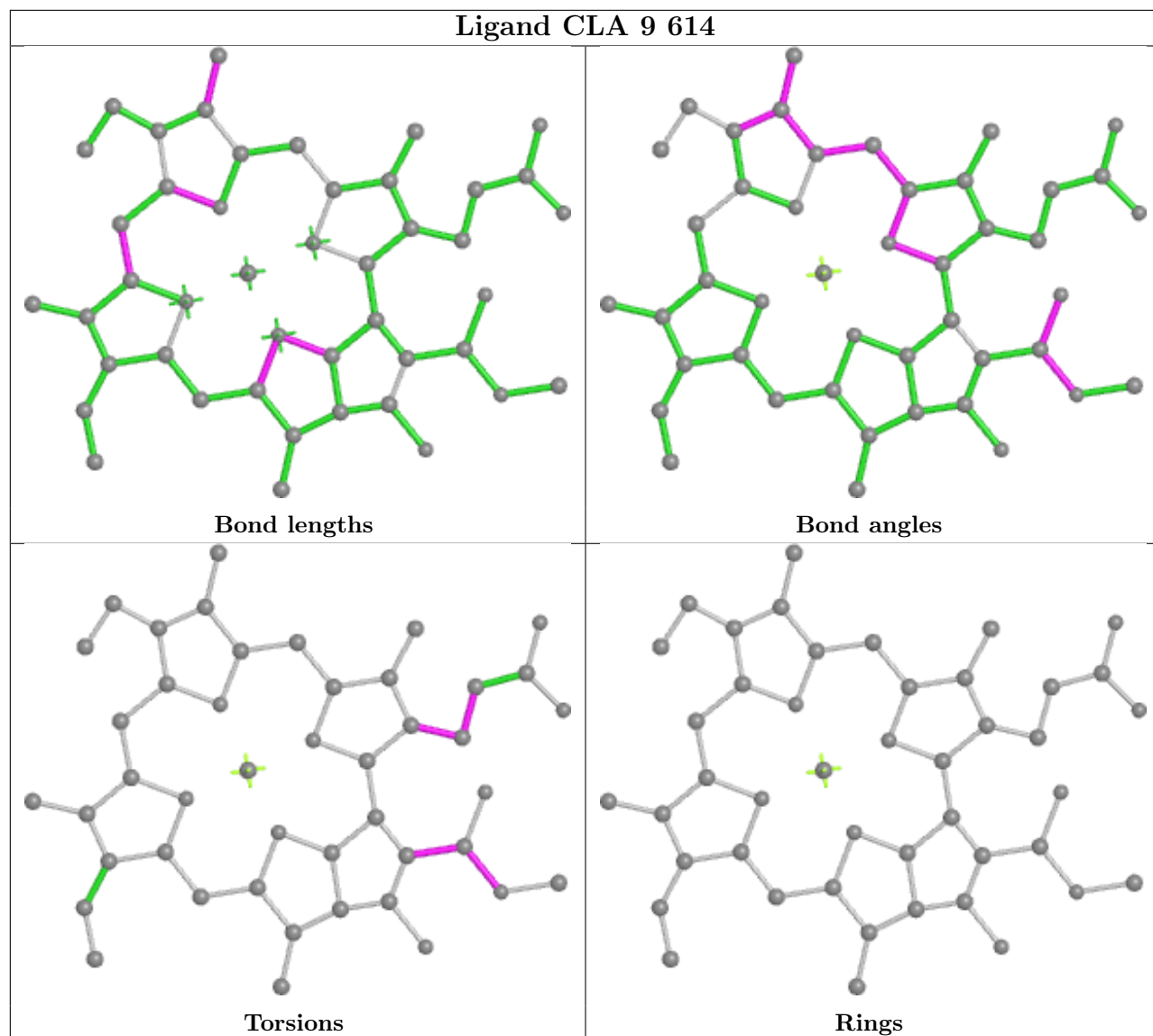
Ligand CLA 2 403**Ligand BCR A 411****Ligand CLA Ba 313**



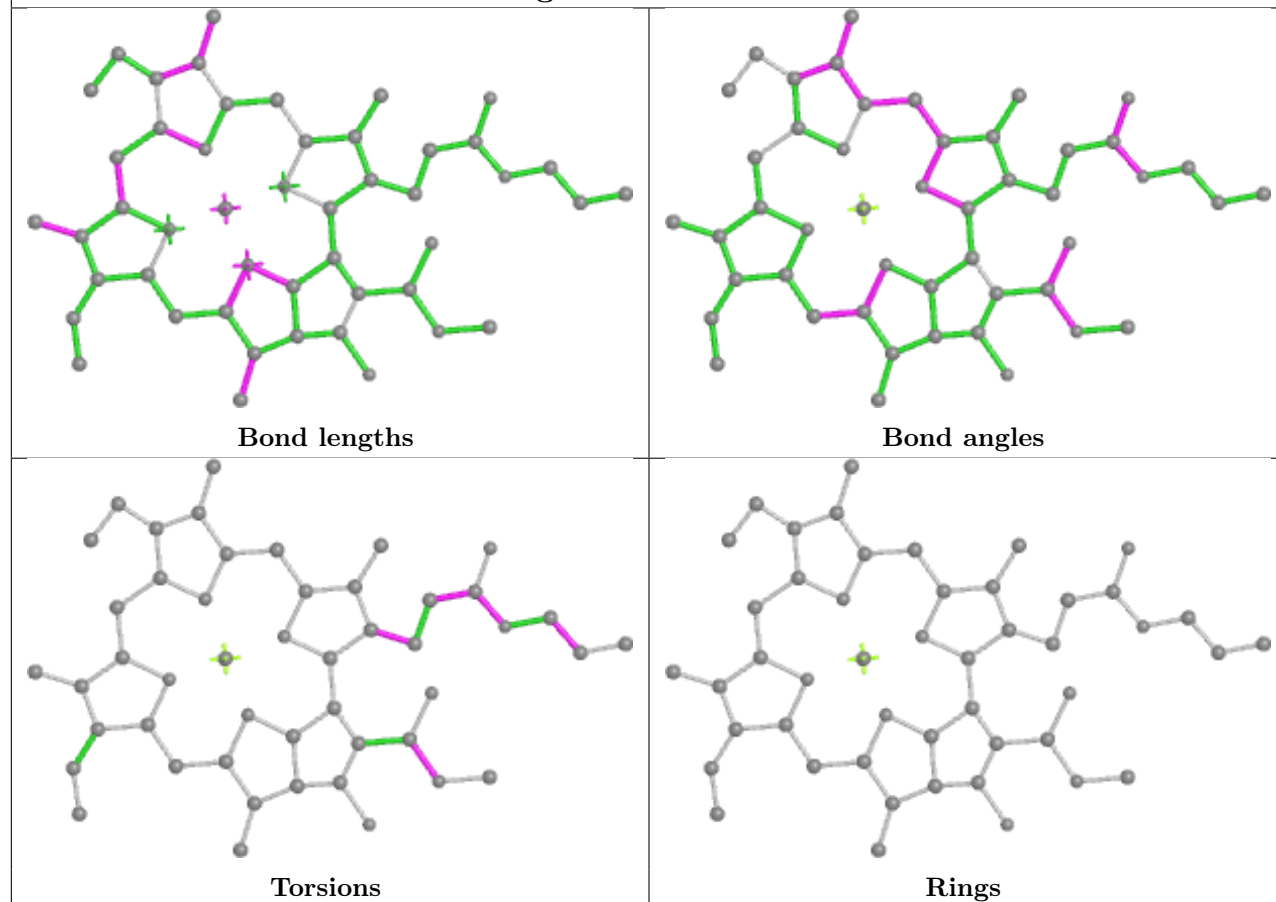
Ligand CLA 8 302



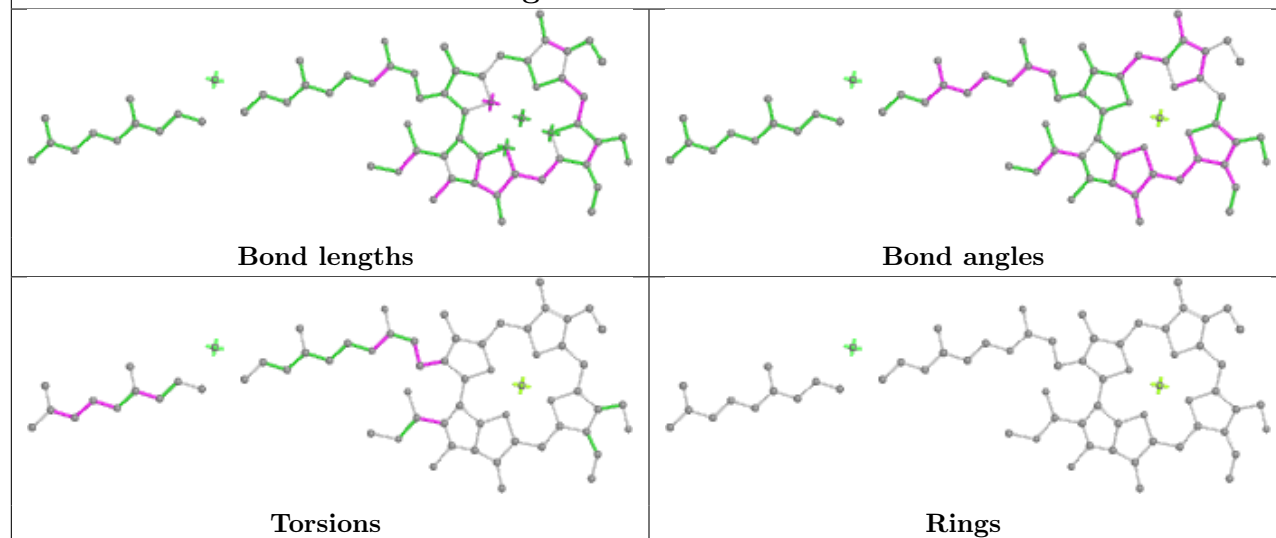
Ligand CLA 9 614

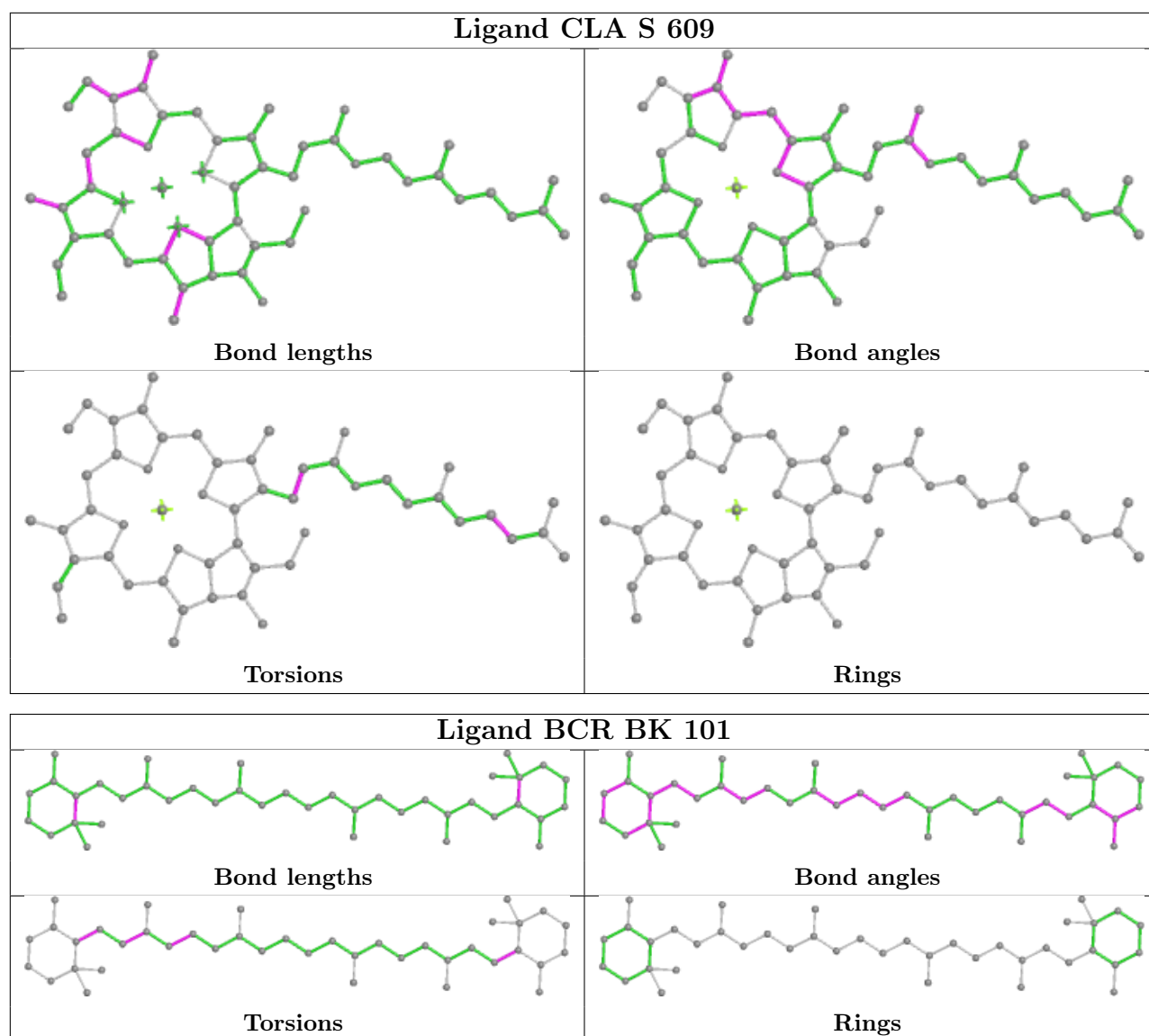


Ligand CLA 0 614

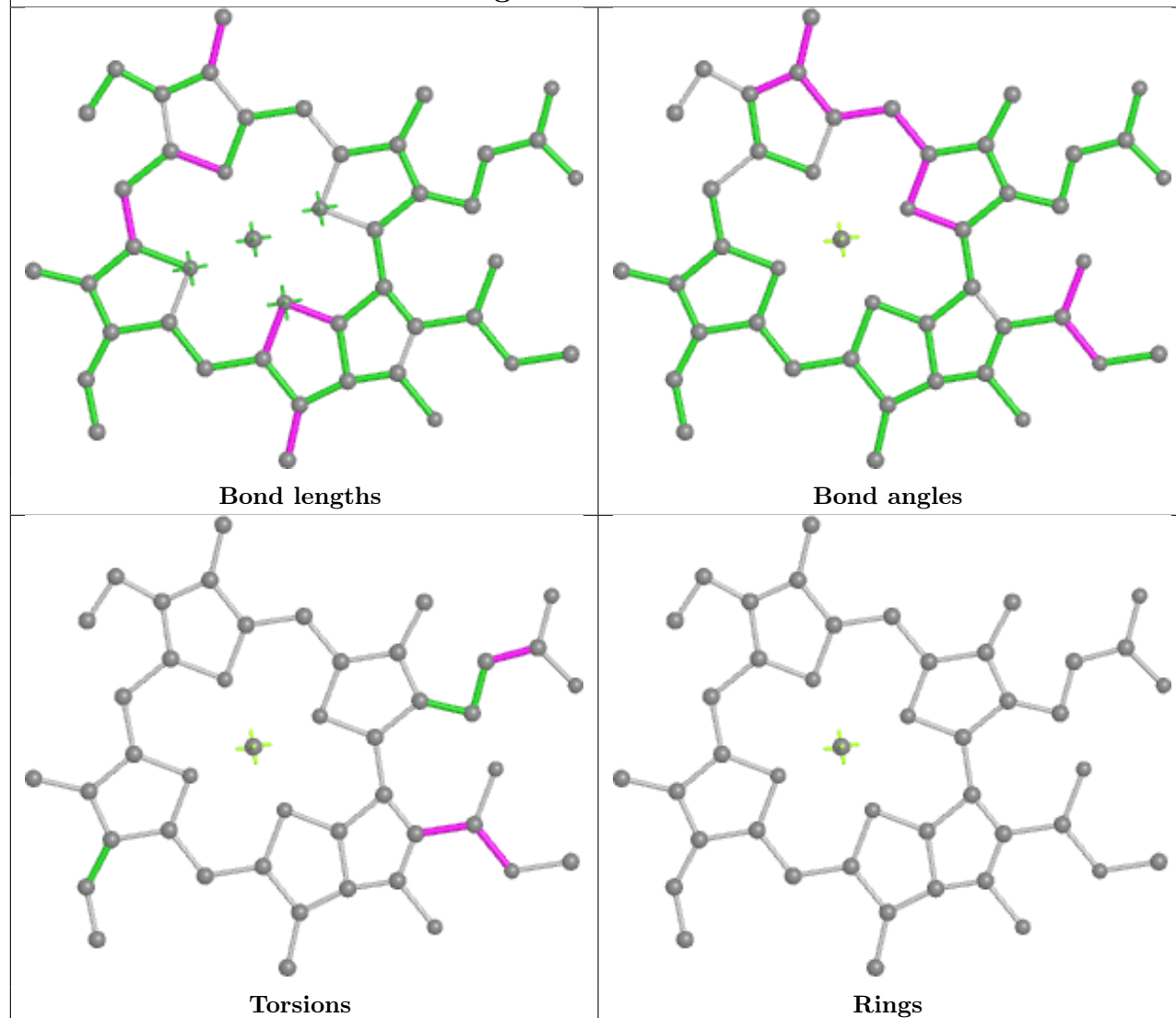


Ligand CHL A2 609

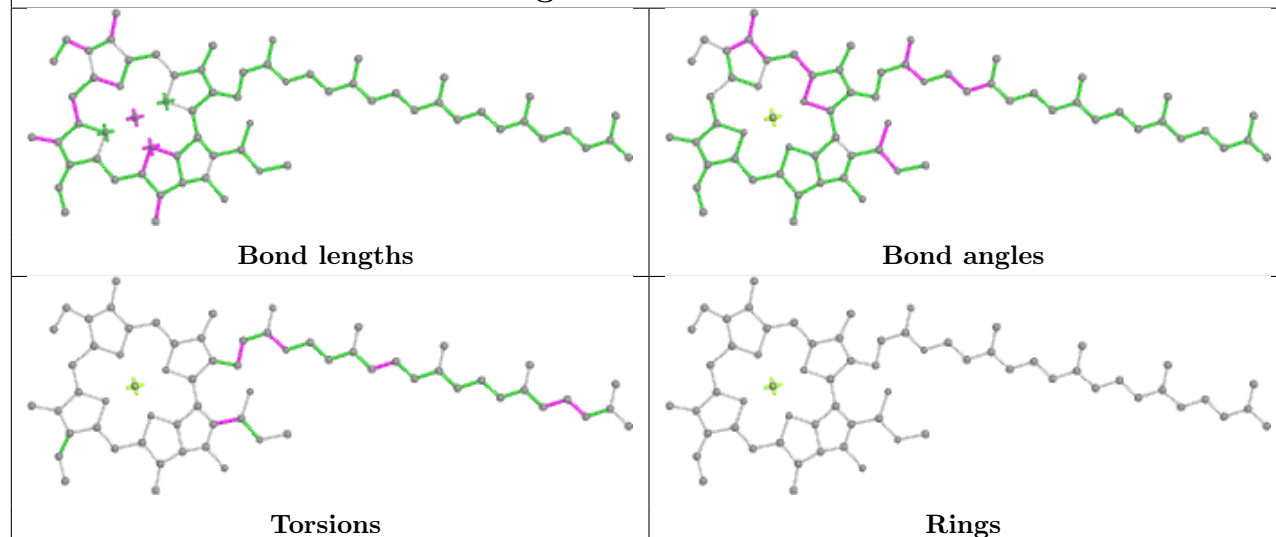


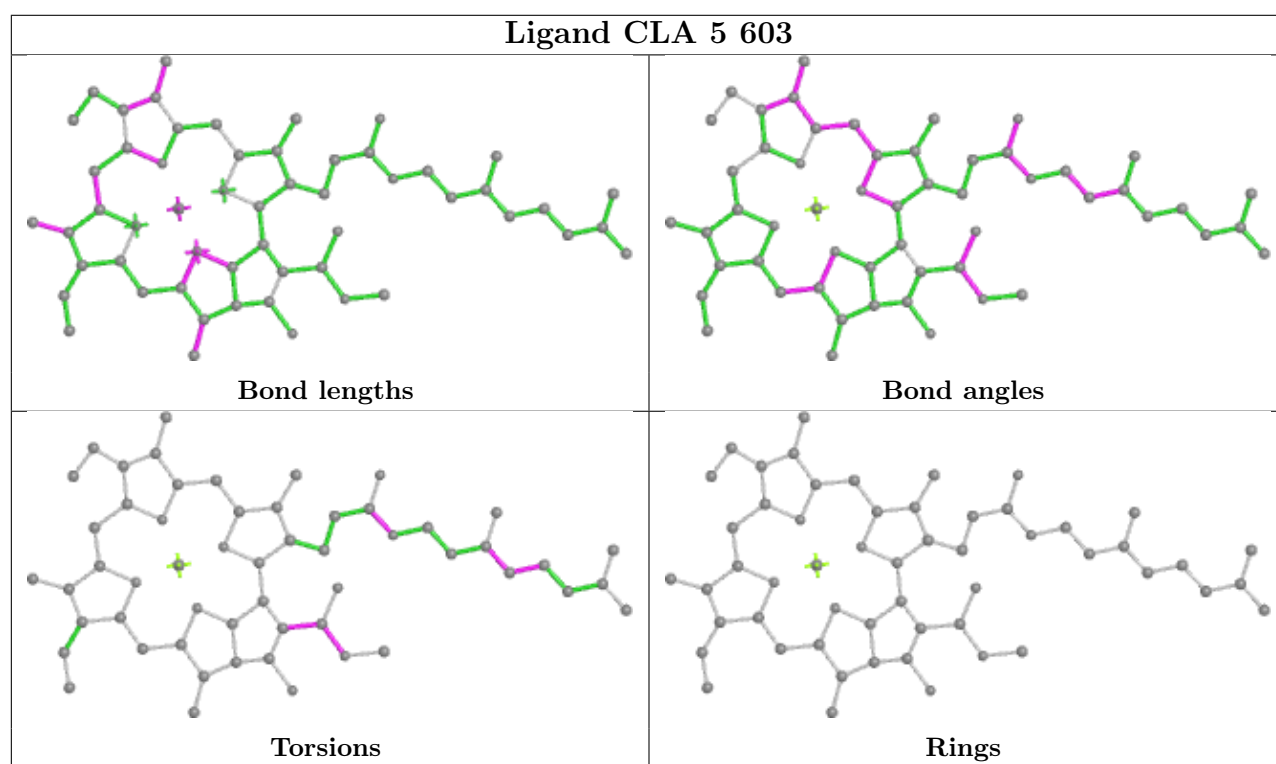
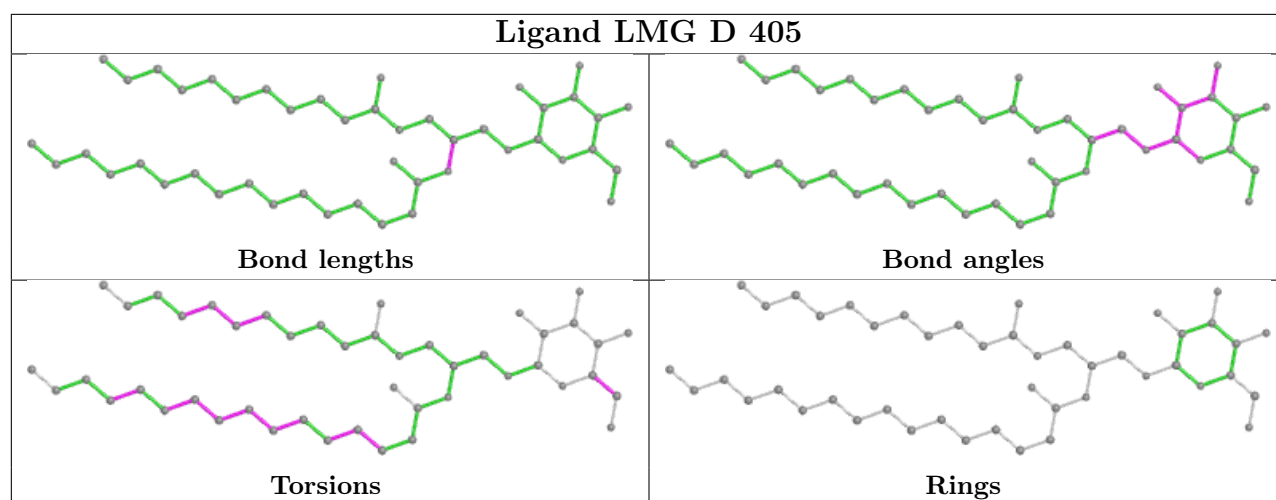


Ligand CLA 7 313

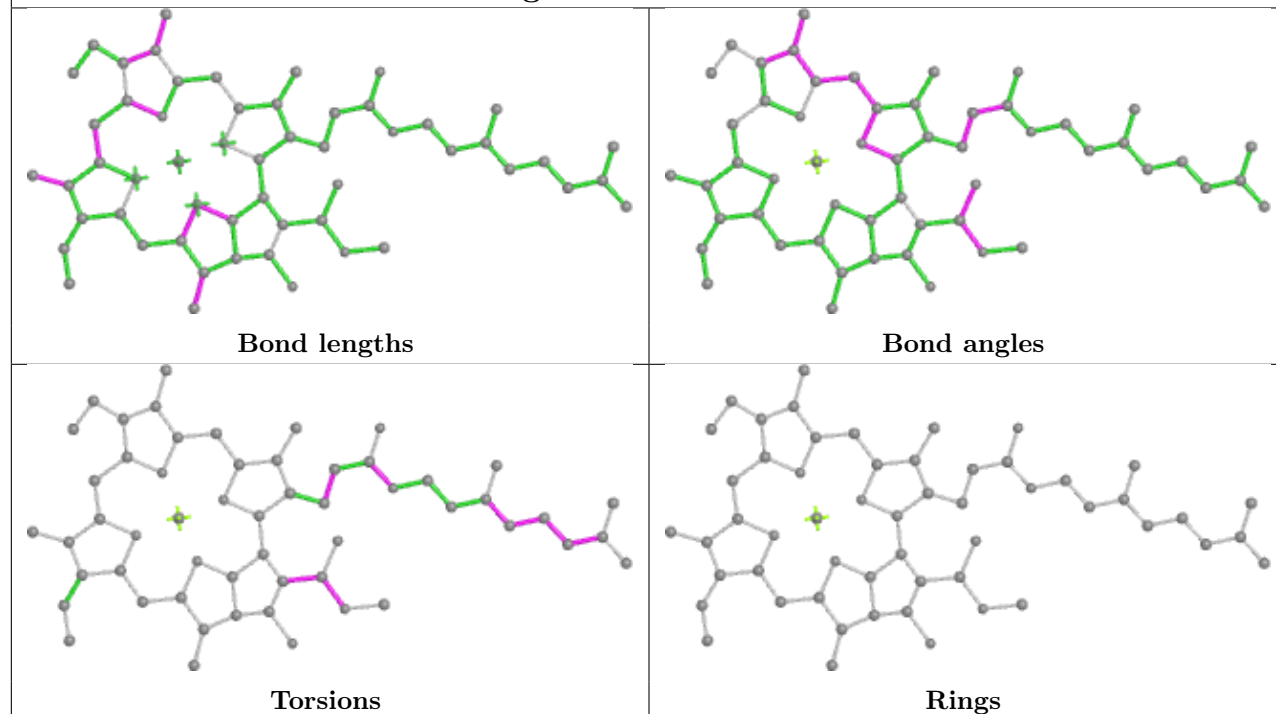


Ligand CLA a 405

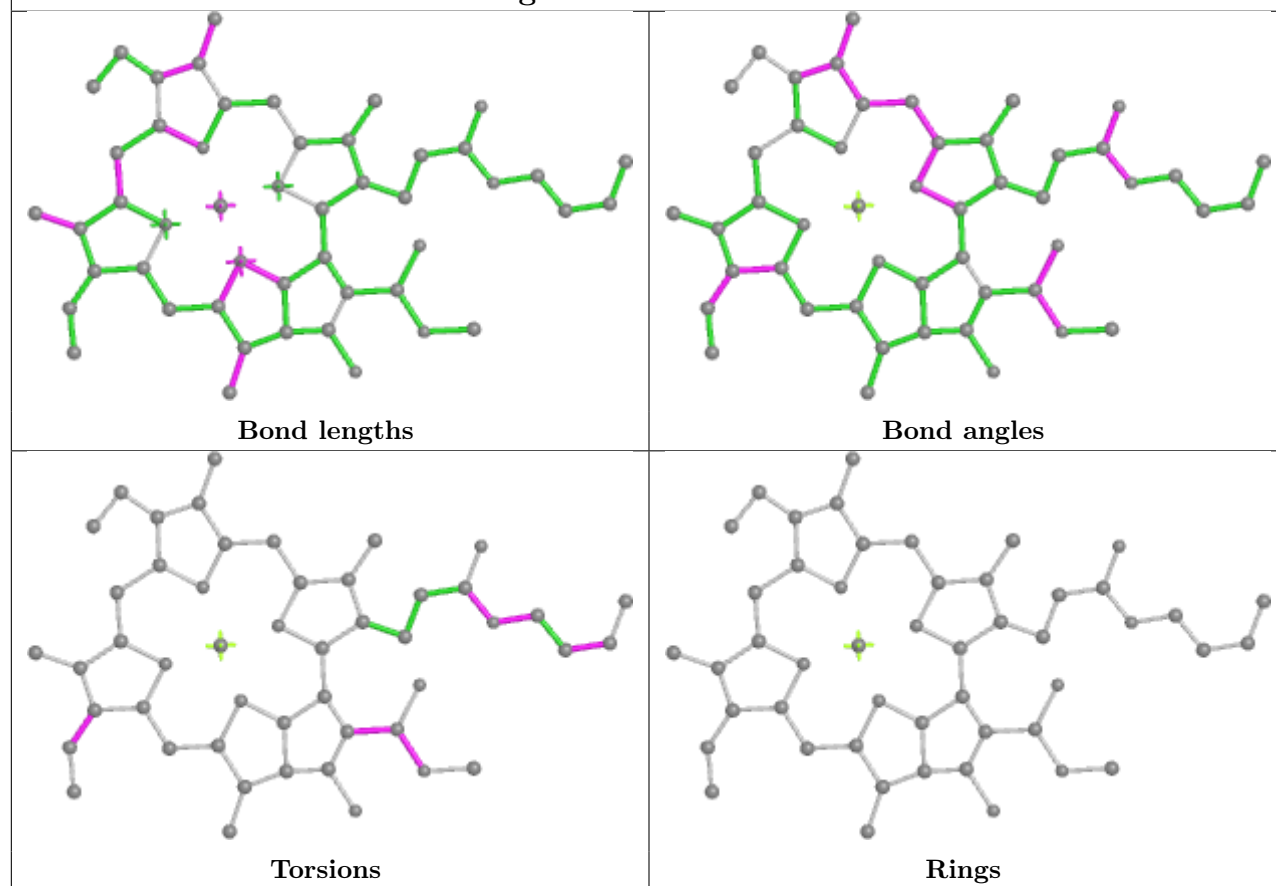


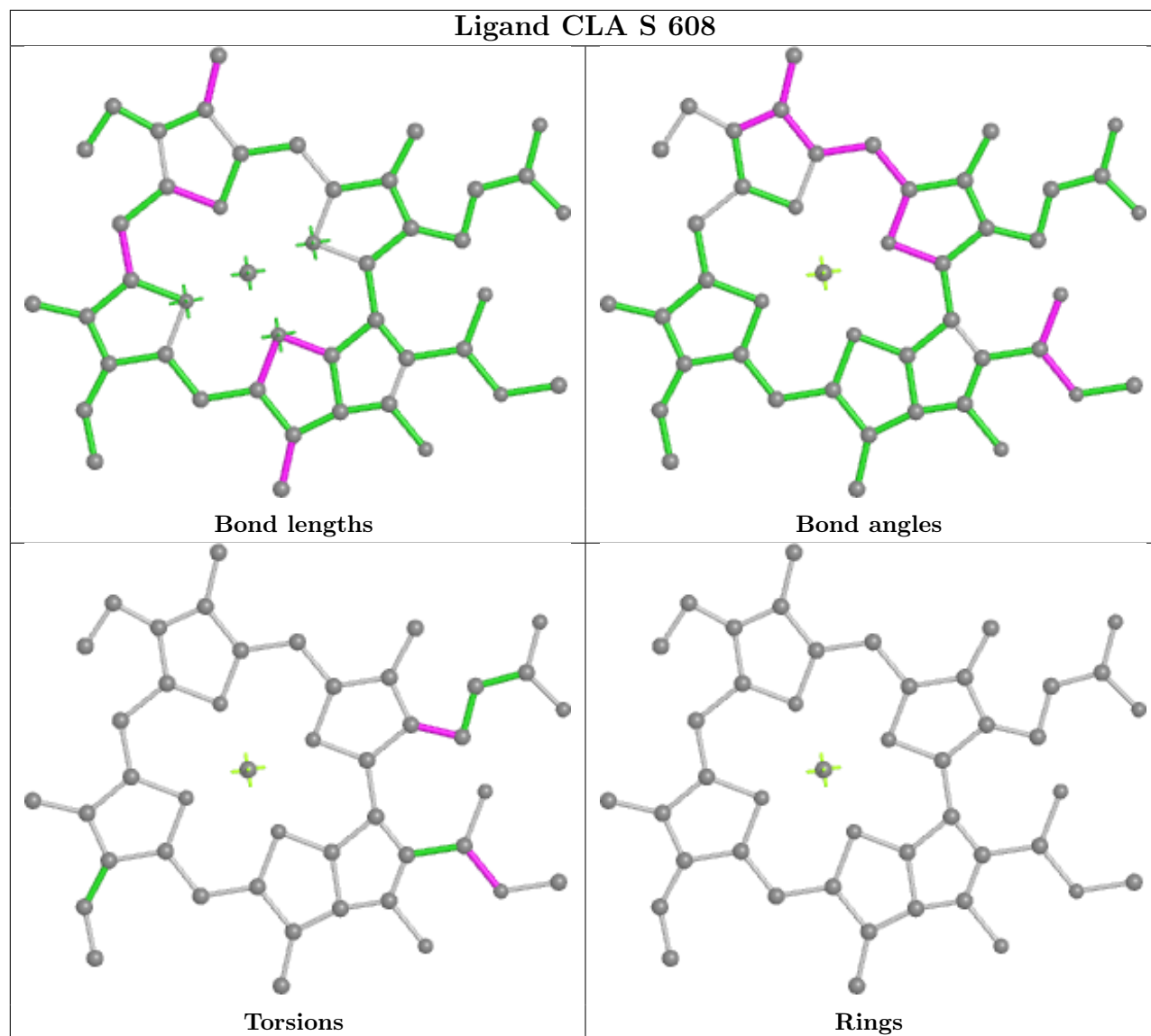
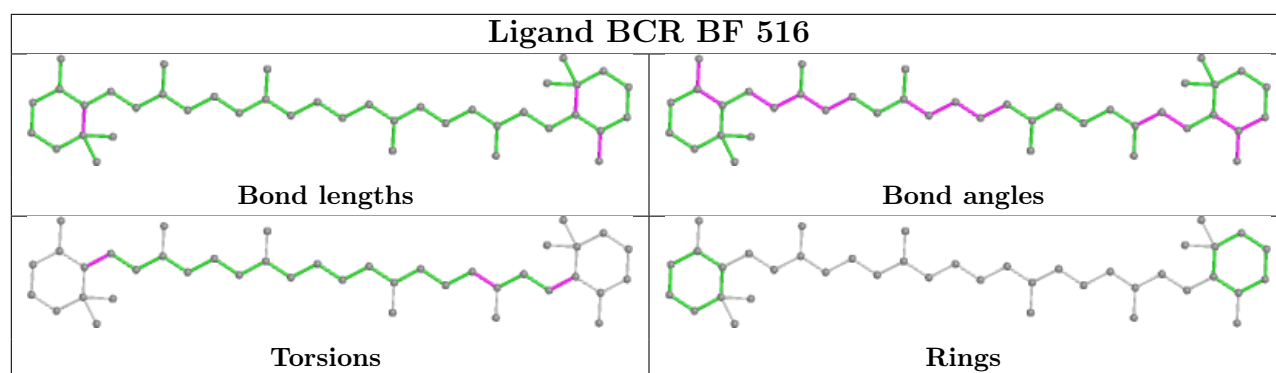


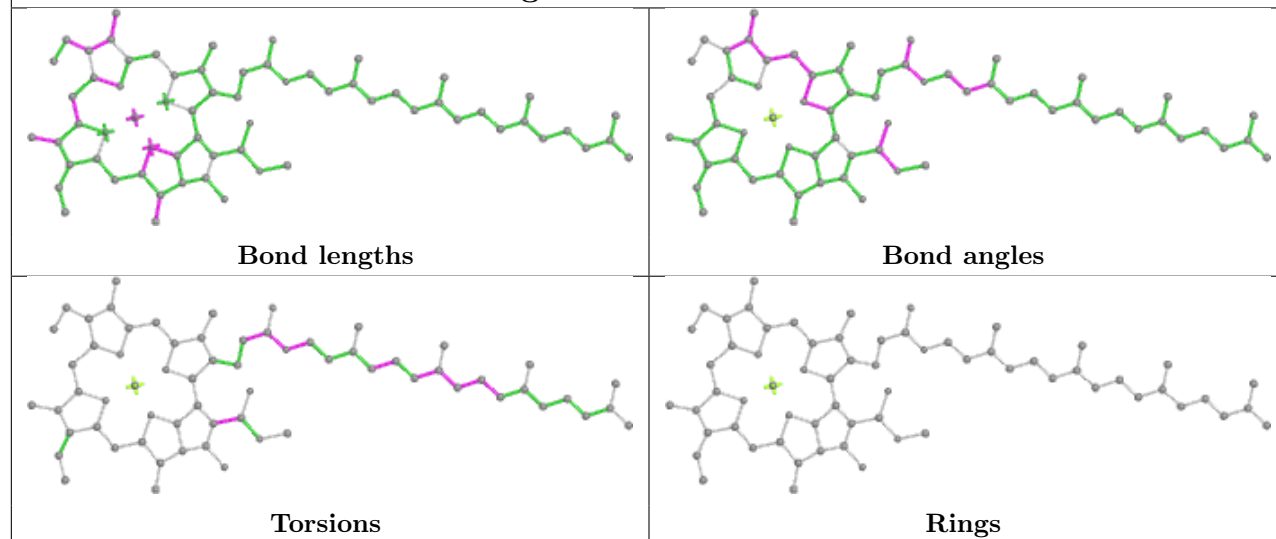
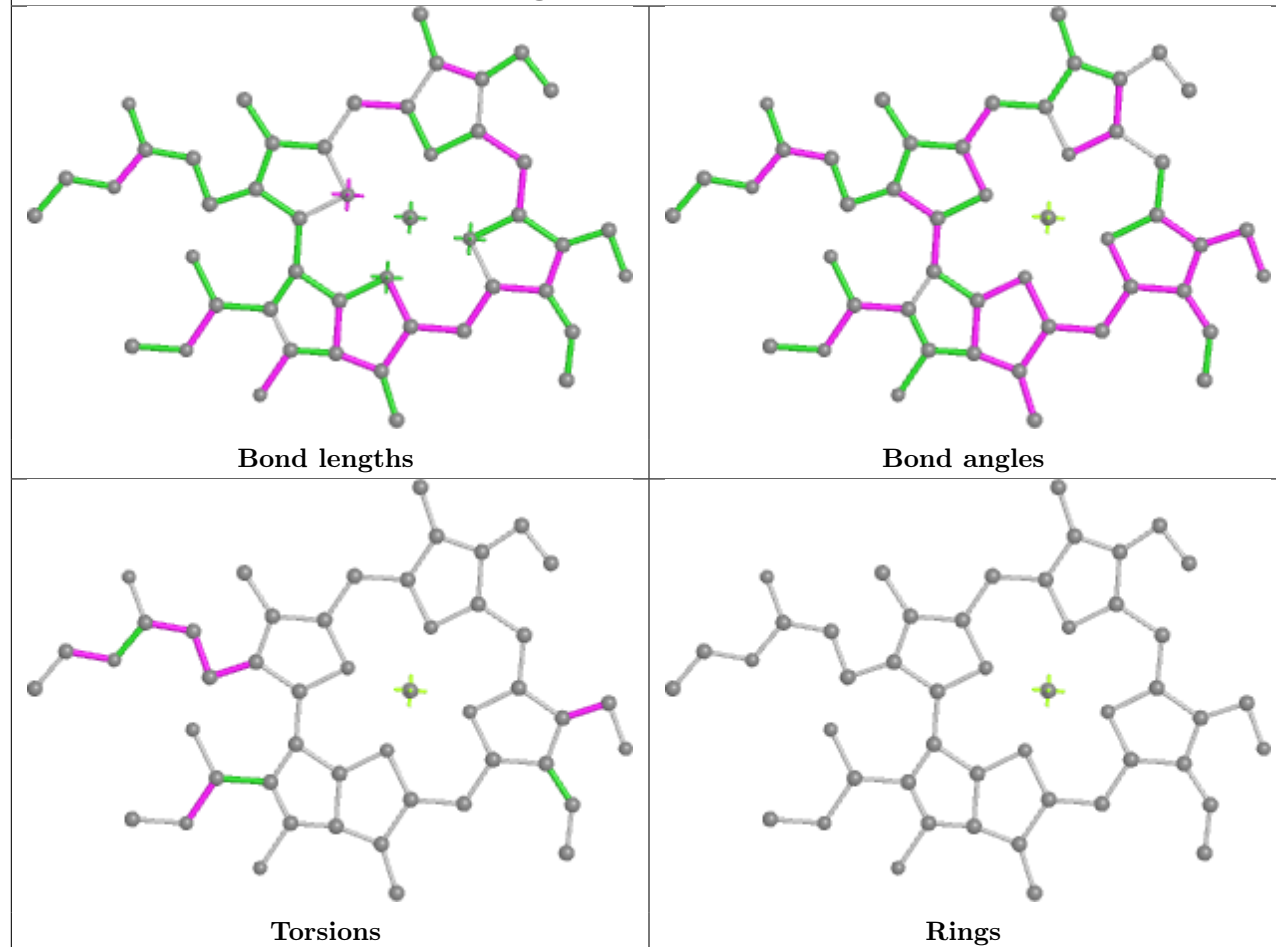
Ligand CLA A6 612

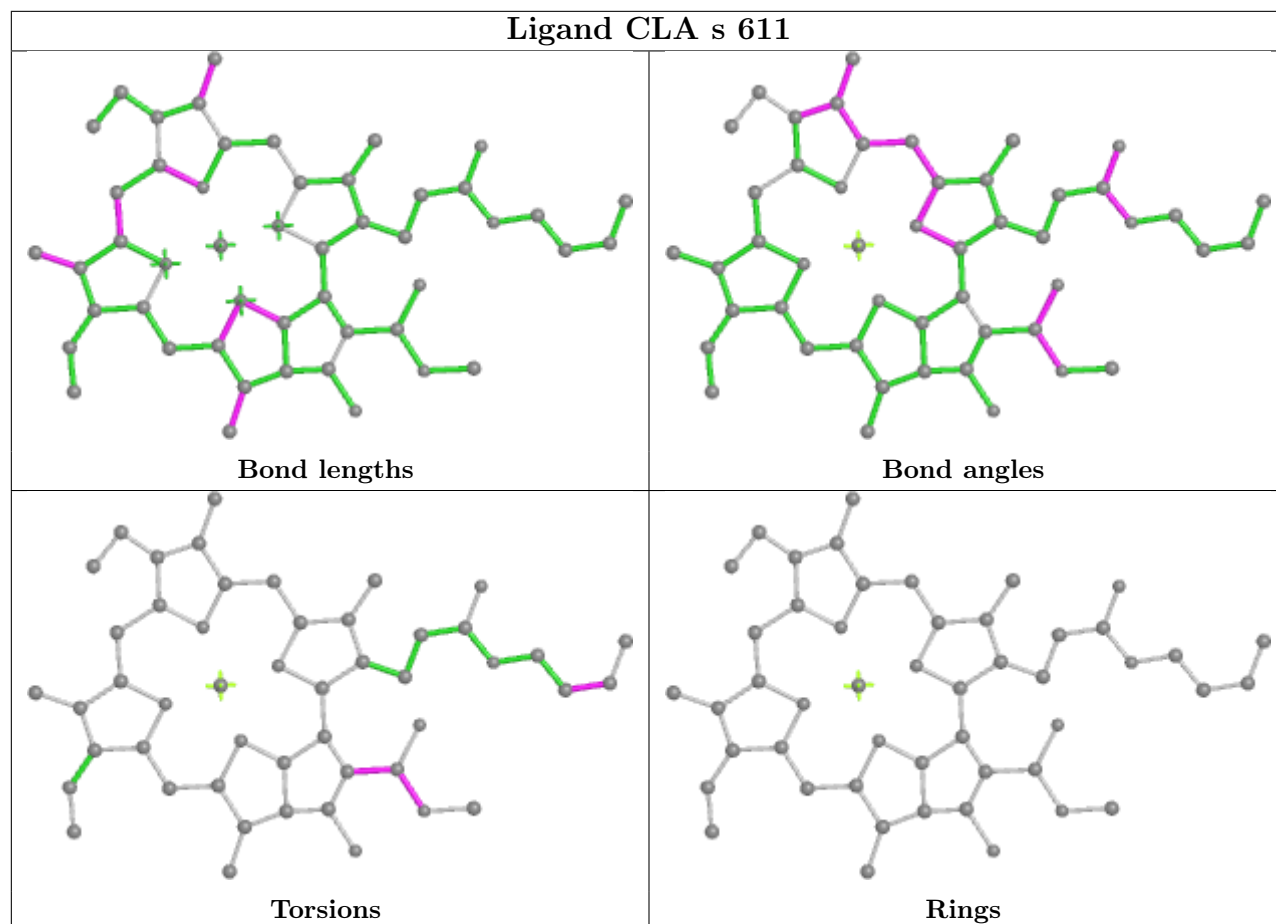
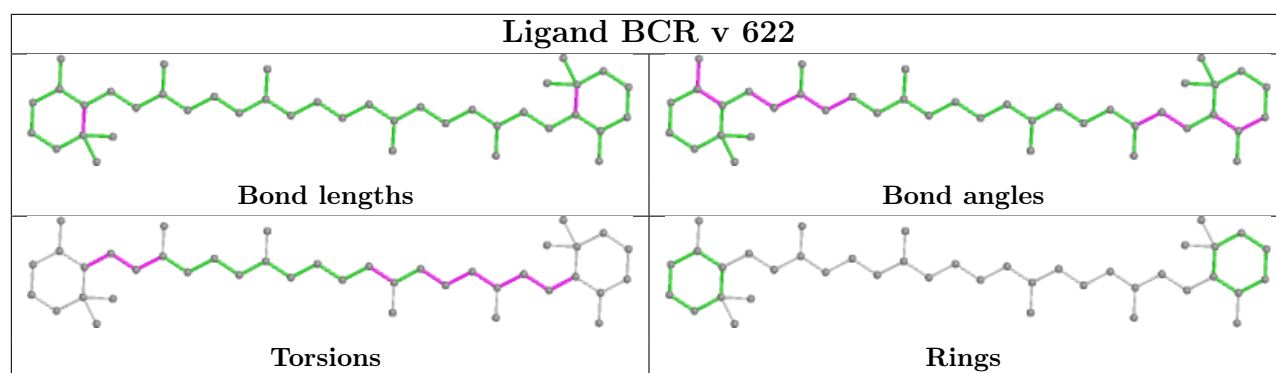


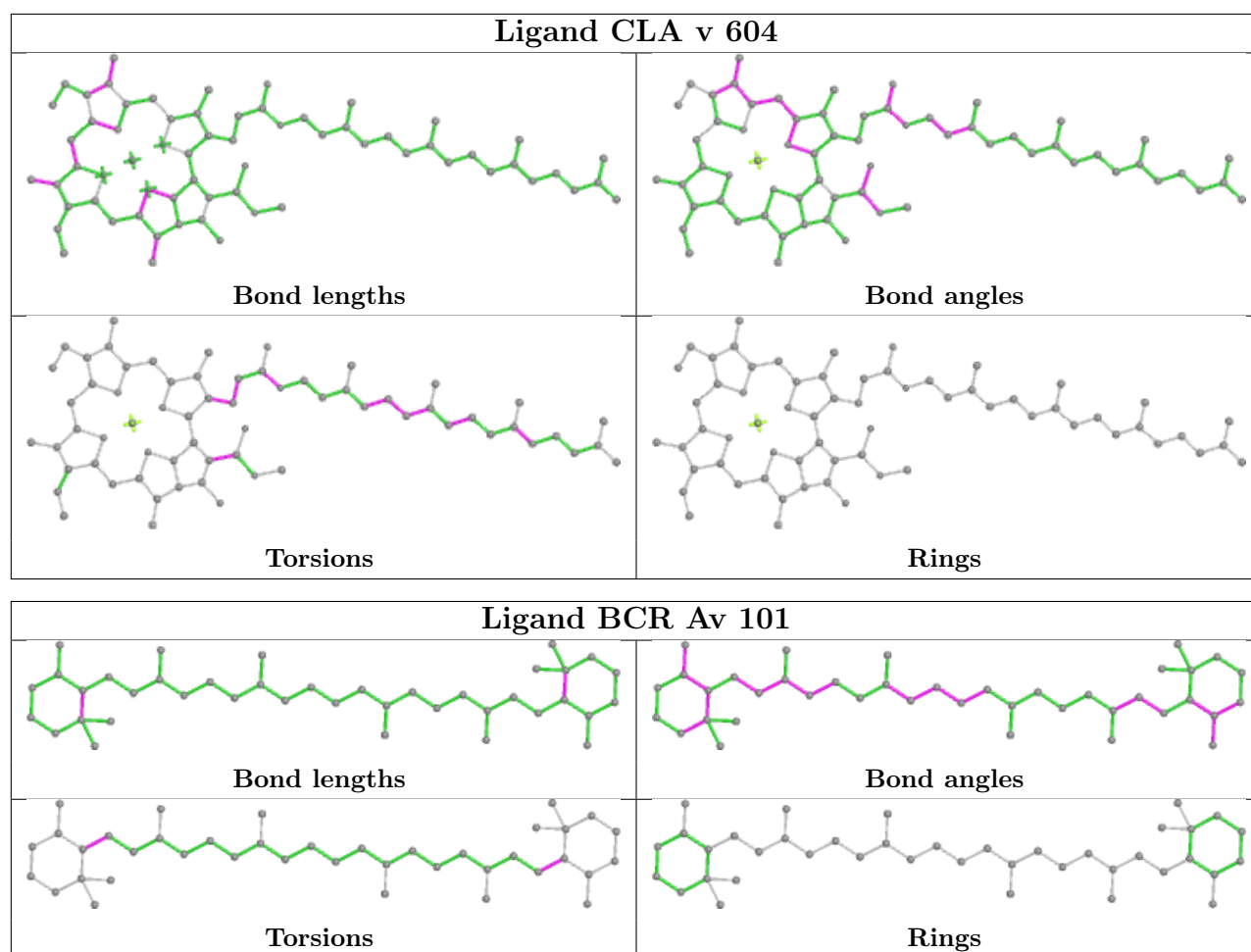
Ligand CLA BU 601



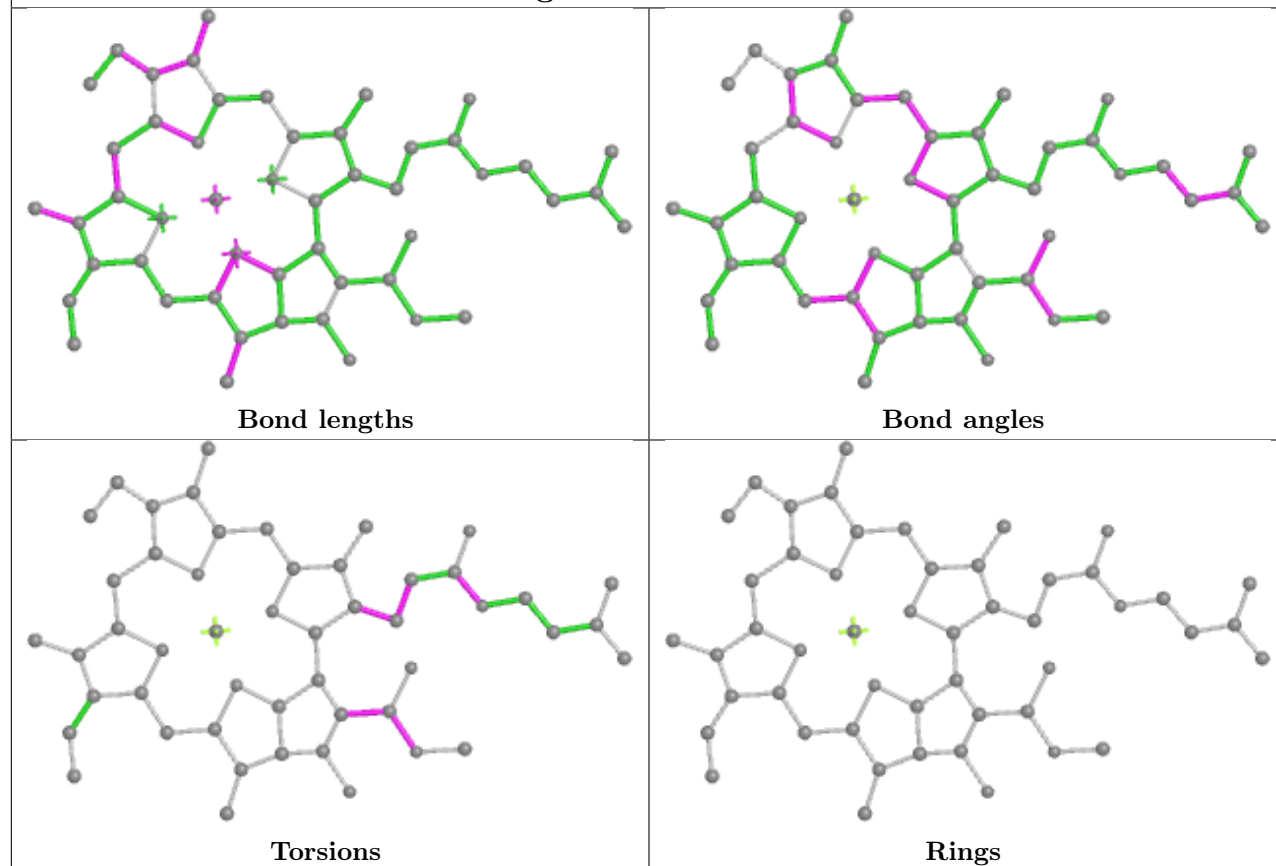


Ligand CLA BF 513**Ligand CHL N 605**

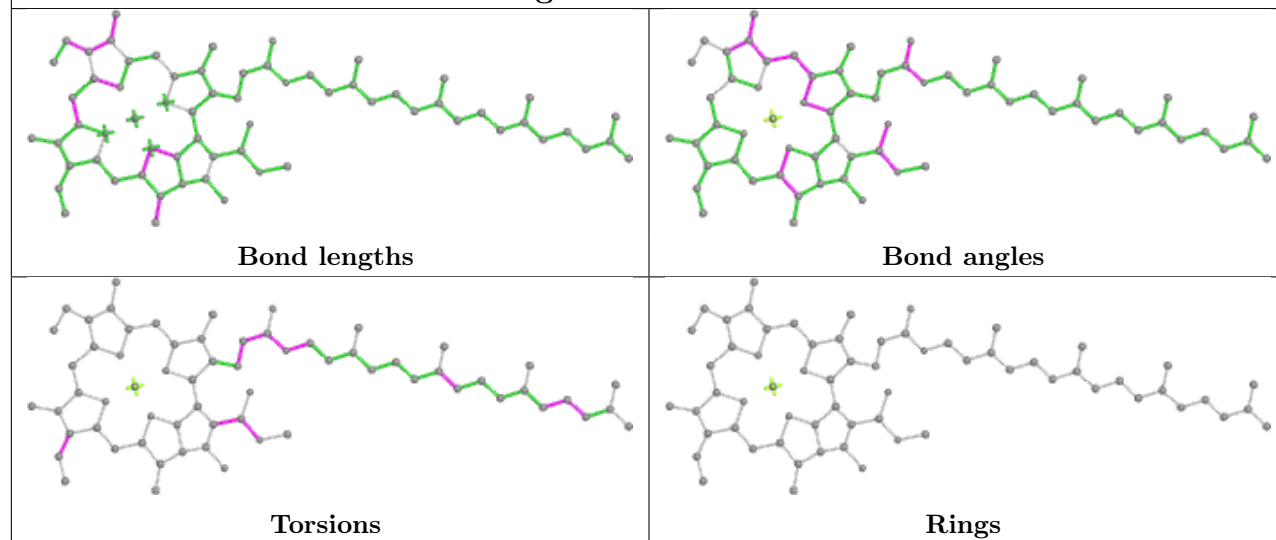


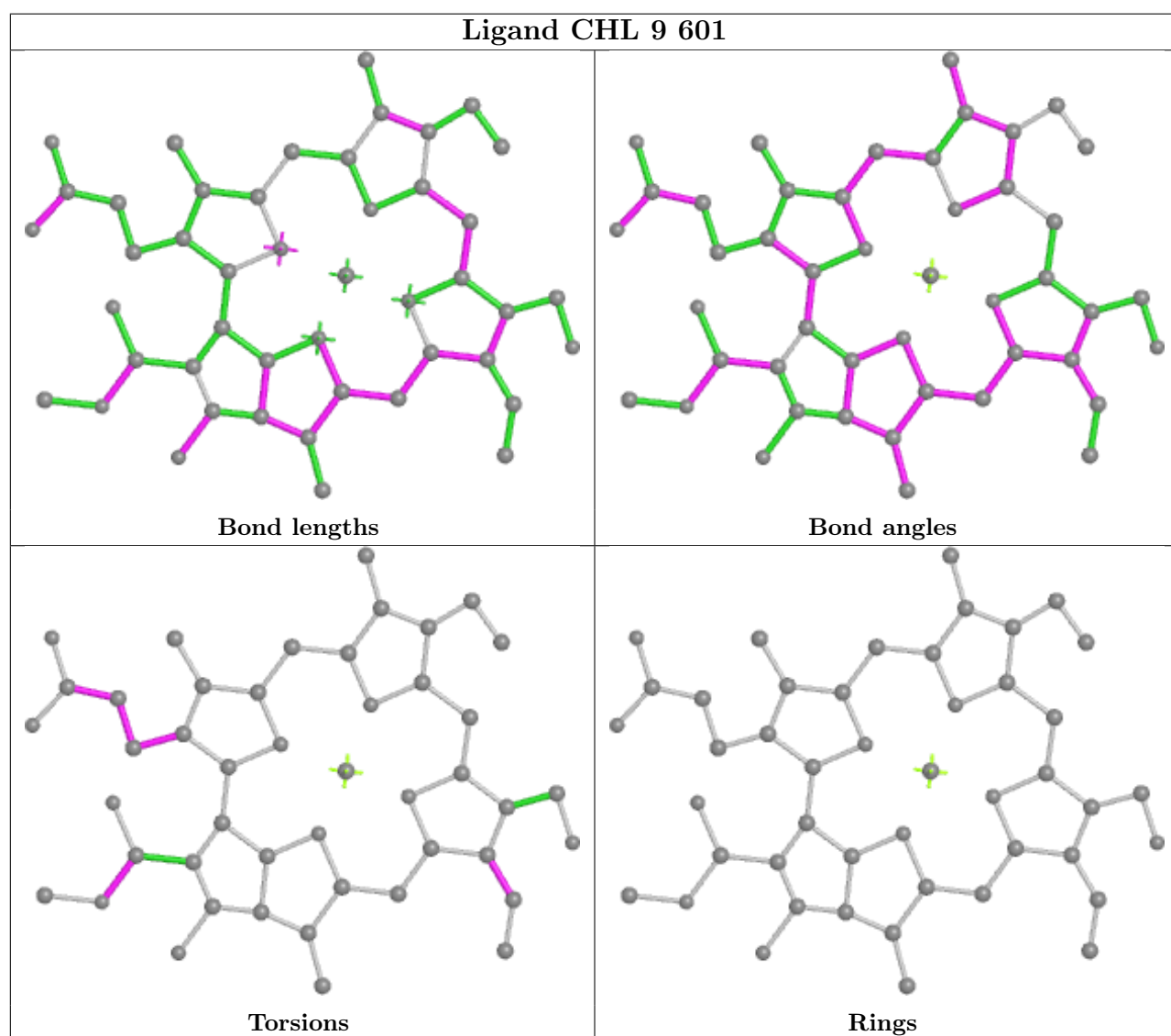
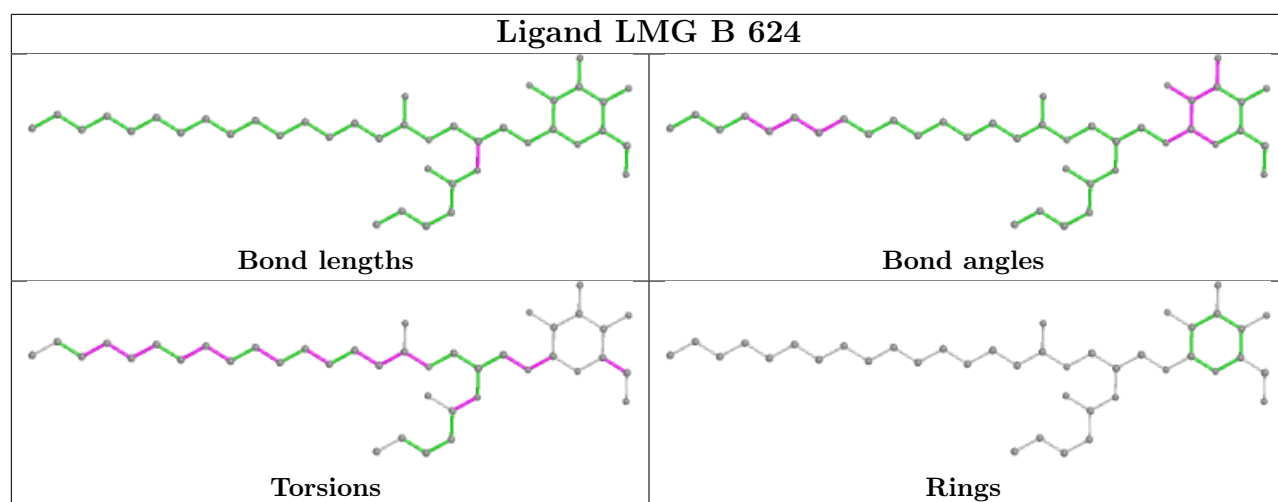


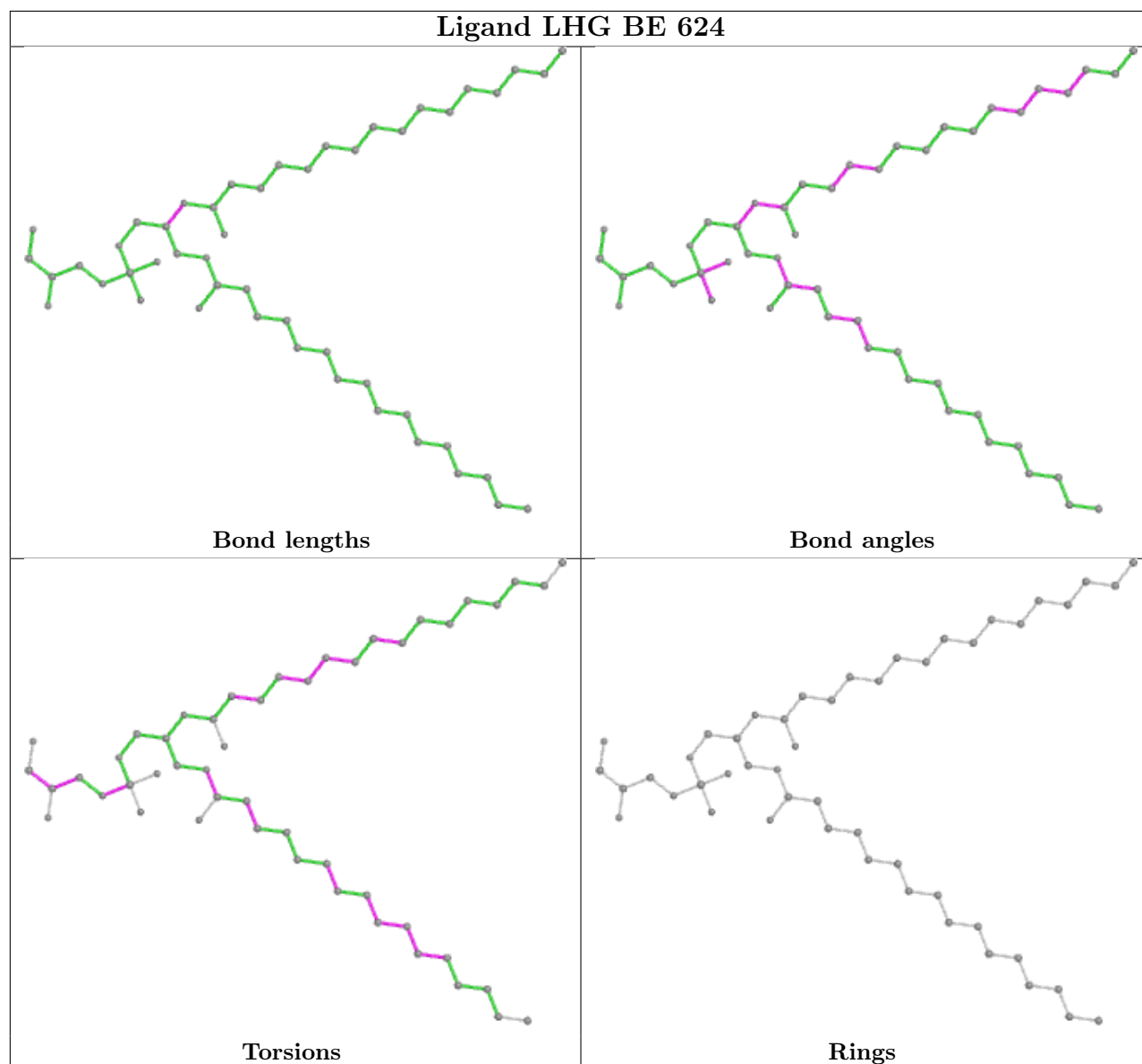
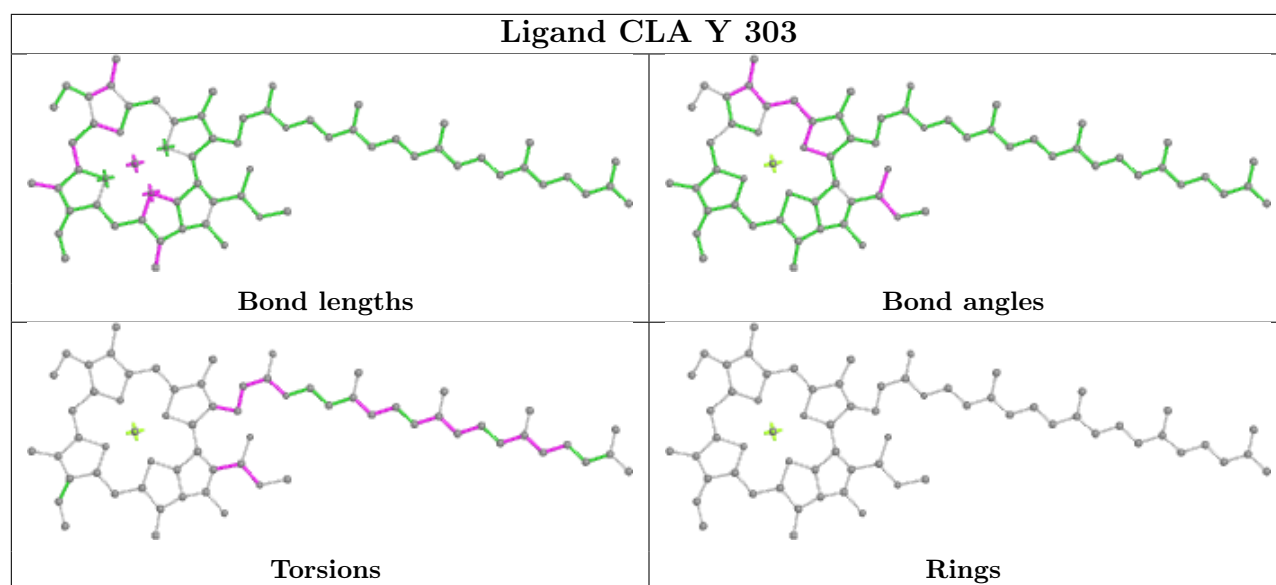
Ligand CLA 9 604

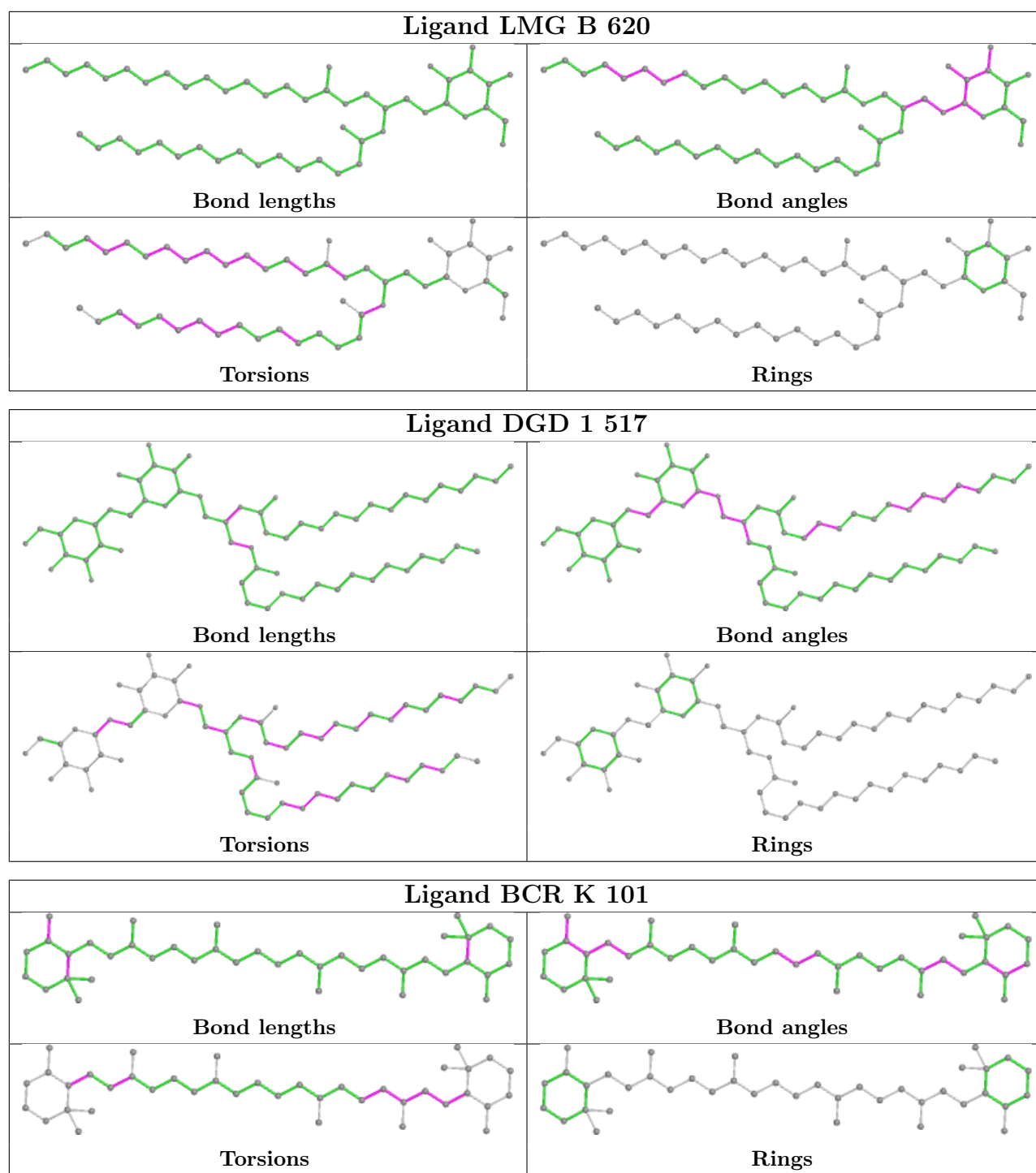


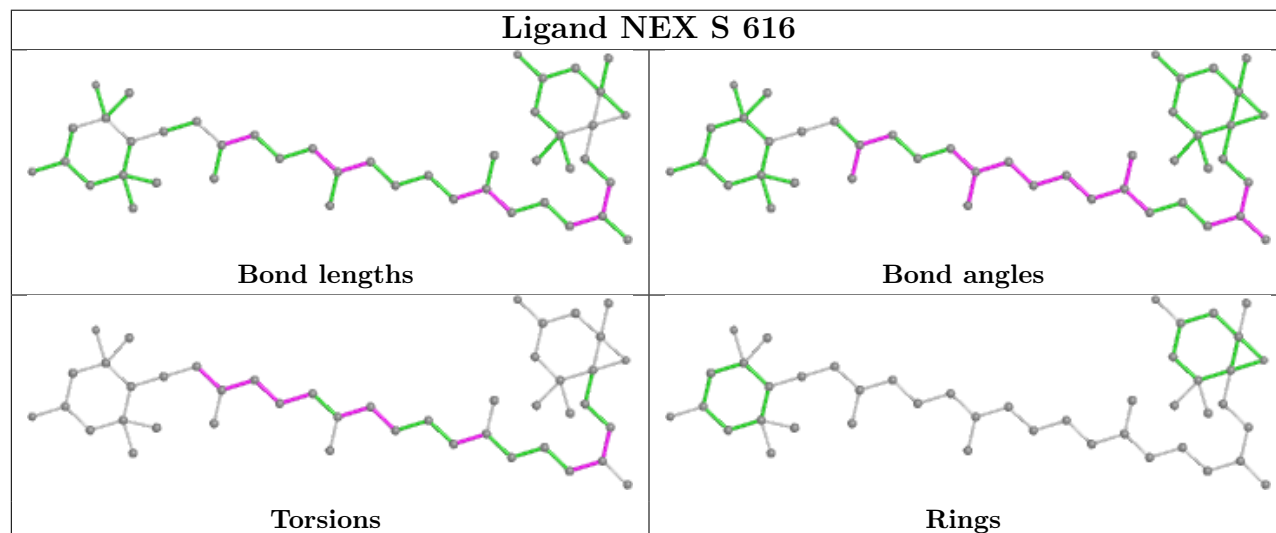
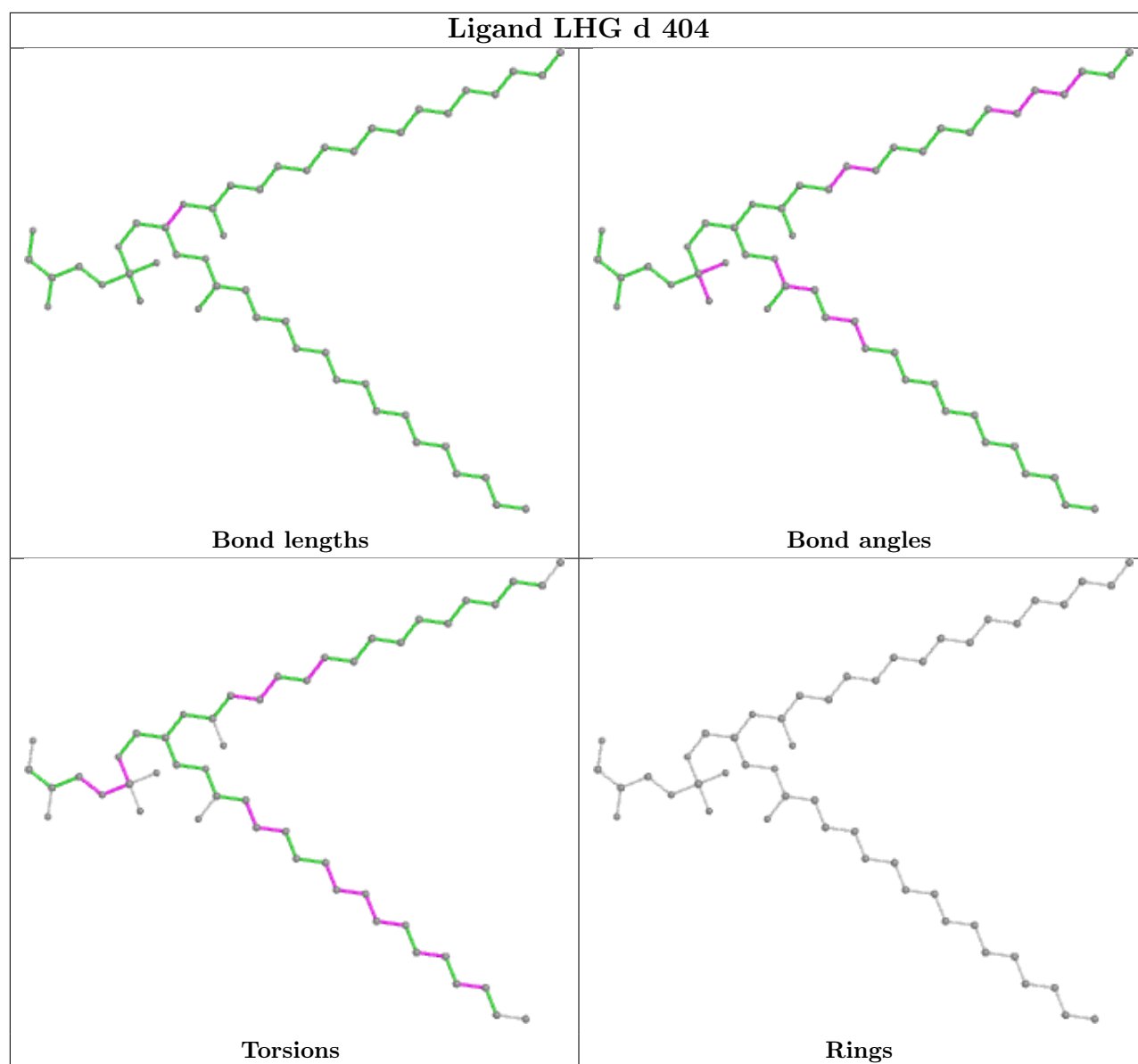
Ligand CLA v 610

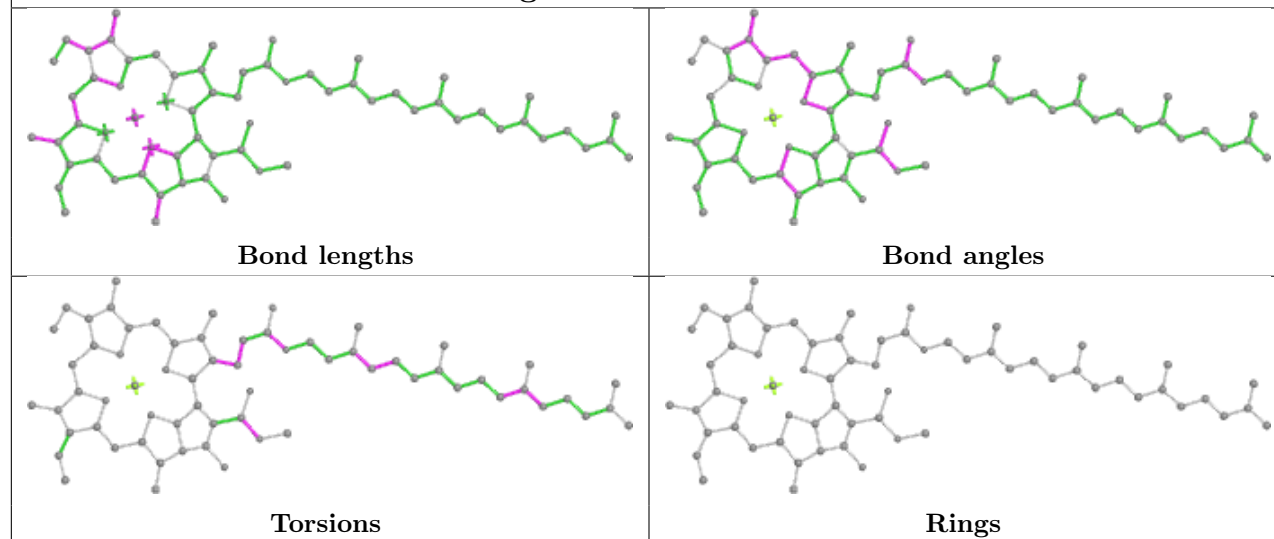
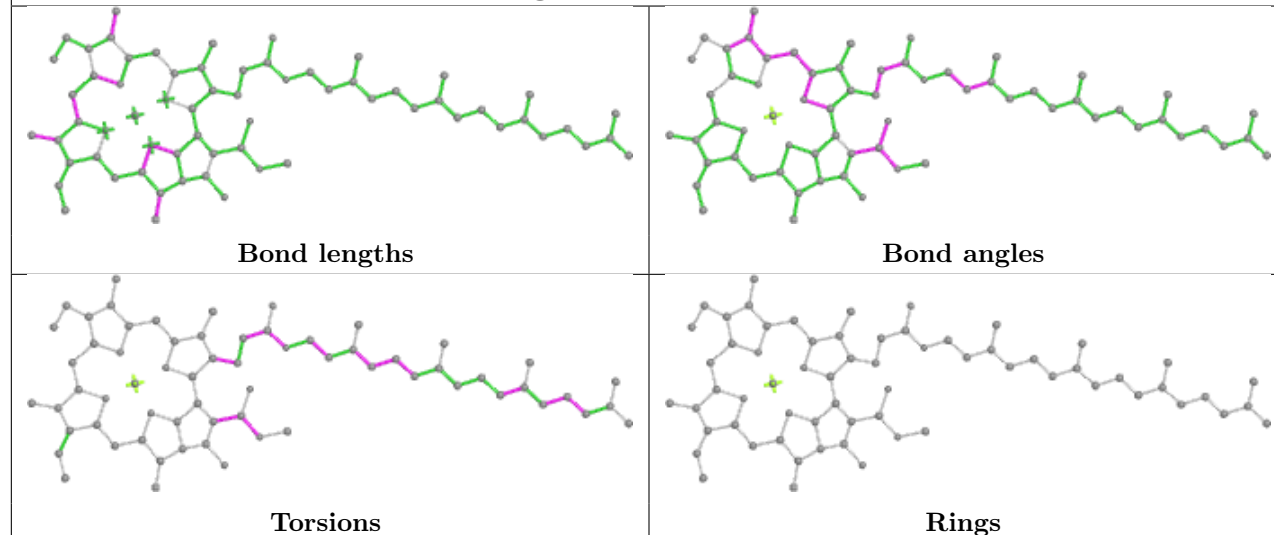
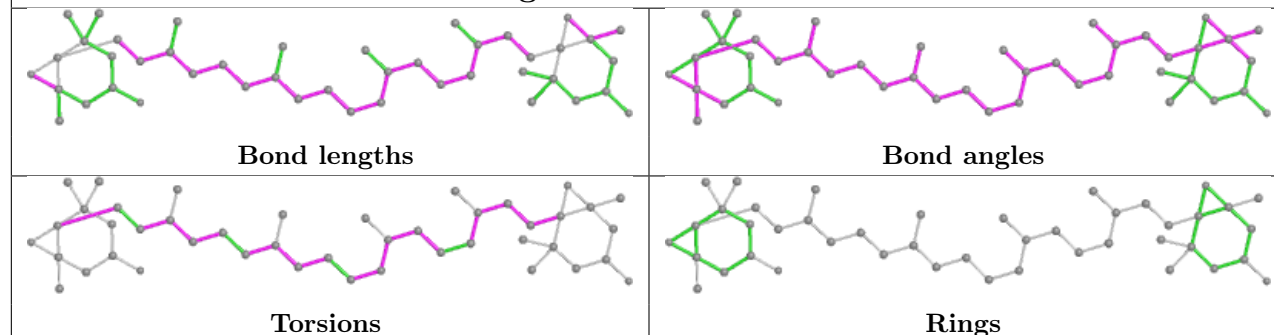




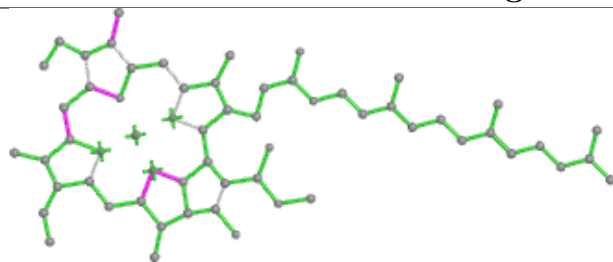




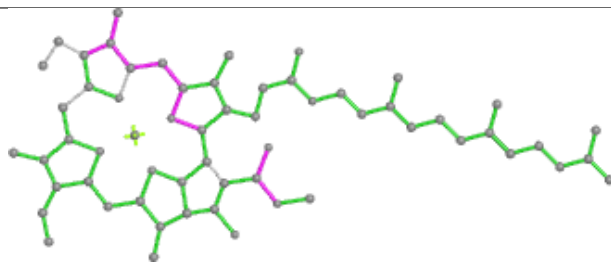


Ligand CLA BB 314**Ligand CLA N 610****Ligand XAT BB 301**

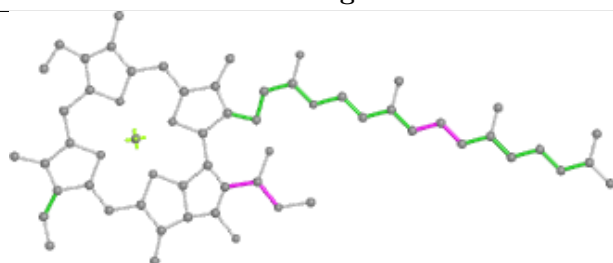
Ligand CLA BJ 612



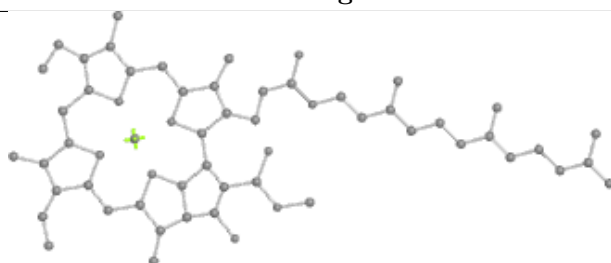
Bond lengths



Bond angles

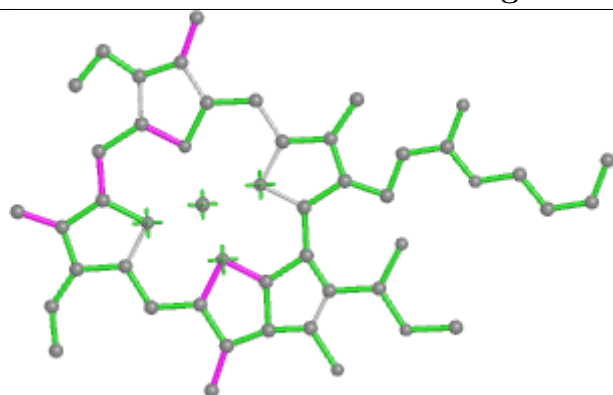


Torsions

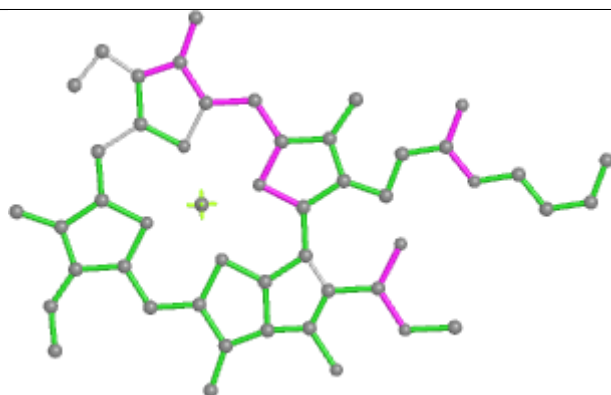


Rings

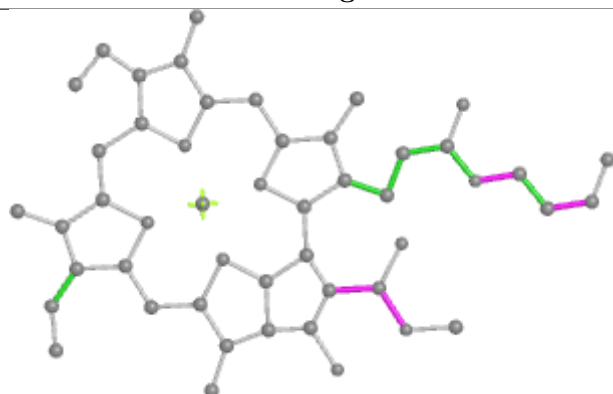
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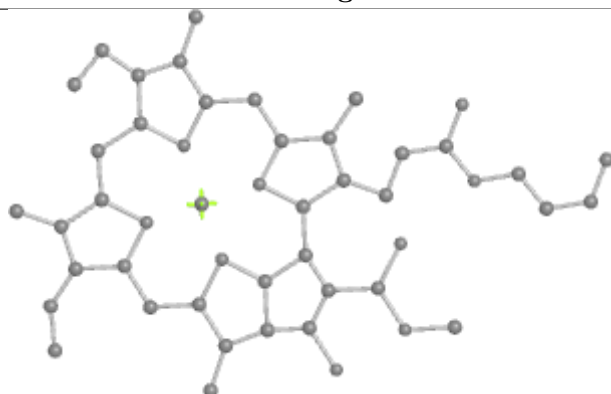
Bond lengths



Bond angles

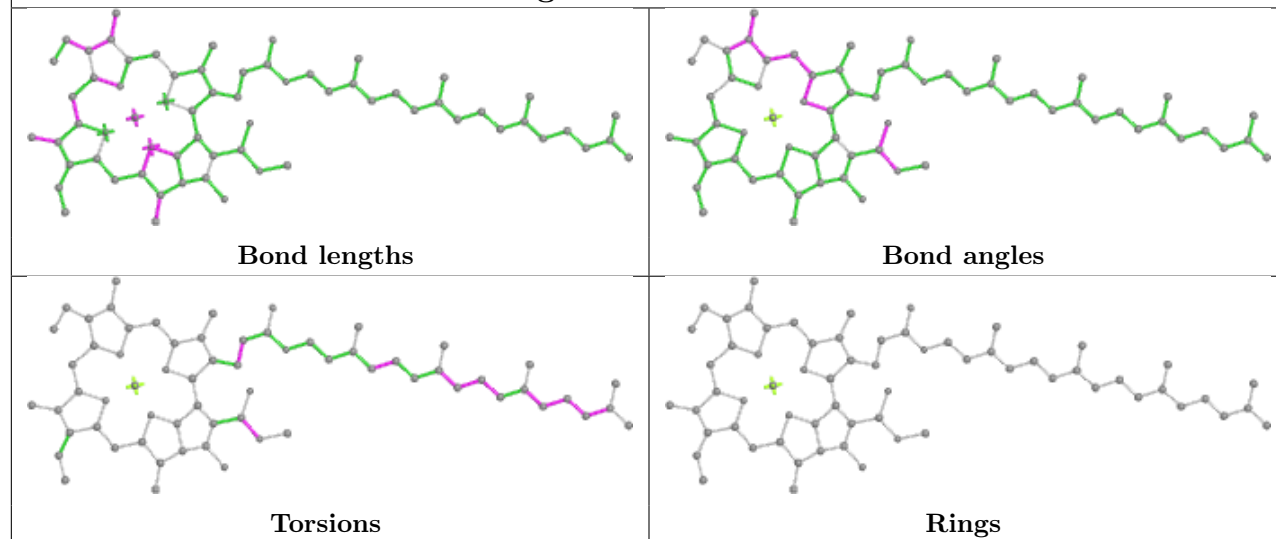


Torsions

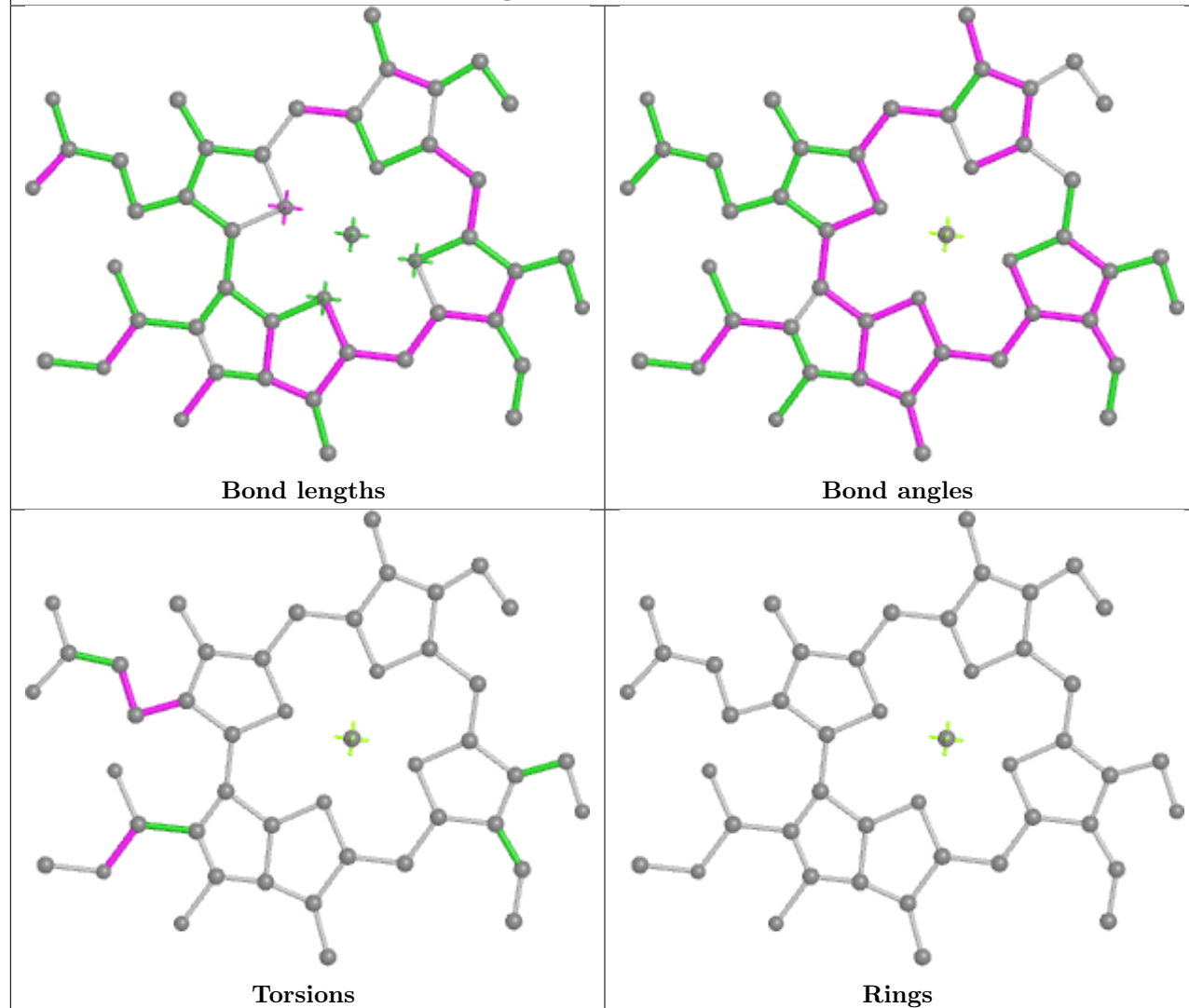


Rings

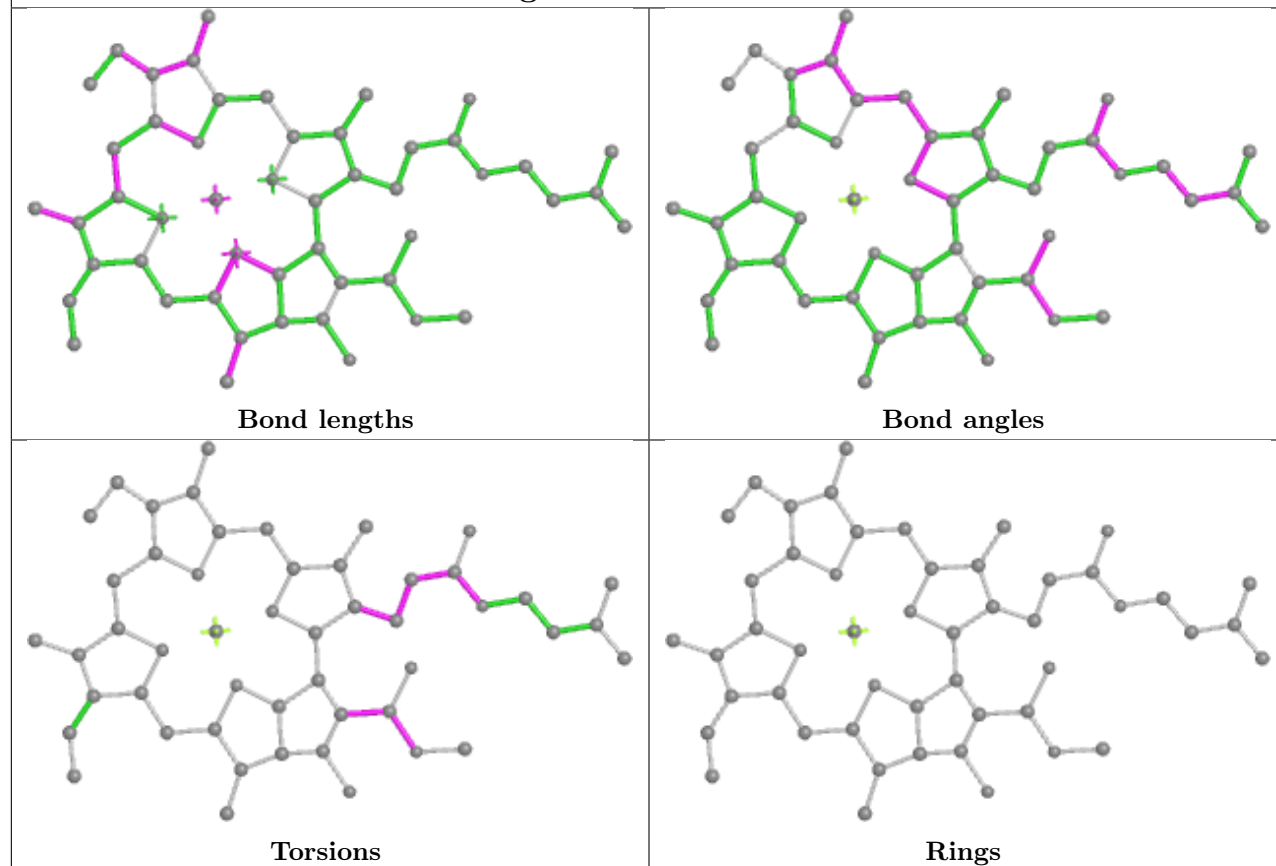
Ligand CLA c 508



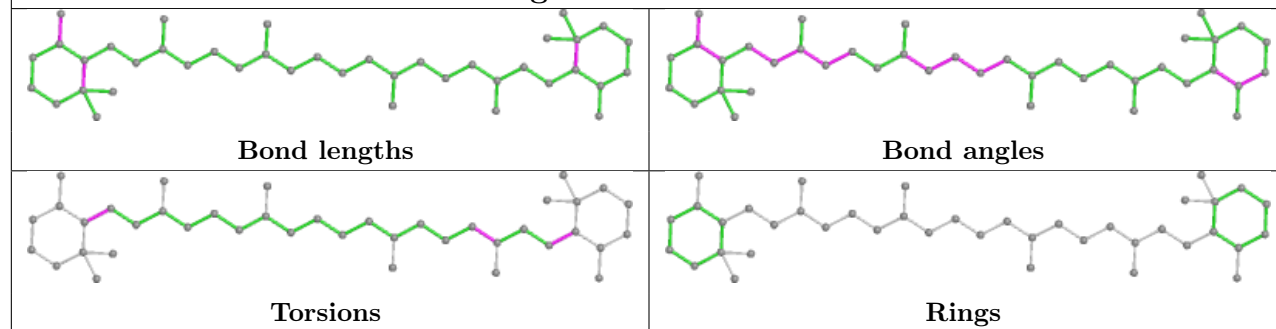
Ligand CHL 5 605



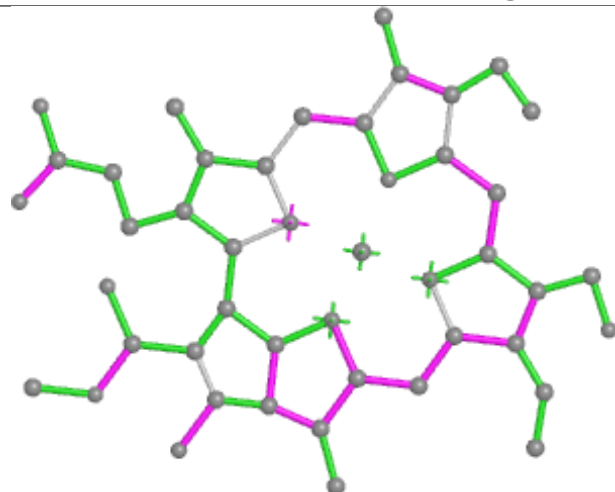
Ligand CLA BB 305



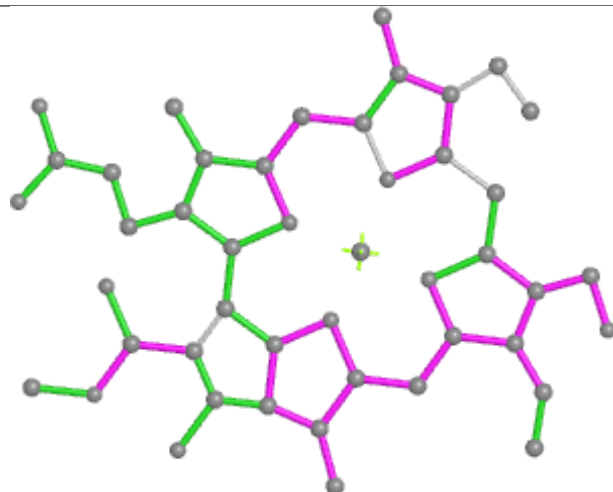
Ligand BCR C 515



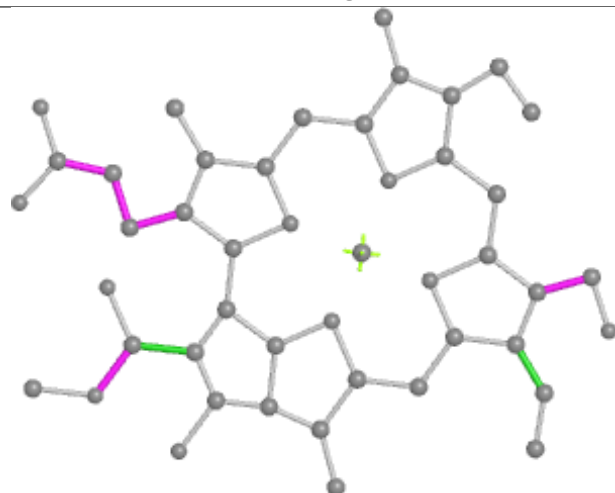
Ligand CHL AA 309



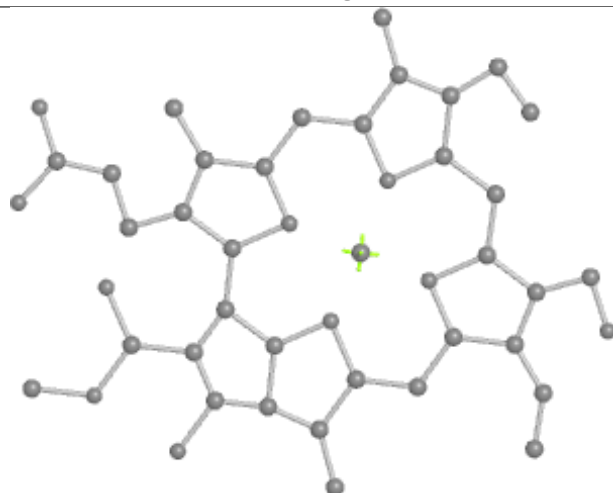
Bond lengths



Bond angles

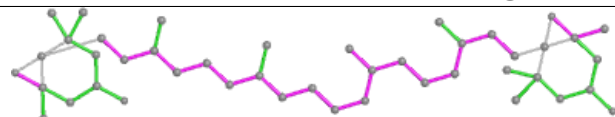


Torsions

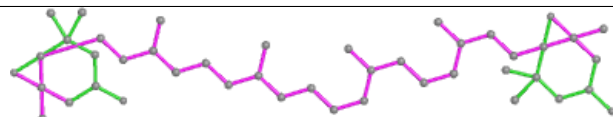


Rings

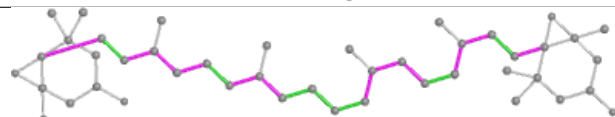
Ligand XAT AA 318



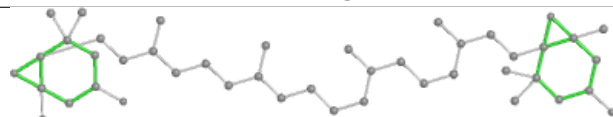
Bond lengths



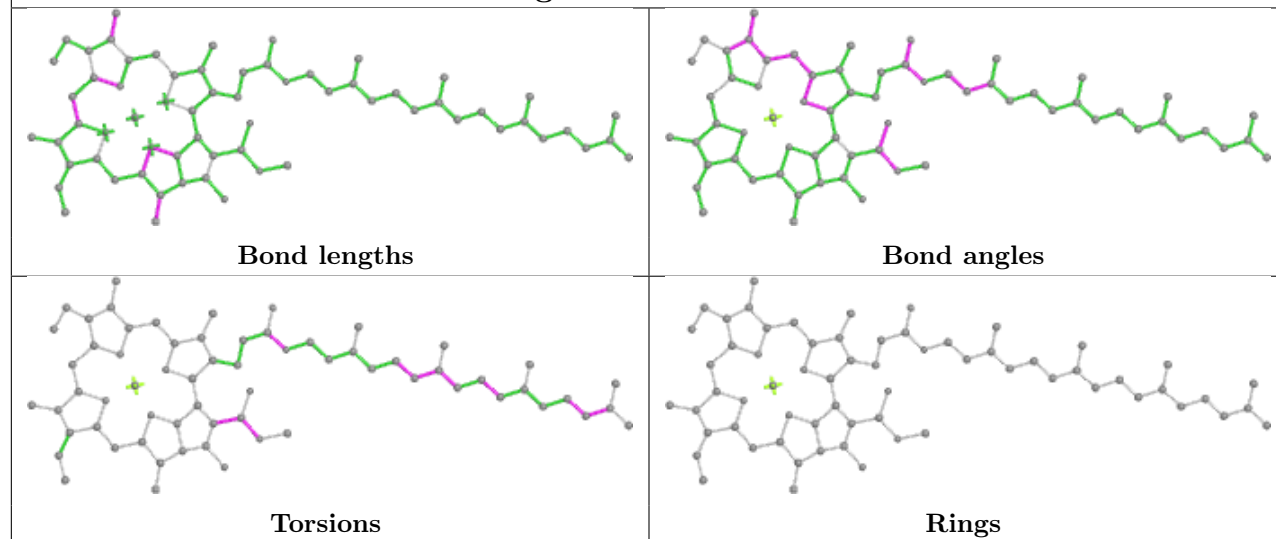
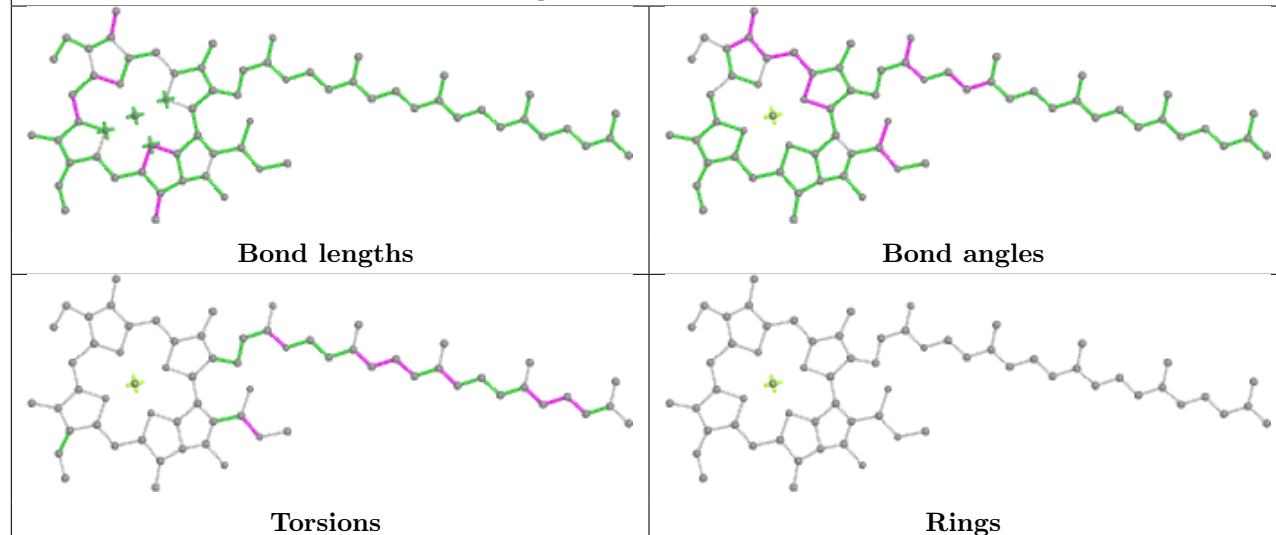
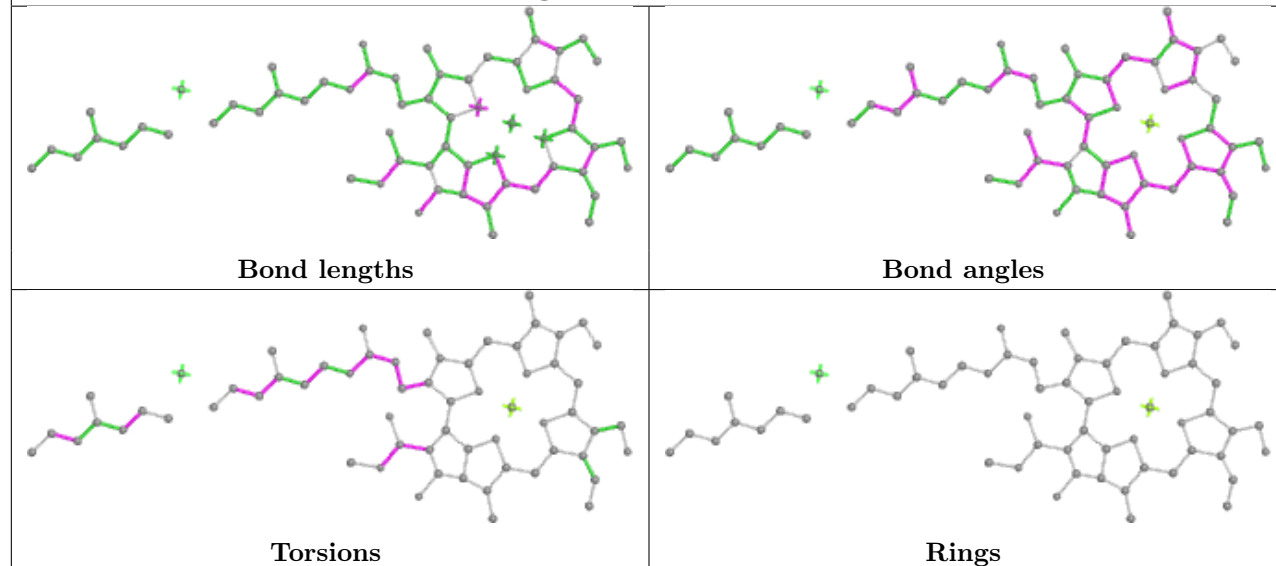
Bond angles

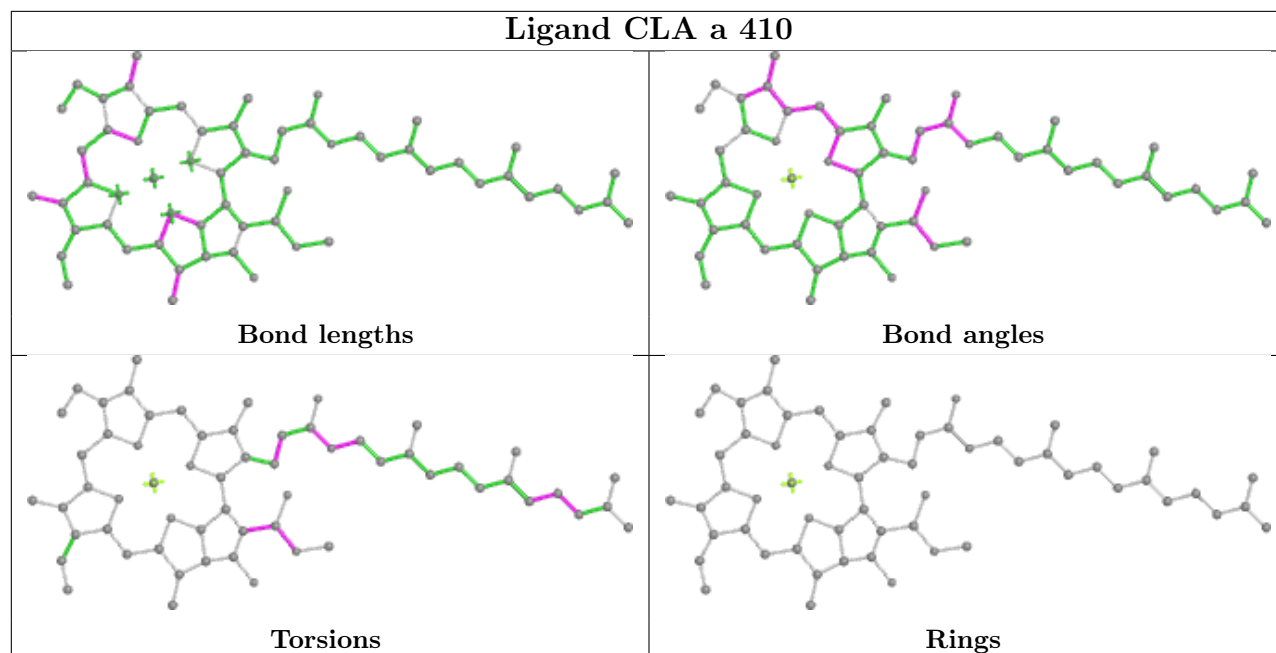
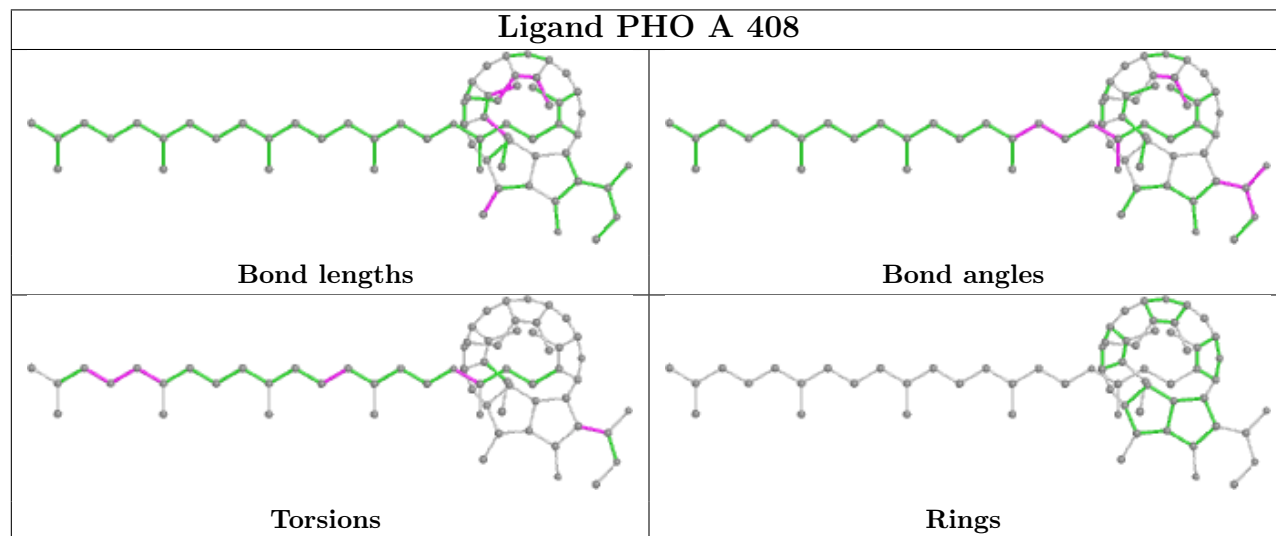


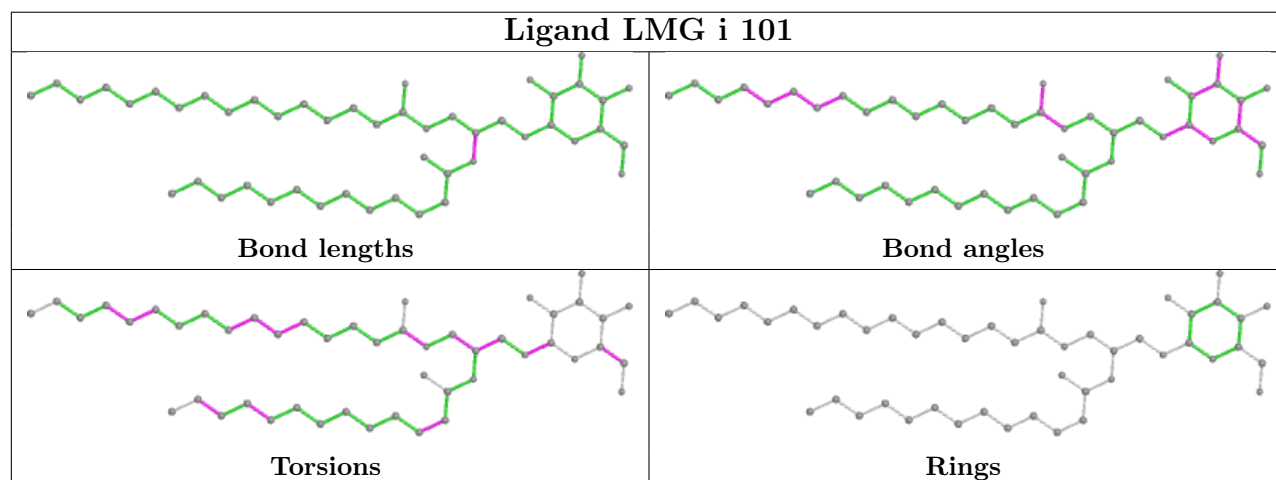
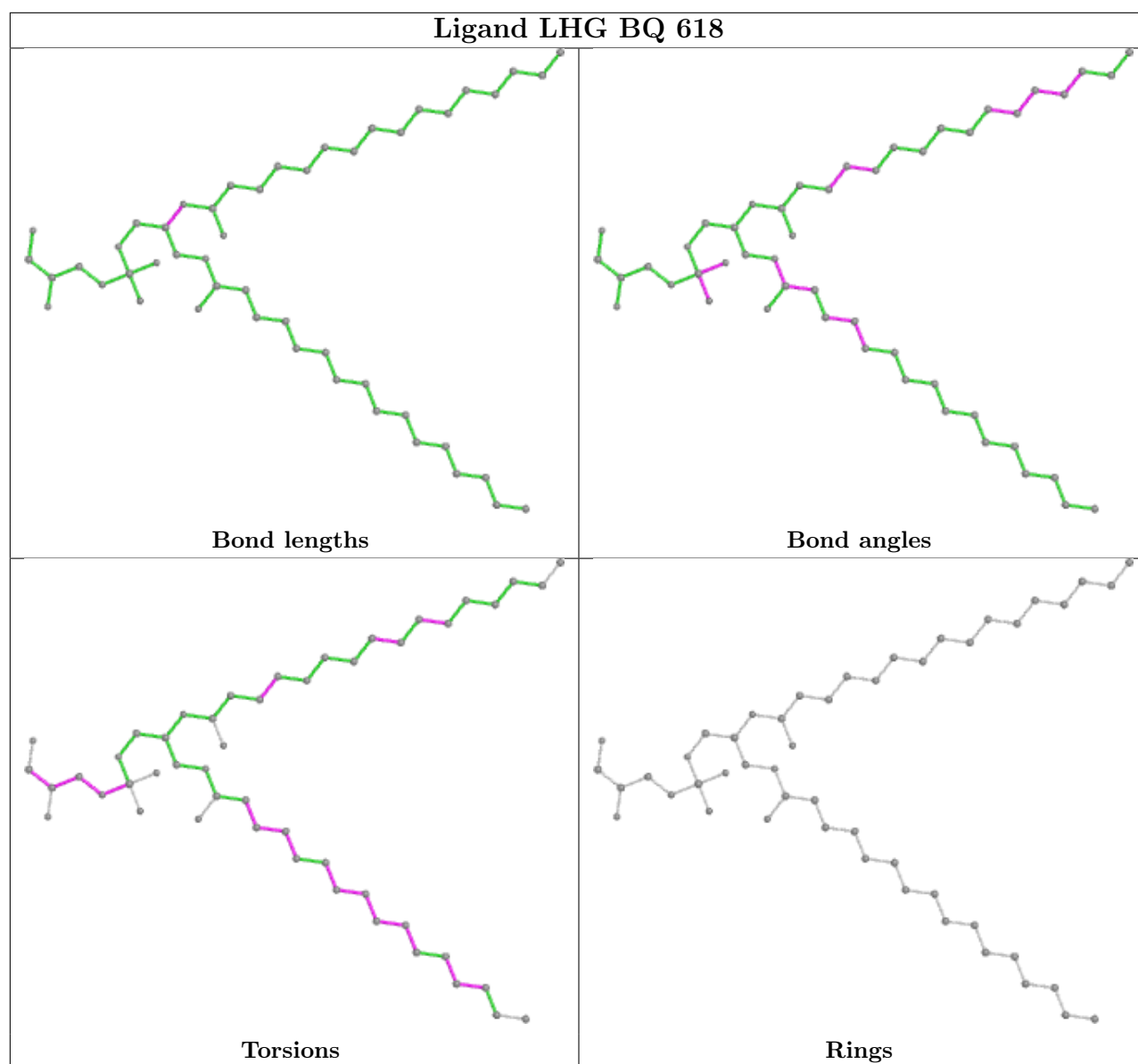
Torsions

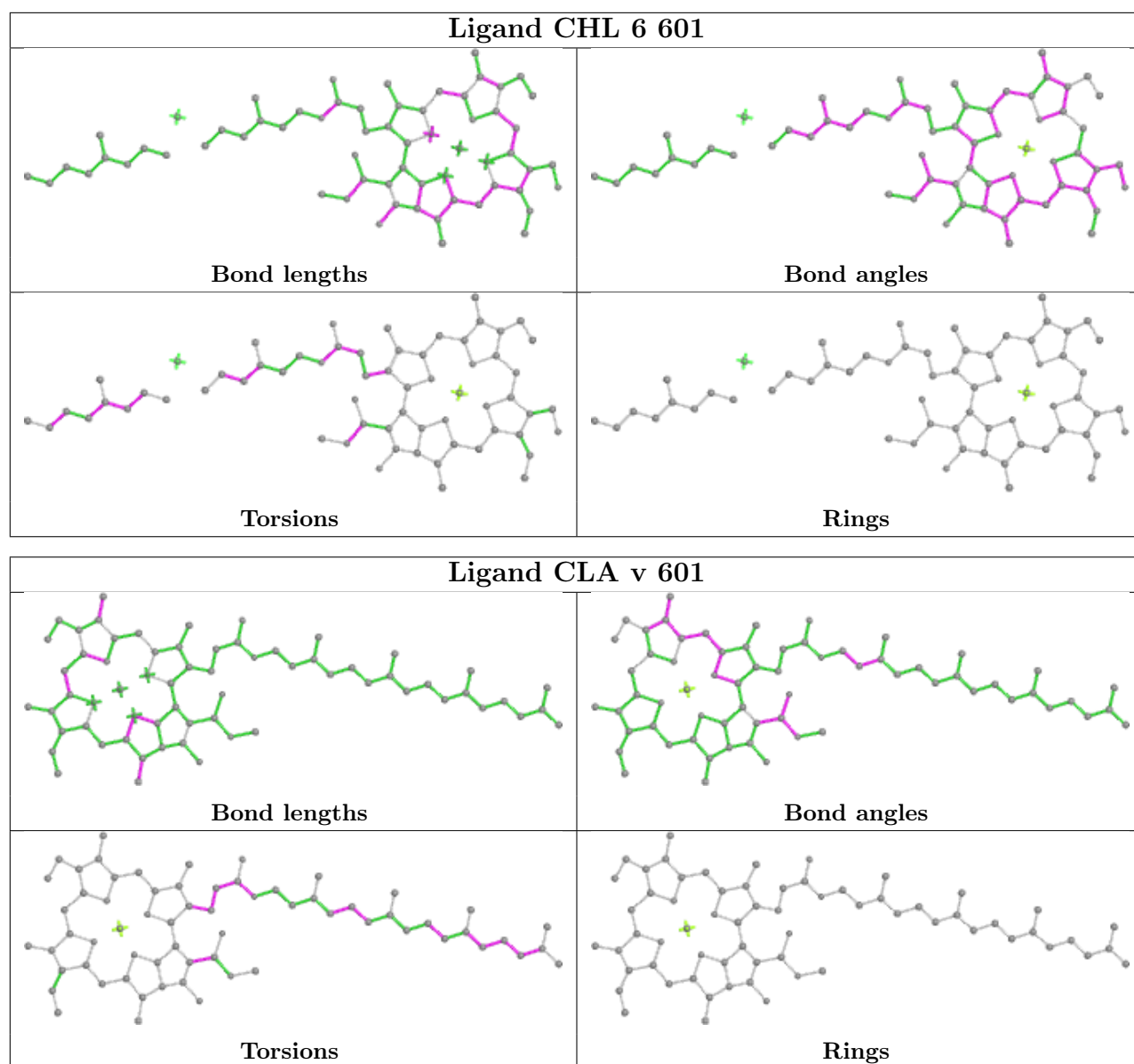


Rings

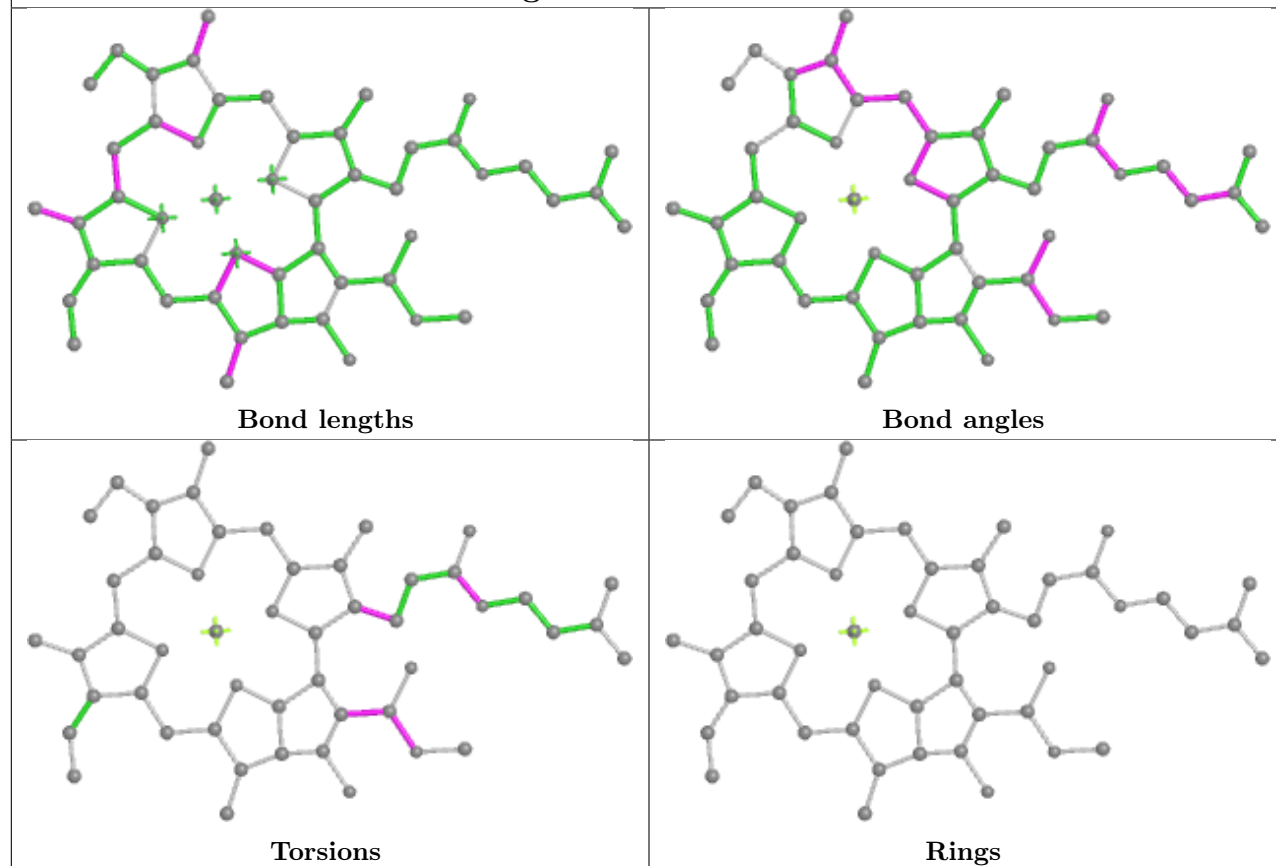
Ligand CLA n 603**Ligand CLA C 504****Ligand CHL 9 607**

Ligand CLA a 410**Ligand PHO A 408**

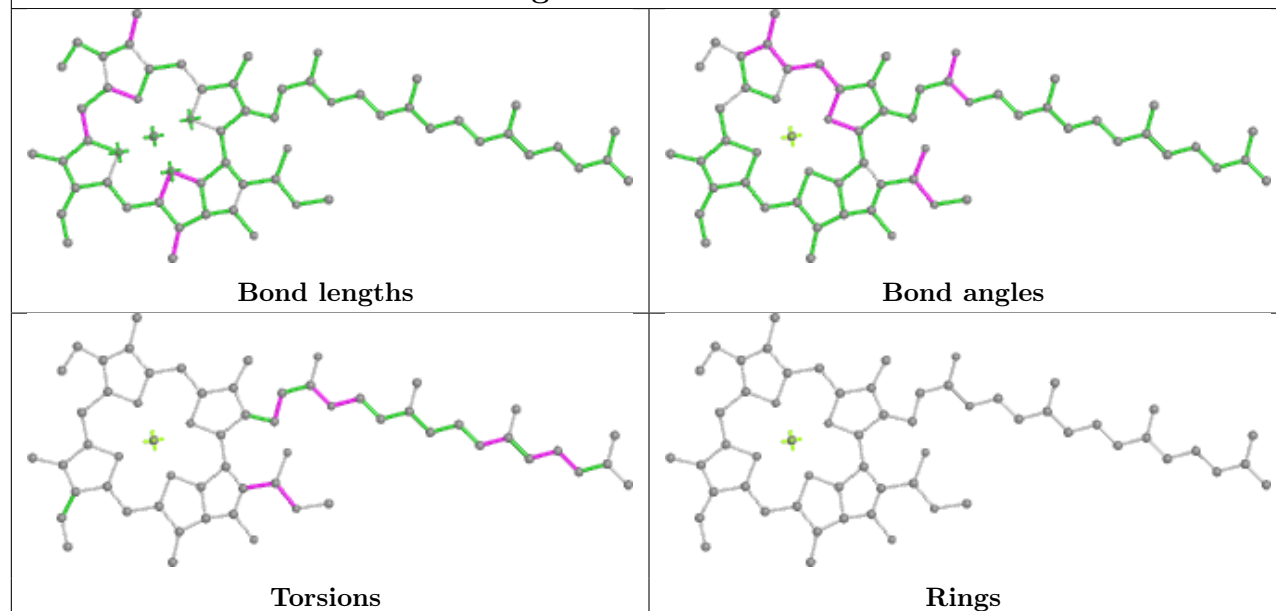


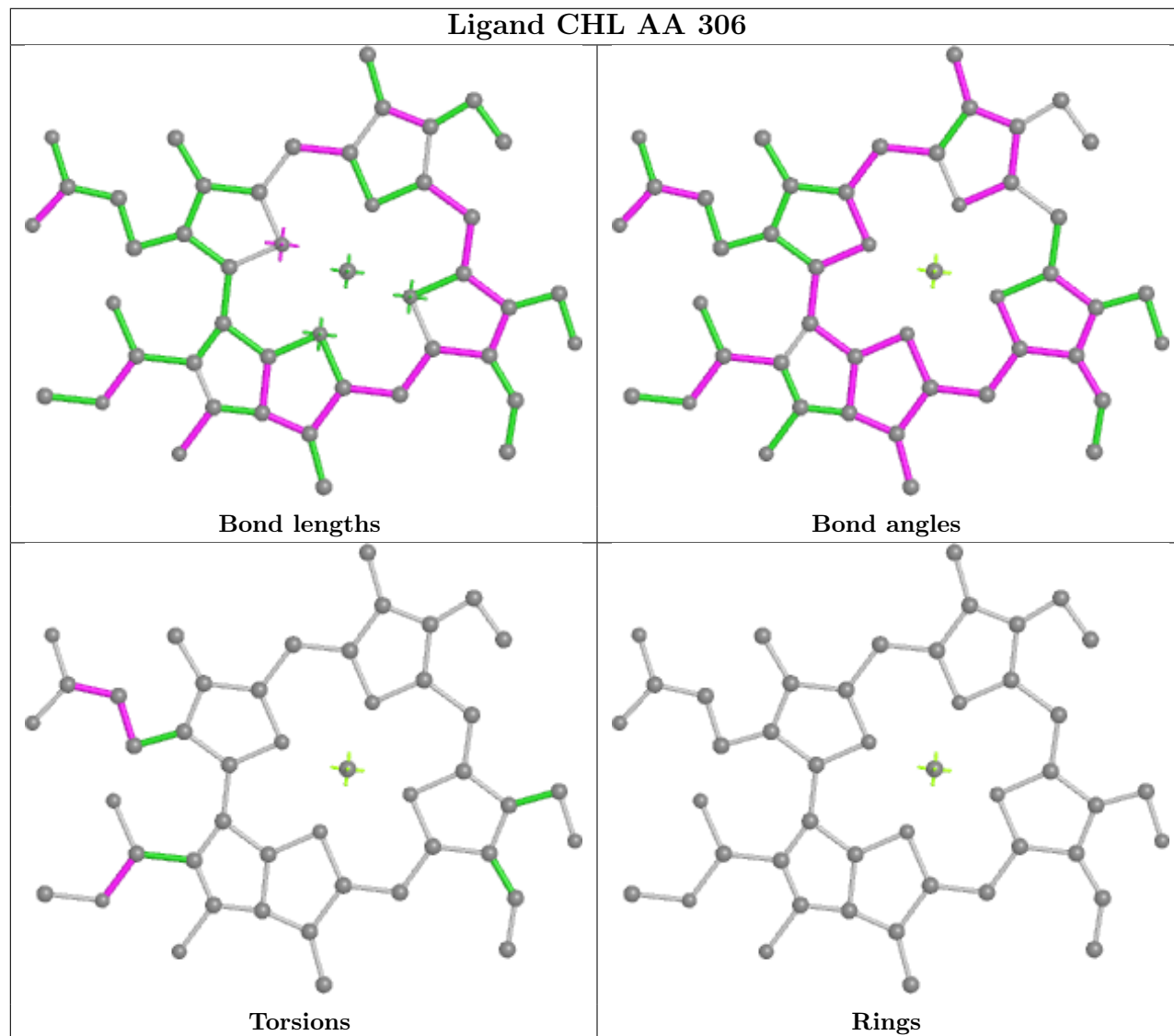
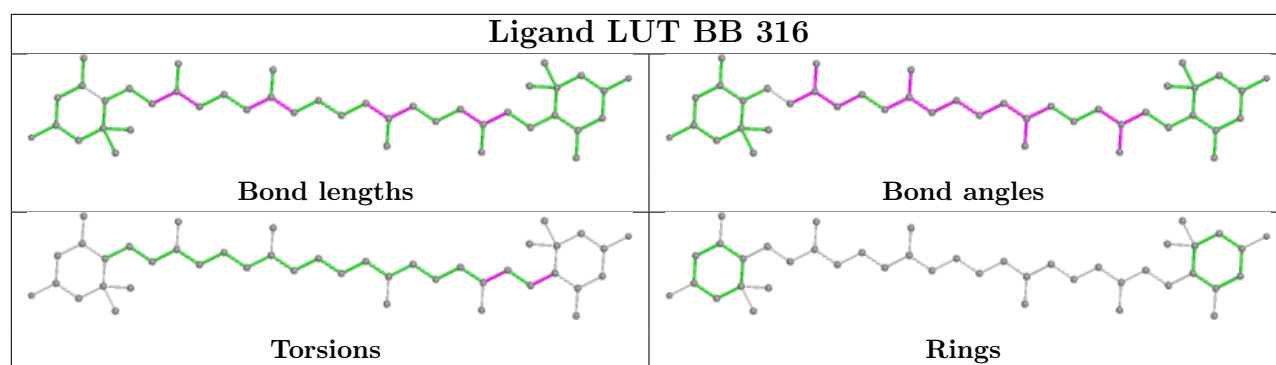


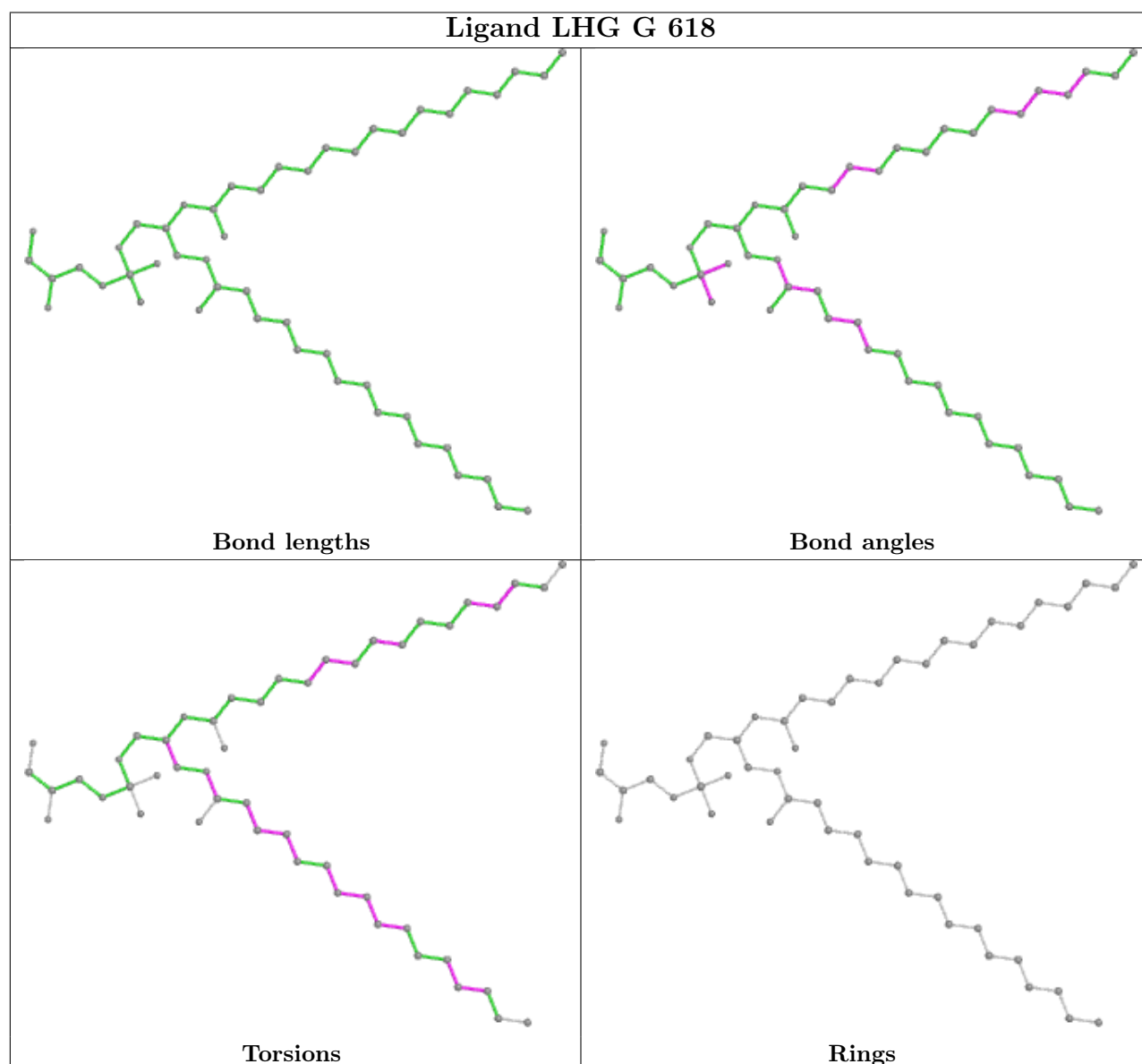
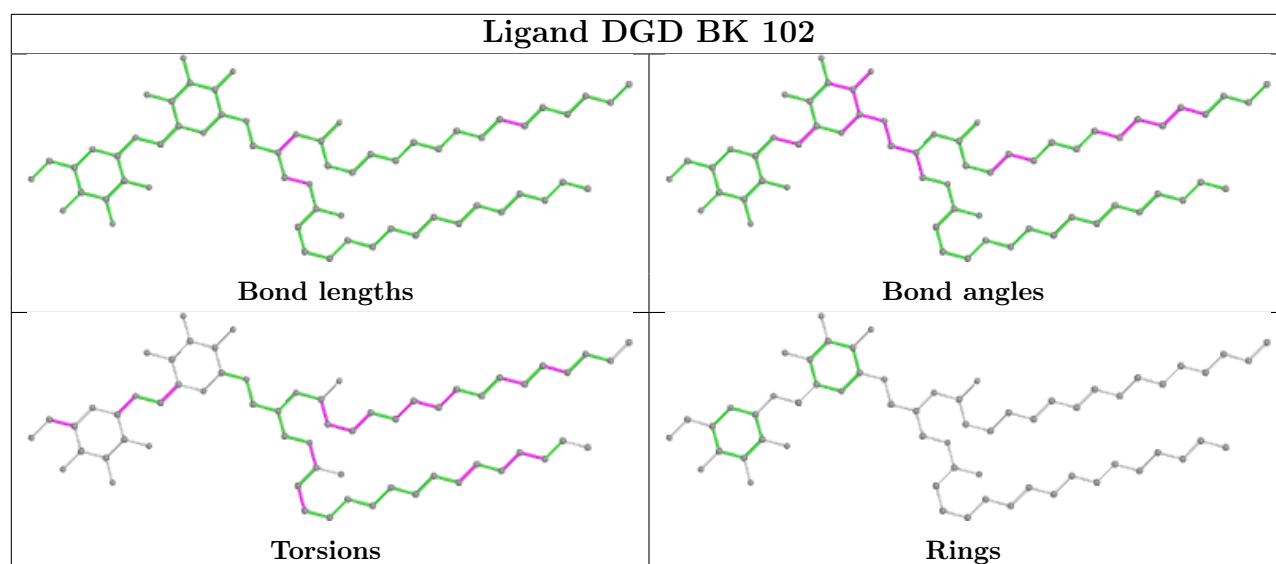
Ligand CLA A2 604

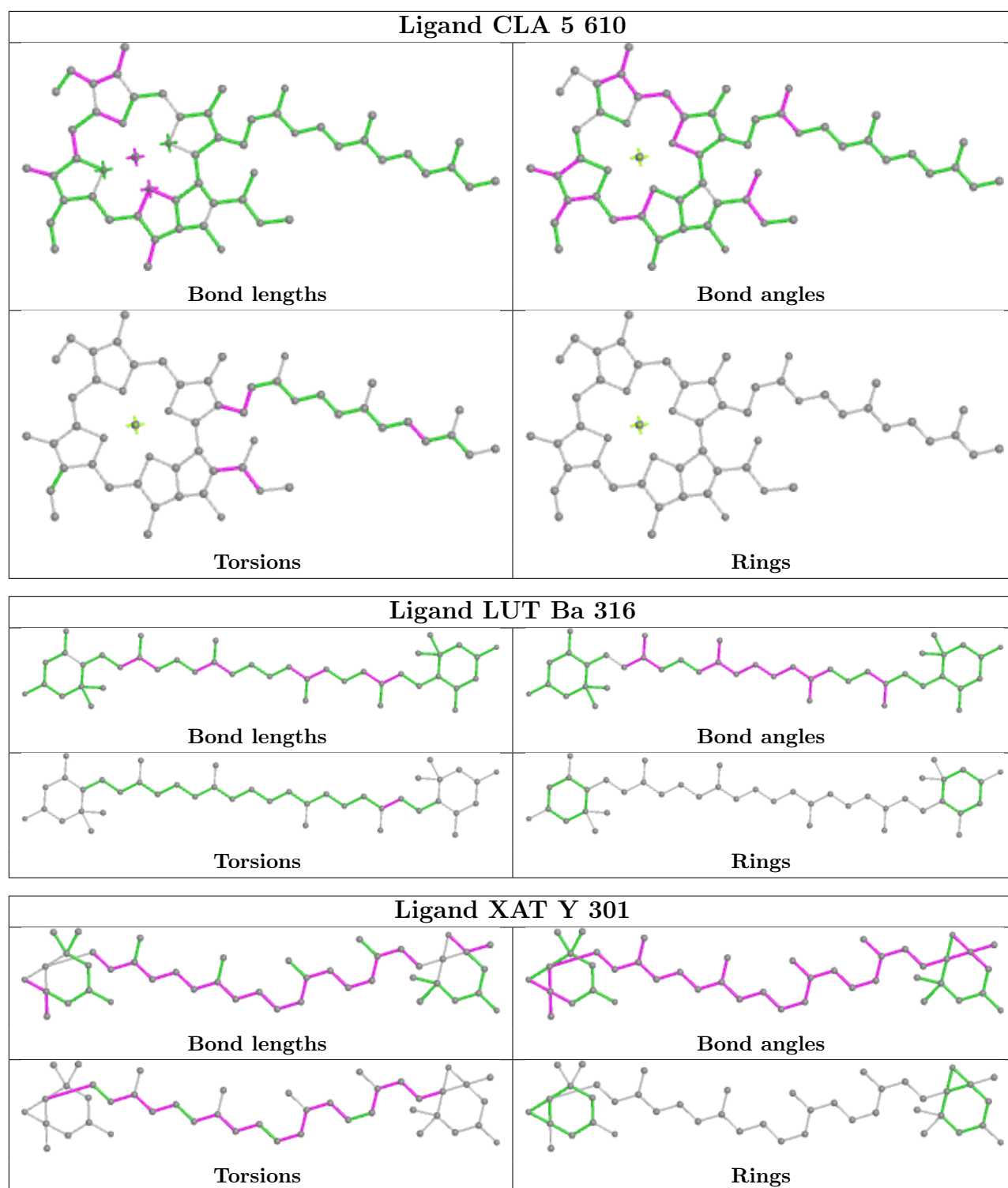


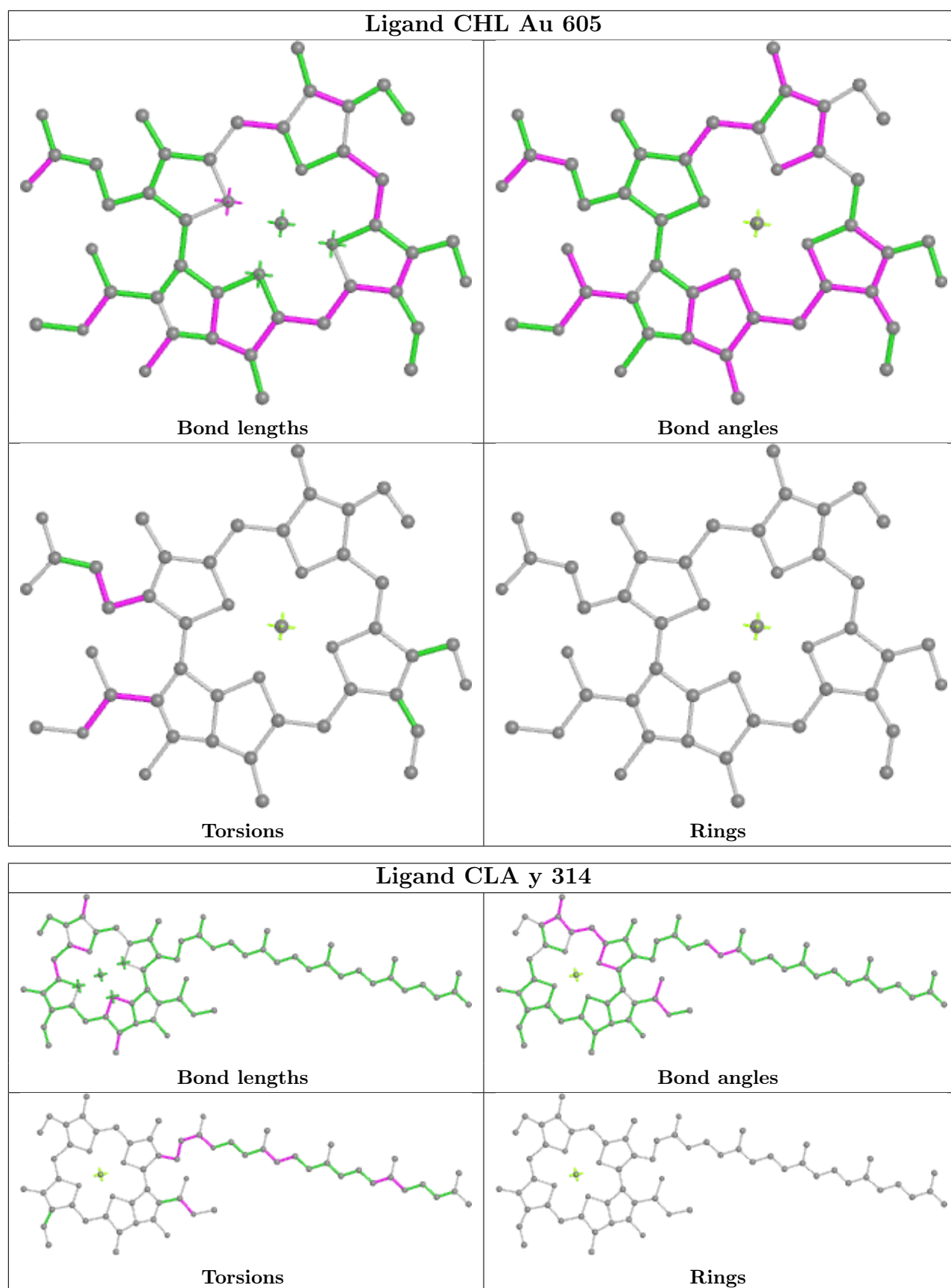
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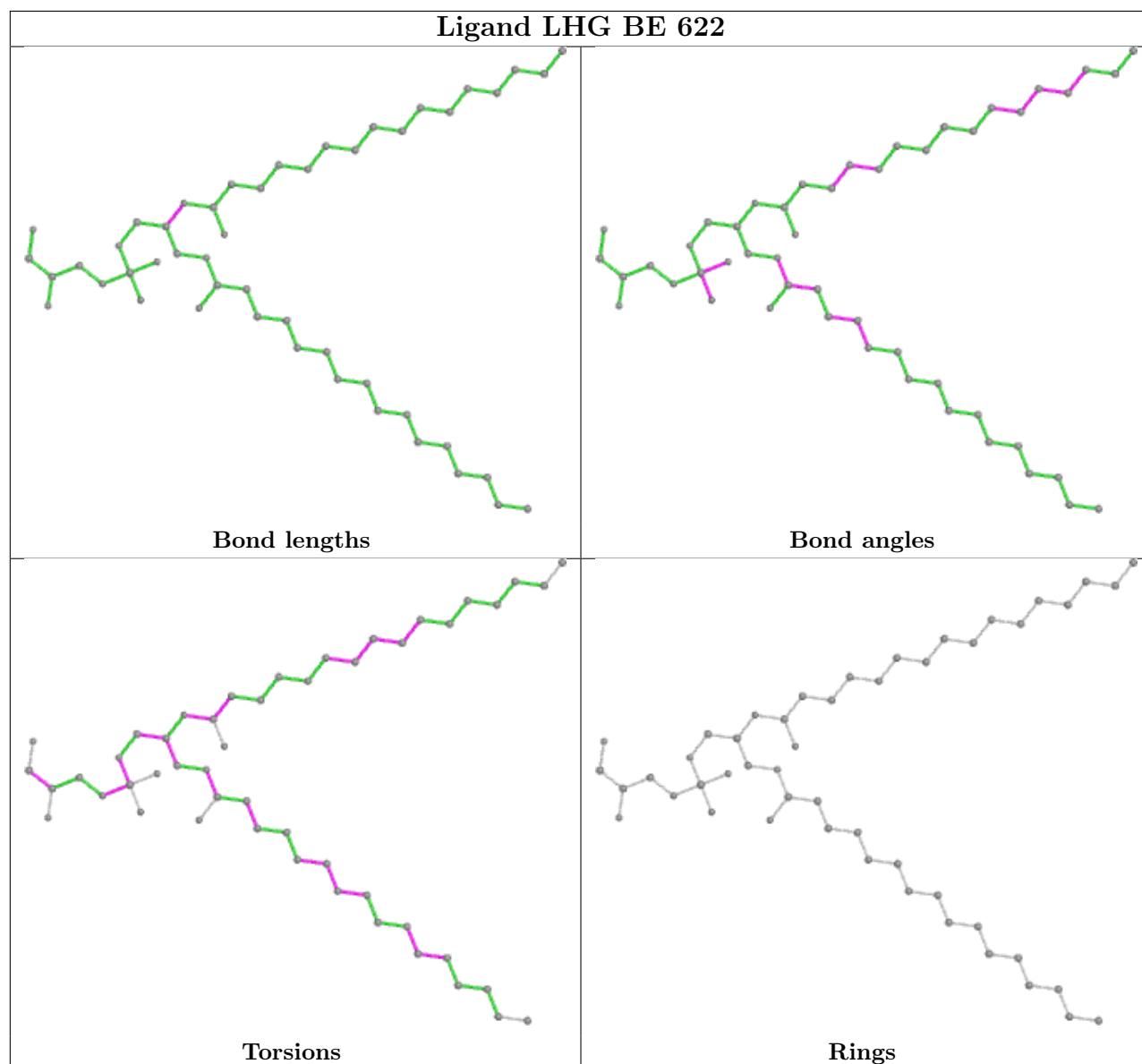
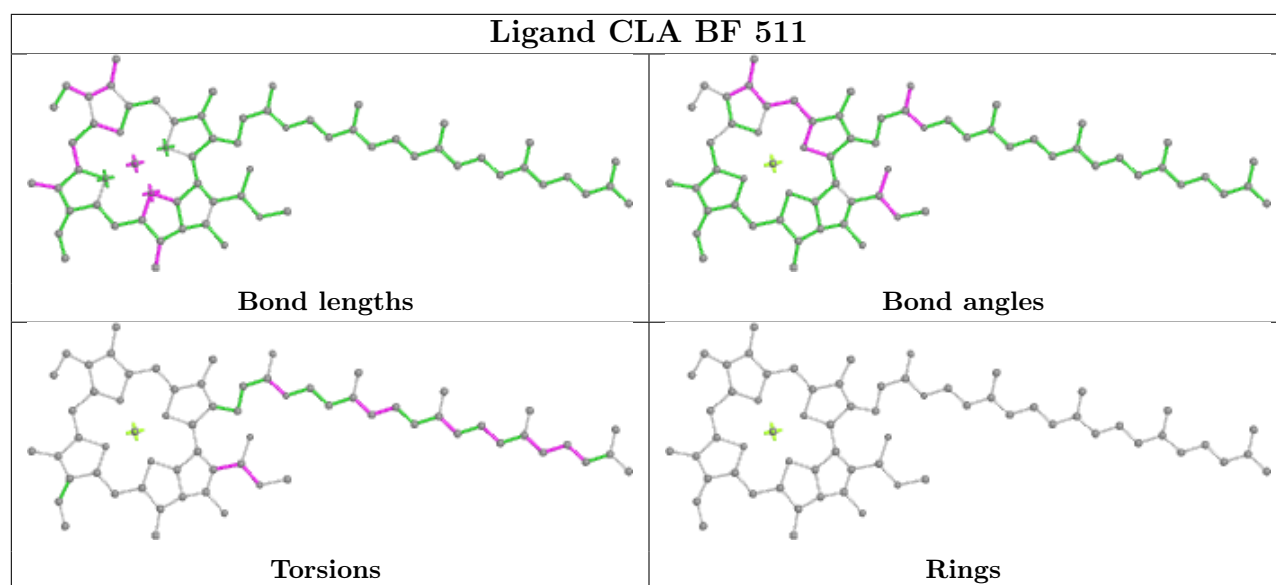




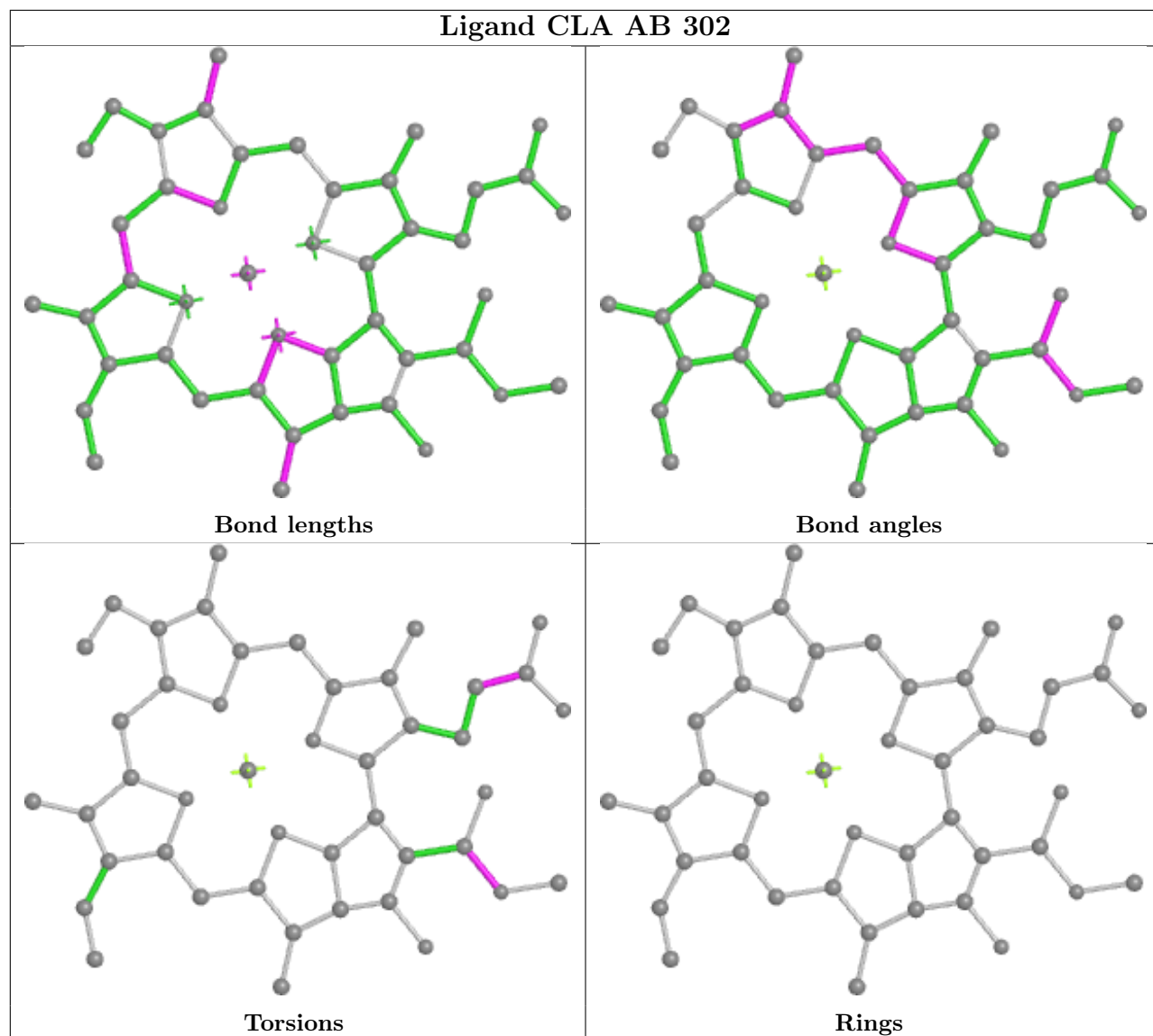




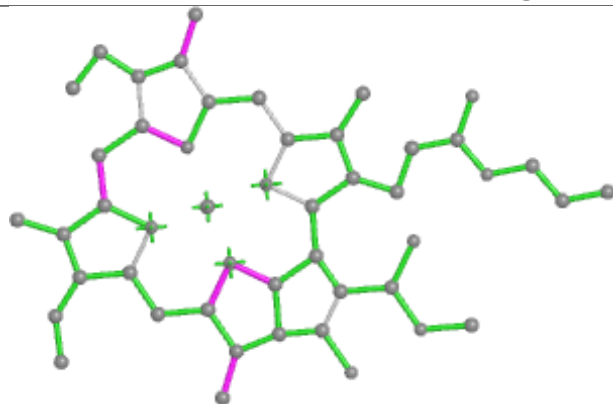




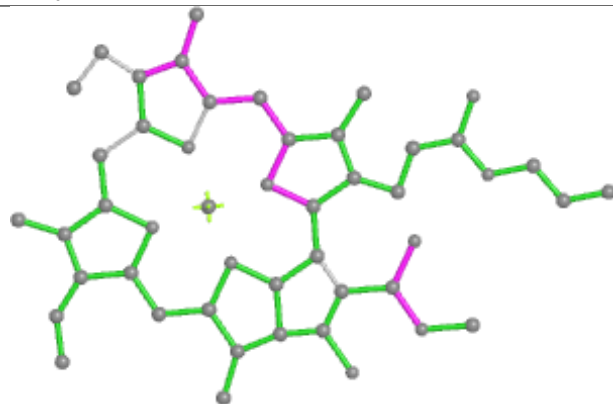
Ligand CLA AB 302



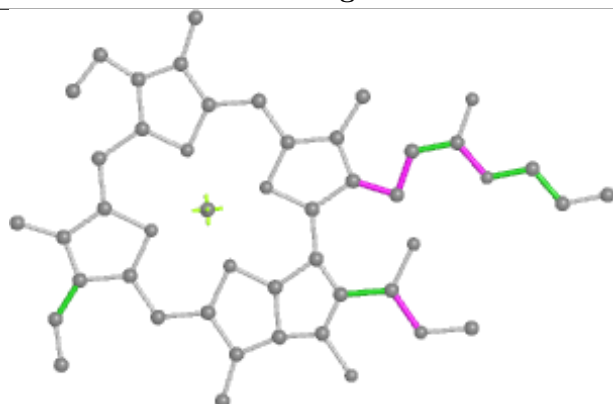
Ligand CLA y 315



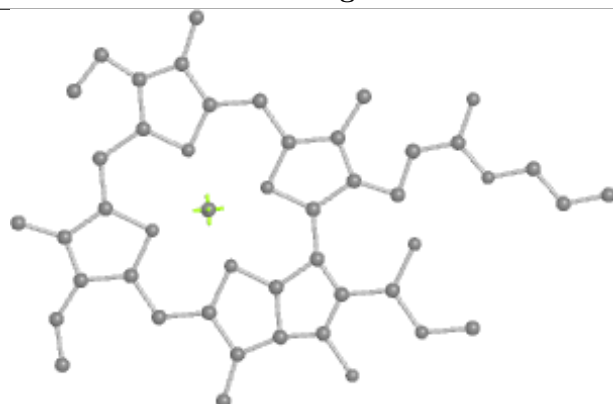
Bond lengths



Bond angles

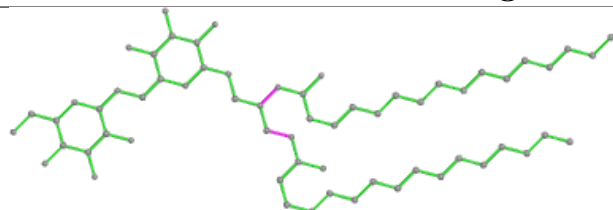


Torsions

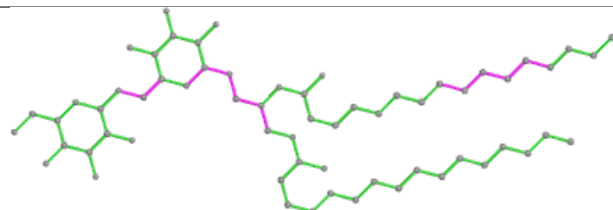


Rings

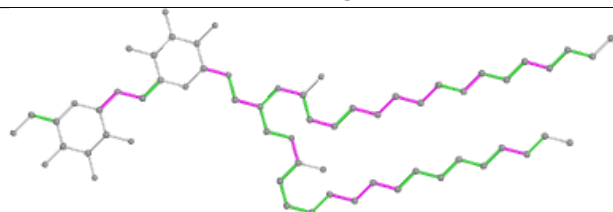
Ligand DGD BF 518



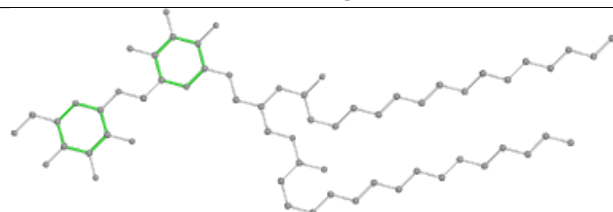
Bond lengths



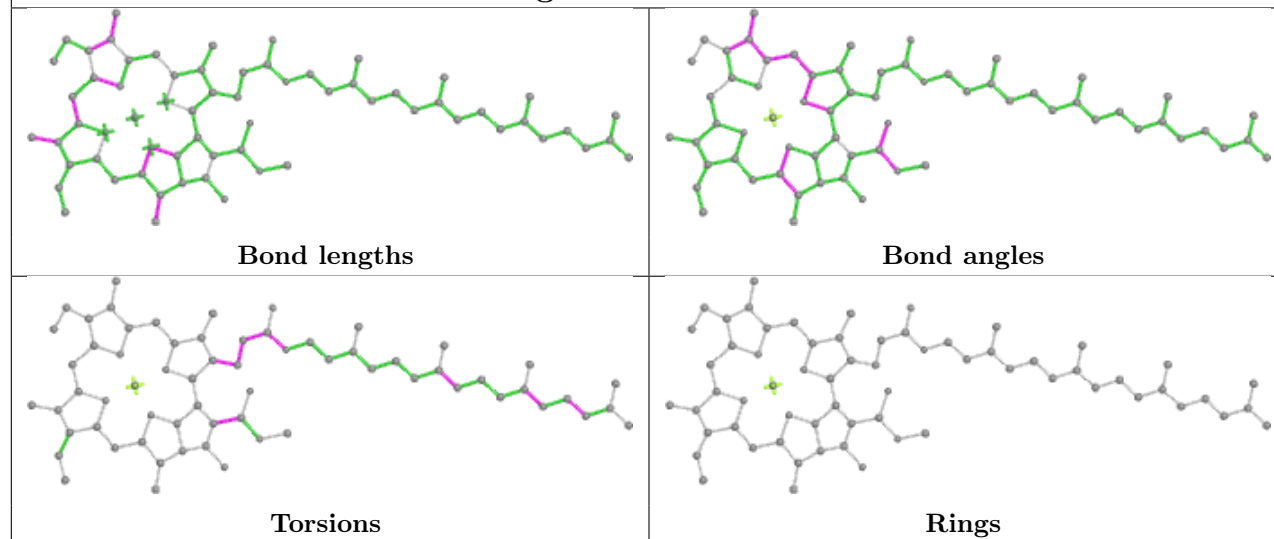
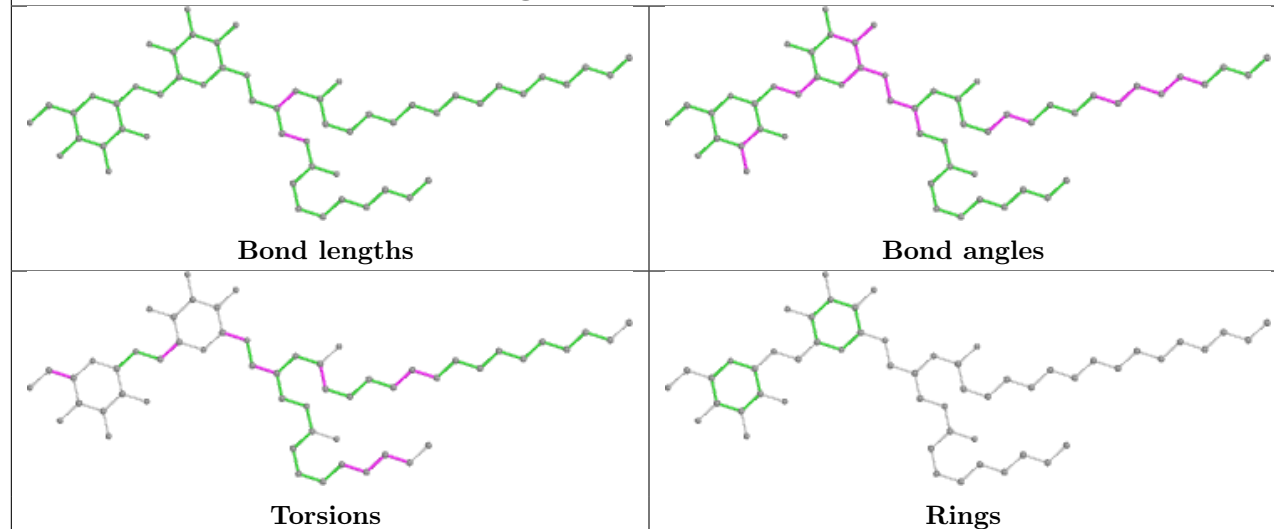
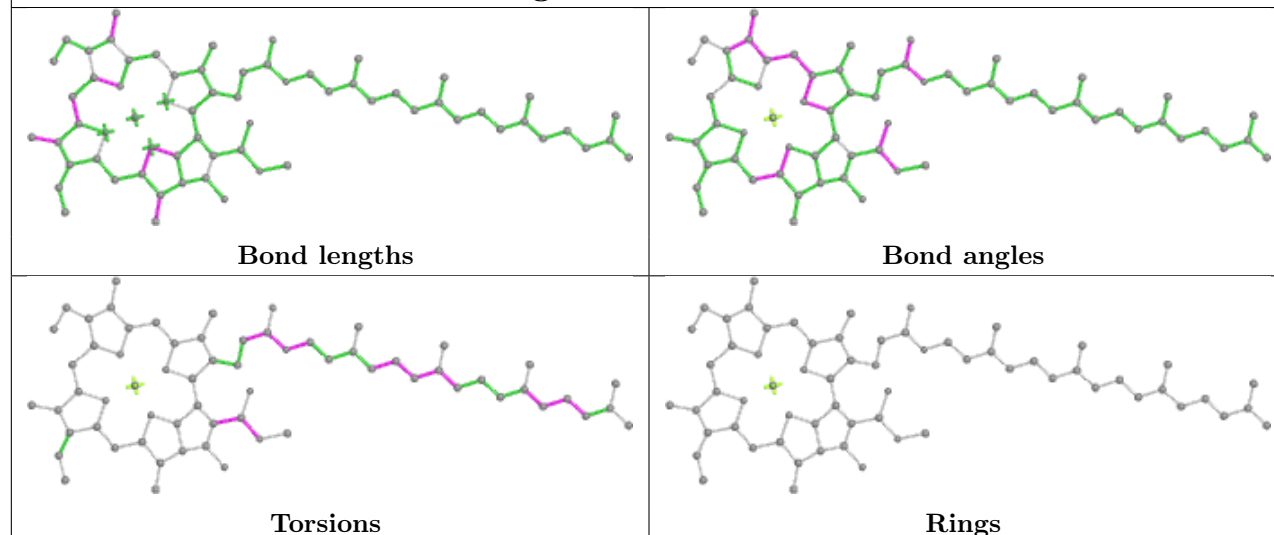
Bond angles

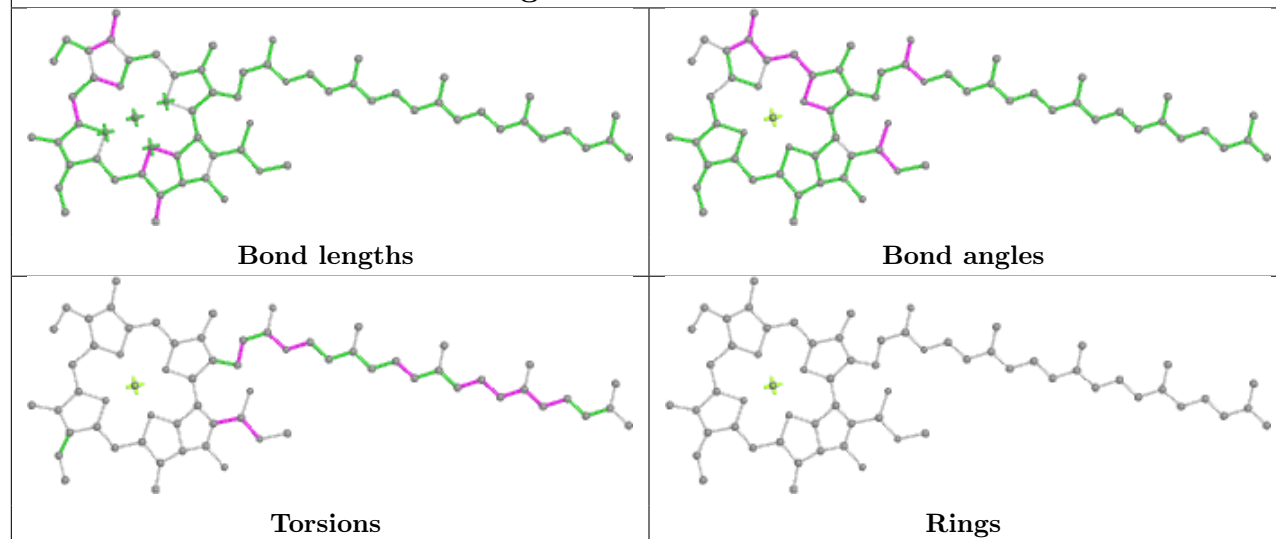
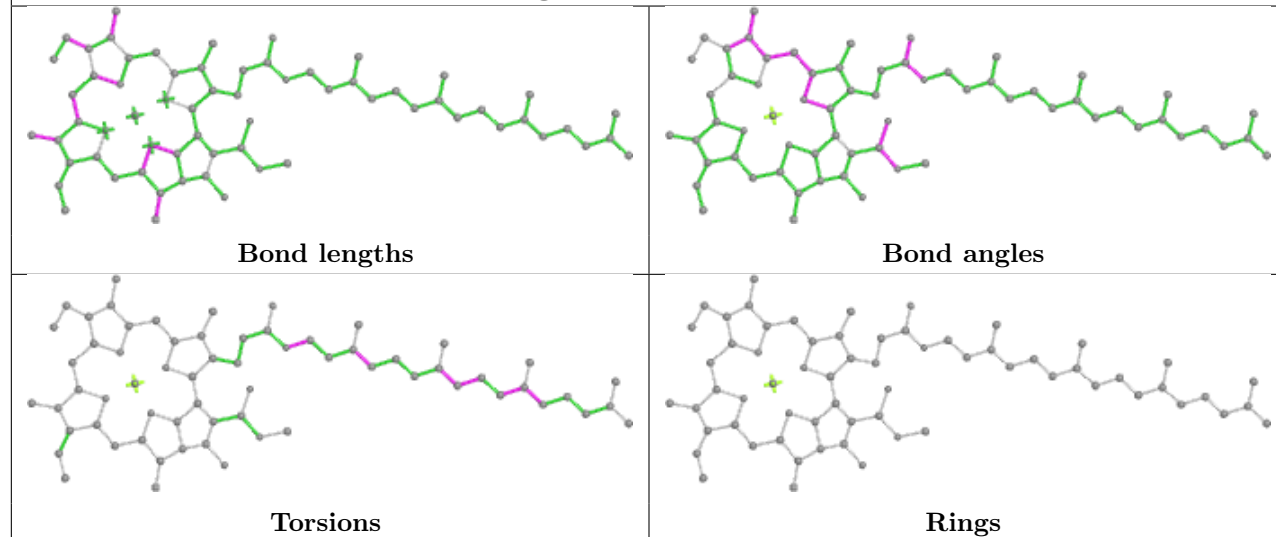


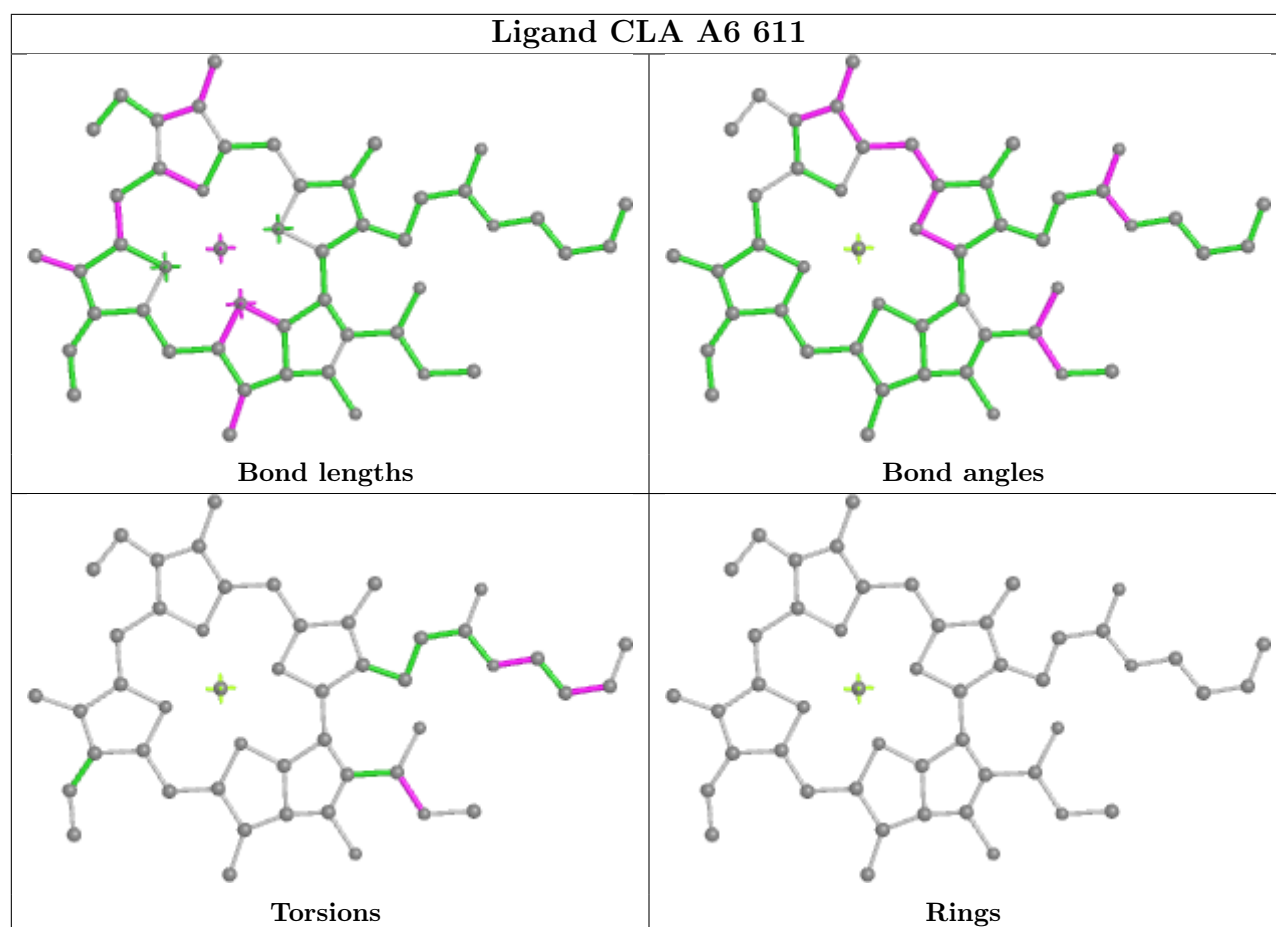
Torsions

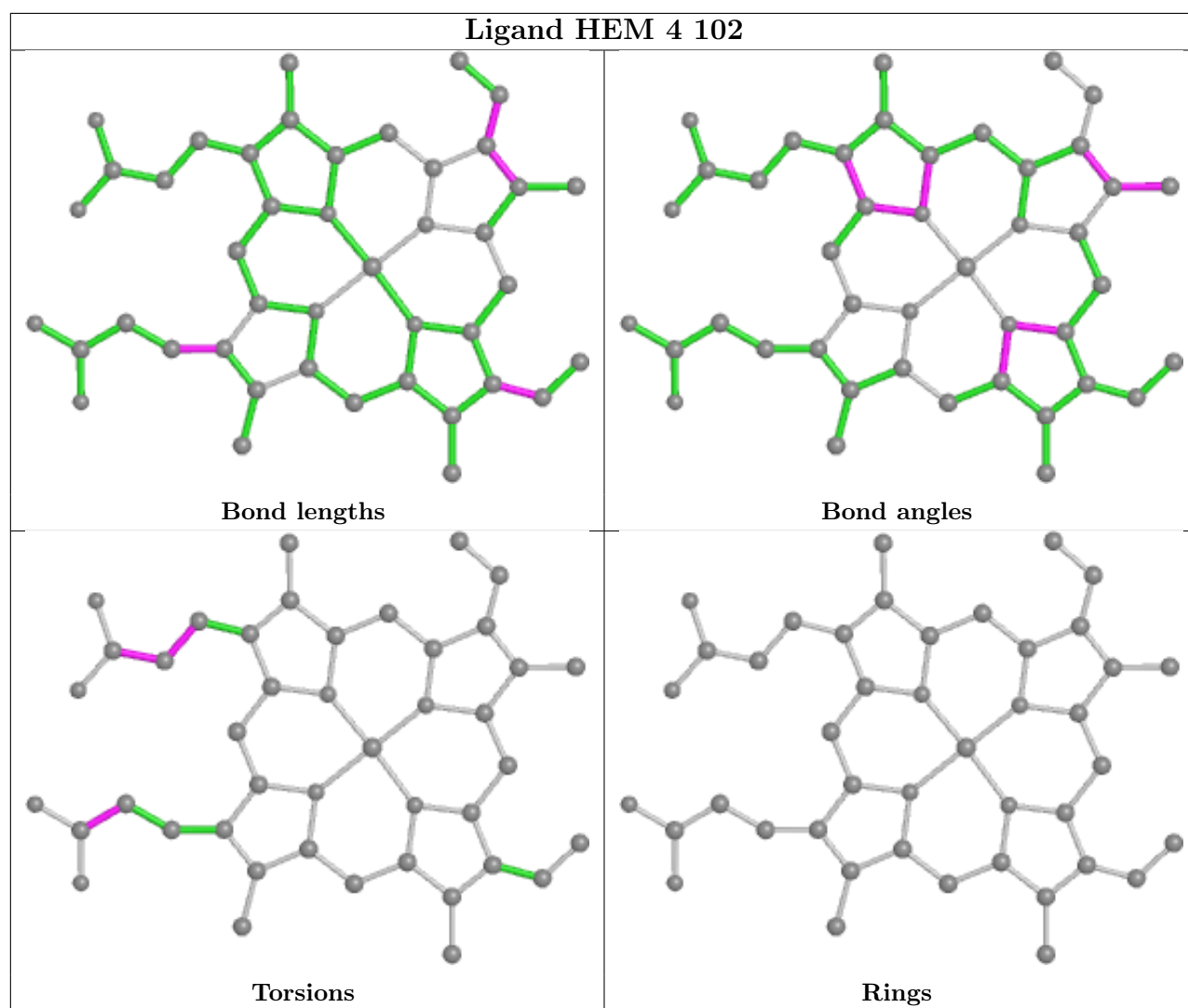


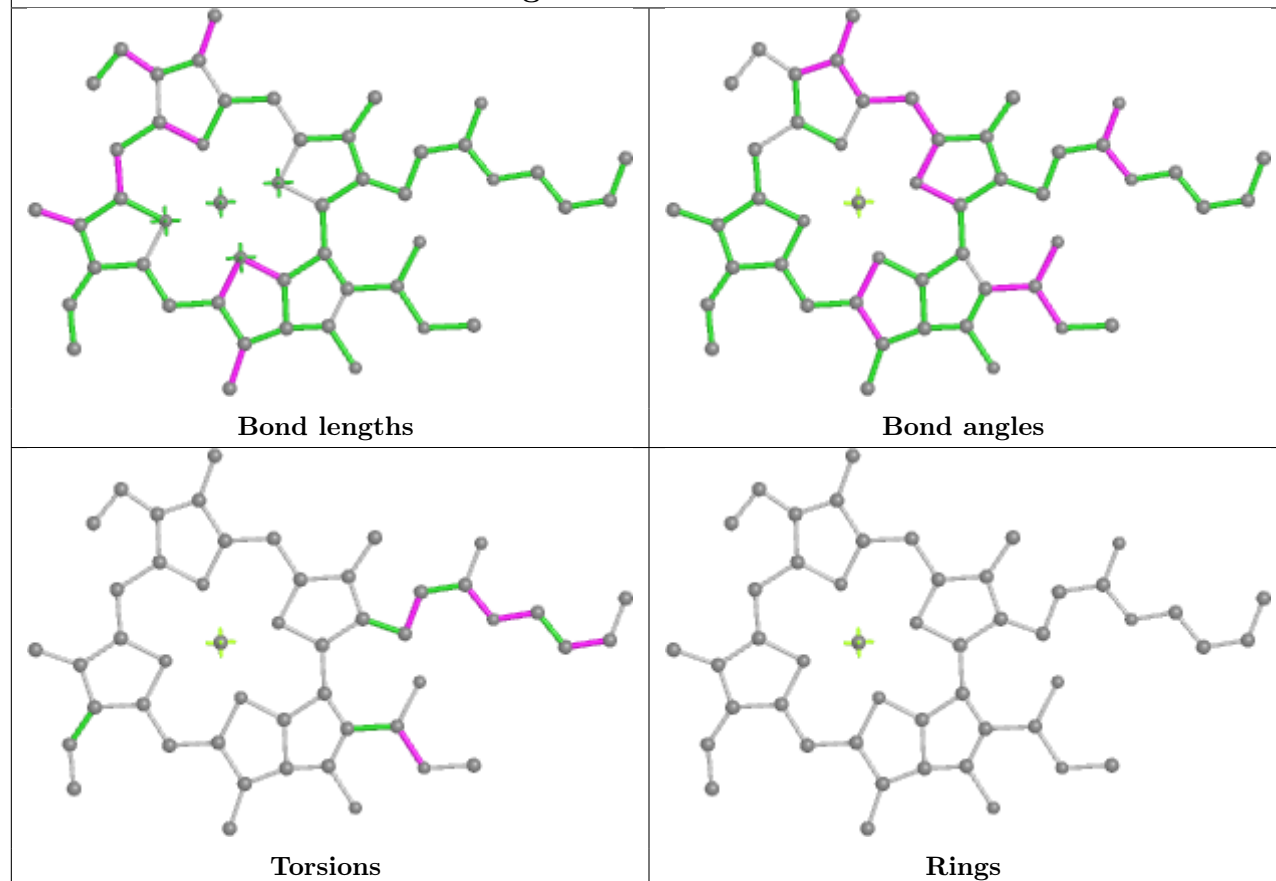
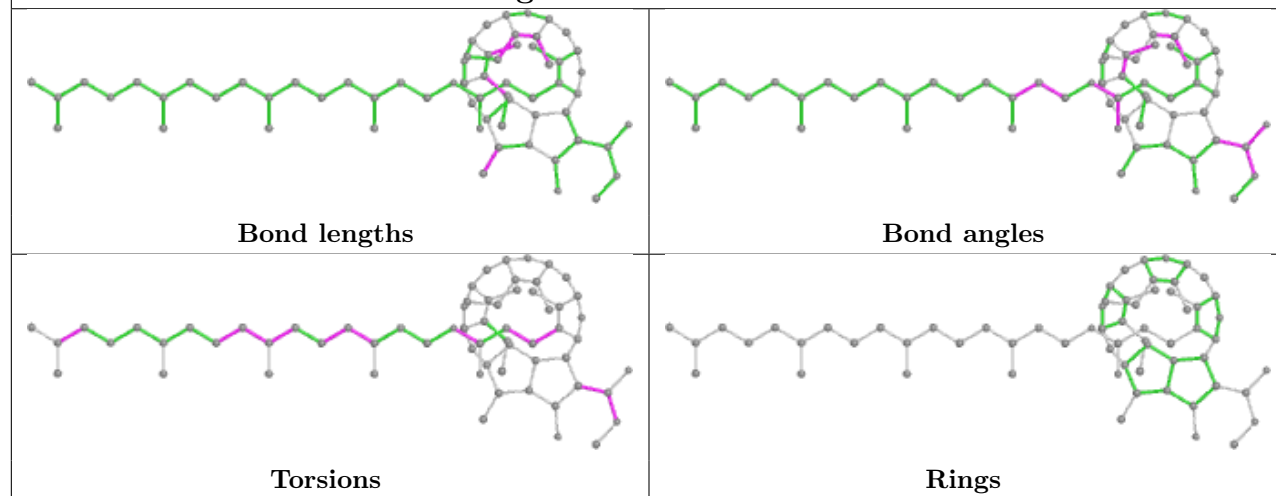
Rings

Ligand CLA 1 502**Ligand DGD BF 517****Ligand CLA B 616**

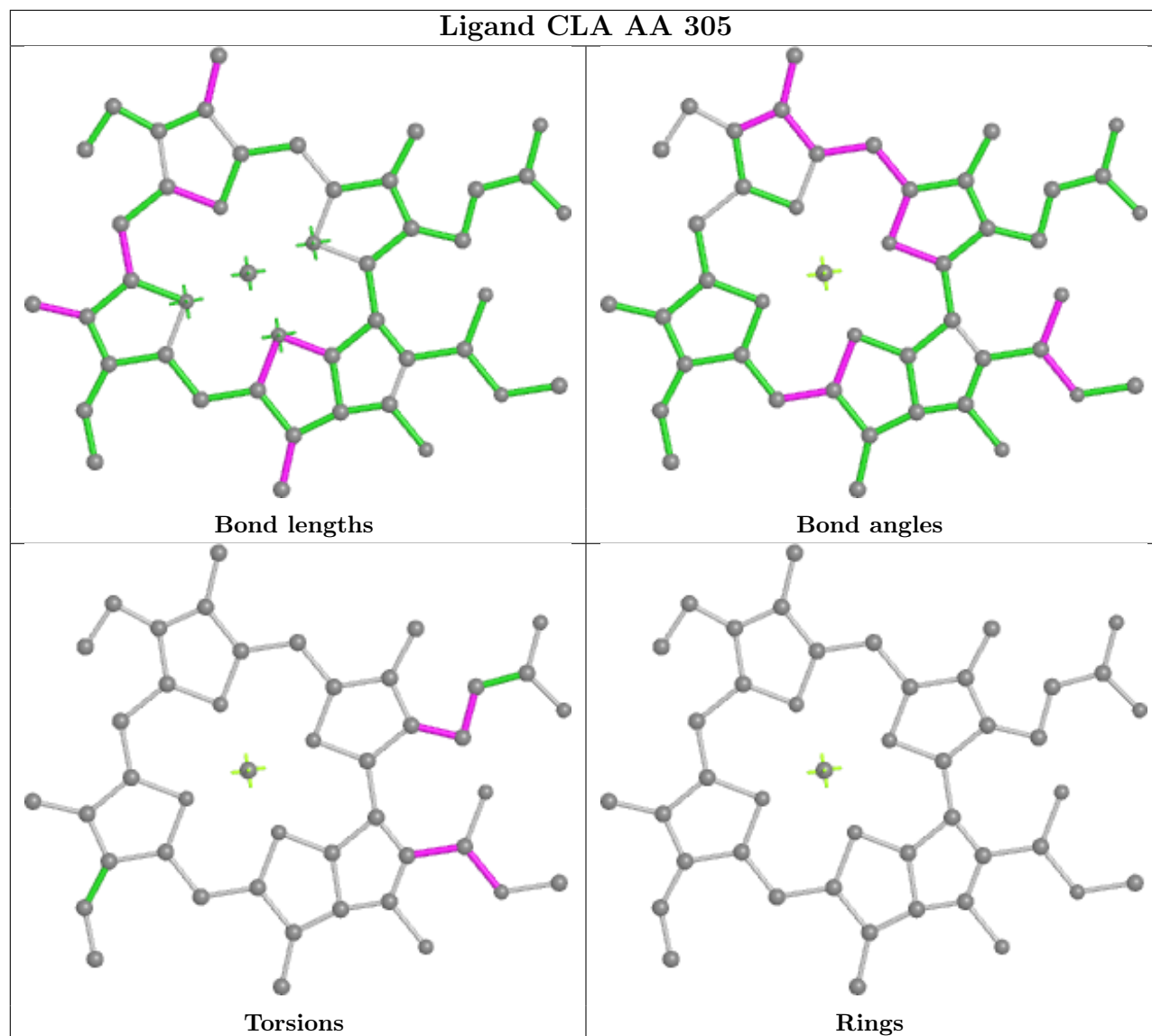
Ligand CLA BE 607**Ligand CLA b 616**

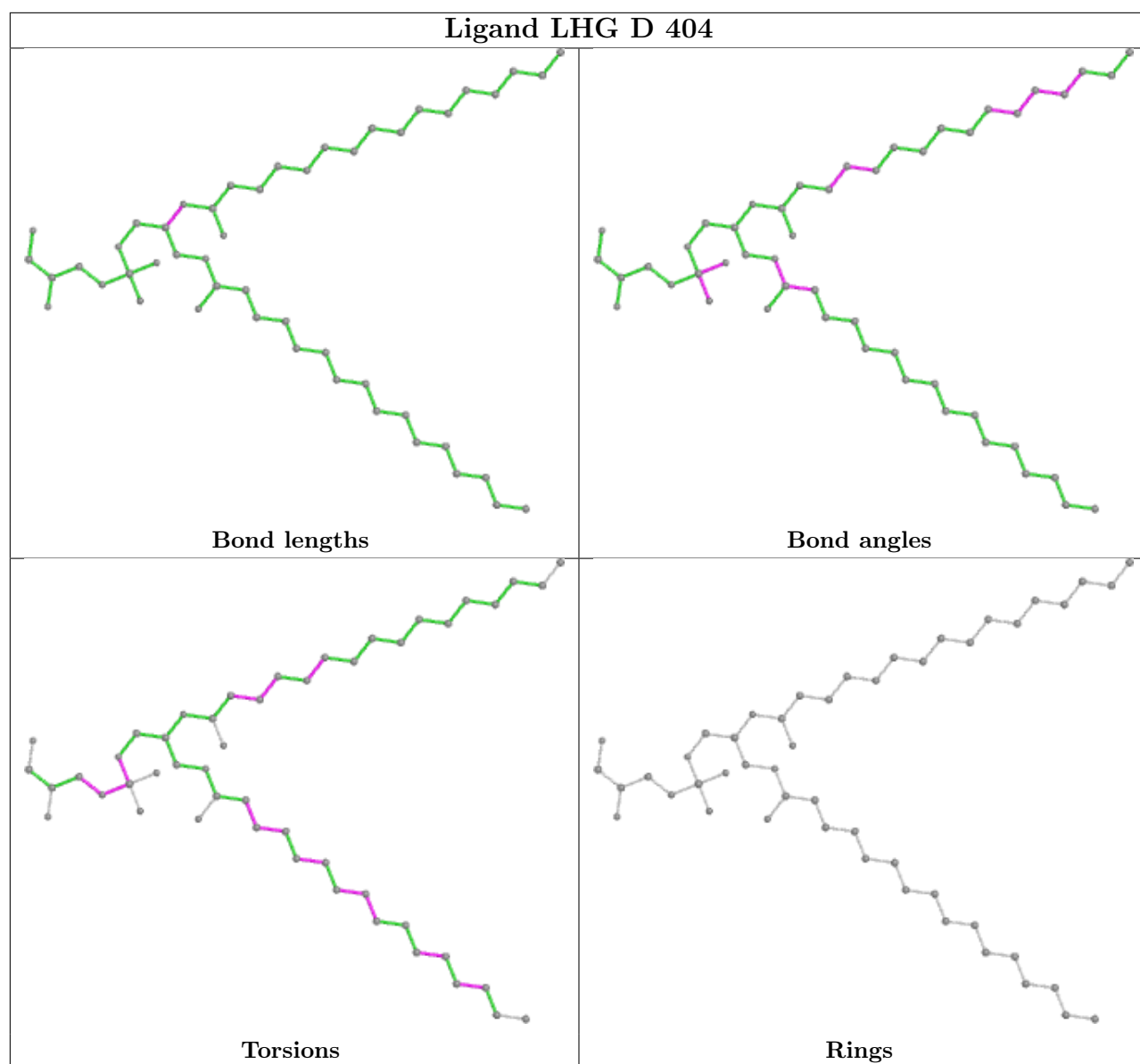


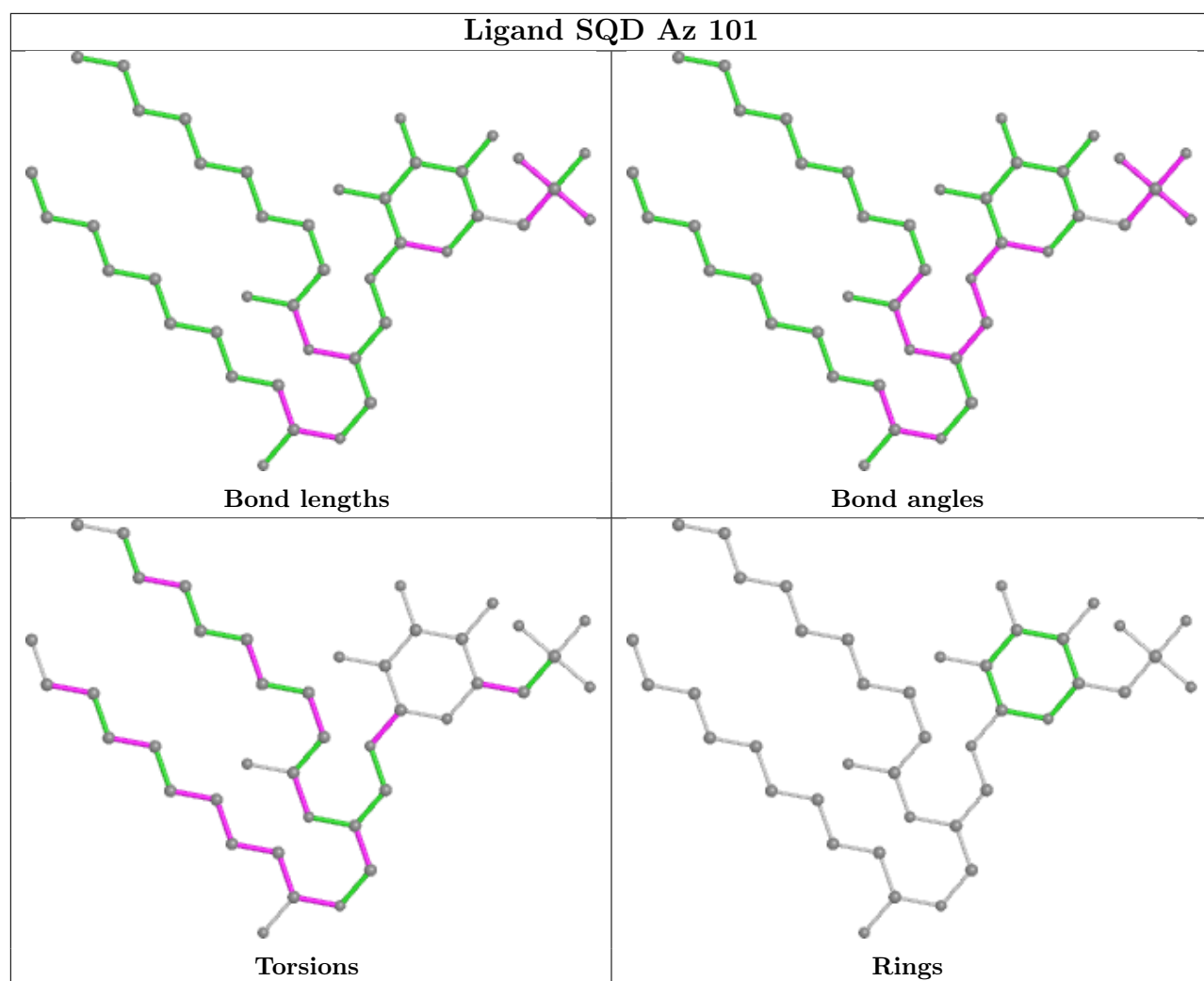


Ligand CLA A6 613**Ligand PHO BD 409**

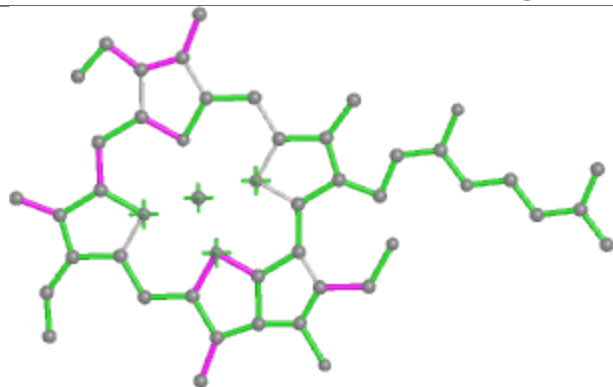
Ligand CLA AA 305



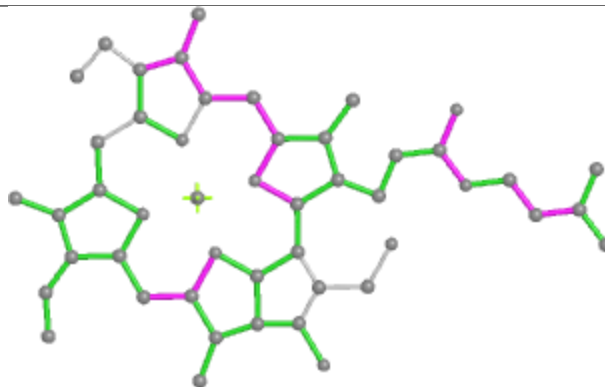




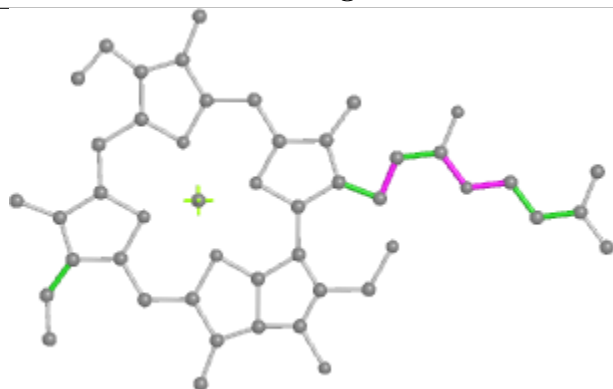
Ligand CLA 7 311



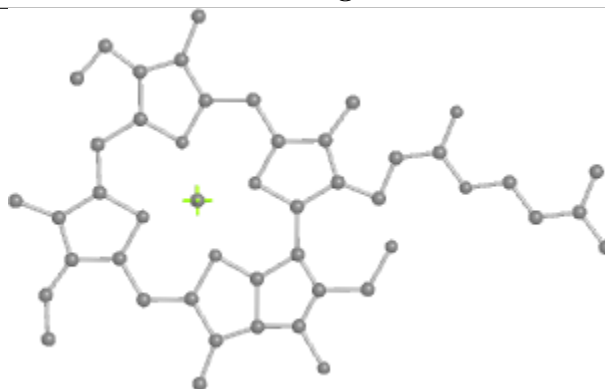
Bond lengths



Bond angles

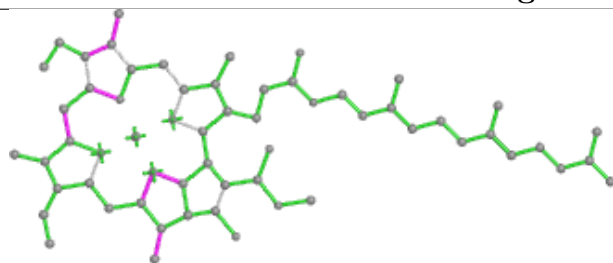


Torsions

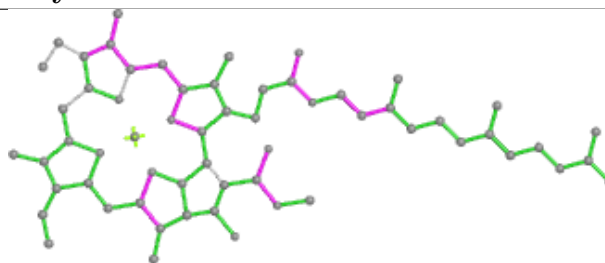


Rings

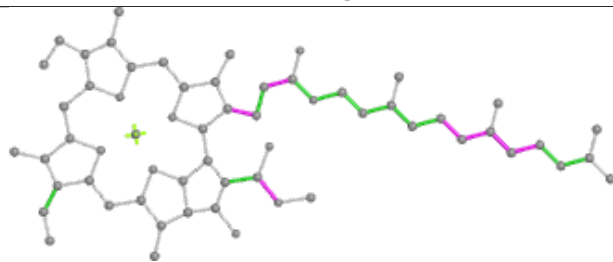
Ligand CLA y 312



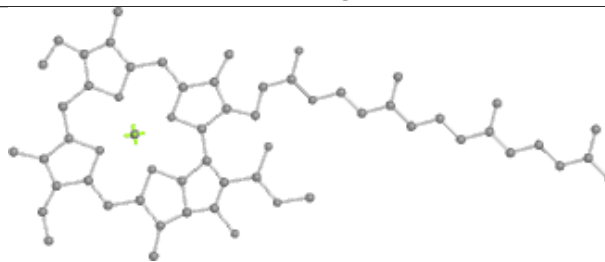
Bond lengths



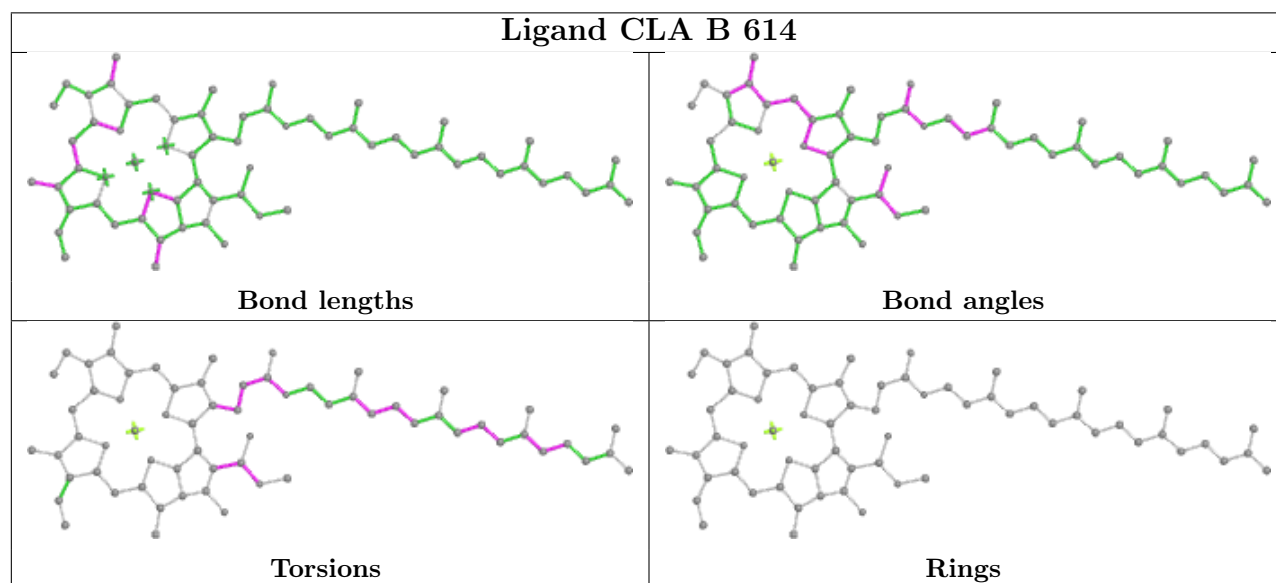
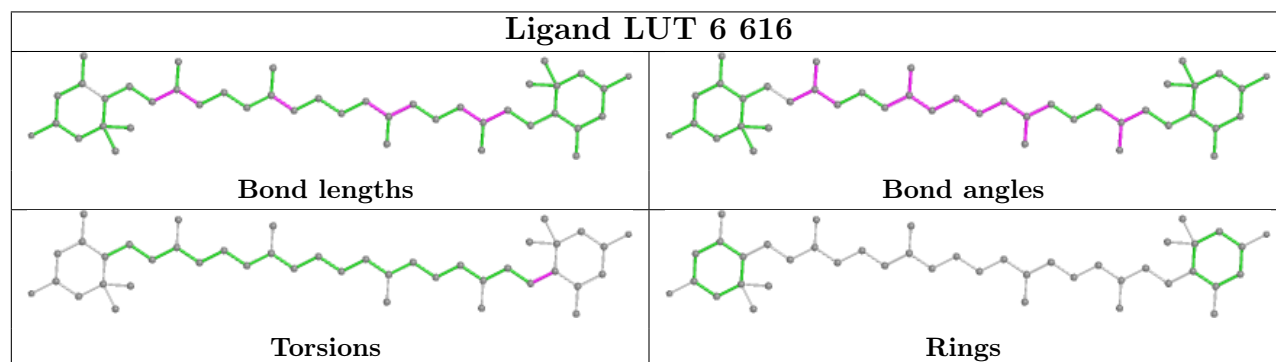
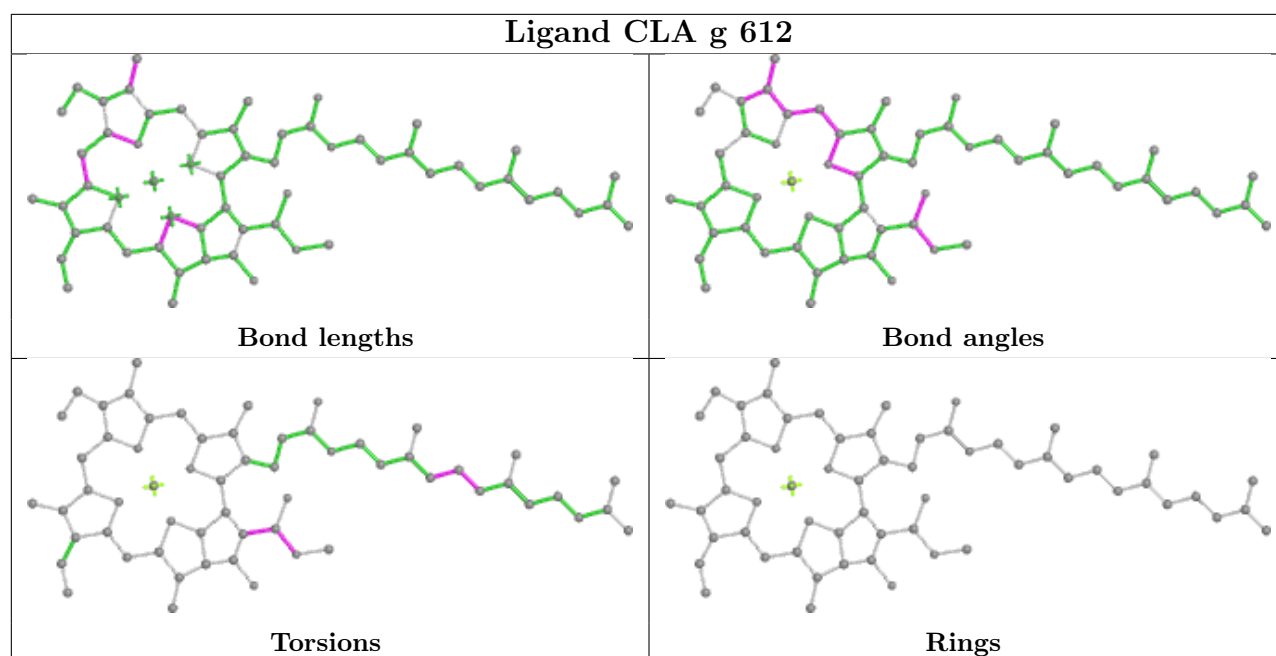
Bond angles

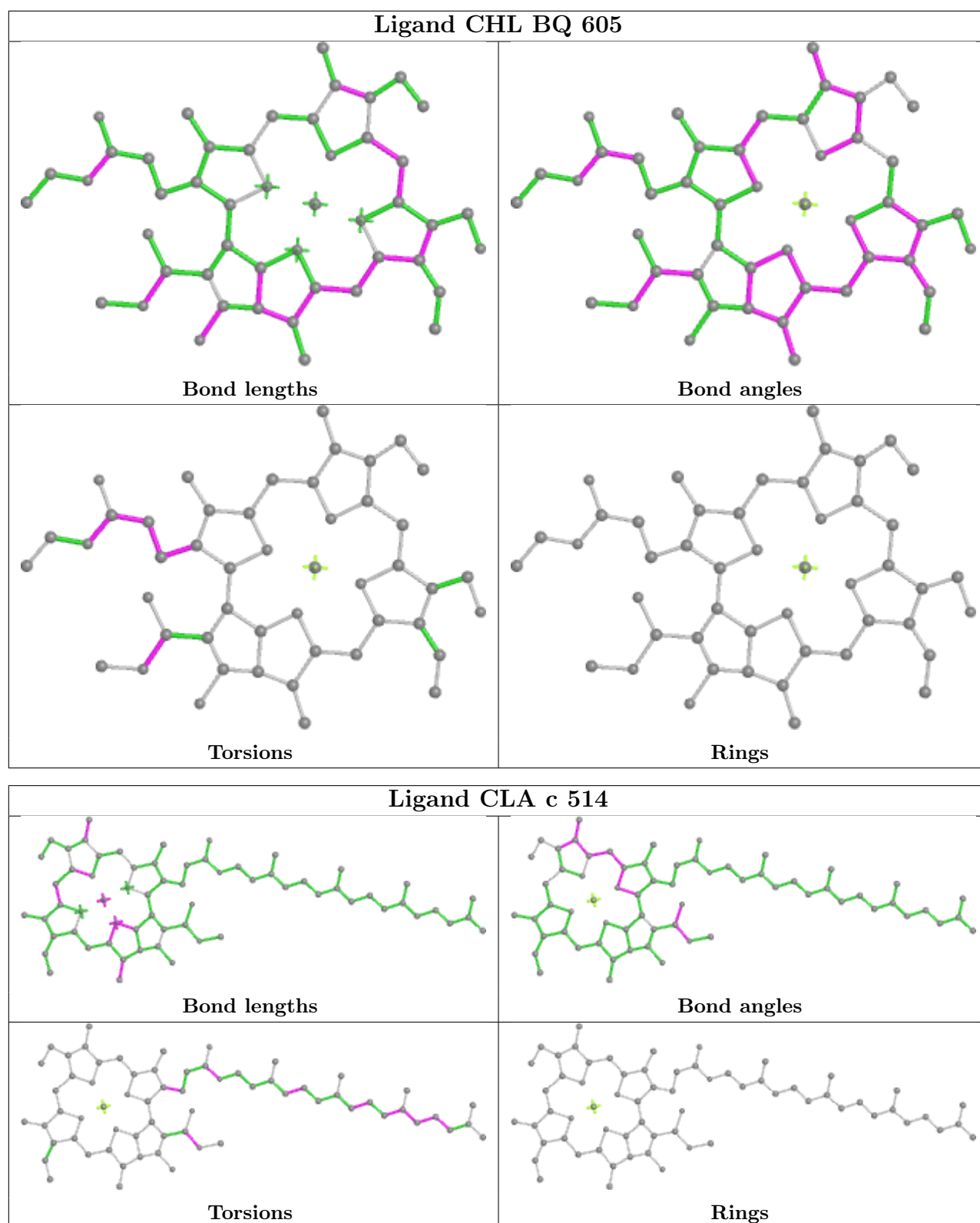


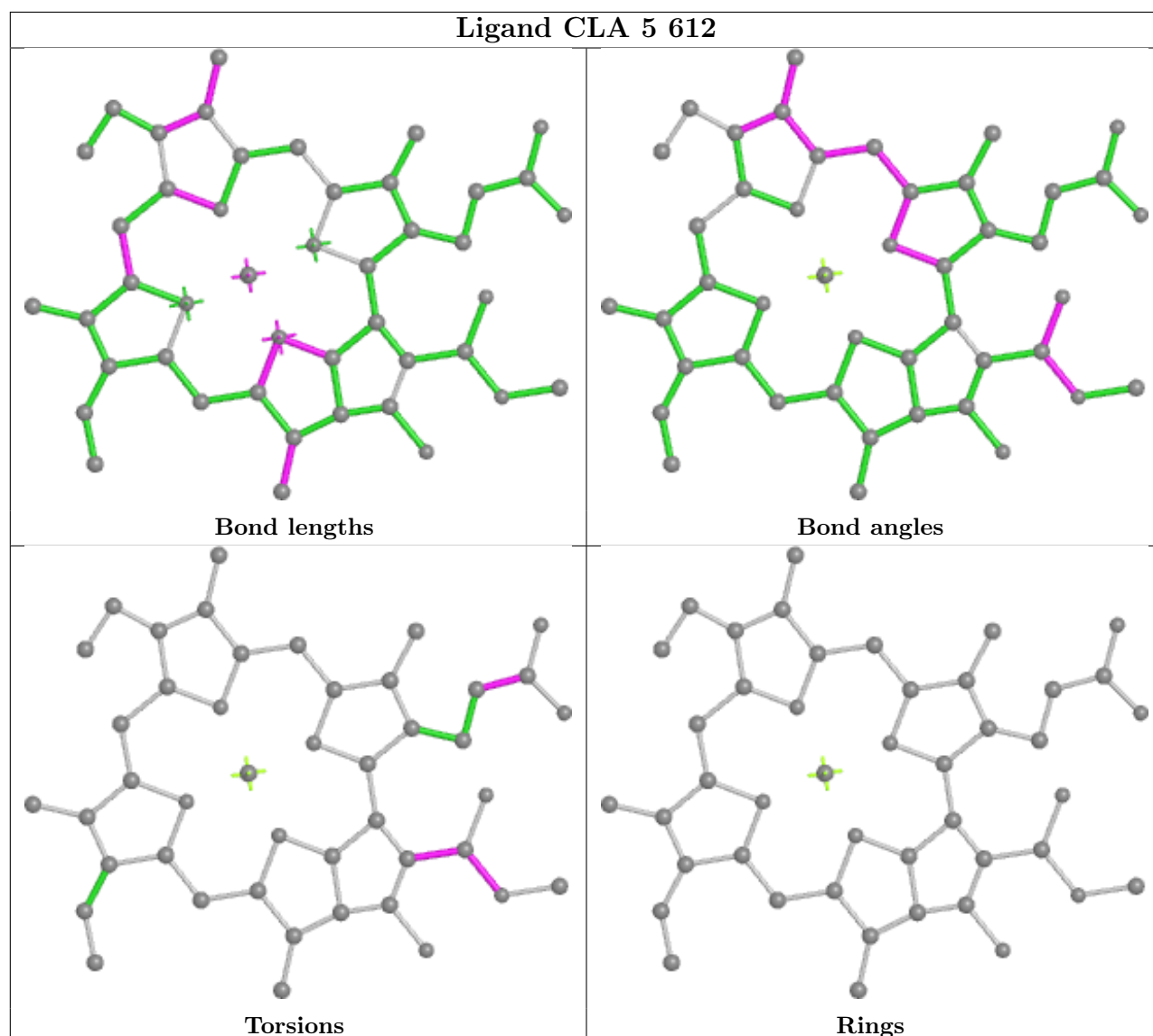
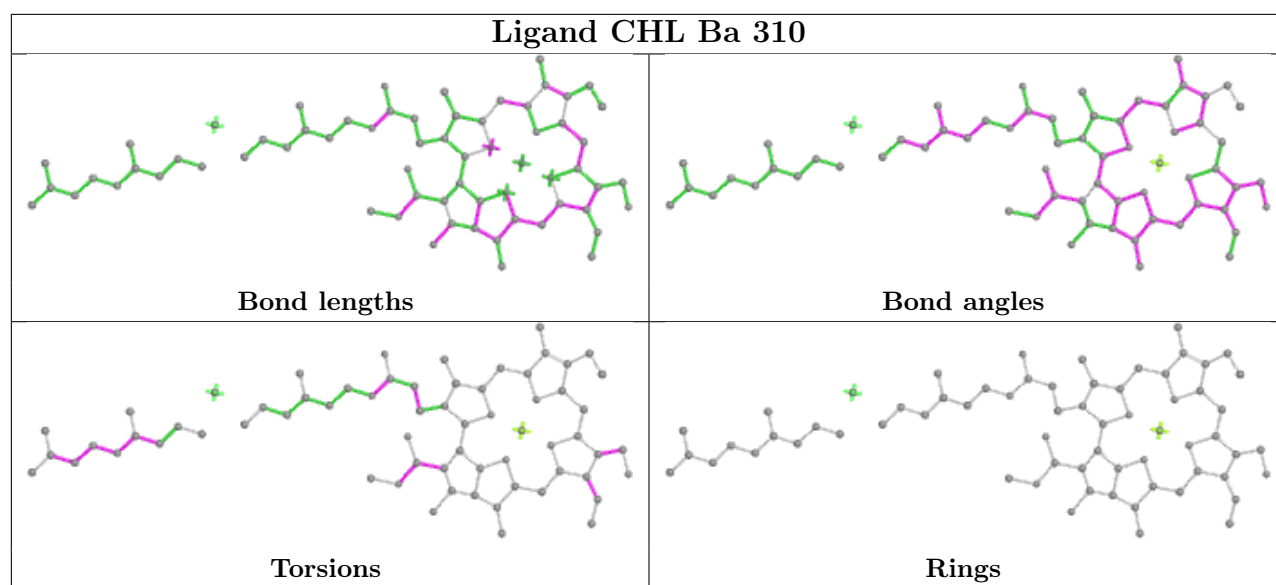
Torsions

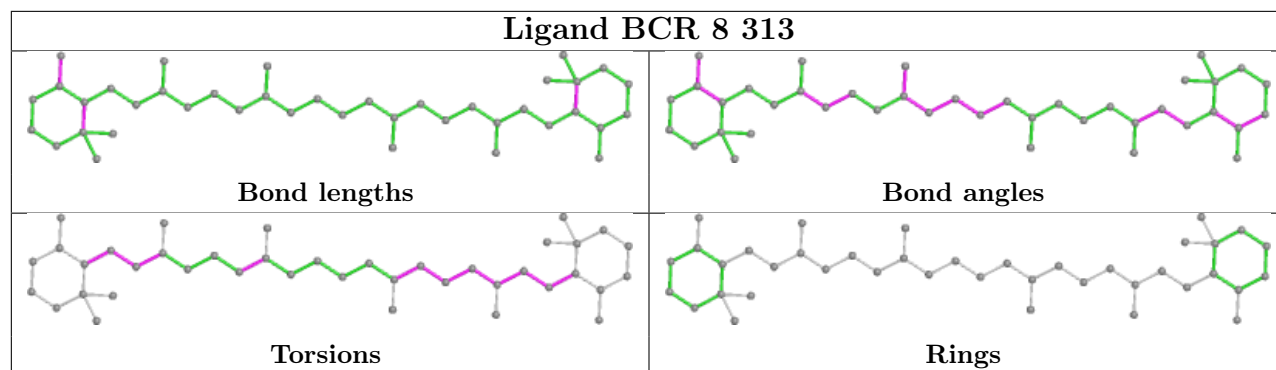
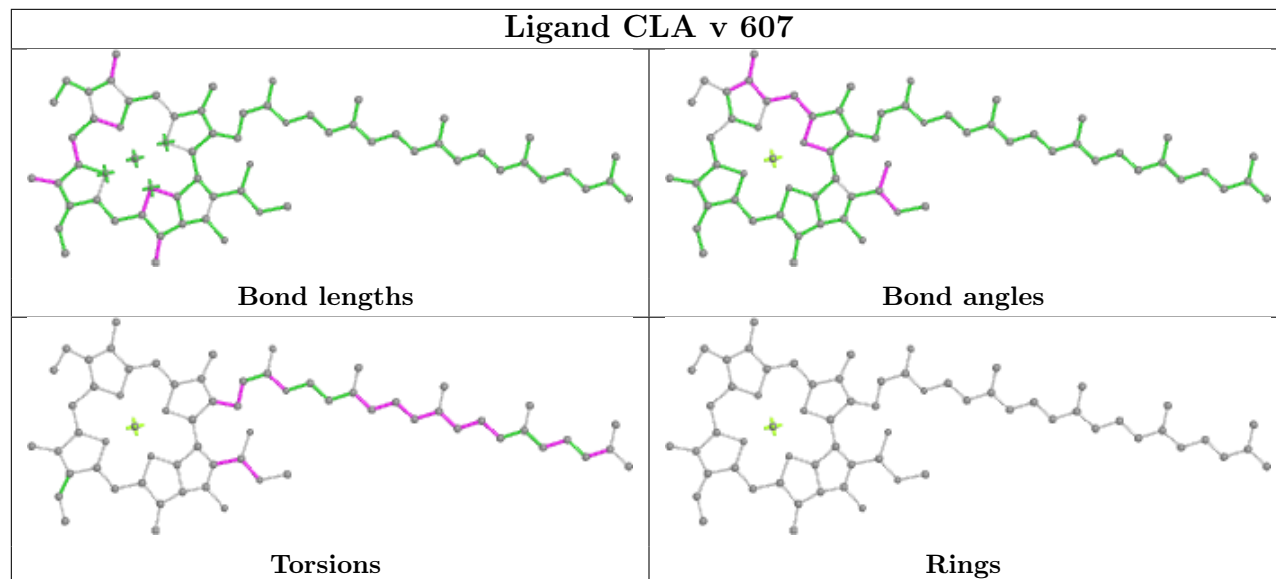
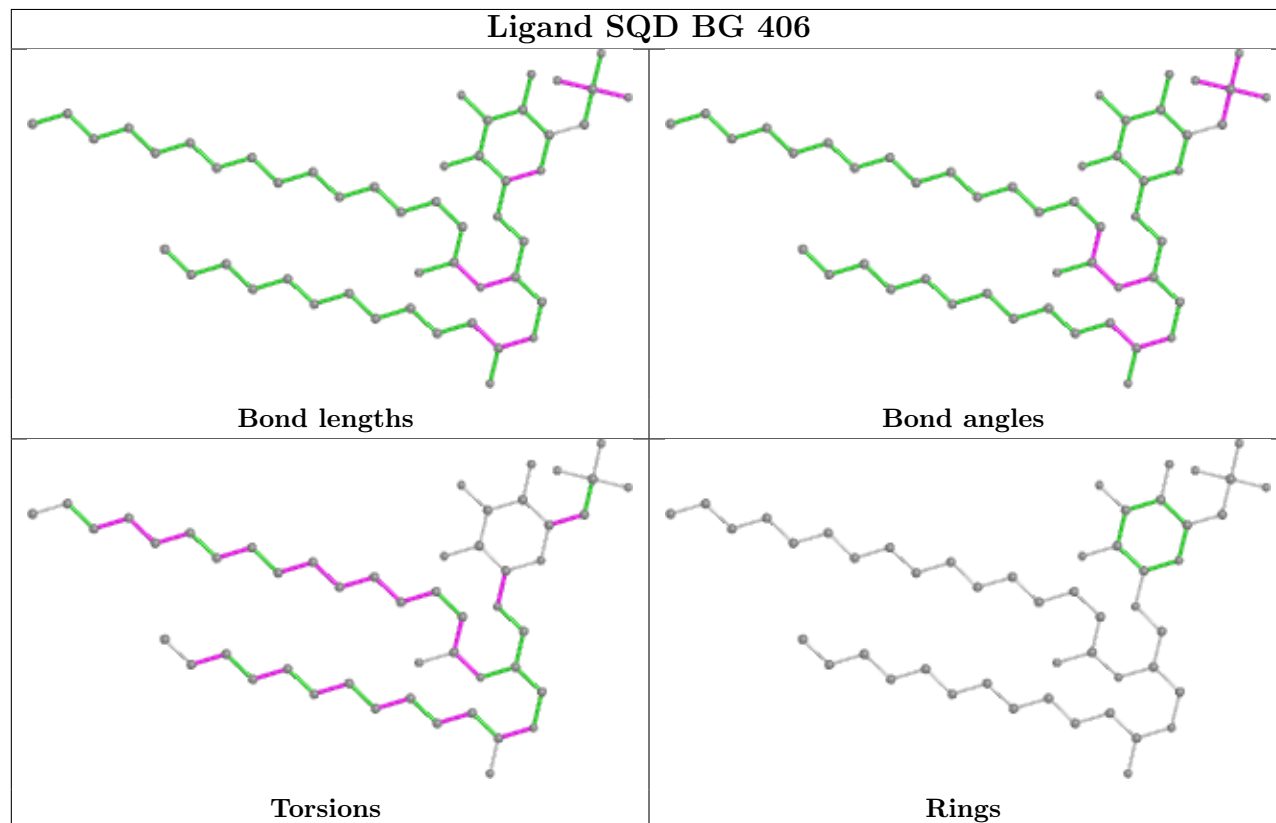


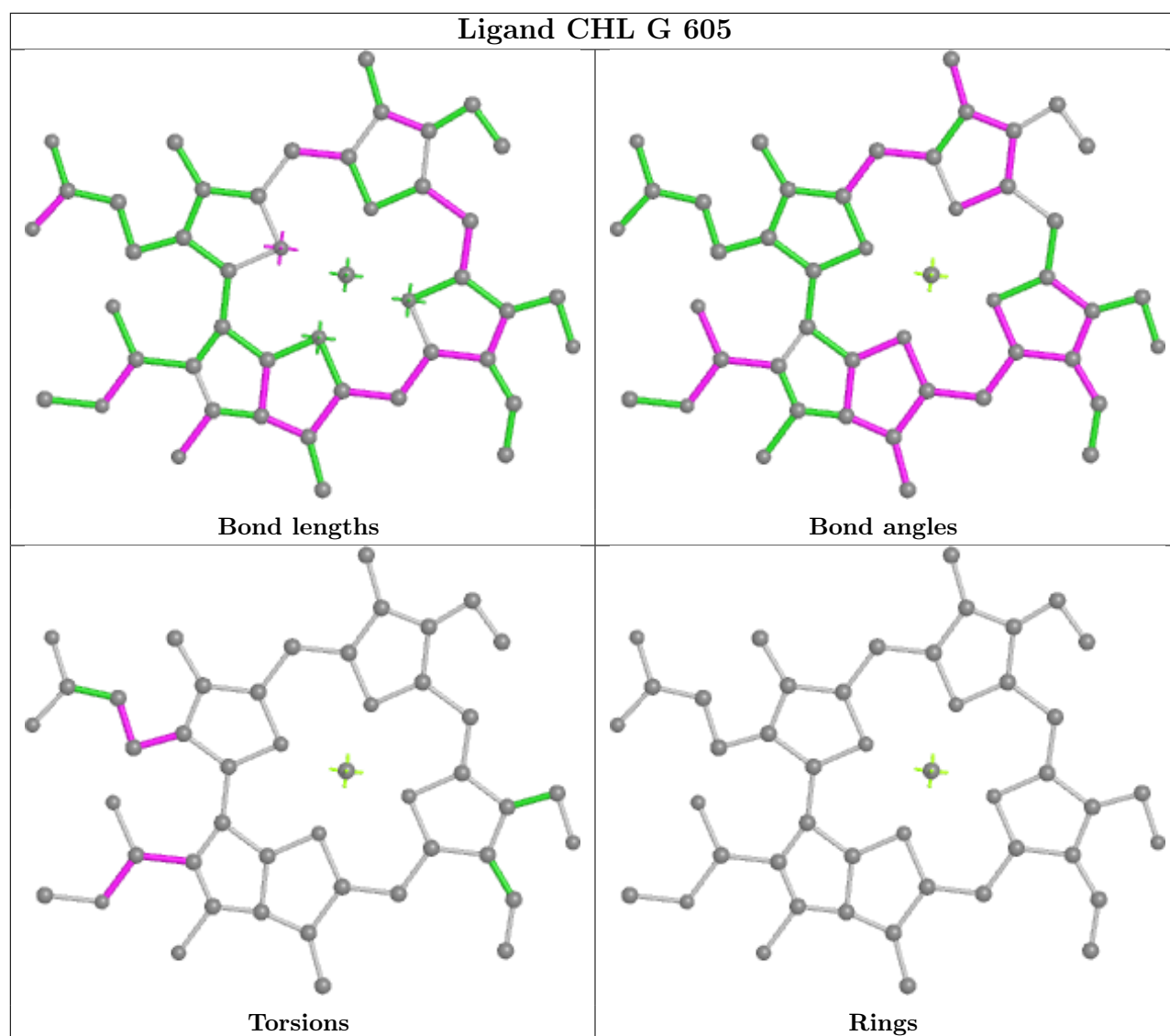
Rings

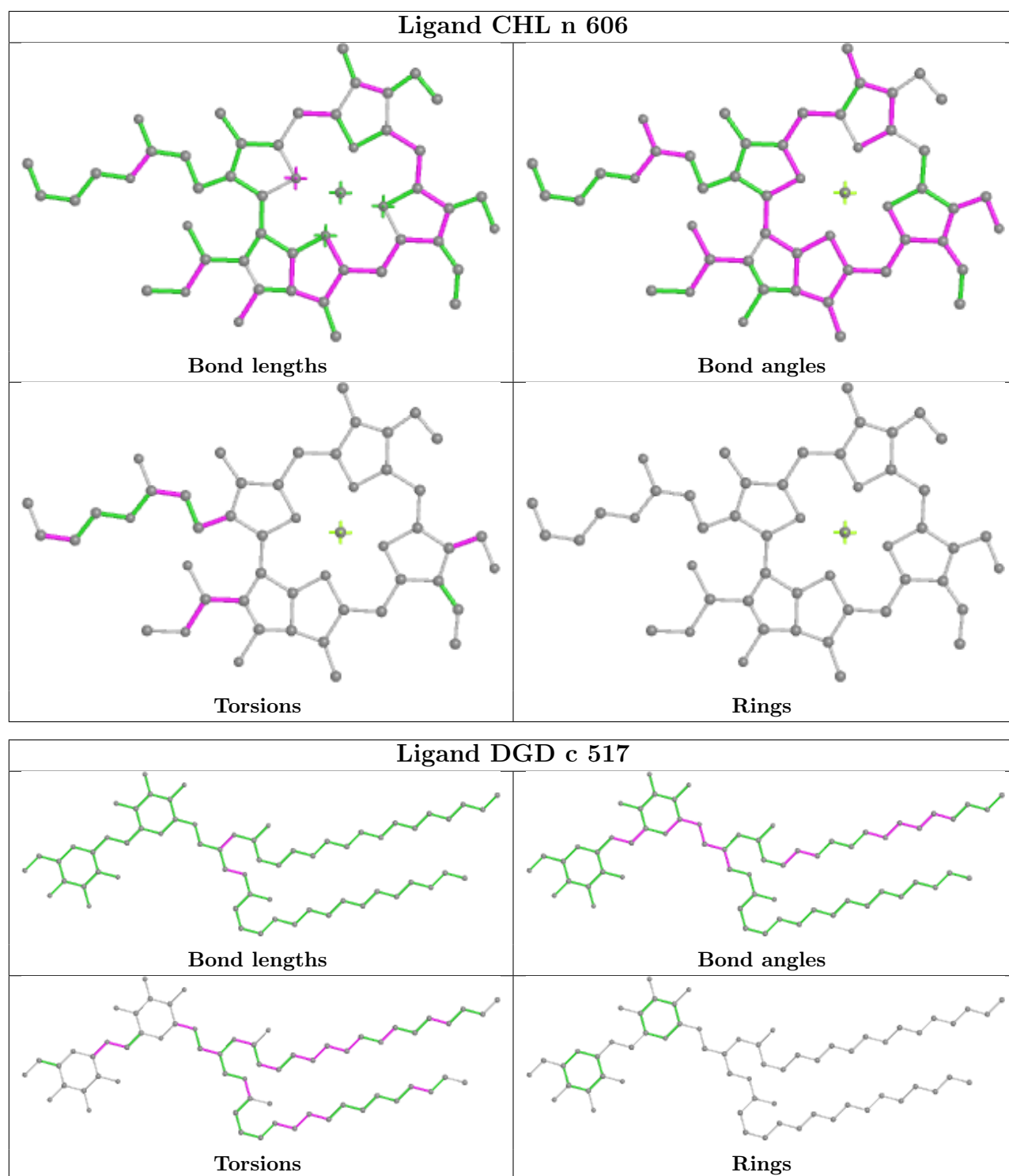




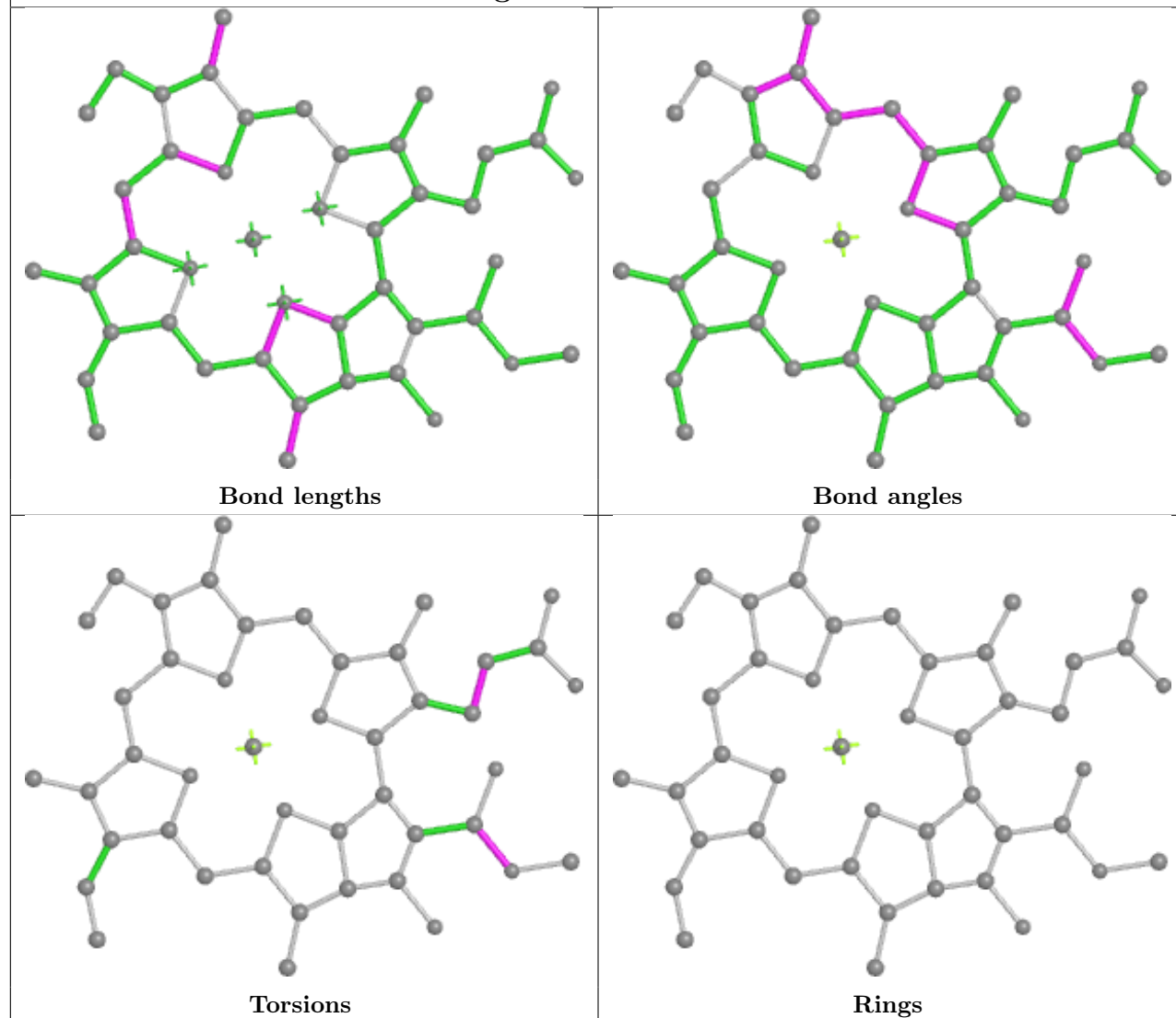


Ligand BCR 8 313**Ligand CLA v 607****Ligand SQD BG 406**

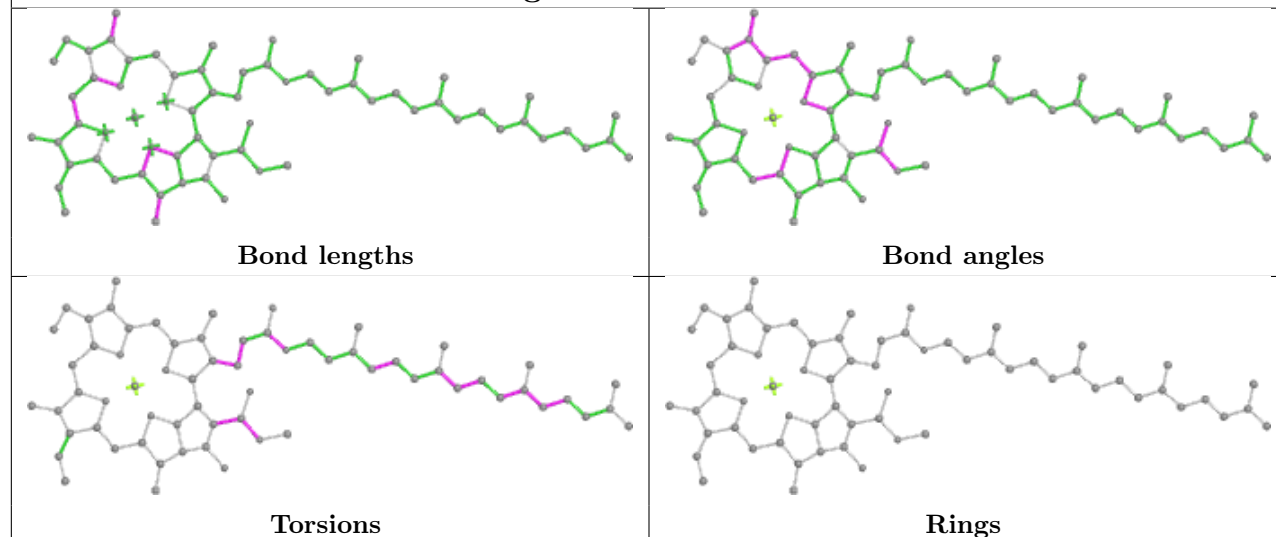




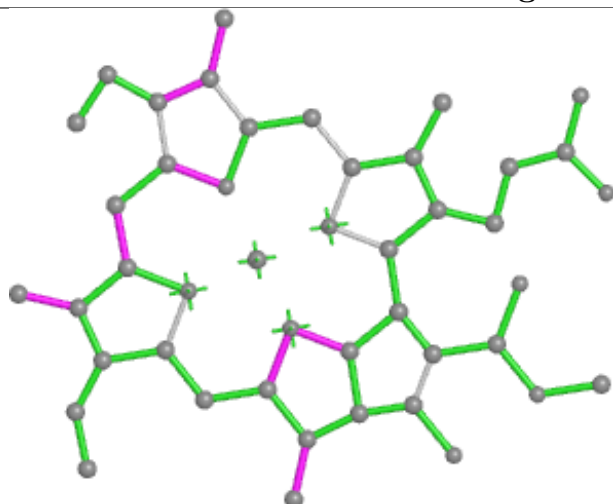
Ligand CLA 7 315



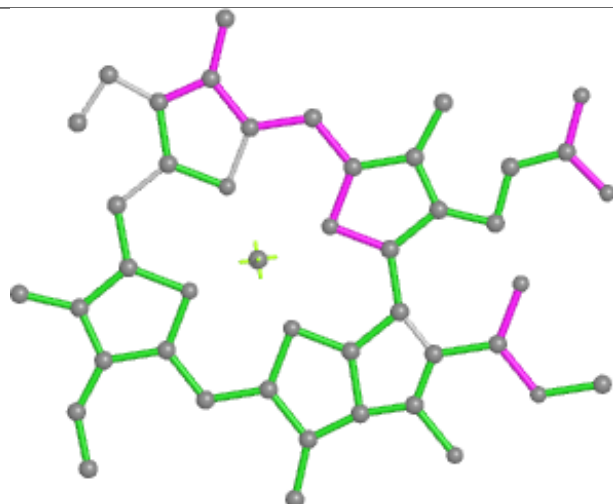
Ligand CLA Ba 303



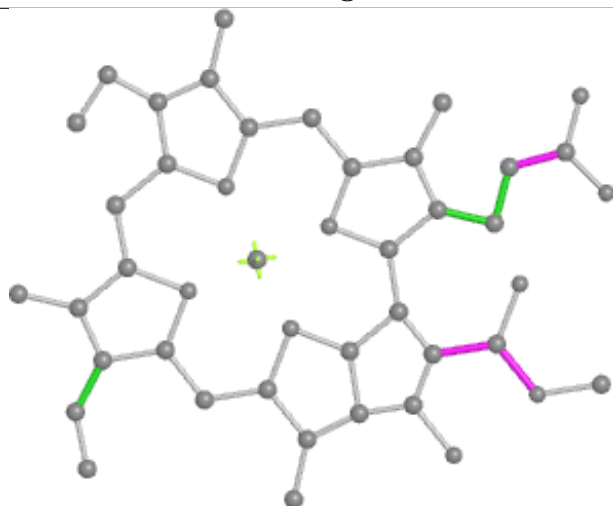
Ligand CLA 6 612



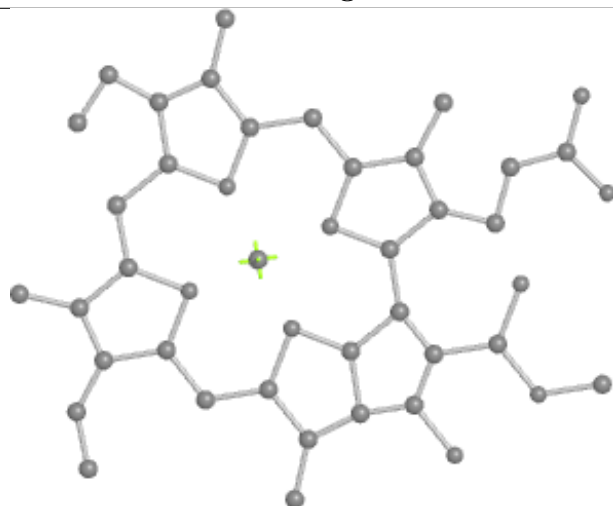
Bond lengths



Bond angles

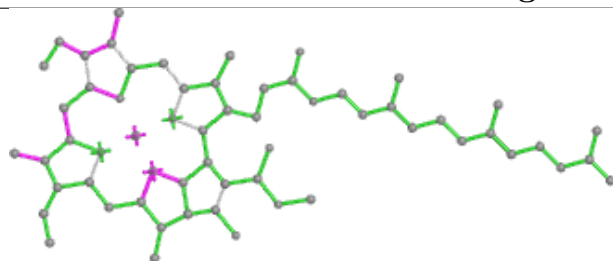


Torsions

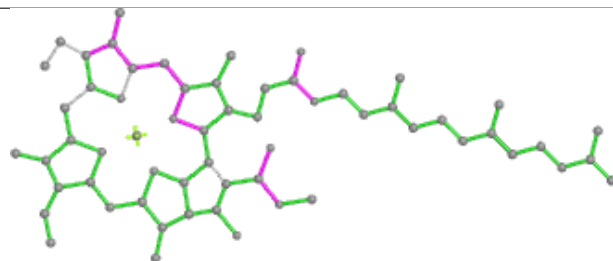


Rings

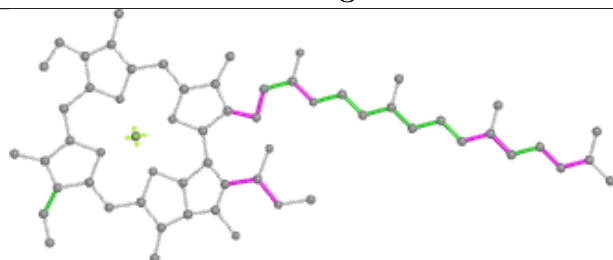
Ligand CLA 6 602



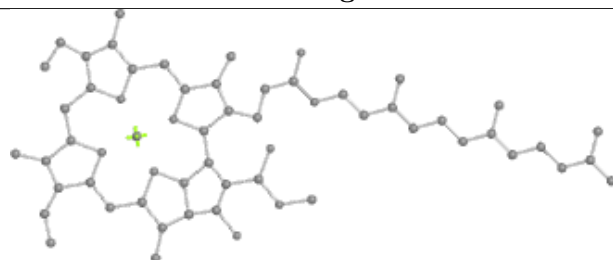
Bond lengths



Bond angles

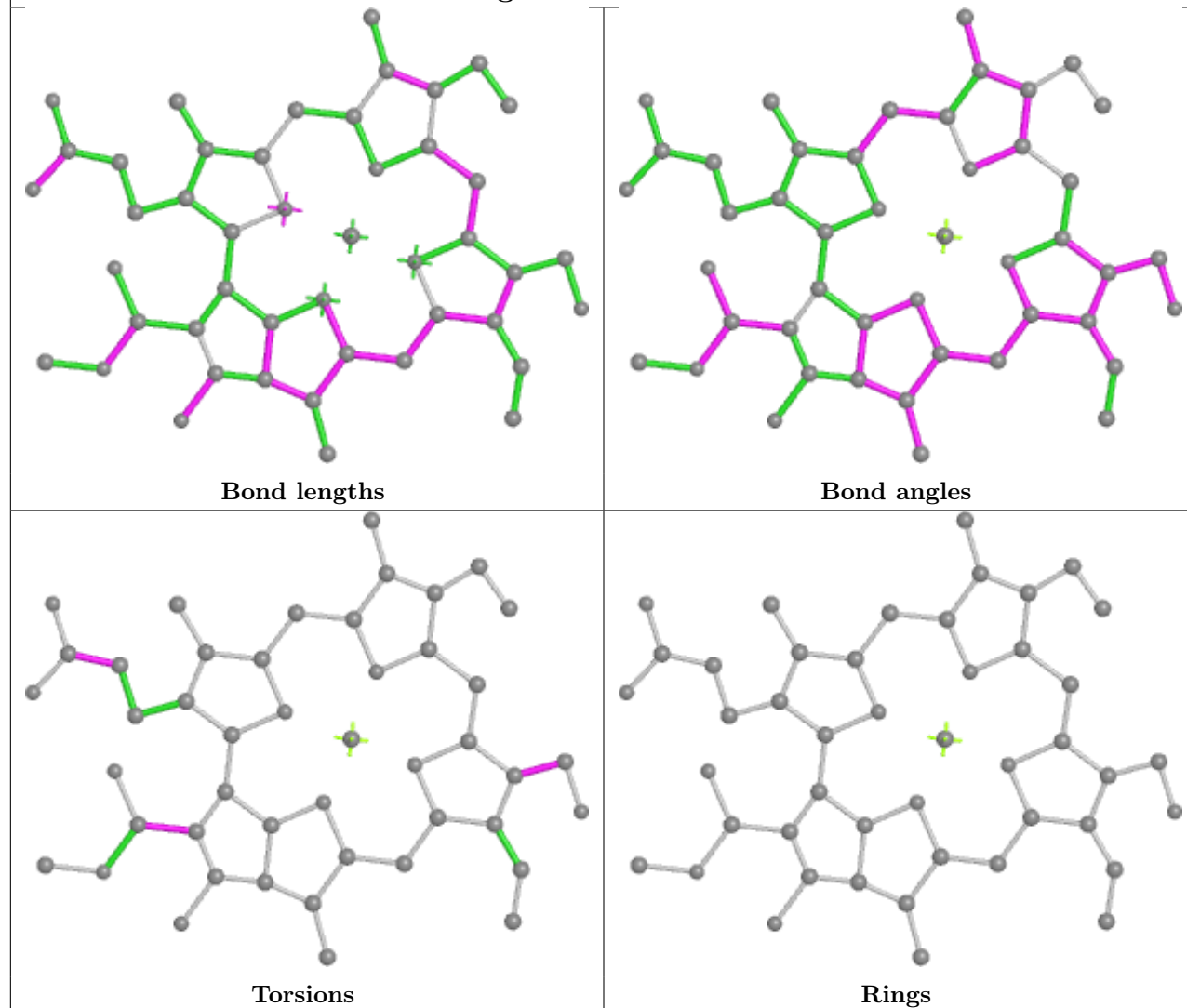


Torsions

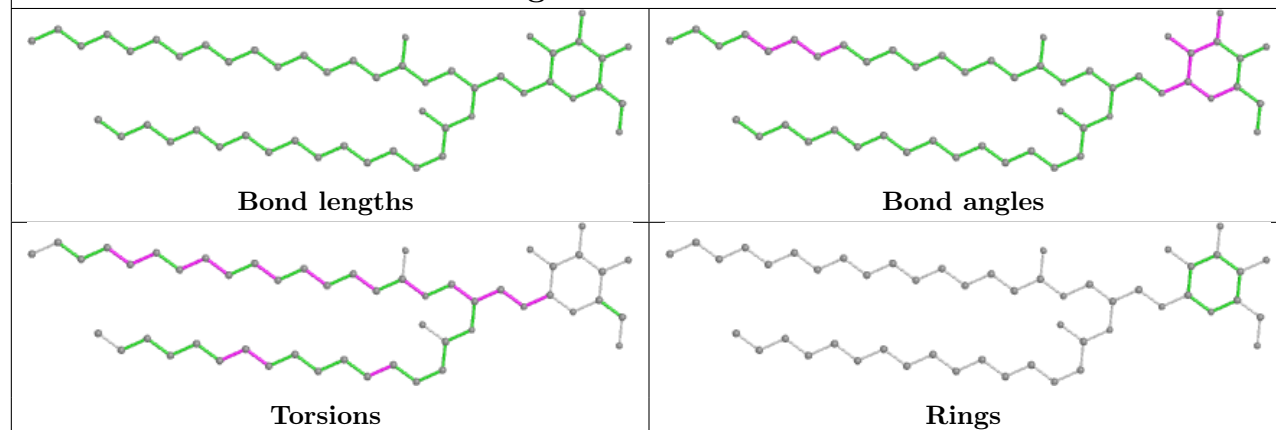


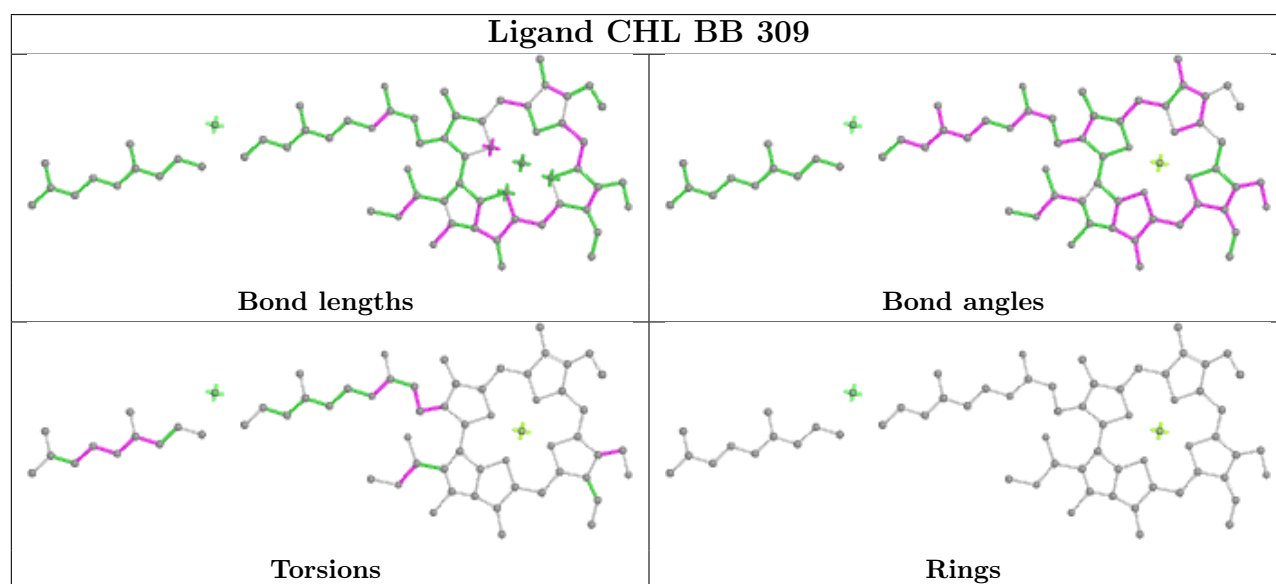
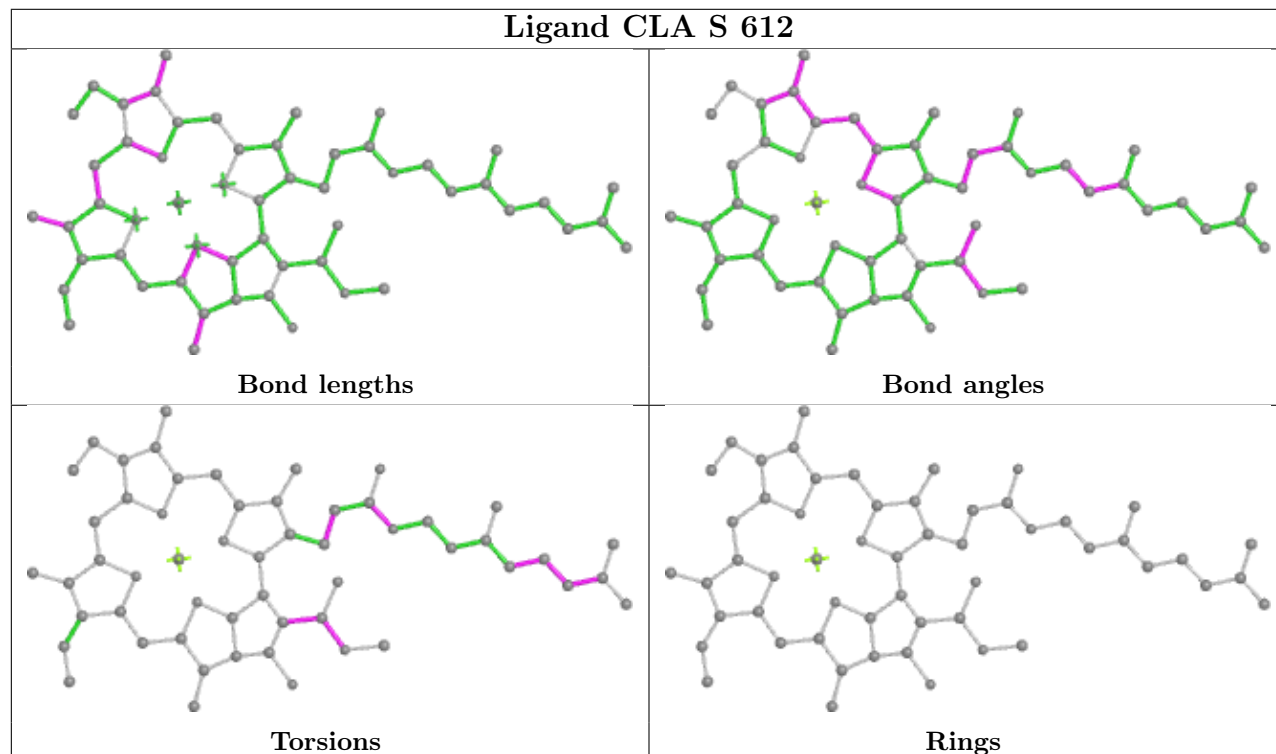
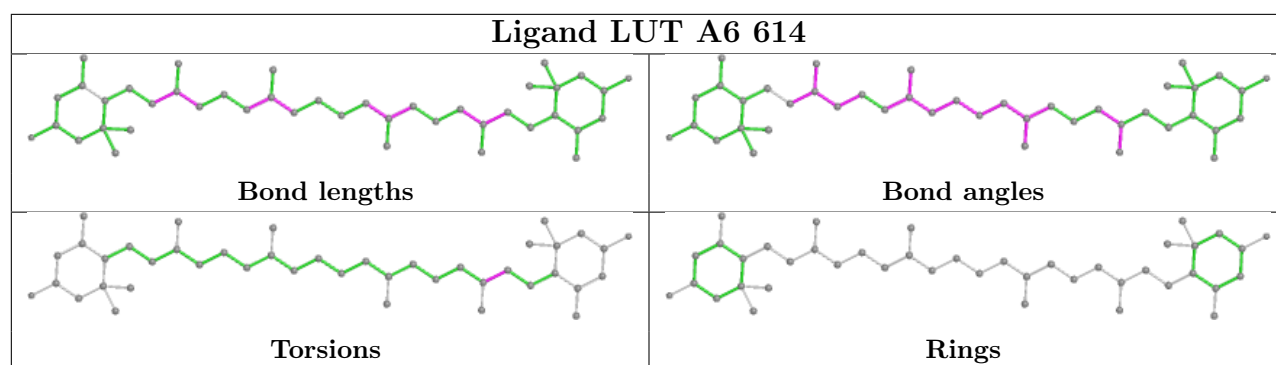
Rings

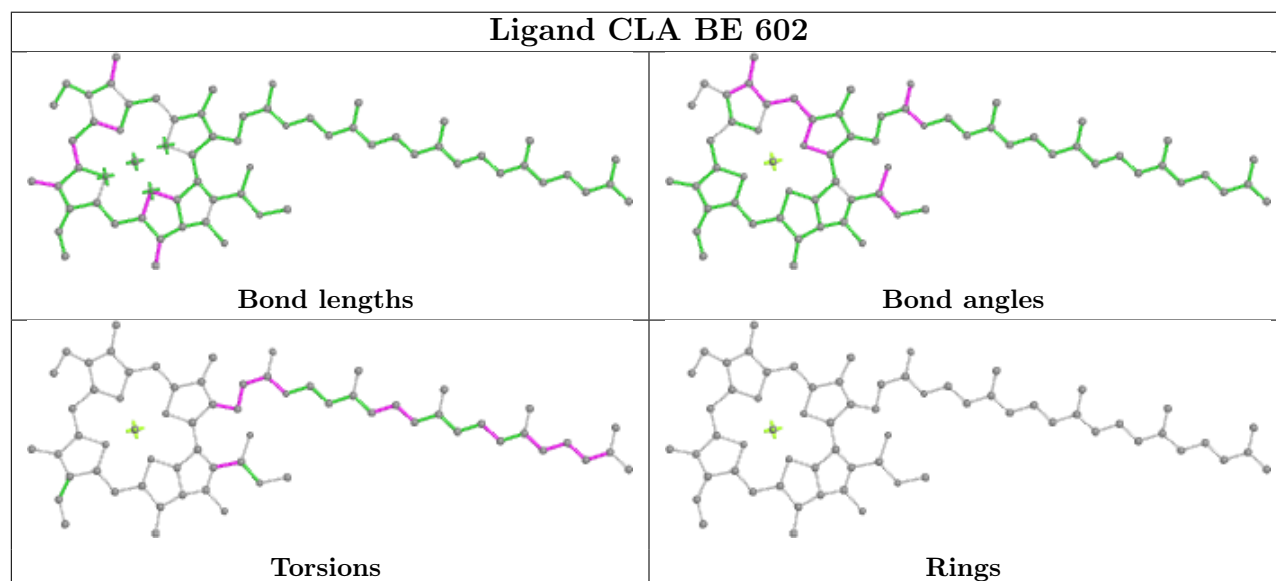
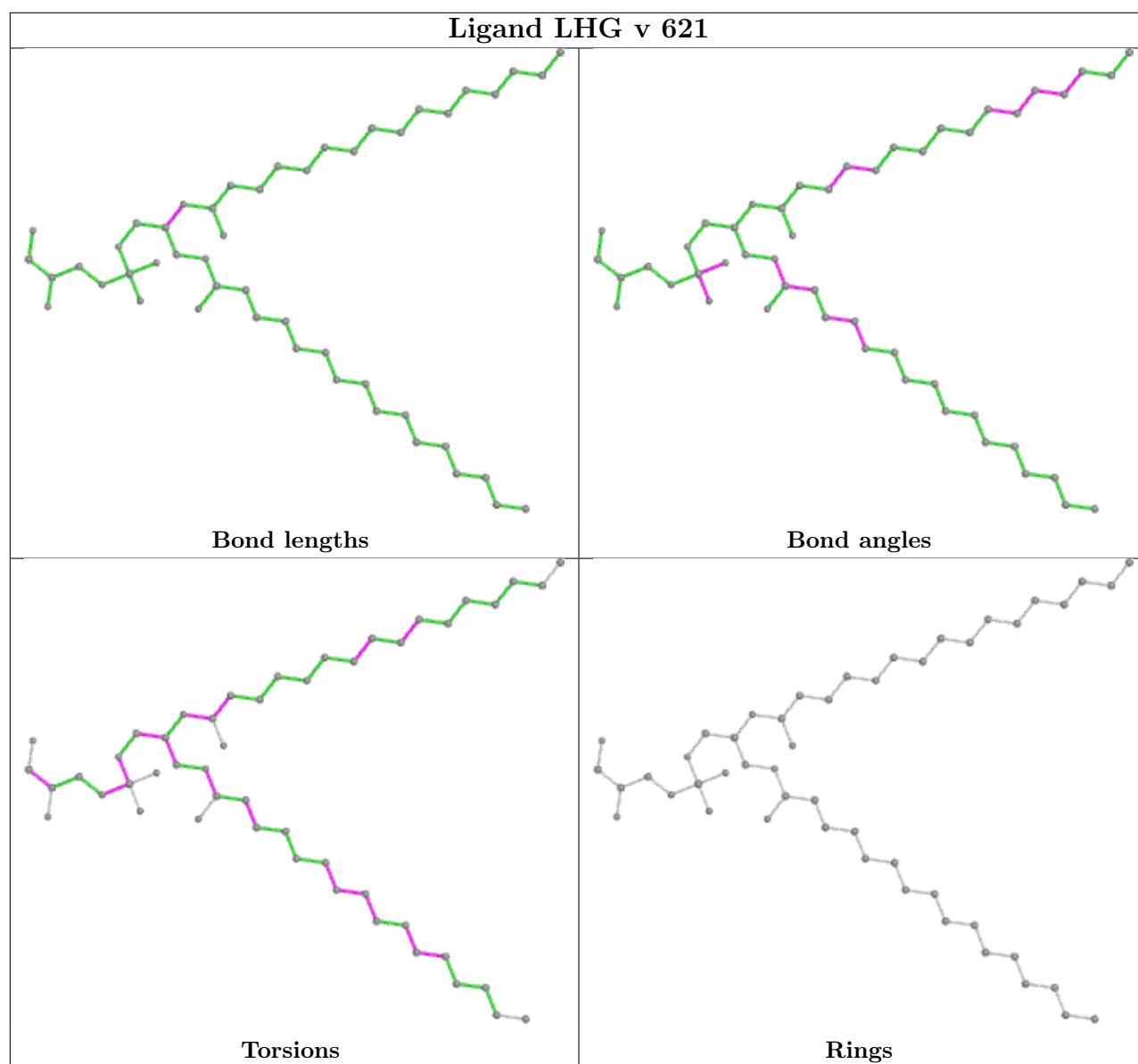
Ligand CHL S 601

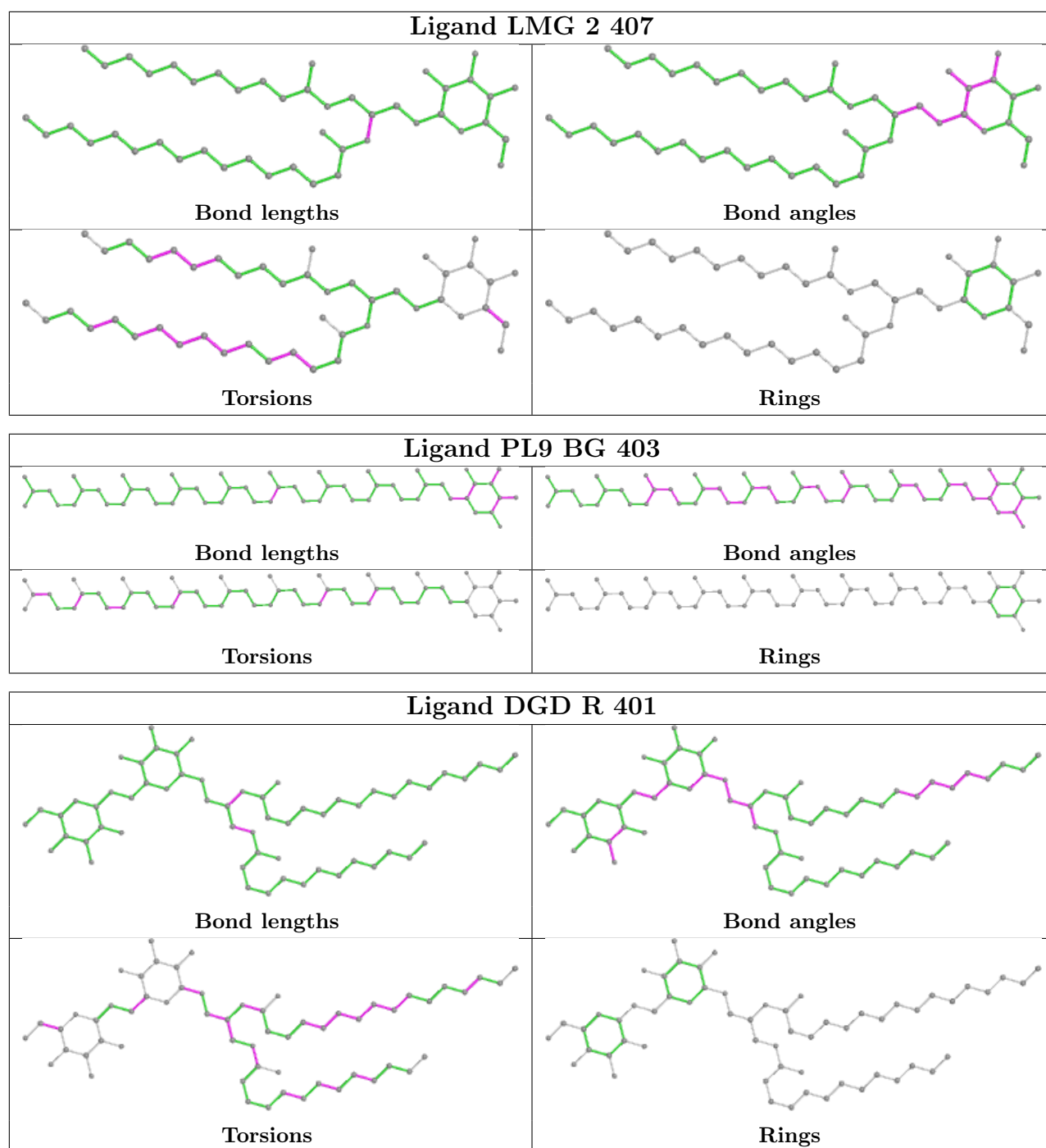


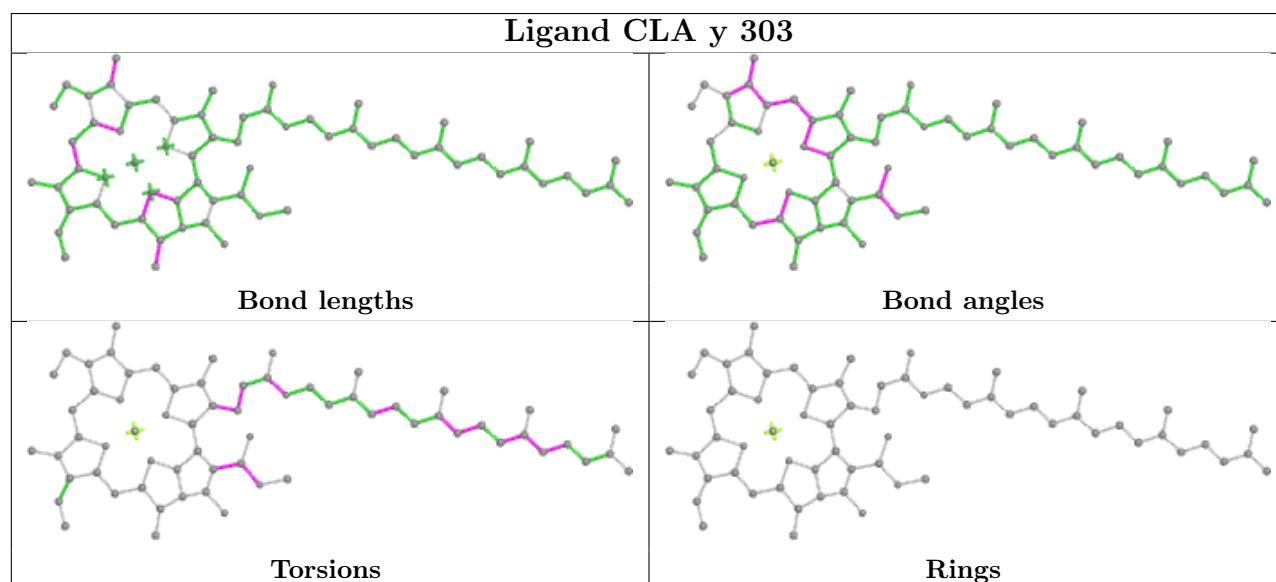
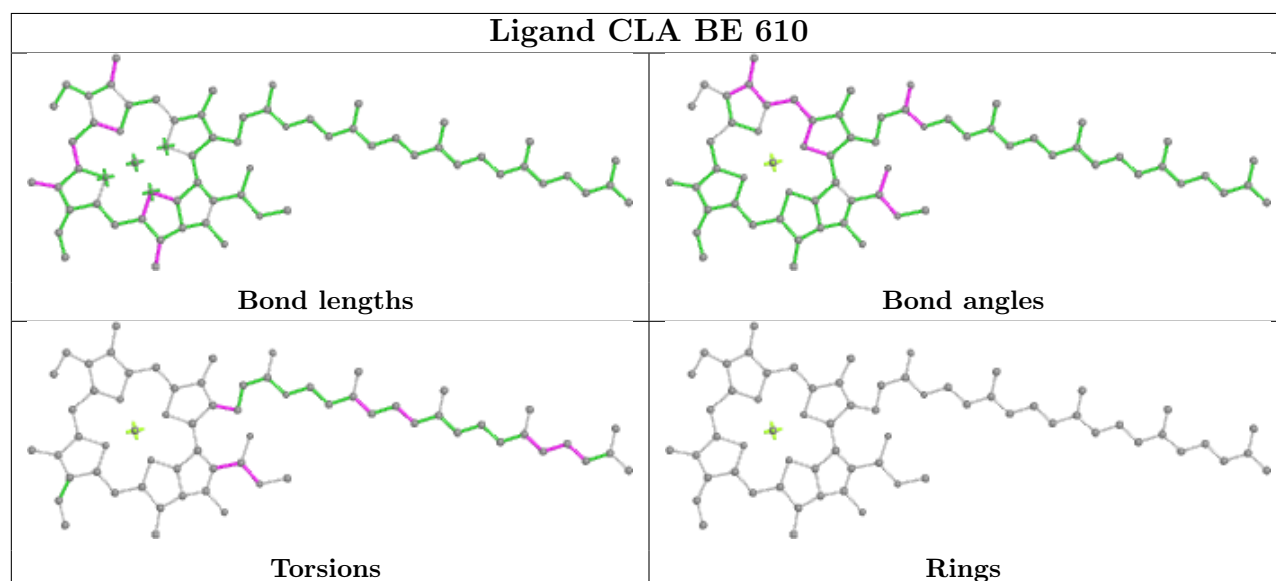
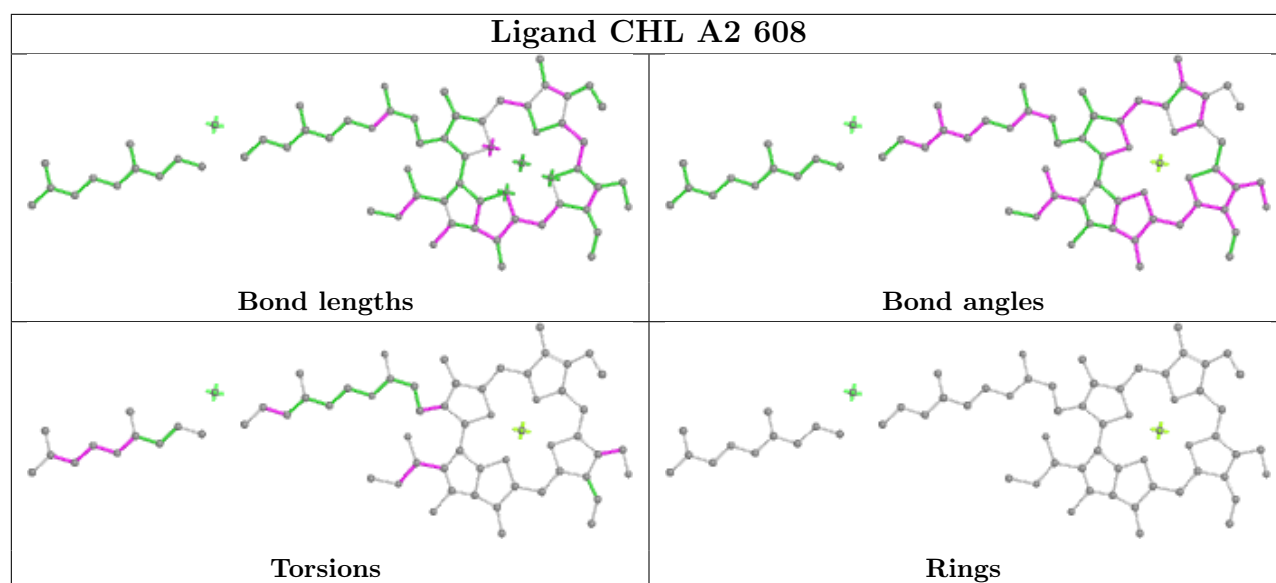
Ligand LMG C 501



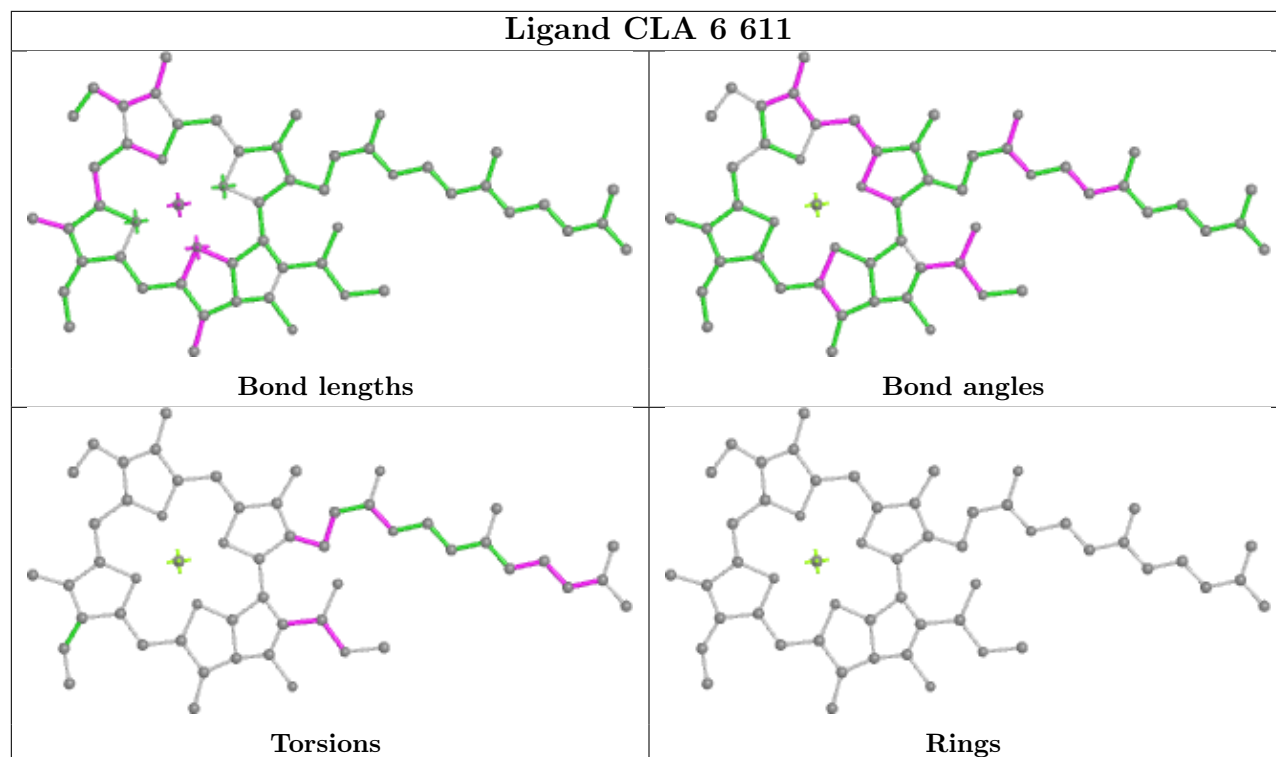




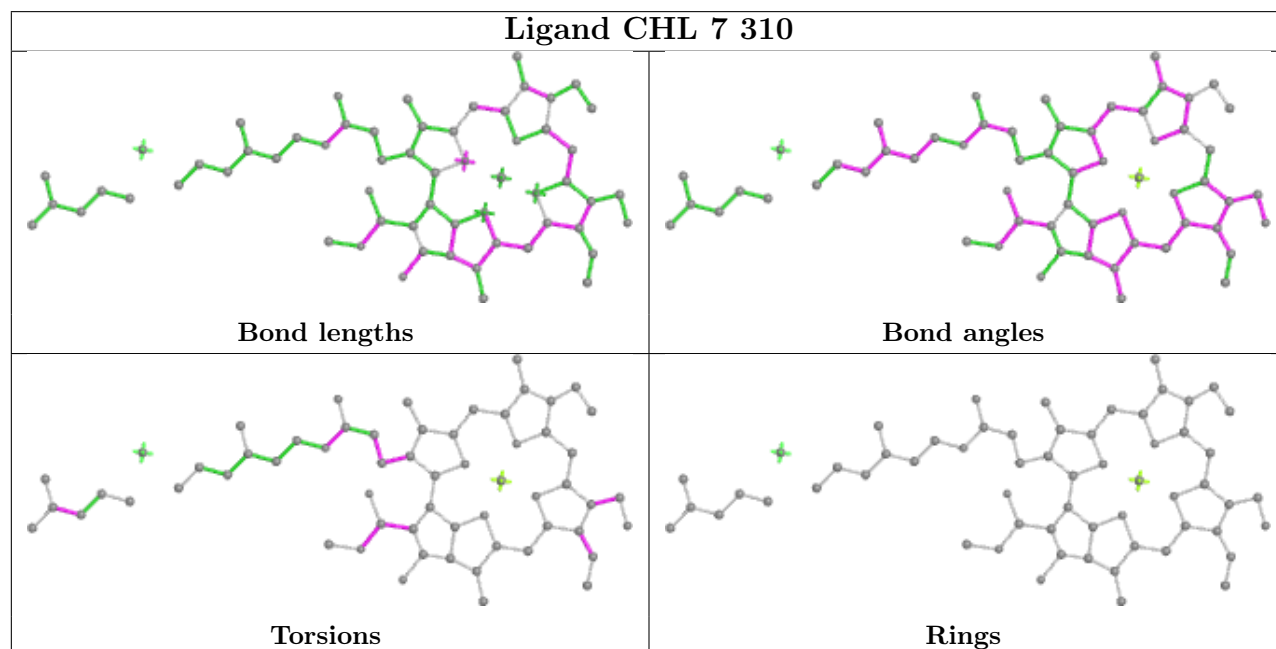


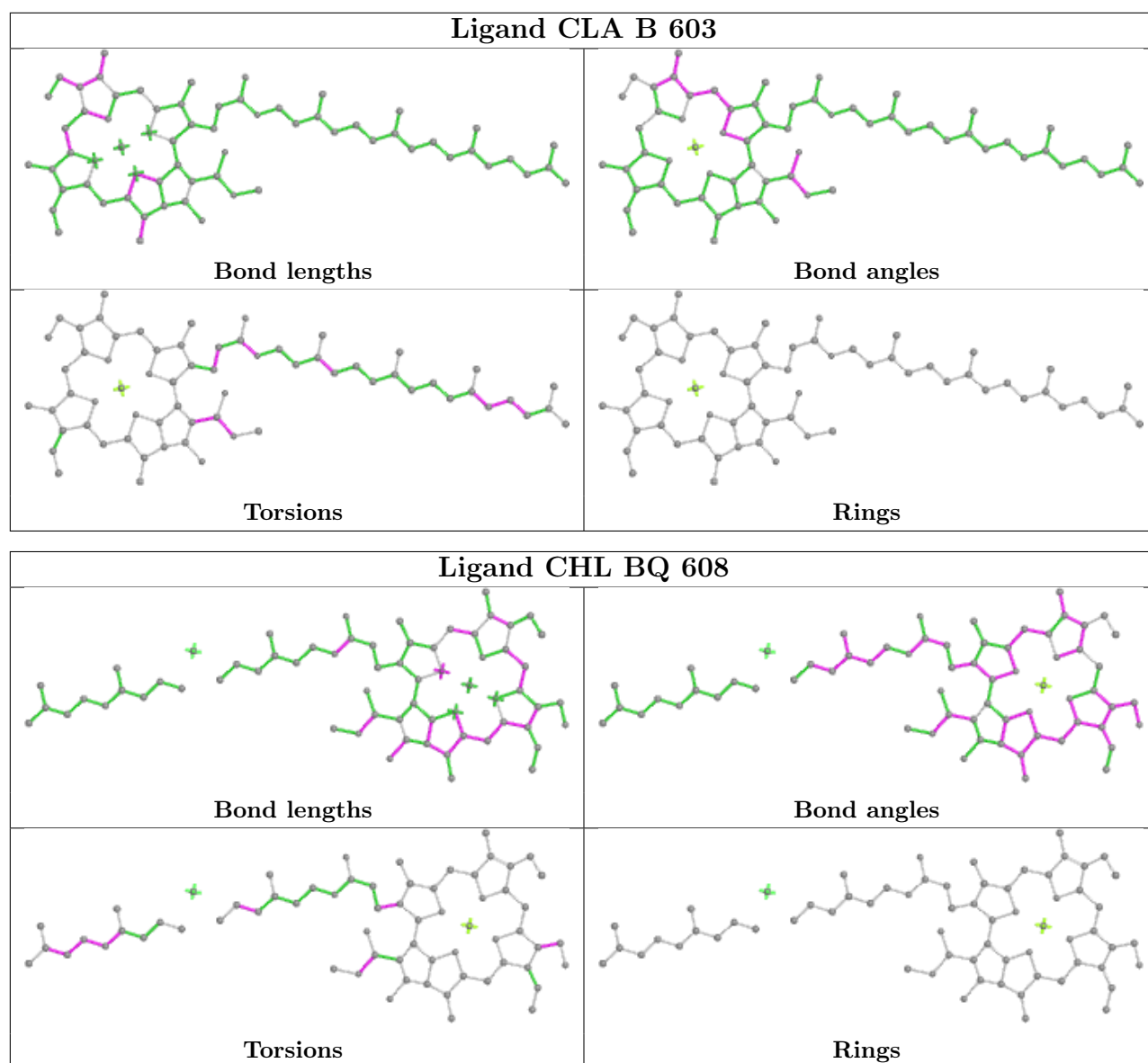


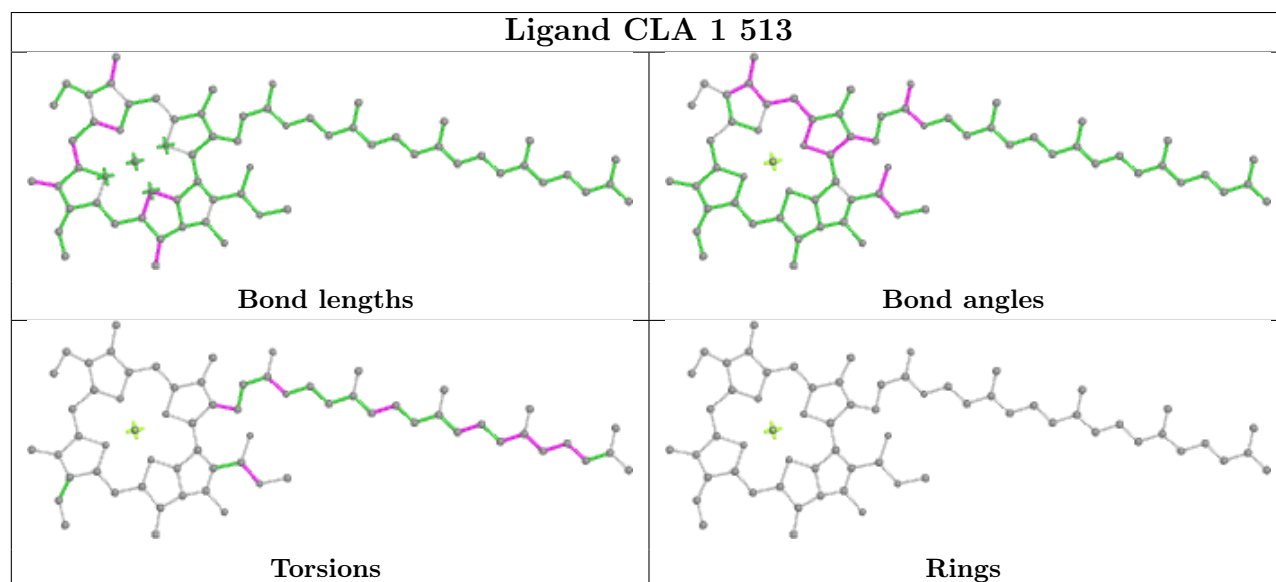
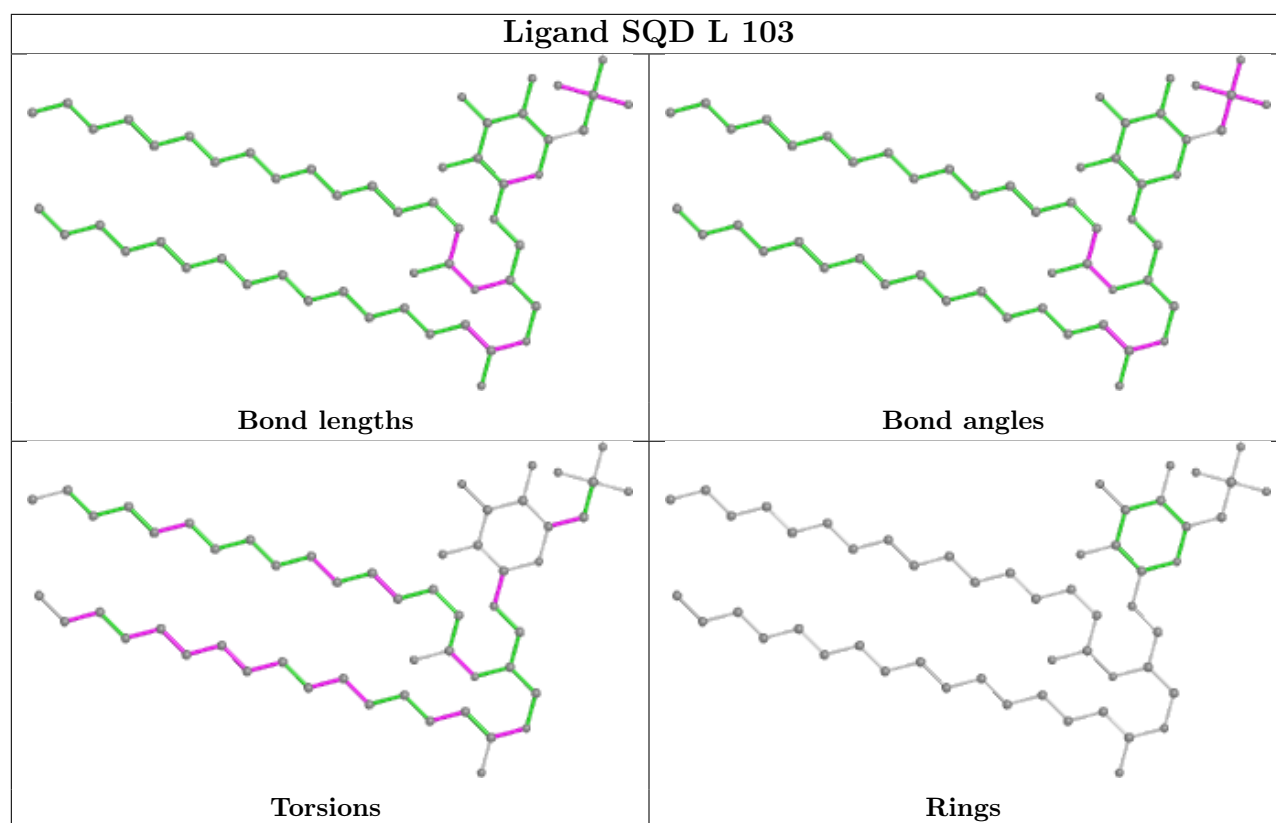
Ligand CLA 6 611



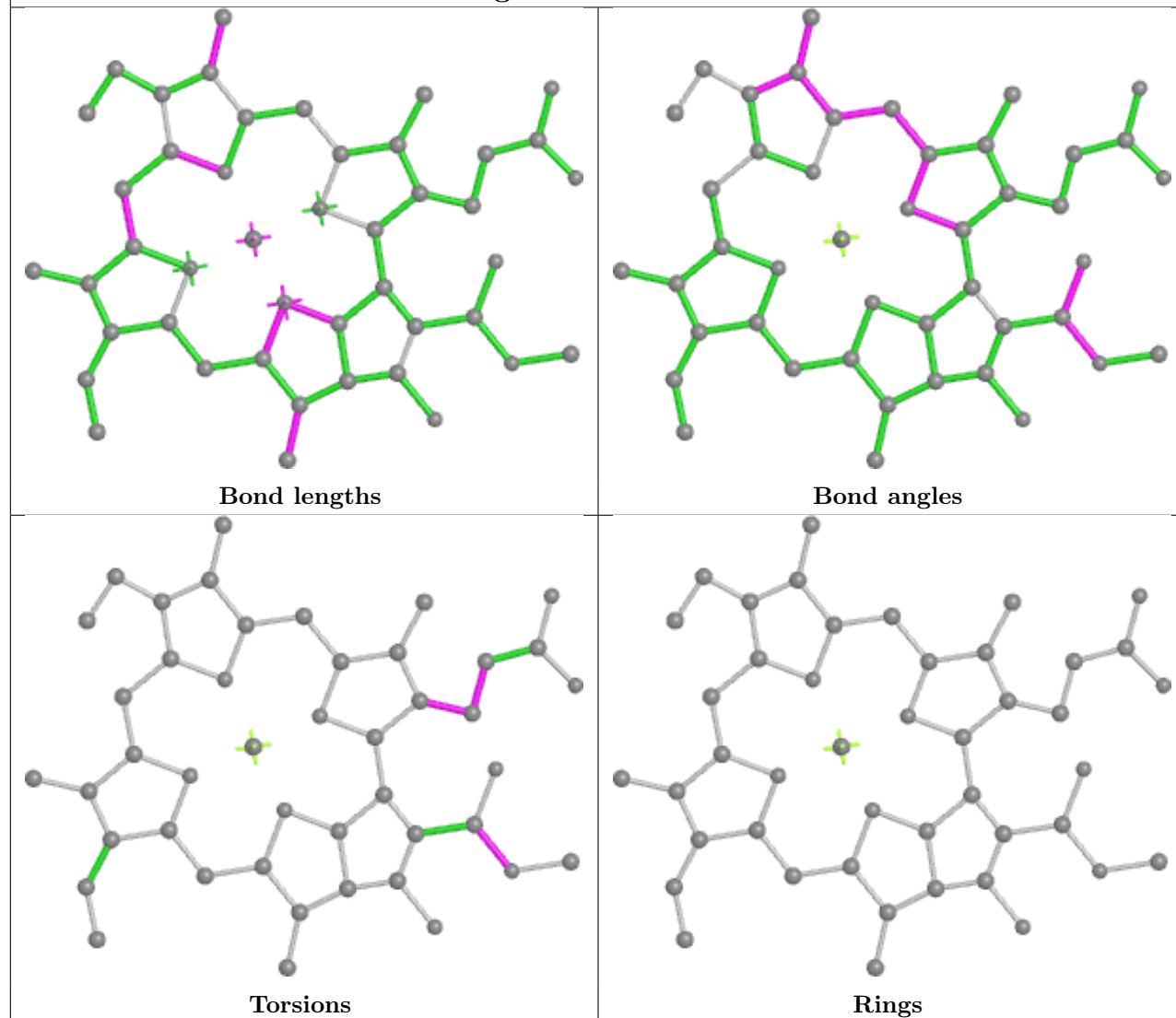
Ligand CHL 7 310



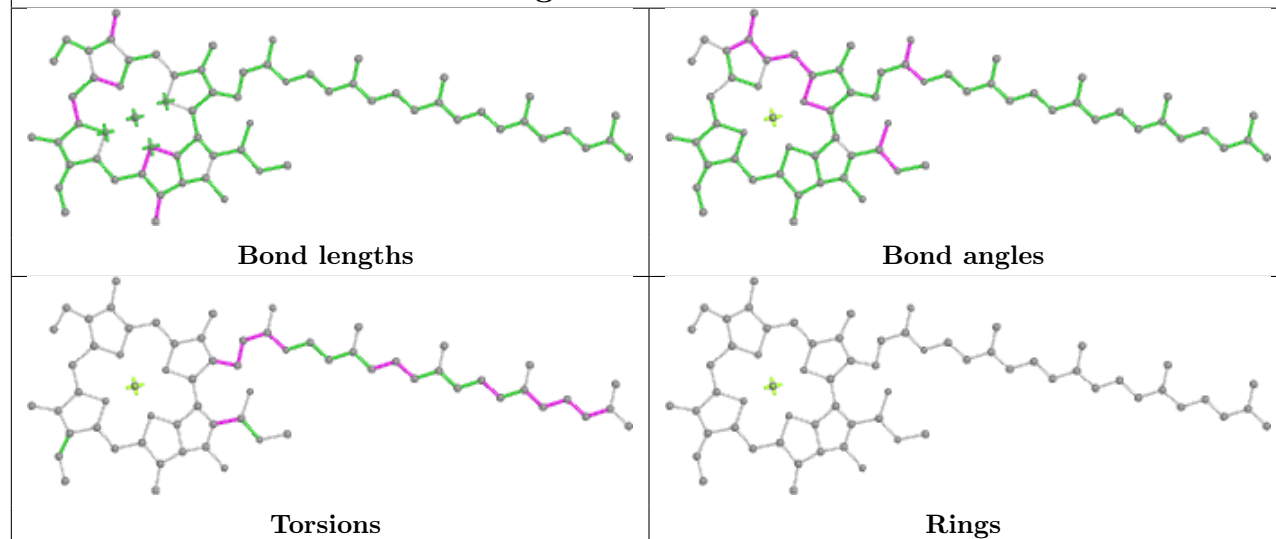


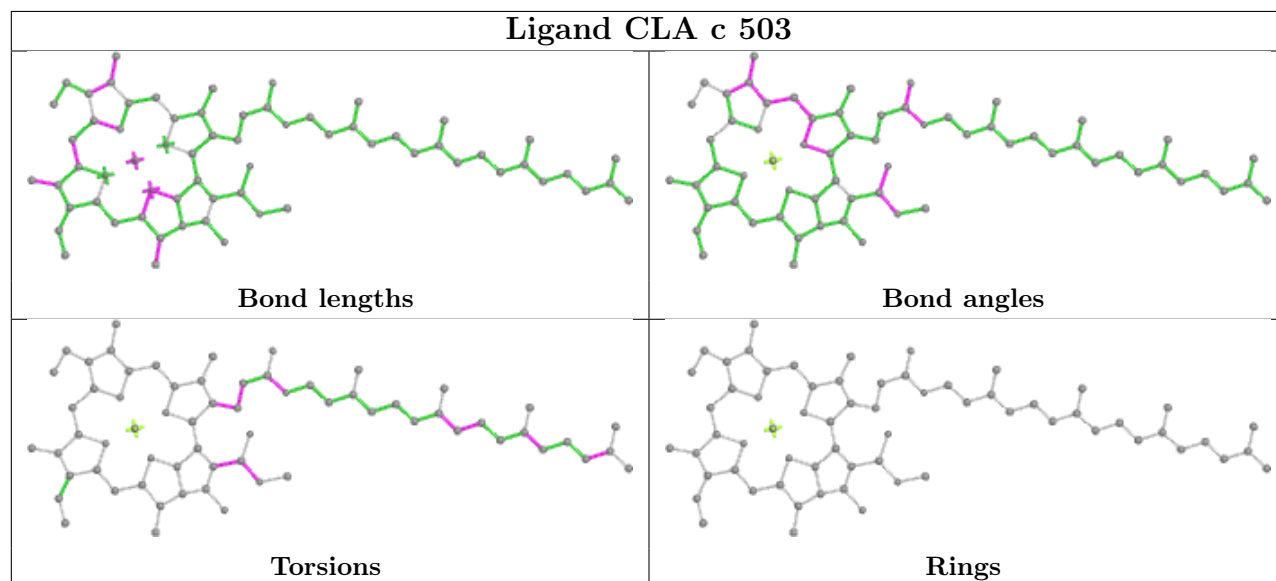
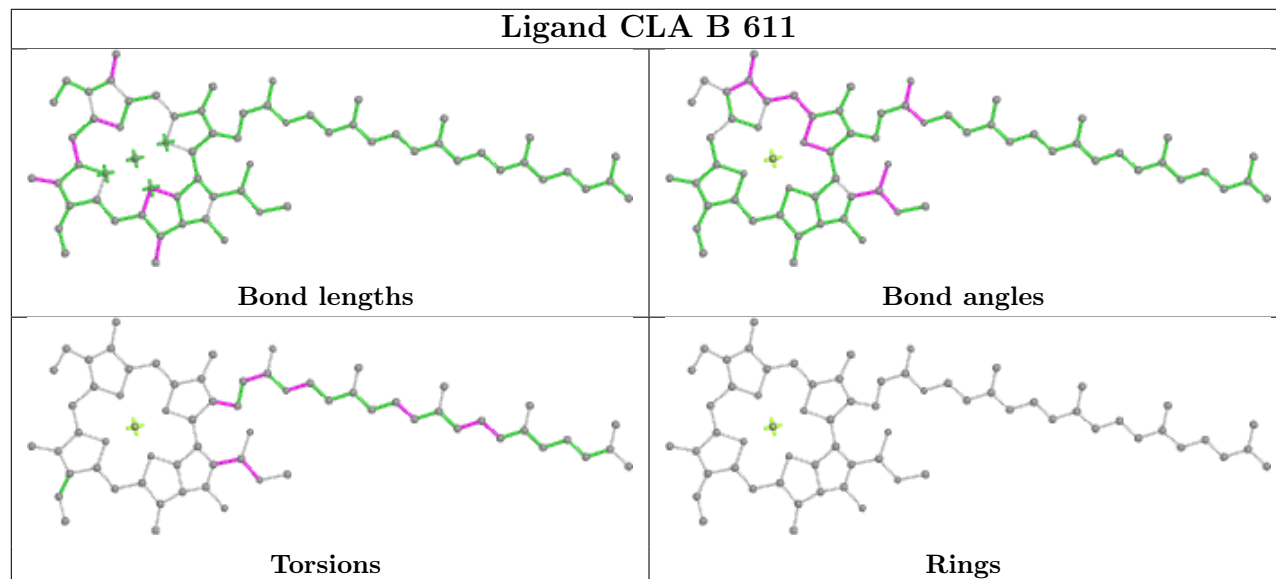
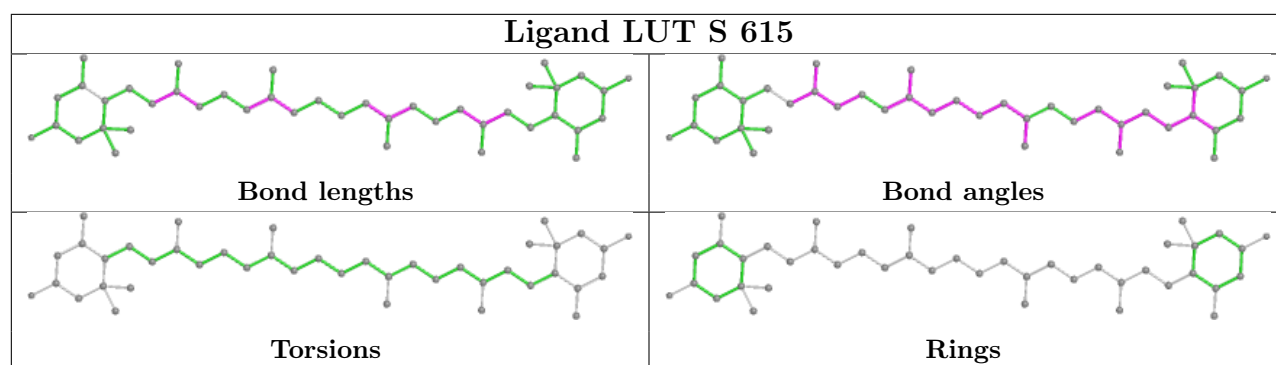


Ligand CLA 8 309

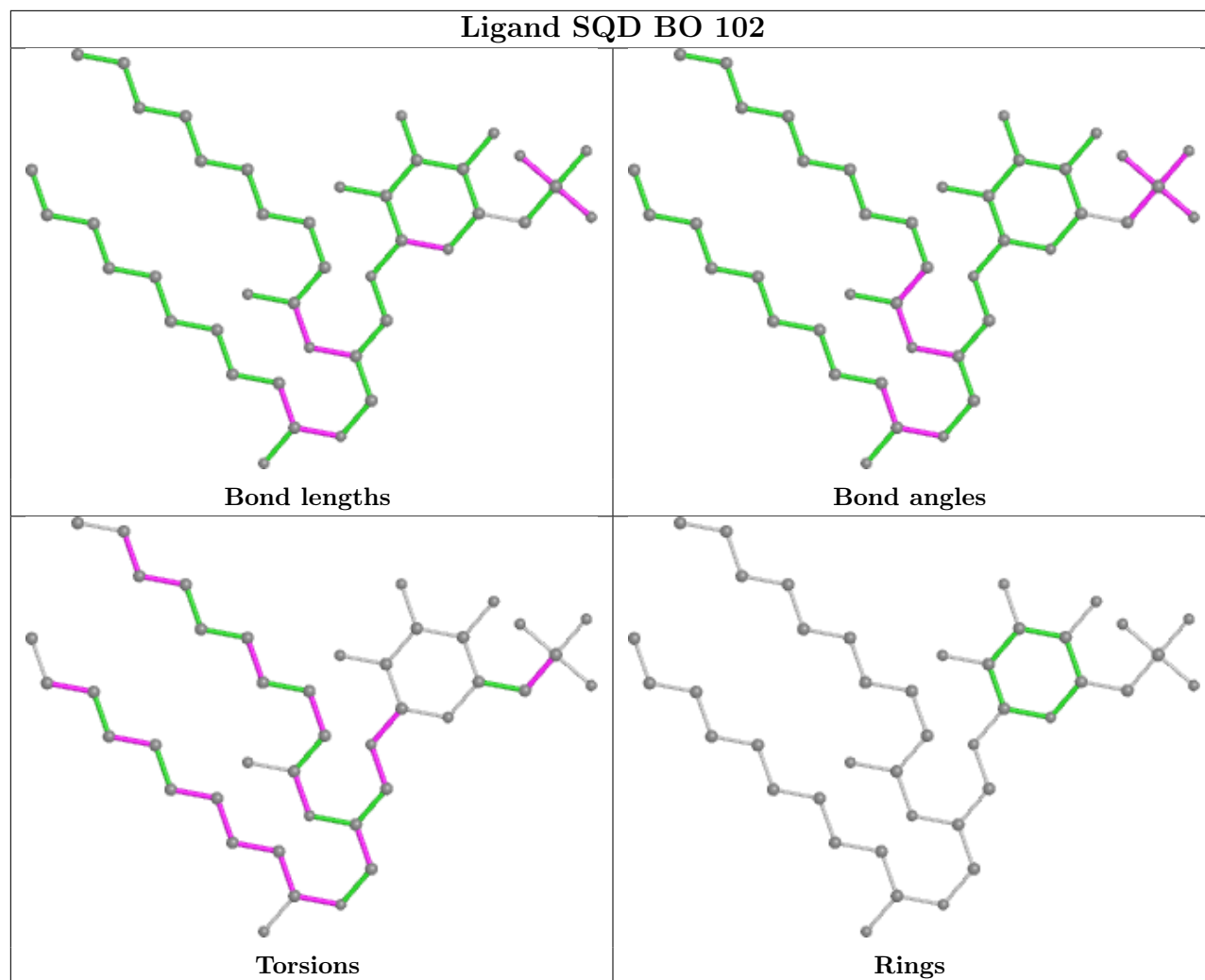


Ligand CLA b 602

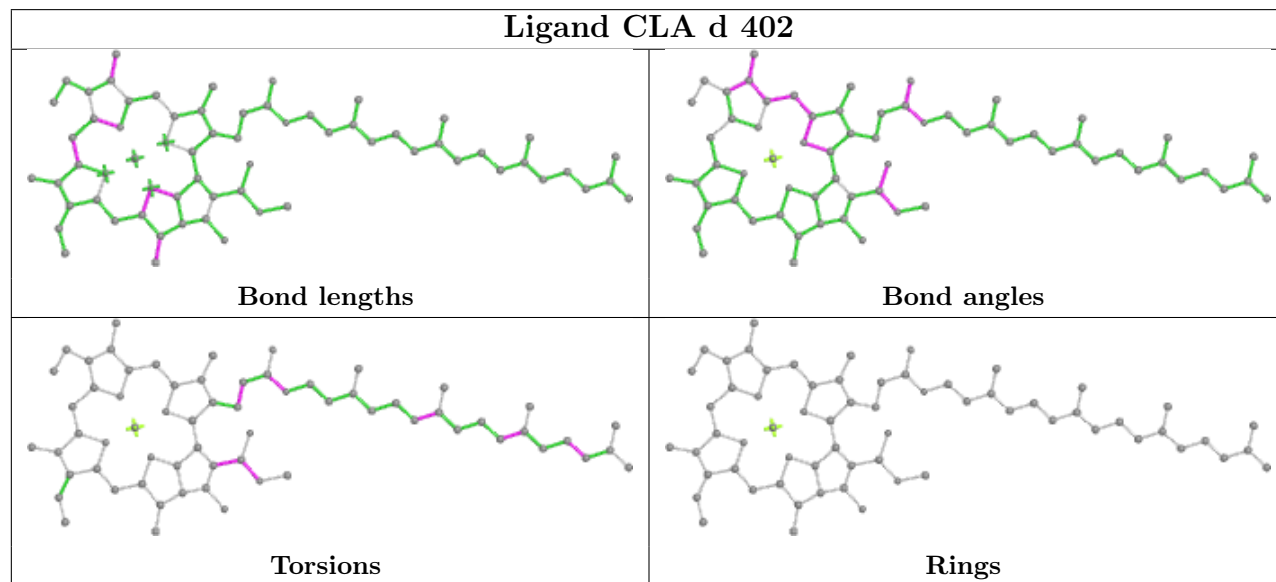




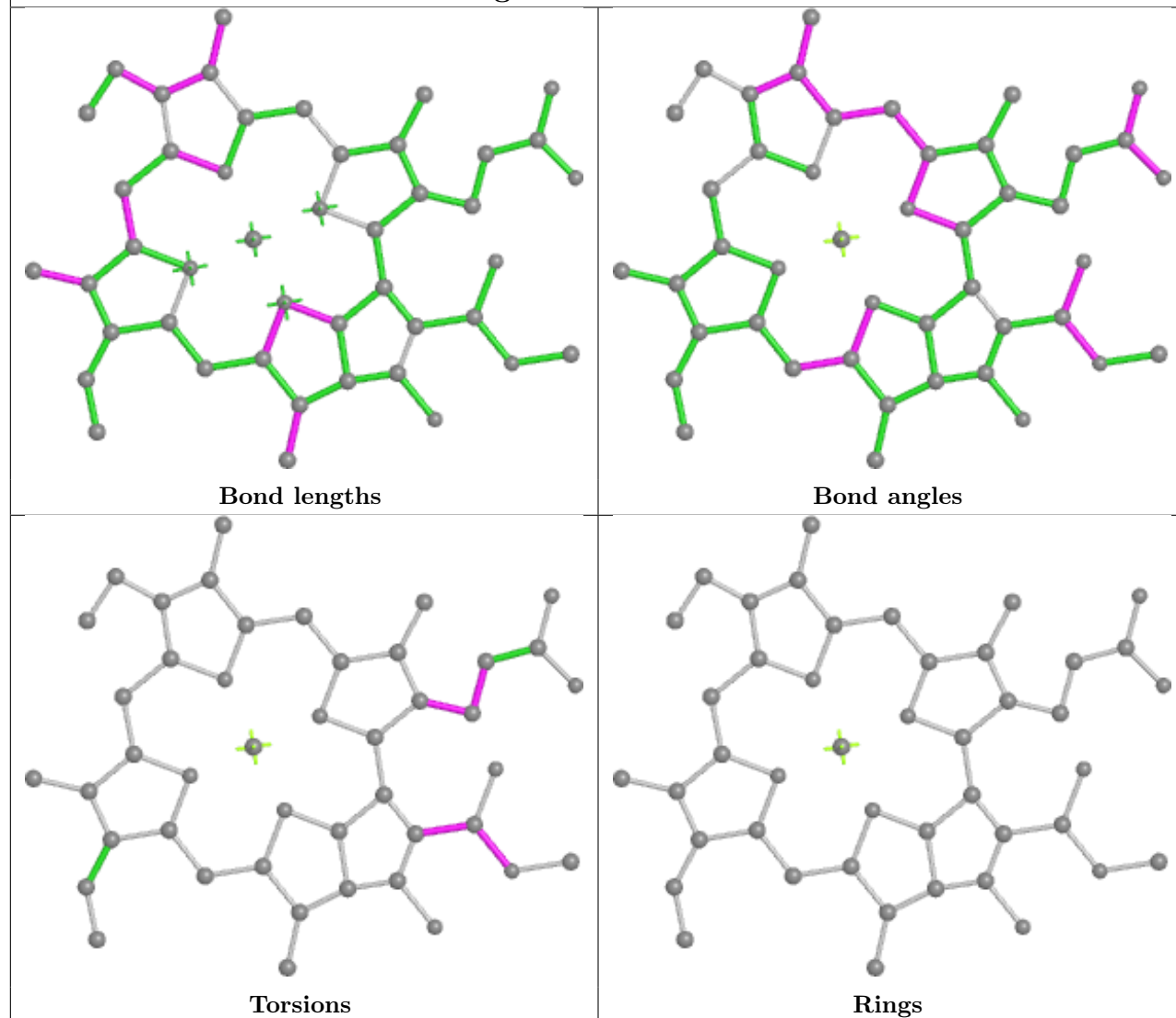
Ligand SQD BO 102



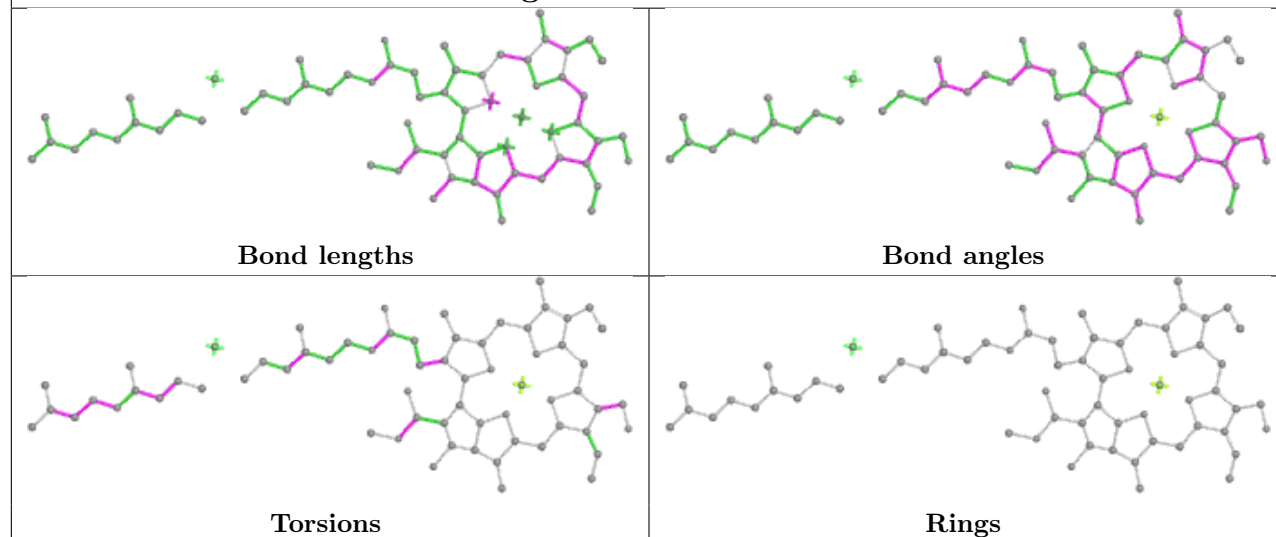
Ligand CLA d 402

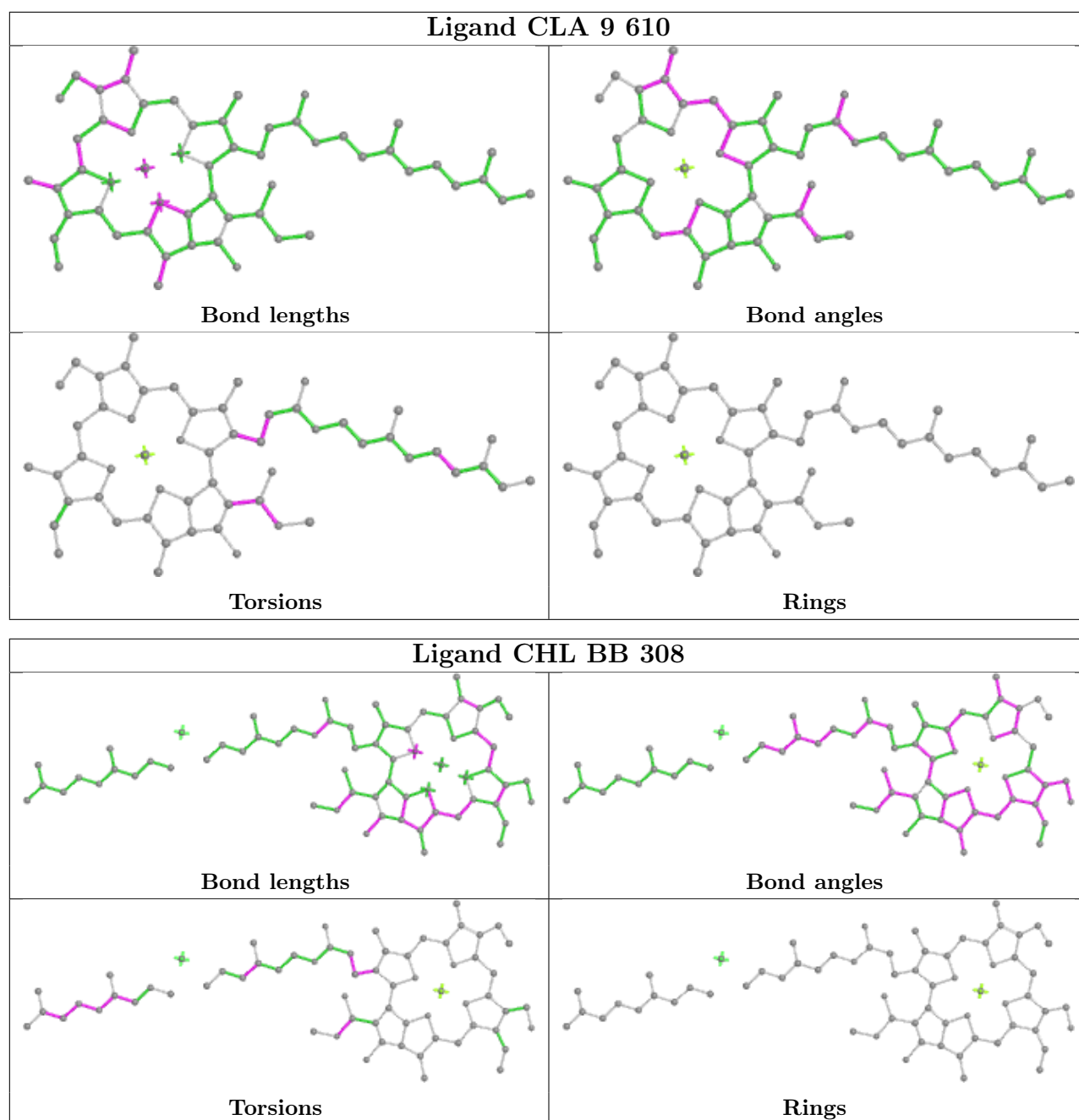


Ligand CLA 0 604

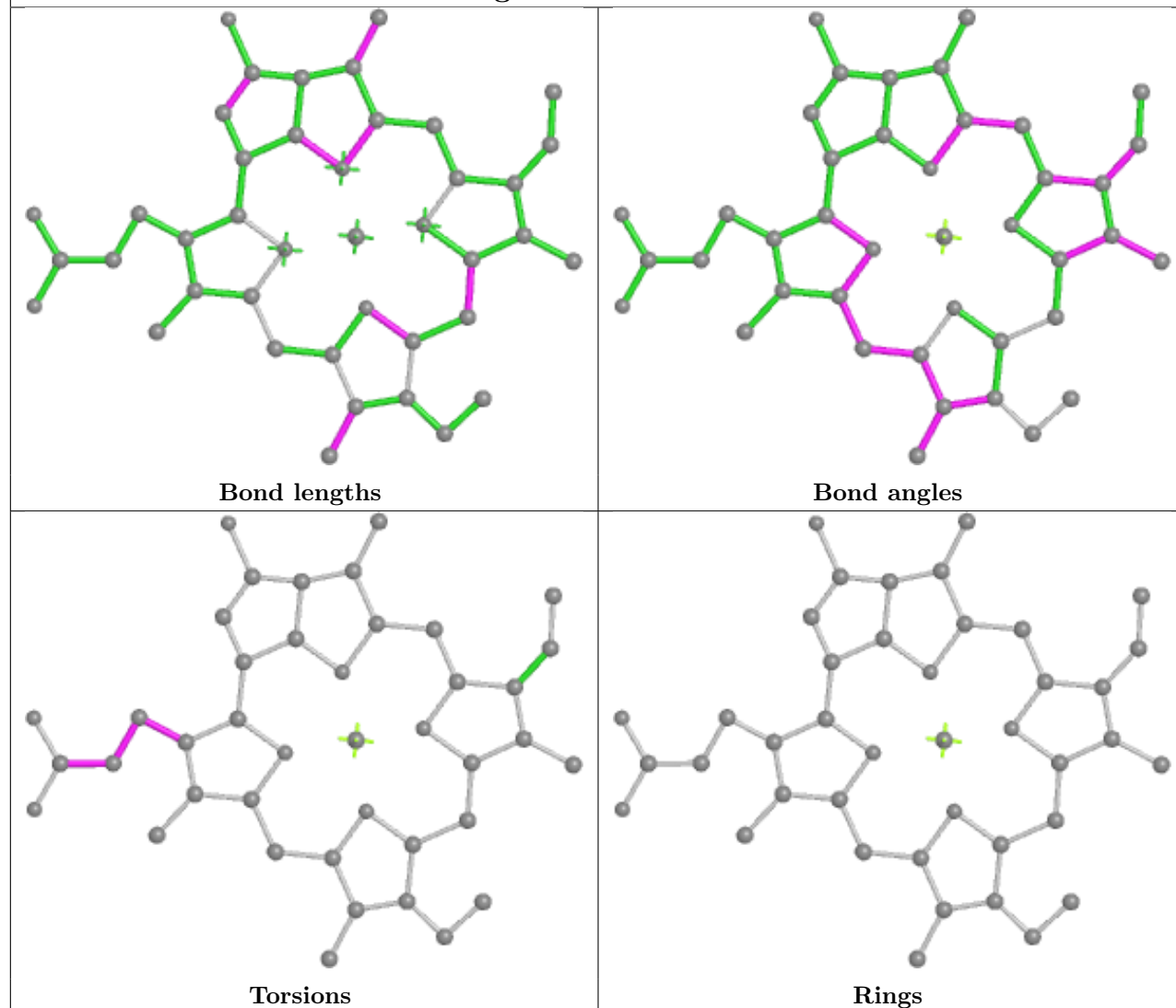


Ligand CHL Au 601

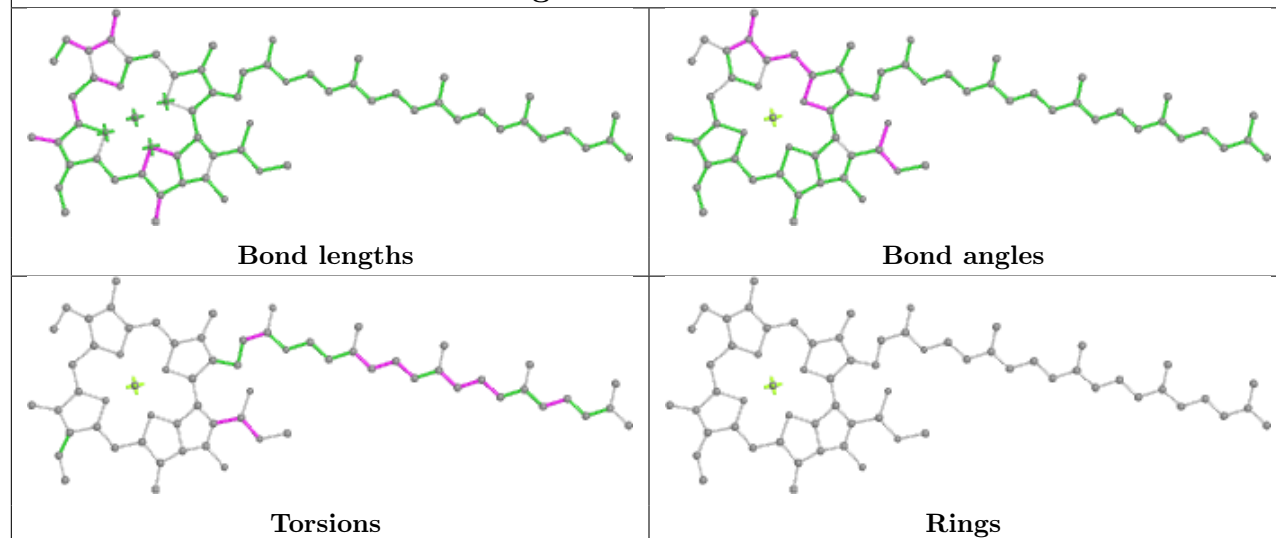


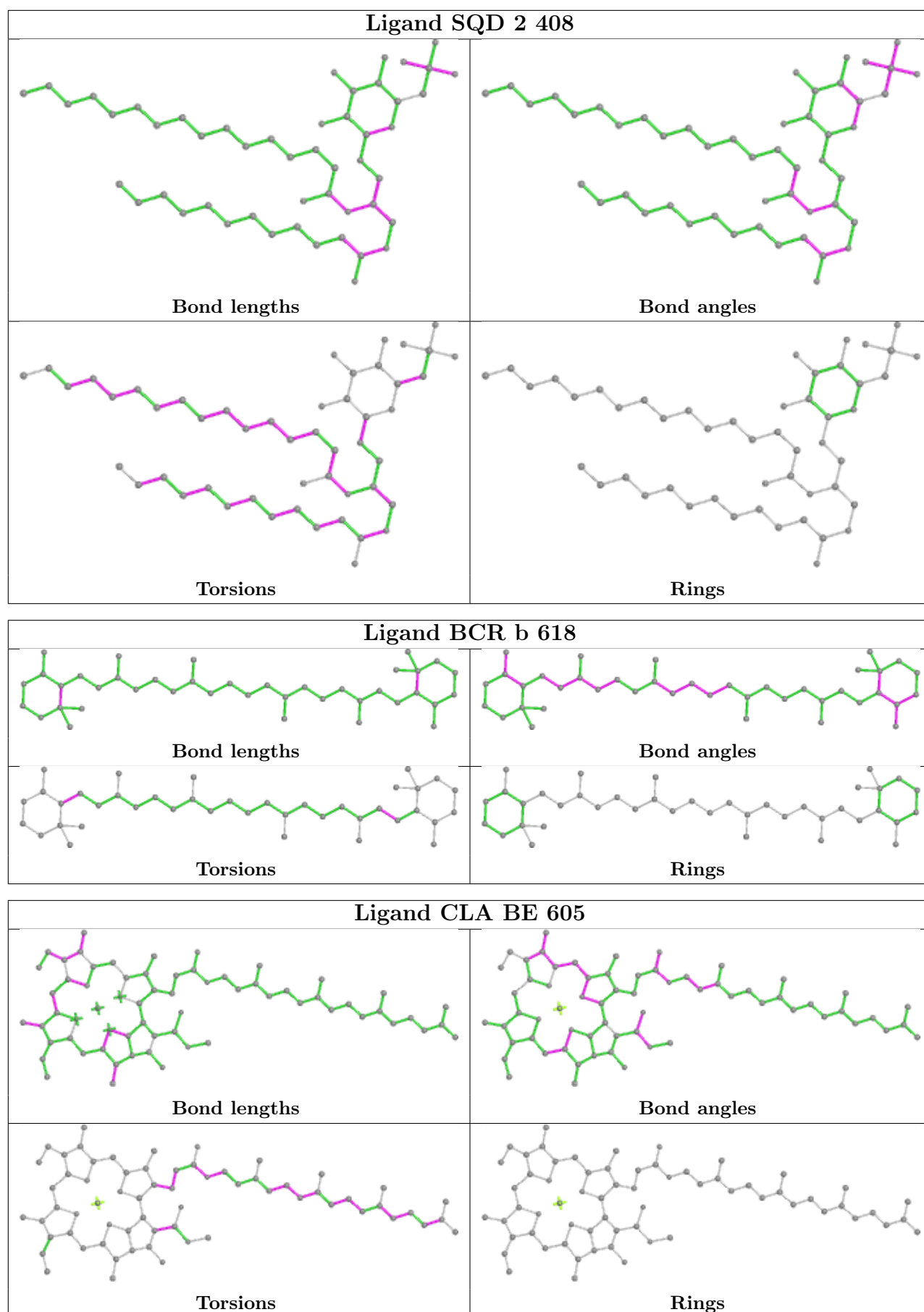


Ligand CLA 8 301

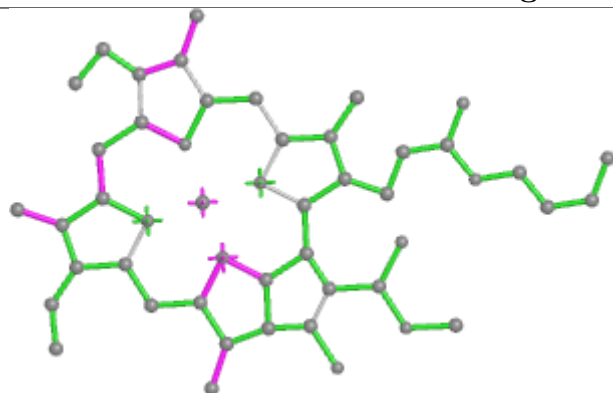


Ligand CLA B 613

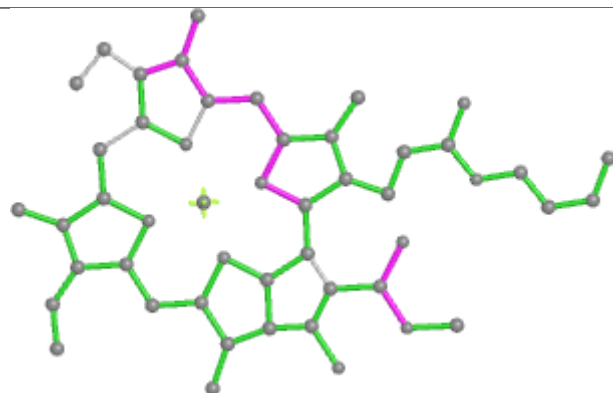




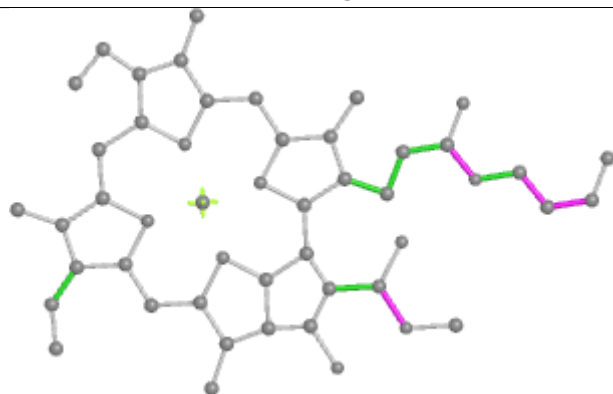
Ligand CLA r 611



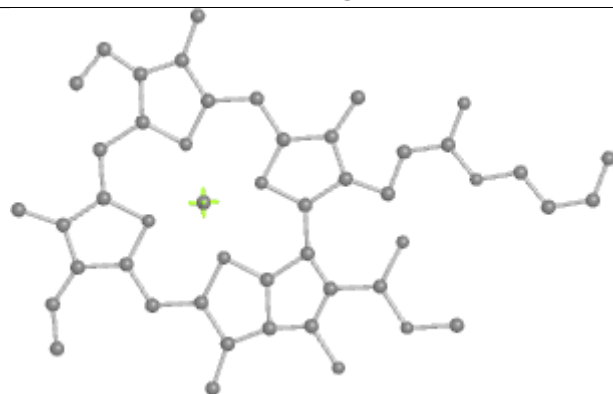
Bond lengths



Bond angles

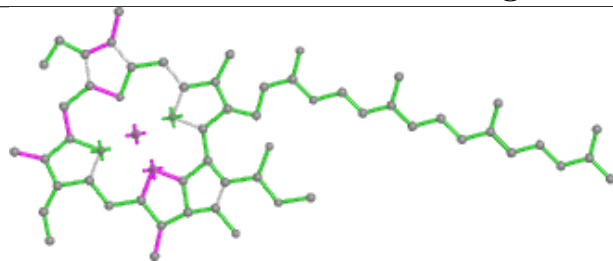


Torsions

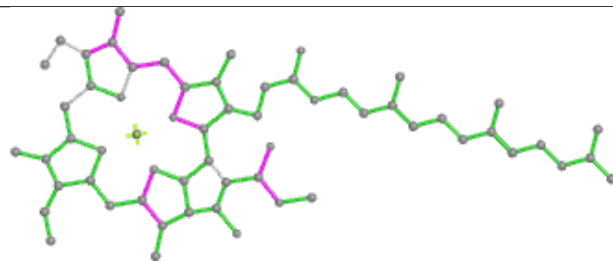


Rings

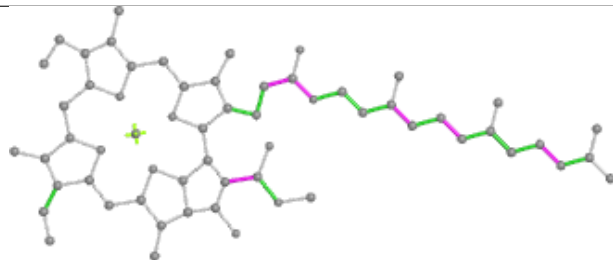
Ligand CLA BB 313



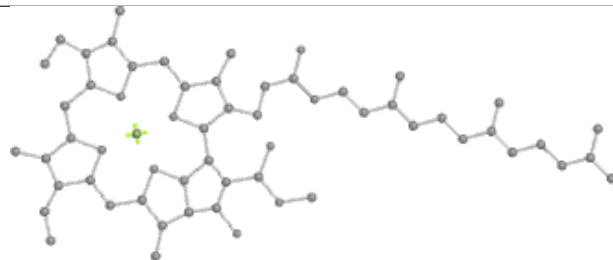
Bond lengths



Bond angles

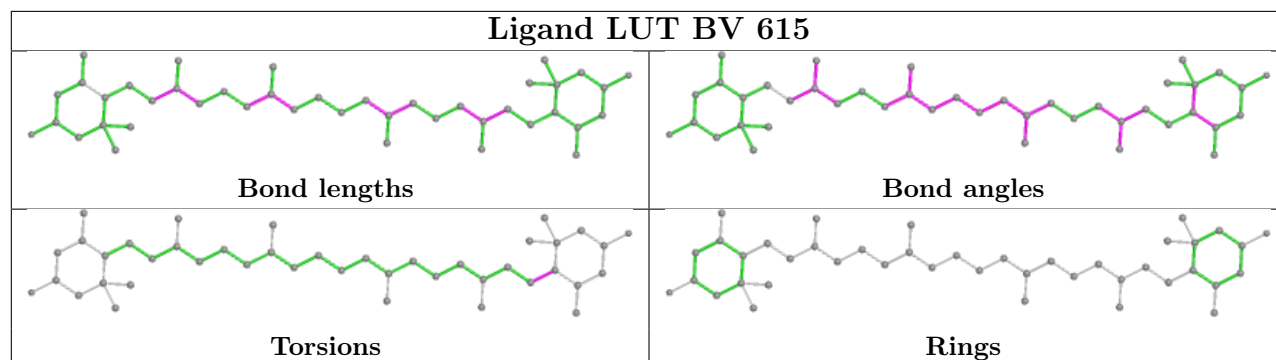


Torsions

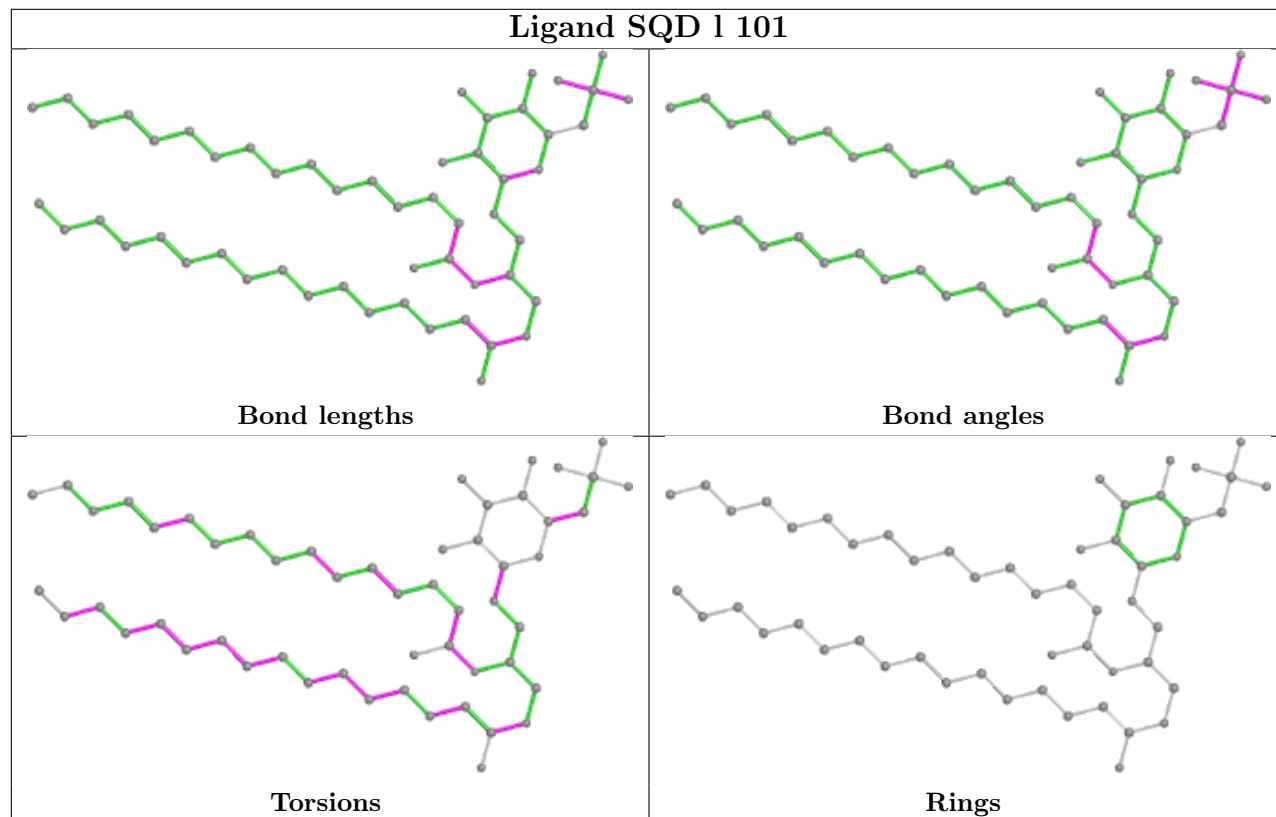


Rings

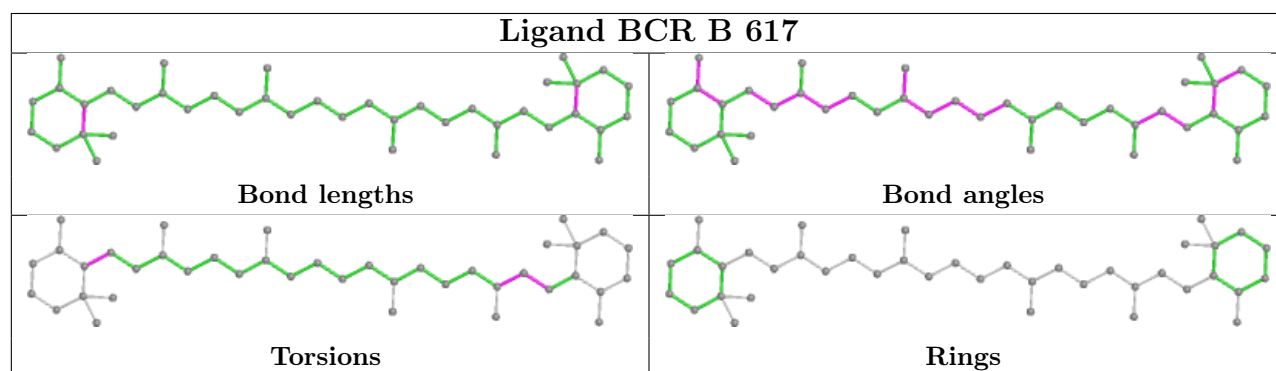
Ligand LUT BV 615

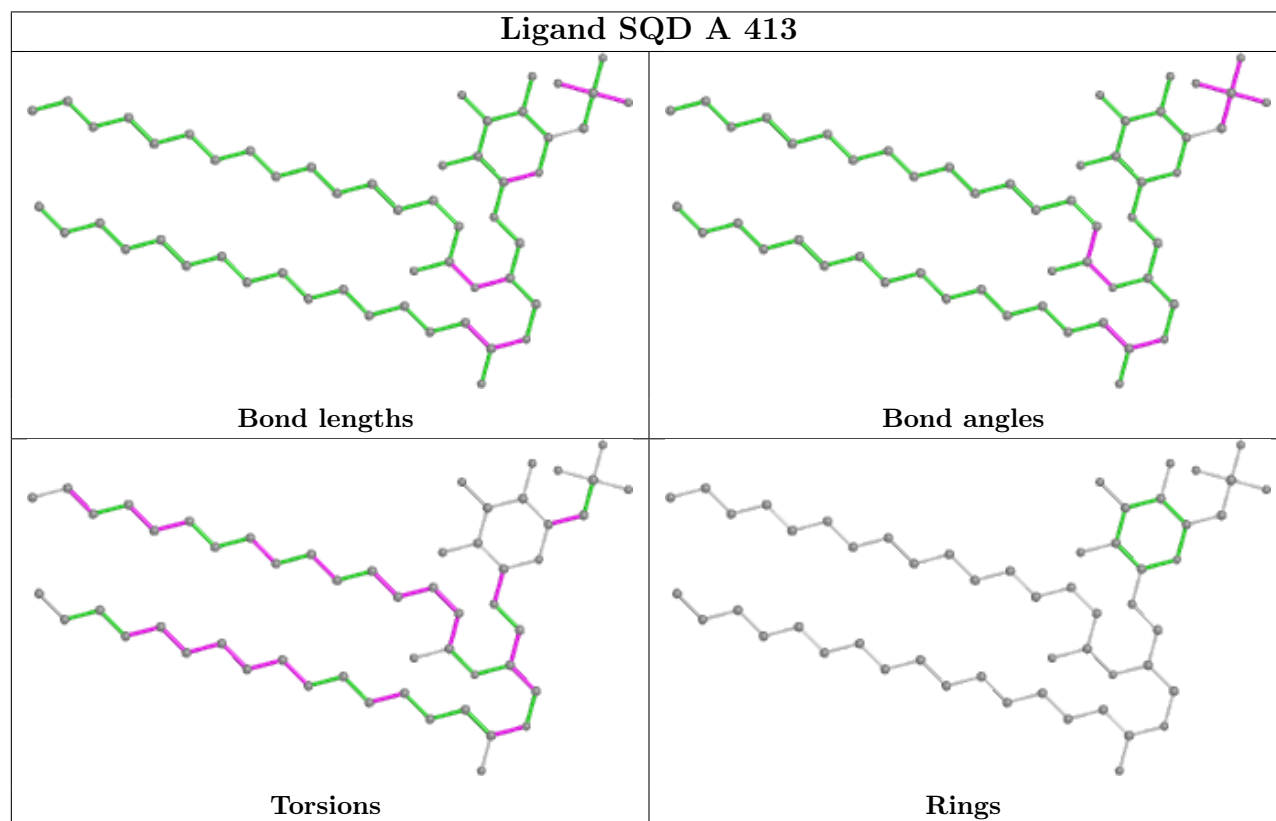
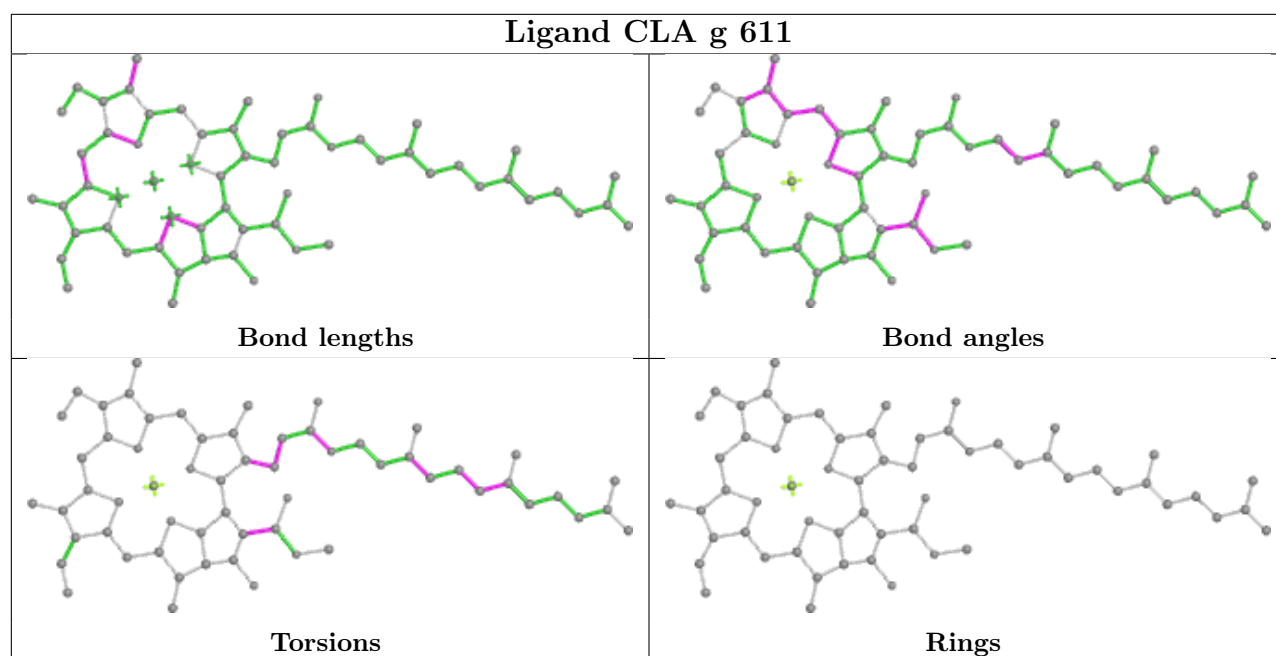


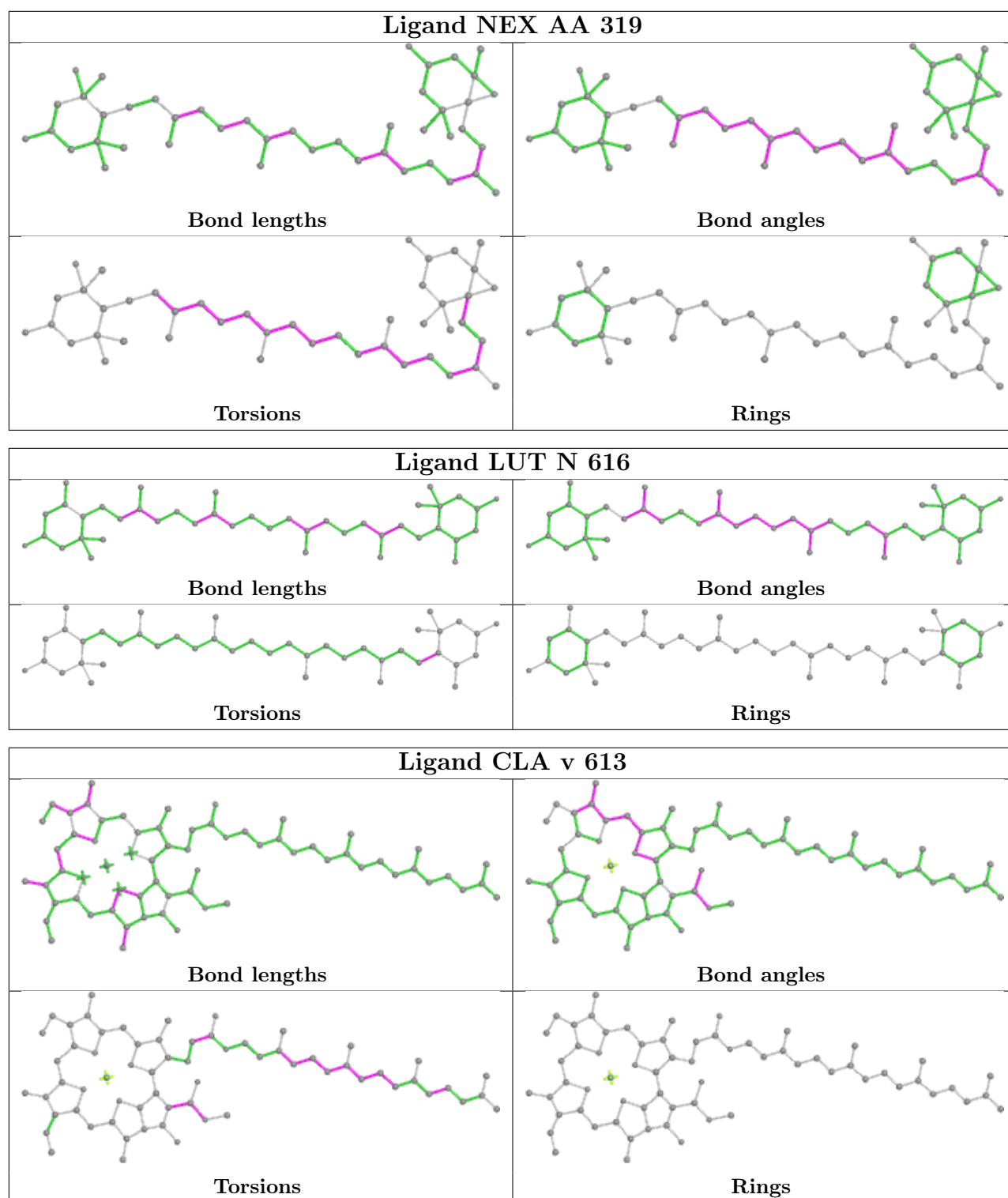
Ligand SQD 1 101

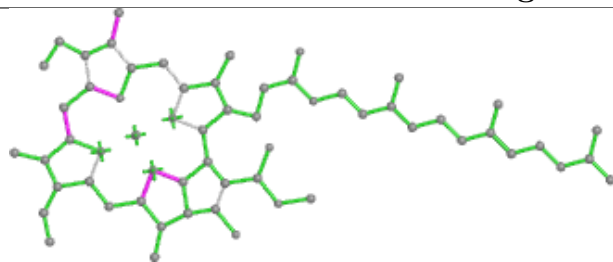


Ligand BCR B 617

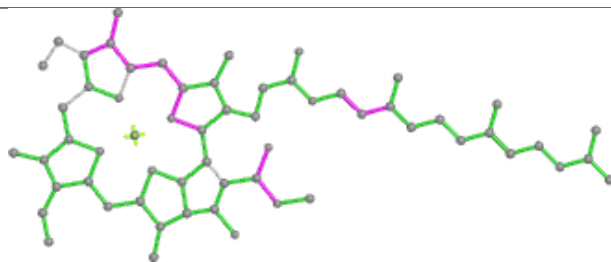




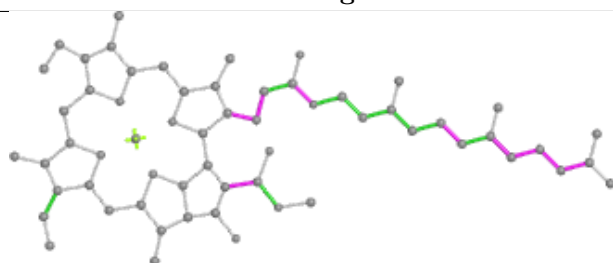


Ligand CLA n 611

Bond lengths



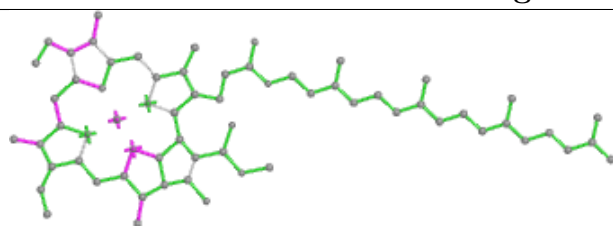
Bond angles



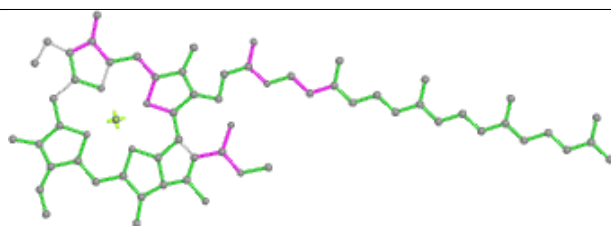
Torsions



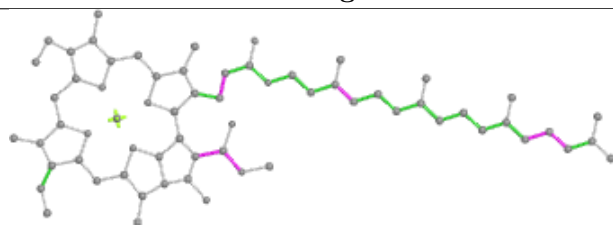
Rings

Ligand CLA A 405

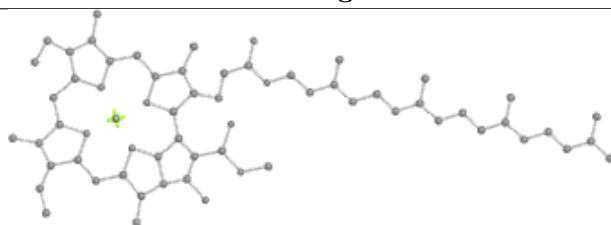
Bond lengths



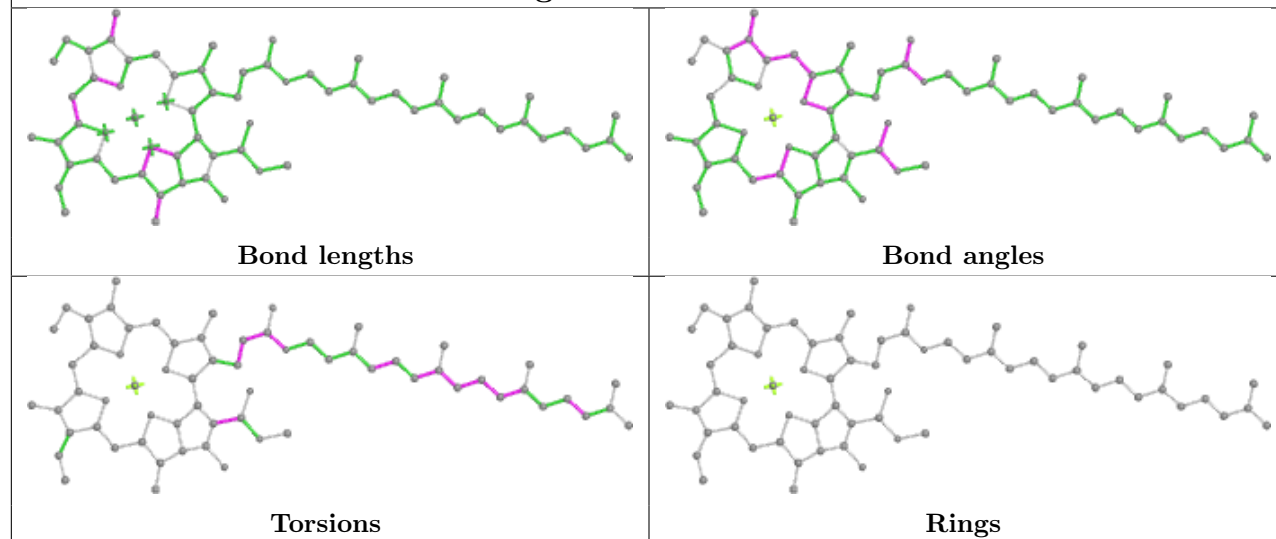
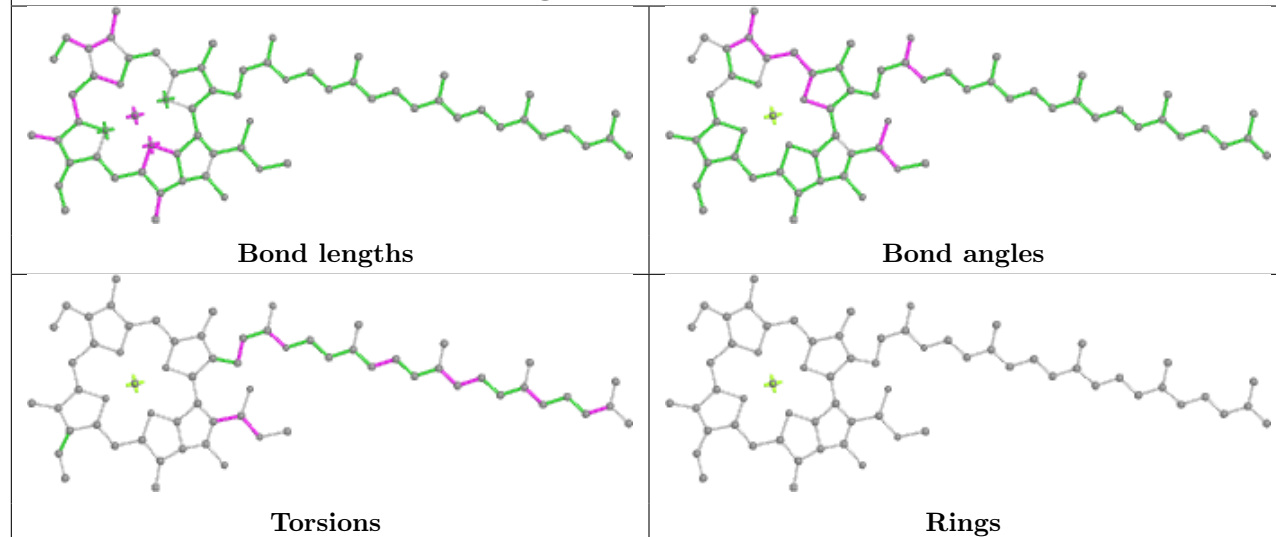
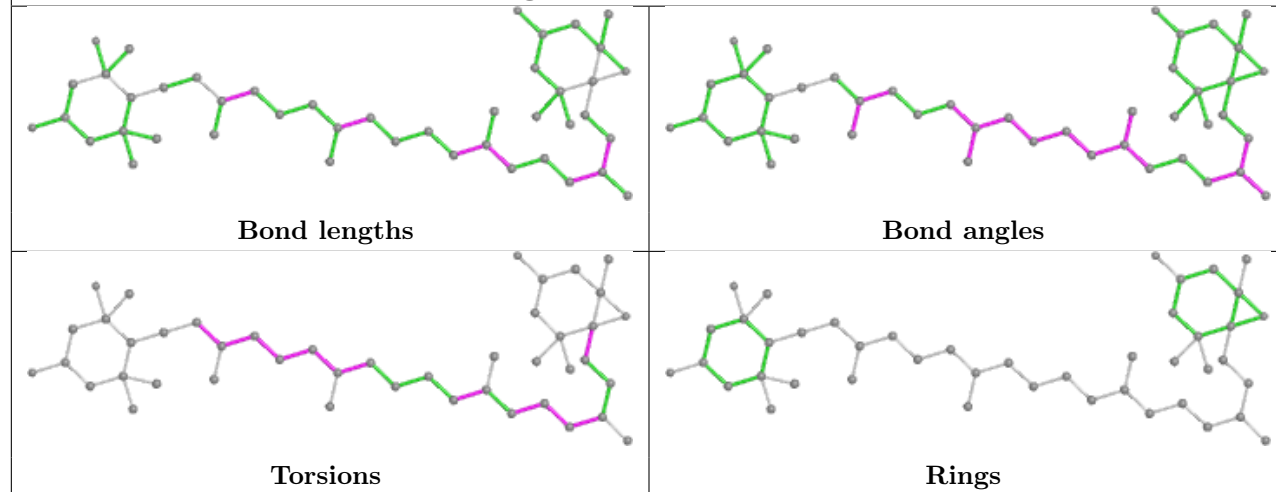
Bond angles

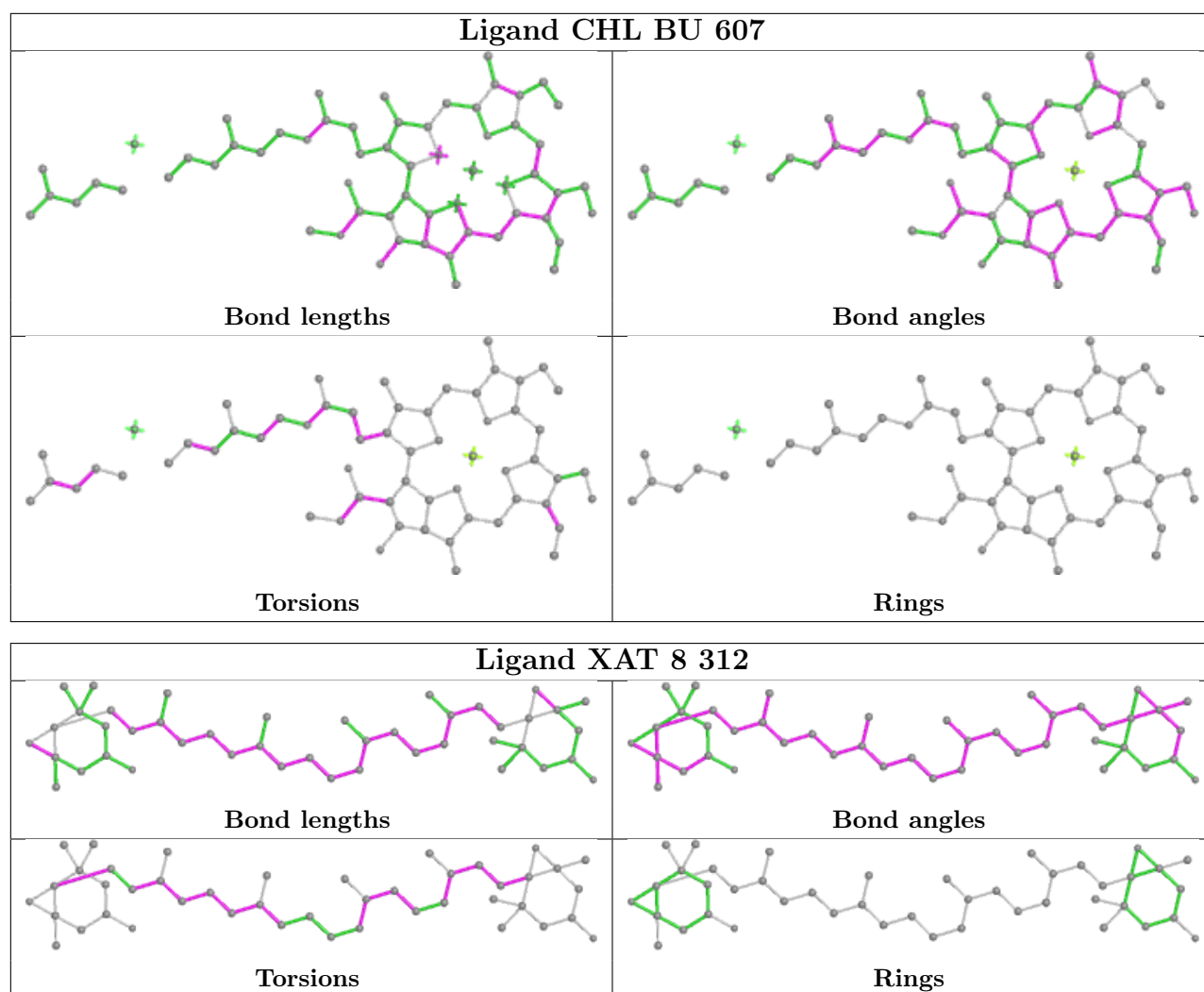


Torsions

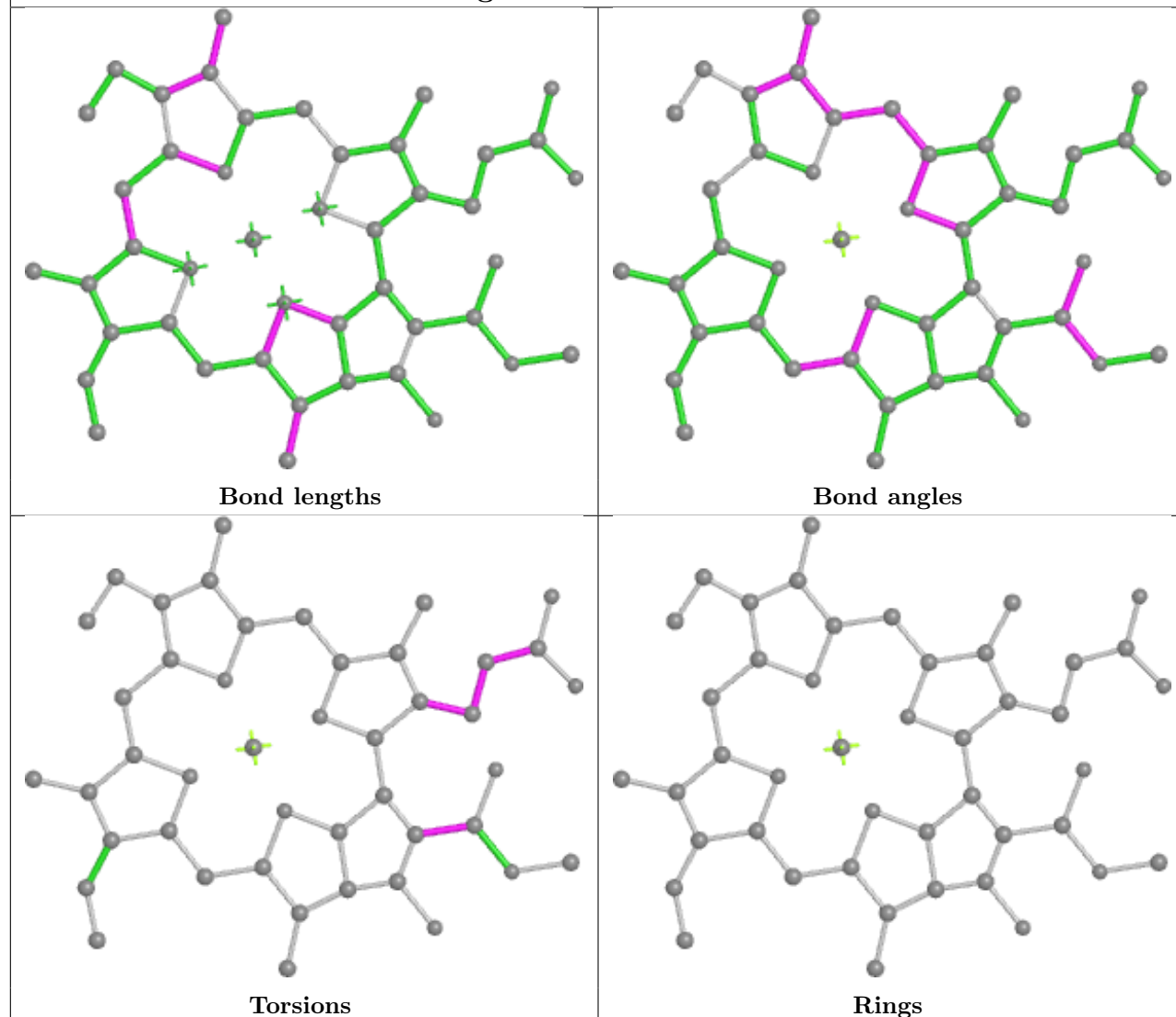


Rings

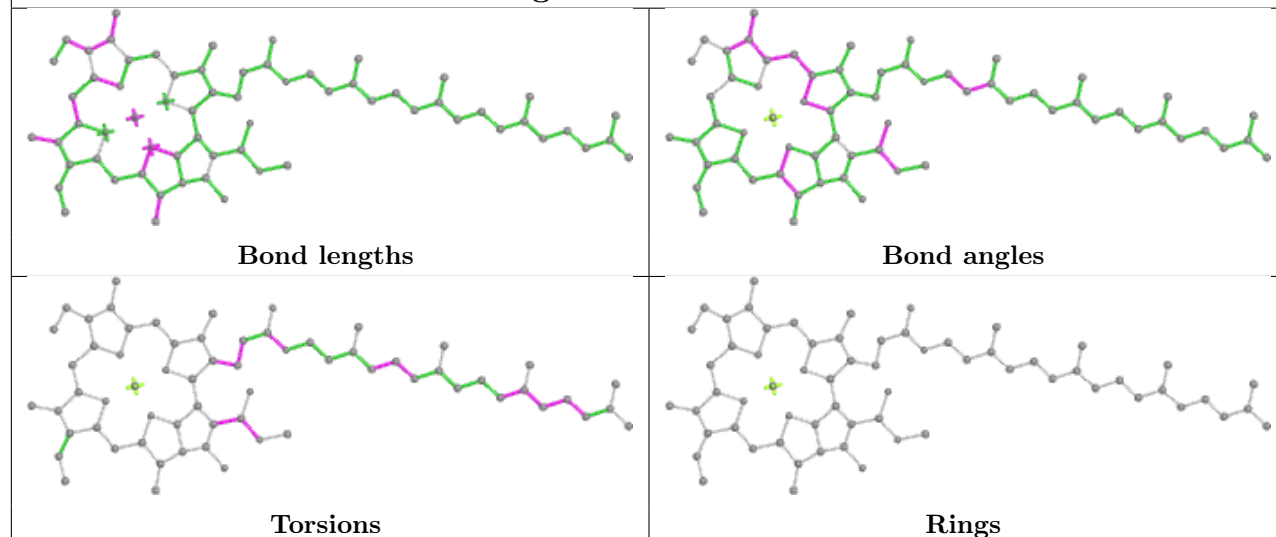
Ligand CLA n 602**Ligand CLA 1 503****Ligand NEX BJ 617**



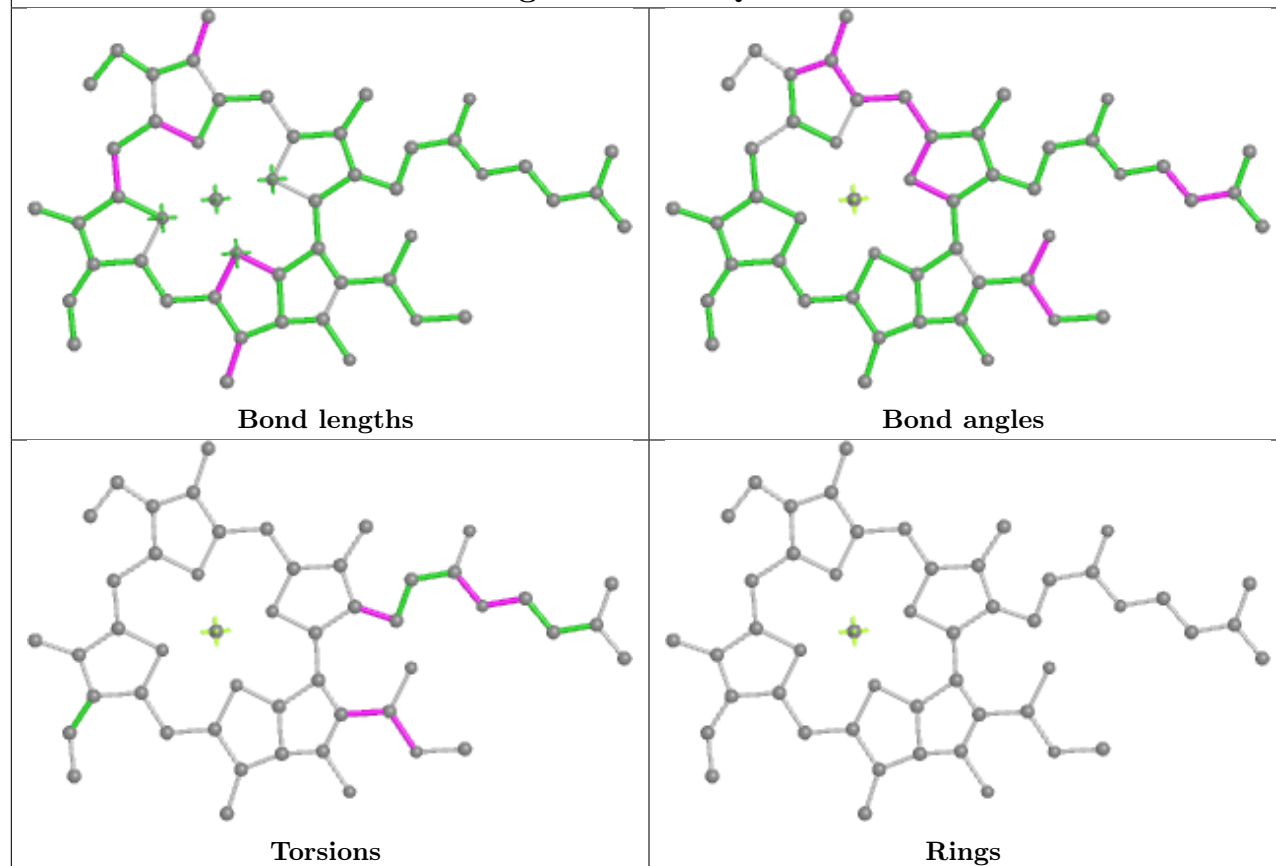
Ligand CLA AA 312



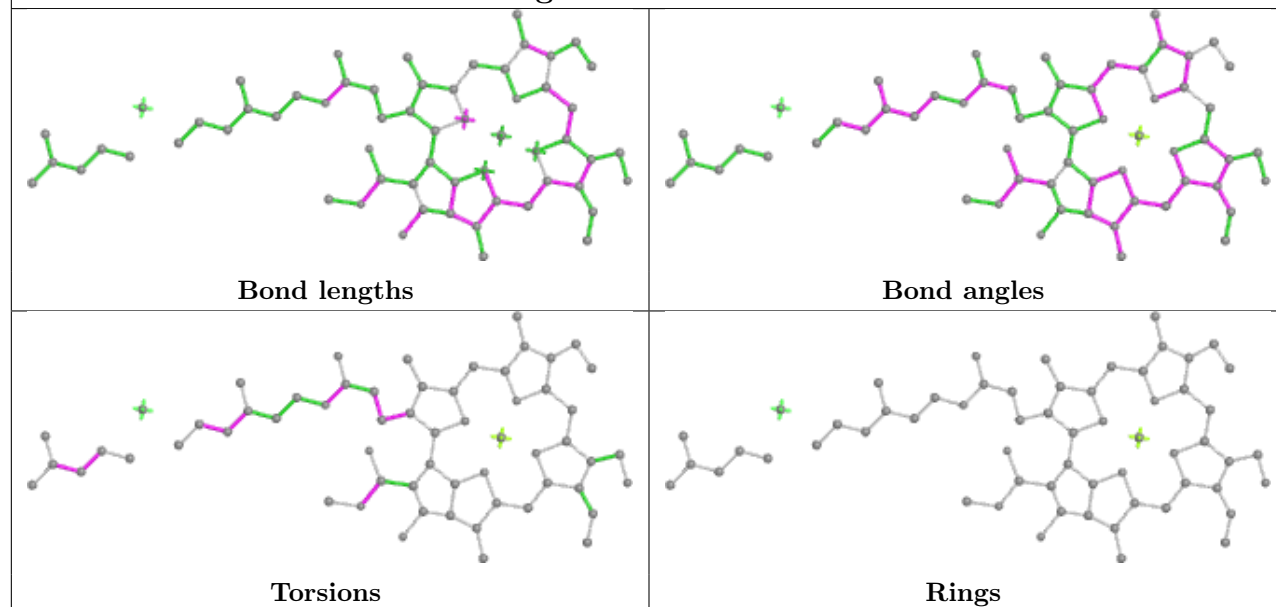
Ligand CLA C 506



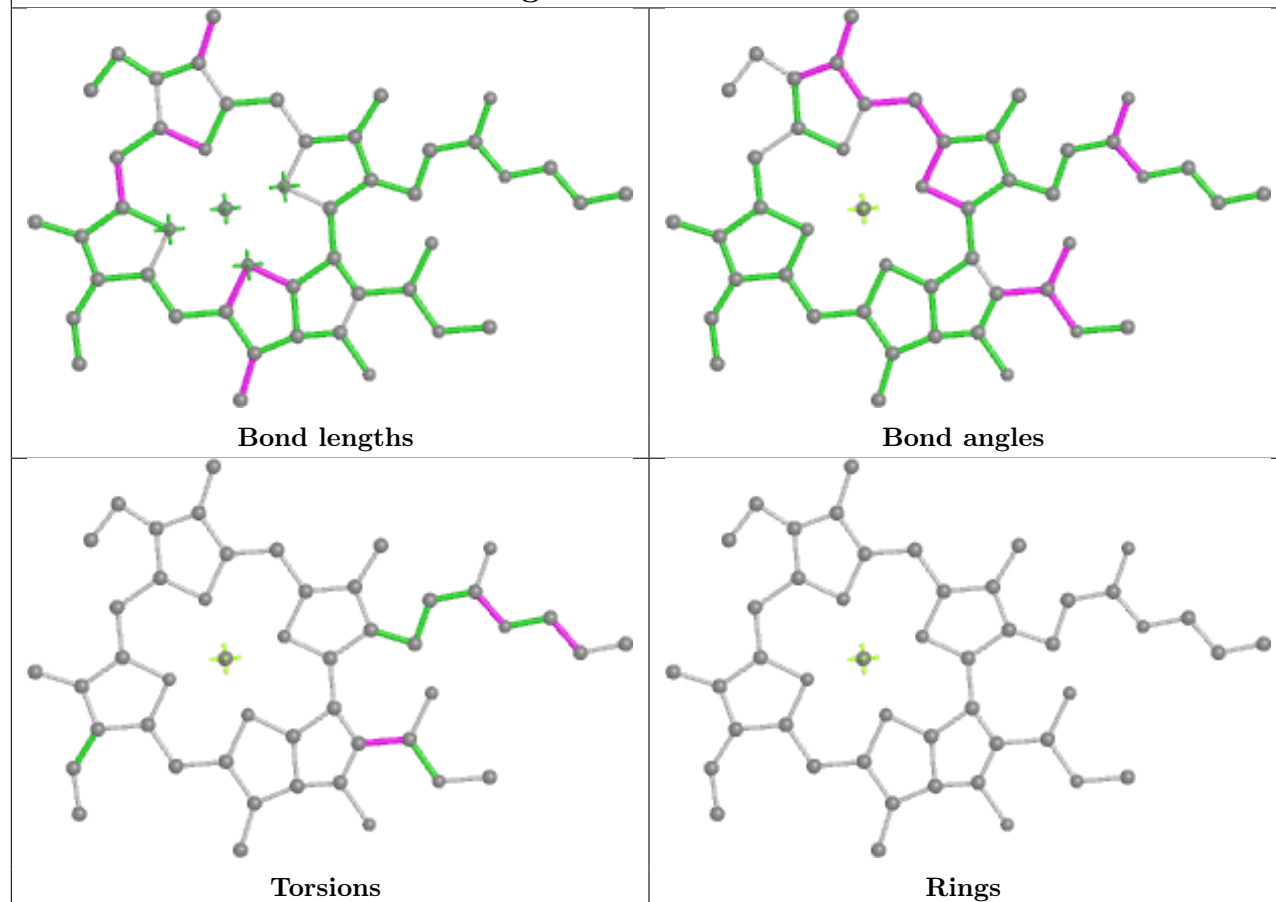
Ligand CLA BQ 604



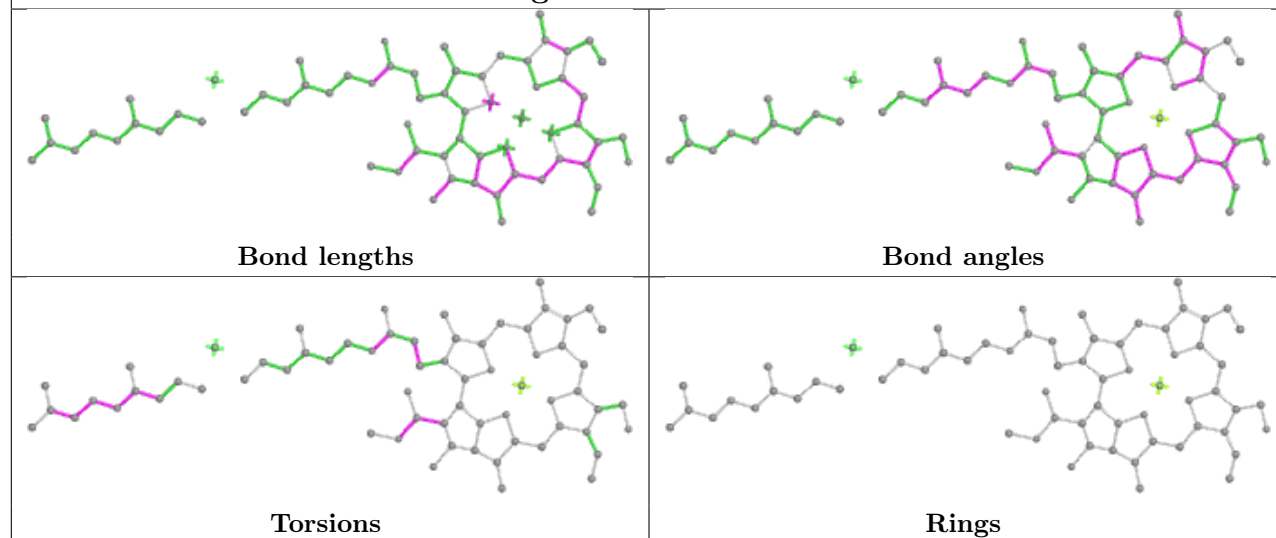
Ligand CHL 7 308

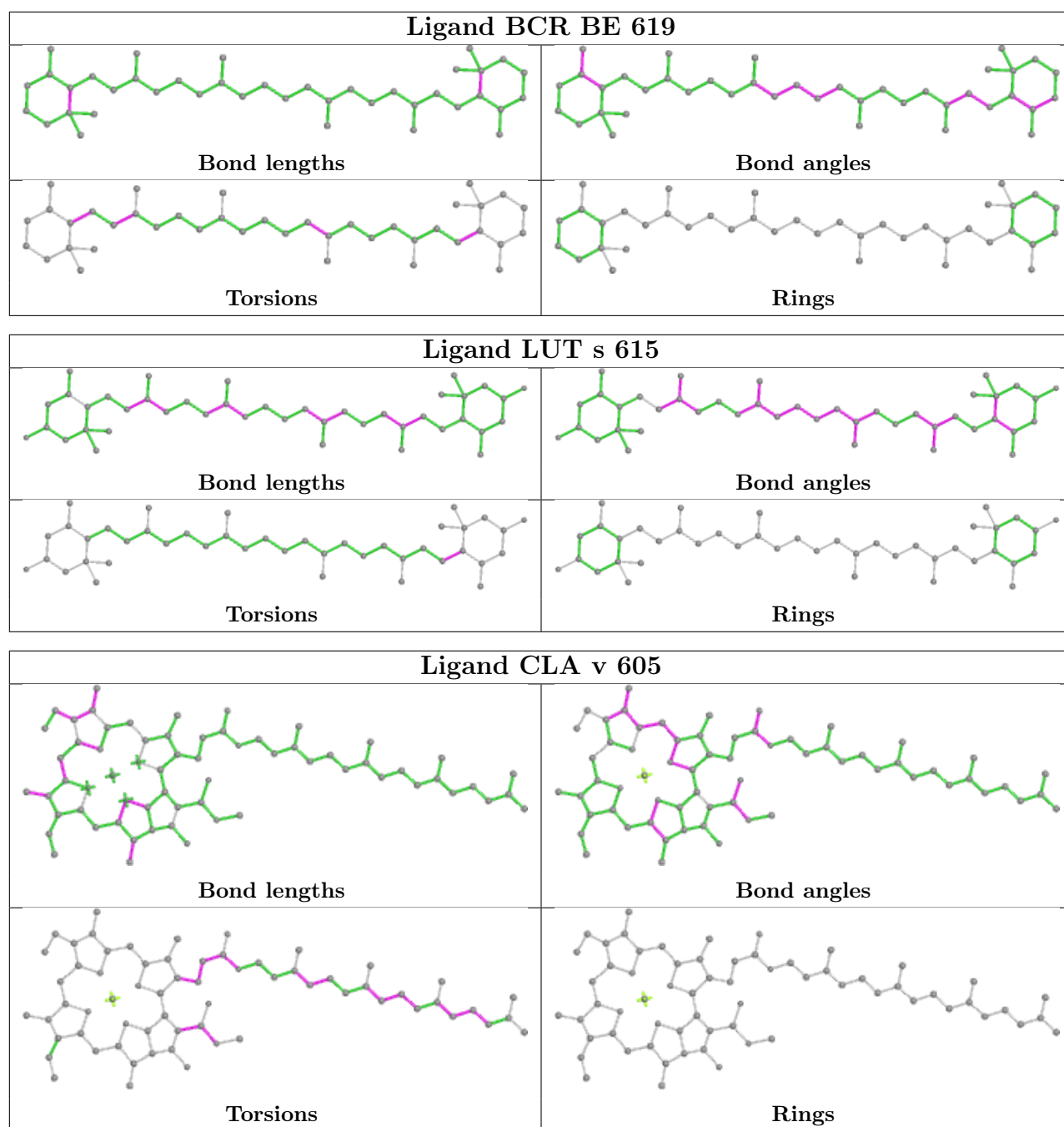


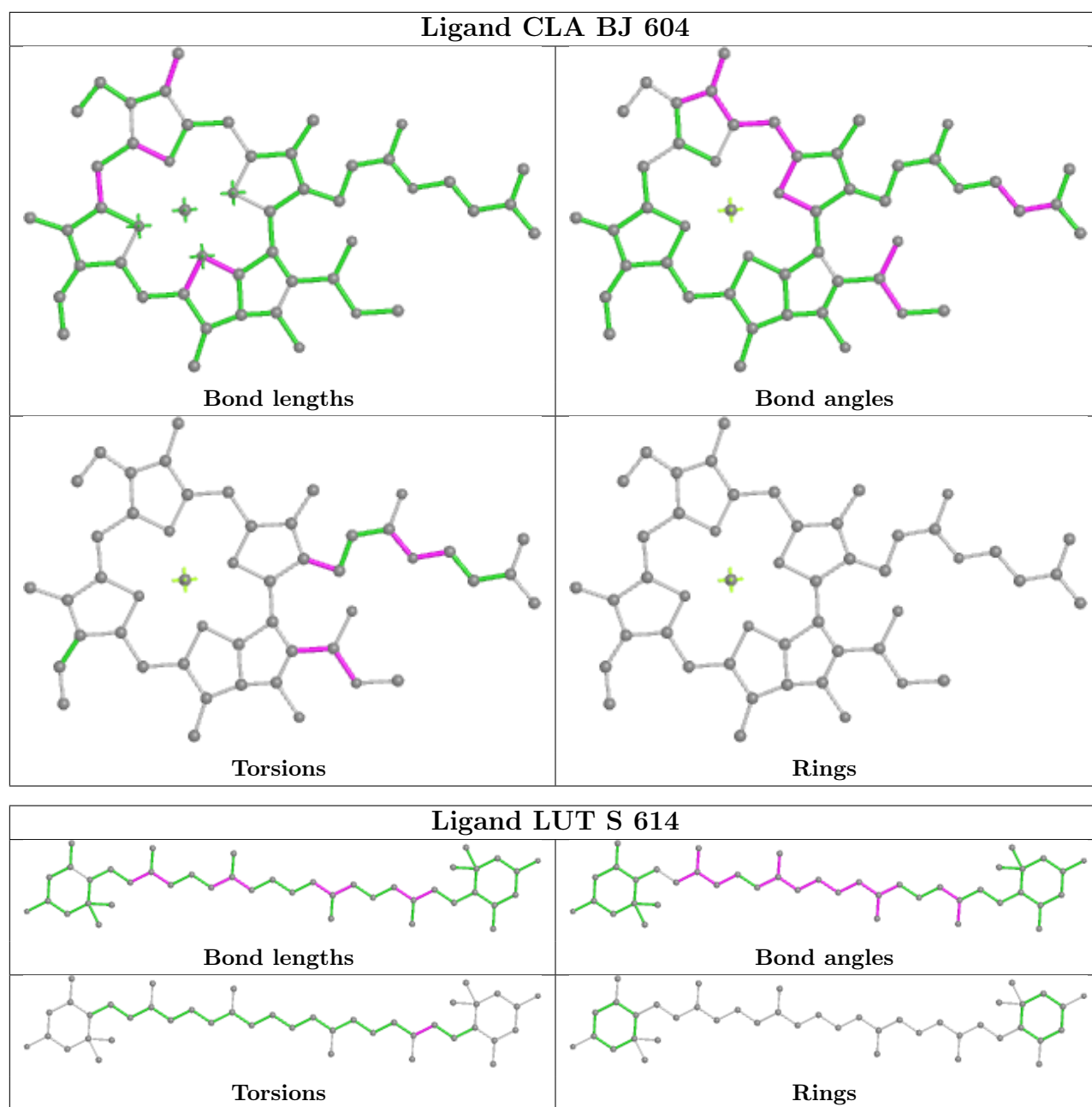
Ligand CLA Au 614



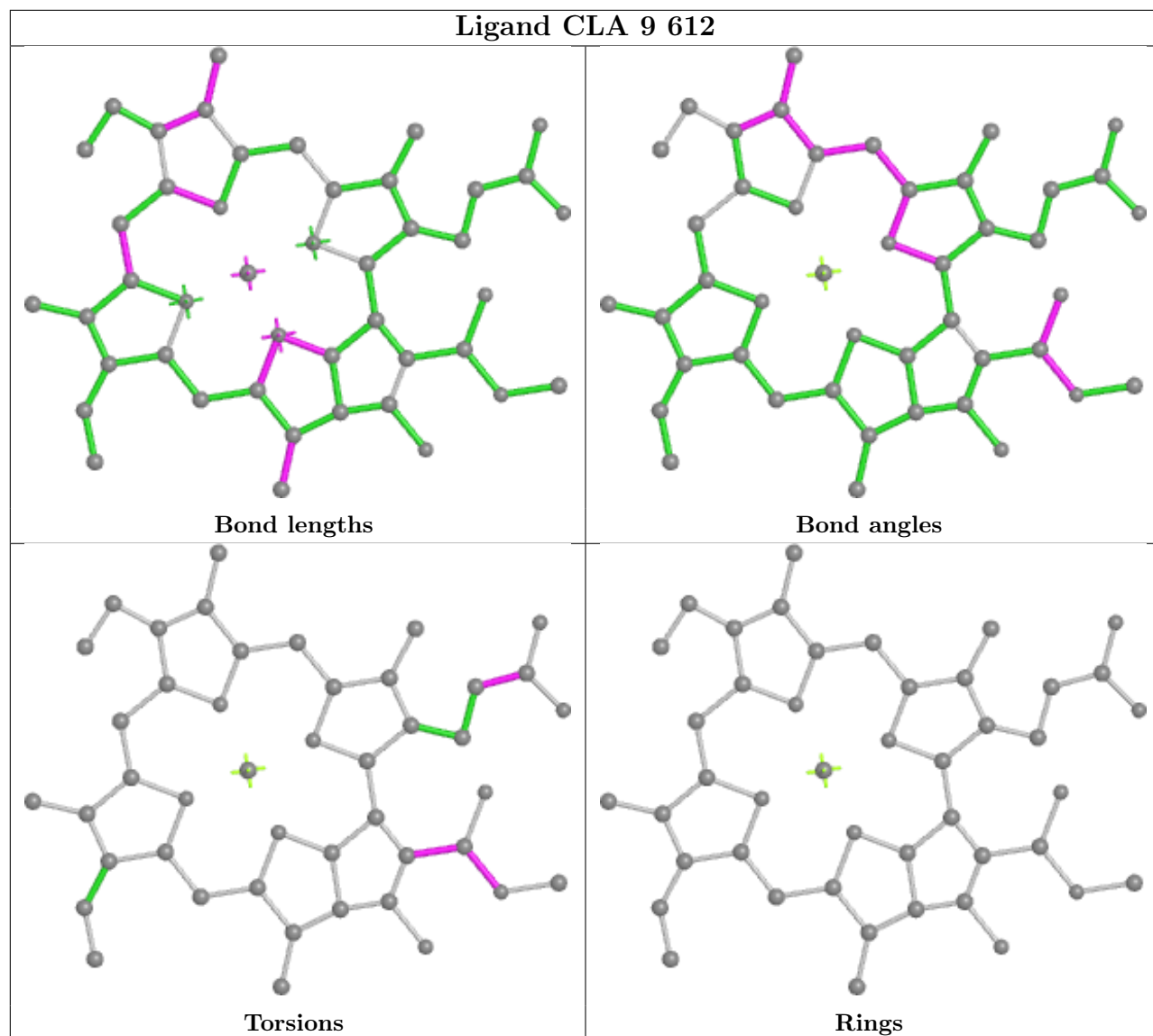
Ligand CHL Y 310

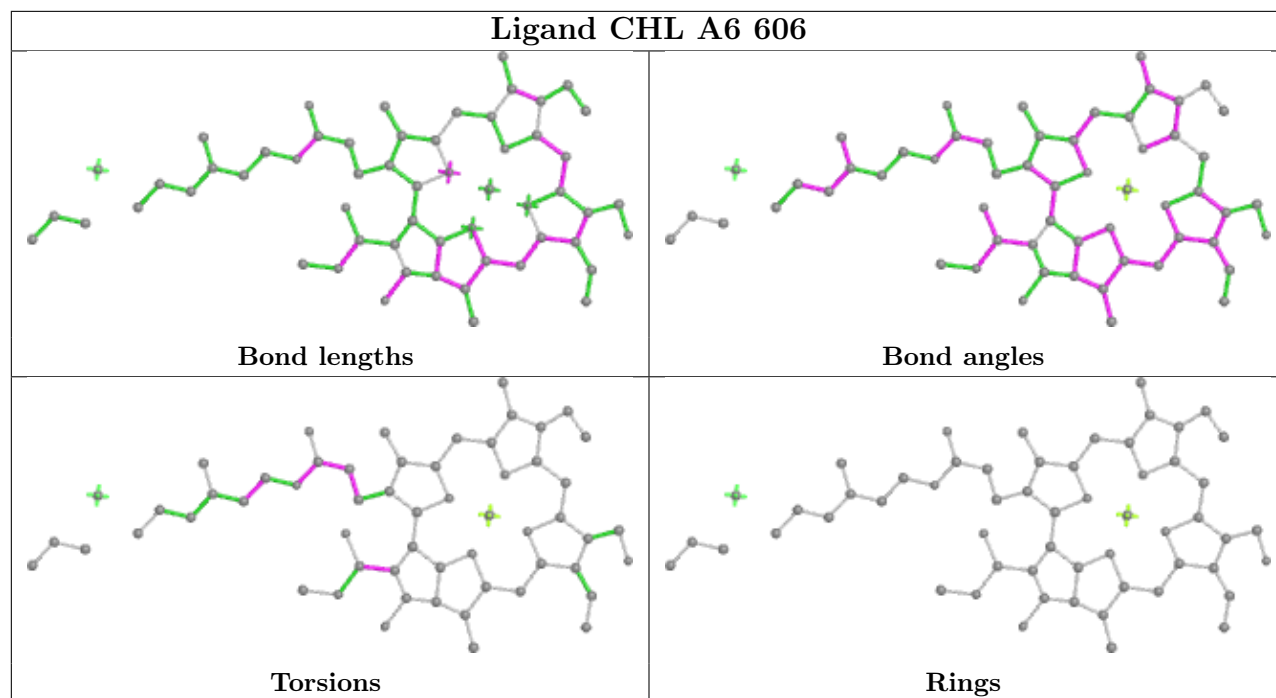


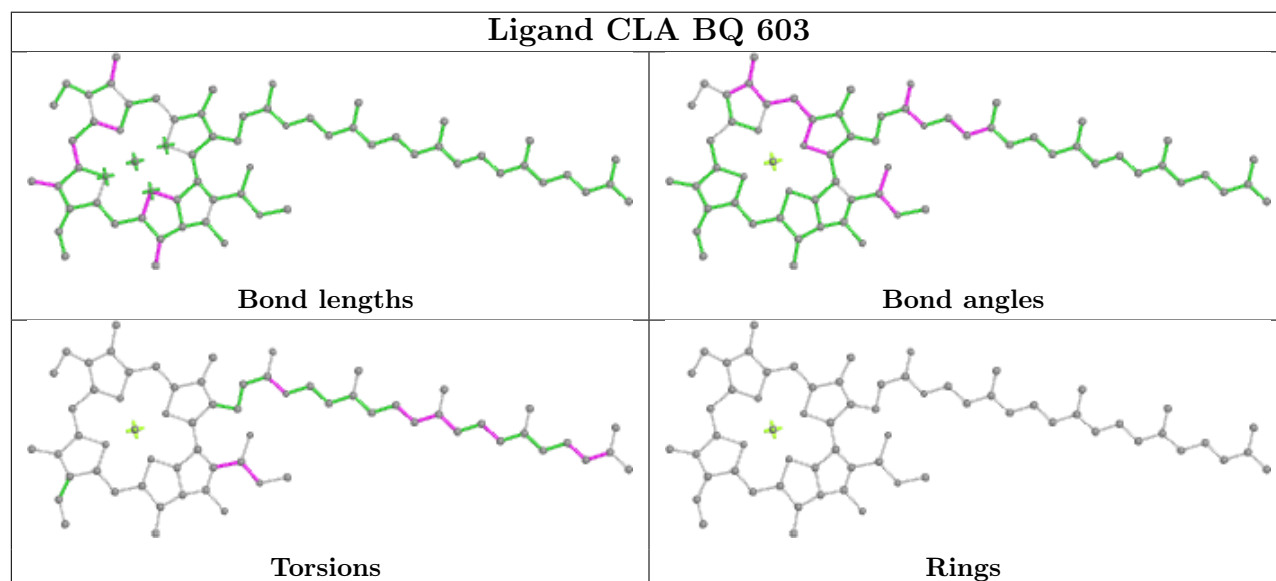
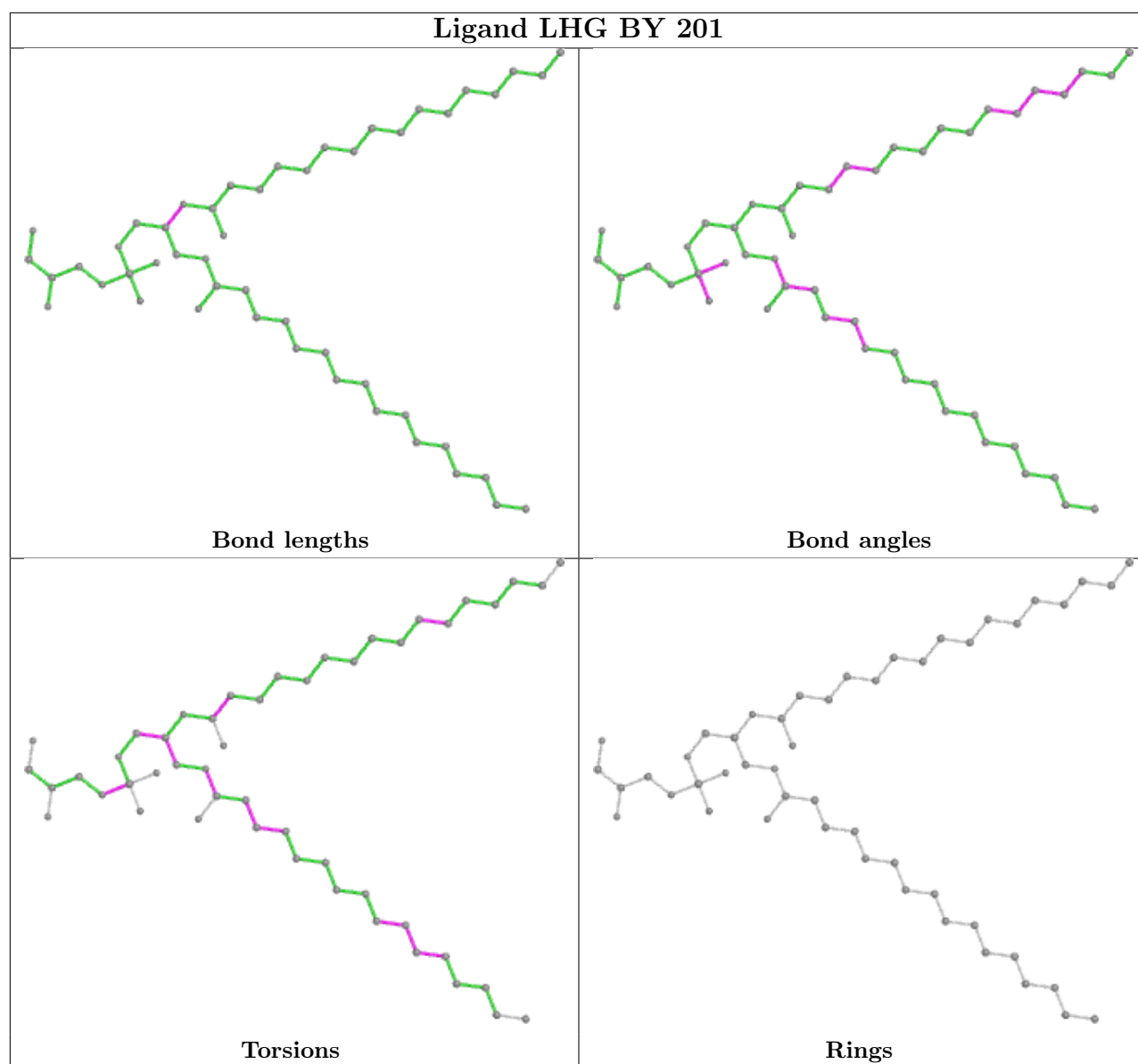


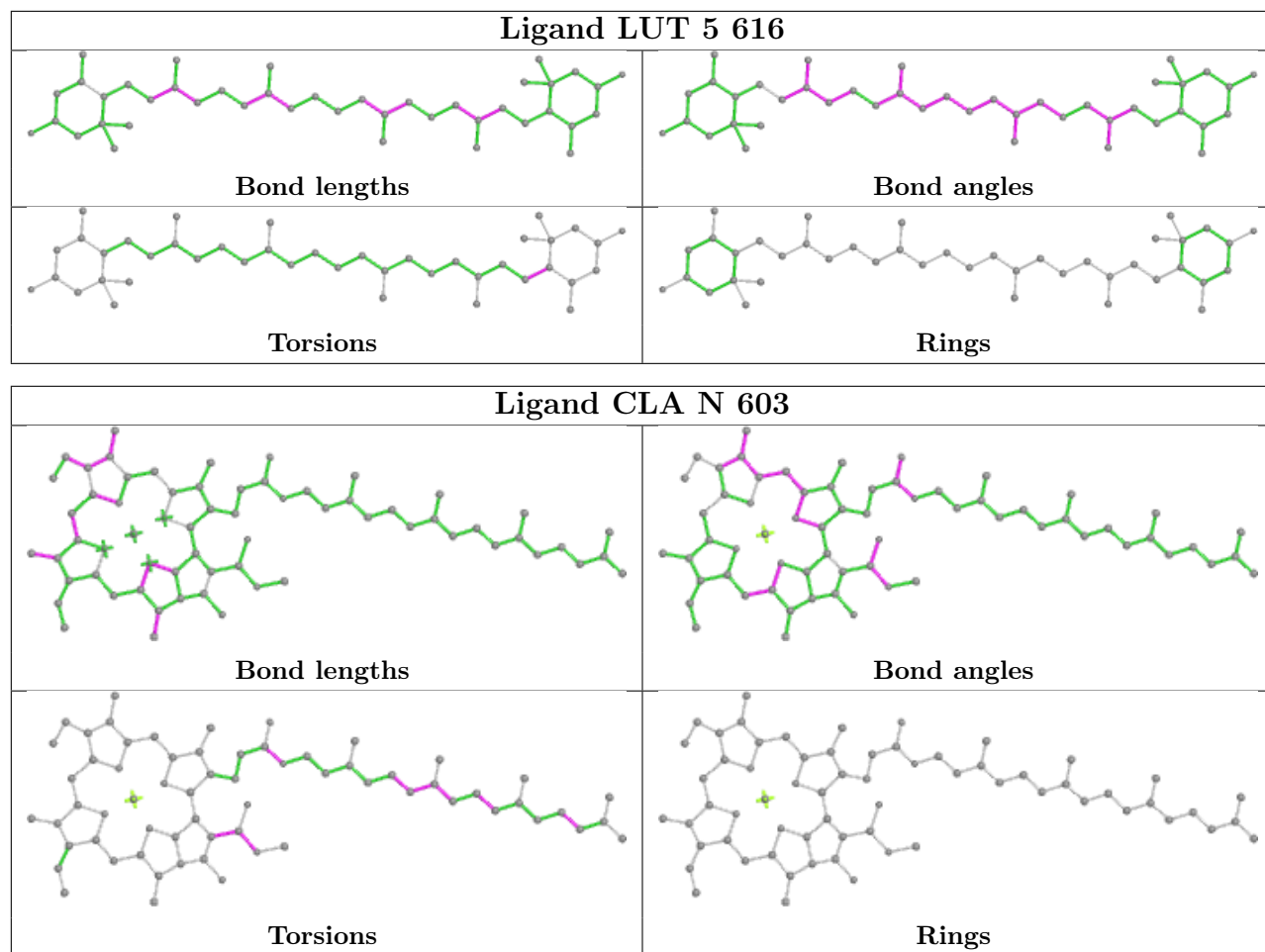


Ligand CLA 9 612

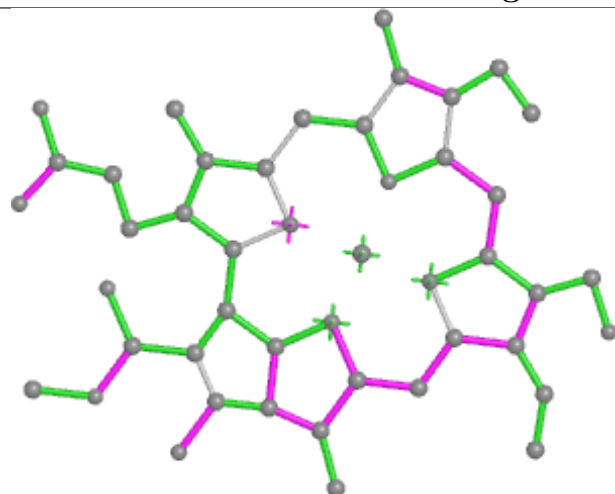




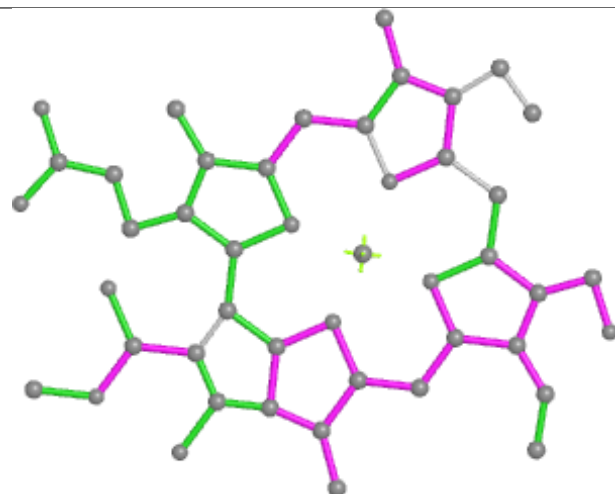




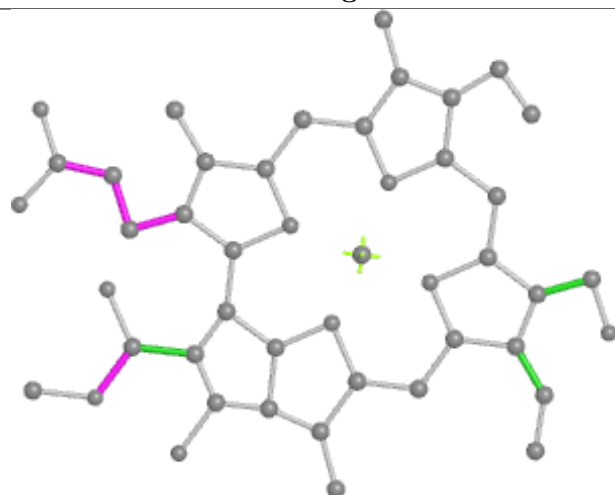
Ligand CHL AB 305



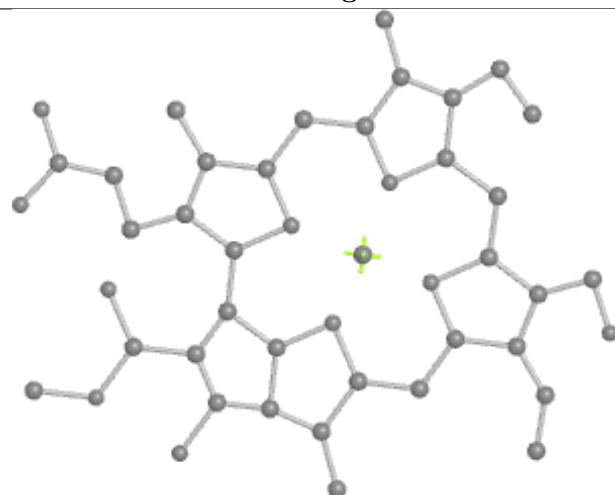
Bond lengths



Bond angles

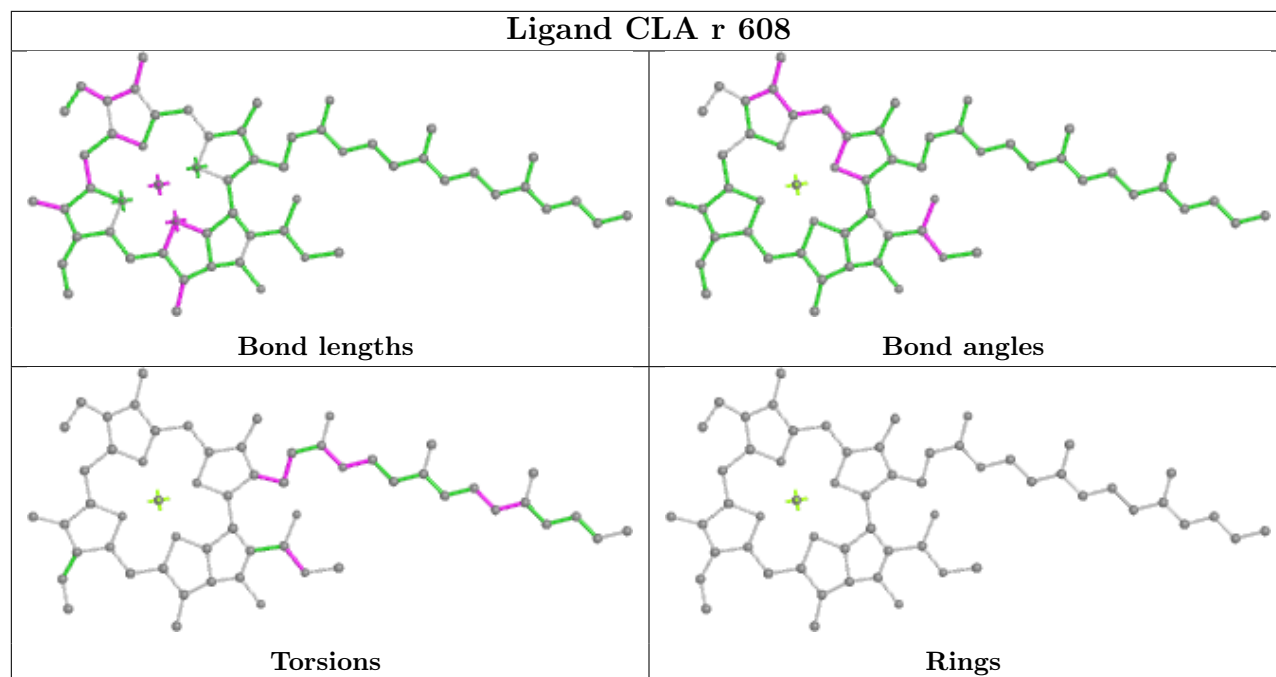


Torsions

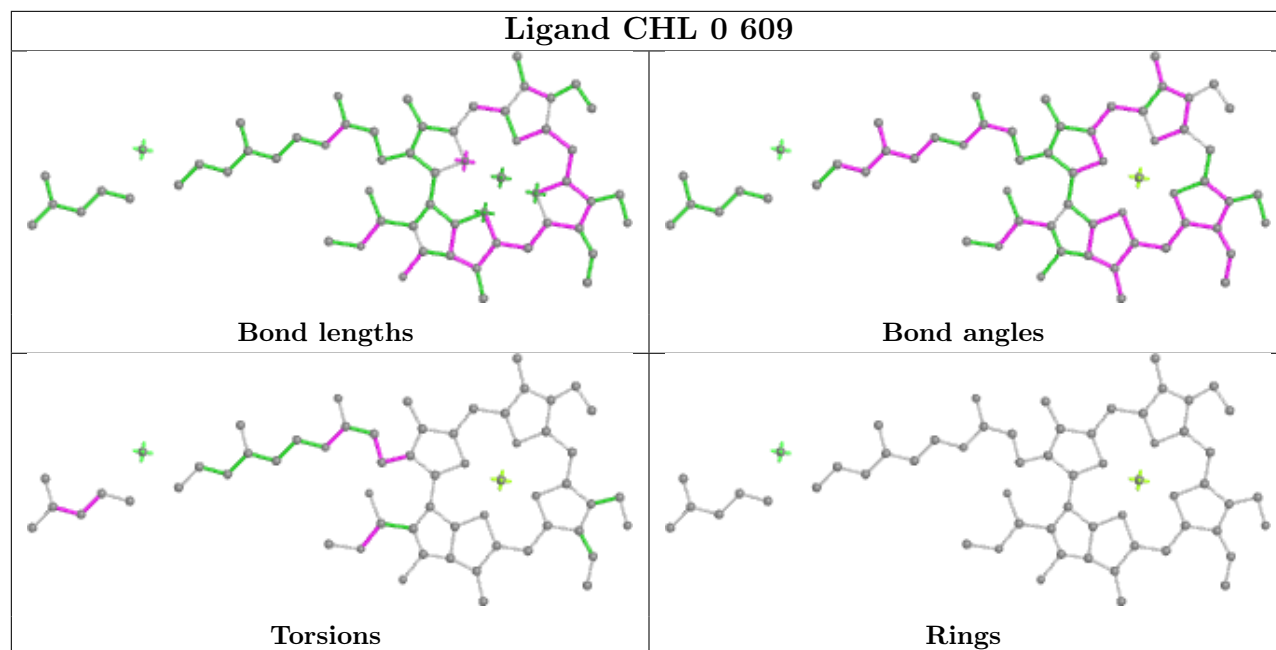


Rings

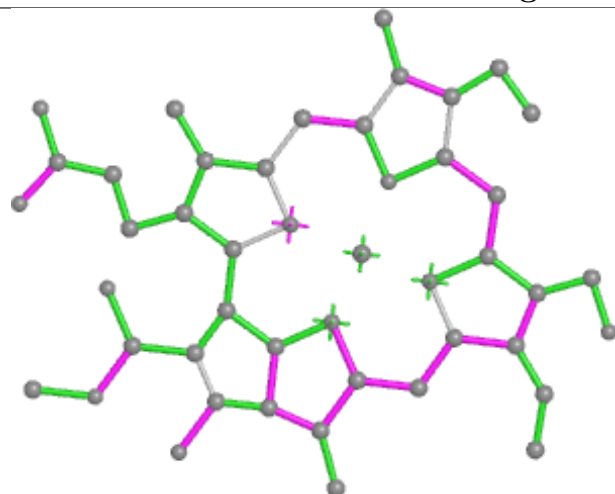
Ligand CLA r 608



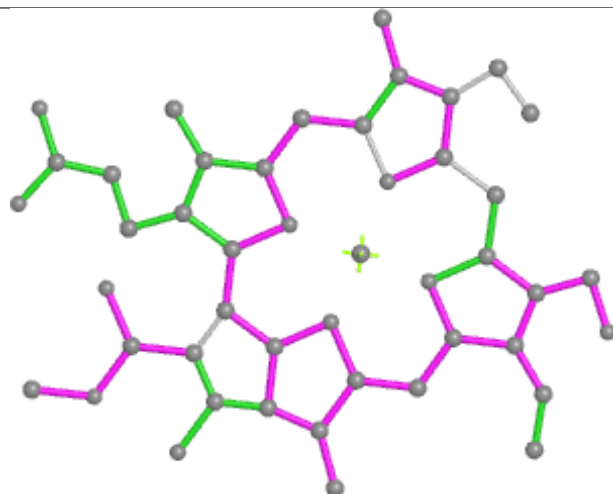
Ligand CHL 0 609



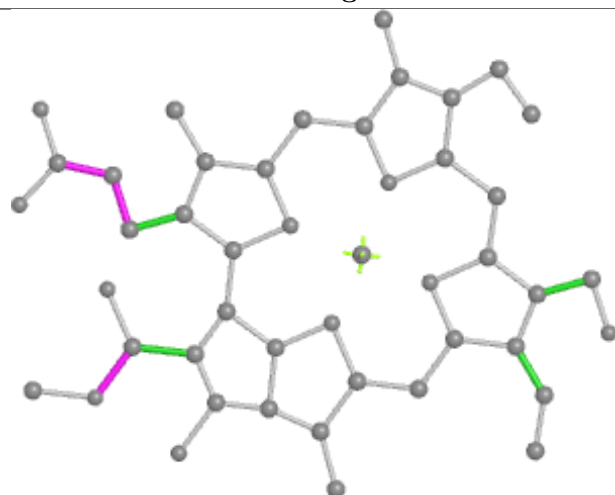
Ligand CHL 0 605



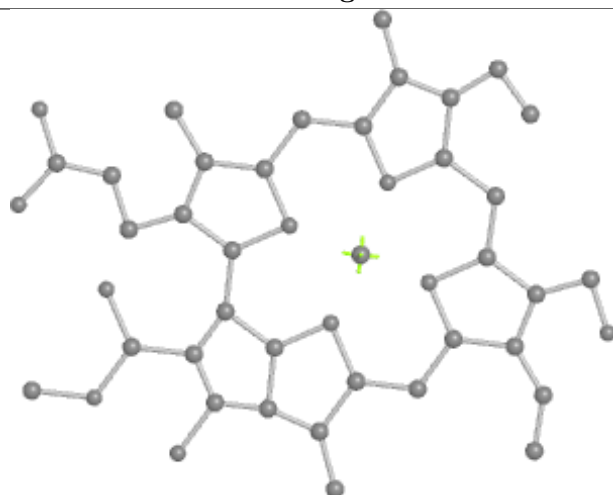
Bond lengths



Bond angles

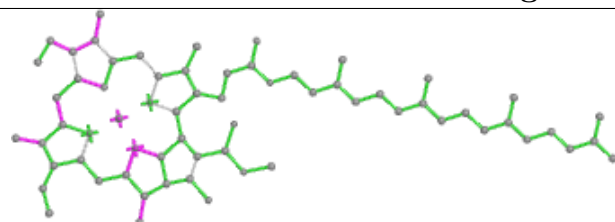


Torsions

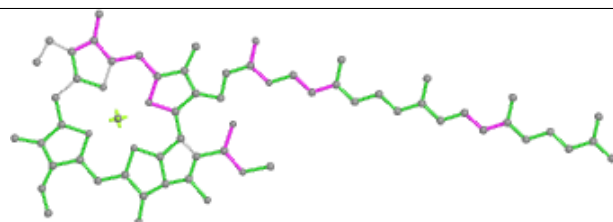


Rings

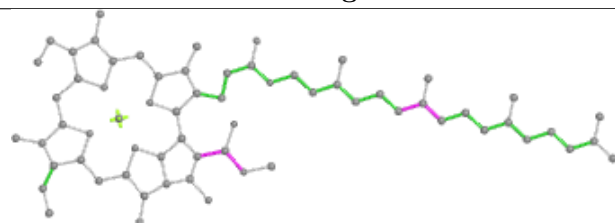
Ligand CLA 1 509



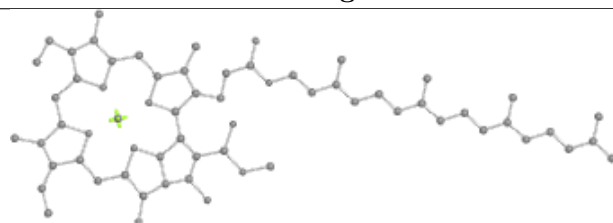
Bond lengths



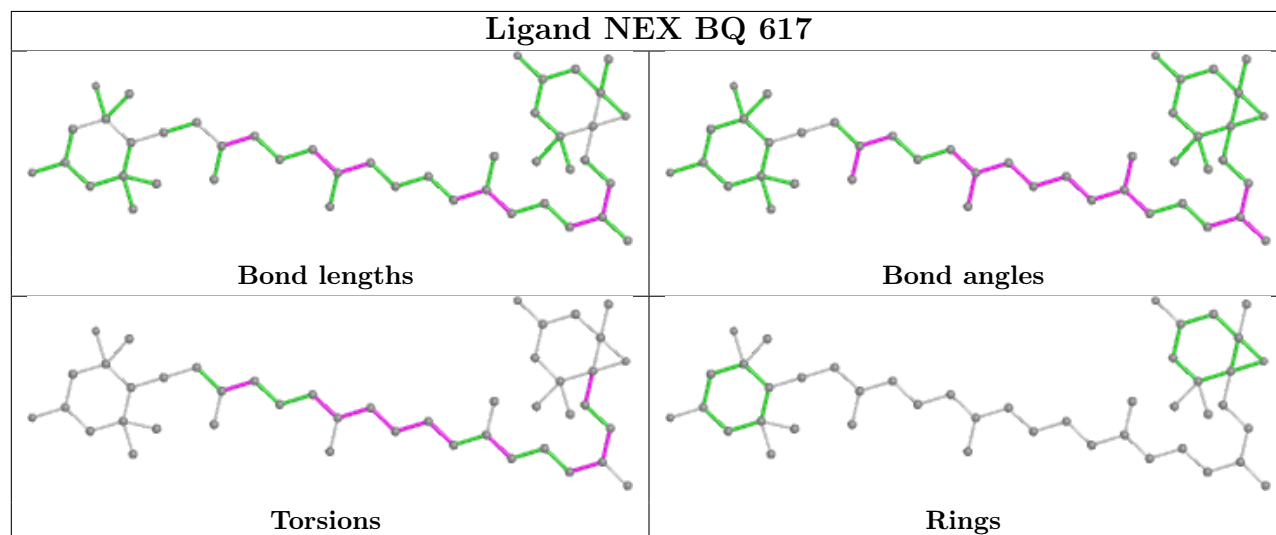
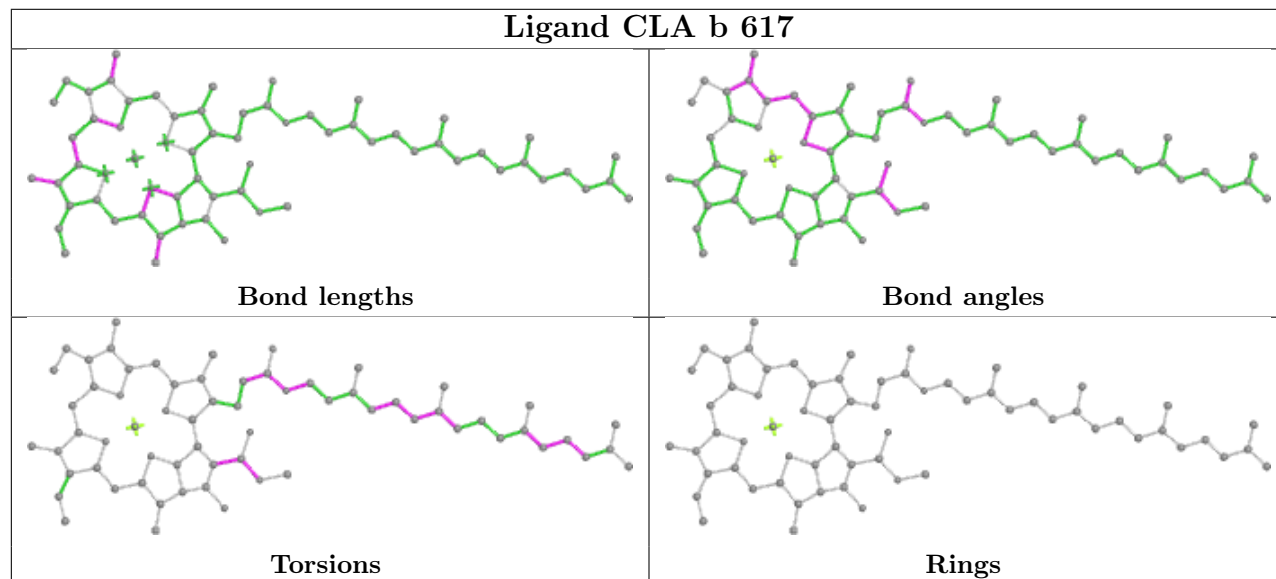
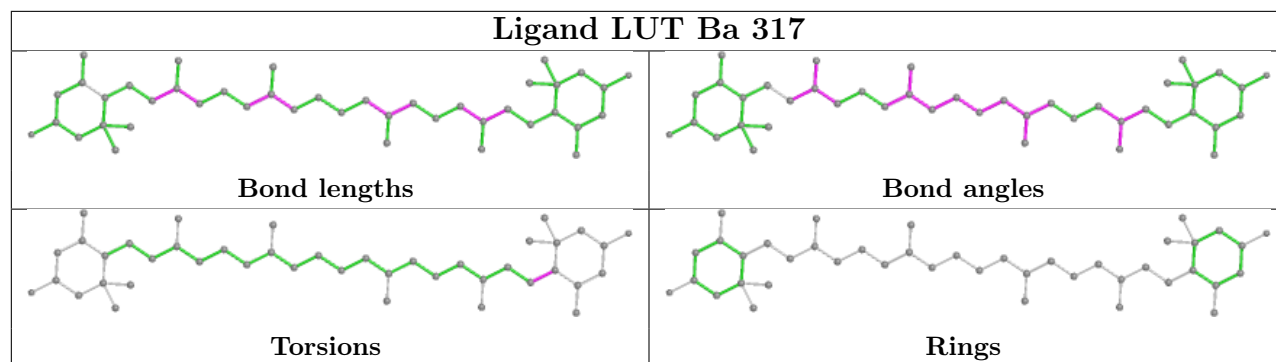
Bond angles

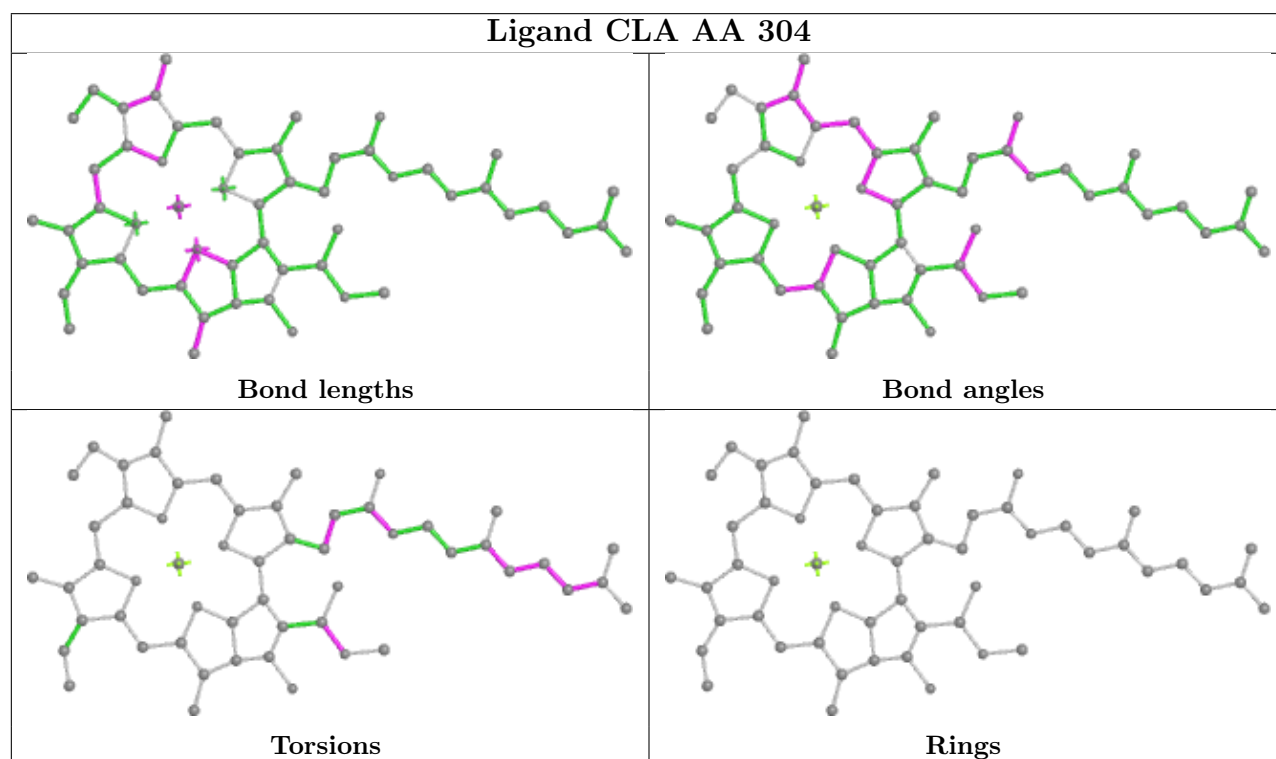
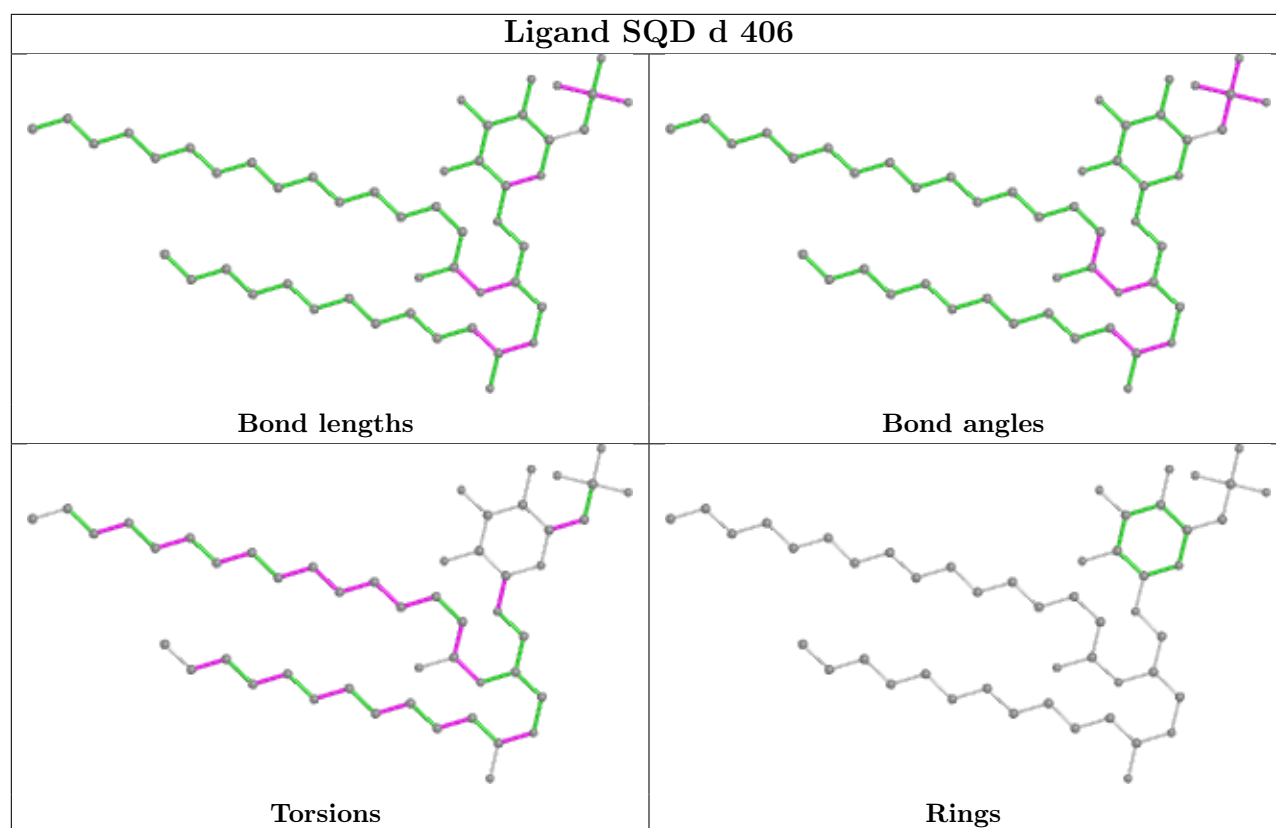


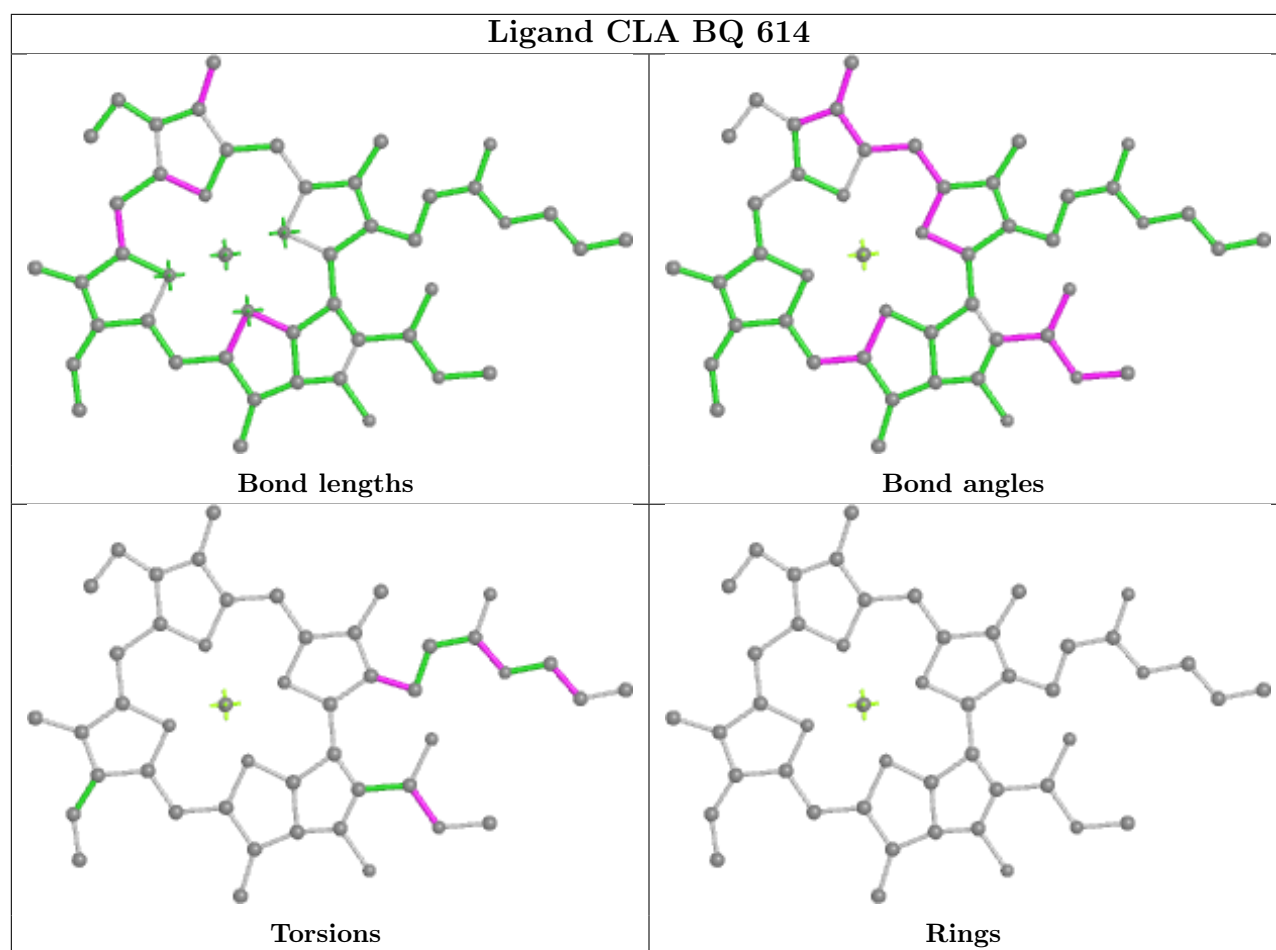
Torsions

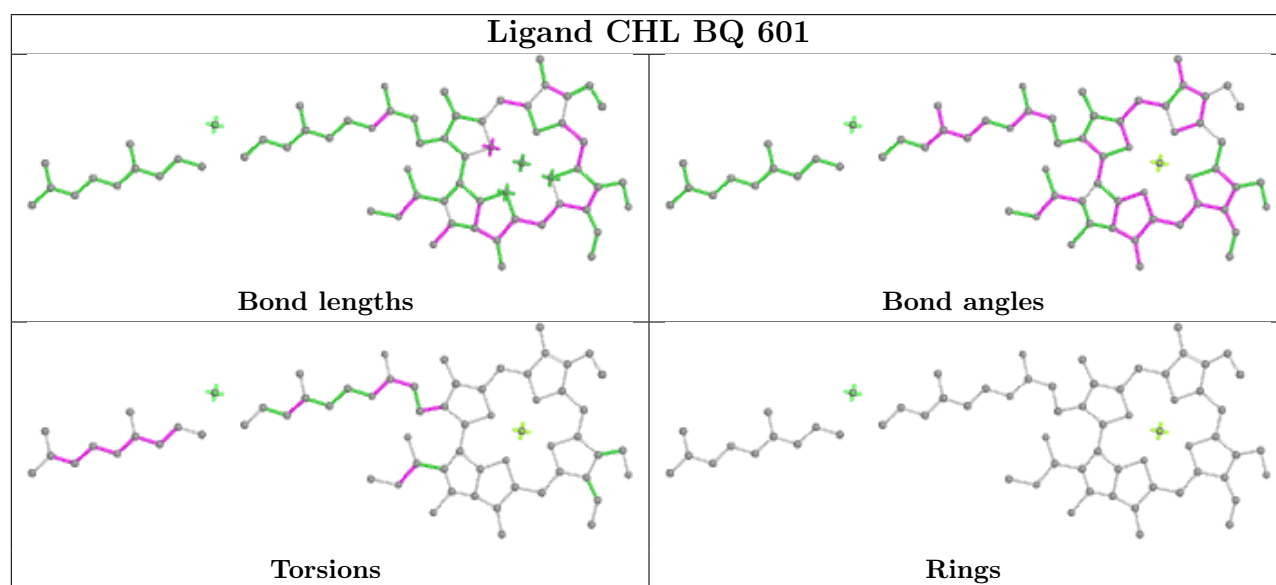
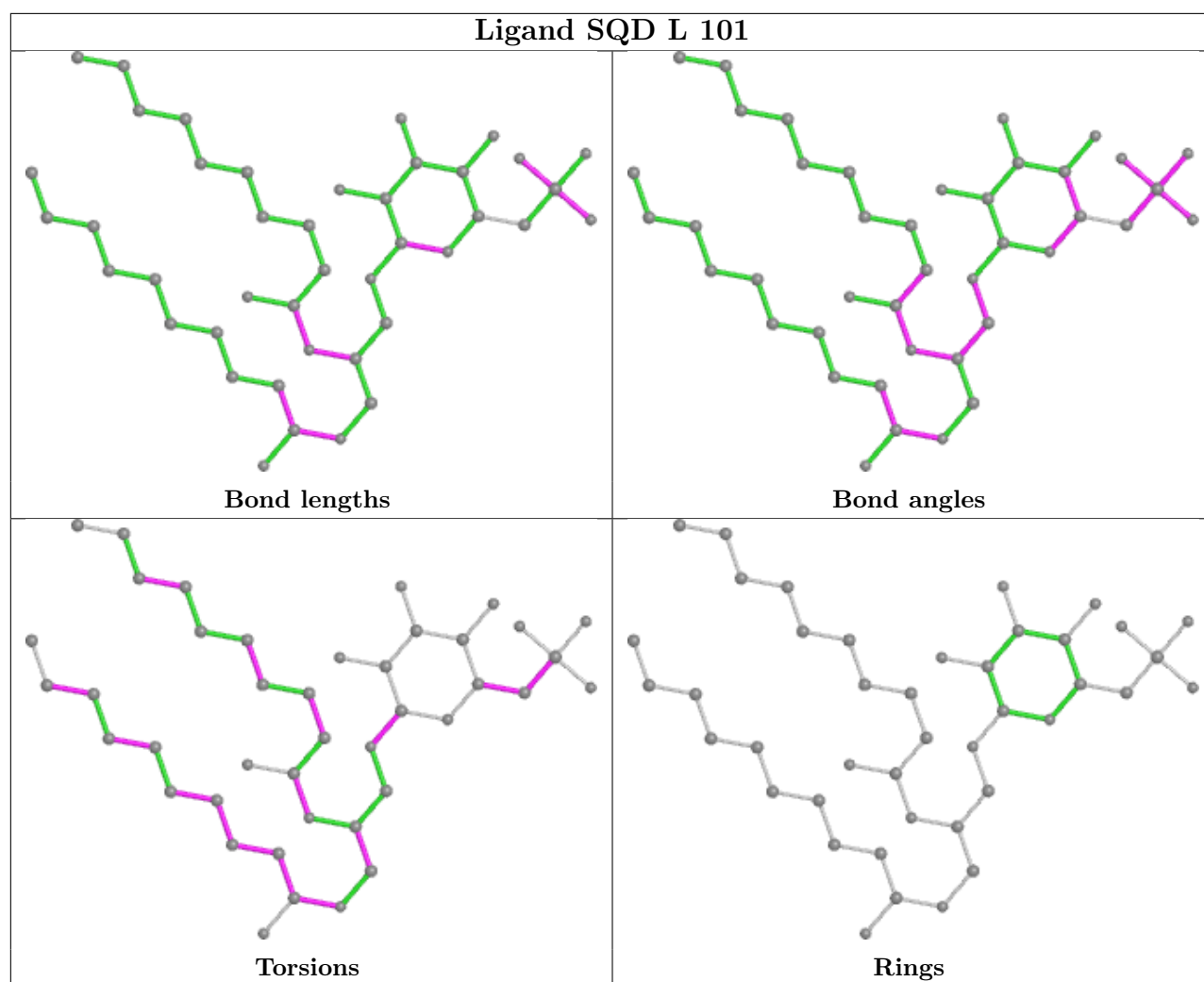


Rings

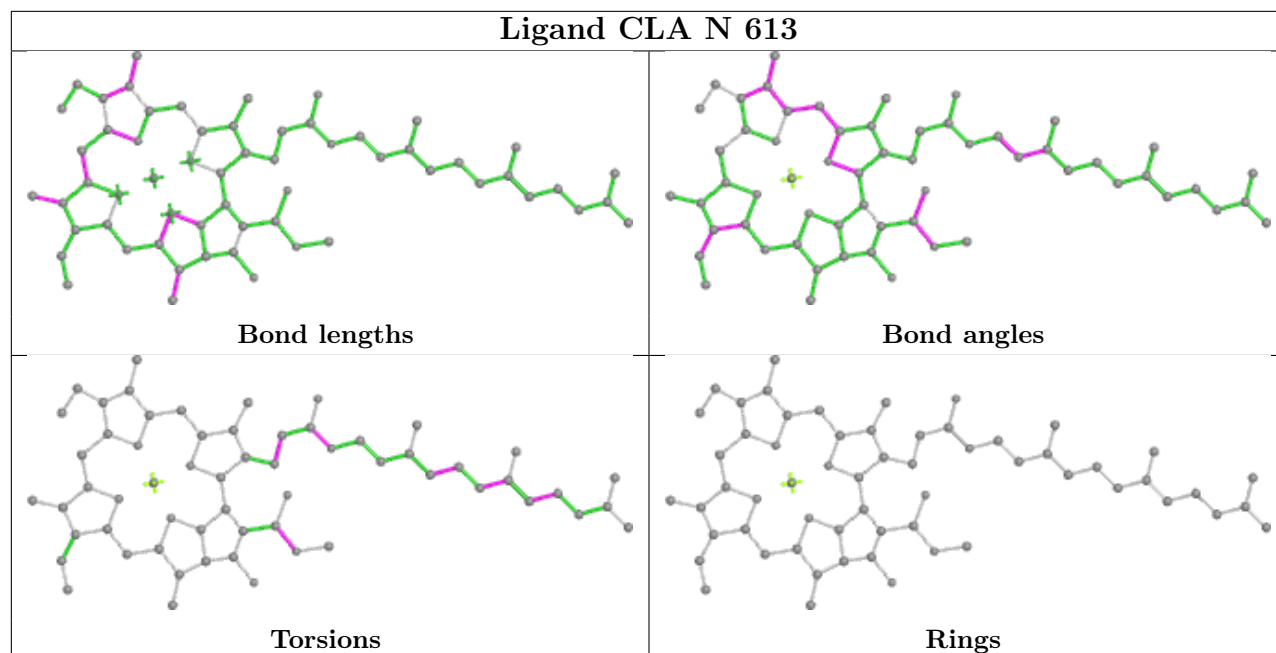




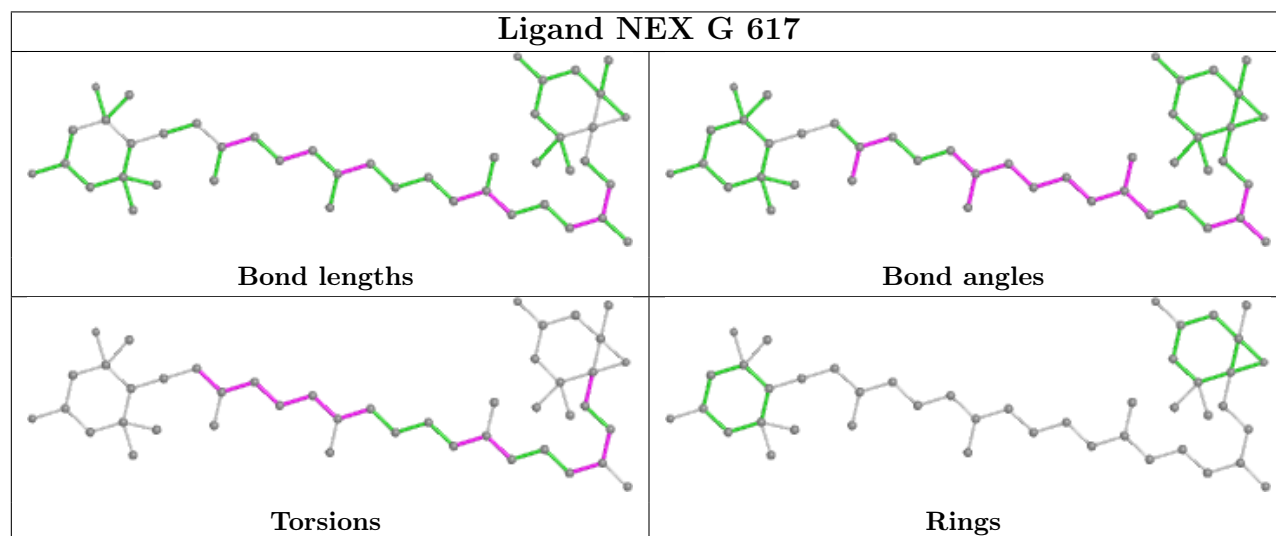




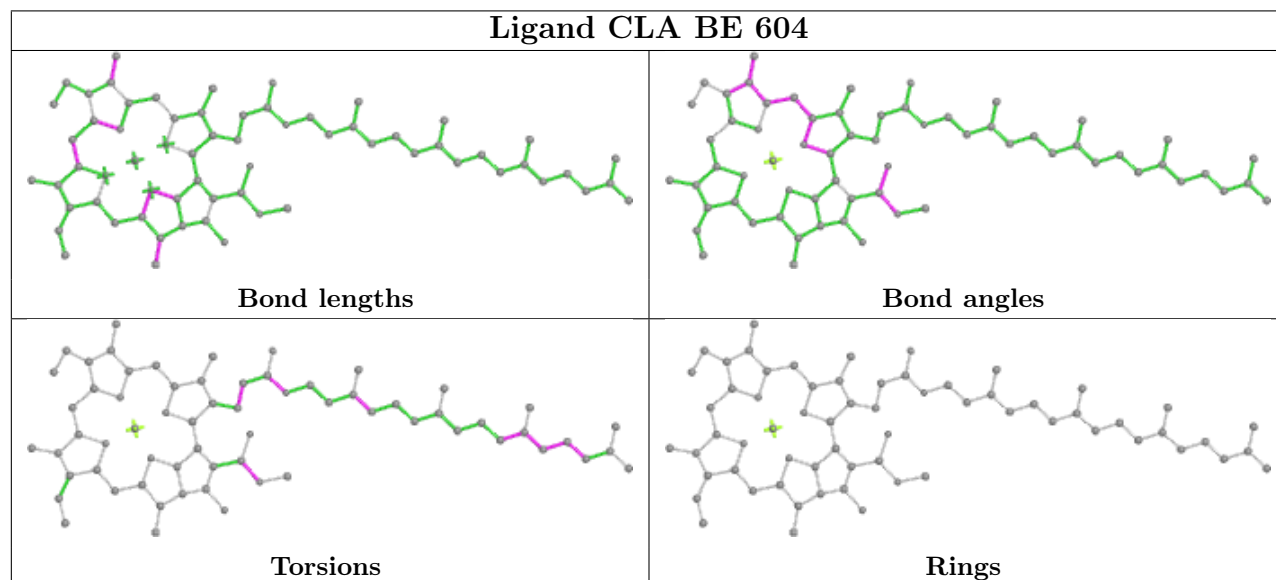
Ligand CLA N 613

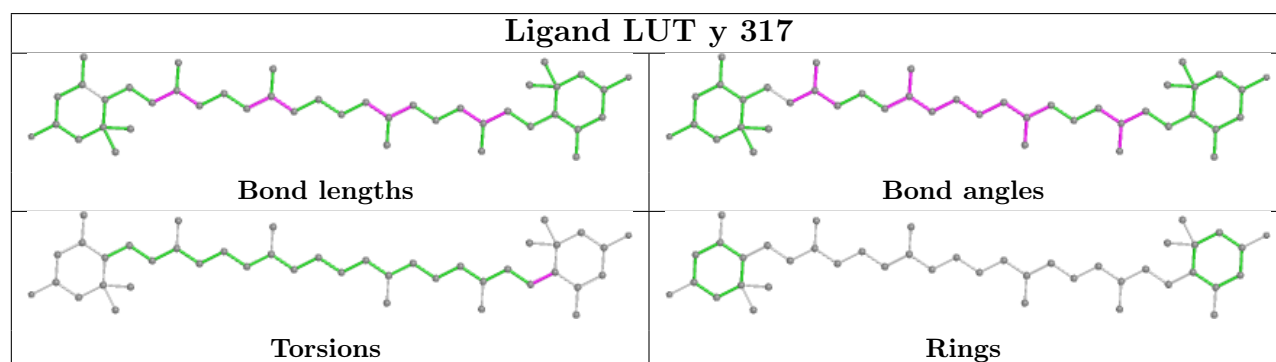
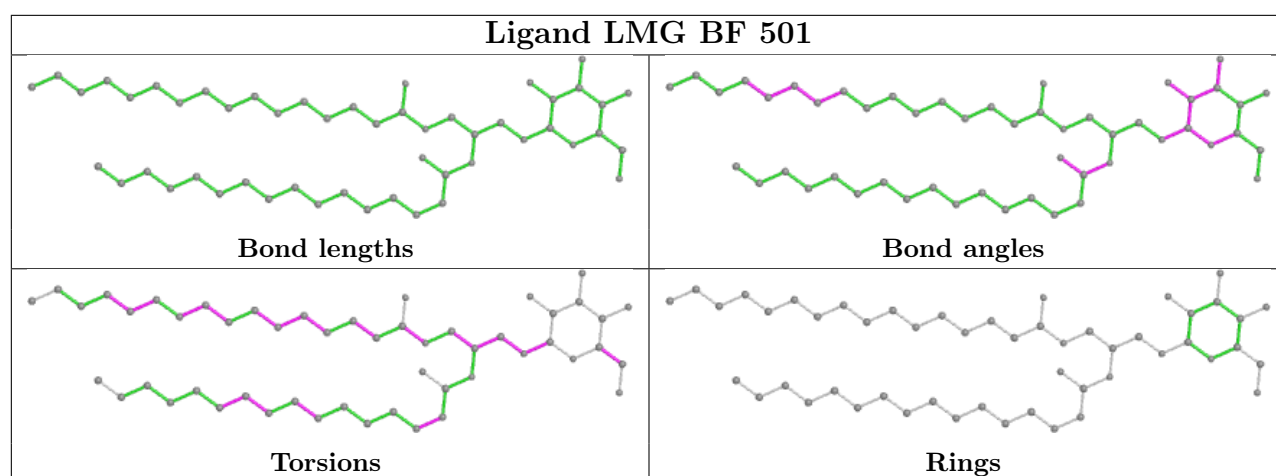
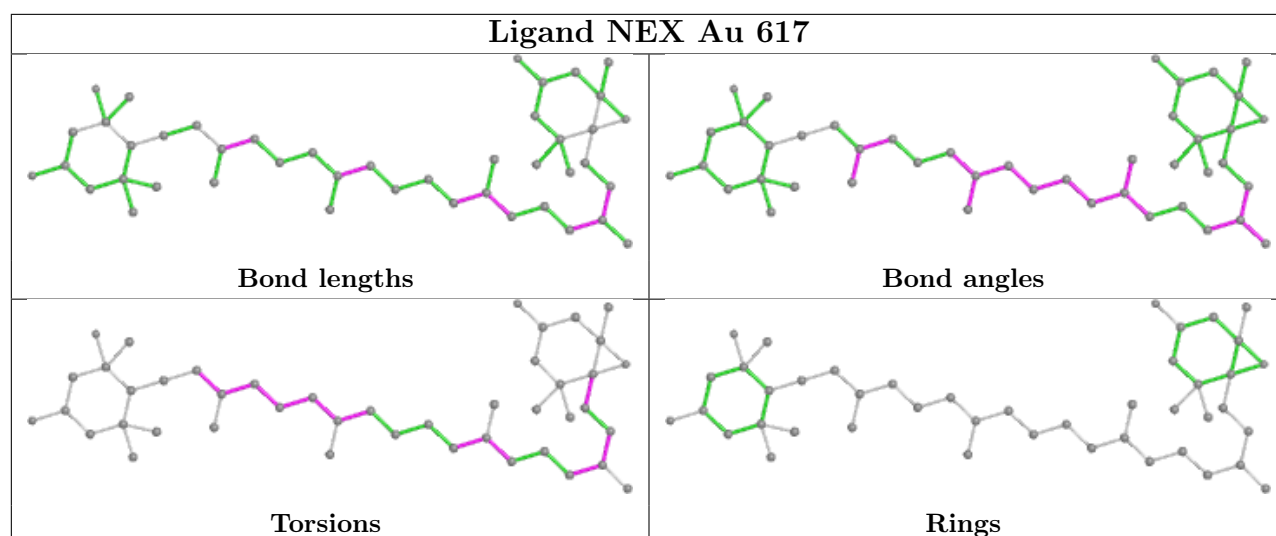


Ligand NEX G 617

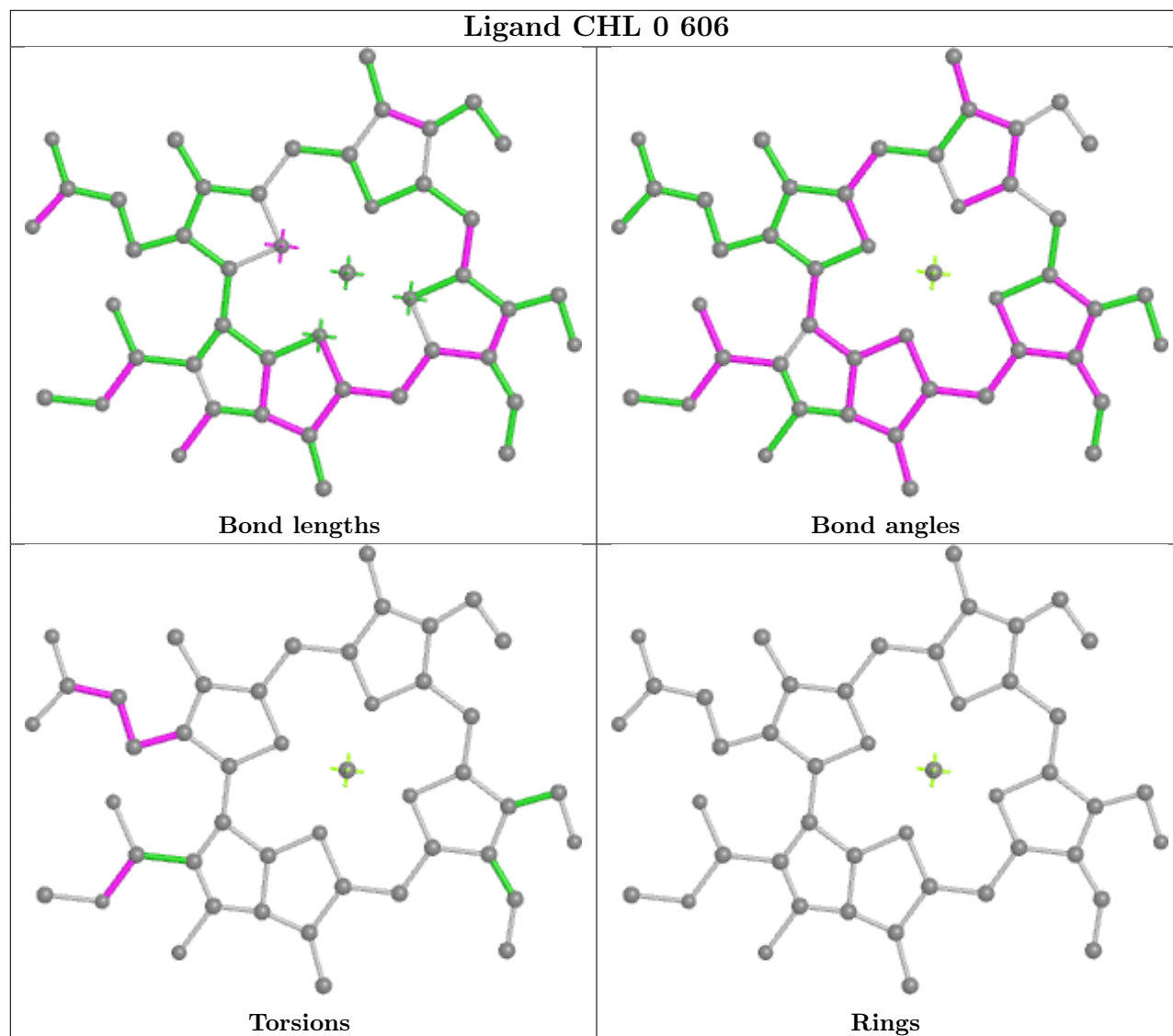


Ligand CLA BE 604

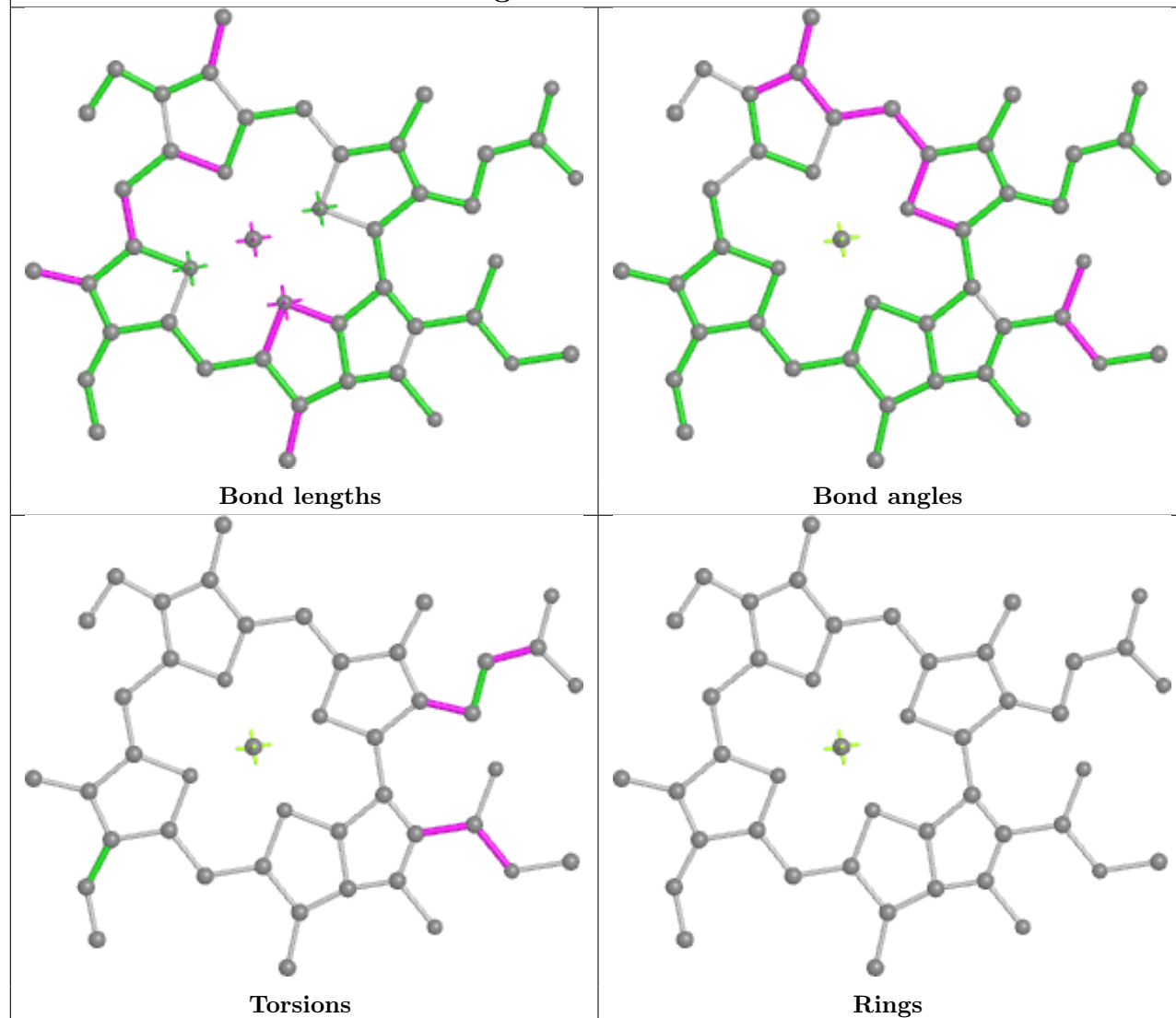




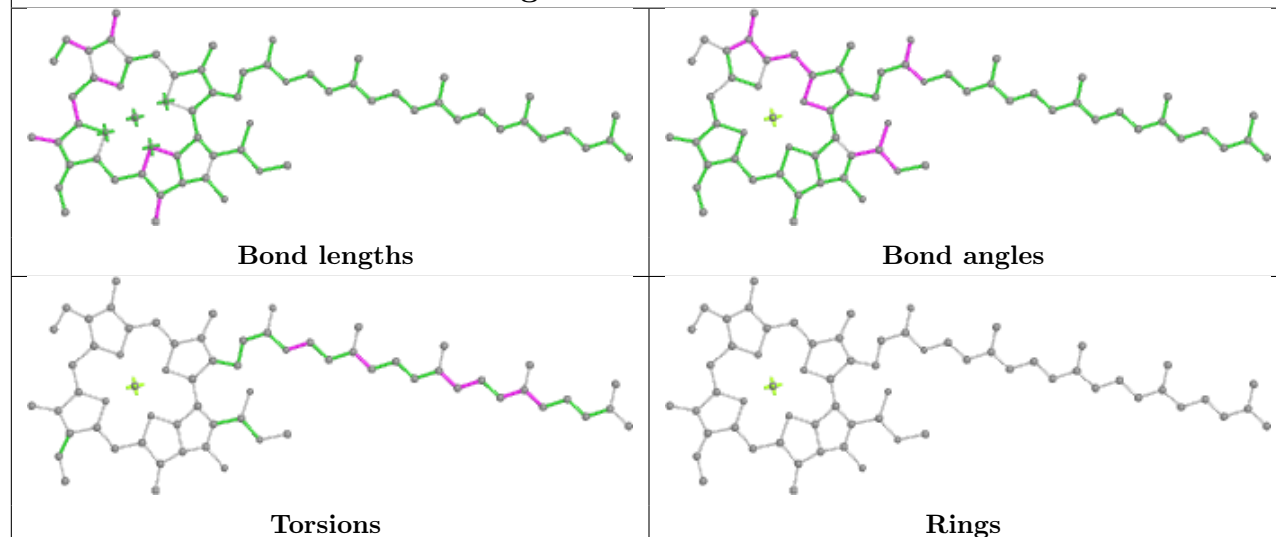
Ligand CHL 0 606

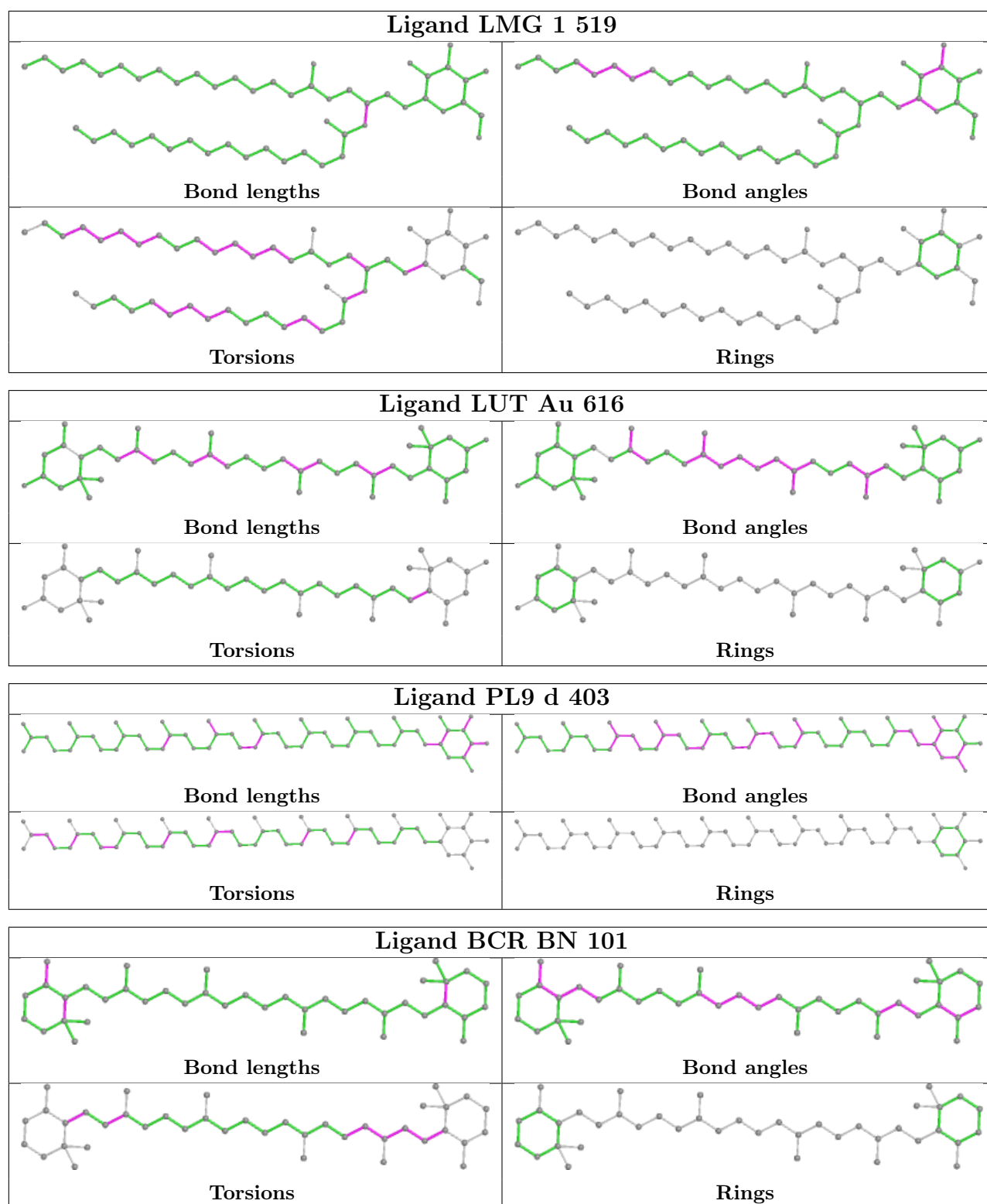


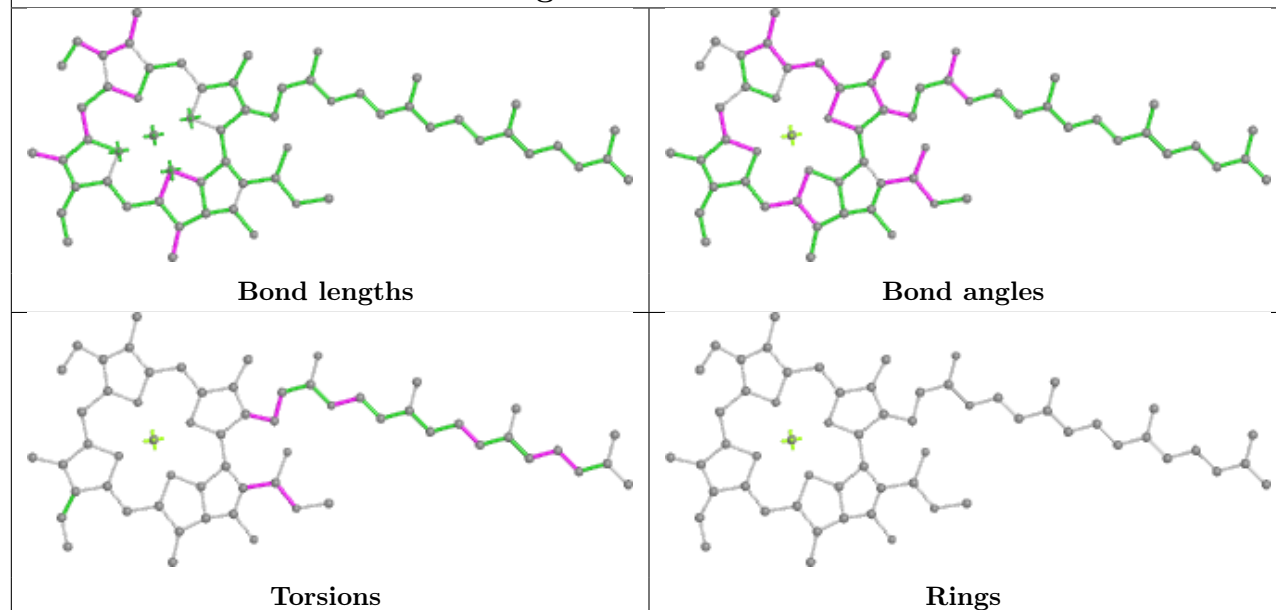
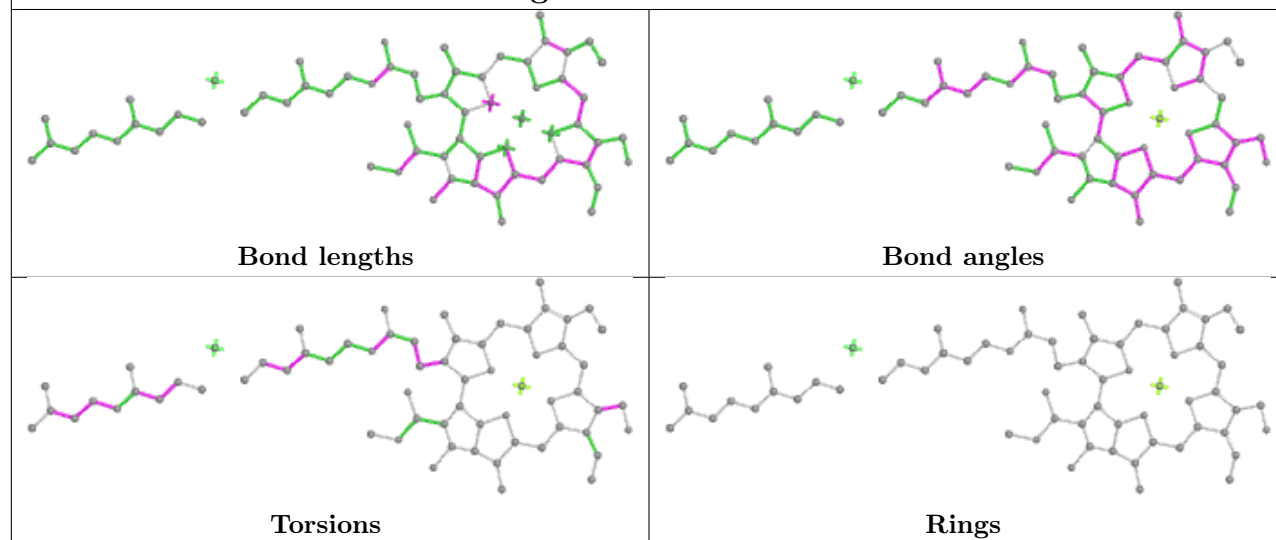
Ligand CLA 7 314



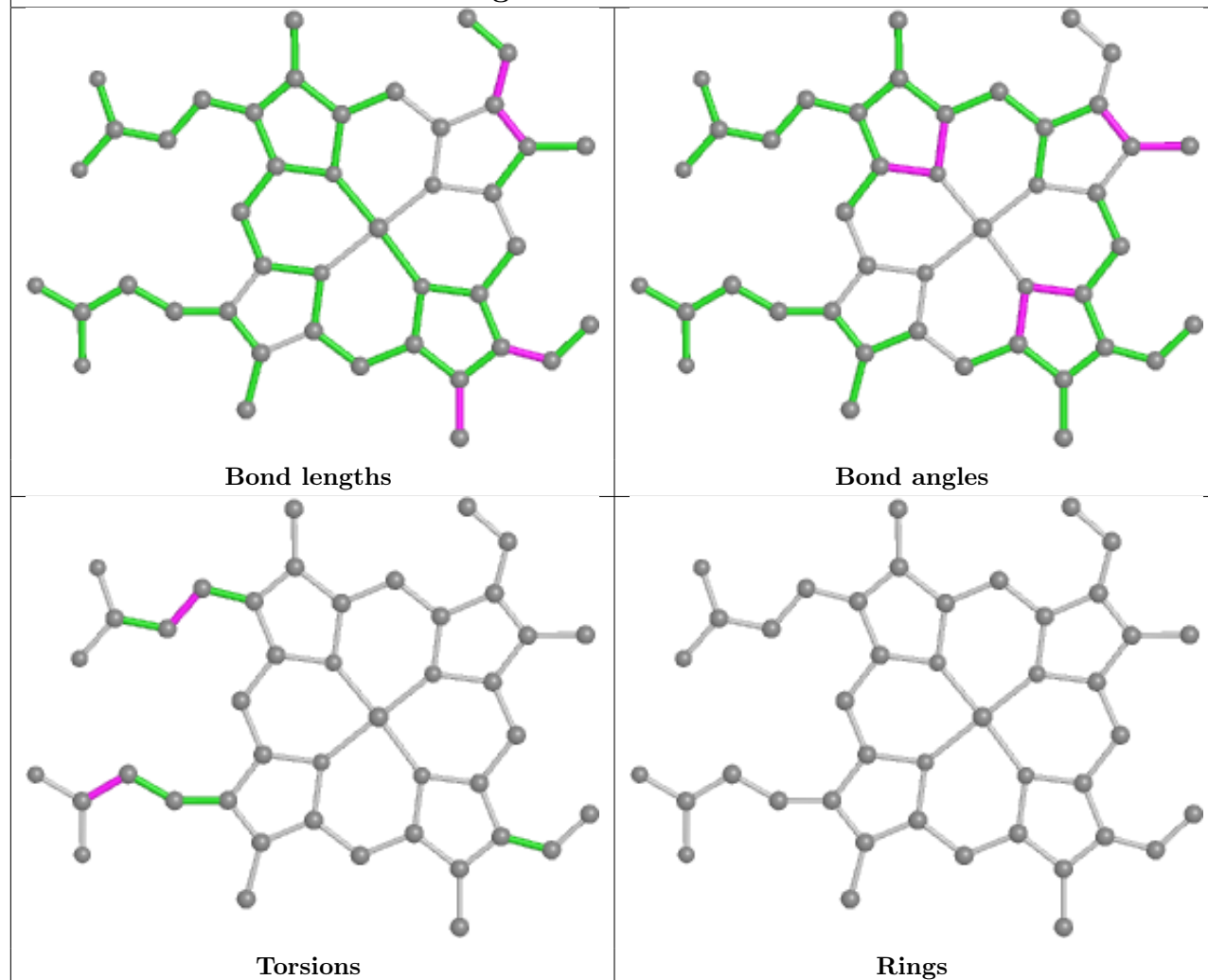
Ligand CLA BE 616



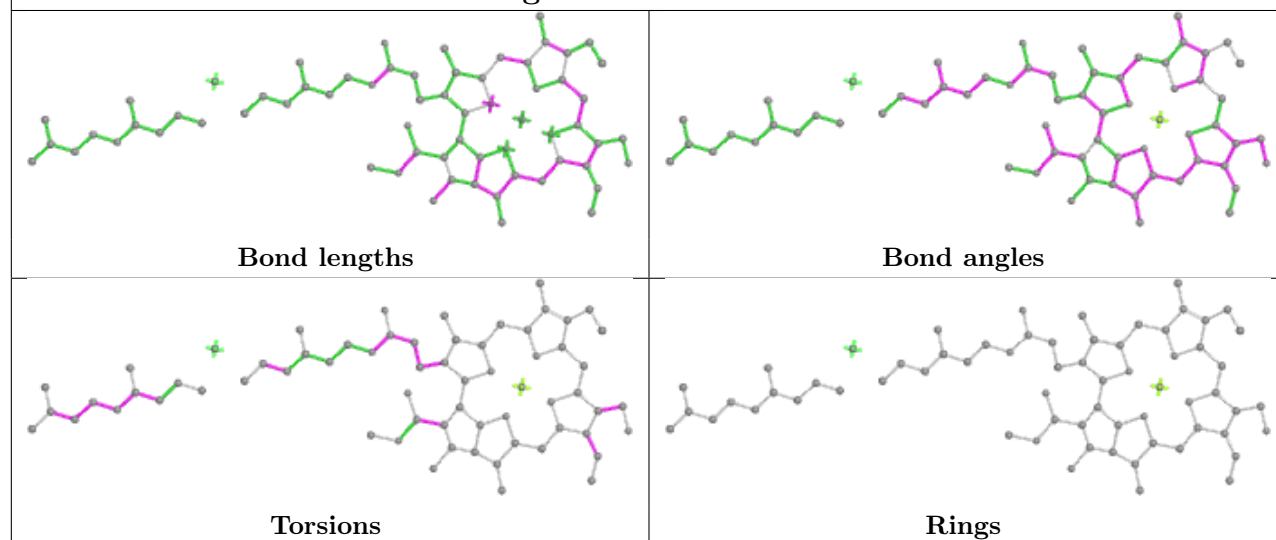


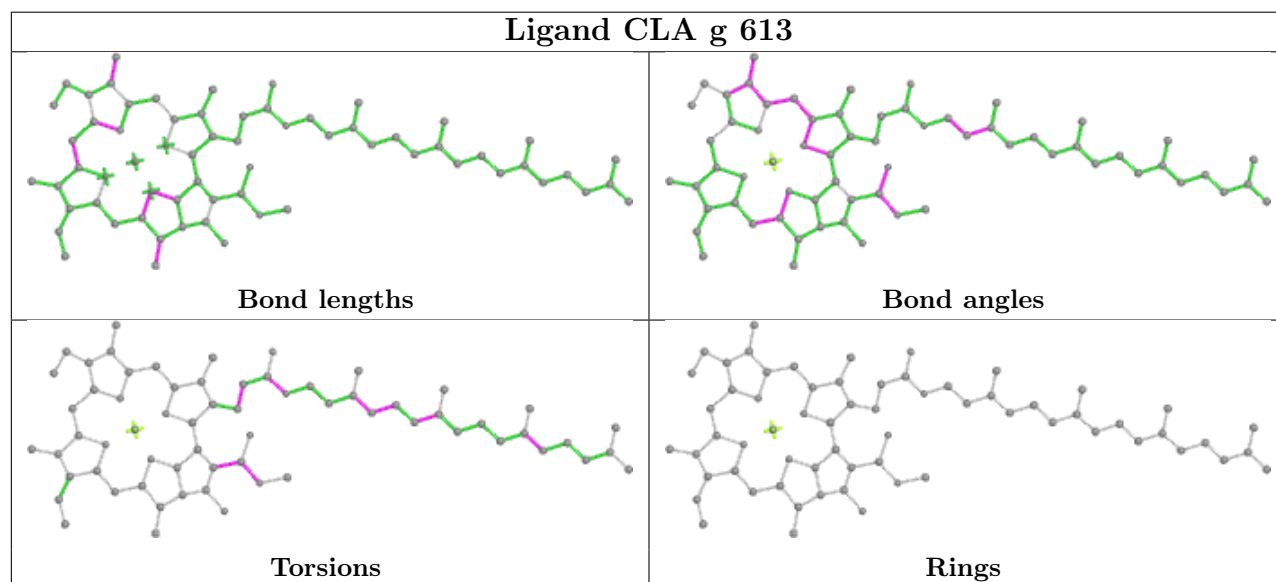
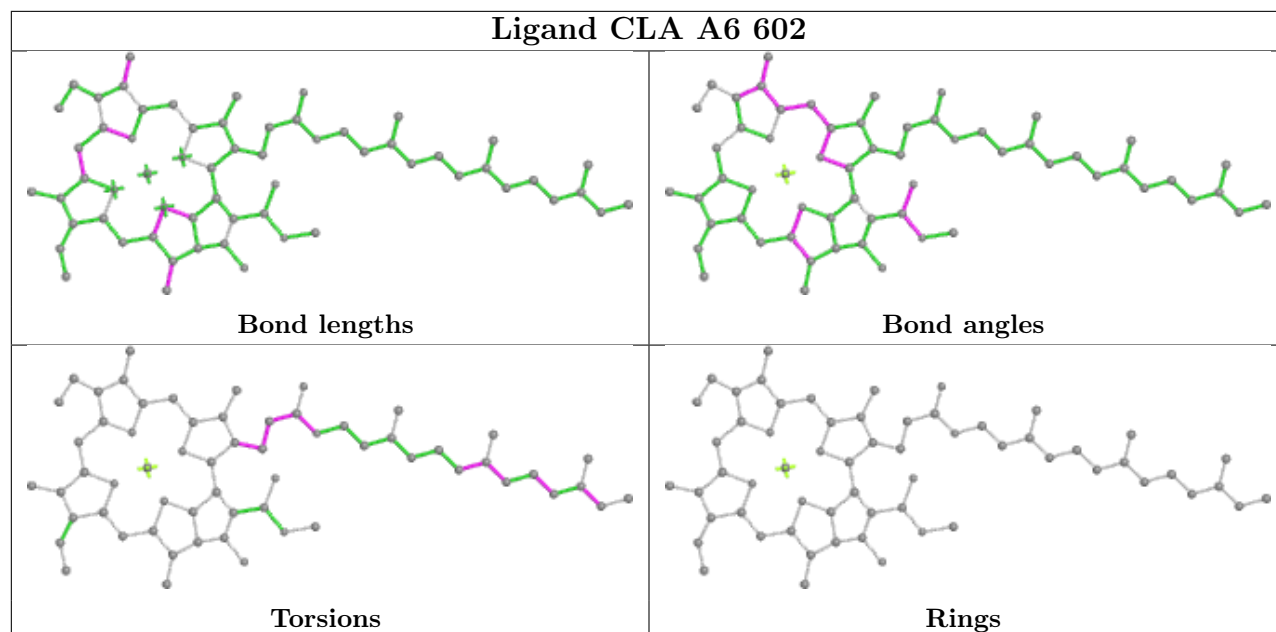
Ligand CLA 0 610**Ligand CHL N 601**

Ligand HEM BI 102

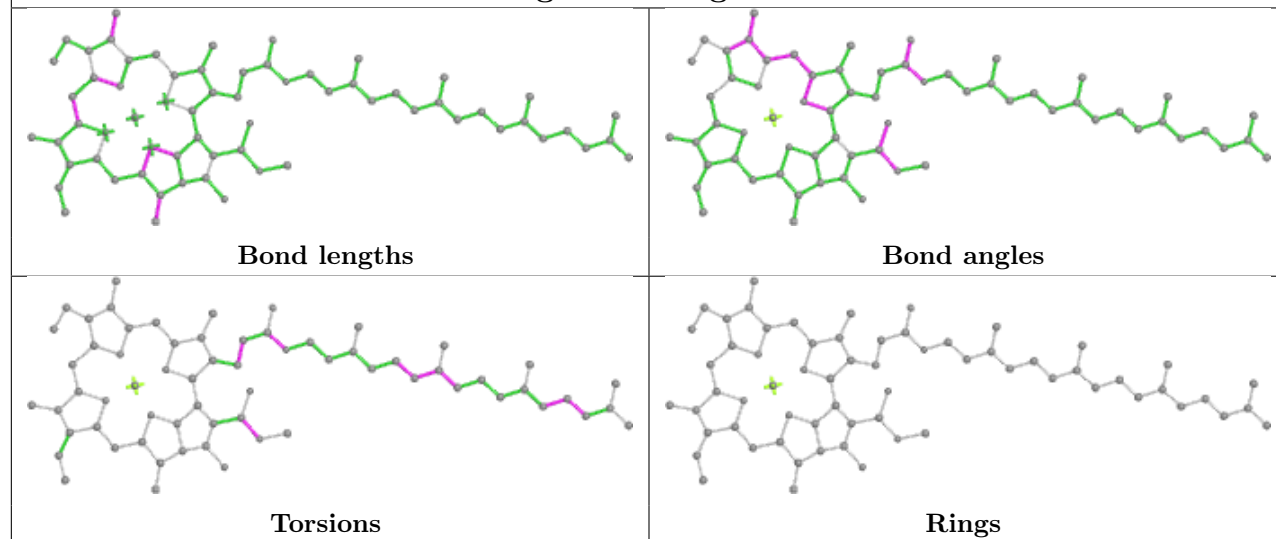


Ligand CHL BJ 608

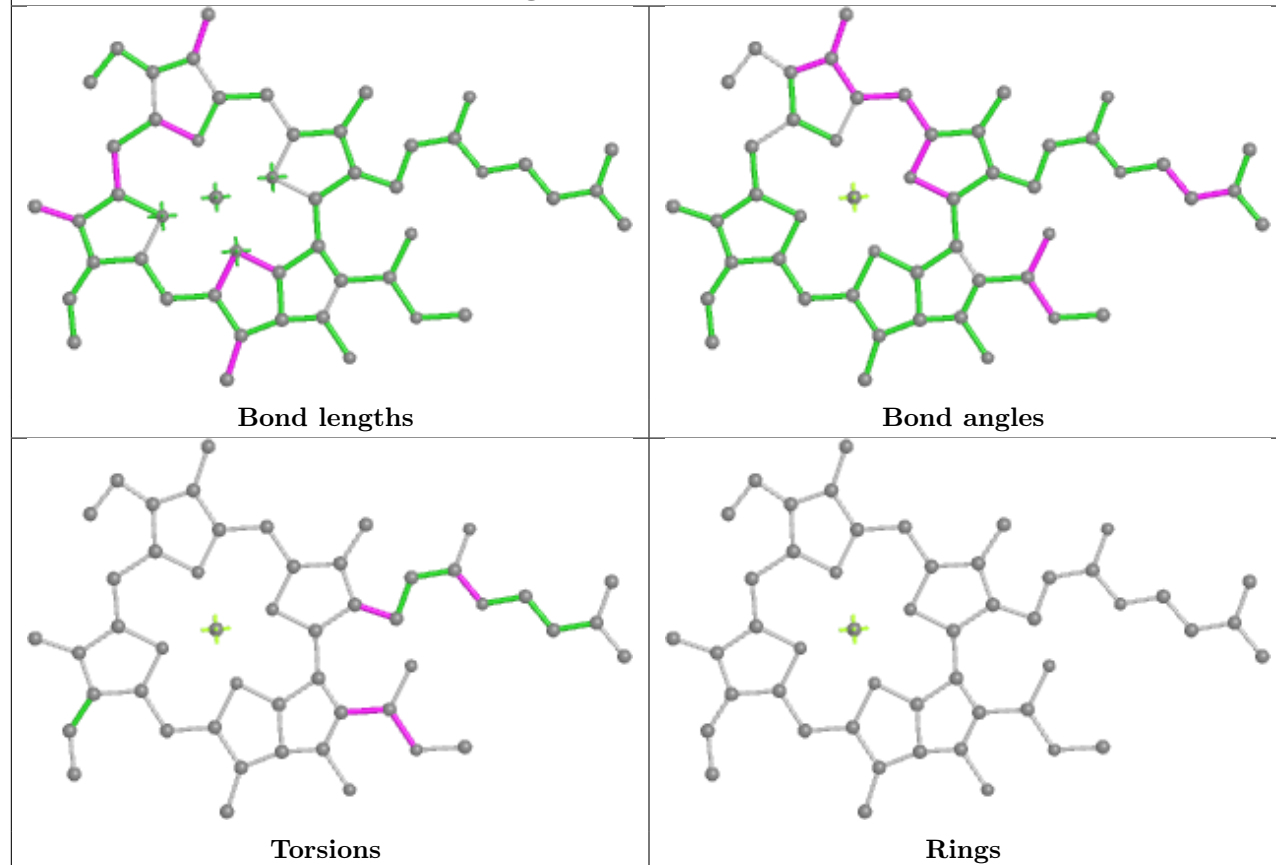


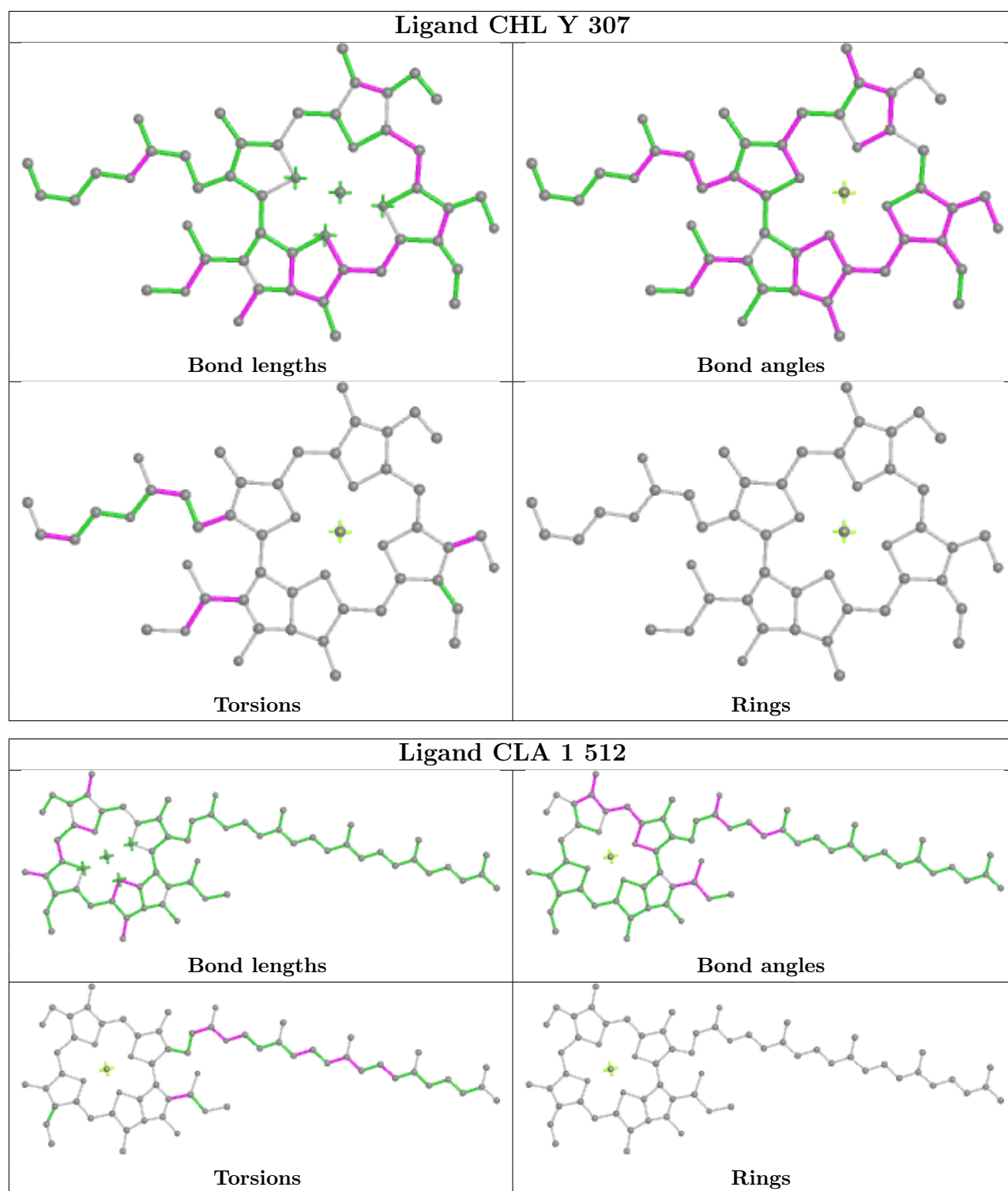


Ligand CLA g 603

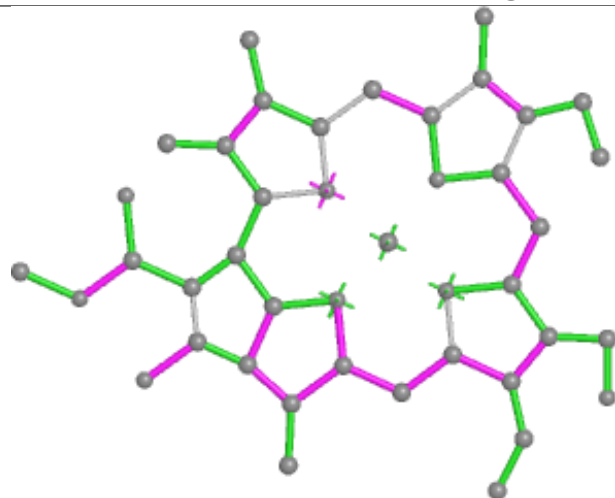


Ligand CLA A6 604

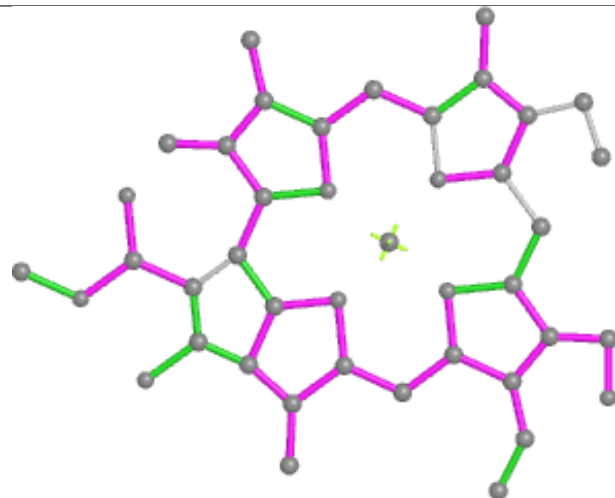




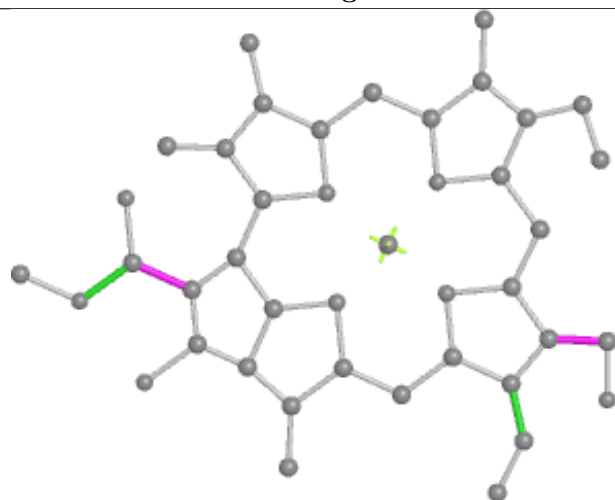
Ligand CHL BU 613



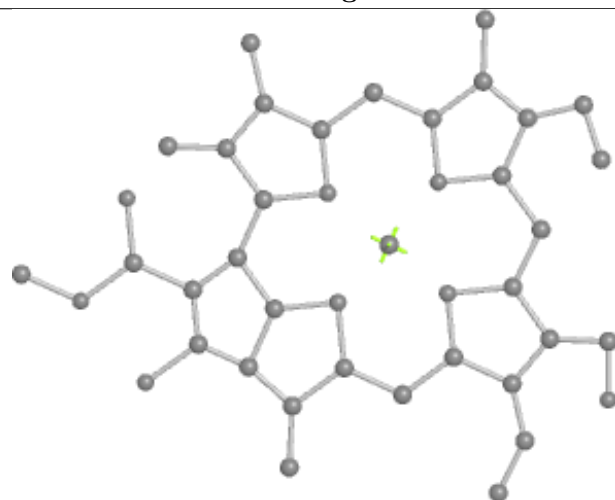
Bond lengths



Bond angles

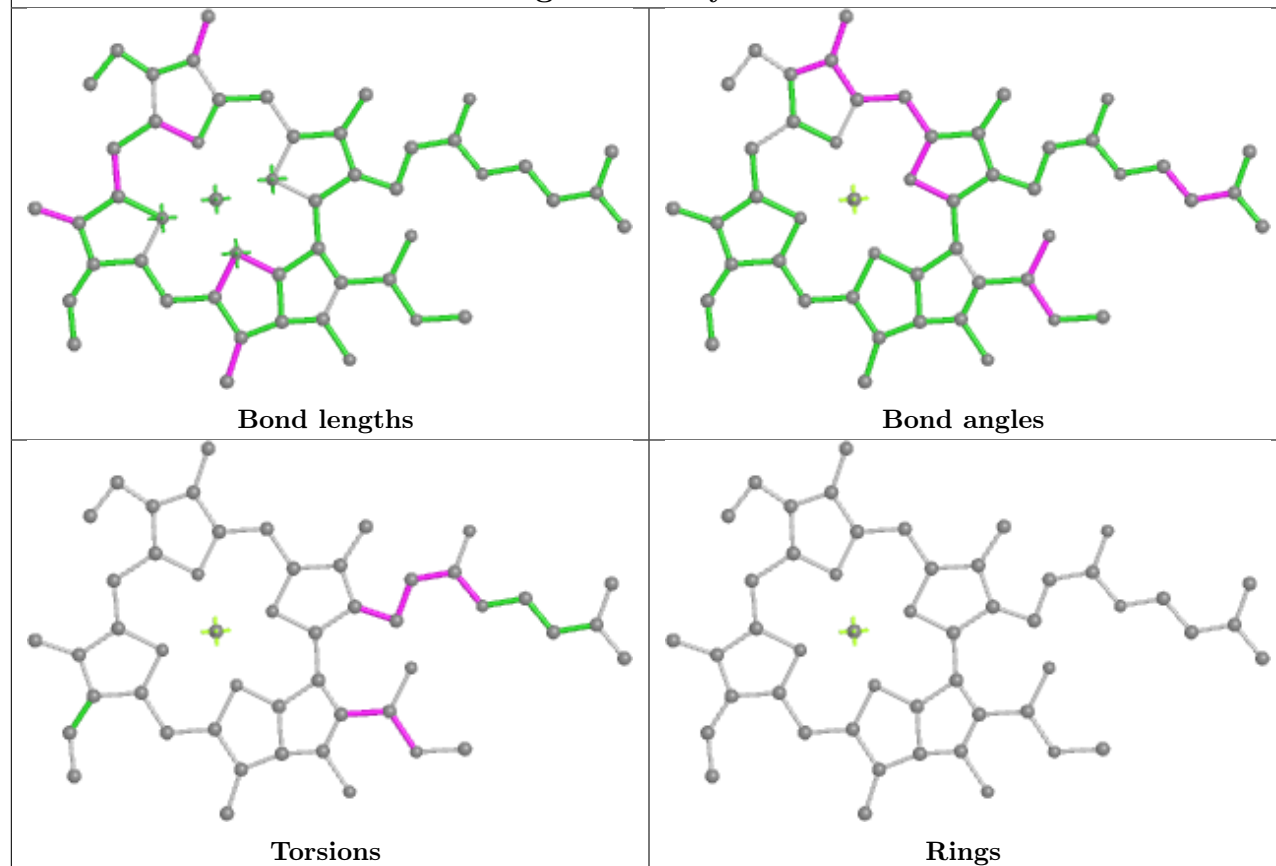


Torsions

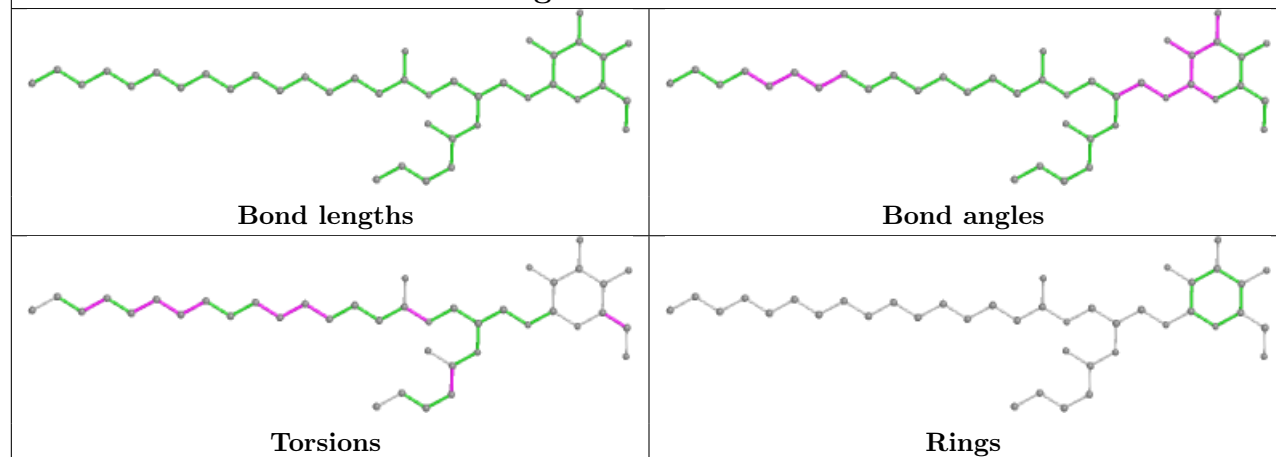


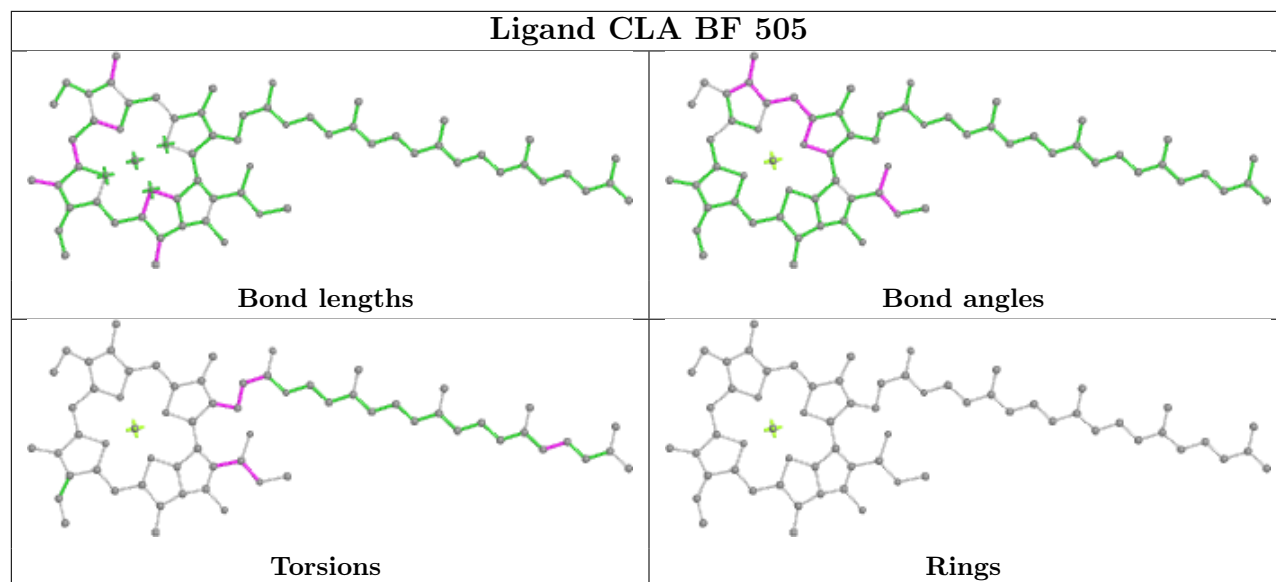
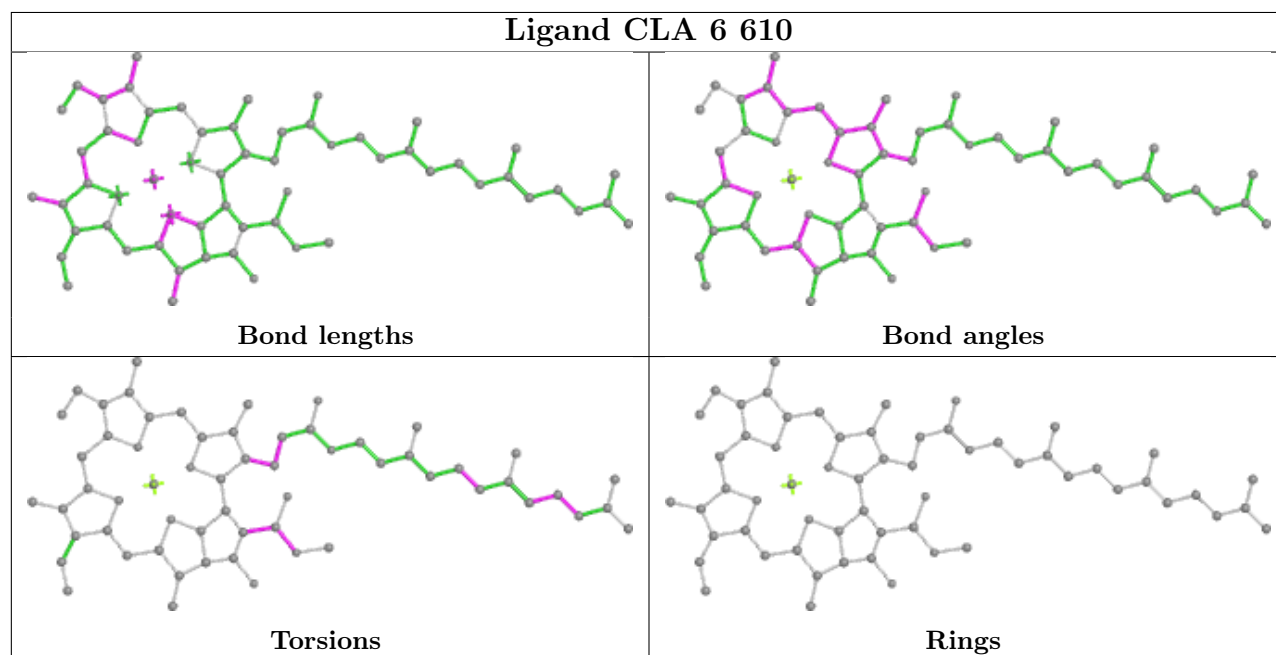
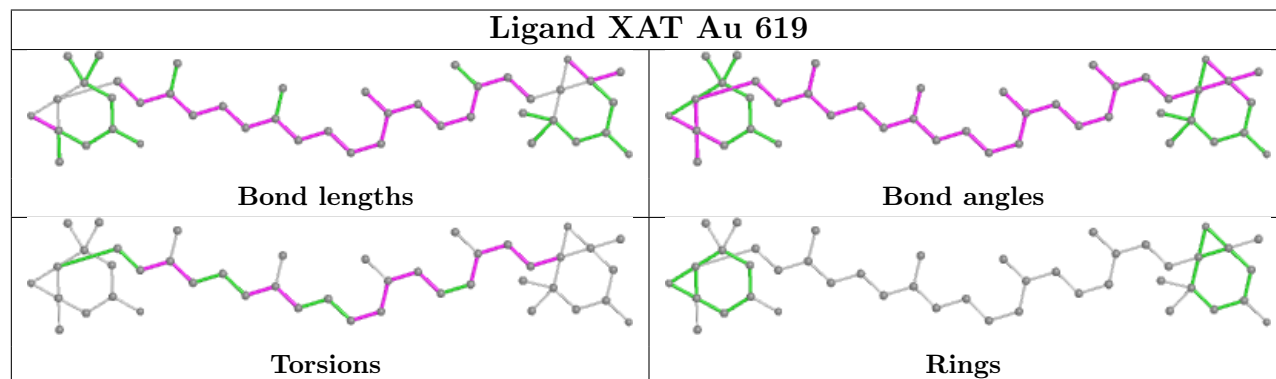
Rings

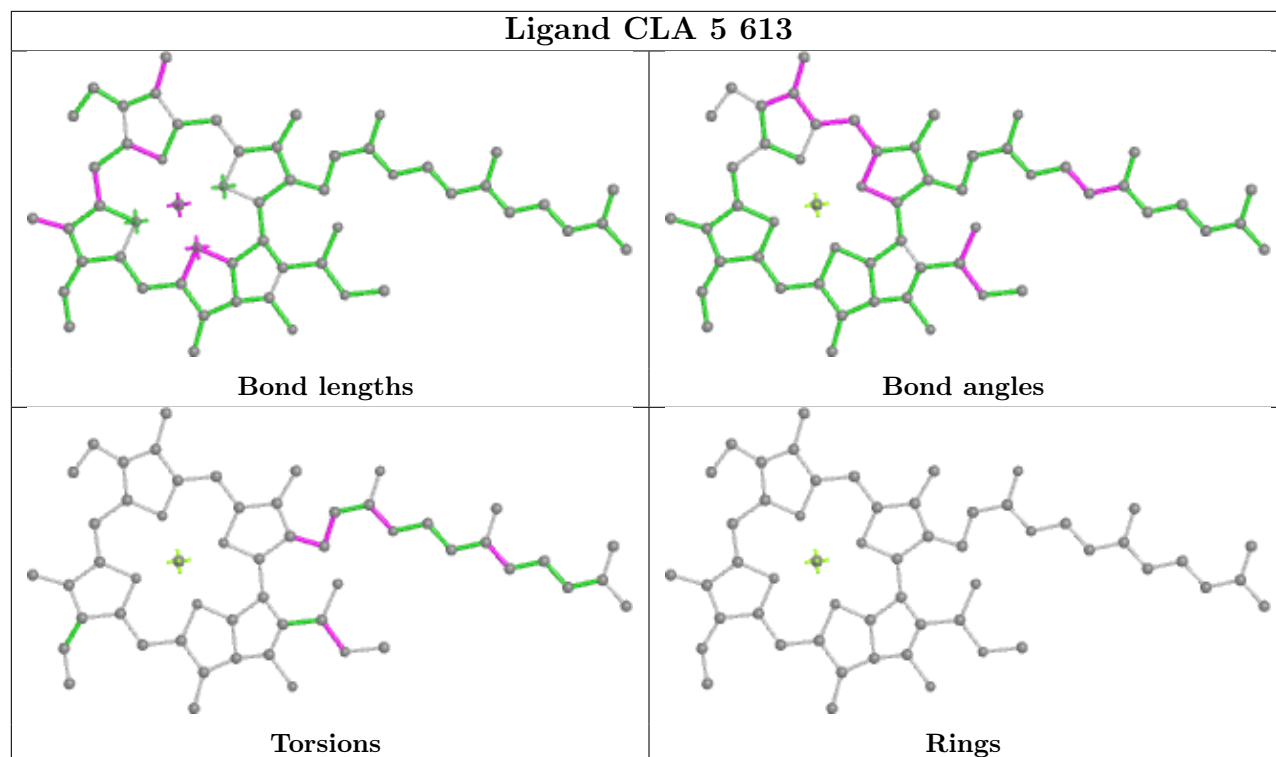
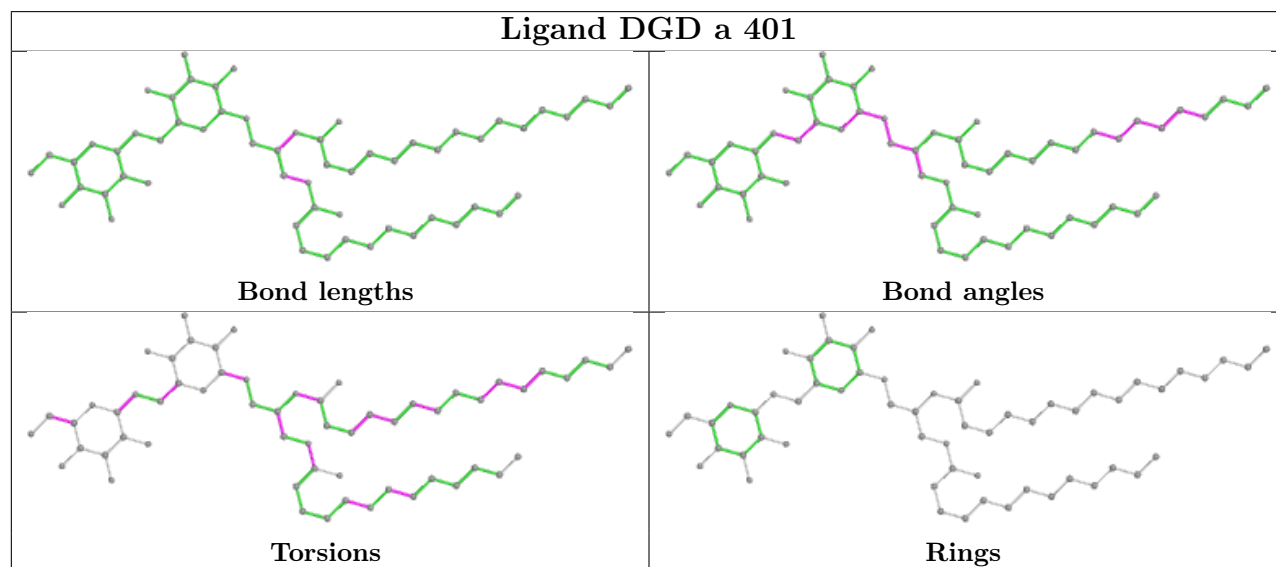
Ligand CLA y 305

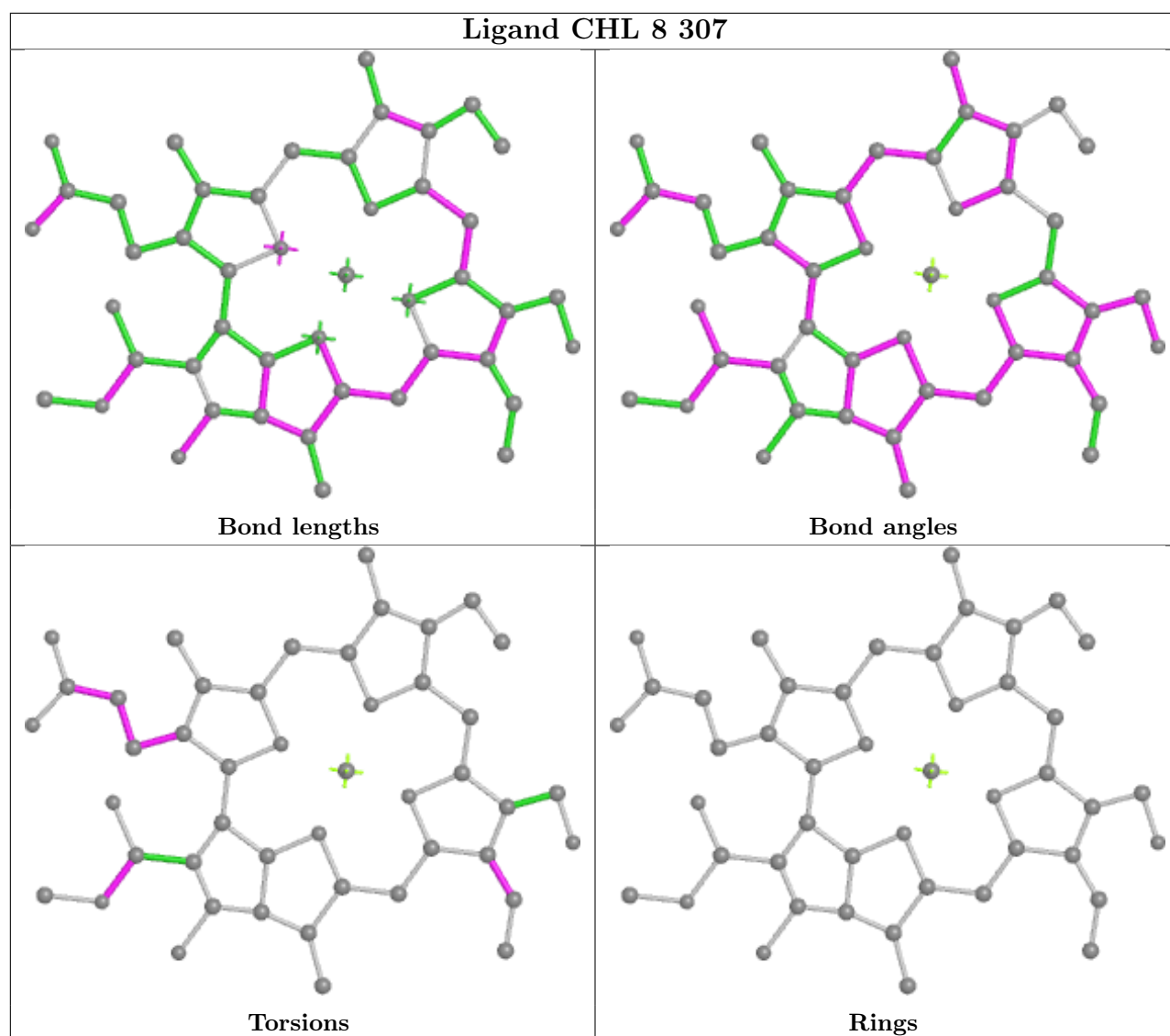


Ligand LMG I 101



Ligand CLA BF 505**Ligand CLA 6 610****Ligand XAT Au 619**

Ligand CLA 5 613**Ligand DGD a 401**



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.

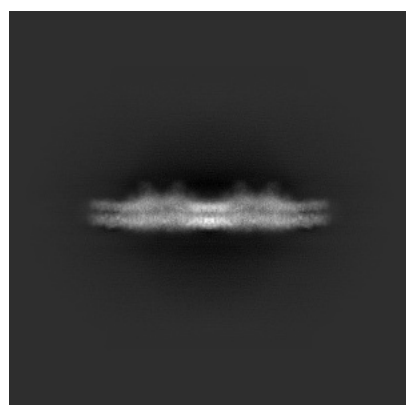
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63017. These allow visual inspection of the internal detail of the map and identification of artifacts.

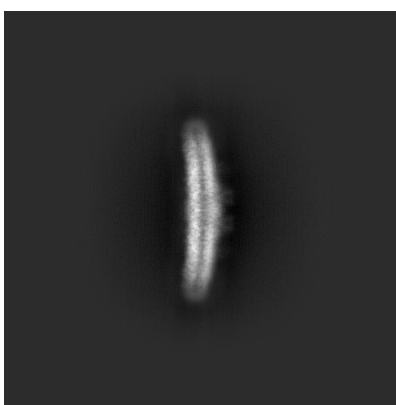
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

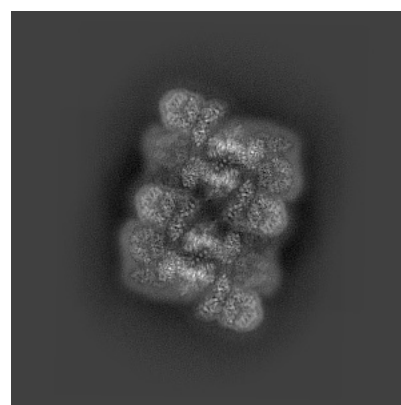
6.1.1 Primary map



X



Y

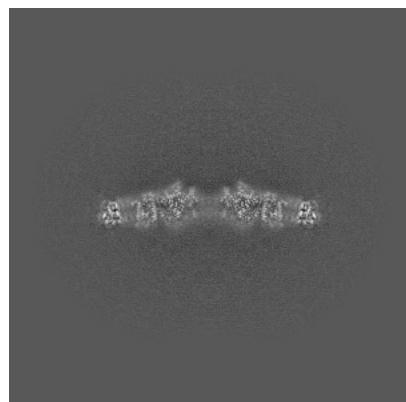


Z

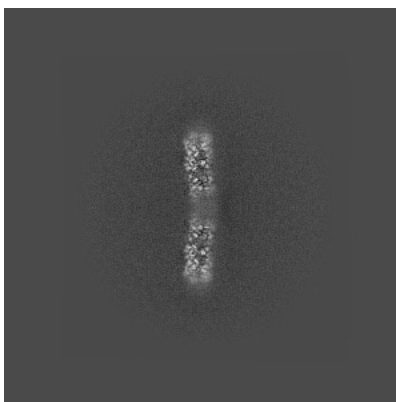
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

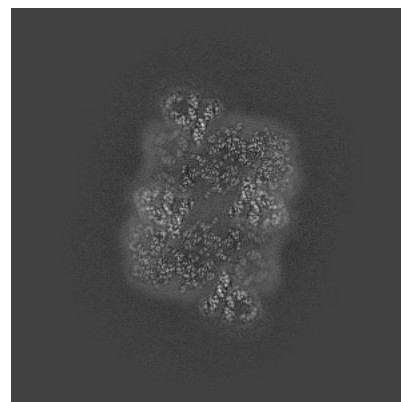
6.2.1 Primary map



X Index: 360



Y Index: 360

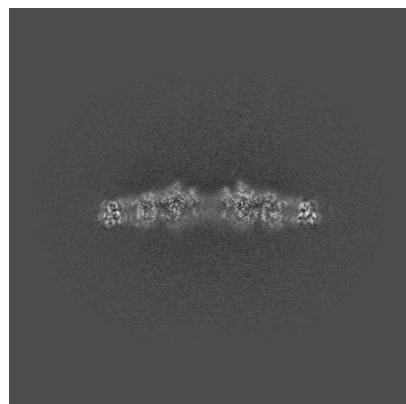


Z Index: 360

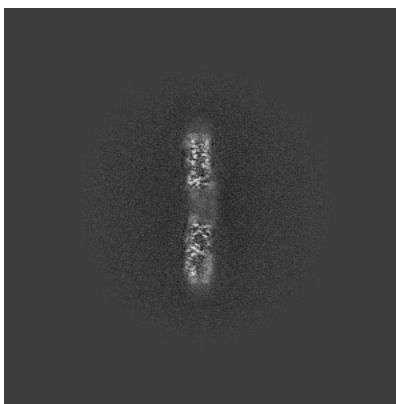
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

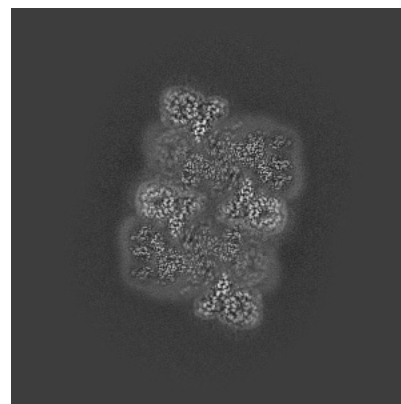
6.3.1 Primary map



X Index: 361



Y Index: 367

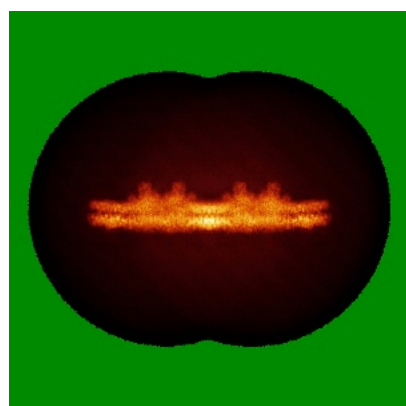


Z Index: 342

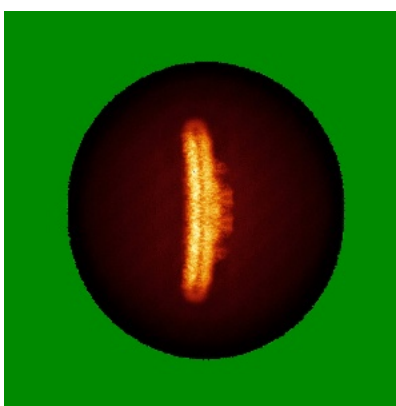
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

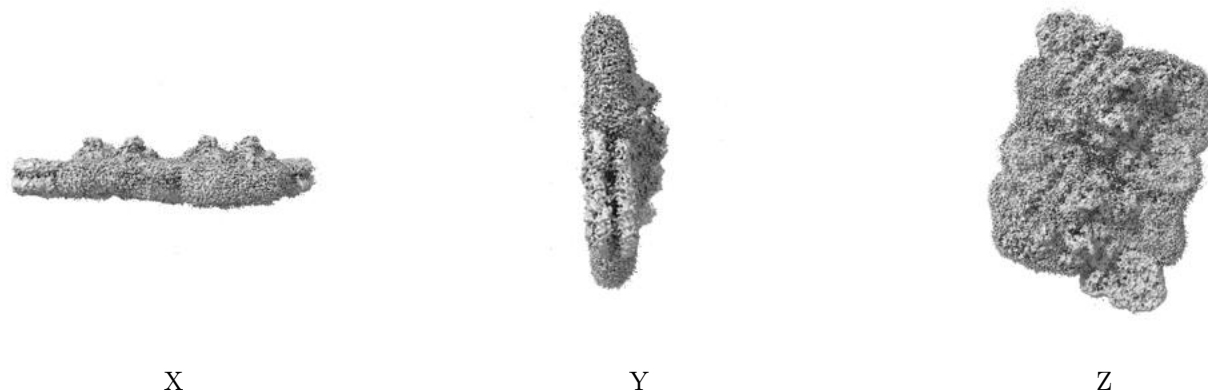


Z

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

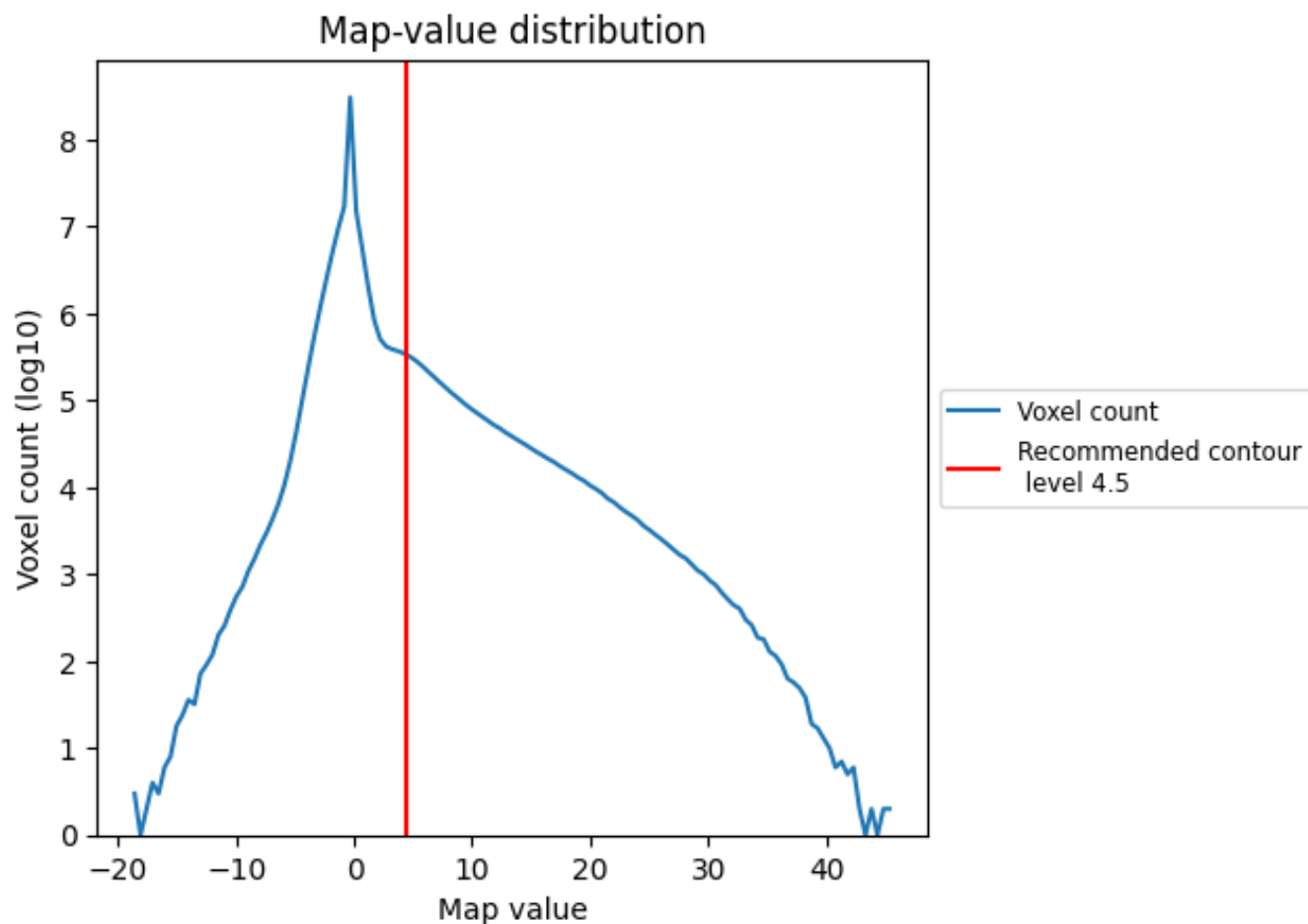
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

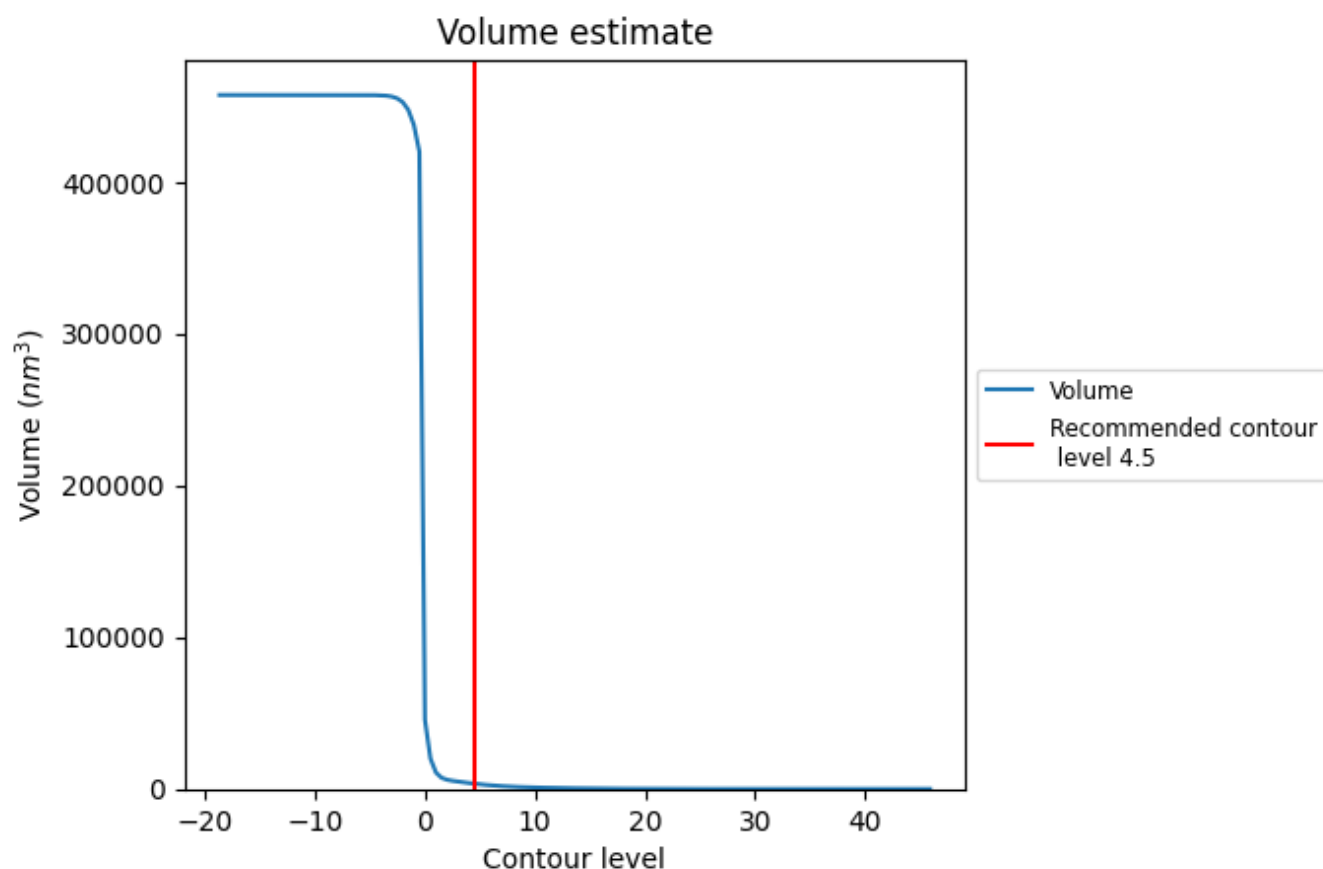
This section contains the results of statistical analysis of the map.

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.

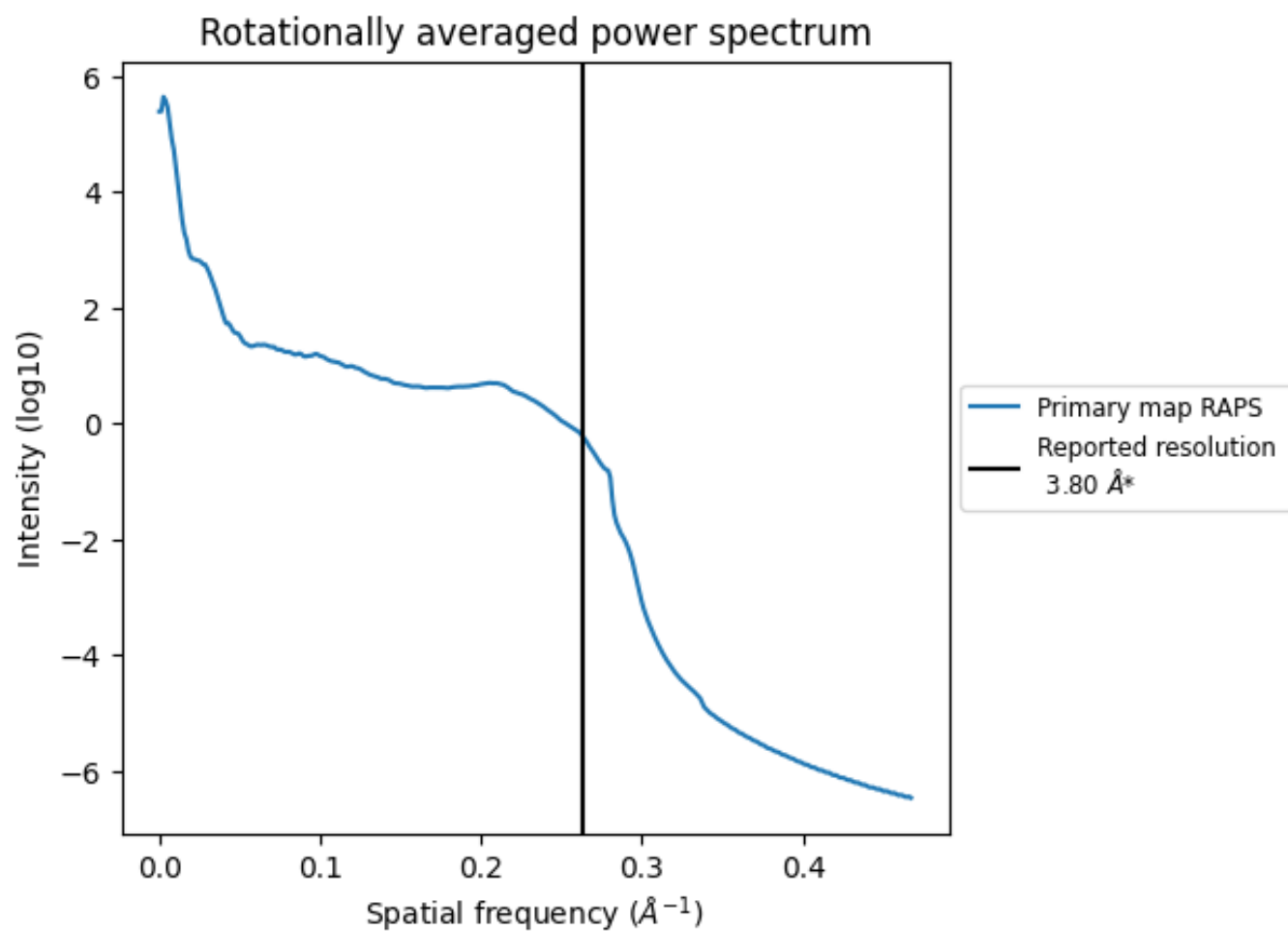
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3500 nm^3 ; this corresponds to an approximate mass of 3162 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 Å⁻¹

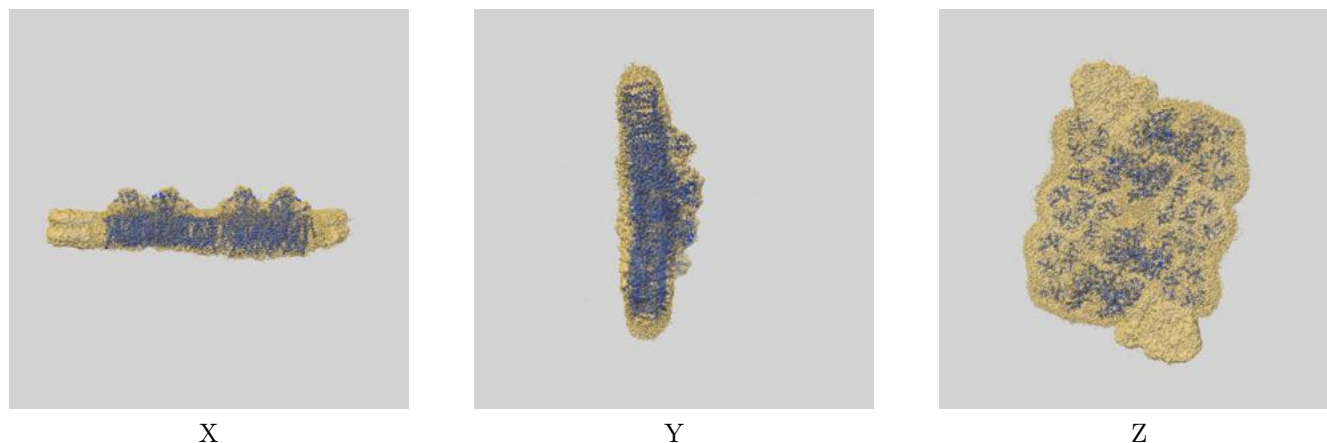
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

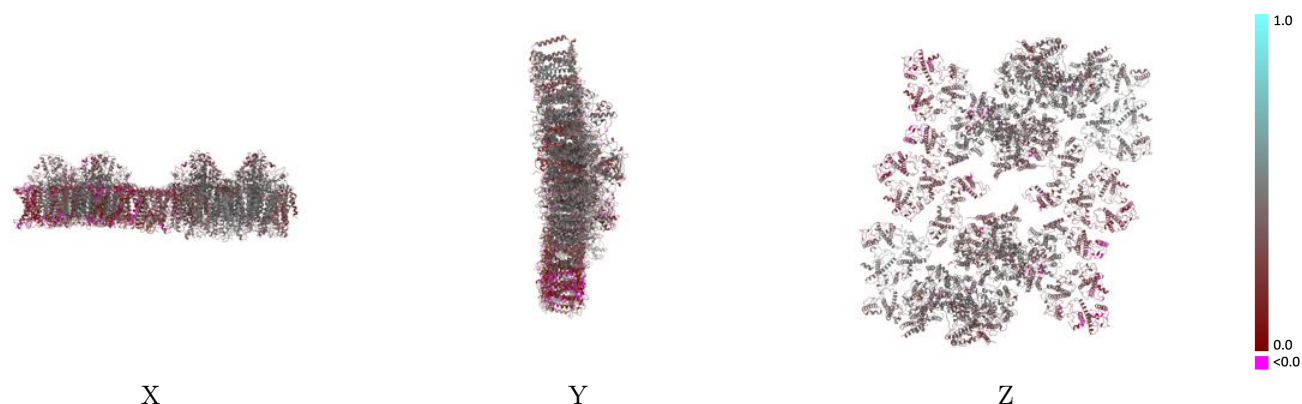
This section contains information regarding the fit between EMDB map EMD-63017 and PDB model 9LE7. Per-residue inclusion information can be found in section [3](#) on page [70](#).

9.1 Map-model overlay [i](#)



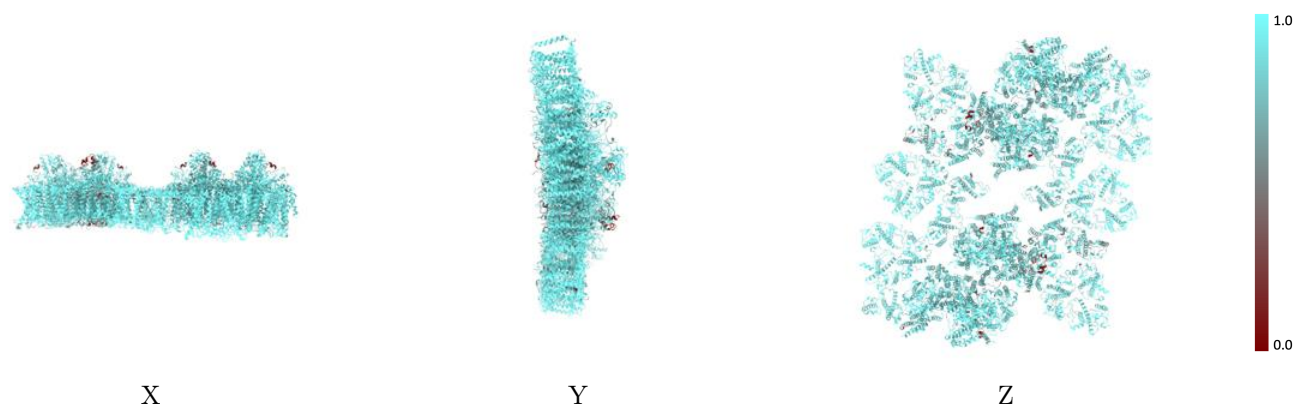
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



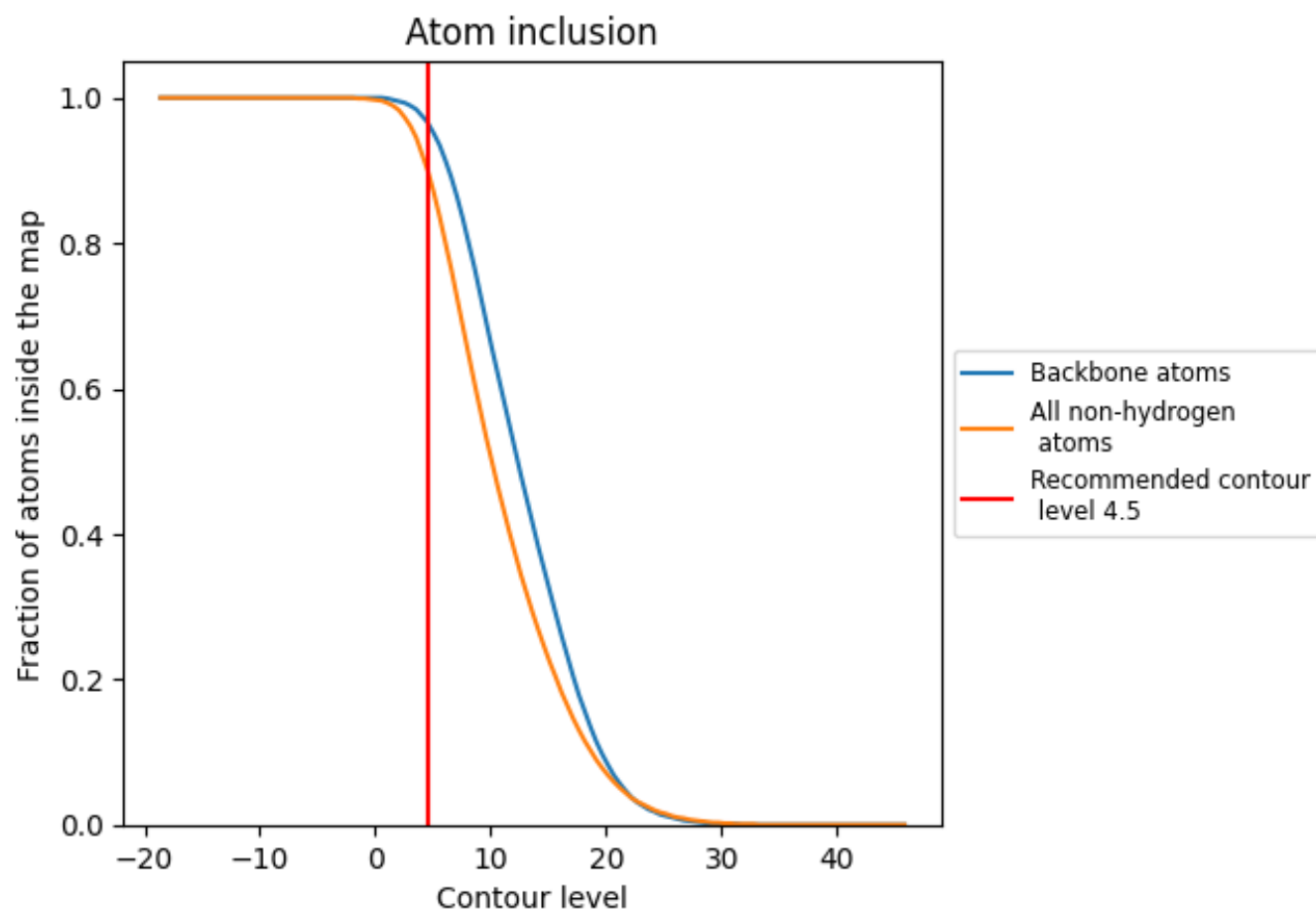
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 90% 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 (4.5) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.9020 |  0.3560 |
| 0 |  0.9480 |  0.3160 |
| 1 |  0.9370 |  0.4360 |
| 2 |  0.9520 |  0.4400 |
| 3 |  0.9320 |  0.3050 |
| 4 |  0.8930 |  0.3100 |
| 5 |  0.9690 |  0.2760 |
| 6 |  0.9510 |  0.3040 |
| 7 |  0.9720 |  0.1710 |
| 8 |  0.9130 |  0.2480 |
| 9 |  0.9670 |  0.2830 |
| A |  0.9210 |  0.4230 |
| A0 |  0.8670 |  0.3990 |
| A1 |  0.8980 |  0.3770 |
| A2 |  0.9450 |  0.4500 |
| A6 |  0.8890 |  0.4040 |
| A7 |  0.8350 |  0.4330 |
| A8 |  0.6400 |  0.2120 |
| AA |  0.9690 |  0.1720 |
| AB |  0.9110 |  0.2560 |
| Au |  0.9410 |  0.3990 |
| Av |  0.9380 |  0.3490 |
| Aw |  0.9420 |  0.4570 |
| Ay |  0.9050 |  0.4320 |
| Az |  0.8940 |  0.4450 |
| B |  0.9210 |  0.4060 |
| BA |  0.8270 |  0.2090 |
| BB |  0.9290 |  0.4590 |
| BC |  0.8680 |  0.3250 |
| BD |  0.9040 |  0.4230 |
| BE |  0.9140 |  0.3960 |
| BF |  0.8370 |  0.4210 |
| BG |  0.9130 |  0.4230 |
| BH |  0.9210 |  0.2950 |
| BI |  0.8260 |  0.3230 |































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| BJ |  0.8500 |  0.1420 |
| BK |  0.8970 |  0.3390 |
| BL |  0.8870 |  0.4330 |
| BN |  0.8080 |  0.3960 |
| BO |  0.9110 |  0.4230 |
| BP |  0.9160 |  0.3920 |
| BQ |  0.8550 |  0.1890 |
| BU |  0.9390 |  0.3370 |
| BV |  0.7600 |  0.2290 |
| BW |  0.8640 |  0.4060 |
| BX |  0.7990 |  0.2080 |
| BY |  0.8310 |  0.3500 |
| BZ |  0.7580 |  0.2340 |
| Ba |  0.8710 |  0.3090 |
| Bb |  0.9200 |  0.3420 |
| C |  0.9310 |  0.4240 |
| D |  0.9480 |  0.4270 |
| E |  0.9320 |  0.2950 |
| F |  0.8800 |  0.2980 |
| G |  0.9380 |  0.3880 |
| H |  0.9210 |  0.3270 |
| I |  0.9320 |  0.4500 |
| K |  0.8860 |  0.4190 |
| L |  0.8960 |  0.4270 |
| M |  0.8550 |  0.3610 |
| N |  0.9350 |  0.4410 |
| R |  0.9280 |  0.4320 |
| S |  0.8790 |  0.3960 |
| T |  0.8390 |  0.4080 |
| U |  0.6450 |  0.2100 |
| W |  0.8690 |  0.3810 |
| X |  0.8270 |  0.2140 |
| Y |  0.9250 |  0.4470 |
| Z |  0.8600 |  0.3170 |
| a |  0.8980 |  0.4140 |
| b |  0.9080 |  0.3850 |
| c |  0.8280 |  0.4060 |
| d |  0.9010 |  0.4090 |
| e |  0.9230 |  0.2840 |
| f |  0.8130 |  0.3050 |
| g |  0.8530 |  0.1340 |
| h |  0.8620 |  0.3220 |

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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| i |  0.8690 |  0.4210 |
| k |  0.7780 |  0.3800 |
| l |  0.8880 |  0.4130 |
| m |  0.9080 |  0.3870 |
| n |  0.8570 |  0.1790 |
| r |  0.9370 |  0.3280 |
| s |  0.7480 |  0.2090 |
| t |  0.8520 |  0.3960 |
| u |  0.8040 |  0.2000 |
| v |  0.9260 |  0.4160 |
| w |  0.8310 |  0.3380 |
| x |  0.7420 |  0.2240 |
| y |  0.8680 |  0.2970 |
| z |  0.9120 |  0.3420 |